

Supporting Information

Conformational analysis of a model synthetic prodiginine

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Single crystal X-Ray crystallography.

Crystallographic data are presented in Tables S1. Single crystals of **1.HCl** or **1.MeSO₃H** were coated in **high-vacuum grease** and mounted on a glass fibre. X-ray measurements were made using a Bruker SMART CCD area-detector diffractometer with Mo-K α radiation ($\lambda = 0.71073$ Å).ⁱ Intensities were integratedⁱⁱ from several series of exposures, each exposure covering 0.3° in ω , and the total data set being a **hemisphere**. Absorption corrections were applied, based on multiple and symmetry-equivalent measurements.ⁱⁱⁱ The structure was solved by **direct methods** and refined by least squares on weighted F² values for all reflections (see Table S1).^{iv} All non-hydrogen atoms were assigned anisotropic displacement parameters and refined without positional constraints. All other hydrogen atoms were constrained to ideal geometries and refined with fixed isotropic displacement parameters. Refinement proceeded smoothly to give the residuals shown in Table S1. Complex neutral-atom scattering factors were used.^v

Table S1: selected crystal data for **1.HCl** and **1.MeSO₃H**.

Compound reference	1.HCl	1.MeSO₃H
Empirical formula	C18 H22 Cl N3 O	C38 H50 N6 O8 S2
Formula weight	331.84	782.96
Temperature	298(2) K	298(2) K
Wavelength	0.71073 Å	0.71073 Å
Crystal system	Monoclinic	Triclinic
Space group	P2(1)/n	P-1
Unit cell dimensions	a = 10.1195(11) Å $\alpha = 90^\circ$ b = 12.7149(13) Å $\beta = 92.809(2)^\circ$ c = 13.6180(14) Å $\gamma = 90^\circ$	a = 9.5644(9) Å $\alpha = 83.838(2)^\circ$ b = 10.5005(10) Å $\beta = 86.955(2)^\circ$ c = 19.7780(19) Å $\gamma = 89.422(2)^\circ$
Volume	1750.1(3) Å ³	1972.0(3) Å ³
Z	4	2
Density (calculated)	1.259 Mg/m ³	1.319 Mg/m ³
Absorption coefficient	0.226 mm ⁻¹	0.194 mm ⁻¹
F(000)	704	832
Crystal size	0.20 x 0.20 x 0.20 mm	0.70 x 0.10 x 0.10 mm
θ range for data collection	2.19 to 25.00°	1.04 to 25.00°
Index ranges	-12 ≤ h ≤ 12, -15 ≤ k ≤ 15, -16 ≤ l ≤ 16	-11 ≤ h ≤ 11, -12 ≤ k ≤ 12, -23 ≤ l ≤ 23
Reflections collected	16619	19585
Independent reflections	3087 [R _{int} = 0.0394]	6936 [R _{int} = 0.0643]
Completeness to $\theta = 25.00^\circ$	100.0 %	99.7 %
Absorption correction	None	None
Refinement method	Full-matrix least-squares on F ²	Full-matrix least-squares on F ²
Data / restraints / parameters	3087 / 0 / 212	6936 / 0 / 497

Goodness-of-fit on F^2	$S = 0.978$	$S = 0.975$
R indices [for reflections with $I > 2\sigma(I)$]	$R_1 = 0.0411, wR_2 = 0.1042$	$R_1 = 0.0644, wR_2 = 0.1461$
R indices (for all data)	$R_1 = 0.0639, wR_2 = 0.1113$	$R_1 = 0.1151, wR_2 = 0.1728$
Weighting scheme	$w^{-1} = \sigma^2(F_o^2) + (aP)^2 + (bP)$, where $P = [\max(F_o^2, 0) + 2F_c^2]/3$ $a = 0.061100, b = 0.0000$	$w^{-1} = \sigma^2(F_o^2) + (aP)^2 + (bP)$, where $P = [\max(F_o^2, 0) + 2F_c^2]/3$ $a = 0.076200, b = 0.0000$
Largest diff. peak and hole	0.176 and -0.167 $e\text{\AA}^{-3}$	0.407 and -0.307 $e\text{\AA}^{-3}$

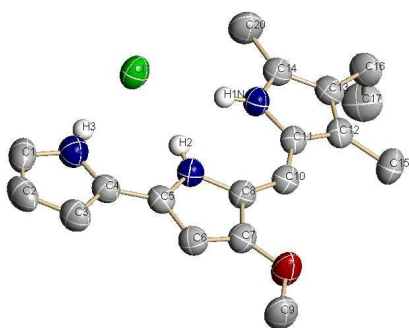


Figure S1: ORTEP diagram (35 % probability level) of the molecular structure of **1.HCl**.

Table S1. Hydrogen bonds [$\text{\AA}$ and $^\circ$] for **1.HCl**.

D-H...A	d(D-H)	d(H...A)	d(D...A)	$\angle(\text{DHA})$
N(3)-H(3)...Cl(1)#1	0.86	2.40	3.2313(19)	164.1
N(2)-H(2)...Cl(1)#1	0.86	2.33	3.1834(17)	169.7
N(1)-H(1N)...Cl(1)#1	0.86	2.35	3.1876(18)	166.0

Symmetry transformations used to generate equivalent atoms: #1 $x+1, y, z$

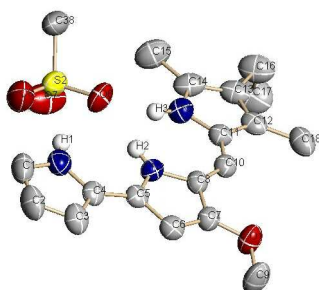


Figure S2. ORTEP diagram (35 % probability level) of the molecular structure of **1.MeSO₃H**.

Table S2. Hydrogen bonds [$\text{\AA}$ and $^\circ$] for **1**.MeSO₃H.

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1)...O(8)	0.86	2.18	2.916(4)	143.4
N(1)-H(1)...O(6)	0.86	2.48	3.288(4)	155.8
N(1)-H(1)...S(2)	0.86	2.82	3.674(3)	171.3
N(2)-H(2)...O(6)	0.86	1.97	2.823(4)	175.3
N(3)-H(3)...O(6)	0.86	2.02	2.856(4)	165.1
N(4)-H(4)...O(5)#1	0.86	2.18	2.907(4)	142.1
N(4)-H(4)...O(4)#1	0.86	2.46	3.266(4)	156.5
N(4)-H(4)...S(1)#1	0.86	2.80	3.654(3)	171.4
N(5)-H(5)...O(4)#1	0.86	1.94	2.798(4)	172.3
N(6)-H(6)...O(4)#1	0.86	1.99	2.839(4)	170.2

Symmetry transformations used to generate equivalent atoms: #1 x,y-1,z

NMR Studies.

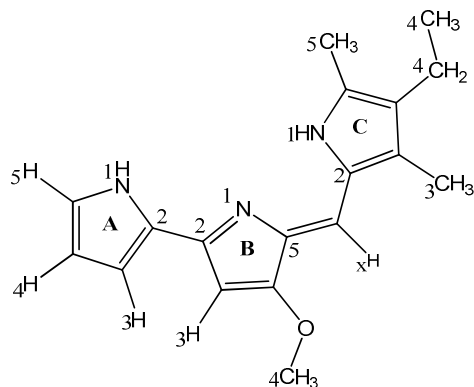


Figure S3. Structure of compound **1** showing the atom numbering scheme.

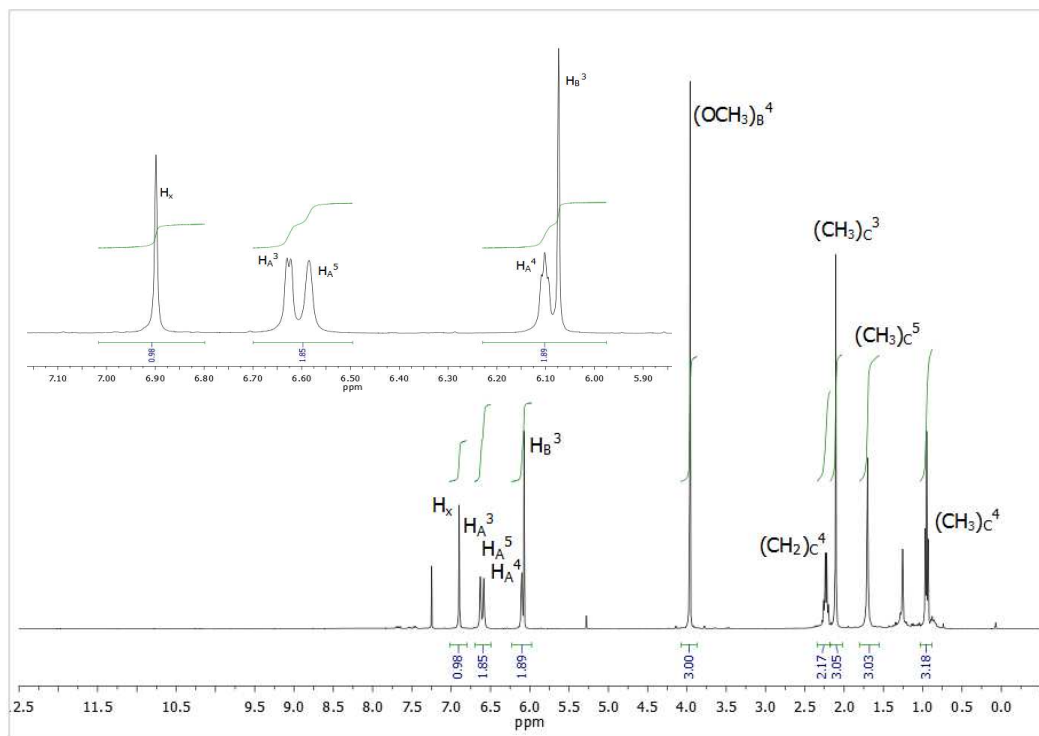


Figure S4. ¹H NMR (CDCl₃, 400 MHz), 25°C of **1**.

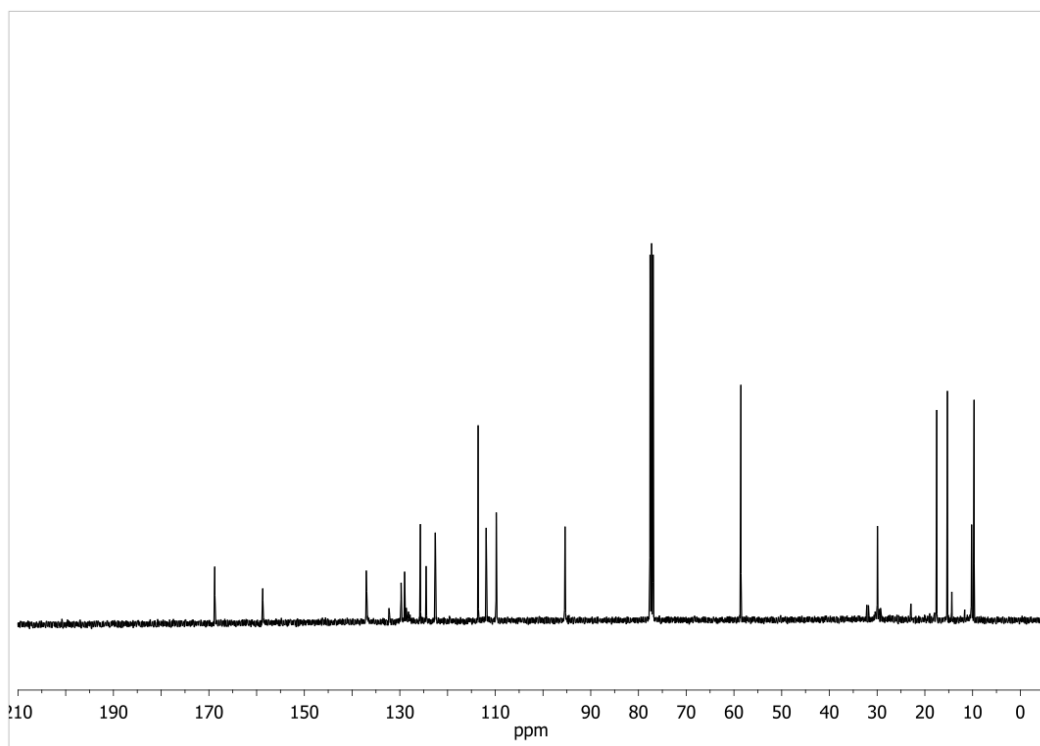


Figure S5. ^{13}C NMR (CDCl_3 , 100 MHz), 25°C of **1**.

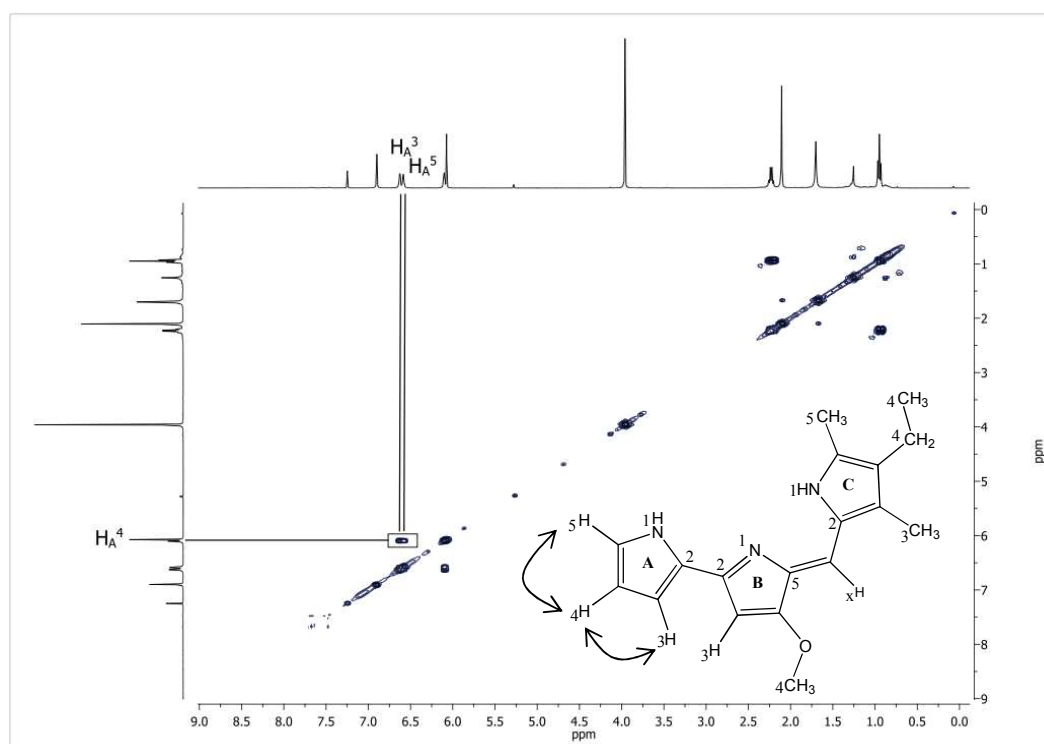


Figure S6. COSY (CDCl_3), 25°C of **1**.

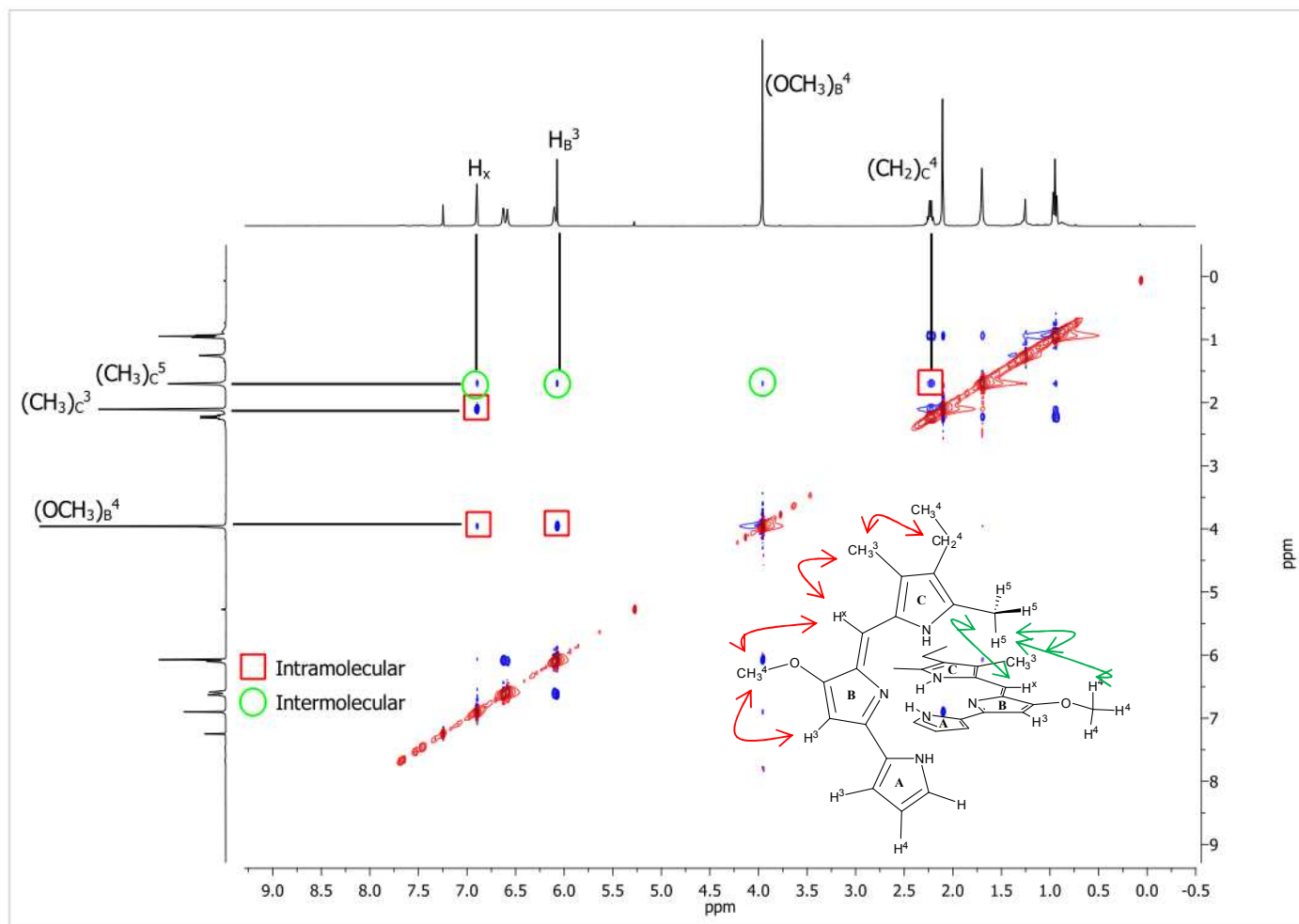


Figure S7. NOESY (CDCl_3), 25°C of **1**.

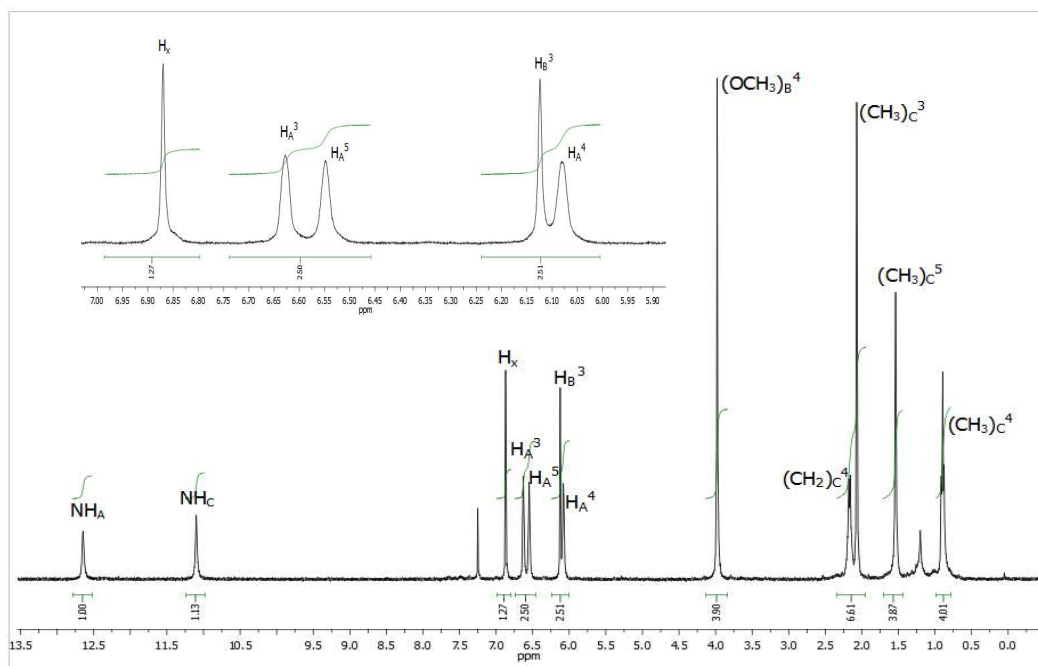


Figure S8. ^1H NMR (CDCl_3 , 400 MHz). -50°C of **1**.

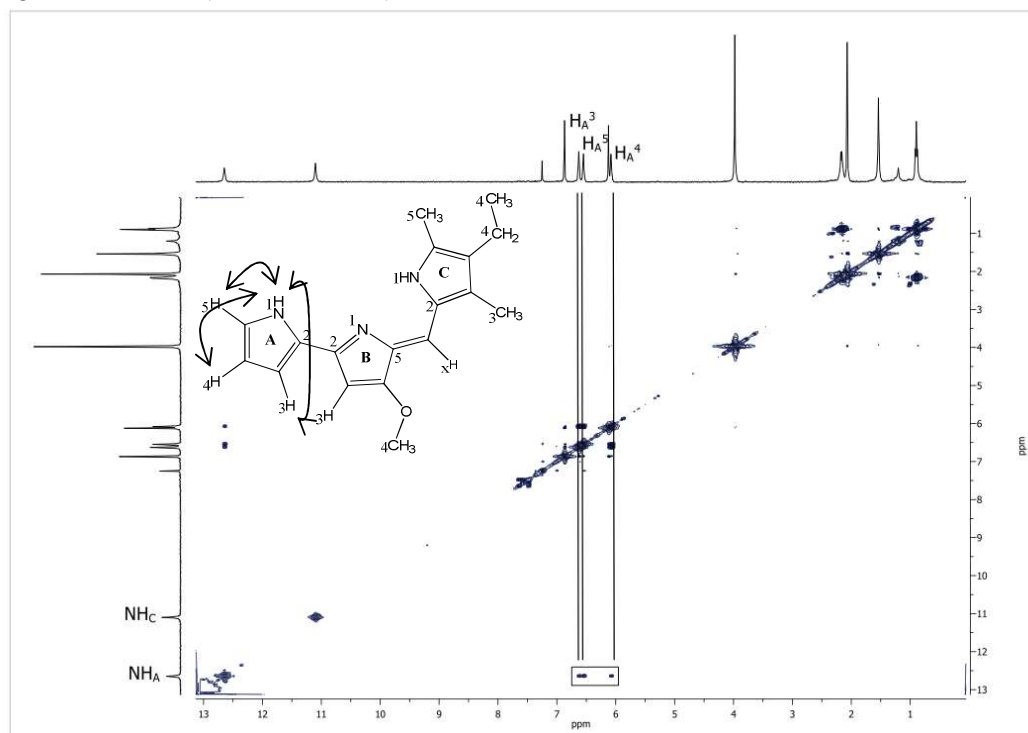


Figure S9. COSY (CDCl_3), -50°C of **1**.

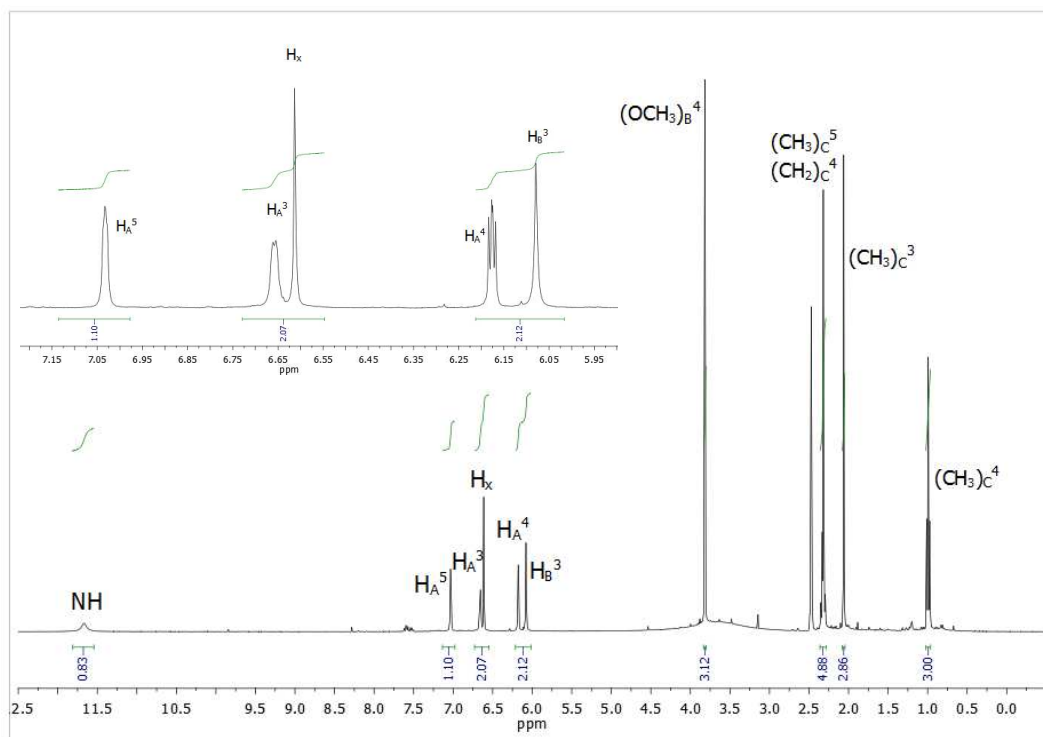


Figure S10. ^1H NMR (DMSO- d_6 , 400 MHz) of **1**.

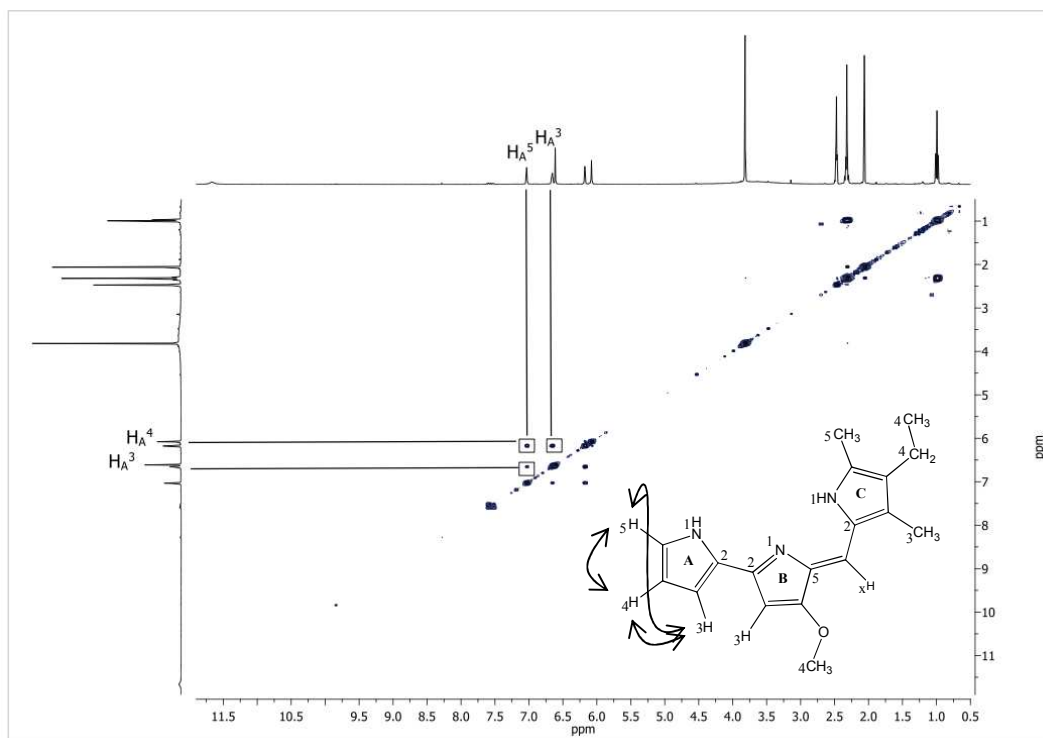


Figure S11. COSY (DMSO- d_6) of **1**.

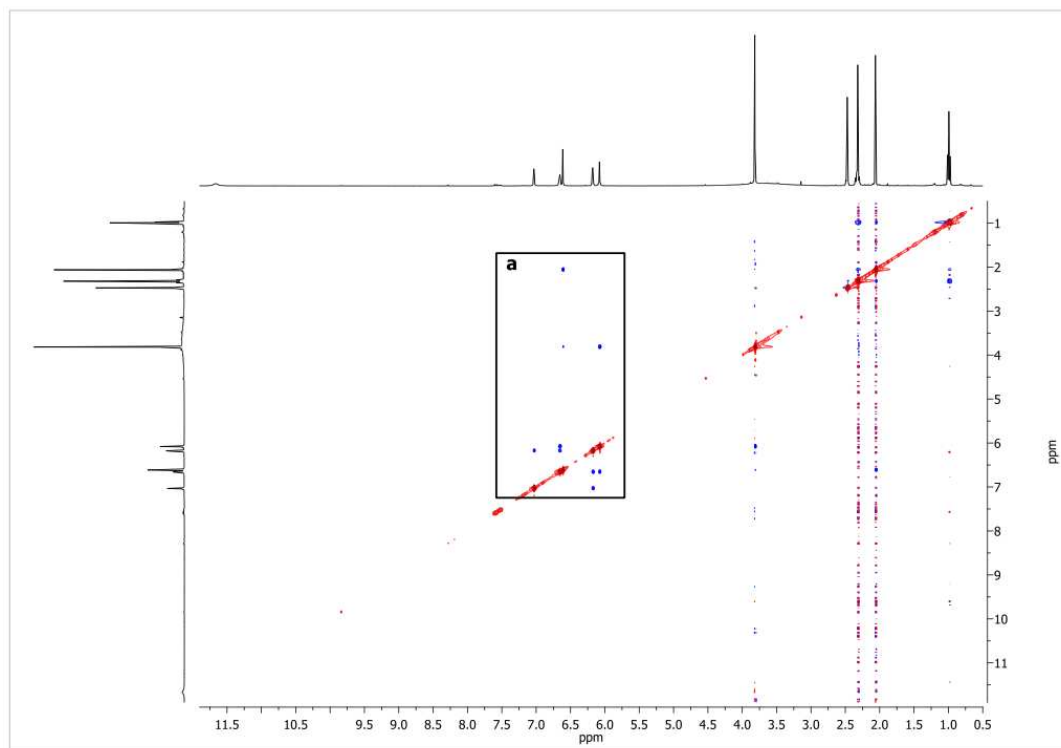


Figure S12. NOESY (DMSO- d_6) of **1**.

