Supporting Information

For

Reverse Turn and Loop Secondary Structures in Stereodefined Cyclic Peptoid Scaffolds

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1.0 List of abbreviations

ACN: acetonitrile

Ar: aryl

Bn: benzyl

c: cis amide bond

COSY: correlation spectroscopy

DCM: dichloromethane

DMSO: dimethyl sulfoxide

DIC*: N,N'*-diisopropylcarbodiimide

DIPEA: *N,N*-diisopropylethylamine

DMF: dimethylformamide

EDC: *N*-(3-Dimethylaminopropyl)-*N'*-ethylcarbodiimide hydrochloride

ESI: electrospray ionisation

FTICR-MS: Fourier transform ion cyclotron resonance mass spectrometry

HATU: *O*-(7-azabenzotriazol-1-yl)-*N,N,N',N'*-tetramethyluronium hexafluorophosphate

HFIP: hexafluoroisopropanol

HMBC: heteronuclear multiple bond correlation

HOBt: 1-Hydroxybenzotriazole hydrate

HSQC: heteronuclear single quantum correlation

HRMS: high resolution mass spectrometry

Ph: phenyl

PyBOP: (Benzotriazol-1-yloxy)tripyrrolidinophosphonium hexafluorophosphate

ROESY: rotating-frame nuclear Overhauser effect correlation spectroscopy

RP HPLC: reversed-phase high-performance liquid chromatography

t: trans amide bond

TCDE: tetrachlorodideuteroethane

TEA: triethylamine

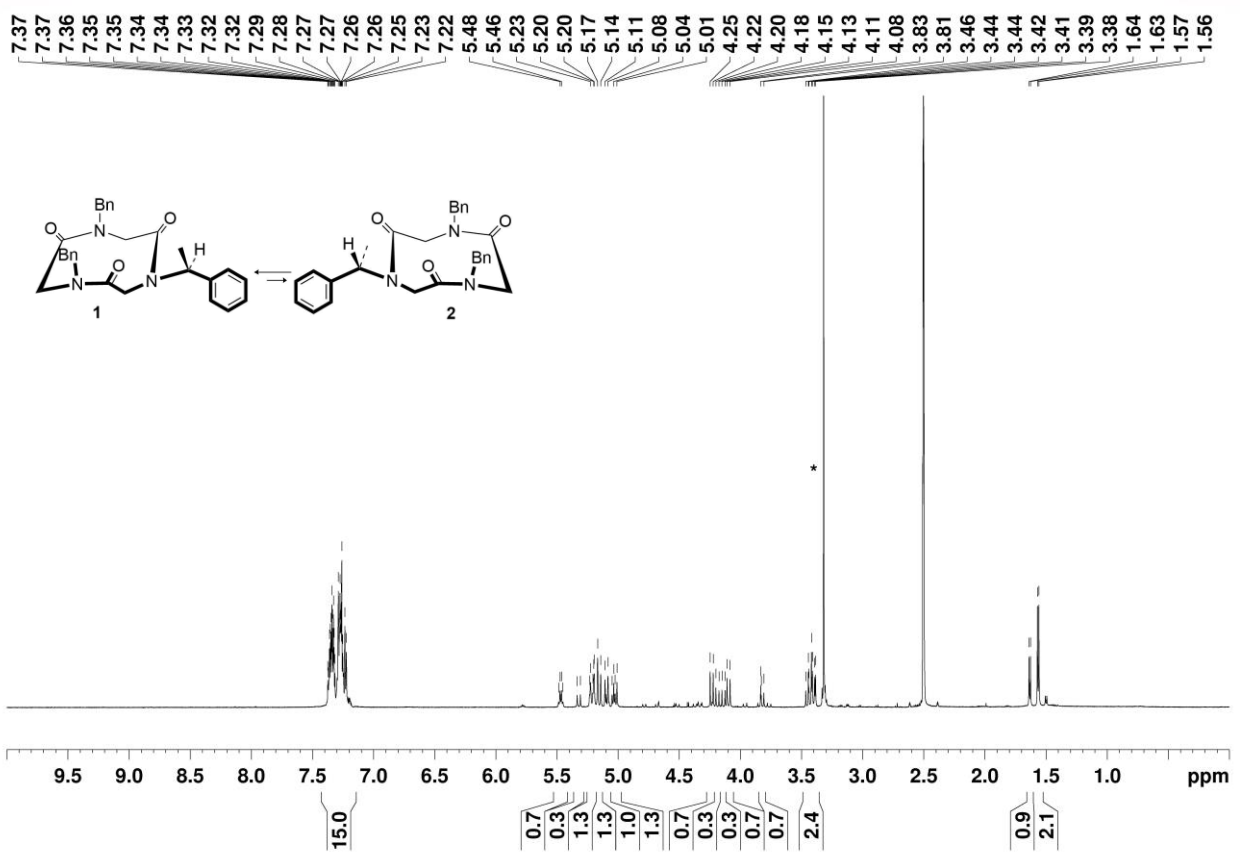
TFA: trifluoroacetic acid

TFPB: tetrakis[3,5-bis(trifluoromethyl)phenyl]borate

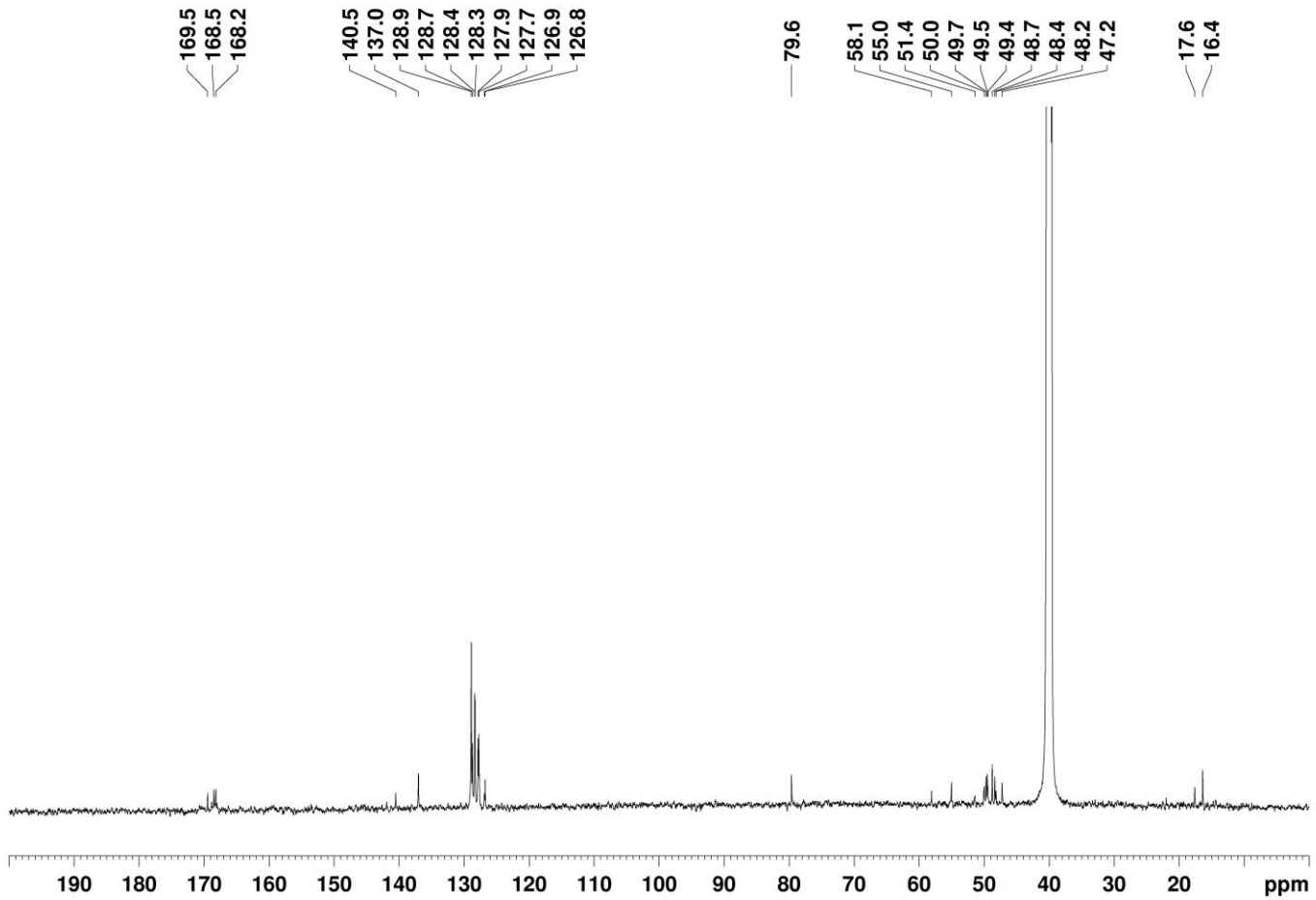
TLC: thin layer chromatography

2.0 ^{1}H-, ^{13}C NMR and two-dimensional spectra

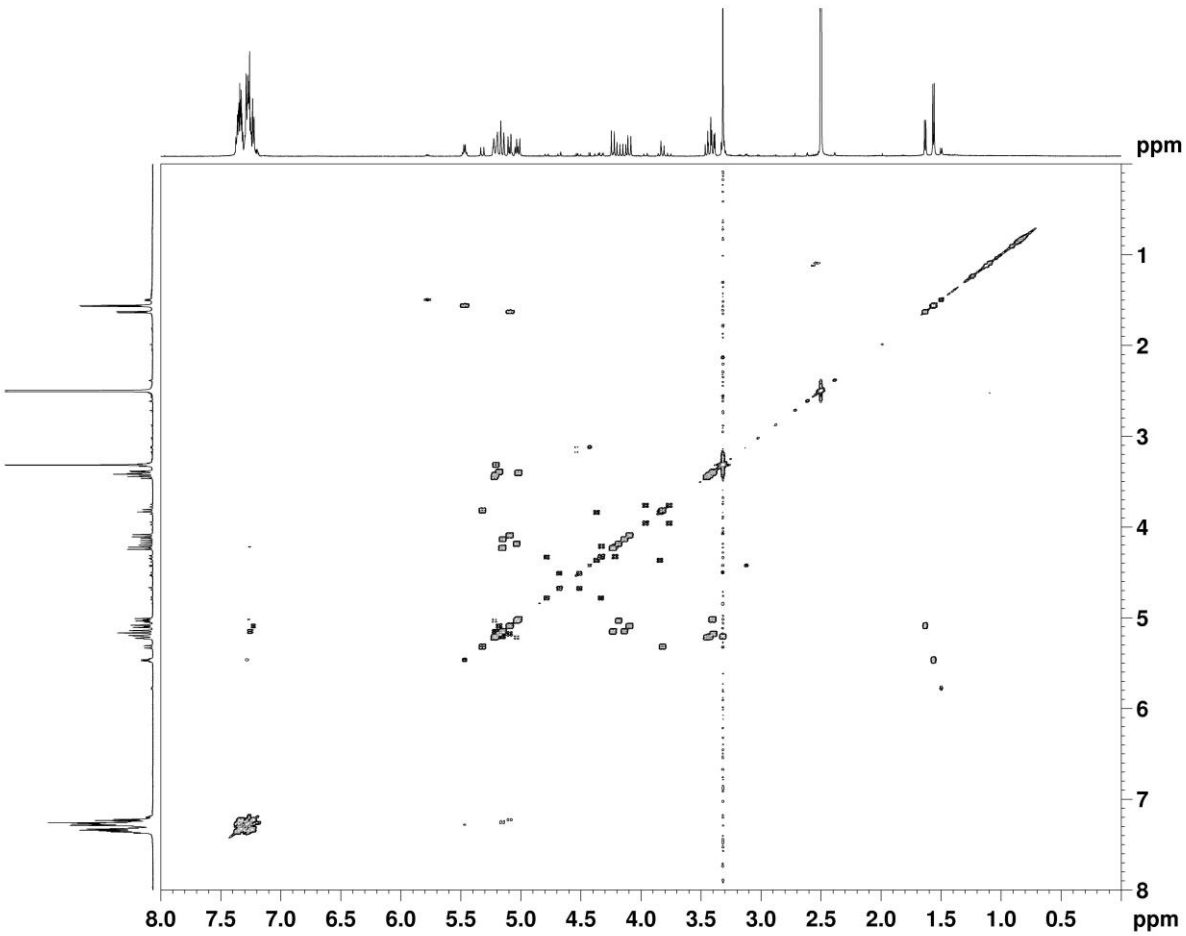
2.1 1D and 2D spectra of cyclic derivatives 1/2, 8, 9, 16/17, 19, 27, 28, 30, 34, 35, 36 and their complexes



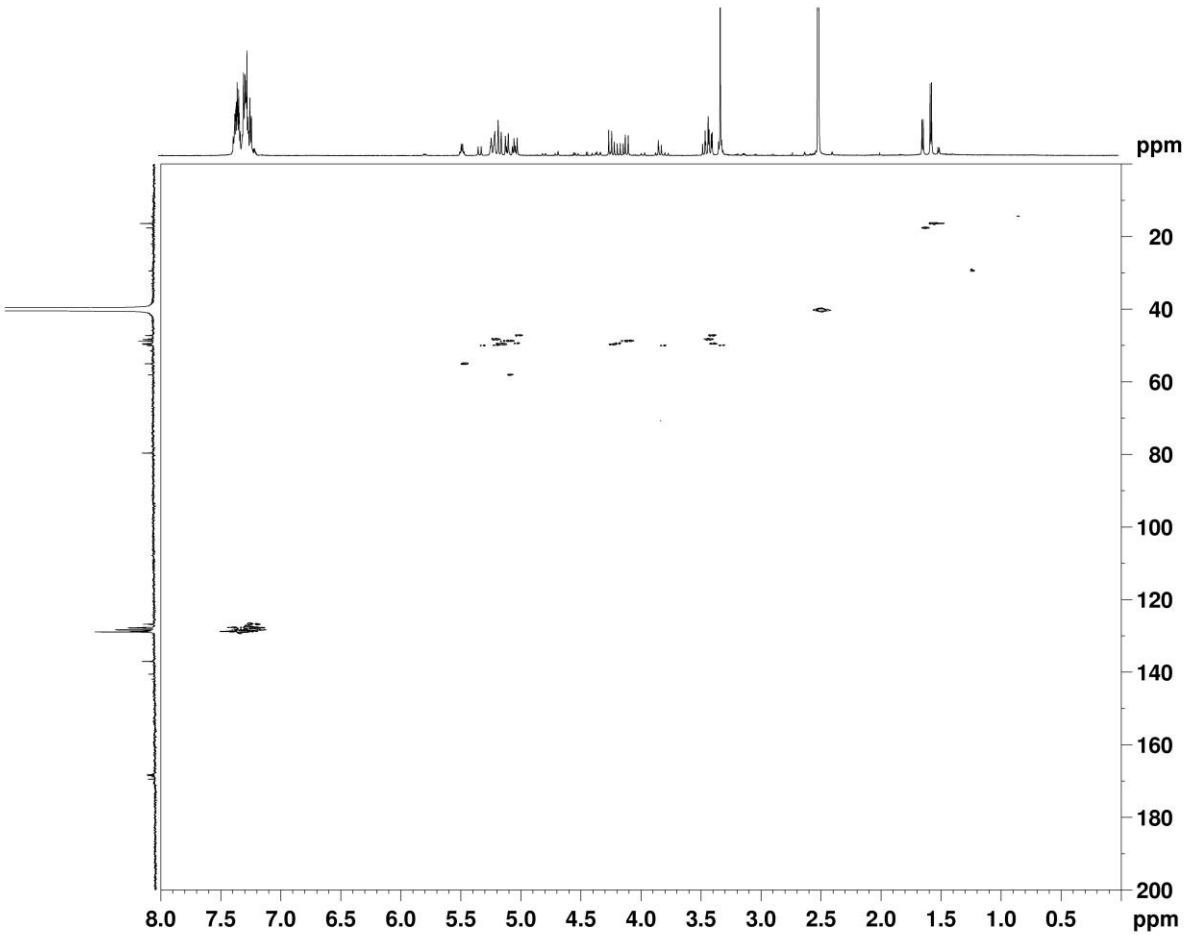
1/**2** (70:30 ratio): ^{1}H NMR (600 MHz, $(CD_3)_2SO$). Water impurities are labelled with a black asterisk.



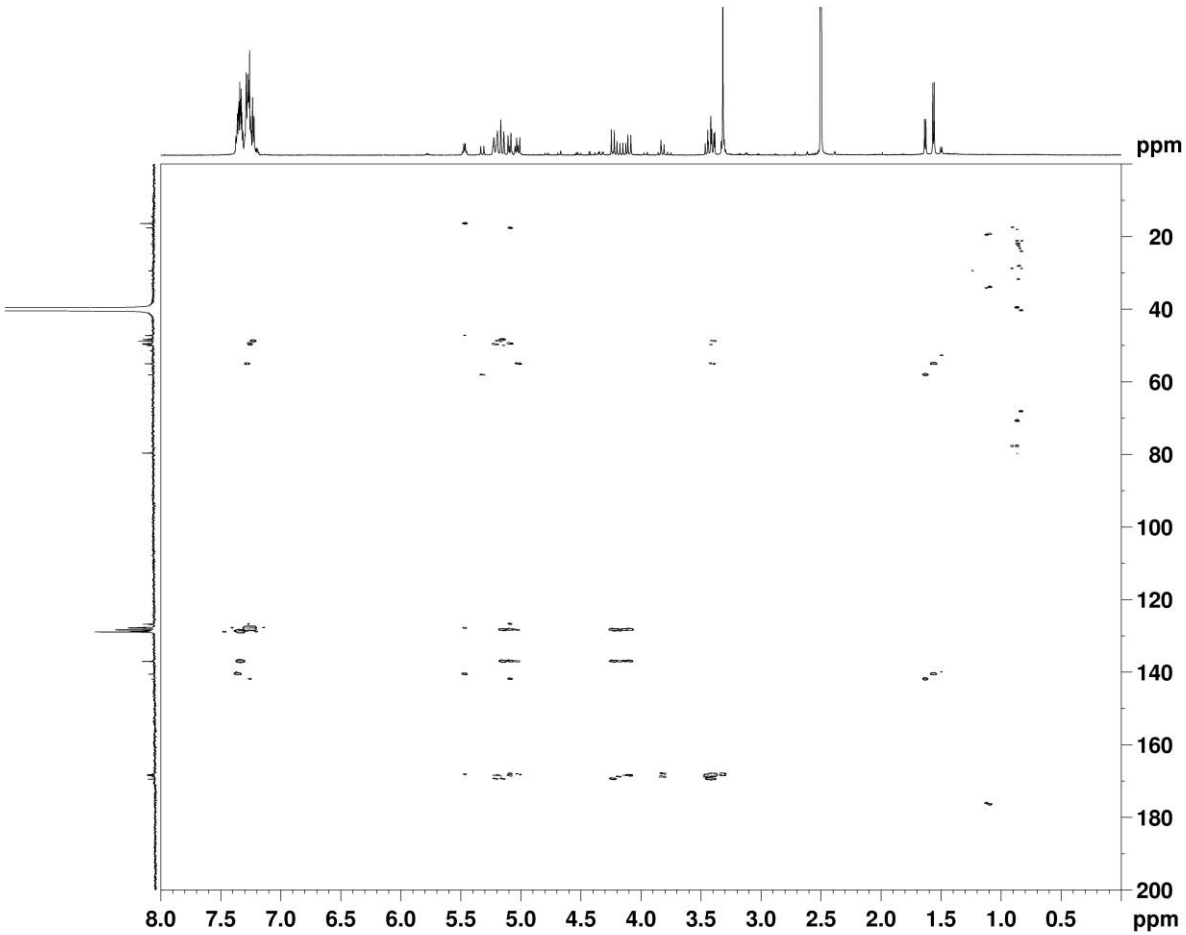
1/2: ^{13}C NMR (150 MHz, $(CD_3)_2SO$)



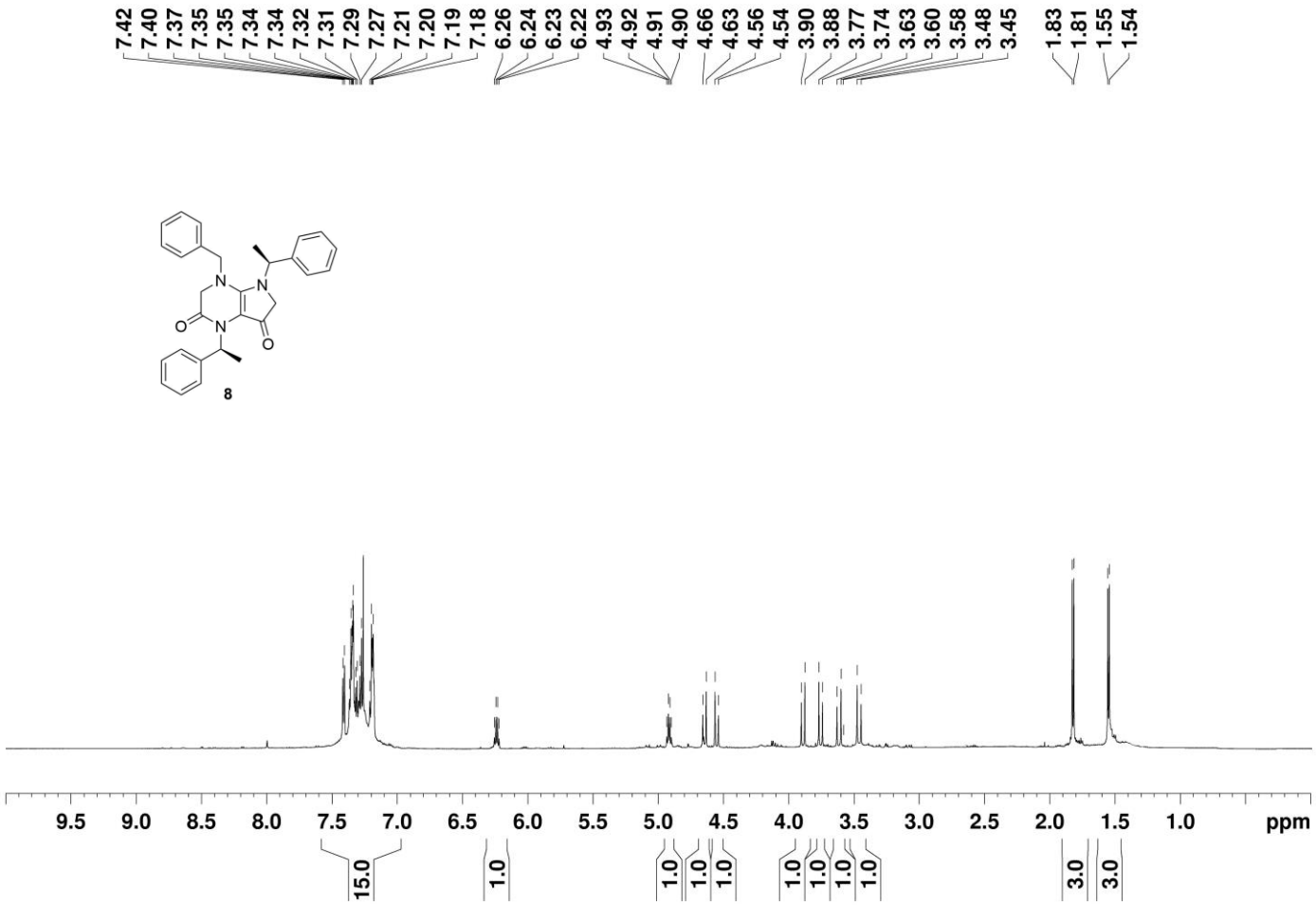
1/2: COSY SPECTRUM (600 MHz, $(CD_3)_2SO$)



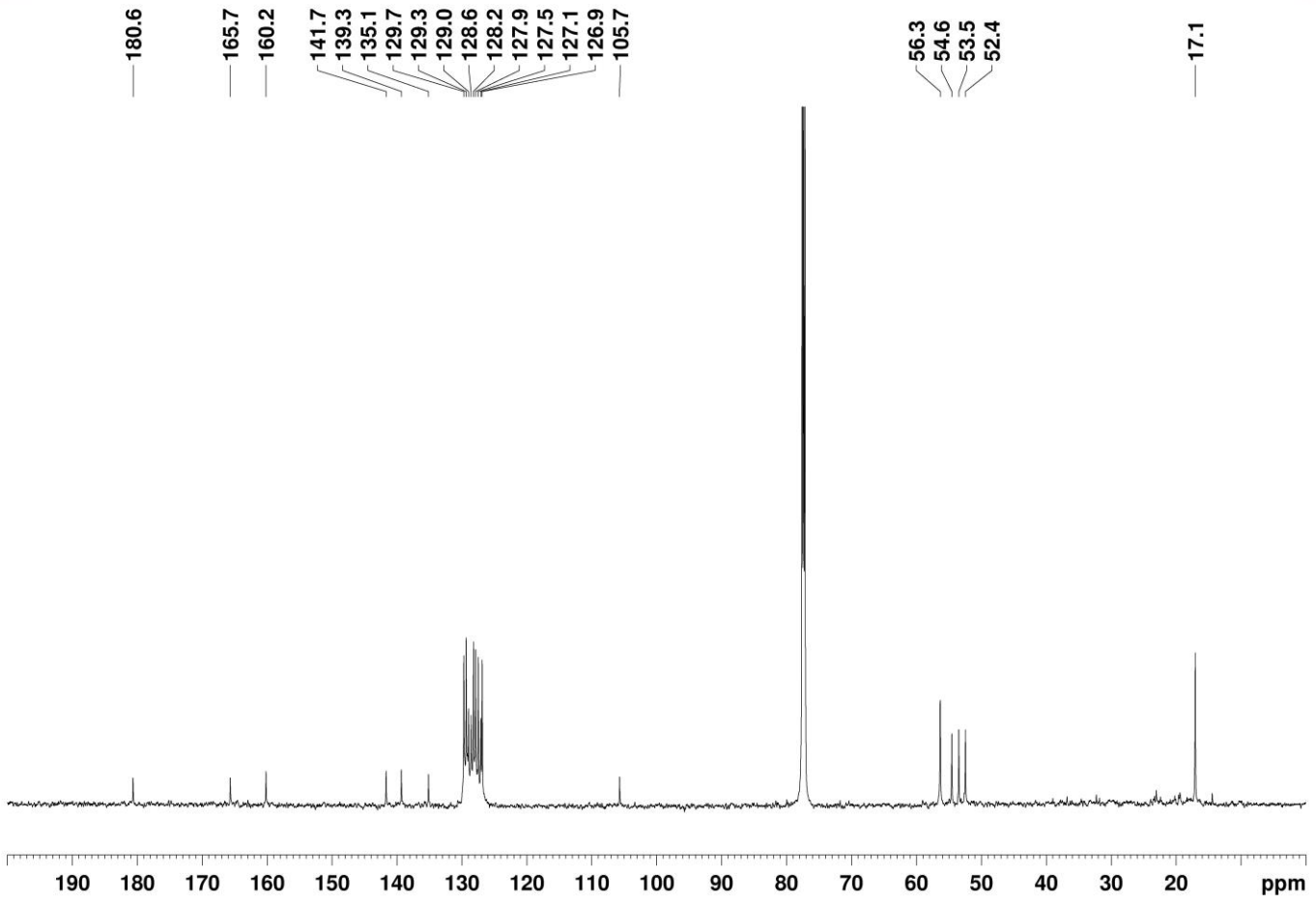
1/2: HSQC SPECTRUM (600 MHz, $(CD_3)_2SO$)



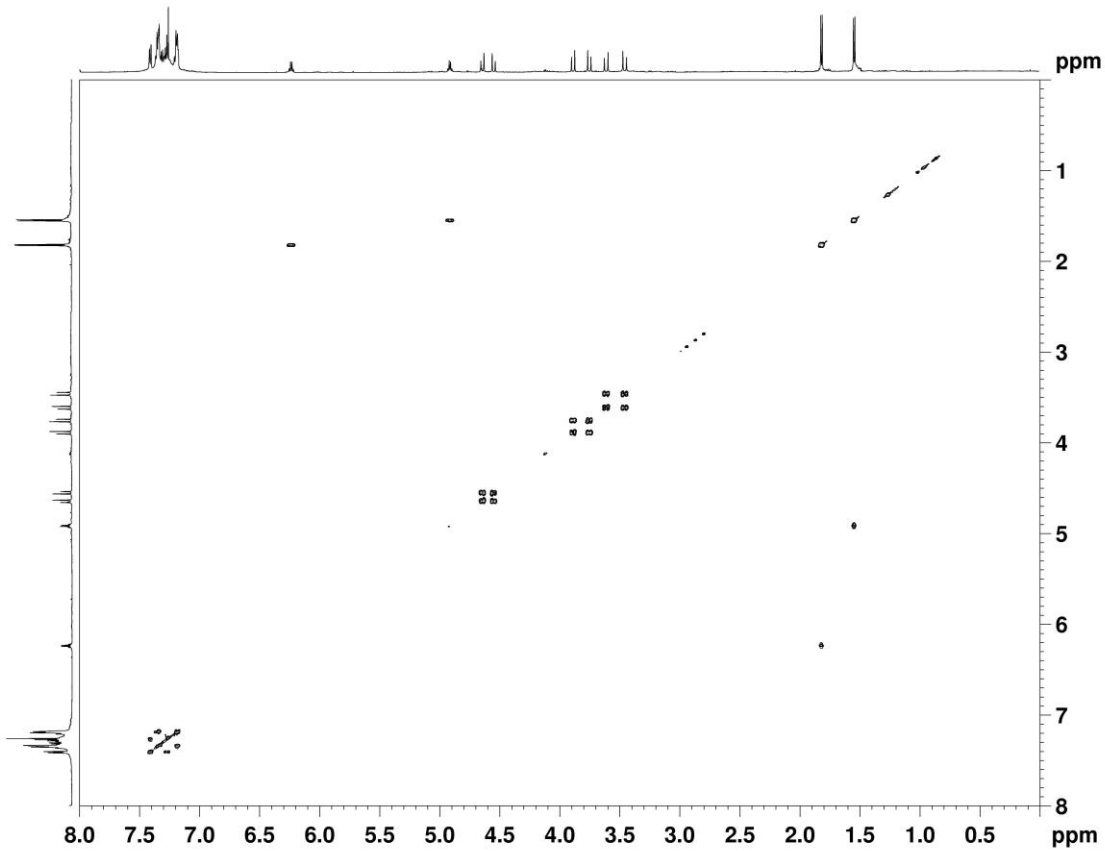
1/2: HMBC SPECTRUM (600 MHz, $(CD_3)_2SO$)



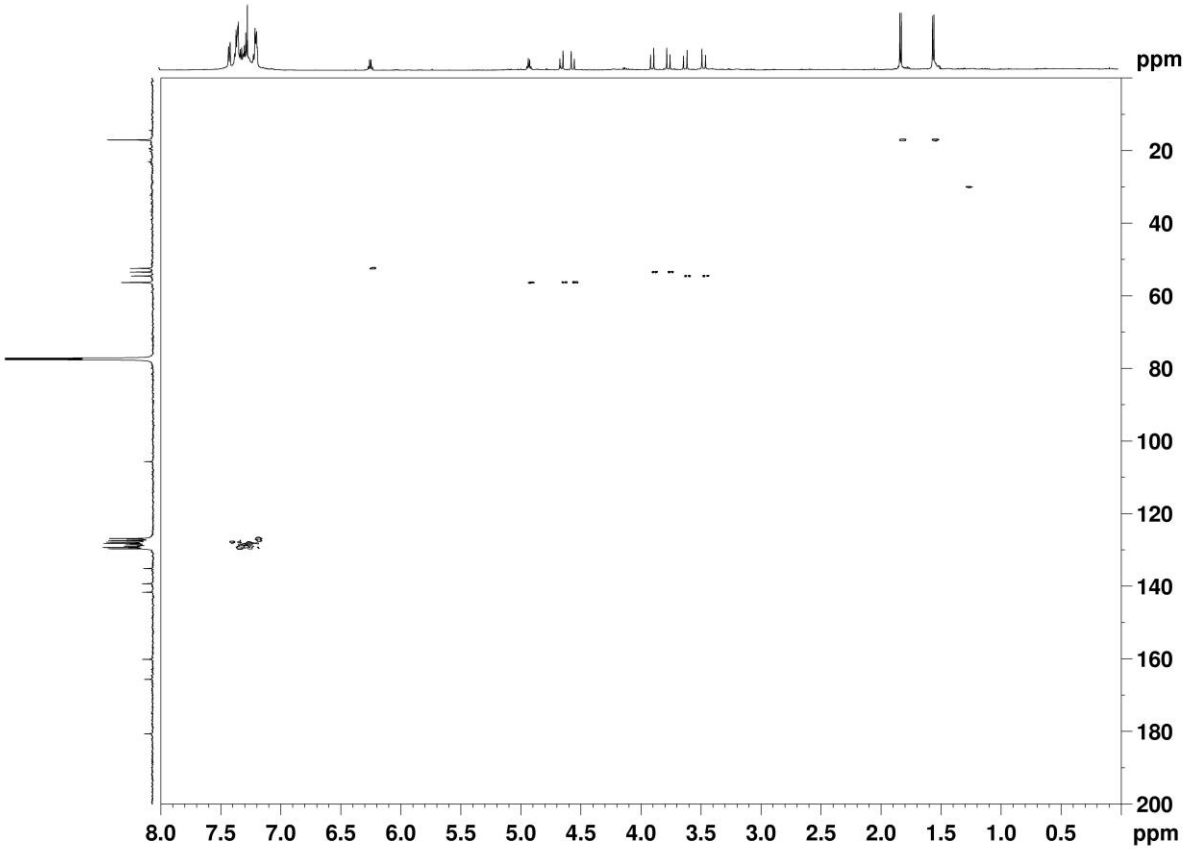
8:^{1}H NMR (600 MHz, $CDCl_3$)



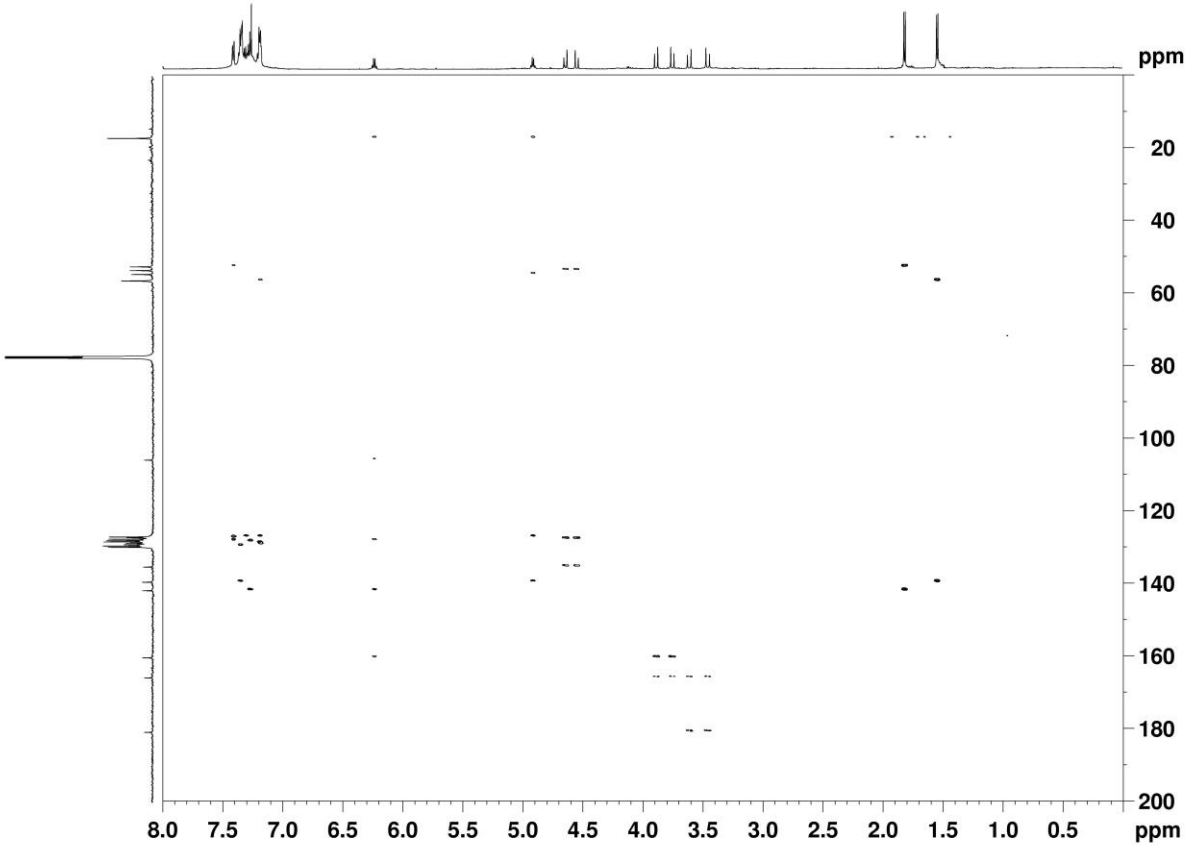
8:^{13}C NMR (150 MHz, $CDCl_3$)



8: COSY SPECTRUM (600 MHz, $CDCl_3$)



8: HSQC SPECTRUM (600 MHz, $CDCl_3$)



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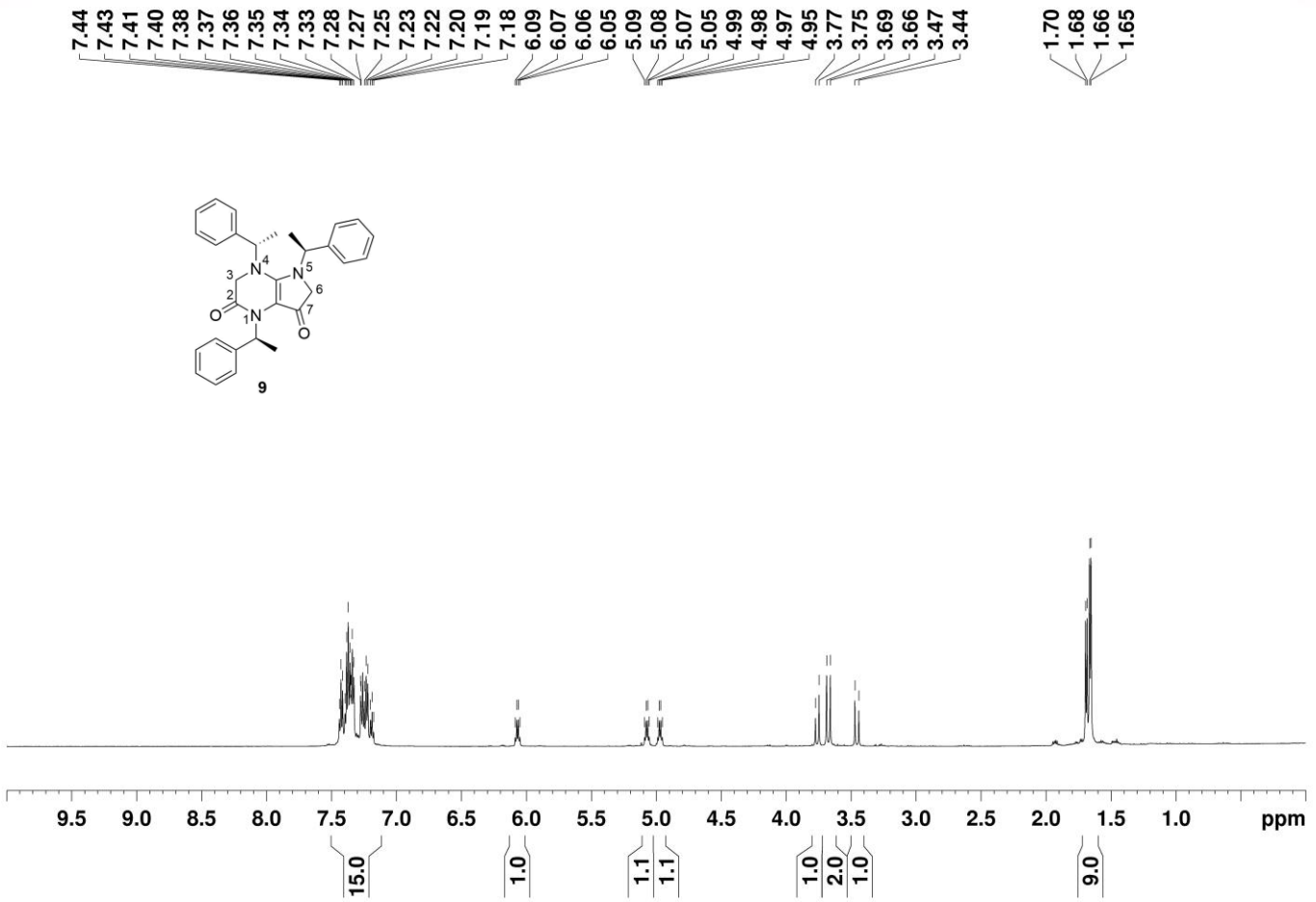
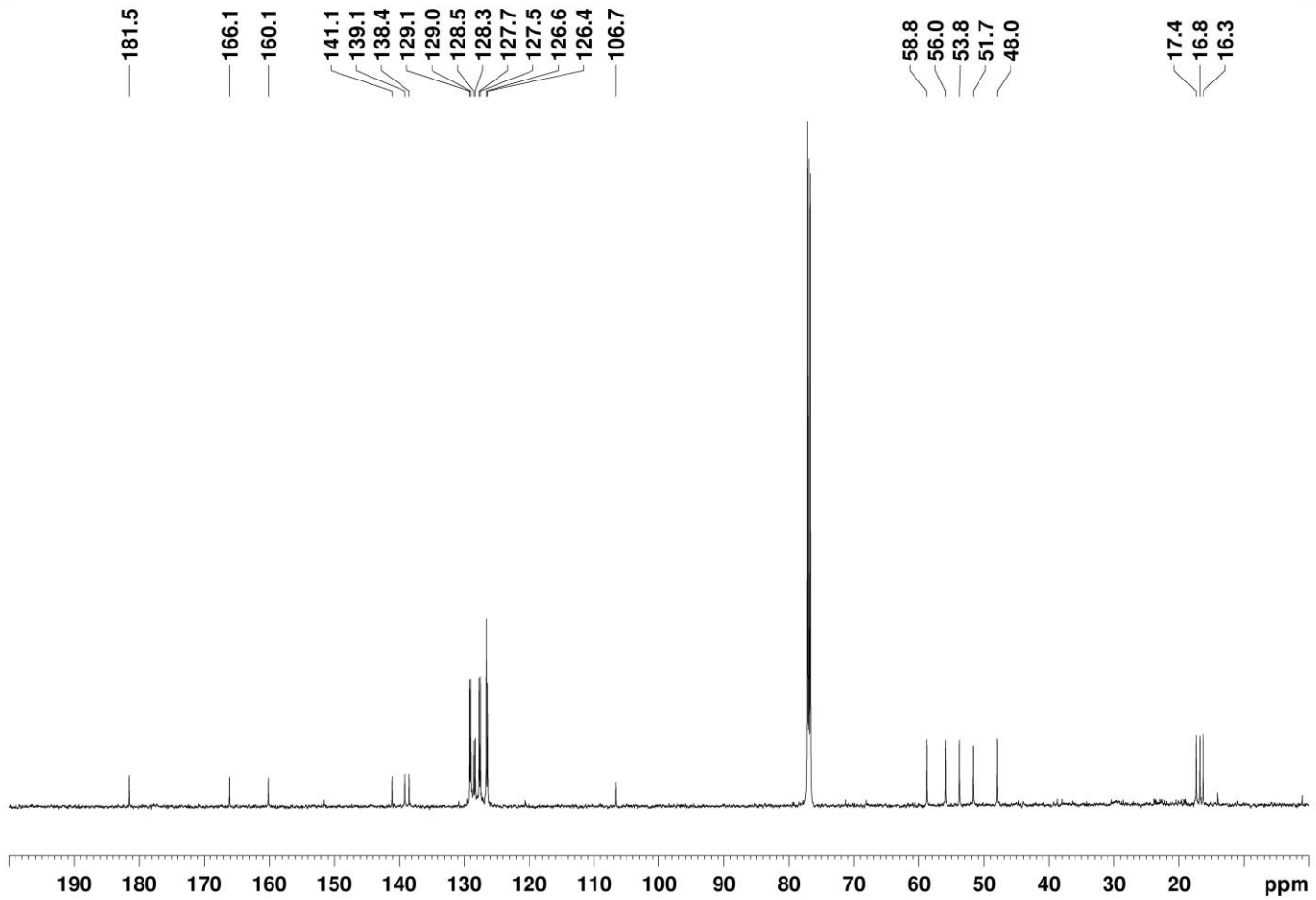
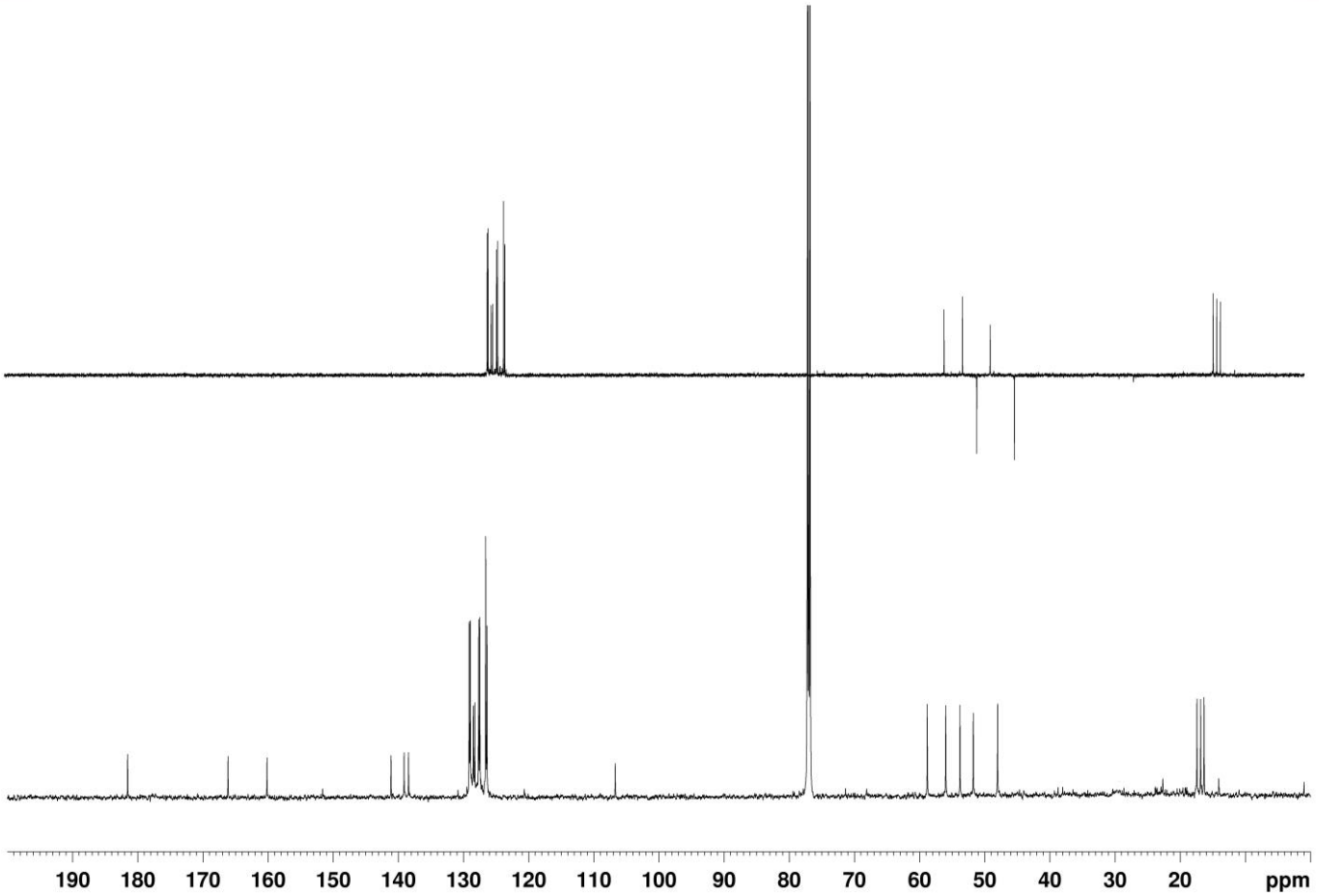


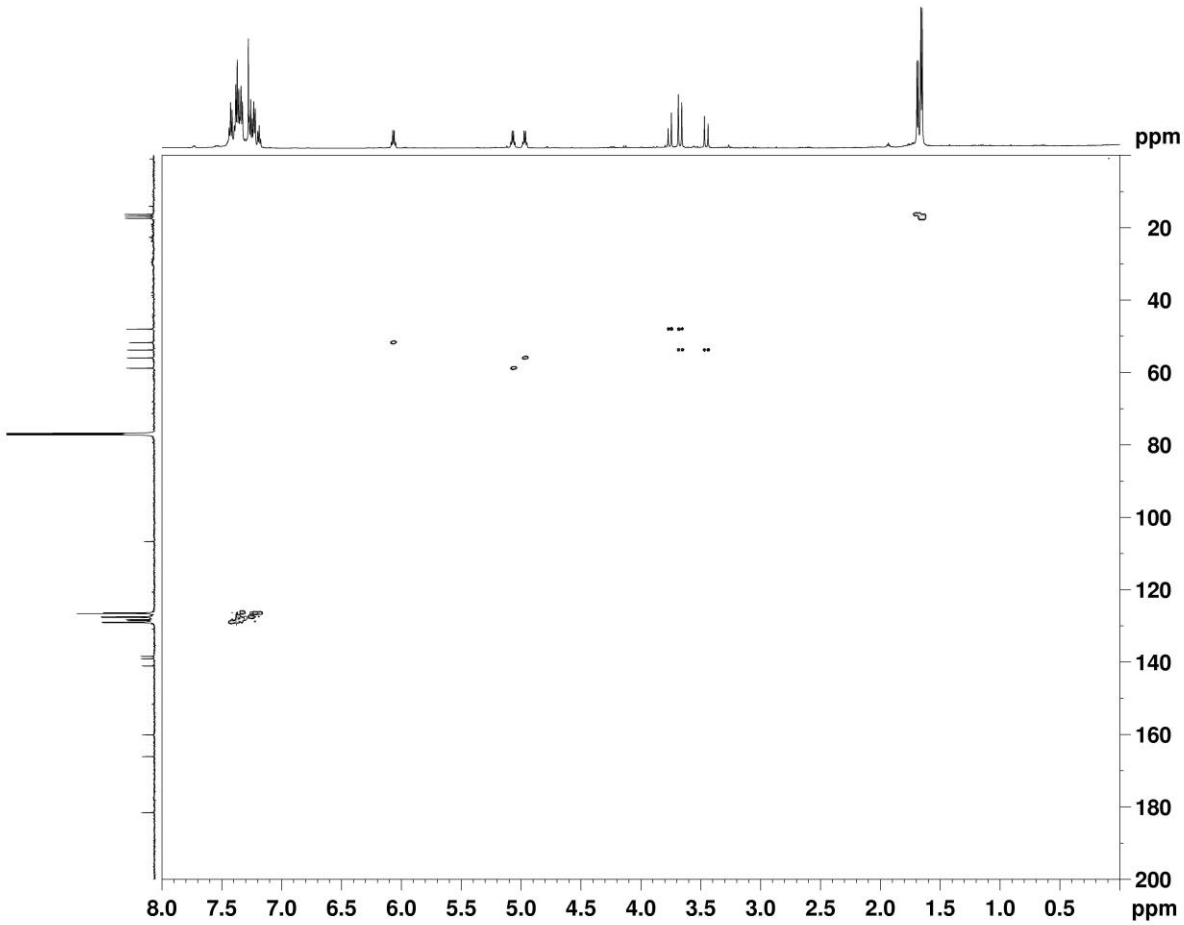
9:^{1}H NMR (600 MHz, $CDCl_3$)



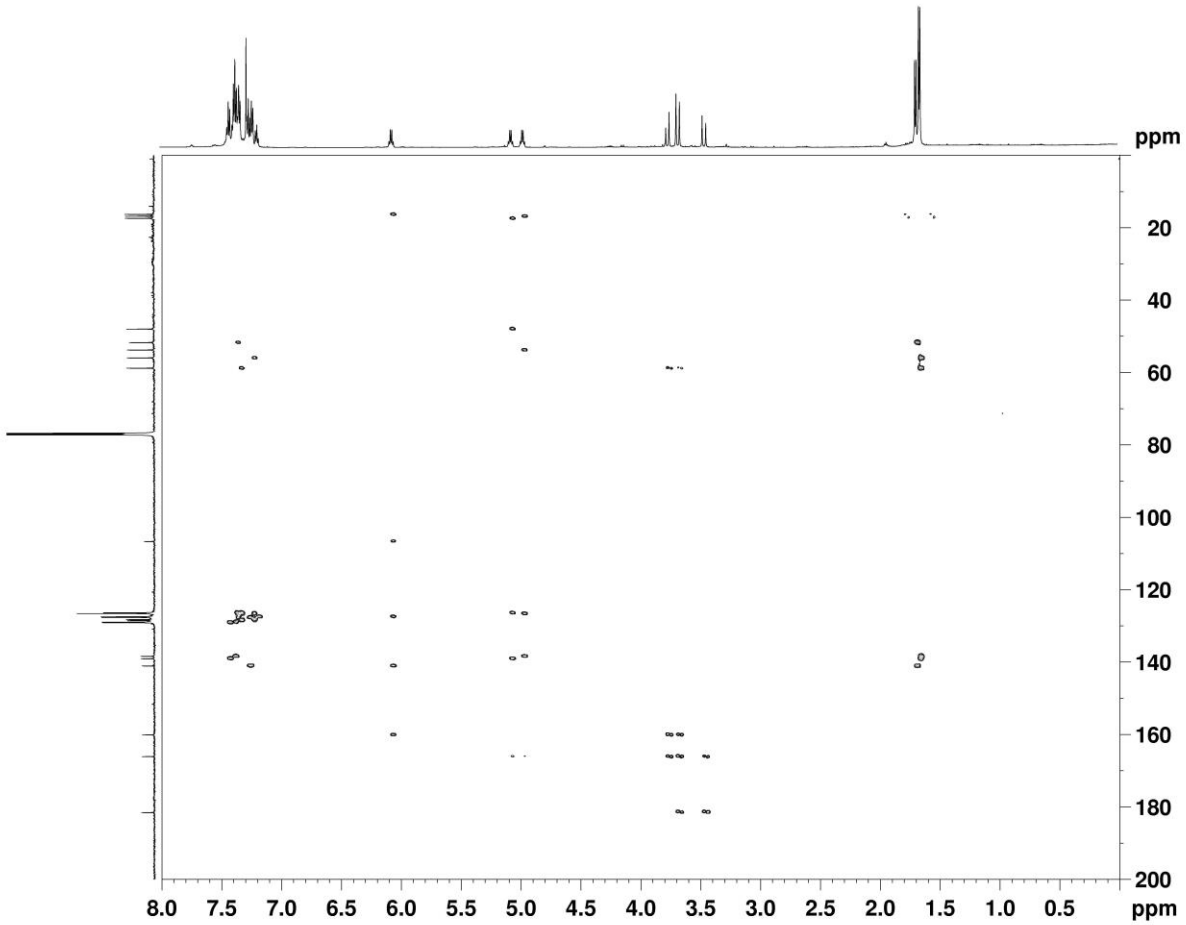
9:^{13}C NMR (600 MHz, $CDCl_3$)



