

An induced-fit model for asymmetric organocatalytic reactions: a case study of the activation of olefins *via* chiral Brønsted acid catalysts – Supporting Information

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Dependency of transition state geometry on computational settings

Here we discuss the influence of different density functionals as well as basis sets on key internal coordinates of the low energy conformers.

Table S1. Key bond lengths for the transition state conformers **TS1-1** and **TS1-2'** for different density functionals and basis sets. All bond lengths are in Å.

TS1-1	PBE-D3/ def2-SVP	PBE-D3/ def2-TZVP(-f)	B3LYP-D3/ def2-TZVP(-f)
N-H	0.1337	0.1358	0.1363
C-H	0.1370	0.1360	0.1364
C-O	0.2686	0.2855	0.2886
H---O	0.1792	0.1891	0.1900
RMSD	0.1210	0.0000	0.1010

TS1-2'	PBE-D3/ def2-SVP	PBE-D3/ def2-TZVP(-f)	B3LYP-D3/ def2-TZVP(-f)
N-H	0.1367	0.1370	0.1368
C-H	0.1330	0.1329	0.1337
C-O	0.2787	0.2868	0.2858
H---O	0.1800	0.1924	0.2004
RMSD	0.4560	0.0000	0.2540

From **Table S1** it can be seen that the basis set size has a larger impact on the geometry than the density functional. While the bond lengths of the TS mode (N-H/C-H bonds) are quite unaffected of both basis set and density functional, the C-O bond length is affected the most. However, the overall changes in geometry are quite small as reflected by the RMSD values. For the larger def2-TZVP(-f) basis set, we seem to be justified in using the computationally less demanding PBE density functional. The constrained geometry optimizations as well as the transition state optimizations were performed *in vacuo* and implicit solvation corrections added to the final Gibbs free energy were obtained from DFT single point energy calculations. In **Table S2** we show the influence of implicit solvation on the transition state geometry of **TS1-1**. For this, the TS geometry was reoptimized using implicit solvation with Cyclohexane as solvent.

Table S2. Important bond lengths for the most stable TS conformer **TS1-1** optimized with and without implicit solvation at the PBE-D3/def2-TZVP(-f) level of theory. All bond lengths are in Å.

TS1-1	Vacuum	CPCM(Cyclo- hexane)
N-H	0.1358	0.1367

C-H	0.1360	0.1354
C-O	0.2855	0.2929
H---O	0.1891	0.1887
RMSD	0.0000	0.0760

The influence of implicit solvation on the TS geometry is fairly small as reflected by the RMSD values. The critical internal coordinates show some moderate changes, but overall the conformation of the system is unchanged. This justifies the use of *in vacuo* optimized geometries for further calculations and analyzes.

Energy ordering of the most stable transition states at different levels of theories

In **Table S3** we introduce 9 different low-energy conformers leading to the major or minor enantiomeric product, respectively. In the main manuscript we discussed the most stable major **TS1-1** and the two two most stable minor conformers **TS1-1'** and **TS1-2'**. We showed there only the DLPNO-CCSD(T) electronic energies. Here, we discuss the electronic energy ordering at different levels of theories. The results can be found in **Table S3**.

Table S3. Relative electronic energies of low-energy transition states at various levels of theory. All energies are obtained for the PBE-D3/def2-TZVP(-f) optimized geometries. All energies are in kcal mol⁻¹.

	Hartree-Fock/ def2-TZVP	DLPNO- CCSD/ def2-TZVP	DLPNO- CCSD(T)/ def2-TZVP	PBE-D3/ def2-TZVP(- f)	B3LYP-D3/ def2-TZVP
TS1-1	0.0	0.0	0.0	0.0	0.0
TS1-2	10.2	9.7	9.4	7.8	8.0

TS1-3	1.0	0.4	0.2	-0.1	0.0
TS1-4	5.2	3.3	2.8	1.2	1.6
TS1-1'	17.7	8.4	6.9	4.6	3.6
TS1-2'	17.7	10.1	8.7	5.8	4.4
TS1-3'	13.5	9.0	8.0	4.9	4.6
TS1-4'	13.3	10.7	10.1	8.3	8.9
TS1-5'	10.0	8.9	8.5	6.9	7.1

We first discuss the results for the transition states leading to major enantiomeric product (**TS1-1** – **TS1-4**). All methods predict the guess conformer **TS1-2** (reoptimized at the PBE-D3/def2-TZVP(-f) level of theory) to be highly disfavored in energy with respect to the other conformers, reflecting the potential importance of exploration of the conformational space for large and flexible systems. Correlated wave function methods (DLPNO-CCSD and DLPNO-CCSD(T)) as well as DFT predict smaller relative energy differences for **TS1-2** accordingly with respect to Hartree-Fock. For the conformers **TS1-3** and **TS1-4**, the DLPNO-CCSD(T) and DFT almost yield the same relative energies as well. It is important to note that the low-energy conformers (**TS1-1**, **TS1-3**, **TS1-4**) show quite similar structural features. For the transition states leading to the minor enantiomeric product (**TS1-1'** – **TS1-5'**), we see that Hartree-Fock predicts very high relative energies, indicating the inclusion of correlation stabilizes the minor enantiomers relative to the major transition states. The initial guess conformer **TS1-4'** is significantly higher in energy for Coupled-Cluster and DFT methods. This effect is considerably large for the B3LYP functional, predicting **TS1-4'** to be 5.3 kcal mol⁻¹ higher in energy than the most stable transition state leading to minor enantiomeric product (**TS1-1'**). In total, DFT and DLPNO-CCSD(T) predict the same energy ordering of the major transition states, while for the minor conformers DFT predicts smaller relative energies. Interestingly, **TS1-1'** is the most stable

minor transition state at both, DFT and DLPNO-CCSD(T) level of theory, while for the other minor conformers the energy ordering might change with respect to the method.

Thermochemical corrections at the r2SCAN-3c level of theory

In order to test the reliability of the thermochemical corrections calculated at the PBE-D3/def2-TZVP(-f) level of theory, the frequencies and thermochemical corrections were also computed at the r2SCAN-3c level.¹ The r2SCAN-3c calculations were carried out with ORCA 5.0.3.²

Table S4. Difference of thermochemical corrections between the major (TS1-1) and minor (TS1-1', TS1-2', TS1-3', TS1-4', TS1-5') transition states. All energies are in kcal mol⁻¹.

	PBE-D3(BJ)/def2-TZVP(-f)	r2SCAN-3c
TS1-1' - TS1-1	1.26	1.32
TS1-2' - TS1-1	-0.03	0.04
TS1-3' - TS1-1	1.02	0.34
TS1-4' - TS1-1	-0.04	-0.38
TS1-5' - TS1-1	0.30	0.63

For all transition state conformers, the difference in thermochemical correction between PBE-D3/def2-TZVP(-f) and r2SCAN-3c is rather small. The largest influence is on TS1-3' – TS1-1 (-0.68 kcal mol⁻¹), while for all other transition states the difference between the methods is below 0.5 kcal mol⁻¹.

Extrapolation of the DLPNO-CCSD(T) energies to the basis set limit

The DLPNO-CCSD(T) energies of TS1-1, TS1-1' and TS1-2' were extrapolated to the basis set limit in order to quantify the error of incomplete basis set to the stereoselectivity. The extrapolation was

performed with ORCA 5.0.3 and the def2-SVP (cardinal number X=2) and def2-TZVP (X=3) basis sets were used. The triples amplitudes were computed iteratively (T1) and implicit solvation was included *via* SMD. The results are shown in **Table S5**.

Table S5. Difference of electronic energies at the DLPNO-CCSD(T) level between the major (**TS1-1**) and minor (**TS1-1'**, **TS1-2'**) transition states. All energies are in kcal mol⁻¹.

	TS1-1'-TS1-1	TS1-2'- TS1-1
ORCA 4.2.1 def2-TZVP	6.880	8.743
ORCA 5.0.3 def2-TZVP	7.086	8.433
ORCA 5.0.3 (2/3)-extrapolated	6.228	8.299

As can be seen, the ORCA version has a rather small influence on the stereoselectivity. For both minor transition states, basis set extrapolation reduces the stereoselectivity and therefore brings it closer to the experimental value, while in general the stereoselectivity still is overestimated.

Extrapolation of the DLPNO-CCSD energies to the pair natural orbital space limit

In addition to the extrapolation towards the basis set limit, extrapolation towards the pair natural orbital (PNO) space limit was carried out (Complete PNO Space, CPS).³ For this, the PNO(6/7)-scheme was used: DLPNO-CCSD calculations with the def2-SVP basis set were carried out once with TCutPNO = 1e-6 and again with TCutPNO=1e-7. The correlation energy was extrapolated *via*:

$$E_{corr,PNO(6,7)} = E_{corr,PNO6} + 1.5 * [E_{corr,PNO7} - E_{corr,PNO6}]. \quad (I)$$

The results are shown in **Table S6**.

Table S6. Difference of correlation energies at the DLPNO-CCSD/def2-SVP level between the major (**TS1-1**) and minor (**TS1-1'**, **TS1-2'**) transition states for different values of TCutPNO. All energies are in kcal mol⁻¹.

	TS1-1'-TS1-1	TS1-2'- TS1-1
TcutPNO=1e-6	-8.016	-7.120
TCutPNO=1e-7	-7.997	-7.263
PNO(6/7)-extrapolation	-7.987	-7.335

The influence of the extrapolation of the TCutPNO value on the difference in correlation energy is only marginally for **TS1-1'** (0.010 kcal mol⁻¹ with respect to TCutPNO=1e-7) while for **TS1-2'** there is a larger, but in total still small influence (-0.072 kcal mol⁻¹ with respect to TCutPNO=1e-7). The value of TCutPNO used in the DLPNO-CCSD(T) calculations reported in the main manuscript was 3.33e-7, so that the net stabilization of **TS1-2'** with respect to **TS1-1** due to the CPS-extrapolation is expected to be around 0.1 kcal mol⁻¹.

Transition state optimizations at the B3LYP-D3(BJ)/def2-TZVP(-f) level of theory

The most stable major transition state and the low-energy minor transition states were reoptimized using ORCA 5.0.3 and the B3LYP functional. In **Table S7** the relative energies of the reoptimized transition states at the B3LYP-D3/def2-TZVP(-f) level of theory are compared to the previously obtained transition states at the PBE-D3/def2-TZVP(-f) level of theory.

Table S7. Relative electronic energies of low-energy transition states. Geometries and energies are at the PBE-D3/def2-TZVP(-f) or B3LYP-D3/def2-TZVP(-f) level of theory, respectively. All energies are in kcal mol⁻¹.

	PBE-D3/def2-TZVP(-f)	B3LYP-D3/def2-TZVP(-f)
TS1-1	0.0	0.0
TS1-1'	4.6	4.3
TS1-2'	5.8	5.1
TS1-3'	4.9	5.2
TS1-4'	8.3	9.0
TS1-5'	6.9	7.1

As **Table S7** demonstrates, for both methods quite similar relative energies are obtained. Noticeably, the most stable minor conformers in terms of free energies (**TS1-1'** and **TS1-2'**) show lower relative energies at the B3LYP-D3 level of theory with respect to the PBE-D3 level of theory.

Local Energy Decomposition for most stable transition states

In **Table S8** we report the LED results for the transition state conformers listed in **Table S3**. In the main manuscript conformers **TS1-1**, **TS1-1'** and **TS1-2'** were considered (see **Table 1**).

Table S8. Decomposition of the reaction barriers for 9 transition state conformers at the DLPNO-CCSD(T) level of theory into geometric preparation, dispersive and non-dispersive interaction contributions. For the definition of the symbols, see the main manuscript. All energies are in kcal mol⁻¹.

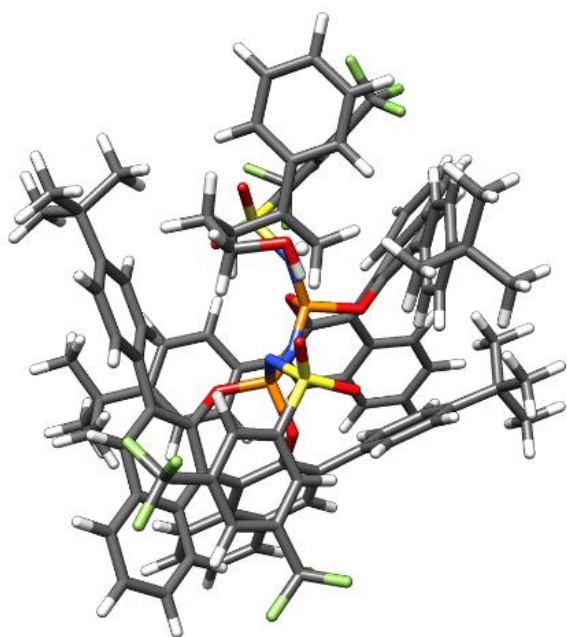
	TS1-1	TS1-2	TS1-3	TS1-4	TS1-1'	TS1-2'	TS1-3'	TS1-4'	TS1-5'
ΔG^\ddagger	20.0	29.1	21.1	23.3	28.1	28.4	28.6	28.8	29.1
ΔG_{corr}^\ddagger	20.0	19.7	20.8	20.5	21.2	19.6	20.5	18.6	20.5
ΔE^\ddagger	0.0	9.5	0.3	2.9	6.9	8.8	8.1	10.2	8.6
$\Delta E_{geo-prep}^\ddagger$	50.4	57.5	51.0	49.8	56.6	63.6	61.4	58.6	64.9

Cat.	41.3	46.9	43.0	40.6	43.2	50.0	49.3	48.8	55.6
Substrate	9.2	10.6	8.0	9.2	13.4	13.6	12.1	9.8	9.3
ΔE_{int}^\ddagger	-50.4	-49.4	-52.1	-48.3	-49.7	-54.8	-54.7	-49.8	-56.4
E_{disp}^\ddagger	-38.2	-38.8	-39.6	-41.0	-43.2	-45.4	-45.7	-38.0	-38.3
$\Delta E_{non-disp}^\ddagger$	-12.2	-10.6	-12.5	-7.4	-6.5	-9.4	-9.0	-11.8	-18.1

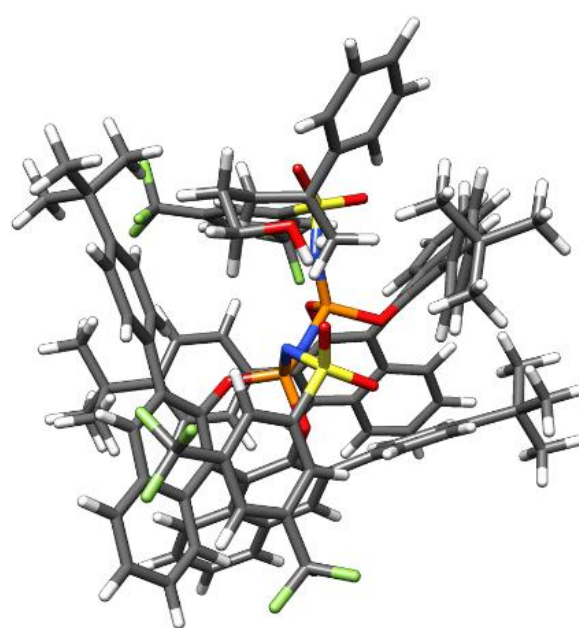
We start by discussing the conformers leading to the major enantiomeric product. The conformers **TS1-1**, **TS1-3** and **TS1-4** have DLPNO-CCSD(T) energies in the same range and it can be seen that geometric preparation is cancelled by the interaction energy between the catalyst and substrate (see main manuscript for detailed discussion). For the guess conformer **TS1-2** we see that the high relative DLPNO-CCSD(T) energy is mostly caused by geometric preparation. The increased geometric preparation for **TS1-2** is caused by the Ph-(CF₃)₂ group at the amine group of the catalyst, which does not allow for attractive π - π interactions (this is the same effect that causes the increased geometric preparation of **TS1-2'**, see *vide infra* and **Figure 6** for details). For the minor transition state conformers, it can be seen that geometric preparation is the most significant contribution to the difference in electronic energies with respect to **TS1-1**. In fact, the interaction between the catalyst and the substrate is even stronger for most of the minor transition states with respect to **TS1-1**. Interestingly, the most stable minor conformer **TS1-1'**, has the lowest geometric preparation energies of all minor TS conformers, but also the weakest interactions between the two fragments. For **TS1-2'** and **TS1-3'** the geometric preparation but also the attractive interactions between catalyst and substrate are increased with respect to **TS1-1'**. The stabilization is carried out by dispersive attraction between the catalyst and the substrate, while the non-dispersive interactions are decreased with respect to **TS1-1**. In conclusion, the geometric preparation is significantly increased for all minor conformers with respect to the major TS conformers. The strengthened attractive interactions for the minor conformers cannot counteract the geometric preparation leading to large energy differences

between the major and the minor TSs.

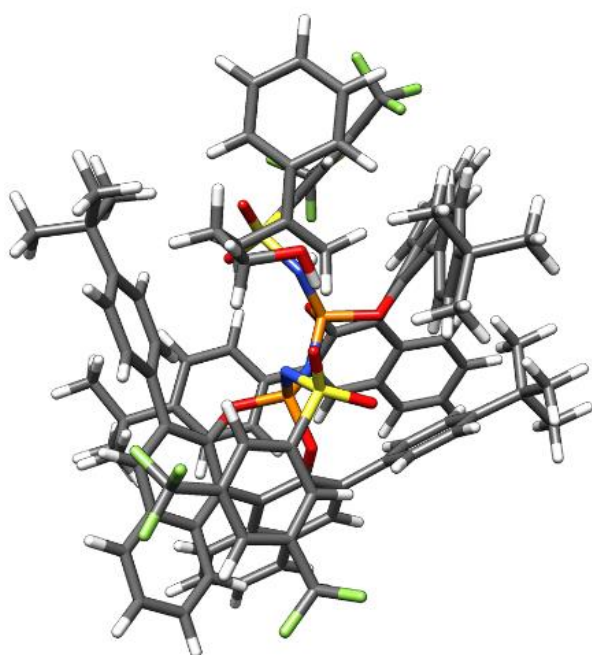
Visualization of discussed transition state conformers



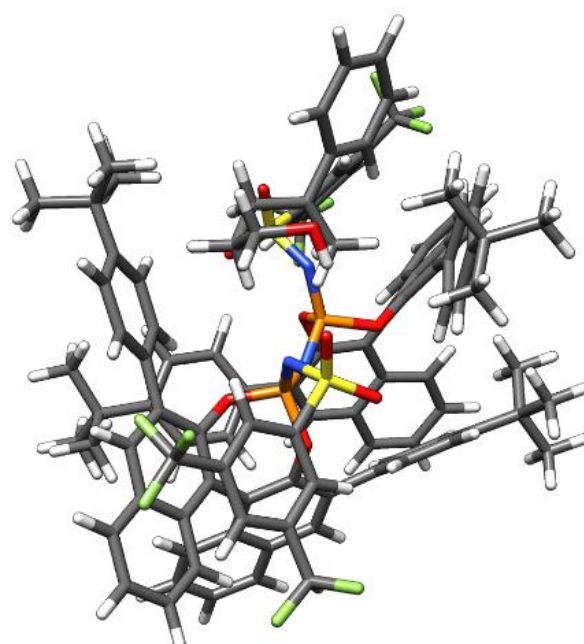
TS1-1



TS1-2



TS1-3



TS1-4

Figure S1. Four different transition state conformers leading to major enantiomeric product.

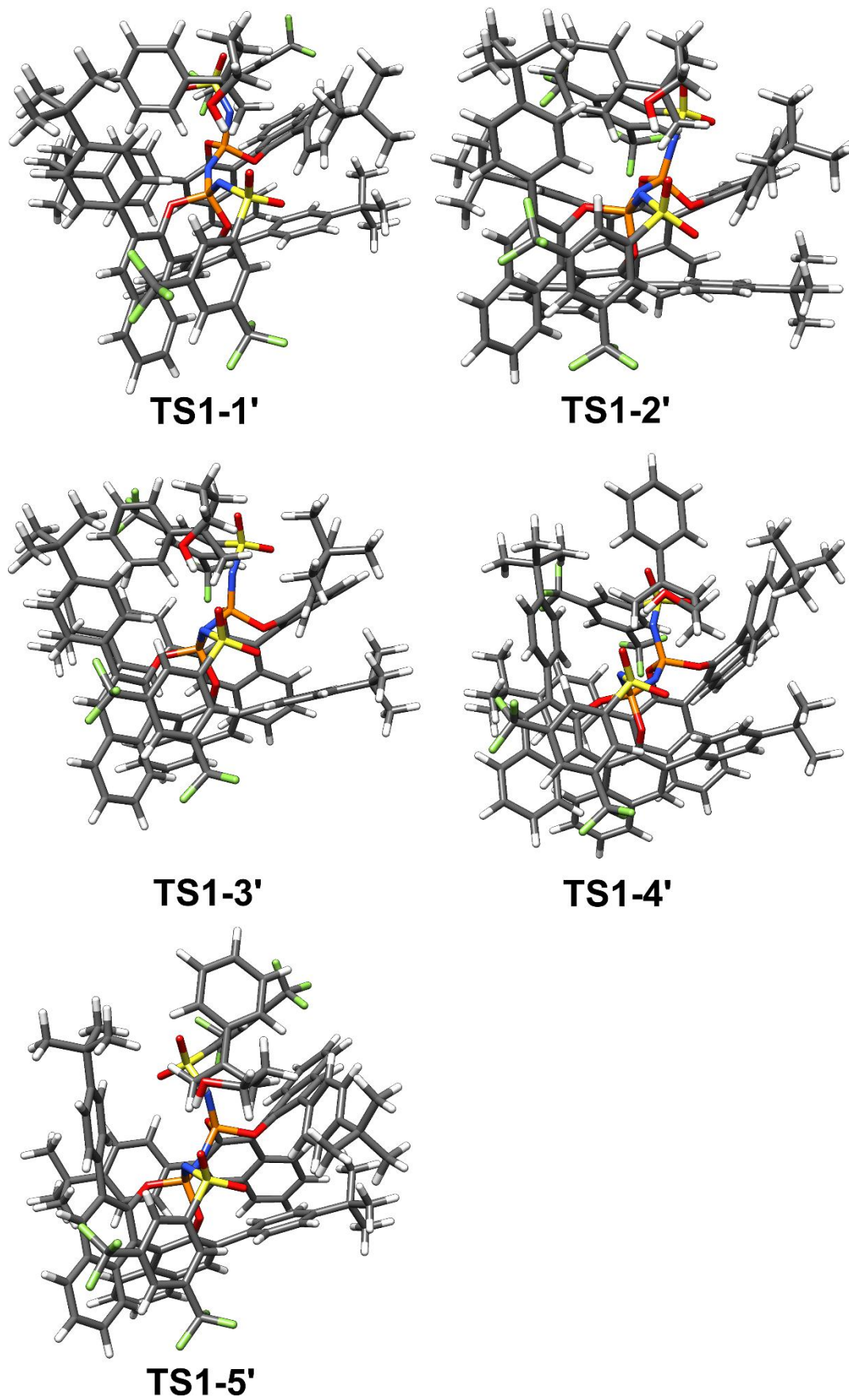


Figure S2. Five different transition state conformers leading to the minor enantiomeric product.

Confinement analysis

We now discuss the results from the confinement analysis of the transition state conformers **TS1-1**, **TS1-1'** and **TS1-2'**. In the main manuscript we have already discussed the general procedure for the deconstruction of the catalyst and how we achieved analysis of the noncovalent interactions (see **Figure 5** and **Figure 6**). In **Table S9** we present the geometric preparation energies for TS conformers **TS1-1** and **TS1-1'** for the different deconstruction points labeled as **3b**, **3b_1**, **3b_2**, **3b_3**, **3b_4**, **3b_5**. The corresponding results for the comparison of **TS1-1** and **TS1-2'** can be found in **Table S10**. For measuring the influence of London dispersion, the geometric preparation was calculated with and without Grimme's D3(BJ) dispersion correction.

Table S9. Geometric preparation energies for TS conformers **TS1-1** and **TS1-1'** obtained from B3LYP-D3/def2-TZVP calculations. During the calculations only the relaxation of the newly added hydrogen atoms was allowed. For definition of the structures **3b** to **3b_5** see **Figure 5** of the main manuscript. In order to obtain the geometric preparation of the catalyst backbone, the geometric preparation energies given below were obtained by subtracting the needed energy for the N-H bond elongation (30.2 kcal mol⁻¹ for **TS1-1**, 29.0 kcal mol⁻¹ for **TS1-1'** with D3BJ, 30.6 kcal mol⁻¹ for **TS1-1**, 29.2 kcal mol⁻¹ for **TS1-1'** without D3BJ) from the total geometric preparation energy. All energies are in kcal mol⁻¹.

	Geo-prep (with D3BJ)			Geo-prep (without D3BJ)		
	TS1-1	TS1-1'	TS1-1' - TS1-1	TS1-1	TS1-1'	TS1-1' - TS1-1
3b	12.5	14.5	2.0	4.4	9.4	5.0
3b_1	13.3	14.2	0.9	4.7	11.0	6.3
3b_2	13.6	10.4	-3.2	4.8	9.0	4.2
3b_3	11.7	9.0	-2.7	3.4	7.0	3.6

3b_4	8.7	5.9	-2.8	2.8	5.7	2.9
3b_5	7.2	3.6	-3.6	2.3	5.2	2.9

It can be seen, that London dispersion has a large impact on the total geometric preparation. For **3b**, 65% for **TS1-1** and 35% for **TS1-1'** of geometric preparation stems from London dispersion. This underlines, that geometric preparation must not be exclusively understood as steric hindrance, since weakened or strengthened noncovalent interactions contribute to geometric preparation as well.

Interestingly, without the D3 dispersion correction, the difference in geometric preparation between **TS1-1'** and **TS1-1** remains much more constant for all six different structures and the difference always remains positive. When dispersive interactions are taken into account, the difference in geometric preparation becomes smaller from step to step and starting from **3b_2** even becomes negative. Starting from **3b_2**, the difference in geometric preparation remains negative and varies within a window of 0.5 kcal mol⁻¹. While substituting groups with hydrogen atoms, the difference in geometric preparation (and therefore the stereoselectivity) becomes smaller, the difference of non-dispersive geometric preparation remains constant. This illustrates, that for the major TS conformer **TS1-1** the removed groups must have had additional dispersive interactions that were not present for the minor TS conformer **TS1-2'**. If the group is removed, the additional dispersive interactions for **TS1-1** cease, leading to decreased difference in geometric preparation.

For all involved groups that are replaced during the deconstruction procedure, we now determine the attractive interactions for **TS1-1** and **TS1-1'** by using NCI plots. In order to analyze the interactions of a particular group, we use the 3D structure of the subsystem before this group is removed. The atomic color code for the **Figures S3 – S12** is: Grey, hydrogen; cyan, carbon; red, oxygen; gold, phosphorus; pink, fluorine; yellow, sulfur.

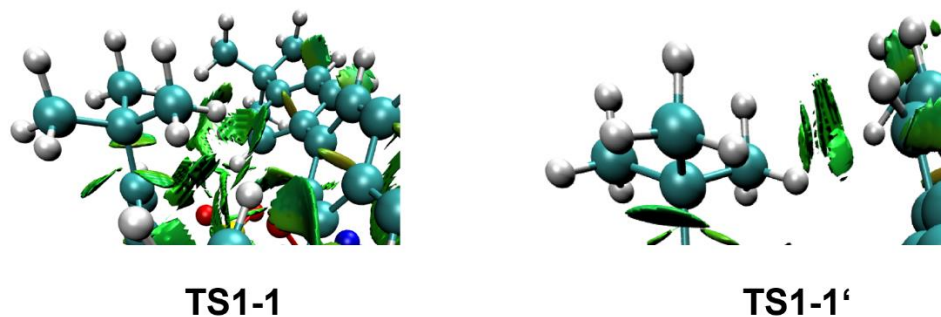


Figure S3. Noncovalent interactions of the *t*-Bu group of the BINOL aryl-substituent that does not form the catalyst pocket with the BINOL backbone (**3b_1**, see **Figure 5**). It can be seen, that for **TS1-1** additional dispersive interactions are present, which is why removal of this group leads do a relative stabilization of **TS1-1'**.

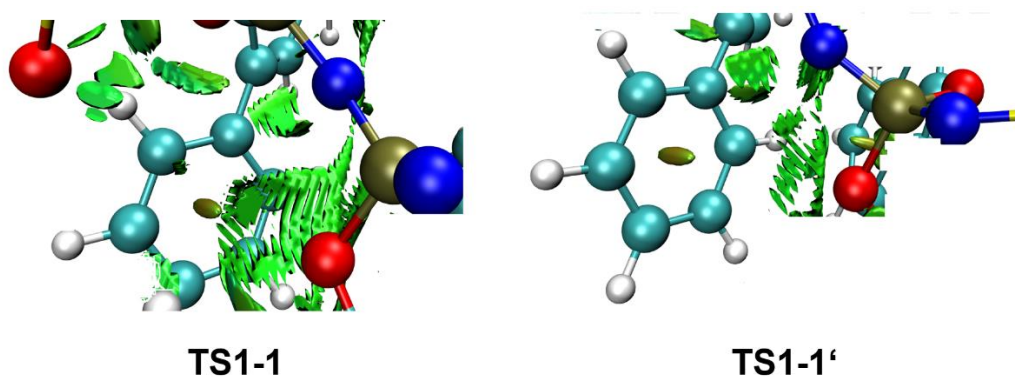
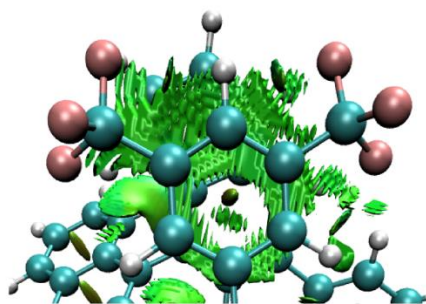
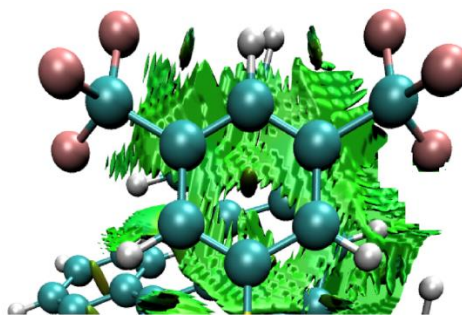


Figure S4. Noncovalent interactions of the Ph-ring bound to the BINOL substituent that is not forming the catalyst pocket (**3b_2**, see **Figure 5**). Due to geometric distortion, **TS1-1** is able to form stronger interactions with the catalyst's backbone, especially with the core catalyst's oxygen atom. Only for **TS1-1** strong attractive interactions of this group are present. Its removal therefore energetically favors **TS1-1'** with respect to **TS1-1**.

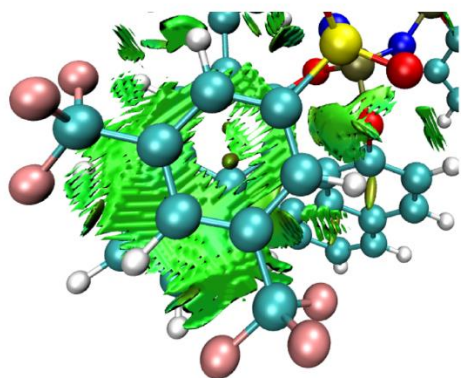


TS1-1

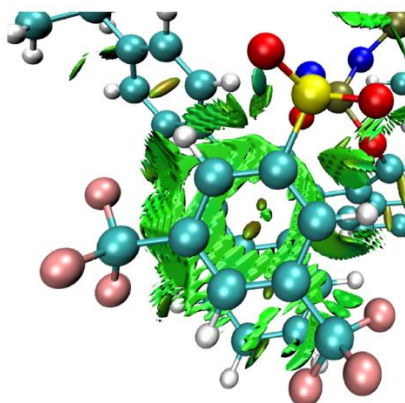


TS1-1'

Figure S5. Noncovalent interactions between the aminyl-Ph-(CF₃)₂ group and the residue (**3b_3**, see **Figure 5**). For both conformers there are equally strong interactions with the ligands Ph-rings. That is why removal of this group does not affect the difference in geometric preparation.



TS1-1



TS1-1'

Figure S6. Noncovalent interactions between the iminyl-Ph-(CF₃)₂ group with the residue (**3b_4**, see **Figure 5**). For both TS conformers π - π interactions with the phenyl-rings of the residue are present which is why the stereoselectivity is not significantly affected by the removal of this group.

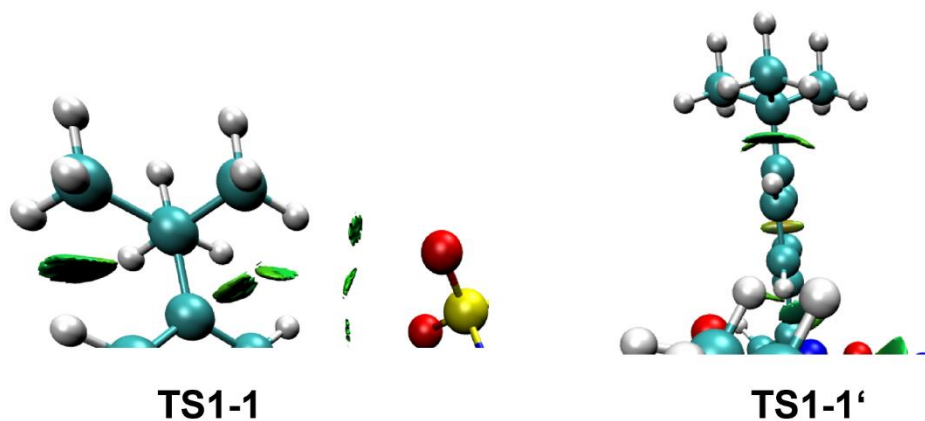


Figure S7. Non-covalent interactions between the *t*-Bu group of the pocket forming substituent with the residue (**3b_5**, see **Figure 5**). For the major TS conformer **TS1-1** additional attractive interactions with the SO₂ group of the core catalyst are present. These stabilizing interactions are missing for the minor TS conformer **TS1-1'**. Removing this group therefore energetically favors **TS1-1'**.

