Hydrogen Bond Network between Amino Acid Radical Intermediates on the PCET Pathway of *E. Coli* α2 Ribonucleotide Reductase

Supplementary Results

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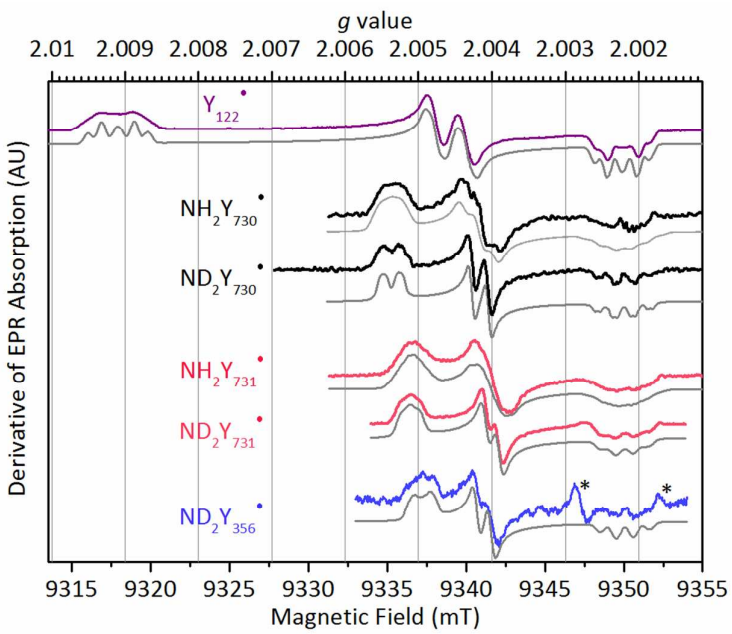
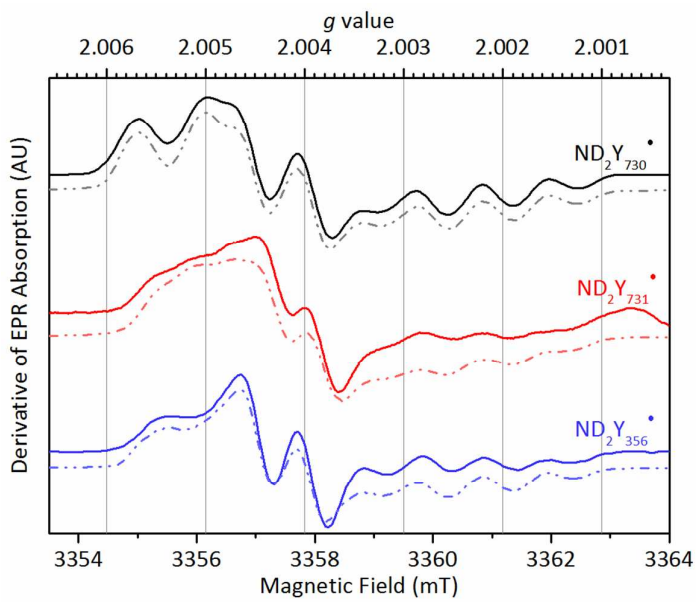
Figure S1. 263-GHz EPR spectra and simulations of the transient $NH_2Y^{\bullet}$s in the single mutants. The derivative of the absorptive 263-GHz EPR spectra of the $ND_2Y^{\bullet}$ from Figure 2 is generated here for comparison with simulations (grey lines). The spectrum of $Y_{122}^{\bullet}$ (top spectrum) was used as an external field/*g* factor standard. The values for the simulation of the *g* tensor of $Y_{122}^{\bullet}$ were taken from ref.1. In the spectrum of $ND_2Y_{356}^{\bullet}$ the lower-field asterisk (*) marks a quartz tube signal and the higher-field asterisk is a Mn^{2+} line. Simulation parameters were the *g* tensor and the hf coupling of the C-β protons. The hf tensor for ^{14}N in the amino group was kept fixed with values A_x= 2.4 MHz, A_y=1.6-5 MHz, A_z= 30.7 MHz.[2] The resulting parameters are given in Table 1. The hf interaction of the weakly coupled C-β proton is visible only in the spectrum of $ND_2Y_{731}^{\bullet}$ (A_x= 13 MHz, A_y= 5 MHz, A_z= 10 MHz, hf axes were taken collinear with *g* axes) and together with the stronger C-β coupling gives rise to the triplet structure on the low field side of the $ND_2Y_{731}^{\bullet}$ spectrum. This coupling was also observed in a previous ^1H ENDOR spectrum at 34 GHz.[3]



Additionally, spectra for the transient $NH_2Y^{\bullet}$s in protonated buffer were also recorded for a control. The spectra are broadened by hf coupling to the amino protons. In the simulation, the hf couplings of the amino protons were taken from previous ^2H ENDOR spectra[4] and multiplied by a factor $\gamma^H/\gamma^D \approx$ 6.5. For the amino proton most distant to the phenolic oxygen, the hf tensor values agree with those from Ref. 4 but the largest component is found here perpendicular to the ring plane ($B \parallel g_z$). The smallest hf coupling ($A \approx 0$) lies along the N-H bond. Most importantly, the simulations of the spectra in protonated and deuterated buffer could be generated with a consistent set of *g* values.

Figure S2. 94-GHz EPR spectra and simulations for the transient $NH_2Y^{\bullet}$s in the single mutants. The echo-detected EPR spectra were recorded in D_2O exchanged buffer at 70 K, where the echo signal of $Y_{122}^{\bullet}$ is not detectable in the pulse experiment. In order to generate the derivative spectra (solid lines), the absorption spectra were smoothed by a 4 points adjacent average. Simulations (dashed/dotted lines) were performed using the same parameters as the simulations at 263 GHz, reported in Table 1. Experimental parameters (94 GHz): $\pi/2$ = 16-32 ns; τ = 260 ns; repetition time = 3-6 ms; shots/point= 50; number of scans = 50-700.



Simulations gave A_{iso}(C-β) couplings (Table 1), that for α-$NH_2Y_{730}^{\bullet}$ are consistent with C_α-C_β-C_1-C_2 dihedral from both the crystal (pdB: 2XO4)[5] and DFT/EPR structure[4] (106.5° *vs*. 107.1°).

More specifically, the observed values of A_{iso}(C-β) depend not only on the dihedral angle, but also on the spin density at the carbon atom C_1. A semi empirical relationship is commonly used to estimate the dihedral angles from A_{iso} (C-β) if the spin density at C_1 is known:[6]

$$A_{iso}(C\text{-}\beta) \approx B_1 \cdot \rho_{C1} \cdot \cos^2(\theta) \quad \Rightarrow \theta = (\arccos(A_{iso}(C\text{-}\beta) \cdot (B_1 \cdot \rho_{C1})^{-1}))^{1/2} \qquad \text{Eq.1}$$

where B_1 = 162 MHz is a semi empirical constant and ρ_{C1} the p_z spin density at carbon C_1 in the aromatic ring (the carbon bonded to the peptide chain). The angle θ is defined as the dihedral between the p_z-orbital at C_1 and the C_α-C_β vector. However, in the present case, the spin density at C_1 is sensitive to the hydrogen bond environment and thus it cannot be inserted in Eq. 1 *a priori* to obtain the dihedral angles. The DFT calculation for the three models of $NH_2Y_{731}^{\bullet}$ illustrates this. If we compare the experimental large A_{iso}(C-β) for $NH_2Y_{731}^{\bullet}$ with the calculated ones (Table 1) we note that model 1 (defined in main text) overestimates the experimental value by more than 50%, model 2 by about 25% and model 3 matches the experimental value. However, the observed weaker but still visible

coupling of the second C-β proton is compatible only with model 2 (A_{iso} = 12 vs 4 and 3 MHz for model 1 and 3, respectively). Although the discrepancies in the A_{iso}(C-β) appear significant, the structural differences illustrated by the three DFT models are subtle (Figure 5). All three models generate a stacked orientation of the $NH_2Y_{731}^{\bullet}$ and Y_{730} with a H bond located between these residues, which is consistent with the ENDOR data. For $NH_2Y_{356}^{\bullet}$ no structural comparison is available.

Figure S3. Kinetics of $NH_2Y^{\bullet}$ formation in $NH_2Y_{731}/Y_{730}F$-α2 and $NH_2Y_{730}/C_{439}A$-α2/ wt-β2/CDP/ATP by SF Vis spectroscopy. SF kinetics was performed on an Applied Photophysics DX. 17MV instrument equipped with the Pro-Data upgrade. All reactions were maintained at 25 °C by Lauda water bath circulation. A syringe containing 10 µM of pre-reduced[7] NH_2Y_{731}/ $Y_{730}F$-α2 (**A**) or NH_2Y_{730} /$C_{439}A$-α2 (**B**), 6 mM ATP in 50 mM Hepes, 15 mM $MgSO_4$, 1 mM EDTA, pH 7.6 (assay buffer) was rapidly mixed with an equal volume from the second syringe containing 10 µM wt-β2 and 2 mM CDP in assay buffer. The reaction was monitored at 320 nm (red) for $NH_2Y_{731}^{\bullet}$ (ε ~ 11,000 $M^{-1}cm^{-1}$), 325 nm (red) for $NH_2Y_{730}^{\bullet}$, (ε ~ 10,500 M^{-1} cm^{-1}) and 410 nm (blue) for $Y_{122}^{\bullet}$ (ε = 3700 $M^{-1}cm^{-1}$) using PMT detection. Double exponential fits in **A** or mono exponential fits in **B** to the data are shown in black. Residuals for the fit for $NH_2Y^{\bullet}$ formation is in magenta for $Y^{\bullet}$ disappearance is in cyan. All results represent the average of 6 to 8 spectra and fits were calculated with OriginPro software to minimize residuals. Equation 2 was used for double exponential fitting, where y_0 is a constant, A_1 and A_2, amplitudes, and R_1 and R_2 rate constants for the phases. Equation 3 was used for single exponential fitting.

