Supporting Information for:

Unravelling Unidirectional Threading of α-Cyclodextrin in a [2]Rotaxane Through Spin Labeling Approach

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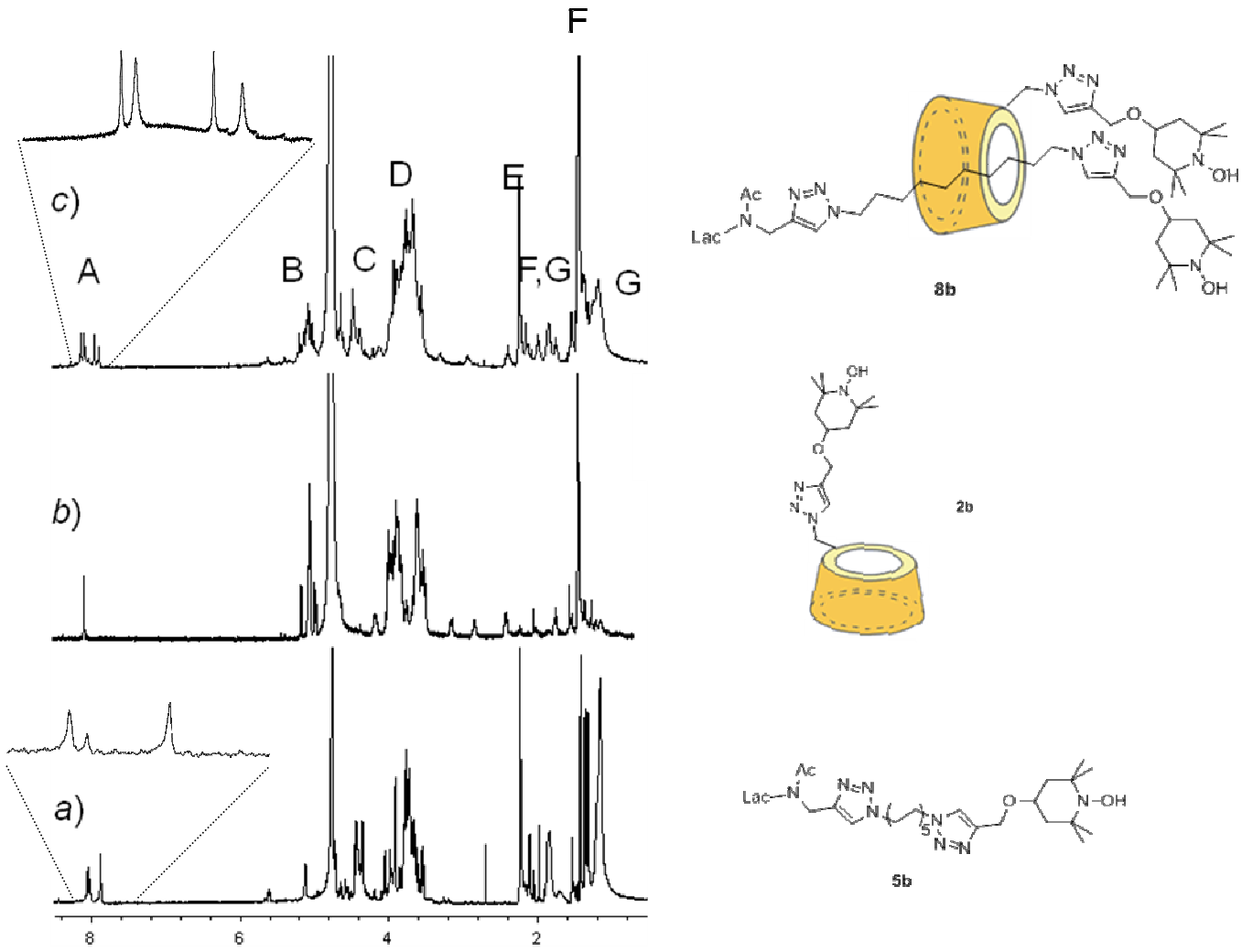

Figure S1. ^{1}H NMR spectra (600 MHz, 298 K, D_2O, 2 mM) of thread **5b** (*a*), host **2b** (*b*) and rotaxanes **8b** (*c*). A: H triazole; B: H1 CD, C*H*$_2$OTEMPOH, H1 Glu; C: H1 Gal, N-C*H*$_2$-triazolyl, C*H*$_2$OTEMPOH and H decane; D: H-2,3,4,5,6 lactosyl moiety and CD; E: CH_3-CO; F: TEMPOH; G: H decane. Signal assignments was achieved by measuring the 2D ROESY spectrum of rotaxanes **8b**.