The same analyses were performed for the second most stable minor transition state conformer (**TS1-2'**) which is only 0.3 kcal mol⁻¹ less stable than **TS1-1'** and therefore should be significantly occupied as well.

Table S10. Geometric preparation energies for TS conformers **TS1-1** and **TS1-2'** obtained from B3LYP-D3/def2-TZVP calculations. During the calculations only the relaxation of the newly added hydrogen atoms was allowed. For definition of the structures **3b** to **3b_5** see **Figure 5** of the main manuscript. In order to obtain the geometric preparation of the catalyst backbone, the geometric preparation energies given below were obtained by subtracting the needed energy for the N-H bond elongation (30.2 kcal mol⁻¹ for **TS1-1**, 31.3 kcal mol⁻¹ for **TS1-2'** with D3BJ, 30.6 kcal mol⁻¹ for **TS1-1**, 31.8 kcal mol⁻¹ for **TS1-2'** without D3BJ) from the total geometric preparation energy. All energies are in kcal mol⁻¹.

	Geo-prep (with D3BJ)			Geo-prep (without D3BJ)		
	TS1-1	TS1-2'	TS1-2' - TS1-1	TS1-1	TS1-2'	TS1-2' - TS1-1
3b	12.5	18.5	6.0	4.4	10.8	6.4
3b_1	13.3	17.9	4.6	4.7	13.2	8.5
3b_2	13.6	16.3	2.7	4.8	10.6	5.8
3b_3	11.7	9.1	-2.6	3.4	9.0	5.6
3b_4	8.7	5.9	-2.8	2.8	7.5	4.7
3b_5	7.2	3.1	-4.1	2.3	6.2	3.9

As for **TS1-1'**, London dispersion has a large impact on the total geometric preparation. For **3b**, 65% for **TS1-1** and 42% for **TS1-2'** of geometric preparation stems from London dispersion.

Again, without the D3 dispersion correction, the difference in geometric preparation between **TS1-2'** and **TS1-1** almost remains constant for all six different structures. When dispersive interactions are taken into account, the difference in geometric preparation becomes smaller from step to step and starting from **3b_3** even becomes negative. This already hints to the great importance of dispersive interactions for the geometric preparation and for stereoselectivity as well.

For all involved groups that are replaced during the deconstruction procedure, we now determine the attractive interactions for **TS1-1** and **TS1-2'** by using NCI plots. In order to analyze the interactions of a particular group, we use the 3D structure of the subsystem before this group is removed.

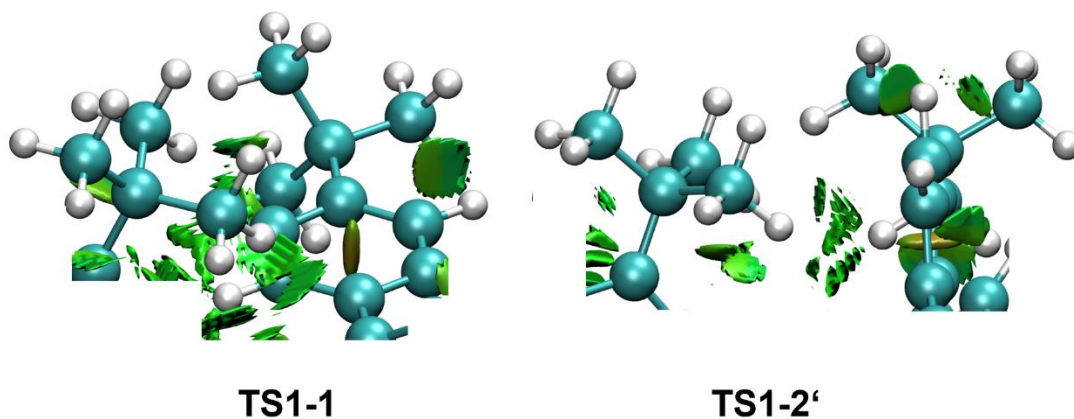


Figure S8. Noncovalent interactions of the *t*-Bu group of the BINOL aryl-substituent that does not form the catalyst pocket with the BINOL backbone (**3b_1**, see **Figure 5**). It can be seen, that for **TS1-1** additional dispersive interactions are present, which is why removal of this group leads do a relative stabilization of **TS1-2'**.

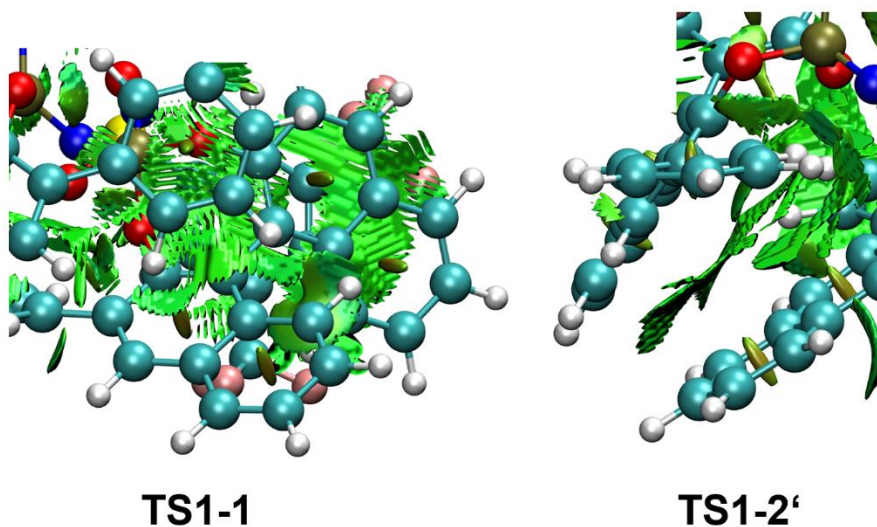


Figure S9. Noncovalent Interactions of the Ph-ring bound to the BINOL substituent that is not forming the catalyst pocket (**3b_2**, see **Figure 5**). Due to geometric distortion, **TS1-1** forms stronger interactions with the catalyst's backbone. For **TS1-2'** the distance to the next aryl-ligand is too large to allow for dispersive interactions. For **TS1-1** more attractive interactions of this group are present. Its removal therefore energetically favors **TS1-2'**.

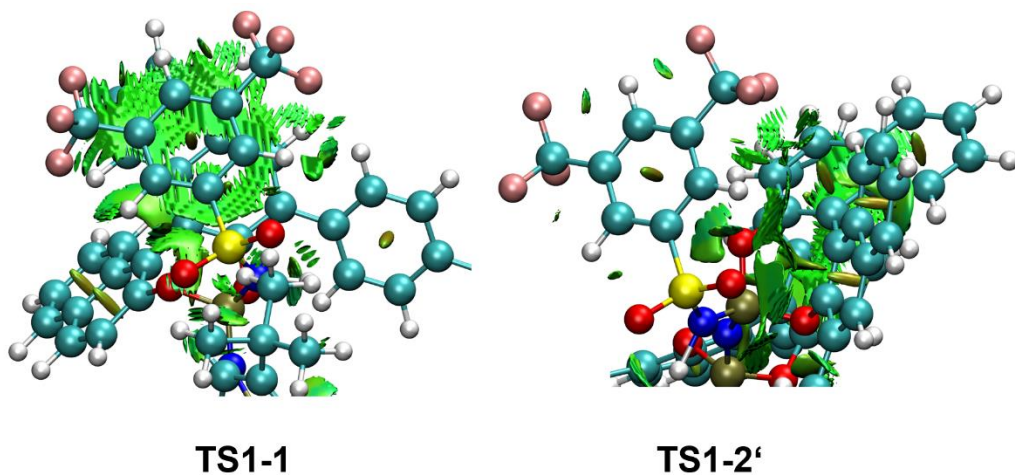


Figure S10. Noncovalent interactions between the aminyl-Ph-(CF₃)₂ group and the residue (**3b_3**, see **Figure 5**). The aminyl-Ph-(CF₃)₂ group of **TS1-1** has strong attractive interactions with the phenyl-rings of the BINOL substituents. For **TS1-2'** the corresponding aminyl-Ph-(CF₃)₂ group has rotated and therefore does not allow for such interaction. Because of the strong interactions only present for **TS1-1**, the removal of this group has large influence on the stereoselectivity.

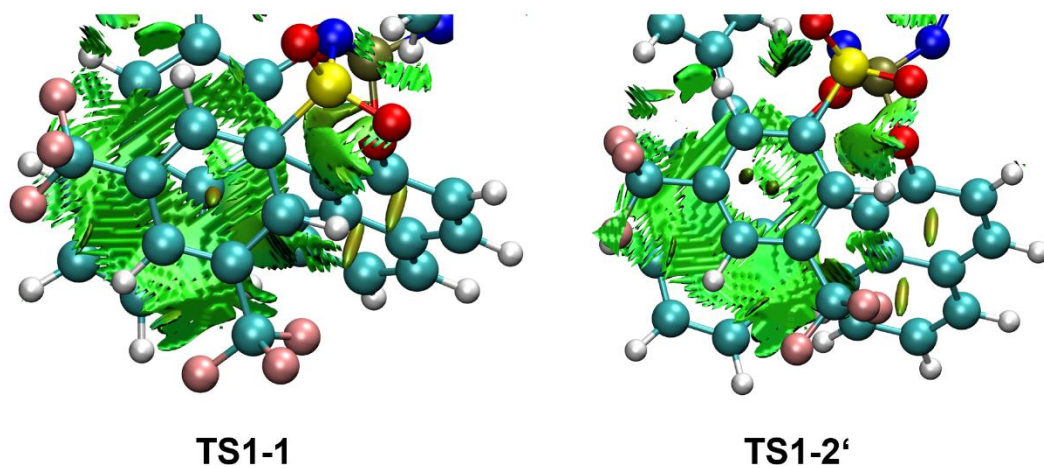


Figure S11. Noncovalent interactions between the iminyl-Ph-(CF₃)₂-group with the residue (**3b_4**, see **Figure 5**). For both TS conformers π - π interactions with the phenyl-rings of the residue are present, which is why the stereoselectivity is not affected by the removal of this group.

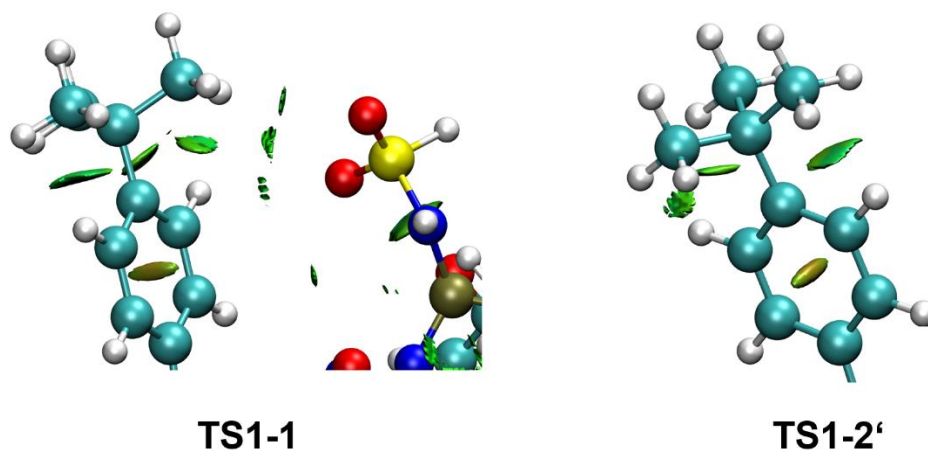


Figure S12. Non-covalent interactions between the *t*-Bu group of the pocket forming substituent with the residue (**3b_5**, see **Figure 5**). For the major TS conformer **TS1-1** additional attractive interactions with the SO₂ group of the core catalyst are present. These stabilizing interactions are missing for the minor TS conformer **TS1-2'**. Removing this group therefore energetically favors **TS1-2'**.

Literature

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- (2) Neese, F. Software update: The ORCA program system—Version 5.0. *WIREs Computational Molecular Science* *n/a* (n/a), e1606. DOI: <https://doi.org/10.1002/wcms.1606>.
- (3) Altun, A.; Neese, F.; Bistoni, G. Extrapolation to the Limit of a Complete Pair Natural Orbital Space in Local Coupled-Cluster Calculations. *Journal of Chemical Theory and Computation* **2020**, *16* (10), 6142-6149. DOI: 10.1021/acs.jctc.0c00344.

Cartesian coordinates of important structures

26

1

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176
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128
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H	-3.64008141229183	1.16889276199719	7.00820676225327
H	-2.54459177083547	0.37126753838788	5.86256916142939
H	-1.92459779544028	1.62102893292275	6.97673164883353
H	-4.18534709176582	1.01443694447765	4.00877125399833
H	-5.21156086812596	1.80913219196911	5.22436795000562
H	-4.67371714232959	2.70754042144367	3.78795414316991

H	-3.74699306017891	4.52130330699713	5.37302494882200
H	-4.27953690632525	3.55855220315746	6.77282207424939
H	-2.57836275665559	4.07786356994138	6.63809976393018
C	0.14634352976968	-4.62377337683356	4.68261584273254
C	-1.90115608401468	-6.04245333650917	4.78810317201999
C	-1.61732721024663	-4.16657312065333	6.41132363228301
C	6.13837222935769	-1.72135097611354	1.39709979702190
H	7.80206654149382	-0.54168075756744	2.11821144156892
C	3.98247684100442	-1.10663375158713	2.24504897043115
H	3.90363809963310	0.53287460538196	3.63494185479020
H	0.59276182474653	-3.62527992956950	4.77234747589027
H	0.65137213541438	-5.28972962062063	5.39852815122887
H	0.35829609332148	-4.99024894245826	3.66904661463760
H	-1.36366434285678	-6.71517322804146	5.47181035466721
H	-2.97239037705628	-6.11170898155148	5.02678727726650
H	-1.74905916663360	-6.41727109185472	3.76518529806112
H	-1.13267027104500	-4.86568508076754	7.10973233484738
H	-1.21114943411012	-3.16277459046658	6.59768745263440
H	-2.69354549631346	-4.14339612119895	6.63578530267177
C	4.76335172425545	-1.93749769771202	1.43764329545532
C	7.01948395844714	-2.64285804843046	0.58829209171066
H	4.30645839312001	-2.74634965327013	0.86551513786618
F	8.07746908646257	-1.98266794750635	0.04074016125948
F	6.34368825685879	-3.23880022236090	-0.42639992138374
F	7.53483456932064	-3.63587286156759	1.36494558606762
C	-4.87323084285720	-2.31154212431041	-1.63618523574949
C	-3.99637563493113	-1.42561938044107	-2.26031232370833
H	-4.47885530553030	-3.16597491855333	-1.08624951504677
C	-6.24817372488763	-2.09956349526638	-1.75023638316616
C	-4.47265685555574	-0.34243346929167	-2.99244240444552
C	-6.74480922654180	-1.00886097288958	-2.46737396819888
C	-7.18983681596791	-3.10701613209496	-1.14141357222567
C	-5.85073695573819	-0.13396182022536	-3.08383377564006
H	-3.76776533800844	0.32108726126255	-3.49053403042259
H	-7.81705106326888	-0.84021568799552	-2.53873926439423
F	-6.83258443306759	-3.43250110275580	0.13690728788447
F	-7.19263808766865	-4.27243575014596	-1.84764420644723
F	-8.47285031037170	-2.66503093470191	-1.09752904047579
C	-6.34517818495426	1.03222271701744	-3.90067429953458
F	-7.67912007544844	1.24275525386369	-3.75967009872229
F	-5.71216942354698	2.19115579485649	-3.55762312622306
F	-6.10859137161848	0.84240292489236	-5.23061029311870
H	-1.16574373625030	-4.93735748564060	-2.15785176118222
H	-2.06868043308664	-7.11094548318294	-0.66578668440184
H	0.05273021085180	-6.63855786250945	0.48489129657112
H	-0.90394778634984	-3.71718841044267	0.37227327707068

228

A-TS1

C	0.954186	-4.171081	-0.174685
C	-0.229143	-4.264120	0.735844
C	-0.957058	-5.616705	0.718866
C	-1.756069	-5.814272	-0.565051
O	-0.927735	-5.660601	-1.720360
H	0.149875	-4.073884	1.754547
H	-1.643318	-5.661073	1.579062
H	-2.588634	-5.091851	-0.599696
C	2.023372	-5.174769	-0.082946
C	2.750157	-5.523315	-1.235735

C	2.352001	-5.800537	1.134090
C	3.779188	-6.458369	-1.174882
H	2.476709	-5.073270	-2.189029
C	3.394119	-6.720903	1.197482
H	1.823048	-5.521464	2.043884
C	4.109663	-7.055552	0.044045
H	4.322098	-6.727123	-2.082693
H	3.652953	-7.178678	2.153309
H	4.921011	-7.783323	0.095715
C	1.117247	-3.063159	-0.994723
H	1.958299	-3.035399	-1.689802
H	0.215593	-2.523445	-1.293692
H	2.784268	5.304498	-5.192393
C	2.612879	4.488197	-5.908068
C	2.519183	3.123694	-5.192966
H	3.446099	4.483804	-6.627371
H	1.684815	4.707380	-6.455551
C	1.350768	3.174119	-4.202585
C	3.838184	2.858455	-4.441033
C	2.340034	2.028414	-6.253692
C	2.408096	-0.730613	-3.400324
C	1.369900	4.092159	-3.138952
C	0.218357	2.357187	-4.316767
H	4.030929	3.626027	-3.679853
H	3.819403	1.881441	-3.940489
H	4.682151	2.862265	-5.147433
H	1.435404	2.189469	-6.857815
H	3.201892	2.036792	-6.936621
H	2.283807	1.027517	-5.801879
C	3.623415	-0.959372	-2.725251
C	1.853747	-1.702168	-4.224771
H	1.881250	0.213905	-3.282667
C	0.305472	4.200629	-2.251677
H	2.236967	4.736666	-2.987575
C	-0.854302	2.460983	-3.430915
H	0.151872	1.618866	-5.115322
C	4.266871	0.067925	-1.874758
C	4.250376	-2.198729	-2.929407
C	2.481685	-2.940646	-4.440137
H	0.892577	-1.487053	-4.694253
C	-0.839181	3.395879	-2.385758
H	0.372992	4.904887	-1.421367
H	-1.707827	1.800307	-3.565591
C	3.519227	0.998163	-1.097136
C	5.646948	0.195795	-1.834703
C	3.697203	-3.159393	-3.777351
H	5.176531	-2.428729	-2.400669
C	1.820982	-3.982494	-5.345845
C	-1.976391	3.583840	-1.457215
O	2.127872	0.871620	-1.110429
C	4.083851	2.051291	-0.388107
H	6.260965	-0.468787	-2.444071
C	6.294377	1.159606	-1.028804
H	4.225657	-4.104346	-3.901198
C	1.605767	-3.370258	-6.745530
C	0.456498	-4.379495	-4.744731
C	2.675542	-5.248307	-5.498523
C	-2.720593	2.495154	-0.923814

C	-2.355200	4.851295	-1.044042
P	1.349177	0.460578	0.243678
C	5.511786	2.104428	-0.285448
C	3.216001	3.100875	0.210787
C	7.710646	1.211490	-0.937544
H	2.563523	-3.068648	-7.194369
H	1.129711	-4.107322	-7.409311
H	0.955838	-2.485804	-6.704577
H	-0.198487	-3.509325	-4.603171
H	-0.057267	-5.088178	-5.411460
H	0.581065	-4.870388	-3.768961
H	2.826967	-5.759763	-4.536250
H	2.164541	-5.956001	-6.166593
H	3.661270	-5.027298	-5.934241
O	-2.374500	1.207099	-1.337670
C	-3.773146	2.625537	-0.029418
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C	-3.396884	5.063362	-0.110935
O	2.024695	1.392234	1.371541
N	-0.129392	0.816102	-0.054768
N	1.761509	-1.052754	0.707041
C	6.183800	3.029382	0.554049
C	3.359364	4.483378	-0.146248
C	2.185716	2.753968	1.069821
H	8.296105	0.490567	-1.511261
C	8.333755	2.131198	-0.122087
P	-1.573727	0.247791	-0.306532
C	-4.456382	1.414074	0.499647
C	-4.117895	3.942354	0.422392
C	-3.721427	6.372576	0.335420
S	2.299072	-1.483176	2.199772
H	1.470549	-2.119631	-0.081854
C	7.560861	3.039264	0.637119
H	5.597006	3.725173	1.152208
C	4.303423	4.944406	-1.100602
C	2.467726	5.440975	0.444229
C	1.282904	3.674927	1.667810
H	9.422177	2.152731	-0.051568
O	-2.319964	0.525870	1.102713
N	-1.786389	-1.258658	-0.781752
C	-3.712515	0.410129	1.107705
C	-5.875625	1.242118	0.410416
C	-5.103516	4.189268	1.413924
H	-3.171110	7.215794	-0.087599
C	-4.693949	6.577744	1.289298
O	2.291085	-2.939355	2.204185
O	1.624925	-0.760164	3.266427
H	8.055816	3.745714	1.304559
H	4.967742	4.227991	-1.580132
C	4.381918	6.280162	-1.437599
C	2.586850	6.810945	0.087377
C	1.465860	5.010047	1.344928
C	0.191591	3.252907	2.572820
S	-2.234912	-1.708122	-2.255402
C	-4.278027	-0.717304	1.767180
C	-6.476213	0.113994	1.062045
C	-6.708345	2.116946	-0.333436
C	-5.383052	5.472293	1.837914

H	-5.639930	3.348410	1.849938
H	-4.928106	7.587963	1.627830
H	5.110462	6.606390	-2.181355
C	3.523090	7.226379	-0.833785
H	1.907288	7.528683	0.551775
H	0.812291	5.757780	1.798337
C	0.367912	2.278172	3.564573
C	-1.069899	3.864802	2.477884
O	-1.614100	-0.934101	-3.328730
O	-2.110874	-3.168027	-2.313054
C	-5.661105	-0.813804	1.749945
C	-3.460660	-1.724044	2.482507
C	-7.884107	-0.056886	0.989600
C	-8.070585	1.909448	-0.403390
H	-6.256122	2.950379	-0.869229
H	-6.140335	5.632917	2.606810
H	3.598210	8.280415	-1.104474
C	-0.668597	1.945591	4.436391
H	1.321847	1.765829	3.667629
C	-2.096580	3.531013	3.353367
H	-1.257083	4.593241	1.687617
H	-6.144266	-1.636213	2.279165
C	-2.300385	-1.385350	3.204748
C	-3.876967	-3.063685	2.524587
H	-8.330510	-0.916808	1.492524
C	-8.667877	0.821632	0.273325
H	-8.688866	2.583822	-0.997294
F	5.439173	2.655943	3.789567
C	-1.921477	2.567774	4.361308
H	-0.477906	1.183516	5.191307
H	-3.058791	4.030795	3.235408
C	-1.627769	-2.336886	3.963557
H	-1.924255	-0.364306	3.192732
C	-3.204620	-4.008199	3.300983
H	-4.744911	-3.375670	1.940648
H	-9.746597	0.670269	0.213746
C	6.207477	1.545116	3.967616
C	-3.060436	2.265664	5.340961
C	-2.075553	-3.665273	4.057124
H	-0.732527	-2.021740	4.502584
H	-3.583589	-5.030021	3.315269
F	6.081451	1.191897	5.279190
C	5.779671	0.418189	3.060588
F	7.500758	1.908104	3.775487
C	-2.709073	1.130283	6.312734
C	-4.332601	1.864546	4.569139
C	-3.349813	3.542492	6.158401
C	-1.360582	-4.650870	4.987830
C	6.718032	-0.308228	2.329124
C	4.424357	0.081270	3.012629
H	-3.559087	0.949931	6.986614
H	-2.499862	0.190373	5.781560
H	-1.838418	1.380012	6.936459
H	-4.172042	0.948333	3.985775
H	-5.157020	1.679305	5.274216
H	-4.652380	2.655107	3.877475
H	-3.646316	4.375475	5.505486
H	-4.167524	3.359721	6.872274

H	-2.460308	3.855405	6.724160
C	0.109959	-4.817206	4.557255
C	-2.022937	-6.035319	4.990412
C	-1.405850	-4.088448	6.424819
C	6.293080	-1.382483	1.542528
H	7.770950	-0.036390	2.363832
C	4.022729	-0.988570	2.220043
H	3.683494	0.632972	3.589646
H	0.632415	-3.854862	4.475936
H	0.649571	-5.439536	5.287208
H	0.168997	-5.318494	3.580705
H	-1.479765	-6.701120	5.676460
H	-3.068270	-5.987477	5.328674
H	-2.002526	-6.499597	3.993285
H	-0.914977	-4.786129	7.120100
H	-0.890592	-3.120923	6.495471
H	-2.444596	-3.944042	6.755317
C	4.943786	-1.730078	1.480029
C	7.300056	-2.234053	0.810562
H	4.609408	-2.576288	0.878848
F	8.496145	-1.610573	0.657267
F	6.863795	-2.584480	-0.433388
F	7.539399	-3.397697	1.479153
C	-4.880812	-2.274145	-1.706850
C	-4.003911	-1.393929	-2.339036
H	-4.489316	-3.135812	-1.166555
C	-6.254803	-2.046926	-1.796886
C	-4.479656	-0.297987	-3.052105
C	-6.750824	-0.944451	-2.496400
C	-7.196387	-3.052156	-1.184589
C	-5.856900	-0.073656	-3.118635
H	-3.775490	0.364013	-3.553531
H	-7.822093	-0.763051	-2.548533
F	-6.817714	-3.402992	0.080560
F	-7.226101	-4.206886	-1.909496
F	-8.472914	-2.597529	-1.109384
C	-6.351700	1.106617	-3.915178
F	-7.682114	1.325978	-3.754872
F	-5.705093	2.255702	-3.566571
F	-6.133464	0.930006	-5.250128
H	-1.169615	-4.795344	-2.111482
H	-2.187532	-6.829526	-0.582516
H	-0.233482	-6.438018	0.832519
H	-0.928704	-3.445667	0.511028

228

A-P

C	0.35000118224245	-4.40574651798565	-0.84692258760425
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C	-0.93422331025604	-5.42219940956308	0.90656330180369
C	-1.70489247886237	-5.66381149924050	-0.38796231432321
O	-0.96330918742090	-4.92632000951641	-1.45091546040406
H	0.77947481178347	-4.07778700379730	1.26796744249500
H	-1.61572374398652	-5.24317351480055	1.74620289875251
H	-2.71284757018176	-5.23200499870241	-0.38180248062186
C	1.38427709014258	-5.50476640951105	-1.02190200666280
C	1.20319028418002	-6.58440169386709	-1.89259754650338
C	2.59862144390027	-5.37984915722037	-0.33073498900035
C	2.21656401494228	-7.53126059746390	-2.06565939538685

H	0.27126849540155	-6.68299946095524	-2.44948444430524
C	3.60902565484700	-6.32333872480482	-0.51034337407854
H	2.75325618116512	-4.53992192890302	0.35008825656178
C	3.42300822454206	-7.40305435193345	-1.37780361507609
H	2.06093152964411	-8.36778147416125	-2.74887662693589
H	4.54848533666780	-6.21279859604333	0.03378823903000
H	4.21486666585052	-8.14076208768321	-1.51560719990820
C	0.74145928245590	-3.17053540362282	-1.62593890209375
H	0.79444139502581	-3.38397863074405	-2.69842222936459
H	0.05682113731927	-2.33871545528036	-1.43600250186020
H	2.73510767081449	5.07836282358726	-5.38427283482570
C	2.58423739427331	4.22408065724782	-6.05880476789047
C	2.53392961066001	2.89294586447318	-5.27847086996594
H	3.41391551286026	4.20907095645156	-6.78204193579743
H	1.64746318538670	4.38977519331718	-6.61036257644176
C	1.37096158922147	2.96088217698761	-4.28256977327317
C	3.86607848924172	2.70401758540647	-4.52460607563385
C	2.37658386309259	1.74768054079980	-6.28831082464818
C	2.79007985189853	-0.88217447225085	-3.43168624652731
C	1.38133051592542	3.93175368399615	-3.26795329866175
C	0.25330982453440	2.11768524330003	-4.34260808473999
H	4.04434342408082	3.51884541511557	-3.81017502460401
H	3.88000225659939	1.75837607575155	-3.96671033231382
H	4.70382532058116	2.69029911954459	-5.23809194542816
H	1.46011282341888	1.85588001651344	-6.88643177912717
H	3.22971619498613	1.75170541308097	-6.98208296959771
H	2.35758429236545	0.76592412625967	-5.79499849637168
C	3.844444450266045	-1.08122434530609	-2.52250845913299
C	2.42787358574365	-1.88078611602993	-4.32848203655134
H	2.26001489846489	0.06929672822905	-3.44951478382405
C	0.32129893756708	4.06963215024855	-2.38179110723764
H	2.23834286406452	4.59643572787777	-3.15372911681070
C	-0.81734595672214	2.25015782232549	-3.45597886939515
H	0.19513050753129	1.33710889916011	-5.10111078897661
C	4.37278767758972	0.01914970543218	-1.68523691647677
C	4.45802331288398	-2.34202897861605	-2.50619728643791
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228

B-E

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C	7.87865348501551	-3.35059763644335	-0.91032280668866
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C	7.14350633670143	-3.39561419184761	-2.11731956746422
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H	-6.58455957546795	-1.53025231832885	-5.66180412073619
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H	-7.76203452276240	3.29956921252805	-0.70049677635395
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F	6.03056724603364	-0.59717955644897	-4.19120169677407
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228

B-TS1

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C	2.69873709569998	-4.28328092656919	-2.56797302466290
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H	7.80560203927562	-3.03737233699607	1.20206087717608
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O	-2.16952837565687	0.68286096345060	-1.35301936542422
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228

B-P

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228

C-TS1

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228

C-I

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H	0.73047762694225	3.82017062356110	0.07760504248180

228

C-TS2

C	-0.95153073487245	4.31938910520483	-0.66747169331128
C	0.36603602397297	4.52473419208399	-0.00575032884305
C	0.97405182270756	5.95230031718352	-0.04329823462844
C	2.42949457638411	5.94472067112743	-0.48449412634635
O	2.46076938188640	5.64659071334896	-1.88084852001359
H	0.22170220284703	4.21006037984426	1.04575348224125
H	0.91663381764551	6.42242662512774	0.94853992159207
H	2.99376990717822	5.19555094082539	0.10154486990506
C	-2.06215717916510	5.22220539444815	-0.45927312008763
C	-3.19085412412044	5.19021099322233	-1.31380930162019
C	-2.08046591210765	6.10961186307361	0.64209429555895
C	-4.29246401752818	5.99799046320576	-1.06515160915018
H	-3.19427993378387	4.53317906064546	-2.18254602813940
C	-3.19048747567375	6.90218181645499	0.89650017938119
H	-1.23944576242638	6.13003049166825	1.33026518165932
C	-4.29954043933261	6.84876613857370	0.04501977474468
H	-5.15655921401788	5.95641849615624	-1.72872743324074
H	-3.20054361590929	7.55701926709464	1.76848660345605
H	-5.17341511333139	7.46957093693608	0.24884661553722
C	-1.09028164823127	3.14369705657084	-1.47493952085561
H	-2.00870818157326	3.04448128082743	-2.05514644728284
H	-0.17461970161890	2.91958155472371	-2.04780170214071
H	-3.38457142250058	-2.35517596849984	-3.82144286613898
C	-3.50216659144429	-3.41866617281647	-4.06760402272193
C	-2.22961807407808	-3.97424919767606	-4.73501721241616
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C	-1.95918676706047	-3.15919521158761	-6.00741755967593
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C	-3.94504397077036	1.83474452971955	-3.38443355740085
C	0.08644040939413	-3.14352696888347	-3.97643604033572
C	-1.10890801316732	-4.64787272096852	-2.54801243366148
H	-1.82088240098779	-2.09098066546259	-5.78492117615323
H	-1.06891754975525	-3.52077117007701	-6.54250618588541
H	-2.81867623957740	-3.24732651538998	-6.68785232910573
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H	-1.57353106956663	-5.87428323735947	-5.60560451335609
C	-3.36959158318696	0.61956888141849	-2.96305449367821
C	-3.28446723723212	2.67927987445964	-4.27196075176718
H	-4.91583639224680	2.13612278835819	-2.99029904153347
C	1.14535329836173	-3.11714496503838	-3.07009907504884
H	0.17307484987036	-2.54284585728932	-4.88109376641123
C	-0.05459990602291	-4.62933344483438	-1.64101772087841
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C	-2.10806013438700	0.29586648470198	-3.49348140187603
C	-2.00698910957848	2.37279533290662	-4.77477377384304
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H	2.00964842826630	-2.49444672394322	-3.29177421255357
H	-0.14271521654521	-5.18564894767716	-0.70634844407505
C	-3.46164222234903	-1.16318993828672	-1.13523752520647
C	-5.49968528745519	-0.30893998202449	-2.05032710014637
C	-1.44599135575251	1.15582858018344	-4.36965659422906
H	-1.61745399726480	-0.63624941598162	-3.22330397817465
C	-1.27879732657444	3.35649414295459	-5.69463715231498
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H	-0.45423636090025	0.86304670999978	-4.71077349102220
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C	-2.15104282922691	3.63592682351170	-6.93503929494686
C	0.08059115474467	2.81392798276620	-6.15834716209390
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P	-1.31851349156972	-0.62193804459194	0.25685486028529
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H	-1.97476806530191	5.11770744658348	-4.57107714200017
H	-0.37067098627986	4.51282824128817	-4.07070928455706
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H	0.56090547174098	3.55185748449451	-6.81724892515627
H	0.75527797554834	2.62991553854824	-5.31056967711696
H	-0.02907162204700	1.87912408105858	-6.72740219399563
O	2.46129170639095	-1.48685104250875	-1.11745608285250
C	3.92542400629138	-2.61537071817127	0.37902934524551