$$y = y_0 + A_1 e^{-R_1 x} + A_2 e^{-R_2 x} \qquad \text{Eq. 2}$$

$$y = y_0 + A_1 e^{-R_1 x} \qquad \text{Eq. 3}$$

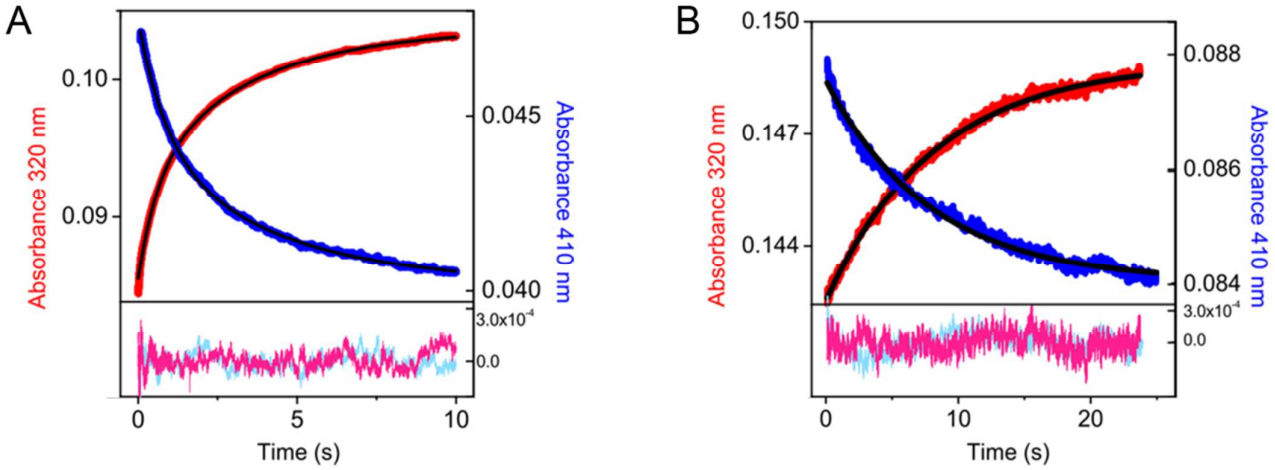


Table S1. Kinetics of $NH_2Y^{\bullet}$ formation for α2 mutants.

	$NH_2Y^{\bullet}$ formation				
Mutant [a]	k_1 (s^{-1})	$\%A_1$	k_2 (s^{-1})	$\%A_2$	$\%NH_2Y^{\bullet}$
NH_2Y_{731}-α2	9.6 ± 0.6	27 ± 2	0.8 ± 0.1	13 ± 1	32 ± 3
NH_2Y_{730}-α2	12 ± 1	20 ± 2	2.4 ± 0.2	19 ± 2	39 ± 4
$NH_2Y_{731}/Y_{730}F$-α2	1.5 ± 0.1	14 ± 2	0.3 ± 0.03	20 ± 1	34 ± 3
$NH_2Y_{730}/C_{439}A$-α2	0.13 ± 0.01	14 ± 1	-	-	14 ± 2

a) Rates were obtained from double exponential fits of 6-8 spectra of SF UV-vis spectra of the reaction with 5 μM NH_2 Y_{731} α2 and 5 μM wt-β2 with CDP/ATP (1 mM/3 mM) in assay buffer. The rate constants for NH_2Y_{730} and NH_2Y_{731}-α2 have been reported previously.[8]

Figure S4. **9-GHz EPR spectroscopy to monitor the reaction of $NH_2Y_{731}/Y_{730}F$-α2 and $NH_2Y_{730}/C_{439}A$-α2 with wt-β2/CDP/ATP.** A reaction mix contained in a final volume of 300 μL: 3 mM ATP, 1 mM CDP, 30 μM $NH_2Y_{731}/Y_{730}F$-α2 and 30 μM wt-β2 (or 100 μM $(His)_6$-NH_2Y_{730} /$C_{439}A$-α2) in assay buffer. The reaction was aged for 30 s and quenched in liquid isopentane. CW EPR spectra were obtained with a Bruker EMX X-band (9 GHz) spectrometer equipped with a quartz finger dewar cooled with liquid N_2 at 77 K at the MIT Department of Chemistry Instrumentation Facility. EPR parameters used were: microwave frequency, 9.34 GHz; power, 100 μW; modulation amplitude, 1.5 G; modulation frequency,100 kHz; time constant, 5.12 ms; scan time, 41.9 s. WinEPR (Bruker) was used for EPR spin quantitation by measuring the normalized double integral intensity of the spectrum, and correcting for power, number of scans, and modulation amplitude, and compared to a standard with a known concentration [$Y_{122}^{\bullet}$].[9] The spectrum of the unreacted $Y_{122}^{\bullet}$ (green) was subtracted from the composite spectrum (blue) to yield the spectrum and amount of the $NH_2Y^{\bullet}$ radical (red). A representative spectrum for double mutant $NH_2Y_{731}/Y_{730}F$-α2 is displayed below.

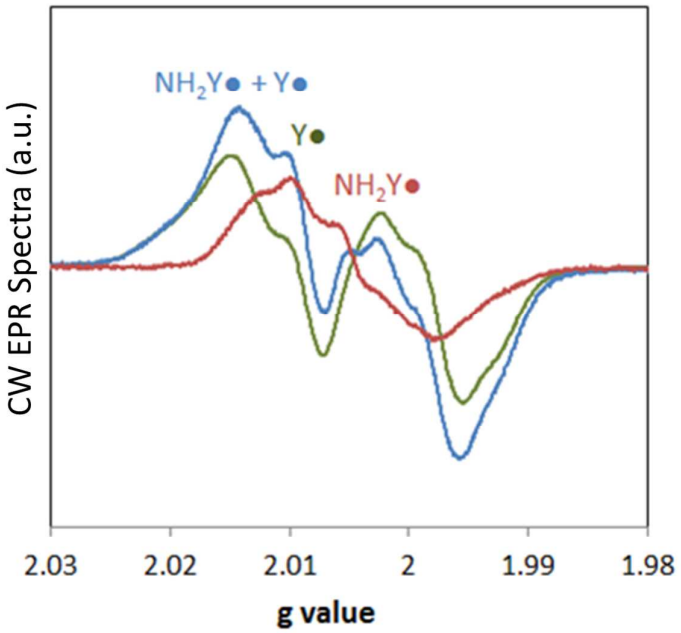


Figure S5. 34-GHz distance measurements between $NH_2Y_{731}^{\bullet}$ and $Y_{122}^{\bullet}$ in the $NH_2Y_{731}/Y_{730}F$ double mutant. To exclude large conformational changes in the structure of $NH_2Y_{731}^{\bullet}$ formed in the double mutant, we have measured its diagonal distance to $Y_{122}^{\bullet}$.[10] The two radicals are located in diagonally opposite monomers of α and β. (**A**) 34-GHz spin-echo detected EPR spectrum (recorded on Bruker Elexsys E580 spectrometer) after reaction of $NH_2Y_{731}/Y_{730}F$-α2:wt-β2 (130 μM, 20 vol% glycerol added 20 s after initial mixing, total reaction time was ~ 40 s) with ATP/CDP. The spectrum of unreacted $Y_{122}^{\bullet}$ (blue) has been subtracted from the observed spectrum (purple), yielding the $NH_2Y^{\bullet}$ (28%) spectrum (red). Pump (P) and detect (D) frequencies are indicated by arrows. The frequency difference was kept constant to $\Delta\nu$ = 55 MHz. (**B**) Normalized and background corrected four-pulse PELDOR traces at 5 K with a pump pulse of π = 46 ns and detection pulses with π/2(π) = 30(58) ns. Three consecutive traces (1, 2, 3) were taken with excitation on the spectrum in 11 G steps (points marked in **A**). **C**) Average trace as sum of the three normalized traces. The red line describes a fit using DeerAnalysis[11] and Tikhonov regularization procedure. **D**) Distance distribution obtained from the analysis in (**C**). The measured distance, 3.84 ± 0.15 nm, is consistent with the distance of (3.8 ± 0.1) nm previously measured in the single mutant $NH_2Y_{731}^{\bullet}$.[10]