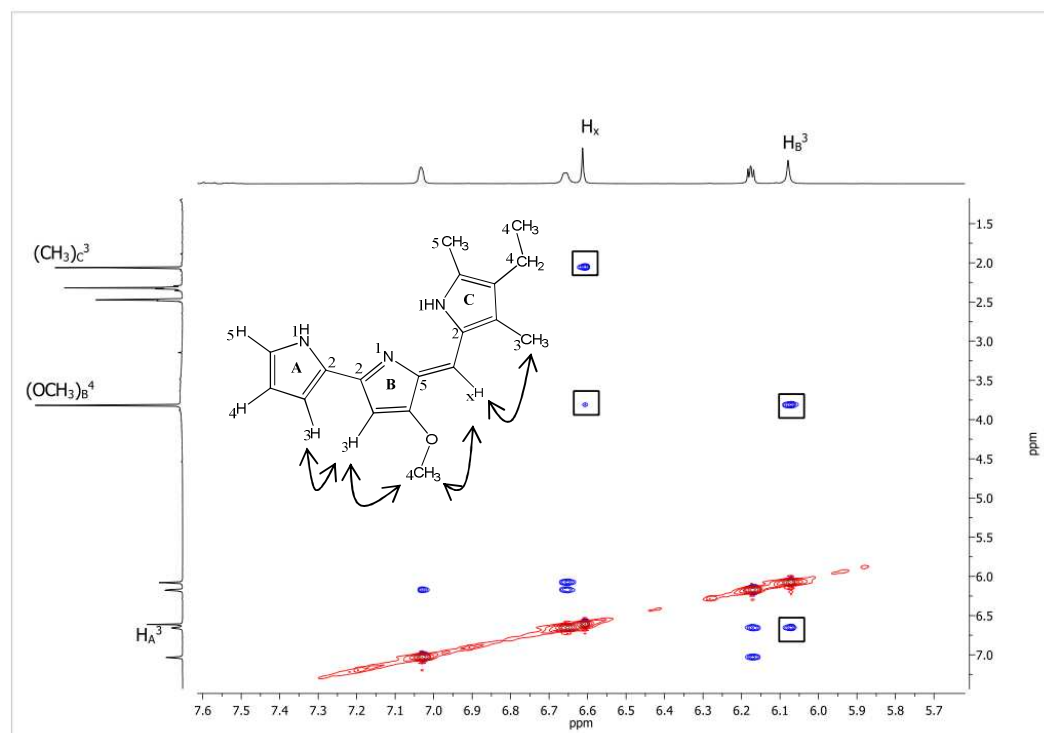


Figure S13. NOESY (DMSO- d_6). Region (a) of **1**.

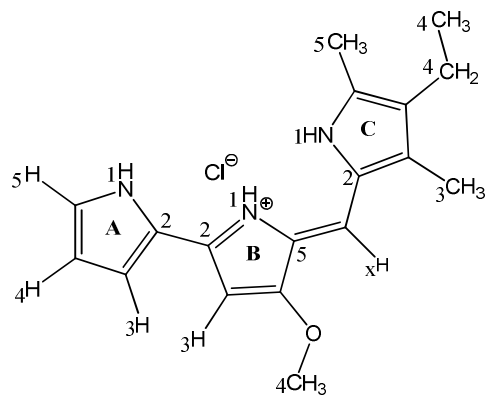


Figure S14. Structure of compound **1.HCl** showing the atom numbering scheme.

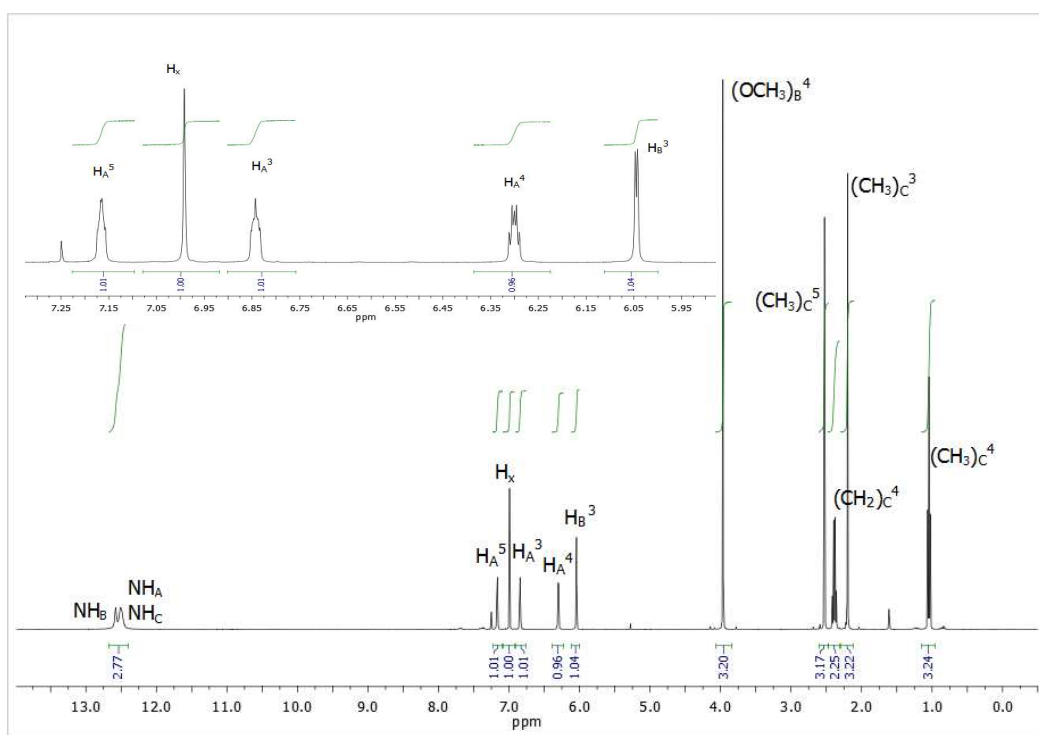


Figure S15. ¹H NMR (CDCl₃, 400 MHz) of **1.HCl**

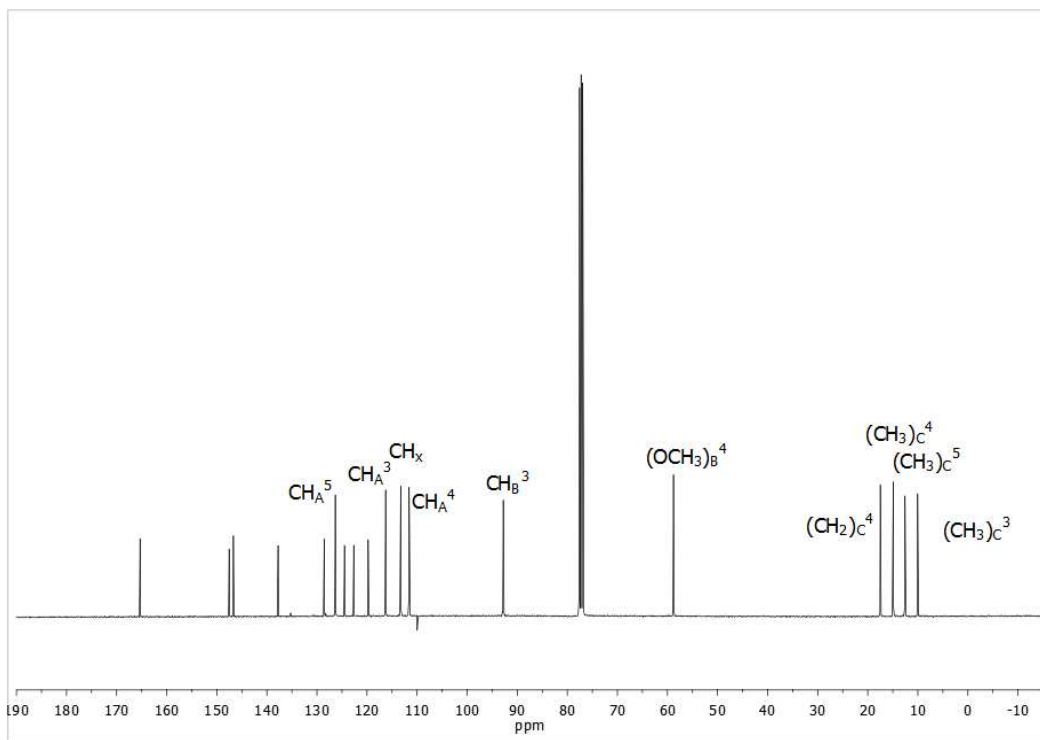


Figure S16. ^{13}C NMR (CDCl_3 , 100 MHz) of **1.HCl**

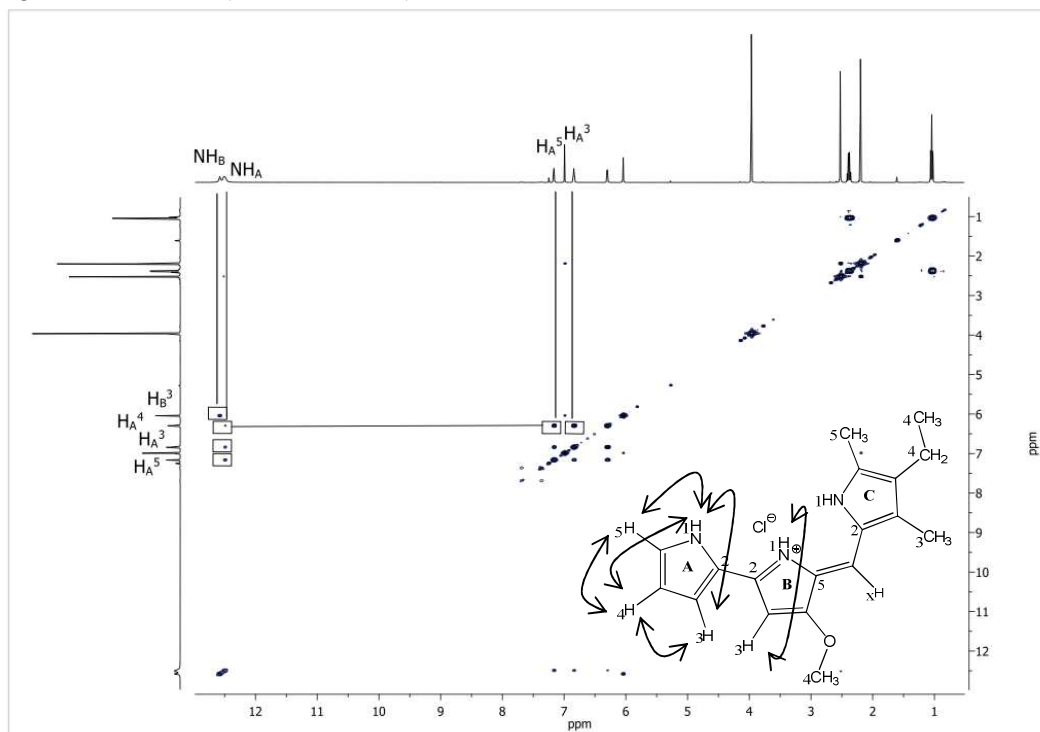


Figure S17. COSY (CDCl_3) of **1.HCl**

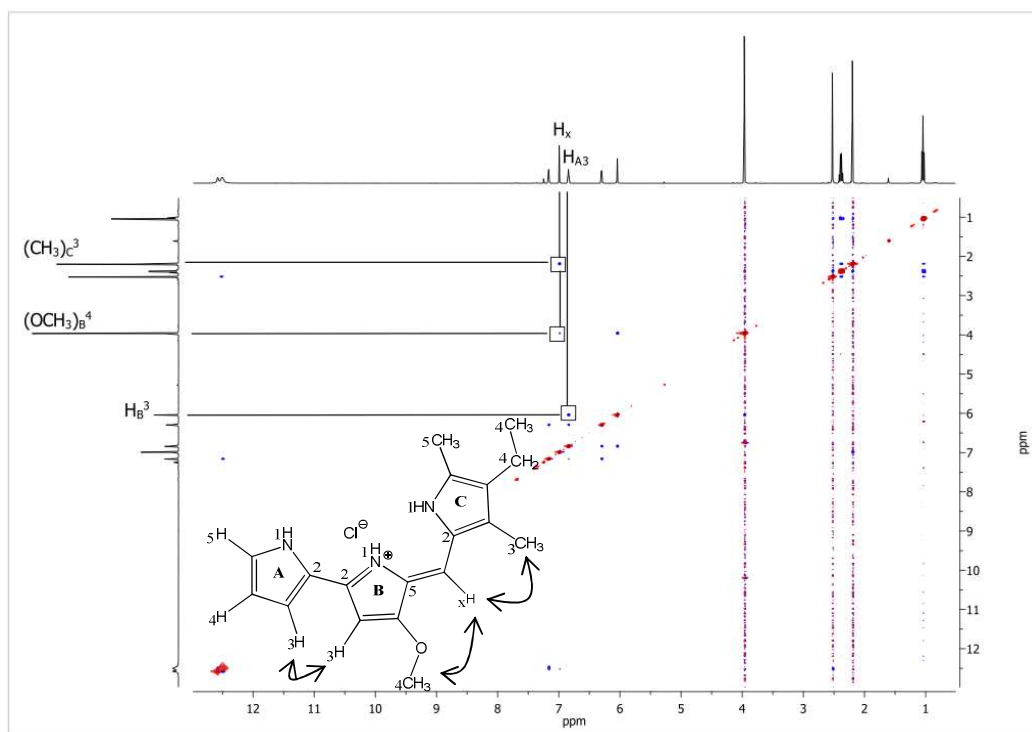


Figure S18. NOESY (CDCl₃) of **1.HCl**

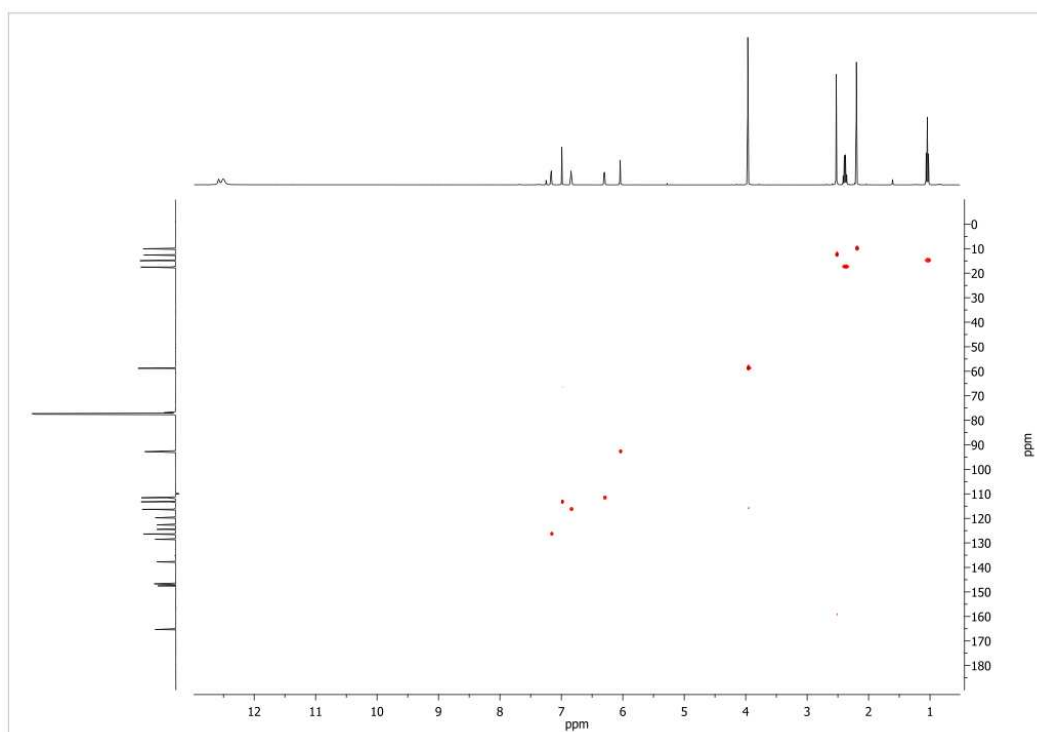


Figure S19. HMQC (CDCl₃) of **1.HCl**

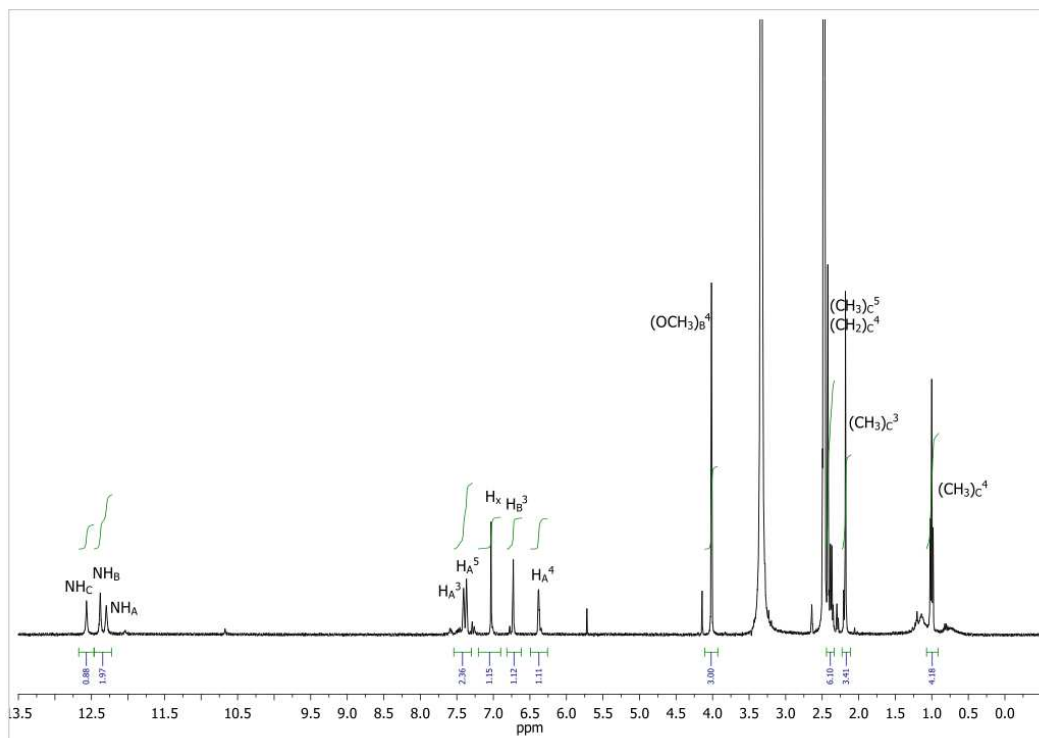


Figure S20. ^1H NMR (DMSO- d_6 , 400 MHz) of **1.HCl**

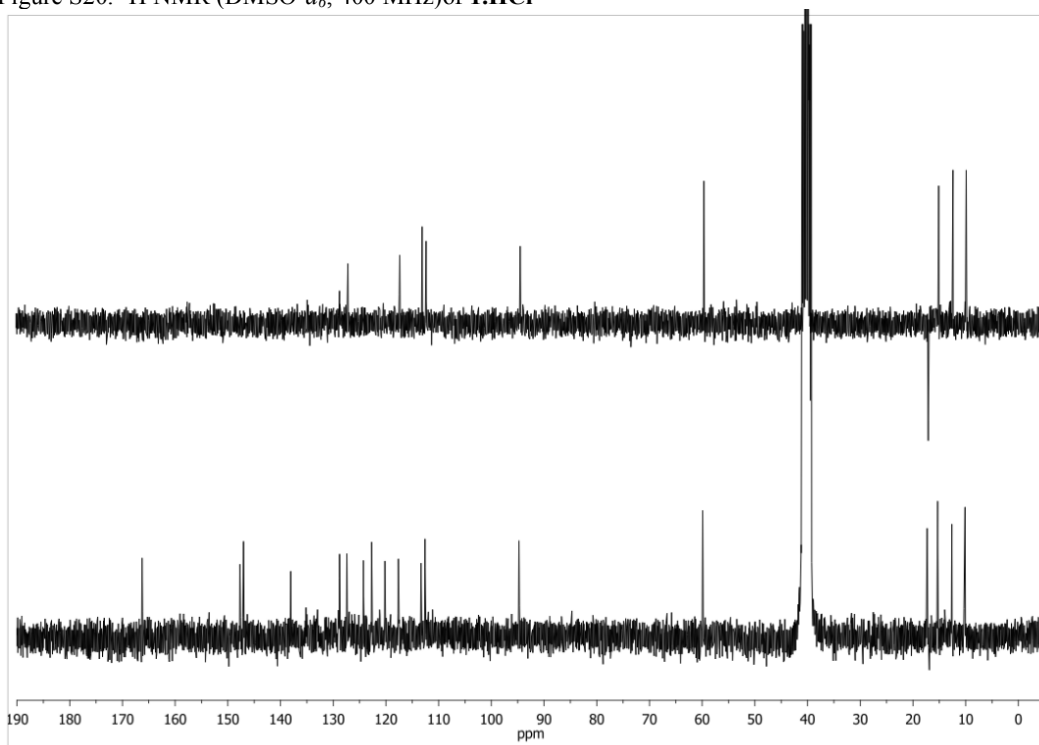


Figure S21. ^{13}C NMR (DMSO- d_6 , 100 MHz) of **1.HCl**

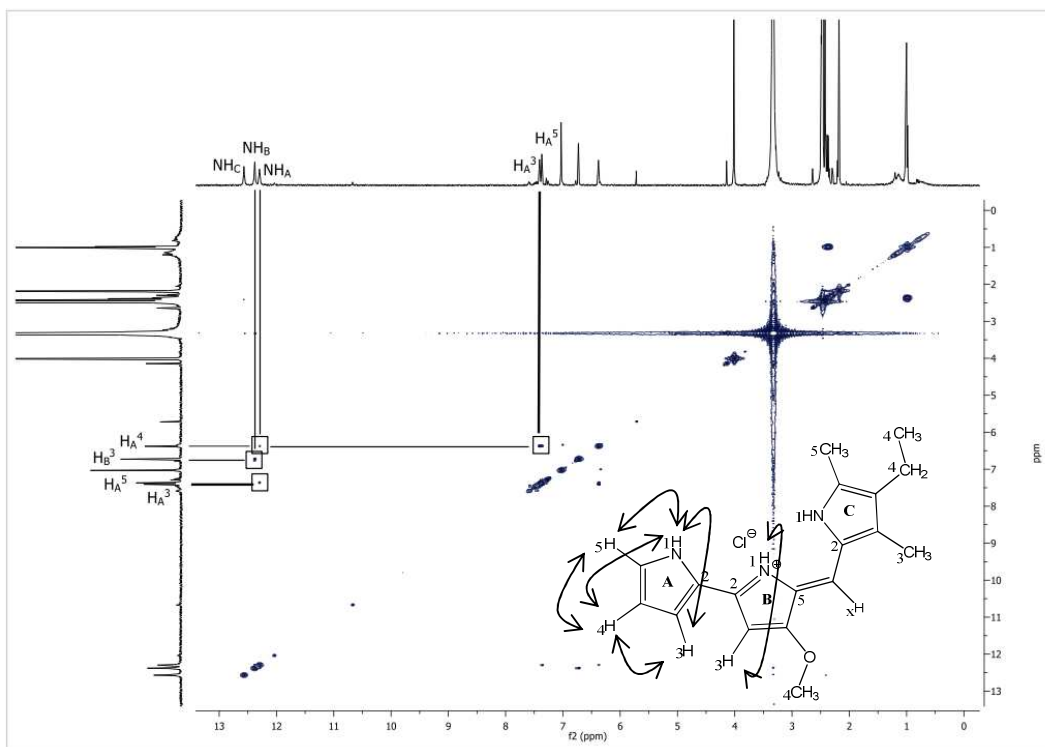


Figure S22. COSY (DMSO- d_6) of **1.HCl**

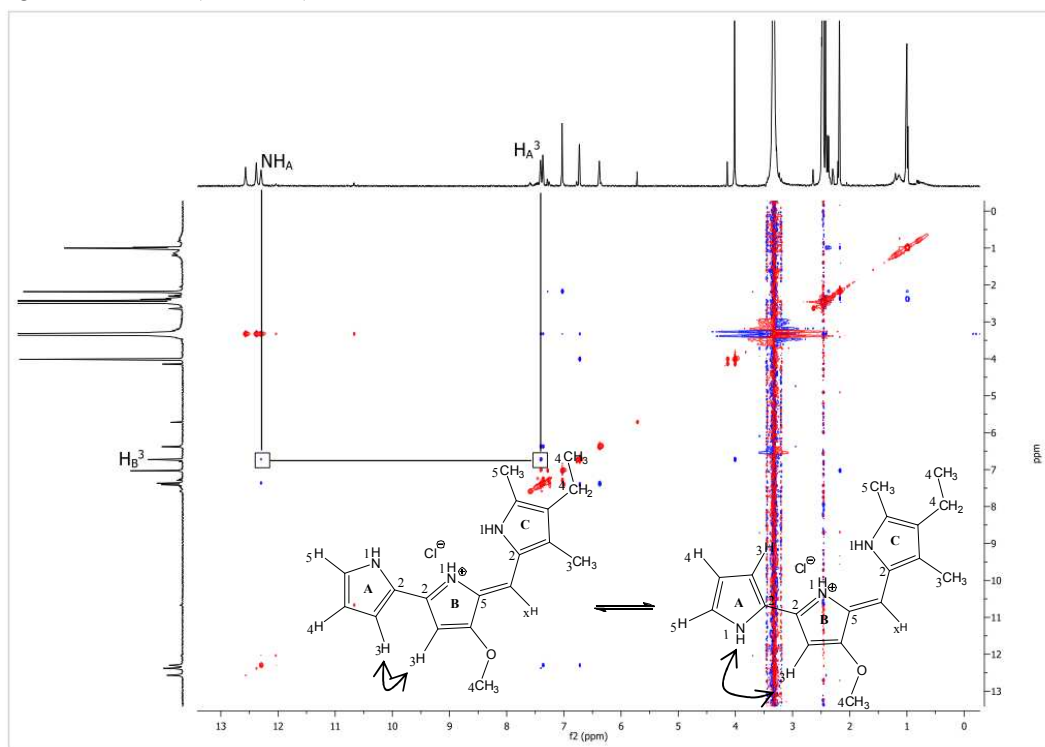


Figure S23. NOESY (DMSO- d_6) of **1.HCl**

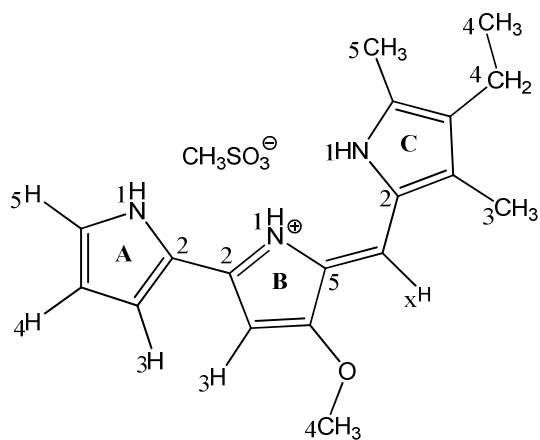


Figure S24. Structure of compound **1.MeSO₃H** showing the atom numbering scheme.