9: Top spectrum: DEPT 135 (150 MHz, $CDCl_3$), lower trace: ^{13}C NMR (600 MHz, $CDCl_3$)



9: HSQC SPECTRUM (600 MHz, $CDCl_3$)



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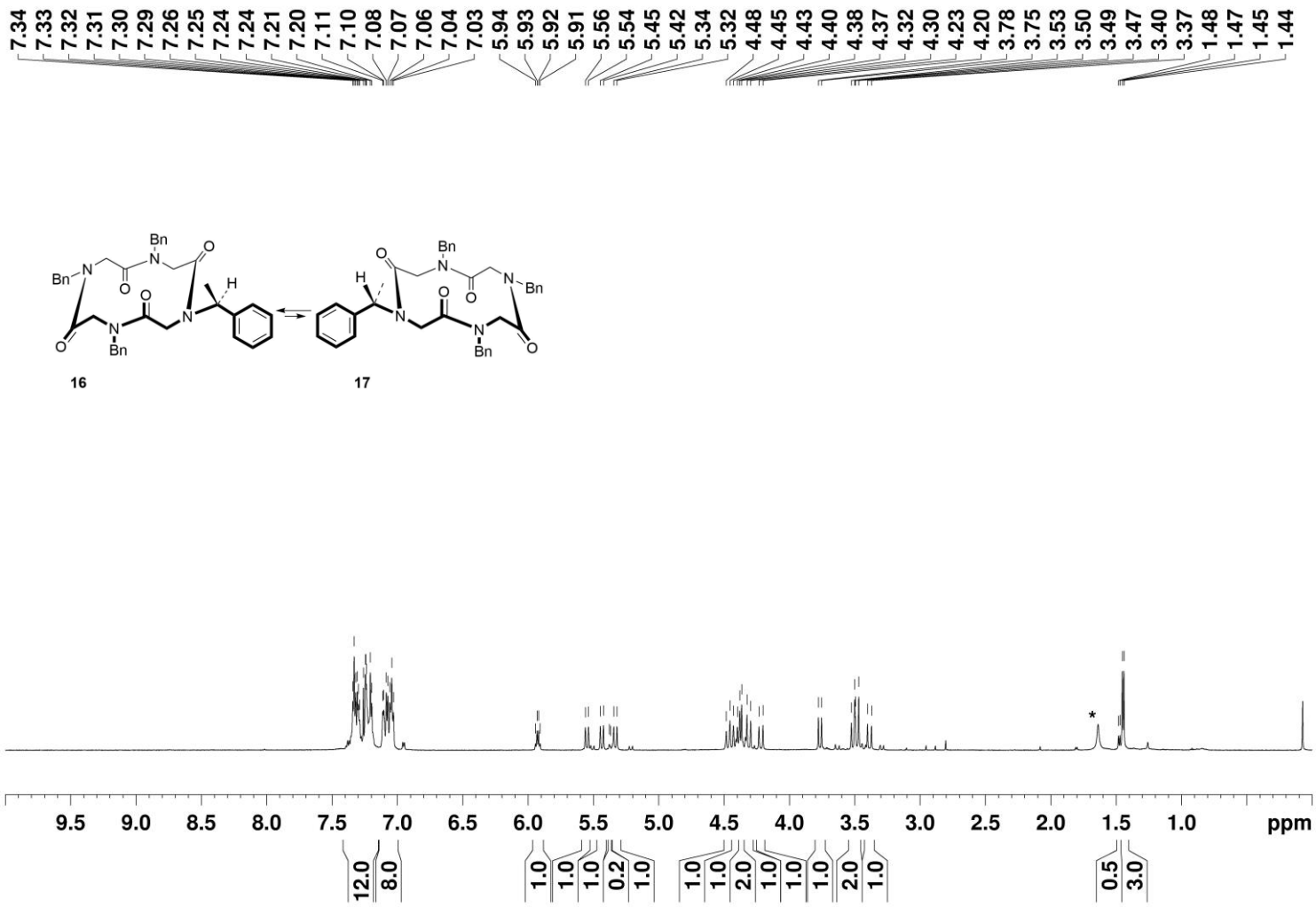
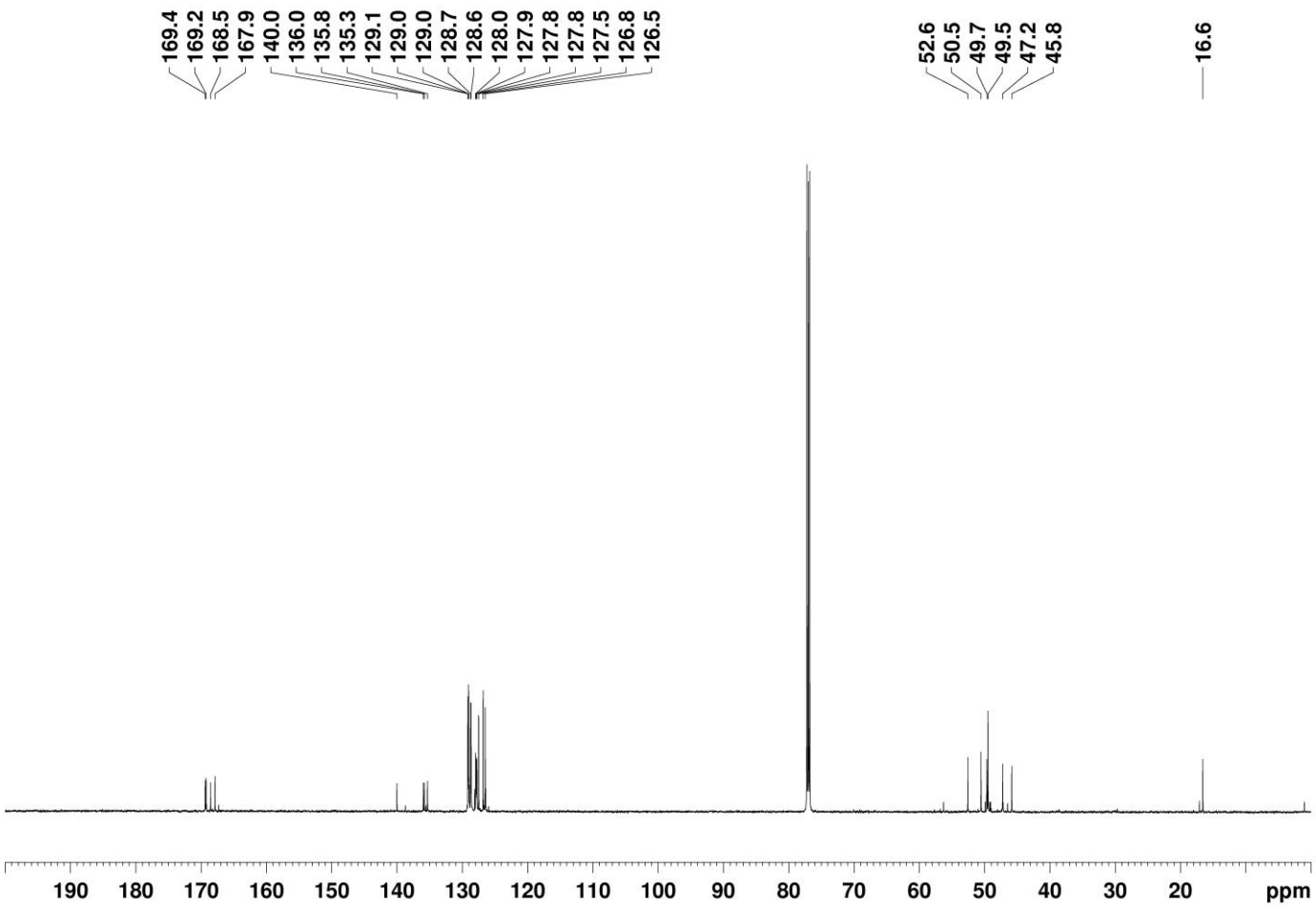
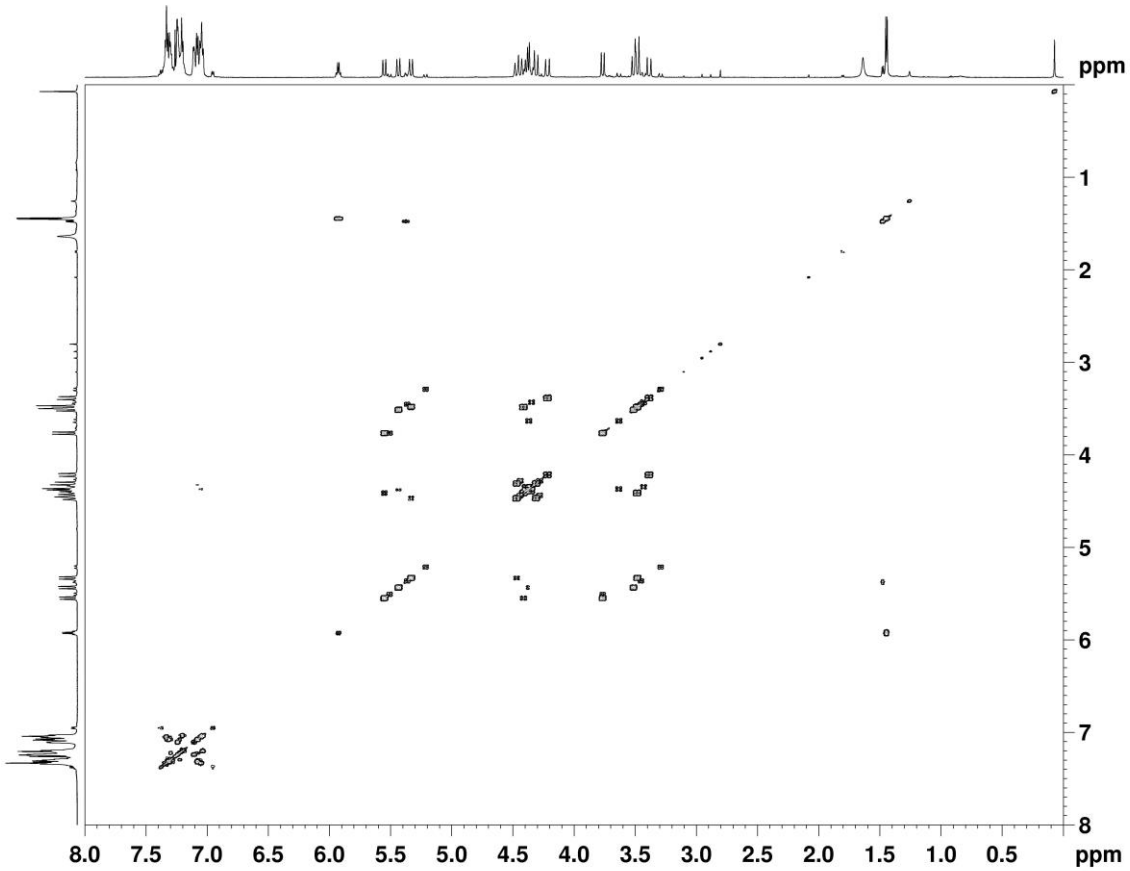


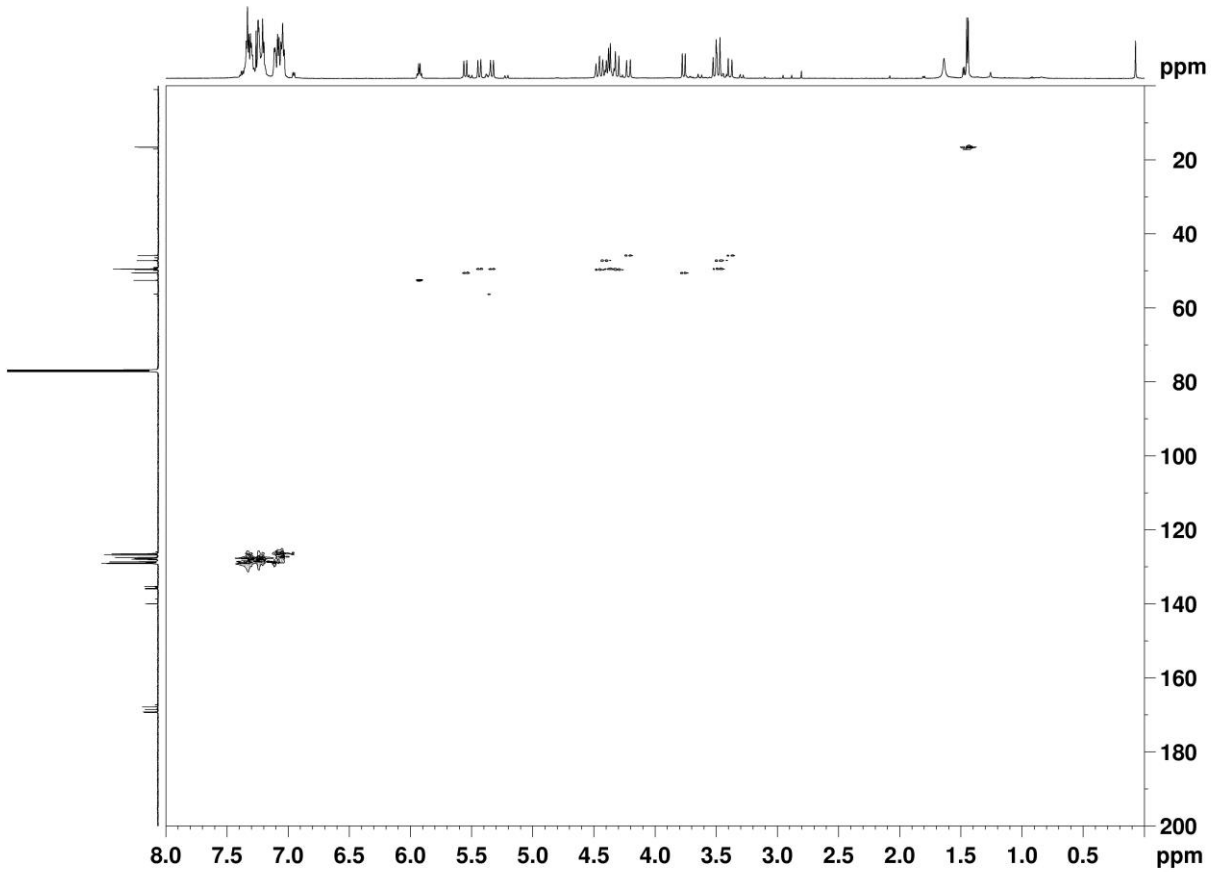
16/**17** (85:15 ratio): ^{1}H NMR (600 MHz, $CDCl_3$). Water impurities are labelled with a black asterisk.



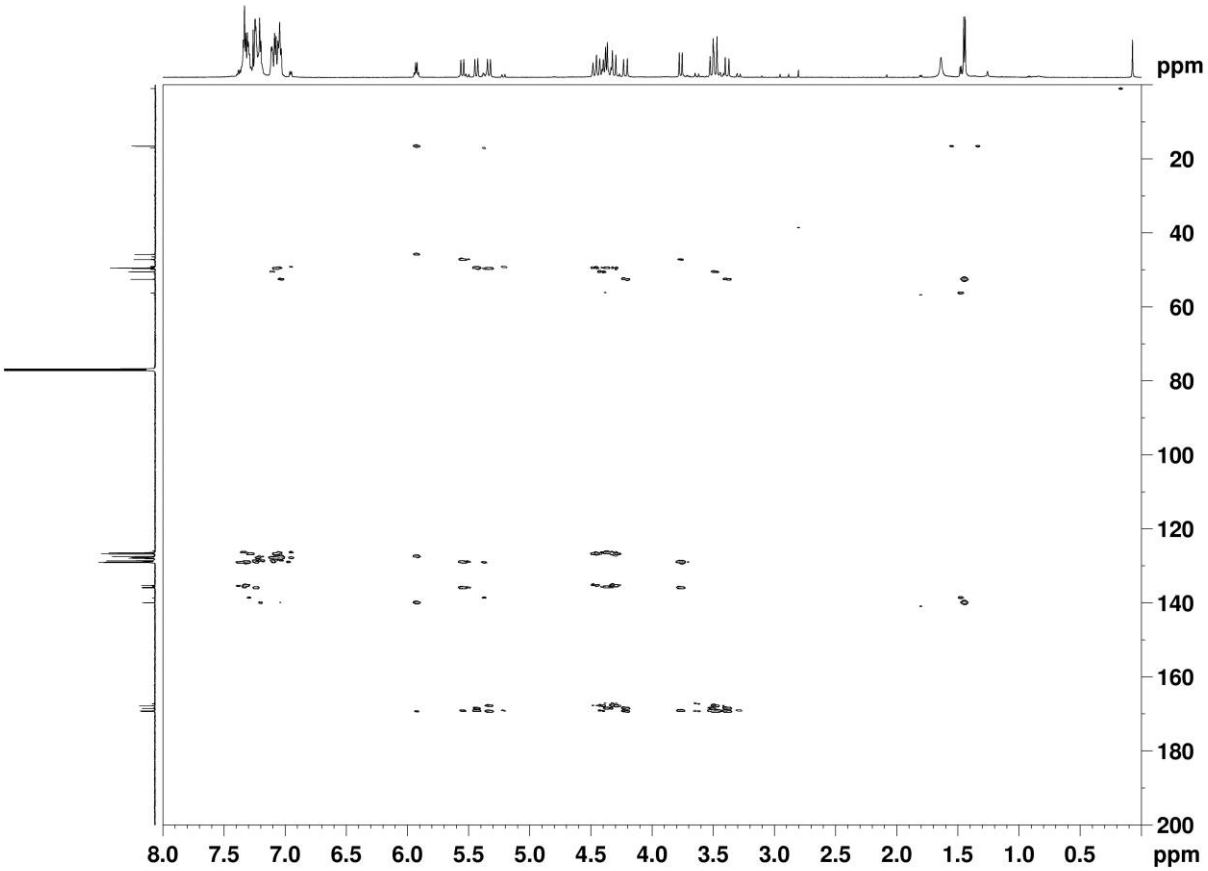
16/17: ^{13}C NMR (150 MHz, $CDCl_3$)



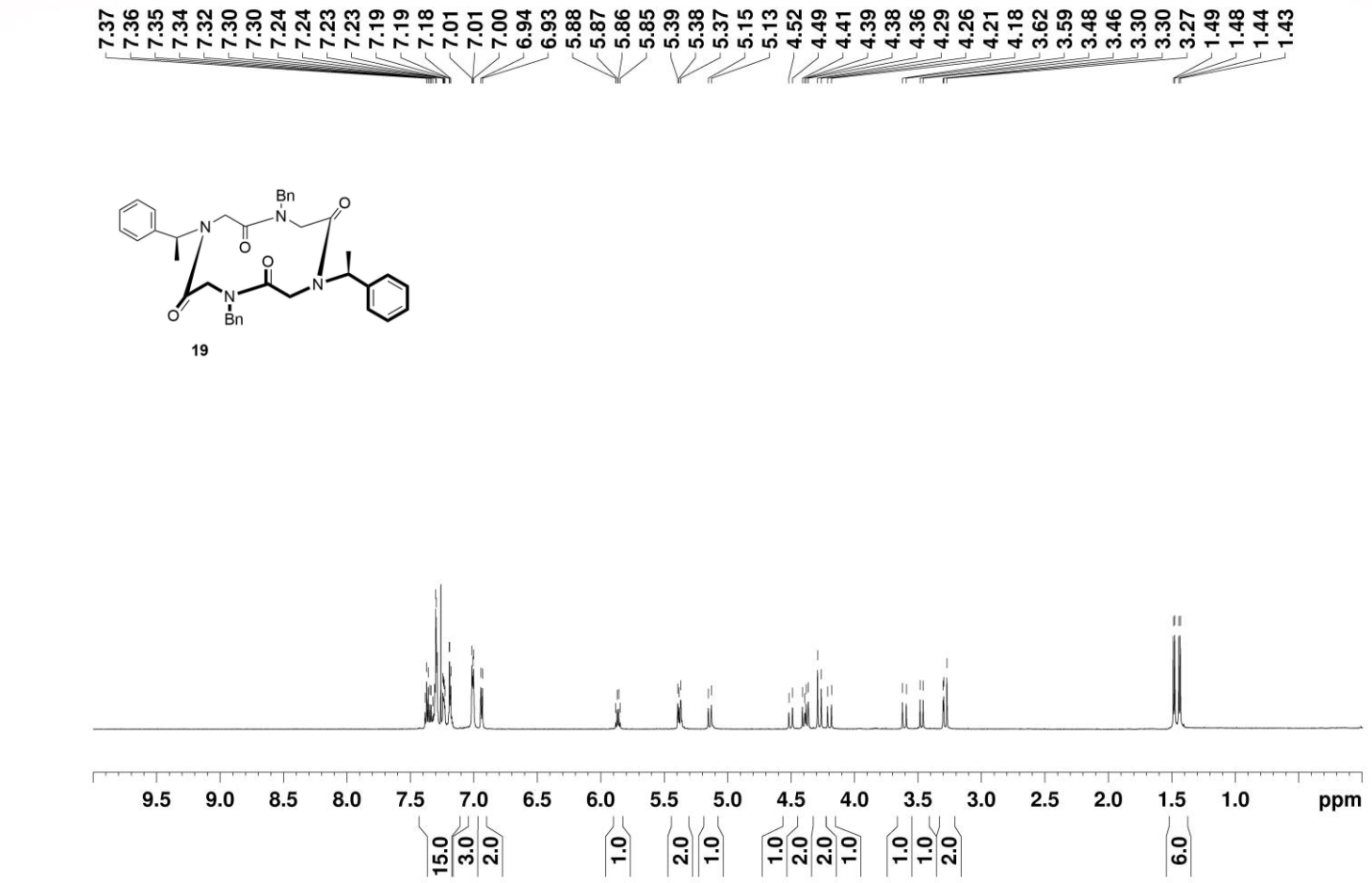
16/17: COSY SPECTRUM (600 MHz, $CDCl_3$)



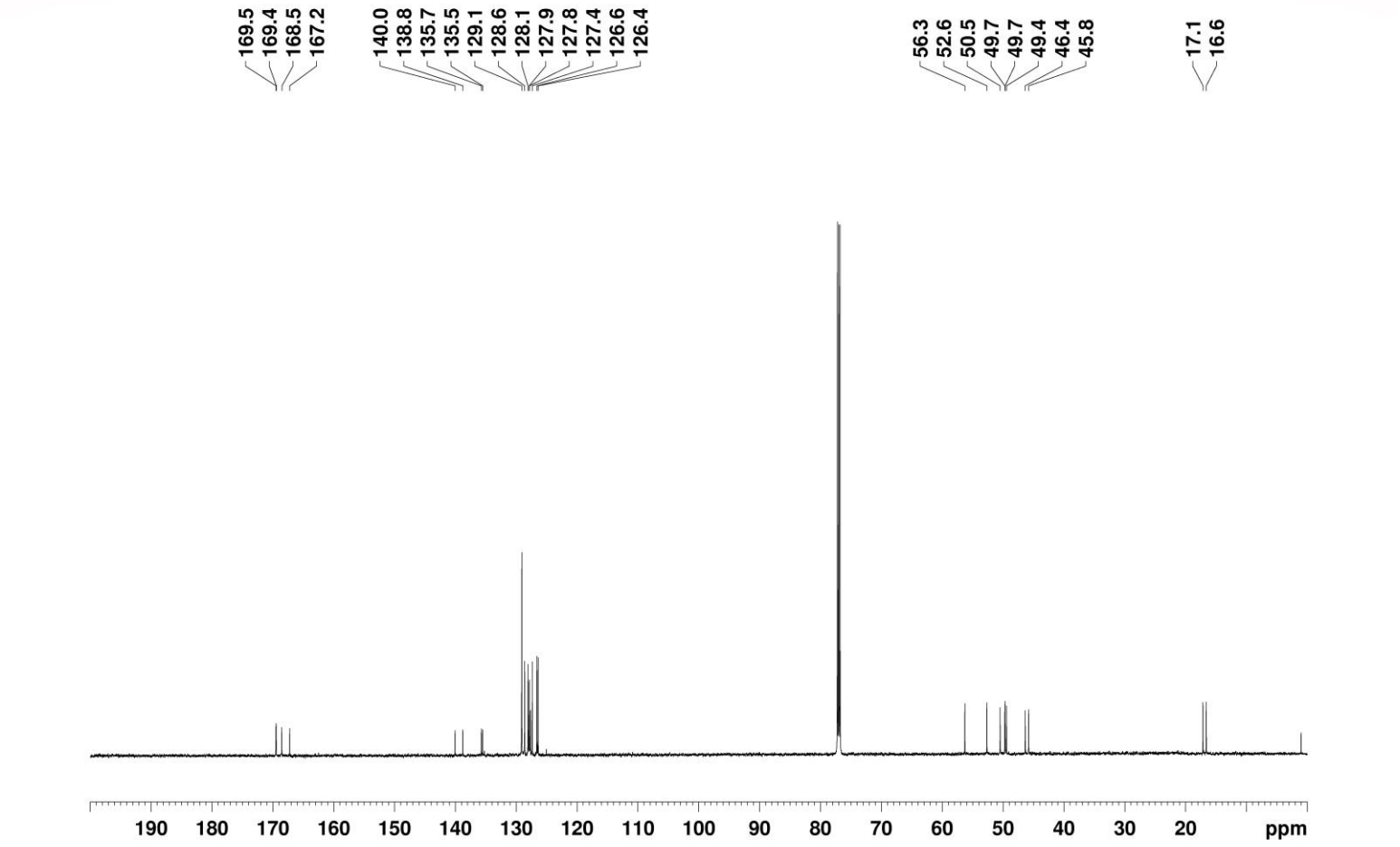
16/17: HSQC SPECTRUM (600 MHz, $CDCl_3$)



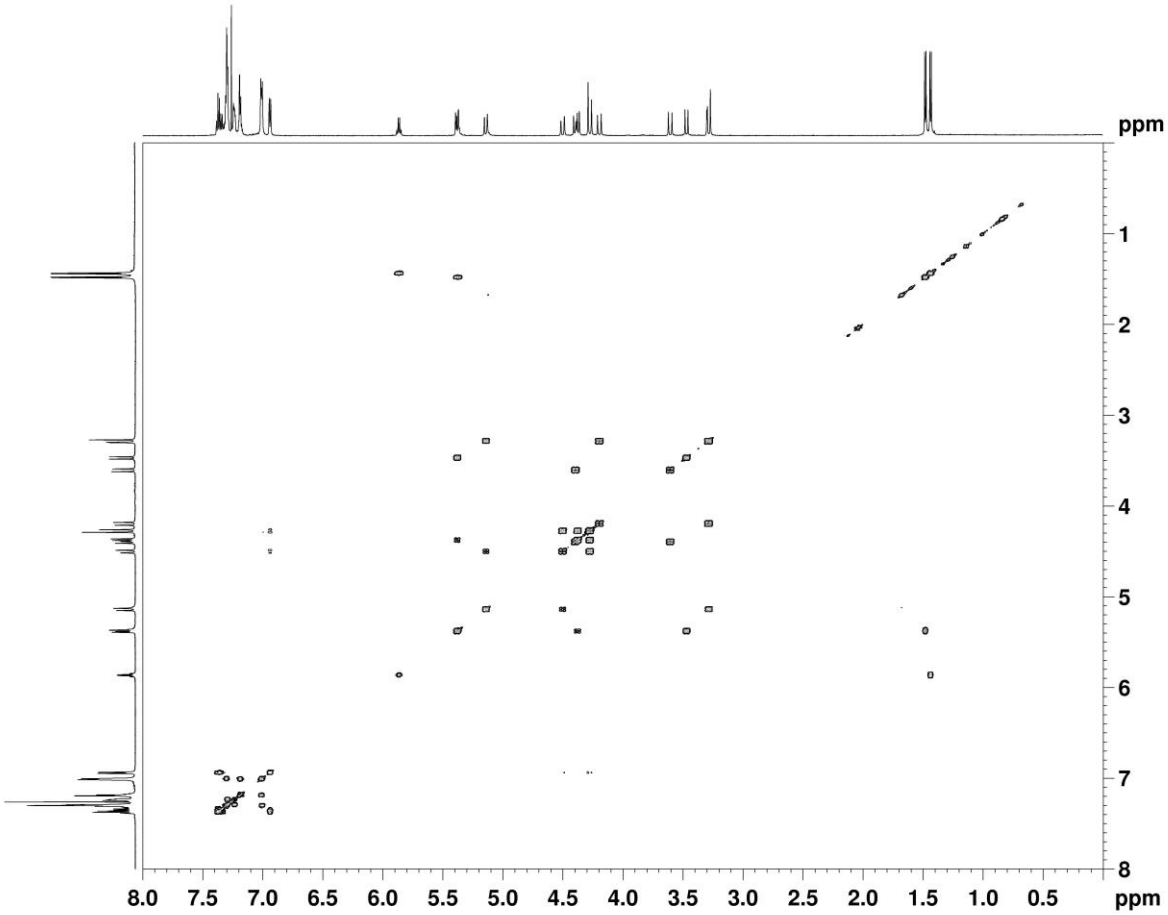
16/17: HMBC SPECTRUM (600 MHz, $CDCl_3$)



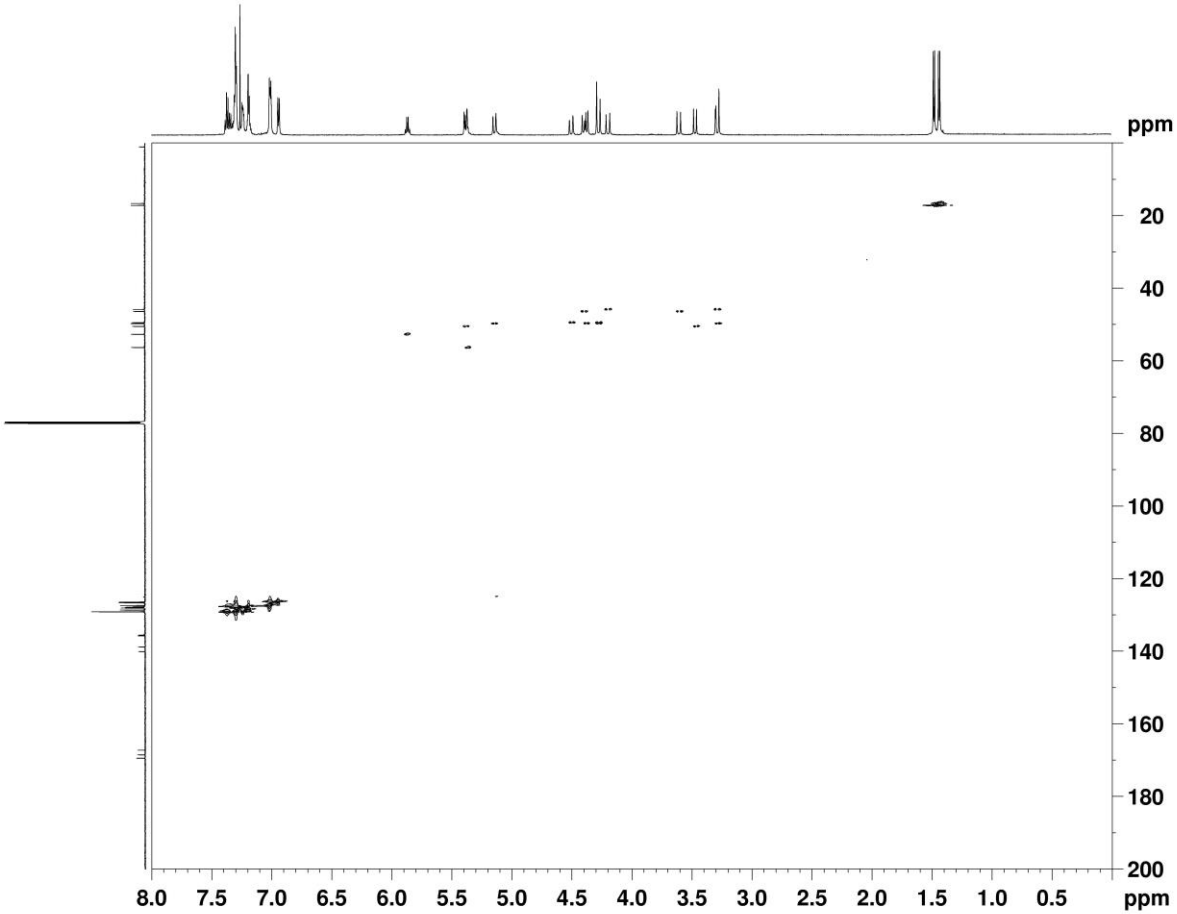
19: ^{1}H NMR (600 MHz, $CDCl_3$)



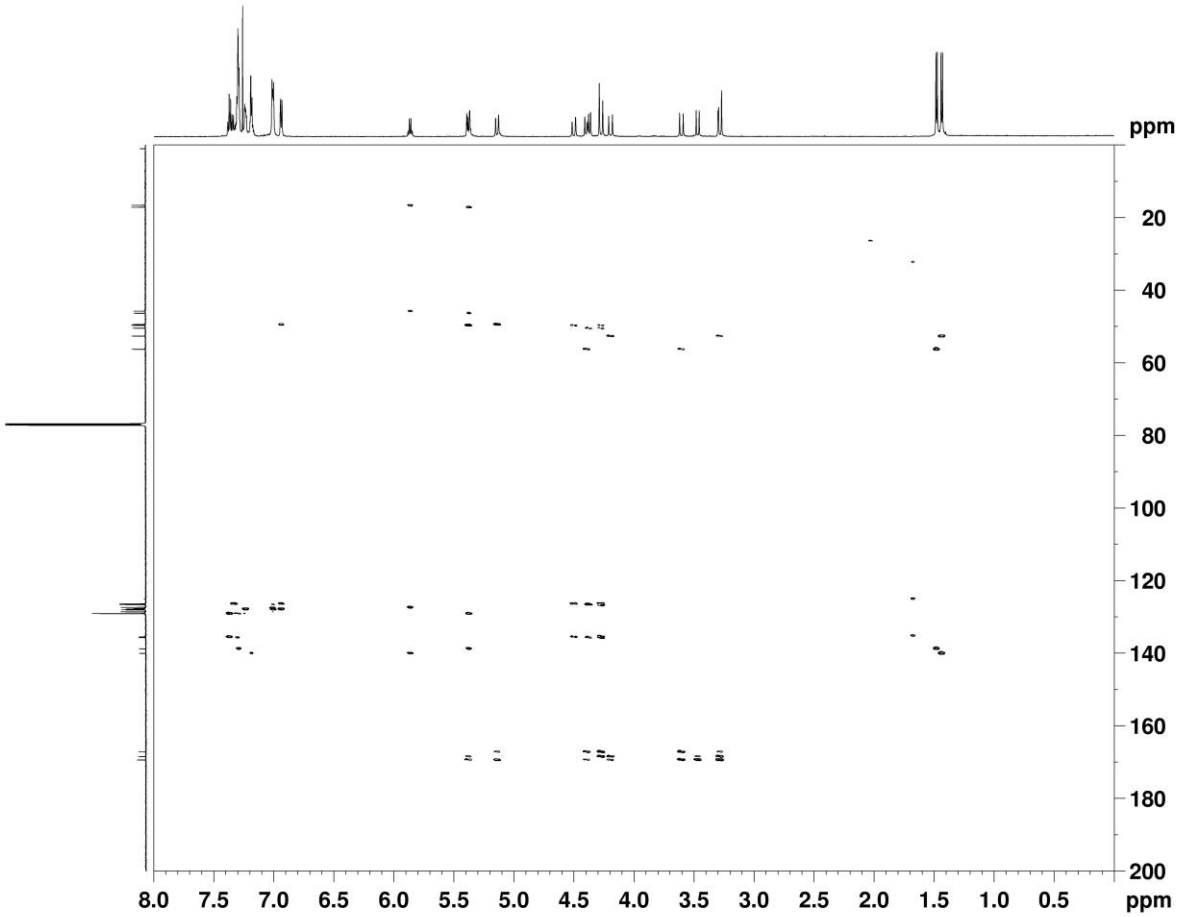
19: ^{13}C NMR (150 MHz, $CDCl_3$)



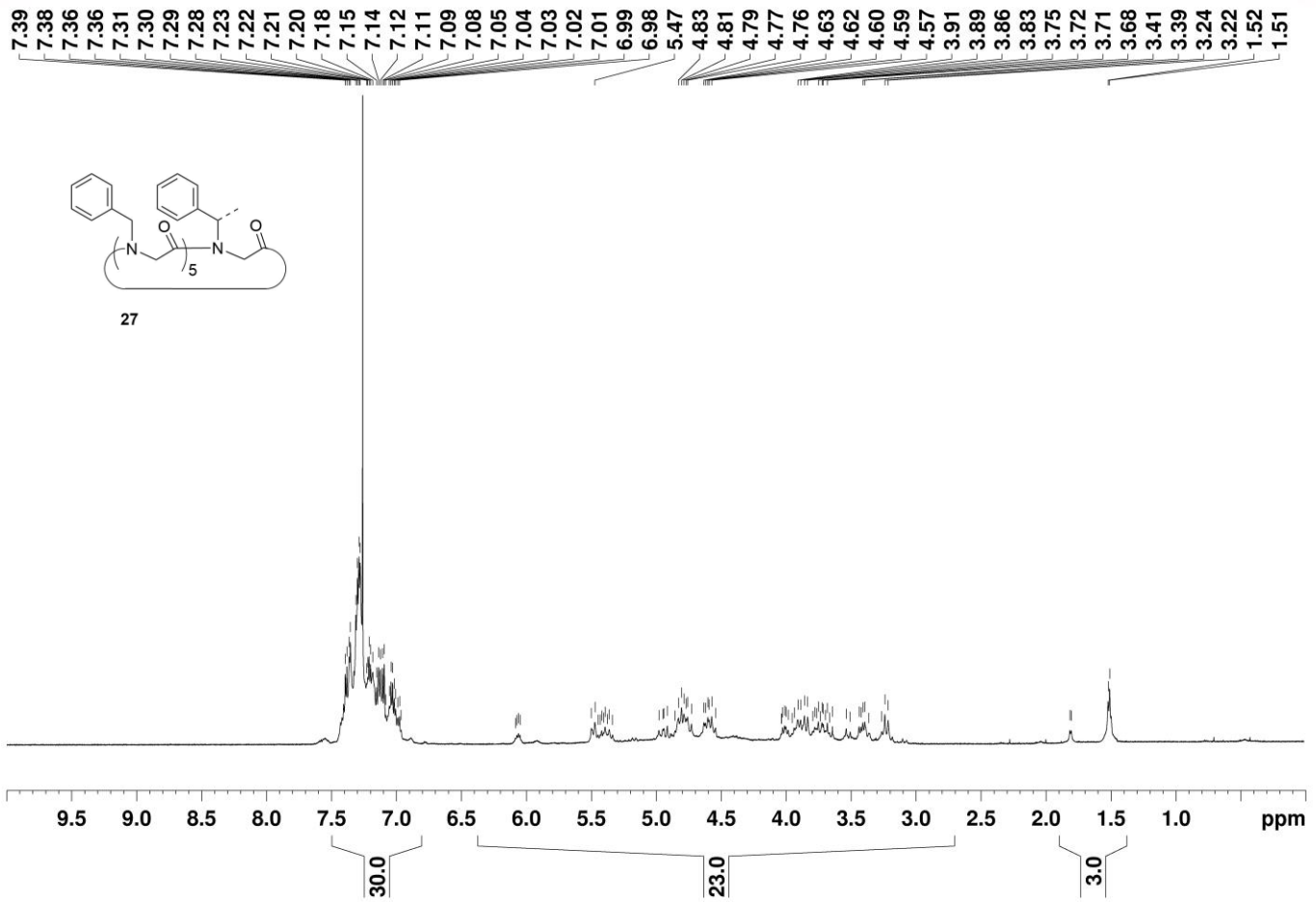
19: COSY SPECTRUM (600 MHz, $CDCl_3$)



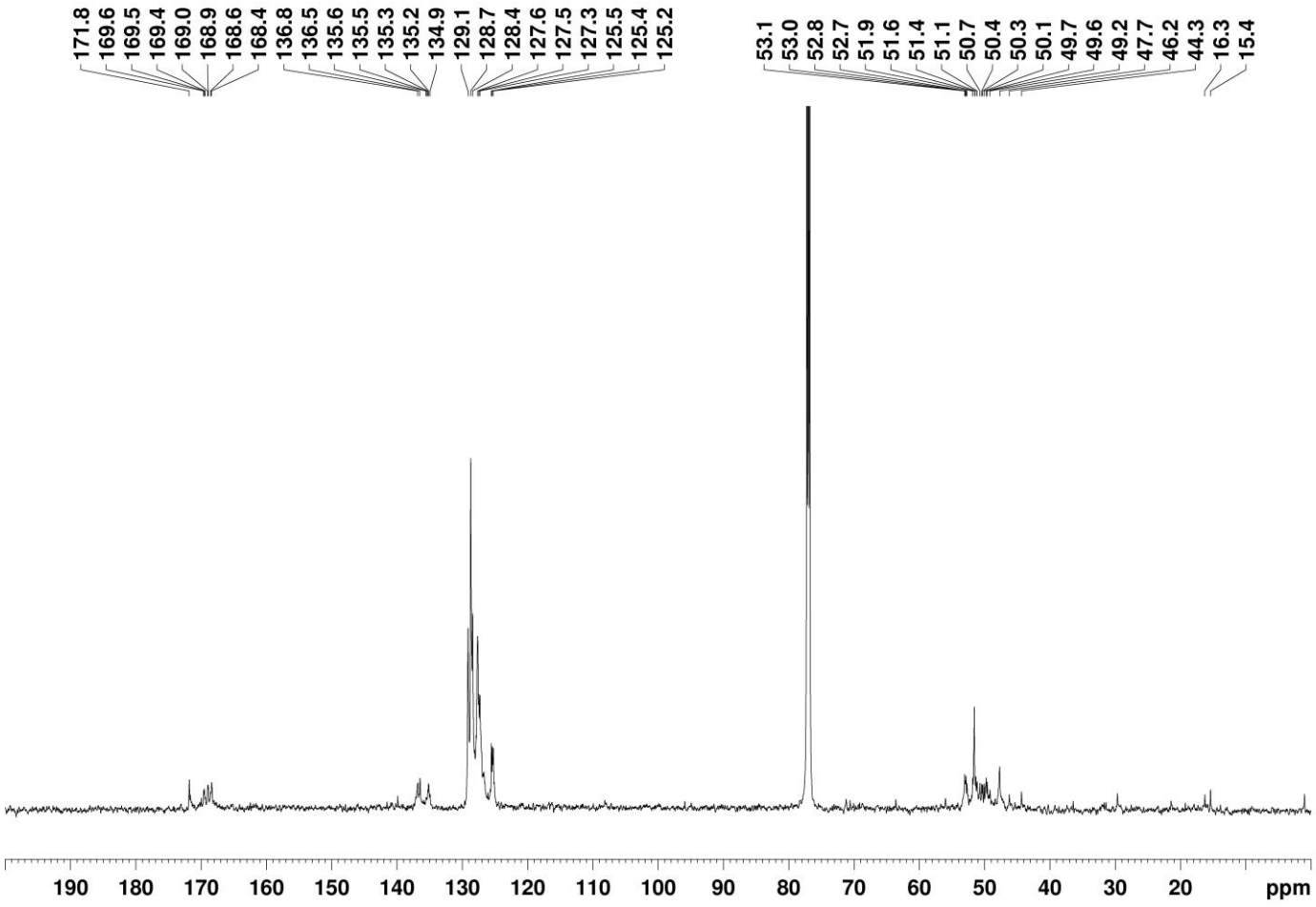
19: HSQC SPECTRUM (600 MHz, $CDCl_3$)



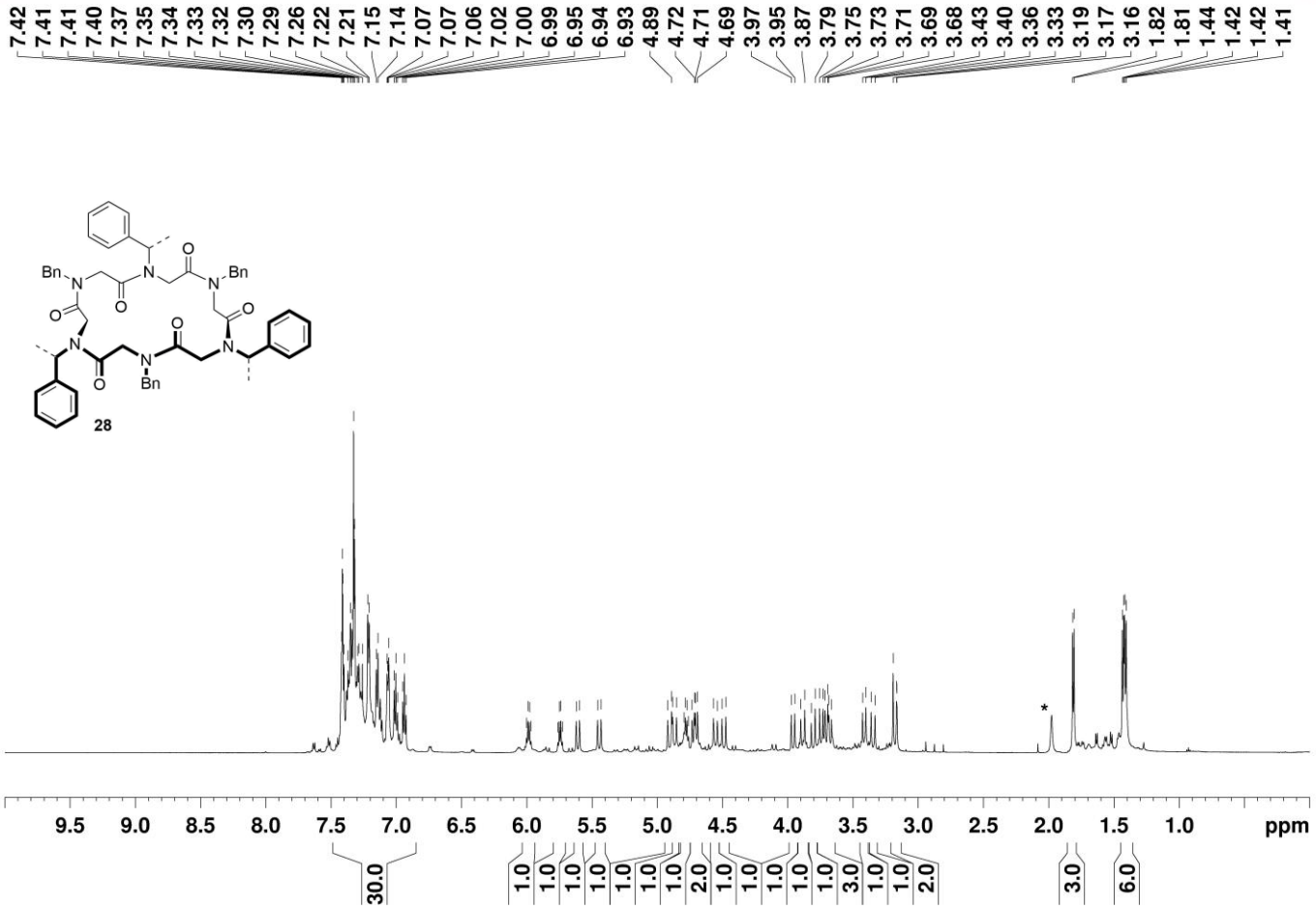
19: HMBC SPECTRUM (600 MHz, $CDCl_3$)



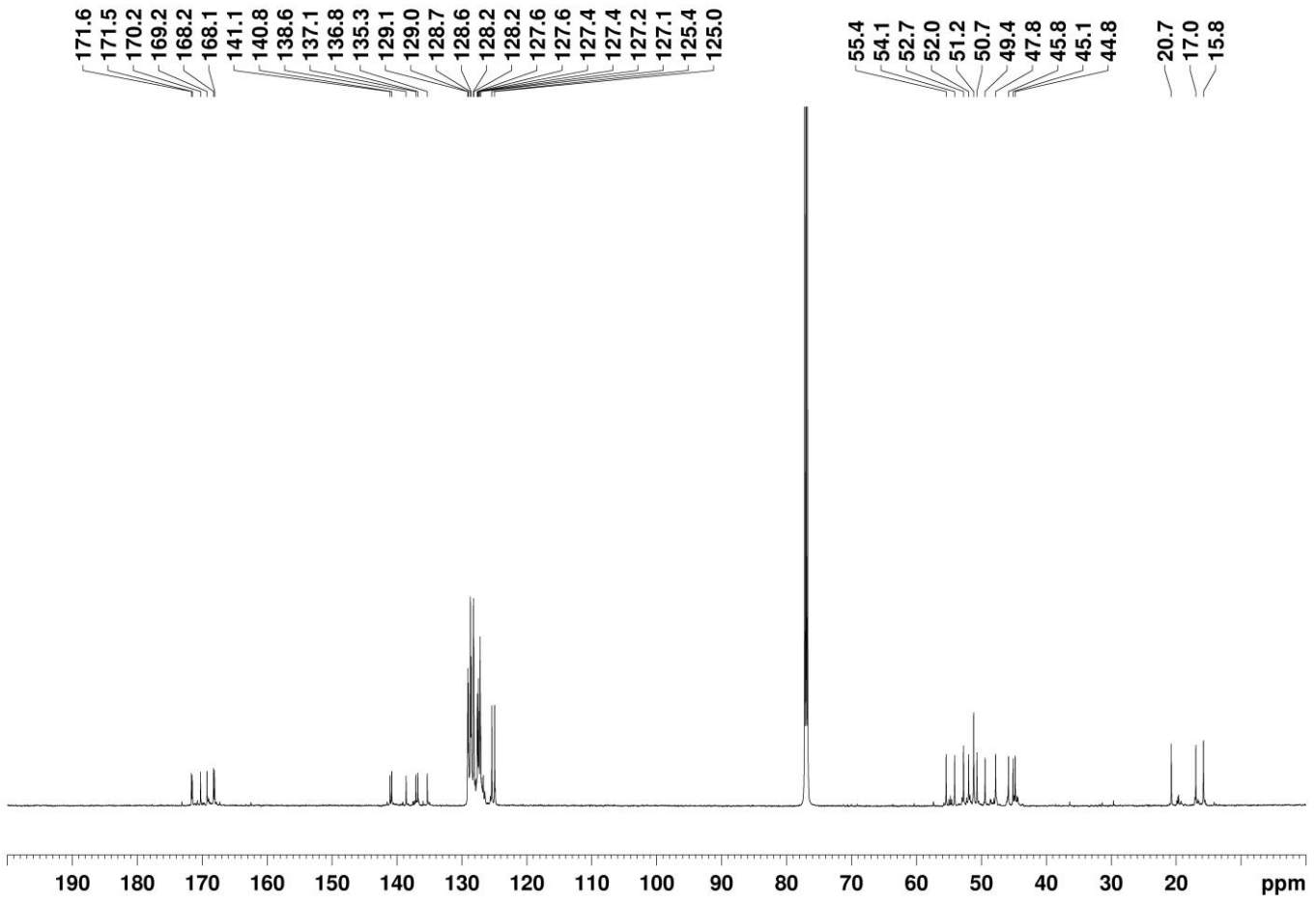
27: ^{1}H NMR (600 MHz, $CDCl_3$)



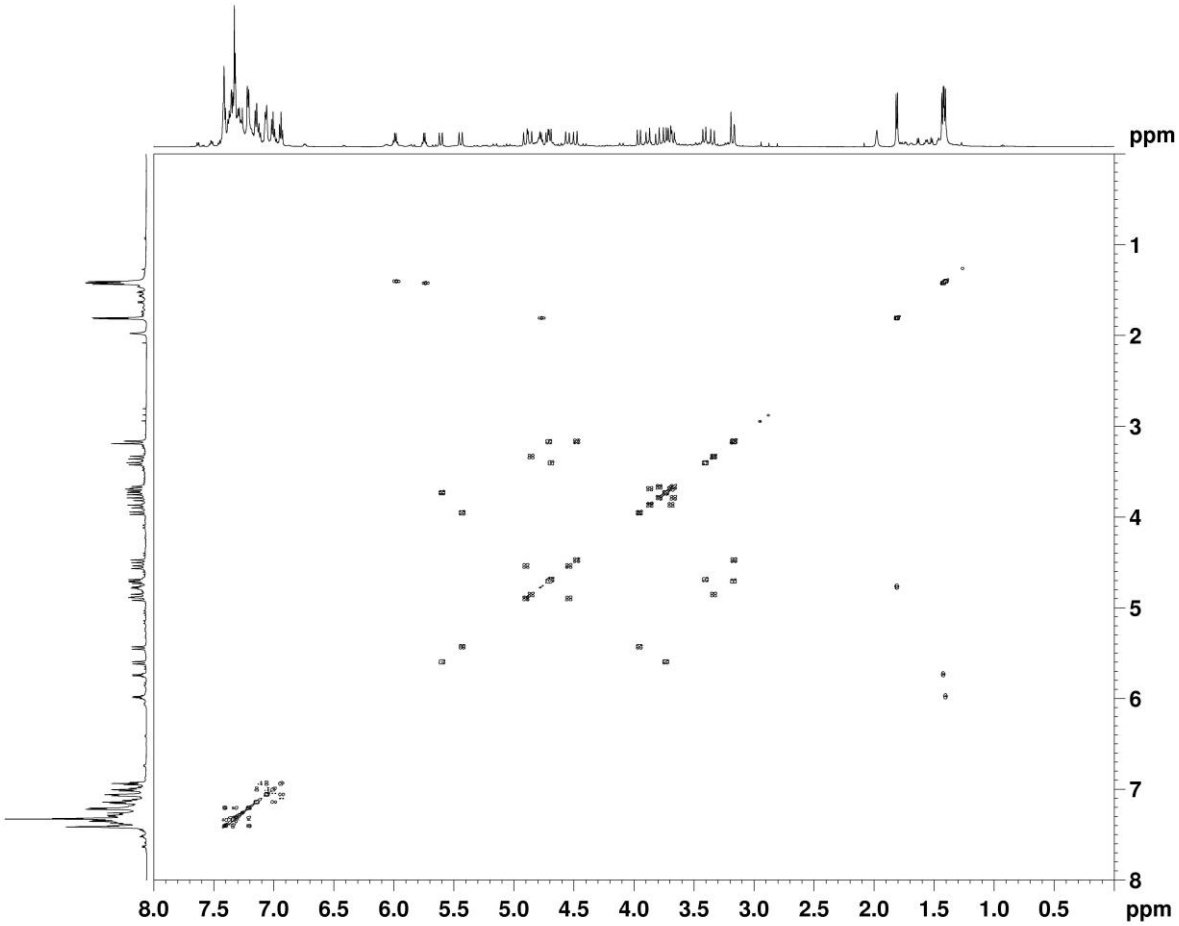
27: ^{13}C NMR (150 MHz, $CDCl_3$)



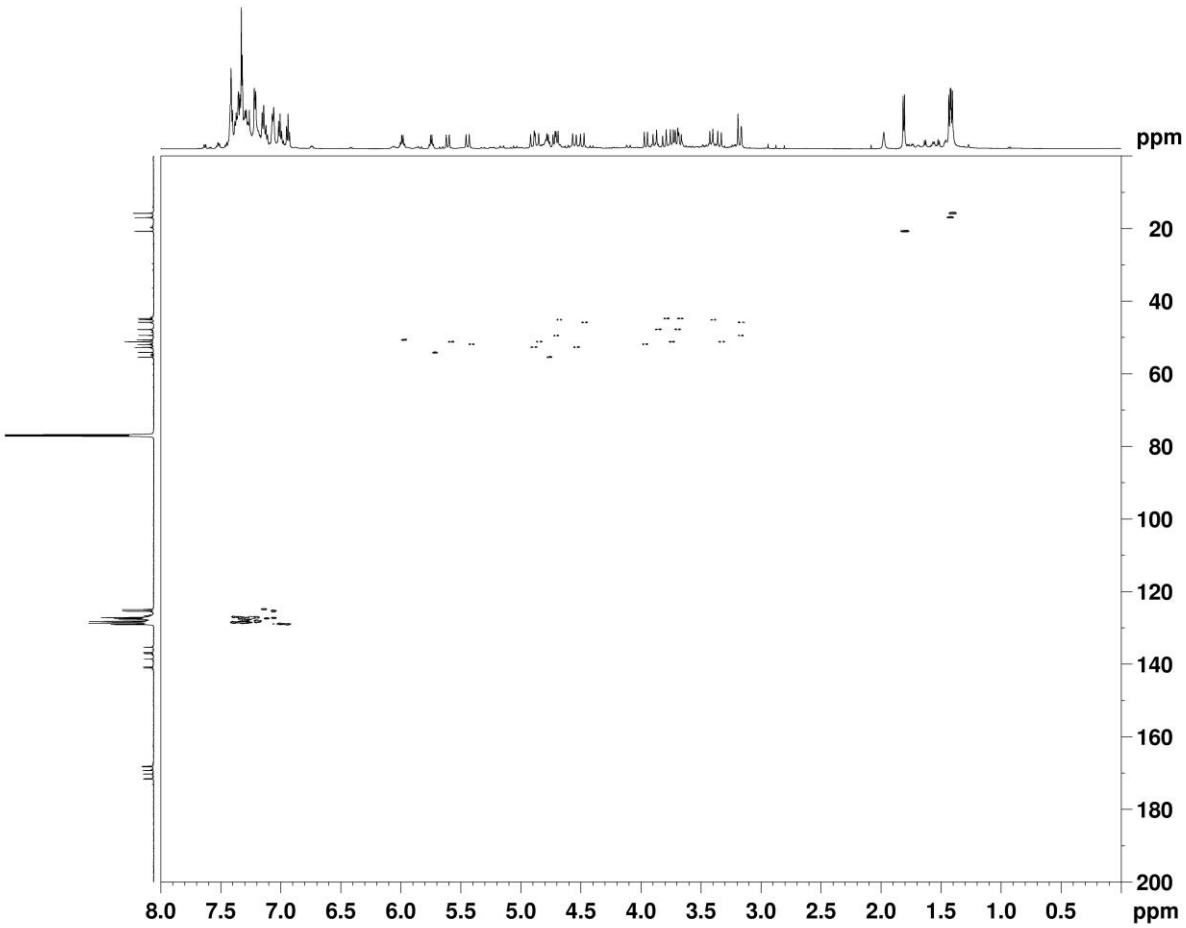
28: ^{1}H NMR (600 MHz, $CDCl_3$). Water impurities are labelled with a black asterisk.