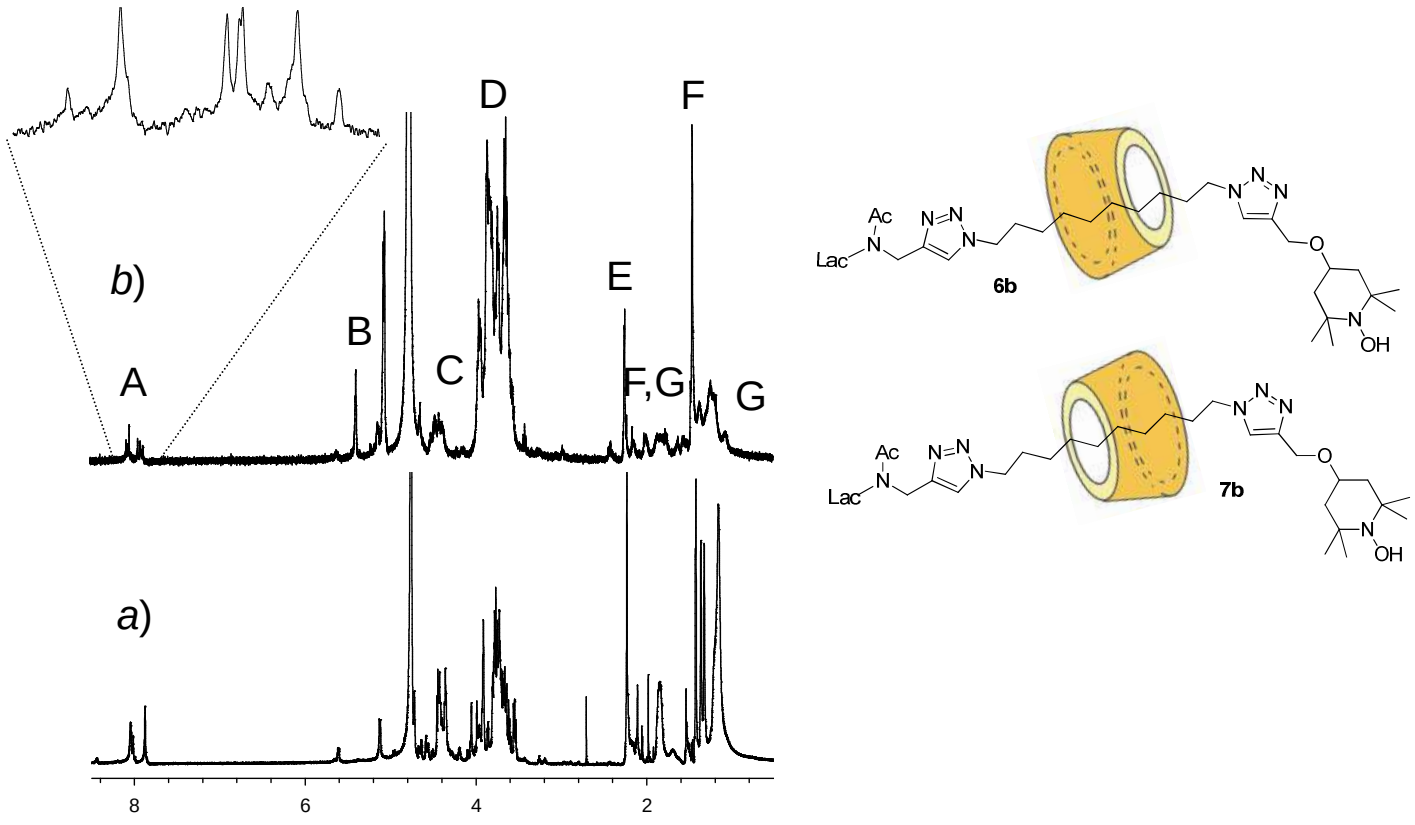

Figure S2. ^{1}H NMR spectra (600 MHz, 298 K, D_2O, 2 mM) of thread **5b** (*a*) and rotaxanes **6b**/**7b** (*b*). A: H triazole; B: H1 CD and Glu; C: C*H*$_2$OTEMPOH, H1 Gal, N-C*H*$_2$-triazolyl and H decane; D: H-2,3,4,5,6 lactosyl moiety and CD; E: CH_3-CO; F: TEMPOH; G: H decane. Signal assignments was achieved by measuring the 2D ROESY spectrum of rotaxanes **6b**/**7b**.

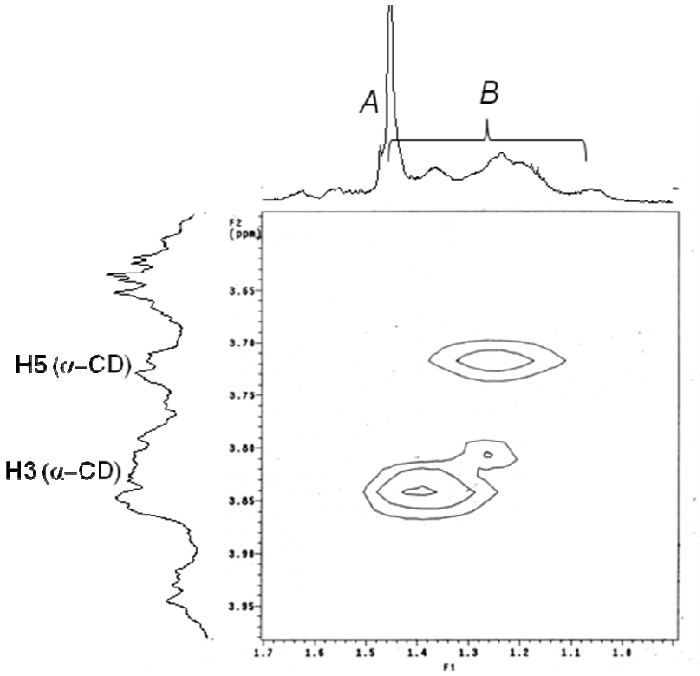

Figure S3. Partial 2D ROESY spectrum (600 MHz, 298 K, D_2O, 1.5 mM) of rotaxanes **6b**/**7b**. (X range from 0.90 to 1.70 ppm, Y range from 3.50 to 3.98 ppm). *A*: TEMPOH; *B*: decyl chain. The cross peaks connect the central part of the decamethylene chain with H3 and H5 protons of α-CD, indicating the encapsulation of the thread into the CD.