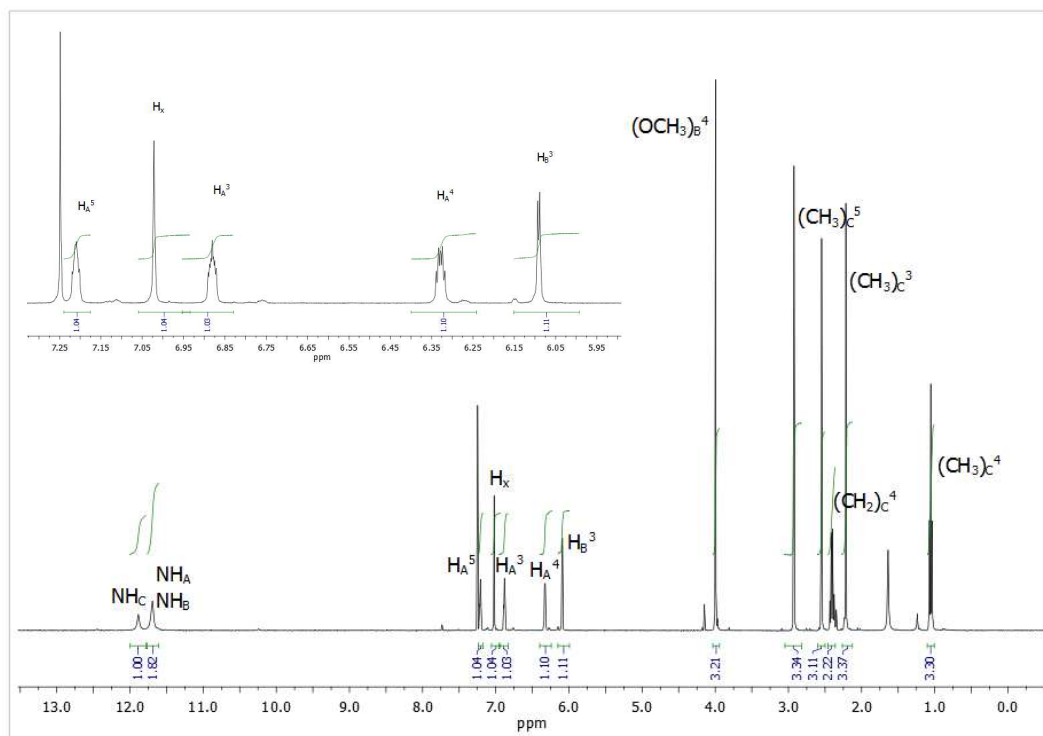


Figure S25. ¹H NMR (CDCl₃, 400 MHz) of **1.MeSO₃H**

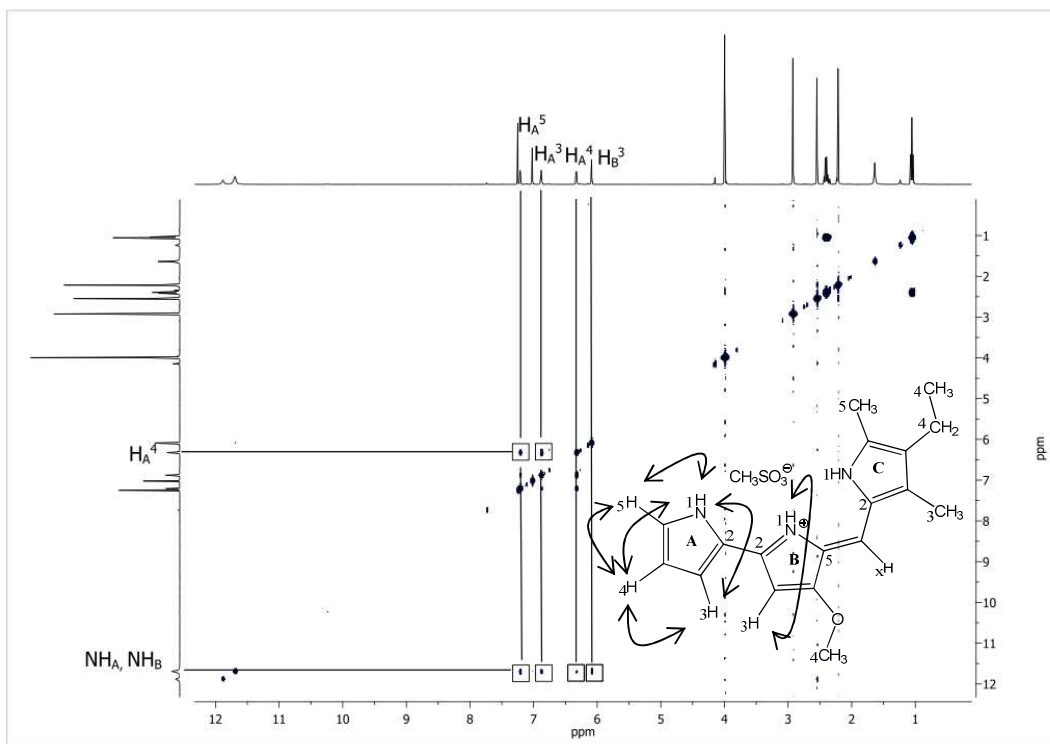


Figure S26. COSY (CDCl₃) of **1.MeSO₃H**

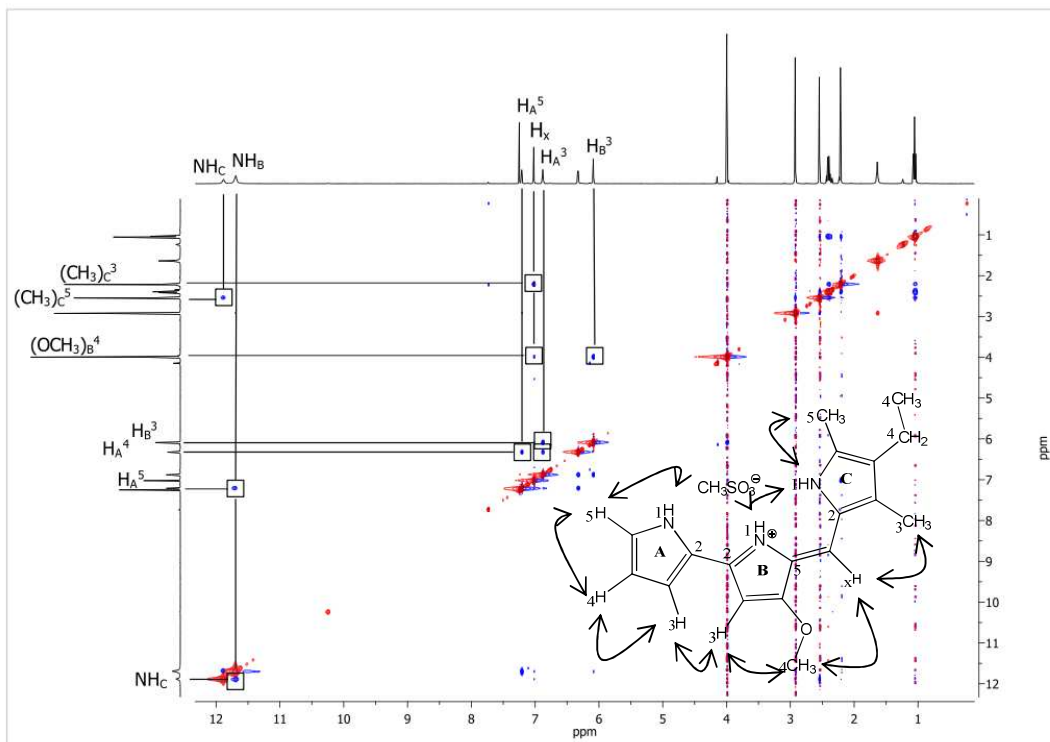


Figure S27. NOESY (CDCl₃) of **1.MeSO₃H**

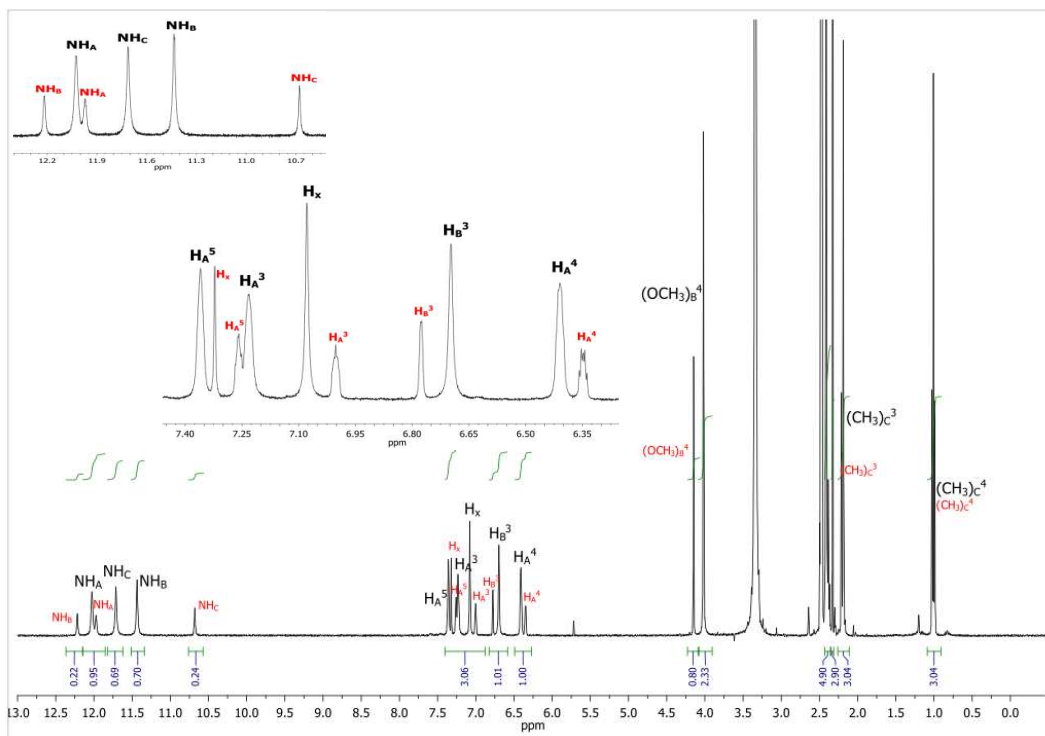


Figure S28. ¹H NMR (DMSO-*d*₆, 400 MHz) of **1.MeSO₃H**

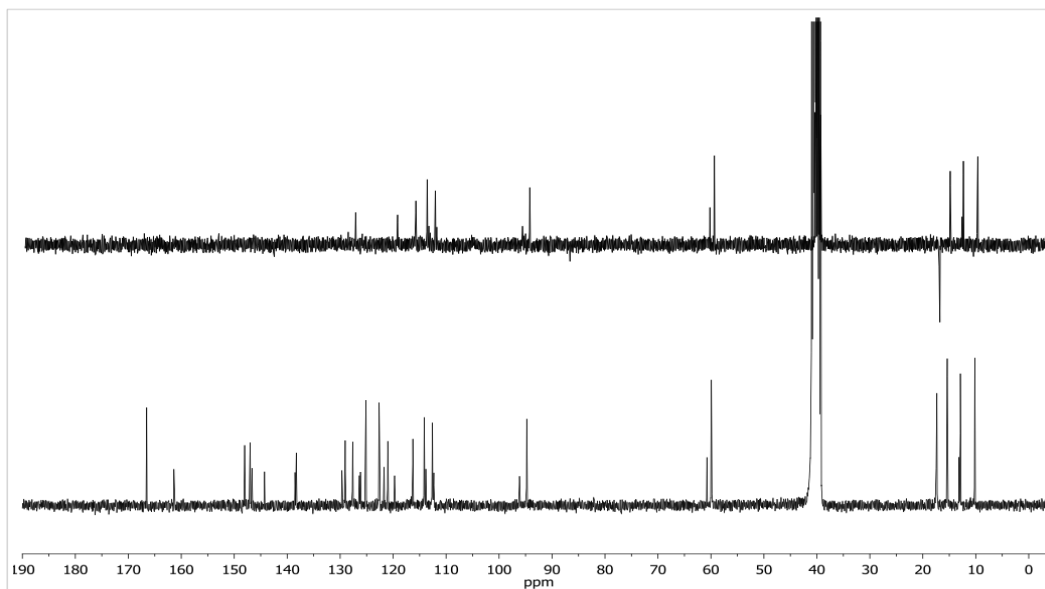


Figure S29. ¹³C NMR (DMSO-*d*₆, 100 MHz) of **1.MeSO₃H**

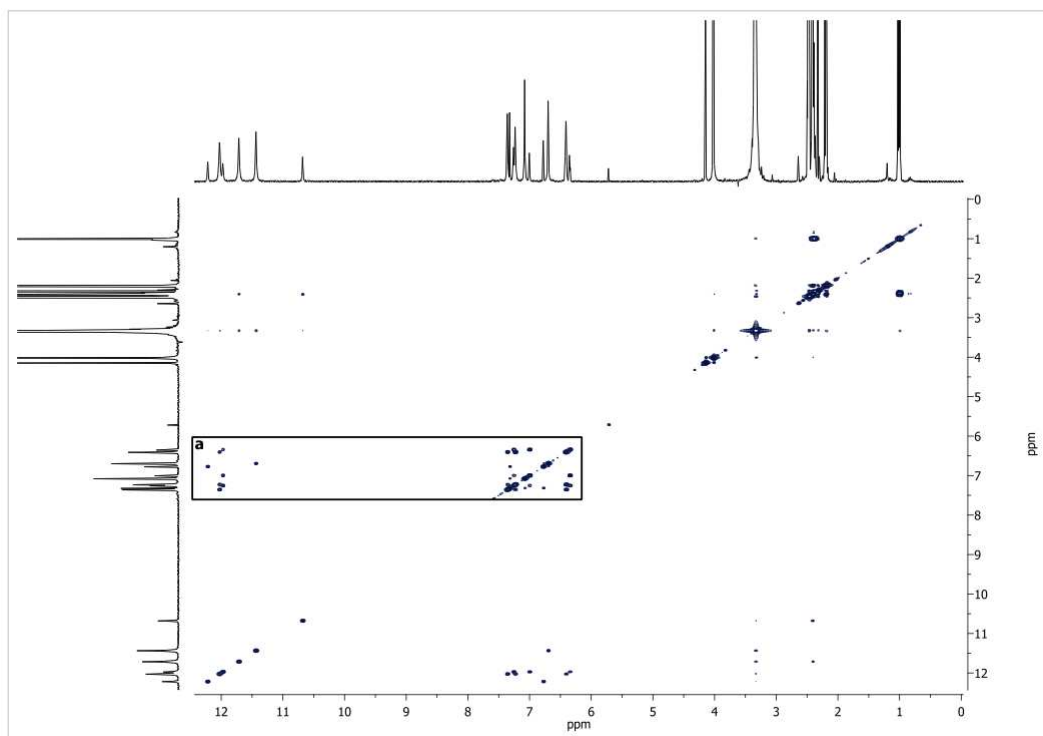


Figure S30. COSY (DMSO- d_6) of **1.MeSO₃H**

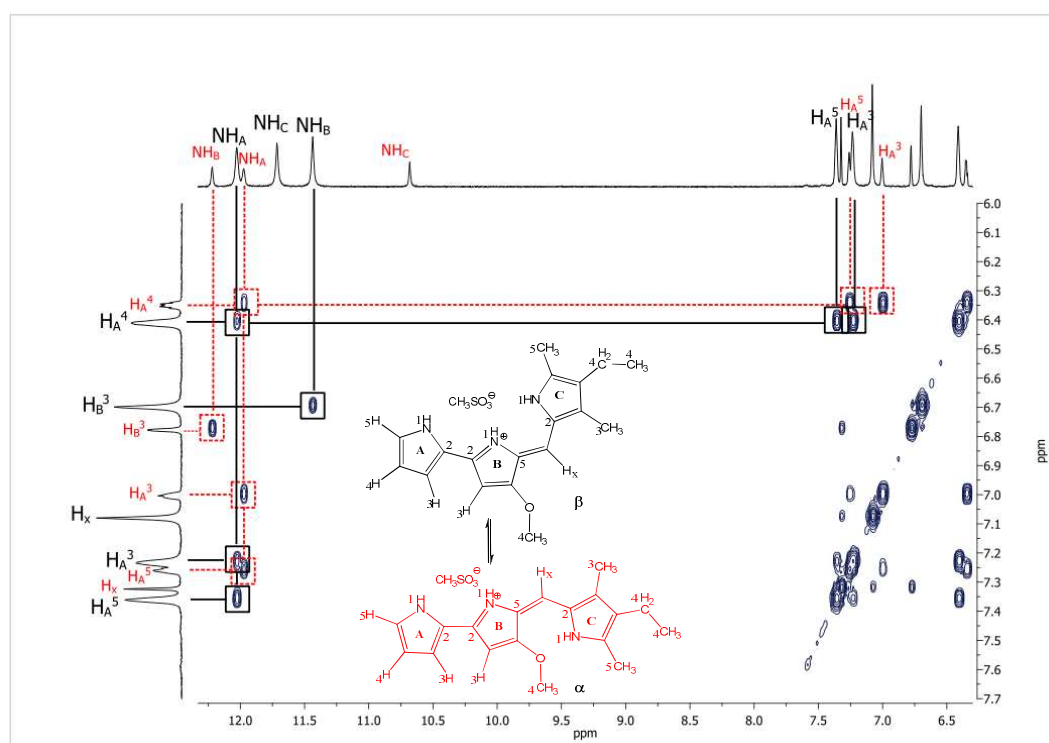


Figure S31. COSY (DMSO- d_6). Region (a) of **1.MeSO₃H**

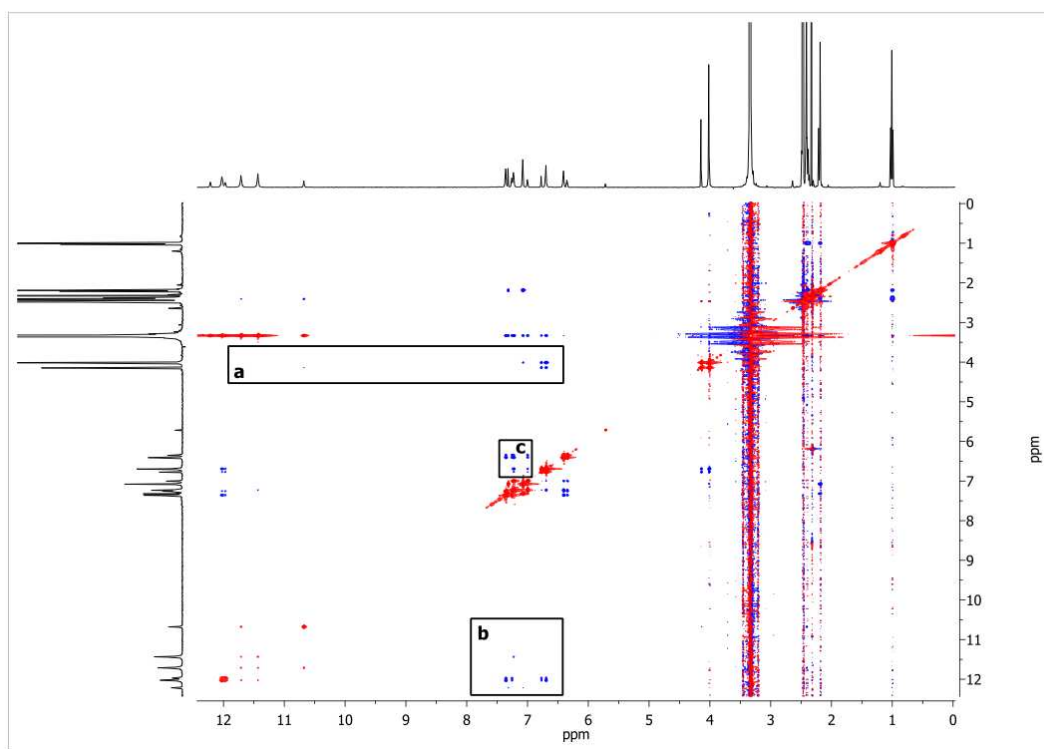


Figure S32. NOESY (DMSO- d_6) of **1.MeSO₃H**

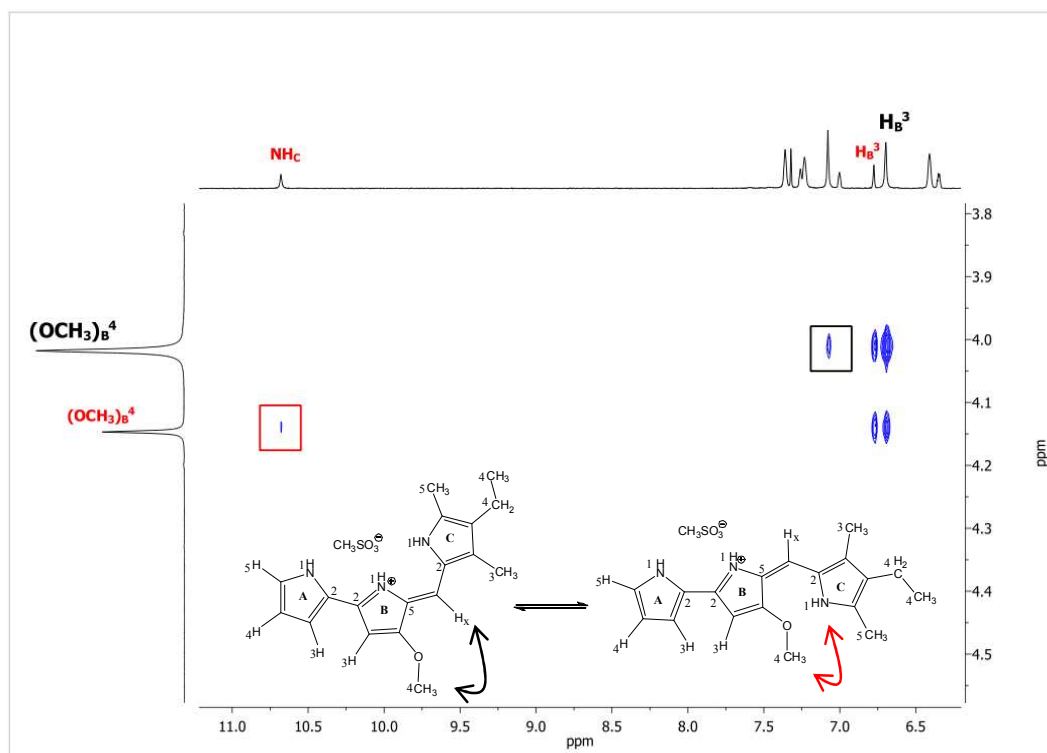


Figure S33. NOESY (DMSO- d_6). Region (a) of **1.MeSO₃H**

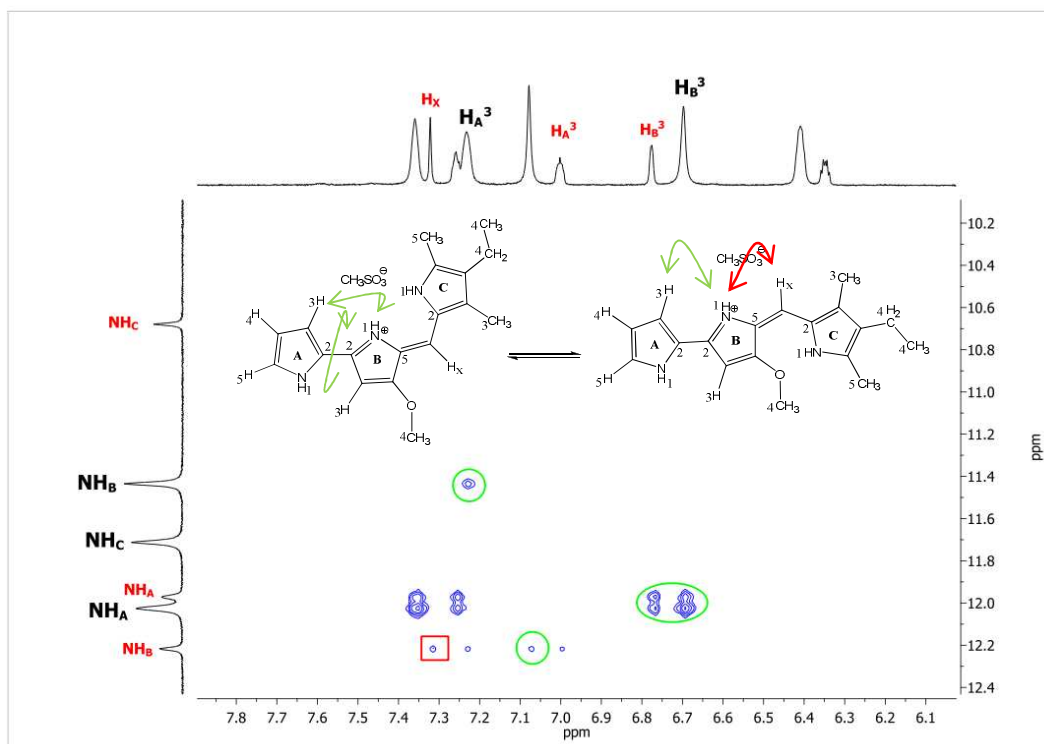


Figure S34. NOESY (DMSO- d_6). Region (b) of **1.MeSO₃H**

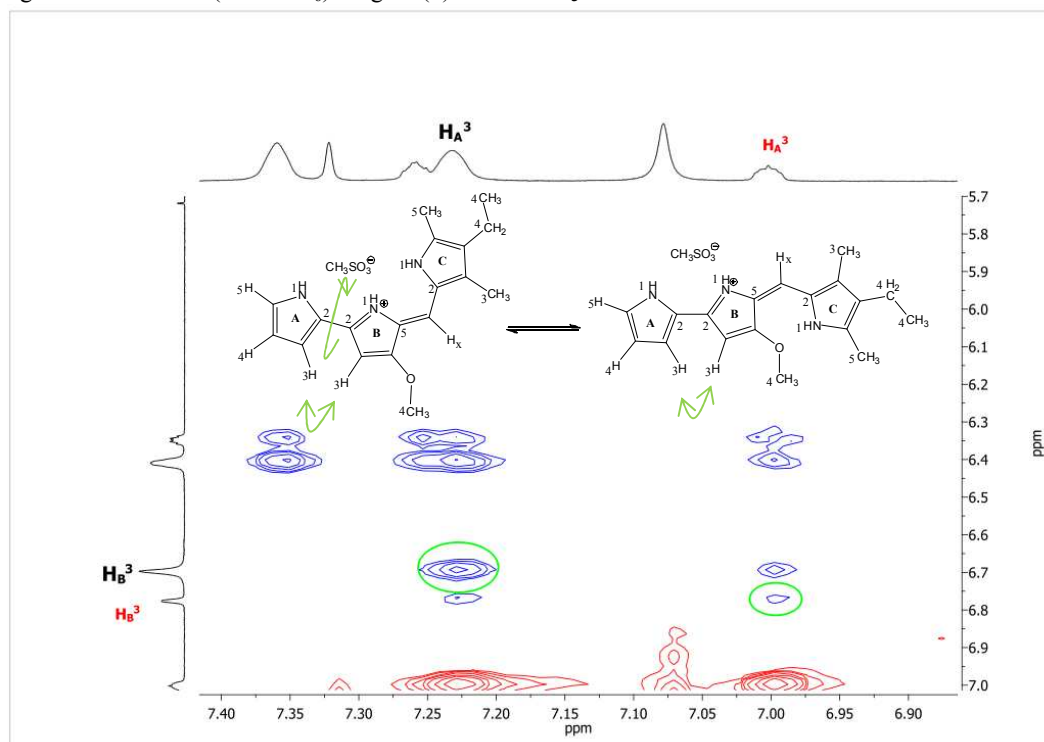


Figure S35. NOESY (DMSO- d_6). Region (c) of **1.MeSO₃H**

Anion binding experiments

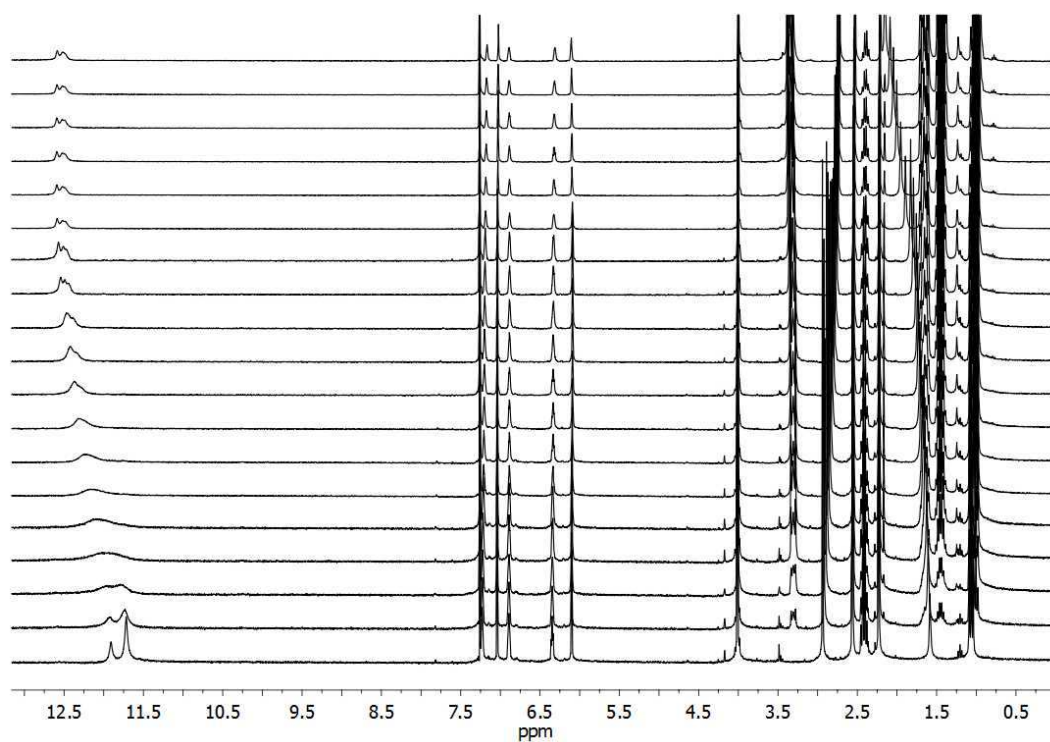


Figure S36. Stack plot of ¹H-NMR (CDCl₃, 300MHz) of compound **1a**.MeSO₃H upon addition of increasing ammounts of TBACl.

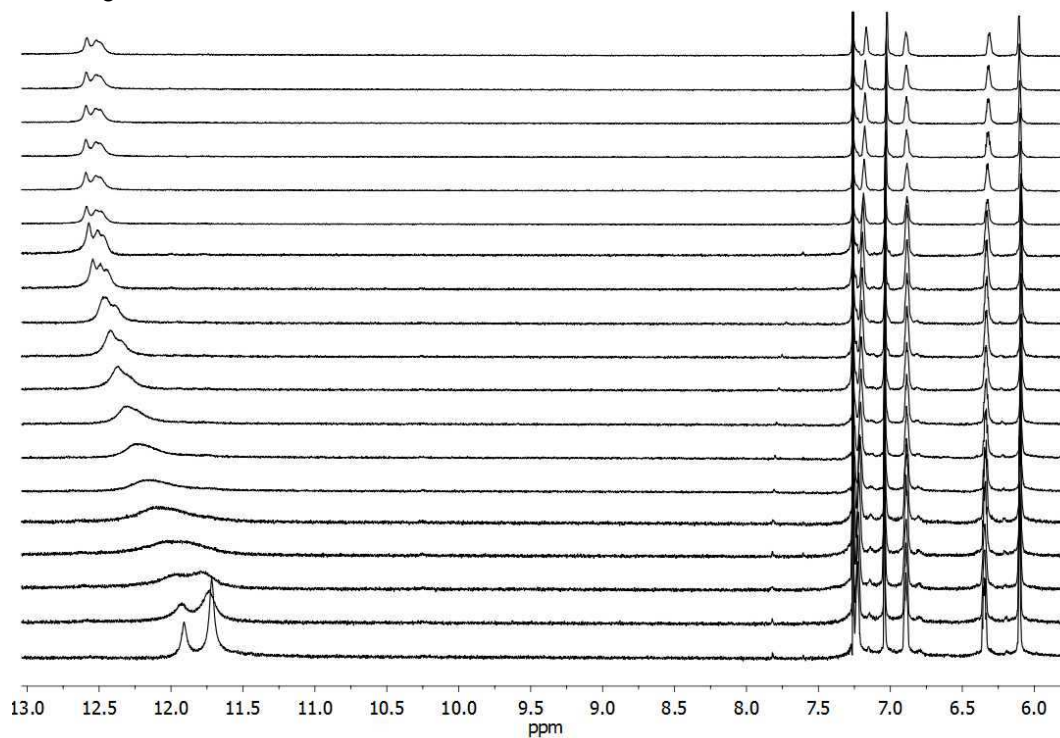


Figure S37. Stack plot of ¹H-NMR (CDCl₃, 300MHz) of compound **1**.MeSO₃H upon addition of increasing ammounts of TBACl (downfield region).

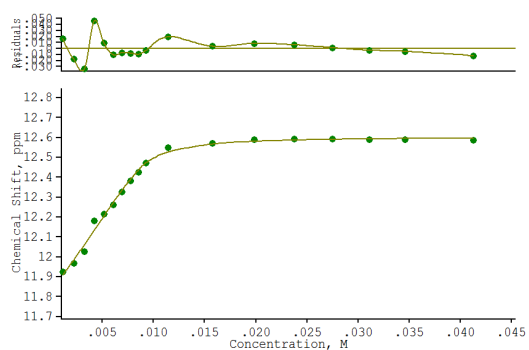


Figure S38. Changes in the chemical shift corresponding to NH1 (Figure S10) are fitted to a 1:1 model using WinEQNMR2. $K_a = 2544 (\pm 379) \text{ M}^{-1}$.