H	2.17588536778379	-5.99113107359203	-0.58878465917531
C	3.68208320741513	-5.05721539892565	0.65333032213208
O	-2.11830660766963	-1.39754061770082	1.43255008513089
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C	-6.32440407693697	-2.83312658764079	0.59004445814106
C	-3.55190095146515	-4.53946161055901	0.13794643660970
C	-2.33787511232313	-2.76600586646779	1.24682829188279
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P	1.52719790433126	-0.49863897424823	-0.23307568567547
C	4.48909801320420	-1.29185748069952	0.76565100229671
C	4.34021332864266	-3.83236115892678	1.01509977861958
C	4.06028378628421	-6.26327817782186	1.30095502979549
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H	-1.10446511524949	2.28168096174826	-0.72533910941477
C	-7.70026595732339	-2.73788076387759	0.61787844089955
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C	-4.49429282378479	-5.03997838846389	-0.79803423793624
C	-2.71437732549006	-5.48159829989990	0.82642373783906
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O	2.26625192473906	-0.52687839952127	1.21370084785071
N	1.59435977273979	0.94735476379702	-0.90695968125987
C	3.64015986168019	-0.30328881139003	1.24909768318418
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C	-0.40975851580746	-3.21381661742557	2.84086390572204
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C	6.36154823053596	0.25991027965169	1.19675877292976
C	6.81353955040808	-1.85520365192737	0.04003739905060
C	5.66250879121779	-5.06463966431907	2.65191129523943
H	5.82519131917619	-2.95544371432002	2.33057385467439
H	5.30155131597821	-7.20483352440857	2.77661400513352
H	-5.33932741253862	-6.75004230058905	-1.76938196351446
C	-3.80375107850730	-7.32107513213675	-0.34276086894305
H	-2.23509117382418	-7.57298746715261	1.10554748568463
H	-1.10777977735088	-5.75559531729413	2.24909838507362
C	0.84785546070427	-3.83996248911068	2.80113944465061
C	-0.59040512897489	-2.17380514449796	3.76269980459353
O	1.73723655547322	0.18371880794128	-3.37286867460411
O	1.69297818322198	2.60464013734645	-2.73898202837058
C	5.45192035501033	1.15824380748002	1.80206917942687
C	3.15316284713818	1.85414364449376	2.49195054288567
C	7.74310163104802	0.57081249179426	1.09314187553706
C	8.14718556405401	-1.51567374942427	-0.05863160793033
H	6.45429881070442	-2.78894915459716	-0.39154361476997
H	6.41937599328523	-5.06851347270958	3.43780040758117

H	-3.90947878057347	-8.38929971949240	-0.53688650858579
C	1.86836005108486	-3.45656904125868	3.66444415480313
H	1.03903208005802	-4.61637476649529	2.05853813277499
C	0.43602460889698	-1.79854637947616	4.62904784813497
H	-1.54028655348125	-1.64466271439245	3.81235436434176
H	5.84312488031926	2.06709220576743	2.26137175057154
C	2.07819774269178	1.38760799118942	3.26435689379649
C	3.35193436573472	3.24451260227161	2.43289278098379
H	8.09331295386822	1.52343437600235	1.49619747601683
C	8.62029394301337	-0.29676800891896	0.47803246424211
H	8.83856245254318	-2.18638739893192	-0.57012143295062
F	-8.07316692552213	2.21264639030196	-0.38371484725138
C	1.68476104370676	-2.43330719745658	4.61073772883664
H	2.83147216506969	-3.96405712212285	3.58784564496938
H	0.24210254942288	-0.98991042763956	5.33307745148518
C	1.26337054276595	2.26608381249273	3.97259750354986
H	1.86966911428230	0.32163235557739	3.32746954236123
C	2.52696795915011	4.11779295990130	3.13877578567811
H	4.16425020562776	3.64584667912992	1.82365329366030
H	9.67765967852372	-0.04105835974454	0.39488122381015
C	-6.90439984357469	2.81207979936043	-0.03842582003098
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C	1.47175091775427	3.64958323076281	3.94195073811571
H	0.43921732098225	1.84598959570752	4.54517837317208
H	2.72103761713651	5.19043517851695	3.06647452816009
F	-7.23055211945486	3.99847101902225	0.55686534837518
C	-6.06010735064239	1.95505669241945	0.86680795321091
F	-6.25908212138386	3.13203945916732	-1.19862056346527
C	4.07228028571795	-1.65634201956779	4.79768993319222
C	3.14287307878326	-3.31509954364807	6.43679565240833
C	2.42837593203489	-0.92219807925185	6.52412273899824
C	0.60395815898787	4.62443479693399	4.74477488514244
C	-6.67831166670420	1.04741335548398	1.73313681811592
C	-4.67714173041734	2.13072618497808	0.88673524977270
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H	3.88748729400430	-0.75677736753137	4.19536117121853
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H	2.26250448787765	-3.64170515668099	7.00915765762010
H	3.47110763743667	-4.15593541316024	5.80987438250314
H	3.95127015427630	-3.08370425275306	7.14722116641765
H	3.26840700804221	-0.70751207533233	7.20055995657715
H	2.20455760060802	0.00055420347503	5.96946849627012
H	1.55675329772342	-1.17616816687372	7.14496747481056
C	1.50464298201882	5.48108121260209	5.65641191243082
C	-0.42617264875115	3.89431069626555	5.61893401308394
C	-0.16506614451523	5.53960276331361	3.77244624090129
C	-5.89668468346253	0.31866408005449	2.62727777020087
H	-7.75711133266412	0.90676069070087	1.70558590911168
C	-3.91174647215650	1.38660103572326	1.78502927100122
H	-4.19439745837593	2.84640892325946	0.22166366881944
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H	0.89271878784414	6.18402942202992	6.24185683817623
H	2.06537964006735	4.84651934298101	6.35764318215234
H	0.06079350950512	3.23166130660091	6.34909760058021
H	-1.01863674920974	4.63219396101652	6.17933606835583
H	-1.11932851273053	3.29349892339084	5.01322263893105
H	-0.77613312915722	6.26544872288404	4.33121262423923
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C	-4.50850767650160	0.48299393275817	2.65791579686005
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H	-3.88763879486834	-0.07489406940920	3.35772511972881
F	-5.88221432760741	-1.80042919761323	3.70925628551297
F	-7.83593069803686	-0.87221890608016	3.34547608072704
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C	4.47644083758819	2.38770546082088	-1.72684576983508
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H	3.84954628876627	3.17612684273246	-1.30977897757764
C	5.86734520062240	2.48554652517866	-1.71644420570657
C	4.64087133952475	0.26302103826933	-2.87793400092593
C	6.65616139087817	1.47530035092649	-2.27324159138244
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H	7.74102501738755	1.55373903321759	-2.26290468828968
F	7.82940739684792	3.78419297272734	-1.32727025541597
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C	6.85153295146284	-0.69383398303685	-3.54413746207600
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H	2.87565488625239	6.93727899888703	-0.28217140010901
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228

C-P

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C	1.73340175607608	5.53516549800805	-1.02885137181888
O	0.67029514668492	4.82832002271685	-1.79702617694667
H	-0.32506010114260	4.26152854474042	1.33393241782899
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C	-1.30519074742387	5.82604469982548	-0.74554297315779
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C	-1.27592763569869	6.78929554688653	-1.76132617331001
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C	-2.07821483600379	7.92932981593626	-1.67883571091416
H	-0.62929116086169	6.64566927459389	-2.62714888631980
C	-2.92799621887856	8.11318885532977	-0.58769107295778
H	-3.64708610588346	7.27061904516720	1.26849663254010
H	-2.04077054939997	8.67301061150216	-2.47652463674233
H	-3.55602193248136	9.00298975429163	-0.52426978754425
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H	-1.71494417084819	3.68618328192346	-2.38099235520767
H	-0.69181377372235	2.49613375667124	-1.50092244884271
H	-3.58669631530235	-2.39471739162606	-3.89521037358457
C	-3.56246847279183	-3.41709986502240	-4.29481386131476
C	-2.20798770815969	-3.72342486776710	-4.96298241689445
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228

TS1-1

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O	2.024695	1.392234	1.371541
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N	1.761509	-1.052754	0.707041
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C	3.359364	4.483378	-0.146248
C	2.185716	2.753968	1.069821
H	8.296105	0.490567	-1.511261
C	8.333755	2.131198	-0.122087
P	-1.573727	0.247791	-0.306532
C	-4.456382	1.414074	0.499647
C	-4.117895	3.942354	0.422392
C	-3.721427	6.372576	0.335420
S	2.299072	-1.483176	2.199772
H	1.470549	-2.119631	-0.081854
C	7.560861	3.039264	0.637119
H	5.597006	3.725173	1.152208
C	4.303423	4.944406	-1.100602
C	2.467726	5.440975	0.444229
C	1.282904	3.674927	1.667810
H	9.422177	2.152731	-0.051568
O	-2.319964	0.525870	1.102713
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C	-3.712515	0.410129	1.107705
C	-5.875625	1.242118	0.410416
C	-5.103516	4.189268	1.413924
H	-3.171110	7.215794	-0.087599
C	-4.693949	6.577744	1.289298
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O	1.624925	-0.760164	3.266427
H	8.055816	3.745714	1.304559
H	4.967742	4.227991	-1.580132
C	4.381918	6.280162	-1.437599
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S	-2.234912	-1.708122	-2.255402
C	-4.278027	-0.717304	1.767180
C	-6.476213	0.113994	1.062045
C	-6.708345	2.116946	-0.333436
C	-5.383052	5.472293	1.837914
H	-5.639930	3.348410	1.849938
H	-4.928106	7.587963	1.627830
H	5.110462	6.606390	-2.181355
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H	1.907288	7.528683	0.551775
H	0.812291	5.757780	1.798337
C	0.367912	2.278172	3.564573
C	-1.069899	3.864802	2.477884
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O	-2.110874	-3.168027	-2.313054
C	-5.661105	-0.813804	1.749945
C	-3.460660	-1.724044	2.482507
C	-7.884107	-0.056886	0.989600
C	-8.070585	1.909448	-0.403390
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H	-6.140335	5.632917	2.606810
H	3.598210	8.280415	-1.104474
C	-0.668597	1.945591	4.436391
H	1.321847	1.765829	3.667629
C	-2.096580	3.531013	3.353367

H	-1.257083	4.593241	1.687617
H	-6.144266	-1.636213	2.279165
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C	-3.876967	-3.063685	2.524587
H	-8.330510	-0.916808	1.492524
C	-8.667877	0.821632	0.273325
H	-8.688866	2.583822	-0.997294
F	5.439173	2.655943	3.789567
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H	-3.058791	4.030795	3.235408
C	-1.627769	-2.336886	3.963557
H	-1.924255	-0.364306	3.192732
C	-3.204620	-4.008199	3.300983
H	-4.744911	-3.375670	1.940648
H	-9.746597	0.670269	0.213746
C	6.207477	1.545116	3.967616
C	-3.060436	2.265664	5.340961
C	-2.075553	-3.665273	4.057124
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H	-3.583589	-5.030021	3.315269
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C	5.779671	0.418189	3.060588
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C	-2.709073	1.130283	6.312734
C	-4.332601	1.864546	4.569139
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C	-1.360582	-4.650870	4.987830
C	6.718032	-0.308228	2.329124
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H	-2.499862	0.190373	5.781560
H	-1.838418	1.380012	6.936459
H	-4.172042	0.948333	3.985775
H	-5.157020	1.679305	5.274216
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H	-2.460308	3.855405	6.724160
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C	-1.405850	-4.088448	6.424819
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H	0.632415	-3.854862	4.475936
H	0.649571	-5.439536	5.287208
H	0.168997	-5.318494	3.580705
H	-1.479765	-6.701120	5.676460
H	-3.068270	-5.987477	5.328674
H	-2.002526	-6.499597	3.993285
H	-0.914977	-4.786129	7.120100
H	-0.890592	-3.120923	6.495471
H	-2.444596	-3.944042	6.755317
C	4.943786	-1.730078	1.480029
C	7.300056	-2.234053	0.810562
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C	-4.479656	-0.297987	-3.052105
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H	-3.775490	0.364013	-3.553531
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F	-7.226101	-4.206886	-1.909496
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F	-5.705093	2.255702	-3.566571
F	-6.133464	0.930006	-5.250128
H	-1.169615	-4.795344	-2.111482
H	-2.187532	-6.829526	-0.582516
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228

TS1-2

C	-1.93191756467025	-3.66461720900963	-2.72970872642533
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H	0.61067980187685	-5.21680476299151	1.32422194057757
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O	-0.13367096260293	1.97577211914020	-2.55109356168980
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S	-2.73273496598308	0.20314783495269	-2.86779323239483
H	-1.24616217854593	-1.67347436005262	-2.26066454488254
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C	0.39575897026458	5.16128066600022	1.13337753796967
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C	6.45228073824287	-2.98881948331819	-5.18605218830564
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O	1.68919200230988	-4.96964854817919	-1.30646600404209
C	5.19618340629011	-3.22168545343239	-5.79089868434283
C	2.76099148991418	-2.80930144314647	-6.08163146291278
C	7.59479769810169	-3.75049849325163	-5.54743290222119
C	8.92351655521821	-2.56643475700827	-3.91261651209978
H	7.93477578493189	-1.05392170690892	-2.76154096011482
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H	0.16649208787405	2.73866505596533	-4.86035732479143
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H	1.04721337668652	1.93261084457157	-6.99442255374863
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228

TS1-3

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H	-1.93592300506614	6.54164802737925	-3.76388312016828
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C	6.96384775351490	2.68357974850794	-0.44167236074431
H	4.25507534297188	2.77852639294387	-0.68878526369274
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228

TS1-4

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H	-1.47735548579194	-2.14599076345834	-0.19364981522272
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C	-0.26359512871430	2.45312537570372	-3.45822284873157
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C	7.93372017847007	-0.08860625554715	-0.96280634261172
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H	6.25186834860037	5.64273393706309	-2.20081208679239
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H	1.39702560914610	4.61085851349734	-1.43147524133086
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H	7.81196913091574	-1.17712073344250	2.45376873155983
F	8.36088674540352	-2.87932612603659	0.81648337074375
F	6.64274818085523	-3.56605981234180	-0.35844093498563
F	7.11217673344045	-4.51820716973616	1.55111158159702
C	6.43977112595738	0.61058764415319	4.01637559530223
F	6.24185822429673	0.32284281061546	5.33499162369592
F	7.77398303793870	0.79584754613362	3.84534244391088
F	5.82989504396466	1.80830736095270	3.78618307752876
H	1.03568840547221	-4.96410109683211	1.80575274618838
H	1.42853269838976	-6.79206947015166	-0.31297548159399
H	1.93838750125204	-4.79366457592284	-1.69900083681896
H	-0.29941057837203	-3.92700928015770	-2.02406019942364
228			
TS1-1'			
C	0.14941323787541	-4.41026946214439	-0.81157055844671
C	0.49324290974072	-5.66309673084176	-1.55506659404388
C	-0.77548814980113	-6.48046113283091	-1.90752828607213
C	-1.83832243109286	-5.68070524384267	-2.65262844583548
O	-2.45199743514897	-4.74601720975968	-1.76395875431854
H	1.02221663849773	-5.39428747358371	-2.48039898035230
H	-1.22838490093546	-6.87991952575085	-0.98682970233849
H	-2.60143216220595	-6.37789358230407	-3.04670877036953
C	-0.31085135603640	-4.50042119992982	0.57499594750443
C	-0.09543032687650	-5.66323793646572	1.34368734794442
C	-0.89666038645556	-3.39002124414029	1.20912923013183
C	-0.42462989850006	-5.69506946768045	2.69433038541335
H	0.37431136051337	-6.53715601048900	0.89471397391996
C	-1.22268523193125	-3.41840270649616	2.55744858428478
H	-1.11724835224546	-2.49687131307562	0.63252042418962
C	-0.98035335318883	-4.56899700174699	3.30842552376341
H	-0.23335520011371	-6.59774747341909	3.27609815703395
H	-1.66703082350877	-2.53679493644472	3.01619626155668
H	-1.22656172653154	-4.59253482430710	4.37148393011844
C	0.36416401900140	-3.18290910525563	-1.42704990366125
H	0.69704929360963	-3.18260829511599	-2.46645010187903
H	-0.29808454110911	-2.34872168826616	-1.16697160904508
H	5.20980109780950	2.03742245724744	-5.81132336085419
C	4.52621314475165	2.08742792353728	-4.95031867456363
C	3.29291835561707	2.93919775914696	-5.31251006733976
H	5.08429234312480	2.50822447023384	-4.10270299471144
H	4.22895271795443	1.06376111827397	-4.68615390141222
C	2.36649037589295	3.07373955955689	-4.09964753413444
C	2.59160557379832	2.27434097660452	-6.50557794052690
C	3.75484170111558	4.35057676527381	-5.73204799644134
C	4.08276619655316	-1.92381884514826	-3.26999776642414
C	1.00345470466508	2.75320332238612	-4.14476691135021
C	2.86334189348547	3.55872676688261	-2.87793945853738
H	1.73460946312566	2.86528198960207	-6.85982027596350
H	3.29958280622063	2.18295326670416	-7.34198662800572
H	2.23873800570706	1.26395150397985	-6.25197458704564
H	2.89439956952572	4.98053421117348	-6.00033874961801
H	4.29977345389548	4.85092366952464	-4.91906080579897

H	4.42395786619301	4.28882244868055	-6.60383297158800
C	3.48270163647995	-0.76174925055975	-2.75982687854833
C	3.47742607294476	-2.66682493040101	-4.28437306292539
H	5.03776570141514	-2.25998869761975	-2.86255208657838
C	0.17764302517051	2.89830926396299	-3.03048207471982
H	0.56175065295034	2.36371878057547	-5.06097394157520
C	2.04324868013039	3.71801101837316	-1.76720894232307
H	3.92063304353681	3.81426588781475	-2.78352590741999
C	4.19477590352611	0.04805609757089	-1.74703963918980
C	2.23198108530875	-0.39341961425490	-3.28739895113181
C	2.24612047343362	-2.28397663842913	-4.83352402837195
H	3.98640748155208	-3.55978008341943	-4.64663920892398
C	0.67885202541805	3.38812424312774	-1.81532259928872
H	-0.87187367472770	2.62733920481000	-3.11902564511525
H	2.47342799124229	4.08572414833686	-0.83654148295107
C	3.52793720732409	0.71389749887137	-0.68194855490660
C	5.57268466172494	0.18885135671197	-1.79576767689090
C	1.63679498220840	-1.13695320512578	-4.29922201274447
H	1.72630653722527	0.50038651647903	-2.93338883429378
C	1.56086711767665	-3.04372321264485	-5.97238885251626
C	-0.19559478369018	3.64606281287418	-0.64932246111745
O	2.13013944599050	0.62583095922543	-0.63797590122982
C	4.16727105207222	1.44993651867338	0.30782589284536
H	6.12370632590718	-0.25897812378968	-2.62373353114918
C	6.29852327934154	0.87506830769538	-0.79610922678320
H	0.66359377001156	-0.80736867963303	-4.66427524829435
C	2.38338134731315	-4.24881728753104	-6.44719488236925
C	1.36538935385715	-2.08381222379437	-7.16484555720085
C	0.18397827075860	-3.54727205162248	-5.49557053475332
C	-1.31585872090577	2.82654133013158	-0.32547654486661
C	-0.00113278957234	4.76520269518433	0.14484509781528
P	1.50049155929193	-0.35112963649979	0.48140822168345
C	5.60036845000168	1.48863133227491	0.29694858756190
C	3.36561965947128	2.16494205353533	1.33679810548463
C	7.71682754260286	0.93692655879114	-0.83384144756374
H	2.53283676678423	-4.98284957862442	-5.64142278116815
H	1.85309127846231	-4.75685533163674	-7.26543929468472
H	3.37069909053322	-3.94597067148738	-6.82568609588506
H	0.87885397037019	-2.61075047987851	-7.99945683508955
H	0.73404092920103	-1.22723362796669	-6.89253315230726
H	2.33215614987014	-1.69597994635291	-7.51774448113423
H	0.30315233381986	-4.27175279144133	-4.67649488683060
H	-0.45538297987457	-2.73133831430572	-5.13249845783201
H	-0.34255566960015	-4.05278617756059	-6.31929383387082
O	-1.47057606865833	1.62721694157208	-1.03215244028726
C	-2.28724280695715	3.16946982786787	0.60198633063363
H	0.83593788670028	5.43156892583353	-0.07019450224946
C	-0.86254408531353	5.08948932877044	1.21828500510245
O	2.23303874766532	0.11324216408918	1.83976982374042
N	-0.03181751257435	-0.10746589024858	0.49322371784865
N	2.03625331485001	-1.87594917771950	0.24356511175395
C	6.36269546677905	2.07489152143221	1.33974083131478
C	3.51403890915058	3.57564720048059	1.55932515932611
C	2.39395818492940	1.49047556475787	2.06574170928490
H	8.23534601622047	0.47204650181468	-1.67449299092643
C	8.42651797875146	1.53941109990112	0.18219683507213
P	-1.38507662291942	0.21400220374781	-0.24329287162203
C	-3.56414898591220	2.41348959065376	0.69348012407200

C	-2.03817067075094	4.30115356898050	1.44758028383357
C	-0.59617421125330	6.19791626405098	2.06498036989750
S	2.78282756271703	-2.84904791794198	1.35250412188977
H	1.32232556552217	-2.60834260583727	-0.64025035408965
C	7.74117204904434	2.09872656153314	1.28432772021725
H	5.84717971884846	2.49731887844090	2.20068379820036
C	4.37702976653450	4.39712974519466	0.78555415617617
C	2.71314556322491	4.20190873449963	2.57123003500079
C	1.54830985519184	2.09502169078702	3.03555212158852
H	9.51645017443481	1.56914608464755	0.14706546271974
O	-2.37614239996699	0.36380933415293	1.03219649901803
N	-1.89246198451745	-0.91132394831383	-1.24249580967814
C	-3.59162409087294	1.04396920813622	0.92601982322726
C	-4.81108539861357	3.10812958387822	0.53400024276888
C	-2.87558364236623	4.63850191771183	2.54286801469373
H	0.29648753075546	6.79488693716672	1.86933606687337
C	-1.43048944854928	6.50067137392857	3.11913559592935
O	2.86004322070678	-4.15084538297030	0.70522888018310
O	2.20218277579181	-2.71725030661130	2.67874861742950
H	8.30571573470409	2.54092106813755	2.10609625257253
H	4.95957077668001	3.94823431657812	-0.01726684935196
C	4.47693539469518	5.75199852225968	1.02596938412380
C	2.86155701332861	5.59399056541188	2.81297976331298
C	1.75913863905440	3.44210011709794	3.28372785880909
C	0.45039402391638	1.37245275112561	3.71726966529968
S	-2.36596637776206	-0.85882990387623	-2.76844131892012
C	-4.79406530874909	0.32123210305289	1.19028877184222
C	-6.03192215186679	2.40120647436493	0.78370408501250
C	-4.89166197834865	4.45464434719503	0.09321891458366
C	-2.57400690913042	5.70571706730120	3.36378525061687
H	-3.75558519567543	4.02868514205907	2.74388679193468
H	-1.21023093107285	7.34947287396222	3.76834843188055
H	5.14094939322743	6.36094184207538	0.41081364345640
C	3.72616481120021	6.35712355501109	2.05985241273261
H	2.25758753266408	6.04807775849686	3.60090990606200
H	1.15017894055937	3.94346025110637	4.03781693769758
C	0.56903696738558	0.06771692391216	4.22531693797036
C	-0.77741277725785	2.02758677883930	3.88847137394978
O	-1.45423991032081	-0.12174925731056	-3.63886874953583
O	-2.70709238265148	-2.23652130049261	-3.14462404597780
C	-5.98026367572072	1.03620910498022	1.14252963375995
C	-4.83983501490238	-1.12176041424241	1.52292759957259
C	-7.27226355083163	3.07403289489198	0.62544274181310
C	-6.11258370621097	5.07667314242731	-0.06609576285106
H	-3.97573214157494	4.99323731590316	-0.14421222333957
H	-3.22274749144509	5.93626788239912	4.21003880715343
H	3.82593694105313	7.42668647104866	2.25042779946102
C	-0.49362789246003	-0.52887451837600	4.89817031534066
H	1.49444433458116	-0.49237692899986	4.10194032236245
C	-1.84107890815190	1.41526487104260	4.54618857696283
H	-0.91524198845309	3.02596863376672	3.47448381431720
H	-6.91771806557488	0.50750446162288	1.32313419993303
C	-5.66555002039189	-1.57074853323268	2.56931390607041
C	-4.15652271254962	-2.09027489919638	0.77876387238098
H	-8.19249662512451	2.51894702419180	0.81731835826263
C	-7.31476558259631	4.38758511610775	0.21172904492340
H	-6.14967378759572	6.10548619844053	-0.42655237416915
F	6.55500268469040	-1.24253405913641	5.09663226822712

C	-1.72412499043938	0.12548090361946	5.08031226033592
H	-0.34810939478351	-1.53608008059189	5.29211324051225
H	-2.77740848115289	1.96552346263050	4.63420470022230
C	-5.78269423217896	-2.92693954286012	2.85664633346207
H	-6.20313408399107	-0.84285039177012	3.18015622772322
C	-4.28939951790007	-3.44911184929917	1.06115142624411
H	-3.51181280716458	-1.79029706100584	-0.04413084815682
H	-8.27314937464053	4.89255930654775	0.08288226364123
C	6.59735443291181	-0.42166061435448	4.00813363820627
C	-2.84856803413238	-0.53542744134740	5.88556270871242
C	-5.09431246629676	-3.90085345295403	2.11281772570144
H	-6.41905392067861	-3.22930546754157	3.69058472205464
H	-3.73690566522088	-4.15355909249715	0.43986181147372
F	7.85851307031875	0.07591959093158	3.93502160453489
C	6.19057440079306	-1.15836903537704	2.75649845124304
F	5.76144954885299	0.62058114214374	4.27570882531745
C	-3.10254330041769	-1.97243650049764	5.39440404600869
C	-4.16808496936914	0.24356518197743	5.77964705078595
C	-2.41617808542914	-0.57757603266848	7.36689296693766
C	-5.22960537404381	-5.38413152439290	2.46695127346276
C	7.14100342012216	-1.53578773646694	1.80790087905585
C	4.84990111231653	-1.51640434017820	2.60123613714242
H	-2.20497962815441	-2.59913434293664	5.48494067525887
H	-3.89342541573227	-2.44097260245654	5.99935479167684
H	-3.43335645234123	-1.98424598120130	4.34741150906560
H	-4.08615971027790	1.25128938997739	6.21168207116232
H	-4.49571889248935	0.33843790060124	4.73424562934532
H	-4.95457651011033	-0.28993490397880	6.33286470186865
H	-2.23400128727307	0.43664588257838	7.75066436570713
H	-3.20152185644018	-1.04482224689236	7.98080944763664
H	-1.49132601558465	-1.15786355210283	7.49384975623546
C	-4.79578414278094	-5.59794861269586	3.93184732153886
C	-4.35361015515502	-6.27182929544879	1.57051935955998
C	-6.70155927455867	-5.81237091204492	2.30068977089997
C	6.73982649931658	-2.27037130982190	0.69028789479906
H	8.18464574440382	-1.25666994789333	1.93522918488787
C	4.46992063672590	-2.24668076580065	1.47847589528634
H	4.10430320265470	-1.25349377012838	3.34990278101440
H	-5.41434047284459	-5.01640499485285	4.62959791823563
H	-4.88826649048421	-6.66062878207873	4.20295848717604
H	-3.74832393608833	-5.29611584051888	4.07257901710870
H	-4.48037049848078	-7.32438978395203	1.86373905657180
H	-4.62945710770489	-6.18183333561511	0.51014300614000
H	-3.28786103329753	-6.01999936947408	1.66753885614235
H	-7.36903476325282	-5.22618086804759	2.94801086055335
H	-7.03212025260628	-5.67430342502409	1.26115794166877
H	-6.82100410393997	-6.87470180421007	2.56287966790457
C	5.40170924816727	-2.62752346097023	0.51440686950298
C	7.76065306811194	-2.76126661350850	-0.30502553764471
H	5.08372390852186	-3.22194220264216	-0.34200247554997
F	7.34560211150341	-2.58103672848391	-1.59385495753882
F	7.99000529620004	-4.09685286845875	-0.15833227644021
F	8.95784790352006	-2.13512591960335	-0.17834503246781
C	-5.08238736168020	-0.55229121151567	-2.31816186259841
C	-3.90990293520503	0.06022855485256	-2.76242246737015
H	-5.07199788228081	-1.59517114132398	-2.00324656888960
C	-6.25958777687146	0.19425095489397	-2.27714554421903
C	-3.90719556109720	1.38556657871290	-3.18518953943324

C	-6.27302638299742	1.53250900562472	-2.68189926516594
C	-7.54438675157961	-0.46602623061124	-1.84275100855667
C	-5.09526270573297	2.11918195730558	-3.14079929842168
H	-2.98250099975424	1.83118400921748	-3.54812228321311
H	-7.19173182637436	2.11401044290011	-2.62955151214807
F	-8.20018074545036	-1.01971019812746	-2.90380554579434
F	-8.40696879722113	0.42177467501970	-1.27109086679046
F	-7.33317499607530	-1.46034622931473	-0.94456454126308
C	-5.08041019527228	3.54123401816154	-3.64159759029449
F	-4.03176603913484	4.24505756563559	-3.12928692377131
F	-4.94742100918278	3.58253950349021	-4.99981313697587
F	-6.21578241134871	4.21586940026496	-3.33263507736292
H	-2.54665088467431	-3.88479785918243	-2.22895215523996
H	-1.39253916825699	-5.15987914488876	-3.51711472727623
H	-0.47042232209341	-7.34256130648161	-2.52195944025223
H	1.17412269581512	-6.29354281553925	-0.96327226011490

228

TS1-2'

C	-1.241367	-1.829752	3.850322
C	-1.422670	-2.807840	4.966844
C	-2.915829	-3.206462	5.136299
C	-3.602267	-3.668036	3.856223
O	-3.901079	-2.535518	3.040398
H	-0.839987	-3.710494	4.735912
H	-3.488423	-2.356687	5.539667
H	-4.534102	-4.202513	4.121602
C	-1.495839	-0.407573	4.074932
C	-1.327818	0.529304	3.033871
C	-1.857119	0.081770	5.348032
C	-1.508405	1.888791	3.251195
H	-1.040232	0.195479	2.041158
C	-2.042319	1.443635	5.565097
H	-1.985168	-0.606548	6.182351
C	-1.868785	2.352679	4.517749
H	-1.361997	2.587604	2.428184
H	-2.318424	1.799805	6.558492
H	-2.005105	3.421063	4.689291
C	-0.777170	-2.307873	2.629251
H	-0.619515	-3.385026	2.535500
H	-1.129114	-1.828826	1.709430
H	1.523781	-6.660347	-4.370763
C	2.189413	-6.692142	-3.496146
C	3.276372	-5.609877	-3.561151
H	2.661534	-7.684958	-3.474790
H	1.577211	-6.590645	-2.587896
C	2.684081	-4.197426	-3.556674
C	4.087128	-5.795325	-4.860936
C	4.209332	-5.798853	-2.347768
C	1.602129	-4.268859	-0.075998
C	1.308887	-3.947799	-3.651011
C	3.527010	-3.076145	-3.472216
H	4.531012	-6.802052	-4.892802
H	3.444153	-5.672481	-5.744503
H	4.901967	-5.060929	-4.931051
H	3.651628	-5.700805	-1.406625
H	4.660962	-6.801915	-2.378366
H	5.025755	-5.064018	-2.334941
C	2.702521	-4.141022	0.786704

C	0.532555	-5.104485	0.240019
H	1.576036	-3.722135	-1.015466
C	0.794603	-2.650961	-3.645750
H	0.603873	-4.775691	-3.713715
C	3.022538	-1.782290	-3.469134
H	4.607031	-3.211902	-3.390479
C	3.855303	-3.258126	0.505241
C	2.679255	-4.878755	1.982533
C	0.510443	-5.854714	1.425426
H	-0.303635	-5.143519	-0.457322
C	1.640425	-1.535473	-3.549509
H	-0.282466	-2.518875	-3.716220
H	3.714489	-0.946834	-3.367913
C	3.693087	-1.953448	-0.031188
C	5.146374	-3.626191	0.841302
C	1.611918	-5.719432	2.286947
H	3.489551	-4.753807	2.702293
C	-0.630121	-6.827354	1.744634
C	1.140421	-0.143105	-3.586922
O	2.394327	-1.562148	-0.390359
C	4.712147	-1.029936	-0.195086
H	5.329947	-4.631460	1.224988
C	6.230954	-2.721645	0.766930
H	1.639898	-6.268069	3.229042
C	-0.947669	-6.837600	3.251773
C	-0.177517	-8.242008	1.322237
C	-1.917526	-6.468871	0.985014
C	-0.129714	0.249037	-3.071990
C	1.896234	0.860833	-4.176281
P	1.657081	-0.569898	0.635546
C	6.018442	-1.387606	0.281806
C	4.445759	0.291024	-0.821322
C	7.525028	-3.094414	1.217313
H	-0.106512	-7.205149	3.854962
H	-1.207094	-5.830386	3.609249
H	-1.805248	-7.497985	3.446770
H	0.041123	-8.274283	0.245167
H	0.731478	-8.543686	1.862602
H	-0.968215	-8.977641	1.536311
H	-2.248739	-5.441621	1.192114
H	-1.798481	-6.560552	-0.102769
H	-2.724196	-7.153566	1.285077
O	-0.884092	-0.704373	-2.361413
C	-0.679896	1.510962	-3.235818
H	2.866171	0.611026	-4.609043
C	1.463038	2.204308	-4.237278
O	2.620326	0.724517	0.698328
N	0.251540	-0.273356	0.053573
N	1.569528	-1.078406	2.172409
C	7.095790	-0.466658	0.344434
C	5.238042	0.740088	-1.933460
C	3.435994	1.131584	-0.364942
H	7.676616	-4.115922	1.572163
C	8.558441	-2.183402	1.239047
P	-1.070054	-0.461575	-0.771256
C	-2.094893	1.785427	-2.873393
C	0.154526	2.549274	-3.766221
C	2.303028	3.224589	-4.757231