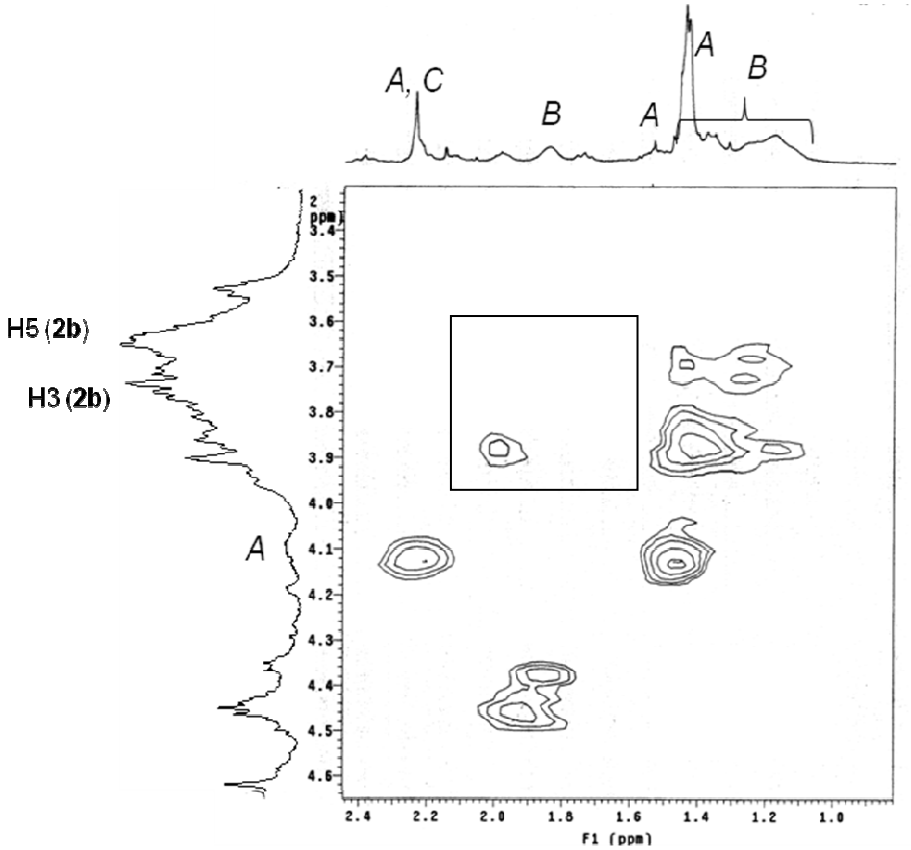

Figure S4. Partial 2D ROESY spectrum (600 MHz, 298 K, D_2O, 1.5 mM) of rotaxane **8b**. (X range from 0.80 to2.40 ppm, Y range from 3.30 to 4.65 ppm). *A*: TEMPOH; *B*: decyl chain; *C*: CH_3CO. The cross peaks in the square connect the central part of the decamethylene chain with H3 and H5 protons of **2b**, indicating the encapsulation of the thread into the CD.

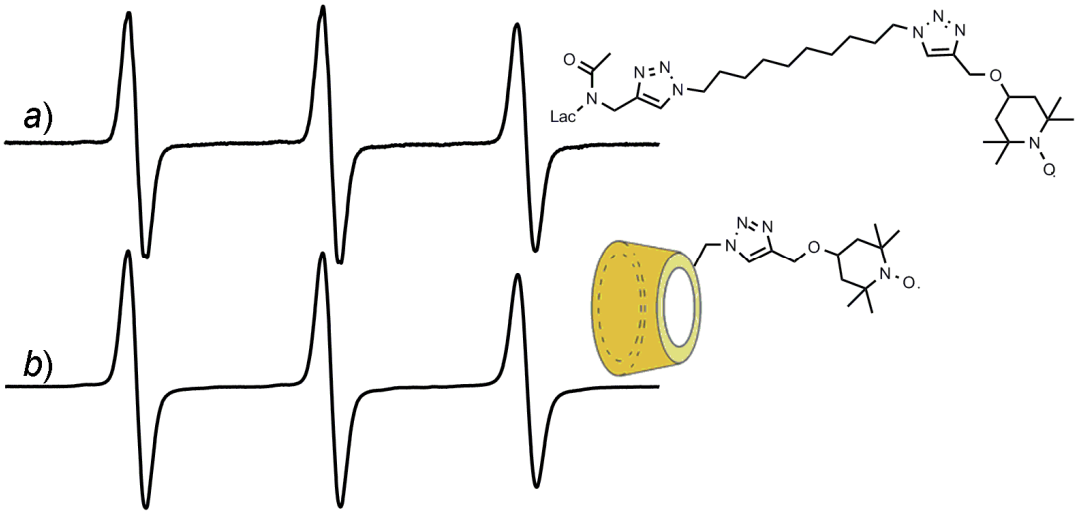

Figure S5. ESR spectra of the thread **5a** and spin-labeled α-CD **2a** (0.05 mM) recorded in water at 328K.

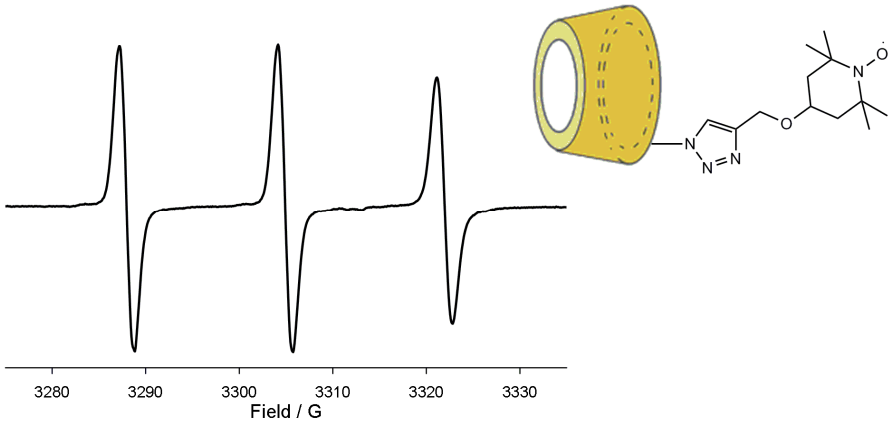

Figure S6. ESR spectra of the spin-labeled α-CD **3a** (0.05 mM) recorded in water at 328K.

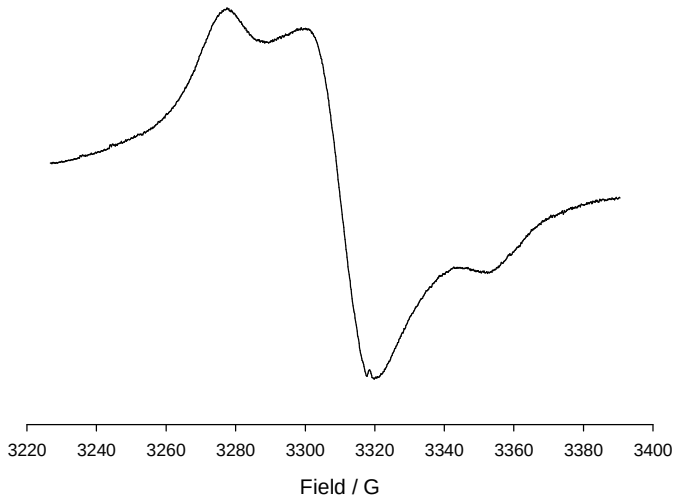

Figure S7. ESR spectrum of rotaxane **8a** at 203 K in H_2O.[S1]

[S1] It should be mentioned that under the reported experimental conditions expulsion of rotaxane radicals from ice could result in shortening of spin-spin distances (see: Bowman, K. H. in *Electron Paramagnetic Resonance: a practitioner's toolkit*; *Brustolon, M.; Giamello, E. Ed.s*, JohnWiley & Sons Inc., Hoboken, 2009; pp 386-388).