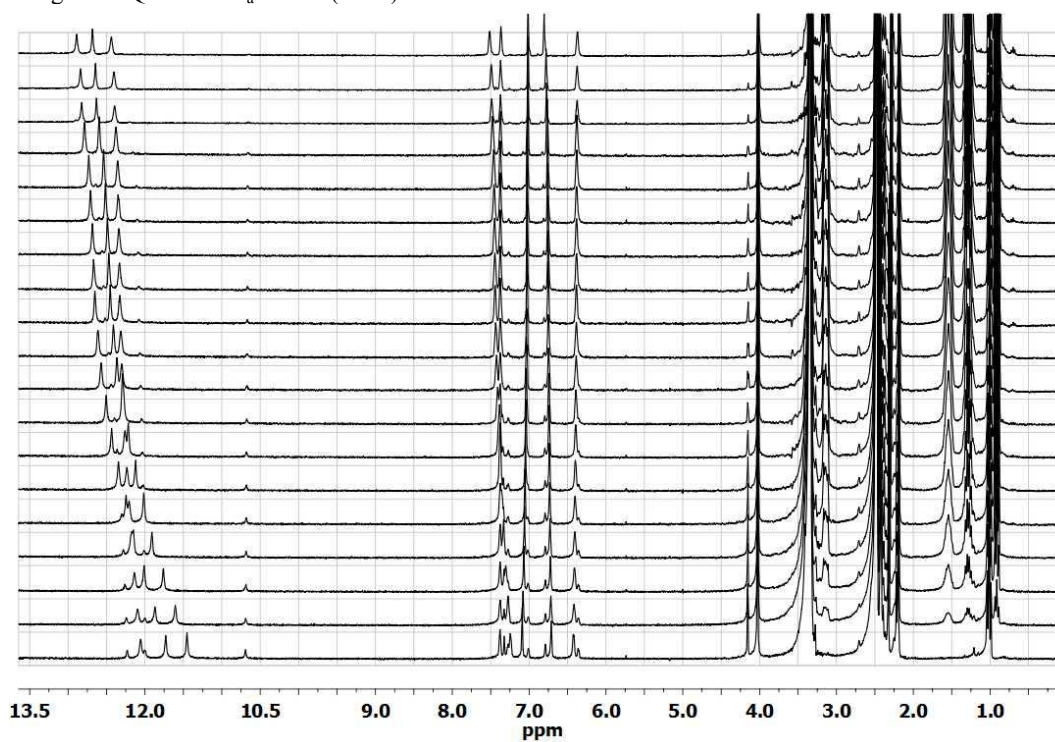


Figure S39. Stack plot of ¹H-NMR (*d*₆-DMSO, 300MHz) of compound **1**.MeSO₃H upon addition of increasing amounts of TBACl.

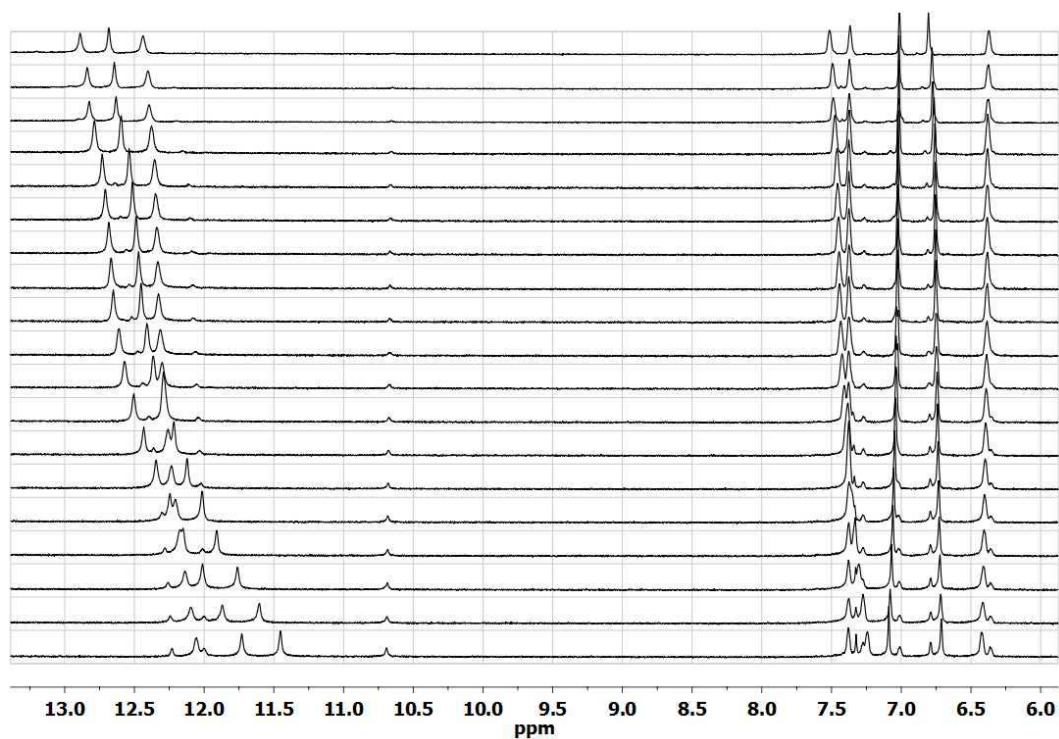


Figure S40. Stack plot of ^1H -NMR (d_6 -DMSO, 300MHz) of compound **1**.MeSO₃H upon addition of increasing amounts of TBACl (downfield region).

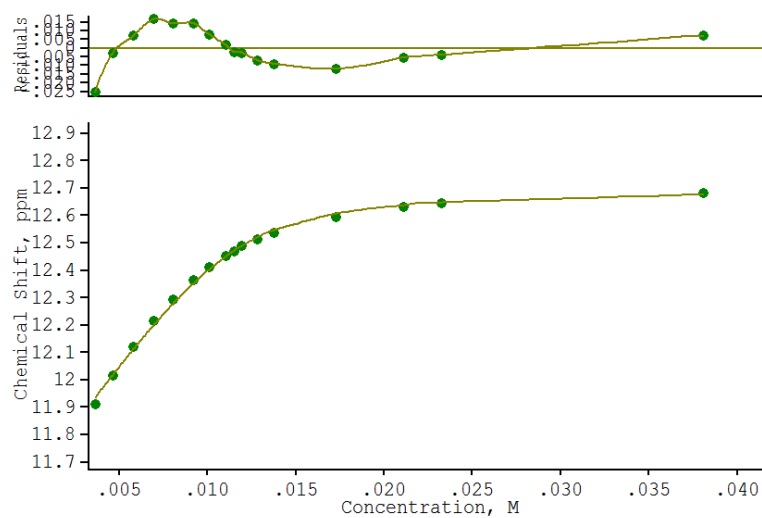


Figure S41. ^1H NMR titration of compound **1**.MeSO₃H with TBACl in d_6 -DMSO. Changes in NH chemical shift at 11.9 ppm are fitted to a 1:1 model using WinEQNMR2. $K_a = 1520 (\pm 177) \text{ M}^{-1}$.

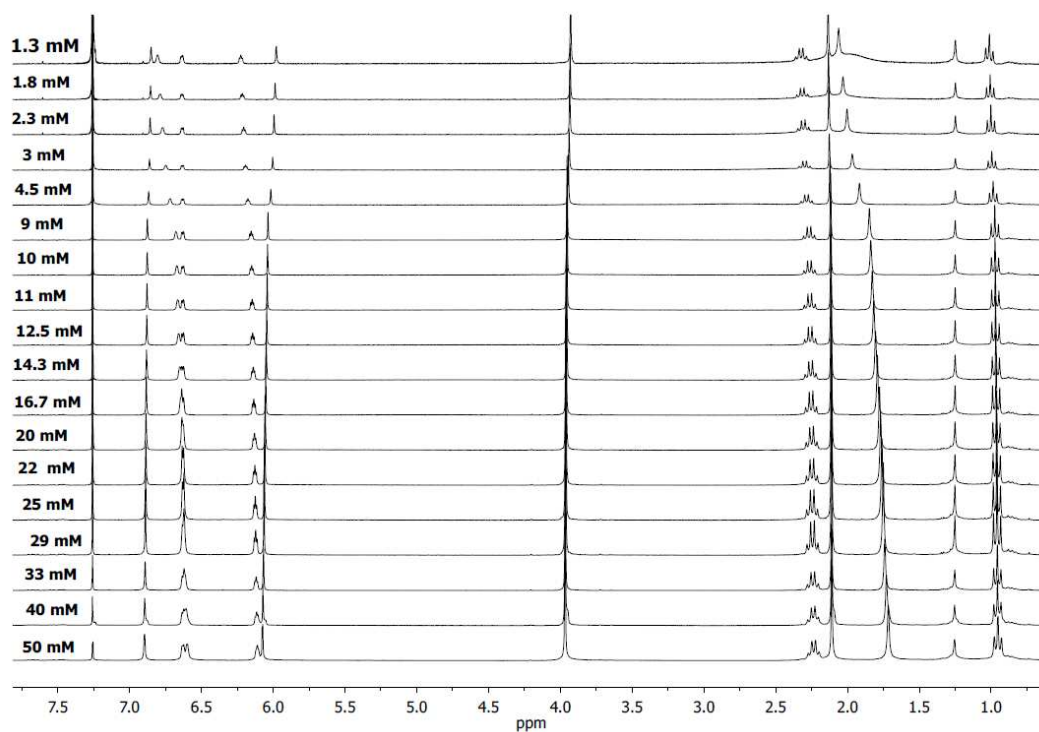


Figure S42. Stack plot of ^1H -NMR (CDCl_3 , 300MHz) of compound **1** at different concentrations.

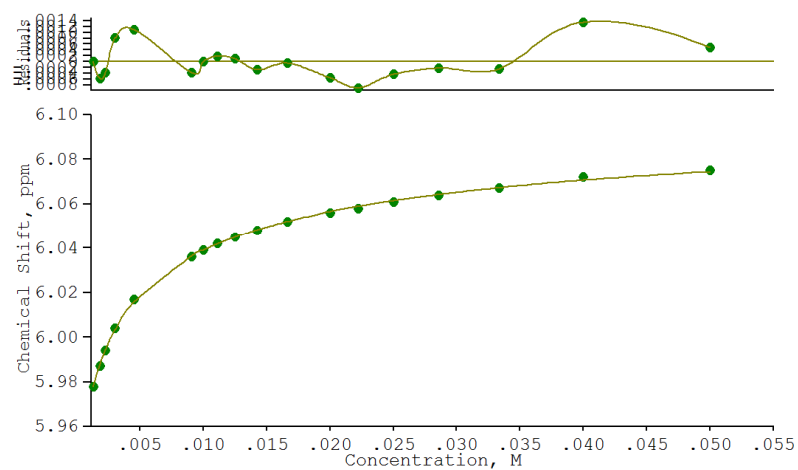


Figure S43. Changes in the chemical shift corresponding to NH1 (Figure S10) are fitted using WinEQNMR2. $K_D = 361 (\pm 22) \text{ M}^{-1}$.

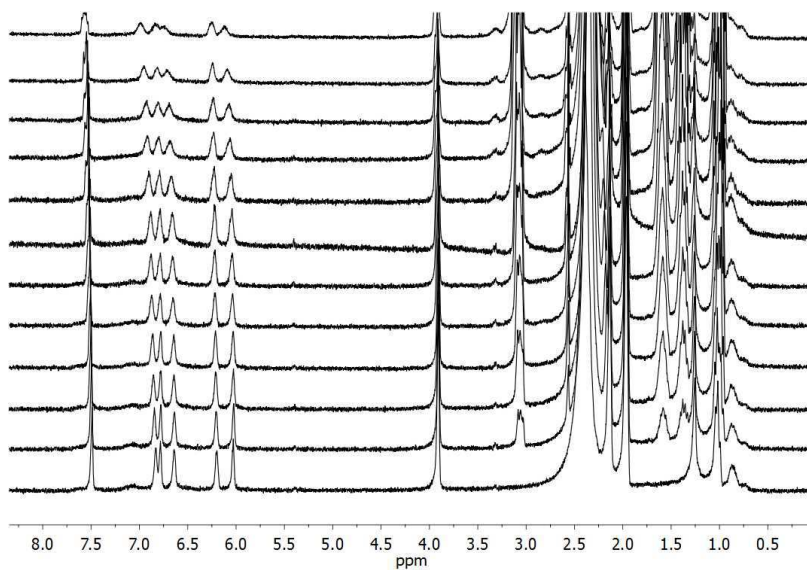


Figure S44. Stack plot of ^1H -NMR (CD_3CN , 300MHz) of compound **1** upon addition of increasing amounts of TBACl.

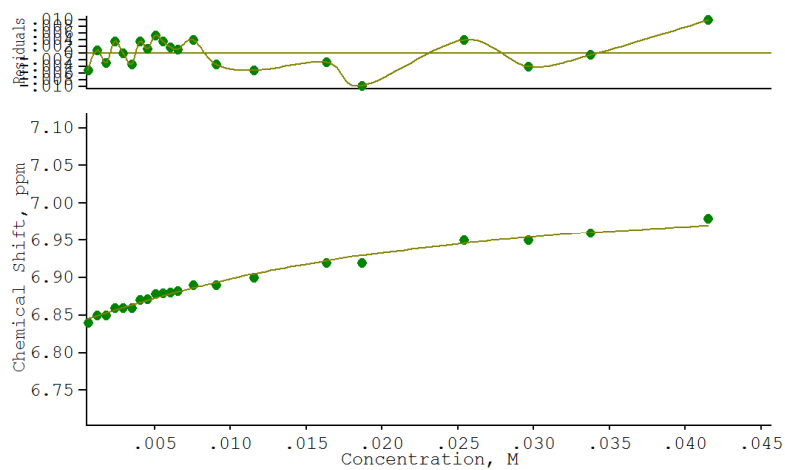


Figure S45. ^1H NMR titration of compound **1**. with TBACl in CD_3CN . Changes in CH chemical shift at 7.37 ppm are fitted to a 1:1 model using winEQNMR2 $K_a = 67 (\pm 8) \text{ M}^{-1}$.

Table S3. Absolute energies (in hartrees) of all compounds in gas phase, water and DMSO solutions at the RI-BP86/def2-QZVP level.

Compound	E(Gas phase)	E(H₂O)	E(DMSO)
Cl⁻	-460.348106	-460.466402	-460.462624
MeSO₃⁻	-664.090874	-664.198192	-664.193846
Iα	-938.488444	-938.508699	
Iβ	-938.496209	-938.513685	
Iγ	-938.481175	-938.505738	
Iδ	-938.492014	-938.511659	
IIα	-938.463372	-938.491870	
IIβ	-938.489023	-938.506633	
IIγ	-938.465618	-938.492999	
IIδ	-938.488423	-938.507694	
IIIα	-938.476700	-938.501979	
IIIβ	-938.476768	-938.500021	
IIIγ	-938.472202	-938.500372	
IIIδ	-938.470909	-938.497073	
IVα	-938.903546	-938.976705	
IVβ	-938.898332	-938.973002	
IVγ	-938.905811	-938.977016	-938.972430
IVδ	-938.901444	-938.971554	
IVα·Cl⁻	-1399.417677	-1399.452287	-1399.449021
IVα·MeSO₃⁻	-1603.146206	-1603.182120	-1603.177958
IVβ·Cl⁻	-1399.432942	-1399.455093	-1399.45246
IVβ·MeSO₃⁻	-1603.158289	-1603.183876	-1603.180463
IVγ·Cl⁻	-1399.400153	-1399.448349	-1399.443546
IVγ·MeSO₃⁻	-1603.129301	-1603.178213	-1603.172145
IVδ·Cl⁻	-1399.417443	-1399.449971	-1399.446796
IVδ·MeSO₃⁻	-1603.141972	-1603.178726	-1603.174255

CARTESIAN COORDINATES OF ALL COMPOUNDS

***GAS PHASE**

MeSO₃⁻

S	0.3002469	0.5481579	-0.6137406
O	1.7549560	0.2866192	-0.7245653
O	0.0016029	1.9152865	-0.1251833
O	-0.4373155	0.2113056	-1.8547212
C	-0.3145820	-0.5758457	0.6455327
H	0.1987463	-0.3620490	1.5886874
H	-1.3925963	-0.4198957	0.7562813
H	-0.1110584	-1.6035788	0.3277090

Ia

C	2.6163558	1.9822990	0.2239578
C	3.8495224	2.6417377	0.2083053
C	3.6107535	3.9900332	-0.1536268
C	2.2424102	4.1301248	-0.3517533
N	1.6603781	2.9144082	-0.1208486
H	0.6778126	2.6702668	-0.1779532
H	4.8090791	2.1908423	0.4342681
H	4.3482020	4.7773060	-0.2600598
H	1.6530991	4.9936291	-0.6355234
C	0.9177033	-1.1042730	0.7879570
C	2.2899226	-1.5380396	1.0639506
C	3.1150395	-0.4552299	0.8929705
C	2.2287817	0.6274268	0.5142639
N	0.9520420	0.2507159	0.4526889
H	4.1912736	-0.4011784	1.0104070
C	-0.3012963	-1.7586233	0.8039922
H	-1.1287347	-1.0974919	0.5395711
C	-0.5376425	-5.2728147	1.6504243
C	-1.8973980	-4.9993422	1.4269620
C	-1.9988428	-3.6298223	1.0757040
C	-0.6903681	-3.0859662	1.0918122
N	0.1626507	-4.1216416	1.4465663
H	1.1711901	-3.9901576	1.5241158
C	0.1421504	-6.5406045	2.0453419
H	1.0029369	-6.7576386	1.3963175
H	0.5133742	-6.5013706	3.0810699
H	-0.5490536	-7.3875239	1.9766212
C	-3.0306058	-5.9761840	1.5585940
H	-3.7741940	-5.7767079	0.7719646
H	-2.6647724	-6.9964630	1.3691298
O	2.6194763	-2.8162248	1.4233891
C	4.0134549	-3.0480002	1.6555367
H	4.1128402	-4.1014569	1.9336057
H	4.5939382	-2.8449926	0.7440635
H	4.3782437	-2.4092007	2.4729672

C	-3.2589511	-2.8913759	0.7500247
H	-3.7701298	-2.5293097	1.6553142
H	-3.0704597	-2.0187686	0.1133951
H	-3.9701791	-3.5385113	0.2187999
C	-3.7302383	-5.9380965	2.9296166
H	-3.0267920	-6.1783130	3.7373570
H	-4.1405502	-4.9413058	3.1358430
H	-4.5577503	-6.6595324	2.9726830

IP

C	2.6118270	1.9092929	0.4682696
C	3.8793003	2.4383959	0.7349714
C	3.7824403	3.8484665	0.6674758
C	2.4634366	4.1592827	0.3615181
N	1.7740356	2.9833825	0.2455816
H	0.7921835	2.8678277	0.0295813
H	4.7688809	1.8591773	0.9531358
H	4.5804180	4.5653359	0.8225379
H	1.9753968	5.1159847	0.2199572
C	0.7295244	-1.1033486	0.1474540
C	2.0375141	-1.6742272	0.4503606
C	2.9188293	-0.6297768	0.6126477
C	2.1232395	0.5588135	0.4023950
N	0.8369395	0.2870431	0.1288302
H	3.9759806	-0.6636790	0.8464059
C	-0.4277038	-1.8207943	-0.0801129
H	-0.3518610	-2.9065744	-0.0282240
C	-3.1902649	0.3749967	-0.7527927
C	-3.8818921	-0.8465454	-0.8574076
C	-2.9464149	-1.8848810	-0.6167081
C	-1.6966429	-1.2719740	-0.3691119
N	-1.8901286	0.0967847	-0.4606100
H	-1.0890711	0.7225288	-0.3132881
C	-3.6794932	1.7755466	-0.9087412
H	-3.6823327	2.3166036	0.0498371
H	-3.0508555	2.3479023	-1.6062972
H	-4.7039983	1.7867524	-1.2962402
C	-5.3453617	-1.0167439	-1.1490871
H	-5.7051884	-0.1715493	-1.7550206
H	-5.4882933	-1.9115755	-1.7741859
O	2.2220748	-3.0113263	0.5299543
C	3.5567244	-3.4291385	0.8288023
H	3.5401968	-4.5225184	0.8523779
H	4.2555375	-3.0828810	0.0522954
H	3.8766718	-3.0393609	1.8067535
C	-3.2233599	-3.3551605	-0.6270169
H	-2.2979303	-3.9421991	-0.6571196
H	-3.7844397	-3.6747113	0.2644981
H	-3.8258554	-3.6427647	-1.5005781
C	-6.2217033	-1.1428237	0.1110451

H	-6.1432227	-0.2436016	0.7356956
H	-7.2788761	-1.2830972	-0.1529844
H	-5.9103153	-1.9978225	0.7250935

Iy

C	1.4507835	3.8980279	-0.8075971
C	0.6663741	4.9939864	-1.1743159
C	1.5261114	6.0995000	-1.3701863
C	2.8232959	5.6705457	-1.1225729
N	2.7634440	4.3431017	-0.7844075
H	3.5613807	3.7677494	-0.5538151
H	-0.4110775	4.9640008	-1.2796105
H	1.2402996	7.1042755	-1.6599808
H	3.7680737	6.1990263	-1.1603455
C	-0.1794468	0.7801186	-0.1795632
C	1.2029982	0.3745924	0.0790015
C	2.0009432	1.4739529	-0.1171741
C	1.0829302	2.5395166	-0.4947762
N	-0.1821100	2.1298393	-0.5283543
H	3.0797586	1.5305239	-0.0112658
C	-1.3855475	0.1012991	-0.1432621
H	-2.2263288	0.7454311	-0.4078779
C	-1.5481755	-3.4066815	0.7433068
C	-2.9126883	-3.1651487	0.5109029
C	-3.0419112	-1.8027681	0.1424362
C	-1.7449705	-1.2311729	0.1546638
N	-0.8711310	-2.2443708	0.5245788
H	0.1328396	-2.0890413	0.6123307
C	-0.8426670	-4.6559801	1.1514336
H	-0.2409729	-5.0739607	0.3295778
H	-0.1632581	-4.4789822	1.9978586
H	-1.5617234	-5.4243680	1.4545536
C	-4.0207376	-4.1740780	0.6121078
H	-3.7426607	-4.9598488	1.3301179
H	-4.9150541	-3.6905962	1.0346203
O	1.5649441	-0.8921425	0.4488127
C	2.9658197	-1.0963868	0.6580002
H	3.0901031	-2.1450825	0.9441402
H	3.5266339	-0.8928447	-0.2659314
H	3.3340137	-0.4436865	1.4632007
C	-4.3146884	-1.0952680	-0.2025395
H	-4.2502107	-0.0177119	-0.0101557
H	-4.5806349	-1.2205869	-1.2634653
H	-5.1560713	-1.4851707	0.3862176
C	-4.3927714	-4.8268462	-0.7318977
H	-3.5342052	-5.3587890	-1.1623241
H	-5.2128234	-5.5472072	-0.6084638
H	-4.7118244	-4.0723426	-1.4621501

C	2.5490571	1.8805065	0.5047297
C	1.8513019	3.0858745	0.3877763
C	2.7707065	4.1439208	0.5718675
C	4.0181531	3.5777805	0.7987187
N	3.8702152	2.2164311	0.7564441
H	4.6170096	1.5473641	0.8829692
H	0.7894267	3.1649780	0.1909530
H	2.5567069	5.2062437	0.5445143
H	4.9833173	4.0329926	0.9842337
C	0.7614415	-1.1867172	0.1334867
C	2.0887800	-1.7291776	0.3873817
C	2.9423098	-0.6612692	0.5612396
C	2.1051582	0.5136405	0.4070935
N	0.8266589	0.2026959	0.1560225
H	4.0058408	-0.6929860	0.7714519
C	-0.3901716	-1.9174707	-0.0930554
H	-0.3015006	-3.0034432	-0.0810977
C	-3.1782657	0.2772716	-0.6289626
C	-3.8652677	-0.9463106	-0.7635422
C	-2.9192498	-1.9842532	-0.5787384
C	-1.6678311	-1.3695494	-0.3347704
N	-1.8721333	0.0007000	-0.3732837
H	-1.0673954	0.6264780	-0.2195770
C	-3.6812623	1.6782520	-0.7257385
H	-3.6616906	2.1856748	0.2506604
H	-3.0717754	2.2779399	-1.4167525
H	-4.7153219	1.6949710	-1.0869165
C	-5.3334300	-1.1144174	-1.0319510
H	-5.4856420	-1.9963080	-1.6729872
H	-5.7059774	-0.2574705	-1.6133050
O	2.3168902	-3.0621580	0.4227868
C	3.6679171	-3.4487964	0.6819580
H	3.6840245	-4.5424926	0.6737123
H	4.3407447	-3.0608819	-0.0982355
H	3.9974170	-3.0789362	1.6647231
C	-3.1847888	-3.4556608	-0.6329518
H	-2.2568141	-4.0323908	-0.7250960
H	-3.7033147	-3.8141402	0.2695567
H	-3.8223738	-3.7160156	-1.4898021
C	-6.1863622	-1.2688635	0.2409432
H	-7.2479861	-1.4061392	-0.0065148
H	-5.8618153	-2.1356757	0.8313737
H	-6.0982841	-0.3826199	0.8826704

IIα

C	1.3374189	3.9216680	-0.3290898
C	2.4517957	4.6784093	0.0299647
C	2.1309340	6.0464941	-0.1641436
C	0.8329237	6.1082029	-0.6384739
N	0.3550717	4.8201973	-0.7207955

H	-0.5080408	4.5584738	-1.1790014
H	3.3756871	4.2762133	0.4289182
H	2.7717454	6.8975847	0.0347849
H	0.2172193	6.9521828	-0.9236614
C	-0.0420831	0.5267387	-0.1757497
C	1.3403615	0.2386740	-0.3419170
C	2.0528013	1.4552827	-0.4282288
C	1.1252059	2.4977649	-0.3182062
N	-0.1178199	1.9306196	-0.2066845
H	3.1111459	1.5849366	-0.6148090
C	-1.2434562	-0.2094755	-0.0288175
H	-2.1360184	0.4239660	-0.0742380
C	-1.2733415	-3.6642412	0.5316910
C	-2.7225274	-3.4311442	0.5184517
C	-2.8769638	-2.0834450	0.2917602
C	-1.5192069	-1.5441054	0.1761563
N	-0.5741817	-2.5638854	0.3285052
C	-0.6090964	-4.9884551	0.7317086
H	-0.9470028	-5.7242124	-0.0143679
H	0.4766561	-4.8749192	0.6471102
H	-0.8417256	-5.4146979	1.7196388
C	-3.7794279	-4.4736791	0.7335952
H	-3.4757119	-5.4122689	0.2434305
H	-4.7128283	-4.1644082	0.2388386
O	1.8221040	-1.0109404	-0.4538315
C	3.2320574	-1.1272045	-0.6407258
H	3.4386784	-2.1996674	-0.6905750
H	3.5511564	-0.6450839	-1.5781495
H	3.7821328	-0.6842196	0.2038204
H	-0.9279390	2.4242933	0.1474483
C	-4.1511814	-1.3054281	0.1778901
H	-4.2659242	-0.5779730	0.9965825
H	-4.2066998	-0.7411280	-0.7650408
H	-5.0257069	-1.9674642	0.2128211
C	-4.0732652	-4.7608215	2.2190282
H	-4.8378583	-5.5424480	2.3283912
H	-3.1705176	-5.0971394	2.7455715
H	-4.4335266	-3.8569553	2.7272464

IIβ

C	2.5033150	1.8786101	-0.0174201
C	3.7697021	2.4698380	-0.0083780
C	3.5957991	3.8742957	-0.0104593
C	2.2327326	4.1245149	-0.0208072
N	1.5841304	2.9150538	-0.0245489
H	0.5789370	2.8010471	-0.0346471
H	4.7107324	1.9326919	0.0004111
H	4.3761427	4.6261371	-0.0046717
H	1.6796060	5.0555195	-0.0259174
C	0.7555399	-1.3107801	-0.0151867

C	2.1025822	-1.7679136	-0.0227059
C	2.9508423	-0.6505182	-0.0244265
C	2.1202462	0.4951364	-0.0182079
N	0.8253140	0.0743838	-0.0126611
H	4.0328946	-0.6373298	-0.0306194
C	-0.4694424	-1.9960033	-0.0072236
H	-0.4185622	-3.0846604	-0.0069899
C	-3.1852730	0.2247852	0.0115800
C	-3.9463921	-1.0120677	0.0287376
C	-3.0125511	-2.0344693	0.0215809
C	-1.7164878	-1.3885783	0.0037089
N	-1.8735040	0.0077055	-0.0027970
C	-3.7567871	1.6060259	-0.0057519
H	-4.3191222	1.8247982	0.9146875
H	-2.9563307	2.3476415	-0.1038267
H	-4.4591596	1.7408922	-0.8417927
C	-5.4427864	-1.1178674	0.0715905
H	-5.7608193	-2.0582930	-0.4041862
H	-5.8876938	-0.3114276	-0.5322138
O	2.4061175	-3.0873955	-0.0269532
C	3.7999149	-3.4030084	-0.0327515
H	3.8659903	-4.4946535	-0.0346658
H	4.2901684	-3.0008356	-0.9322460
H	4.2970065	-3.0035285	0.8641963
H	-0.0868453	0.5731725	-0.0081691
C	-3.2581802	-3.5108344	0.0391902
H	-2.6221444	-4.0399293	-0.6843914
H	-3.0524655	-3.9494347	1.0280530
H	-4.3017355	-3.7447710	-0.2069129
C	-6.0286920	-1.0570261	1.4953632
H	-7.1250852	-1.1254707	1.4767342
H	-5.6456269	-1.8812009	2.1110456
H	-5.7581044	-0.1187071	1.9976728

Иγ

C	1.3292242	3.9227966	-0.3432721
C	0.4326519	4.9736024	-0.5496669
C	1.1618717	6.1877424	-0.4764543
C	2.4849115	5.8647022	-0.2290322
N	2.5741914	4.4956259	-0.1572055
H	3.4085136	3.9776377	0.0838816
H	-0.6233850	4.8702245	-0.7736230
H	0.7685815	7.1894841	-0.6037268
H	3.3587558	6.4907993	-0.0992779
C	-0.0253663	0.5305345	-0.1308991
C	1.3499797	0.2357244	-0.3467326
C	2.0623235	1.4494395	-0.4587413
C	1.1378309	2.4972253	-0.3162794
N	-0.0900099	1.9306263	-0.1418856
H	3.1153672	1.5631209	-0.6851139