S	2.636937	-1.002619	3.431724
H	0.416442	-1.734685	2.513104
C	8.333187	-0.853906	0.816734
H	6.935295	0.563608	0.030368
C	6.146729	-0.110372	-2.617299
C	5.074026	2.080316	-2.412922
C	3.252540	2.466946	-0.826173
H	9.543992	-2.479351	1.601226
O	-1.696075	1.035487	-0.638424
N	-2.071383	-1.535786	-0.186748
C	-2.566717	1.571352	-1.585763
C	-3.000957	2.302763	-3.858496
C	-0.234687	3.913180	-3.781991
H	3.291862	2.943957	-5.125492
C	1.891588	4.539246	-4.769223
O	3.860459	-1.737846	3.160237
O	1.836027	-1.332154	4.602001
H	9.141225	-0.123087	0.871668
H	6.257549	-1.142093	-2.286352
C	6.873004	0.345787	-3.698024
C	5.854642	2.527172	-3.511955
C	4.107290	2.919183	-1.815031
C	2.193644	3.366583	-0.312900
S	-2.881105	-2.753059	-0.832181
C	-3.845548	2.012963	-1.136282
C	-4.310552	2.710969	-3.443193
C	-2.671538	2.390746	-5.235685
C	0.617689	4.885274	-4.261924
H	-1.210279	4.191846	-3.386290
H	2.549957	5.317292	-5.159034
H	7.554450	-0.331695	-4.214523
C	6.738993	1.680505	-4.143945
H	5.726569	3.556315	-3.854212
H	3.977102	3.932437	-2.198152
C	2.485430	4.687252	0.055599
C	0.852232	2.963980	-0.287239
O	-2.040223	-3.664064	-1.600979
O	-3.707422	-3.311997	0.245299
C	-4.676101	2.591150	-2.083783
C	-4.304564	1.918578	0.268737
C	-5.223965	3.207253	-4.410407
C	-3.584026	2.870126	-6.152342
H	-1.692067	2.053021	-5.570913
H	0.306954	5.930971	-4.246184
H	7.327137	2.032239	-4.992712
C	1.465942	5.577248	0.404435
H	3.524601	5.023139	0.070246
C	-0.156653	3.855370	0.051913
H	0.587486	1.951886	-0.574684
H	-5.672638	2.916014	-1.780243
C	-4.176418	0.756883	1.040526
C	-4.978555	3.010271	0.846314
H	-6.219661	3.508481	-4.078602
C	-4.869322	3.288459	-5.739404
H	-3.315598	2.911238	-7.208791
F	2.276088	5.170623	5.022613
C	0.119263	5.188266	0.391927
H	1.738424	6.595011	0.682880

H	-1.188113	3.501881	0.022849
C	-4.740990	0.668171	2.313108
H	-3.644141	-0.106296	0.645920
C	-5.530922	2.919630	2.119564
H	-5.062856	3.944674	0.287623
H	-5.581274	3.663502	-6.475980
C	1.634463	4.037153	4.631169
C	-1.039812	6.149164	0.675157
C	-5.444048	1.739136	2.877361
H	-4.618317	-0.268251	2.856998
H	-6.049982	3.790215	2.524804
F	0.710917	4.411166	3.698857
C	2.587957	3.004613	4.084429
F	0.945265	3.571042	5.706313
C	-1.941704	5.585400	1.792112
C	-1.874844	6.293189	-0.616276
C	-0.549717	7.538680	1.102833
C	-6.137955	1.643823	4.239432
C	3.833570	3.405661	3.598306
C	2.206997	1.661240	4.048271
H	-2.778845	6.274387	1.981365
H	-2.373689	4.612145	1.521286
H	-1.378469	5.465015	2.727745
H	-2.290525	5.326021	-0.933450
H	-2.713682	6.986809	-0.452501
H	-1.258393	6.683636	-1.439244
H	0.053410	8.018588	0.318344
H	-1.413084	8.189431	1.302915
H	0.052976	7.488685	2.021588
C	-5.700160	2.812593	5.144028
C	-5.814175	0.326611	4.959419
C	-7.662981	1.720689	4.014875
C	4.721879	2.449683	3.104549
H	4.118496	4.455709	3.626767
C	3.103747	0.727356	3.532984
H	1.232288	1.342864	4.418329
H	-5.951903	3.788032	4.705527
H	-6.206108	2.744059	6.118937
H	-4.615393	2.785716	5.315263
H	-6.322516	0.307722	5.934722
H	-6.151461	-0.548503	4.386505
H	-4.734202	0.220909	5.134424
H	-7.949223	2.663723	3.527983
H	-8.004789	0.893652	3.376206
H	-8.193978	1.657579	4.977122
C	4.366259	1.100859	3.076174
C	6.060200	2.875049	2.554235
H	5.050095	0.341152	2.697547
F	6.454294	4.082489	3.038883
F	6.024009	2.990925	1.192011
F	7.037823	1.979156	2.845814
C	-3.638980	-1.930331	-3.345459
C	-4.004343	-1.982161	-2.003410
H	-2.722390	-2.418259	-3.672805
C	-4.453844	-1.243812	-4.248157
C	-5.185765	-1.391215	-1.554059
C	-5.624749	-0.623874	-3.815633
C	-4.053114	-1.215217	-5.701485

C	-5.988752	-0.709317	-2.468729
H	-5.464496	-1.453380	-0.502923
H	-6.243439	-0.069334	-4.518974
F	-4.227821	-2.436786	-6.285115
F	-2.736401	-0.898423	-5.853174
F	-4.774600	-0.321851	-6.422964
C	-7.287044	-0.094623	-2.008447
F	-7.630719	0.991705	-2.757811
F	-8.319422	-0.981592	-2.110184
F	-7.235401	0.306928	-0.714184
H	-3.833588	-2.800378	2.095401
H	-2.961350	-4.383669	3.311881
H	-2.961585	-4.013886	5.883877
H	-1.044108	-2.410751	5.919204

228

TS1-3'

C	-0.20760560643525	-3.35153875511674	-2.89580763102848
C	-0.00031610808882	-4.12841192505947	-4.15641012995329
C	-1.34298592932869	-4.39190380344053	-4.89400943937952
C	-2.21171292642461	-3.15571403356906	-5.09321542078389
O	-2.83434464522066	-2.80131079622505	-3.85780382542032
H	0.65861633108891	-3.54674692555536	-4.81547047495867
H	-1.93736241190664	-5.13506163035865	-4.33983205808451
H	-2.98343726423800	-3.37854870339141	-5.85384521351249
C	-0.61234265597763	-4.03914107512709	-1.66951768564295
C	-0.76943954318949	-3.32896189650073	-0.46114166116145
C	-0.80607974778874	-5.43682523485738	-1.64237968586125
C	-1.10251962680379	-3.98129948779715	0.71911478276729
H	-0.62244770204030	-2.25277066940276	-0.43510941594208
C	-1.14674422337127	-6.08925894241662	-0.46183465889548
H	-0.68590431437798	-6.02275666516861	-2.55257388639068
C	-1.29495802065425	-5.36409016825058	0.72364488500652
H	-1.20976916052936	-3.40030012731918	1.63524352399625
H	-1.29181863852988	-7.17024219498446	-0.46302993134033
H	-1.55232959105407	-5.87999075372892	1.64968253790964
C	0.05296003768513	-1.98622515835953	-2.91321742484749
H	0.34839041816841	-1.53856272568554	-3.86508459923047
H	-0.54744043836972	-1.32720284974178	-2.27423170768933
H	5.33236542099059	4.33950723643367	-2.92995423971369
C	4.68293604528600	4.40430887705419	-3.81345624412377
C	3.48949281131830	5.35421486626322	-3.58863492266009
H	4.33477872087480	3.39054581707565	-4.05228784079922
H	5.29385949800531	4.76657997892146	-4.65407602171349
C	2.66614177595906	4.89239087557585	-2.38234220171047
C	2.65802982534186	5.38410901742876	-4.87902181569841
C	4.01676419865588	6.77616277227185	-3.30356360232357
C	2.22253669032869	1.44292300093240	-3.58499798688411
C	3.28597276365569	4.68042936257319	-1.13921044548063
C	1.28213574582090	4.68360399583642	-2.44214967117947
H	2.25119909596071	4.39029238252650	-5.11750974917840
H	1.82302176227291	6.09662554964383	-4.81396660235688
H	3.29597553995780	5.69695617839282	-5.71823440053216
H	4.65159442090367	6.79419674499705	-2.40636169568883
H	4.61595928407541	7.13758168076931	-4.15323600897454
H	3.18510109422764	7.47756639548837	-3.14356461187113
C	3.45499872424470	0.78694841050837	-3.44635322799802
C	1.41136615637820	1.22202817003058	-4.69749819525076
H	1.88741611154110	2.14789384614231	-2.82769979463835

C	2.56349712745245	4.28143423251416	-0.02144951922351
H	4.36381890356896	4.82008953288422	-1.03720955147044
C	0.55200149798077	4.27537562761758	-1.32656902667849
H	0.74589073235105	4.82323569713563	-3.37982257491766
C	4.35452593560984	0.98896575522081	-2.28997996384175
C	3.83277700064164	-0.10974735076232	-4.46180517195393
C	1.78996658351420	0.34175638146847	-5.72034535082507
H	0.45685421844882	1.74394240656370	-4.73806148247420
C	1.17712723137140	4.06462051952131	-0.08840353259056
H	3.09048802115552	4.11023691582299	0.91613622589516
H	-0.51908195842282	4.12160569209997	-1.43384843877400
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C	5.72971868794730	1.01748141780577	-2.45023137574178
C	3.02137637125006	-0.31908415928491	-5.57239553123940
H	4.75573150601207	-0.68084559407044	-4.35244252322166
C	0.93528463277427	0.13089304567611	-6.97462867732834
C	0.41703293355726	3.71024052765271	1.13067477619508
O	2.47785620792570	1.05332448940448	-0.77069607617851
C	4.67967822332622	1.14704840586035	0.16776904145312
H	6.14635866022063	0.99074235853258	-3.45874301438372
C	6.61834128967591	1.01825690275106	-1.35107436895272
H	3.35676811385360	-1.02584108200823	-6.33311959837043
C	-0.48191102062658	0.70044748633512	-6.80899285182498
C	0.81559943124833	-1.36948432476364	-7.30426517814224
C	1.62722860221146	0.84836758787690	-8.15333550570558
C	-0.74982220354306	2.89228010991928	1.10459488274407
C	0.77844977670752	4.22317130850604	2.36685289226204
P	1.83773009439055	-0.31475767304268	-0.20888183744925
C	6.09678285461932	1.04374883459564	-0.01486496549887
C	4.07227687027006	1.29881262104469	1.51527017276267
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H	-1.07206454260442	0.48382079630881	-7.71141870134471
H	-1.00642133993942	0.26456517528938	-5.94629291414120
H	-0.47251668887047	1.79122163781657	-6.67613819204701
H	1.79135227147393	-1.83198580319099	-7.50499739682982
H	0.34603379123778	-1.91663648253534	-6.47449619124675
H	0.19024845668591	-1.50858770374851	-8.19861502063620
H	1.71855874607329	1.92550282729618	-7.95222199757143
H	2.63722813546502	0.44899667259926	-8.32454624582419
H	1.04357009603259	0.71786437848992	-9.07763658074996
O	-1.07810271756451	2.26027372084651	-0.10184601071857
C	-1.60658927804652	2.72136514065048	2.18029871595329
H	1.65851604570767	4.86399554144285	2.44124971087378
C	0.03927243037965	3.95659228338106	3.54233634421224
O	2.72728687339345	-0.64030379960698	1.09690720795135
N	0.34488746143500	-0.04258737987848	0.12949370980375
N	2.04742536437123	-1.62060693933248	-1.15383891722999
C	7.00295240538098	0.91419310313380	1.06969584190824
C	4.42302043493492	2.39090138696939	2.37809968182812
C	3.09506297300434	0.41481711243902	1.94893486263158
H	8.41074229535132	0.93829422625320	-2.56201529300557
C	8.88019162420728	0.84719381021888	-0.46574030882052
P	-1.03682490196405	0.64347357328196	-0.18298916613063
C	-2.93608072732953	2.07916316878568	2.00298173618524
C	-1.18651877138542	3.21661079962334	3.45872527132605
C	0.48148574795397	4.42188785719069	4.80923622198913
S	3.33588322693705	-2.62983781493638	-1.34767666855011
H	1.08893996583771	-1.87190913701298	-2.09614217341325

C	8.36113707105937	0.81365555773167	0.84884448951616
H	6.61296988749358	0.87997702460577	2.08670278648236
C	5.32303906032204	3.41991525560787	1.99292569437138
C	3.79423013491300	2.48627910540196	3.66378657623971
C	2.44429714021060	0.49288601907199	3.21010709430054
H	9.95690438879324	0.77646788157508	-0.62630536741890
O	-1.90891158198370	0.12254793634138	1.08526644977898
N	-1.71790011020646	0.22182975101533	-1.55253348625361
C	-3.06795245479978	0.79781886256588	1.47952069206059
C	-4.12210751035825	2.80243746176567	2.36579208730497
C	-1.89999297118484	2.95108224667540	4.65657269165351
H	1.41178547661707	4.99153718737541	4.85461216284901
C	-0.23334186888534	4.14546685603947	5.95451714135886
O	4.57741849575203	-1.91181759657697	-1.57850519335047
O	2.87741798858468	-3.62770662923419	-2.30376372632477
H	9.03898096758209	0.70039482609514	1.69608973765493
H	5.78109607257366	3.38114667021615	1.00587160187250
C	5.60933339665541	4.46950954499839	2.84128779658470
C	4.12835356289272	3.56770982816741	4.52215890610193
C	2.83049584158921	1.52653302236145	4.04664219639922
C	1.37435344699291	-0.44222918734963	3.62063570638030
S	-2.31422004782702	1.06507315111400	-2.77192211216328
C	-4.31144804839414	0.09670753397976	1.43652555909184
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O	-2.77274096538805	0.08378188182071	-3.76459537399535
C	-5.42951624884855	0.78125267833048	1.88916865998577
C	-4.48927532690927	-1.29323478319544	0.95238988436902
C	-6.56663435169401	2.82698322548975	2.66818301908283
C	-5.27866687828182	4.83534462718436	3.04312982307322
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H	-1.98548367729992	3.16572444358447	6.78539352546089
H	5.26118995469087	5.37061672049585	4.78911104131732
C	0.44253269471521	-2.67205414144753	3.89270494198171
H	2.33798981716626	-2.26257174908037	2.96876872838359
C	-0.78979322219227	-0.77642326660921	4.67803672361481
H	0.12075078320098	1.14322076222675	4.38238217567368
H	-6.39943533590633	0.28335947430671	1.84680961872991
C	-3.92466447316947	-1.76967354119365	-0.23673233947246
C	-5.35376476760096	-2.15863132269394	1.64862994222671
H	-7.51872968926943	2.29448493565970	2.62409450905432
C	-6.51799310934551	4.15609514036047	3.02741611070323
H	-5.24665088352507	5.89634205504002	3.29417679805759
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C	-0.70712972188976	-2.16908591139080	4.51690707816289
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H	-1.67060858811856	-0.33138569156016	5.14465089496170
C	-4.23834690251063	-3.03593007182371	-0.73274154214953

H	-3.24914011525560	-1.13948489843979	-0.81055420134857
C	-5.65160043595958	-3.42455157853089	1.15809383465719
H	-5.78476893270719	-1.83608254388178	2.59818996786772
H	-7.43395781950836	4.69033389361416	3.28367506748543
C	2.17185047025492	-6.41484788243242	2.16453047448367
C	-1.84779897490441	-3.06293708299532	5.01162370222679
C	-5.11489608567461	-3.88995891808902	-0.05508945194333
H	-3.78614704059326	-3.33736279909365	-1.67746145148939
H	-6.32489472114974	-4.06143826825597	1.73521736257238
F	1.11250764002366	-6.08747374664179	2.96789314463970
C	2.97788642169602	-5.19824950821386	1.78222324279116
F	1.66543225211910	-7.05697915160513	1.08374232579516
C	-3.13629288847062	-2.70035035783097	4.24740321029314
C	-2.06272308773461	-2.82804269638920	6.52071281105099
C	-1.55693025359633	-4.55394848674859	4.79368108139745
C	-5.50754622301894	-5.26861856102216	-0.59275327563814
C	3.94743499422372	-4.72510431929251	2.67233060911762
C	2.75208733266743	-4.55434075736045	0.56400554562314
H	-3.97746782682816	-3.31503034969905	4.60274721046476
H	-3.40571289160867	-1.64366009154255	4.38430202956802
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C	-4.80144132768470	-5.59272978118498	-1.91710420376572
C	-7.03145687908091	-5.29675346521850	-0.83085166535113
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H	4.11537653588638	-5.23221827516125	3.62122147228426
C	3.53647470969875	-3.44763082437545	0.23797021804485
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H	-5.64065280816282	-6.19095236757879	1.40051404663475
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H	-5.11734719836918	-6.58687772126699	-2.26624623523402
H	-7.58975561011245	-5.10538101373288	0.09625042390362
H	-7.32450752255895	-4.53269754825047	-1.56513996557122
H	-7.33828608517813	-6.28146750528199	-1.21526986410299
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C	5.74424642797927	-3.05376299608661	3.27683390214483
H	5.14100295833451	-2.12934925549499	0.79967822242257
F	5.31894305634551	-1.87301902002372	3.81488354495096
F	6.92288465656961	-2.79649916190413	2.65041000369757
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C	-3.72738621271127	3.21116259003259	-1.78622881772796
C	-3.78935521238573	1.86384473995480	-2.12828884517987
H	-2.80363401712553	3.76444555115160	-1.94755790368566
C	-4.85668299399925	3.83135449758294	-1.24636180013158
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F	-5.83307935807425	5.72268049550941	-0.17140328113097
F	-4.78630475016952	6.05512965441811	-2.06415764092013
F	-3.64347042956087	5.61839523682542	-0.25321521489985
C	-7.37246364650151	0.99769632478814	-1.26233013468809
F	-7.16537762274093	-0.32968402018802	-1.07813284153515
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H	-2.84620714013321	-1.82015208872577	-3.79054992331479
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H	0.50041953683885	-5.08730206539019	-3.96191946818667
228			
TS1-4'			
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C	-2.83103304066087	-3.05934062890925	1.38076278639125
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C	-1.32978244711739	-4.98469288800443	2.03656205947164
O	-1.40666703574306	-5.54212430082104	0.72584525562789
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C	-1.91031511969424	-2.76441085307626	-0.93333019313532
H	-0.88249645633345	-2.67990793706403	-0.56562455048872
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C	-1.51312279001547	1.31684149337586	6.89387154685143
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H	-1.30255526714046	2.38721319417982	6.76565954020677
H	-2.17272831680207	1.00009389271757	6.07494529216302
C	0.58869684440248	0.65156903171014	5.64672059352618
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C	-3.65723067844851	1.64351989020751	3.05696227941908
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H	-2.70487084005818	-2.47238372902770	5.01992236009170
C	2.27657885509739	1.06180451364138	3.37252559385056
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C	-2.47258796782029	1.99695690541307	2.35262176635868
C	-4.51580060396479	2.67096347482549	3.40154622255728
C	-5.66783912460967	-1.49054597943704	3.70338493632604
H	-6.02191148291827	0.39413420110435	2.72402403970742
C	-5.21480791547905	-3.69141314054440	4.90592866579196
C	3.20050574582448	1.36431020726188	2.25298073540178
O	-1.63041730907288	0.95156495710353	1.97184244591139
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H	-5.42407334385659	2.43547455385760	3.95953227943349
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C	-4.05200091494250	-4.50238573822913	5.49481355179073
C	3.32554477072031	0.56348483261578	1.08039760180914
C	3.98165428284694	2.50974837807753	2.29939447284327
P	-1.22406615463474	0.63940078719031	0.43975974503965
C	-3.04612894638408	4.35081251257435	2.36919798203959
C	-0.77825969170938	3.64339450132099	1.49647959059173
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H	-5.13977420934008	-4.75327965476474	2.98560954590092
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H	-3.58660210392326	-3.99042928127741	6.34952530523490
O	2.62905176058175	-0.64482888302236	1.04847648007189
C	4.13209056898652	0.88816202511658	-0.00670077109539
H	3.95743926039379	3.13356843526178	3.19371561979892
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O	-1.14557266310098	2.08557227692350	-0.28516818217781
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C	-2.84526796127578	5.69884859327588	1.97325369175439
C	0.10560537523332	4.55861805479982	2.15892696830562
C	-0.36988425417418	3.10825935895864	0.28596530165703
H	-6.12078326326858	4.77216573594190	3.86320650899557
C	-4.96710810296802	6.34511221981332	2.95716699315107
P	1.37453306080919	-0.86418321481571	0.04522695546972
C	4.18959732651010	0.00014261777356	-1.19937891294981
C	4.85503126098290	2.12761660580387	0.03120351143403
C	5.50789750105125	4.15065990620497	1.27786814545222
S	-3.87740631478545	0.39975296793721	-0.81568981084991
H	-2.19319194079258	-1.44059753664404	-0.72831305469049
C	-3.78387560971295	6.66934765122745	2.25686992386458
H	-1.94662276970233	5.96318623952139	1.41861429905158

C	-0.13429750663722	5.04146115202690	3.47154997834952
C	1.31266857686964	4.95464965650710	1.49453723396344
C	0.75998148922869	3.56708482927285	-0.45082255129467
H	-5.69829103550602	7.12337526890946	3.18003580357541
O	1.79735645240717	-0.00280774876759	-1.25738558996611
N	1.29231464859050	-2.40736242662765	-0.31195789133566
C	3.01633678271689	-0.39670742330234	-1.82778236826915
C	5.43197723315331	-0.47733533934756	-1.73483657510529
C	5.59176565074349	2.63350874568517	-1.07342938764170
H	5.46061511163679	4.73417241210677	2.19975021303085
C	6.22853218799649	4.60270444758382	0.19459798014419
O	-4.52065033516894	0.99957794388371	0.34348815969583
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H	-3.61375144088342	7.69505040444351	1.92674537875607
H	-1.03504756963368	4.72519969920182	3.99566922533594
C	0.77049843449508	5.87497398323369	4.09602829086923
C	2.21449060275461	5.82842074461086	2.15802754056228
C	1.57817871224982	4.48536603283527	0.18778237048564
C	1.03383701820692	3.16518900841846	-1.84857351845470
S	1.89949050708782	-3.64442224702130	0.49982848070862
C	2.96401281624855	-1.20015104630893	-2.99972462085350
C	5.41310700626896	-1.23927876798991	-2.95075802771811
C	6.67922258479090	-0.26642301606608	-1.09268448242430
C	6.25611458851722	3.84017721996791	-0.99584102650171
H	5.61899062849972	2.06182633081915	-1.99963155996207
H	6.76876357448545	5.54898799288198	0.24774937500179
H	0.57432196683516	6.22096199299716	5.11195013484117
C	1.95373121250896	6.27795406071919	3.43439260370469
H	3.12763606399436	6.12298624603039	1.63703337641636
H	2.45297710258357	4.87308480179384	-0.33673609622518
C	0.01130994044316	2.98413101564463	-2.79149032168126
C	2.35683897987030	3.04412659403525	-2.30203607674654
O	1.88691112815283	-3.45694572806486	1.95018082527276
O	1.27660099598518	-4.85421216746273	-0.04911565407887
C	4.17791791679586	-1.56682734848728	-3.55571767608459
C	1.68817571463146	-1.66068369691598	-3.59052203394769
C	6.64026018013683	-1.68899605512794	-3.50600632812206
C	7.85247166376878	-0.73489415867803	-1.64755647795820
H	6.70311304678024	0.26020167340925	-0.14016027426357
H	6.80603375847975	4.20928250864784	-1.86277010829762
H	2.65852898691664	6.94105835596341	3.93819666488098
C	0.30504520858613	2.69449116623182	-4.12411763125893
H	-1.02848752739256	3.08986878514282	-2.49080390046833
C	2.64129406600503	2.74010908143233	-3.62745912219955
H	3.17839574650133	3.16585500958663	-1.59835197481110
H	4.18683470683755	-2.14864316153475	-4.47866831673676
C	1.58281291506649	-2.97031102958512	-4.08389342706730
C	0.55938268522281	-0.83356552387484	-3.70265682672190
H	6.61120464652131	-2.26323578603918	-4.43392354755177
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C	1.62346715759458	2.55414760581045	-4.57718569841987
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C	1.97383599063501	2.23765061731595	-6.03396502793720
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C	-3.47289521973248	2.47158043303420	-4.28078903281671
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C	2.70739927833879	3.45390206461572	-6.63678912553079
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C	2.89505803224626	1.00258961010458	-6.09803729399660
C	-1.99510066716871	-3.08359428430107	-5.50524231540255
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H	-3.26584031423635	-1.32770860908756	-5.15291954718582
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C	5.33036773132266	-4.49137192668925	-1.50196198850015
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228			
TS1-5'			
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C	-3.59684727492250	-2.08533846693109	-4.79015470255820
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H	-1.42850140234342	-3.92118580317328	-6.80248907364161
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C	-1.39441554137025	1.90417862364601	-4.18576707256842
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C	-3.32126185544684	-0.64289083039902	-1.08314815367192
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H	-4.85067858130742	-3.71853952423447	-2.07465000889486
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H	1.15188584384205	-4.74882160731282	1.38201371904370
H	6.36924054229191	1.21419782863014	2.68789566831024
C	2.47738673942663	1.23000684130437	3.48833175340021
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H	8.52000271810540	0.43108203537781	1.87074687430763
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F	-6.62570605933183	-1.54226413754034	4.96857183583471
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C	3.43047083613117	3.83199245985728	3.35643884330270
H	5.06409235736451	3.02753092819238	2.22126518198550
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C	-6.62035100256780	-1.75182136096274	3.62093770266066
C	2.94885022853554	-2.93004744663476	5.31440807161888
C	2.21594920036227	3.59967320099485	4.02258047992250
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F	-7.90228976879999	-2.00531302779532	3.25298901706063
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C	4.20864545701085	-2.38850482140265	4.61134684751077
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H	-0.44718918883469	5.23527837427802	5.57528702014443
H	-0.56180277848793	3.94985084382229	4.35188782077180
H	0.11970375915003	3.59945151386272	5.95174628066021
C	-4.90672137789216	1.67823216530551	1.66965505195497
C	-7.13564515405375	2.39007809005303	0.78981281487387
H	-4.46557392042784	2.56716944755988	1.21781458466479
F	-8.35081373053039	1.87773738406332	0.47034809454290
F	-6.55428042631675	2.80543253506376	-0.37393870194248
F	-7.36119950036301	3.51496471156566	1.52960654904798
C	5.17228737495081	2.37811207678207	-1.03665390862722
C	4.20060550958936	1.64189154904802	-1.71190558110478
H	4.87108065730874	3.20287726503098	-0.39110951118411
C	6.51885037805015	2.05718062508625	-1.22208871755626
C	4.55609436837956	0.60218537182338	-2.56684842016909
C	6.89291630698624	1.00352649436709	-2.05811820370675
C	7.56618701038813	2.90995477838202	-0.55289715288004
C	5.90511747533580	0.27999878921456	-2.72628169703137
H	3.78095654063121	0.05861350059552	-3.10365452265110
H	7.94244734135974	0.74617172228847	-2.18253370570284
F	7.63768936206467	4.14547665199628	-1.12541462097553
F	8.80785836866117	2.36658361984757	-0.62258266923637
F	7.29048397432661	3.11532379193643	0.76968036438433
C	6.26713380305914	-0.83798364811636	-3.67007130919624
F	6.01784531447284	-0.49262160256987	-4.96679939101501
F	7.57793577514888	-1.18309358384739	-3.59535121338541
F	5.53553783417516	-1.96228149400085	-3.42302431799625
O	1.11445993715146	5.99275361842534	-0.52809722290730
C	-2.33014432104772	4.87381023028730	0.68385275424339
C	-3.54757013719036	4.94114229464923	-0.02544506126720
C	-3.37416088995615	6.09323341050321	2.51104887421418
C	-4.66603058355865	5.54439681210326	0.54144309602665
H	-3.62801556642583	4.47968398952199	-1.00987774106933
C	-4.58257552347379	6.12303391657299	1.81130573427162
H	-3.30031786392795	6.55023930992979	3.49857276744466
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H	-5.46033196306139	6.59715962862780	2.25294100009508
H	1.63667359409056	5.16658513550770	-0.48070413221915
H	1.24272110566198	5.45628930230860	-2.53532575291976
C	-0.83871124183052	5.57734798953766	-1.94992007558837
H	-1.49812598498412	6.28347583401397	-1.42359157307748
H	-1.15689484201470	5.56909000115941	-3.00365570278390
C	0.60872823254290	6.05823853950335	-1.86337015051047
C	-2.26262158814227	5.46662978340951	1.95801397711734
H	0.66559543045364	7.10873095127153	-2.19414064220160

H	-0.36365595831629	3.58820918594383	2.01340771632492
C	-0.32307055747841	3.43081488437082	0.93391319425615
C	-1.01545407840515	4.15806461295085	-1.36351365231262
C	-1.17109936665617	4.17322652723253	0.11910705144980
H	-1.92189684771949	3.71310825863138	-1.80457202372522
H	-0.17417363202902	3.51724829539063	-1.65468387802717
H	0.63487771408064	3.09828741948971	0.52913691869699
H	-1.32241108900365	5.45039452964582	2.50595823517038

178

3b_1 (cat)

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H	3.14038002057474	-1.20769964863136	4.03126968370083
C	4.18346009363254	-2.51115981799999	2.65123988277742
C	3.04295995654414	-1.95603055016030	3.24535043827380
C	1.75719000286760	-2.34314024673242	2.86734024475711
C	1.55677999737958	-3.30942970494473	1.87144972999658
C	2.69792999427391	-3.84503988375081	1.24852988451434
C	3.97580993187412	-3.45696007016577	1.63289005666054
H	4.82808001611494	-3.90210000522482	1.11756999813187
H	2.57997999715397	-4.56029004578806	0.43310003073423
C	0.21411000621077	-3.80058002937446	1.49078002131569
C	0.00385999847049	-5.13986001793003	1.19958002004066
C	-1.25098000416396	-5.63645000483450	0.77498001416288
C	-1.41871999958010	-7.00242999861802	0.42254999899408
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C	-2.09426999953968	0.90075999857034	3.24050000150514
C	-1.97207000141611	-0.19689000095123	4.08716000219277
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F	-2.32245000019682	-2.91385000264859	5.01484999856214
F	-4.13309000165747	-2.34638000200486	6.11355000206294
F	-2.18072999890537	-1.57694000023040	6.73761000146427
H	-0.99795999955130	-0.66432000190750	4.22043999775025
N	0.59804000172123	-0.97145999972885	-0.49359999997546
P	1.81167999869161	-0.24308000047971	-1.10150000192416
N	1.75215999842521	1.41528999997400	-1.30400000077469
S	0.95366999881537	2.16173999854198	-2.59887999744994

O	-0.13264999916376	1.26476999874312	-2.93608000143433
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C	-0.61206999746616	6.05265999908062	-0.82377999754938
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H	1.90292999856881	4.80440000132227	-2.75767000146980
C	1.30149999822849	7.30409999747885	-1.89817000233111
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H	-0.98633000122086	6.99271999936673	-0.42033999832491
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C	2.71401000804876	-2.18009000142933	-2.46266004185341
C	4.04334000158507	-2.32257000143535	-2.08784000404728
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C	6.34145999977606	-5.19102999844482	-1.29079000029687
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C	0.40791001208731	-3.10508002440095	-3.07293005924321
C	-0.06047012744577	-2.14470964196150	-3.97946961490966
C	-1.40744971577765	-2.10687043395825	-4.34481038964537
C	-2.34065016115907	-3.01112999281197	-3.81932002796306
C	-1.86976992916399	-3.93845964583022	-2.87473963684160
C	-0.53112994509182	-3.98603034872615	-2.50875036519765
H	-0.20879000526465	-4.70337994974800	-1.75257994446999
H	-2.55932002713453	-4.64240006125913	-2.40653005185115
H	-4.67200000094689	-6.95709000037051	-0.56761000040493
H	-3.86202999940497	-4.15828000095510	2.86885000031901
H	-7.84941999989145	-2.71999000151314	3.63982999798595
H	-7.58139999906255	-0.98772999768818	1.88250999781247
H	-0.56222999814523	-7.67307999770123	0.52027000280579
H	-2.73901000039503	-8.52142999987500	-0.32035999944649
H	-5.96823999914387	-4.28470999820337	4.14412000212743
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H	-4.44671000168075	-4.58554999793370	0.05819999840802
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H	-2.57613000245310	1.44568999758833	-4.25899000152788
H	-2.67631005852049	-0.32322992152489	-2.60375992138203
H	-1.72382004542424	-1.35446993811079	-5.06681996297808
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H	1.75479999919296	-5.39903000113506	-2.84527999351165
H	3.57260999846410	-6.91953999857597	-2.28938000251376
H	5.88614000233804	-7.30862000164184	-1.47566000219055
H	7.35029999849976	-5.36348999892716	-0.91294000082438