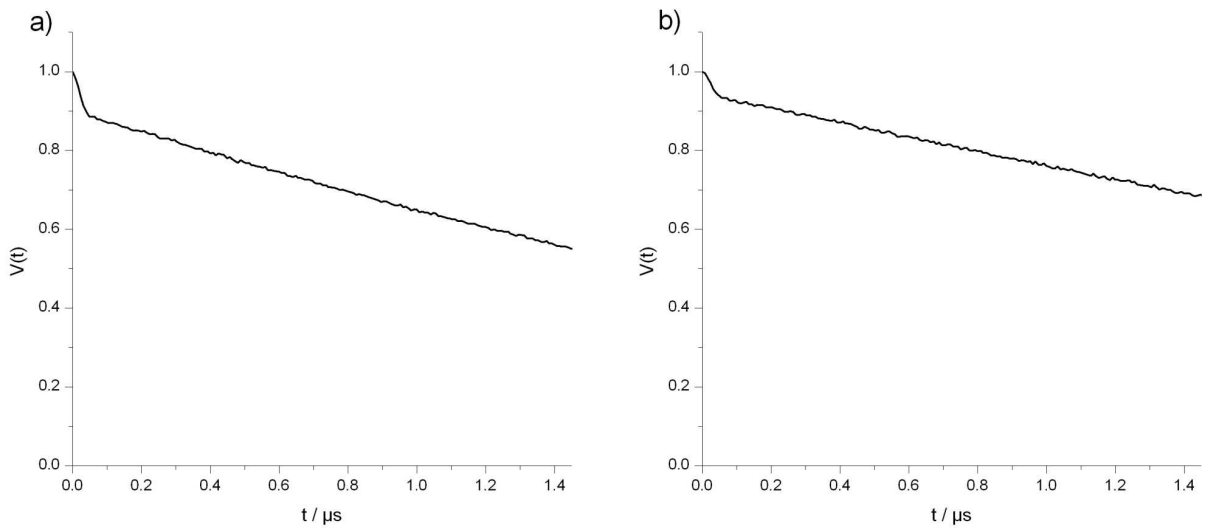

Figure S8. PELDOR signal decay for the frozen glassy solution of bis-labelled rotaxane **8a** in H_2O (10% glycerol) at 40 K. The effect of the mw pulse duration on the oscillation amplitude was investigated recording the data using 12 ns (*a*) or 36 ns (*b*) as pump pulse.[S2-S3] All experiments were carried out using the four-pulse, dead time free, PELDOR sequence given by: $\pi/2(\upsilon_{obs})–t_1–\pi(\upsilon_{obs})–t–\pi(\upsilon_{pump})–(t_1+t_2–t)–\pi(\upsilon_{obs})\ t_2–$echo.[S4] The ELDOR pulse (υ_{pump}, 12 or 36 ns) was positioned at the maxima of the echo-detected nitroxide spectrum, whereas the $\pi/2$ and π observe pulses (υ_{obs}, 16 and 32 ns) were positioned at the low field side of the spectrum ($\upsilon_{obs}–\upsilon_{pump} \approx 75$ MHz). The delay time between the first and second observe pulses was set to 204 ns and varied in 8 ns steps within 8 time intervals to suppress contribution of proton nuclear modulation. The interpulse separation time between the second and third observe pulses was set to 2004 ns. The PELDOR traces were recorded at the temperature of 40 K with an experiment repetition time of 10 ms, a video amplifier bandwidth of 20 MHz and an amplifier gain of 48 dB. The signal was accumulated with 448 data points and a time increment of 4 ns for approximate 5 h. The PELDOR time domain data were analyzed using DeerAnalysis 2011 software package[S5] and fit using Tikhonov regularization method.[S6]

[S2] Milov, A. D.; Naumov, B. D.; Tsvetkov, Yu. D. *Appl. Magn. Reson.* **2004**, *26*, 587-599.
[S3] Milov, A. D.; Grishin, Y. A.; Dzuba, S. A.; Tsvetkov, Y. D. *Appl. Magn. Reson.* **2011**, *41*, 59-67.
[S4] Martin, R. E.; Pannier, M.; Diederich, F.; Gramlich, V.; Hubrich, M.; Spiess, H. W. *Angew. Chem. Int. Ed.* **1998**, *37*, 2833 –2837.
[S5] Jeschke, G.; Chechik, V.; Ionita, P.; Godt, A.; Zimmermann, H.; Banham, J.; Timmel, C. R.; Hilger, D.; Jung, H. *Appl. Magn. Reson.* **2006**, *30*, 473–498.
[S6] Chiang, Y.W.; Borbat, P. P.; Freed J.H. *J. Magn. Reson.* **2005,** *172*, 279–295.

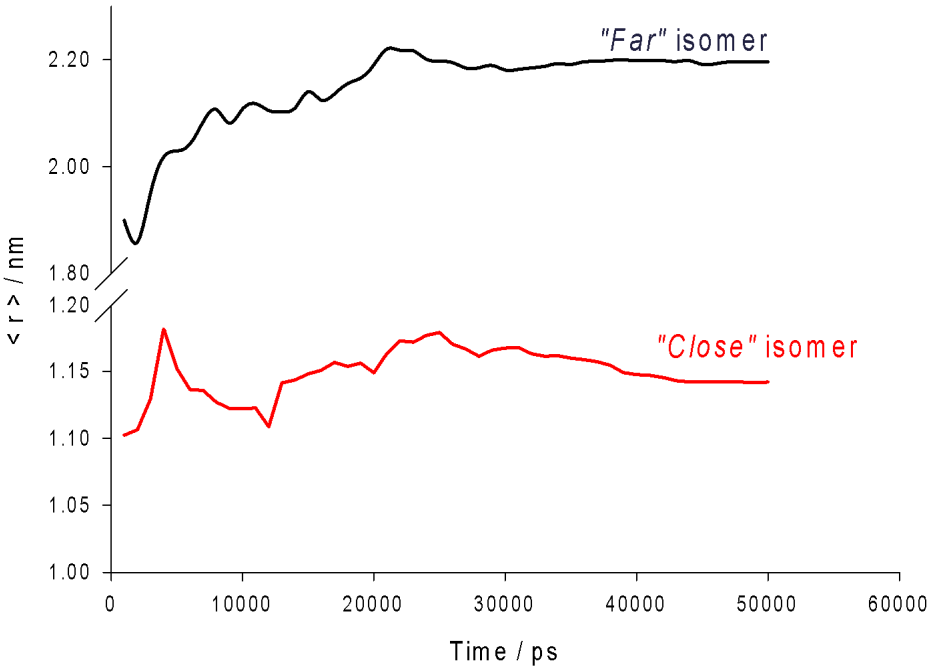

Figure S9. Variation of spin labels mean distance during MD simulation of **8a** and **9a**.