C	-1.2255142	-0.2003137	0.0528656
H	-2.1120042	0.4426492	0.0708819
C	-1.2764231	-3.6725415	0.4935733
C	-2.7205597	-3.4194898	0.5653662
C	-2.8658058	-2.0627022	0.3947819
C	-1.5075289	-1.5376619	0.2271715
N	-0.5715520	-2.5753704	0.2935656
C	-0.6238038	-5.0124158	0.6105633
H	-1.0107299	-5.7149978	-0.1436690
H	0.4579220	-4.9110953	0.4745325
H	-0.8129821	-5.4720730	1.5928392
C	-3.7810009	-4.4543687	0.7990560
H	-3.5199166	-5.3780674	0.2583102
H	-4.7344399	-4.1132745	0.3679125
O	1.8244834	-1.0171293	-0.4617429
C	3.2242052	-1.1392305	-0.7041647
H	3.4259290	-2.2125513	-0.7566515
H	3.5074366	-0.6635293	-1.6565598
H	3.8100387	-0.6940535	0.1154785
H	-0.9226311	2.4477339	0.1089634
C	-4.1316697	-1.2634300	0.3761432
H	-4.1906430	-0.5627863	1.2236753
H	-4.2287310	-0.6662210	-0.5428402
H	-5.0136273	-1.9137188	0.4361888
C	-3.9987903	-4.7933613	2.2867237
H	-4.7705507	-5.5660256	2.4086734
H	-3.0751541	-5.1639844	2.7499669
H	-4.3145429	-3.9038184	2.8472865

IIδ

C	2.5289511	1.9090121	-0.0595722
C	1.7641075	3.0779531	-0.0851500
C	2.6534648	4.1795153	-0.1043072
C	3.9438048	3.6744016	-0.0903421
N	3.8553906	2.3051326	-0.0633134
H	4.6438567	1.6731401	-0.0493261
H	0.6810735	3.1210219	-0.0883648
H	2.3861507	5.2294528	-0.1256118
H	4.9046850	4.1739437	-0.0973443
C	0.7440327	-1.2523312	0.0044040
C	2.0783702	-1.7380291	0.0241463
C	2.9516075	-0.6372685	0.0023276
C	2.1439557	0.5251730	-0.0309259
N	0.8427076	0.1292117	-0.0292366
H	4.0344252	-0.6630256	0.0113722
C	-0.4884582	-1.9299326	0.0185757
H	-0.4398256	-3.0183545	0.0503893
C	-3.1927117	0.2931112	-0.0553109
C	-3.9605139	-0.9437723	-0.0076779
C	-3.0310607	-1.9668397	0.0241965

C	-1.7315392	-1.3218278	-0.0008056
N	-1.8839570	0.0732731	-0.0503683
C	-3.7595981	1.6743718	-0.1225535
H	-4.3457616	1.9166978	0.7768340
H	-2.9536910	2.4098007	-0.2186577
H	-4.4400627	1.7878942	-0.9797984
C	-5.4576438	-1.0414986	0.0246146
H	-5.8922938	-0.2630564	-0.6220168
H	-5.7755010	-2.0022980	-0.4081577
O	2.3546798	-3.0643197	0.0592364
C	3.7397375	-3.4100470	0.0785292
H	3.7823006	-4.5025895	0.1062758
H	4.2500393	-3.0441023	-0.8257823
H	4.2361988	-2.9987142	0.9708985
H	-0.0393358	0.6694105	-0.0516904
C	-3.2767906	-3.4420015	0.0800908
H	-2.6942188	-3.9823145	-0.6799075
H	-3.0000784	-3.8667311	1.0573041
H	-4.3352232	-3.6772411	-0.0877047
C	-6.0573022	-0.9086168	1.4376478
H	-5.7881276	0.0522451	1.8959190
H	-7.1537605	-0.9739466	1.4110381
H	-5.6835537	-1.7029486	2.0967437

III α

C	2.5567427	2.0066616	0.2799270
C	3.8173579	2.6878226	0.2387209
C	3.5133850	4.0054120	-0.0563231
C	2.0841085	4.0614417	-0.1802351
N	1.5053503	2.8764542	0.0181065
H	4.8001322	2.2563388	0.4050668
H	4.2073343	4.8329831	-0.1719055
H	1.4862650	4.9429428	-0.4089080
C	0.9378213	-1.1853510	0.8201933
C	2.3338336	-1.5552603	1.0032094
C	3.1364000	-0.4484051	0.8340887
C	2.2765896	0.6597571	0.5374571
N	0.9979920	0.1815819	0.5380351
H	4.2146026	-0.3881984	0.9042137
C	-0.2659647	-1.8604749	0.8760454
H	-1.1366350	-1.2287701	0.6877336
C	-0.3886896	-5.4170245	1.5901020
C	-1.7610209	-5.1580248	1.4605189
C	-1.9052114	-3.7754263	1.1727880
C	-0.6079982	-3.2102023	1.1330616
N	0.2808241	-4.2423151	1.3914474
H	1.2880668	-4.1014092	1.4182654
C	0.3365876	-6.6852802	1.8897698
H	1.1432837	-6.8727752	1.1660153
H	0.7908117	-6.6724971	2.8927399

H	-0.3481840	-7.5392522	1.8518754
C	-2.8694786	-6.1584998	1.6215982
H	-2.4980735	-7.1648089	1.3773189
H	-3.6593769	-5.9478486	0.8845030
O	2.7044713	-2.8308217	1.2973004
C	4.1148157	-3.0448703	1.4534202
H	4.2402078	-4.1053780	1.6877350
H	4.6458956	-2.8020661	0.5223812
H	4.5078297	-2.4310138	2.2759785
H	0.2169210	0.8030486	0.3516311
C	-3.1931024	-3.0439277	0.9566333
H	-3.5966782	-2.6282948	1.8928203
H	-3.0804486	-2.2087924	0.2534651
H	-3.9616142	-3.7121149	0.5465886
C	-3.4908868	-6.1781481	3.0302143
H	-4.3011737	-6.9170686	3.0956758
H	-2.7384611	-6.4300236	3.7887488
H	-3.9069815	-5.1969077	3.2921817

IIIβ

C	3.2383514	-1.0197544	0.2556978
C	4.6663448	-1.1407232	0.2773308
C	4.9194529	-2.4748063	0.5419477
C	3.6341186	-3.1019199	0.6716438
N	2.6267525	-2.2457571	0.5019465
H	5.3909112	-0.3476363	0.1182575
H	5.8882068	-2.9571080	0.6352148
H	3.4434925	-4.1531191	0.8850648
C	0.4513012	1.2428916	-0.0254492
C	1.5546793	2.1734121	-0.1966370
C	2.7507840	1.4842297	-0.1678837
C	2.4345356	0.1050694	0.0514378
N	1.0614328	-0.0063502	0.0845537
H	3.7529859	1.8775883	-0.2785724
C	-0.8895720	1.5392251	-0.0208602
H	-1.1277052	2.6014336	-0.0373359
C	-3.1418396	-1.3069915	-0.2035985
C	-4.0688422	-0.3103131	0.1116588
C	-3.3563749	0.9165561	0.2273055
C	-1.9941922	0.6462172	-0.0090159
N	-1.8987285	-0.7244000	-0.2467828
C	-3.3253617	-2.7617092	-0.4733041
H	-4.3539112	-3.0654271	-0.2516246
H	-3.1274553	-3.0131760	-1.5268297
H	-2.6527742	-3.3771083	0.1414050
C	-5.5495531	-0.4941010	0.2865394
H	-5.9022313	0.1610514	1.0980215
H	-5.7598403	-1.5206876	0.6209433
O	1.3038045	3.4840728	-0.3767793
C	2.4549314	4.3178358	-0.5581394

H	2.0766233	5.3354948	-0.6849580
H	3.1114202	4.2701600	0.3226928
H	3.0167017	4.0131483	-1.4531701
H	0.6619654	-0.8531379	0.4790085
H	-1.0819193	-1.1760128	-0.6411789
C	-3.9438568	2.2447942	0.5884291
H	-3.1708905	3.0092920	0.7273981
H	-4.6362121	2.6095309	-0.1847266
H	-4.5165566	2.1887829	1.5260040
C	-6.3658026	-0.2005911	-0.9855472
H	-6.0785292	-0.8761306	-1.8016535
H	-7.4417104	-0.3252051	-0.8029151
H	-6.2002629	0.8267151	-1.3350934

III_y

C	2.5929601	2.0132111	0.2418882
C	1.7845729	3.1522221	-0.0914123
C	2.6710687	4.2022679	-0.2434213
C	3.9770862	3.6529697	0.0037442
N	3.9425399	2.3556213	0.2925255
H	0.7038034	3.1895460	-0.2029573
H	2.4355080	5.2320882	-0.4973468
H	4.9231332	4.1922531	-0.0280168
C	0.8612488	-1.1510504	0.8038603
C	2.2545288	-1.5114917	1.0172275
C	3.0554313	-0.4086533	0.8379572
C	2.2053252	0.6957421	0.5048647
N	0.9213078	0.2154126	0.4929261
H	4.1303451	-0.3136066	0.9160529
C	-0.3418016	-1.8250675	0.8504780
H	-1.2122233	-1.2023046	0.6308570
C	-0.4676799	-5.3642924	1.6473532
C	-1.8375234	-5.1151883	1.4795013
C	-1.9806138	-3.7402949	1.1548553
C	-0.6857086	-3.1708269	1.1316213
N	0.2012808	-4.1913060	1.4356638
H	1.2075714	-4.0444330	1.4799781
C	0.2562848	-6.6209115	1.9956110
H	1.0859035	-6.8175358	1.3008317
H	0.6797220	-6.5838949	3.0113607
H	-0.4213792	-7.4804190	1.9549910
C	-2.9454679	-6.1166576	1.6378752
H	-2.5612832	-7.1276800	1.4368504
H	-3.7133678	-5.9340716	0.8705496
O	2.6224444	-2.7800828	1.3432867
C	4.0332082	-2.9825909	1.5243101
H	4.1601180	-4.0373613	1.7824537
H	4.5753975	-2.7544490	0.5964397
H	4.4101151	-2.3481257	2.3382370
H	0.1065555	0.7796451	0.2942826

C	-3.2659407	-3.0199251	0.8902567
H	-3.6827108	-2.5640890	1.8017266
H	-3.1440203	-2.2167487	0.1518383
H	-4.0285665	-3.7059883	0.4994591
C	-3.6101998	-6.0965307	3.0264304
H	-4.4181065	-6.8382743	3.0899644
H	-2.8803549	-6.3198137	3.8153136
H	-4.0398006	-5.1103498	3.2446162

IIIδ

C	3.2696930	-1.0167483	0.2652385
C	2.9745971	-2.4052445	0.4964851
C	4.2002547	-3.0248429	0.6410563
C	5.1859522	-1.9858347	0.4903184
N	4.6462270	-0.7931874	0.2673720
H	1.9960569	-2.8773517	0.5367137
H	4.3890416	-4.0790259	0.8243552
H	6.2673798	-2.1079541	0.5421131
C	0.4226450	1.2177248	-0.0365680
C	1.5400144	2.1266142	-0.2157116
C	2.7223571	1.4205010	-0.1716083
C	2.3932986	0.0493021	0.0650309
N	1.0069288	-0.0550226	0.0768157
H	3.7407592	1.7689237	-0.2822932
C	-0.9118735	1.5306779	-0.0159045
H	-1.1386193	2.5955305	-0.0248883
C	-3.1824903	-1.2995402	-0.2403729
C	-4.0967080	-0.3148389	0.1354491
C	-3.3769686	0.9072574	0.2817459
C	-2.0244943	0.6437112	0.0029732
N	-1.9350555	-0.7194221	-0.2834264
C	-3.3788721	-2.7410564	-0.5670415
H	-4.4152588	-3.0383015	-0.3755746
H	-3.1655858	-2.9570058	-1.6254898
H	-2.7279299	-3.3901889	0.0369713
C	-5.5738293	-0.4996962	0.3386373
H	-5.9037567	0.1229489	1.1845163
H	-5.7816439	-1.5381346	0.6356890
O	1.3086898	3.4366835	-0.4198727
C	2.4763143	4.2487619	-0.6089126
H	2.1149607	5.2700276	-0.7544159
H	3.1272556	4.2030064	0.2755639
H	3.0369947	3.9185252	-1.4950187
H	0.5520566	-0.7971291	0.5962639
H	-1.1383317	-1.1348755	-0.7528693
C	-3.9507971	2.2209036	0.7117905
H	-3.1754694	2.9877355	0.8220470
H	-4.6916725	2.5985080	-0.0081179
H	-4.4642175	2.1377210	1.6813749
C	-6.4178465	-0.1505986	-0.9008028

H	-6.1539693	-0.7941196	-1.7500159
H	-7.4899094	-0.2767985	-0.6979765
H	-6.2541794	0.8889735	-1.2126921

IV α

C	2.5341364	2.0197776	0.2387612
C	3.7832474	2.5553425	-0.1054673
C	3.6156908	3.9339330	-0.3357587
C	2.2757827	4.2311118	-0.1225640
N	1.6268501	3.0722180	0.2057243
H	0.6715229	3.0403538	0.5381956
H	4.7007069	1.9883728	-0.2120512
H	4.3800462	4.6419042	-0.6320598
H	1.7440872	5.1738501	-0.1704936
C	0.8909735	-1.1918238	0.8612188
C	2.2732318	-1.5301906	1.0601022
C	3.0574613	-0.3976185	0.8622189
C	2.1863722	0.6693448	0.5359222
N	0.9117349	0.1818422	0.5615673
H	4.1295885	-0.3061207	0.9742882
C	-0.3174697	-1.8840100	0.9096236
H	-1.1980187	-1.2642479	0.7231384
C	-0.3888424	-5.4189190	1.5795905
C	-1.7795582	-5.1778432	1.4351533
C	-1.9386674	-3.8099014	1.1661900
C	-0.6338568	-3.2202167	1.1482636
N	0.2691896	-4.2482057	1.4052728
H	1.2759848	-4.0993632	1.4547411
C	0.3255538	-6.6871581	1.8848687
H	1.3212932	-6.7112077	1.4253618
H	0.4549248	-6.8176093	2.9701380
H	-0.2419905	-7.5510398	1.5216364
C	-2.8583394	-6.2114098	1.5759448
H	-2.4859687	-7.1816713	1.2169484
H	-3.6965366	-5.9507317	0.9143218
O	2.6662417	-2.7724236	1.4125990
C	4.0852759	-2.9616260	1.6125559
H	4.2134839	-4.0100827	1.8903450
H	4.6305615	-2.7504438	0.6839028
H	4.4423043	-2.3136807	2.4231583
H	0.1024356	0.6658880	0.1932770
C	-3.2266949	-3.0854472	0.9462153
H	-3.6069738	-2.6450054	1.8796972
H	-3.1274338	-2.2731473	0.2152872
H	-4.0011197	-3.7665911	0.5753400
C	-3.3783330	-6.3678190	3.0172586
H	-4.1645132	-7.1313534	3.0640137
H	-2.5752150	-6.6694393	3.7017752
H	-3.7986863	-5.4262573	3.3919655

IV β

C	2.7847679	1.9885877	0.0710217
C	4.0977892	2.4019759	0.3436691
C	4.1153438	3.8080667	0.3586795
C	2.8233993	4.2434663	0.0875041
N	2.0246453	3.1447703	-0.0660063
H	1.0713428	3.1832483	-0.4024250
H	4.9331715	1.7417658	0.5455837
H	4.9690985	4.4464087	0.5508106
H	2.4227278	5.2447864	-0.0156955
C	0.7151401	-1.0127780	0.0103878
C	2.0303809	-1.5742574	-0.1202427
C	2.9671458	-0.5374926	-0.1519725
C	2.2555148	0.6705699	-0.0196222
N	0.9008779	0.3857968	0.0157094
H	4.0372144	-0.6151536	-0.2936644
C	-0.4772349	-1.7054043	0.1140947
H	-0.3584294	-2.7817960	0.2413370
C	-3.5501461	0.1524788	-0.2655130
C	-4.0753990	-1.0632534	0.2107453
C	-2.9884174	-1.9410027	0.4169863
C	-1.7971127	-1.2398011	0.0856784
N	-2.1855916	0.0511694	-0.2925199
C	-4.2476815	1.3944438	-0.6955653
H	-4.3166429	2.1215775	0.1279447
H	-3.7262466	1.8853217	-1.5280251
H	-5.2702787	1.1737929	-1.0195885
C	-5.5264777	-1.3504745	0.4665209
H	-6.1445313	-0.7740256	-0.2366511
H	-5.7278904	-2.4076822	0.2435361
O	2.1961937	-2.8904531	-0.2358244
C	3.5518434	-3.3698392	-0.3728790
H	3.4763311	-4.4572006	-0.4346299
H	4.0038599	-2.9718546	-1.2905652
H	4.1483099	-3.0835847	0.5031773
H	0.2619162	0.9782217	0.5375212
H	-1.6004393	0.6678593	-0.8448741
C	-3.0611465	-3.3400288	0.9330604
H	-2.2072143	-3.9464791	0.6086163
H	-3.0786938	-3.3637128	2.0326611
H	-3.9754407	-3.8378556	0.5875640
C	-5.9728071	-1.0410049	1.9075069
H	-5.8278327	0.0193298	2.1504245
H	-7.0360072	-1.2750250	2.0412940
H	-5.4037713	-1.6313145	2.6364621

IV γ

C	2.0304393	4.3000263	-0.8927101
C	1.1951290	5.3559540	-1.2885699
C	1.9882310	6.5113008	-1.4133940

C	3.2942475	6.1551228	-1.0938719
N	3.3092331	4.8264255	-0.7867704
H	4.1315474	4.3138139	-0.4960500
H	0.1295891	5.2920629	-1.4804505
H	1.6567850	7.4997875	-1.7069233
H	4.2004898	6.7477113	-1.0635629
C	0.4526625	1.0576373	-0.3514329
C	1.8338502	0.7175511	-0.1483828
C	2.6161864	1.8575274	-0.3166050
C	1.7407891	2.9292032	-0.6283147
N	0.4761627	2.4275857	-0.6457248
H	3.6942110	1.9215372	-0.2446514
C	-0.7567200	0.3647503	-0.3086028
H	-1.6333936	0.9811226	-0.5219184
C	-0.8477832	-3.1510542	0.4529627
C	-2.2366324	-2.9063297	0.2963030
C	-2.3869073	-1.5460070	-0.0128876
C	-1.0785587	-0.9639045	-0.0409094
N	-0.1824017	-1.9889888	0.2502353
H	0.8257606	-1.8474896	0.2859743
C	-0.1409405	-4.4146226	0.7929669
H	0.8393721	-4.4737512	0.3038080
H	0.0223890	-4.4974321	1.8783299
H	-0.7310827	-5.2852703	0.4874012
C	-3.3219739	-3.9290627	0.4632265
H	-2.9547492	-4.9113556	0.1327625
H	-4.1567508	-3.6821769	-0.2077511
O	2.2305068	-0.5381198	0.1491659
C	3.6501731	-0.7370652	0.3256111
H	3.7797165	-1.7946944	0.5655256
H	4.1849701	-0.4966954	-0.6023060
H	4.0196372	-0.1186198	1.1538666
H	-0.3565553	2.9798990	-0.8072682
C	-3.6691439	-0.8193009	-0.2571580
H	-4.0401117	-0.3356064	0.6585221
H	-3.5654446	-0.0400418	-1.0226281
H	-4.4518502	-1.5080597	-0.5945181
C	-3.8461574	-4.0410481	1.9071735
H	-4.6366033	-4.7986164	1.9740793
H	-3.0461720	-4.3269780	2.6020111
H	-4.2621460	-3.0867277	2.2534371

IV8

C	2.7479960	1.9926463	0.0491368
C	2.0661699	3.2196416	0.0106514
C	3.0186139	4.2478141	0.1269484
C	4.2682153	3.6449652	0.2368623
N	4.0958357	2.2940820	0.1820109
H	4.8387304	1.6144925	0.2856916
H	0.9978681	3.3500296	-0.1222658

H	2.8307111	5.3145391	0.1229397
H	5.2536994	4.0801466	0.3508566
C	0.7293508	-1.0283698	0.0206756
C	2.0416653	-1.5923065	-0.1305563
C	2.9784536	-0.5549078	-0.1777348
C	2.2658140	0.6554057	-0.0332010
N	0.9222215	0.3622043	0.0336344
H	4.0447502	-0.6471030	-0.3408650
C	-0.4671512	-1.7175829	0.1216521
H	-0.3547266	-2.7952830	0.2428674
C	-3.5269850	0.1629070	-0.2430761
C	-4.0595400	-1.0526200	0.2287704
C	-2.9789985	-1.9385198	0.4252084
C	-1.7827334	-1.2430567	0.0942402
N	-2.1644821	0.0522623	-0.2769619
C	-4.2187019	1.4115599	-0.6621060
H	-4.3352651	2.1067619	0.1831902
H	-3.6643768	1.9385877	-1.4494277
H	-5.2227690	1.1920204	-1.0411989
C	-5.5119621	-1.3285055	0.4888234
H	-6.1273687	-0.7422282	-0.2084819
H	-5.7239662	-2.3826176	0.2611166
O	2.2046750	-2.9097059	-0.2465480
C	3.5553334	-3.3901592	-0.4119892
H	3.4782705	-4.4776306	-0.4710030
H	3.9884947	-2.9943193	-1.3399158
H	4.1712293	-3.1045051	0.4510679
H	0.2654192	0.9938019	0.4785072
H	-1.5788982	0.6735863	-0.8240705
C	-3.0583059	-3.3398888	0.9338833
H	-2.2163852	-3.9532669	0.5912687
H	-3.0576851	-3.3703709	2.0334594
H	-3.9834329	-3.8256647	0.6005278
C	-5.9493127	-1.0225780	1.9334061
H	-5.7921123	0.0346515	2.1819494
H	-7.0144167	-1.2460257	2.0700379
H	-5.3836452	-1.6231883	2.6565235

IV α -Cl⁻

C	2.5277208	1.9930520	0.2581176
C	3.7833437	2.6294205	0.2165182
C	3.5578963	3.9811995	-0.0909762
C	2.1755150	4.1437745	-0.2306144
N	1.5684805	2.9506934	-0.0199277
H	0.5310011	2.7616902	-0.0598906
H	4.7410385	2.1517634	0.3911563
H	4.3032459	4.7601668	-0.2020504
H	1.5926722	5.0270151	-0.4647037
C	0.9287558	-1.2123335	0.8248222
C	2.3204609	-1.5702675	1.0098058

C	3.1008852	-0.4446527	0.8286708
C	2.2041899	0.6321700	0.5264998
N	0.9455930	0.1504741	0.5320722
H	4.1778084	-0.3604165	0.8960353
C	-0.2840560	-1.8808743	0.8802795
H	-1.1417849	-1.2322076	0.6860009
C	-0.3872224	-5.4210917	1.5913297
C	-1.7664608	-5.1699095	1.4610018
C	-1.9190837	-3.7937104	1.1763498
C	-0.6194471	-3.2201378	1.1377744
N	0.2774067	-4.2497099	1.3967875
H	1.2851751	-4.1043674	1.4243308
C	0.3349153	-6.6892980	1.8949495
H	1.2030539	-6.8270866	1.2353681
H	0.7023076	-6.7100649	2.9324008
H	-0.3269454	-7.5520066	1.7643098
C	-2.8657451	-6.1801457	1.6211746
H	-2.5053389	-7.1730453	1.3135119
H	-3.6851019	-5.9331556	0.9299069
O	2.7128989	-2.8362503	1.3147955
C	4.1267823	-3.0256641	1.4797180
H	4.2688771	-4.0813359	1.7256647
H	4.6574685	-2.7839420	0.5483440
H	4.5043651	-2.3969024	2.2980502
H	0.0604765	0.7365672	0.3361586
Cl	-1.3582388	1.9477188	-0.0350875
C	-3.2090117	-3.0689735	0.9605724
H	-3.6943770	-2.8126580	1.9142700
H	-3.0739998	-2.1332157	0.4065371
H	-3.9190401	-3.6884008	0.3965680
C	-3.4248426	-6.2664543	3.0534069
H	-4.2333186	-7.0069447	3.1167573
H	-2.6423109	-6.5565791	3.7666093
H	-3.8265444	-5.2989153	3.3796120

IV α ·MeSO₃⁻

C	-0.7007552	0.0484200	-0.0961140
C	-0.4644684	1.4729850	-0.0365163
C	0.8992088	1.7004471	-0.0166752
C	1.5337226	0.4175578	-0.0608235
N	0.5725894	-0.5271738	-0.1164882
H	1.4178810	2.6468059	0.0629560
C	-1.8154865	-0.7763612	-0.1035704
H	-1.5643864	-1.8395920	-0.1256570
C	-5.1375155	0.6374538	-0.0216139
C	-5.4651317	-0.7327137	-0.0292316
C	-4.2517961	-1.4560465	-0.0650291
C	-3.1922221	-0.5084515	-0.0799128
N	-3.7819995	0.7500168	-0.0543469
H	-3.2367930	1.6098884	-0.0346736

C	-6.0205976	1.8382552	0.0114067
H	-5.7145303	2.5433670	0.7974125
H	-6.0018185	2.3820943	-0.9452367
H	-7.0588235	1.5497141	0.2058251
O	-1.4777167	2.3782152	0.0140751
C	-1.0779969	3.7549306	0.0948903
H	-2.0001651	4.3415596	0.1182505
H	-0.4979562	3.9327411	1.0110445
H	-0.4803004	4.0329725	-0.7843839
H	0.6920414	-1.5719512	-0.2805872
C	4.0051011	1.0476686	-0.1879061
C	2.9334621	0.1501533	-0.0192672
C	5.1947254	0.3109483	-0.0664927
N	3.4737646	-1.1044627	0.2009981
C	4.8277162	-1.0136048	0.1839810
H	2.9602161	-1.9828357	0.4683000
H	3.9128207	2.1064604	-0.4025294
C	-4.0993499	-2.9433899	-0.0818066
H	-4.1677536	-3.3456605	-1.1039272
H	-3.1377636	-3.2686718	0.3316971
H	-4.8924354	-3.4246371	0.5052751
S	1.0724610	-3.9852285	0.5037001
O	2.3484791	-3.4482041	1.0481849
O	0.0447107	-4.2463795	1.5070068
O	0.5922856	-3.1387610	-0.6383146
C	1.4915613	-5.5644710	-0.2439025
H	1.8762386	-6.2174969	0.5456923
H	0.5829744	-5.9899417	-0.6807318
H	2.2508836	-5.4017653	-1.0144567
H	6.2083246	0.6851755	-0.1501930
H	5.4389632	-1.8898153	0.3658446
C	-6.8513022	-1.3103357	-0.0203353
H	-6.8550812	-2.2253858	0.5901657
H	-7.5406158	-0.6150351	0.4811438
C	-7.3947798	-1.6399173	-1.4225157
H	-6.7478788	-2.3618286	-1.9369987
H	-8.4025679	-2.0719710	-1.3628360
H	-7.4475381	-0.7389846	-2.0476240

IVβ-CI⁻

C	-3.4342689	-0.8914602	-0.0805491
C	-4.8374308	-0.7871522	-0.0665234
C	-5.3595093	-2.0901957	-0.1417103
C	-4.2722885	-2.9641979	-0.2000256
N	-3.1260996	-2.2374332	-0.1624760
H	-2.1589262	-2.6251119	-0.1932629
H	-5.4010223	0.1369063	-0.0071343
H	-6.4047690	-2.3758847	-0.1525882
H	-4.2404839	-4.0452619	-0.2654535
C	-0.4190332	1.1314792	0.0291821

C	-1.4396166	2.1504809	0.0883980
C	-2.6868393	1.5453119	0.0580283
C	-2.4541214	0.1430757	-0.0226365
N	-1.1100675	-0.0764189	-0.0375258
H	-3.6610921	2.0151693	0.0871799
C	0.9445797	1.3789634	0.0469020
H	1.1714689	2.4443764	0.1067128
C	3.4185852	-1.2426349	-0.0830008
C	4.2673024	-0.1098636	-0.0083395
C	3.4375635	1.0196538	0.0486269
C	2.0826927	0.5627774	0.0093460
N	2.1329990	-0.8244361	-0.0704421
C	3.7666546	-2.6888918	-0.1788394
H	4.3473452	-3.0165814	0.6951748
H	2.8611055	-3.3030205	-0.2427530
H	4.3853740	-2.8853797	-1.0663082
C	5.7681452	-0.1553522	0.0300429
H	6.1206842	-1.0280951	-0.5397202
H	6.1771040	0.7242611	-0.4888815
O	-1.1071041	3.4540323	0.1604627
C	-2.2022007	4.3759678	0.2213518
H	-1.7571396	5.3728883	0.2756153
H	-2.8279902	4.2955216	-0.6792232
H	-2.8155548	4.1919065	1.1152588
H	-0.6870815	-1.0332067	-0.1006914
H	1.3342569	-1.4956349	-0.1237376
Cl	-0.0893162	-2.9963002	-0.2336766
C	3.8669525	2.4517954	0.1310129
H	3.4614770	3.0500743	-0.6975338
H	3.5356468	2.9265254	1.0660904
H	4.9591332	2.5378796	0.0924179
C	6.3471822	-0.2156007	1.4557084
H	5.9889297	-1.1040822	1.9919606
H	7.4445454	-0.2522940	1.4349692
H	6.0472236	0.6640128	2.0400785

IVβ·MeSO₃⁻

C	-0.4343452	1.2819608	-0.0115970
C	-1.4548456	2.2959039	0.0954608
C	-2.6960913	1.6854882	0.1600393
C	-2.4639638	0.2834143	0.0975892
N	-1.1206983	0.0640370	-0.0014264
H	-3.6665512	2.1486370	0.2786161
C	0.9206946	1.5730881	-0.0699458
H	1.0954189	2.6490769	-0.0210471
C	3.5675331	-0.8684499	-0.3134313
C	4.3326117	0.3177960	-0.1936766
C	3.4261831	1.3844782	-0.1021107
C	2.1066696	0.8337995	-0.1564893
N	2.2535109	-0.5429420	-0.2829593

C	4.0243035	-2.2754289	-0.4872412
H	5.0008310	-2.4296665	-0.0136324
H	3.3023364	-2.9794151	-0.0533155
H	4.1371520	-2.5223821	-1.5548706
O	-1.1271642	3.6019994	0.1375908
C	-2.2217020	4.5164689	0.2743382
H	-1.7814282	5.5168490	0.2888148
H	-2.9124297	4.4254002	-0.5764362
H	-2.7653317	4.3343806	1.2127845
H	-0.6894534	-0.8660489	-0.1834571
H	1.4891680	-1.2392052	-0.3958755
C	-4.8667089	-0.5425424	0.0159141
C	-3.4759539	-0.7227191	0.1453197
C	-5.4725428	-1.8048502	0.1303449
N	-3.2556944	-2.0744653	0.3347823
C	-4.4473297	-2.7285494	0.3355902
H	-2.3552324	-2.5606420	0.5427654
H	-5.3640748	0.4028812	-0.1683410
C	3.7632445	2.8338137	0.0556132
H	3.0896694	3.4809009	-0.5215586
H	3.7032212	3.1566070	1.1060106
H	4.7857383	3.0369977	-0.2856405
S	0.1053846	-3.6000888	0.0883607
O	1.3601004	-3.8975100	0.7719872
O	-1.1014216	-3.6540236	0.9409586
O	0.1502118	-2.3038186	-0.6827348
C	-0.1168374	-4.8568315	-1.1745970
H	-0.1808914	-5.8264823	-0.6712480
H	-1.0380270	-4.6476256	-1.7269458
H	0.7473517	-4.8318256	-1.8450911
H	-6.5306757	-2.0310832	0.0703743
H	-4.4842572	-3.7995319	0.4965753
C	5.8322345	0.3828862	-0.1435295
H	6.1767954	1.3009870	-0.6433522
H	6.2548148	-0.4488749	-0.7256334
C	6.4019270	0.3430423	1.2863369
H	7.4989828	0.3913155	1.2759376
H	6.0305700	1.1867772	1.8823069
H	6.1072750	-0.5793226	1.8036718