H	6.53259000172360	-3.06034999794870	-1.20374999601896
C	4.84322000163842	-1.10947999900451	-1.78278999775828
C	4.36894000305807	-0.19738999891793	-0.85309000149841
C	5.02716000023744	1.01551999671414	-0.51570000131872
C	6.24496000184022	1.25895000242013	-1.12899000162514
C	6.78779999893832	0.38108000302951	-2.09557999971440
C	8.01576000241321	0.67436999858528	-2.74621999844299
C	8.49931999766975	-0.14132999770693	-3.74512000060336
C	7.76275000213623	-1.28032999954203	-4.14386000128606
C	6.57636000102056	-1.60423000227337	-3.51933999875449
C	6.06735000057200	-0.80503000005876	-2.46268000248183
H	6.01408000133345	-2.48043999916973	-3.83953999983228
H	8.13314000067957	-1.90620000193269	-4.95699000063925
H	9.43318580944408	0.09568413988305	-4.23744193187144
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H	6.79534000178492	2.16644000299293	-0.87298000071015
C	4.39842999887643	2.01494998468125	0.37810000467888
C	3.78358998989949	1.66779996335562	1.59158003263320
C	3.18859000004897	2.63856999923313	2.39446000153651
C	3.16945000313552	3.99032000063984	2.02518999800660
C	3.76858999963976	4.33097999995200	0.80008999776253
C	4.37343000136138	3.37069999853280	-0.00671999946450
H	4.81604000075315	3.66402000232685	-0.96133999985982
H	3.75809000163112	5.36763000266770	0.45896999782067
C	2.52661000150522	5.07371999980042	2.89489000050841
C	1.92416000119686	4.49951000172117	4.18461999747363
H	1.12889000242371	3.77332000240045	3.96824999952119
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C	3.60036999955967	6.11633999911462	3.26808999945078
H	4.03366999735001	6.59202000061402	2.37694999801112
H	4.41849000249882	5.65146999778584	3.83745999994386
H	3.15472000050519	6.90726000233492	3.88971000000911
C	1.39861000089390	5.75801999825824	2.09723000002381
H	1.78180000242613	6.22557000160566	1.17979000246695
H	0.93234999923035	6.54613999767550	2.70753000039429
H	0.62354999963765	5.02841000049866	1.82893000096419
H	2.70195000157184	2.31523000409552	3.31196000112617
H	3.75503998881884	0.62660999723969	1.91117002853448
O	3.13487000263839	-0.46195999665461	-0.21738000173632
O	-1.88954000032930	-1.10326999884195	-0.58293999909809
C	-3.13794999891617	-1.28838999787820	0.02787000093935
C	-3.28483999674846	-2.37625000183495	0.87928999598116
C	-4.50320000163619	-2.50726999729083	1.61734000275400
C	-4.68084000178240	-3.47850999789736	2.63580999885453
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C	-6.92161999839666	-2.65479999989381	3.06965000155089
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C	-5.39177000166417	-0.57661999823582	0.37926999938509
C	-4.18919999993614	-0.37805999864472	-0.28381999960054
C	-4.05546999782197	0.70639999959422	-1.28257000136050
C	-3.26420000195416	0.57658999923792	-2.43855999936525
C	-3.21494999774351	1.59119000157911	-3.38689999841246
C	-3.93565000053565	2.78637000118280	-3.23810999919438
C	-4.72109999953055	2.91275000183555	-2.08504000089845
C	-4.77976999838882	1.89882999747165	-1.13001000074535
H	-5.37322999760371	2.05755999783639	-0.22900999897346

H	-5.28610999799197	3.82625000004837	-1.90383999851573
C	-3.83478999941811	3.87792000039227	-4.30792000167097
C	-2.36741999790031	4.33714999908042	-4.43634000160866
H	-2.02133000196683	4.79850999953391	-3.50070999773511
H	-2.27214000109702	5.08282000104918	-5.24002999813074
H	-1.69662999968439	3.49859999886980	-4.66889000031592
C	-4.30711000070216	3.30215999979280	-5.65895000235310
H	-5.35117999824411	2.96319999997955	-5.59471000068195
H	-3.69272000039391	2.44639999787027	-5.97093999890247
H	-4.24092999834347	4.07101000081785	-6.44361999943940
C	-4.69626999949720	5.10302000215619	-3.97288999989800
H	-4.59044999922835	5.85510999789026	-4.76807999755179
H	-4.38848999923209	5.57072000065674	-3.02653999822580
H	-3.38236499952091	-2.97548246671822	-4.10454042273669

178

3b_1 (TS1-1)

C	-4.003909999712461	-1.39392999994943	-2.33904000198956
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F	8.49614999857050	-1.61057000025432	0.65727000209471
H	4.60941000057161	-2.57628999920015	0.87884999855348
C	1.35076989636650	3.17412001502987	-4.20258992577151
C	-6.25479999872846	-2.04693000251425	-1.79688999856430
C	7.30005999938426	-2.23405000028294	0.81056000259785
C	2.40810000216670	-0.73061000323221	-3.40031999870106
C	1.36989994988677	4.09216031583102	-3.13895032152058
C	0.21836027401115	2.35718966734238	-4.31676984433466
H	-2.72422617167005	2.30418997135886	5.03480681673432
C	-4.88080999911161	-2.27413999988235	-1.70684999913735
H	-4.48932000132836	-3.13581000107450	-1.16656000065983
H	-2.44460000159546	-3.94403999935323	6.75532000158842
C	4.94378999808254	-1.73008000008594	1.48003000002737
H	-0.89059000126896	-3.12092000217433	6.49546999941751
C	3.62342000180992	-0.95937000098658	-2.72525000187360
C	1.85374999919982	-1.70216999868728	-4.22477000003485
H	1.88124999903093	0.21391000401955	-3.28267000091559
C	0.30547015857369	4.20062967035391	-2.25167972392979
H	2.23696999001205	4.73666994016985	-2.98757993931835
C	-0.85430020784029	2.46098033411595	-3.43092024414573
H	0.15186995212857	1.61887006463738	-5.11532000745702
C	4.26687000017849	0.06792000041178	-1.87476000174828
C	4.25038000267338	-2.19872999857173	-2.92940999826555
C	2.48169000014875	-2.94065000200516	-4.44014000239441
H	0.89257999809159	-1.48705000114346	-4.69424999796702
C	-0.83918001975987	3.39588000758632	-2.38575998992795
H	0.37298997145025	4.90489005207335	-1.42137003157614
H	-1.70782997112242	1.80030995079992	-3.56558996322507
C	3.51922999878385	0.99816000135814	-1.09713999969048
C	5.64694999881907	0.19579000026458	-1.83470000120277
C	3.69719999873412	-3.15938999961527	-3.77734999911723
H	5.17652999768815	-2.42872999798593	-2.40067000114522
C	1.82098000257948	-3.98248999921152	-5.34584000250531
C	-1.97638999995114	3.58383999938157	-1.45721000856015
O	2.12787000074982	0.87161999878646	-1.11042999931859
C	4.08384999929216	2.05128999920021	-0.38810999946995
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178			
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C	-1.72468023891522	0.12568999815766	5.08022998633896
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H	-2.77775008774860	1.96592998257709	4.63442996848397
C	-5.78232001812365	-2.92723000113988	2.85673998369287
H	-6.20282992893849	-0.84316998929275	3.18029005041621
C	-4.28968000125698	-3.44937999961548	1.06069999812879
H	-3.51264000840939	-1.79052000189966	-0.04495000552260
H	-8.27339000046384	4.89252999889354	0.08353999918379
C	6.59883999912468	-0.42512999932259	4.00832999768377
H	-2.54799272886839	-0.35467110512550	5.58900758116212
C	-5.09409997486391	-3.90112999603351	2.11275002161473
H	-6.41834999077117	-3.22960999918479	3.69092000622525
H	-3.73735000796762	-4.15380999914894	0.43923999657515
F	7.86018999966972	0.07195999860447	3.93518000121694
C	6.19109000000549	-1.16013000018315	2.75599000094859
F	5.76353999898667	0.61724000061588	4.27739000109571
F	-8.20007000054775	-1.01836000224596	-2.90388999838384
H	-7.19068999794552	2.11568000159300	-2.62885000151870
F	-4.94538000096564	3.58475000074760	-4.99834999920050
C	-5.22899999684151	-5.38436999750120	2.46720999935983

C	7.14099000259480	-1.53709999968177	1.80670000200690
C	4.85019999842448	-1.51757000078753	2.60100999873374
C	-6.27224000206443	1.53382000061332	-2.68162999890483
F	-7.33308000096557	-1.45878000022363	-0.94457999912741
H	-2.98168000040474	1.83159000020389	-3.54799000215955
C	-7.54418000265511	-0.46458000139531	-1.84292999786095
C	-5.09429000164731	2.12021999808559	-3.14039999953984
F	-8.40663000042974	0.42340999869094	-1.27140999798052
C	-5.07880000056256	3.54261000038699	-3.64021000000001
F	-6.21404000251921	4.21741999909693	-3.33116000090022
F	-4.03006999971878	4.24575999981584	-3.12713999867418
C	-4.79483000137969	-5.59785000154634	3.93204999526197
C	-4.35302000455071	-6.27206000306524	1.57076999989586
C	-6.70090000230556	-5.81293999811677	2.30130999970171
C	6.73910000042168	-2.27073999926451	0.68870000085577
H	8.18478000184593	-1.25841999924004	1.93380000121396
C	4.46954999911459	-2.24695000191668	1.47792000110293
H	4.10501999825648	-1.25498999967094	3.35019999810486
H	-5.41358999904828	-5.01659000184764	4.62986000101002
H	-4.88678000138239	-6.66056000031553	4.20320000198959
H	-3.74748999999953	-5.29552000139679	4.07263999874842
H	-4.47955999961955	-7.32461000078187	1.86413000091226
H	-4.62904999993537	-6.18226000108354	0.51042999857833
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H	-7.36840000211937	-5.22688999912727	2.94872000224927
H	-7.03166000172890	-5.67497000124388	1.26183000127755
178			
3b_1	(TS1-2')		
C	6.06020000169310	2.87504999930436	2.55422999838886
F	6.02401000105706	2.99092000080527	1.19201000060770
H	3.07735423394003	-5.20350017576578	-3.54056647609182
C	-3.63898000168433	-1.93033000094335	-3.34545999894997
F	6.45429000058934	4.08248999763768	3.03887999797976
C	2.68407994893277	-4.19742986119626	-3.55666998171864
H	5.05008999913552	0.34114999968820	2.69754999866985
H	-2.72238999806709	-2.41825999981535	-3.67279999760546
C	1.60212999728106	-4.26885999446855	-0.07600002098782
C	1.30889001748081	-3.94780018218218	-3.65101055041806
C	3.52701007102591	-3.07614013629842	-3.47221963701100
F	7.03782000009680	1.97916000252984	2.84581000044230
H	-8.19398000167819	1.65758000261057	4.97712000229431
C	4.36626000024886	1.10085999905424	3.07616999923519
C	-5.18576000205479	-1.39121999893874	-1.55406000227581
C	-4.00434000165381	-1.98215999813073	-2.00340999792748
C	-4.45383999785150	-1.24380999863716	-4.24815999838497
C	2.70251999935700	-4.14102000102130	0.78669999868765
C	0.53256000220287	-5.10449000058773	0.24002000088561
H	1.57604001731228	-3.72213999012302	-1.01546984167039
C	0.79460002693129	-2.65095991842677	-3.64575019299740
H	0.60386999486316	-4.77568995410473	-3.71371979888220
C	3.02253994302635	-1.78228996166148	-3.46912984250611
H	4.60702998165798	-3.21189996778880	-3.39048018693103
C	3.85529999829326	-3.25813000094231	0.50524000011216
C	2.67924999728155	-4.87875000139702	1.98253000000883
C	0.51044000036763	-5.85470999638152	1.42543000013254
H	-0.30363000180485	-5.14351999745273	-0.45732000161450
C	1.64043000310893	-1.53547001088135	-3.54950991626358
H	-0.28247001120491	-2.51887001584726	-3.71621989611227

H	3.71449001412749	-0.94683000613804	-3.36791009858091
C	3.69309000106792	-1.95345000249116	-0.03119000139404
C	5.14636999805810	-3.62619000037515	0.84130000196278
C	1.61192000017184	-5.71942999916169	2.28694999914177
H	3.48954999980300	-4.75380999877996	2.70228999824829
C	-0.63011999977112	-6.82734999916909	1.74463000288935
C	1.14041998724060	-0.14311001000996	-3.58692006065035
O	2.39432999770640	-1.56214999982627	-0.39035999742568
C	4.71214999938164	-1.02993999770752	-0.19508999899939
H	5.32995000125932	-4.63145999971954	1.22499000205297
C	6.23094999783794	-2.72164999876564	0.76692999770845
H	1.63990000173503	-6.26807000150871	3.22904000244956
C	-0.94767000233851	-6.83759999851924	3.25176999978339
C	-0.17751999817171	-8.24200999849227	1.32223999827941
C	-1.91752999804868	-6.46887000232688	0.98501000036039
C	-0.12970998008485	0.24904001127612	-3.07198995410554
C	1.89622998886877	0.86082999653675	-4.17628002394803
P	1.65707999919644	-0.56989999801185	0.63554999781394
C	6.01843999810596	-1.38760999986813	0.28180999875593
C	4.44576000283892	0.29102000096019	-0.82131999930028
C	7.52503000023340	-3.09441000205499	1.21730999999308
H	-0.10650999968684	-7.20514999797162	3.85496000148236
H	-1.20709000056074	-5.83038999794481	3.60925000052323
H	-1.80524999829247	-7.49798000131785	3.44677000183263
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H	0.73147999866388	-8.54368999836588	1.86260000151700
H	-0.96822000138789	-8.97764000063505	1.53631000166137
H	-2.24874000190168	-5.44161999747395	1.19210999925976
H	-1.79848000139081	-6.56055000105275	-0.10276999747528
H	-2.72419999793357	-7.15357000008710	1.28507999989498
O	-0.88409000330480	-0.70437000342759	-2.36141000474257
C	-0.67990000046104	1.51096000141807	-3.23581999917344
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C	1.46304000135884	2.20430999929198	-4.23727999176747
O	2.62033000181088	0.72452000145298	0.69833000153767
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C	7.09578999798842	-0.46666000125835	0.34442999863623
C	5.23804000258101	0.74008999822570	-1.93345999799345
C	3.43598999922468	1.13158000117701	-0.36494000257464
H	7.67661999777762	-4.11592000048622	1.57216000060334
C	8.55843999809475	-2.18339999958236	1.23905000197493
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C	-2.09489000071925	1.78542999834067	-2.87339000525230
C	0.15452999944931	2.54926999872239	-3.76622000195999
C	2.30303000198893	3.22458999810928	-4.75722999993740
S	2.63693999917383	-1.00262000191127	3.43172000090084
H	0.41643999936175	-1.73469000143999	2.51310000146269
C	8.33318999898182	-0.85390999839583	0.81673000246163
H	6.93529000038216	0.56361000194824	0.03036999858291
C	6.14673000278173	-0.11036999749311	-2.61729999963780
C	5.07403000156432	2.08031999865680	-2.41291999952074
C	3.25253999795026	2.46695000394469	-0.82616999806194
H	9.54398999741010	-2.47934999994065	1.60123000133982
O	-1.69606999803313	1.03548999733473	-0.63842000086580
N	-2.07137999999515	-1.53579000054020	-0.18675000212836
C	-2.56671999859949	1.57134999965810	-1.58575999723079
C	-3.00096000076896	2.30275999855506	-3.85850000072549

C	-0.23469000222550	3.91317999843695	-3.78198999985354
H	3.29185999928856	2.94396000045063	-5.12548999893280
C	1.89159000020989	4.53924999761422	-4.76922000123538
O	3.86045999950679	-1.73784999903131	3.16024000130634
O	1.83602999805515	-1.33215000040070	4.60200000087147
H	9.14123000148950	-0.12309000008522	0.87167000048804
H	6.25754999965051	-1.14209000005341	-2.28635000212042
C	6.87300000073564	0.34579000007025	-3.69802000111734
C	5.85463999847449	2.52716999782145	-3.51195000235459
C	4.10728999350009	2.91918000077606	-1.81503000126307
C	2.19364001881515	3.36657998753570	-0.31289999894038
S	-2.88109999778473	-2.75305999975627	-0.83217999790225
C	-3.84554999780242	2.01296000065003	-1.13627999929105
C	-4.31055000159866	2.71097000193600	-3.44319000143656
C	-2.67154000207219	2.39074999772991	-5.23568999877927
C	0.61769000054281	4.88527000189081	-4.26192000039922
H	-1.21028000273399	4.19184999762308	-3.38629000064682
H	2.54995999861229	5.31728999759899	-5.15903000192429
H	7.55444999816761	-0.33170000086929	-4.21452000233768
C	6.73899000061829	1.68050000114296	-4.14394999834639
H	5.72657000187076	3.55631999767502	-3.85420999851536
H	3.97710000075991	3.93244000004320	-2.19815000065468
C	2.48543001794428	4.68724991944895	0.05560015801195
C	0.85223001218825	2.96398005389716	-0.28724017041708
O	-2.04021999851242	-3.66406000093772	-1.60098000222380
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C	-4.67609999748667	2.59114999893101	-2.08377999826661
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C	-5.22395999755942	3.20724999840840	-4.41041000090226
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H	-1.69207000030642	2.05302000125858	-5.57091000176387
H	0.30694999354308	5.93097000475724	-4.24618001911368
H	7.32713999743932	2.03224000082330	-4.99271000201179
C	1.46593992165321	5.57725017081984	0.40442988639550
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C	-0.15665011623027	3.85537000679814	0.05191019286244
H	0.58749000288065	1.95188999153525	-0.57467997851595
H	-5.67264000195326	2.91600999799996	-1.78023999861818
C	-4.17641999992323	0.75688000195943	1.04052999779912
C	-4.97855999931071	3.01027000043461	0.84630999766217
H	-6.21966000207259	3.50848000187284	-4.07860000011613
C	-4.86932000081564	3.28845999879356	-5.73939999838519
H	-3.31560000022196	2.91123999990205	-7.20879000160964
F	2.27609000204768	5.17061999864082	5.02261000135884
C	0.11926011292656	5.18826989952377	0.39192995858058
H	1.73842001656134	6.59500995837293	0.68288001150924
H	-1.18810996759005	3.50187999520035	0.02284997283303
C	-4.74098999805470	0.66816999952852	2.31311000125073
H	-3.64413999805759	-0.10630000103938	0.64591999765709
C	-5.53092000070902	2.91962999874664	2.11955999766354
H	-5.06285999768264	3.94467000068798	0.28761999965085
H	-5.58127000028915	3.66349999914907	-6.47598000067003
C	1.63446000169066	4.03714999918988	4.63117000012776
H	-0.66984623479791	5.87891166432416	0.65232869869812
C	-5.44405000032489	1.73914000076956	2.87736000068414
H	-4.61832000062127	-0.26825000241616	2.85699999755708
H	-6.04998000225911	3.79020999997523	2.52479999845295
F	0.71091999779941	4.41117000057849	3.69885999843140

C	2.58796000243106	3.00461000034315	4.08442999840363
F	0.94526999859588	3.57103999825531	5.70631000253076
F	-8.31941999835751	-0.98159000221384	-2.11017999826908
C	-4.05310999966100	-1.21521999867909	-5.70148000103372
F	-4.22781999817309	-2.43679000218250	-6.28512000062785
C	-6.13794999804306	1.64381999816755	4.23942999791780
C	3.83357000253033	3.40566000251619	3.59830999737118
C	2.20700000131388	1.66123999854763	4.04827000207701
F	-7.63071999753538	0.99170000159299	-2.75781000032441
C	-7.28704000163371	-0.09462000168810	-2.00844999805064
F	-7.23540000032401	0.30692999879522	-0.71417999982534
C	-5.62474999912659	-0.62386999831594	-3.81563000086901
H	-5.46450000064395	-1.45338000076106	-0.50292000142203
C	-5.98874999765554	-0.70931999928268	-2.46873000073626
H	-6.24343999812555	-0.06932999843085	-4.51897000137585
F	-2.73639999849275	-0.89841999829918	-5.85317000246521
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C	-5.70016000024583	2.81259000158471	5.14402999752614
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H	4.11849999864739	4.45570999885612	3.62676999961645
C	3.10375000095135	0.72735999958494	3.53298000173761
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H	-5.95190000185912	3.78803000154627	4.70552999738047
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H	-6.32252000199023	0.30772000215362	5.93471999920305
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H	-8.00479000023677	0.89365000022392	3.37620999967973

158

3b_2 (cat)

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C	-2.36741999816402	4.33714999886984	-4.43634000114878
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H	1.17063269562912	-3.39937002067521	1.78821672276092
C	-3.26420013820579	0.57659011285153	-2.43855998956466
C	-4.72109999127303	2.91275000100417	-2.08503999715241
C	-3.93564998303981	2.78637000037042	-3.23810999189347
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C	-2.62642999419112	-7.47150999800136	-0.04642002131309
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C	-3.59716999851470	-5.25799999371927	0.16882998685392
C	-2.37046001421994	-4.74485000254013	0.66550002396500
C	-2.18320003138302	-3.36683006110494	1.00670006039647
C	-0.91757992364262	-2.94596984851212	1.37970993898938
O	-0.75090002440230	-1.58188003439794	1.64662997293190
P	-0.68402000093389	-0.59112999986219	0.36668000722059
N	-0.93473999740708	0.90381000291796	0.82916999860601

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O	-0.73286999945068	2.92170999852615	2.24804000111647
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C	-2.09426999972221	0.90075999842887	3.24050000173838
C	-1.97207000161178	-0.19689000084250	4.08716000241501
C	-3.10503000125171	-0.68644000137489	4.74160999796871
C	-4.34557999837240	-0.07403000226688	4.56952999963857
C	-4.44295000173602	1.04567999804419	3.73976000184860
C	-3.32273000157096	1.53683999907351	3.06691000144668
H	-3.39683999961033	2.40640000072082	2.41580999920628
C	-5.75377000133027	1.77555000157240	3.59659000206841
F	-6.02273000058178	2.09389999906862	2.29624000019429
F	-6.80789000009731	1.05245000012759	4.05673000055064
F	-5.74567999833597	2.95142000200247	4.28670000107427
H	-5.22807000053779	-0.46736000213886	5.06947999927831
C	-2.94619000079946	-1.87879999978646	5.64912999738346
F	-2.32245000014082	-2.91385000247531	5.01484999857772
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F	-2.18072999892961	-1.57694000019892	6.73761000148848
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C	-0.82239000260178	3.63976999959167	-1.04691000158290
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F	0.69568999784513	8.40451000010137	-1.39012999969761
F	2.56096000008247	7.25491000201459	-1.36740000237172
F	1.45234999958225	7.49898999936428	-3.23601999793933
H	-0.98633000120603	6.99271999938803	-0.42033999834772
C	-2.54070000088585	4.95645999798764	0.28420999761804
F	-2.30560999917715	5.58442999785871	1.46547000132634
F	-3.09591999873437	3.75817999889126	0.55029999916704
F	-3.48715000112872	5.70547000249000	-0.36816999967465
H	-1.33501000230726	2.70473000195449	-0.81917999761618
H	2.56958000245643	1.93409000087610	-0.94894000410872
O	2.20455000824694	-0.86057998492754	-2.53798015690352
C	2.71401007204487	-2.18009015721417	-2.46265987474602
C	4.04333994744278	-2.32256997425334	-2.08783986148678
C	4.57380998129936	-3.64339999335872	-1.93364995061473
C	5.88489999030822	-3.89940999831760	-1.45339997669342
C	6.34145999335463	-5.19102999840323	-1.29078998770964
C	5.51135999025466	-6.29221999660122	-1.60360997989940
C	4.22883995999696	-6.07785999894299	-2.05820989298824
C	3.72150011379737	-4.76053999794747	-2.22047018908263
C	2.38508011603998	-4.53627017576390	-2.62187039413806
C	1.83752974338638	-3.26588969080622	-2.73055983800397
H	0.80878339869015	-3.08367939569727	-2.99968435232182
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H	-3.86202999943979	-4.15828000090517	2.86885000053991
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H	7.35030000038595	-5.36348999929369	-0.91294000396459
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C	4.84322001478985	-1.10947999321720	-1.78279005021583
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C	6.24496000268372	1.25895000067999	-1.12898999937611
C	6.78780000190090	0.38107999898558	-2.09557999252523
C	8.01576000309362	0.67436999708621	-2.74621999644674
C	8.49931999773067	-0.14132999808081	-3.74512000022107
C	7.76275000199034	-1.28032999994321	-4.14386000022612
C	6.57636000191764	-1.60423000262018	-3.51933999621086
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H	6.01408000024083	-2.48043999865612	-3.83954000065978
H	8.13314000014730	-1.90620000141411	-4.95699000107094
H	9.43318999979115	0.09568000264522	-4.23744000163067
H	8.56146000121323	1.57172000081928	-2.44752000236099
H	6.79534000130959	2.16644000302229	-0.87298000099731
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C	3.18859003008044	2.63857002432951	2.39446001554866
C	3.16945002177276	3.99032000768469	2.02519001313439
C	3.76858999643633	4.33097999795425	0.80008999699024
C	4.37343002555527	3.37070000516580	-0.00671999071204
H	4.81603999326143	3.66401999845523	-0.96134000274417
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C	1.92415999997511	4.49951000131395	4.18461999700240
H	1.12889000211864	3.77332000273749	3.96824999978569
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H	3.15472000066275	6.90726000203309	3.88971000023552
C	1.39860999888741	5.75801999720710	2.09722999949985

H	1.78180000256774	6.22557000107336	1.17979000229701
H	0.93235000011441	6.54613999818549	2.70753000015877
H	0.62354999932632	5.02841000065285	1.82893000137718
H	2.70194998981156	2.31522999697085	3.31195999322153
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O	3.13487000046991	-0.46195999309916	-0.21737999862385
O	-1.88954000109652	-1.10326999786885	-0.58293999781617
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C	-3.28483999537004	-2.37624999754621	0.87928998908138
C	-4.50319999980367	-2.50726999524605	1.61734000570819
C	-4.68084000188365	-3.47850999833855	2.63580999879426
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158

3b_2 (TS1-1)

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C	-6.25479999873253	-2.04693000243884	-1.79688999860239
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C	2.40809992347119	-0.73060992606646	-3.40031996287246
F	-6.13345999821167	0.93000999903296	-5.25013000134815
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C	1.85375000245670	-1.70216999923834	-4.22477000298188
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C	5.64694999901646	0.19579000535818	-1.83470000682861
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H	5.17652999942916	-2.42872999901915	-2.40067000053505
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C	4.38192001730571	6.28016000797563	-1.43759998174177

C	2.58685000465469	6.81094997951518	0.08738001791858
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C	-6.70833999702404	2.11694999724194	-0.33344000144239
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H	3.68349000157443	0.63296999929509	3.58965000201824
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H	-0.91498000145626	-4.78612999969895	7.12010000276513
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H	-1.92425979970650	-0.36430966567484	3.19272993077215
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H	-4.74490998953283	-3.37567000168215	1.94064999312608
H	-9.74660000169724	0.67027000187088	0.21374999870489
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F	-7.22610000207969	-4.20689000232351	-1.90949999874492
C	-2.07554998564237	-3.66526998074762	4.05711998272179
H	-0.73252998532843	-2.02173998422212	4.50258000769731
H	-3.58359001392139	-5.03002000009359	3.31527001494786
F	6.08145000152816	1.19190000048599	5.27919000057885
C	5.77966999762390	0.41818999894603	3.06059000097400
F	7.50076000195619	1.90810000204546	3.77548999928557
H	-7.82208999740651	-0.76305000189472	-2.54852999788277
F	-6.81770999950120	-3.40299000203011	0.08056000191600
F	-5.70509000037739	2.25569999989111	-3.56657000118129
C	-1.36057998533424	-4.65086999775546	4.98782998005855
C	6.71803000025968	-0.30823000198421	2.32911999839288
C	4.42436000117555	0.08126999802484	3.01262999857574

C	-5.85689999796567	-0.07366000155701	-3.11862999837043
C	-4.47965999832441	-0.29798999974960	-3.05210999962553
C	-7.19638999860712	-3.05216000160595	-1.18458999968444
C	-6.75082000029010	-0.94445000147304	-2.49639999966639
158			
3b_2	(TS1-1')		
C	-3.90652000175618	1.38616000101102	-3.18522000205713
C	-6.25928000229378	0.19539000036243	-2.27747000087781
F	-4.03006999970638	4.24575999991357	-3.12713999836285
H	-5.07235000254065	-1.59459000224319	-2.00435999798327
H	-6.82006000163494	-6.87530000076802	2.56350999915987
C	-4.79483000064584	-5.59785000064402	3.93204999745498
H	5.08231999739615	-3.22116999955159	-0.34347000256289
C	-5.08236999927680	-0.55159000104286	-2.31888000136166
C	4.08321998878670	-1.92355999137354	-3.26974999692563
C	-4.35302000234566	-6.27206000235856	1.57077000037064
C	-5.07880000053279	3.54261000037828	-3.64020999996234
C	5.40083999828935	-2.62742000053541	0.51319999906458
F	7.34327999788461	-2.58014999773156	-1.59612000170654
C	7.75920000104610	-2.76097999944047	-0.30767000001652
F	8.95648999949682	-2.13490999975237	-0.18149999815917
C	-3.90969000094343	0.06064999993752	-2.76297999847459
F	7.98870000211352	-4.09664000042145	-0.16180000074798
C	3.48302999638045	-0.76144998161104	-2.75979999008561
C	3.47794999987969	-2.66679999657320	-4.28399999986669
H	5.03823999965493	-2.25956999969625	-2.86222000479749
C	6.73910000054002	-2.27073999936749	0.68870000090794
C	-6.70089999954074	-5.81293999845176	2.30131000042905
F	-8.40663000042321	0.42340999859049	-1.27140999809442
F	-6.21404000251730	4.21741999908996	-3.33116000093332
C	4.19491000107824	0.04851000338938	-1.74698999526739
C	2.23232008267435	-0.39329017150526	-3.28750008423358
C	2.24661999899357	-2.28414998925111	-4.83324999256767
H	3.98699000222689	-3.55980000076825	-4.64607000232659
H	0.47568937832622	3.35665745967665	-1.44333825706061
H	8.18478000189905	-1.25841999924867	1.93380000117911
C	-5.09429000166881	2.12021999795901	-3.14039999951144
C	3.52788000059605	0.71427000564481	-0.68197000937747
C	5.57281000335063	0.18945999732197	-1.79557999939134
C	1.63722000058433	-1.13703998911834	-4.29920999077991
H	1.72657988512914	0.50055023976013	-2.93365988273830
C	1.56144999874874	-3.04417999681911	-5.97197999926820
C	-0.19587979710135	3.64597949853738	-0.64962021277913
O	2.13007000812685	0.62617999899299	-0.63817999388219
C	4.16705995941975	1.45026999580677	0.30792996286801
H	6.12395000121329	-0.25828999687829	-2.62352000331548
C	6.29849000358513	0.87567999321483	-0.79579999635214
H	0.66401999524352	-0.80757999537011	-4.66437000431782
C	2.38396999946509	-4.24942000095379	-6.44640000009552
C	1.36609999935777	-2.08457999757754	-7.16469999888810
C	0.18449999931496	-3.54756999936606	-5.49516999998585
C	-1.31615007761488	2.82643025695016	-0.32581971386982
C	-0.00144014736055	4.76508030652956	0.14459008089840
P	1.50029999629262	-0.35086002160890	0.48107002582271
C	5.60014999737592	1.48906000341296	0.29724999944918
C	3.36525013128410	2.16518006901696	1.33683006998669
C	7.71678999873774	0.93778999818147	-0.83341000093833
H	2.53340000116242	-4.98322999910828	-5.64041999999774

H	1.85369999761641	-4.75767999894689	-7.26451999797873
H	3.37130999866538	-3.94669999875582	-6.82495000156960
H	0.87952000023724	-2.61169999797438	-7.99917000098723
H	0.73482999754657	-1.22787000144668	-6.89262000242396
H	2.33290000117167	-1.69693000126361	-7.51770000201806
H	0.30356000253093	-4.27188000201066	-4.67592999959844
H	-0.45484999853280	-2.73153000188881	-5.13234000218393
H	-0.34198999986007	-4.05324000284034	-6.31883000174335
O	-1.47088998322398	1.62715996475256	-1.03258012307929
C	-2.28753003807026	3.16926997672220	0.60167984686511
H	0.83562002976676	5.43146993503438	-0.07040999729434
C	-0.86288009110690	5.08933012097409	1.21802987816098
O	2.23271003555509	0.11341009518095	1.83954991085921
N	-0.03200000130246	-0.10731998929340	0.49277000156151
N	2.03608999014368	-1.87564000654343	0.24308000374698
C	6.36228999873271	2.07526000079560	1.34021000170700
C	3.51361000344428	3.57588000151464	1.55943999706623
C	2.39355986454524	1.49062978189072	2.06565015222322
H	8.23546000142731	0.47306999992905	-1.67405999983607
C	8.42629999876770	1.54030999854626	0.182739999832992
P	-1.38527999540977	0.21389998763606	-0.24379999398237
C	-3.56438997932627	2.41321997683092	0.69319003247645
C	-2.03848991245320	4.30094990246409	1.44731008374274
C	-0.59653995132637	6.19774993955983	2.06473004451023
S	2.78232000027558	-2.84892000113618	1.35202999661252
H	1.32232000002801	-2.60768999834058	-0.64105000382194
C	7.74077000292329	2.09929999820802	1.28491999840500
H	5.84664999988832	2.49751000176729	2.20116000131796
C	4.37658999666516	4.39742999476781	0.78573000597126
C	2.71270002756897	4.20204001613478	2.57137988329565
C	1.54784019406119	2.09509011499453	3.03545990634493
H	9.51623000117342	1.57034000257313	0.14768000182295
O	-2.37639999634388	0.36348999940930	1.03169001326845
N	-1.89255000551230	-0.91140999830711	-1.24305999602893
C	-3.59185000129609	1.04368000472600	0.92564999892022
C	-4.81134999902790	3.10789000677620	0.53388001062280
C	-2.87588998039438	4.63825998489114	2.54261002260914
H	0.29611000607733	6.79473999618931	1.86909000253231
C	-1.43085997546603	6.50046996795925	3.11890002632621
O	2.85941999966931	-4.15070999876582	0.70470999786590
O	2.20164000176912	-2.71711999884251	2.67825000115115
H	8.30517999839045	2.54144000303415	2.10681000149220
H	4.95913998683749	3.94860000126984	-0.01712000946748
C	4.47648000793377	5.75227999868802	1.02626000855805
C	2.86109002759692	5.59409999451435	2.81325004772276
C	1.75867964978147	3.44213995855283	3.28378004040211
H	0.80116041099009	1.50675501096177	3.54619517238450
S	-2.36599999793069	-0.85883999723792	-2.76903999895192
C	-4.79429999725154	0.32097000186168	1.19003999998969
C	-6.03216999812731	2.40101999774106	0.78378999968881
C	-4.89193000257231	4.45439999886537	0.09310999803138
C	-2.57434002204685	5.70547002506244	3.36354998100945
H	-3.75588001383383	4.02842001591020	2.74362998286295
H	-1.21062001858394	7.34926002368903	3.76812998007273
H	5.14048999909665	6.36127999905905	0.41116000221823
C	3.72570000122444	6.35731000021155	2.06018999883635
H	2.25711000335941	6.04812000461583	3.60121000508524
H	1.14972012413596	3.94342998943093	4.03791000263319