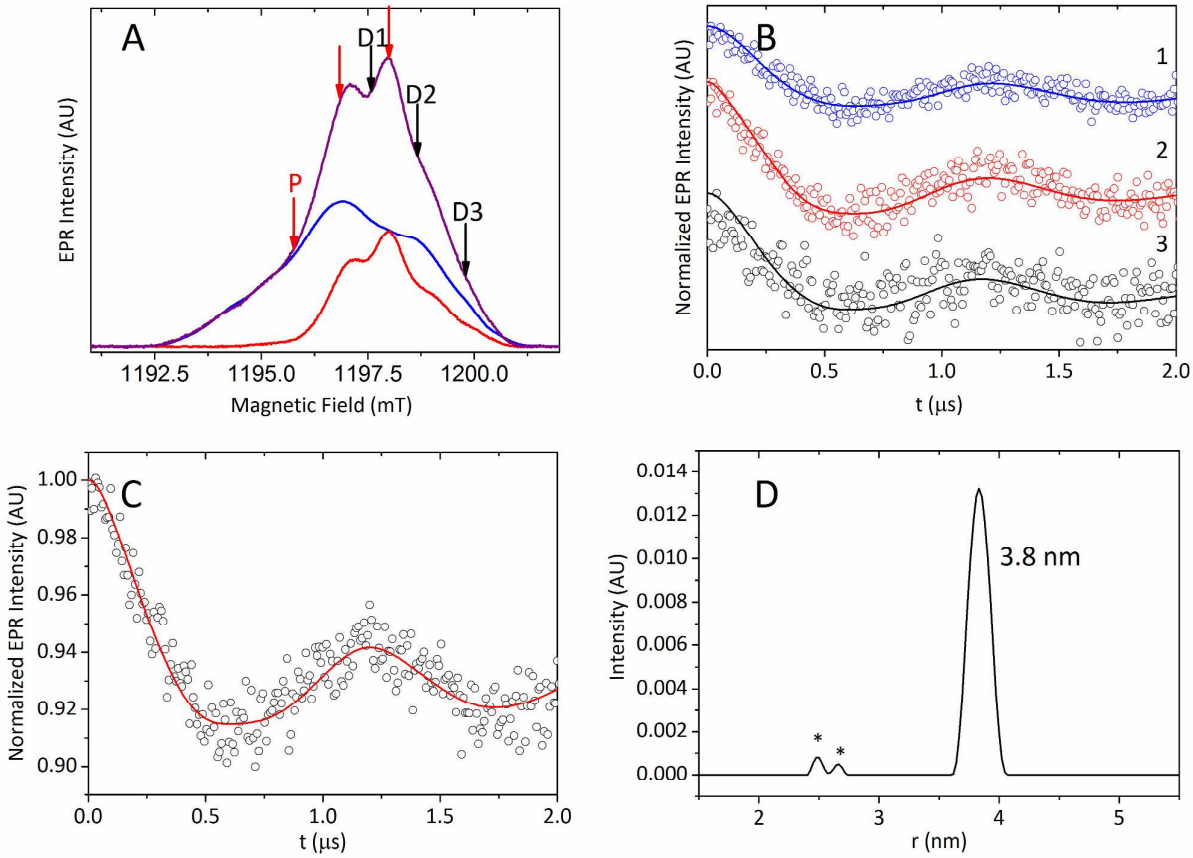


Figure S6. 34-GHz distance measurements between $NH_2Y_{730}^{\bullet}$ and $Y_{122}^{\bullet}$ in the $NH_2Y_{730}/C_{439}A$ double mutant. PELDOR measurements were also performed for $NH_2Y_{730}/C_{439}A$-α2:wt-β2, CDP/ATP (130 µM, 20 vol% glycerol added after 25 s, total reaction time 1 min), similarly as in Figure S5. (**A**) The composite EPR spectrum at 5 K (purple) followed by subtraction of the $Y_{122}^{\bullet}$ (blue) gives the $NH_2Y^{\bullet}$ spectrum (red) in 13% yield. **B**) The PELDOR traces at 20 K were taken with detection pulses (π/2(π) = 20(40) ns) separated by 50 MHz from the pump pulse (π = 56 ns). **B**) Three consecutive traces (1, 2, 3) were measured at D1, D2 and D3 (see A), respectively, with 11 G spacing. **C**) The averaged traces were summed and fit by DeerAnalysis[11] using Tikhonov regularization. **D**) In the distance distribution the distance of (3.29 ± 0.15) nm arises from $Y_{122}^{\bullet}$-$Y_{122}^{\bullet}$ located on different β monomers.[12] The second distance distribution at 3.9 ± 0.1 nm is consistent with the distance previously measured in the single mutant ($NH_2Y_{730}^{\bullet}$)[10] and the much lower $NH_2Y^{\bullet}$ yield in this double mutant reaction. To support the assignment of a long distance the effect a simulated trace with suppression of the long distance component (cut off distance 3.5 nm) is shown in B2 and C in green, which fits the data less satisfactorily. However, due to the absence of a clear modulation from the second distance in the time traces, the assignment remains uncertain.

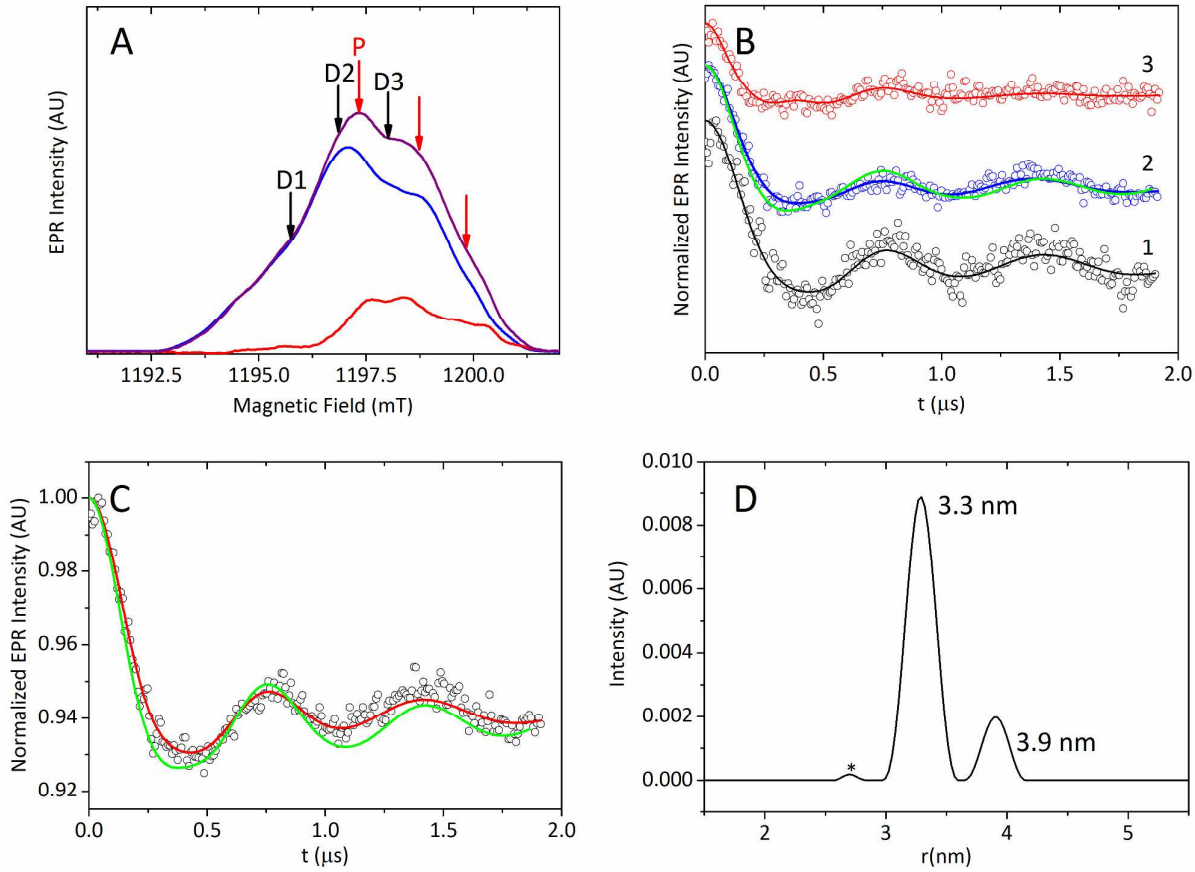
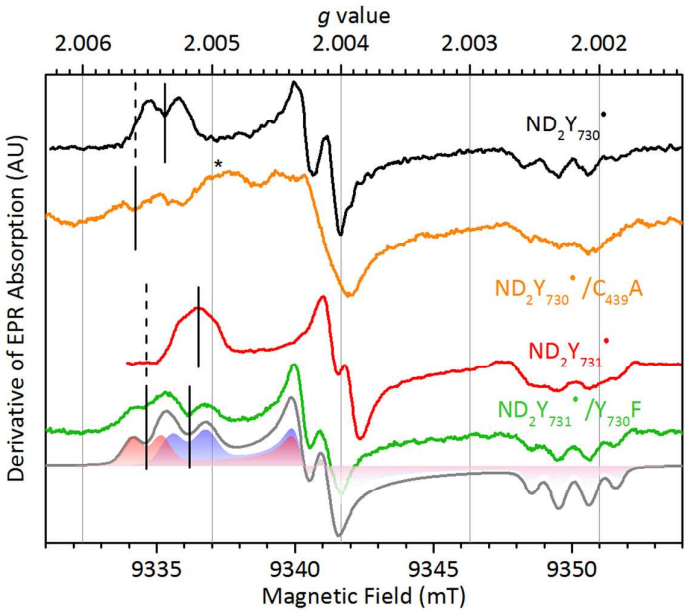


Figure S7. 263- and 94-GHz spectra of $NH_2Y_{730}^{\bullet}/C_{439}A$ and $NH_2Y_{731}^{\bullet}/Y_{730}F$. The spectra of $NH_2Y_{730}^{\bullet}/C_{439}A$ and $NH_2Y_{731}^{\bullet}/Y_{730}F$ (orange and green, respectively) are compared with their corresponding single mutant spectra of $NH_2Y_{730}^{\bullet}$ (black) and $NH_2Y_{731}^{\bullet}$ (red) in D_2O exchanged buffer. The echo-detected EPR spectra were recorded at 70 K, where the echo signal of $Y_{122}^{\bullet}$ is not detectable in the pulse experiment. Experimental parameters (263 GHz): Stimulated echo $\pi/2$ = 110 ns; τ = 220 ns; repetition time = 6 ms; number of transients = 7500 and 8750. (94 GHz): electron spin echo $\pi/2$ = 18 ns; τ = 260 ns; repetition time = 6 ms; shots/point = 100; number of scans = 15-110. To build the derivative spectra, the absorption spectra were smoothed by a 5 point, second order Savitzky-Golay filter. For the 263 GHz spectrum of $ND_2Y_{730}^{\bullet}/C_{439}A$ 10 G pseudo modulation was used. The positions of the observed g_x values are marked by bars. The asterisk (*) denotes the presence of a background signal, which could not be assigned and is visible due to the low yield of the $ND_2Y_{730}^{\bullet}$ in the double mutant reaction. In the $ND_2Y_{730}^{\bullet}$, g_x is located in the center of the doublet splitting at the low field site. The g_x shift observed at 94 GHz and 263 GHz is well consistent in size.

For the $ND_2Y_{731}^{\bullet}$ in the double mutant, the low field side of the 263-GHz spectrum (green spectrum) shows a distinct triplet. As compared to the single mutant (red spectrum), the dominant C–β coupling increases ($A_{iso} \approx 26$ MHz, Table 1). However, this hf coupling in combination with a weaker coupling to the second C–β proton ($A_{iso} < 26$ MHz) is not sufficient to generate the large triplet splittings (peak separation of ~ 1.1 and 1.4 mT). Since no other large hf couplings are expected in deuterated buffer (the amino protons are exchanged to deuterons), we assign the triplet to the contribution of two $ND_2Y_{731}^{\bullet}$ with slightly different g_x values, i.e. electrostatic environments. A simulation (grey) in support of this interpretation requires the addition of two components with a weight of 55% (blue) and 45% (red) (Table 1). These two contributions cannot be resolved at 94 GHz, where the spectral region around g_x shows only broadening (area marked in grey in the spectrum). The results indicate that, as expected, removal of the hydrogen bond to Y_{730} perturbs the electrostatic environment at $NH_2Y_{731}^{\bullet}$ and destabilizes the radical.

263 GHz



94 GHz

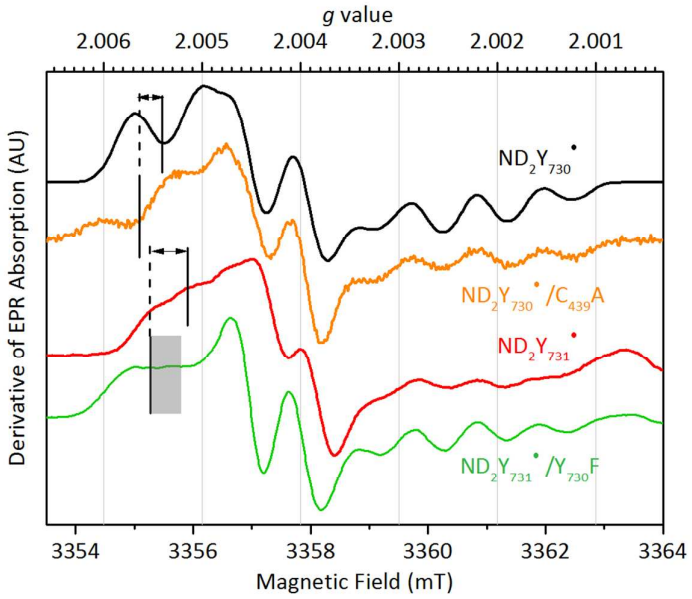


Figure S8. Large DFT models for $NH_2Y_{731}^{\bullet}$. The 210 to 216 atoms large model 1 (wine red), model 2 (green) and model 3 (purple) are depicted. The GDP is modeled by an (3*R*, 4*S*)-tetrahydrofuran-3,4-diol.