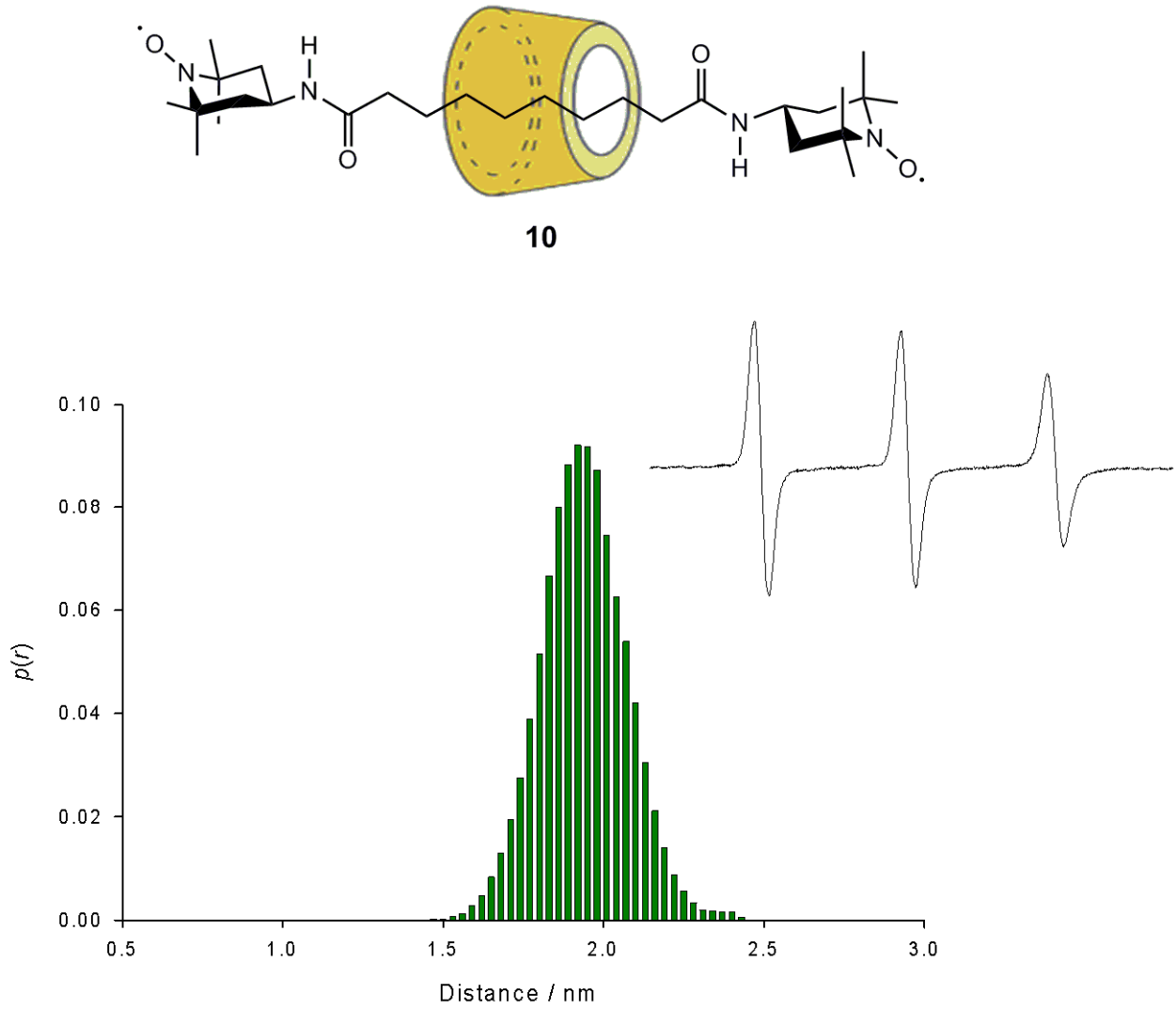

Figure S10. Molecular dynamic determined distance distribution calculated at 328 K in water for rotaxane **10**. Inset: corresponding ESR spectrum at 328K in water (see ref 18).

Absolute energies and coordinates of the atoms in the optimized starting geometry for the MD simulation of 8a carbonyl analogue.

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Total energy:             449.6741 kJ/mol ( 1.031422182e+23 Hartrees )
 Force-field terms:       570.1899 kJ/mol ( 1.307850531e+23 Hartrees )
  Stretch:                 23.4490 kJ/mol ( 5.378521631e+21 Hartrees )
  Bend:                   343.8795 kJ/mol ( 7.887600022e+22 Hartrees )
  Proper torsion:         598.7905 kJ/mol ( 1.373452026e+23 Hartrees )
  Out-of-plane:            48.5918 kJ/mol ( 1.114555194e+22 Hartrees )
  Van der Waals:         -146.0232 kJ/mol (-3.349349396e+22 Hartrees )
  Electrostatic:         -298.4977 kJ/mol (-6.846672934e+22 Hartrees )
 All solvation:          -120.5158 kJ/mol (-2.764283497e+22 Hartrees )
  Solvation Term 1:        38.6160 kJ/mol ( 8.857392269e+21 Hartrees )
  Solvation Term 2:      -159.1317 kJ/mol (-3.650020430e+22 Hartrees )