H	4.10501999780524	-1.25498999959501	3.35019999791135
H	-5.41358999929602	-5.01659000203082	4.62986000084524
O	-1.45409999877014	-0.12194999901179	-3.63945000135092
O	-2.70739999651056	-2.23646000039643	-3.14521999963729
C	-5.98048000026735	1.03599000097897	1.14254000104708
C	-4.84004999768227	-1.12203999925346	1.52262999868088
C	-7.27250000053152	3.07392000072332	0.62583000039870
C	-6.11285000126399	5.07650000023605	-0.06595000166721
H	-3.97601999841635	4.99293000236633	-0.14453000019253
H	-3.22307999807043	5.93597999811774	4.20981000741828
H	3.82545998863555	7.42685000402815	2.25085998970627
H	-3.28731000141904	-6.02001999962379	1.66762999855959
C	4.46954999838731	-2.24695000131471	1.47792000139940
H	-3.74749000019977	-5.29552000174346	4.07263999892190
H	-4.88678000172791	-6.66056000076918	4.20320000205858
H	-6.91792000205319	0.50730999719753	1.32329999789797
C	-5.66540000037268	-1.57104000250477	2.56929000070640
C	-4.15701999812615	-2.09055000039491	0.77818999993246
H	-8.19273000049699	2.51891999841216	0.81793000179451
C	-7.31501000167212	4.38749000261068	0.21215000078918
H	-6.14995999754226	6.10532000015429	-0.42639999781681
F	6.55660000017035	-1.24716000250712	5.09594999883477
H	-7.36840000255069	-5.22688999887785	2.94872000232477
H	-4.62904999988340	-6.18226000067983	0.51042999972356
H	-4.47955999975503	-7.32461000117395	1.86413000104158
C	-5.78232000070196	-2.92722999953565	2.85674000205170
H	-6.20283000262014	-0.84316999774361	3.18029000146940
C	-4.28967999889236	-3.44937999909766	1.06069999967685
H	-3.51264000145063	-1.79052000154414	-0.04495000028850
H	-8.27339000047715	4.89252999886285	0.08353999905032
C	6.59883999919074	-0.42512999936044	4.00832999770614
H	-7.03166000166079	-5.67497000093234	1.26183000129651
C	-5.09410000080293	-3.90112999853493	2.11275000016068
H	-6.41834999915121	-3.22961000028583	3.69091999885219
H	-3.73735000180568	-4.15380999880264	0.43924000158544
F	7.86018999968903	0.07195999866727	3.93518000120008
C	6.19108999983721	-1.16013000015997	2.75599000117806
F	5.76353999897075	0.61724000031815	4.27739000134174
F	-8.20007000054344	-1.01836000220681	-2.90388999835779
H	-7.19068999792437	2.11568000161272	-2.62885000145609
F	-4.94538000098139	3.58475000073822	-4.99834999923757
C	-5.22899999777067	-5.38436999803985	2.46720999742924
C	7.14099000263807	-1.53709999980180	1.80670000204657
C	4.85019999750588	-1.51757000038486	2.60100999925520
C	-6.27224000199381	1.53382000064753	-2.68162999867398
F	-7.33308000099669	-1.45878000016268	-0.94457999913306
H	-2.98168000056002	1.83159000011360	-3.54799000228947
C	-7.54418000261860	-0.46458000141888	-1.84292999786460
158			
3b_2 (TS1-2')			
C	6.06019999894810	2.87505000115963	2.55422999155941
F	6.02401000006571	2.99092000190782	1.19201000240159
H	-6.32252000196920	0.30772000216465	5.93471999921449
C	-3.63898000169679	-1.93033000088456	-3.34545999914363
F	6.45429000271960	4.08248999642201	3.03888000083302
H	-4.61538999933990	2.78572000223638	5.31525999968578
H	5.05008999725560	0.34114999997391	2.69754999435163
H	-2.72239000010899	-2.41825999967756	-3.67279999752652

C	1.60212996768540	-4.26885984608892	-0.07600010174136
H	-6.15145999800704	-0.54849999763496	4.38650000188790
H	-5.95190000186085	3.78803000155010	4.70552999738393
F	7.03782000080104	1.97916000053447	2.84580999842301
H	-8.19398000167603	1.65758000262129	4.97712000229865
C	4.36626000967158	1.10085999811010	3.07617002229445
C	-5.18576000205224	-1.39121999877934	-1.55406000244102
C	-4.00434000169836	-1.98215999764148	-2.00340999795396
C	-4.45383999772291	-1.24380999863505	-4.24815999845827
C	2.70252000875507	-4.14102003419911	0.78670001430380
C	0.53256000254646	-5.10449002989307	0.24002001098616
H	1.57604002181541	-3.72214016435141	-1.01546985540441
H	-7.94922000090145	2.66372000134813	3.52798000213978
H	-4.73419999829314	0.22090999986846	5.13442000183281
H	1.23228999954181	1.34286000237421	4.41832999592355
H	-6.20611000158532	2.74406000261947	6.11894000005908
C	3.85529999328486	-3.25812999513241	0.50524000473740
C	2.67925000832003	-4.87875001487269	1.98252999789448
C	0.51044000363022	-5.85471001709926	1.42542999641131
H	-0.30363000153470	-5.14351998789789	-0.45731999785782
H	1.48207752872803	-1.16102578803036	-3.47970983095009
H	-8.00479000023399	0.89365000021942	3.37620999968918
C	3.10375000403583	0.72735999817779	3.53298000960570
C	3.69308999797595	-1.95345000022088	-0.03118998999781
C	5.14636999875566	-3.62618999987976	0.84130000066074
C	1.61191999990123	-5.71942999800690	2.28694999926069
H	3.48954999828332	-4.75380999442494	2.70228999875841
C	-0.63012000057907	-6.82734999939191	1.74463000407919
C	1.14041990224555	-0.14310977917984	-3.58692053395116
O	2.39432999815312	-1.56215000084551	-0.39035999891484
C	4.71214998531532	-1.02994001628306	-0.19509003154313
H	5.32995000071917	-4.63145999930555	1.22499000231273
C	6.23094999933409	-2.72164999893887	0.76692999534534
H	1.63990000000073	-6.26806999708892	3.22904000221868
C	-0.94767000307476	-6.83759999737733	3.25176999981889
C	-0.17751999861776	-8.24200999743865	1.32223999867641
C	-1.91752999864082	-6.46887000165721	0.98501000036283
C	-0.12970995900237	0.24903982436754	-3.07198968967710
C	1.89623016247622	0.86082992305976	-4.17627944319277
P	1.65707998579537	-0.56989998720377	0.63554998952047
C	6.01843999473999	-1.38760999643137	0.28181000812665
C	4.44576002078157	0.29102000377876	-0.82132002423273
C	7.52503000036276	-3.09441000211488	1.21731000023185
H	-0.10650999939178	-7.20514999713243	3.85496000119954
H	-1.20709000113877	-5.83038999801038	3.60925000093349
H	-1.80524999779231	-7.49798000139412	3.44677000159600
H	0.04112000069372	-8.27428000246814	0.24517000189752
H	0.73147999890137	-8.54368999794411	1.86260000119511
H	-0.96822000113627	-8.97764000024616	1.53631000188665
H	-2.24874000231390	-5.44161999712557	1.19210999912106
H	-1.79848000122770	-6.56055000060764	-0.10276999759084
H	-2.72419999749640	-7.15357000015554	1.28507999973149
O	-0.88408998228650	-0.70436991868963	-2.36141000521720
C	-0.67990001609329	1.51096004166054	-3.23582014187860
H	2.86616996013717	0.61103000294582	-4.60904013633161
C	1.46303999326181	2.20431000413156	-4.23728000616195
O	2.62033004869726	0.72451996936533	0.69832999068932
N	0.25153999633953	-0.27336000126743	0.05356999934679

N	1.56952999431754	-1.07840999539501	2.17240999931150
C	7.09579000004543	-0.46666000183763	0.34442999480289
C	5.23803995944986	0.74008997889550	-1.93346004263675
C	3.43599002102345	1.13158009028643	-0.36493982977144
H	7.67661999760789	-4.11592000040935	1.57216000114142
C	8.55843999749726	-2.18339999920183	1.23905000380785
P	-1.07005001085297	-0.46158000689697	-0.77126002026846
C	-2.09489000285644	1.78542999003549	-2.87338999950912
C	0.15452995923377	2.54927000032799	-3.76622007247137
C	2.30302994973662	3.22458998924921	-4.75723012245745
S	2.63693999710375	-1.00262000188536	3.43171999649488
H	0.41644000055126	-1.73469000233306	2.51310000184873
C	8.33318999898990	-0.85390999787328	0.81673000397095
H	6.93528999950959	0.56361000331079	0.03037000109901
C	6.14672999985364	-0.11036999729471	-2.61729999736382
C	5.07403004256932	2.08031998774768	-2.41291997986196
C	3.25253984424538	2.46694987050156	-0.82617032005105
H	9.54398999768834	-2.47935000023194	1.60123000013557
O	-1.69606999905599	1.03548999111469	-0.63842000272938
N	-2.07137999584595	-1.53579000467954	-0.18674999786559
C	-2.56671999917612	1.57135000257748	-1.58575999508682
C	-3.00095999936886	2.30276000181140	-3.85850000019042
C	-0.23468998405506	3.91317999831593	-3.78198996309158
H	3.29186000137684	2.94396000052014	-5.12548999324707
C	1.89159001197772	4.53925000370515	-4.76921997765920
O	3.86045999994826	-1.73784999846520	3.16024000122531
O	1.83602999861363	-1.33215000056508	4.60200000079420
H	9.14123000154975	-0.12309000029690	0.87166999991331
H	6.25755000901131	-1.14208999637146	-2.28634999470003
C	6.87300000097420	0.34579000068361	-3.69801999946611
C	5.85463995906460	2.52716998212009	-3.51195004470686
C	4.10729012353229	2.91918013467265	-1.81502976426354
H	2.46852891685362	3.07748464941809	-0.40416759329426
S	-2.88109999672931	-2.75305999994801	-0.83217999676080
C	-3.84554999929749	2.01295999695878	-1.13628000007406
C	-4.31055000275726	2.71096999918323	-3.44319000213835
C	-2.67154000252510	2.39074999611990	-5.23568999893712
C	0.61768999664949	4.88526999735629	-4.26192000659711
H	-1.21027998648182	4.19184999579497	-3.38628997653561
H	2.54996000697925	5.31728999934404	-5.15902998134721
H	7.55444999917699	-0.33170000049060	-4.21452000191709
C	6.73898999598992	1.68049999964915	-4.14395000194455
H	5.72657000057831	3.55631999732389	-3.85420999931873
H	3.97709996887199	3.93243996221375	-2.19815005225821
C	4.72188000215060	2.44968000561721	3.10455000497089
H	-5.46450000051504	-1.45338000080197	-0.50292000144839
O	-2.04021999861344	-3.66406000076103	-1.60098000215947
O	-3.70741999865714	-3.31200000180614	0.24529999933034
C	-4.67609999778369	2.59114999790790	-2.08377999833265
C	-4.30456000227845	1.91858000170086	0.26873999912909
C	-5.22395999744742	3.20724999847925	-4.41041000085143
C	-3.58403000198462	2.87013000118496	-6.15233999829996
H	-1.69207000018207	2.05302000151786	-5.57091000175720
H	0.30695000041731	5.93097000010748	-4.24618000653324
H	7.32714000925451	2.03224000572564	-4.99270999095945
C	-5.81417000209512	0.32660999861870	4.95941999836013
H	4.11850004924153	4.45571003140977	3.62677011445411
H	-6.24343999810000	-0.06932999849012	-4.51897000135578

C	-5.98874999766694	-0.70931999933503	-2.46873000076256
H	-5.67264000118754	2.91600999990967	-1.78023999823863
C	-4.17641999977638	0.75688000252805	1.04052999784615
C	-4.97855999866360	3.01027000120229	0.84630999790447
H	-6.21966000163606	3.50848000296362	-4.07860000002317
C	-4.86932000038130	3.28845999980693	-5.73939999825225
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F	2.27609000243528	5.17061999758683	5.02261000489050
C	-5.70016000025607	2.81259000157935	5.14402999752077
C	-7.66298000016105	1.72068999926774	4.01486999825369
F	-2.73639999857570	-0.89841999851699	-5.85317000250621
C	-4.74098999792324	0.66816999960029	2.31311000127739
H	-3.64413999801489	-0.10630000103767	0.64591999759638
C	-5.53092000040279	2.91962999886180	2.11955999780642
H	-5.06285999753568	3.94467000078059	0.28761999981316
H	-5.58127000056442	3.66349999847752	-6.47598000077605
C	1.63445999856043	4.03715000100424	4.63116999343474
F	-4.77460000050731	-0.32185000198377	-6.42296000044569
C	-5.44405000032057	1.73914000072466	2.87736000069409
H	-4.61832000079544	-0.26825000251905	2.85699999748830
H	-6.04998000253844	3.79020999983489	2.52479999832277
F	0.71092000158706	4.41117000056601	3.69886000142376
C	2.58796000416522	3.00461000544481	4.08443000216600
F	0.94526999599140	3.57103999712819	5.70631000215282
F	-8.31941999837395	-0.98159000223118	-2.11017999825931
C	-4.05310999967204	-1.21521999872262	-5.70148000105225
F	-4.22781999812368	-2.43679000215244	-6.28512000061254
C	-6.13794999812640	1.64381999811898	4.23942999787709
C	3.83356995944869	3.40565998449536	3.59830990164858
C	2.20700001192853	1.66123999644485	4.04827002435791
F	-7.63071999762145	0.99170000150441	-2.75781000026090
C	-7.28704000165039	-0.09462000180268	-2.00844999803245
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142

3b_3 (cat)

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C	-2.36741999793564	4.33714999905846	-4.43634000166718
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C	-4.77976999831995	1.89882999740375	-1.13001000077668
H	1.17062999763714	-3.39937000143240	1.78822000294882
C	-3.26420000176072	0.57658999918237	-2.43855999927845
C	-4.72109999950110	2.91275000178443	-2.08504000088907
C	-3.93565000049872	2.78637000118879	-3.23810999918243
C	-3.21494999771065	1.59119000155829	-3.38689999836841
C	0.21410999840857	-3.80057999947133	1.49077999189209
C	0.00385999809966	-5.13986000220092	1.19958000339127
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C	-1.41871999939660	-7.00242999884724	0.42255000051203
C	-2.62642999997451	-7.47151000154142	-0.04642000188851
C	-3.72117000105195	-6.58703999816880	-0.18108000120518
C	-3.59717000104520	-5.25799999892351	0.16882999789113
C	-2.37045999994433	-4.74485000253410	0.66550000035732
C	-2.18320000728067	-3.36683000114652	1.00670000769152
C	-0.917579998732923	-2.94597000215749	1.37970999722010
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O	-0.73287003761643	2.92171007096277	2.24803999065169
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H	0.62355001090274	5.02841001419696	1.82892999956492
H	3.75503999908567	0.62660999869675	1.91117000244686
C	-4.68084000171046	-3.47850999810856	2.63580999935998
C	-6.92161999831353	-2.65479999976468	3.06965000160416
C	-5.85993999927609	-3.54590000085607	3.34896999966194
O	3.13487000117738	-0.46195999614629	-0.21738000095583
H	2.70195000136234	2.31523000150746	3.31196000192436
C	-4.05546999777297	0.70639999961591	-1.28257000091684
O	-1.88954001954769	-1.10327000677584	-0.58294000690144
C	-4.18919999966334	-0.37805999876371	-0.28381999707350
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C	-6.77716000206116	-1.69605000022565	2.09030999749346
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N	0.59803995910659	-0.97146001592974	-0.49359998774524
P	1.81168001112678	-0.24307999905507	-1.10149998606720
N	1.75215999733785	1.41528999959843	-1.30400000292593
S	0.95366999796456	2.16173999889022	-2.59887999756060
O	-0.13264999895458	1.26476999931535	-2.93608000198545
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C	-1.28556000086220	4.85708000474989	-0.54988999961057
C	-0.61207000846867	6.05266000336399	-0.82378001670856
C	0.53838999724137	6.03751000004927	-1.60443000193725
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F	-3.48715000901547	5.70547000533321	-0.36817000358548
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C	2.71400999685499	-2.18009000105700	-2.46265999954382
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C	6.34146000041113	-5.19102999842868	-1.29079000189226
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H	-2.02133000210594	4.79850999956599	-3.50070999776009
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H	1.75480000021392	-5.39903000054823	-2.84527999819249
H	3.57260999822655	-6.91953999857081	-2.28938000179003
H	5.88614000217182	-7.30862000164869	-1.47566000172911
H	7.35029999886772	-5.36348999893700	-0.91294000174783
H	6.53259000255370	-3.06034999791520	-1.20374999804162
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C	6.24496000148652	1.25895000193728	-1.12899000113187
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C	3.78358999853527	1.66780000205497	1.59157999993522
C	3.18858999843896	2.63857000249809	2.39446000084328
C	3.16945000224333	3.99032000143961	2.02519000040284
C	3.76858999917773	4.33097999912430	0.80008999860126
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H	4.81604000018153	3.66402000029410	-0.96133999904620
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H	1.12889000277917	3.77332000206287	3.96824999973484
H	1.48180999839254	5.31670999827748	4.77237000005832
H	2.68826999804008	4.01532000062366	4.81062999954441
C	3.60036999929092	6.11633999876761	3.26808999924231
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H	3.15472000046660	6.90726000210766	3.88970999965876
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142			
3b_3	(TS1-1)		
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C	-7.19638999851149	-3.05216000165714	-1.18458999952417
H	-0.73252991553918	-2.02173994814966	4.50257995686790
C	-2.02294000284768	-6.03531999981806	4.99041000242051
C	-6.25479999869711	-2.04693000253021	-1.79688999860552
C	-4.47965999835009	-0.29798999961334	-3.05210999968325
C	2.40809999834243	-0.73060999988145	-3.40032000096212
F	-6.13345999818042	0.93000999904247	-5.25013000130587
C	-1.40585000224214	-4.08844999879387	6.42482000013742
H	-1.47975999779403	-6.70111999979861	5.67645999983034
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H	-4.48932000126985	-3.13581000111675	-1.16656000069039
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C	3.62342000051868	-0.95936999996777	-2.72525000145177
C	1.85374999967741	-1.70216999834080	-4.22477000065400
H	1.88125000014278	0.21391000126354	-3.28267000088899
C	-6.35169999745051	1.10661999771612	-3.91518000261547
F	-7.68210999963154	1.32598000046835	-3.75487000081580
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H	-3.77548999924612	0.36401000000039	-3.55353000066445
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H	0.89257999874361	-1.48705000143911	-4.69424999783602
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C	5.64694999775280	0.19579000104231	-1.83470000143412
C	3.69719999886735	-3.15938999987766	-3.77734999900272
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C	-1.97638999785664	3.58384000115345	-1.45720999998426
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C	6.29437999790648	1.15960999938629	-1.02880000196626
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C	1.60576999785604	-3.37025999996224	-6.74553000101876
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H	-0.19848999990268	-3.50932999862882	-4.60317000174599
H	-0.05727000237373	-5.08818000034396	-5.41145999827576
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H	2.82697000039692	-5.75976000157928	-4.53625000275671
H	2.16454000222056	-5.95599999810530	-6.16659000019122
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O	-2.37449999785005	1.20710000062053	-1.33767000420438
C	-3.77314999893944	2.62553999821136	-0.02941999822247
H	-1.83197000218311	5.71948000081124	-1.44956999879461
C	-3.39688000010981	5.06336000135711	-0.11094000139989
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C	6.18380000104409	3.02938000246759	0.55404999721044
C	3.35936000184523	4.48337999732015	-0.14625000219015
C	2.18571999383740	2.75396999853992	1.06982000271711
H	8.29611000160492	0.49057000012013	-1.51126000148637
C	8.33376000214525	2.13120000163272	-0.12208999801869
P	-1.57373000308580	0.24778999728418	-0.30653001697520
C	-4.45638000121106	1.41406999788256	0.49964999847427
C	-4.11789000030701	3.94234999797265	0.42238999923681
C	-3.72143000176490	6.37258000185201	0.33542000011122
S	2.29907024074650	-1.48317977200074	2.19976995587449
H	1.47054989415172	-2.11962999501319	-0.08184994993115
C	7.56086000149516	3.03926000006703	0.63711999756164
H	5.59701000063522	3.72516999873524	1.15221000071908
C	4.30342000022530	4.94440999797242	-1.10059999834364
C	2.46772999845202	5.44096999820863	0.44423000004647
C	1.28290000147426	3.67493000070423	1.66781000007311
H	9.42217999760347	2.15272999997802	-0.05157000192156
O	-2.31996000178951	0.52586999945540	1.10271000054386
N	-1.78639000321720	-1.25866000381514	-0.78175000153552
C	-3.71251000135745	0.41013000107113	1.10770000114950
C	-5.87562999797090	1.24212000227124	0.41041999984604
C	-5.10352000058989	4.18926999951464	1.41392000244544
H	-3.17110999966003	7.21579000007909	-0.08760000027039
C	-4.69395000196840	6.57773999997216	1.28929999765436
O	2.29108009058855	-2.93935006532835	2.20417998805226
O	1.62491976700549	-0.76016015728999	3.26643007383800
H	8.05581999772621	3.74571000149421	1.30456000239322
H	4.96773999731143	4.22799000145978	-1.58013000239710
C	4.38191999955597	6.28016000141109	-1.43759999988580
C	2.58685000039700	6.81094999891519	0.08738000064831
C	1.46585999961675	5.01005000124678	1.34492999998818
H	-3.58359000291552	-5.03002000055998	3.31527000110557
S	-2.23490999852835	-1.70811999819716	-2.25539999798845
C	-4.27802999986192	-0.71730000145712	1.76718000211454
C	-6.47621000216585	0.11398999869244	1.06203999797741
C	-6.70833999835106	2.11695000048262	-0.33343999887793
C	-5.38305000255727	5.47229000243052	1.83791000060947
H	-5.63992999764344	3.34840999786021	1.84993999777562
H	-4.92811000120705	7.58796000258323	1.62782999857892
H	5.11046000092001	6.60638999799705	-2.18134999880488
C	3.52309000259512	7.22638000014127	-0.83378000207046
H	1.90729000130746	7.52868000004164	0.55178000204472
H	0.81228999978013	5.75778000039990	1.79834000295344

H	-2.00252999738293	-6.49960000001810	3.99328999828237
H	3.57183974367837	-1.03166278417744	2.14164448569612
O	-1.61409999820179	-0.93409999904260	-3.32872999776880
O	-2.11086999751089	-3.16802999778334	-2.31304999786219
C	-5.66110999781380	-0.81380000104811	1.74995000116400
C	-3.46066000134147	-1.72403999740271	2.48251000021677
C	-7.88411000015493	-0.05689000023427	0.98959999877939
C	-8.07057999897521	1.90945000191257	-0.40339000251675
H	-6.25611999947245	2.95037999954852	-0.86923000129259
H	-6.14034000047950	5.63291999775826	2.60680999832106
H	3.59820999883690	8.28041000191054	-1.10446999836880
H	-3.06826999731148	-5.98747999897381	5.32867000112449
C	0.10996000172008	-4.81721000072441	4.55724999765031
H	0.64956999747063	-5.43953999740607	5.28720999878746
C	-2.07554999720748	-3.66527000226981	4.05711999748009
H	-6.14426999859734	-1.63621000150633	2.27916000230247
C	-2.30037999728303	-1.38535000155790	3.20474999940307
C	-3.87697000190430	-3.06367999828289	2.52459000163377
H	-8.33051000216754	-0.91681000161802	1.49252000035044
C	-8.66787999912269	0.82162999829073	0.27332000165421
H	-8.68886999824508	2.58382000029331	-0.99729000215415
C	-1.36057999741654	-4.65086999865949	4.98782999729662
H	0.16900000172217	-5.31849000188309	3.58070999743577
H	-0.91498000107648	-4.78612999926905	7.12010000208199
H	0.63240999762069	-3.85485999735272	4.47593999919642
C	-1.627769998228857	-2.33688999610623	3.96355999480355
H	-1.92425999821747	-0.36431000259152	3.19272999763028
C	-3.20461999982925	-4.00819999966017	3.30097999970998
H	-4.74490999909241	-3.37567000094062	1.94064999821822
H	-9.74660000163639	0.67027000223678	0.21374999930371
F	-6.81770999980204	-3.40299000190130	0.08056000143323
F	-7.22610000195442	-4.20689000233701	-1.90949999861856
142			
3b_3 (TS1-1')			
C	-3.90652000175041	1.38616000135118	-3.18522000215061
C	-6.25928000235236	0.19539000025262	-2.27747000112363
F	-4.03006999972050	4.24575999986133	-3.12713999826639
H	-5.07235000240471	-1.59459000229814	-2.00435999802825
H	-6.82006000163409	-6.87530000076644	2.56350999918266
C	-4.79483000066817	-5.59785000064744	3.93204999744025
H	-6.41834999938861	-3.22961000028482	3.69091999859293
C	-5.08236999933856	-0.55159000087746	-2.31888000173162
C	4.08321999960808	-1.92355998856768	-3.26974999392278
C	-4.35302000235986	-6.27206000236675	1.57077000036127
C	-5.07880000053832	3.54261000039944	-3.64020999990321
C	-5.09410000078646	-3.90112999856097	2.11275000011493
H	-3.73735000190215	-4.15380999889626	0.43924000147561
F	-4.94538000097521	3.58475000076806	-4.99834999917931
C	-5.22899999777123	-5.38436999805285	2.46720999740316
C	-3.90969000109285	0.06065000146744	-2.76297999837536
F	-7.33308000099778	-1.45878000016830	-0.94457999910726
C	3.48303002210250	-0.76145002473806	-2.75980001268179
C	3.47794999668470	-2.66679998976432	-4.28399999551550
H	5.03823999485349	-2.25956999589702	-2.86222000297359
F	-8.20007000052236	-1.01836000218619	-2.90388999833314
C	-6.70089999955882	-5.81293999846240	2.30131000041302
F	-8.40663000046450	0.42340999830196	-1.27140999832882
F	-6.21404000250225	4.21741999908986	-3.33116000085361

C	4.19490999520958	0.04851000169291	-1.74698999182056
C	2.23232006379270	-0.39329013808632	-3.28750006899975
C	2.24661999438791	-2.28414999528084	-4.83325000075124
H	3.98698999939778	-3.55979999795360	-4.64607000020896
H	0.47585142960412	3.35641484053141	-1.44312162015330
H	-7.19068999788107	2.11568000159941	-2.62885000140471
C	-5.09429000169361	2.12021999799287	-3.14039999959378
C	3.52788000110865	0.71427000469759	-0.68196999392382
C	5.57281000087799	0.18946000354602	-1.79558000086173
C	1.63722001849180	-1.13704004109001	-4.29921002078045
H	1.72657985729260	0.50055030241955	-2.93365985214025
C	1.56144999681542	-3.04417999417603	-5.97197999859451
C	-0.19587982732770	3.64597949158632	-0.64962028698200
O	2.13006999781172	0.62617999406877	-0.63818000164717
C	4.16706000166439	1.45026999663572	0.30793000500761
H	6.12395000108085	-0.25828999664044	-2.62352000414208
C	6.29849000234158	0.87567999574857	-0.79580000083189
H	0.66401999827011	-0.80757998505872	-4.66436999514571
C	2.38396999914004	-4.24941999950500	-6.44639999893730
C	1.36609999917205	-2.08457999636772	-7.16469999815314
C	0.18449999891753	-3.54756999850156	-5.49516999943262
C	-1.31615005229427	2.82643018069871	-0.32581975260488
C	-0.00144000229472	4.76508012185517	0.14459012575504
P	1.50029997843962	-0.35086000911689	0.48107000492728
C	5.60015000581061	1.48905999892216	0.29725000154885
C	3.36525000859522	2.16518006926351	1.33682997336663
C	7.71678999835777	0.93778999992269	-0.83341000200450
H	2.53340000146279	-4.98322999905708	-5.64042000000195
H	1.85369999768855	-4.75767999840101	-7.26451999764936
H	3.37130999889910	-3.94669999891217	-6.82495000128168
H	0.87952000176686	-2.61169999849998	-7.99917000081198
H	0.73482999665783	-1.22787000148154	-6.89262000298235
H	2.33290000124496	-1.69693000003944	-7.51770000105587
H	0.30356000220030	-4.27188000157072	-4.67592999997272
H	-0.45484999930189	-2.73153000182134	-5.13234000268049
H	-0.34198999872816	-4.05324000354983	-6.31883000126210
O	-1.47088998967246	1.62716000805916	-1.03258005790761
C	-2.28753006029003	3.16927003888336	0.601679990384659
H	0.83561998854845	5.43147000965023	-0.07041001435116
C	-0.86288008409748	5.08933013614959	1.21802996367709
O	2.23271007482438	0.11341005297287	1.83954999479200
N	-0.03200000779839	-0.10731999748481	0.49277001238292
N	2.03609005334123	-1.87563997896706	0.24307999059412
C	6.36228999806933	2.07525999873010	1.34020999975566
C	3.51361000319424	3.57588000586269	1.55943999429978
C	2.39355983542758	1.49062984861576	2.06565005116000
H	8.23546000158617	0.47306999903874	-1.67405999891856
C	8.42629999858416	1.54030999902507	0.18273999825874
P	-1.38527999213820	0.21389999447392	-0.24380002341842
C	-3.56438998183672	2.41321996472631	0.69319001217918
C	-2.03848998163919	4.30094996124001	1.44730999916283
C	-0.59654000735488	6.19775000596170	2.06472999839747
S	2.78231993317110	-2.84892004321736	1.35203000722286
H	1.32231999189325	-2.60769000306668	-0.64104999525985
C	7.74077000188421	2.09929999954261	1.28491999716581
H	5.84664999905880	2.49751000103067	2.20116000183675
C	4.37658999417147	4.39742999890778	0.78572999876220
C	2.71270007605223	4.20203998872032	2.57137997489829

C	1.54784014448573	2.09509010400877	3.03545989977516
H	9.51623000128259	1.57034000143308	0.14768000248090
O	-2.37639999601459	0.36349000410446	1.03169000505730
N	-1.89254999163097	-0.91141000974579	-1.24305999626538
C	-3.59185000215307	1.04367999463018	0.92564999377803
C	-4.81134999416603	3.10788999816411	0.53387999828654
C	-2.87588997334669	4.63825997089420	2.54261001930806
H	0.29611001315932	6.79473998337014	1.86909000630710
C	-1.43085997157860	6.50046996306474	3.11890002744592
O	2.85942001391572	-4.15070998594039	0.70470999573935
O	2.20164002178749	-2.71711998349773	2.67824999635479
H	8.30517999821069	2.54144000281659	2.10681000162813
H	4.95914000382332	3.94859999711005	-0.01711999491628
C	4.47647999753467	5.75228000197079	1.02625999914994
C	2.86108999601653	5.59410000394738	2.81325000900193
C	1.75867984939601	3.44213992759738	3.28378016435827
H	0.80209192354271	1.50610111108616	3.54672814840253
S	-2.36600000222843	-0.85883999737550	-2.76903999569108
C	-4.79429999817253	0.32097000313657	1.19004000361321
C	-6.03216999778477	2.40102000102886	0.78379000668060
C	-4.89193000149884	4.45440000118921	0.09311000324999
C	-2.57433999613141	5.70546999645521	3.36355000526136
H	-3.75588000039680	4.02842000377726	2.74362999732406
H	-1.21062000618837	7.34926000854618	3.76812998917238
H	5.14048999838719	6.36127999845321	0.41116000262159
C	3.72569998940115	6.35731000445238	2.06018998735115
H	2.25710999252474	6.04812000577523	3.60120999525434
H	1.14972003432534	3.94343001243402	4.03790993613090
C	-7.54418000258219	-0.46458000146719	-1.84292999791904
H	-5.41358999929157	-5.01659000203375	4.62986000085507
O	-1.45410000200664	-0.12194999858584	-3.63944999922667
O	-2.70739999788455	-2.23645999952347	-3.14521999904070
C	-5.98048000020189	1.03599000263590	1.14254000465267
C	-4.84004999732329	-1.12203999804486	1.52263000120902
C	-7.27250000051462	3.07392000220593	0.62583000462369
C	-6.11285000140907	5.07650000118783	-0.06594999966373
H	-3.97601999886223	4.99293000222122	-0.14453000192576
H	-3.22308001348985	5.93598001640585	4.20980999102928
H	3.82546000726815	7.42684999997926	2.25086000659251
H	-3.28731000141147	-6.02001999961352	1.66762999855668
H	3.99991598283204	-2.26140956841129	1.36171211044009
H	-3.74749000019494	-5.29552000173659	4.07263999892984
H	-4.88678000171500	-6.66056000077152	4.20320000206541
H	-6.91792000201511	0.50730999664376	1.32329999624818
C	-5.66540000011842	-1.57104000244088	2.56929000092709
C	-4.15701999782188	-2.09055000005761	0.77819000019238
H	-8.19273000062709	2.51891999809067	0.81793000035569
C	-7.31501000181514	4.38749000260854	0.21215000059943
H	-6.14995999777924	6.10531999974089	-0.42639999942190
H	-2.98168000056263	1.83159000010261	-3.54799000237144
H	-7.36840000254453	-5.22688999887275	2.94872000232649
H	-4.62904999988787	-6.18226000068665	0.51042999973704
H	-4.47955999972675	-7.32461000117182	1.86413000106522
C	-5.78232000086431	-2.92722999955827	2.85674000182449
H	-6.20283000255946	-0.84316999782891	3.18029000138219
C	-4.28967999893680	-3.44937999907346	1.06069999963119
H	-3.51264000102785	-1.79052000157243	-0.04495000017494
H	-8.27339000058954	4.89252999854532	0.08353999813326