IV γ -Cl⁻

C	0.8875724	-1.1493924	0.8082392
C	2.2599278	-1.5214380	1.0580908
C	3.0610914	-0.4059946	0.8732926
C	2.1829713	0.6675730	0.5052144
N	0.9243454	0.2020720	0.4759332
H	4.1373664	-0.3463980	0.9829071
C	-0.3447820	-1.7905596	0.8300455
H	-1.1689052	-1.1117186	0.5718567
C	-0.5664198	-5.2976406	1.6471544

C	-1.9317068	-5.0172064	1.4384320
C	-2.0349214	-3.6493228	1.1039345
C	-0.7188979	-3.1085278	1.1133056
N	0.1383491	-4.1519368	1.4509513
H	1.1471201	-4.0321983	1.5211713
C	0.1024623	-6.5738231	2.0290700
H	1.0349867	-6.7237418	1.4676890
H	0.3552547	-6.5952137	3.1003407
H	-0.5526138	-7.4290154	1.8306373
O	2.6242389	-2.7834342	1.4137410
C	4.0270906	-2.9885852	1.6316400
H	4.1457802	-4.0392089	1.9100306
H	4.5933460	-2.7803953	0.7128775
H	4.3875955	-2.3445565	2.4462753
H	-0.0143764	0.7374848	0.2268680
Cl	-1.7011650	1.3153912	-0.1303796
C	1.6617738	3.0929220	-0.1539464
C	2.4995617	2.0298842	0.2041145
C	2.4760745	4.2296901	-0.3401462
N	3.7956961	2.5250977	0.2317280
C	3.7918170	3.8533510	-0.0959374
H	4.6209354	1.9869220	0.4565922
H	0.5813519	3.0176329	-0.2596034
C	-3.2898863	-2.8996166	0.7926288
H	-3.9003838	-2.7490608	1.6951070
H	-3.0916257	-1.9094246	0.3667873
H	-3.9122538	-3.4546428	0.0766950
C	-3.0636322	-5.9946786	1.5735709
H	-3.8451469	-5.7408082	0.8426060
H	-2.7180242	-7.0042238	1.3045386
C	-3.6848422	-6.0315945	2.9822492
H	-4.0723746	-5.0458823	3.2685222
H	-4.5160288	-6.7478845	3.0273884
H	-2.9419874	-6.3258725	3.7350479
H	4.7122625	4.4236791	-0.1302399
H	2.1464990	5.2228129	-0.6218117

IV γ -MeSO₃⁻

C	-0.6112715	0.0631475	-0.1244530
C	-0.4033368	1.4874262	-0.0260730
C	0.9603182	1.7400645	-0.0074633
C	1.6102191	0.4691741	-0.0983560
N	0.6688533	-0.4885827	-0.1788042
H	1.4504044	2.6976119	0.1182548
C	-1.7144526	-0.7854066	-0.1185438
H	-1.4521904	-1.8490007	-0.1218065
C	-5.0506241	0.5792528	0.0404376
C	-5.3578847	-0.7967583	0.0285345
C	-4.1368634	-1.5016935	-0.0418476
C	-3.0901667	-0.5356204	-0.0697072

N	-3.6998448	0.7151689	-0.0236619
H	-3.1682120	1.5832159	0.0017146
C	-5.9519837	1.7644447	0.1166408
H	-5.7270751	2.3869641	0.9952188
H	-5.8544051	2.4036004	-0.7732493
H	-6.9983300	1.4508546	0.1878714
O	-1.4291607	2.3760865	0.0647223
C	-1.0526371	3.7537863	0.1998580
H	-1.9841758	4.3238705	0.2499252
H	-0.4724299	3.9053542	1.1208221
H	-0.4640499	4.0783833	-0.6699125
H	0.8305655	-1.5376658	-0.3874503
C	3.6742639	-1.0368460	0.1769441
C	3.0093230	0.1710746	-0.0645465
C	5.0595563	-0.7701328	0.1435484
N	3.9830829	1.1471118	-0.2295025
C	5.2253931	0.5845006	-0.1181163
H	3.8037342	2.1077184	-0.4882190
H	3.1890944	-1.9858332	0.3902883
C	-3.9622162	-2.9847534	-0.0843702
H	-4.0914622	-3.3691664	-1.1081020
H	-2.9706193	-3.3040899	0.2604582
H	-4.7171236	-3.4830445	0.5386874
S	0.6515044	-3.9556999	0.3212901
O	1.6629429	-3.8219920	1.3737319
O	-0.7490241	-3.8802766	0.7770737
O	0.9064058	-3.0188747	-0.8310045
C	0.8608925	-5.5920555	-0.3968097
H	0.6807289	-6.3280078	0.3931026
H	0.1386107	-5.7171322	-1.2091658
H	1.8845808	-5.6786305	-0.7734806
H	5.8587126	-1.4838418	0.3054242
H	6.1219374	1.1815200	-0.2335765
C	-6.7344781	-1.3959856	0.0639131
H	-6.7086833	-2.3137102	0.6696248
H	-7.4244766	-0.7148426	0.5834610
C	-7.3006985	-1.7292520	-1.3283505
H	-6.6518888	-2.4379461	-1.8583120
H	-8.2993971	-2.1790700	-1.2498631
H	-7.3819144	-0.8270452	-1.9488338

IVδ-CI⁺

C	-4.1501255	-1.0925722	-0.2007623
C	-4.0579951	-2.4888292	-0.2626669
C	-5.3716180	-3.0022173	-0.2820360
C	-6.2484717	-1.9251624	-0.2328638
N	-5.5047083	-0.7798399	-0.1840535
H	-5.8854233	0.1553183	-0.1441906
H	-3.1226461	-3.0439179	-0.2928614
H	-5.6563881	-4.0467193	-0.3274207

H	-7.3312696	-1.8890535	-0.2297640
C	-1.1045044	0.8826773	-0.1135742
C	-2.1016466	1.9201789	-0.0515331
C	-3.3608185	1.3368847	-0.0734302
C	-3.1516327	-0.0693599	-0.1523000
N	-1.8138628	-0.3158728	-0.1736538
H	-4.3183404	1.8412970	-0.0350456
C	0.2621251	1.1420915	-0.0958124
H	0.4643993	2.2128538	-0.0378341
C	2.8083926	-1.3949106	-0.2095466
C	3.6266851	-0.2350553	-0.1255861
C	2.7650041	0.8668058	-0.0757869
C	1.4216391	0.3640651	-0.1263491
N	1.5144354	-1.0193206	-0.2064404
C	3.2005270	-2.8296612	-0.3020908
H	3.7080443	-3.1615543	0.6155585
H	2.3174309	-3.4609416	-0.4543445
H	3.9017121	-2.9915498	-1.1328852
C	5.1271345	-0.2360410	-0.0749956
H	5.5106479	-1.0974760	-0.6419920
H	5.5135466	0.6571120	-0.5890709
O	-1.7491284	3.2197940	0.0187571
C	-2.8269561	4.1587420	0.0916509
H	-2.3654703	5.1482358	0.1460934
H	-3.4614444	4.0939312	-0.8045121
H	-3.4365060	3.9830845	0.9902727
H	-1.3983377	-1.2878547	-0.2509785
H	0.7235746	-1.7219168	-0.2762782
Cl	-0.6207705	-3.1421412	-0.4122097
C	3.1553517	2.3081515	0.0252105
H	2.5288602	2.9513392	-0.6067701
H	3.0715017	2.6842963	1.0562832
H	4.1966942	2.4549285	-0.2869994
C	5.6968950	-0.2792951	1.3550991
H	5.3619831	-1.1787165	1.8881379
H	6.7950180	-0.2826605	1.3424274
H	5.3664618	0.5908523	1.9371479

IVδ-MeSO₃⁻

C	-0.4559002	1.2173547	0.0647035
C	-1.4694420	2.2337982	0.1749240
C	-2.7166643	1.6256257	0.2113035
C	-2.4843350	0.2248740	0.1314026
N	-1.1433983	0.0030574	0.0445004
H	-3.6799030	2.1038729	0.3367371
C	0.9016859	1.5164512	0.0058447
H	1.0669266	2.5930066	0.0753578
C	3.5892611	-0.8544645	-0.3664070
C	4.3290441	0.3549135	-0.2602331
C	3.4011157	1.3899601	-0.1093900

C	2.0934867	0.8004492	-0.1190664
N	2.2710037	-0.5706983	-0.2754630
C	4.0870038	-2.2399710	-0.5821259
H	5.0936172	-2.3619927	-0.1655081
H	3.4108932	-2.9745916	-0.1235009
H	4.1506195	-2.4665033	-1.6585785
O	-1.1400848	3.5392598	0.2380625
C	-2.2321991	4.4567322	0.3619053
H	-1.7884690	5.4552988	0.3911360
H	-2.9080570	4.3756876	-0.5020792
H	-2.7932590	4.2720788	1.2896883
H	-0.7092452	-0.9416826	-0.0885743
H	1.5112531	-1.2910018	-0.3378386
C	-3.3842587	-2.1913946	0.3573713
C	-3.4717191	-0.8098340	0.1513107
C	-4.6962297	-2.7099198	0.3130435
N	-4.8212028	-0.5081272	-0.0030241
C	-5.5652936	-1.6516649	0.0794596
H	-5.1860171	0.4040545	-0.2408938
H	-2.4749589	-2.7560880	0.5571795
C	3.6944007	2.8494821	0.0458487
H	3.1409987	3.4601226	-0.6815843
H	3.4267637	3.2168665	1.0474090
H	4.7614909	3.0520182	-0.1005416
S	0.2950764	-3.7094941	0.1077138
O	1.6181740	-3.9251116	0.6974977
O	-0.8501192	-4.0238213	0.9627699
O	0.1808171	-2.3223683	-0.5002268
C	0.1815175	-4.8025459	-1.3169525
H	0.2553466	-5.8308164	-0.9492906
H	-0.7824388	-4.6414088	-1.8093870
H	1.0056858	-4.5815589	-2.0018342
H	-6.6423940	-1.6269531	-0.0350138
H	-4.9825094	-3.7459659	0.4499442
C	5.8273875	0.4567924	-0.2806049
H	6.1253121	1.4014904	-0.7598014
H	6.2390644	-0.3410922	-0.9156427
C	6.4680205	0.3745705	1.1173320
H	7.5618479	0.4483869	1.0547072
H	6.1084078	1.1860039	1.7634981
H	6.2190485	-0.5733292	1.6120562

WATER SOLUTION

MeSO₃⁻

S	0.3107701	0.5684482	-0.6364655
O	1.7560997	0.2727709	-0.7131048
O	-0.0044683	1.9126571	-0.1110506
O	-0.4473544	0.2007206	-1.8497272
C	-0.3139276	-0.5740418	0.6435909

H	0.2000742	-0.3581645	1.5874900
H	-1.3935725	-0.4198201	0.7539308
H	-0.1076214	-1.6025703	0.3253364

Iα

C	2.5809667	1.9926655	0.2369820
C	3.8377931	2.6110756	0.2277362
C	3.6438989	3.9749891	-0.1083396
C	2.2789992	4.1648680	-0.2974170
N	1.6552081	2.9654858	-0.0863866
H	0.6579235	2.7918835	-0.1508334
H	4.7822534	2.1218319	0.4410978
H	4.4083254	4.7388379	-0.2037736
H	1.7133438	5.0505969	-0.5621852
C	0.8935998	-1.1203795	0.7842651
C	2.2706328	-1.5410945	1.0365557
C	3.0839609	-0.4432045	0.8656118
C	2.1871135	0.6332736	0.5116156
N	0.9074652	0.2427003	0.4614519
H	4.1614473	-0.3850289	0.9709510
C	-0.3199742	-1.7942701	0.8134476
H	-1.1677947	-1.1511318	0.5657918
C	-0.5007613	-5.3111441	1.6490758
C	-1.8719187	-5.0477232	1.4502066
C	-1.9926429	-3.6813521	1.1059457
C	-0.6837926	-3.1246264	1.1002212
N	0.1853254	-4.1562745	1.4364496
H	1.1953239	-4.0205934	1.4984500
C	0.1922681	-6.5732831	2.0332609
H	1.0935180	-6.7357238	1.4264256
H	0.5059122	-6.5545761	3.0879989
H	-0.4694545	-7.4356472	1.8992348
C	-2.9894992	-6.0394517	1.6046415
H	-2.6177951	-7.0508575	1.3847457
H	-3.7654033	-5.8312076	0.8529456
O	2.6123347	-2.8129272	1.3747251
C	4.0190513	-3.0511602	1.5882342
H	4.1139940	-4.1077501	1.8501951
H	4.5826711	-2.8373804	0.6706012
H	4.3886580	-2.4238087	2.4101611
C	-3.2641600	-2.9486228	0.8117310
H	-3.7170762	-2.5339985	1.7252125
H	-3.1076230	-2.1129389	0.1187767
H	-4.0082141	-3.6192527	0.3623292
C	-3.6337970	-6.0336096	3.0036763
H	-4.4485488	-6.7681593	3.0624656
H	-2.8958830	-6.2812988	3.7781801
H	-4.0505162	-5.0461902	3.2425319

Iβ

C	2.6195877	1.9181894	0.4712119
C	3.9012732	2.4263282	0.7239020
C	3.8216002	3.8396233	0.6728046
C	2.4994089	4.1702738	0.3910794
N	1.7920098	3.0066086	0.2732968
H	0.8016665	2.9306239	0.0711323
H	4.7867210	1.8316489	0.9209624
H	4.6318627	4.5450794	0.8225992
H	2.0173150	5.1330714	0.2675954
C	0.7320498	-1.0984408	0.1516596
C	2.0423968	-1.6684211	0.4448291
C	2.9255920	-0.6204398	0.6031932
C	2.1282339	0.5672037	0.4021382
N	0.8373971	0.2932790	0.1360383
H	3.9845802	-0.6583130	0.8304426
C	-0.4317087	-1.8127649	-0.0745322
H	-0.3621402	-2.8997133	-0.0267969
C	-3.2224818	0.3561634	-0.7491094
C	-3.8963789	-0.8790824	-0.8462777
C	-2.9466369	-1.9017497	-0.6024613
C	-1.7013294	-1.2688295	-0.3597242
N	-1.9176465	0.0994577	-0.4580822
H	-1.1417636	0.7540839	-0.3211964
C	-3.7340103	1.7472539	-0.9064059
H	-3.7959231	2.2652301	0.0625401
H	-3.0770524	2.3443389	-1.5539253
H	-4.7365224	1.7442340	-1.3474041
C	-5.3587533	-1.0697842	-1.1331091
H	-5.7281998	-0.2350436	-1.7467333
H	-5.4923491	-1.9761304	-1.7427619
O	2.2340916	-3.0031465	0.5221882
C	3.5817017	-3.4213728	0.8137117
H	3.5640970	-4.5139324	0.8358269
H	4.2689791	-3.0716291	0.0308291
H	3.9017504	-3.0301135	1.7891614
C	-3.2043981	-3.3758716	-0.6029289
H	-2.2726592	-3.9534274	-0.6079353
H	-3.7807794	-3.6888397	0.2808110
H	-3.7895844	-3.6769419	-1.4835290
C	-6.2290480	-1.1869071	0.1326877
H	-6.1614085	-0.2755822	0.7414911
H	-7.2841901	-1.3431398	-0.1301097
H	-5.9074075	-2.0307580	0.7576390

Iy

C	1.4476792	3.9250310	-0.7334879
C	0.6621763	5.0508201	-1.0107170
C	1.5314960	6.1582281	-1.1665477
C	2.8307982	5.6961987	-0.9837550
N	2.7641751	4.3542056	-0.7248894

H	3.5689039	3.7637041	-0.5506791
H	-0.4193739	5.0506448	-1.0872097
H	1.2506506	7.1826937	-1.3871429
H	3.7835530	6.2114765	-1.0171747
C	-0.1917248	0.7809491	-0.2099882
C	1.1957635	0.3560411	-0.0445590
C	1.9958283	1.4640468	-0.2169545
C	1.0782438	2.5511045	-0.4859922
N	-0.2000174	2.1528055	-0.4830148
H	3.0783225	1.5104003	-0.1635636
C	-1.4006182	0.0996107	-0.1411445
H	-2.2630695	0.7464720	-0.3203710
C	-1.5395582	-3.4450848	0.5732597
C	-2.9196683	-3.1742467	0.4489383
C	-3.0535228	-1.7967843	0.1623748
C	-1.7450287	-1.2408952	0.1140611
N	-0.8623731	-2.2838678	0.3703247
H	0.1494105	-2.1494032	0.3889741
C	-0.8301226	-4.7227649	0.8655538
H	-0.1031995	-4.9668267	0.0776159
H	-0.2779128	-4.6672772	1.8153013
H	-1.5402403	-5.5525844	0.9398519
C	-4.0269959	-4.1747480	0.6275294
H	-3.6755406	-5.1710399	0.3225491
H	-4.8550770	-3.9277819	-0.0527411
O	1.5569783	-0.9256543	0.2297150
C	2.9734054	-1.1684741	0.3586705
H	3.0824140	-2.2338320	0.5759277
H	3.4869327	-0.9204186	-0.5795883
H	3.3865153	-0.5711580	1.1821879
C	-4.3282088	-1.0411073	-0.0582614
H	-4.4833840	-0.2677576	0.7078015
H	-4.3397338	-0.5348014	-1.0339183
H	-5.1940285	-1.7122088	-0.0248208
C	-4.5639437	-4.2491354	2.0692164
H	-5.3682337	-4.9929575	2.1502129
H	-3.7682798	-4.5307138	2.7719775
H	-4.9649437	-3.2787471	2.3910428

I8

C	2.5623617	1.8948136	0.5111674
C	1.8604372	3.1013391	0.3890600
C	2.7789835	4.1594944	0.5868023
C	4.0255085	3.5883477	0.8261043
N	3.8798776	2.2299979	0.7776809
H	4.6338612	1.5672818	0.9162409
H	0.8001042	3.1855944	0.1797027
H	2.5660119	5.2228941	0.5598905
H	4.9907098	4.0393349	1.0244062
C	0.7652120	-1.1700627	0.1245284

C	2.0942686	-1.7133404	0.3752175
C	2.9504222	-0.6451343	0.5535203
C	2.1166528	0.5280750	0.4057868
N	0.8310254	0.2219613	0.1528298
H	4.0144219	-0.6738927	0.7608354
C	-0.3878870	-1.9034148	-0.1021671
H	-0.2970927	-2.9897846	-0.0931050
C	-3.2221798	0.2447004	-0.6371227
C	-3.8819080	-0.9961351	-0.7645743
C	-2.9136199	-2.0130868	-0.5791707
C	-1.6715647	-1.3709941	-0.3410228
N	-1.9081326	-0.0029255	-0.3846464
H	-1.1334961	0.6542227	-0.2383940
C	-3.7568531	1.6327029	-0.7330764
H	-3.7822672	2.1228696	0.2517713
H	-3.1361241	2.2560204	-1.3915771
H	-4.7775632	1.6284678	-1.1299622
C	-5.3480121	-1.1959755	-1.0252262
H	-5.4847779	-2.0877656	-1.6551239
H	-5.7395114	-0.3499760	-1.6090803
O	2.3256680	-3.0433448	0.4048848
C	3.6885804	-3.4332831	0.6626647
H	3.7008800	-4.5260855	0.6495046
H	4.3537604	-3.0400781	-0.1186816
H	4.0130512	-3.0648358	1.6454368
C	-3.1505458	-3.4899355	-0.6272447
H	-2.2108553	-4.0527976	-0.6713092
H	-3.7038023	-3.8427303	0.2562984
H	-3.7492794	-3.7683932	-1.5061781
C	-6.1894452	-1.3549533	0.2552610
H	-7.2484694	-1.5154626	0.0113057
H	-5.8459458	-2.2111766	0.8512544
H	-6.1177339	-0.4589448	0.8859510

II α

C	1.3051837	3.9306630	-0.4359752
C	2.5084641	4.6408440	-0.5280750
C	2.1906987	6.0165784	-0.6370527
C	0.8064368	6.1262817	-0.6108149
N	0.2853780	4.8648860	-0.4888881
H	-0.7078602	4.6677523	-0.4534886
H	3.4998540	4.2013125	-0.5137103
H	2.8896120	6.8412288	-0.7246621
H	0.1563708	6.9910692	-0.6695497
C	-0.0329028	0.5340425	-0.0745675
C	1.3715399	0.2701106	-0.1425154
C	2.0562253	1.4872694	-0.2853053
C	1.0911735	2.5154068	-0.3076621
N	-0.1312288	1.9303286	-0.1832100
H	3.1256913	1.6330582	-0.3687349

C	-1.2222910	-0.2106484	0.0688471
H	-2.1110337	0.4280765	0.0820918
C	-1.3148783	-3.7197009	0.3532239
C	-2.7430277	-3.4478817	0.4548495
C	-2.8702128	-2.0750264	0.3532511
C	-1.5126616	-1.5598127	0.1986297
N	-0.5906987	-2.6145654	0.2030689
C	-0.6824446	-5.0750762	0.3897135
H	-1.0990270	-5.7343766	-0.3871243
H	0.3995502	-4.9938498	0.2356599
H	-0.8598603	-5.5795491	1.3519309
C	-3.8193521	-4.4758435	0.6529630
H	-3.5736398	-5.3822886	0.0774524
H	-4.7689660	-4.1027071	0.2412950
O	1.8912694	-0.9710992	-0.0746363
C	3.3253794	-1.0511981	-0.1610924
H	3.5699884	-2.1140463	-0.0904997
H	3.6813453	-0.6493348	-1.1201270
H	3.7975610	-0.5040308	0.6670536
H	-1.0208351	2.4146753	-0.1538387
C	-4.1282516	-1.2620245	0.3996093
H	-4.1944921	-0.6573774	1.3170389
H	-4.2007557	-0.5640256	-0.4472236
H	-5.0166093	-1.9057125	0.3712142
C	-4.0370691	-4.8684626	2.1277387
H	-4.8210420	-5.6328435	2.2199891
H	-3.1178310	-5.2734084	2.5716819
H	-4.3397116	-3.9968366	2.7235358

Πβ

C	2.5415074	1.9023181	-0.0203122
C	3.8334078	2.4446514	-0.0196391
C	3.7095919	3.8545111	-0.0114668
C	2.3521837	4.1522431	-0.0080956
N	1.6611054	2.9704963	-0.0139359
H	0.6501721	2.9061129	-0.0118940
H	4.7543126	1.8720804	-0.0229727
H	4.5165941	4.5789728	-0.0089104
H	1.8288109	5.1009745	-0.0017469
C	0.7427082	-1.2671272	-0.0155176
C	2.0898376	-1.7347556	-0.0217347
C	2.9474561	-0.6257763	-0.0269567
C	2.1272129	0.5281670	-0.0225041
N	0.8255822	0.1211178	-0.0156285
H	4.0300066	-0.6246926	-0.0313738
C	-0.4743745	-1.9635556	-0.0065561
H	-0.4072340	-3.0520508	-0.0067210
C	-3.2509700	0.1915891	0.0182472
C	-3.9777699	-1.0655852	0.0302780
C	-3.0157238	-2.0649907	0.0202123

C	-1.7372198	-1.3838394	0.0049055
N	-1.9295203	0.0084803	0.0032654
C	-3.8597876	1.5568406	0.0041828
H	-4.4729663	1.7360875	0.8998605
H	-3.0792246	2.3249051	-0.0402848
H	-4.5275409	1.6885717	-0.8605669
C	-5.4721226	-1.2091529	0.0735505
H	-5.7665002	-2.1632843	-0.3887482
H	-5.9352734	-0.4198341	-0.5385885
O	2.3833886	-3.0534174	-0.0210558
C	3.7858536	-3.3837119	-0.0255958
H	3.8385572	-4.4752386	-0.0255570
H	4.2728200	-2.9851427	-0.9260724
H	4.2785279	-2.9847648	0.8716286
H	-0.0595105	0.6513464	-0.0105225
C	-3.2211291	-3.5486975	0.0227360
H	-2.7290188	-4.0312644	-0.8346091
H	-2.8093536	-4.0169516	0.9292929
H	-4.2870907	-3.8027618	-0.0215514
C	-6.0589445	-1.1436007	1.4971640
H	-7.1535066	-1.2357168	1.4758147
H	-5.6606370	-1.9543941	2.1218950
H	-5.8101790	-0.1925770	1.9874444

IIγ

C	1.3209791	3.9243145	-0.3772579
C	0.3970346	4.9739281	-0.3064930
C	1.1146675	6.1876565	-0.4475020
C	2.4565240	5.8619675	-0.6012819
N	2.5662548	4.4983733	-0.5566674
H	3.4376880	3.9890017	-0.6472393
H	-0.6740294	4.8702335	-0.1668708
H	0.7029573	7.1909931	-0.4381266
H	3.3316955	6.4859027	-0.7376913
C	0.0024134	0.5298721	-0.0601719
C	1.3965580	0.2485897	-0.2104420
C	2.0920023	1.4620706	-0.3529447
C	1.1409071	2.5011576	-0.2913960
N	-0.0805030	1.9282737	-0.1214061
H	3.1595583	1.5877855	-0.4853295
C	-1.1902763	-0.2040256	0.1161361
H	-2.0695430	0.4452177	0.1726697
C	-1.3150642	-3.7133776	0.3747493
C	-2.7374058	-3.4260143	0.5148395
C	-2.8513549	-2.0515930	0.4256094
C	-1.4921856	-1.5506893	0.2380579
N	-0.5825494	-2.6159247	0.2111904
C	-0.6978185	-5.0760060	0.3903100
H	-1.1375594	-5.7252301	-0.3822222
H	0.3817731	-5.0064030	0.2152905

H	-0.8625154	-5.5843849	1.3526857
C	-3.8199326	-4.4430279	0.7347785
H	-3.5961917	-5.3511463	0.1530982
H	-4.7741717	-4.0595081	0.3439169
O	1.9004345	-1.0006921	-0.2103553
C	3.3263905	-1.0982402	-0.3778063
H	3.5574779	-2.1661650	-0.3544312
H	3.6363469	-0.6707562	-1.3417912
H	3.8512454	-0.5851609	0.4403145
H	-0.9538492	2.4359823	-0.0383849
C	-4.0982379	-1.2244958	0.5080961
H	-4.1268048	-0.6124916	1.4225898
H	-4.1915074	-0.5320594	-0.3412522
H	-4.9938947	-1.8584894	0.5147663
C	-4.0100057	-4.8348224	2.2136645
H	-4.7991386	-5.5917003	2.3218941
H	-3.0854298	-5.2487209	2.6378244
H	-4.2916464	-3.9608049	2.8162057

IIδ

C	2.5456544	1.9262058	-0.0570430
C	1.7826092	3.1004351	-0.0848421
C	2.6797183	4.1958138	-0.0997267
C	3.9693406	3.6769698	-0.0808114
N	3.8739104	2.3128140	-0.0552488
H	4.6667311	1.6819334	-0.0376937
H	0.6991370	3.1517331	-0.0926241
H	2.4208008	5.2487227	-0.1215151
H	4.9357815	4.1669227	-0.0834701
C	0.7334698	-1.2232040	-0.0022339
C	2.0713554	-1.7147349	0.0191896
C	2.9500724	-0.6198622	0.0010799
C	2.1490480	0.5466234	-0.0314443
N	0.8417382	0.1614349	-0.0329942
H	4.0327551	-0.6470680	0.0115583
C	-0.4938421	-1.9033914	0.0095932
H	-0.4395124	-2.9921344	0.0412369
C	-3.2464340	0.2790543	-0.0649301
C	-3.9871470	-0.9697101	-0.0133814
C	-3.0358187	-1.9783033	0.0187109
C	-1.7495777	-1.3102930	-0.0105627
N	-1.9272352	0.0827376	-0.0627198
C	-3.8407922	1.6492370	-0.1300630
H	-4.4202849	1.8819021	0.7762312
H	-3.0537447	2.4038509	-0.2393523
H	-4.5371284	1.7446431	-0.9766059
C	-5.4827569	-1.0976045	0.0240811
H	-5.9347240	-0.3255414	-0.6177919
H	-5.7822724	-2.0650112	-0.4065932
O	2.3418512	-3.0375892	0.0524078

C	3.7378929	-3.3934627	0.0746028
H	3.7700703	-4.4854743	0.1001905
H	4.2440601	-3.0251163	-0.8281862
H	4.2259195	-2.9832405	0.9692191
H	-0.0207570	0.7222563	-0.0559600
C	-3.2584959	-3.4578684	0.0857168
H	-2.6184515	-4.0011143	-0.6237794
H	-3.0369455	-3.8599777	1.0864624
H	-4.3006303	-3.7140543	-0.1430593
C	-6.0791227	-0.9782784	1.4402094
H	-5.8279835	-0.0118390	1.8979499
H	-7.1740418	-1.0644976	1.4138359
H	-5.6906134	-1.7687590	2.0962619

III α

C	1.4788803	4.0132655	-0.7455942
C	2.7641968	4.6290400	-0.7712605
C	2.5331888	5.9750246	-1.0628235
C	1.1230348	6.1067883	-1.1987600
N	0.4791019	4.9367802	-1.0104830
H	3.7213811	4.1441207	-0.5986224
H	3.2733771	6.7645659	-1.1661415
H	0.5690640	7.0172246	-1.4271144
C	-0.1434441	0.7990569	-0.2115286
C	1.2491694	0.4381942	-0.0300547
C	2.0409028	1.5604440	-0.1998817
C	1.1691603	2.6540784	-0.4920677
N	-0.1032246	2.1711986	-0.4922939
H	3.1190796	1.6260813	-0.1293722
C	-1.3465535	0.1156146	-0.1593446
H	-2.2221305	0.7396658	-0.3528347
C	-1.4355888	-3.4294646	0.5647086
C	-2.8174527	-3.1804336	0.4204949
C	-2.9691871	-1.8058039	0.1290261
C	-1.6687746	-1.2305112	0.0977094
N	-0.7734049	-2.2575479	0.3685497
H	0.2354667	-2.1149595	0.4027865
C	-0.7090938	-4.6937964	0.8705094
H	0.0374021	-4.9236110	0.0967902
H	-0.1762927	-4.6280303	1.8306714
H	-1.4051495	-5.5364648	0.9310049
C	-3.9107728	-4.1982503	0.5853358
H	-3.5391957	-5.1885832	0.2850281
H	-4.7339008	-3.9644918	-0.1054204
O	1.6260000	-0.8253685	0.2597183
C	3.0466761	-1.0454780	0.4165347
H	3.1625351	-2.1068396	0.6460462
H	3.5708931	-0.8003550	-0.5156765
H	3.4332853	-0.4351600	1.2424282
H	-0.9163503	2.7509577	-0.6708589