Atomic      Coordinates
      ------------------------------------------

Atom  Coordinates
Type  X           Y           Z

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H2    15.7893     20.7442     -14.0722
H2    16.4031     17.7284     -14.922
H1    10.9290     18.8506     -11.204
H2    15.5715     17.2991     -4.3462
H2    20.0818     17.4720     -5.5568
H2    10.5977     18.6186     -13.4116
H1    14.1513     14.5678     -12.0482
H2    21.2112     20.4324     -5.8024
H1    11.5719     20.4761     -11.4924
H1    13.3464     18.7127     -11.2275
H1    13.1813     20.0884     -13.9561
H2    11.9902     16.9922     -9.1414
H1    16.2261     18.6232     -2.5745
H1    15.1268     19.8598     -3.2123
H1    16.4602     19.7634     -5.3863
H1    18.4242     18.2782     -3.5625
H1    16.7145     15.7972     -10.9539
H1    18.9007     19.3528     -6.3673
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H2    16.4093     15.7358     -13.2481
H1    15.9377     12.8683     -11.2798
H2    18.1252     13.5312     -11.692
H1    15.6266     18.8863     -12.6093
H1    14.0717     17.8901     -15.0356
H2    13.7390     24.2471     -5.8681
H1    12.0281     22.5622     -8.9957
H2    16.5353     23.1960     -13.9291
H1    13.4371     23.2036     -8.1526
H2    17.4430     24.1400     -11.0329
H1    13.5403     15.9455     -13.6421
O3    15.7406     19.8431     -14.421
O3    15.8695     17.0637     -14.4686
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H1    14.7467     24.6848     -10.5374
H1    16.2420     22.1905     -11.4264
H1    14.5835     24.1535     -13.0737
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O3    16.9357     24.0705     -11.8542
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H1    12.2302     14.9136     -8.9894
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C3	15.9061	13.7366	-9.31
H1	15.9682	25.5088	-8.8919
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H2	20.4198	15.0615	-6.0418
H1	13.9400	14.9910	-7.2131
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O3	17.8467	13.4161	-10.7727
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C2	5.2368	26.0793	-10.5664
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C3	4.8030	28.2618	-9.3799
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H1	4.4588	23.4712	-11.1999
H1	5.8272	24.5763	-12.8177
H1	7.2584	25.5108	-12.3958
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H1	4.3757	27.7085	-8.5425
H1	9.7524	27.9450	-9.6855
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C3	22.9405	9.8124	-11.9967
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H1	25.6562	18.2434	-9.6914
H1	24.6160	17.1696	-10.5955
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H1	27.3507	18.2176	-8.1099
H1	24.4965	12.4393	-9.0995
H1	27.1132	17.8895	-6.3873
H2	21.2555	16.1506	-9.3466
H1	25.8237	18.6749	-7.3048
H2	26.6835	14.4222	-8.4236
H2	26.3379	12.1415	-10.54
H1	22.318	13.6508	-8.8144
H1	24.3342	14.6376	-7.9985
O3	21.8635	7.7171	-11.5254
O3	24.0187	9.5464	-11.0959
C3	19.2018	11.5238	-13.2555
O3	20.6738	8.9515	-13.6335
H1	23.6027	11.7164	-12.6846
H1	3.5697	19.6315	-12.9229
H1	4.3022	20.4771	-11.549
H1	4.2823	18.7124	-11.5926
H1	5.7811	21.8015	-12.9581
H1	6.7152	21.0478	-14.2629
H1	4.9451	21.0919	-14.3479
H1	5.6814	15.2138	-12.7473
H1	4.4945	16.1008	-13.7186
H1	4.8435	16.6081	-12.0619
H1	6.2371	16.1608	-15.4614
H1	7.7745	16.9987	-15.1857
H1	7.4592	15.4401	-14.4009
H1	6.7011	20.3206	-11.1374
H1	7.8119	19.9232	-12.4502
H1	8.4082	17.6549	-12.9618
H1	7.7557	16.2823	-12.0676
H1	6.2588	17.8916	-10.798
H1	8.3689	16.3483	-9.8982
H1	7.3962	17.3703	-8.8156
H1	9.9773	19.7074	-8.6239
H1	11.3676	20.0193	-6.2808
H1	12.4628	18.7199	-5.7873
H1	12.7091	20.1916	-8.4517
H1	13.528	20.7193	-6.9689
O3	19.1635	12.9503	-13.2321
H2	24.5961	10.3239	-11.1003
H1	19.3234	11.1842	-14.2845
H1	18.268	11.1316	-12.8514
H2	19.9496	13.2577	-13.6968
H2	22.7071	7.5372	-11.0916
H2	20.9303	8.0325	-13.4826

Absolute energies and coordinates of the atoms in the optimized starting geometry for the MD simulation of 9a carbonyl analogue.

```
Total energy:              452.4327 kJ/mol ( 1.037749611e+23 Hartrees )
  Force-field terms:       574.7620 kJ/mol ( 1.318337605e+23 Hartrees )
  Stretch:                  23.3127 kJ/mol ( 5.347258358e+21 Hartrees )
  Bend:                    342.7095 kJ/mol ( 7.860763610e+22 Hartrees )
  Proper torsion:          589.1520 kJ/mol ( 1.351344098e+23 Hartrees )
  Out-of-plane:             52.6613 kJ/mol ( 1.207897741e+22 Hartrees )
  Van der Waals:          -139.0793 kJ/mol (-3.190076436e+22 Hartrees )
  Electrostatic:          -293.9942 kJ/mol (-6.743375684e+22 Hartrees )
All solvation:            -122.3293 kJ/mol (-2.805879936e+22 Hartrees )
  Solvation Term 1:         42.0873 kJ/mol ( 9.653607977e+21 Hartrees )
  Solvation Term 2:       -164.4166 kJ/mol (-3.771240734e+22 Hartrees )
```

Atomic Coordinates

Atom Type	Coordinates X	Y	Z
O3	14.2972	24.2402	-5.0628
H2	14.7118	22.4538	-4.3416
H2	14.8670	19.8187	-2.5401
H1	20.0797	21.1728	-6.5326
H2	16.0239	15.7842	-12.1929
H2	11.4977	15.6915	-10.7135
H2	20.3108	21.8096	-4.3961
H1	18.1072	16.6548	-4.2349
H2	9.7713	18.2263	-11.6676
H1	18.9939	22.5444	-6.8069
H1	17.7813	20.3874	-6.4155
H1	17.3907	22.5354	-4.2652
H2	20.5883	18.5981	-6.9583
H1	15.1723	16.3941	-14.2083
H1	16.0158	17.9434	-14.0283
H1	14.6405	18.3517	-11.9351
H1	13.0692	15.9748	-13.0392
H1	15.3958	16.7262	-5.6176
H1	12.2887	17.8565	-10.7717
H1	11.0613	17.6600	-13.5526
H2	15.533	17.4939	-3.4420
H1	16.8127	14.3548	-4.3271
H2	14.4931	14.6261	-4.2004
H1	15.4724	20.3399	-5.1323
H1	17.0476	20.6506	-2.5384
H2	16.4526	23.1324	-13.1621
H1	18.2205	23.4619	-9.7479
H2	13.3851	24.5161	-5.2168
H1	16.7661	23.3602	-10.7366
H2	12.4738	24.2325	-8.2873
H1	18.2031	18.6040	-3.2199
O3	14.9539	21.7458	-3.7280
O3	15.5903	19.2189	-2.7626
H1	15.3698	20.5211	-13.3854
H1	14.9501	25.1999	-8.9855
H1	14.0601	22.8696	-7.2527
H1	15.0817	25.6117	-6.3924
O3	17.0744	24.1491	-7.4838
O3	12.9108	24.5470	-7.4829
O3	16.3000	22.4963	-6.0683