28: ^{13}C NMR (150 MHz, $CDCl_3$)



28: COSY SPECTRUM (600 MHz, $CDCl_3$)



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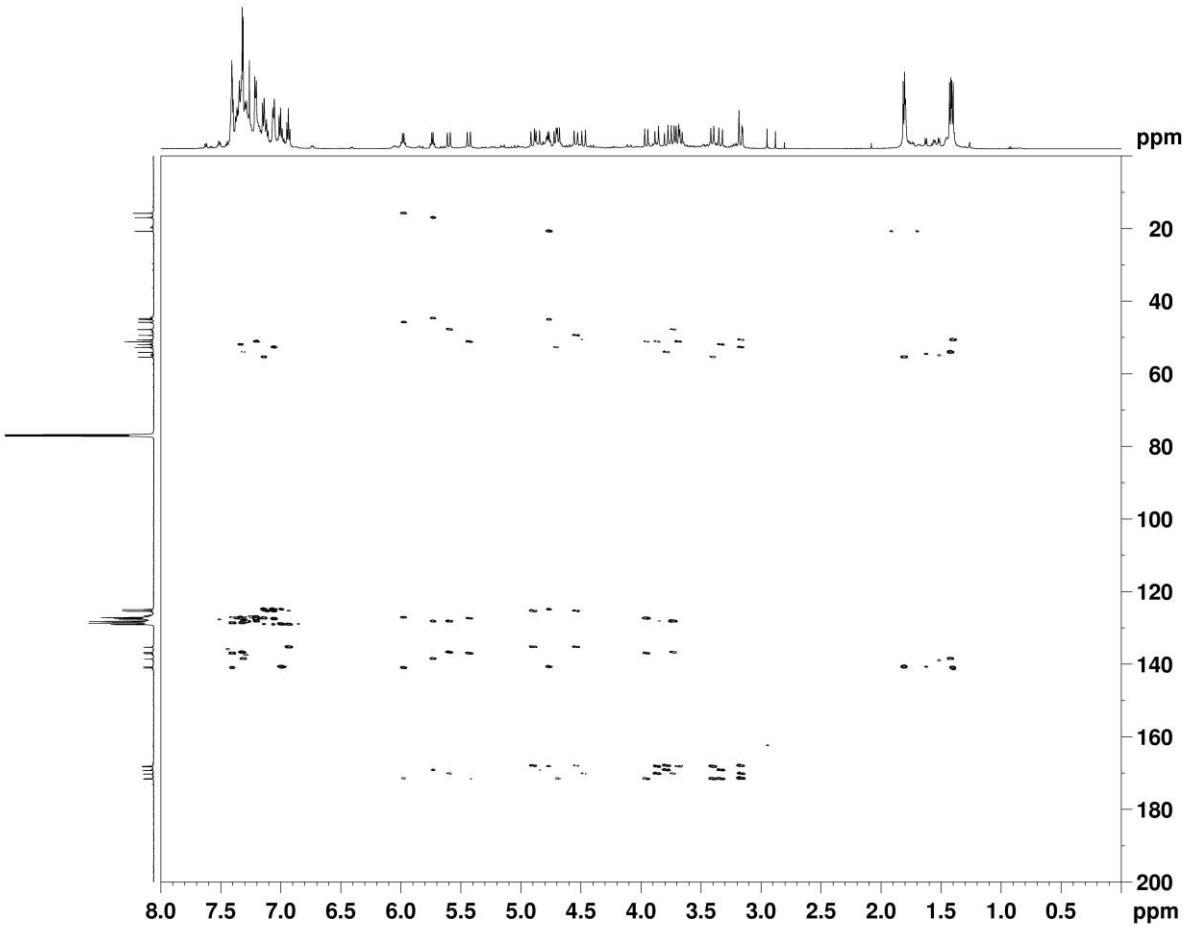
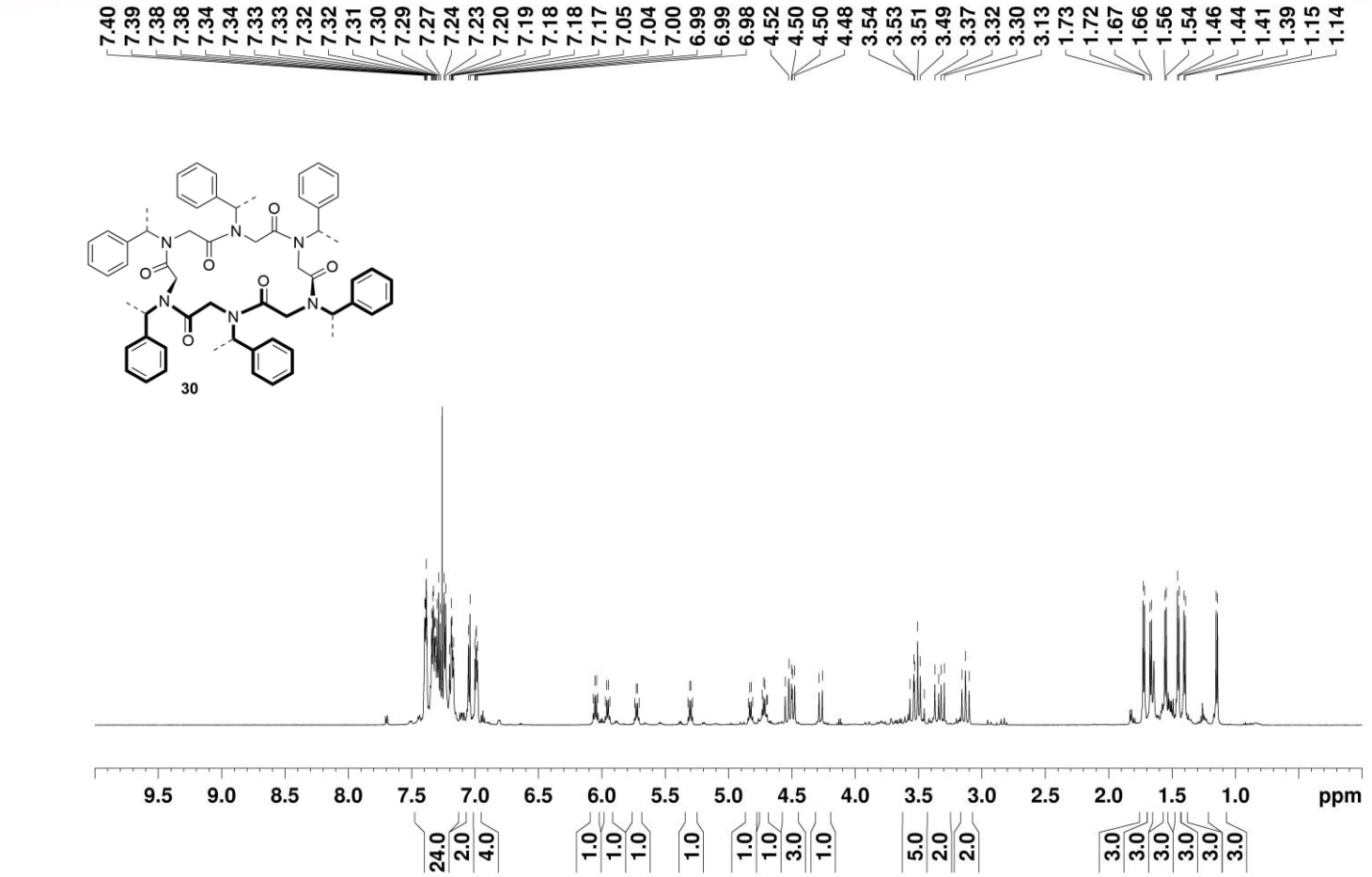
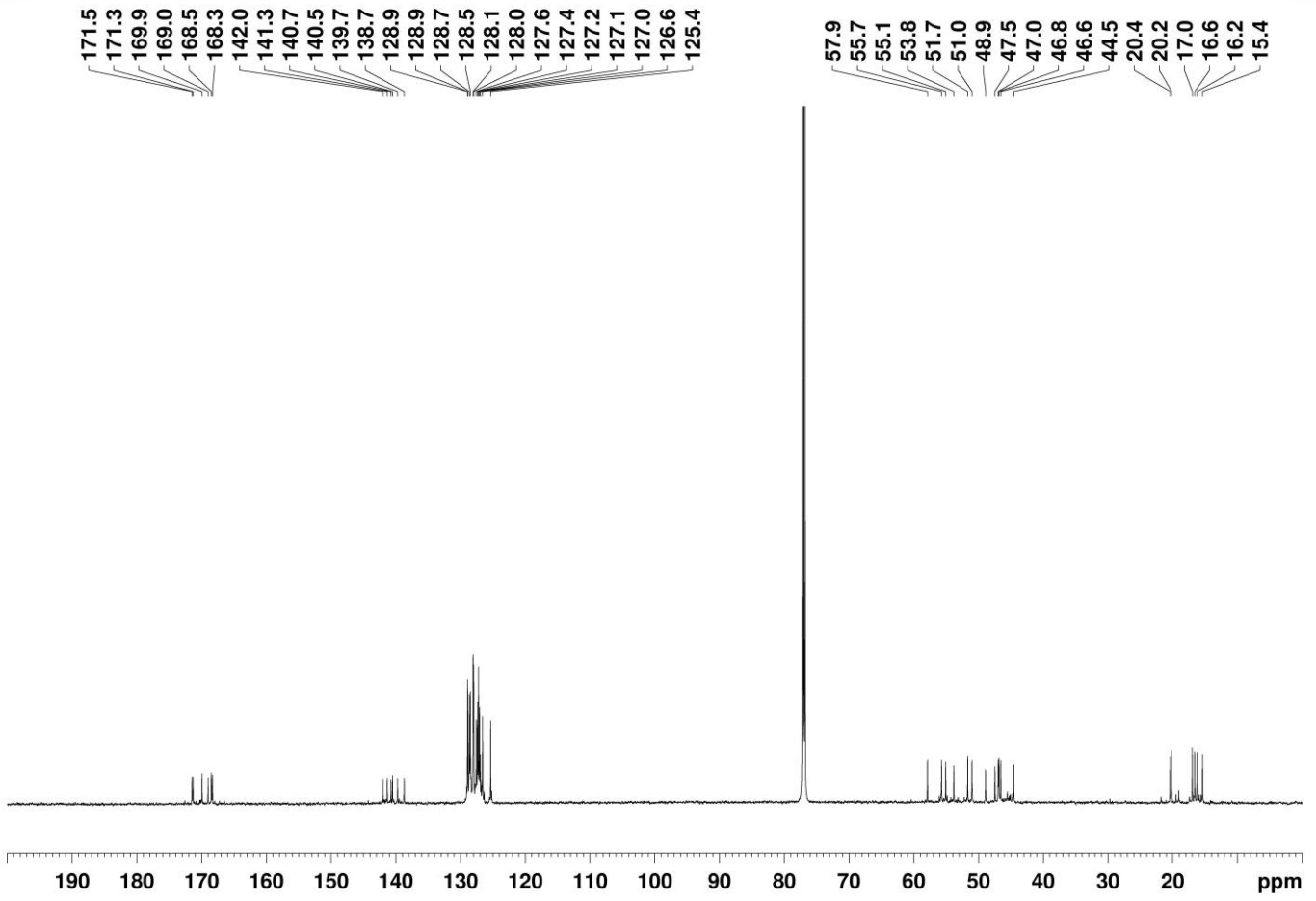


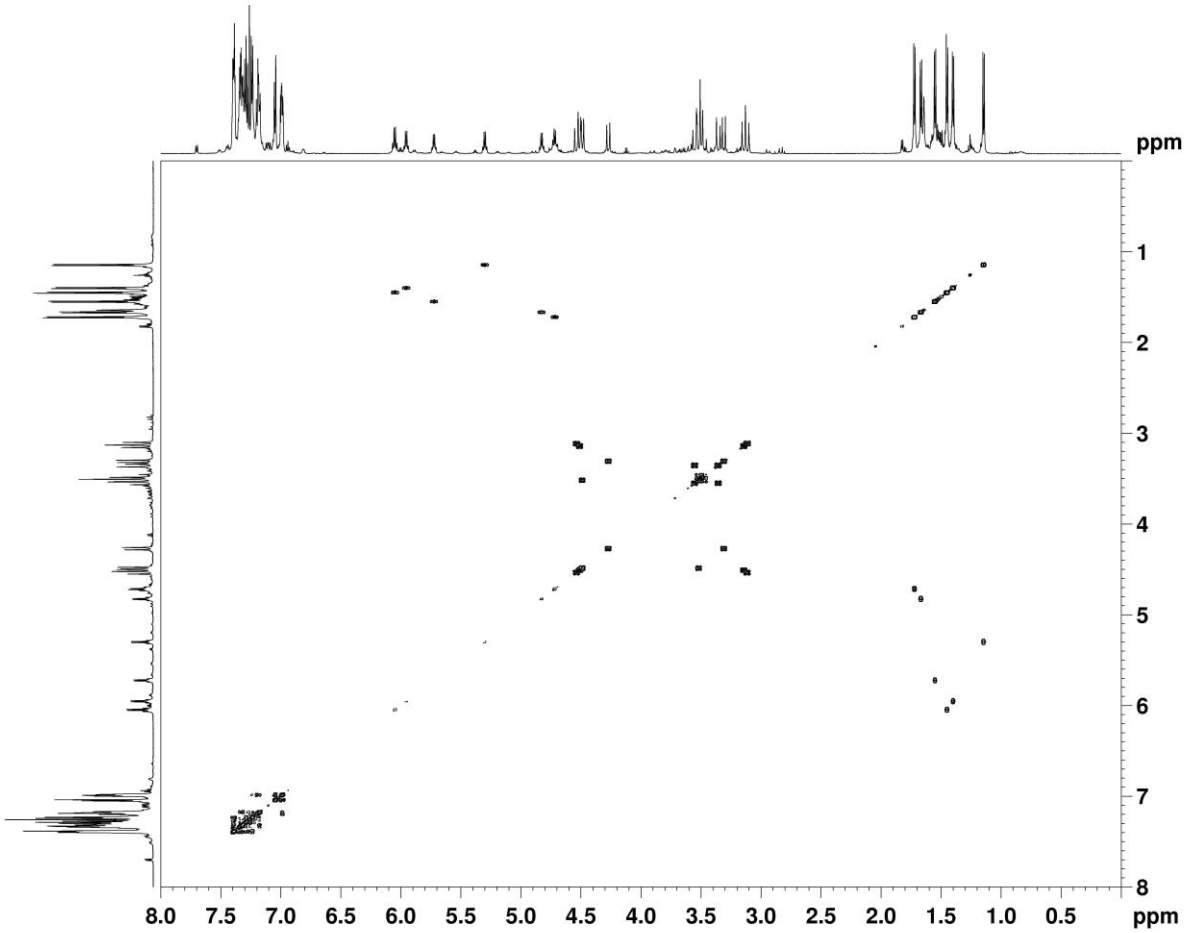
28: HMBC SPECTRUM (600 MHz, $CDCl_3$)



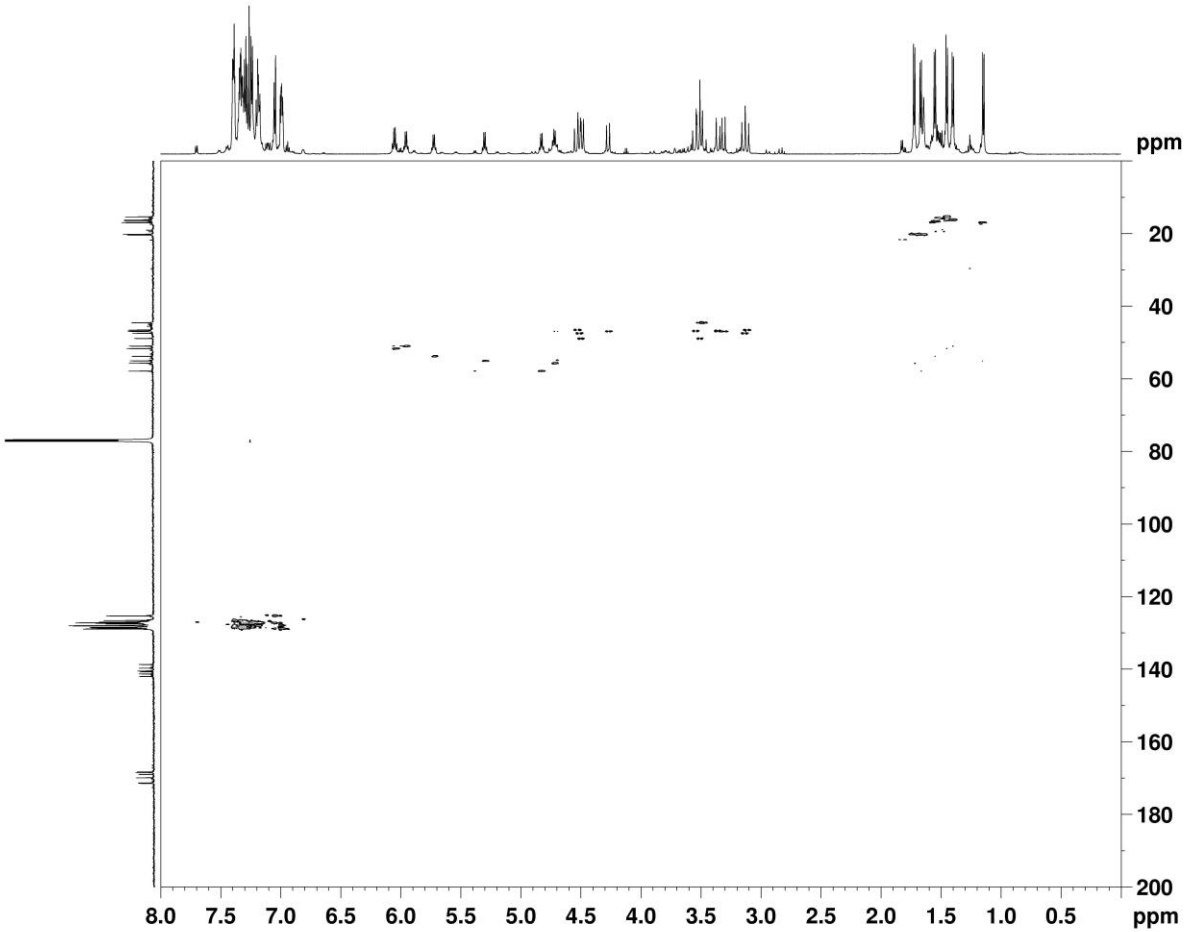
30: ^{1}H NMR (600 MHz, $CDCl_3$)



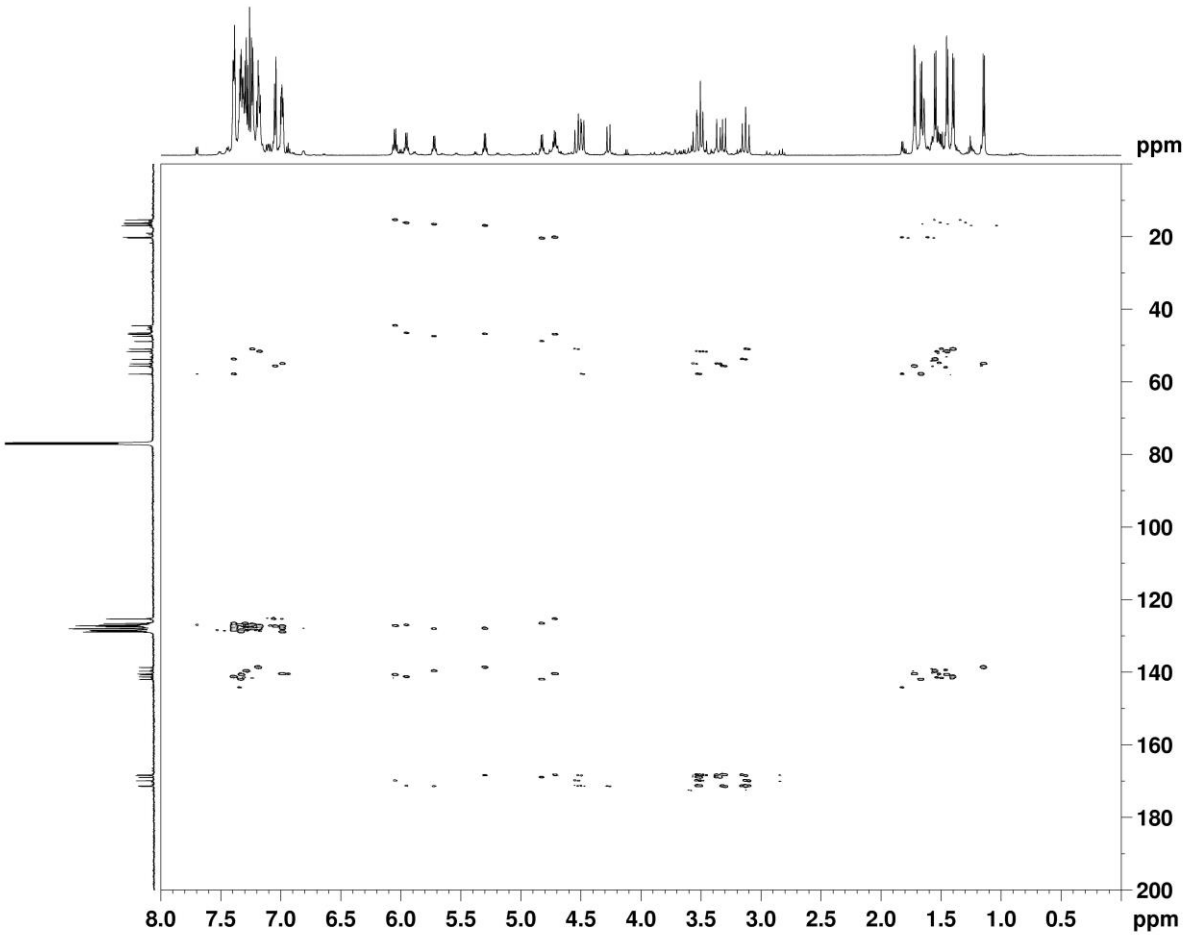
30: ^{13}C NMR (150 MHz, $CDCl_3$)



30: COSY SPECTRUM (600 MHz, $CDCl_3$)



30: HSQC SPECTRUM (600 MHz, $CDCl_3$)



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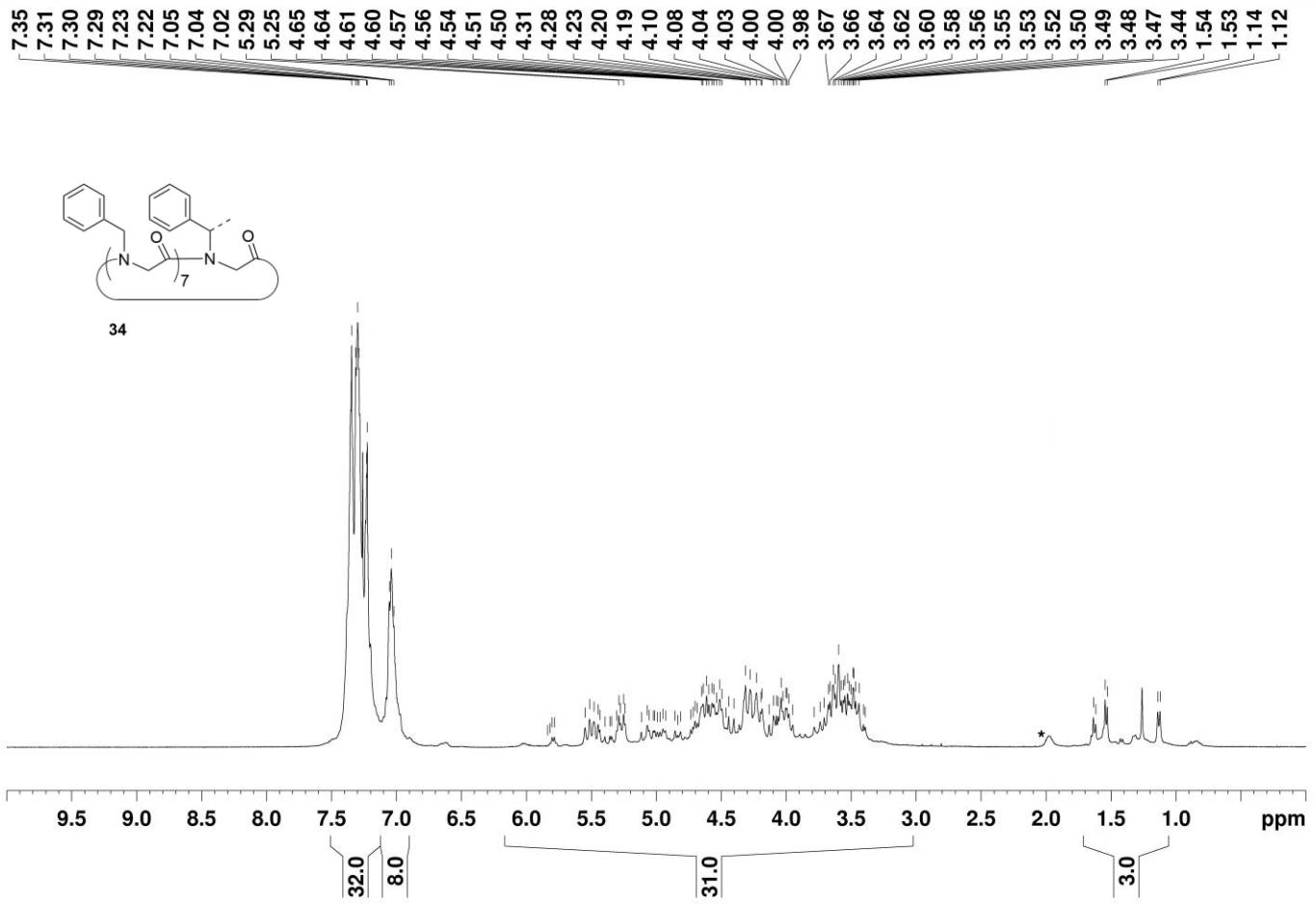
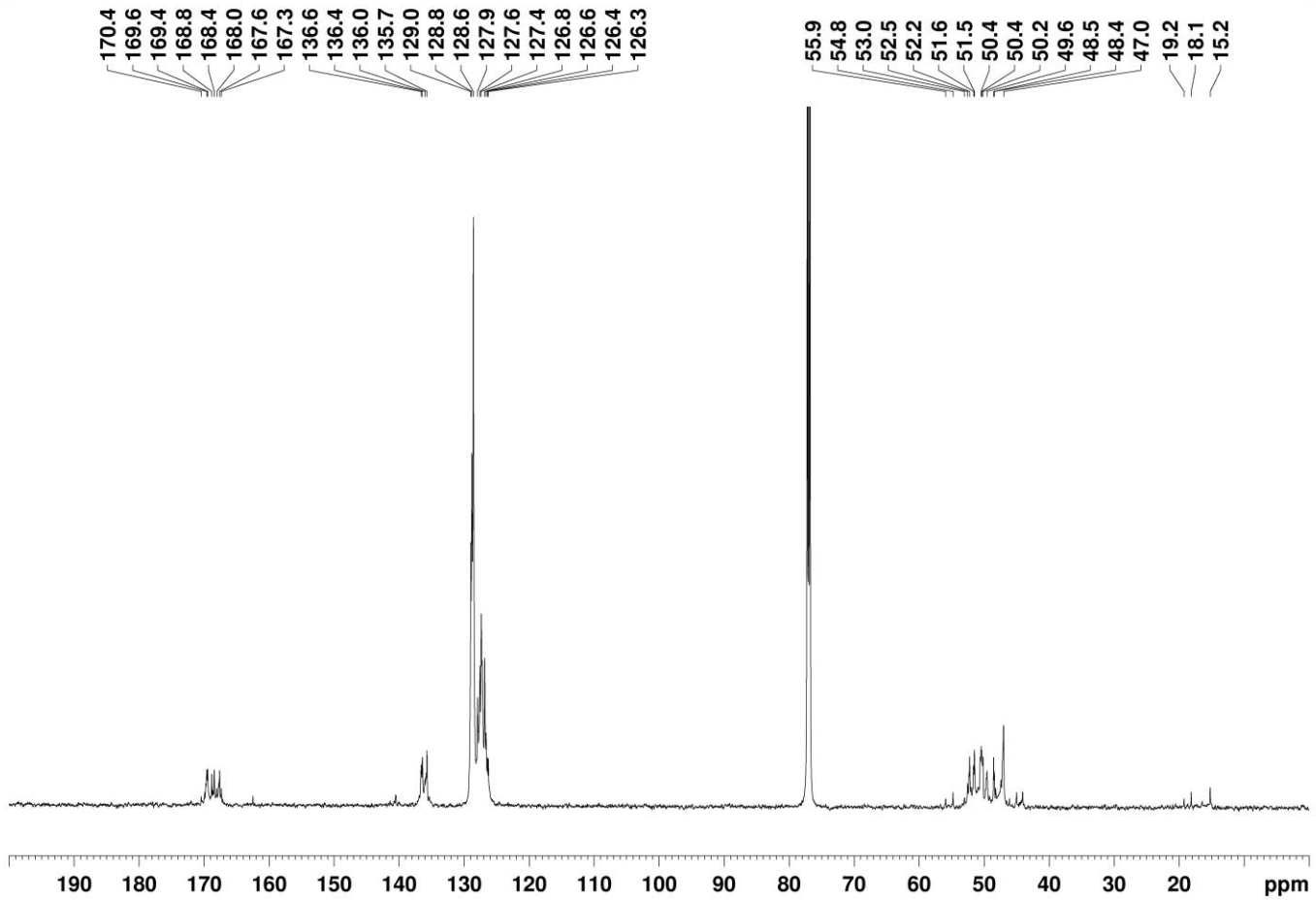
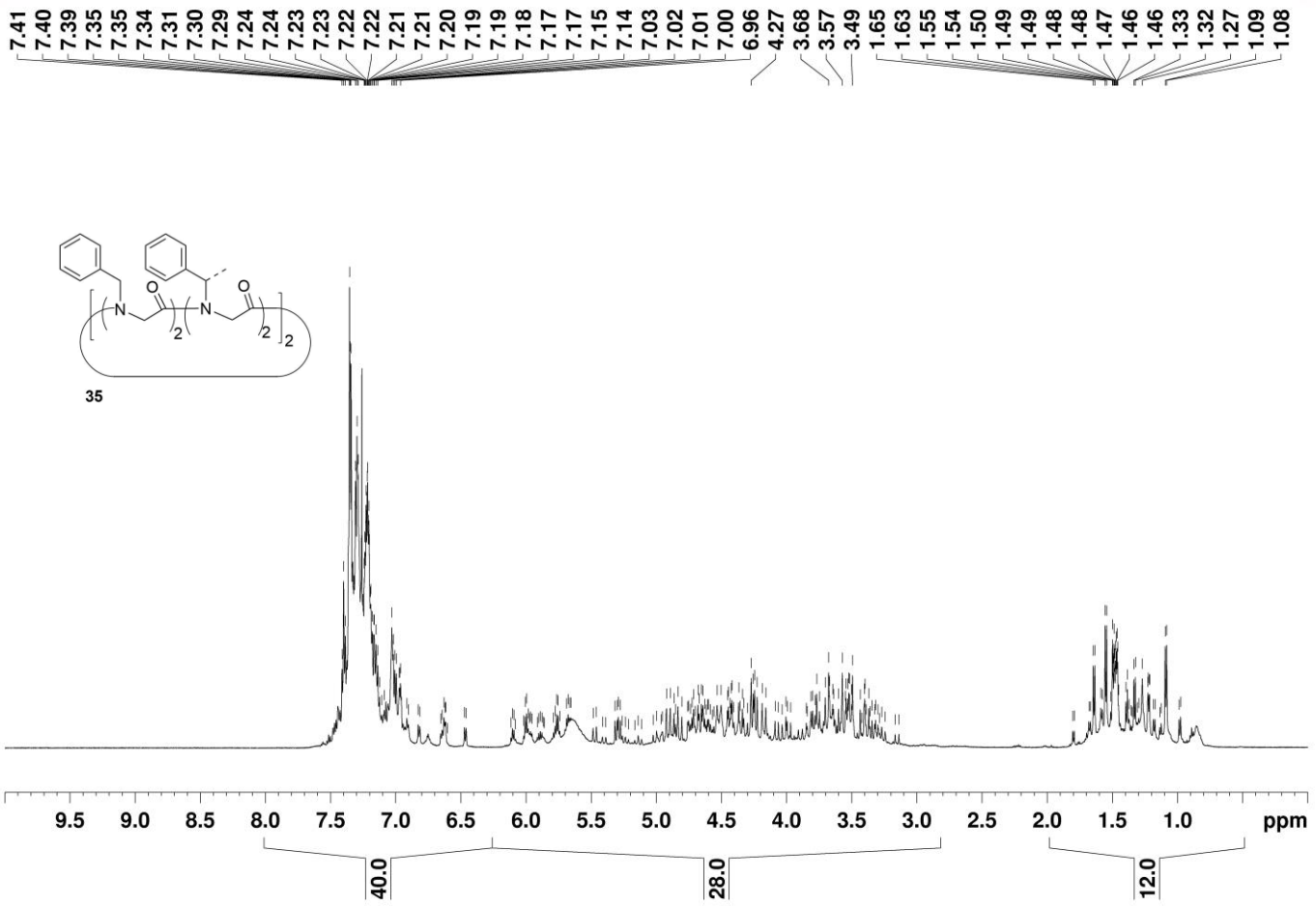


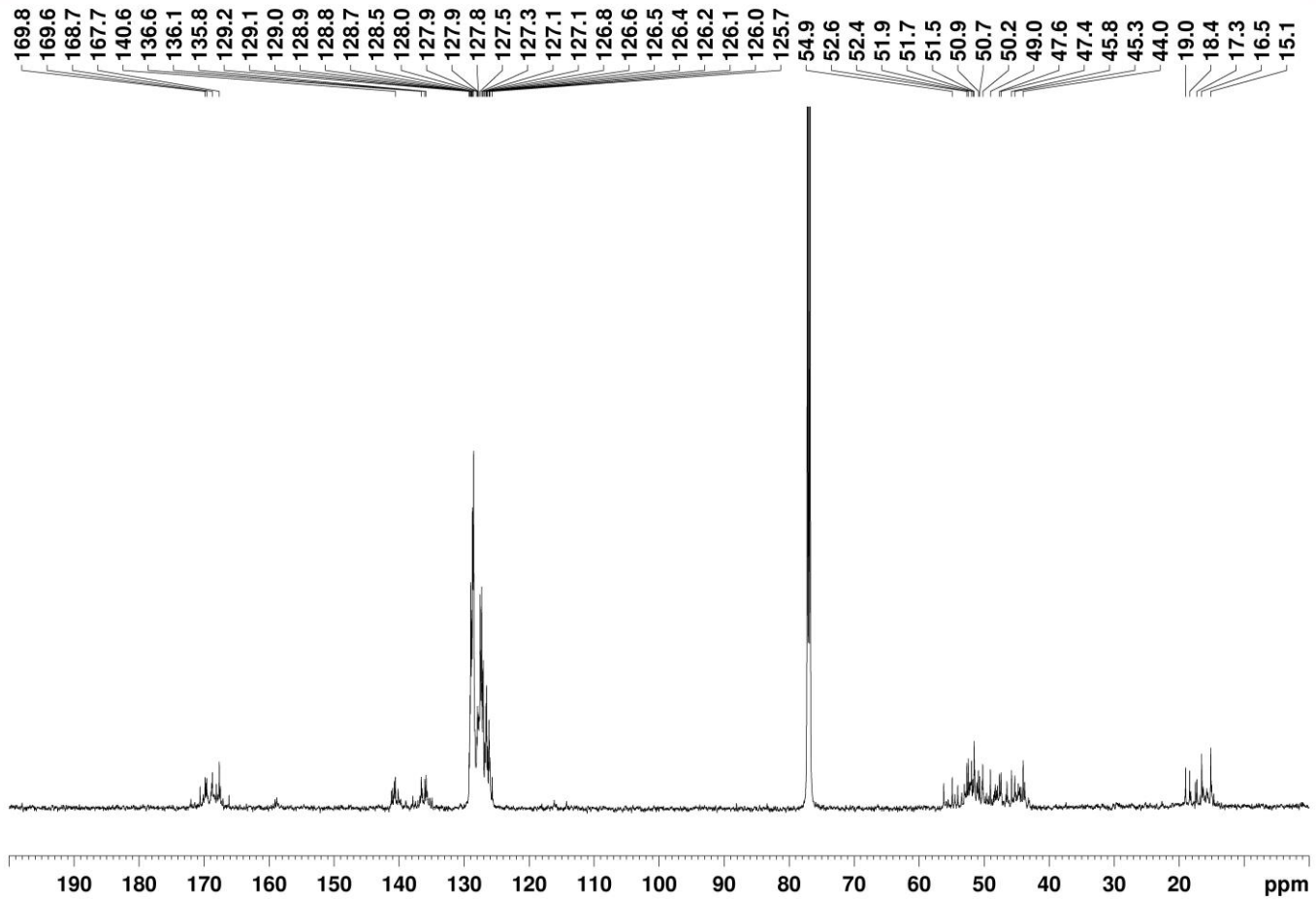
34: ^{1}H NMR (400 MHz, $CDCl_3$). Water impurities are labelled with a black asterisk.



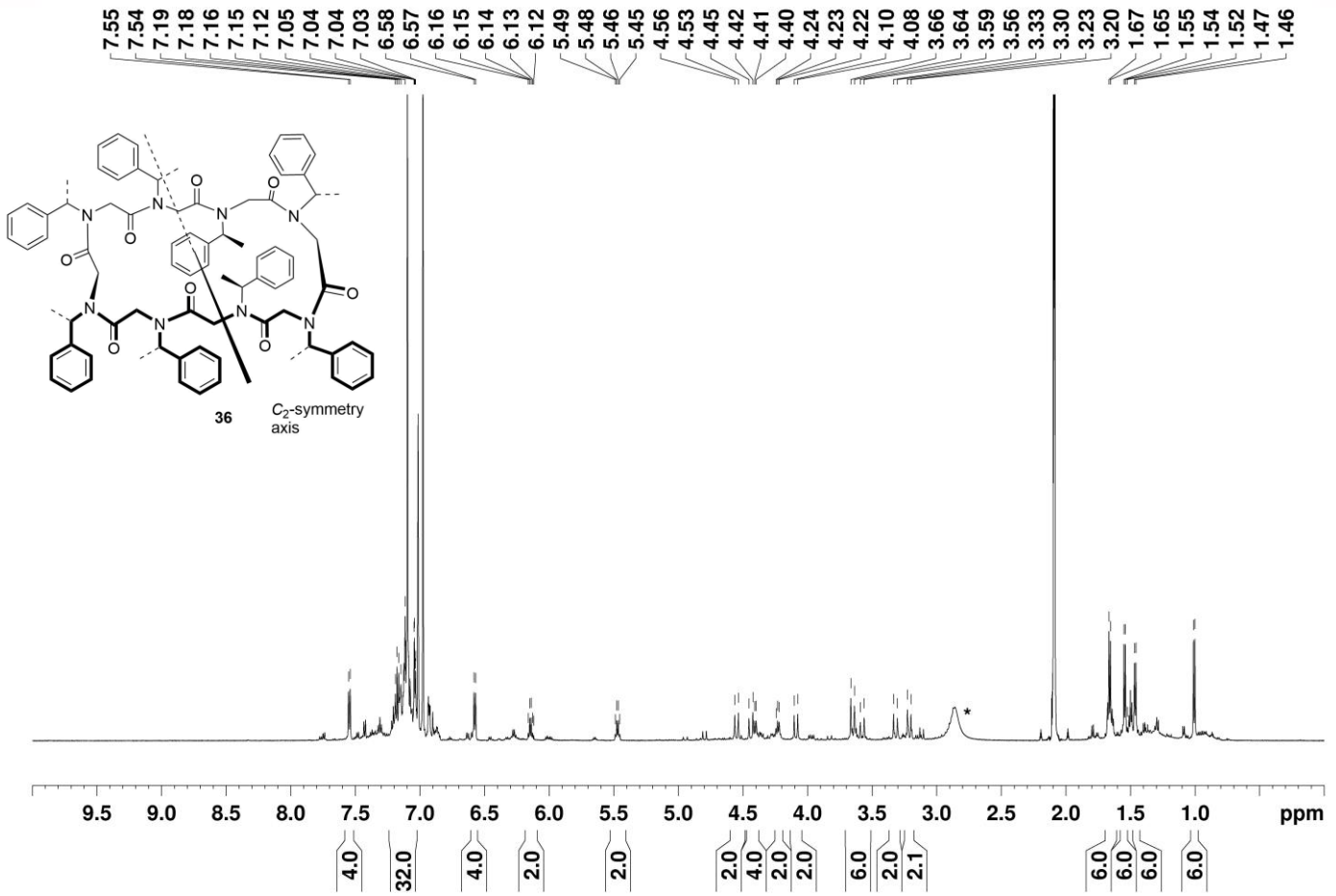
34: ^{13}C NMR (150 MHz, $CDCl_3$)



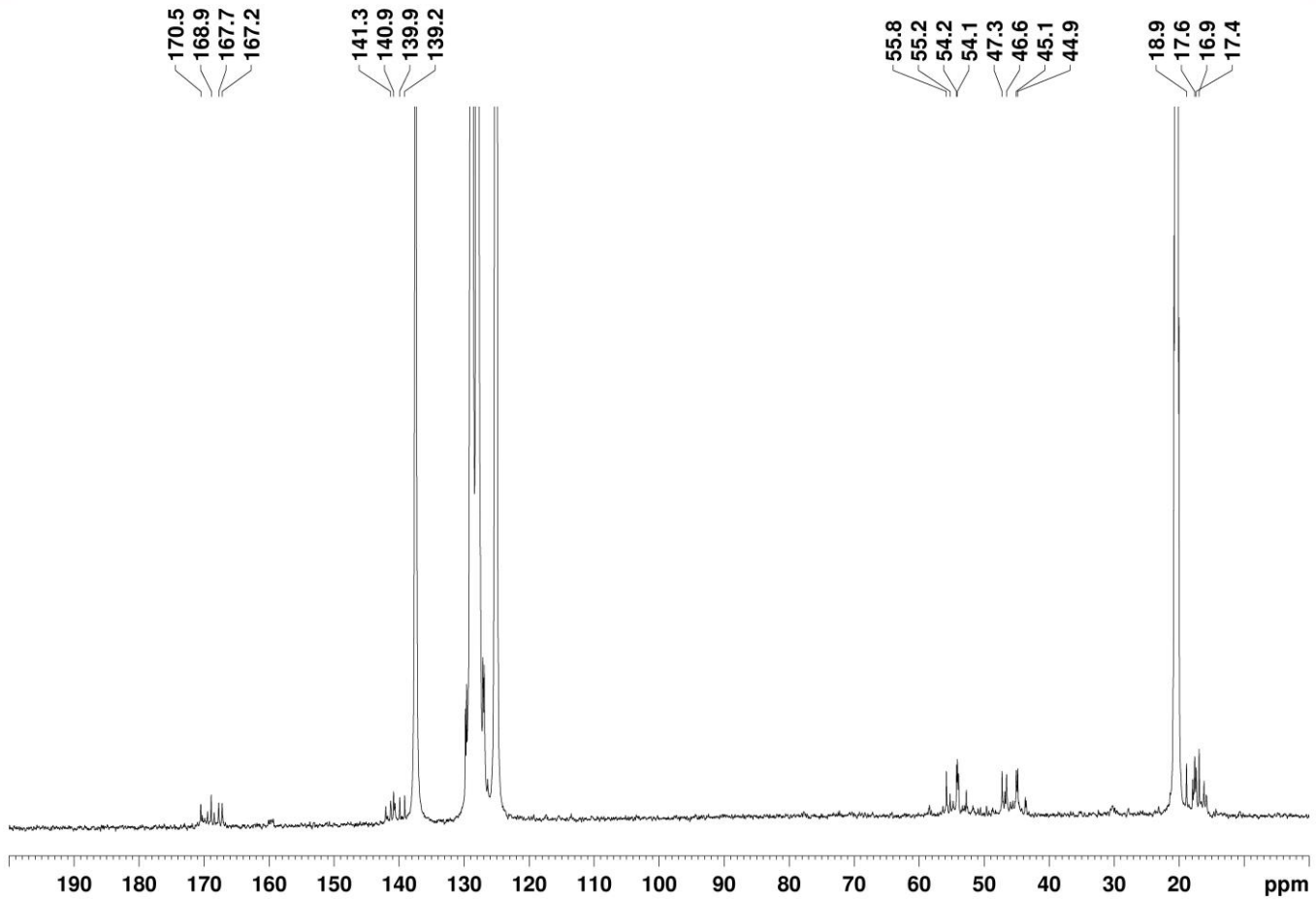
35: ^{1}H NMR (600 MHz, $CDCl_3$)



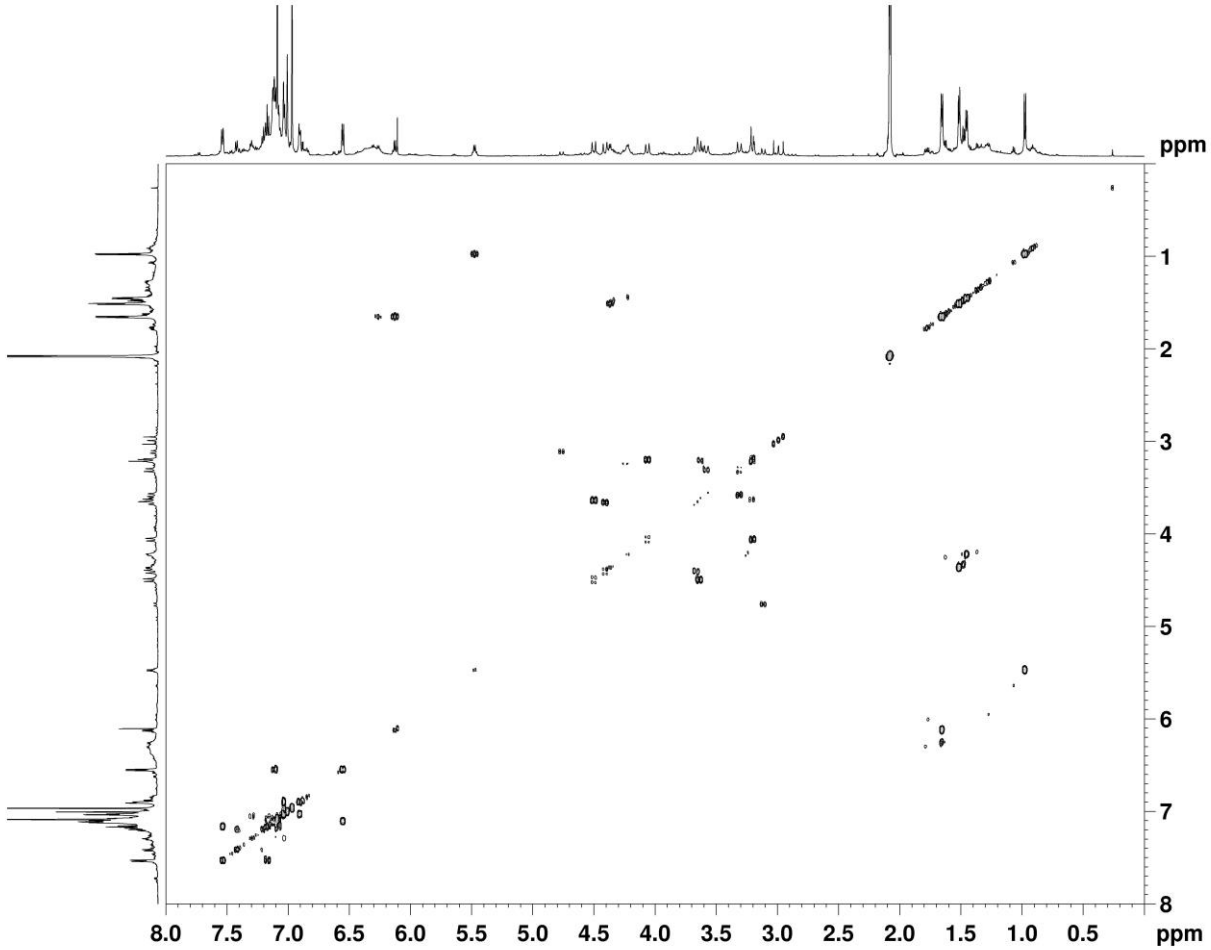
35: ^{13}C NMR (150 MHz, $CDCl_3$)



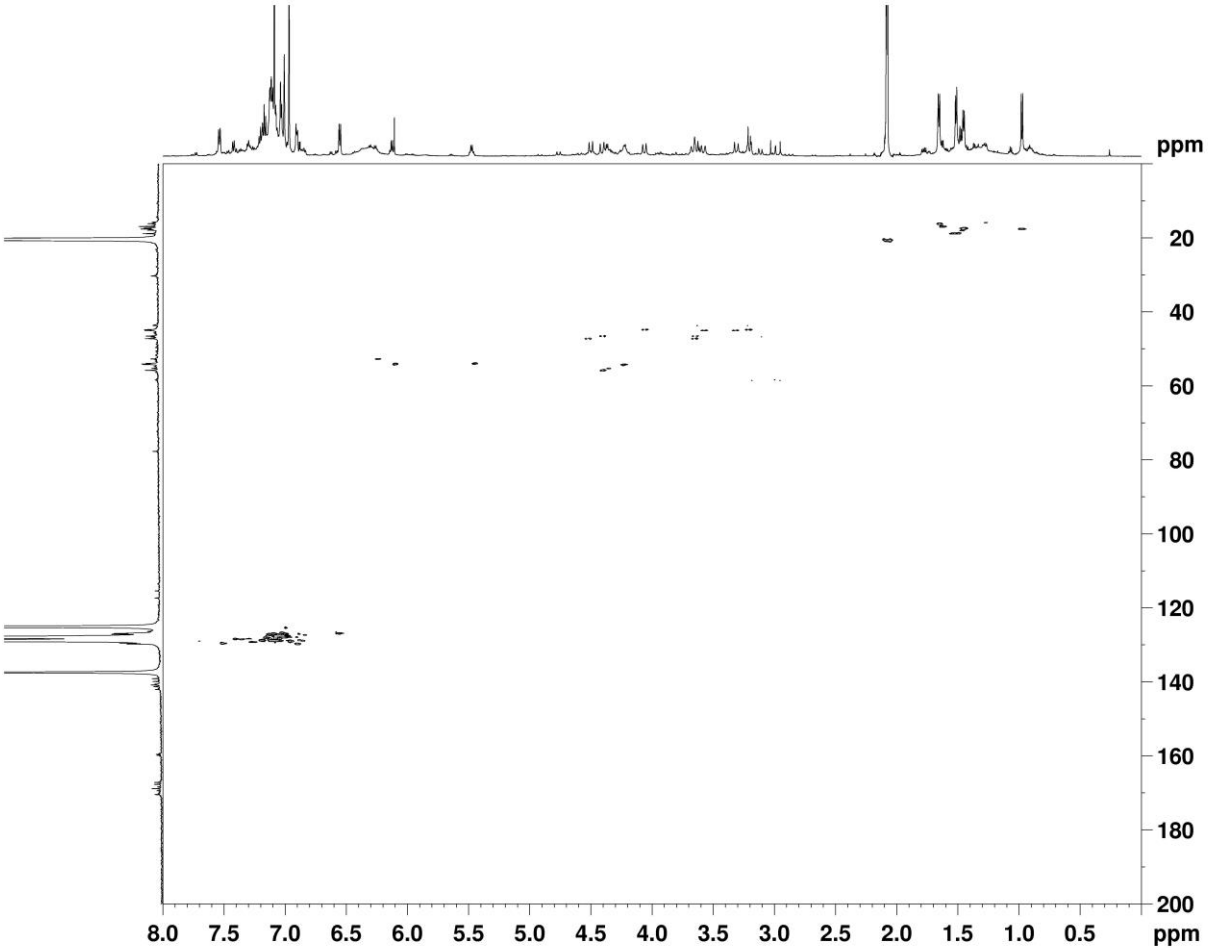
36: ^{1}H NMR (600 MHz, $C_6D_5CD_3$)