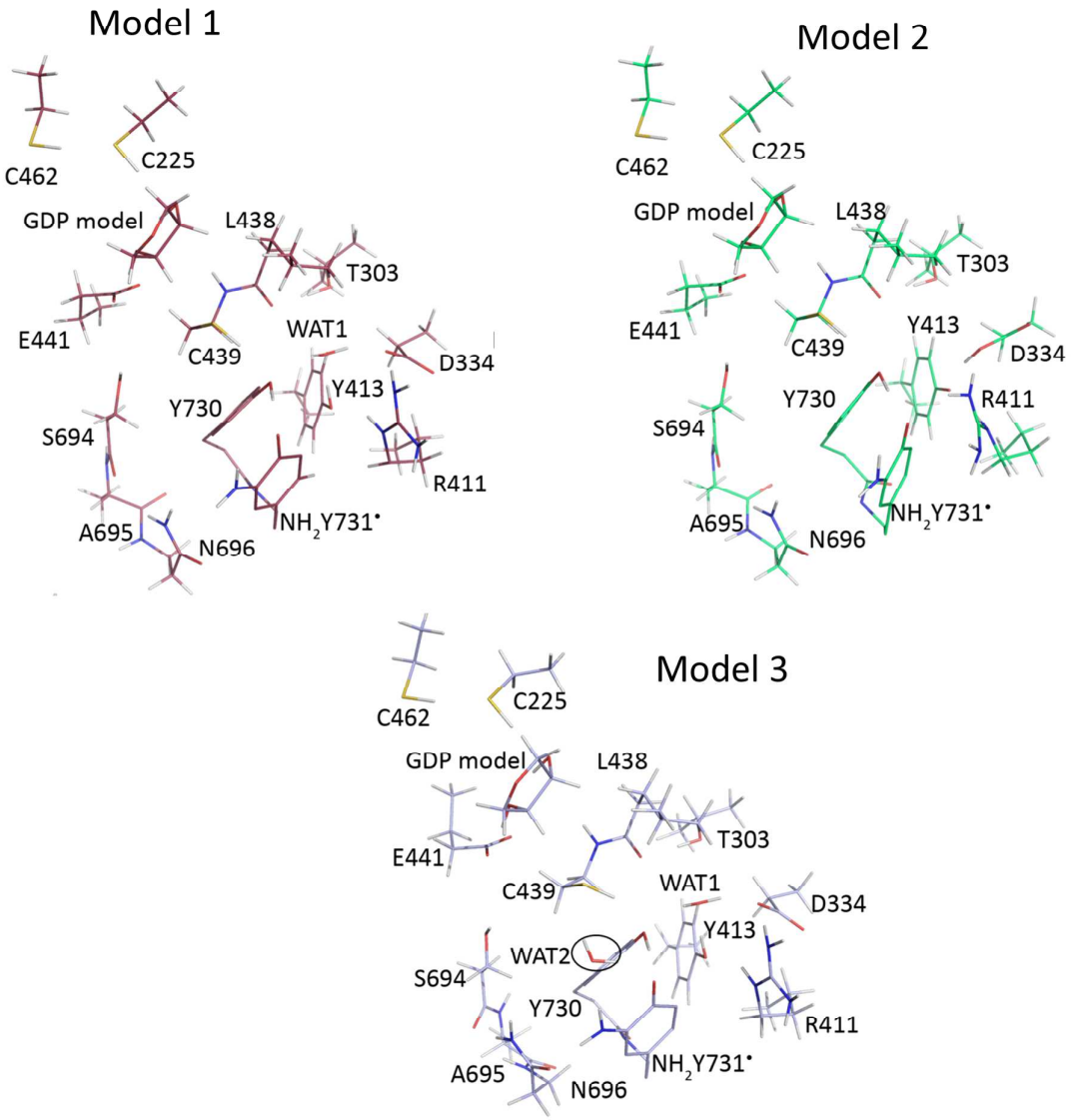


Figure S9: X-ray structures displaying water molecules in α subunit.[5] Crystal structures of: **A** wild-type α, pdb 2X0X, molecule C, 2.3 Å resolution; (**B**) NH_2Y_{730}-α, pdb: 2X04, molecule B, 2.7 Å resolution; (**C**) NH_2Y_{731}-α, pdb 2X05, molecule C, 2.5 Å resolution. Only water oxygen atoms (red spheres), which are near to the phenolic oxygen (≤ 5.5 Å) of the tyrosines, are displayed. The distances are given in Å.

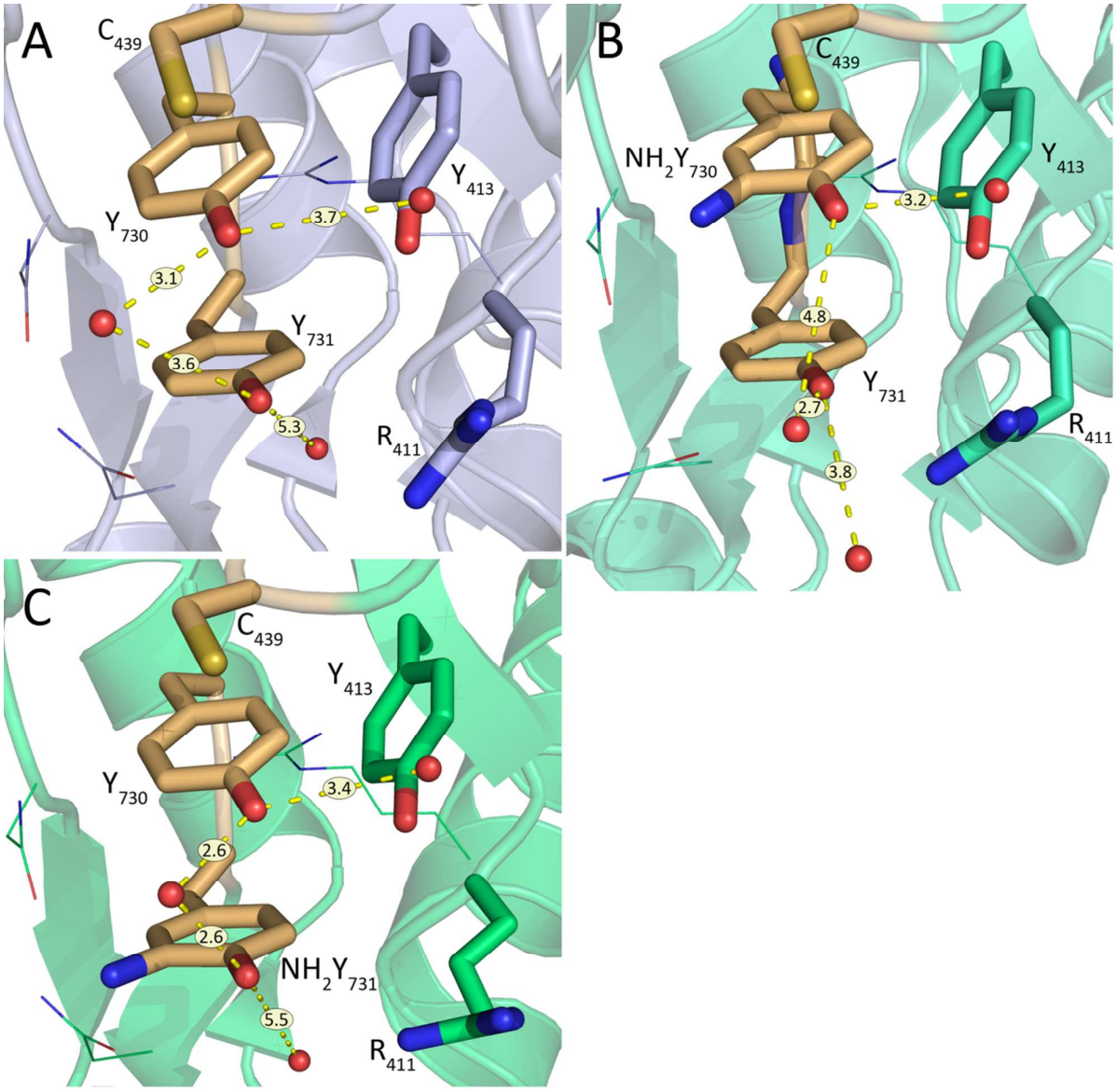


Table S2. EPR parameters for the *strong* hydrogen bond to $NH_2Y_{730}^{\bullet}$. Values for the single mutant are from the simulation of the ENDOR spectra in Ref.4,[a] values for the double mutant are from the simulation in Figure 3B[b].

$NH_2Y_{730}^{\bullet}$	A_x [MHz]	A_y [MHz]	A_z [MHz]	α [°]	β [°]	γ [°]	Q_1 [MHz]	Q_2 [MHz]	Q_3 [MHz]
Y_{731}-O**D**	0.73	-1.15	-1.25	14 111	133 134	126 -110	-0.02	-0.03	0.06
$NH_2Y_{730}^{\bullet}/C_{439}A$-α2	A_x [MHz]	A_y [MHz]	A_z [MHz]	α [°]	β [°]	γ [°]	Q_1 [MHz]	Q_2 [MHz]	Q_3 [MHz]
Y_{731}-O**D**[b]	0.67	-1.06	-1.19	5 115	140 130	120 -100	-0.06	-0.07	0.13

a) With respect to Ref. 4, the A- and Q tensor are here defined such that $|A_x|<|A_y|<|A_z|$. Within this more convenient definition, for both the amino and H bond deuterons, the A_x direction results along the bond direction. In Ref.2, the tensor directions were defined from the DFT calculation such that the Euler angles are minimized.

b) The signs of the couplings from the simulation are only relative to each other within one tensor. The Euler angles (α, β, γ) are defined from the A or Q to the g tensor based on the y convention (positive sign for a rotation is counterclockwise, second rotation is around the y axis). Euler angles from DFT (in ORCA output positive rotations are defined clockwise) were transformed into the magnetic resonance convention, for comparison. The simulation for the double mutant has a line width of 70 kHz (full width half maximum).