C	-6.27224000197864	1.53382000059920	-2.68162999875303
H	-7.03166000164771	-5.67497000094484	1.26183000130220
142			
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C	-6.13794999802205	1.64381999818774	4.23942999793021
C	-4.05310999963789	-1.21521999867901	-5.70148000102835
H	-6.32252000199961	0.30772000214860	5.93471999919727
C	-3.63898000170229	-1.93033000110804	-3.34545999875631
F	-8.31941999837062	-0.98159000221573	-2.11017999826930
H	-4.61538999934424	2.78572000222750	5.31525999969200
H	-6.04998000214290	3.79021000005836	2.52479999852235
H	-2.72239000022104	-2.41825999973913	-3.67279999753880
C	1.60213002201370	-4.26886015236330	-0.07599986867012
H	-6.15145999800281	-0.54849999764421	4.38650000187628
H	-5.95190000185908	3.78803000154371	4.70552999737838
F	-7.63071999745531	0.99170000171833	-2.75781000041479
H	-8.19398000167906	1.65758000260525	4.97712000229263
H	-4.61832000057567	-0.26825000238574	2.85699999758519
C	-5.18576000196339	-1.39121999912861	-1.55406000210936
C	-4.00434000116355	-1.98215999873358	-2.00340999786301
C	-4.45383999772759	-1.24380999859243	-4.24815999828844
C	2.70252000051628	-4.14101999026093	0.78669997519396
C	0.53256000546777	-5.10448998069934	0.24001998780314
H	1.57603998204031	-3.72213980408472	-1.01547018434060
H	-7.94922000090783	2.66372000135204	3.52798000214450
H	-4.73419999830433	0.22090999986912	5.13442000184000
C	-5.62474999904958	-0.62386999828351	-3.81563000085366
H	-6.20611000159426	2.74406000261821	6.11894000005301
C	3.85529999994224	-3.25812999811144	0.50523999581163
C	2.67924998415499	-4.87874998199268	1.98253000058383
C	0.51043999710263	-5.85470997356296	1.42542999970016
H	-0.30363000442271	-5.14352000487115	-0.45732000762365
H	1.48190005333077	-1.16110942881478	-3.47989941413119
H	-8.00479000023685	0.89365000022690	3.37620999967291
H	2.92206228247112	0.31876722180506	3.40202209137018
C	3.69309000637825	-1.95345000052466	-0.03119000686265
C	5.14636999745008	-3.62619000156231	0.84130000276966
C	1.61191999827658	-5.71942999640440	2.28695000035619
H	3.48955000013829	-4.75381000247871	2.70228999650490
C	-0.63011999966159	-6.82734999702404	1.74463000278288
C	1.14042006290814	-0.14311032122830	-3.58691948009260
O	2.39433000379625	-1.56215001685836	-0.39036000177281
C	4.71214998909488	-1.02994000156099	-0.19509000245492
H	5.32995000185430	-4.63146000051519	1.22499000111032
C	6.23094999667786	-2.72164999777879	0.76693000204880
H	1.63990000476834	-6.26807000764522	3.22904000113022
C	-0.94767000150697	-6.83760000112027	3.25176999946461
C	-0.17751999752330	-8.24200999953339	1.32223999702752
C	-1.91752999732362	-6.46887000314357	0.98501000026407
C	-0.12971000337575	0.24904027107744	-3.07199025634404
C	1.89622990761082	0.86083015903657	-4.17628042930709
P	1.65707997004495	-0.56989994022552	0.63555002157663
C	6.01844000042115	-1.38760999909451	0.28180999827280
C	4.44576000833770	0.29102000687412	-0.82131999019591
C	7.52503000009006	-3.09441000209546	1.21731000002084
H	-0.10651000026724	-7.20514999905178	3.85496000179583
H	-1.20708999746405	-5.83038999136945	3.60924999908388
H	-1.80524999867298	-7.49798000167874	3.44677000192104

H	0.04112000081461	-8.27428000247368	0.24517000207826
H	0.73147999850328	-8.54368999886894	1.86260000200048
H	-0.96822000165892	-8.97764000089587	1.53631000149701
H	-2.24874000147150	-5.44161999782932	1.19210999948105
H	-1.79848000160164	-6.56055000148051	-0.10276999735420
H	-2.72419999821764	-7.15357000006571	1.28508000005389
O	-0.88409002081585	-0.70437010565406	-2.36140998935739
C	-0.67990004747138	1.51095990254598	-3.23581999448252
H	2.86617001946000	0.61102998072348	-4.60903990169170
C	1.46303996869244	2.20430997205948	-4.23728009001613
O	2.62032999682851	0.72451997605551	0.69832998748248
N	0.25154000919843	-0.27336001688575	0.05356999404126
N	1.56953002084148	-1.07841002737911	2.17240998640462
C	7.09578999771258	-0.46666000079078	0.34443000061580
C	5.23803998996963	0.74008999122041	-1.93346000719097
C	3.43599002787847	1.13158001685710	-0.36493998012970
H	7.67661999796287	-4.11592000061228	1.57215999994309
C	8.55843999827693	-2.18339999975172	1.23905000123005
P	-1.07004999136309	-0.46157999711717	-0.77125998779345
C	-2.09488998210891	1.78543001355376	-2.87338996310452
C	0.15453006483904	2.54927000852954	-3.76621986396566
C	2.30303004496592	3.22459000269221	-4.75722989127263
S	2.63693999732484	-1.00262000185899	3.43172000367404
H	0.41643999156663	-1.73469000589191	2.51310000532978
C	8.33318999910346	-0.85390999863719	0.81673000176991
H	6.93529000050111	0.56361000168832	0.03036999781310
C	6.14673000692528	-0.11036999586168	-2.61729999487926
C	5.07402998724991	2.08031999781451	-2.41292001338763
C	3.25253998530250	2.46694999902745	-0.82617000932558
H	9.54398999732777	-2.47934999983126	1.60123000172366
O	-1.69606999606659	1.03549000750431	-0.63841999868093
N	-2.07138000610234	-1.53578999356685	-0.18675000567804
C	-2.56671999881040	1.57135000234153	-1.58576000157599
C	-3.00095999616319	2.30276000875460	-3.85850000349270
C	-0.23469000014234	3.91318000113868	-3.78199000422656
H	3.29186000079274	2.94396000086087	-5.12548999969850
C	1.89159000348997	4.53924999719229	-4.76921998783443
O	3.86045999632358	-1.73784999766759	3.16024000161671
O	1.83602999758087	-1.33214999409717	4.60200000077106
H	9.14123000149313	-0.12309000010565	0.87167000035158
H	6.25754999803002	-1.14209000057804	-2.28635000393018
C	6.87300000669019	0.34579000237143	-3.69801999675013
C	5.85463999651778	2.52716999653967	-3.51195000244343
C	4.10729000589069	2.91917999482967	-1.81502999624266
H	2.46735514769331	3.07727894642063	-0.40622556711096
S	-2.88109999875766	-2.75305999937585	-0.83217999900443
C	-3.84554999706283	2.01296000160082	-1.13628000028599
C	-4.31055000273087	2.71096999974250	-3.44319000243599
C	-2.67154000331572	2.39074999666894	-5.23569000041012
C	0.61768999825533	4.88526999955605	-4.26192001089144
H	-1.21028001301096	4.19184999590989	-3.38629002113446
H	2.54995998722733	5.31728999447072	-5.15903002959057
H	7.55444999554355	-0.33170000197746	-4.21452000472511
C	6.73899000615093	1.68050000333166	-4.14394999352931
H	5.72657000303722	3.55631999844425	-3.85420999692770
H	3.97710000403822	3.93244000603287	-2.19814999573235
C	-5.44405000036230	1.73914000078153	2.87736000068664
H	-5.46450000074378	-1.45338000075310	-0.50292000143033

O	-2.04021999804166	-3.66406000135999	-1.60098000237862
O	-3.70741999743379	-3.31200000308425	0.24529999987768
C	-4.67609999793412	2.59114999762331	-2.08377999829640
C	-4.30456000165987	1.91858000106954	0.26873999922717
C	-5.22395999876299	3.20724999586866	-4.41041000112770
C	-3.58403000305720	2.87012999883339	-6.15233999903298
H	-1.69207000024834	2.05302000187123	-5.57091000135588
H	0.30695000321139	5.93097000223074	-4.24617999757756
H	7.32713999392804	2.03223999942039	-4.99271000526962
C	-5.81417000207480	0.32660999862994	4.95941999836703
F	-7.23540000033084	0.30692999880781	-0.71417999983516
H	-6.24343999811384	-0.06932999846284	-4.51897000138790
C	-5.98874999754079	-0.70931999927278	-2.46873000072044
H	-5.67264000213254	2.91600999756323	-1.78023999857915
C	-4.17641999985609	0.75688000177197	1.04052999792858
C	-4.97855999971208	3.01027000007185	0.84630999753044
H	-6.21966000211934	3.50848000194623	-4.07859999997533
C	-4.86932000108545	3.28845999812834	-5.73939999841518
H	-3.31559999987254	2.91124000059068	-7.20879000143290
C	-7.28704000159408	-0.09462000160617	-2.00844999806804
C	-5.70016000023606	2.81259000159023	5.14402999753227
C	-7.66298000013885	1.72068999927819	4.01486999825888
F	-2.73639999841614	-0.89841999812373	-5.85317000249211
C	-4.74098999807019	0.66816999949835	2.31311000129926
H	-3.64413999815592	-0.10630000105222	0.64591999768194
C	-5.53092000077441	2.91962999873123	2.11955999766174
H	-5.06285999775508	3.94467000062312	0.28761999957340
H	-5.58126999992971	3.66349999990925	-6.47598000051600
F	-4.22781999815483	-2.43679000219815	-6.28512000061844
F	-4.77460000052134	-0.32185000202460	-6.42296000047223

126

3b_4 (cat)

H	0.83586000205982	-5.83991000158813	1.29773999796600
H	-5.37322999642427	2.05755999832441	-0.22900999830064
C	-3.83478999872539	3.87792000105662	-4.30792000116123
C	-2.36741999826033	4.33714999925507	-4.43634000125379
H	-5.28610999865416	3.82624999985184	-1.90383999863348
C	-4.77977000006314	1.89882999650986	-1.13001000177550
H	1.17062999788576	-3.39937000081245	1.78822000156203
C	-3.26420000195208	0.57659000036354	-2.43855999845453
C	-4.72110000237550	2.91275000058920	-2.08504000248541
C	-3.93564999790142	2.78637000292610	-3.23810999911359
C	-3.21494998279081	1.59119000353372	-3.38689999085477
C	0.21410999860924	-3.80057999974305	1.49078000198106
C	0.00385999856754	-5.13986000155356	1.19958000176201
C	-1.25098000045699	-5.63645000120697	0.77498000018564
C	-1.41871999961438	-7.00242999896555	0.42255000111777
C	-2.62643000007118	-7.47151000165869	-0.04642000141536
C	-3.72117000119640	-6.58703999834469	-0.18108000087127
C	-3.59717000146397	-5.2579999883905	0.16882999817453
C	-2.37045999919971	-4.74485000171716	0.66549999859962
C	-2.18320000237062	-3.36683000001659	1.00670000076051
C	-0.91758000177033	-2.94597000036258	1.37970999895508
O	-0.75089999833857	-1.58188000184857	1.64663000173169
P	-0.68401999698214	-0.59113000217619	0.36668001021758
N	-0.93474000188054	0.90381000187728	0.82917000330405
S	-0.65496000072604	1.46619999724840	2.31421999816338
O	-0.73287001854595	2.92170997012838	2.24804000636995

O	0.51071999971057	0.85799999944324	2.95701000193575
H	0.62354999387986	5.02840994028883	1.82892994209106
H	3.75504000158871	0.62660999947992	1.91117000302842
C	-4.68084000178470	-3.47850999793181	2.63580999929500
C	-6.92161999839474	-2.65479999986764	3.06965000152491
C	-5.85993999932372	-3.54590000085795	3.34896999964525
O	3.13487001087560	-0.46195999735352	-0.21738001196132
H	2.70194999956321	2.31522999753013	3.31196000579233
C	-4.05547000118149	0.70639999789134	-1.28257000341021
O	-1.88953999951562	-1.10326999922423	-0.58293999534363
C	-4.18920000055377	-0.37805999958984	-0.28382000038779
C	-5.56817000147287	-1.58425999722534	1.35374999810174
C	-5.39177000133880	-0.57661999823783	0.37926999943750
C	-4.50320000210803	-2.50726999808394	1.61734000213521
C	-3.13794999845340	-1.28838999777078	0.02787000225470
C	-6.77716000216713	-1.69605000018508	2.09030999745340
C	-3.28483999810087	-2.37625000207751	0.87928999919734
H	0.93234998647590	6.54613992503951	2.70752993166686
N	0.59803999690283	-0.97145999800904	-0.49360000280046
P	1.81168003840415	-0.24307996769040	-1.10149999651104
N	1.75216000806815	1.41528995555062	-1.30400009271037
S	0.95366999126015	2.16173974707594	-2.59888026906380
O	-0.13265008295583	1.26477002920608	-2.93607999610850
O	1.94282999862792	2.56892003747926	-3.57842996827440
H	0.47236579549226	3.25080170372426	-1.95860593324610
C	4.37343000030512	3.37069999945117	-0.00671999865530
C	1.92415999730324	4.49950998907320	4.18461998204284
C	3.60036998724617	6.11633998774023	3.26808999232133
H	4.41849000297235	5.65146999842279	3.83745999593990
H	3.75808999195386	5.36762999745769	0.45896999996071
C	2.52660998789828	5.07371997040396	2.89488997834870
H	1.78180008727552	6.22557024465267	1.17979025934890
H	-1.73750000045200	1.04910999981937	3.01212999900730
H	4.03367002317862	6.59201998994645	2.37694998471953
C	1.39861001562634	5.75802007712106	2.09723005872957
H	3.15471999891989	6.90726000659329	3.88970996556682
H	1.48180999073785	5.31671001142635	4.77236999883605
H	2.68827000659639	4.01532003941310	4.81063001941497
H	4.81604000128078	3.66402000235001	-0.96133999789091
H	1.12889001619628	3.77332000585487	3.96825000930820
C	3.76858998846541	4.33097998764748	0.80008999914331
H	2.56957994817805	1.93409008628545	-0.94893982704568
O	2.20454999184876	-0.86057999330879	-2.53797999964251
C	2.71400998149077	-2.18009000574029	-2.46266000297673
C	4.04333999646063	-2.32257000053428	-2.08784000317248
C	4.57381000102997	-3.64340000127163	-1.93365000011610
C	5.88490000273521	-3.89940999799500	-1.45339999814850
C	6.34146000055153	-5.19102999859693	-1.29079000179028
C	5.51136000250095	-6.29221999780116	-1.60361000247388
C	4.22883999797564	-6.07785999987789	-2.05821000240470
C	3.72150000179054	-4.76054000012848	-2.22046999997231
C	2.38508000169271	-4.53627000059384	-2.62186999949254
C	1.83752999443905	-3.26589000177172	-2.73055999828833
H	0.80877999914157	-3.08367999787804	-2.999679999890942
H	-4.38848999920214	5.57072000063356	-3.02653999815688
C	-4.69626999984733	5.10302000208928	-3.97289000002589
H	-3.69272000084250	2.44639999778907	-5.97093999878803
C	-4.30711000056583	3.30215999972032	-5.65895000253565

H	-2.27214000117130	5.08282000082164	-5.24002999827836
H	-1.69662999986866	3.49859999861944	-4.66889000056090
H	-5.35117999866619	2.96320000021928	-5.59471000085132
H	-4.67200000125399	-6.95709000053506	-0.56760999946630
H	-3.86202999945741	-4.15828000094267	2.86885000034581
H	-7.84941999987742	-2.71999000150928	3.63982999794642
H	-7.58139999905805	-0.98772999769630	1.88250999774976
H	-0.56222999775227	-7.67307999805929	0.52027000233585
H	-2.73901000103255	-8.52143000035441	-0.32035999769240
H	-5.96823999915717	-4.28470999822379	4.14412000208801
H	-2.02133000206182	4.79850999918236	-3.50070999785171
H	-4.44671000162096	-4.58554999820891	0.05819999944032
H	-6.23703000052933	0.07337999813507	0.14973999936400
H	-5.76228999780160	4.84271999851875	-3.89926999889735
H	-2.57612995123019	1.44568998975771	-4.25898997320068
H	-2.67630999826598	-0.32322999983759	-2.60376000014373
H	-4.59044999903032	5.85510999807389	-4.76807999743789
H	-4.24092999849856	4.07101000082497	-6.44361999949998
H	1.75480000044488	-5.39903000027313	-2.84527999801576
H	3.57260999833283	-6.91953999858494	-2.28938000203596
H	5.88614000215935	-7.30862000172810	-1.47566000158292
H	7.35029999896187	-5.36348999908907	-0.91294000161477
H	6.53259000272858	-3.06034999810816	-1.20374999774294
C	4.84322000216542	-1.10947999795251	-1.78279000120367
C	4.36894000647517	-0.19739000506983	-0.85309001184275
C	5.02715999860683	1.01551999761030	-0.51570000194510
C	6.24496000129203	1.25895000219016	-1.12898999992648
C	6.78779999918543	0.38108000235381	-2.09557999860892
C	8.01576000267579	0.67436999825609	-2.74621999781465
C	8.49931999769485	-0.14132999772147	-3.74512000049454
C	7.76275000231436	-1.28032999982338	-4.14386000084049
C	6.57636000117194	-1.60423000250349	-3.51933999814341
C	6.06735000036222	-0.80502999910168	-2.46268000262920
H	6.01408000153221	-2.48043999937452	-3.83953999938543
H	8.13314000046398	-1.90620000175396	-4.95699000077997
H	9.43319000015135	0.09568000205712	-4.23744000075887
H	8.56146000172724	1.57172000056955	-2.44752000151601
H	6.79534000168931	2.16644000236600	-0.87297999969305
C	4.39842999983833	2.01494999955895	0.37809999989292
C	3.78358999746574	1.66780000091259	1.59158000260457
C	3.18858998997670	2.63856998987595	2.39446000212764
C	3.16945001179118	3.99031998903222	2.02518998504307

126

3b_4 (TS1-1)

C	-2.30037999801528	-1.38535000000019	3.20475000148716
H	-1.92425999997510	-0.36431000109305	3.19273000043088
C	-1.62777000035786	-2.33689000262934	3.96356000229681
H	0.63240999768910	-3.85485999756045	4.47593999900587
H	-0.73252999726357	-2.02173999788886	4.50258000188742
C	-2.02294000246769	-6.03531999969203	4.99041000213017
H	-0.91498000106172	-4.78612999928306	7.12010000204313
C	-8.66787999895249	0.82162999824349	0.27332000164666
C	2.40809999545348	-0.73060999998011	-3.40031999907950
H	-4.74491000002606	-3.37567000076955	1.94064999919927
C	-1.40585000245678	-4.08844999881324	6.42482000013178
H	-1.47975999793818	-6.70111999969997	5.67645999993484
H	-8.33051000201408	-0.91681000157334	1.49252000034072
H	-3.55657585090036	-1.40956714114968	-2.28320256216272

H	-2.44460000160277	-3.94403999933401	6.75532000158638
C	-1.36057999824208	-4.65086999765441	4.98782999860925
H	-0.89059000127030	-3.12092000217477	6.49546999941559
C	3.62341999970352	-0.95937000039389	-2.72525000086235
C	1.85374999945389	-1.70216999658054	-4.22477000170068
H	1.88124999958194	0.21391000086348	-3.28266999850464
H	-9.74660000153357	0.67027000228719	0.21374999947218
H	0.16900000177779	-5.31849000212644	3.58070999736523
H	-8.68886999821365	2.58382000039491	-0.99729000203233
C	-3.87697000020294	-3.06367999903322	2.52459000014014
C	4.26687000013278	0.06791999998271	-1.87476000192236
C	4.25038000243618	-2.19872999870773	-2.92940999821160
C	2.48168999749381	-2.94065000162773	-4.44014000089112
H	0.892580005750070	-1.487050001338648	-4.69425002856839
H	-1.17136000031445	3.39906999885451	-2.15176000255192
C	-3.20461999811836	-4.00820000013958	3.30097999800089
H	0.50307000212134	3.32400000041687	2.32592000047092
C	3.51922999637620	0.99815999998172	-1.09713999949097
C	5.64694999906748	0.19579000047401	-1.83470000166146
C	3.69719999700561	-3.15939000001525	-3.77734999795915
H	5.17652999867529	-2.42872999777698	-2.40067000237678
C	1.82098000119338	-3.98248999940735	-5.34584000173705
C	-1.97639000485445	3.58384000078591	-1.45721000091410
O	2.12786999430547	0.87162000050948	-1.11042999574973
C	4.08384999831027	2.05128999879297	-0.38811000035146
H	6.26096000260480	-0.46878999745434	-2.44406999911986
C	6.29437999849272	1.15960999904090	-1.02880000206301
H	4.22566000290649	-4.10435000051673	-3.90119999923031
C	1.60576999727585	-3.37025999995797	-6.74553000058301
C	0.45649999951440	-4.37949999873215	-4.74473000008431
C	2.67553999960528	-5.24831000202804	-5.49851999900502
C	-2.72059002433627	2.49514999360415	-0.92380998968993
C	-2.35520000000011	4.85129999857295	-1.04403999840928
P	1.34917999213011	0.46058000546968	0.24368000172773
C	5.51179000098684	2.10443000104359	-0.28544999777750
C	3.21600000148196	3.10087000103413	0.21078999876993
C	7.71064999760802	1.21148999792907	-0.93754000020501
H	2.56352000030247	-3.06864999917205	-7.19437000151034
H	1.12970999969462	-4.10731999775106	-7.40930999932145
H	0.95584000047331	-2.48579999827806	-6.70457999845124
H	-0.19848999987886	-3.50932999844999	-4.60317000102982
H	-0.05727000218297	-5.08818000039399	-5.41145999742747
H	0.58106999731614	-4.87039000304491	-3.76896000027900
H	2.82697000057386	-5.75976000168271	-4.53625000274500
H	2.16454000234077	-5.95599999794157	-6.16659000020469
H	3.66126999872813	-5.02729999812037	-5.93423999828084
O	-2.37450002128469	1.20710000590401	-1.33766997944293
C	-3.77315000640354	2.62553999774652	-0.02941999621005
H	-1.83197000093329	5.71948000069219	-1.44956999805058
C	-3.39688000027919	5.06336000175131	-0.11094000174060
O	2.02468999659483	1.39223000215234	1.37154000317958
N	-0.12939000119123	0.81610005167799	-0.05477003947611
N	1.76150999344383	-1.05275000155405	0.70704000312068
C	6.18380000151427	3.02938000239161	0.55404999748463
C	3.35936000228004	4.48337999757201	-0.14625000180208
C	2.18572000200530	2.75396999887298	1.06981999905217
H	8.29611000165758	0.49057000025315	-1.51126000146615
C	8.33376000220300	2.13120000177434	-0.12208999800228

P	-1.57372947118225	0.24778997505143	-0.30653011478384
C	-4.45638001061401	1.41406999580833	0.49964999807066
C	-4.11789000205905	3.94234999843604	0.42238999876210
C	-3.72143000123540	6.37258000192005	0.33542000065227
S	2.29906999867731	-1.48318000180873	2.19977000123847
H	1.47054999803457	-2.11963000369879	-0.08184999659551
C	7.56086000159794	3.03926000009850	0.63711999765743
H	5.59701000059719	3.72516999879011	1.15221000065893
C	4.30342000022802	4.94440999794063	-1.10059999859339
C	2.46772999860442	5.44096999841938	0.44422999967424
C	1.28290000166945	3.67492999929225	1.66780999815298
H	9.42217999761845	2.15272999983841	-0.05157000169067
O	-2.31995998490948	0.52587001087785	1.10271002086008
N	-1.78639058201518	-1.25866002888418	-0.78174980492725
C	-3.71251001550810	0.41012999063773	1.10770000468646
C	-5.87563000080848	1.24212000213090	0.41041999869880
C	-5.10352000067042	4.18926999984315	1.41392000252905
H	-3.17110999930414	7.21579000009960	-0.08760000001989
C	-4.69395000165201	6.57773999991678	1.28929999791164
O	2.29108000229864	-2.93934999919684	2.20417999932966
O	1.62492000041013	-0.76016000208717	3.26643000152729
H	8.05581999778315	3.74571000151190	1.30456000253962
H	4.96773999750583	4.22799000159101	-1.58013000221561
C	4.38191999960568	6.28016000147745	-1.43759999991492
C	2.58685000026648	6.81094999901981	0.08738000027133
C	1.46585999979244	5.01005000139250	1.34493000046643
H	-3.58359000189145	-5.03002000106585	3.31526999982801
S	-2.23490999625798	-1.70812001598219	-2.25540010066108
C	-4.27803000398394	-0.71730000510420	1.76718000185707
C	-6.47621000280080	0.11398999853038	1.06203999810276
C	-6.70833999886852	2.11695000061184	-0.33343999914467
C	-5.38305000209696	5.47229000243399	1.83791000109756
H	-5.63992999766751	3.34840999788692	1.84993999756387
H	-4.92811000119728	7.58796000254929	1.62782999852253
H	5.11046000095426	6.60638999796617	-2.18134999871287
C	3.52309000258740	7.22638000018652	-0.83378000210011
H	1.90729000118017	7.52868000005005	0.55178000216355
H	0.81228999984484	5.75778000026140	1.79834000298492
H	-2.00252999737657	-6.49959999998548	3.99328999825032
H	3.57183999832611	-1.03165999678467	2.14164000088489
O	-1.61410006071477	-0.93410000132650	-3.32872995739472
O	-2.11086980907772	-3.16802996164781	-2.31305002275417
C	-5.66110999934392	-0.81380000321692	1.74995000106822
C	-3.46065999925303	-1.72403999783227	2.48250999854840
C	-7.88411000005561	-0.05689000014097	0.98959999889991
C	-8.07057999899100	1.90945000204682	-0.40339000259860
H	-6.25611999935041	2.95037999953477	-0.86923000135931
H	-6.14034000019094	5.63291999766229	2.60680999850605
H	3.59820999883256	8.28041000181971	-1.10446999825202
H	-3.06826999740792	-5.98747999876003	5.32867000103127
C	0.10996000227642	-4.81721000021958	4.55724999798377
H	0.64956999744786	-5.43953999760192	5.28720999867142
C	-2.07555000136052	-3.66527000172708	4.05711999858658
H	-6.14426999905615	-1.63621000188837	2.27916000242696
126			
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C	-5.78232000079431	-2.92722999951843	2.85674000210048

H	-8.19273000055075	2.51891999797100	0.81793000087137
H	-6.20283000261766	-0.84316999768318	3.18029000162473
H	-6.82006000163423	-6.87530000076818	2.56350999915788
C	-4.79483000066449	-5.59785000064840	3.93204999743356
H	-6.41834999900656	-3.22961000031424	3.69091999900227
C	-4.28967999889870	-3.44937999913239	1.06069999977925
C	4.08321999062278	-1.92355998892124	-3.26974999621812
C	-4.35302000237269	-6.27206000236436	1.57077000034758
H	-6.14995999747779	6.10531999991980	-0.42639999832362
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H	-3.73735000173851	-4.15380999877081	0.43924000162892
C	-4.15701999808542	-2.09055000058722	0.77818999963972
C	-5.22899999770382	-5.38436999803486	2.46720999747488
H	-3.52015671472549	-0.14843287472646	-2.73909567393208
H	-7.03166000167042	-5.67497000093026	1.26183000128969
C	3.48302999901320	-0.76144998580133	-2.75979999591494
C	3.47794999913893	-2.66679999585483	-4.28399999843465
H	5.03823999901036	-2.25957000015746	-2.86222000440248
H	-4.47955999976507	-7.32461000117424	1.86413000103301
C	-6.70089999956299	-5.81293999845248	2.30131000041208
H	-3.51264000169472	-1.79052000155867	-0.04495000030816
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C	2.24661999762605	-2.28414998810447	-4.83324999157513
H	3.98699000221665	-3.55980000144119	-4.64607000246958
H	0.47494071576566	3.35584820268969	-1.44367726071073
H	-4.62904999987927	-6.18226000068303	0.51042999971204
H	-7.36840000255074	-5.22688999887642	2.94872000232346
C	3.52788000225724	0.71426999889823	-0.68196999205529
C	5.57281000238472	0.18946000102387	-1.79558000237846
C	1.63722000329987	-1.13703999773846	-4.29920999382023
H	1.72657988202225	0.50055024698355	-2.93365987919941
C	1.56144999825624	-3.04417999548961	-5.97197999895423
C	-0.19587979295870	3.64597948799028	-0.64962020965711
O	2.13007000432139	0.62617999397351	-0.63818000073926
C	4.16706001364288	1.45026998773944	0.30793001907459
H	6.12395000220084	-0.25828999896475	-2.62352000201319
C	6.29849000089794	0.87567999926509	-0.79580000280714
H	0.66401999513832	-0.80757999327639	-4.66437000361978
C	2.38396999960079	-4.24942000095124	-6.44639999995082
C	1.36609999952388	-2.08457999748089	-7.16469999881746
C	0.18449999940588	-3.54756999929467	-5.49516999988948
C	-1.31615013529845	2.82643030360430	-0.32581978296216
C	-0.00144009562817	4.76508025994899	0.14459012161708
P	1.50029996709216	-0.35086000921417	0.48106999624880
C	5.60015000257314	1.48905999639800	0.29725000076613
C	3.36524998856585	2.16518004386776	1.33682996145097
C	7.71678999809006	0.93779000118562	-0.83341000218370
H	2.53340000112479	-4.98322999915775	-5.64042000005083
H	1.85369999762546	-4.75767999901096	-7.26451999808880
H	3.37130999868723	-3.94669999880522	-6.82495000168260
H	0.87952000031335	-2.61169999802779	-7.99917000110065
H	0.73482999750967	-1.22787000159687	-6.89262000242981
H	2.33290000118126	-1.69693000127693	-7.51770000208239
H	0.30356000250127	-4.27188000210201	-4.67592999970341
H	-0.45484999846620	-2.73153000195880	-5.13234000237621
H	-0.34198999986960	-4.05324000297701	-6.31883000182238

O	-1.47088994898565	1.62715994033848	-1.03258008368147
C	-2.28753004251090	3.16926998393751	0.60167985573094
H	0.83561999973700	5.43146996443732	-0.07041002629336
C	-0.86288004185671	5.08933006901082	1.21802995555246
O	2.23271007050582	0.11341001968516	1.83955001152702
N	-0.03200000211378	-0.10731999401489	0.49277000113969
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C	6.36228999658471	2.07526000154054	1.34020999794281
C	3.51360999141399	3.57588000062774	1.55943999701475
C	2.39355989448677	1.49062994503607	2.06565000140882
H	8.23546000160663	0.47306999829424	-1.67405999856282
C	8.42629999875622	1.54030999952919	0.18273999805729
P	-1.38527998853233	0.21389999528239	-0.24380001518315
C	-3.56438996820177	2.41321996323563	0.69319003972964
C	-2.03848994576601	4.30094993667817	1.44731003674207
C	-0.59653997937698	6.19774997031086	2.06473000812825
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H	1.32231999501561	-2.60769000056469	-0.64104999922090
C	7.74077000181105	2.09929999990643	1.28491999691164
H	5.84664999944163	2.49751000166537	2.20116000194794
C	4.37658999462031	4.39742999797764	0.78573000061535
C	2.71270006588414	4.20203999405769	2.57138000397875
C	1.54784005017466	2.09509004470562	3.03545995296310
H	9.51623000148746	1.57034000108001	0.14768000260897
O	-2.37639999527771	0.36349000407544	1.03169001842384
N	-1.89255002424613	-0.91140999786361	-1.24305998751504
C	-3.59185000319496	1.04368000094422	0.92565000433472
C	-4.81134999616049	3.10789000496967	0.53388000445799
C	-2.87588998445137	4.63825998922410	2.54261001692341
H	0.29611000956445	6.79473999388906	1.86909000621232
C	-1.43085998249667	6.50046997429408	3.11890001733657
O	2.85942000235159	-4.15070999536999	0.70470999762119
O	2.20164000804952	-2.71711999427391	2.67824999916520
H	8.30517999853627	2.54144000178993	2.10681000225096
H	4.95914000693655	3.94859999726933	-0.01711999350491
C	4.47647999610351	5.75228000258209	1.02625999706652
C	2.86108997675621	5.59410000835590	2.81324999279043
C	1.75867997778604	3.44213995080137	3.28378011609355
H	0.80186059333219	1.50592046227726	3.54617520888219
S	-2.36599998837643	-0.85884000113280	-2.76904000227595
C	-4.79429999815745	0.32097000343998	1.19004000063467
C	-6.03216999903437	2.40101999964617	0.78379000180528
C	-4.89193000327548	4.45440000147834	0.09311000105853
C	-2.57434000822661	5.70547001005183	3.36354999735875
H	-3.75588000549401	4.02842000699108	2.74362999252742
H	-1.21062000924034	7.34926001367737	3.76812999061204
H	5.14048999717493	6.36127999966134	0.41116000090057
C	3.72569999362274	6.35731000194442	2.06018999046179
H	2.25710999160626	6.04812000561000	3.60120999319401
H	1.14971999432759	3.94343001238236	4.03790994943429
H	-8.27339000033386	4.89252999911360	0.08353999996678
H	-5.41358999929451	-5.01659000202780	4.62986000084420
O	-1.45410000215292	-0.12194999699069	-3.63945000036557
O	-2.70739999519371	-2.23646000031359	-3.14521999954130
C	-5.98048000029237	1.03599000118327	1.14254000132625
C	-4.84004999719532	-1.12203999920975	1.52262999754588
C	-7.27250000089912	3.07392000061464	0.62583000083627
C	-6.11285000158166	5.07650000055137	-0.06595000198446