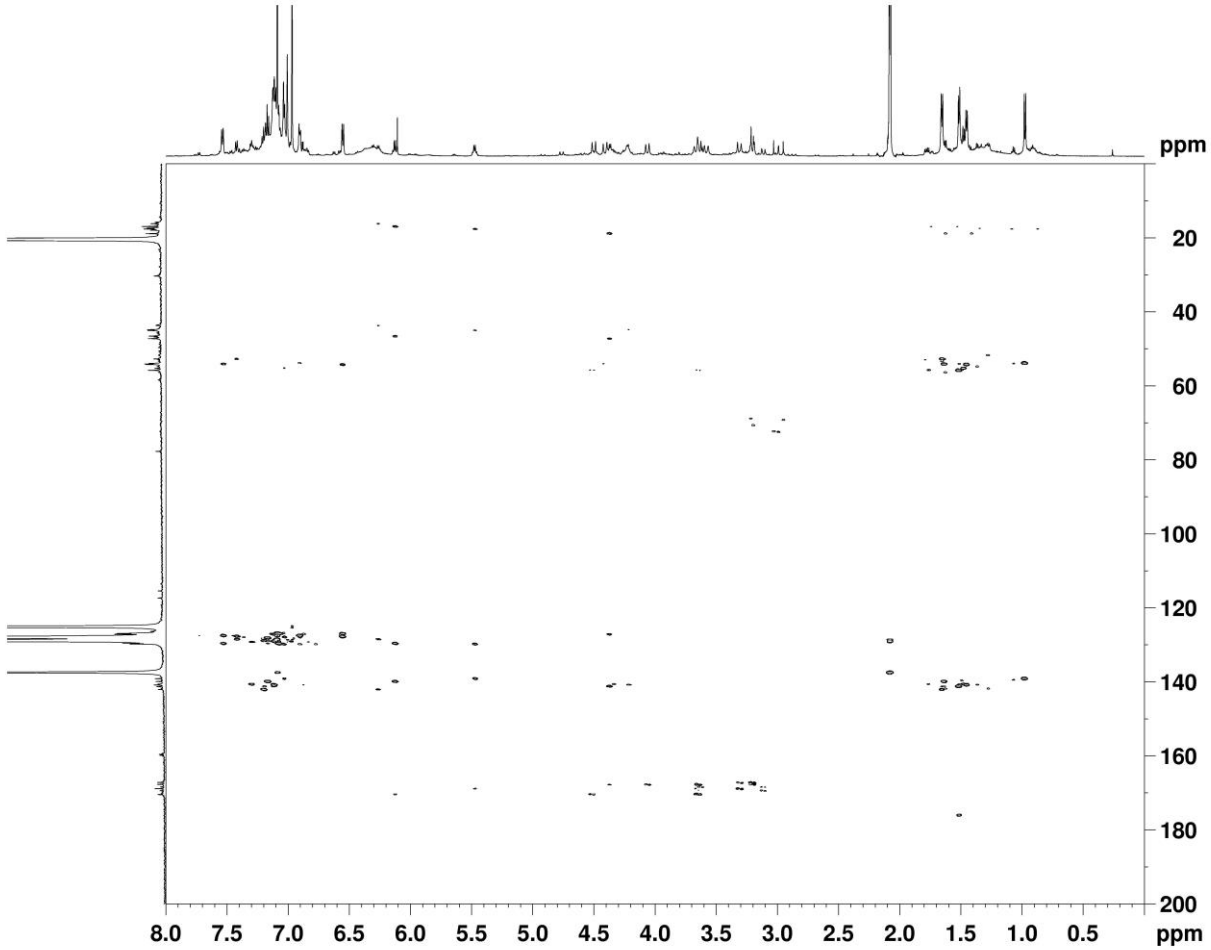
36: ^{13}C NMR (150 MHz, $C_6D_5CD_3$)



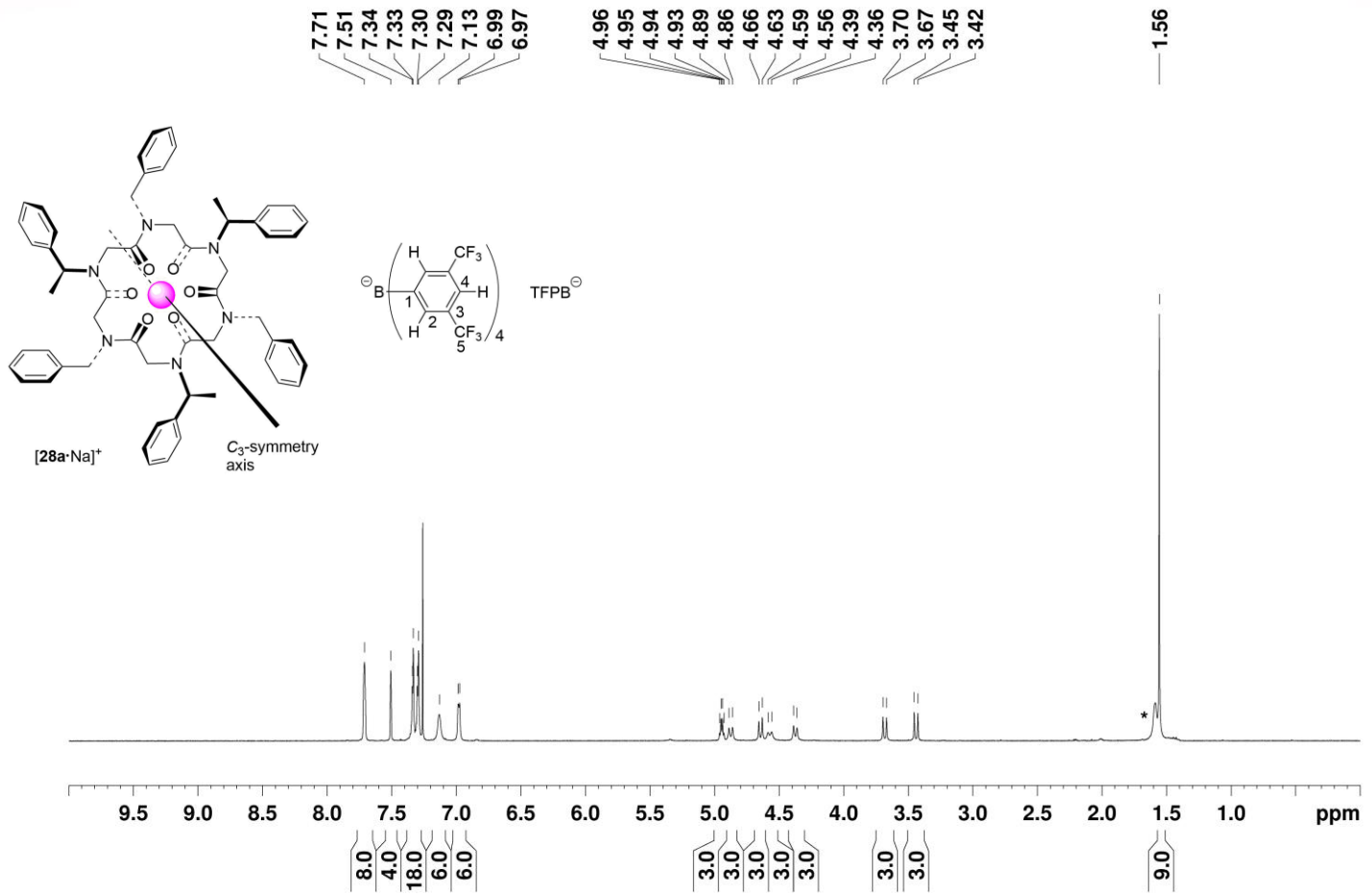
36: COSY SPECTRUM (600 MHz, $C_6D_5CD_3$)



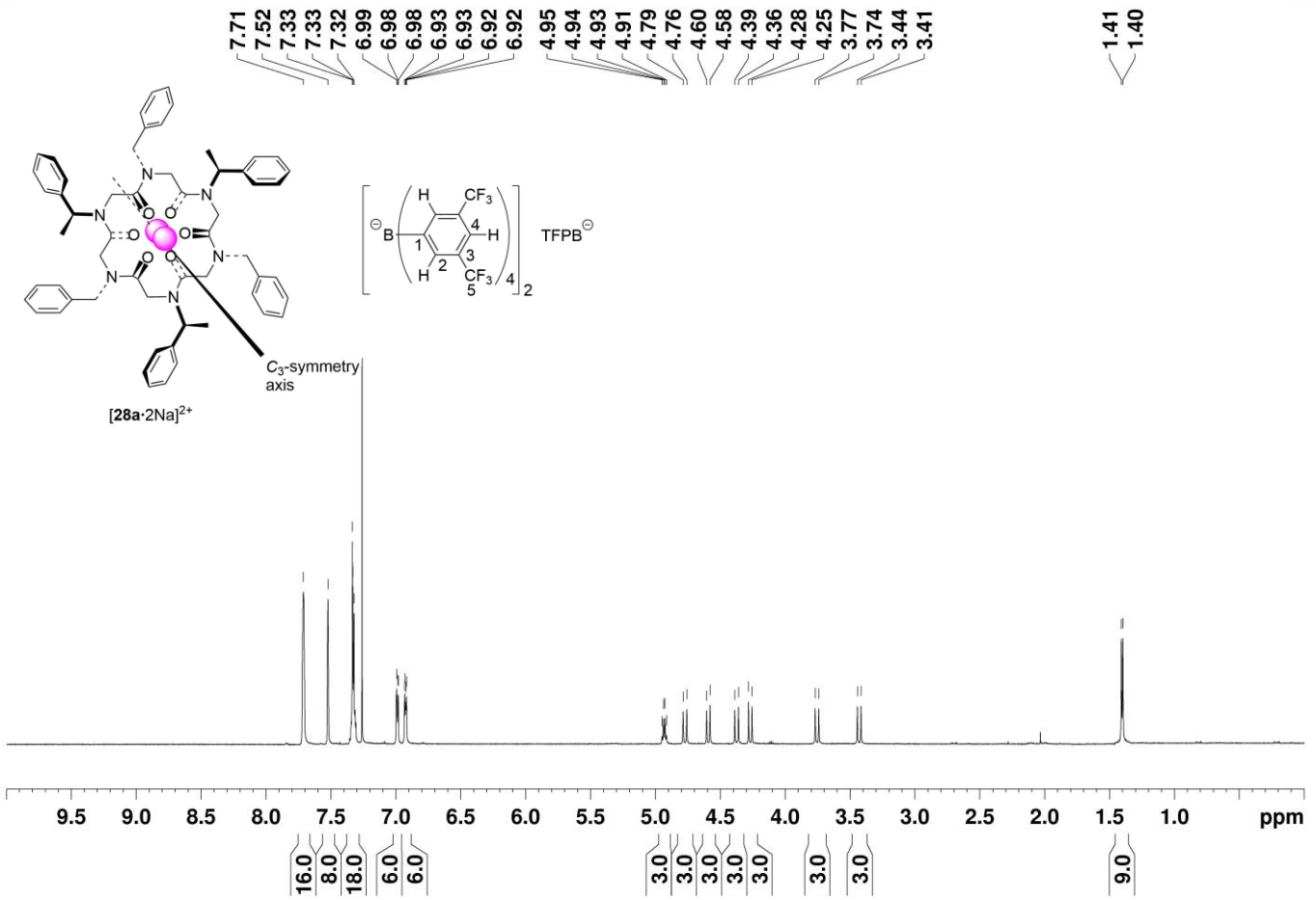
36: HSQC SPECTRUM (600 MHz, $C_6D_5CD_3$)



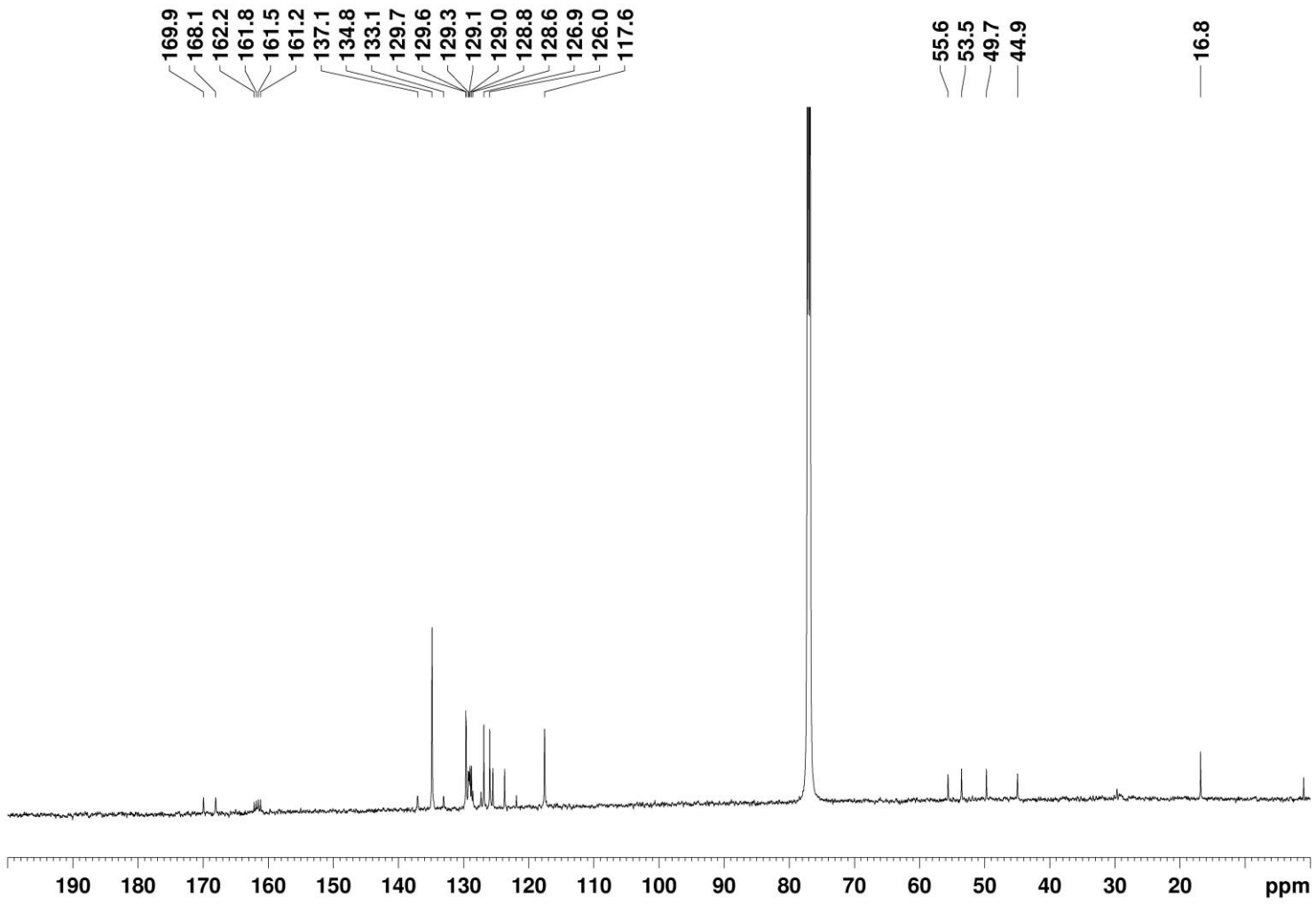
36: HMBC SPECTRUM (600 MHz, $C_6D_5CD_3$)



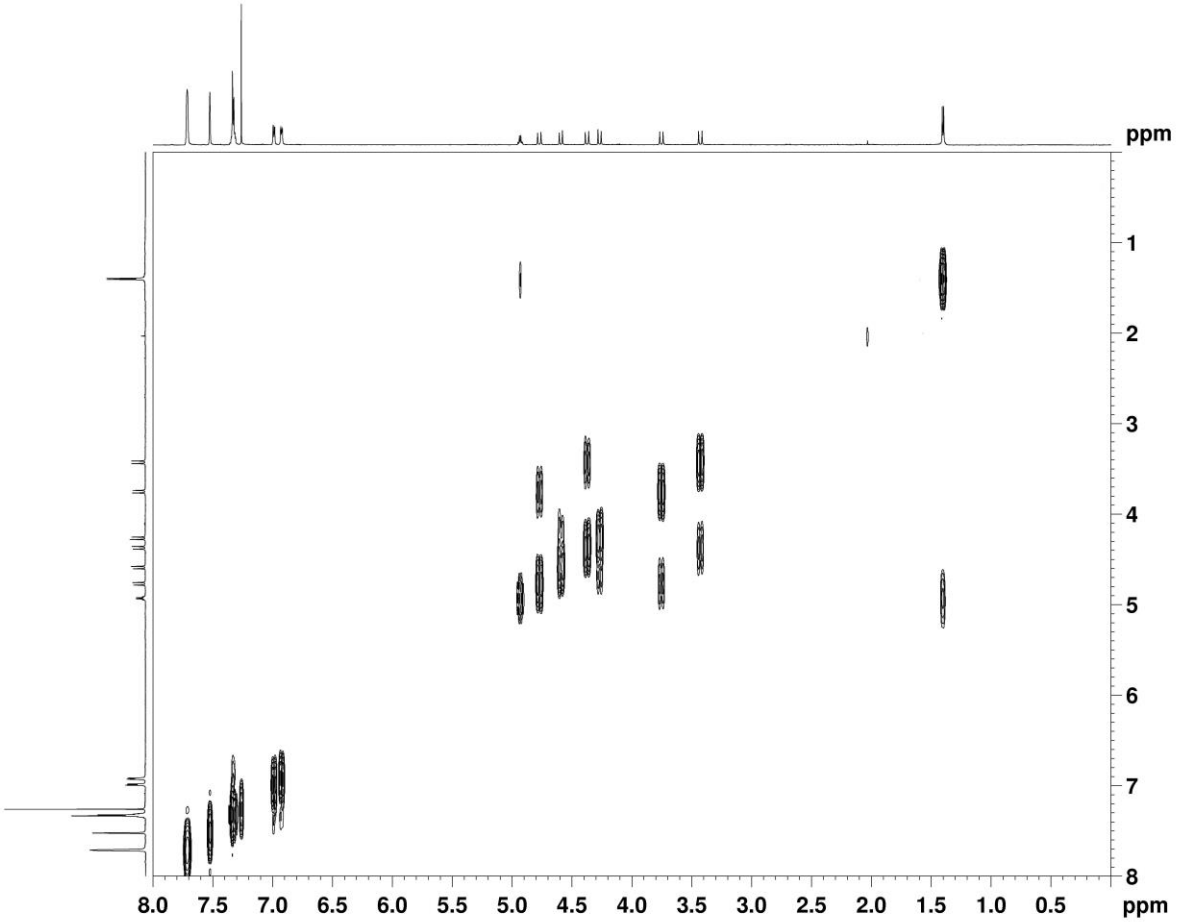
[**28a**·Na]$^{+}$[TFPB]$^{-}$: ^{1}H NMR (600 MHz, $CDCl_3$). Water impurities are labelled with a black asterisk.



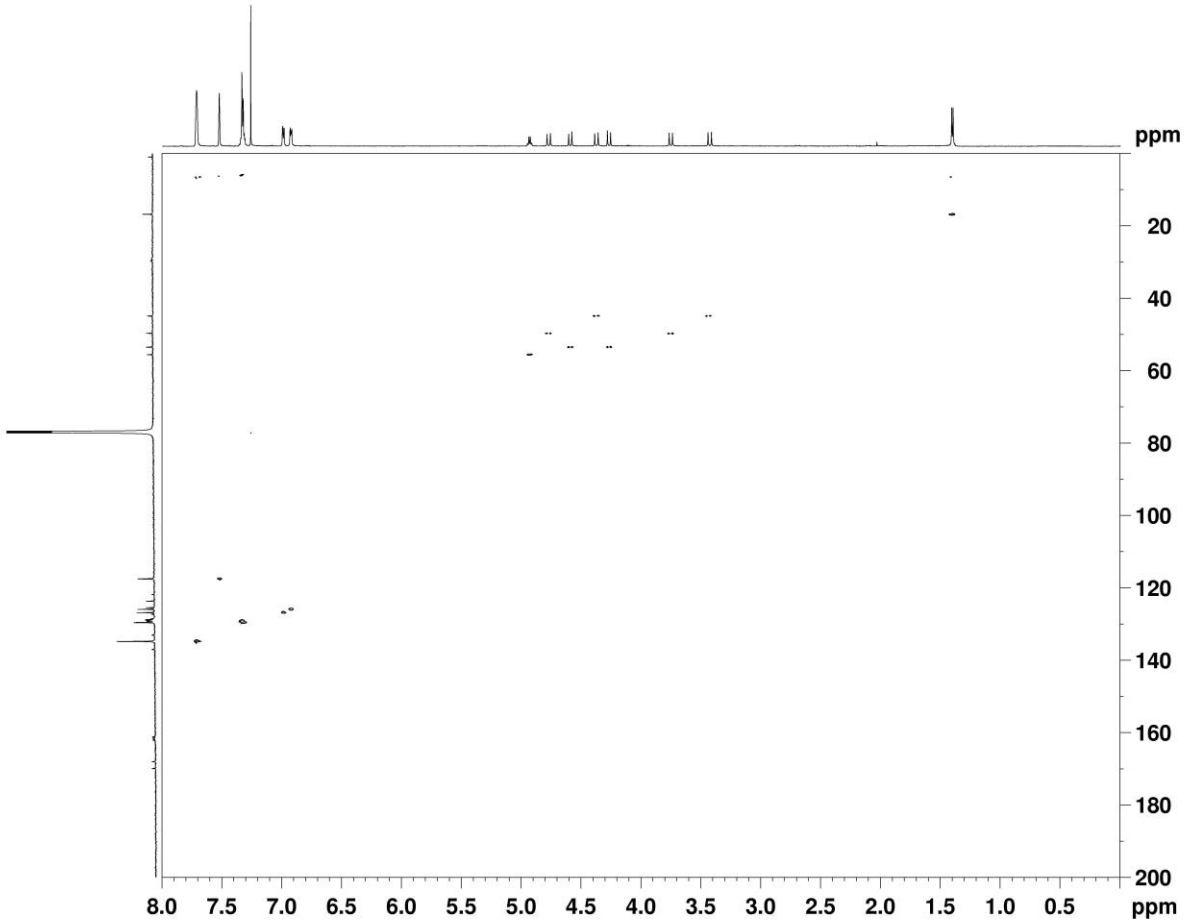
[**28a**·2Na]$^{2+}$2[TFPB]$^{-}$: ^{1}H NMR (600 MHz, $CDCl_3$)



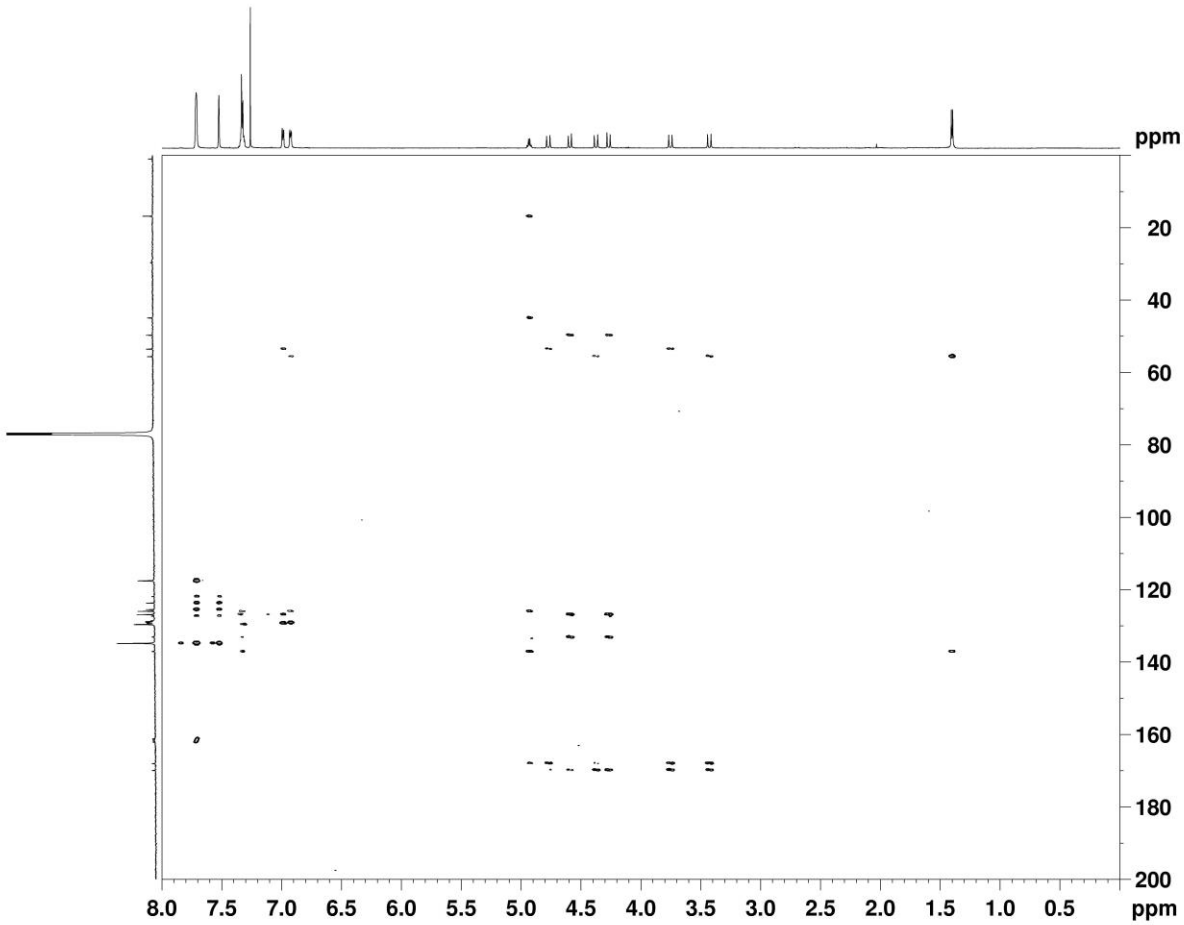
[**28a**·2Na]$^{2+}$2[TFPB]$^{-}$: ^{13}C NMR (600 MHz, $CDCl_3$)



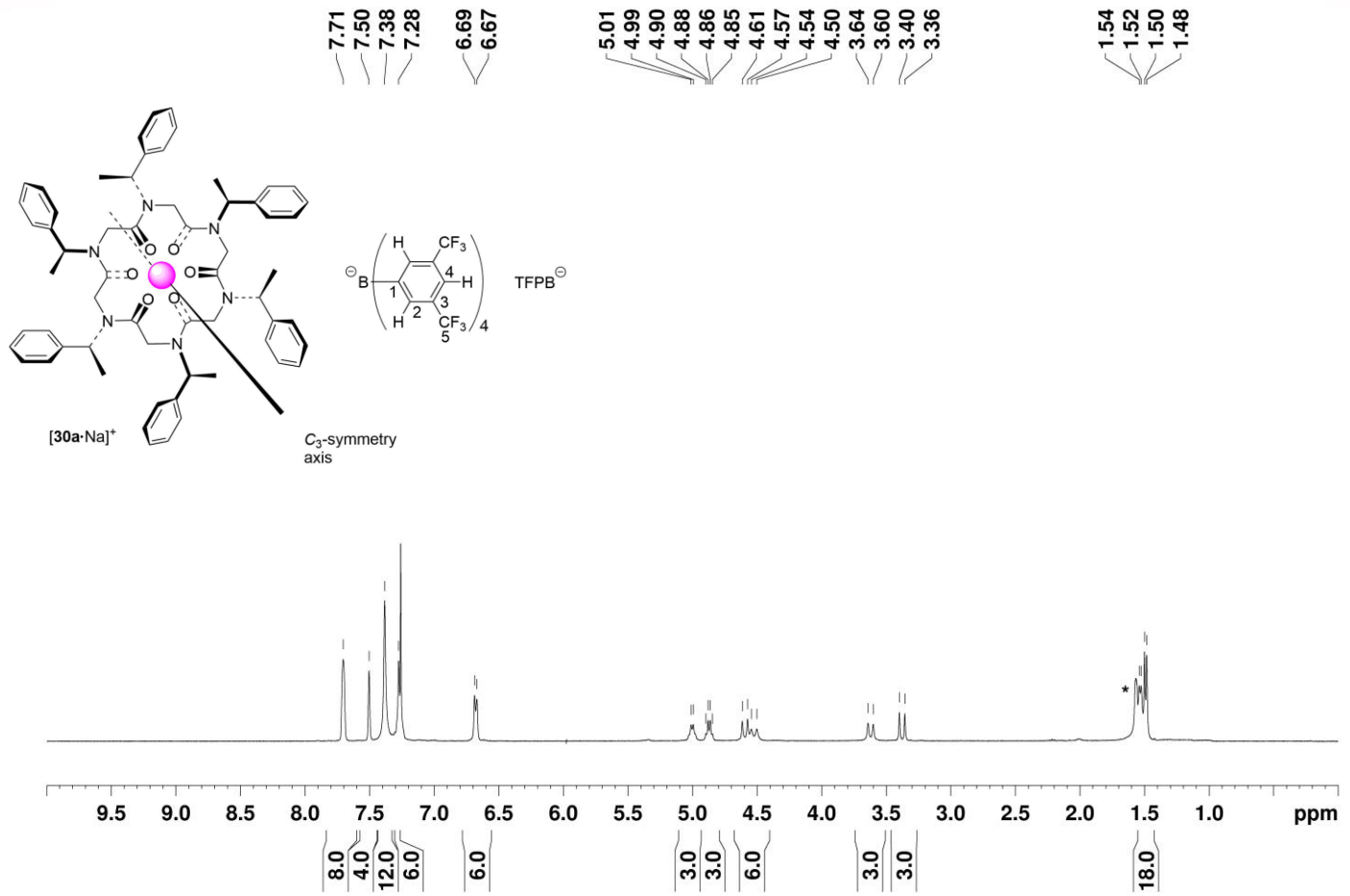
[**28a**·2Na]$^{2+}$2[TFPB]$^{-}$: COSY SPECTRUM (600 MHz, $CDCl_3$)



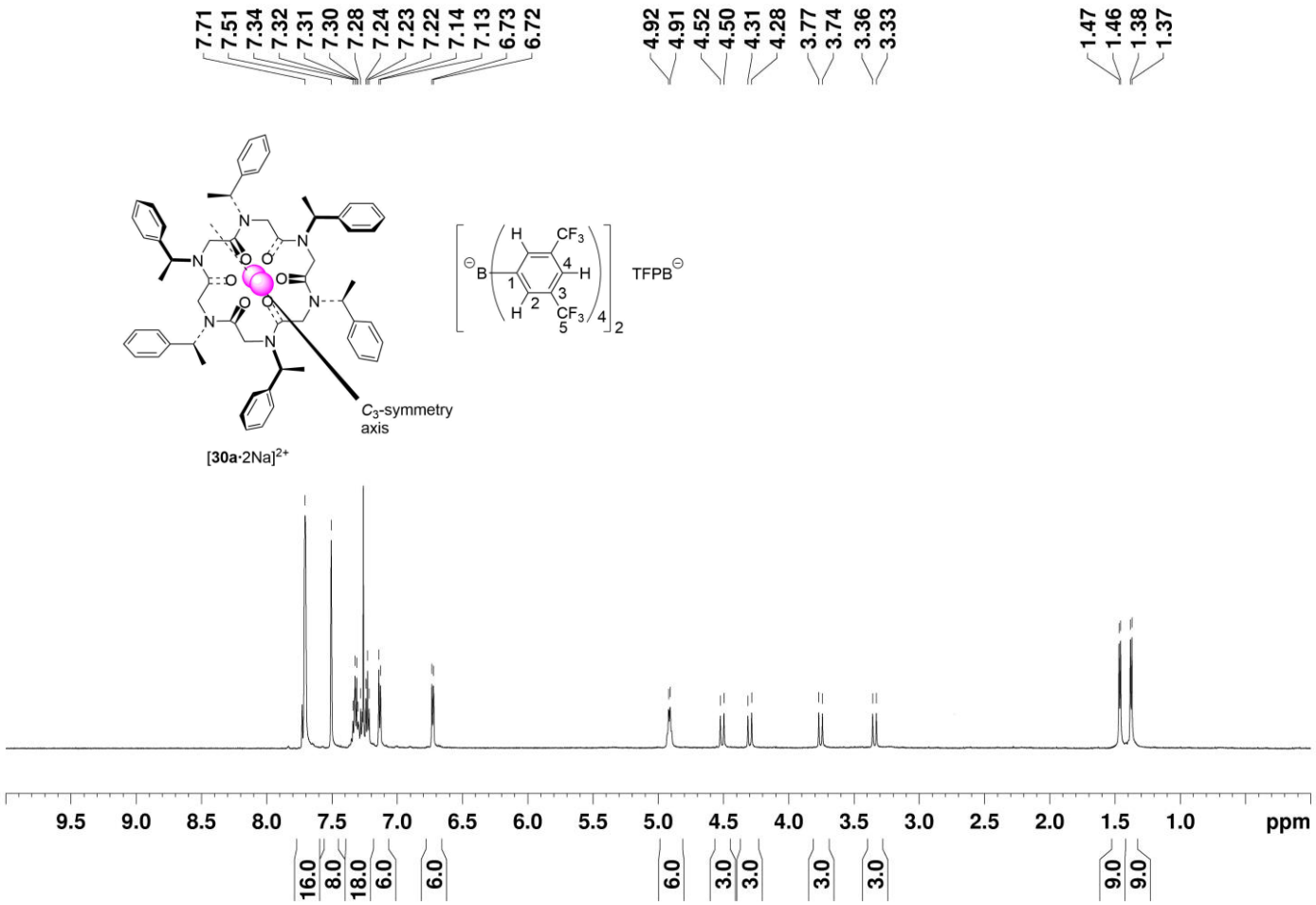
[**28a**·2Na]$^{2+}$2[TFPB]$^{-}$: HSQC SPECTRUM (600 MHz, $CDCl_3$)



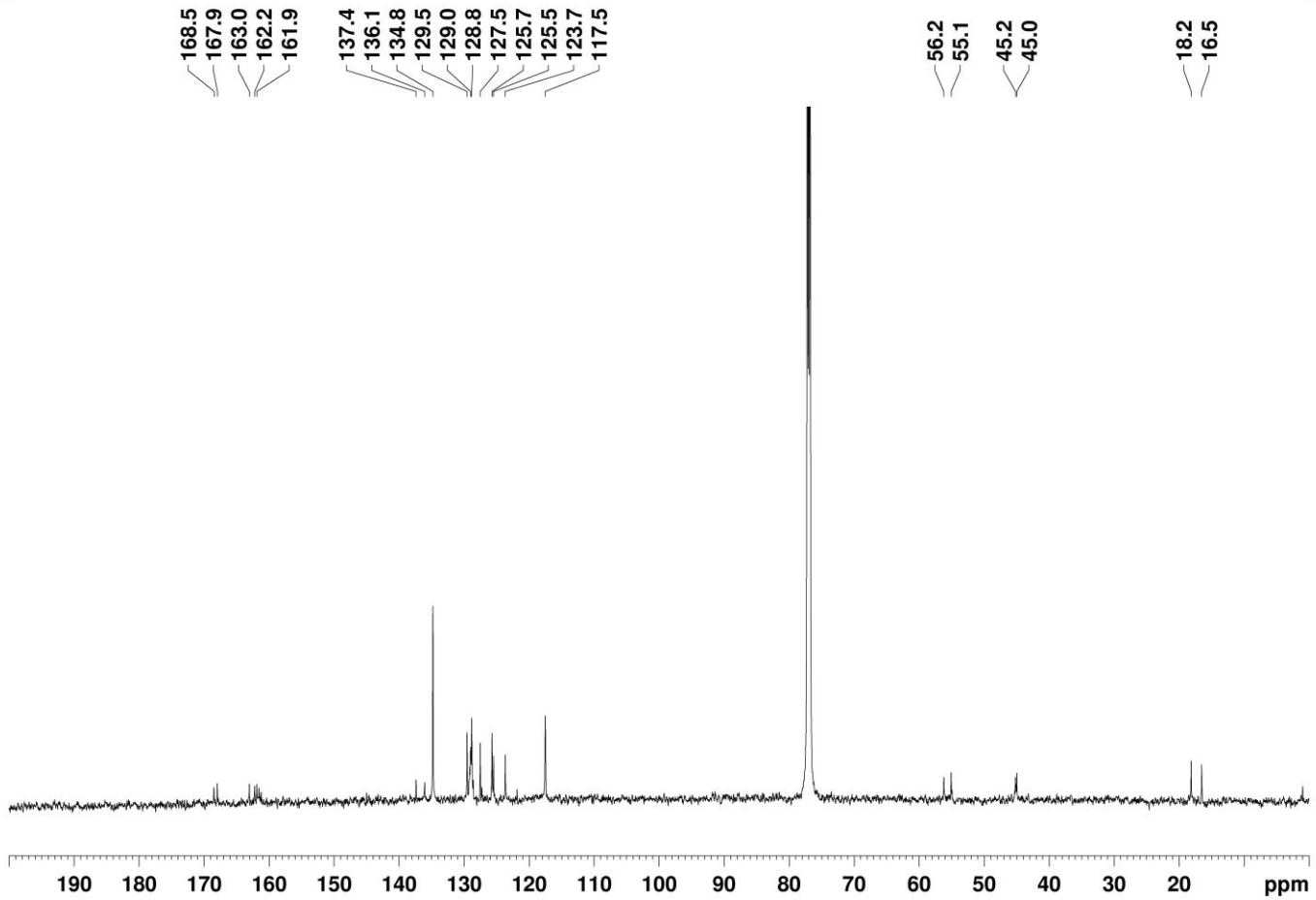
[**28a**·2Na]$^{2+}$2[TFPB]$^{-}$: HMBC SPECTRUM (600 MHz, $CDCl_3$)



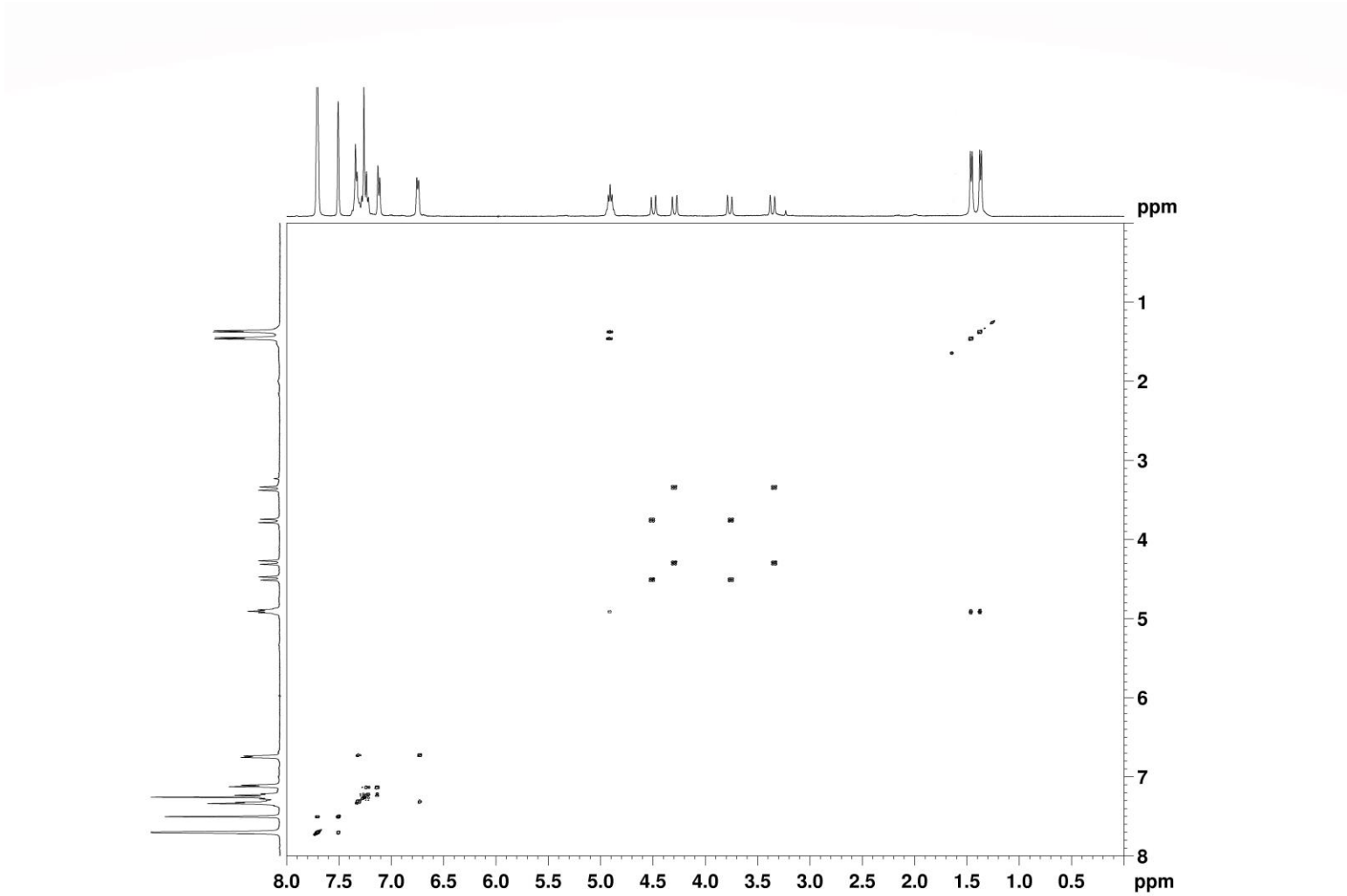
[**30a**·Na]$^{+}$[TFPB]$^{-}$: ^{1}H NMR (400 MHz, $CDCl_3$)



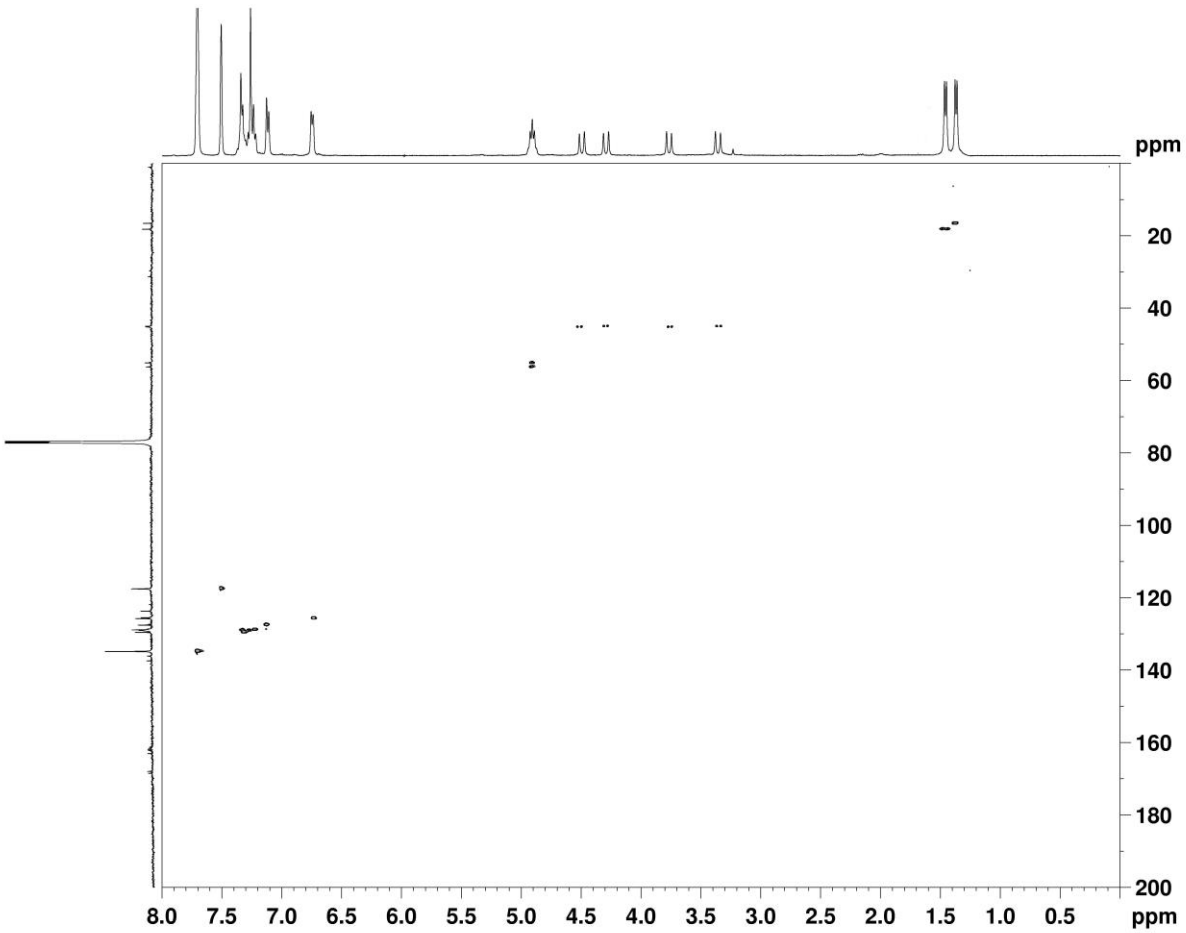
[**30a**·2Na]$^{2+}$2[TFPB]$^{-}$: ^{1}H NMR (600 MHz, $CDCl_3$)



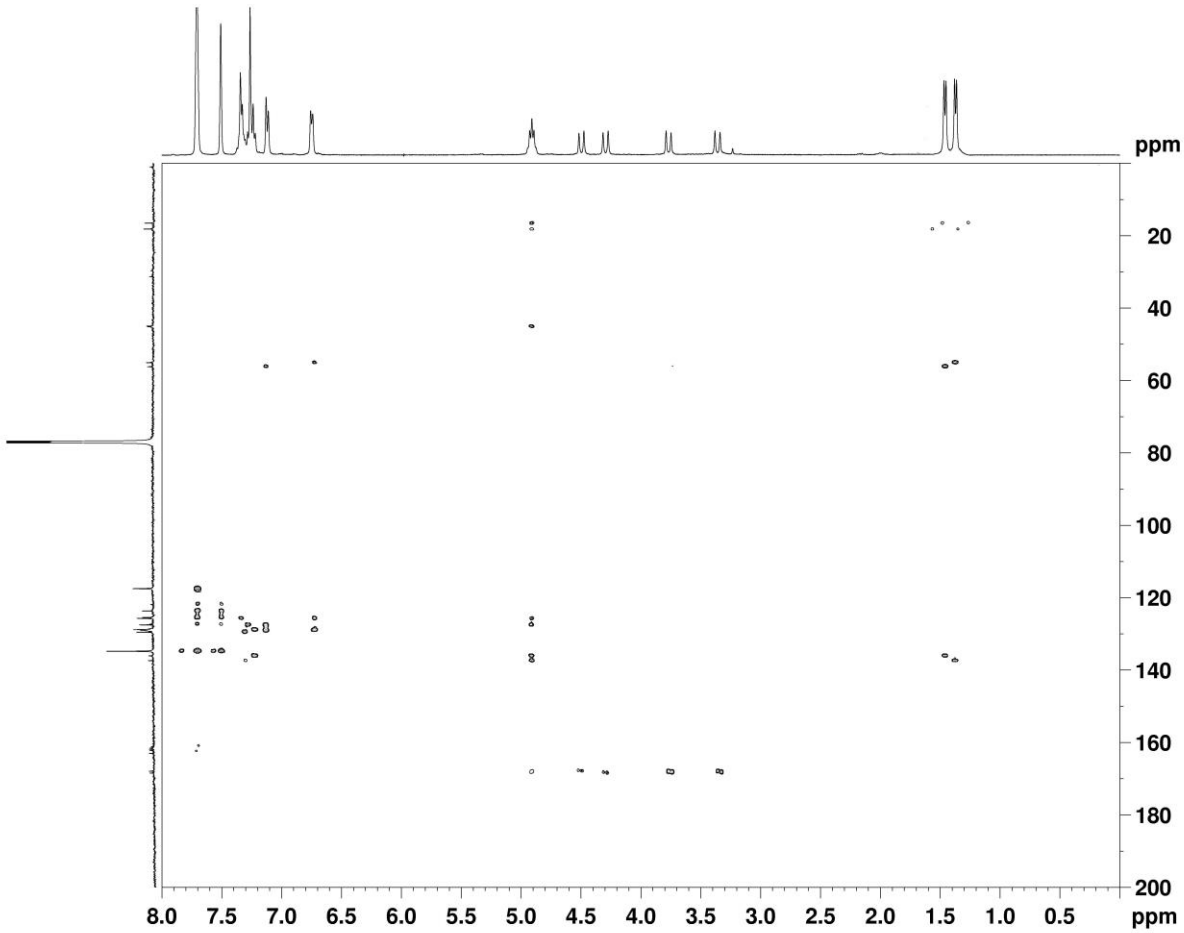
[**30a**·2Na]$^{2+}$2[TFPB]$^{-}$: ^{13}C NMR (150 MHz, $CDCl_3$)



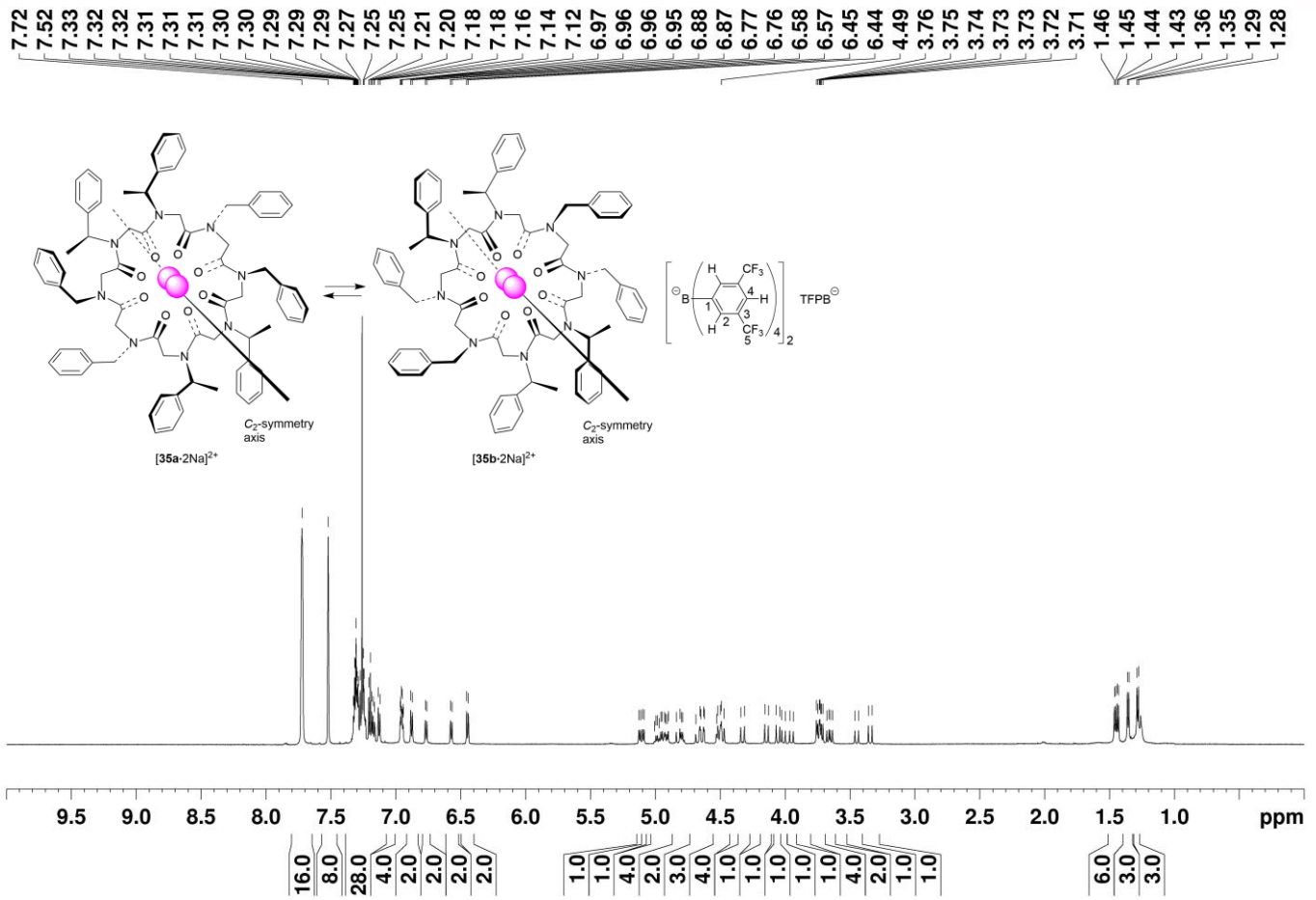
[**30a**·2Na]$^{2+}$2[TFPB]$^{-}$: COSY SPECTRUM (600 MHz, $CDCl_3$)