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Figure S10. Comparison of orientation of the hydrogen bond to $NH_2Y_{731}^{\bullet}$ from the DFT models and the ENDOR simulation. The directions of the ^2H hyperfine tensor A (A_x, A_y, A_z mintgreen), g tensor (g_x, g_y, g_z, blue) and quadrupole tensor Q (Q_z, green) of the $NH_2Y_{731}^{\bullet}$–DOY_{730} bond from the DFT calculations for the three DFT models (model 1 in A, model 2 in B and model 3 in C, left column) are compared with those obtained from the ENDOR simulation (right column). For proper comparison, the hf tensor orientation (defined by the Euler angles α, β and γ) from the ENDOR simulation was plotted with respect to the g tensor calculated for each considered model. Tensor values are from Table 2. All orientations are not distinguishable within an estimated error of about 20% in Euler angles. The experiment is entirely consistent with a hydrogen bond contributed by Y_{730} and directed between the two tyrosine rings, as predicted by the DFT for all three models independently on the number of water molecules (one H_2O in model 1, none in model 2 and two in model 3) around $NH_2Y_{731}^{\bullet}$. The assignment is further consistent with the direction of the Q_z tensor component, which lies along the OD bond of Y_{730} (illustrated in **A**).

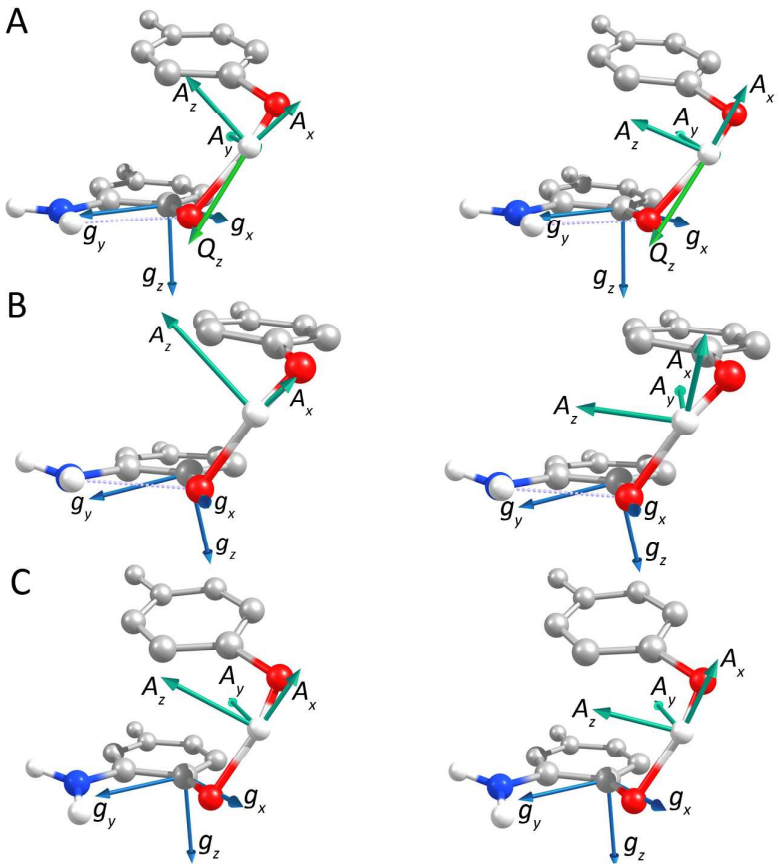

Figure S11. Small DFT models for $NH_2Y_{731}^{\bullet}$. Small models were constructed from DFT model 2 in order to check for the effect of individual amino acid residues on the *g* values of $NH_2Y_{731}^{\bullet}$. For geometry optimization the functional (B3LYP) and the Ahlrichs' TZVPP basis set of triple-ζ quality were used. For deriving the EPR parameters, the EPR II basis set was used (Online Methods). Solvent effects were taken into account by a conductor like screening model (COSMO) with the polarizability of ethanol. **A**) This first small model is built from model 2 by considering residues only in the first interaction sphere. No further geometry optimization was carried out. The *g* tensor with R_{411} is g_{xyz} = [2.0050, 2.0041, 2.0022]. If R_{411} is removed the *g* tensor becomes g_{xyz} = [2.0055, 2.0044, 2.0021], i.e. the g_x value shifts by Δg_x = + 0.5 ppt. **B**) Small model A after additional geometry optimization, g_{xyz} = [2.0052, 2.0042, 2.0022]. **C**) Small model which mimics the double mutant $NH_2Y_{731}^{\bullet}/Y_{730}F$. The *g* tensor results to g_{xyz} = [2.0060, 2.0046, 2.0023]. **D**) Small model C after geometry optimization. The *g* tensor is g_{xyz} = [2.0052, 2.0043, 2.0023,], i.e. the computed g_x lowers by 0.8 ppt.

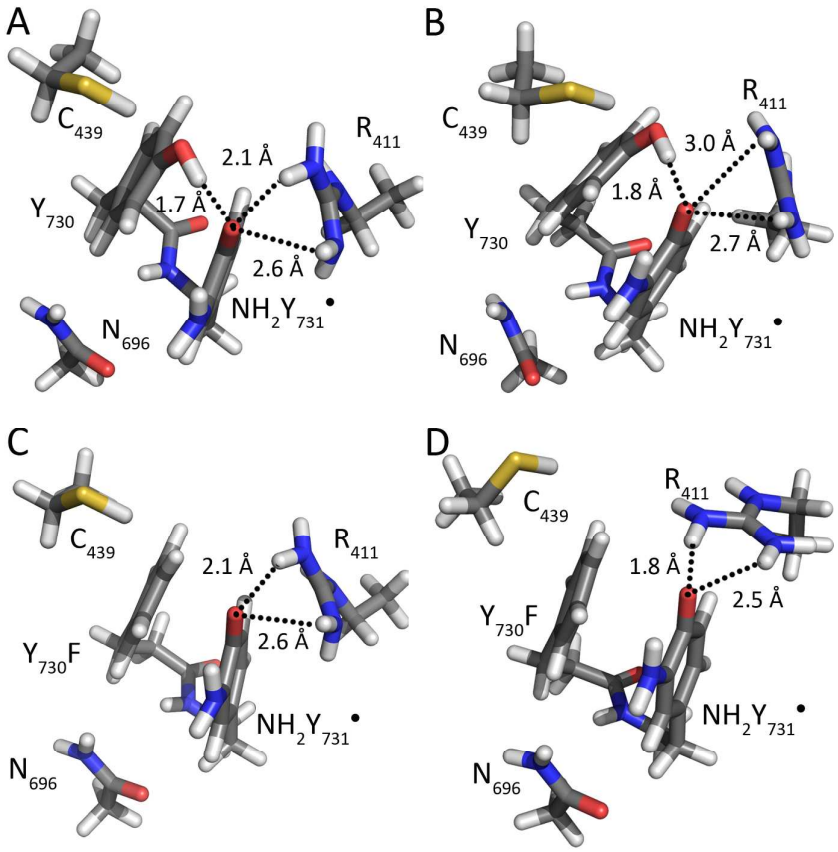

Table S3: Geometries of the optimized models in Å as XYZ coordinates.

	Model 1: 214 Atoms (Total energy = -5588.283194607 Eh)				**Model 2:** 211 Atoms (Total Energy = -5511.849573802 Eh)			
#		**x**	**y**	**z**		**x**	**y**	**z**
1	C	-7.853360321	92.96559023	19.0698462	C	-7.853361594	92.96701963	19.0699451
2	O	-8.040357692	93.82311006	20.2045798	O	-8.039245944	93.82589856	20.20391762
3	C	-6.811342302	93.7209967	20.94770132	C	-6.811008806	93.72224639	20.94795222
4	C	-5.670376241	93.68088007	19.90919078	C	-5.669598792	93.68068102	19.91014506
5	C	-6.416249953	93.22837898	18.58956503	C	-6.414759083	93.22415301	18.59106603
6	O	-4.691300239	92.70644439	20.18198323	O	-4.689967154	92.70736908	20.18637944
7	O	-5.765756935	92.08294909	18.04450403	O	-5.766953216	92.07393747	18.05255157
8	O	-2.652364864	93.32774271	21.54164844	O	-2.640569055	93.33084275	21.53428974
9	C	-1.632354783	92.64724808	21.12392114	C	-1.629125119	92.63772737	21.11818909
10	O	-1.213658941	92.62574445	19.94157029	O	-1.213944507	92.60285093	19.93451576
11	C	-0.928068999	91.78406101	22.19482102	C	-0.92753797	91.77823996	22.19467801
12	C	0.570000003	92.076	22.398	C	0.569999982	92.07600001	22.398
13	C	1.454181825	91.67758411	21.21098141	C	1.45653401	91.66730519	21.21627926
14	O	0.478770741	95.34859789	22.35321764	C	-1.983998995	95.64399895	19.268001
15	C	1.144999997	96.343001	23.132999	S	-3.572328993	96.4577667	18.77976988
16	C	2.608000002	95.894001	23.24	C	-0.976999888	95.53399904	18.12599906
17	C	3.413665285	97.08313054	23.77061782	N	-1.521439673	94.75839056	17.01760311
18	N	4.766782235	96.94190848	23.83801687	C	-1.332516294	95.05024878	15.71534901
19	C	5.583	98.037001	24.335	O	-0.52931701	95.93370717	15.33602033
20	C	7.039000002	97.574001	24.409	C	-2.177000018	94.25199896	14.72800008
21	O	2.889509952	98.14074689	24.15779317	C	-3.676999993	94.49799903	14.86999992
22	C	5.516426189	99.26618371	23.42386531	C	-4.077365991	95.98247865	14.82020555
23	N	5.475029536	100.4443233	24.11567249	C	-5.560200058	96.135672	15.17728463
24	C	5.570000002	101.741	23.470999	C	-3.756964368	96.62418298	13.46441574
25	C	4.509999995	102.725001	23.959999	O	-0.087554928	96.22558859	12.66845629
26	C	3.074460956	102.4663869	23.47493211	C	0.398999979	95.02399799	12.05299992
27	O	2.361547511	103.409148	23.1050789	C	1.931869013	95.00452301	12.05472105
28	O	5.574585175	99.18600438	22.20093652	C	-0.173585376	94.97172014	10.64005611
29	N	2.62654749	101.1846479	23.48798936	O	0.485630351	95.36683403	22.32358431
30	C	3.307947529	98.51768922	20.03127949	C	1.145000031	96.34299898	23.13300002
31	C	1.94191381	98.71104687	19.4104087	C	2.607999974	95.89400002	23.24
32	C	1.68090788	98.32578528	18.08313224	C	3.411091638	97.07368955	23.79588042
33	C	0.424315331	98.48677893	17.51328873	N	4.767117796	96.93897465	23.84384238
34	C	-0.61548397	99.05434956	18.26226147	C	5.583	98.037	24.33499999
35	C	-0.399502055	99.38132835	19.60959056	C	7.039000014	97.57399999	24.40900001
36	C	0.87555617	99.22686261	20.16012852	O	2.885701955	98.11788697	24.21486945
37	O	-1.83746207	99.23460422	17.64977934	C	5.504883955	99.26426802	23.41856411
38	C	4.501000994	98.999	19.188999	N	5.476562919	100.4425241	24.11104055
39	C	4.708330125	100.4887082	19.00750396	C	5.569999994	101.741	23.47099995
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42	C	2.629249383	103.5287067	19.60637052	O	2.37418226	103.4191694	23.08330387
43	C	1.217365449	103.0462807	19.37514277	O	5.5385738	99.18444292	22.19352284
44	C	0.798101418	102.6239841	18.07712847	N	2.624303318	101.1927966	23.4674182
45	C	-0.473554869	102.1623892	17.84405017	C	3.167532253	99.37136513	19.95435402
46	C	-1.430853016	102.0748538	18.90587807	C	1.790522385	99.36170046	19.3340655
47	C	-0.995277226	102.5493138	20.23112876	C	1.577978721	98.82639476	18.04761823
48	C	0.316987187	103.0054477	20.43606171	C	0.310106968	98.78654118	17.47835125
49	O	-2.59035096	101.550779	18.78499244	C	-0.782821883	99.29786306	18.19153165
50	O	5.7987846	100.9467282	18.64310996	C	-0.6009263	99.78057493	19.50076773
51	O	-1.046173555	98.97837328	14.84606255	C	0.67848206	99.82143806	20.05045053
52	O	0.860533292	100.6152944	15.23184466	O	-2.009239277	99.33245924	17.58568263
53	C	2.036001659	99.92557832	15.08456892	C	4.281837608	99.91650488	19.0534576