H1	20.1227	16.6993	-5.6372
H1	20.0109	16.5115	-7.3932
H1	17.5418	16.9910	-7.2240
H1	14.8221	21.9871	-14.2349
C3	17.2194	23.8709	-9.8893
H2	10.6817	20.7505	-11.4933
H1	13.6002	12.8462	-9.8867
H1	13.6545	14.1074	-12.0125
H2	17.9034	14.0823	-11.9135
O3	19.6783	18.4031	-6.7116
O3	15.9781	15.0864	-7.4984
O3	19.9307	22.4889	-4.9646
O3	18.6884	20.0816	-4.5644
C3	18.1578	20.967	-5.5722
C3	17.0095	21.8375	-5.0117
C3	15.9548	20.9442	-4.3621
C3	16.6119	20.0376	-3.3289
C3	17.7157	19.2021	-3.9908
C3	19.5647	16.9954	-6.5259
C3	18.0999	16.5432	-6.4034
C3	17.4588	16.9667	-5.0546
C3	16.0887	16.3012	-4.8896
C3	16.1878	14.7955	-5.1053
C3	16.7996	14.5116	-6.4785
H1	13.8126	25.030	-10.8806
H2	13.8929	14.2175	-6.6930
O3	18.0961	15.1096	-6.5571
O3	17.1752	18.3766	-5.0314
H2	11.7418	13.9811	-8.9420
H1	18.2067	14.7521	-9.1836
O3	16.5680	22.1757	-13.1558
C3	15.2720	21.6034	-13.3187
O3	15.5565	16.5377	-3.5840
O3	14.8682	14.2589	-5.0106
H1	17.6803	13.2167	-9.9095
H2	10.5966	23.6262	-10.0526
H1	14.8619	21.5265	-11.2230
H1	16.1695	15.8644	-9.9419
H1	12.5683	21.8411	-13.2292
O3	14.4916	23.4196	-11.9743
O3	10.7195	21.7087	-11.3588
C3	12.0527	17.2984	-11.6796
C3	11.4223	18.2392	-12.7016
O3	11.4654	24.0363	-9.9592
O3	16.4136	16.5827	-12.5670
H1	12.404	21.6250	-10.1995
O3	18.1989	14.7017	-11.2355
O3	13.6008	18.6000	-13.7198
H1	11.8528	24.0325	-11.9882
C3	14.4184	21.9858	-12.1057
C3	12.9604	21.5039	-12.2687
C3	12.4504	19.2616	-13.1901
H1	16.3445	22.5162	-8.5173
C3	12.0887	22.0640	-11.1461
O3	13.9303	15.9819	-11.1111
O3	14.1956	23.3555	-9.6806
H1	16.9853	24.3752	-5.4379
O3	11.0996	16.2857	-11.3625
H1	11.9946	19.8555	-13.9836
C3	12.2357	23.5807	-11.072
O3	12.0169	14.1534	-9.8518
C3	16.3904	23.5980	-8.6273

C3	14.9465	24.1367	-8.7440
C3	13.7143	23.9436	-10.8922
O3	10.3232	18.9085	-12.0801
O3	12.8738	20.0837	-12.0999
O3	15.4909	14.2872	-11.0942
H1	16.9026	13.4329	-6.6036
O3	13.4033	13.9265	-7.4753
C3	17.6305	14.303	-9.991
C3	16.1744	14.7767	-9.9179
C3	14.2037	23.9375	-7.4231
C3	15.0048	24.5305	-6.2685
C3	15.5224	14.2934	-8.6018
H1	15.7133	13.2283	-8.4638
C3	15.4927	17.1510	-13.4918
C3	14.2777	17.7545	-12.7716
H1	13.8108	15.5991	-8.5914
C3	13.3308	16.6576	-12.2298
C3	14.0138	14.5277	-8.6203
C3	13.4225	13.9226	-9.8848
C3	16.4080	23.9128	-6.2397
C3	19.3315	21.8174	-6.0709
C3	14.0831	14.5566	-11.1156
N2	17.3156	25.2994	-10.1591
C2	18.2961	26.1201	-9.6249
C2	18.1972	27.2941	-10.3505
N2	17.1663	27.0742	-11.3022
N2	16.7377	25.8748	-11.146
C3	18.9971	28.5767	-10.256
O3	20.3943	28.3099	-10.2376
C3	20.9323	27.9327	-11.4971
C3	22.1826	27.0698	-11.3063
C3	23.3929	27.7976	-10.6886
C2	23.6264	29.1817	-11.3176
C3	22.4373	30.017	-11.8218
C3	21.2976	29.1378	-12.3716
O2	24.7637	29.6259	-11.4065
C3	23.2672	27.9105	-9.1588
C3	24.6136	26.8921	-10.9384
C3	21.9359	30.9707	-10.7229
C3	22.8847	30.922	-12.9851
H1	19.0071	25.8992	-8.8403
H1	20.2127	27.3208	-12.0443
H1	21.1023	31.5675	-11.0938
H1	25.501	27.303	-10.4553
H1	24.1808	28.3396	-8.7459
H1	22.4371	28.551	-8.8726
H1	23.1143	26.9244	-8.7195
H1	23.3109	30.3185	-13.7875
H1	18.7299	29.2456	-11.0743
H1	21.9262	26.2008	-10.6989
H1	22.7415	31.6422	-10.4238
H1	24.8081	26.8113	-12.0087
H1	22.4684	26.7080	-12.2952
H1	22.0335	31.4789	-13.3781
H1	20.4146	29.7512	-12.5498
H1	18.7309	29.0631	-9.3173
H1	21.6135	28.7370	-13.336
H1	23.6397	31.6337	-12.6484
H1	21.6082	30.4265	-9.8412
H1	24.4304	25.8944	-10.5379
H1	20.2461	9.2373	-11.9789
H1	22.3849	9.9852	-11.0751