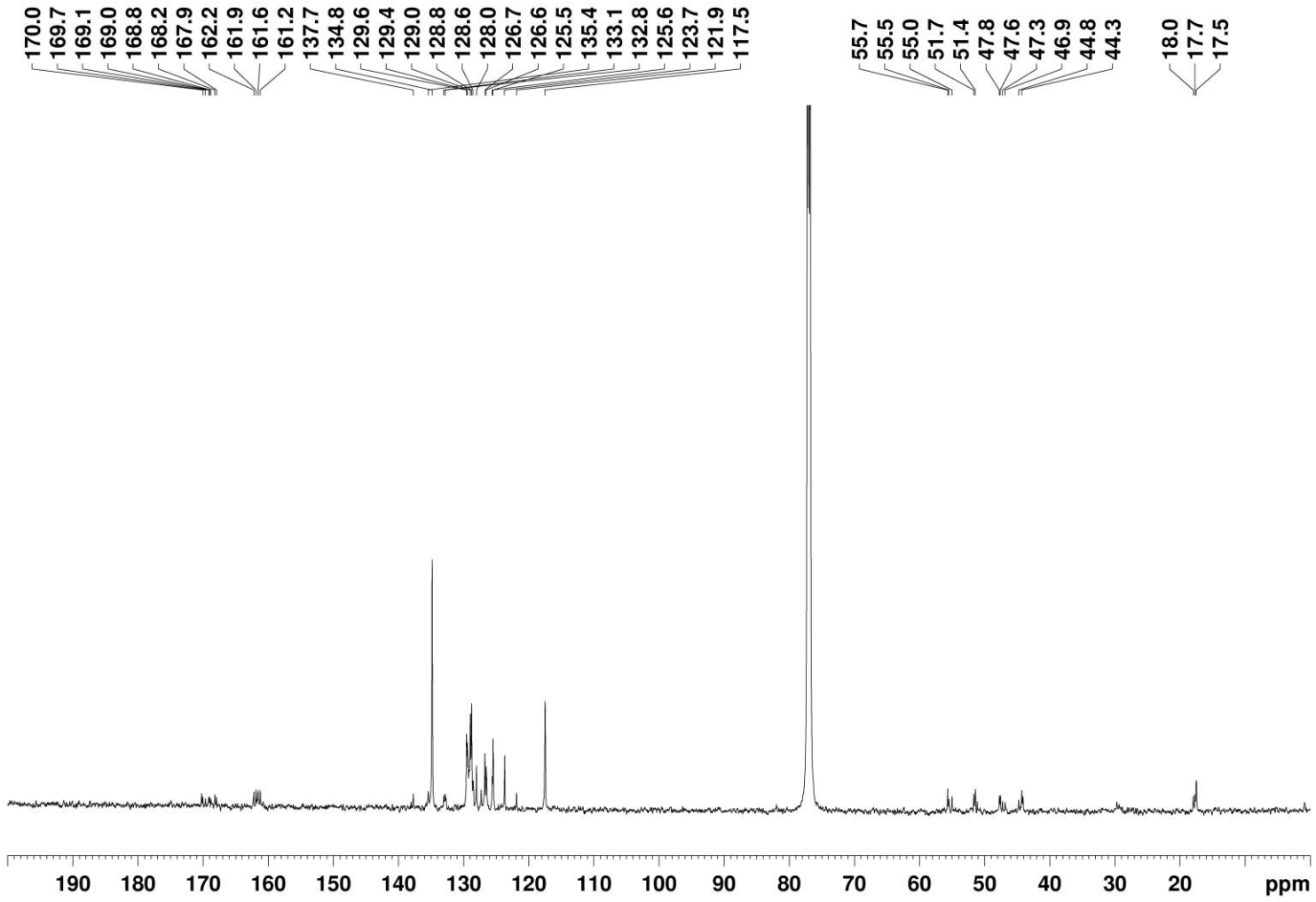
[**30a**·2Na]$^{2+}$2[TFPB]$^{-}$: HSQC SPECTRUM (600 MHz, $CDCl_3$)



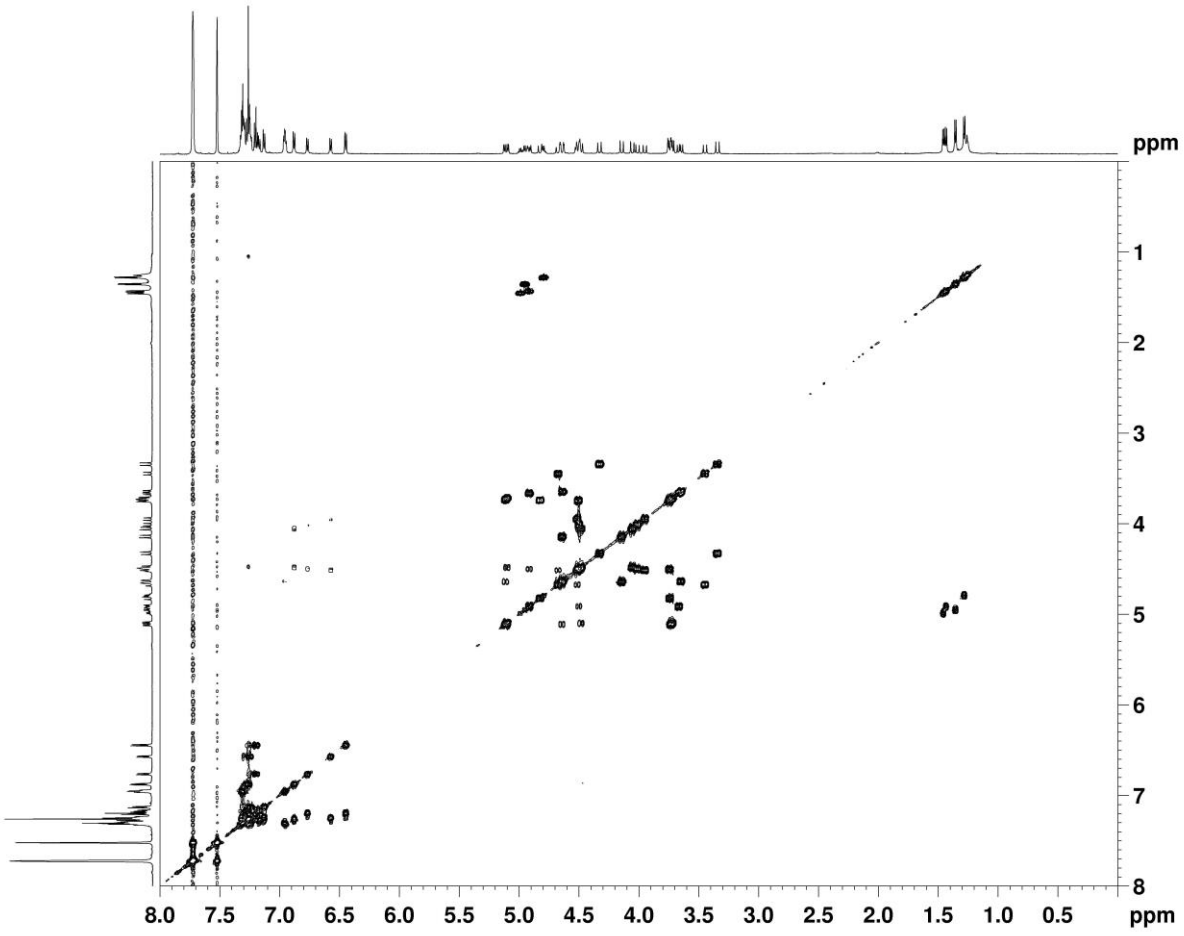
[**30a**·2Na]$^{2+}$2[TFPB]$^{-}$: HMBC SPECTRUM (600 MHz, $CDCl_3$)



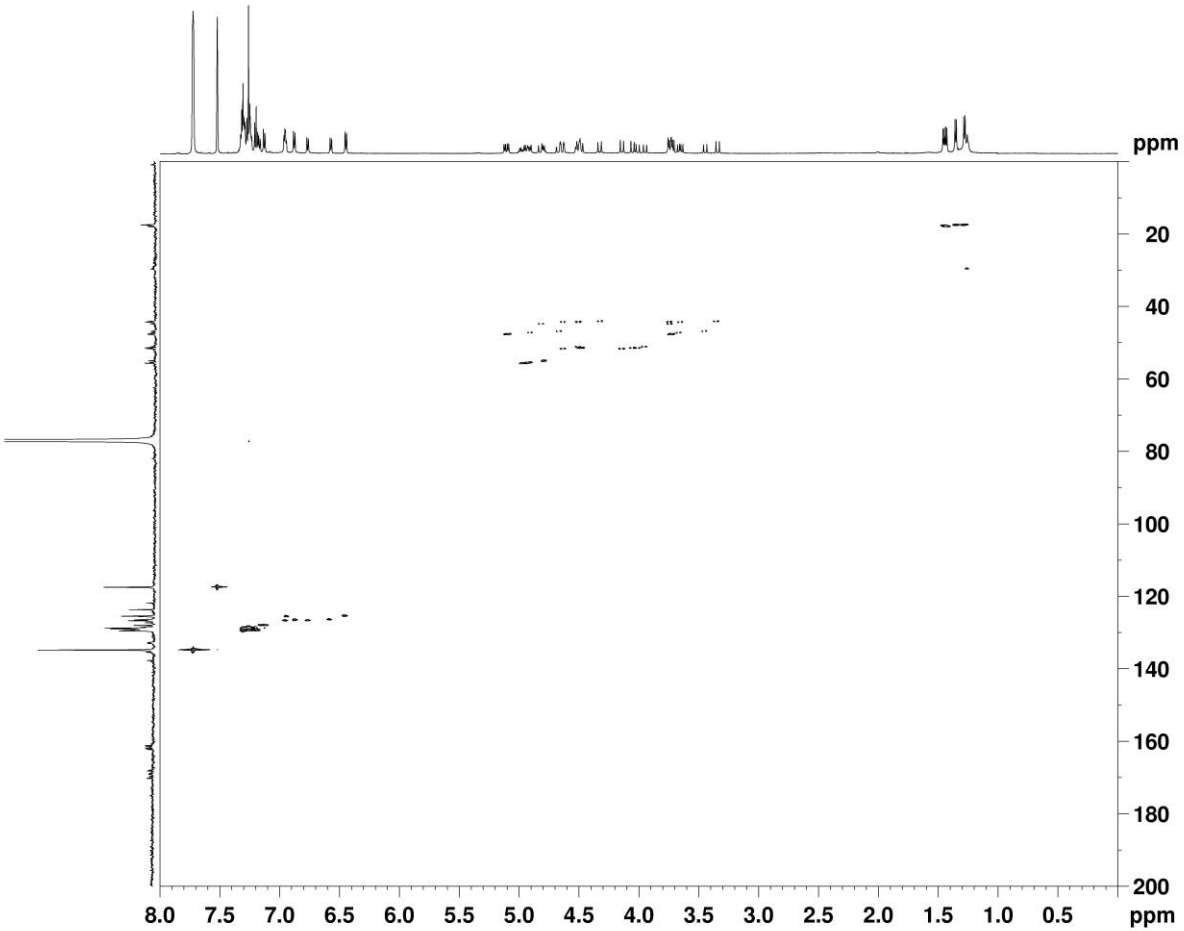
[**35a**·2Na]$^{2+}$ 2[TFPB]$^{-}$ and [**35b**·2Na]$^{2+}$ 2[TFPB]$^{-}$ (50:50 ratio): ^{1}H NMR (600 MHz, $CDCl_3$)



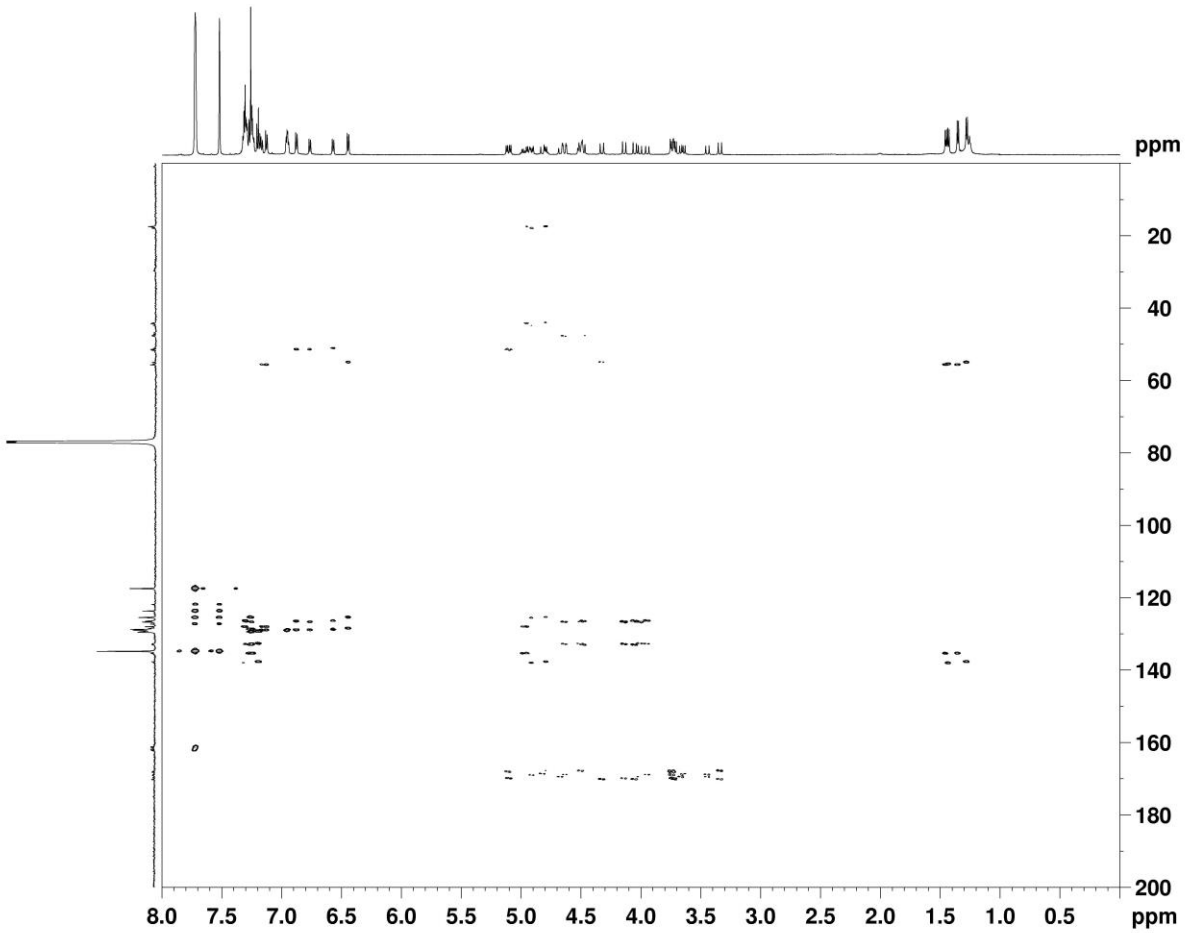
[**35a**·2Na]$^{2+}$ 2[TFPB]$^{-}$ and [**35b**·2Na]$^{2+}$ 2[TFPB]$^{-}$: ^{13}C NMR (600 MHz, $CDCl_3$)



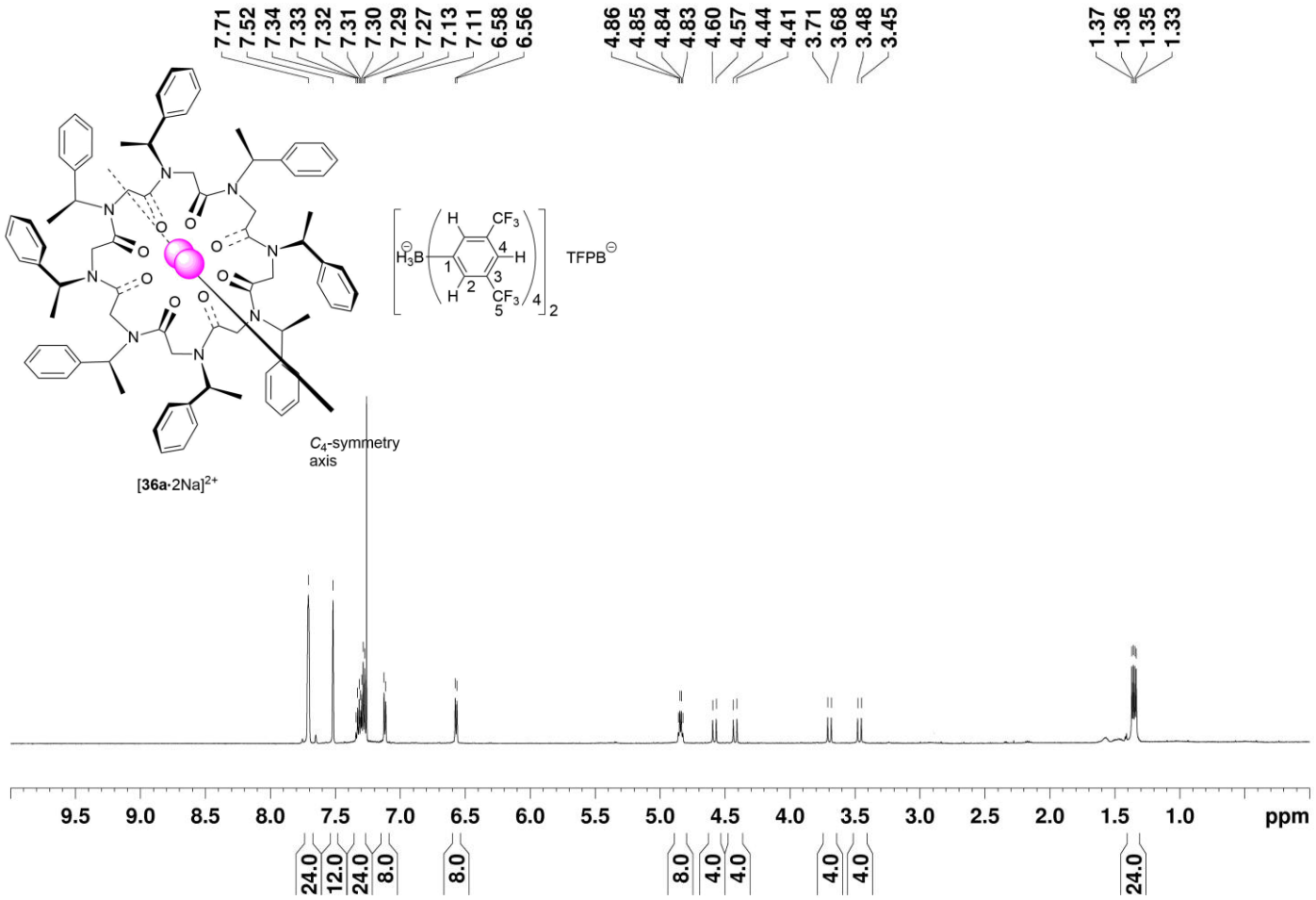
[**35a**·2Na]$^{2+}$ 2[TFPB]$^{-}$ and [**35b**·2Na]$^{2+}$ 2[TFPB]$^{-}$: COSY SPECTRUM (600 MHz, $CDCl_3$)



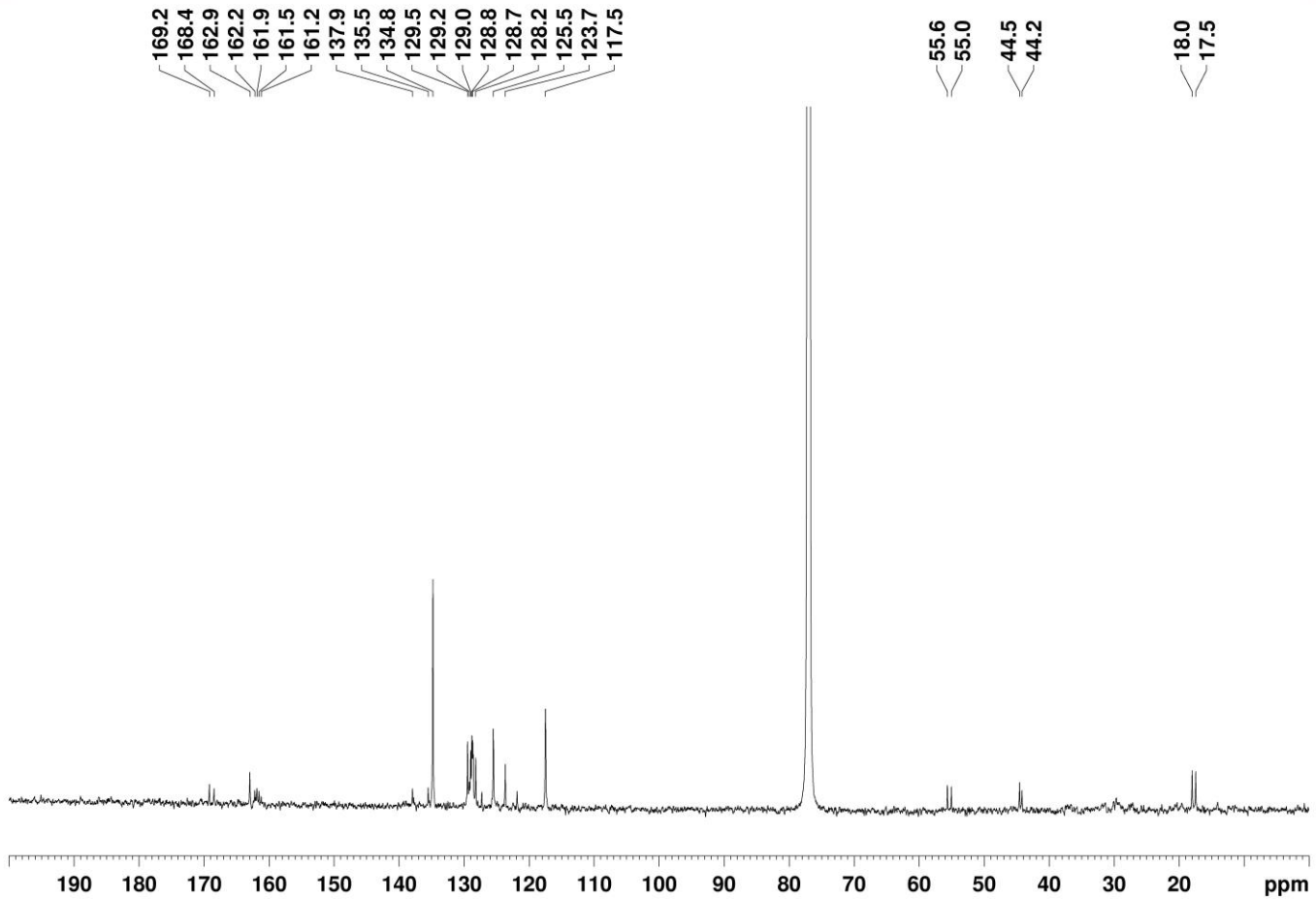
[**35a**·2Na]$^{2+}$ 2[TFPB]$^{-}$ and [**35b**·2Na]$^{2+}$ 2[TFPB]$^{-}$: HSQC SPECTRUM (600 MHz, $CDCl_3$)



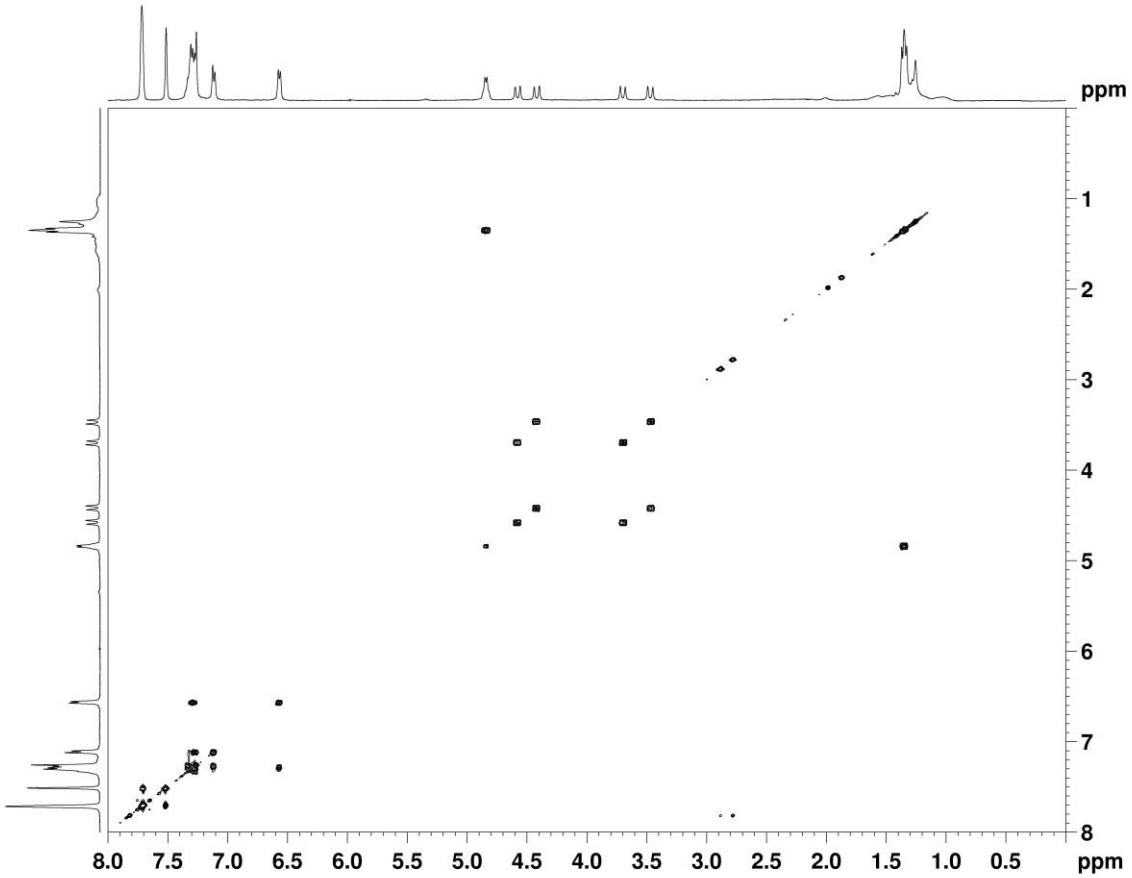
[**35a**·2Na]$^{2+}$ 2[TFPB]$^{-}$ and [**35b**·2Na]$^{2+}$ 2[TFPB]$^{-}$: HMBC SPECTRUM (600 MHz, $CDCl_3$)



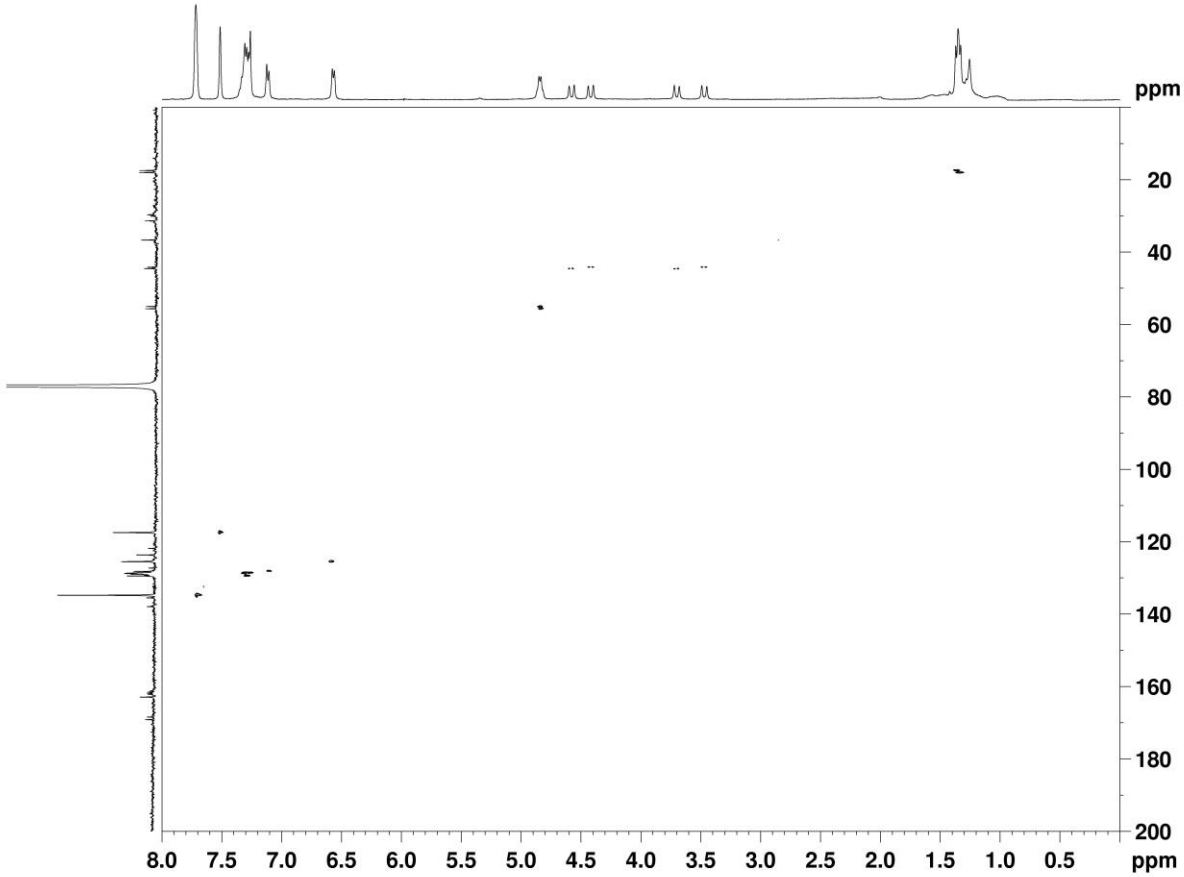
[**36a**·2Na]$^{2+}$2[TFPB]$^{-}$: ^{1}H NMR (600 MHz, $CDCl_3$)



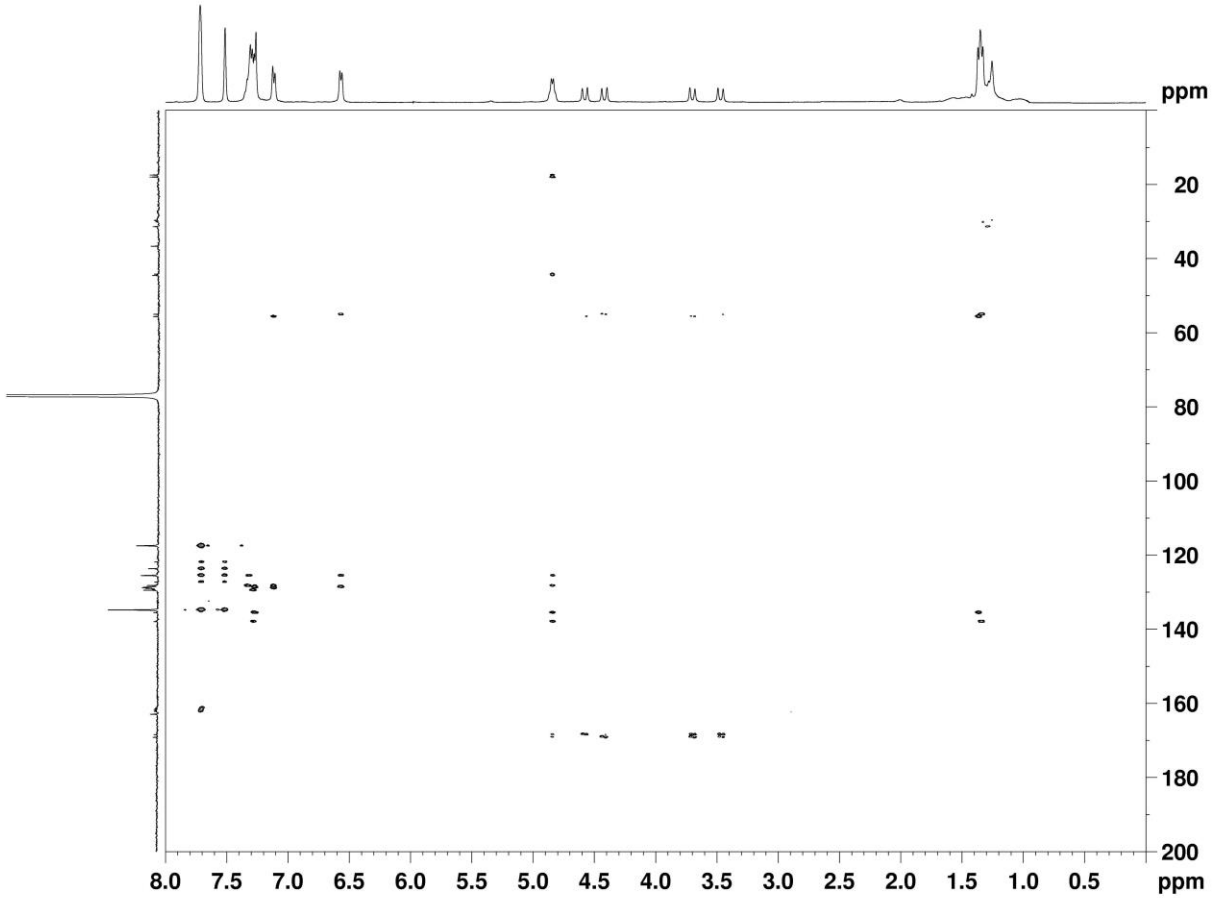
[**36a**·2Na]$^{2+}$2[TFPB]$^{-}$: ^{13}C NMR (150 MHz, $CDCl_3$)



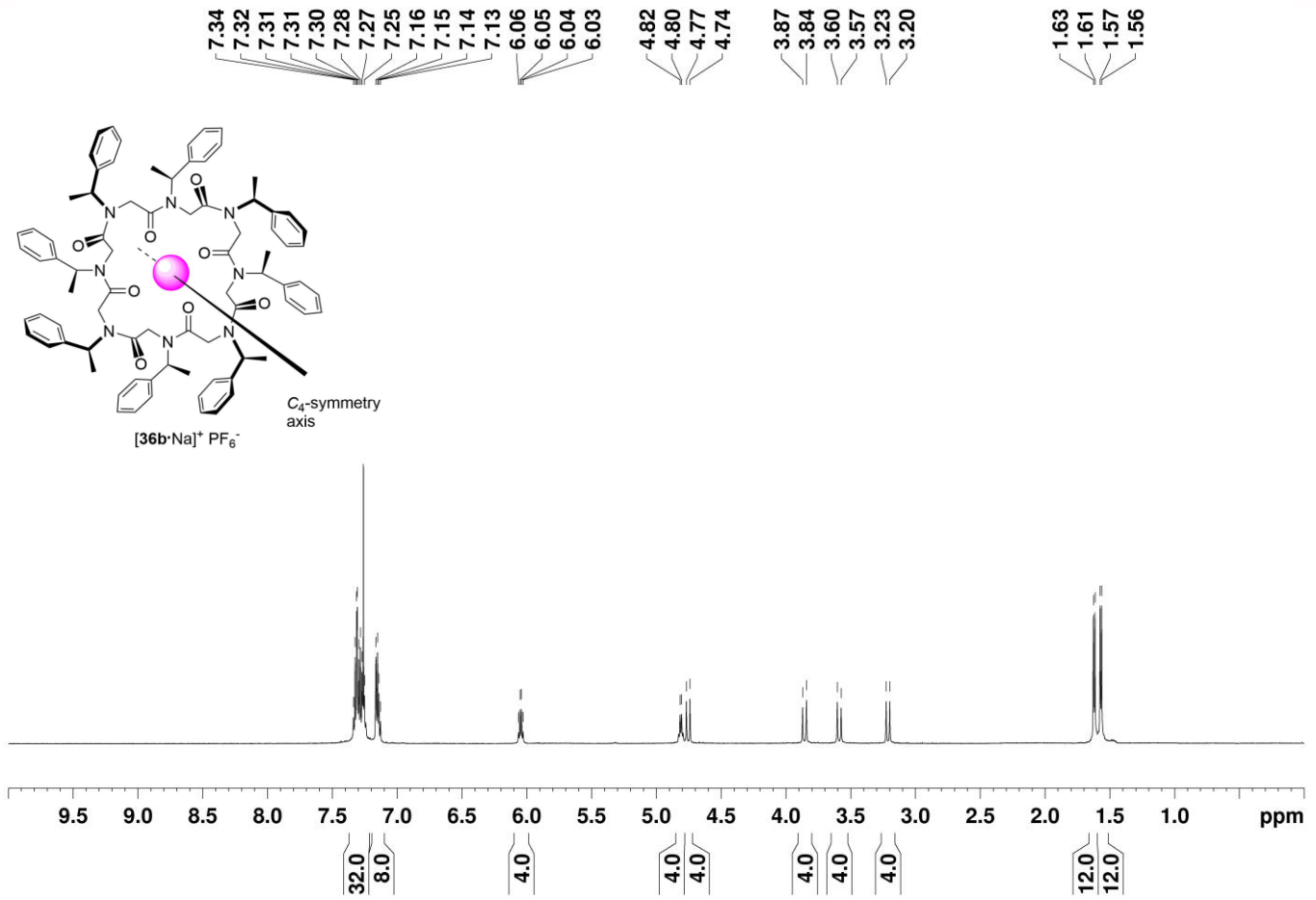
[**36a**·2Na]$^{2+}$2[TFPB]$^{-}$: COSY SPECTRUM (600 MHz, $CDCl_3$)



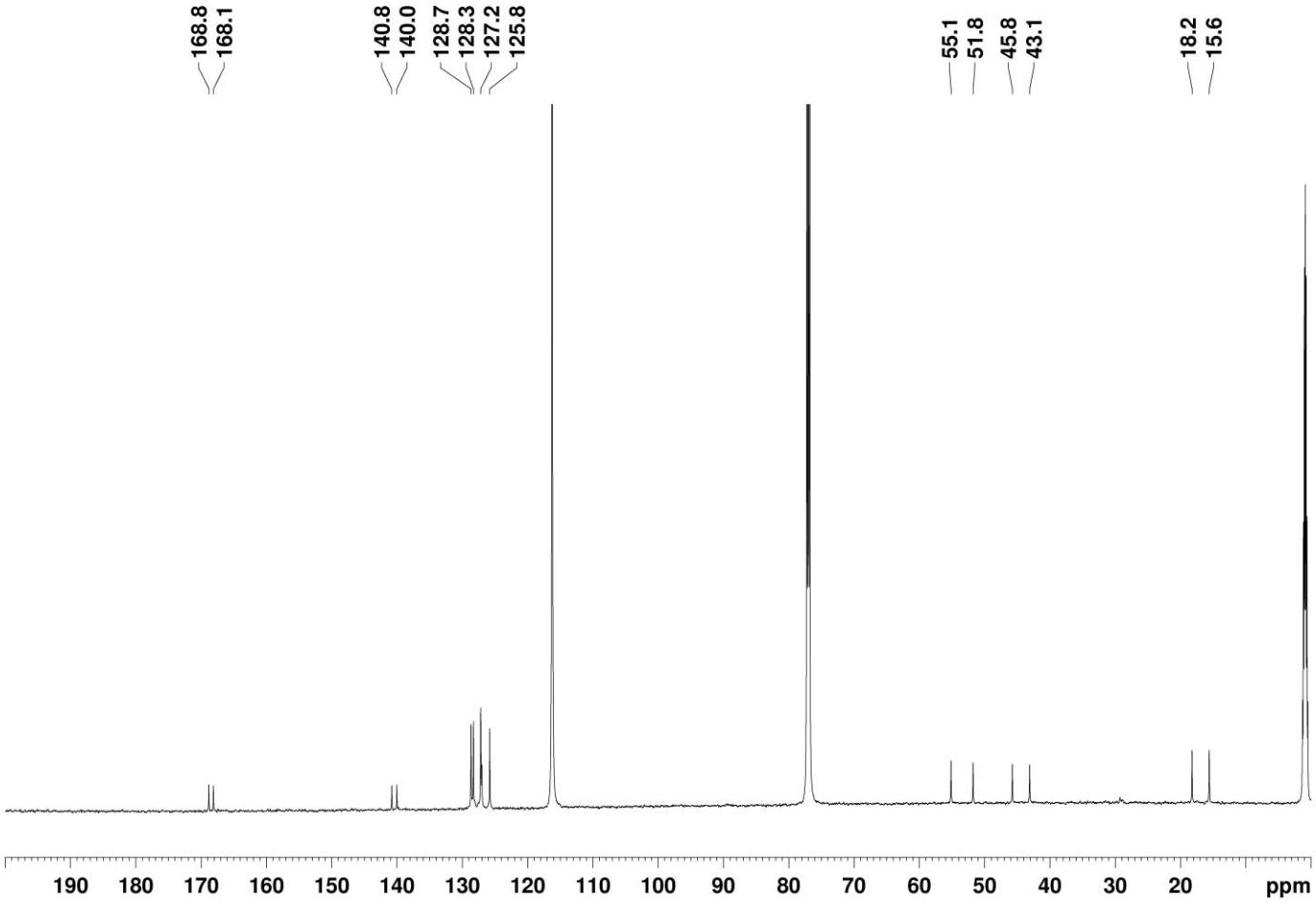
[**36a**·2Na]$^{2+}$2[TFPB]$^{-}$: HSQC SPECTRUM (600 MHz, $CDCl_3$)



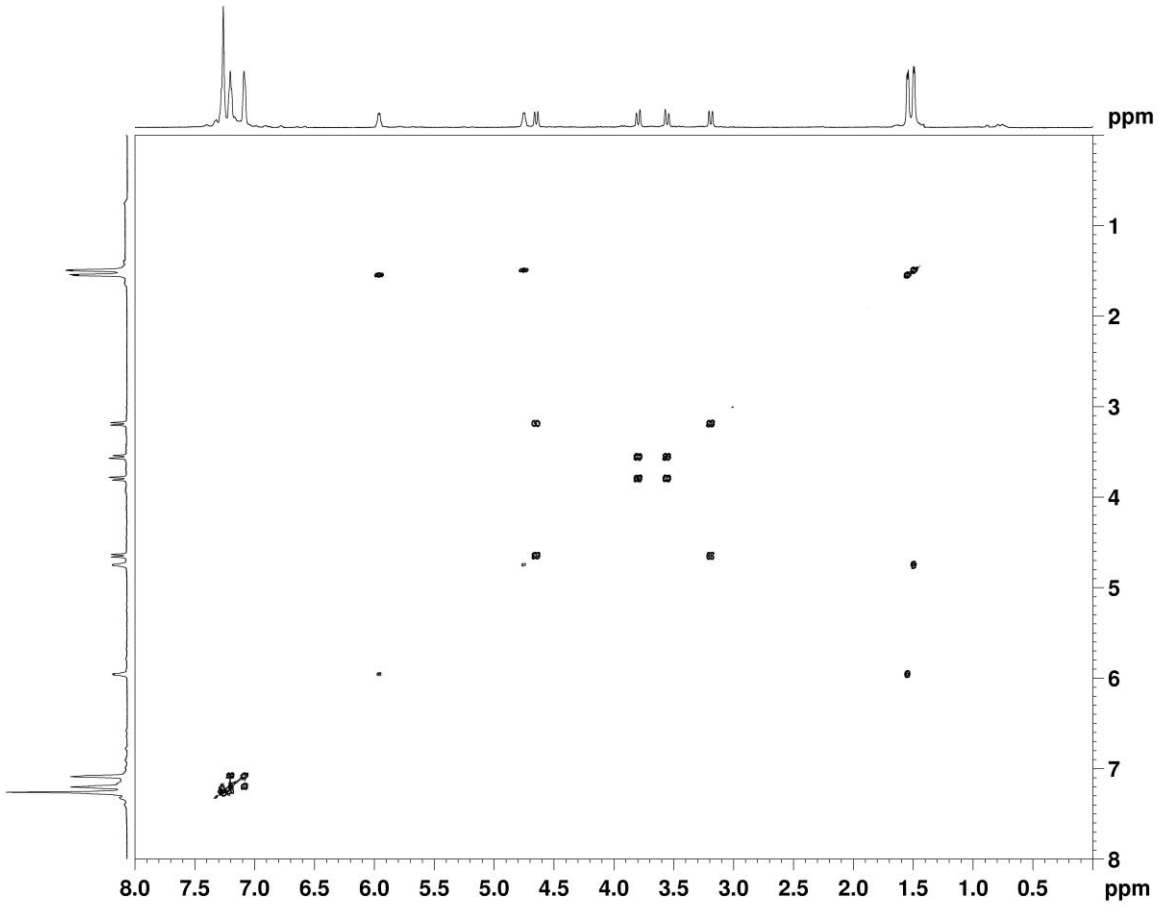
[**36a**·2Na]$^{2+}$2[TFPB]$^{-}$: HMBC SPECTRUM (600 MHz, $CDCl_3$)



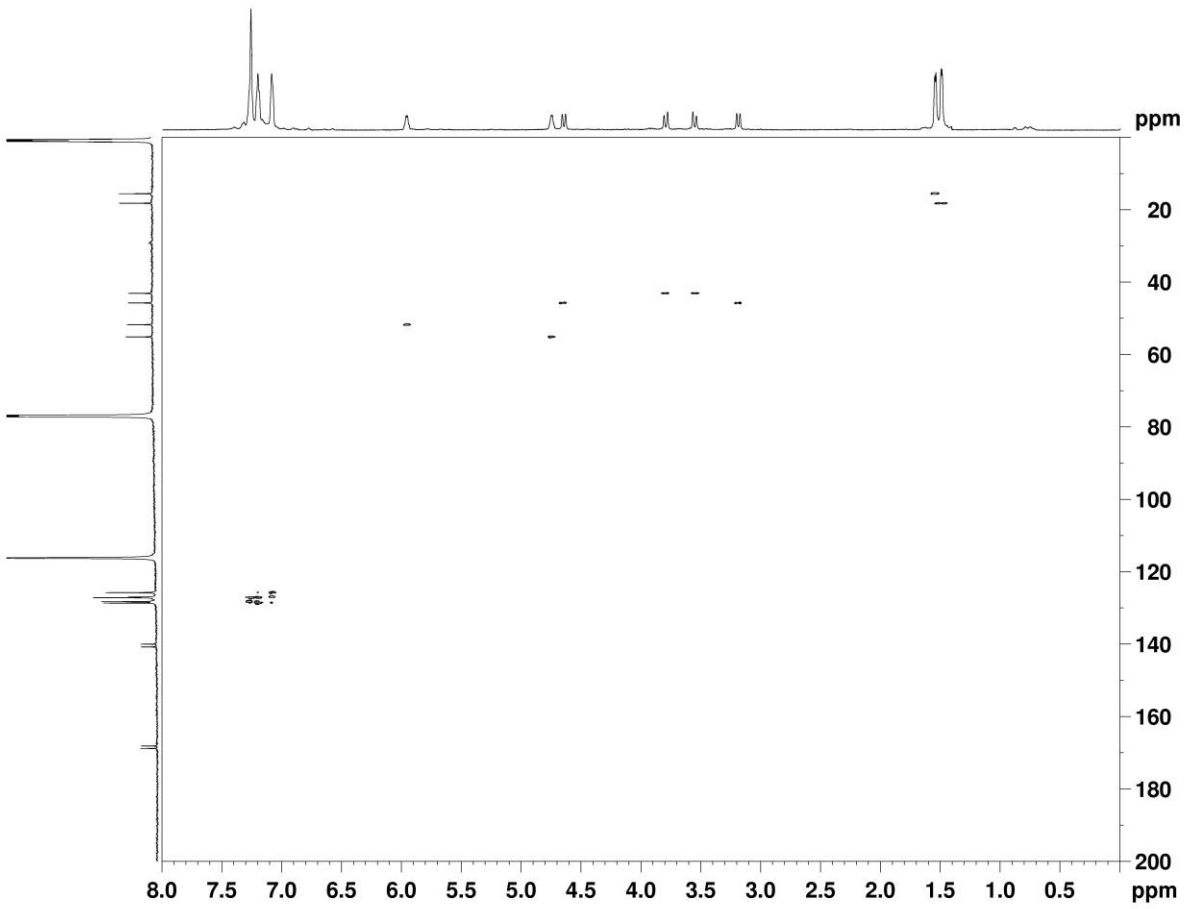
[**36b**·Na]$^{+}$ PF_6^{-}: ^{1}H NMR (600 MHz, $CDCl_3$:CD_3CN = 9:1)



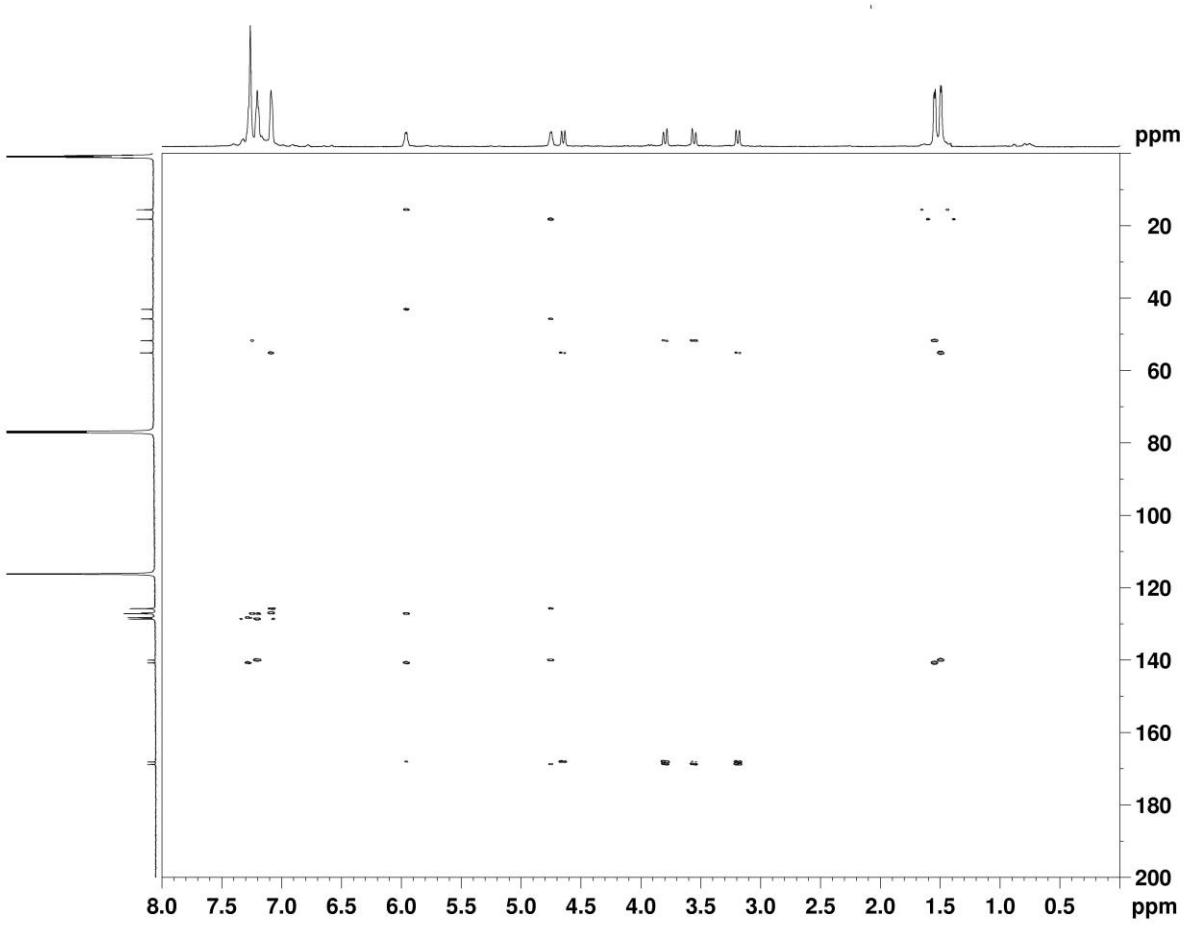
[**36b**·Na] $^{+}PF_6^{-}$: ^{13}C NMR (150 MHz, $CDCl_3$:CD_3CN = 9:1)



[**36b**·Na] $^{+}PF_6^{-}$: COSY SPECTRUM (600 MHz, $CDCl_3$:CD_3CN = 9:1)



[**36b**·Na] $^{+}PF_6^{-}$: HSQC SPECTRUM (600 MHz, $CDCl_3$:CD_3CN = 9:1)



[**36b**·Na]$^{+}PF_6^{-}$: HMBC SPECTRUM (600 MHz, $CDCl_3$:CD_3CN = 9:1)

2.2 ^{1}H NMR titration with NaTFPB and $NaPF_6$ (Figure S1-S7)

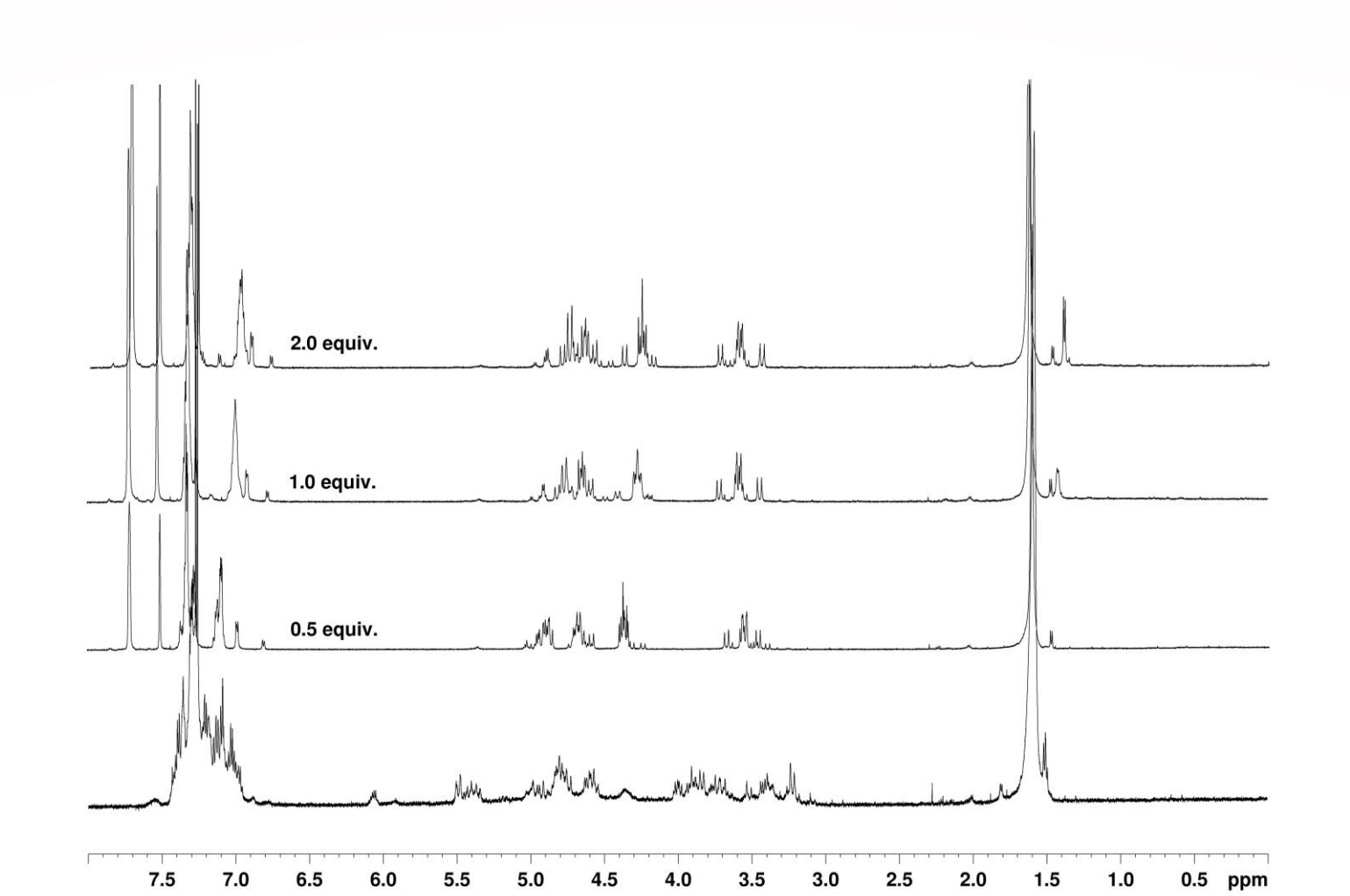


Figure S1. Stepwise addition of NaTFPB to **27** (600 MHz, $CDCl_3$)