54	C	3.198845309	100.4272391	15.68316899	C	4.36540172	101.4053874	18.76742891
55	C	4.412805036	99.75023801	15.55369773	N	3.765290322	102.2516762	19.65875976
56	C	4.496374811	98.55188527	14.82582724	C	3.667881603	103.6801948	19.36757532
57	C	3.318105452	98.0567589	14.24894527	C	2.329936692	104.2476691	19.84431935
58	C	2.098430189	98.72097042	14.36814207	C	1.089445456	103.5611024	19.30978737
59	C	5.792002003	97.783	14.681	C	1.089276822	102.7938416	18.11631359
60	C	7.012003	98.65	14.351001	C	-0.069765841	102.2090515	17.63356902
61	O	-1.479645171	100.2567245	12.63208957	C	-1.320372727	102.3848113	18.29669062
62	C	-0.616244572	100.6709255	11.72628924	C	-1.303107161	103.1520733	19.53603376
63	O	-0.676940789	101.793576	11.20191475	C	-0.109279811	103.7048718	20.01614027
64	C	0.513003001	99.699	11.364999	O	-2.462070807	101.9120393	17.88523623
65	C	0.753003002	99.676	9.868999003	O	5.008981501	101.837477	17.80187535
66	N	-2.565889419	102.2569684	13.7223205	N	-2.183761461	101.9755026	14.97164591
67	C	-1.721253154	103.2315807	14.03055426	C	-1.387946796	103.0450305	15.08858151
68	N	-2.107543137	104.5505298	14.00198701	N	-1.850744517	104.1278923	15.78996804
69	N	-0.45677919	102.9535375	14.3789981	N	-0.194383869	103.0795159	14.4960352
70	C	0.612728998	103.936251	14.495325	C	0.643841995	104.268574	14.41719299
71	C	1.172809001	104.386509	13.131074	C	1.190788997	104.471209	12.99457901
72	C	1.991079137	103.3161527	12.39854529	C	2.157556873	103.3688982	12.53317302
73	C	3.298261189	102.9409351	13.10024243	C	3.509290934	103.3964299	13.25067709
74	C	-1.984000038	95.64400002	19.26799998	O	0.823947063	100.5589981	14.59251451
75	S	-3.571125799	96.46409116	18.78735571	C	1.962294411	99.89638694	14.6835614
76	C	-0.97699999	95.53399998	18.126	C	3.111586787	100.4697146	15.29063706
77	N	-1.540314485	94.75582357	17.02763561	C	4.33364028	99.80484239	15.2950354
78	C	-1.304693304	95.00737125	15.72492959	C	4.471947791	98.52566009	14.71938043
79	O	-0.427305159	95.81853404	15.35328571	C	3.313848596	97.92606004	14.18740207
80	C	-2.176999998	94.251999	14.728	C	2.084843257	98.56975063	14.182344
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82	C	-4.066945753	95.98686034	14.87070554	C	7.011997968	98.64999797	14.35099701
83	C	-5.553843199	96.14211267	15.20813564	O	-1.115683573	100.1530199	13.10090983
84	C	-3.715826357	96.68048283	13.54846891	C	-0.892824621	100.1341904	11.76526993
85	O	-0.149330169	96.19525635	12.67151337	O	-1.774227285	100.4220729	10.97439592
86	C	0.399000002	95.023999	12.053	C	0.512997003	99.698999	11.36499897
87	C	1.931554999	95.077887	12.053514	C	0.752997003	99.675999	9.868999031
88	C	-0.170293165	94.95011847	10.63976226	S	-6.736310356	89.02408301	19.11919705
89	S	-6.733457129	89.02957856	19.11777811	C	-6.171000004	88.36199997	17.485
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96	H	-5.930414867	87.30500066	17.66742394	H	0.03634733	94.14200313	12.6173092
97	H	0.080275612	94.12088019	12.61260733	H	0.659072734	98.69218497	11.79057912
98	H	0.280672957	98.69771922	11.75523368	H	1.239032498	100.3457052	11.88361937
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122	H	-1.523693134	96.20830285	20.09027094	H	0.906758164	91.54547885	23.30760308
123	H	0.906358829	91.53456214	23.30130298	H	0.695042044	93.15101472	22.59129811
124	H	0.697745622	93.14817501	22.60299366	H	-1.468498345	91.91520799	23.14185773
125	H	-1.467231219	91.91684055	23.14369942	H	-1.052308443	90.72260505	21.89409355
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131	H	0.707437297	96.4444559	24.14115262	H	1.104589241	97.34198115	22.6673233
132	H	1.103828641	97.32943485	22.64220231	H	5.218817837	96.17764853	23.34501297
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144	H	2.471561727	97.88773965	17.47230265	H	0.818401342	100.2281911	21.05484381
145	H	1.044609513	99.49680994	21.2059407	H	0.153911663	98.38984668	16.475498
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153	H	1.514107984	102.6179186	17.25510941	H	-0.110949471	104.2555035	20.96105926
154	H	0.653337273	103.298308	21.43538304	H	-0.022079421	101.5561472	16.76237681
155	H	-0.759672162	101.7871803	16.86339833	N	-2.518722157	103.305592	20.14750918
156	N	-1.925366496	102.4511828	21.20895024	H	-6.777911847	92.77935074	21.52776008
157	H	-6.776204888	92.77785908	21.52691443	H	-5.224601205	94.68887502	19.76924788
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164	H	-3.494949558	102.5538176	13.43490639	H	3.145993189	100.3818029	23.80023583
165	H	3.169955371	100.3698198	23.77229438	H	1.663537102	101.036761	23.17618285
166	H	1.690383871	101.01359	23.13398051	H	-0.205928794	96.08640943	13.65357279
167	H	-0.187497786	96.06777112	13.66419909	H	-3.848811865	93.07268494	20.69000441
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169	H	0.074812125	99.94655942	15.1074539	H	-6.409443565	90.33595696	18.84033495
170	H	-6.404634519	90.34002284	18.83607107	H	-3.025248001	97.57677839	18.21731852
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174	H	2.308800307	95.12181327	13.08502717	H	2.32545875	94.10189161	11.5598264
175	H	2.368070057	94.19142643	11.56530382	H	2.315978185	95.89056348	11.52717218
176	H	2.272174125	95.97777685	11.51944833	H	1.772279211	99.32537785	9.649975385
177	H	1.626524429	99.05565061	9.615982288	H	0.626460775	100.6725225	9.421771716
178	H	0.92116974	100.69221	9.486952988	H	0.041108518	99.00470825	9.370343843
179	H	-0.11616886	99.25915659	9.338057926	H	-0.482372864	95.45742734	22.38589011
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181	H	3.868373092	102.2142149	12.50366235	H	4.041411703	104.3423166	13.05706111
182	H	3.938512833	103.8241791	13.26001307	H	3.401684399	103.2894306	14.33929195
183	H	3.128161591	102.4628991	14.07465396	H	-5.537288502	87.52272502	20.77013097
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185	H	7.679512512	98.368531	24.81490015	H	7.131481289	96.69374412	25.0602941
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187	H	7.404998207	97.32748486	23.40194798	H	7.928234048	98.04160043	14.31337796
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189	H	7.215906685	99.37864296	15.14846277	H	6.888578974	99.14462023	13.37581664
190	H	6.851806156	99.212816	13.41889742	H	-2.685414604	96.58208998	13.22181056
191	H	-2.641601743	96.63518384	13.31933728	H	-4.309499106	96.11596255	12.65562746
192	H	-4.26180255	96.21554332	12.70969591	H	-4.0483163	97.68442701	13.45226706
193	H	-3.999398686	97.74345662	13.57652512	H	-5.763684542	95.74175268	16.18452886
194	H	-5.78052883	95.71589697	16.19691598	H	-6.198132315	95.59139837	14.46119307
195	H	-6.184185427	95.63021193	14.46203362	H	-5.862911647	97.19361093	15.16229781
196	H	-5.847098222	97.20291685	15.22582451	H	-1.271719602	94.96712897	10.67400443
197	H	-1.266684057	94.8837314	10.67358328	H	0.171959467	94.07549332	10.10200888
198	H	0.224128955	94.07796497	10.09620854	H	0.145015842	95.86178572	10.07538968
199	H	0.098245729	95.86084405	10.08198802	H	2.508930379	91.95135261	21.38671654
200	H	2.507781661	91.95524704	21.38451831	H	1.098516248	92.14614383	20.29554901
201	H	1.098076154	92.1685884	20.29599894	H	1.422994754	90.57700015	21.05479722
202	H	1.416322255	90.5894456	21.03632416	H	-6.853455075	88.06919277	15.43849239
203	H	-6.8548248	88.06588315	15.43948758	H	-8.152932087	87.98687168	16.66121102
204	H	-8.154283632	87.99014544	16.66270553	H	-7.456892471	89.55943152	16.20794727
205	H	-7.454072059	89.55962767	16.20527067	H	-6.897985475	85.13252379	19.59796088
206	H	-6.897677722	85.13256309	19.59742836	H	-6.544637122	84.00489136	20.92182778
207	H	-6.545006273	84.00547738	20.92194072	H	-5.93686646	83.66368997	19.27615697
208	H	-5.936790354	83.66332365	19.27659414	H	-8.627190904	93.21889902	18.3325996
209	H	-1.366822497	99.29061201	13.94527485	H	-6.76623151	94.57963709	21.63238833
210	H	-1.750786868	99.02668387	15.51951456	H	-3.254889529	102.7090812	19.76825925
211	H	-8.629213741	93.21509949	18.33377618	H	-2.566051504	103.5769656	21.12228468
212	H	-6.76735861	94.57799779	21.63266609				
213	H	-2.81907617	102.036598	20.94555543				
214	H	-1.726687627	102.6934789	22.17119455				