C	-4.2512949	-1.0695633	-0.1111045
H	-4.4334843	-0.3035184	0.6563521
H	-4.2536363	-0.5585414	-1.0843957
H	-5.1062465	-1.7550820	-0.0973167
C	-4.4645143	-4.2813479	2.0201470
H	-5.2584005	-5.0373131	2.0903790
H	-3.6737261	-4.5514662	2.7327424
H	-4.8842066	-3.3173694	2.3372979

IIIβ

C	3.3553150	-1.0251912	0.2083497
C	4.7818477	-1.0082834	0.2296364
C	5.1719883	-2.3295417	0.4452204
C	3.9656417	-3.0810024	0.5447170
N	2.8701379	-2.3109481	0.4038516
H	5.4232662	-0.1402263	0.1040875
H	6.1856590	-2.7144706	0.5225260
H	3.8754506	-4.1538733	0.7137999
C	0.4572044	1.1347786	-0.0531865
C	1.5270857	2.1038417	-0.1908509
C	2.7480450	1.4500816	-0.1500238
C	2.4708503	0.0631190	0.0345025
N	1.1078096	-0.0978002	0.0504712
H	3.7375080	1.8812207	-0.2347224
C	-0.8931133	1.4089631	-0.0472403
H	-1.1315834	2.4727919	-0.0611167
C	-3.2583770	-1.3394314	-0.1231194
C	-4.1455094	-0.2689725	0.0891935
C	-3.3734147	0.9161501	0.1433818
C	-2.0130667	0.5514792	-0.0241467
N	-1.9903444	-0.8341410	-0.1665420
C	-3.5191696	-2.7996774	-0.2649399
H	-4.5460981	-2.9829850	-0.5981442
H	-2.8353565	-3.2574065	-0.9919836
H	-3.3817451	-3.3260880	0.6921762
C	-5.6402854	-0.3833062	0.2040495
H	-6.0062248	0.3421402	0.9455440
H	-5.9033766	-1.3748752	0.5990358
O	1.2443891	3.4054348	-0.3502385
C	2.3802482	4.2867262	-0.4879466
H	1.9672854	5.2916124	-0.6001721
H	3.0124506	4.2357875	0.4080524
H	2.9652045	4.0164853	-1.3768785
H	0.6986108	-0.9724255	0.3597932
H	-1.1909894	-1.3799249	-0.4643087
C	-3.8747624	2.3097796	0.3670582
H	-3.4088165	2.7758575	1.2464640
H	-3.6635936	2.9618511	-0.4930527
H	-4.9592675	2.3165908	0.5248422
C	-6.3779209	-0.1567424	-1.1286803

H	-7.4644094	-0.2445339	-0.9942200
H	-6.1654747	0.8420625	-1.5327964
H	-6.0672214	-0.8936344	-1.8814768

IIIy

C	1.5747277	4.0061284	-0.8005457
C	0.7142808	5.0910311	-1.1424962
C	1.5469271	6.1993313	-1.3066472
C	2.8684802	5.7328763	-1.0571721
N	2.8991384	4.4215755	-0.7530263
H	-0.3671750	5.0630967	-1.2523917
H	1.2518137	7.2120993	-1.5699914
H	3.7870206	6.3184784	-1.0922827
C	-0.0978131	0.8124429	-0.2279369
C	1.2874076	0.4564345	0.0042689
C	2.0853518	1.5725365	-0.1758761
C	1.2265149	2.6599467	-0.5246028
N	-0.0478198	2.1764821	-0.5488481
H	3.1603588	1.6494208	-0.0802555
C	-1.3054123	0.1368856	-0.1916870
H	-2.1696428	0.7602147	-0.4318147
C	-1.4374832	-3.3820473	0.6435775
C	-2.8122092	-3.1325285	0.4522864
C	-2.9494702	-1.7675338	0.1108501
C	-1.6460571	-1.1979404	0.0991386
N	-0.7637975	-2.2192729	0.4294551
H	0.2445698	-2.0815864	0.4885484
C	-0.7296816	-4.6368494	1.0221350
H	0.1787412	-4.7802501	0.4215806
H	-0.4249403	-4.6223371	2.0795813
H	-1.3781406	-5.5072533	0.8758103
C	-3.9191238	-4.1351307	0.6110409
H	-4.7005276	-3.9333275	-0.1366823
H	-3.5386004	-5.1425770	0.3885349
O	1.6513059	-0.7993769	0.3395030
C	3.0663365	-1.0189747	0.5413822
H	3.1715341	-2.0736326	0.8044335
H	3.6165700	-0.8019744	-0.3826768
H	3.4325253	-0.3862306	1.3596439
H	-0.8710907	2.7280592	-0.7600695
C	-4.2296701	-1.0479193	-0.1759274
H	-4.6949466	-0.6614840	0.7436178
H	-4.0831016	-0.1946001	-0.8492855
H	-4.9599336	-1.7197529	-0.6457957
C	-4.5564795	-4.1361858	2.0133231
H	-4.9811346	-3.1528999	2.2551197
H	-5.3641886	-4.8781618	2.0750667
H	-3.8126742	-4.3779638	2.7839894

IIIδ

C	3.3200415	-1.0349359	0.2148308
C	3.0061506	-2.4171848	0.3913939
C	4.2293016	-3.0702941	0.5281794
C	5.2256726	-2.0551852	0.4278106
N	4.6959137	-0.8341869	0.2401073
H	2.0180963	-2.8710771	0.4066976
H	4.3958476	-4.1343450	0.6763530
H	6.3053978	-2.1913826	0.4878524
C	0.4424049	1.1713692	-0.0569519
C	1.5327233	2.1116975	-0.2049335
C	2.7376443	1.4278667	-0.1611032
C	2.4323547	0.0500910	0.0380979
N	1.0601186	-0.0820127	0.0468358
H	3.7399148	1.8241002	-0.2577616
C	-0.9040438	1.4616754	-0.0400428
H	-1.1385356	2.5263600	-0.0328515
C	-3.2484736	-1.3006546	-0.1771360
C	-4.1386989	-0.2531459	0.1167486
C	-3.3781516	0.9384010	0.2024765
C	-2.0209731	0.5989718	-0.0243672
N	-1.9865150	-0.7795978	-0.2316282
C	-3.4996510	-2.7542398	-0.3876337
H	-4.5128569	-2.9266991	-0.7664121
H	-2.7873164	-3.1806877	-1.1059010
H	-3.3972879	-3.3182478	0.5522016
C	-5.6271318	-0.3930821	0.2764038
H	-5.9767462	0.2919057	1.0629187
H	-5.8639275	-1.4055961	0.6328797
O	1.2808876	3.4168261	-0.3824104
C	2.4370363	4.2704000	-0.5297035
H	2.0468491	5.2830452	-0.6530557
H	3.0677312	4.2148134	0.3669376
H	3.0153696	3.9769082	-1.4154761
H	0.6081308	-0.8881579	0.4621437
H	-1.1988276	-1.2881550	-0.6158984
C	-3.8865220	2.3124010	0.5140554
H	-3.4113570	2.7301994	1.4125955
H	-3.6914183	3.0147878	-0.3094134
H	-4.9685704	2.3013068	0.6870515
C	-6.4123754	-0.1153242	-1.0189577
H	-7.4925718	-0.2241446	-0.8526615
H	-6.2259720	0.9038966	-1.3827434
H	-6.1186621	-0.8122952	-1.8152678

IV α

C	1.4903983	3.8798407	-0.7425582
C	2.7647873	4.4681682	-0.7733980
C	2.5986422	5.8342492	-1.0798993
C	1.2329865	6.0621165	-1.2314316
N	0.5784412	4.8828244	-1.0264303

H	-0.4287885	4.7811356	-1.0786444
H	3.6998391	3.9500074	-0.5920460
H	3.3793545	6.5795238	-1.1821770
H	0.6843565	6.9663210	-1.4671341
C	-0.1528949	0.6659616	-0.1797657
C	1.2329531	0.3156478	0.0036898
C	2.0172421	1.4483068	-0.1782588
C	1.1379633	2.5216052	-0.4776898
N	-0.1300275	2.0359897	-0.4727603
H	3.0944970	1.5246848	-0.1100013
C	-1.3620163	-0.0188490	-0.1236556
H	-2.2372637	0.6049369	-0.3176639
C	-1.4232673	-3.5492616	0.5902508
C	-2.8145348	-3.3094170	0.4578072
C	-2.9780899	-1.9425174	0.1737034
C	-1.6748966	-1.3552536	0.1351984
N	-0.7698892	-2.3796499	0.3965138
H	0.2396166	-2.2340478	0.4271669
C	-0.7000918	-4.8114385	0.8994735
H	0.2552706	-4.8651288	0.3626728
H	-0.4800955	-4.8859338	1.9753467
H	-1.3041101	-5.6833438	0.6254758
C	-3.8934362	-4.3397664	0.6227260
H	-3.5253974	-5.3154867	0.2738679
H	-4.7411905	-4.0829372	-0.0287174
O	1.6216364	-0.9378235	0.3044306
C	3.0457334	-1.1474504	0.4634295
H	3.1658648	-2.2047557	0.7076421
H	3.5660452	-0.9125961	-0.4731490
H	3.4271339	-0.5237873	1.2812285
H	-0.9723216	2.5698832	-0.6538313
C	-4.2687319	-1.2190697	-0.0386504
H	-4.6521600	-0.7953689	0.9015937
H	-4.1653923	-0.3909403	-0.7505774
H	-5.0390998	-1.8981980	-0.4238433
C	-4.3952252	-4.4787568	2.0725237
H	-5.1817575	-5.2421761	2.1394919
H	-3.5798965	-4.7717023	2.7473040
H	-4.8093134	-3.5305069	2.4393992

IV β

C	2.7949060	1.9881306	0.0562927
C	4.1403663	2.3844237	0.1433160
C	4.1689521	3.7912411	0.2006502
C	2.8490679	4.2359616	0.1454446
N	2.0349702	3.1462850	0.0628810
H	1.0269584	3.2013922	-0.0259377
H	4.9916120	1.7134798	0.1730276
H	5.0463813	4.4234670	0.2755649
H	2.4356654	5.2375633	0.1536446

C	0.7091479	-0.9974789	0.0195301
C	2.0257226	-1.5712289	-0.0805843
C	2.9674676	-0.5449380	-0.1134814
C	2.2530427	0.6716131	-0.0117336
N	0.9111946	0.3892884	0.0238416
H	4.0415363	-0.6314363	-0.2138791
C	-0.4894762	-1.6846623	0.0911385
H	-0.3793265	-2.7637684	0.2054559
C	-3.5711407	0.1600182	-0.2673521
C	-4.0908992	-1.0887325	0.1407917
C	-2.9984126	-1.9585861	0.3249003
C	-1.8102037	-1.2230756	0.0451253
N	-2.2140468	0.0700952	-0.2901022
C	-4.2796247	1.4136574	-0.6386877
H	-4.5694796	1.9837221	0.2568881
H	-3.6457125	2.0616514	-1.2552512
H	-5.1993927	1.1919094	-1.1935886
C	-5.5457982	-1.3943899	0.3505683
H	-6.1483356	-0.7925435	-0.3450810
H	-5.7372859	-2.4450289	0.0896128
O	2.1913206	-2.8953090	-0.1613298
C	3.5565181	-3.3630657	-0.2608906
H	3.4948191	-4.4525673	-0.2985490
H	4.0219184	-2.9777710	-1.1769087
H	4.1310308	-3.0466081	0.6190586
H	0.2209627	1.0408896	0.3801964
H	-1.6257130	0.7666444	-0.7338620
C	-3.0470462	-3.3835183	0.7738429
H	-2.3108608	-4.0033083	0.2455437
H	-2.8361774	-3.4752878	1.8495499
H	-4.0391339	-3.8165922	0.5985520
C	-6.0284013	-1.1359634	1.7900080
H	-5.8864595	-0.0844055	2.0720234
H	-7.0959893	-1.3729528	1.8896033
H	-5.4746030	-1.7538317	2.5090129

IV γ

C	1.4127556	3.8972150	-0.7344509
C	0.5751265	4.9728137	-1.0680250
C	1.3874683	6.1173425	-1.2078450
C	2.7023478	5.7276025	-0.9592573
N	2.7033122	4.3948698	-0.6777150
H	3.5323540	3.8554630	-0.4555103
H	-0.5011174	4.9245441	-1.1956495
H	1.0619595	7.1199077	-1.4615173
H	3.6247149	6.2961541	-0.9623600
C	-0.1705803	0.6619434	-0.2084015
C	1.2128784	0.3183476	0.0010076
C	1.9951319	1.4574523	-0.1638619
C	1.1139052	2.5243401	-0.4775393

N	-0.1498705	2.0298402	-0.5006477
H	3.0716919	1.5302656	-0.0758848
C	-1.3768537	-0.0311229	-0.1716041
H	-2.2521748	0.5847260	-0.3902201
C	-1.4422400	-3.5480664	0.6047456
C	-2.8312580	-3.3143242	0.4311132
C	-2.9895968	-1.9544853	0.1148591
C	-1.6868476	-1.3653269	0.0968336
N	-0.7864609	-2.3813241	0.4018906
H	0.2214601	-2.2308633	0.4511530
C	-0.7185843	-4.8031745	0.9424141
H	0.0316741	-5.0454567	0.1765533
H	-0.1893184	-4.7087600	1.9017561
H	-1.4128180	-5.6452478	1.0200198
C	-3.9116997	-4.3445887	0.5951326
H	-3.5333849	-5.3264249	0.2765867
H	-4.7444166	-4.1084345	-0.0822378
O	1.6037515	-0.9333395	0.3038128
C	3.0262835	-1.1363542	0.4869665
H	3.1481232	-2.1951319	0.7238052
H	3.5617184	-0.8907578	-0.4381891
H	3.3889868	-0.5177597	1.3169644
H	-0.9853495	2.5738376	-0.6851925
C	-4.2687498	-1.2294021	-0.1596673
H	-4.4545067	-0.4403562	0.5826936
H	-4.2589966	-0.7489759	-1.1480505
H	-5.1228328	-1.9147678	-0.1321052
C	-4.4440946	-4.4499147	2.0366311
H	-5.2238666	-5.2198315	2.1076996
H	-3.6406295	-4.7142830	2.7369698
H	-4.8755614	-3.4961003	2.3678215

IVδ

C	2.7436360	1.9896175	0.0431575
C	2.0514825	3.2116101	0.0748360
C	3.0087119	4.2415968	0.1639628
C	4.2665351	3.6387986	0.1857059
N	4.0937715	2.2906671	0.1101928
H	4.8480758	1.6133817	0.1221942
H	0.9745939	3.3333487	0.0253278
H	2.8171486	5.3078723	0.2051555
H	5.2587736	4.0697539	0.2503161
C	0.7246488	-1.0242051	-0.0063556
C	2.0430135	-1.5918571	-0.1145050
C	2.9820476	-0.5601592	-0.1431673
C	2.2601216	0.6509185	-0.0348384
N	0.9220946	0.3603856	0.0043150
H	4.0560353	-0.6499792	-0.2460229
C	-0.4732338	-1.7140487	0.0693513
H	-0.3639483	-2.7938567	0.1741644

C	-3.5417446	0.1591572	-0.2519417
C	-4.0713916	-1.0875998	0.1460428
C	-2.9861181	-1.9699615	0.3185828
C	-1.7916709	-1.2445933	0.0385242
N	-2.1844774	0.0564652	-0.2809702
C	-4.2356785	1.4246406	-0.6088067
H	-4.3632799	2.0676684	0.2753336
H	-3.6654529	1.9958635	-1.3517805
H	-5.2337026	1.2215220	-1.0134050
C	-5.5273790	-1.3863110	0.3583008
H	-6.1294628	-0.7890643	-0.3417506
H	-5.7206524	-2.4389434	0.1067967
O	2.2138954	-2.9153693	-0.2032406
C	3.5815389	-3.3786195	-0.3028798
H	3.5216658	-4.4679300	-0.3468386
H	4.0467758	-2.9867069	-1.2160026
H	4.1523152	-3.0658476	0.5806351
H	0.2389395	1.0193759	0.3587287
H	-1.5939927	0.7446480	-0.7343154
C	-3.0560580	-3.3963173	0.7571267
H	-2.1951712	-3.9785438	0.4079884
H	-3.0798606	-3.4778063	1.8541172
H	-3.9660893	-3.8791452	0.3797275
C	-6.0103326	-1.1144013	1.7950152
H	-5.8726487	-0.0594472	2.0653369
H	-7.0769182	-1.3539494	1.8970082
H	-5.4545916	-1.7219232	2.5208273

IV α ·Cl⁻

C	2.5272300	2.0040312	0.2741682
C	3.7953275	2.6088370	0.2490265
C	3.6079265	3.9739529	-0.0486042
C	2.2363383	4.1793326	-0.1996165
N	1.5974019	2.9920724	-0.0040448
H	0.5729255	2.8473633	-0.0540742
H	4.7381359	2.1035169	0.4281609
H	4.3767361	4.7326251	-0.1452355
H	1.6786652	5.0798167	-0.4302788
C	0.8932986	-1.2073581	0.8185485
C	2.2804720	-1.5639191	1.0038317
C	3.0656263	-0.4330848	0.8273455
C	2.1819674	0.6415427	0.5311826
N	0.9135445	0.1619629	0.5306103
H	4.1429518	-0.3572334	0.8980097
C	-0.3148777	-1.8936274	0.8701884
H	-1.1896282	-1.2699230	0.6708466
C	-0.3791114	-5.4222643	1.6070668
C	-1.7681779	-5.1849365	1.4557134
C	-1.9296030	-3.8188844	1.1592541
C	-0.6285363	-3.2314248	1.1305000

N	0.2746775	-4.2517615	1.4098940
H	1.2827997	-4.0986217	1.4464241
C	0.3496373	-6.6817089	1.9192784
H	1.0946583	-6.9116544	1.1444719
H	0.8850235	-6.6036986	2.8768021
H	-0.3430159	-7.5260168	1.9878279
C	-2.8485851	-6.2155867	1.6198498
H	-2.4767428	-7.1940047	1.2835346
H	-3.6891821	-5.9688700	0.9558661
O	2.6679419	-2.8209433	1.3005663
C	4.0915789	-3.0307609	1.4598599
H	4.2134436	-4.0900028	1.6952486
H	4.6132726	-2.7875251	0.5260981
H	4.4716888	-2.4133325	2.2830781
H	0.0605329	0.7273425	0.3462963
Cl	-1.4935932	2.1347248	-0.0708606
C	-3.2129194	-3.0906811	0.9109965
H	-3.3896016	-2.3106247	1.6650073
H	-3.2182059	-2.5998478	-0.0723919
H	-4.0666561	-3.7764503	0.9425092
C	-3.3644408	-6.3395824	3.0657386
H	-4.1548155	-7.0990624	3.1331291
H	-2.5561967	-6.6286709	3.7507454
H	-3.7773151	-5.3858339	3.4199632

IV α ·MeSO₃⁻

C	-0.7754555	0.0478005	0.0311125
C	-0.5079373	1.4658986	0.0233867
C	0.8651443	1.6646876	0.0507998
C	1.4708009	0.3774780	0.0777730
N	0.4880822	-0.5574437	0.0723188
H	1.3976691	2.6064590	0.0768047
C	-1.9218538	-0.7389161	0.0089465
H	-1.7214399	-1.8126144	0.0301371
C	-5.1816528	0.7986804	-0.1047952
C	-5.5622330	-0.5661770	-0.0967227
C	-4.3810569	-1.3301604	-0.0565094
C	-3.2827690	-0.4181586	-0.0378842
N	-3.8280877	0.8608948	-0.0704090
H	-3.2531694	1.7034623	-0.0540537
C	-6.0202189	2.0282352	-0.1355838
H	-5.8251050	2.6638034	0.7399460
H	-5.8089257	2.6300158	-1.0311135
H	-7.0844863	1.7737215	-0.1412208
O	-1.4931297	2.3866951	0.0089133
C	-1.0741154	3.7722717	0.0090781
H	-1.9924990	4.3626056	-0.0089418
H	-0.5007696	3.9906819	0.9184452
H	-0.4706936	3.9818413	-0.8827031
H	0.6035631	-1.5853334	-0.0379195

C	3.9431256	0.9837446	-0.0868865
C	2.8722078	0.0957464	0.1139431
C	5.1366811	0.2438388	0.0313218
N	3.4156353	-1.1563727	0.3481887
C	4.7760258	-1.0742136	0.3087650
H	2.9078162	-2.0178751	0.6235888
H	3.8503326	2.0402217	-0.3139289
C	-4.2710291	-2.8220848	-0.0381125
H	-3.8655749	-3.2109501	-0.9833534
H	-3.6118547	-3.1728541	0.7676498
H	-5.2526150	-3.2854679	0.1115734
S	1.1904751	-4.2501385	0.5231935
O	2.2831856	-3.5666070	1.2695724
O	0.2683677	-4.9819457	1.4068849
O	0.5001968	-3.3059789	-0.3998050
C	1.9797821	-5.4689985	-0.5245563
H	2.5108360	-6.1810245	0.1151253
H	1.2050913	-5.9818335	-1.1034742
H	2.6803501	-4.9579514	-1.1921671
H	6.1496808	0.6163260	-0.0738988
H	5.3899292	-1.9494559	0.4887304
C	-6.9731116	-1.0793044	-0.1519498
H	-7.6448377	-0.3623510	0.3414559
H	-7.0434943	-2.0084234	0.4312788
C	-7.4758413	-1.3423344	-1.5836491
H	-8.5067780	-1.7202897	-1.5704912
H	-7.4575665	-0.4227808	-2.1834224
H	-6.8471696	-2.0856200	-2.0916176

IV β -CT

C	-4.1577984	-1.0288817	-0.1938622
C	-5.5574887	-0.8988181	-0.1604376
C	-6.1062123	-2.1944662	-0.2331375
C	-5.0397386	-3.0910229	-0.3098628
N	-3.8774898	-2.3818112	-0.2846678
H	-2.9291169	-2.7896864	-0.3363113
H	-6.1019450	0.0364479	-0.0891219
H	-7.1577285	-2.4593139	-0.2302459
H	-5.0302801	-4.1726239	-0.3806568
C	-1.1160451	0.9692081	-0.1112778
C	-2.1324420	1.9940455	-0.0458918
C	-3.3851498	1.3935784	-0.0626689
C	-3.1626622	-0.0055832	-0.1437273
N	-1.8169610	-0.2367960	-0.1683891
H	-4.3552060	1.8721876	-0.0239427
C	0.2476598	1.2145694	-0.0983909
H	0.4730766	2.2806005	-0.0424476
C	2.7556472	-1.3855258	-0.2128086
C	3.5863011	-0.2429512	-0.1301945
C	2.7423575	0.8789410	-0.0803998

C	1.3921607	0.4080658	-0.1309138
N	1.4606163	-0.9816026	-0.2095452
C	3.1328319	-2.8239366	-0.2929515
H	3.5467763	-3.1775143	0.6627744
H	2.2656259	-3.4475986	-0.5377479
H	3.9064281	-2.9825661	-1.0561365
C	5.0869622	-0.2633486	-0.0782331
H	5.4599984	-1.1381607	-0.6307159
H	5.4823210	0.6191837	-0.6025059
O	-1.7973225	3.2900504	0.0203814
C	-2.8944598	4.2268398	0.1001576
H	-2.4375461	5.2178051	0.1446734
H	-3.5308621	4.1437820	-0.7902810
H	-3.4864299	4.0419640	1.0058948
H	-1.4012641	-1.1799043	-0.2467513
H	0.6756032	-1.6480067	-0.2822233
Cl	-0.8034782	-3.2599808	-0.4417708
C	3.1657430	2.3100745	0.0238722
H	2.5149870	2.9779857	-0.5545119
H	3.1501512	2.6619298	1.0663697
H	4.1901998	2.4414037	-0.3455633
C	5.6520616	-0.2918973	1.3543306
H	5.3102669	-1.1830157	1.8976748
H	6.7499756	-0.3042383	1.3393826
H	5.3298760	0.5905883	1.9227828

IV β -MeSO₃⁻

C	-0.4306373	1.2971747	0.0554845
C	-1.4553345	2.3098396	0.1605699
C	-2.6986752	1.6951218	0.1999410
C	-2.4640072	0.2978931	0.1272060
N	-1.1169746	0.0773533	0.0478937
H	-3.6705257	2.1606053	0.2999425
C	0.9231340	1.5897320	-0.0117352
H	1.1003859	2.6650253	0.0469001
C	3.5709054	-0.8408231	-0.3855942
C	4.3335628	0.3465664	-0.2847139
C	3.4270987	1.4087346	-0.1331995
C	2.1077425	0.8539350	-0.1361162
N	2.2551378	-0.5227759	-0.2865744
C	4.0284749	-2.2399760	-0.6105251
H	5.0090053	-2.4094214	-0.1505991
H	3.3137266	-2.9603287	-0.1945700
H	4.1330154	-2.4496987	-1.6864999
O	-1.1341367	3.6100984	0.2156797
C	-2.2394644	4.5332771	0.3307073
H	-1.7939364	5.5301341	0.3547676
H	-2.9061261	4.4380367	-0.5360848
H	-2.7967788	4.3456956	1.2577086
H	-0.6872846	-0.8469084	-0.1160441

H	1.4980363	-1.2202875	-0.3647923
C	-4.8632027	-0.5287380	-0.0245412
C	-3.4777193	-0.7108813	0.1390162
C	-5.4726487	-1.7960117	0.0509362
N	-3.2630482	-2.0678993	0.3089131
C	-4.4563330	-2.7258378	0.2669153
H	-2.3763996	-2.5445385	0.5499777
H	-5.3556149	0.4210144	-0.2023537
C	3.7699791	2.8558544	0.0262264
H	3.0268142	3.5127292	-0.4430279
H	3.8345039	3.1426921	1.0865820
H	4.7437602	3.0778312	-0.4278953
S	0.1000516	-3.6647064	0.2205577
O	1.3477475	-3.9329790	0.9489285
O	-1.1041948	-3.6884535	1.0875060
O	0.1519511	-2.3949264	-0.5767729
C	-0.1037286	-4.9687625	-0.9844993
H	-0.1649194	-5.9207482	-0.4478076
H	-1.0236940	-4.7864155	-1.5482756
H	0.7632037	-4.9618592	-1.6522900
H	-6.5294891	-2.0200272	-0.0429698
H	-4.5010442	-3.8004047	0.4033195
C	5.8335117	0.4226719	-0.3129088
H	6.1418327	1.3470164	-0.8239216
H	6.2315205	-0.4044479	-0.9178239
C	6.4760511	0.3839139	1.0864610
H	7.5699351	0.4460823	1.0145498
H	6.1275878	1.2224552	1.7038271
H	6.2220933	-0.5461841	1.6126420

IV γ -Cl⁻

C	0.8411031	-1.1640315	0.8079467
C	2.2248912	-1.5144711	1.0152651
C	3.0092064	-0.3836386	0.8214371
C	2.1240761	0.6800782	0.4918699
N	0.8583277	0.1975748	0.4891216
H	4.0866379	-0.3123496	0.9022952
C	-0.3696333	-1.8482118	0.8643045
H	-1.2368845	-1.2191566	0.6441883
C	-0.4424685	-5.3613817	1.6646540
C	-1.8309056	-5.1249861	1.5083138
C	-1.9903461	-3.7650978	1.1871018
C	-0.6875086	-3.1785539	1.1502057
N	0.2136887	-4.1964749	1.4489327
H	1.2228316	-4.0500815	1.4875817
C	0.2766892	-6.6152533	2.0159266
H	1.2488507	-6.6723019	1.5106112
H	0.4623456	-6.6736435	3.0992479
H	-0.3140692	-7.4944322	1.7356922
O	2.6117170	-2.7630187	1.3427057

C	4.0333351	-2.9678855	1.5220878
H	4.1528822	-4.0210291	1.7843180
H	4.5651835	-2.7468082	0.5884927
H	4.4045626	-2.3307776	2.3343821
H	-0.0126149	0.7359797	0.2860382
Cl	-1.9148115	1.5736650	-0.0817395
C	1.6097798	3.1282977	-0.1280842
C	2.4383030	2.0451038	0.2024434
C	2.4379701	4.2563109	-0.3118694
N	3.7386700	2.5214604	0.2151704
C	3.7525834	3.8492297	-0.0923748
H	4.5648551	1.9713927	0.4208307
H	0.5282006	3.0813771	-0.2191733
C	-3.2798015	-3.0499028	0.9412755
H	-3.6960541	-2.6382533	1.8728944
H	-3.1617615	-2.2147153	0.2402644
H	-4.0326002	-3.7317023	0.5262459
H	4.6842799	4.4010815	-0.1321971
H	2.1231476	5.2601593	-0.5746414
C	-2.9141231	-6.1488573	1.6856049
H	-2.5376024	-7.1376813	1.3860706
H	-3.7444307	-5.9187069	1.0023232
C	-3.4547620	-6.2300365	3.1258917
H	-3.8754304	-5.2672505	3.4443654
H	-4.2455497	-6.9882600	3.2018475
H	-2.6584770	-6.4979193	3.8329023

IV γ -MeSO₃⁻

C	-0.5563017	0.0134347	0.0103794
C	-0.3651694	1.4433207	-0.0096796
C	0.9969048	1.7170930	0.0007762
C	1.6683481	0.4643762	0.0210335
N	0.7379278	-0.5216539	0.0308152
H	1.4688920	2.6915369	-0.0003055
C	-1.6624721	-0.8323387	0.0298061
H	-1.4084103	-1.8942014	0.0912520
C	-4.9937684	0.5462940	-0.0324121
C	-5.3103830	-0.8329096	0.0111896
C	-4.0954642	-1.5418935	0.0340071
C	-3.0379951	-0.5798544	0.0060910
N	-3.6448862	0.6724064	-0.0377751
H	-3.1148282	1.5442799	-0.0504716
C	-5.8934892	1.7303838	-0.0813372
H	-5.4856965	2.5657718	0.5018249
H	-6.0262626	2.0831847	-1.1153051
H	-6.8849720	1.4822716	0.3131018
O	-1.3959532	2.3113218	-0.0245057
C	-1.0518159	3.7171137	-0.0306959
H	-2.0007052	4.2570013	-0.0458731
H	-0.4864274	3.9691124	0.8750568