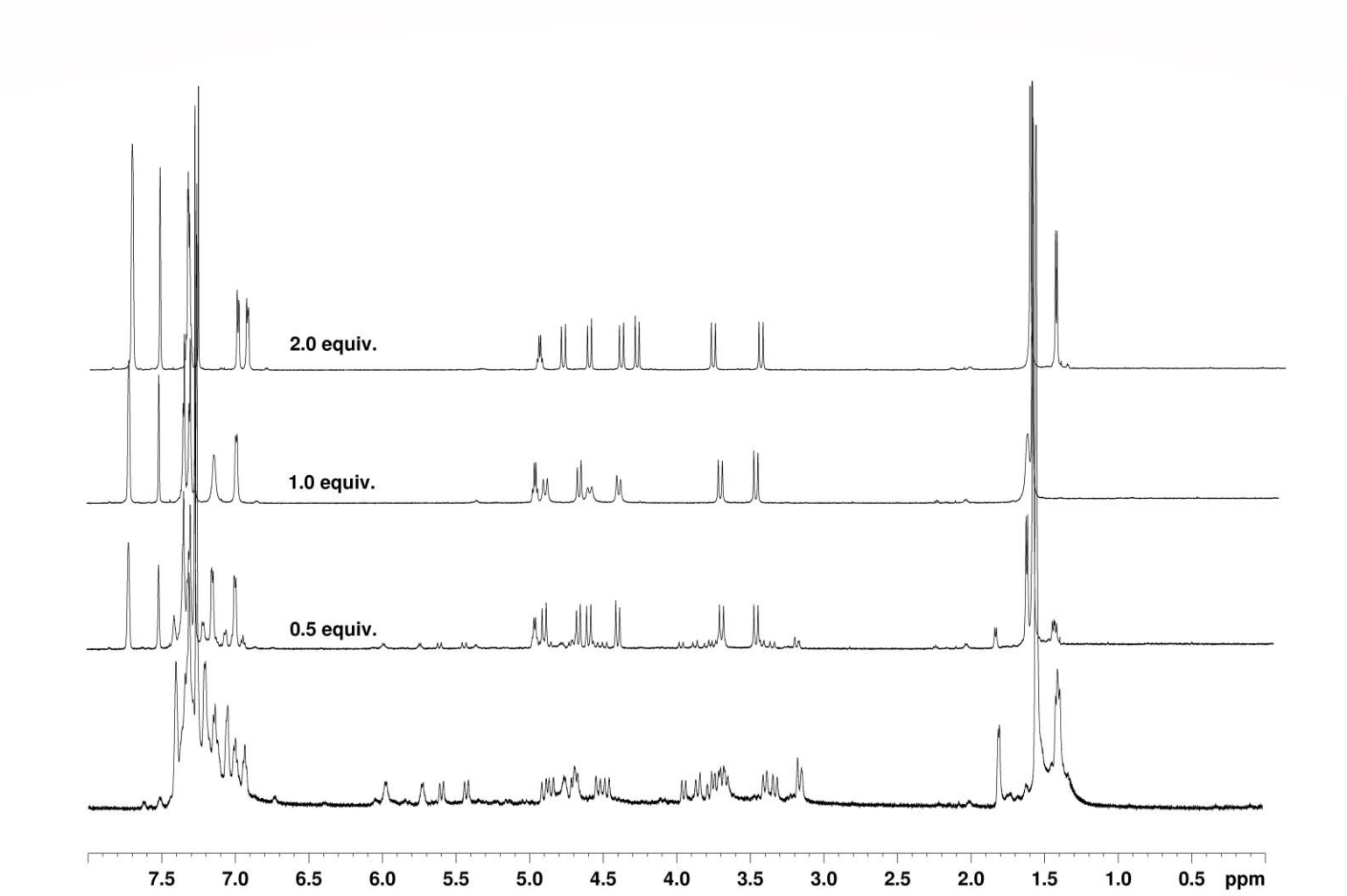


Figure S2. Stepwise addition of NaTFPB to **28** (600 MHz, $CDCl_3$)

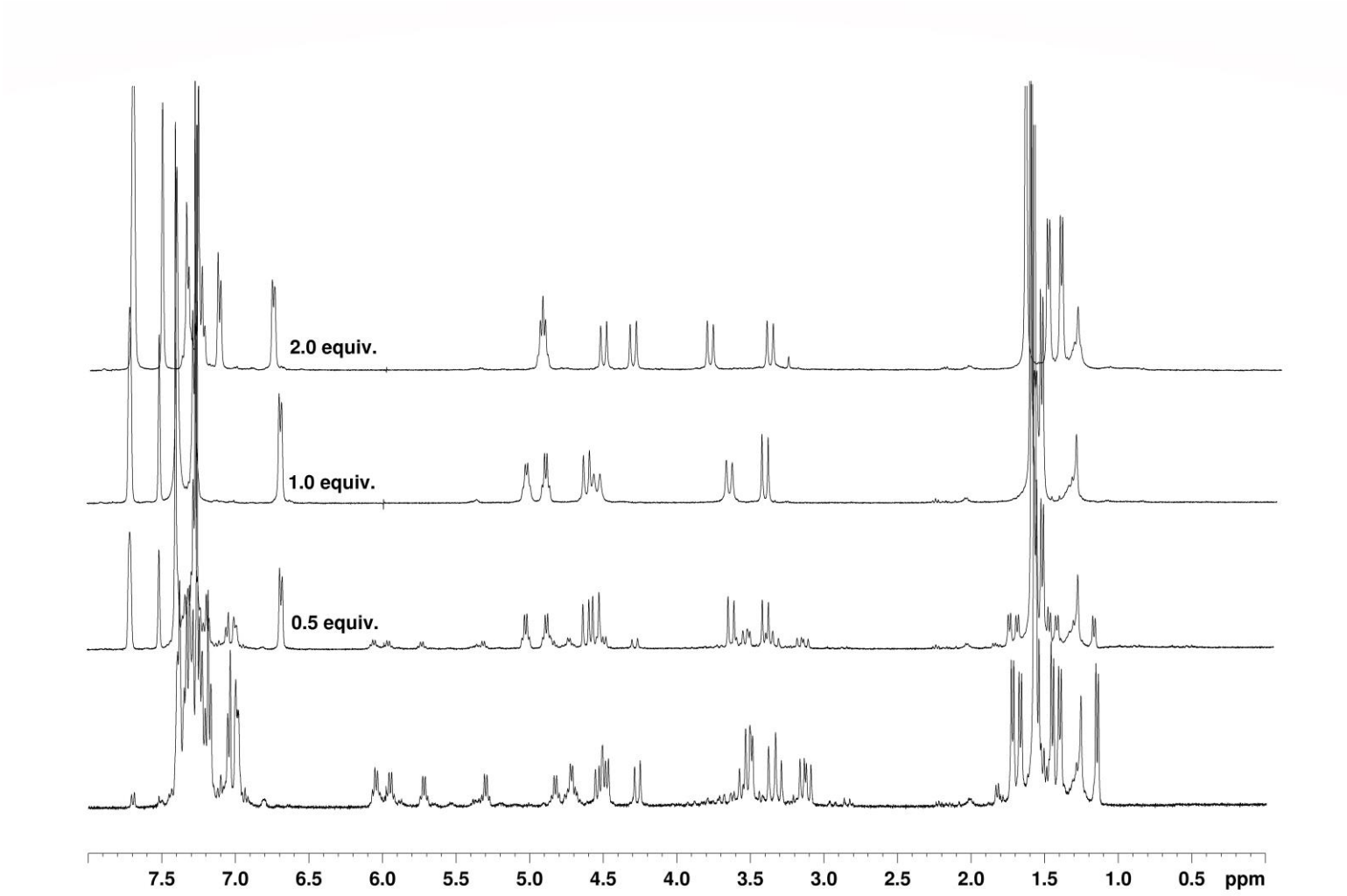


Figure S3. Stepwise addition of NaTFPB to **30** (400 MHz, $CDCl_3$)

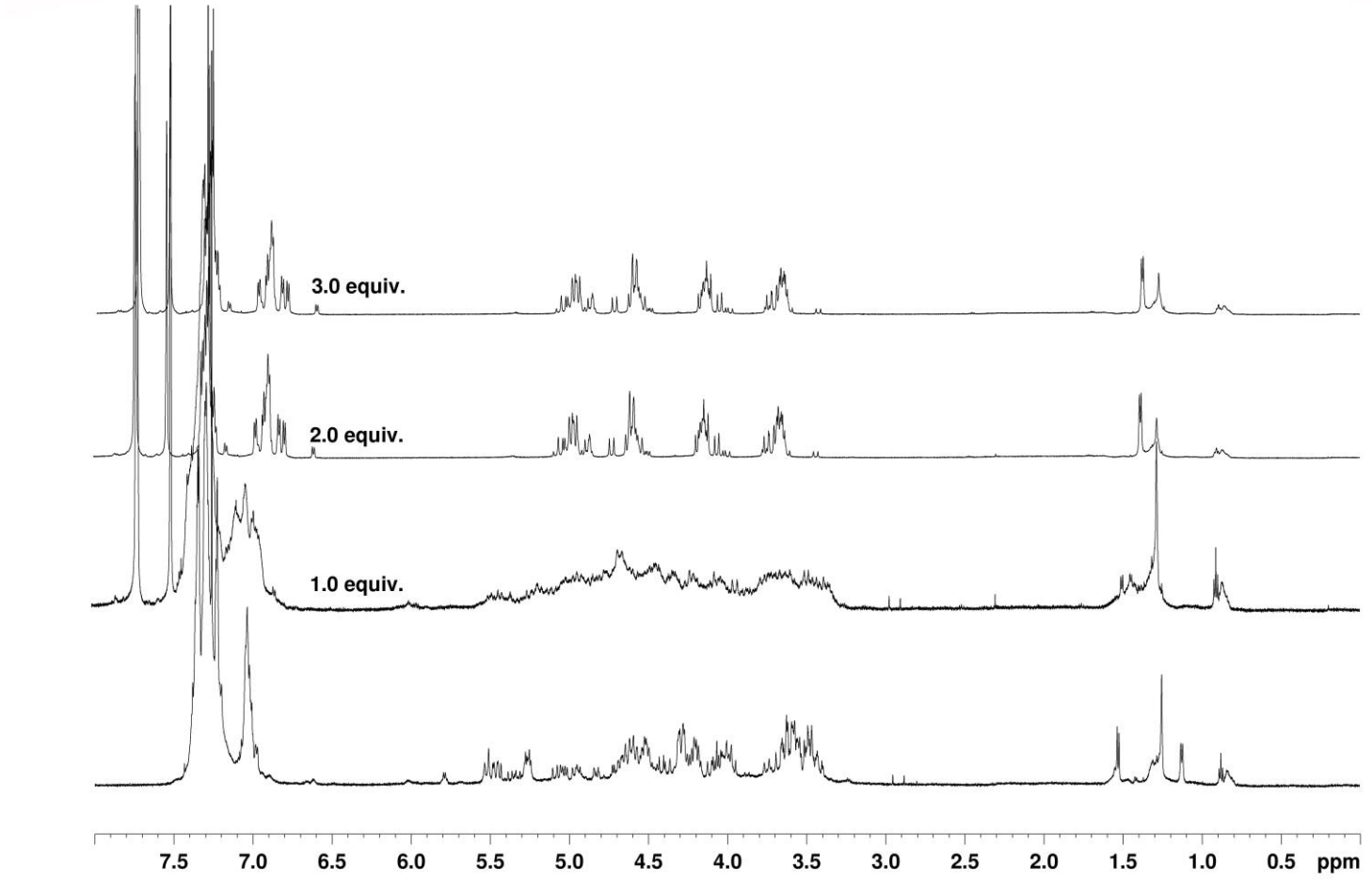


Figure S4. Stepwise addition of NaTFPB to **34** (600 MHz, $CDCl_3$)

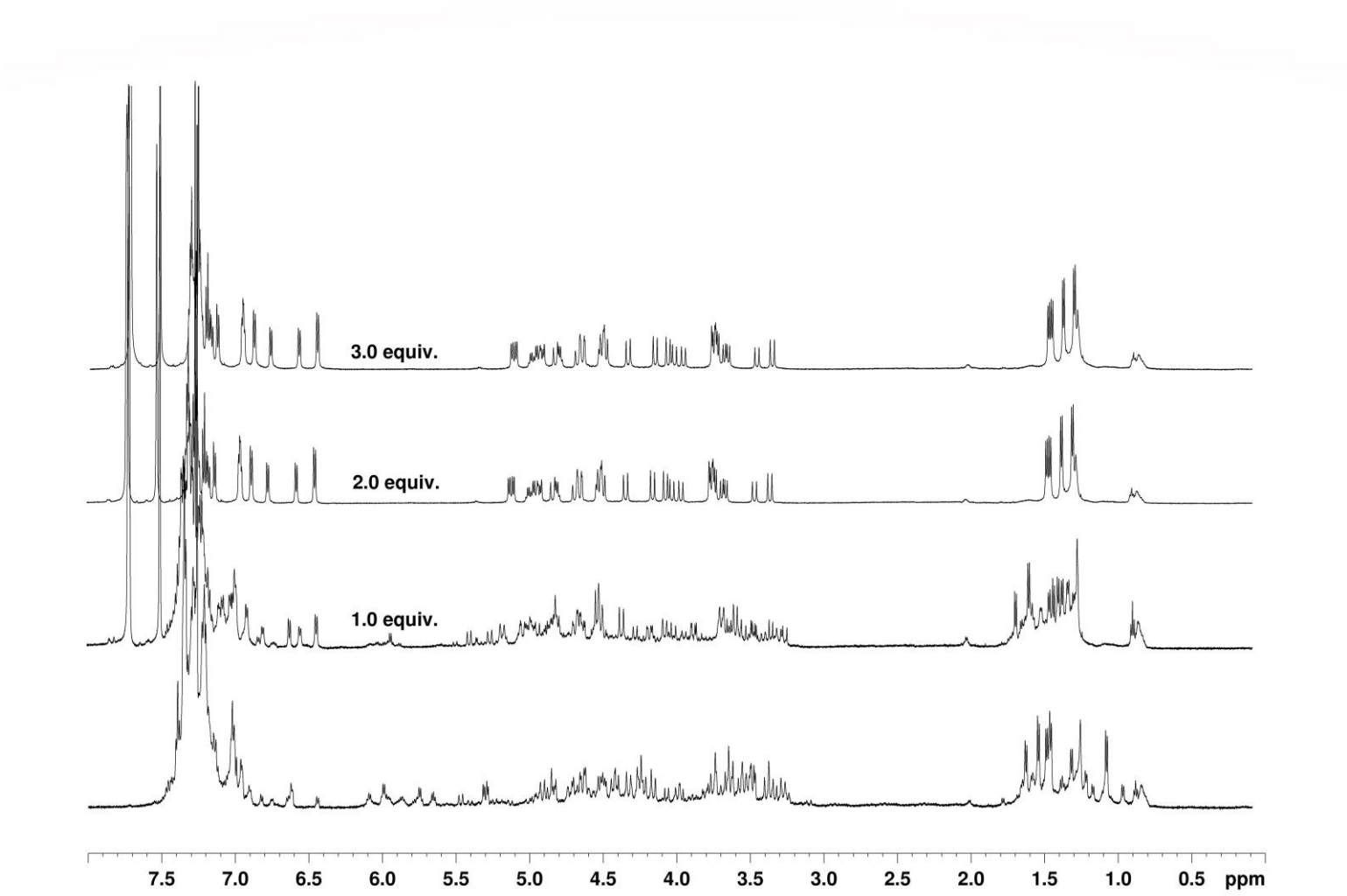


Figure S5. Stepwise addition of NaTFPB to **35** (600 MHz, $CDCl_3$)

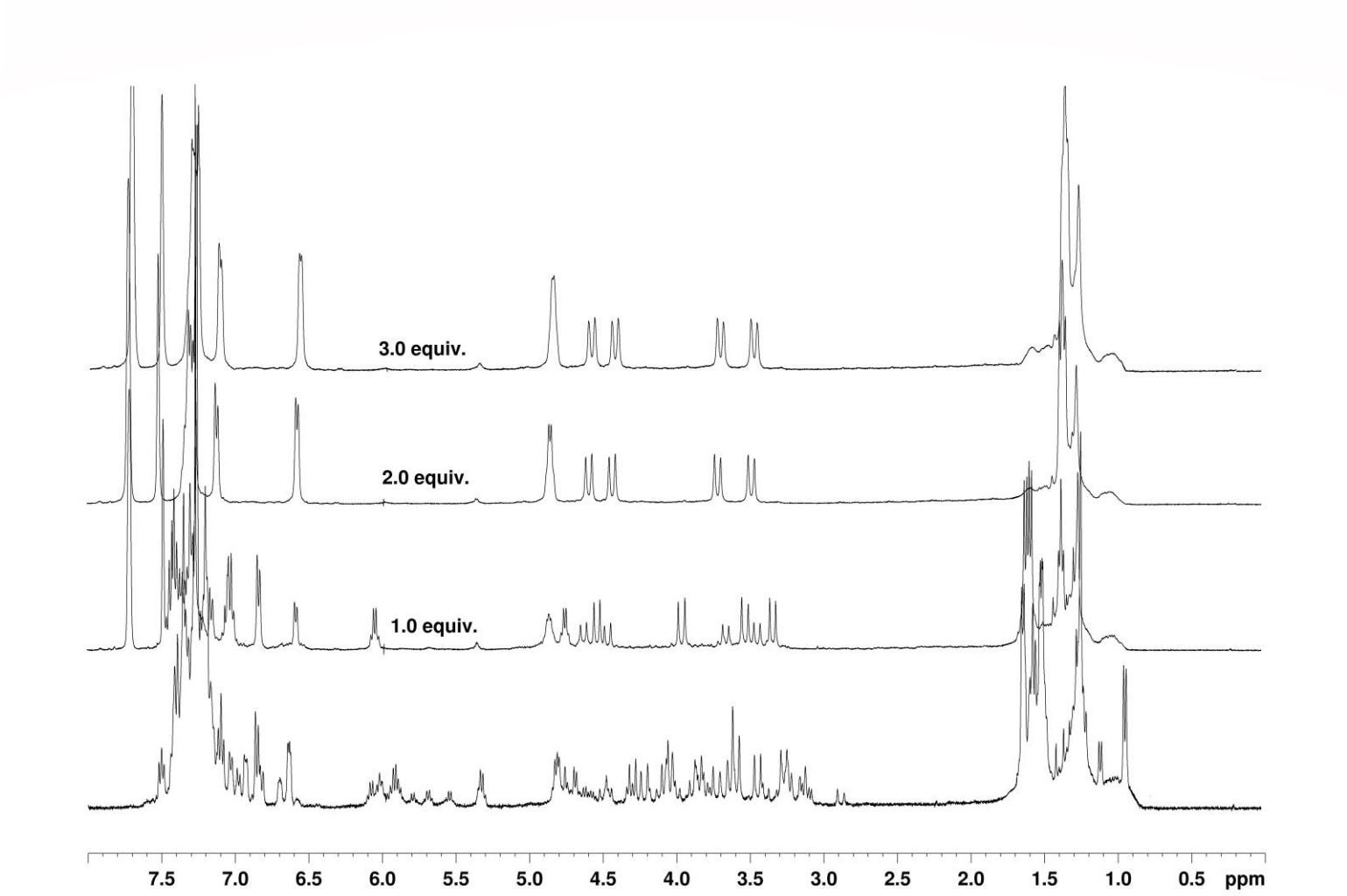


Figure S6. Stepwise addition of NaTFPB to **36** (400 MHz, $CDCl_3$)

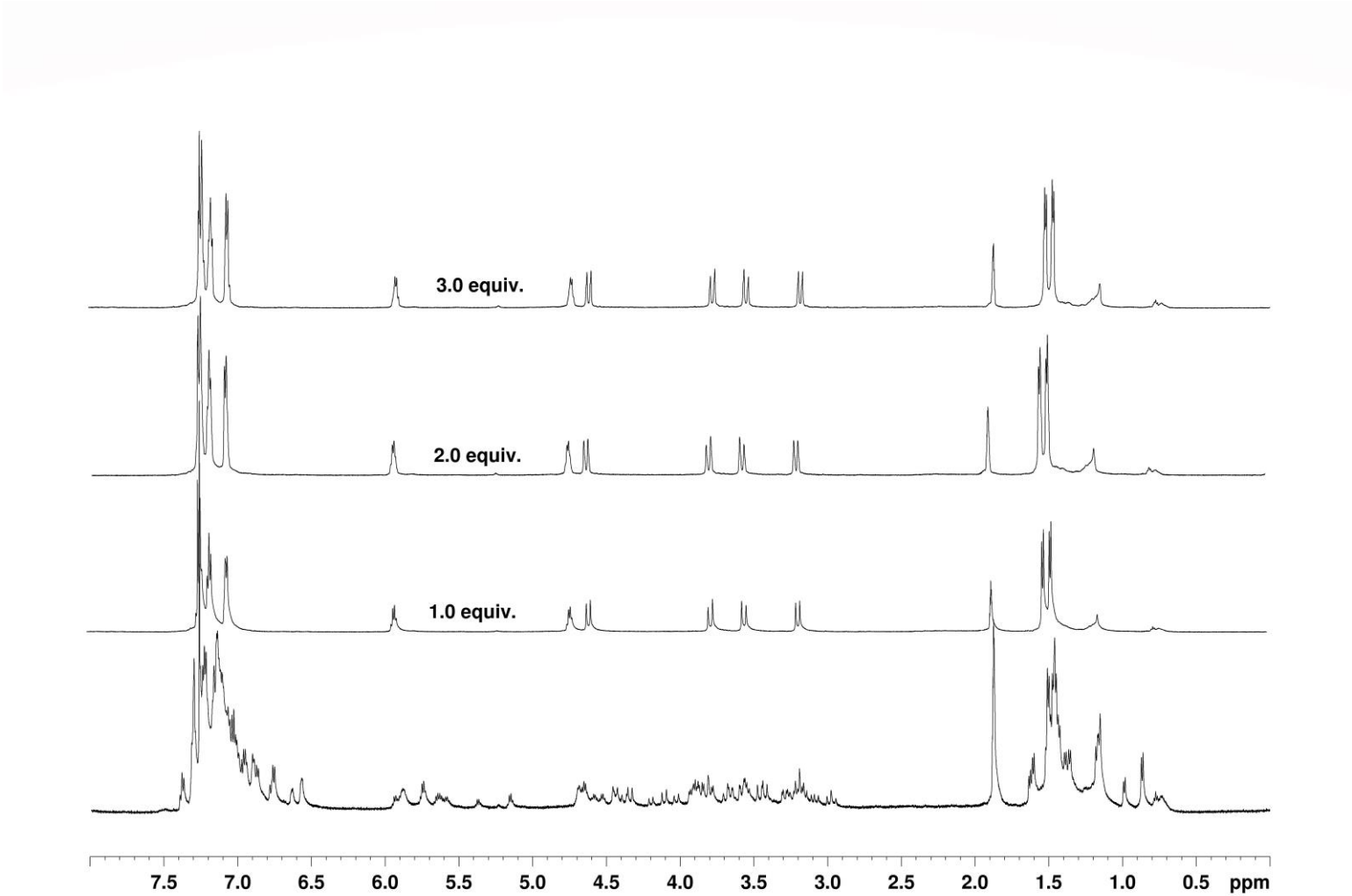


Figure S7. Stepwise addition of $NaPF_6$ to **36** (600 MHz, $CDCl_3$:CD_3CN = 9:1)

2.3 ^{1}H NMR variable temperature experiments (Figure S8-S13)

The cyclopeptoids were dissolved in $C_2D_2Cl_4$ (TCDE, 5.0 mM solution), then ^{1}H NMR spectra were acquired at different temperatures, increasing 20 Kelvin each time.

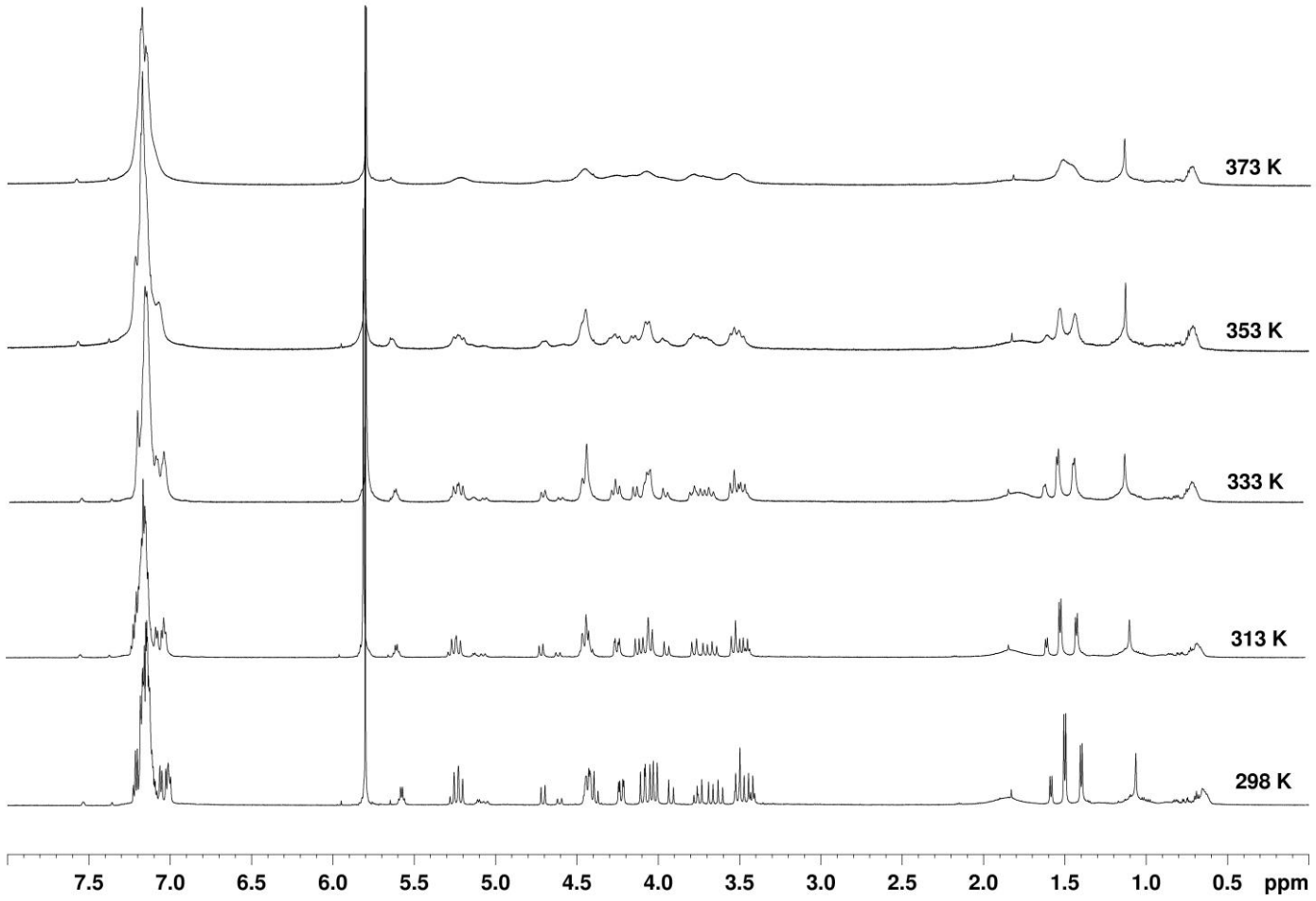


Figure S8. Variable temperature ^{1}H NMR spectra of compound **1/2** (600 MHz, $C_2D_2Cl_4$, 5.0 mM solution)

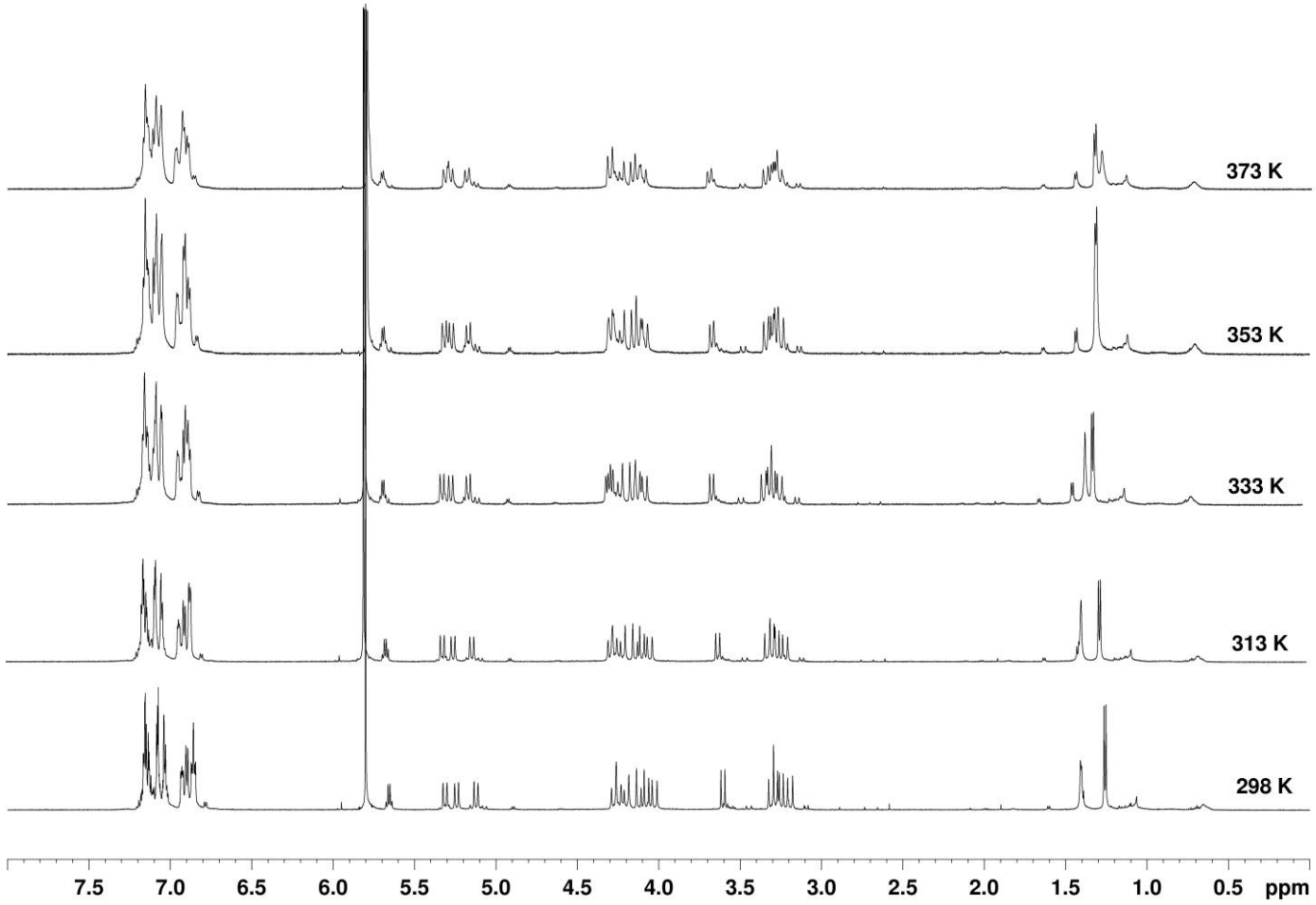


Figure S9. Variable temperature ^{1}H NMR spectra of compound **16/17** (600 MHz, $C_2D_2Cl_4$, 5.0 mM solution)

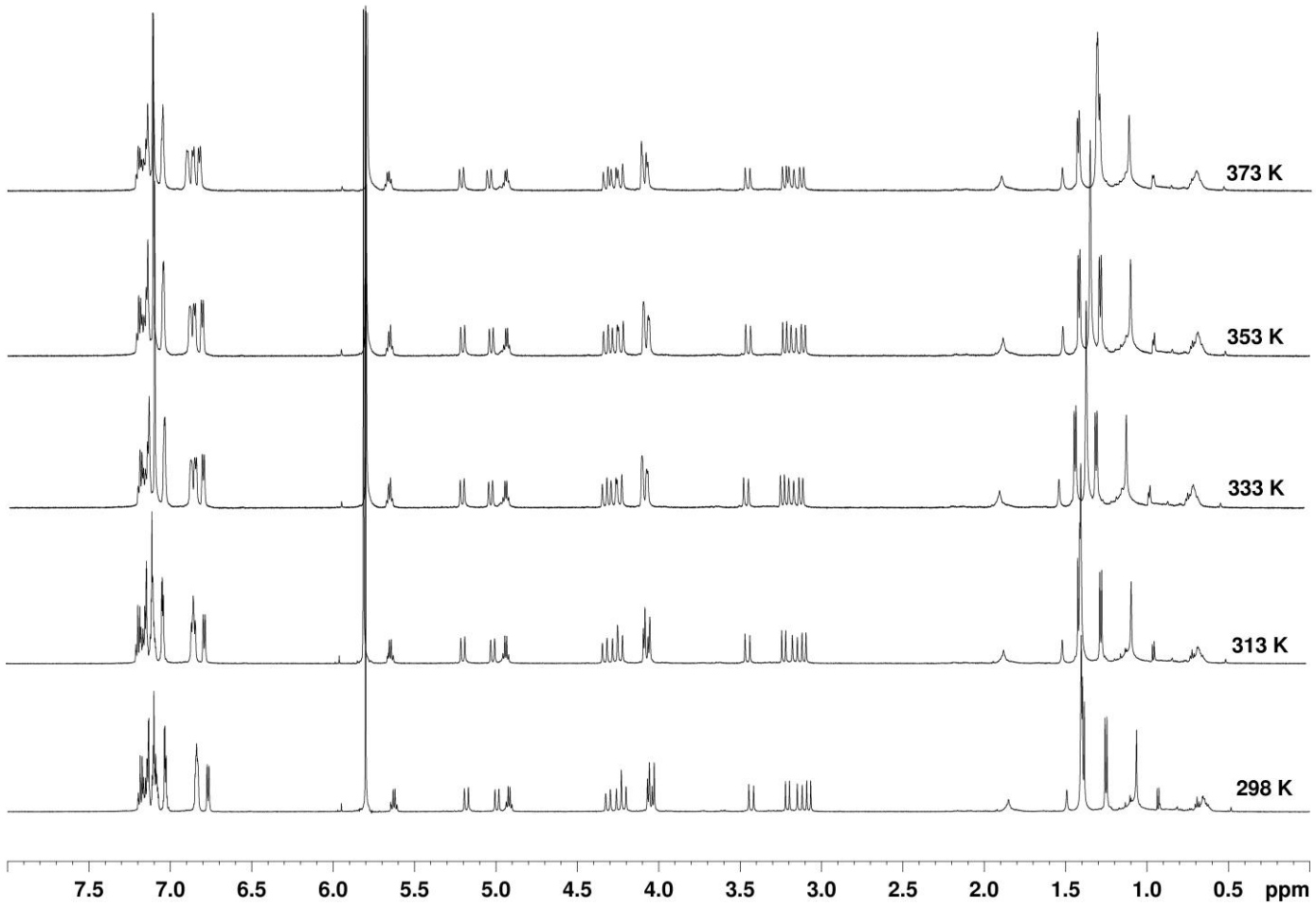


Figure S10. Variable temperature ^{1}H NMR spectra of compound **19** (600 MHz, $C_2D_2Cl_4$, 5.0 mM solution)

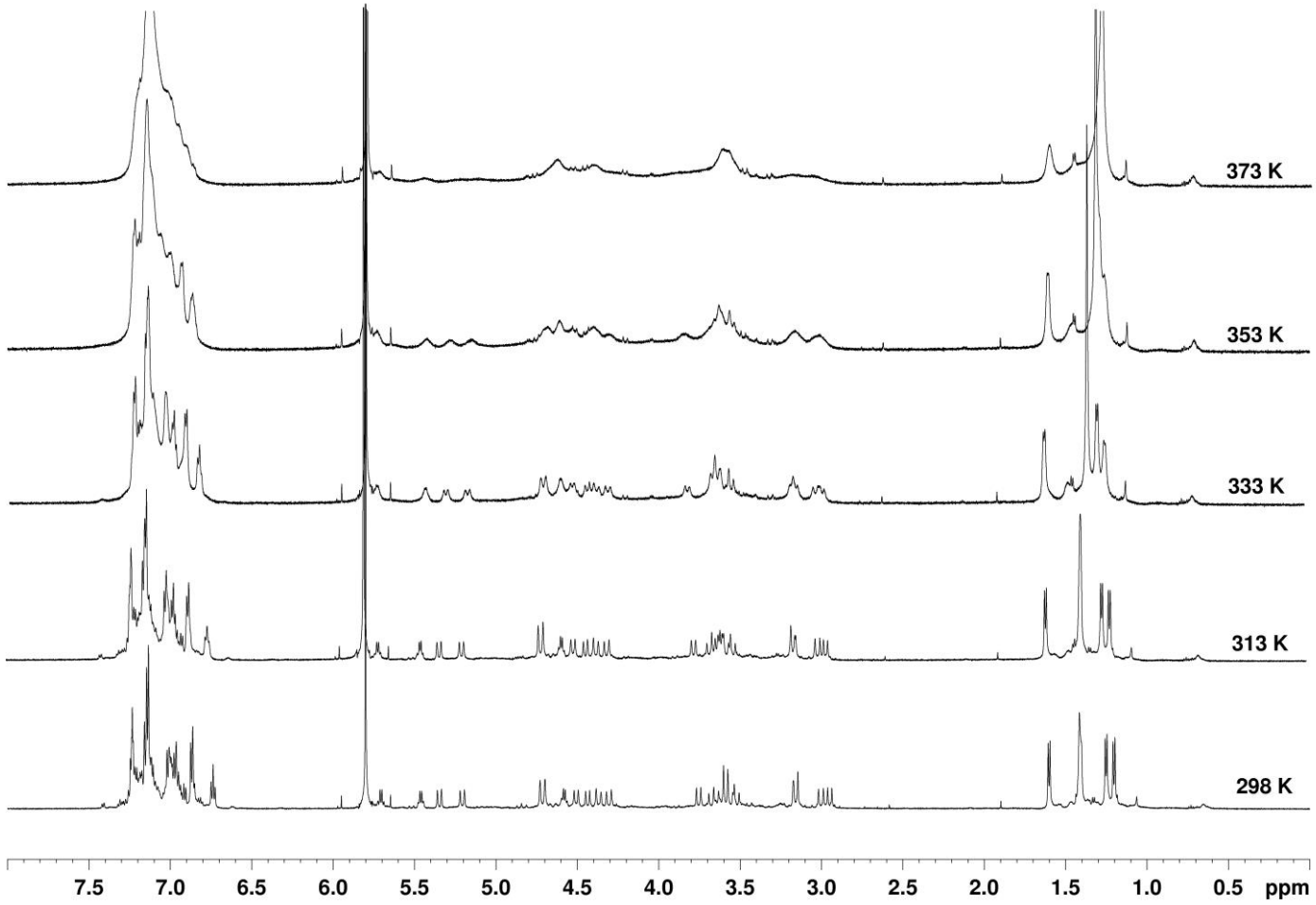


Figure S11. Variable temperature ^{1}H NMR spectra of compound **28** (600 MHz, $C_2D_2Cl_4$, 5.0 mM solution)

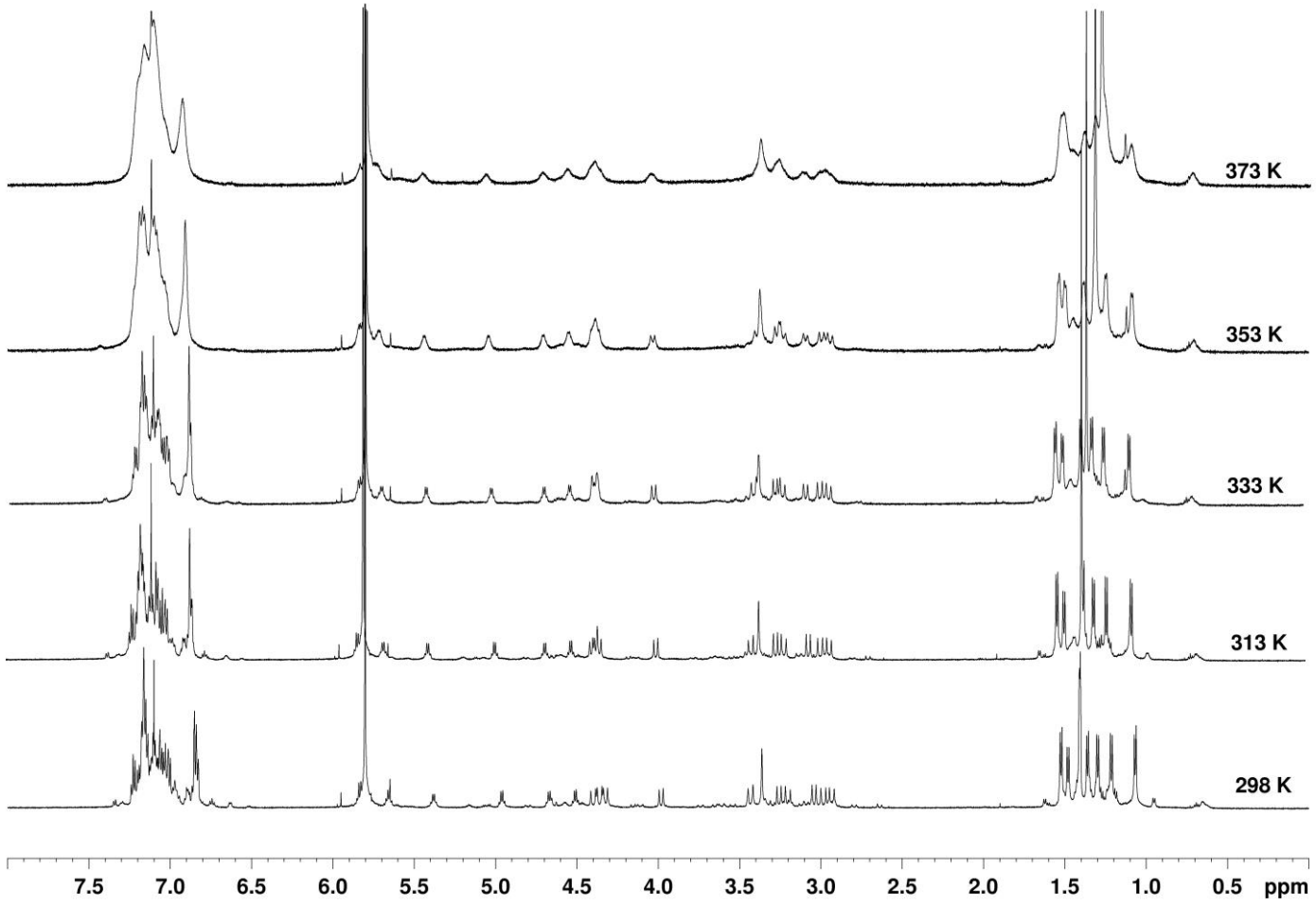


Figure S12. Variable temperature ^{1}H NMR spectra of compound **30** (600 MHz, $C_2D_2Cl_4$, 5.0 mM solution)

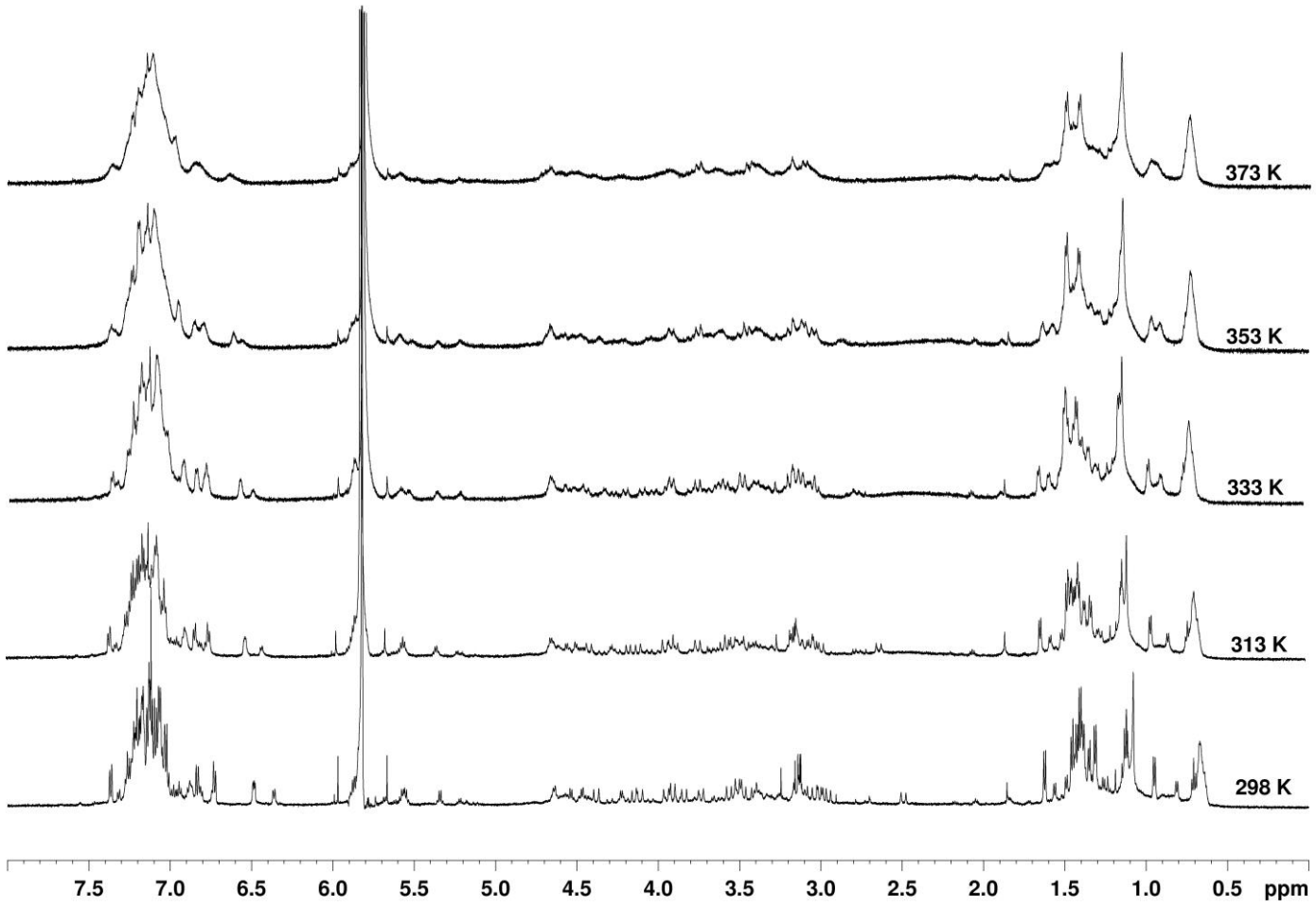


Figure S13. Variable temperature ^{1}H NMR spectra of compound **36** (600 MHz, $C_2D_2Cl_4$, 5.0 mM solution)

3.0 HPLC chromatograms

3.1 HPLC chromatograms of linear peptoids 3, 6, 7, 18, 21, 22, 24, 25, 26, 31, 32, 33 as crude mixtures (Figure S14-S25)

Conditions: 5 → 100% A in 30 min (A, 0.1% TFA in acetonitrile, B, 0.1% TFA in water); flow: 1 mL min^{-1}, 220 nm.