	Model 3: 217 Atoms (Total energy = -5664.720887123 Eh)					**Small model figure S11 B:** 59 Atoms (Total energy = -1681.114019327 Eh)			
#		**x**	**y**	**z**	**#**				
1	C	2.088760274	98.65326441	14.31585678	1	C	-2.021743583	96.04799768	19.10197141
2	C	2.009950719	99.89263898	14.97144478	2	S	-3.444873045	96.87320834	18.28991063
3	C	3.159987691	100.4360778	15.5580198	3	C	-0.977000001	95.533999	18.125999
4	C	4.383162975	99.77280297	15.46406604	4	C	4.501922023	102.8198163	23.10849686
5	C	4.483833016	98.54175502	14.77835598	5	C	3.077691991	102.4764149	23.46328492
6	C	3.315520536	97.99578949	14.23233959	6	O	2.225118117	103.342357	23.6607071
7	O	0.823862687	100.5690599	15.08579199	7	N	2.774953888	101.162065	23.50094484
8	C	5.817808403	97.84835085	14.62817937	8	C	3.167531995	99.37136505	19.95435406
9	C	6.54397211	98.2460942	13.33089216	9	C	1.945281293	99.37927459	19.06003607
10	O	-1.03380113	98.86190844	14.73011806	10	C	2.000521299	99.66319528	17.69227202
11	O	-1.482262032	100.2666701	12.62379804	11	C	0.846900658	99.74843038	16.92241596
12	C	-0.584470963	100.6968819	11.77328899	12	C	-0.395547768	99.53556339	17.5111624
13	C	0.488070592	99.67944363	11.38680363	13	C	-0.461908805	99.17581164	18.85255272
14	C	1.01893805	99.85949762	9.964709897	14	C	0.694122756	99.11724675	19.61399249
15	O	-0.575860017	101.85376	11.312317	15	O	-1.528328213	99.70520013	16.76212366

16	N	-2.610693	102.341184	13.70493999	16	C	4.316974387	100.2818081	19.52081456
17	C	-1.736496584	103.2904268	14.02832498	17	C	4.088378599	101.7822183	19.45775988
18	N	-0.480038342	102.975435	14.36649474	18	N	2.873526947	102.257577	19.78636591
19	C	0.612727999	103.936251	14.49532499	19	C	2.543864486	103.6711811	19.69439165
20	C	1.172808999	104.386509	13.131075	20	C	1.280922713	103.9993382	20.49016485
21	C	2.065950063	103.3419736	12.44814267	21	C	0.07568877	103.2101014	20.06845938
22	C	3.390625192	103.0933256	13.17147669	22	C	-0.478912585	103.412007	18.76949222
23	N	-2.103996252	104.611936	14.03526271	23	C	-1.557861857	102.7006336	18.33777949
24	O	-1.817473879	99.14308012	17.51194781	24	C	-2.170524361	101.7072744	19.16569266
25	C	-0.618768111	99.01755583	18.1573192	25	C	-1.622215228	101.5452328	20.51613788
26	C	0.457460338	98.48854435	17.4298802	26	C	-0.495905538	102.2876557	20.91419471
27	C	1.693940412	98.31262651	18.03577181	27	O	-3.101356406	100.9481492	18.769742
28	C	1.896447921	98.64700276	19.38558094	28	O	5.015596396	102.5317848	19.13913396
29	C	0.798536721	99.12358393	20.11623926	29	H	-0.181091442	95.02098963	18.67123977
30	C	-0.458502843	99.28407623	19.52424523	30	H	-2.473336962	95.23323081	19.66749393
31	C	3.241318099	98.44034998	20.04982674	31	H	-1.57665542	96.73829886	19.81629098
32	C	4.464556325	98.87057816	19.22601861	32	H	5.202369887	102.0289068	23.37085011
33	C	4.649391065	100.3541507	18.92748234	33	H	4.76547302	103.737372	23.62293902
34	O	5.713235895	100.7824065	18.47349969	34	H	5.158433943	100.1438169	20.2026124
35	N	3.588667505	101.1785804	19.19601169	35	H	4.695691772	99.99099026	18.53959186
36	C	3.659295905	102.5862276	18.83966908	36	H	3.567316807	98.35542166	20.01629636
37	C	2.562913931	103.3889465	19.54396689	37	H	2.860296873	99.62883914	20.97003769
38	C	1.164319	102.880435	19.28530699	38	H	2.94989334	99.86592272	17.21532496
39	C	0.740060432	102.5848643	17.95341096	39	H	0.618094758	98.8848005	20.66918556
40	C	-0.533934659	102.1485057	17.68237189	40	H	0.899128138	100.0229978	15.87726577
41	C	-1.485696	101.92723	18.72489702	41	H	-1.4245211	98.98813906	19.30038278
42	C	-1.03819004	102.2150658	20.09991846	42	H	2.11005981	101.6067946	19.88226587
43	C	0.269564296	102.7147288	20.32484834	43	H	2.425419932	103.9609836	18.6468281
44	O	-2.643685468	101.4095677	18.50769162	44	H	3.379576191	104.243965	20.09231931
45	N	-1.85332222	101.9330517	21.13466398	45	H	1.472594773	103.8349486	21.54909556
46	O	5.849160654	100.2883542	21.93414226	46	H	1.08195696	105.0645638	20.34484927
47	C	5.21550518	99.67994569	22.79434568	47	H	-0.021310354	104.1464917	18.11918749
48	N	4.077261282	100.1353449	23.38004873	48	H	-0.08229246	102.1288307	21.90330249
49	C	3.412396508	101.3686558	22.98383282	49	H	-1.966263011	102.8424996	17.34633126
50	C	2.308029797	101.7423829	23.9866607	50	N	-2.204406137	100.6373997	21.30439691
51	C	0.950279044	101.0867019	23.74158323	51	H	3.492646993	100.4591136	23.46843845
52	N	0.852833126	99.74377076	23.90903546	52	H	1.854539296	100.8756773	23.79277287
53	C	5.649081812	98.28454021	23.34021418	53	H	-2.736651331	97.73889345	17.54622496
54	C	7.019463696	97.88931636	22.8123587	54	H	-2.249240608	100.0154193	17.34549068
55	N	4.658721644	97.25578328	22.98653218	55	H	-2.999704414	100.1270828	20.95248965
56	C	3.476176799	97.07520483	23.62015774	56	H	-1.870659125	100.4396292	22.23226762
57	O	3.112424086	97.8173834	24.56308735	57	H	-1.415957587	94.83477096	17.41371337
58	C	2.613502452	95.93512633	23.12608609	58	H	-0.525909618	96.35572459	17.56934231
59	C	1.145001037	96.34299912	23.1329987	59	H	4.572256987	103.0017375	22.03454318
60	O	0.393014949	95.27274687	22.57872435		**Small model figure S11 D:** 74 Atoms (Total energy = -1890.268720222 Eh)			
61	O	-0.021650449	101.7746054	23.39167282	1	C	-1.94656918	96.52963234	18.73876
62	C	-0.007712148	90.67366177	21.68279349	2	S	-3.195088986	97.15480888	17.55084
63	C	-0.7713816	89.5471872	20.97902271	3	C	-0.976999989	95.53399901	18.126
64	C	-0.928067907	91.78405904	22.19481887	4	C	4.525662105	102.0790202	23.61884
65	C	-1.590700102	92.62666596	21.09289109	5	C	3.077691997	102.476415	23.46328
66	O	-1.157718188	92.57291533	19.91871507	6	O	2.714671348	103.650772	23.45167
67	O	-2.578961684	93.37031443	21.48737305	7	N	2.203645049	101.4590062	23.28312
68	O	-4.660924532	92.72812809	20.15799614	8	C	3.167531992	99.371365	19.95435
69	C	-5.667767894	93.68923644	19.91657869	9	C	1.832870157	99.63287462	19.2926
70	C	-6.78499899	93.69199801	20.99299999	10	C	1.58208981	99.25562492	17.9721
71	O	-8.041737	93.45618599	20.364989	11	C	0.327391973	99.45019643	17.40232
72	C	-7.833984647	92.87335024	19.06815896	12	C	-0.698267633	100.0240243	18.14441
73	C	-6.415633085	93.24007196	18.5962777	13	C	-0.458665319	100.411792	19.45627
74	O	-5.741834001	92.10935	18.029694	14	C	0.797137694	100.2209193	20.01879