O3	22.8747	12.6163	-11.7721
O3	23.3142	16.0943	-10.63
C3	24.7268	16.123	-10.4075
O3	26.8386	15.266	-11.3103
C3	24.886	13.9159	-11.5713
C3	26.6095	19.3324	-9.4705
O2	5.8115	17.1177	-15.7509
C3	7.7592	15.2283	-15.1761
O3	21.4091	12.0489	-13.492
N2	10.2522	16.011	-8.15
C3	23.2781	10.5252	-12.9648
C3	23.3681	13.9608	-11.7818
C3	22.7682	11.9704	-13.0449
H1	23.3356	10.1307	-13.9804
C2	6.1332	17.0619	-14.5715
C3	21.2508	14.9332	-10.7502
C3	25.4412	15.3421	-11.5266
O3	20.8418	15.8870	-9.7881
O2	26.9579	17.0037	-9.1002
C3	4.3643	17.9187	-12.9724
C3	5.5928	19.5201	-14.382
C3	5.9667	14.7457	-13.5574
C3	6.8000	18.4244	-12.5237
C3	6.9205	15.8498	-14.0448
O3	8.2310	17.4787	-10.8737
C3	20.9163	9.7847	-12.6431
C3	20.5091	11.2692	-12.6827
C3	7.2625	17.1289	-11.8526
C3	7.9012	16.2401	-12.9259
H1	20.5111	11.6610	-11.6645
C3	22.3448	9.6613	-12.1162
C3	22.7655	14.7724	-10.625
H1	23.1361	14.4584	-12.7253
O3	25.5387	13.1865	-12.5977
C3	5.7362	18.1956	-13.611
C3	8.3566	16.5081	-9.8403
C2	9.8287	18.1863	-8.4471
N2	10.8557	17.9467	-7.5486
C3	12.4646	19.7908	-7.4453
C3	13.7067	18.9523	-7.7656
C3	14.6655	19.7322	-8.6680
C3	11.4218	18.9699	-6.6800
C2	9.4315	16.9275	-8.8610
C3	16.8722	19.5718	-9.9057
C3	18.1492	18.7392	-10.0688
C3	19.4652	20.6798	-11.1588
C3	20.2822	21.0191	-9.9026
N2	22.6829	18.5589	-9.1816
C3	19.0154	19.2125	-11.2438
C3	15.9566	18.9343	-8.8569
N2	21.6377	19.2632	-8.9342
N2	21.4771	20.1907	-9.8050
C2	22.4434	20.1097	-10.7954
C2	26.2502	17.8579	-9.6321
C3	24.4204	18.4892	-11.1565
N2	25.1855	17.5131	-10.3733
C2	23.2329	19.0489	-10.3962
N2	11.0274	16.6887	-7.3834
H1	14.2083	18.6897	-6.8334
H1	13.4144	18.0376	-8.2813
H1	14.1868	19.8890	-9.6338
H1	14.8957	20.6957	-8.2152

H1	16.4793	18.8868	-7.9024
H1	15.6992	17.9259	-9.1757
H1	16.3525	19.6175	-10.8621
H1	17.1279	20.5803	-9.5860
H1	18.7258	18.7671	-9.1460
H1	17.8728	17.7022	-10.2626
H1	19.8938	18.5689	-11.3049
H1	18.4446	19.0854	-12.1647
H1	20.0645	20.9025	-12.0421
H1	18.5898	21.3272	-11.193
H1	20.5843	22.0660	-9.9540
H1	19.6629	20.8899	-9.0150
H1	22.5425	20.7017	-11.695
H1	25.0507	19.3184	-11.476
H1	24.0490	18.0195	-12.068
H1	20.9961	15.2968	-11.7465
H1	20.7561	13.9783	-10.5721
H1	25.2571	15.8371	-12.4815
H1	27.0644	19.7073	-10.3875
H1	25.1025	13.4296	-10.6182
H1	27.3279	19.4416	-8.6576
H2	21.4769	16.6146	-9.8277
H1	25.7248	19.9201	-9.2260
H2	27.0544	15.8921	-10.6041
H2	26.4764	13.4113	-12.5255
H1	22.9884	14.2852	-9.6650
H1	24.9230	15.6406	-9.4471
O3	22.7767	8.3015	-12.2106
O3	24.5871	10.4900	-12.3908
C3	19.0908	11.4366	-13.2414
O3	20.8765	9.1752	-13.9336
H1	23.3743	12.4869	-13.7908
H1	3.6188	17.7687	-13.7543
H1	4.0590	18.7659	-12.3575
H1	4.3877	17.0314	-12.3447
H1	5.3663	20.3348	-13.6935
H1	6.5217	19.7508	-14.9052
H1	4.7878	19.4491	-15.1145
H1	6.5337	13.8596	-13.2704
H1	5.2782	14.4747	-14.3588
H1	5.3852	15.0720	-12.6987
H1	7.1101	14.8476	-15.9657
H1	8.4256	15.9788	-15.6033
H1	8.3602	14.4035	-14.7917
H1	6.4025	19.0982	-11.7634
H1	7.6694	18.9027	-12.9769
H1	8.7339	16.7891	-13.3659
H1	8.2997	15.3322	-12.4741
H1	6.4128	16.6357	-11.3811
H1	8.6244	15.5338	-10.2486
H1	7.4170	16.4182	-9.2934
H1	9.4049	19.1338	-8.7501
H1	10.6254	19.6350	-6.3423
H1	11.8851	18.5133	-5.8037
H1	12.0184	20.1618	-8.3678
H1	12.7613	20.6424	-6.8319
O3	18.7512	12.8224	-13.2318
H2	25.0082	11.3405	-12.5823
H1	19.0360	11.0644	-14.2648
H1	18.3814	10.8902	-12.6192
H2	19.3480	13.2580	-13.8506
H2	23.7235	8.3029	-12.0213

H2	21.3358	8.3299	-13.8445