H	-3.97601999860535	4.99293000202441	-0.14453000000247
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H	-3.28731000142907	-6.02001999962047	1.66762999856338
H	4.00013773781635	-2.26182605390236	1.36222548668138
H	-3.74749000020513	-5.29552000174636	4.07263999891333
H	-4.88678000173416	-6.66056000076691	4.20320000205979
H	-6.91792000192657	0.50730999672141	1.32329999696892
126			
3b_4 (TS1-2')			
C	-6.13794999801448	1.64381999818290	4.23942999793042
H	-6.21966000176910	3.50848000265154	-4.078600000000057
H	-6.32252000200267	0.30772000214675	5.93471999919723
C	-5.70016000024481	2.81259000158140	5.14402999752568
C	-4.17641999992521	0.75688000183525	1.04052999792785
H	-4.61538999935020	2.78572000222299	5.31525999969100
H	-6.04998000214563	3.79021000003344	2.52479999853449
H	-5.58126999998160	3.66349999984571	-6.47598000054856
C	1.60213003243036	-4.26886014933219	-0.07599990565743
H	-6.15145999800497	-0.54849999765004	4.38650000187896
H	-5.95190000185887	3.78803000154383	4.70552999737800
H	-5.06285999767576	3.94467000078889	0.28761999962866
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H	-3.64413999821306	-0.10630000098787	0.64591999760019
H	-3.72107237450367	-2.16684932543409	-1.71992089002055
H	-3.31559999980568	2.91124000078868	-7.20879000138129
C	2.70251999067110	-4.14101996762403	0.78669997547876
C	0.53255999806787	-5.10448995929462	0.24001998253430
H	1.57603998256741	-3.72213984596760	-1.01547013324691
H	-7.94922000090657	2.66372000134978	3.52798000214150
H	-4.73419999830800	0.22090999987365	5.13442000183675
C	-4.97855999965143	3.01027000019531	0.84630999752744
H	-6.20611000159895	2.74406000262292	6.11894000005168
C	3.85530000255627	-3.25813000521197	0.50523999773624
C	2.67924998252121	-4.87874998684543	1.98253000401195
C	0.51043999761193	-5.85470997785012	1.42543000360435
H	-0.30363000112410	-5.14352001059417	-0.45732000234863
H	1.48090294254384	-1.16142938476549	-3.47984485279670
H	-8.00479000024337	0.89365000022179	3.37620999967466
H	2.92251869092317	0.31862934101880	3.40246448420290
C	3.69309000313773	-1.95345000123704	-0.03119000013649
C	5.14636999757776	-3.62619000157301	0.84130000228015
C	1.61192000113438	-5.71943000316860	2.28694999940027
H	3.48955000333363	-4.75381000472933	2.70228999612890
C	-0.63011999719571	-6.82735000234126	1.74463000177531
C	1.14042010686351	-0.14311021146168	-3.58691947287493
O	2.39432999780548	-1.56215000387248	-0.39035999844549
C	4.71214999427610	-1.02994000031200	-0.19509000247733
H	5.32995000168292	-4.63145999991492	1.22499000151648
C	6.23094999699869	-2.72164999809834	0.76693000012711
H	1.63990000335420	-6.26807000426963	3.22904000200458
C	-0.94767000161360	-6.83760000062667	3.25176999961234
C	-0.17751999784103	-8.24200999985981	1.32223999736565
C	-1.91752999746547	-6.46887000339839	0.98501000047415
C	-0.12971005993611	0.24904018163923	-3.0719903407802
C	1.89622984153226	0.86083009378737	-4.17628054419869
P	1.65707999259779	-0.56989997930150	0.63555000715960

C	6.01843999920393	-1.38760999887901	0.28180999921367
C	4.44576000602640	0.29102000411364	-0.82131999332282
C	7.52503000038902	-3.09441000229416	1.21730999915120
H	-0.10651000017570	-7.20514999855968	3.85496000156323
H	-1.20708999960936	-5.83038999680269	3.60925000039579
H	-1.80524999911427	-7.49798000046932	3.44677000181900
H	0.04112000084431	-8.27428000225352	0.24517000219482
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H	-0.96822000163750	-8.97764000062380	1.53631000145476
H	-2.24874000153390	-5.44161999738225	1.19210999905821
H	-1.79848000166014	-6.56055000150799	-0.10276999739440
H	-2.72419999832669	-7.15356999966947	1.28508000032706
O	-0.88409001126281	-0.70437008754915	-2.36140997004783
C	-0.67990000462360	1.51095993364832	-3.23581989988187
H	2.86617003412667	0.61102999142435	-4.60903986973821
C	1.46304000094049	2.20430997637770	-4.23727998866228
O	2.62032999250857	0.72451999561294	0.69832999380633
N	0.25154000191227	-0.27336001064435	0.05356999399563
N	1.56953000929909	-1.07841002223120	2.17240999295768
C	7.09578999787889	-0.46666000120846	0.34442999922498
C	5.23803999665908	0.74008999472122	-1.93346000339229
C	3.43599001262123	1.13158000420801	-0.36493999714062
H	7.67661999784422	-4.11592000053030	1.57216000040122
C	8.55843999823411	-2.18339999969213	1.23905000152632
P	-1.07004998111602	-0.46157999972834	-0.77125998259125
C	-2.09488998589116	1.78543001889253	-2.87338998355433
C	0.15453006330540	2.54927001533779	-3.76621988125184
C	2.30303005701614	3.22459000687975	-4.75722987094454
S	2.63693999701903	-1.00261999233510	3.43172000163736
H	0.41643999704191	-1.73468999804824	2.51310000290356
C	8.33318999918364	-0.85390999862779	0.81673000172146
H	6.93529000042725	0.56361000184702	0.03036999830428
C	6.14673000451471	-0.11036999658124	-2.61729999677729
C	5.07402999523590	2.08031999866902	-2.41292000430911
C	3.25254000265831	2.46695000238868	-0.82616999369660
H	9.54398999731505	-2.47934999982113	1.60123000176437
O	-1.69606999454642	1.03549000482995	-0.63841999736143
N	-2.07138002701058	-1.53578997960524	-0.18675001528287
C	-2.56671999779814	1.57135000338828	-1.58576000153644
C	-3.00095999988206	2.30276000266698	-3.85850000477011
C	-0.23469001509756	3.91317999738989	-3.78199004042228
H	3.29185999693300	2.94396000086018	-5.12549000964825
C	1.89158998394459	4.53924999204324	-4.76922003527221
O	3.86045999896774	-1.73785000108675	3.16024000176914
O	1.83602999783258	-1.33215000045690	4.60200000152290
H	9.14123000140305	-0.12309000001262	0.87167000072839
H	6.25754999829694	-1.14209000057957	-2.28635000358102
C	6.87300000213361	0.34579000054621	-3.69802000019409
C	5.85464000181949	2.52716999899051	-3.51194999853726
C	4.10728999232145	2.91917999576754	-1.81503000765323
H	2.46723429396866	3.07710962082426	-0.40622343390981
S	-2.88109998682143	-2.75306001275520	-0.83217999009667
C	-3.84554999741056	2.01296000114600	-1.13627999953028
C	-4.31055000340362	2.71096999770645	-3.44319000234138
C	-2.67154000383579	2.39074999507352	-5.23569000010147
C	0.61768999950847	4.88527000085694	-4.26192000390145
H	-1.21028001310954	4.19184999650046	-3.38629001726274
H	2.54995999332918	5.31728999695503	-5.15903001565412

H	7.55444999796884	-0.33170000100598	-4.21452000270336
C	6.73899000203968	1.68050000171740	-4.14394999732337
H	5.72657000025428	3.55631999730926	-3.85420999935545
H	3.97710000551442	3.93244000428898	-2.19814999456939
C	-5.44405000031407	1.73914000080745	2.87736000068716
C	-5.53092000070691	2.91962999880306	2.11955999766780
O	-2.04022000249252	-3.66405999608165	-1.60098000637884
O	-3.70741999599050	-3.31200000246788	0.24529999906872
C	-4.67609999805735	2.59114999724892	-2.08377999825235
C	-4.30456000191684	1.91858000084629	0.26873999929501
C	-5.22395999846018	3.20724999634137	-4.41041000108588
C	-3.58403000273573	2.87012999940505	-6.15233999873949
H	-1.69207000005767	2.05302000195977	-5.57091000136329
H	0.30695000728427	5.93097000209414	-4.24617998893146
H	7.32713999570165	2.03224000011498	-4.99271000359242
C	-5.81417000208479	0.32660999862181	4.95941999836278
C	-4.86932000096839	3.28845999826066	-5.73939999839288
C	-7.66298000014965	1.72068999927214	4.01486999825425
C	-4.74098999803586	0.66816999956427	2.31311000129402
H	-5.67264000178857	2.91600999836576	-1.78023999853085
102			
3b_5 (cat)			
H	0.83586000199111	-5.83991000173270	1.29773999825967
H	-5.37322994287511	2.05756004166397	-0.22900995998877
H	-3.88429807313255	3.57301712250496	-3.97762351136187
H	5.88614000217293	-7.30862000163624	-1.47566000174185
H	-5.28610982287517	3.82625000336274	-1.90383987359691
C	-4.77977005220027	1.89882986279005	-1.13001002319170
H	1.17062999761299	-3.39937000111421	1.78822000138320
C	-3.26419993270446	0.57659002294265	-2.43855985262479
C	-4.72110035791889	2.91275007683380	-2.08504034270111
C	-3.93565000013086	2.78636983055249	-3.23810983445819
C	-3.21494963837623	1.59119031104259	-3.38690002546308
C	0.21410999890661	-3.80057999970630	1.49078000230246
C	0.00385999856955	-5.13986000173042	1.19958000231787
C	-1.25098000056445	-5.63645000131689	0.77498000060805
C	-1.41871999965619	-7.00242999899889	0.42255000112582
C	-2.62643000004625	-7.47151000168032	-0.04642000156477
C	-3.72117000118377	-6.58703999831845	-0.18108000090080
C	-3.59717000151994	-5.25799999880271	0.16882999848584
C	-2.37045999911029	-4.74485000156596	0.66549999914012
C	-2.18320000233527	-3.36683000008334	1.00670000053912
C	-0.91758000184597	-2.94597000042494	1.37970999798610
O	-0.75089999766151	-1.58188000162358	1.64662999839576
P	-0.68401999951542	-0.59113000011628	0.36668000130997
N	-0.93474000213369	0.90381000170383	0.82917000086083
S	-0.65496000032577	1.46620000130045	2.31421999809618
O	-0.73286999907488	2.92170999843228	2.24804000102969
O	0.51072000429065	0.85800000161618	2.95701000327464
C	4.39843000031299	2.01494999821511	0.37809999911903
H	3.75503998993512	0.62660999727028	1.91116999755028
C	-4.68084000163272	-3.47850999769608	2.63580999977241
C	-6.92161999835352	-2.65479999979451	3.06965000169450
C	-5.85993999942922	-3.54590000103770	3.34896999959264
O	3.13487000232815	-0.46195999712740	-0.21738000208826
H	2.70194998288446	2.31522999616784	3.31195999317896
C	-4.05547001039803	0.70639999183300	-1.28257000196520
O	-1.88954000030223	-1.10326999861255	-0.58293999862532

C	-4.18919999482345	-0.37805999655889	-0.28381999944254
C	-5.56817000158387	-1.58425999806769	1.35374999658186
C	-5.39176999366615	-0.57661998059710	0.37927001685896
C	-4.50320000196136	-2.50726999799002	1.61734000246296
C	-3.13795000768321	-1.28839001232081	0.02786998188915
C	-6.77716000215415	-1.69605000032870	2.09030999731665
C	-3.28483999840106	-2.37625000179737	0.87928999846716
C	3.18859002364302	2.63857000646110	2.39446001564561
N	0.59804000169409	-0.97145999998225	-0.49359999946581
P	1.81167999832609	-0.24308000105436	-1.10150000163750
N	1.75215999690242	1.41528999942079	-1.30400000169529
S	0.95366999659216	2.16173999888188	-2.59887999863074
O	-0.13264993558475	1.26476999773340	-2.93607996869054
O	1.94282999593467	2.56891999846654	-3.57843000001135
H	0.47236999715381	3.25080000123333	-1.95860999825754
C	4.37342998588472	3.37069999761118	-0.00672000884123
H	9.43319000042390	0.09568000183181	-4.23744000053795
H	6.01408000134374	-2.48043999915697	-3.83953999985798
C	7.76275000206312	-1.28032999944313	-4.14386000142932
H	3.75809001549303	5.36763000358368	0.45897000547245
H	2.67994024496636	4.73165080521294	2.63937574818293
H	6.79534000182581	2.16644000217923	-0.87297999954908
H	-1.73750000158868	1.04910999771770	3.01213000009248
C	6.57636000101762	-1.60423000222687	-3.51933999885550
C	3.78359001526082	1.66780000434285	1.59158000888194
H	8.13314000061743	-1.90620000186418	-4.95699000074403
C	3.16945000323125	3.99032000227239	2.02519000041117
C	6.06735000071266	-0.80503000024401	-2.46268000237146
H	4.81604000890548	3.66402000192264	-0.96133999438796
H	8.56146000181571	1.57172000044349	-2.44752000146187
C	3.76858997309596	4.33097999418017	0.80008998432056
H	2.56957999996751	1.93409000045665	-0.94894000190535
O	2.20455000045016	-0.86058000190790	-2.53797999825619
C	2.71400999773217	-2.18009000134813	-2.46265999957702
C	4.04334000198609	-2.32257000161104	-2.08783999910943
C	4.57381000061825	-3.64340000194787	-1.93365000043352
C	5.88490000233068	-3.89940999796678	-1.45339999835645
C	6.34146000041514	-5.19102999842953	-1.29079000190768
C	5.51136000238131	-6.29221999765528	-1.60361000230826
C	4.22883999770362	-6.07785999979019	-2.05821000201344
C	3.72150000128905	-4.76054000022870	-2.22047000066550
C	2.38508000173380	-4.53627000034442	-2.62187000066987
C	1.83752999986839	-3.26588999888858	-2.73055999890294
H	0.80878000088866	-3.08367999987636	-2.99968000062844
C	8.49931999751837	-0.14132999753345	-3.74512000081326
C	6.78779999947561	0.38108000214141	-2.09557999839303
H	7.35029999888117	-5.36348999893050	-0.91294000177863
C	4.36894000204742	-0.19738999880847	-0.85309000226602
H	6.53259000254795	-3.06034999791791	-1.20374999806107
H	1.75479999998052	-5.39903000048909	-2.84527999786181
C	5.02715999888077	1.01551999806292	-0.51570000166629
H	-4.67200000122265	-6.95709000051260	-0.56760999961575
H	-3.86202999939738	-4.15828000088855	2.86885000054922
H	-7.84941999996057	-2.71999000156706	3.63982999793980
H	-7.58139999935868	-0.98772999822620	1.88250999721229
H	-0.56222999770798	-7.67307999804953	0.52027000218719
H	-2.73901000101906	-8.52143000033674	-0.32035999774536
H	-5.96823999920087	-4.28470999826281	4.14412000206794

H	3.57260999824363	-6.91953999856241	-2.28938000186199
H	-4.44671000164095	-4.58554999822779	0.05819999949423
H	-6.23703000164197	0.07337999644610	0.14973999789247
C	8.01576000242630	0.67436999853395	-2.74621999830770
H	-2.57613023865033	1.44568989159824	-4.25899006155222
H	-2.67631006186975	-0.32323003543018	-2.60376005128241
C	6.24496000201728	1.25895000152772	-1.12898999998908
C	4.84322000145764	-1.10947999900377	-1.78278999835789
102			
3b_5 (TS1-1)			
C	-2.30038003909945	-1.38534998290798	3.20475006105602
H	-1.92425997693424	-0.36431001262571	3.19272996773912
C	-1.62777007881329	-2.33688996784289	3.96356010609144
C	-5.66110999824971	-0.81379999841564	1.74995000532266
H	-0.73252994100054	-2.02174000680986	4.50257993947881
C	-2.07555000250054	-3.66527000346298	4.05712000138578
C	-3.46065999854893	-1.72403999909031	2.48250999816625
C	-8.66787999906861	0.82162999795357	0.27332000127136
C	2.40810000039807	-0.73061002220613	-3.40031985927539
H	-4.74491002357614	-3.37566999244169	1.94065003101619
H	3.59820999872923	8.28041000182106	-1.10446999839091
H	-6.14426999852396	-1.63621000035721	2.27916000383627
H	-8.33051000215680	-0.91681000181817	1.49252000009716
H	-3.55657999654591	-1.40957000096270	-2.28320000196701
H	-6.14034000050080	5.63291999773208	2.60680999826298
H	-1.55175310714614	-4.39561533855804	4.65706954641806
H	-6.25611999950415	2.95037999949150	-0.86923000134514
C	3.62341999488128	-0.95937000814619	-2.72524998408568
C	1.85374964964304	-1.70217028496727	-4.22476982559500
H	1.88125003660406	0.21391003467559	-3.28267007352521
H	-9.74660000165055	0.67027000219965	0.21374999935584
C	-7.88411000014670	-0.05689000010364	0.98959999889637
H	-8.68886999829564	2.58382000039482	-0.99729000199701
C	-3.87696995882485	-3.06368001232833	2.52458994058857
C	4.26686999962083	0.06792000502700	-1.87476000540429
C	4.25038007528287	-2.19872985841675	-2.92941008364877
C	2.48169009205318	-2.94064984259474	-4.44013988296142
H	0.89258019860860	-1.48704991121966	-4.69425013926681
H	-1.17135999948041	3.39907000231772	-2.15176000152603
C	-3.20461991751937	-4.00820003271992	3.30097988978155
H	0.50307000273053	3.32400000121156	2.32591999999030
C	3.51922999806156	0.99816001602178	-1.09714001990557
C	5.64694999915466	0.19578998176375	-1.83469998112159
C	3.69720014448772	-3.15939006698109	-3.77735043091132
H	5.17652995709835	-2.42873004305927	-2.40066993301453
H	2.03878538760045	-3.69262603385015	-5.07672883578432
C	-1.97638999882502	3.58384000182310	-1.45720999984223
O	2.12787000050777	0.87161999812686	-1.11042999981395
C	4.08384999908808	2.05128999909574	-0.38811000099770
H	6.26096000276896	-0.46878999643329	-2.44407000066184
C	6.29437999798287	1.15960999724077	-1.02880000055388
H	4.22565990449568	-4.10435000849554	-3.90119981140453
H	1.90729000106423	7.52868000005207	0.55178000199399
H	-5.63992999760364	3.34840999784403	1.84993999776725
H	3.57183999903492	-1.03165999821301	2.14164000072617
C	-2.72058999891523	2.49514999853255	-0.92381000004152
C	-2.35519999993298	4.85129999825816	-1.04403999829374
P	1.34918000245966	0.46057999809840	0.24367999822968

C	5.51179000115979	2.10443000130927	-0.28544999782681
C	3.21600000170900	3.10087000105409	0.21078999961030
C	7.71064999746297	1.21148999886966	-0.93754000143573
H	0.81228999922298	5.75778000039433	1.79834000220911
C	3.52309000261036	7.22638000021499	-0.83378000212611
H	5.11046000084644	6.60638999795871	-2.18134999887076
C	-6.70833999829420	2.11695000046662	-0.33343999881705
H	-4.92811000115835	7.58796000255301	1.62782999860411
C	-5.38305000252297	5.47229000243513	1.83791000064025
O	-2.11086999758465	-3.16802999815921	-2.31304999765163
C	-8.07057999900030	1.90945000191027	-0.40339000253678
O	-1.61410005105122	-0.93409998867037	-3.32872996850547
O	-2.37449999724166	1.20710000208932	-1.33767000126057
C	-3.77314999892876	2.62553999799314	-0.02941999866989
H	-1.83197000242137	5.71948000069633	-1.44956999919171
C	-3.39687999998521	5.06336000140054	-0.11094000123833
O	2.02469000222631	1.39223000231654	1.37153999941887
N	-0.12938999736891	0.81610000124639	-0.05476999933662
N	1.76150999897292	-1.05275000101968	0.70704000230158
C	6.18380000165975	3.02938000241049	0.55404999764595
C	3.35936000262591	4.48337999761426	-0.14625000135143
C	2.18572000243007	2.75396999926552	1.06981999882927
H	8.29611000166467	0.49057000061201	-1.51126000186401
C	8.33376000222969	2.13120000209157	-0.12208999832757
P	-1.57373000050091	0.24779000087525	-0.30652999880075
C	-4.45638000043462	1.41406999667497	0.49964999655842
C	-4.11789000006528	3.94234999793866	0.42238999940537
C	-3.72143000174667	6.37258000182296	0.33542000009527
S	2.29906999714359	-1.48318000191416	2.19977000230844
H	1.47055000202582	-2.11963000263237	-0.08184999806496
C	7.56086000166600	3.03926000002115	0.63711999784784
H	5.59701000063400	3.72516999858519	1.15221000099467
C	4.30342000041214	4.94440999792508	-1.10059999833978
C	2.46772999869044	5.44096999840339	0.44422999984963
C	1.28290000120282	3.67492999890901	1.66780999845304
H	9.42217999765364	2.15272999963113	-0.05157000144755
O	-2.31995999914161	0.52586999750968	1.10271000079907
N	-1.78639000054010	-1.25866000198307	-0.78175000303995
C	-3.71250999991800	0.41012999764607	1.10769999634979
C	-5.87562999773339	1.24212000236394	0.41041999999166
C	-5.10352000044425	4.18926999948551	1.41392000259727
H	-3.17110999972489	7.21579000005100	-0.08760000039043
C	-4.69395000192446	6.57773999989903	1.28929999761685
O	2.29107999995368	-2.93934999851239	2.20417999995765
O	1.62491998456461	-0.76016000937960	3.26643001043390
H	8.05581999781759	3.74571000157987	1.30456000248256
H	4.96773999765656	4.22799000162243	-1.58013000209719
C	4.38191999958691	6.28016000146636	-1.43759999993054
C	2.58685000026422	6.81094999903334	0.08738000022291
C	1.46585999938108	5.01005000128826	1.34493000043572
H	-3.58359004398266	-5.03001998427652	3.31527005597662
S	-2.23490999686799	-1.70811999824783	-2.25539999926971
C	-4.27802999929056	-0.71730000208014	1.76718000030140
C	-6.47621000231993	0.11399000007612	1.06204000006556
102			
3b_5	(TS1-1')		
C	-5.66539998403837	-1.57104000107526	2.56929001574639
C	-5.78231993878081	-2.92722999326225	2.85674005119866

H	-8.19273000026991	2.51891999869551	0.81793000282040
H	-6.20283001468927	-0.84316999855710	3.18028999203320
C	-5.98048000078547	1.03598999846221	1.14253999179143
H	-3.22308000071564	5.93598000108699	4.20981000239055
H	-6.41835002945628	-3.22961000325919	3.69091997484448
C	-4.28968006714962	-3.44938000443398	1.06069994512769
C	4.08322002401749	-1.92355986208637	-3.26974995132675
H	-3.97601999825399	4.99293000135961	-0.14453000156711
H	-6.14995999735176	6.10532000013109	-0.42639999713222
C	-5.09409999756750	-3.90112999880126	2.11275000282321
H	-3.73734997037565	-4.15380999617539	0.43924002682939
C	-4.15702001359838	-2.09055000186422	0.77818998850285
H	-5.19009449754324	-4.95313717178858	2.34190539010608
H	-3.51877204999413	-0.14658964344874	-2.73658319877957
H	3.82546000248152	7.42685000095319	2.25086000260307
C	3.48302999294826	-0.76144999805885	-2.75979999806834
C	3.47795003206833	-2.66680010369846	-4.28400036919297
H	5.03823998893384	-2.25957003951464	-2.86221998560231
C	-4.84004999530796	-1.12204000002348	1.52262999650114
H	4.00019029836059	-2.26207819407834	1.36258857522450
H	-3.51263998917773	-1.79052000029922	-0.04494998994160
C	-7.31501000141840	4.38749000219384	0.21215000005787
C	4.19490999518146	0.04850999456861	-1.74699001195855
C	2.23232009853242	-0.39329004138150	-3.28749989707887
C	2.24662011313312	-2.28414985653473	-4.83324981278260
H	3.98698995625719	-3.55979998481869	-4.64606987136631
H	0.47428919296285	3.35562548645349	-1.44417233068518
C	-6.11285000125623	5.07650000027230	-0.06595000208989
H	-6.91792000160632	0.50730999809716	1.32330000160877
C	3.52787999629325	0.71427001392480	-0.68197000890926
C	5.57281000382404	0.18945998318790	-1.79557999038424
C	1.63721969997422	-1.13704022065762	-4.29921007601719
H	1.72657997678336	0.50055007637771	-2.93366001398431
H	1.77352556054365	-2.85662399156179	-5.61800790103799
C	-0.19587997908274	3.64597991560914	-0.64962009973306
O	2.13007000429626	0.62617999808191	-0.63817999544073
C	4.16705999988054	1.45026999744131	0.30793000301928
H	6.12395000102676	-0.25828999522823	-2.62352000279127
C	6.29849000179940	0.87567999909674	-0.79580000025072
H	0.66402014037842	-0.80757993693178	-4.66437002283287
H	-3.75587999725162	4.02841999653392	2.74363000017556
H	1.14972000463250	3.94343000234960	4.03790998964682
O	-1.45410002606133	-0.12194999092962	-3.63944998772978
C	-1.31615006789702	2.82643009654359	-0.32581992830473
C	-0.00143994332635	4.76507997606975	0.14459015953260
P	1.50030000115223	-0.35086000374819	0.48106999841914
C	5.60015000036737	1.48906000080369	0.29724999889227
C	3.36525000455234	2.16518001029024	1.33682999947437
C	7.71678999856592	0.93779000072392	-0.83341000205973
H	-1.21062000015963	7.34926000340129	3.76813000113085
C	-4.89193000378214	4.45440000163649	0.09311000210243
C	-2.57434001894172	5.70547002133142	3.36354998393184
C	3.72570000173772	6.35731000045657	2.06018999841074
H	5.14048999780103	6.36127999951999	0.41116000131804
H	2.25710999918725	6.04812000243679	3.60121000081442
C	-7.27250000065169	3.07392000055424	0.62583000145158
O	-2.70739999694666	-2.23646000015972	-3.14521999948149
H	-8.27339000040287	4.89252999913403	0.08353999983844

O	-1.47088993721488	1.62715994956649	-1.03258000335352
C	-2.28753005401581	3.16927004246697	0.60167986203428
H	0.83561996830972	5.43147002109387	-0.07041005281866
C	-0.86288000376101	5.08933000926188	1.21802997761174
O	2.23271001670509	0.11341000764293	1.83954999776106
N	-0.03199999704501	-0.10731999483853	0.49276999916874
N	2.03608998309177	-1.87564000927293	0.24308000471253
C	6.36228999742395	2.07526000232510	1.34020999873769
C	3.51360999710505	3.57588000137293	1.55943999732470
C	2.39355997584307	1.49062998106761	2.06565000882050
H	8.23546000164024	0.47306999917810	-1.67405999933135
C	8.42629999882953	1.54030999992843	0.18273999763869
P	-1.38528002258591	0.21390000736094	-0.24380001802925
C	-3.56438996347766	2.41321996685549	0.69319007384449
C	-2.03848997443753	4.30094997329613	1.44731003470176
C	-0.59654002670157	6.19775002519962	2.06472996384797
S	2.78232001044334	-2.84891999485885	1.35202999578502
H	1.32232000266512	-2.60768999695027	-0.64105000225842
C	7.74077000225544	2.09929999867079	1.28491999771089
H	5.84664999957139	2.49751000128251	2.20116000180669
C	4.37658999922178	4.39742999767443	0.78573000330103
C	2.71270001187447	4.20203999860725	2.57137999601493
C	1.54784001730705	2.09509001525200	3.03545998641555
H	9.51623000137439	1.57034000079540	0.14768000279226
O	-2.37639999176418	0.36349000484112	1.03169001447250
N	-1.89255000465648	-0.91141000088586	-1.24305999515601
C	-3.59185000476295	1.04368000244953	0.92565000365652
C	-4.81134999982736	3.10789000503379	0.53387999145813
C	-2.87588999197878	4.63825999384083	2.54261001385679
H	0.29611000481019	6.79473999703549	1.86909000397490
C	-1.43085998041029	6.50046997539439	3.11890002473341
O	2.85941999784419	-4.15071000100181	0.70470999784585
O	2.20164000003314	-2.71712000029961	2.67825000147126
H	8.30517999844906	2.54144000211878	2.10681000204914
H	4.95914000062074	3.94859999869354	-0.01711999889235
C	4.47647999743057	5.75228000226047	1.02625999843032
C	2.86108999341511	5.59410000362264	2.81325000066755
C	1.75867998130216	3.44213998693581	3.28378002191476
H	0.80207086459602	1.50584483769203	3.54636312145454
S	-2.36599999473393	-0.85883999873194	-2.76904000000971
C	-4.79429999939220	0.32097000154130	1.19003999406281
C	-6.03216999970047	2.40101999744962	0.78378999601219

102

3b_5 (TS1-2')

H	-5.88637229401531	1.67074488638763	3.86131467272458
H	-6.21966000171070	3.50848000278409	-4.07859999998796
H	-1.69207000015405	2.05302000161682	-5.57091000144963
C	-5.22395999791386	3.20724999763508	-4.41041000081289
C	-4.17642002314395	0.75687998841451	1.04052999876470
C	-4.67610000044060	2.59114999227056	-2.08377999937028
H	-6.04998003320304	3.79020999187400	2.52479999066198
H	-5.58127000016636	3.66349999939871	-6.47598000063525
C	1.60213001907348	-4.26886013048203	-0.07599993751862
H	0.30695000657286	5.93097000173792	-4.24617999039668
C	-4.30455999995089	1.91858000155315	0.26873999918272
H	-5.06286001067212	3.94466999464739	0.28761999259522
C	-4.74099004958745	0.66816998368431	2.31310995128649
H	-4.61831997404280	-0.26824999459925	2.85700001665273

H	-3.64413998405734	-0.10629999406148	0.64592000268377
H	-3.71706580767362	-2.16419807263155	-1.72215560583864
H	-3.3155999981894	2.91124000078166	-7.20879000139483
C	2.70251999274219	-4.14101997097730	0.78669998040642
C	0.53256004641327	-5.10448998742989	0.24001996298687
H	1.57603998409575	-3.72213987511281	-1.01547009380758
C	-4.86932000085134	3.28845999853955	-5.73939999835625
H	7.32713999682791	2.03224000061168	-4.99271000257559
C	-4.97855998313888	3.01027001224508	0.84631001407174
C	-3.58403000257004	2.87012999976540	-6.15233999864446
C	3.85530000294774	-3.25813000415555	0.50523999775944
C	2.67924997093710	-4.87874998864801	1.98253001855726
C	0.51043998165815	-5.85471000226428	1.42543000861230
H	-0.30363002312393	-5.14351999178359	-0.45731999574010
H	1.48046798692489	-1.16162403110537	-3.48029817452967
H	-5.67264000128468	2.91600999951612	-1.78023999827187
H	2.92284462616987	0.31855055195509	3.40232018334851
C	3.69309000254387	-1.95344999995881	-0.03118999749466
C	5.14636999810478	-3.62619000331017	0.84129999857718
C	1.61192000130221	-5.71942995067124	2.28695000515835
H	3.48955000773085	-4.75381000882787	2.70228999075186
H	-0.32562546409579	-6.49368194367327	1.67028160891133
C	1.14042008750593	-0.14311016053903	-3.58691959104874
O	2.39432999841473	-1.56215000474372	-0.39035999805477
C	4.71214999418186	-1.02993999881524	-0.19508999902423
H	5.32995000150376	-4.63145999950690	1.22499000222159
C	6.23094999747606	-2.72164999840655	0.76692999870499
H	1.63990000878808	-6.26807002575636	3.22903999708827
O	-2.04021999892773	-3.66405999906941	-1.60098000466864
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H	2.54995999480658	5.31728999724877	-5.15903001178077
C	-0.12971005384356	0.24904014128051	-3.07199027511932
C	1.89622987236218	0.86083007530356	-4.17628042537312
P	1.65707998849666	-0.56989997825854	0.63555000429933
C	6.01843999900970	-1.38760999956121	0.28180999800876
C	4.44576000545408	0.29102000124805	-0.82132000049318
C	7.52503000016649	-3.09441000199523	1.21731000004946
O	-3.70741999571798	-3.31200000262322	0.24529999915821
H	5.72657000083877	3.55631999738926	-3.85420999894786
C	-5.53091993438257	2.91963001567597	2.11956000408131
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C	-5.44405000614702	1.73914000056733	2.87736001898755
C	-2.67154000369859	2.39074999530443	-5.23568999989664
C	0.61768999999438	4.88527000012341	-4.26192000404876
H	-1.21028000536537	4.19184999569706	-3.38629000795999
O	-0.88409000702690	-0.70437006852605	-2.36140997135359
C	-0.67990000460640	1.51095994314088	-3.23581992330289
H	2.86617002704557	0.61102999217558	-4.60903989903807
C	1.46304000408115	2.20430997784607	-4.23727998237969
O	2.62033000244897	0.72451999307526	0.69832999649786
N	0.25154000200693	-0.27336001101755	0.05356999330416
N	1.56953000779289	-1.07841001831247	2.17240999396028
C	7.09578999799898	-0.46666000110998	0.34442999921890
C	5.23803999507482	0.74008999511386	-1.93346000420007
C	3.43599000777301	1.13158000774068	-0.36493998905502
H	7.67661999781770	-4.11592000052481	1.57216000048814
C	8.55843999815663	-2.1833999964436	1.23905000176361

P	-1.07004997952258	-0.46158000488960	-0.77125998548259
C	-2.09488998624549	1.78543002018228	-2.87338998423404
C	0.15453005271475	2.54927001460387	-3.76621990248691
C	2.30303004491358	3.22459000530573	-4.75722989882044
S	2.63693999739329	-1.00261999504521	3.43172000205479
H	0.41643999776411	-1.73468999821777	2.51310000254123
C	8.33318999908131	-0.85390999850166	0.81673000215715
H	6.93529000040934	0.56361000184808	0.03036999834264
C	6.14673000290146	-0.11036999716942	-2.61729999775505
C	5.07403000061901	2.08031999850700	-2.41292000163590
C	3.25253999039148	2.46694999818088	-0.82617001288014
H	9.54398999740194	-2.47934999990675	1.60123000144798
O	-1.69606999468432	1.03549000403478	-0.63841999740546
N	-2.07138003164078	-1.53578997581422	-0.18675001577775
C	-2.56671999725055	1.57135000657506	-1.58576000037938
C	-3.00096000031078	2.30276000159421	-3.85850000485503
C	-0.23469001834143	3.91317999807664	-3.78199004014970
H	3.29185999689141	2.94396000069014	-5.12549000890192
C	1.89158998745073	4.53924999368534	-4.76922002879445
O	3.86045999898599	-1.73785000033199	3.16024000160137
O	1.83602999793288	-1.33214999998978	4.60200000122719
H	9.14123000142327	-0.12309000004257	0.87167000062921
H	6.25754999988748	-1.14209000001293	-2.28635000234245
C	6.87300000150661	0.34579000033638	-3.69802000064034
C	5.85463999615135	2.52716999710358	-3.51195000393450
C	4.10729000564244	2.91918000518117	-1.81502998823742
H	2.46728488014687	3.07711564037095	-0.40612471218038
S	-2.88109998415075	-2.75306001488558	-0.83217998862635
C	-3.84554999789365	2.01296000042652	-1.13628000095253
C	-4.31055000392909	2.71096999617396	-3.44319000244954