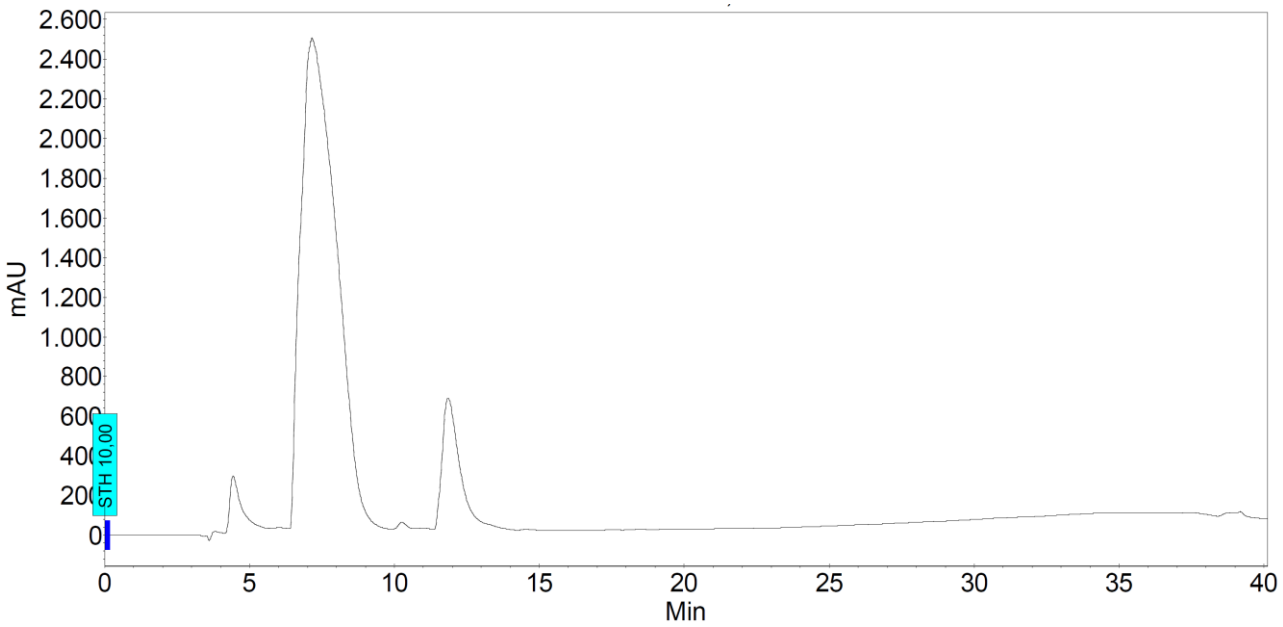


Figure S14. HPLC analysis of **3**

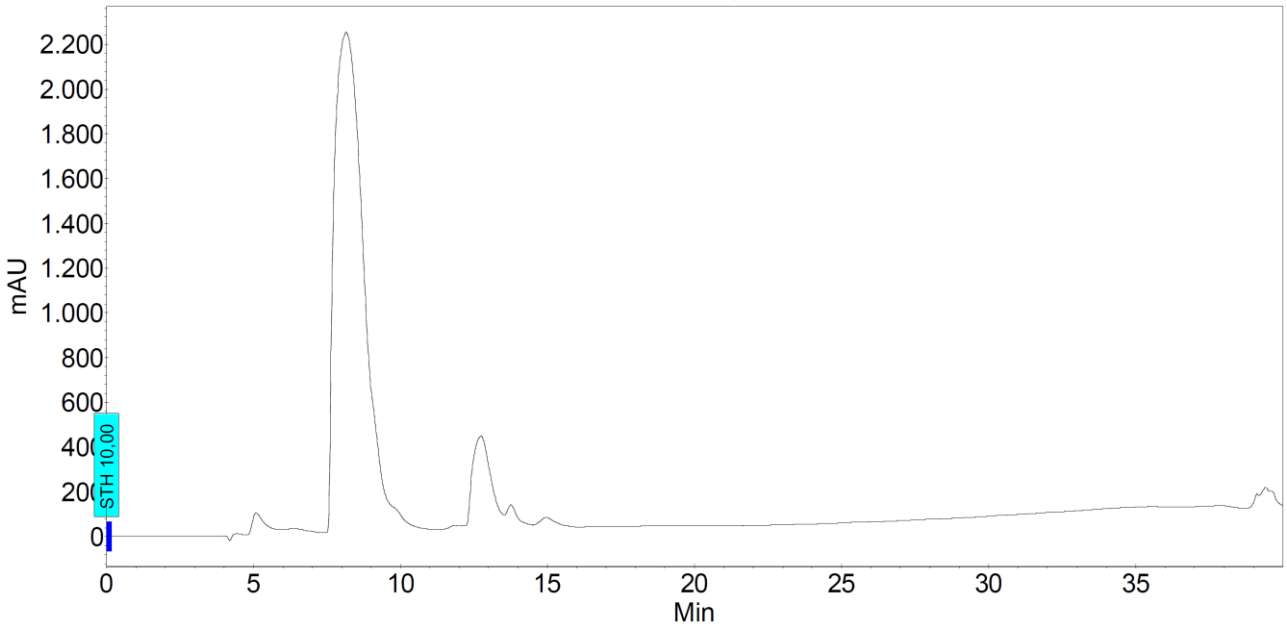


Figure S15. HPLC analysis of **6**

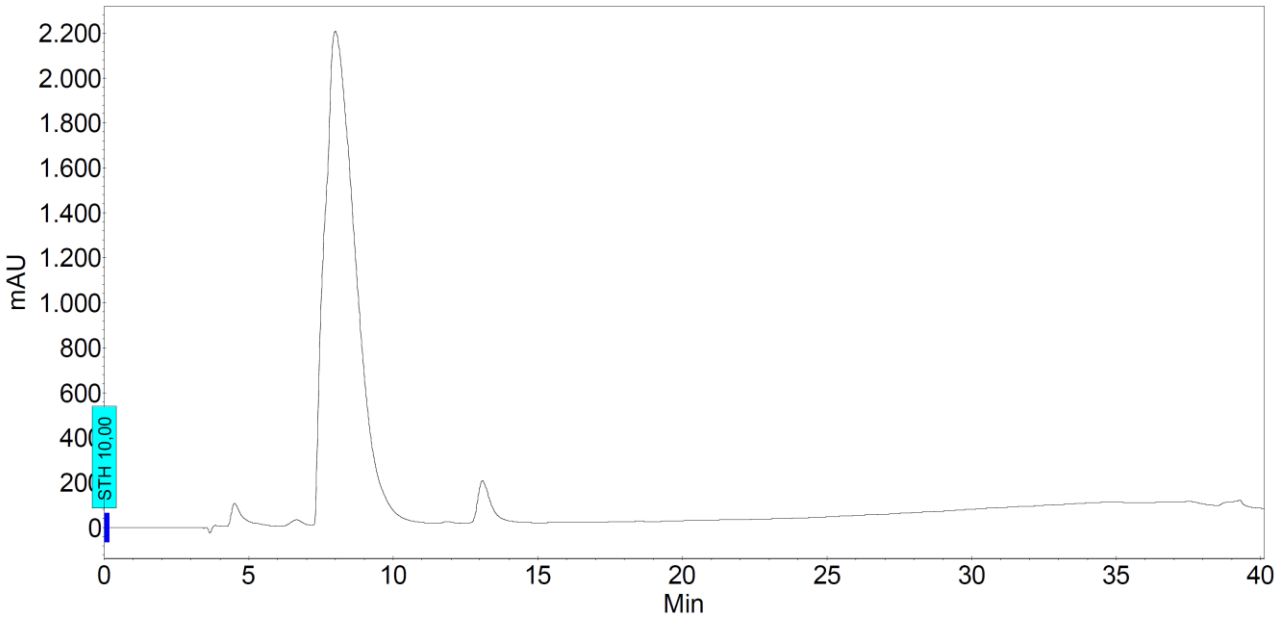


Figure S16. HPLC analysis of **7**

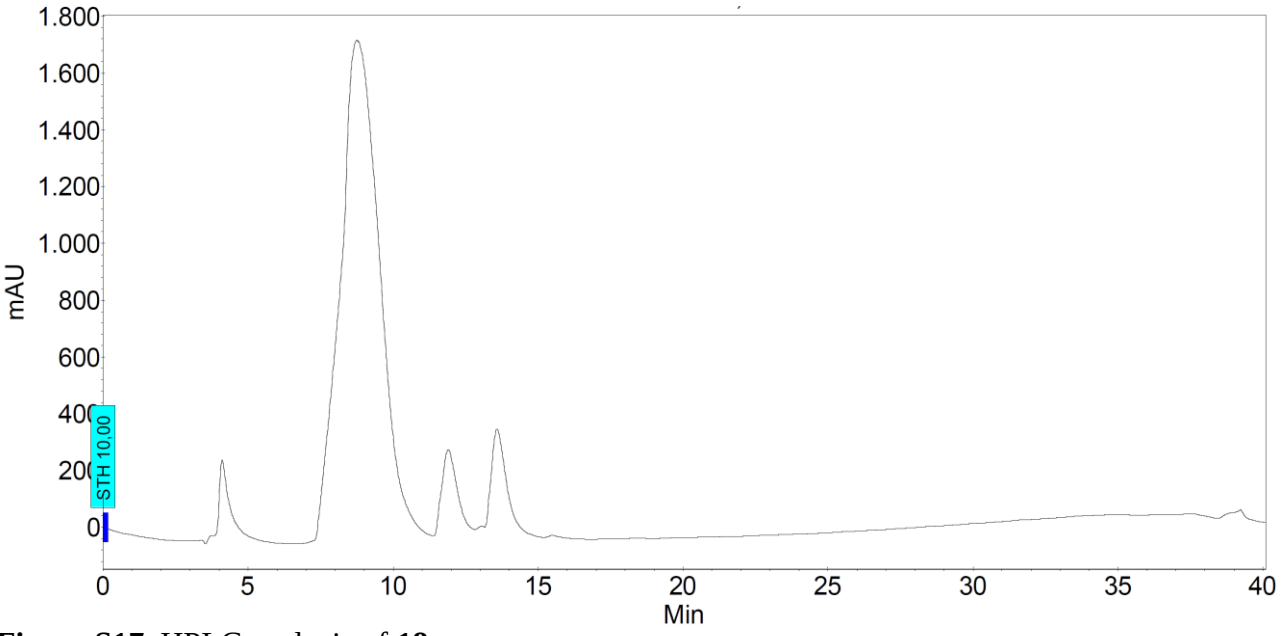


Figure S17. HPLC analysis of **18**

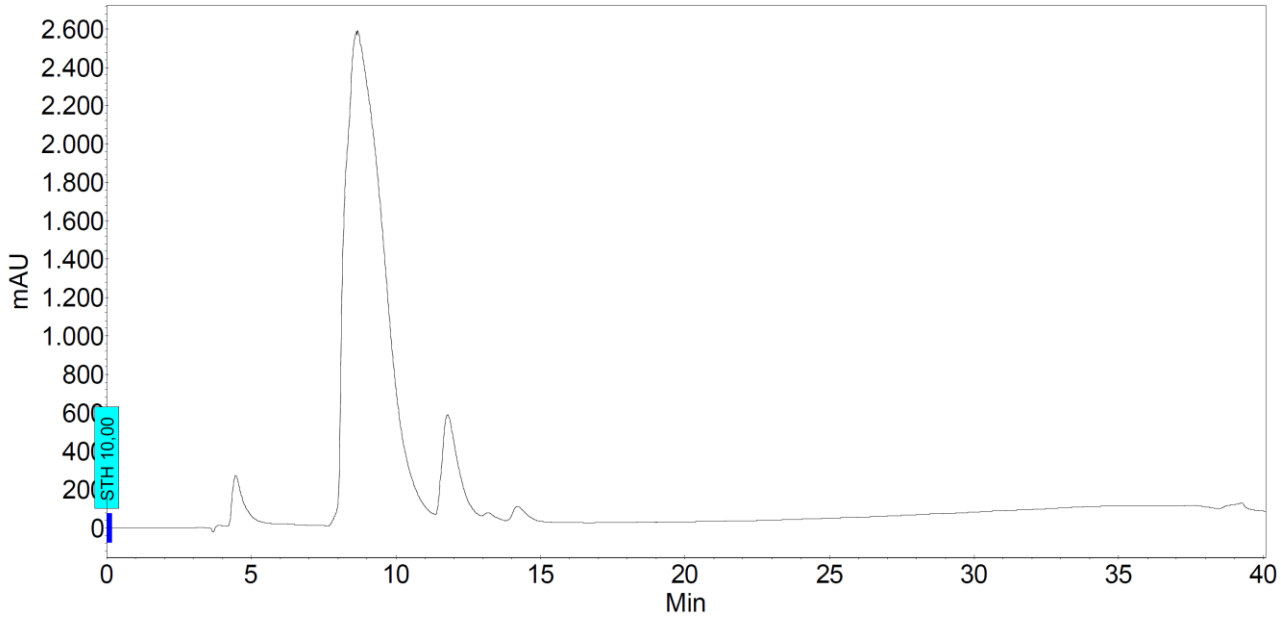


Figure S18. HPLC analysis of **21**

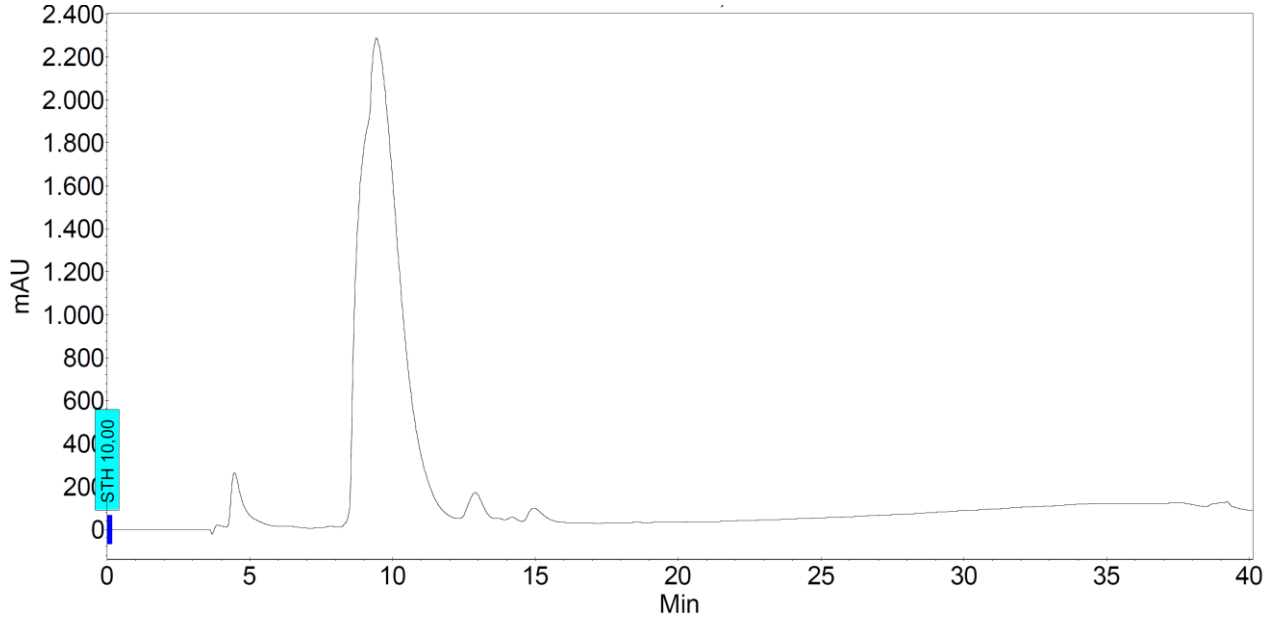


Figure S19. HPLC analysis of **22**

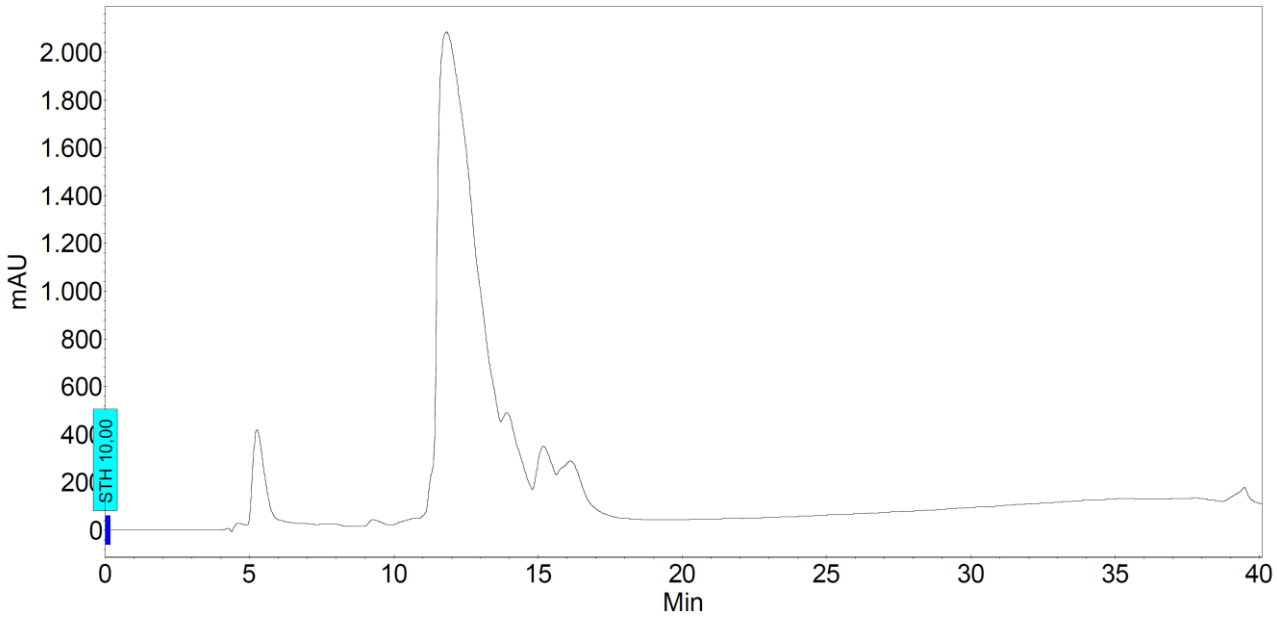


Figure S20. HPLC analysis of **24**

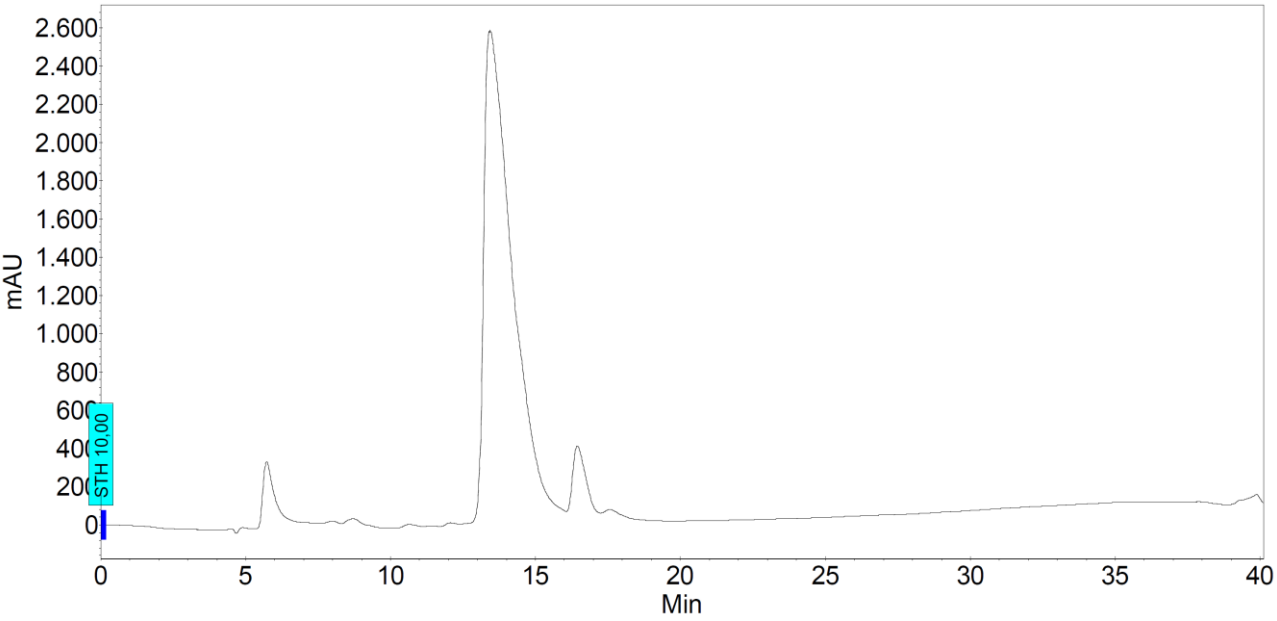


Figure S21. HPLC analysis of **25**

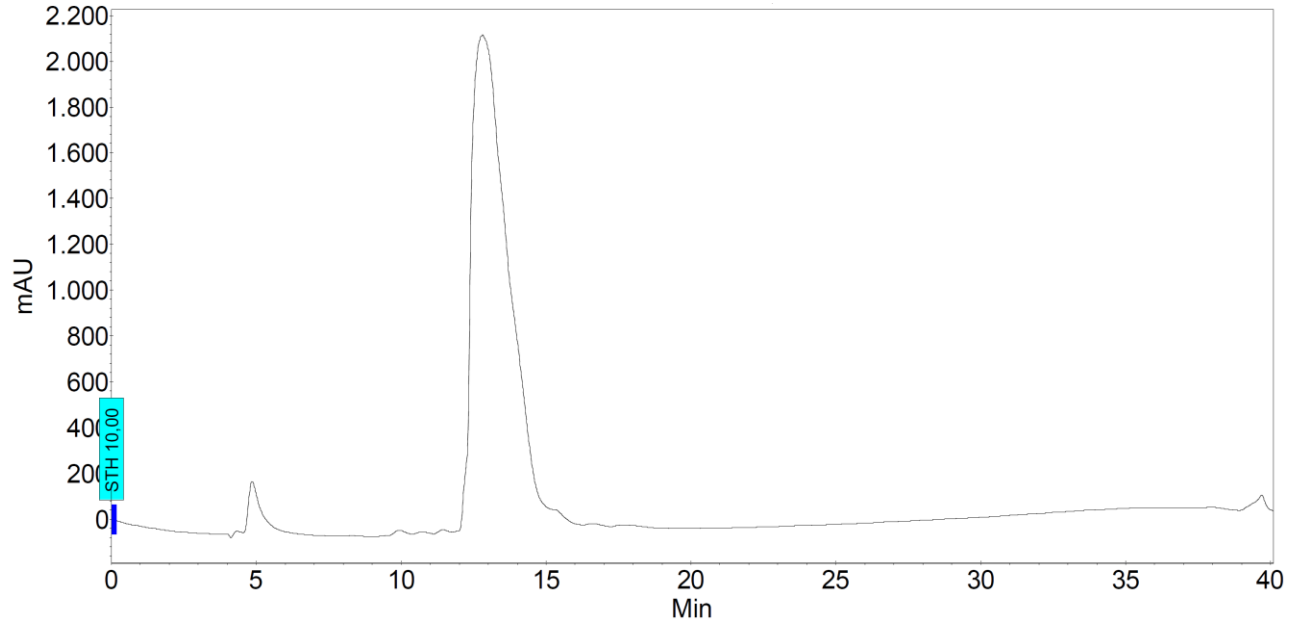


Figure S22. HPLC analysis of **26**

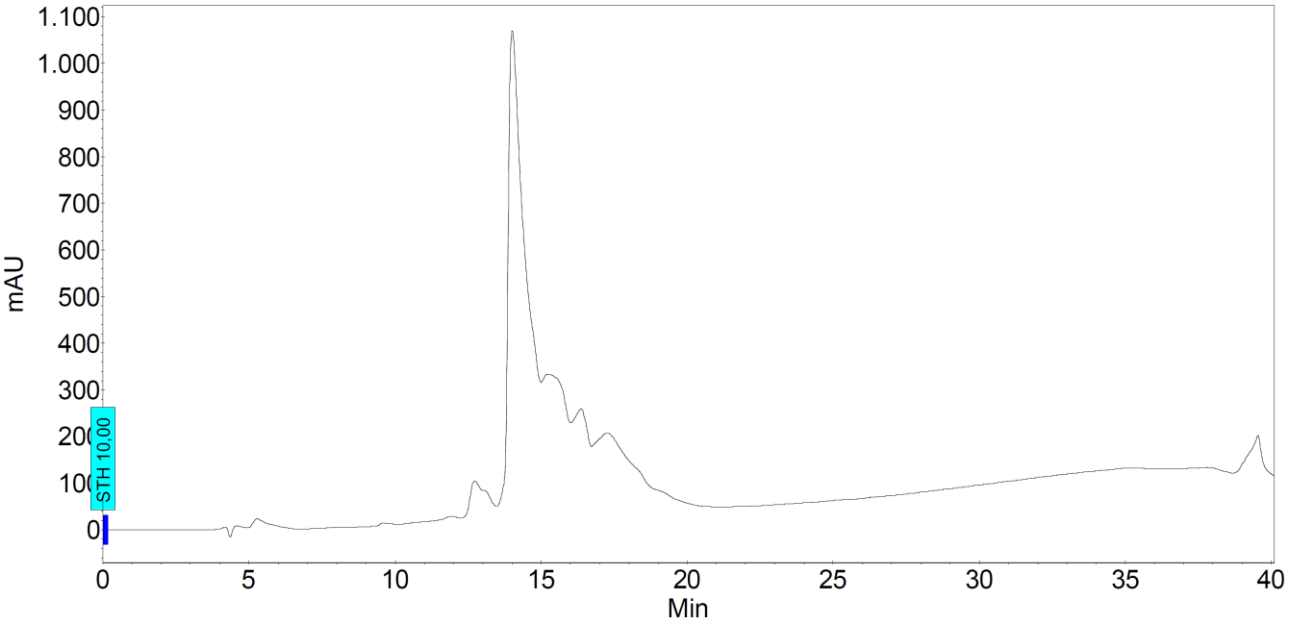


Figure S23. HPLC analysis of **31**

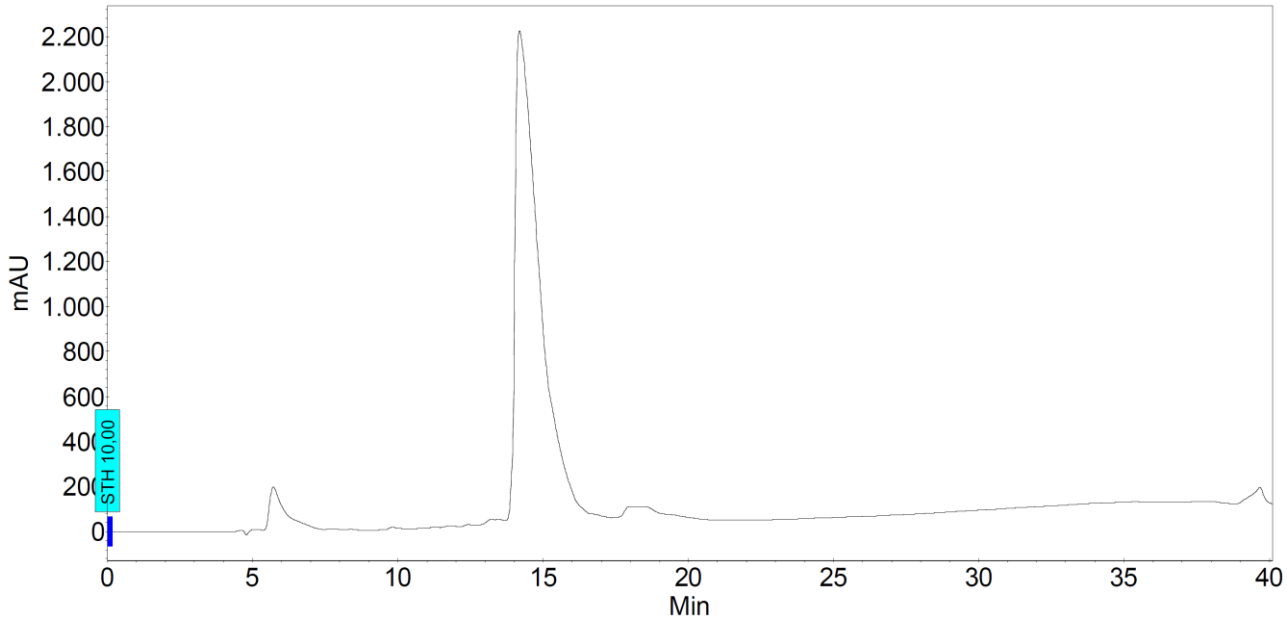


Figure S24. HPLC analysis of **32**

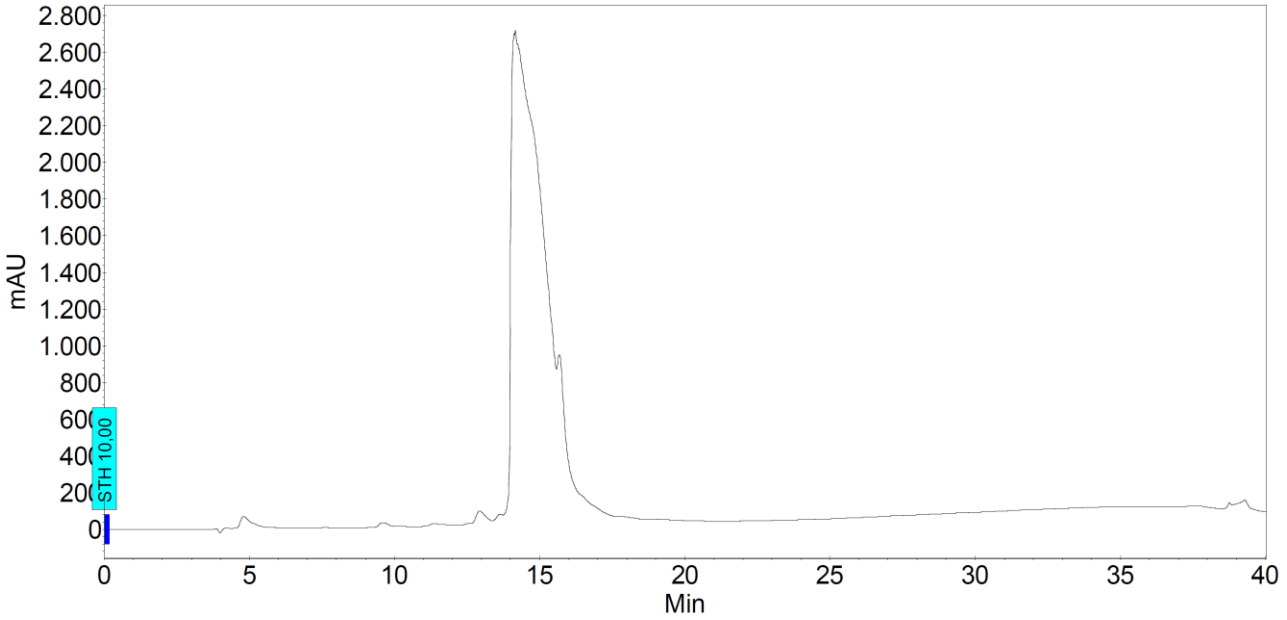


Figure S25. HPLC analysis of **33**

3.2 HPLC chromatograms of cyclic derivatives **1/2, 8, 9, 30, 34, 35, 36** (Figure S26-S32)

Note: **16/17**, **19**, **27**, **28** chromatograms are not reported due to the insolubility of the compounds in the acetonitrile solutions. Their analytical purity was corroborated by the elemental analysis (see experimental section).

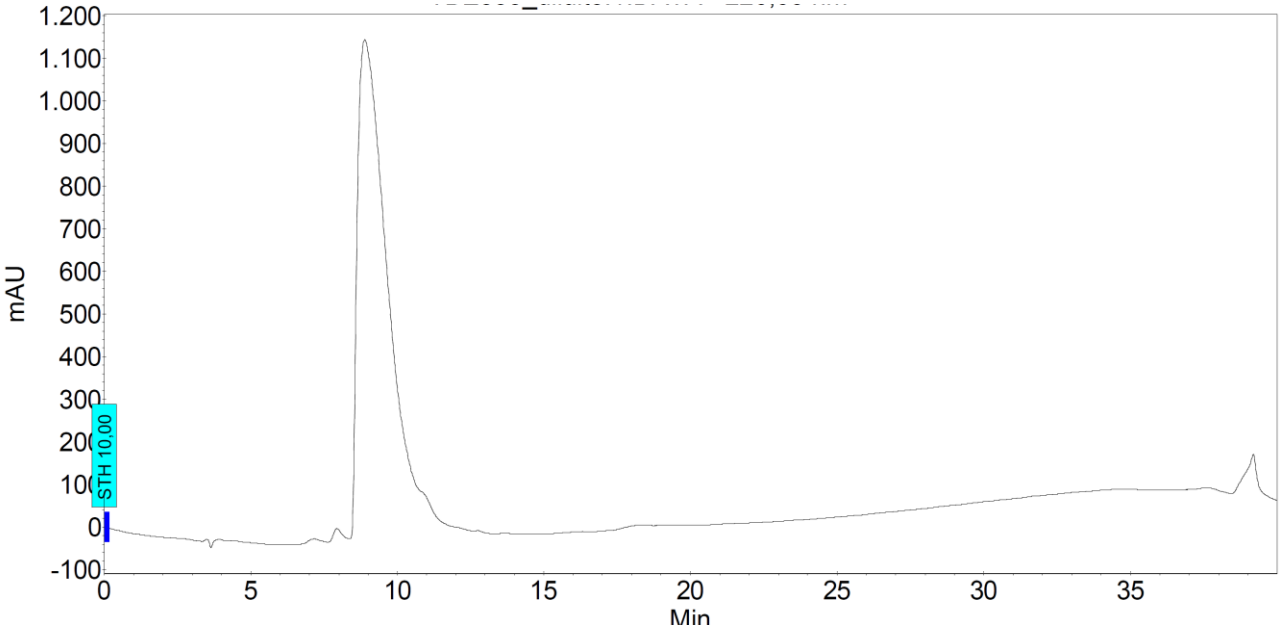


Figure S26. HPLC analysis of **1/2**

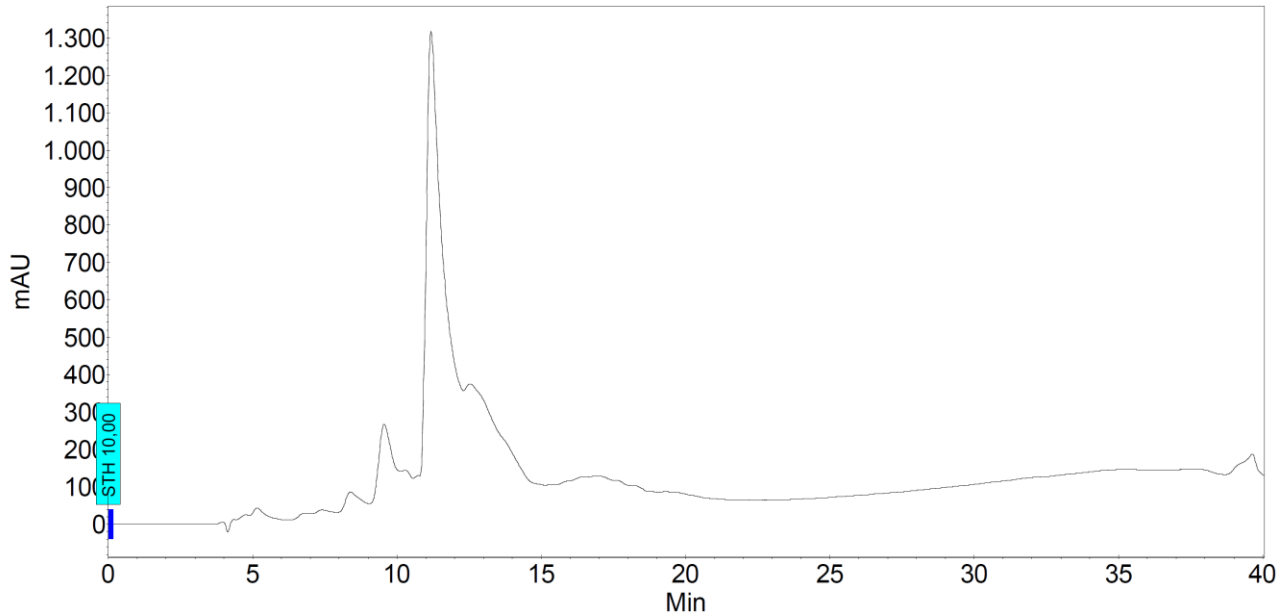


Figure S27. HPLC analysis of **8**

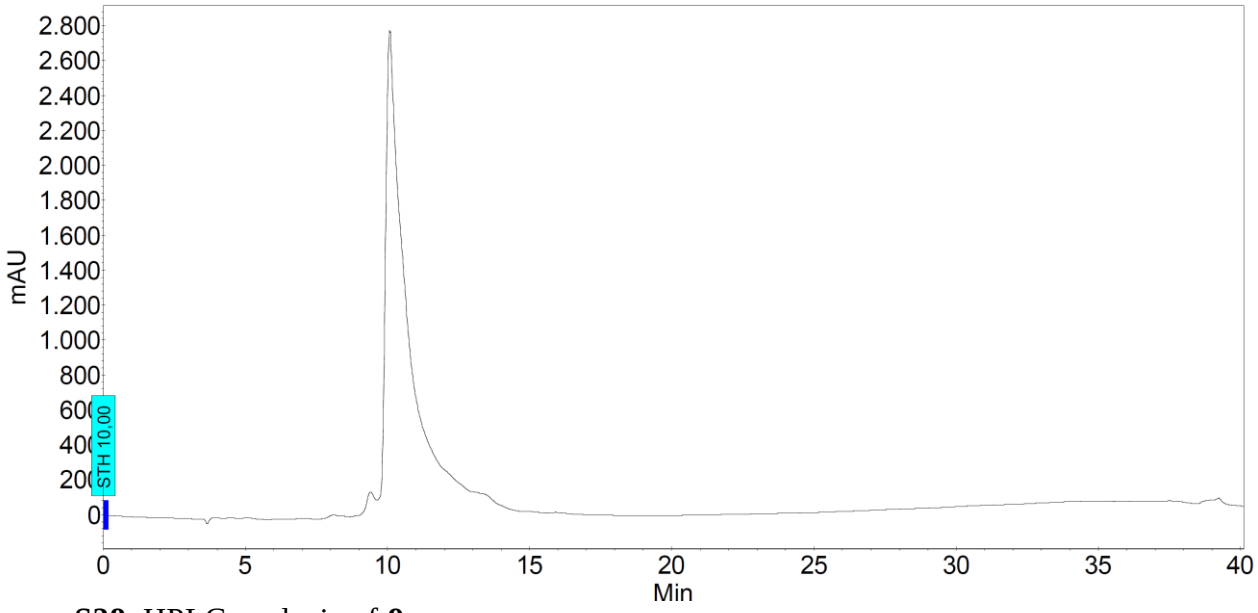


Figure S28. HPLC analysis of **9**

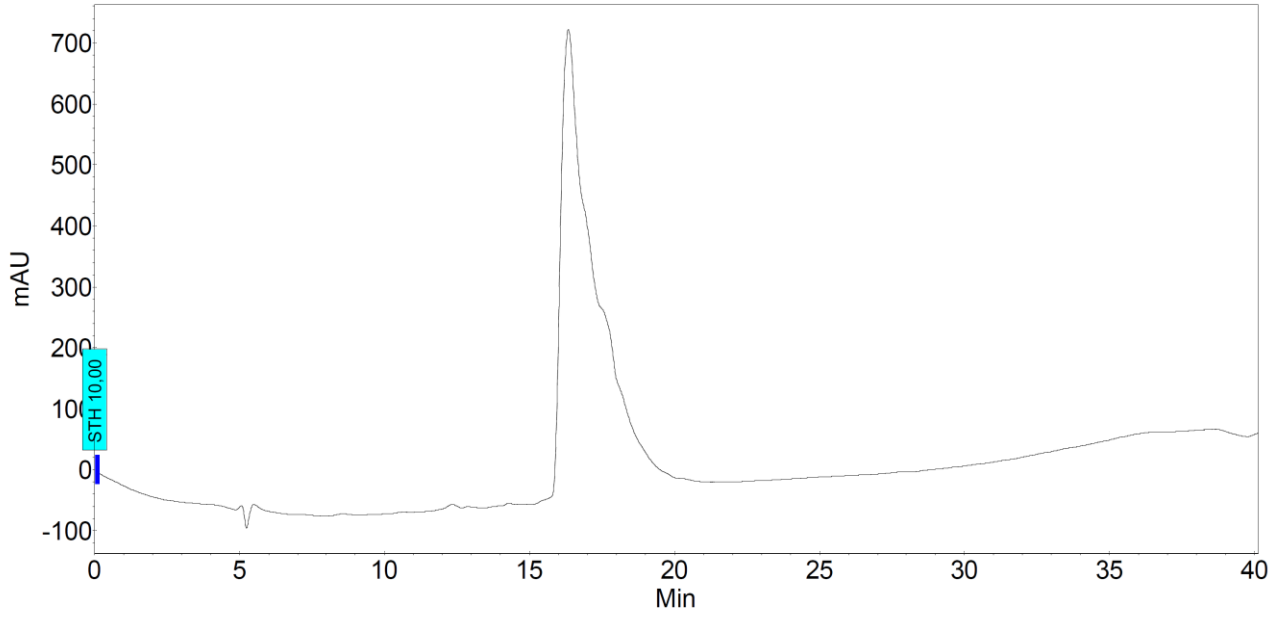


Figure S29. HPLC analysis of **30**

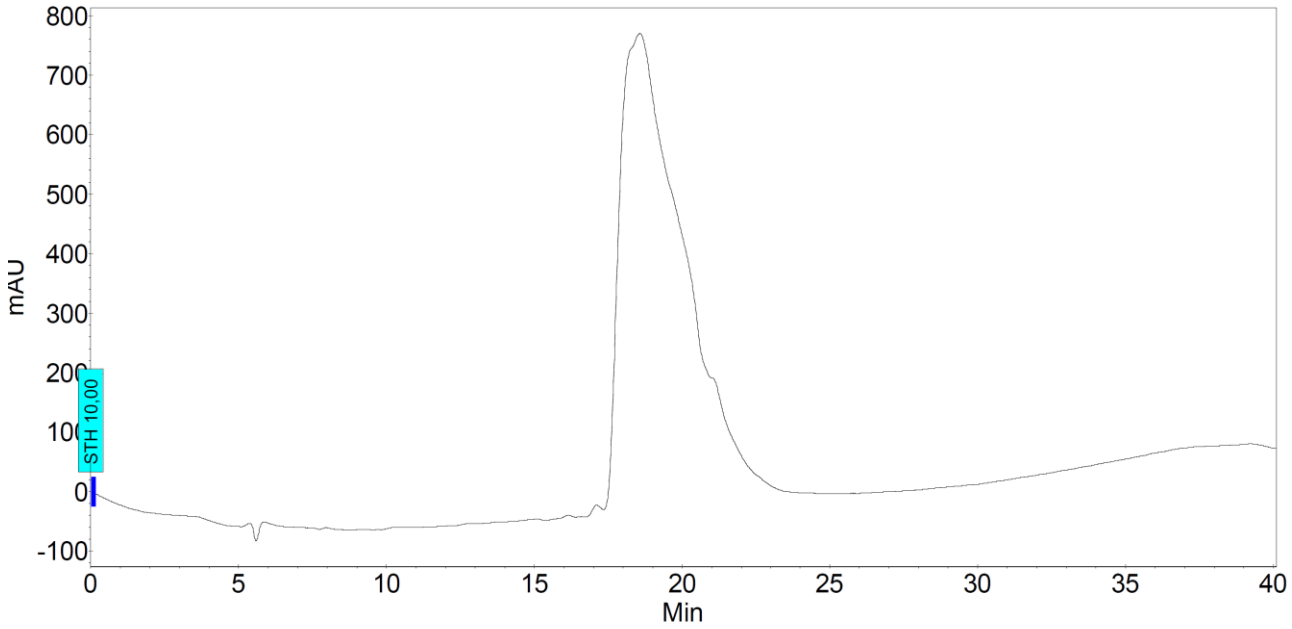


Figure S30. HPLC analysis of **34**

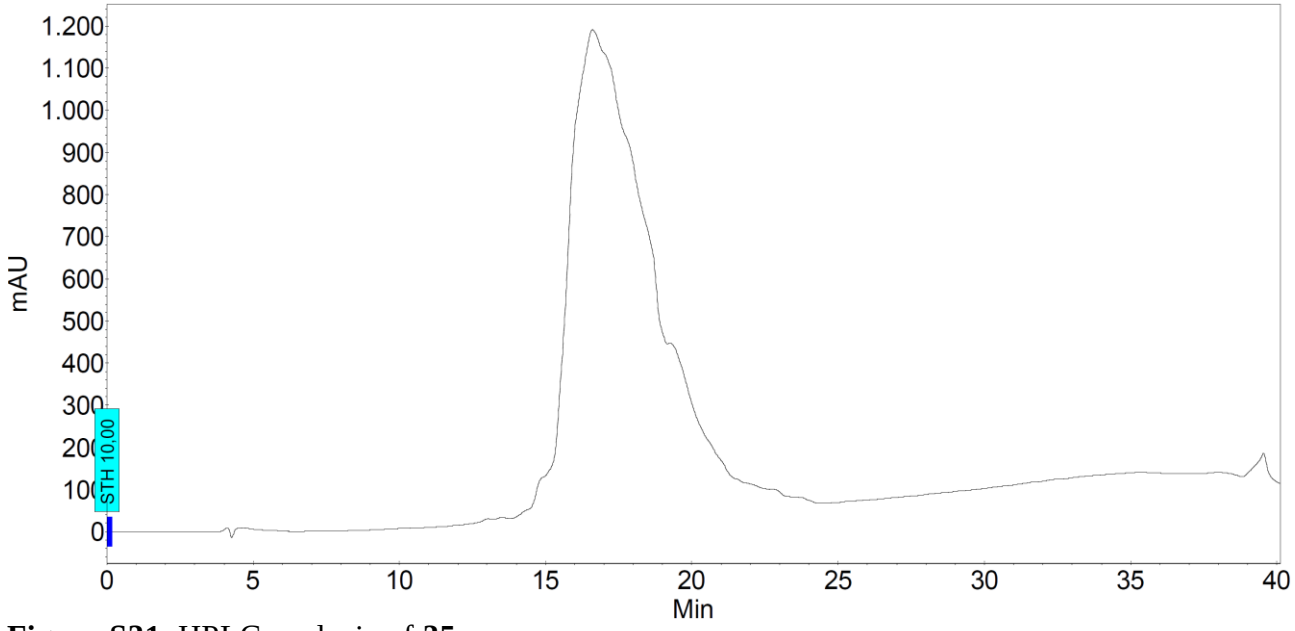


Figure S31. HPLC analysis of **35**

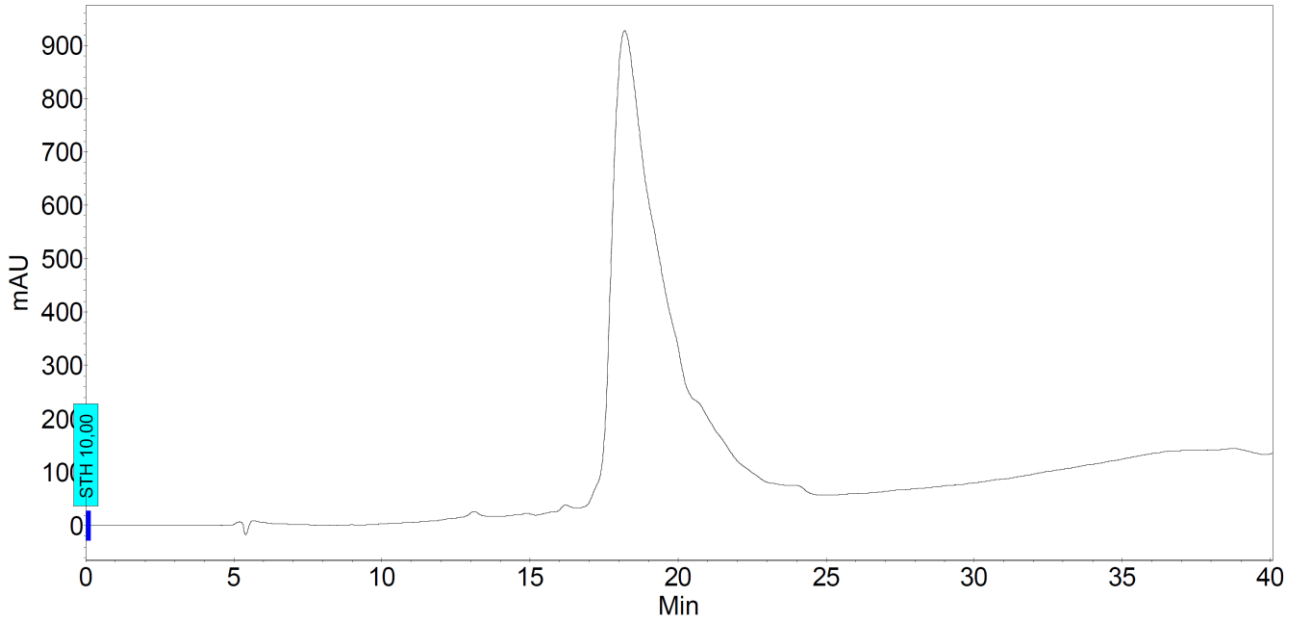


Figure S32. HPLC analysis of **36**

4.0 Computational details

Cartesian coordinates and energies of calculated structures

63
1 E(gas)=-1474.86864574 G(gas)=-1474.430086 E(DMSO)=-1474.88554588

C	-1.695652	0.605853	0.258917
C	-1.450332	-0.658038	-0.598100
N	-0.778455	1.630422	0.224870
C	0.436234	1.674019	-0.598710
C	1.678667	1.278330	0.224704
N	2.094276	-0.031414	0.198776
C	1.488955	-1.097509	-0.607993
C	0.530564	-1.981135	0.216914
N	-0.828003	-1.766877	0.139199
O	2.236206	2.141211	0.915000
O	1.019363	-2.872930	0.923177
O	-2.713308	0.662504	0.960910
C	3.214023	-0.444910	1.079099
C	-0.977947	2.794874	1.123344
C	-1.697350	-2.715286	0.923060
H	-2.449409	-0.991315	-0.908950
H	-0.885810	-0.455783	-1.514864
H	0.301002	1.089484	-1.513365
H	0.591491	2.718987	-0.903678
H	2.301313	-1.766827	-0.928043
H	1.041862	-0.682643	-1.515794
H	2.872608	-1.298171	1.684075
H	3.409013	0.410046	1.739539
C	4.457215	-0.821583	0.298295
H	-1.063152	-3.609131	1.013941
C	-2.932268	-3.110350	0.123841
C	-1.970709	-2.204683	2.343575
C	-1.314510	4.063565	0.366037
H	-0.054111	2.933278	1.704737
H	-1.793356	2.515704	1.802714
C	-0.394005	5.121086	0.300718
C	-0.705449	6.295403	-0.396217
C	-1.941678	6.422020	-1.036821
C	-2.866557	5.370954	-0.977267
C	-2.555679	4.200429	-0.280625
H	0.573511	5.018879	0.800000
H	0.019946	7.111149	-0.437372
H	-2.187408	7.337814	-1.579101
H	-3.837146	5.469089	-1.469148
H	-3.281528	3.384897	-0.225149
C	-4.186119	-2.508002	0.319385
C	-5.295438	-2.911225	-0.433840
C	-5.168868	-3.922325	-1.391628
C	-3.924167	-4.530380	-1.595136
C	-2.818494	-4.126733	-0.841664

H	-4.293109	-1.706078	1.051890
H	-6.262958	-2.431569	-0.268842
H	-6.036510	-4.238728	-1.974960
H	-3.817448	-5.327206	-2.334870
H	-1.849699	-4.610900	-0.994958
C	4.886884	-2.156349	0.239011
C	6.037319	-2.503531	-0.480684
C	6.768476	-1.517596	-1.149933
C	6.346831	-0.182315	-1.096176
C	5.199917	0.163216	-0.376950
H	4.312122	-2.926586	0.760633
H	6.360833	-3.546282	-0.517684
H	7.666833	-1.786134	-1.710313
H	6.920266	0.592717	-1.610083
H	4.877339	1.206514	-0.325406
H	-2.543558	-2.960099	2.902273
H	-1.015113	-2.048720	2.864025
H	-2.529816	-1.260384	2.345207

63

2 E(gas)=-1474.86645315 A.U. G(gas)=-1474.426844 E(DMSO)=-1474.88351959

C	1.420869	1.427749	0.293496
C	1.904250	0.249554	-0.575634
N	0.123413	1.863132	0.162493
C	-0.875368	1.322998	-0.767570
C	-1.841489	0.347516	-0.050108
N	-1.481744	-0.971725	0.068362
C	-0.413541	-1.605532	-0.723780
C	0.830376	-1.923715	0.132709
N	1.859945	-1.013826	0.171087
O	-2.869396	0.817400	0.454733
O	0.850633	-2.976326	0.784200
O	2.209019	1.923707	1.109066
C	-2.244846	-1.941197	0.933426
C	-0.365929	2.928042	1.072778
C	3.000081	-1.259909	1.087459
H	2.958540	0.455924	-0.810038
H	1.380931	0.149002	-1.531488
H	-0.388763	0.906384	-1.654539
H	-1.499750	2.160859	-1.108731
H	-0.791958	-2.575906	-1.077841
H	-0.195674	-1.009548	-1.614523
H	-1.506836	-2.737437	1.114767
C	-2.622723	-1.382266	2.311381
C	-3.409231	-2.575831	0.180634
H	2.703531	-2.107925	1.718445
C	4.285337	-1.561447	0.343247
H	3.122379	-0.366175	1.717339
C	-0.624583	4.234479	0.349682
H	-1.291373	2.568457	1.546983
H	0.408326	3.048801	1.841390
C	5.346773	-0.643270	0.346187

C	6.533506	-0.922997	-0.343353
C	6.669108	-2.125424	-1.043611
C	5.614936	-3.048648	-1.050951
C	4.431849	-2.768893	-0.362649
H	5.240245	0.296173	0.895808
H	7.352229	-0.199922	-0.331256
H	7.594573	-2.346543	-1.580009
H	5.720195	-3.993419	-1.589380
H	3.613187	-3.493346	-0.359826
C	-1.937047	4.683529	0.135384
C	-2.177488	5.888402	-0.536892
C	-1.105491	6.655813	-1.002188
C	0.208115	6.215800	-0.791502
C	0.447338	5.014074	-0.119999
H	-2.774323	4.080831	0.498240
H	-3.204039	6.226316	-0.695940
H	-1.290465	7.596762	-1.525206
H	1.048765	6.816865	-1.145949
H	1.472321	4.675783	0.053225
C	-3.370318	-3.949557	-0.110216
C	-4.427002	-4.571881	-0.786033
C	-5.538725	-3.822930	-1.182098
C	-5.587917	-2.452519	-0.895729
C	-4.534774	-1.831628	-0.218289
H	-2.504008	-4.539407	0.203783
H	-4.379246	-5.641713	-1.002065
H	-6.365660	-4.303945	-1.709488
H	-6.456302	-1.863100	-1.199798
H	-4.572740	-0.763478	0.003943
H	-2.968061	-2.219744	2.935711
H	-1.742102	-0.936089	2.797607
H	-3.413677	-0.627664	2.256583

69

5 E(gas)=-1553.50955844 G(gas)=-1553.016967 E(DMF)=-1553.52515285

C	0.723931	-1.845311	0.213025
C	1.515912	-0.810371	-0.619012
N	-0.650018	-1.876038	0.130757
C	-1.455815	-0.909983	-0.626656
C	-1.961990	0.294161	0.200339
N	-1.296846	1.497235	0.127800
C	-0.055498	1.712886	-0.625954
C	1.238676	1.551282	0.204281
N	1.950364	0.375085	0.130801
O	-2.983508	0.151271	0.885563
O	1.622793	2.507365	0.891125
O	1.356333	-2.651648	0.908068
C	-1.902154	2.643781	0.894623
C	-1.342197	-2.972675	0.898033
C	3.248101	0.328694	0.894468
H	2.421896	-1.345324	-0.934879
H	0.996475	-0.504311	-1.532887

H	-0.925481	-0.614385	-1.537971
H	-2.369308	-1.428519	-0.948189
H	-0.048235	2.763018	-0.948528
H	-0.060735	1.104081	-1.535824
C	-1.296552	2.779000	2.297575
H	-2.948120	2.328458	1.017739
C	-1.904807	3.919434	0.062221
H	3.499368	1.392461	1.013070
C	4.351190	-0.309660	0.060309
C	3.065813	-0.257818	2.299901
C	-2.445103	-3.610979	0.063827
C	-1.765075	-2.515082	2.299754
H	-0.547403	-3.721901	1.022693
C	-3.798474	-3.259642	0.200038
C	-4.778240	-3.881345	-0.583780
C	-4.421179	-4.863511	-1.513081
C	-3.075497	-5.222133	-1.657459
C	-2.099343	-4.600532	-0.873893
H	-4.087330	-2.482669	0.910273
H	-5.825888	-3.595373	-0.464928
H	-5.187592	-5.350794	-2.120013
H	-2.787466	-5.994099	-2.374858
H	-1.049926	-4.889678	-0.981658
C	4.734975	-1.652759	0.210193
C	5.762967	-2.191847	-0.573074
C	6.422595	-1.397622	-1.516169
C	6.048142	-0.057850	-1.675303
C	5.022622	0.478391	-0.891871
H	4.216400	-2.287006	0.931449
H	6.048278	-3.238350	-0.443293
H	7.227551	-1.818500	-2.122873
H	6.563167	0.572546	-2.403935
H	4.739479	1.528267	-1.010529
C	-0.929270	4.920035	0.205474
C	-0.980646	6.082138	-0.574042
C	-2.007301	6.262051	-1.506374
C	-2.984591	5.270959	-1.658832
C	-2.931438	4.112072	-0.879598
H	-0.114922	4.782843	0.919073
H	-0.213655	6.850008	-0.449430
H	-2.048718	7.171513	-2.109987
H	-3.794906	5.406110	-2.379016
H	-3.702222	3.344267	-0.992687
H	4.018282	-0.202198	2.848358
H	2.321479	0.336553	2.848850
H	2.728991	-1.301873	2.272955
H	-2.193466	-3.365948	2.850676
H	-0.881224	-2.163036	2.850686
H	-2.503212	-1.703738	2.266173
H	-1.820712	3.574084	2.849085
H	-1.434159	1.836384	2.846477

H -0.224656 3.012643 2.266597
66
9 E(gas)=-1477.02555971 G(gas)=-1476.56018 E(DMF)=-1477.04475022

O	1.491185	1.185452	2.716426
O	1.734939	-2.402987	-1.366848
N	1.320331	-0.866005	0.305745
N	-1.676299	1.108633	1.016146
N	-1.322212	-0.508024	-0.765344
C	-0.877801	0.219796	0.302763
C	0.422899	0.117136	0.791574
C	1.028712	-1.528787	-0.860628
C	-2.651408	-2.571105	-0.349926
C	3.814398	-0.596626	0.301253
C	0.556852	1.005952	1.919328
C	-2.690466	-1.111036	-0.805557
H	-3.261553	-0.560287	-0.044292
C	-2.619579	2.034526	0.308652
H	-2.969578	1.476908	-0.571758
C	4.249074	0.708957	0.591238
H	3.705650	1.294006	1.338677
C	-1.918721	3.287661	-0.220875
C	-3.346924	-0.882621	-2.170570
H	-3.414834	0.193361	-2.387148
H	-4.361875	-1.305277	-2.184339
H	-2.776330	-1.347881	-2.987764
C	-0.260338	-1.102205	-1.591869
H	-0.639079	-2.014354	-2.068635
C	-2.499447	-2.845083	1.021800
H	-2.434806	-2.014402	1.730230
C	-0.818088	1.683710	2.069788
H	-1.219004	1.485903	3.076177
H	-0.715210	2.771664	1.938424
C	2.599899	-1.137849	1.054847
H	2.499864	-0.519958	1.956952
C	-2.738218	-3.650165	-1.242840
H	-2.872737	-3.470705	-2.311477
C	-2.080181	4.553629	0.365663
H	-2.748928	4.680865	1.219457
C	5.363630	1.253402	-0.055177
H	5.689171	2.268167	0.186639
C	-2.511368	-5.228265	0.585267
H	-2.456393	-6.257289	0.946624
C	-3.825422	2.306240	1.211609
H	-4.321392	1.359362	1.467883
H	-4.552797	2.958308	0.706805
H	-3.530245	2.790085	2.154695
C	6.064644	0.496507	-1.000279
H	6.937628	0.917298	-1.505115
C	-1.055952	3.170225	-1.326160
H	-0.921972	2.194372	-1.799905
C	-2.429620	-4.159630	1.486945

H	-2.315517	-4.352274	2.555986
C	2.700345	-2.603587	1.493545
H	1.813675	-2.880889	2.083299
H	3.587162	-2.723331	2.133525
H	2.780122	-3.290905	0.643624
C	-1.398363	5.668983	-0.135431
H	-1.540075	6.645007	0.334207
C	-0.541568	5.536367	-1.231912
H	-0.009383	6.406254	-1.622533
C	-2.665831	-4.969699	-0.778920
H	-2.731531	-5.796661	-1.489359
C	4.527118	-1.350220	-0.646230
H	4.192322	-2.357174	-0.895243
C	-0.372170	4.280958	-1.827142
H	0.292067	4.167322	-2.686691
C	5.642605	-0.805701	-1.291701
H	6.184743	-1.403805	-2.028336
H	0.036829	-0.404472	-2.397391