H	-0.4655876	3.9561336	-0.9266608
H	0.9361356	-1.5434136	-0.0118012
C	3.7996483	-0.9888551	0.0732863
C	3.0768403	0.2130630	0.0335298
C	5.1721877	-0.6601767	0.0748214
N	4.0057636	1.2407961	0.0120745
C	5.2690016	0.7293857	0.0364245
H	3.7881613	2.2303227	-0.0189919
H	3.3588311	-1.9802988	0.0959289
C	-3.9387646	-3.0279650	0.0715012
H	-4.1350059	-3.4738571	-0.9154617
H	-2.9317282	-3.3341606	0.3778102
H	-4.6573561	-3.4783192	0.7700746
S	0.6700068	-4.3245826	0.5559363
O	1.6110665	-4.9196425	1.5268674
O	-0.6045352	-3.8894903	1.1667401
O	1.3028028	-3.2428490	-0.2553206
C	0.2637528	-5.6200625	-0.6158797
H	-0.2021077	-6.4460963	-0.0691061
H	-0.4308896	-5.2156229	-1.3586241
H	1.1864164	-5.9565118	-1.0993057
H	6.1336812	1.3822925	0.0248178
H	6.0075890	-1.3510572	0.1013978
C	-6.6939959	-1.4154405	0.0085221
H	-6.6964025	-2.3395672	0.6045170
H	-7.3856407	-0.7247170	0.5123667
C	-7.2299151	-1.7251807	-1.4020851
H	-6.5805209	-2.4405385	-1.9236634
H	-8.2375421	-2.1584925	-1.3483149
H	-7.2835301	-0.8141652	-2.0125658

IV8-CI⁺

C	-3.5045423	-0.9204238	-0.0809481
C	-3.4255371	-2.3207861	-0.1391469
C	-4.7440809	-2.8211986	-0.1777325
C	-5.6072701	-1.7275164	-0.1425892
N	-4.8530337	-0.5954027	-0.0843562
H	-5.2320839	0.3439983	-0.0505286
H	-2.5002379	-2.8901122	-0.1508294
H	-5.0444748	-3.8620205	-0.2257680
H	-6.6895403	-1.6745197	-0.1551034
C	-0.4349861	1.0296911	0.0397904
C	-1.4323127	2.0722277	0.0905963
C	-2.6955281	1.4945795	0.0522474
C	-2.4968373	0.0924535	-0.0224572
N	-1.1546929	-0.1661701	-0.0287800
H	-3.6520980	2.0013609	0.0765361
C	0.9299615	1.2833138	0.0606900
H	1.1355321	2.3532845	0.1246176
C	3.5235285	-1.2232777	-0.0921391

C	4.3138956	-0.0486868	-0.0122802
C	3.4295517	1.0374515	0.0575570
C	2.0962677	0.5132098	0.0196416
N	2.2161222	-0.8711594	-0.0711168
C	3.9576278	-2.6435965	-0.2008691
H	4.5743692	-2.9353090	0.6607222
H	3.0939735	-3.3158241	-0.2533184
H	4.5735472	-2.7951361	-1.0987774
C	5.8156084	-0.0223194	0.0181422
H	6.2059857	-0.8546138	-0.5857626
H	6.1767162	0.8974329	-0.4639839
O	-1.0783216	3.3629000	0.1613091
C	-2.1607093	4.3188153	0.2082194
H	-1.6876768	5.3017457	0.2617814
H	-2.7739068	4.2436040	-0.6990634
H	-2.7801602	4.1485665	1.0982580
H	-0.7518247	-1.1193240	-0.0841457
H	1.4494366	-1.5704993	-0.1168860
Cl	0.0637482	-3.1526045	-0.1937363
C	3.7864389	2.4880451	0.1508593
H	3.3586277	3.0679789	-0.6793574
H	3.4184242	2.9387514	1.0836799
H	4.8729891	2.6269938	0.1250102
C	6.4021885	-0.1108518	1.4395574
H	6.0901109	-1.0366142	1.9414134
H	7.4997516	-0.0954368	1.4094501
H	6.0663147	0.7329253	2.0569692

IVδ-MeSO₃⁻

C	-0.4603622	1.2457551	0.0820134
C	-1.4799128	2.2638819	0.1746215
C	-2.7273696	1.6544592	0.2189575
C	-2.4964349	0.2568549	0.1608278
N	-1.1508624	0.0303502	0.0805477
H	-3.6933911	2.1361080	0.3027581
C	0.8938538	1.5416119	0.0107323
H	1.0633698	2.6184333	0.0644551
C	3.5784161	-0.8425818	-0.3887496
C	4.3179975	0.3623403	-0.3106390
C	3.3936062	1.4044447	-0.1458675
C	2.0854168	0.8210010	-0.1196167
N	2.2582828	-0.5541912	-0.2651513
C	4.0707583	-2.2286255	-0.6161540
H	5.0480552	-2.3779548	-0.1418334
H	3.3660274	-2.9688196	-0.2185410
H	4.2004730	-2.4242766	-1.6922053
O	-1.1557179	3.5636273	0.2070216
C	-2.2581144	4.4930148	0.2997270
H	-1.8084799	5.4882444	0.3082833
H	-2.9201394	4.3848952	-0.5690744

H	-2.8209134	4.3244946	1.2269978
H	-0.7260423	-0.9059655	-0.0068580
H	1.5124137	-1.2709399	-0.2988727
C	-3.3782345	-2.1749658	0.2735419
C	-3.4822422	-0.7781713	0.1887564
C	-4.6889381	-2.6984820	0.2853278
N	-4.8364394	-0.4777065	0.1540819
C	-5.5711844	-1.6226894	0.2064599
H	-5.2304259	0.4524784	0.0707879
H	-2.4564009	-2.7436328	0.3495362
C	3.7065651	2.8601815	-0.0047537
H	2.9665951	3.4943925	-0.5094372
H	3.7330127	3.1685811	1.0510739
H	4.6893671	3.0905588	-0.4338738
S	0.2997088	-3.8523540	0.1549287
O	1.5971556	-4.0734797	0.8193582
O	-0.8613935	-4.2363554	0.9774142
O	0.1718394	-2.4523036	-0.3739849
C	0.2732943	-4.8987225	-1.2978708
H	0.3638280	-5.9388531	-0.9688550
H	-0.6749911	-4.7461003	-1.8225132
H	1.1151187	-4.6278537	-1.9423906
H	-6.6540733	-1.5902362	0.1820853
H	-4.9715450	-3.7434312	0.3492004
C	5.8151404	0.4663901	-0.3720710
H	6.0955153	1.3976698	-0.8863736
H	6.2143062	-0.3517609	-0.9883245
C	6.4887668	0.4344943	1.0130194
H	7.5796566	0.5144757	0.9173677
H	6.1400735	1.2658154	1.6399603
H	6.2614180	-0.5007261	1.5422241

DMSO SOLUTION

MeSO₃⁻

S	0.3005145	0.5494525	-0.6152716
O	1.7543211	0.2847016	-0.7231166
O	0.0015534	1.9150240	-0.1243142
O	-0.4379343	0.2111071	-1.8542824
C	-0.3145851	-0.5754368	0.6452027
H	0.1988955	-0.3611917	1.5881528
H	-1.3927006	-0.4206824	0.7562435
H	-0.1100646	-1.6029743	0.3273858

IVγ

C	1.4180888	3.8955976	-0.7481806
C	0.5789059	4.9781585	-1.0541115
C	1.3941604	6.1177901	-1.2118968
C	2.7129030	5.7189068	-1.0019167
N	2.7130400	4.3851839	-0.7249354

H	3.5445955	3.8386497	-0.5330837
H	-0.5010008	4.9393905	-1.1497899
H	1.0677838	7.1234097	-1.4515167
H	3.6376984	6.2826094	-1.0298655
C	-0.1702017	0.6633490	-0.2118960
C	1.2130465	0.3183447	-0.0049294
C	1.9969214	1.4554813	-0.1746824
C	1.1177960	2.5240414	-0.4881655
N	-0.1469137	2.0311617	-0.5064072
H	3.0735596	1.5258765	-0.0869801
C	-1.3782414	-0.0268246	-0.1737545
H	-2.2519442	0.5910514	-0.3925856
C	-1.4377244	-3.5426935	0.6024232
C	-2.8273141	-3.3126007	0.4389752
C	-2.9919971	-1.9535233	0.1227378
C	-1.6910830	-1.3598185	0.0970302
N	-0.7861836	-2.3741204	0.3963164
H	0.2219224	-2.2223488	0.4322147
C	-0.7159531	-4.7946657	0.9533532
H	0.2758514	-4.8297473	0.4861853
H	-0.5742340	-4.8767748	2.0416762
H	-1.2827068	-5.6750729	0.6302572
C	-3.9048575	-4.3438885	0.6050635
H	-3.5216817	-5.3279058	0.2983153
H	-4.7337893	-4.1135824	-0.0796176
O	1.6041836	-0.9332676	0.2999401
C	3.0268111	-1.1362382	0.4812577
H	3.1499559	-2.1943114	0.7208542
H	3.5613502	-0.8947088	-0.4454296
H	3.3914419	-0.5167493	1.3096770
H	-0.9806595	2.5759175	-0.6941878
C	-4.2826242	-1.2433605	-0.1283358
H	-4.7071915	-0.8379940	0.8021853
H	-4.1650026	-0.4051039	-0.8254726
H	-5.0291974	-1.9266399	-0.5516925
C	-4.4492395	-4.4391295	2.0430430
H	-5.2341297	-5.2039306	2.1109478
H	-3.6538189	-4.7056801	2.7513622
H	-4.8784840	-3.4821430	2.3671137

IV α -Cl⁻

C	2.5359274	2.0023211	0.2549440
C	3.8042580	2.6066295	0.2224316
C	3.6166856	3.9683696	-0.0881675
C	2.2445984	4.1720189	-0.2392675
N	1.6053956	2.9875113	-0.0311340
H	0.5793566	2.8399412	-0.0791810
H	4.7476323	2.1036716	0.4049701
H	4.3854719	4.7258238	-0.1932772
H	1.6882554	5.0712188	-0.4780387

C	0.8972363	-1.2017026	0.8196327
C	2.2838883	-1.5603845	1.0082043
C	3.0711609	-0.4323964	0.8270809
C	2.1894164	0.6426469	0.5229980
N	0.9207170	0.1659116	0.5245823
H	4.1485048	-0.3581578	0.8979852
C	-0.3139180	-1.8813686	0.8749861
H	-1.1837117	-1.2501690	0.6793421
C	-0.3828139	-5.4141206	1.5910326
C	-1.7712466	-5.1744374	1.4596565
C	-1.9356536	-3.8054198	1.1744662
C	-0.6349013	-3.2183732	1.1344789
N	0.2701297	-4.2421514	1.3955844
H	1.2792051	-4.0933912	1.4173111
C	0.3444179	-6.6749485	1.9004298
H	1.2704573	-6.7559076	1.3167193
H	0.6195081	-6.7242474	2.9648406
H	-0.2789984	-7.5481591	1.6804753
C	-2.8548381	-6.2003790	1.6232289
H	-2.4849492	-7.1822115	1.2940201
H	-3.6912606	-5.9513041	0.9539378
O	2.6685464	-2.8169796	1.3127361
C	4.0901749	-3.0262161	1.4829082
H	4.2113141	-4.0836838	1.7269176
H	4.6194018	-2.7911841	0.5512359
H	4.4657093	-2.4040165	2.3047060
H	0.0671699	0.7335575	0.3337985
Cl	-1.4655441	2.1171338	-0.0858552
C	-3.2314948	-3.0908010	0.9632634
H	-3.6870910	-2.7899609	1.9185886
H	-3.1129327	-2.1838396	0.3587970
H	-3.9566832	-3.7367101	0.4516974
C	-3.3812501	-6.3171295	3.0661755
H	-4.1752757	-7.0729668	3.1307641
H	-2.5792819	-6.6076419	3.7576769
H	-3.7932302	-5.3614084	3.4153046

IV α ·MeSO₃⁻

C	-0.7500585	0.0182092	0.0054434
C	-0.5039899	1.4402562	-0.0117522
C	0.8662507	1.6590825	-0.0106551
C	1.4911159	0.3798435	0.0106782
N	0.5224563	-0.5675625	0.0247982
H	1.3857526	2.6083687	0.0025411
C	-1.8807510	-0.7904524	0.0048164
H	-1.6549056	-1.8590606	0.0186888
C	-5.1687990	0.6877730	-0.0243832
C	-5.5267820	-0.6812606	-0.0172876
C	-4.3328586	-1.4269562	-0.0112422
C	-3.2489138	-0.4979575	-0.0135811

N	-3.8154731	0.7723688	-0.0237123
H	-3.2560620	1.6252411	-0.0111808
C	-6.0314823	1.9005004	-0.0454356
H	-5.5854131	2.7191914	0.5333450
H	-6.1807603	2.2643114	-1.0732921
H	-7.0205816	1.6824487	0.3724297
O	-1.5039802	2.3459179	-0.0118012
C	-1.1058379	3.7366394	-0.0206974
H	-2.0321225	4.3148925	-0.0291655
H	-0.5250472	3.9675289	0.8809446
H	-0.5173279	3.9537853	-0.9207074
H	0.6470413	-1.5984518	-0.0755340
C	3.9563376	1.0040821	-0.2068845
C	2.8955161	0.1117351	0.0248577
C	5.1567369	0.2737303	-0.1014737
N	3.4512087	-1.1340298	0.2651964
C	4.8096479	-1.0427995	0.1997759
H	2.9539753	-1.9956399	0.5642815
H	3.8529212	2.0567949	-0.4462549
C	-4.2158481	-2.9175031	-0.0106225
H	-4.3007336	-3.3298300	-1.0272961
H	-3.2586051	-3.2584647	0.4009928
H	-5.0158758	-3.3730574	0.5871883
S	1.2083111	-4.2040012	0.5798818
O	2.3499567	-3.5227433	1.2527799
O	0.2782118	-4.8322267	1.5289068
O	0.5402308	-3.2933022	-0.3917138
C	1.9172327	-5.5225772	-0.4040850
H	2.4314284	-6.2168513	0.2679822
H	1.1065212	-6.0345384	-0.9319569
H	2.6234002	-5.0891879	-1.1192371
H	6.1649931	0.6514302	-0.2303847
H	5.4335517	-1.9106446	0.3809327
C	-6.9277937	-1.2203937	-0.0366626
H	-6.9640815	-2.1511437	0.5478803
H	-7.6006740	-0.5152994	0.4726263
C	-7.4635832	-1.4951084	-1.4544423
H	-6.8342618	-2.2249245	-1.9804226
H	-8.4852399	-1.8954491	-1.4133787
H	-7.4823291	-0.5759472	-2.0545711

IV β -Cl⁻

C	-3.4614694	-0.8872256	-0.0805313
C	-4.8614317	-0.7583486	-0.0557598
C	-5.4086201	-2.0542645	-0.1295271
C	-4.3408826	-2.9499506	-0.1981210
N	-3.1792691	-2.2401651	-0.1675006
H	-2.2287774	-2.6467416	-0.2094190
H	-5.4077434	0.1761608	0.0101260
H	-6.4599050	-2.3197009	-0.1327731

H	-4.3317720	-4.0317045	-0.2662837
C	-0.4187125	1.1069211	0.0149156
C	-1.4331129	2.1336931	0.0778079
C	-2.6867866	1.5354038	0.0543745
C	-2.4664613	0.1356977	-0.0266794
N	-1.1210371	-0.0976560	-0.0469011
H	-3.6561218	2.0156001	0.0891177
C	0.9452729	1.3501174	0.0295605
H	1.1705047	2.4161364	0.0864763
C	3.4487640	-1.2531208	-0.0894449
C	4.2816184	-0.1116584	-0.0098122
C	3.4395687	1.0111132	0.0417316
C	2.0887055	0.5422220	-0.0045848
N	2.1546642	-0.8474618	-0.0835061
C	3.8224465	-2.6924031	-0.1722962
H	4.2738871	-3.0389336	0.7687837
H	2.9458791	-3.3171041	-0.3777072
H	4.5649836	-2.8585486	-0.9644408
C	5.7824229	-0.1358813	0.0370876
H	6.1508500	-1.0128823	-0.5150448
H	6.1790895	0.7434290	-0.4915729
O	-1.0942977	3.4284401	0.1478542
C	-2.1886161	4.3677815	0.2196580
H	-1.7302080	5.3576498	0.2724272
H	-2.8163661	4.2906930	-0.6775932
H	-2.7908512	4.1828165	1.1187092
H	-0.7065836	-1.0435421	-0.1171232
H	1.3682324	-1.5149895	-0.1477372
Cl	-0.1106857	-3.1074384	-0.2836935
C	3.8631055	2.4426549	0.1413772
H	3.2461536	3.1012295	-0.4834655
H	3.7958693	2.8156678	1.1744034
H	4.9048983	2.5650576	-0.1784622
C	6.3526019	-0.1626684	1.4675753
H	6.0073906	-1.0493733	2.0158643
H	7.4503253	-0.1815950	1.4493425
H	6.0374732	0.7234418	2.0342751

IV β ·MeSO₃⁻

C	-0.4312473	1.2904394	0.0513399
C	-1.4543866	2.3045876	0.1557735
C	-2.6979402	1.6911121	0.2032259
C	-2.4649748	0.2930761	0.1361824
N	-1.1183094	0.0710632	0.0532648
H	-3.6688859	2.1577440	0.3057435
C	0.9222581	1.5830415	-0.0204193
H	1.0964159	2.6591956	0.0294855
C	3.5732550	-0.8469647	-0.3688563
C	4.3347423	0.3420220	-0.2788773
C	3.4270852	1.4047173	-0.1397352

C	2.1083751	0.8485865	-0.1392651
N	2.2572636	-0.5291518	-0.2759347
C	4.0312078	-2.2489407	-0.5756996
H	5.0085773	-2.4146187	-0.1076622
H	3.3126150	-2.9637040	-0.1563703
H	4.1437616	-2.4711305	-1.6483811
O	-1.1304150	3.6043189	0.2047146
C	-2.2332298	4.5289573	0.3202830
H	-1.7872820	5.5256888	0.3409180
H	-2.9023969	4.4337136	-0.5447207
H	-2.7889167	4.3455077	1.2492160
H	-0.6897245	-0.8545830	-0.1128749
H	1.5001776	-1.2282022	-0.3536917
C	-4.8661062	-0.5312215	0.0064088
C	-3.4790823	-0.7147405	0.1565103
C	-5.4762132	-1.7973511	0.0872565
N	-3.2642789	-2.0720119	0.3242649
C	-4.4584750	-2.7280378	0.2929831
H	-2.3750496	-2.5533573	0.5501020
H	-5.3600337	0.4187387	-0.1653157
C	3.7690328	2.8534770	0.0063840
H	3.0276611	3.5063349	-0.4714899
H	3.8324473	3.1516199	1.0636578
H	4.7429447	3.0722527	-0.4489499
S	0.0976949	-3.6645519	0.1949161
O	1.3422396	-3.9504152	0.9189036
O	-1.1111953	-3.7038298	1.0541236
O	0.1540426	-2.3787954	-0.5776494
C	-0.1050976	-4.9415293	-1.0400589
H	-0.1733152	-5.9050839	-0.5254491
H	-1.0201856	-4.7434500	-1.6064097
H	0.7654692	-4.9245944	-1.7027484
H	-6.5341325	-2.0199985	0.0037332
H	-4.5036099	-3.8025008	0.4294700
C	5.8346125	0.4192158	-0.3053118
H	6.1432925	1.3350745	-0.8313050
H	6.2345772	-0.4168290	-0.8965562
C	6.4749818	0.4035954	1.0954293
H	7.5689584	0.4648867	1.0248732
H	6.1251514	1.2515937	1.6988280
H	6.2204856	-0.5175211	1.6367646

IVγ·Cl⁻

C	0.8406208	-1.1323277	0.7843446
C	2.2098710	-1.5077058	1.0406752
C	3.0215281	-0.3940744	0.8637377
C	2.1673389	0.6836949	0.4956670
N	0.8947125	0.2250277	0.4547731
H	4.0968614	-0.3429045	0.9795308
C	-0.3864755	-1.7882439	0.8045455

H	-1.2284036	-1.1395689	0.5456883
C	-0.5578452	-5.2877237	1.6488351
C	-1.9335447	-5.0288412	1.4385989
C	-2.0566308	-3.6705528	1.0922536
C	-0.7436556	-3.1079320	1.0948275
N	0.1273433	-4.1371375	1.4409462
H	1.1371632	-4.0071297	1.5047763
C	0.1253565	-6.5487425	2.0449611
H	1.1116925	-6.6356192	1.5719108
H	0.2752277	-6.5935345	3.1343427
H	-0.4723109	-7.4216831	1.7602891
O	2.5627349	-2.7617537	1.3901077
C	3.9733312	-2.9893887	1.6180208
H	4.0681189	-4.0433678	1.8874523
H	4.5405767	-2.7819226	0.7023605
H	4.3281149	-2.3565504	2.4409609
H	0.0363289	0.7757714	0.2163999
Cl	-1.8222021	1.5985344	-0.2148372
C	1.7121749	3.1327503	-0.1598032
C	2.5136326	2.0405936	0.2052962
C	2.5623808	4.2466760	-0.3266125
N	3.8202023	2.4977480	0.2548797
C	3.8633942	3.8228491	-0.0628684
H	4.6305662	1.9372693	0.4912055
H	0.6332279	3.0988100	-0.2843510
C	-3.3257438	-2.9430945	0.7851993
H	-3.8639063	-2.6667683	1.7042198
H	-3.1498091	-2.0204098	0.2201112
H	-4.0052131	-3.5716138	0.1945083
C	-3.0432530	-6.0286093	1.5879035
H	-3.8446340	-5.7866422	0.8748329
H	-2.6786731	-7.0278478	1.3083068
C	-3.6337273	-6.0866308	3.0096202
H	-4.0427883	-5.1126257	3.3079686
H	-4.4438496	-6.8259936	3.0643333
H	-2.8681500	-6.3668281	3.7449776
H	4.8031541	4.3619628	-0.0783995
H	2.2706580	5.2525965	-0.6072872

IV γ -MeSO₃⁻

C	-0.5646963	0.0022397	0.0380334
C	-0.3729064	1.4320199	-0.0049793
C	0.9885807	1.7050269	-0.0061924
C	1.6597199	0.4517010	0.0315343
N	0.7293335	-0.5330114	0.0629452
H	1.4602321	2.6793601	-0.0272280
C	-1.6711400	-0.8433923	0.0635222
H	-1.4184554	-1.9056454	0.1352510
C	-4.9960769	0.5503820	-0.0195992
C	-5.3200216	-0.8263121	0.0213521

C	-4.1088173	-1.5424681	0.0524133
C	-3.0461523	-0.5867808	0.0315132
N	-3.6460466	0.6688075	-0.0169600
H	-3.1083158	1.5358138	-0.0220622
C	-5.8888263	1.7400584	-0.0746811
H	-5.4783577	2.5759831	0.5059622
H	-6.0213889	2.0897659	-1.1096720
H	-6.8818409	1.5004869	0.3212510
O	-1.4025458	2.3034964	-0.0290003
C	-1.0541625	3.7073391	-0.0581775
H	-2.0007313	4.2516451	-0.0724428
H	-0.4810855	3.9716227	0.8392395
H	-0.4758815	3.9330595	-0.9627356
H	0.9306953	-1.5582584	0.0468491
C	3.7937064	-0.9981163	0.0839563
C	3.0684521	0.2018685	0.0356305
C	5.1653807	-0.6665592	0.0635447
N	3.9952605	1.2312286	-0.0122146
C	5.2598598	0.7222947	0.0036517
H	3.7750670	2.2193560	-0.0547437
H	3.3516789	-1.9888323	0.1264386
C	-3.9609998	-3.0293596	0.0875190
H	-4.1678556	-3.4718476	-0.8988949
H	-2.9542481	-3.3441370	0.3858322
H	-4.6788649	-3.4761042	0.7892567
S	0.6584881	-4.3359751	0.5833954
O	1.5161570	-4.9624940	1.6072569
O	-0.6673348	-3.9260226	1.0950839
O	1.3464039	-3.2272461	-0.1409756
C	0.3621079	-5.5927482	-0.6632263
H	-0.1437917	-6.4394496	-0.1886275
H	-0.2670807	-5.1658940	-1.4504784
H	1.3257045	-5.9087207	-1.0751408
H	6.1238943	1.3752567	-0.0284351
H	6.0026249	-1.3551756	0.0892256
C	-6.7068544	-1.4010359	0.0072263
H	-6.7185517	-2.3270500	0.6000692
H	-7.3981646	-0.7089176	0.5097976
C	-7.2352034	-1.7023032	-1.4080271
H	-6.5863998	-2.4189082	-1.9284211
H	-8.2455632	-2.1301012	-1.3633168
H	-7.2795303	-0.7889534	-2.0157091

IVδ-CI⁺

C	-4.1800013	-1.0810239	-0.1951856
C	-4.1039865	-2.4808912	-0.2633137
C	-5.4235994	-2.9794764	-0.2768589
C	-6.2849251	-1.8855653	-0.2173166
N	-5.5280690	-0.7543127	-0.1689783
H	-5.9043351	0.1851588	-0.1201735

H	-3.1785229	-3.0491645	-0.3017640
H	-5.7263128	-4.0195687	-0.3245662
H	-7.3671559	-1.8328858	-0.2062873
C	-1.1055396	0.8615349	-0.1205755
C	-2.0986428	1.9072740	-0.0563129
C	-3.3637654	1.3330014	-0.0727104
C	-3.1698095	-0.0700865	-0.1507036
N	-1.8289797	-0.3324316	-0.1764414
H	-4.3180141	1.8430306	-0.0324182
C	0.2597708	1.1127928	-0.1052153
H	0.4640445	2.1833091	-0.0479394
C	2.8424703	-1.4056607	-0.2187886
C	3.6389160	-0.2367862	-0.1275281
C	2.7608111	0.8560348	-0.0776634
C	1.4249810	0.3401197	-0.1356189
N	1.5372963	-1.0449549	-0.2194886
C	3.2662018	-2.8304424	-0.3108349
H	3.7572049	-3.1577275	0.6172220
H	2.4064269	-3.4852131	-0.4914987
H	3.9924825	-2.9705881	-1.1231962
C	5.1392626	-0.2147047	-0.0682290
H	5.5394691	-1.0706387	-0.6311964
H	5.5129085	0.6851616	-0.5788352
O	-1.7380145	3.1962393	0.0100971
C	-2.8145393	4.1552700	0.0870574
H	-2.3377097	5.1365950	0.1361406
H	-3.4485752	4.0893640	-0.8066948
H	-3.4148464	3.9827694	0.9899101
H	-1.4297779	-1.2875943	-0.2564736
H	0.7669673	-1.7397555	-0.2970238
Cl	-0.6243332	-3.2905511	-0.4587730
C	3.1354275	2.3002486	0.0333405
H	2.4974015	2.9428124	-0.5871354
H	3.0546366	2.6627139	1.0691933
H	4.1727266	2.4603802	-0.2843713
C	5.6979337	-0.2474352	1.3666986
H	5.3759237	-1.1532847	1.8975539
H	6.7958581	-0.2320916	1.3582207
H	5.3503340	0.6190248	1.9446764

IVδ-MeSO₃⁻

C	-0.4624899	1.2364806	0.0684968
C	-1.4798637	2.2567008	0.1584330
C	-2.7276042	1.6490774	0.2152833
C	-2.4987063	0.2502331	0.1667372
N	-1.1539969	0.0217980	0.0801659
H	-3.6920599	2.1338172	0.2989984
C	0.8916297	1.5326656	-0.0068272
H	1.0573812	2.6104143	0.0380219
C	3.5814127	-0.8490547	-0.3755345

C	4.3192418	0.3576541	-0.3035363
C	3.3927090	1.3996513	-0.1534792
C	2.0852487	0.8142343	-0.1293821
N	2.2605860	-0.5615706	-0.2623471
C	4.0761694	-2.2368811	-0.5868876
H	5.0506449	-2.3814985	-0.1053093
H	3.3689885	-2.9737388	-0.1868261
H	4.2137497	-2.4424902	-1.6601718
O	-1.1524311	3.5558702	0.1786430
C	-2.2509536	4.4875998	0.2758854
H	-1.8003105	5.4824151	0.2743478
H	-2.9216202	4.3770588	-0.5861302
H	-2.8059235	4.3270763	1.2094597
H	-0.7300542	-0.9164375	-0.0097953
H	1.5139202	-1.2799235	-0.2960940
C	-3.3836962	-2.1802545	0.2928022
C	-3.4853602	-0.7833182	0.2090979
C	-4.6954226	-2.6999820	0.3218622
N	-4.8396236	-0.4794988	0.1919171
C	-5.5766209	-1.6227903	0.2549549
H	-5.2317689	0.4518648	0.1198955
H	-2.4633550	-2.7532439	0.3569310
C	3.7029271	2.8568907	-0.0216991
H	2.9681613	3.4869088	-0.5393703
H	3.7205615	3.1750791	1.0313917
H	4.6887193	3.0856887	-0.4445977
S	0.2979174	-3.8408474	0.1257288
O	1.5907157	-4.0712866	0.7939798
O	-0.8714007	-4.2387924	0.9268010
O	0.1743431	-2.4313052	-0.3826930
C	0.2858854	-4.8588253	-1.3481795
H	0.3711652	-5.9055661	-1.0395861
H	-0.6558546	-4.6944323	-1.8807998
H	1.1347572	-4.5773064	-1.9786769
H	-6.6596521	-1.5891381	0.2463921
H	-4.9795756	-3.7441507	0.3894512
C	5.8166386	0.4619799	-0.3552756
H	6.1008824	1.3906964	-0.8720836
H	6.2202299	-0.3583756	-0.9658087
C	6.4807430	0.4355641	1.0344291
H	7.5723790	0.5137829	0.9467776
H	6.1283876	1.2695968	1.6555967
H	6.2486634	-0.4967120	1.5666658

ⁱ SMART diffractometer control software, Bruker Analytical X-ray Instruments Inc., Madison, WI, 2000.

ⁱⁱ SAINT integration software, Siemens Analytical X-ray Instruments Inc., Madison, WI, 2000.

ⁱⁱⁱ G. M. Sheldrick. *SADABS: A program for absorption correction with the Siemens SMART system*;

University of Göttingen: Germany, 2001.

^{iv} *SHELXTL program system version 6.1*; Bruker Analytical X-ray Instruments Inc., Madison, WI, 1998.

^v *International Tables for Crystallography*, Kluwer, Dordrecht, 1992, vol. C.

^{vi} M. J. Hynes, *J. Chem. Soc., Dalton Trans*, **1993**, 311