75	C	-1.84647232	95.81303771	19.34542431	15	C	4.401213762	99.78463848	19.14958
76	C	-0.97699996	95.53400006	18.12599995	16	C	4.592722039	101.256795	18.83875
77	N	-1.6504653	94.78731985	17.07430708	17	N	4.14140627	102.1467203	19.74622
78	C	-1.321658998	94.93760812	15.77012641	18	C	4.383801461	103.5785925	19.63623
79	C	-2.176102865	94.18941461	14.75640894	19	C	3.242458325	104.4058038	20.22048
80	C	-3.677000996	94.49800099	14.86999999	20	C	1.878966612	104.0701529	19.68188
81	C	-4.040648998	95.99299401	14.968884	21	C	1.70201565	103.815436	18.29156
82	C	-3.701722764	96.74792556	13.67711151	22	C	0.472369589	103.5636785	17.76183
83	S	-3.451072277	96.67668002	18.9918318	23	C	-0.701901718	103.5395172	18.57578
84	O	-0.384950356	95.68284024	15.41012152	24	C	-0.501262325	103.7676184	20.00903
85	C	-5.516823318	96.1547596	15.34465203	25	C	0.785385506	104.0295938	20.51564
86	O	-0.149177991	96.16664	12.70938	26	O	-1.871442089	103.3306636	18.13404
87	C	0.39899899	95.024003	12.053	27	O	5.196097287	101.6053112	17.82194
88	C	0.373326665	95.31454306	10.55709336	28	N	-1.743020021	102.3083902	15.515
89	C	1.810402031	94.7161218	12.561678	29	C	-1.399959648	103.3404401	14.73384
90	S	-6.705120014	89.13929701	19.08098704	30	N	-1.648575329	104.5729161	15.17223
91	C	-6.170998988	88.36199999	17.48499695	31	N	-0.840684189	103.1296606	13.54577
92	C	-6.731229388	89.07914145	16.2610962	32	C	-0.272755831	104.1622781	12.67833
93	S	-5.030431006	86.58057701	21.577288	33	C	1.190788998	104.471209	12.99458
94	C	-4.843997996	85.231999	20.325995	34	H	1.551861695	105.2472373	12.31929
95	C	-6.164527387	84.76962907	19.71725514	35	H	1.806463638	103.5830921	12.84944
96	H	-5.072929599	88.33612341	17.4631934	36	H	-0.88793807	105.058181	12.74222
97	H	-6.52691216	87.32359988	17.53946044	37	H	-0.376626541	103.7950536	11.65905
98	H	-0.238373092	94.1339059	12.24736558	38	H	-0.655591759	102.1710638	13.29664
99	H	0.103647662	98.66341492	11.55723054	39	H	-0.310504249	95.13273578	18.89323
100	H	1.313817683	99.81229177	12.10806713	40	H	-2.54142965	96.06642327	19.52581
101	H	2.263867502	103.6845808	11.42027417	41	H	-1.423887626	97.38167103	19.16983
102	H	1.498267847	102.4085452	12.33170564	42	H	4.647044033	101.3431609	24.41402
103	H	1.751630748	105.3147802	13.29072212	43	H	5.11895362	102.9601097	23.84334
104	H	0.328825124	104.6404437	12.4720857	44	H	5.297236353	99.47301518	19.6951
105	H	1.388560496	103.4338326	15.08533373	45	H	4.435326767	99.26480316	18.19446
106	H	0.286325577	104.7965648	15.1033847	46	H	3.259074914	98.30171498	20.15988
107	H	-0.182120065	101.9907763	14.32326149	47	H	3.171482922	99.848482	20.93567
108	H	5.668423966	96.75635981	14.64113586	48	H	2.364820715	98.7963035	17.38253
109	H	6.456426432	98.0928101	15.49235318	49	H	0.978710208	100.5306994	21.03892
110	H	5.263120224	100.2002377	15.95070732	50	H	0.152979645	99.14133823	16.37934
111	H	3.355356587	97.02551878	13.73244048	51	H	-1.246601662	100.8675443	20.03953
112	H	3.077737531	101.3661786	16.12054488	52	H	3.609861849	101.8098879	20.53082
113	H	1.193617991	98.18954524	13.90202527	53	H	4.536602189	103.7980188	18.58222
114	H	-1.798046925	94.46843117	13.76491168	54	H	5.310117039	103.8442488	20.15169
115	H	-2.013162799	93.10542974	14.87582556	55	H	3.229175462	104.3196347	21.3063
116	H	-4.086358749	93.98333941	15.7563097	56	H	3.466441462	105.4538081	19.99538
117	H	-4.194669141	94.05379142	14.00233939	57	H	2.565355924	103.821581	17.64109
118	H	-3.441458185	96.42329186	15.79011142	58	H	0.909842157	104.19724	21.57838
119	H	-2.332937704	94.08393573	17.35149573	59	H	0.369014393	103.3656612	16.70742
120	H	-0.103456035	94.96616016	18.4908808	60	N	-1.585432233	103.6961487	20.78703
121	H	-0.606910478	96.45660229	17.67143621	61	H	-1.484067614	105.3852222	14.60678
122	H	-2.124133446	94.88207362	19.86696198	62	H	-2.044903601	104.7022978	16.08926
123	H	-1.259643009	96.43242732	20.03696244	63	H	-1.38307364	101.3965874	15.2882
124	H	0.570816407	90.2611809	22.5287413	64	H	-1.924431405	102.5201155	16.50281
125	H	0.713803728	91.11760854	20.97807472	65	H	2.4718403	100.5104063	23.48647
126	H	-0.365848192	92.49091009	22.82952403	66	H	1.218265028	101.6705326	23.30047
127	H	-1.729952029	91.37315098	22.83007014	67	H	-2.336517052	97.71922692	16.68763
128	H	-4.355812102	84.41364442	20.8741856	68	H	-2.482023886	103.5307798	20.35722
129	H	-4.142031823	85.56795149	19.55050361	69	H	-1.547032107	103.878168	21.77561
130	H	2.901873264	95.62193413	22.11228055	70	H	-1.509759776	94.70227515	17.66379
131	H	2.75413977	95.06710823	23.79036282	71	H	-0.362966038	96.01341253	17.36226
132	H	0.840360631	96.5718438	24.16991993	72	H	4.894572602	101.6230598	22.69714
133	H	1.032663693	97.26514214	22.52803136	73	H	1.314826024	104.8278538	14.01778
134	H	4.854103938	96.68336978	22.16863283	74	H	-1.681036337	100.1621978	17.71531

135	H	5.65575901	98.34219884	24.44069362					
136	H	3.637735556	99.49637864	24.05526083					
137	H	4.165753698	102.1691661	22.94313818					
138	H	3.004333084	101.2741874	21.96202669					
139	H	2.657260639	101.5204481	25.00904561					
140	H	2.119568347	102.821255	23.93253275					
141	H	5.390740347	98.56998529	19.73724483					
142	H	4.474409354	98.36050322	18.24953564					
143	H	3.353212783	97.36469835	20.27545417					
144	H	3.246564337	98.9577192	21.02111651					
145	H	2.508749596	97.90210079	17.4378342					
146	H	0.922031728	99.36580916	21.17566889					
147	H	0.302421194	98.18229479	16.39752112					
148	H	-1.316919442	99.58349868	20.1229538					
149	H	2.661946783	100.7582049	19.29334083					
150	H	3.589538224	102.714124	17.74357921					
151	H	4.653892614	102.9531892	19.12581318					
152	H	2.748721116	103.3967098	20.62863759					
153	H	2.642971833	104.4358434	19.20174006					
154	H	1.45258276	102.6682219	17.13273193					
155	H	0.570546334	102.9104225	21.35552525					
156	H	-0.827963549	101.8941425	16.66620472					
157	H	-6.543860283	92.8891219	21.71414963					
158	H	-5.223383	94.688623	19.77099799					
159	H	-6.407063998	94.063481	17.852553					
160	H	-7.918618956	91.7733699	19.11201133					
161	H	-1.549397967	105.255817	14.58906562					
162	H	-3.096235144	104.8154075	14.00689355					
163	H	-2.190172904	101.4191432	13.20937526					
164	H	-3.519822475	102.6561998	13.37945817					
165	H	1.605878167	99.13335868	24.23796852					
166	H	-0.05649147	99.31933485	23.74704559					
167	H	-0.191253412	95.99690543	13.69340417					
168	H	-3.819950441	93.09719128	20.65414075					
169	H	0.053643465	99.88084478	14.97081586					
170	H	-6.248038411	90.40254413	18.76715697					
171	H	-2.940402686	97.58727524	18.10956342					
172	H	-4.947553303	92.04101998	18.64699051					
173	H	-2.285706268	99.98128342	17.83485883					
174	H	1.801295017	94.57165627	13.65170814					
175	H	2.216350567	93.80555731	12.09290405					
176	H	2.48043855	95.55807853	12.32745137					
177	H	1.865027142	99.18248369	9.774785132					
178	H	1.350245034	100.894728	9.804628357					
179	H	0.237482268	99.64405941	9.220702967					
180	H	-0.557194564	95.48301707	22.5455661					
181	H	3.999612992	102.3536074	12.63263729					
182	H	3.981055145	104.0199057	13.26184064					
183	H	3.242180275	102.6852194	14.18071055					
184	H	-5.453999675	87.55490379	20.70653922					
185	H	7.762624662	98.64213719	23.10083371					
186	H	7.321053613	96.91336451	23.21627248					
187	H	7.016150332	97.8516772	21.71386712					
188	H	7.509401088	97.7265463	13.23489339					
189	H	6.732584933	99.32934336	13.30927659					
190	H	5.930814242	97.99829977	12.4516801					
191	H	-2.638035087	96.66805271	13.41055731					
192	H	-4.293743265	96.35440914	12.83360324					
193	H	-3.93576549	97.81915824	13.77236445					
194	H	-5.729524596	95.69497025	16.32154855					

195	H	-6.170672245	95.68028512	14.59446825					
196	H	-5.793831639	97.21792008	15.40807983					
197	H	-0.65127891	95.53670653	10.22853194					
198	H	0.752415848	94.45759773	9.980271695					
199	H	1.000535977	96.19178296	10.33659007					
200	H	-0.091695722	88.75557404	20.62598816					
201	H	-1.310906339	89.94744823	20.11001102					
202	H	-1.508911751	89.08187111	21.65278469					
203	H	-6.402106391	88.57957295	15.33462471					
204	H	-7.830452968	89.08844205	16.28246478					
205	H	-6.385623345	90.12174472	16.23377242					
206	H	-6.658034729	85.59257448	19.18072144					
207	H	-6.855690364	84.42305565	20.49844555					
208	H	-5.999716451	83.94599721	19.0021975					
209	H	-1.367352686	99.23602466	13.85250879					
210	H	-1.715825261	98.91653879	15.42648575					
211	H	-8.626412741	93.25799232	18.40878875					
212	H	-6.854723189	94.64899459	21.532546					
213	H	-2.6842613	101.3459105	20.98084221					
214	H	-1.437036074	101.9216275	22.07254246					
215	O	-3.859825652	99.82938578	20.48739747					
216	H	-3.72446987	98.87401305	20.29011254					
217	H	-3.681388714	100.2880487	19.63539969					

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