83

16 E(gas)=-1953.39071123 G(gas)=-1952.804502 E($CHCl_3$)=-1953.40564146

C	-0.998030	0.349275	0.940694
N	-0.665867	1.646402	0.616066
C	0.419269	2.313297	1.346322
C	1.583509	2.726104	0.416145
C	-1.990641	-0.334794	-0.027845
N	2.315519	1.734194	-0.190891
C	2.161420	0.316743	0.085294
C	1.188639	-0.385694	-0.887902
N	0.833763	-1.671095	-0.548522
C	-0.248254	-2.329822	-1.286083
C	-1.444004	-2.740764	-0.393857
N	-2.191283	-1.754585	0.211898
O	0.723269	0.195517	-1.876379
O	-1.691623	-3.945869	-0.258836
O	-0.498541	-0.238244	1.907617
O	1.802184	3.927866	0.219505
C	1.417350	-2.406342	0.587806
C	3.306636	2.108573	-1.219124
C	-3.367959	-2.174172	1.033872
C	-1.279699	2.393443	-0.495395
H	0.733067	1.637718	2.153997
H	0.059964	3.251283	1.793371
H	-1.628604	-0.173853	-1.054492
H	-2.968350	0.171868	0.027612
H	1.799040	0.167019	1.112095
H	3.152861	-0.163080	0.036867
H	-0.547178	-1.652110	-2.098447
H	0.107964	-3.270524	-1.729954
C	-4.665303	-1.856664	0.290282
H	-3.271427	-3.268577	1.069582
C	-3.291608	-1.636369	2.464259

H	-0.655860	3.288899	-0.644924
H	-1.189545	1.816245	-1.429071
C	-2.718089	2.833729	-0.268563
H	3.138716	1.463898	-2.095170
H	3.076465	3.145052	-1.501835
C	4.741277	1.999608	-0.738544
H	0.801616	-3.311011	0.713300
C	2.869966	-2.823079	0.417925
H	1.279028	-1.826965	1.514248
C	5.628777	1.083833	-1.322398
C	6.957594	0.998368	-0.887821
C	7.411581	1.830033	0.139634
C	6.532502	2.748398	0.729147
C	5.208039	2.833373	0.293725
H	5.278018	0.434257	-2.129544
H	7.636324	0.279713	-1.352634
H	8.447671	1.766616	0.479734
H	6.884719	3.406346	1.527094
H	4.525137	3.558926	0.742963
C	-3.563413	3.007473	-1.375785
C	-4.868036	3.482898	-1.211225
C	-5.347874	3.787652	0.067081
C	-4.515327	3.610227	1.177521
C	-3.209137	3.137282	1.010677
H	-3.195879	2.766023	-2.377207
H	-5.513168	3.608928	-2.083516
H	-6.366671	4.158743	0.197579
H	-4.881720	3.845590	2.179430
H	-2.567175	2.998927	1.883843
C	-5.510131	-0.795421	0.649801
C	-6.681624	-0.534692	-0.073535
C	-7.027524	-1.335399	-1.164527
C	-6.195011	-2.401364	-1.530196
C	-5.026967	-2.658318	-0.809302
H	-5.266791	-0.163782	1.506736
H	-7.324687	0.297080	0.222438
H	-7.943363	-1.135920	-1.725475
H	-6.462834	-3.040194	-2.375130
H	-4.382697	-3.495891	-1.090055
C	3.693450	-2.917747	1.550812
C	5.012362	-3.369736	1.440034
C	5.528011	-3.728798	0.190296
C	4.717046	-3.630004	-0.945916
C	3.397188	-3.181310	-0.832640
H	3.296909	-2.633145	2.529619
H	5.640531	-3.433858	2.331287
H	6.558550	-4.078949	0.101315
H	5.112179	-3.907604	-1.925799
H	2.772476	-3.104754	-1.725737
H	-4.136645	-2.031355	3.047727
H	-2.351701	-1.950786	2.934292

H	-3.330095	-0.538260	2.514728

83

17 E(gas)=-1953.38882491 G(gas)=-1952.801607 E($CHCl_3$)=-1953.40357966

C	-1.168225	-0.252758	-0.937004
N	-0.704638	-1.519081	-0.663908
C	0.391869	-2.074809	-1.463968
C	1.645631	-2.426943	-0.620852
C	-2.157326	0.332109	0.096750
N	2.254141	-1.423317	0.090390
C	1.963460	-0.015323	-0.136145
C	0.989135	0.583638	0.902440
N	0.545306	1.856964	0.629065
C	-0.560449	2.416818	1.414750
C	-1.783115	2.766424	0.534667
N	-2.437208	1.742692	-0.109238
O	0.596003	-0.062678	1.881854
O	-2.115779	3.950884	0.407815
O	-0.784068	0.400733	-1.915479
O	2.026408	-3.603703	-0.601391
C	1.054537	2.672918	-0.488750
C	3.346395	-1.687654	1.083591
C	-3.485241	2.076226	-1.093427
C	-1.191756	-2.340477	0.459238
H	0.609151	-1.358698	-2.269143
H	0.088340	-3.026937	-1.922328
H	-1.748879	0.171203	1.104262
H	-3.108106	-0.225404	0.057623
H	1.535586	0.129232	-1.137684
H	2.910578	0.549537	-0.129416
H	-0.796062	1.695792	2.209934
H	-0.259486	3.365499	1.881580
C	-4.888819	1.771183	-0.605553
H	-3.377879	3.150362	-1.299014
H	-3.264793	1.521696	-2.018518
H	-0.500974	-3.195217	0.533701
H	-1.073991	-1.786063	1.403549
C	-2.610408	-2.868828	0.313277
H	3.336169	-0.782693	1.711003
C	3.055624	-2.863003	2.026717
C	4.721591	-1.755195	0.424052
H	0.382779	3.542527	-0.563979
C	2.483809	3.168613	-0.329779
H	0.932094	2.124925	-1.436439
C	5.665136	-0.749219	0.687348
C	6.941662	-0.790421	0.113282
C	7.289826	-1.843476	-0.737162
C	6.356070	-2.852136	-1.006663
C	5.083189	-2.812749	-0.430951
H	5.400208	0.075849	1.355378
H	7.661663	0.001694	0.331386
H	8.284505	-1.880427	-1.187306

H	6.622521	-3.678866	-1.669587
H	4.352725	-3.595019	-0.645451
C	-3.385697	-3.077816	1.464649
C	-4.667487	-3.629627	1.372790
C	-5.194259	-3.974867	0.123879
C	-4.431775	-3.763187	-1.030133
C	-3.148358	-3.215114	-0.936139
H	-2.980856	-2.803901	2.443154
H	-5.258757	-3.782032	2.278404
H	-6.196476	-4.402133	0.049567
H	-4.836395	-4.028846	-2.009434
H	-2.562301	-3.048644	-1.843113
C	-5.697059	0.843212	-1.278355
C	-7.001158	0.579905	-0.840740
C	-7.509157	1.242389	0.280108
C	-6.708926	2.170375	0.960101
C	-5.409495	2.433838	0.520489
H	-5.303077	0.324033	-2.156689
H	-7.618091	-0.145671	-1.375625
H	-8.525972	1.039442	0.623661
H	-7.104059	2.696781	1.832107
H	-4.789962	3.168758	1.040609
C	3.274244	3.363144	-1.473388
C	4.568540	3.882655	-1.367827
C	5.092884	4.209667	-0.112878
C	4.314888	4.012794	1.033620
C	3.019077	3.497022	0.925806
H	2.871689	3.103236	-2.456561
H	5.171163	4.024300	-2.267675
H	6.104492	4.612200	-0.028082
H	4.716766	4.265368	2.017531
H	2.420671	3.342338	1.826786
H	3.813488	-2.861016	2.824326
H	2.066281	-2.734734	2.489023
H	3.088395	-3.827111	1.508843

86

19 E(gas)=-1992.70969065 G(gas)=-1992.096146 E($CHCl_3$)=-1992.72402140

C	1.048086	-0.254012	0.995055
N	0.604098	-1.522355	0.692550
C	-0.516024	-2.095851	1.446562
C	-1.737329	-2.444486	0.555633
C	2.083077	0.333261	0.006564
N	-2.337626	-1.430892	-0.147652
C	-2.066724	-0.026301	0.120328
C	-1.058550	0.597684	-0.868802
N	-0.617846	1.860334	-0.545377
C	0.506024	2.437483	-1.287530
C	1.731236	2.767783	-0.401324
N	2.396554	1.736324	0.223552
O	-0.637300	-0.023448	-1.852819
O	2.075761	3.951281	-0.290109

O	0.609103	0.387717	1.956785
O	-2.099366	-3.625817	0.493234
C	-1.156417	2.649810	0.576760
C	-3.386191	-1.682184	-1.189920
C	3.611769	2.072859	1.027788
C	1.154043	-2.340057	-0.401465
H	-0.765631	-1.392657	2.253493
H	-0.221050	-3.052459	1.901440
H	1.699278	0.187229	-1.014160
H	3.017575	-0.249177	0.061923
H	-1.676905	0.099375	1.139572
H	-3.016617	0.532874	0.089629
H	0.756679	1.737433	-2.097447
H	0.215977	3.398629	-1.735658
C	4.872561	1.683381	0.255224
H	3.585660	3.170659	1.077176
C	3.528812	1.522607	2.452740
H	0.449724	-3.174934	-0.544552
H	1.126643	-1.771235	-1.343769
C	2.543277	-2.909142	-0.152572
H	-3.362039	-0.761846	-1.794120
C	-3.043933	-2.829857	-2.149430
C	-4.784939	-1.780647	-0.586975
H	-0.483609	3.514370	0.691610
C	-2.578918	3.155559	0.391521
H	-1.060975	2.077841	1.513210
C	-5.729480	-0.779276	-0.863743
C	-7.025946	-0.846644	-0.339164
C	-7.393632	-1.922125	0.474162
C	-6.459404	-2.927060	0.755825
C	-5.166396	-2.861352	0.229501
H	-5.449181	0.063058	-1.503351
H	-7.746190	-0.057372	-0.566628
H	-8.403914	-1.979546	0.885774
H	-6.741356	-3.771456	1.389432
H	-4.435812	-3.640988	0.453411
C	3.368306	-3.207086	-1.248703
C	4.621746	-3.797708	-1.060472
C	5.071203	-4.093549	0.231057
C	4.260056	-3.791004	1.330213
C	3.004434	-3.203852	1.139700
H	3.025286	-2.973206	-2.260655
H	5.251369	-4.019897	-1.924847
H	6.049986	-4.554313	0.380552
H	4.603322	-4.017392	2.342338
H	2.379332	-2.969074	2.004475
C	5.659966	0.570689	0.588644
C	6.798087	0.246948	-0.162230
C	7.168291	1.035256	-1.254315
C	6.393797	2.152444	-1.593350
C	5.258529	2.471909	-0.845678

H	5.399062	-0.052118	1.446952
H	7.396861	-0.623915	0.113824
H	8.058501	0.786122	-1.836294
H	6.681642	2.781982	-2.438676
H	4.659972	3.349027	-1.105696
C	-3.396595	3.330909	1.519050
C	-4.685689	3.858540	1.392397
C	-5.177476	4.213435	0.131817
C	-4.372297	4.035880	-0.998899
C	-3.081771	3.511655	-0.869833
H	-3.019405	3.049230	2.506303
H	-5.309733	3.984828	2.279866
H	-6.184972	4.622381	0.030310
H	-4.748739	4.310092	-1.987076
H	-2.461985	3.372169	-1.758773
H	4.407780	1.856808	3.023850
H	2.619266	1.887813	2.945104
H	3.501801	0.423457	2.488785
H	-3.768093	-2.814960	-2.977721
H	-2.037914	-2.678658	-2.566629
H	-3.086976	-3.807330	-1.658029

86

20 E(gas)=-1992.70340276 G(gas)=-1992.089315 E($CHCl_3$)=-1992.71782560

C	1.119084	-0.505506	0.875823
N	0.873651	-1.825232	0.551046
C	-0.224777	-2.511928	1.243983
C	-1.353462	-2.897010	0.257749
C	1.921931	0.306557	-0.162208
N	-2.181063	-1.902806	-0.216108
C	-2.148394	-0.517996	0.226532
C	-1.284898	0.389946	-0.683439
N	-0.965024	1.635668	-0.188648
C	-0.001732	2.452225	-0.939620
C	1.354428	2.743894	-0.243605
N	2.125246	1.696202	0.203014
O	-0.858201	-0.025507	-1.768966
O	1.709823	3.920593	-0.110051
O	0.627511	0.029462	1.875910
O	-1.459931	-4.075217	-0.104087
C	-1.703679	2.222205	0.959881
C	-3.162865	-2.235459	-1.268143
C	3.322156	2.000569	1.014785
C	1.664504	-2.663844	-0.401580
H	-0.557793	-1.861158	2.062562
H	0.127285	-3.460306	1.674477
H	1.367637	0.244951	-1.109343
H	2.904829	-0.159281	-0.342669
H	-1.758293	-0.465325	1.250819
H	-3.183782	-0.138003	0.259869
H	0.160318	1.938872	-1.899804
H	-0.419548	3.445382	-1.151886

C	4.617289	1.987854	0.223602
H	3.156488	2.993241	1.454635
H	3.362697	1.259826	1.828424
H	1.224888	-3.665254	-0.258236
C	1.450779	-2.338201	-1.890063
C	3.131428	-2.783187	0.033043
H	-3.016065	-1.531143	-2.101139
H	-2.904346	-3.245350	-1.615223
C	-4.597389	-2.194010	-0.777283
C	-0.888418	3.281937	1.716672
C	-3.082753	2.756371	0.555510
H	-1.862072	1.405064	1.678682
C	-5.512025	-1.273696	-1.310392
C	-6.840529	-1.245429	-0.867790
C	-7.267768	-2.139365	0.117937
C	-6.361688	-3.062116	0.657794
C	-5.037516	-3.089727	0.213745
H	-5.181469	-0.573601	-2.082975
H	-7.539441	-0.521550	-1.292826
H	-8.303300	-2.120320	0.464932
H	-6.692340	-3.768156	1.423193
H	-4.334835	-3.817875	0.627076
C	4.156474	-2.980703	-0.906673
C	5.480448	-3.178270	-0.496176
C	5.805278	-3.180721	0.862778
C	4.793630	-2.982419	1.809752
C	3.472264	-2.787464	1.398391
H	3.927660	-2.983525	-1.973281
H	6.259554	-3.328906	-1.246779
H	6.837415	-3.337328	1.183562
H	5.032527	-2.983920	2.875825
H	2.695143	-2.631987	2.149473
C	5.561235	0.965757	0.405225
C	6.758729	0.961730	-0.321525
C	7.023351	1.981928	-1.239615
C	6.085963	3.006365	-1.427942
C	4.892099	3.010873	-0.702627
H	5.361070	0.165275	1.123567
H	7.483363	0.159027	-0.167720
H	7.957696	1.982242	-1.805675
H	6.290665	3.809700	-2.139674
H	4.160365	3.810601	-0.839807
C	-4.058414	2.932627	1.552285
C	-5.320058	3.445527	1.240830
C	-5.630026	3.792965	-0.079349
C	-4.671126	3.613756	-1.080181
C	-3.408713	3.095523	-0.765684
H	-3.829098	2.658518	2.586473
H	-6.065617	3.568005	2.029743
H	-6.615266	4.194381	-0.325776
H	-4.903709	3.876268	-2.114827

H	-2.678556	2.945515	-1.563130
H	-1.481749	3.630787	2.573314
H	0.042267	2.841982	2.098569
H	-0.649618	4.154465	1.094918
H	1.705452	-3.217798	-2.499066
H	0.399250	-2.085414	-2.073882
H	2.068015	-1.498723	-2.238499

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28 E(gas)=-2989.06696872 G(gas)=-2988.138771 E($CHCl_3$)=-2989.08932239

O	-0.961648	0.791810	0.842989
N	-3.418414	-0.506392	0.823410
C	-3.182735	0.569854	-0.126360
H	-3.907126	1.374356	0.072378
H	-3.399419	0.235792	-1.154517
O	-0.126134	4.315701	0.133920
N	-1.350698	1.974600	-1.060706
C	-1.743492	1.133162	-0.054915
O	3.238925	2.231347	-1.615105
N	1.719807	3.058463	0.617989
C	-4.206044	-0.208375	2.051432
C	-3.485627	0.794773	2.957927
H	-4.235779	-1.177465	2.572636
O	1.259742	-1.171208	-0.776493
N	3.661503	0.146316	-0.766059
C	-5.641569	0.160642	1.676195
O	0.391615	-4.621231	-0.101428
N	1.594528	-2.292780	1.180065
C	-6.223410	1.391256	2.012861
H	-5.643216	2.140145	2.554788
O	-2.939557	-2.624638	1.561631
N	-1.389296	-3.294422	-0.660224
C	-7.551994	1.675437	1.667669
H	-7.985470	2.640526	1.939527
C	-8.317568	0.731130	0.980578
H	-9.353676	0.950759	0.713380
C	-7.746647	-0.501982	0.637378
H	-8.338380	-1.250237	0.104846
C	-6.423668	-0.782420	0.982697
H	-5.985786	-1.748362	0.717007
C	0.091056	2.264154	-1.108941
H	0.321099	2.714227	-2.084506
H	0.629458	1.310922	-1.048020
C	0.536120	3.289566	-0.048882
C	-2.234454	2.418064	-2.155672
C	2.354085	1.743917	0.601650
H	1.584679	0.976649	0.785868
H	3.059127	1.688704	1.440658
C	3.121752	1.410427	-0.700802
C	2.142095	4.142826	1.554000
C	3.094438	3.658628	2.656981
H	1.209792	4.479339	2.035050

C	2.730331	5.362720	0.841890
C	2.566606	6.625716	1.433853
H	1.966055	6.721103	2.343788
C	3.144615	7.764086	0.865555
H	3.001056	8.739648	1.336309
C	3.892818	7.654496	-0.312406
H	4.341544	8.542711	-0.763200
C	4.046065	6.402250	-0.915790
H	4.614415	6.309198	-1.844530
C	3.469961	5.260719	-0.344261
H	3.563383	4.291944	-0.841657
C	3.432147	-0.869714	0.249544
H	3.604745	-0.455203	1.254807
H	4.187016	-1.661361	0.126251
C	2.009739	-1.473514	0.161997
C	4.251613	-0.310757	-2.038459
C	0.150182	-2.582692	1.162009
H	-0.374280	-1.622816	1.086402
H	-0.142802	-3.043241	2.110363
C	-0.255667	-3.579329	0.062822
C	2.499390	-2.692616	2.298534
C	1.746112	-3.337577	3.471692
H	2.953867	-1.765314	2.693041
C	3.646707	-3.604270	1.858780
C	4.923291	-3.408971	2.409737
H	5.096258	-2.569458	3.091259
C	5.978086	-4.271095	2.092497
H	6.967447	-4.102794	2.523670
C	5.763952	-5.339577	1.215329
H	6.585296	-6.013943	0.962628
C	4.494409	-5.535275	0.659284
H	4.321728	-6.367521	-0.027313
C	3.436551	-4.675659	0.976461
H	2.443979	-4.825546	0.539654
C	-2.051120	-1.996150	-0.612461
H	-2.768651	-1.963689	-1.447469
H	-1.306129	-1.203230	-0.783132
C	-2.835248	-1.746601	0.700663
C	-1.790923	-4.232085	-1.720734
H	-1.588646	2.962903	-2.859870
H	-2.620510	1.543384	-2.710461
C	-3.400824	3.313438	-1.763477
C	-3.228603	4.380150	-0.865772
C	-4.302259	5.229088	-0.578225
C	-5.549778	5.029959	-1.182516
C	-5.724781	3.969252	-2.076718
C	-4.654385	3.114176	-2.361759
H	-2.248762	4.538002	-0.404787
H	-4.159251	6.058996	0.117873
H	-6.383635	5.697967	-0.955034
H	-6.695895	3.800366	-2.547133

H	-4.796652	2.280137	-3.056122
H	-1.524639	-3.804571	-2.704796
H	-1.161494	-5.123062	-1.576583
C	-3.260600	-4.602307	-1.712449
C	-3.985318	-4.609516	-2.915021
C	-5.325271	-5.012921	-2.943638
C	-5.960472	-5.406843	-1.761799
C	-5.248647	-5.391532	-0.555495
C	-3.908458	-4.995133	-0.528793
H	-3.491273	-4.302198	-3.841843
H	-5.872500	-5.015946	-3.889208
H	-7.006461	-5.721345	-1.778666
H	-5.740118	-5.693598	0.372330
H	-3.363733	-4.961822	0.416752
H	3.659423	-1.163262	-2.409193
H	4.126660	0.523502	-2.743063
C	5.713407	-0.692941	-1.914878
C	6.145619	-1.987665	-2.237132
C	7.500128	-2.332737	-2.149788
C	8.438216	-1.383435	-1.735262
C	8.016258	-0.087602	-1.408236
C	6.665085	0.254506	-1.498050
H	5.414348	-2.733618	-2.560926
H	7.819458	-3.346008	-2.403402
H	9.495424	-1.649357	-1.666949
H	8.746031	0.660364	-1.089425
H	6.339273	1.268271	-1.251040
H	3.274855	4.496600	3.344472
H	2.661044	2.832911	3.242715
H	4.075357	3.354198	2.260080
H	2.474155	-3.553156	4.266154
H	0.977242	-2.669780	3.887815
H	1.284892	-4.291005	3.177343
H	-4.036414	0.911414	3.903243
H	-2.474468	0.431460	3.179743
H	-3.387134	1.789036	2.496634

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29 E(gas)=-2989.06160335 G(gas)=-2988.13263 E($CHCl_3$)=-2989.08378567

O	-1.195705	-1.225569	-0.811379
N	-3.738366	-0.211049	-0.652006
C	-3.331679	-1.208465	0.327963
H	-3.992114	-2.080741	0.219965
H	-3.498054	-0.838516	1.350150
O	0.048632	-4.606455	-0.163147
N	-1.274190	-2.414751	1.123803
C	-1.852545	-1.636072	0.156163
O	3.348983	-2.361554	1.278735
N	1.710847	-3.173366	-0.829450
C	-4.386292	-0.709276	-1.879674
H	-3.786158	-1.547386	-2.268781
H	-4.333518	0.115400	-2.604526

O	0.840661	0.914923	0.715286
N	3.371628	-0.155782	0.636272
C	-5.825667	-1.137981	-1.670752
O	-0.318540	4.338813	0.161859
N	1.060528	2.147361	-1.186145
C	-6.234377	-2.447593	-1.960918
H	-5.499606	-3.172831	-2.321794
O	-3.658348	1.927538	-1.467259
N	-2.046957	2.901954	0.594743
C	-7.570900	-2.832760	-1.796517
H	-7.873389	-3.856598	-2.027775
C	-8.513250	-1.909622	-1.335228
H	-9.556416	-2.207159	-1.207118
C	-8.113892	-0.599282	-1.039061
H	-8.847500	0.128415	-0.684193
C	-6.781087	-0.216759	-1.206380
H	-6.472480	0.808540	-0.986653
C	0.189733	-2.522697	1.032287
H	0.571972	-2.899172	1.991809
H	0.593164	-1.513874	0.886546
C	0.633613	-3.522265	-0.050153
C	-1.941071	-3.081842	2.281311
C	2.271546	-1.826536	-0.831810
H	1.466703	-1.098315	-1.019433
H	2.979356	-1.771118	-1.674265
C	3.051512	-1.479155	0.469044
C	2.107604	-4.089367	-1.911298
H	1.742237	-3.691214	-2.875851
H	1.555428	-5.021798	-1.720009
C	3.596319	-4.354727	-2.006281
C	4.225216	-4.347538	-3.261663
H	3.641774	-4.099362	-4.153557
C	5.583369	-4.662095	-3.385084
H	6.056362	-4.654860	-4.369849
C	6.332293	-4.979444	-2.247691
H	7.393091	-5.223370	-2.339280
C	5.715783	-4.976748	-0.990226
H	6.296679	-5.218567	-0.097123
C	4.357887	-4.668619	-0.868030
H	3.885349	-4.641600	0.115672
C	3.018124	0.847942	-0.358773
H	3.186994	0.464193	-1.376625
H	3.701217	1.704376	-0.257881
C	1.551496	1.320260	-0.214490
C	3.960207	0.382314	1.906905
C	-0.397651	2.334963	-1.176519
H	-0.871439	1.345708	-1.161075
H	-0.686472	2.826550	-2.116314
C	-0.891227	3.266701	-0.052015
C	1.874093	2.672512	-2.298409
H	1.168718	3.174181	-2.977152

H	2.310692	1.838506	-2.877351
C	2.976336	3.651072	-1.919137
C	4.232413	3.551101	-2.537057
H	4.425375	2.738745	-3.244708
C	5.241590	4.479321	-2.256843
H	6.215204	4.388046	-2.743437
C	5.001880	5.515139	-1.348313
H	5.787487	6.240355	-1.124419
C	3.751181	5.616599	-0.725909
H	3.557550	6.426980	-0.019207
C	2.738697	4.693823	-1.007631
H	1.758535	4.773234	-0.526667
C	-2.504966	1.516565	0.632729
H	-3.103808	1.384784	1.548294
H	-1.634088	0.850588	0.729973
C	-3.355388	1.107617	-0.595112
C	-2.712559	3.881523	1.502093
H	-1.219607	-3.867001	2.558874
C	-2.057807	-2.140911	3.490103
C	-3.213256	-3.841670	1.902863
C	-3.134799	-4.821132	0.894331
C	-4.257244	-5.582008	0.560143
C	-5.472874	-5.383929	1.228412
C	-5.556639	-4.418197	2.234141
C	-4.432009	-3.652916	2.570589
H	-2.179741	-4.977624	0.383080
H	-4.179365	-6.343089	-0.219854
H	-6.348644	-5.982099	0.967494
H	-6.498634	-4.255906	2.762577
H	-4.517613	-2.906000	3.362360
H	-3.691869	3.418507	1.715041
C	-1.956725	4.006321	2.832924
C	-3.025935	5.203635	0.796571
C	-3.663043	5.175424	-0.456959
C	-4.027915	6.363147	-1.095873
C	-3.772727	7.600203	-0.491443
C	-3.142918	7.635928	0.755449
C	-2.772517	6.446167	1.393749
H	-3.850751	4.211288	-0.938369
H	-4.518262	6.321442	-2.071612
H	-4.060353	8.528413	-0.990614
H	-2.931598	8.594287	1.235929
H	-2.269292	6.499149	2.360296
H	3.680695	1.447158	1.883692
C	3.333006	-0.192734	3.185785
C	5.484351	0.328048	1.903301
C	6.219878	1.521136	1.980758
C	7.619666	1.503204	2.001934
C	8.302159	0.284957	1.942098
C	7.577019	-0.910979	1.864248
C	6.179671	-0.893221	1.848475

H 5.690650 2.477790 2.026842
H 8.174582 2.442321 2.062132
H 9.394284 0.265588 1.955909
H 8.105201 -1.866254 1.817132
H 5.614059 -1.825297 1.789019
H 3.670096 0.417595 4.037222
H 2.237136 -0.130208 3.123019
H 3.625125 -1.233787 3.356382
H -2.373891 -2.697591 4.384592
H -1.079686 -1.686481 3.702129
H -2.777728 -1.325467 3.325769
H -2.537216 4.594647 3.558875
H -1.793141 3.008117 3.265676
H -0.979251 4.481735 2.681063
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36 E(gas)-4142.71316979 G(gas)=-4141.362544 E(Tol)=-4142.73055884
O -1.442403 -1.241853 0.340336
O 3.490017 0.227410 -1.886488
O -3.490075 -0.226692 -1.886343
O 1.442592 1.241840 0.340486
O 0.624077 -3.721026 1.710434
O 4.183388 -3.398538 -0.322911
O -4.183211 3.398662 -0.322239
O -0.623943 3.720784 1.710891
N -3.888103 -2.068344 -0.602862
N 0.215383 2.803607 -0.783722
N -0.215369 -2.803612 -0.784049
N -2.538810 2.460465 1.731710
N 2.539003 -2.460788 1.731237
N 3.888200 2.068731 -0.602584
N -5.290364 1.405284 -0.587135
N 5.290243 -1.404989 -0.587700
C -1.397655 -2.191036 -0.452658
C 1.397743 2.191134 -0.452360
C -1.361607 2.892631 1.166100
C 0.997438 -2.246257 -0.187412
H 0.845501 -1.166634 -0.032527
H 1.825246 -2.375009 -0.898501
C -0.997364 2.246142 -0.187065
H -0.845347 1.166523 -0.032221
H -1.825198 2.374860 -0.898124
C -5.343461 -0.030963 -0.347022
H -6.288014 -0.412928 -0.762237
H -5.390195 -0.245379 0.729478
C 3.440982 -1.538265 1.058322
H 4.083908 -1.089419 1.832342
H 2.873691 -0.700653 0.620447
C -3.440882 1.538128 1.058674
H -4.083782 1.089165 1.832643
H -2.873632 0.700584 0.620605
C 4.158916 0.780029 -1.008912

C	5.343404	0.031187	-0.347204
H	6.288016	0.413215	-0.762221
H	5.390016	0.245327	0.729357
C	-2.681809	-2.663119	-1.173834
H	-2.599196	-2.350647	-2.224550
H	-2.779770	-3.755173	-1.153754
C	-4.327989	2.209425	-0.020429
C	-4.158904	-0.779569	-1.008864
C	4.328053	-2.209317	-0.020959
C	1.361732	-2.892845	1.165676
C	2.681862	2.663649	-1.173315
H	2.599342	2.351789	-2.224217
H	2.779660	3.755708	-1.152584
C	2.957457	-3.052911	3.026445
C	4.101383	-4.059057	2.850733
H	2.063775	-3.614240	3.344913
C	-4.570972	-2.822765	0.487164
C	-4.175921	-2.365507	1.901039
H	-4.156020	-3.839389	0.378626
H	3.840032	-4.777613	2.064324
C	0.066097	4.058509	-1.579486
C	0.568872	5.308694	-0.836956
H	-1.028116	4.175845	-1.647982
C	-6.074489	-2.981677	0.235155
C	-7.019427	-2.860497	1.264664
C	-8.380262	-3.085913	1.019421
C	-0.066189	-4.058448	-1.579977
C	-0.568925	-5.308672	-0.837522
H	1.028013	-4.175797	-1.648568
C	-8.817010	-3.441333	-0.258711
C	4.571151	2.822876	0.487581
C	4.175959	2.365460	1.901368
H	4.156381	3.839587	0.379171
C	-7.882588	-3.568347	-1.294174
C	3.212446	-1.956729	4.062038
C	4.341586	-1.956372	4.896526
C	4.518900	-0.962199	5.868503
C	-2.957172	3.052417	3.027037
C	-4.100942	4.058775	2.851525
H	-2.063400	3.613528	3.345628
C	-6.204769	1.998016	-1.603098
C	-5.934586	1.465416	-3.012861
H	-5.935308	3.065024	-1.587865
C	6.204671	-1.997494	-1.603762
C	5.934662	-1.464399	-3.013366
H	5.935074	-3.064474	-1.588894
C	0.552668	3.908292	-3.025909
C	1.259478	4.928332	-3.680781
C	1.640574	4.792399	-5.022103
C	-3.212320	1.956057	4.062402
C	-4.341617	1.955509	4.896659

C	-4.519075	0.961174	5.868457
C	-7.653169	1.879763	-1.127806
C	-8.609992	1.088806	-1.780379
C	-9.927073	1.017285	-1.305814
C	6.074703	2.981611	0.235689
C	7.653049	-1.879539	-1.128336
C	8.609970	-1.088426	-1.780575
C	9.927023	-1.017158	-1.305901
C	7.019585	2.860135	1.265216
C	8.380455	3.085443	1.020065
C	8.817294	3.441046	-0.257986
C	7.882933	3.568348	-1.293467
C	-0.552917	-3.908025	-3.026326
C	-1.260538	-4.927593	-3.681035
C	-1.641826	-4.791412	-5.022280
C	6.527091	3.341388	-1.047370
H	6.699883	2.587112	2.272161
H	9.099552	2.979580	1.835375
H	9.877974	3.617795	-0.448443
C	1.316423	3.633715	-5.731735
C	0.605015	2.612056	-5.090444
C	0.225732	2.749469	-3.753518
H	1.519500	5.843308	-3.145854
H	8.211695	3.849189	-2.296789
H	-6.568363	1.997104	-3.738712
H	5.804734	3.436823	-1.861907
H	-6.137168	0.387991	-3.108387
H	-4.880765	1.621946	-3.272657
H	-4.274076	4.609548	3.788226
H	-5.044084	3.570748	2.561522
H	-3.839562	4.777323	2.065116
H	3.089834	2.221316	1.952041
H	4.462690	3.129468	2.639101
H	4.655119	1.421650	2.198085
H	4.880945	-1.621113	-3.273482
H	6.568753	-1.995598	-3.739298
H	6.136955	-0.386875	-3.108423
H	4.274673	-4.609875	3.787382
H	5.044424	-3.570851	2.560712
H	-4.462414	-3.129768	2.638606
C	10.307434	-1.741325	-0.173992
C	3.569746	0.051227	6.020627
C	2.440600	0.065379	5.191357
C	2.265585	-0.927502	4.225271
H	5.095221	-2.739861	4.798836
H	5.405213	-0.984306	6.507243
H	3.706131	0.826224	6.778249
H	1.692141	0.853726	5.298561
H	1.387413	-0.903734	3.575777
C	9.361860	-2.539523	0.484012
C	8.050635	-2.605449	0.010244

H	8.335075	-0.524916	-2.674166
H	10.656937	-0.395002	-1.829034
H	11.334967	-1.690385	0.193085
H	9.651924	-3.118730	1.363928
H	7.318044	-3.238017	0.518960
C	-1.317048	-3.632949	-5.731981
C	-0.604818	-2.611756	-5.090851
C	-0.225353	-2.749414	-3.754004
H	-1.521049	-5.842385	-3.146027
H	-2.194779	-5.597263	-5.510722
H	-1.614492	-3.524812	-6.777295
H	-0.341019	-1.703124	-5.636352
H	0.323494	-1.943014	-3.262246
C	-10.307602	1.741027	-0.173676
C	-9.362127	2.539067	0.484663
C	-8.050879	2.605250	0.011001
H	-8.335006	0.525656	-2.674167
H	-10.656915	0.395264	-1.829210
H	-11.335155	1.689897	0.193320
H	-9.652294	3.117946	1.364762
H	-7.318361	3.237688	0.519984
C	-3.569897	-0.052213	6.020621
C	-2.440583	-0.066180	5.191560
C	-2.265429	0.926849	4.225664
H	-5.095281	2.738965	4.798950
H	-5.405517	0.983147	6.507022
H	-3.706371	-0.827334	6.778100
H	-1.692107	-0.854507	5.298807
H	-1.387131	0.903237	3.576332
C	-6.526781	-3.341278	-1.047984
H	-6.699796	-2.587625	2.271674
H	-9.099398	-2.980279	1.834726
H	-9.877660	-3.618170	-0.449252
H	-8.211280	-3.849041	-2.297560
H	-5.804382	-3.436482	-1.862509
H	2.192887	5.598619	-5.510661
H	1.613724	3.525766	-6.777109
H	0.341723	1.703232	-5.635871
H	-0.322458	1.942699	-3.261639
H	-4.655377	-1.421920	2.197986
H	-3.089834	-2.221088	1.951731
H	-1.665800	-5.395313	-0.833815
H	-0.221064	-5.264314	0.202157
H	-0.165576	-6.216302	-1.310758
H	0.164572	6.216307	-1.309416
H	1.665701	5.395977	-0.834334
H	0.221967	5.263717	0.203017

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37 E(gas)=-4142.70983360 G(gas)=-4141.359871 E(Tol)=-4142.72645731

O	1.356920	-1.431955	0.177712
O	-3.728849	0.957755	-1.884123

O	3.728832	-0.957704	-1.884452
O	-1.357060	1.432232	0.178201
O	-0.796595	-3.630961	1.429075
O	-4.768237	-2.820531	-0.359348
O	4.768359	2.820506	-0.359556
O	0.796526	3.630696	1.429491
N	3.697479	-2.685971	-0.396654
N	-0.023466	2.817017	-1.047826
N	0.023263	-2.816939	-1.048016
N	2.723476	2.386242	1.429845
N	-2.723326	-2.386178	1.430027
N	-3.697659	2.686026	-0.396343
N	5.440272	0.624034	-0.445699
N	-5.440182	-0.624064	-0.445536
C	1.240852	-2.399536	-0.582927
C	-1.241042	2.399686	-0.582592
C	1.532660	2.798711	0.888893
C	-1.155551	-2.171392	-0.481860
H	-0.939923	-1.100145	-0.347867
H	-1.989347	-2.267408	-1.192772
C	1.155376	2.171447	-0.481732
H	0.939781	1.100176	-0.347837
H	1.989143	2.267556	-1.192668
C	5.238538	-0.750040	-0.002865
H	6.204032	-1.275617	-0.074093
H	4.961775	-0.771739	1.060068
C	-3.458216	-1.236549	0.924506
H	-3.859156	-0.700448	1.801480
H	-2.784739	-0.520678	0.429304
C	3.458275	1.236578	0.924279
H	3.859145	0.700357	1.801219
H	2.784735	0.520828	0.428992
C	-4.159436	1.476755	-0.850994
C	-5.238586	0.749995	-0.002578
H	-6.204135	1.275481	-0.073778
H	-4.961834	0.771666	1.060355
C	2.494495	-3.194968	-1.041148
H	2.615277	-3.109964	-2.130880
H	2.393112	-4.259861	-0.787234
C	4.617697	1.640628	-0.026424
C	4.159339	-1.476717	-0.851302
C	-4.617619	-1.640639	-0.026225
C	-1.532742	-2.798832	0.888714
C	-2.494695	3.195090	-1.040831
H	-2.615472	3.110092	-2.130561
H	-2.393340	4.259984	-0.786899
C	-3.377805	-3.073592	2.582882
H	-4.448079	-2.856522	2.433317
C	-3.256278	-4.605137	2.558911
C	4.198417	-3.393879	0.810525
H	5.149441	-2.906125	1.070284

C	3.250338	-3.250330	2.007574
H	-2.236891	-4.939554	2.776283
C	0.177633	3.936905	-2.002405
H	-0.827552	4.306948	-2.245770
C	0.946207	5.106279	-1.373172
C	4.558010	-4.840573	0.445042
C	5.550326	-5.069341	-0.525413
C	5.919063	-6.366434	-0.886093
C	-0.177902	-3.937020	-2.002412
H	0.827248	-4.307389	-2.245412
C	-0.946948	-5.106007	-1.372986
C	5.297632	-7.466268	-0.279979
C	-4.198816	3.394037	0.810692
H	-5.149793	2.906166	1.070430
C	-3.250813	3.250757	2.007823
C	4.309699	-7.253029	0.683982
C	-2.986817	-2.470196	3.928219
C	-3.988600	-2.041510	4.813502
C	-3.662666	-1.524873	6.073342
C	3.378092	3.073618	2.582676
H	4.448348	2.856655	2.432862
C	3.256414	4.605152	2.558800
C	6.484257	0.817217	-1.505898
H	6.651463	-0.202595	-1.886038
C	6.011963	1.645639	-2.709098
C	-6.484155	-0.817120	-1.505763
H	-6.651056	0.202685	-1.886055
C	-6.012098	-1.645812	-2.708862
C	0.767927	3.422719	-3.322972
C	0.045620	2.471026	-4.065400
C	0.515680	2.017445	-5.299056
C	2.987414	2.470091	3.928028
C	3.989383	2.041107	4.812966
C	3.663729	1.524335	6.072822
C	7.811235	1.290057	-0.918844
C	8.933592	0.448119	-0.971958
C	10.168772	0.857708	-0.454886
C	-4.558585	4.840615	0.444995
C	-7.811229	-1.289629	-0.918678
C	-8.933563	-0.447700	-0.972223
C	-10.168798	-0.857105	-0.455129
C	-5.550930	5.069124	-0.525489
C	-5.919781	6.366118	-0.886404
C	-5.298437	7.466116	-0.280501
C	-4.310486	7.253140	0.683502
C	-0.767816	-3.423046	-3.323232
C	-0.044973	-2.472052	-4.066055
C	-0.514841	-2.018691	-5.299867
C	-3.944427	5.949214	1.045094
H	-6.031798	4.215355	-1.011150
H	-6.695465	6.521497	-1.639754

H	-5.584697	8.482151	-0.560666
C	1.727379	2.498520	-5.811119
C	2.461000	3.431904	-5.076021
C	1.982213	3.893548	-3.842722
H	-0.892550	2.072097	-3.669918
H	-3.818512	8.103251	1.161473
H	5.888852	2.703313	-2.455262
H	-3.171683	5.803671	1.801518
H	5.055491	1.250037	-3.078331
H	6.764656	1.554484	-3.506974
H	2.237022	4.939471	2.776295
H	3.559249	4.987927	1.573582
H	3.939378	5.015804	3.317876
H	-2.265723	3.699669	1.816077
H	-3.075657	2.189564	2.225408
H	-3.686743	3.729150	2.897660
H	-5.889155	-2.703481	-2.454931
H	-5.055620	-1.250417	-3.078308
H	-6.764870	-1.554633	-3.506664
H	-3.559257	-4.987848	1.573715
H	-3.939179	-5.015742	3.318069
H	2.265201	-3.699139	1.815828
C	-10.295616	-2.121604	0.126696
C	-2.322887	-1.426772	6.460421
C	-1.315789	-1.846302	5.581584
C	-1.642476	-2.365656	4.325803
H	-5.038795	-2.118639	4.514789
H	-4.455907	-1.196568	6.749314
H	-2.063363	-1.024040	7.442271
H	-0.266706	-1.767024	5.875744
H	-0.859636	-2.697602	3.640576
C	-9.183161	-2.971105	0.182539
C	-7.951499	-2.562904	-0.336960
H	-8.842659	0.540756	-1.433616
H	-11.030244	-0.187153	-0.508019
H	-11.256644	-2.446206	0.532077
H	-9.277245	-3.962866	0.631611
H	-7.082974	-3.223221	-0.292346
C	-1.726852	-2.499254	-5.811664
C	-2.460982	-3.431942	-5.076196
C	-1.982398	-3.893383	-3.842749
H	0.893432	-2.073514	-3.670747
H	0.070943	-1.290586	-5.864943
H	-2.096349	-2.145241	-6.776736
H	-3.411641	-3.808312	-5.460685
H	-2.569737	-4.626469	-3.287926
C	10.295527	2.122419	0.126490
C	9.183066	2.971936	0.181888
C	7.951455	2.563549	-0.337598
H	8.842744	-0.540510	-1.432989
H	11.030224	0.187739	-0.507450

H	11.256514	2.447174	0.531849
H	9.277096	3.963864	0.630603
H	7.082934	3.223885	-0.293295
C	2.324044	1.426398	6.460276
C	1.316765	1.846201	5.581776
C	1.643172	2.365693	4.325979
H	5.039505	2.118133	4.513969
H	4.457117	1.195811	6.748513
H	2.064728	1.023586	7.442148
H	0.267750	1.767036	5.876213
H	0.860193	2.697809	3.640992
C	3.943756	-5.949008	1.045341
H	6.031242	-4.215701	-1.011251
H	6.694727	-6.522018	-1.639421
H	5.583798	-8.482381	-0.559957
H	3.817655	-8.103013	1.162108
H	3.171015	-5.803257	1.801725
H	-0.069733	1.288777	-5.863793
H	2.097053	2.144324	-6.776054
H	3.411422	3.808705	-5.460682
H	2.569213	4.627162	-3.288242
H	3.075350	-2.189087	2.225058
H	3.686163	-3.728680	2.897487
H	-1.986323	-4.838207	-1.133032
H	-0.461008	-5.412159	-0.438621
H	-0.966437	-5.958893	-2.067715
H	1.985674	4.838927	-1.133131
H	0.460086	5.412471	-0.438915
H	0.965353	5.959086	-2.068016

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[**28a**·Na]$^+$ E(gas)=-3151.30540577 G(gas)=-3150.376505 E($CHCl_3$)=-3151.35323855

C	-0.984836	2.863756	-0.223088
N	-0.049253	3.748491	0.227715
C	1.314428	3.549320	-0.262547
C	1.973339	2.291028	0.353349
C	-2.419689	2.932228	0.356149
C	-1.961320	-2.280769	-0.207380
N	-3.196467	-1.897544	0.228163
C	-3.699072	-0.626225	-0.291263
C	-2.951247	0.585182	0.317375
N	-3.247686	1.836557	-0.147317
O	-1.346700	-1.617773	-1.059787
O	-2.098139	0.421954	1.203720
O	-0.695334	1.999394	-1.067239
O	1.391094	1.641605	1.235853
C	-3.988622	-2.614941	1.268775
C	-4.095470	2.120421	-1.320658
C	-0.299927	4.793800	1.262792
C	2.965616	-0.561028	-0.177036
N	3.256094	-1.813739	0.278451
C	2.412766	-2.897130	-0.225451

C	0.984806	-2.844539	0.371712
C	3.729150	0.647662	0.418002
N	0.052760	-3.734612	-0.087670
C	-1.314817	-3.550822	0.398474
N	3.208955	1.913604	-0.097672
O	2.086292	-0.379005	-1.036152
O	0.693957	-2.011316	1.243731
C	0.241458	-4.606422	-1.264695
C	3.868884	2.480232	-1.292105
C	4.278981	-2.124170	1.317768
H	1.896532	4.452974	-0.027780
H	1.279489	3.438336	-1.355830
H	-2.916231	3.876551	0.088160
H	-2.370868	2.868914	1.452382
H	-3.563411	-0.618148	-1.382505
H	-4.777175	-0.571817	-0.078681
H	2.905053	-3.851674	0.013370
H	2.347265	-2.810388	-1.319632
H	4.801542	0.603495	0.177651
H	3.618866	0.639622	1.511554
H	-1.293712	-3.459471	1.493511
H	-1.886104	-4.454310	0.139142
Na	0.005012	0.009239	0.092256
C	5.363055	2.681109	-1.116010
C	-5.415631	-2.857863	0.766010
C	5.232700	-3.208300	0.803907
C	0.230751	6.146166	0.777420
C	-5.091199	3.242847	-1.085647
C	-0.323186	-6.002545	-1.073976
C	1.230342	6.854585	1.460108
C	-0.310710	6.708908	-0.392770
C	1.682360	8.092493	0.982880
C	0.137342	7.941738	-0.870205
C	1.139179	8.638478	-0.182152
C	-5.189752	4.298708	-2.003704
C	-5.955562	3.221559	0.021736
C	-6.138209	5.313021	-1.824451
C	-6.898209	4.236216	0.205730
C	-6.993158	5.284094	-0.718885
C	5.869445	3.453755	-0.057223
C	6.259988	2.123926	-2.039422
C	7.244824	3.661025	0.074673
C	7.638234	2.335746	-1.912440
C	8.132919	3.103466	-0.854338
C	-5.606327	-3.614684	-0.404517
C	-6.545657	-2.372254	1.440039
C	-6.888968	-3.875619	-0.889707
C	-7.834602	-2.631742	0.954524
C	-8.010225	-3.382295	-0.209917
C	5.955188	-2.971670	-0.380069
C	5.432992	-4.421743	1.477976

C	6.848116	-3.921449	-0.878888
C	6.328934	-5.377394	0.979058
C	7.037341	-5.131510	-0.199062
C	0.052828	-6.789783	0.027588
C	-1.203393	-6.540784	-2.024266
C	-0.444561	-8.087044	0.174923
C	-1.697894	-7.842907	-1.881421
C	-1.320424	-8.617648	-0.780892
H	1.661077	6.451866	2.378533
H	-1.091839	6.171868	-0.938226
H	2.458418	8.631437	1.530415
H	-0.299489	8.365203	-1.777118
H	1.488628	9.604505	-0.551831
H	-4.524330	4.323671	-2.871456
H	-5.887698	2.406544	0.747386
H	-6.206541	6.127015	-2.549102
H	-7.565411	4.208156	1.069825
H	-7.731900	6.075202	-0.576132
H	5.181456	3.892463	0.670603
H	5.876010	1.525097	-2.870290
H	7.626680	4.265234	0.900326
H	8.324522	1.899765	-2.641363
H	9.207148	3.269584	-0.752430
H	-4.737539	-4.002753	-0.943516
H	-6.432254	-1.795175	2.359200
H	-7.016728	-4.470627	-1.796500
H	-8.702295	-2.248248	1.495414
H	-9.014453	-3.587604	-0.585837
H	5.813595	-2.031306	-0.920024
H	4.898407	-4.631838	2.406054
H	7.403438	-3.716632	-1.796675
H	6.473545	-6.315124	1.519676
H	7.737230	-5.875012	-0.585492
H	0.735292	-6.381192	0.777771
H	-1.499619	-5.938053	-2.887586
H	-0.143799	-8.690155	1.034247
H	-2.378942	-8.250588	-2.631324
H	-1.705375	-9.632905	-0.666837
H	-0.222514	-4.127370	-2.144239
C	-3.886778	-1.921488	2.632315
H	-3.522418	-3.606709	1.360737
C	3.629550	-2.413458	2.675740
H	4.878950	-1.208762	1.422453
C	0.202188	4.352707	2.642614
H	-1.393657	4.894475	1.319229
H	3.397238	3.446366	-1.513551
H	3.675613	1.818932	-2.154325
H	-3.445809	2.364098	-2.178958
H	-0.073287	5.098337	3.402605
H	-0.241140	3.386499	2.915700
H	1.293745	4.224771	2.663385

H	4.401958	-2.532566	3.449365
H	2.966158	-1.586748	2.960502
H	3.020449	-3.328579	2.654613
H	-4.392209	-2.522654	3.402051
H	-2.833977	-1.794398	2.915155
H	-4.343542	-0.921611	2.621141
H	1.318407	-4.676006	-1.465806
H	-4.637307	1.201958	-1.581330

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[**28b**·Na]$^+$ E(gas)=-3151.28287101 G(gas)=-3150.354805 E($CHCl_3$)=-3151.33076505

C	-2.811372	1.156428	0.431610
N	-3.728907	0.266423	-0.051576
C	0.885634	3.713589	0.493932
C	-2.406687	-1.828632	-0.036296
O	1.769844	1.355579	1.375074
N	-1.637754	3.345367	0.379065
C	-3.659584	-1.089874	0.493138
C	2.406641	1.855660	0.433132
N	2.094855	3.095262	-0.050466
C	-0.380526	2.998088	-0.035961
C	-2.712893	2.553007	-0.228710
C	-4.493634	0.456765	-1.298156
C	-0.854509	-3.625657	-0.227524
C	0.403365	-3.012390	0.433783
N	1.633300	-3.362603	-0.048221
C	1.851236	-4.119990	-1.294829
C	2.642378	3.661832	-1.297266
C	2.772766	-2.624215	0.496980
O	-0.237071	2.085052	-0.870197
O	1.924392	-0.838053	-0.868208
C	2.786591	-1.170268	-0.033648
O	-1.687130	-1.247935	-0.870106
C	3.567294	1.072068	-0.226456
C	4.772785	-0.303999	1.436250
C	-2.123906	4.283075	1.435876
C	-2.648984	-3.981066	1.434969
N	3.715779	-0.255100	0.381579
N	-2.078817	-3.090879	0.379192
O	-2.059699	0.855489	1.373587
O	0.287394	-2.210831	1.375570
H	-4.581733	-1.617852	0.213090
H	-0.869129	-4.720640	-0.122177
H	-3.616988	-1.022355	1.584376
H	-2.501603	2.428412	-1.299374
H	-3.653730	3.113486	-0.124032
H	0.889979	4.776118	0.213727
H	0.922690	3.642901	1.585186
H	4.522924	1.606789	-0.121197
H	3.354466	0.951260	-1.297255
H	3.691258	-3.159208	0.218334
H	2.691513	-2.620097	1.588133

H	-0.851381	-3.381102	-1.298363
Na	-0.000334	-0.000235	0.359326
C	7.802876	-1.073073	-0.802418
C	8.785728	-0.260720	-0.225620
C	2.955671	-6.098152	-0.134107
C	2.998371	5.133682	-1.183596
C	2.557414	6.039167	-2.159833
C	3.805652	5.604200	-0.134363
C	2.920157	7.389892	-2.095166
C	4.162918	6.953247	-0.064517
C	3.722483	7.849471	-1.046712
C	-2.849567	5.476695	0.814295
C	-4.053745	5.922973	1.380905
C	-2.317731	6.173777	-0.281106
C	-4.710326	7.047898	0.870532
C	-2.973197	7.297186	-0.794827
C	-5.945968	0.028123	-1.184559
C	-6.508909	-0.806573	-2.161192
C	-6.757495	0.490910	-0.135176
C	-7.859763	-1.168792	-2.096757
C	-8.104150	0.124577	-0.065465
C	-8.659371	-0.704866	-1.048124
C	-3.547275	-3.331000	2.494637
C	4.660905	-1.407835	2.495141
C	-4.170214	7.738343	-0.219329
C	-4.188090	-5.091090	-0.285344
C	-3.110647	-6.471111	1.380005
H	-5.886828	-1.170818	-2.983820
H	-6.329170	1.137620	0.635283
H	-8.286058	-1.815680	-2.866311
H	-8.725413	0.491264	0.754402
H	-9.712523	-0.987684	-0.994837
H	-2.433681	-6.574805	2.233631
H	-3.582140	-8.579217	1.320104
H	-5.505922	-6.116359	-1.655716
H	-5.127075	-8.356832	-0.627369
H	-4.351242	-4.116532	-0.752166
H	-4.682114	8.614446	-0.622187
H	-2.548743	7.829846	-1.648504
H	-5.647174	7.381648	1.321484
H	-4.481955	5.385825	2.232851
H	4.005065	8.902679	-0.993259
H	4.791857	7.307181	0.755109
H	2.573412	8.082949	-2.864481
H	4.151303	4.909468	0.635813
H	1.930513	5.683231	-2.982456
H	9.799740	-0.255565	-0.630151
H	8.049437	-1.704171	-1.658903
H	9.220102	1.190659	1.319568
H	5.740793	-1.707430	-0.753513
H	6.910698	1.179947	2.234726

H	5.719452	-7.909745	-0.992895
H	3.941765	-7.802236	0.753405
H	5.722020	-6.257068	-2.861506
H	2.179938	-6.054257	0.635049
C	-4.834907	-6.218988	-0.800235
H	-1.390238	5.831328	-0.746770
H	-1.759656	-4.336981	1.982759
H	4.636319	0.643685	1.984840
H	-2.875373	3.689556	1.984236
H	-4.449582	1.520799	-1.566157
C	-3.758064	-7.600748	0.868350
C	-4.623123	-7.476527	-0.223655
C	2.950208	-5.161839	-1.181568
C	3.956097	-5.228021	-2.156948
C	-3.321643	-5.204830	0.812350
C	4.947518	-6.214483	-2.092912
C	3.948433	-7.079090	-0.064906
C	4.946188	-7.140852	-1.045974
C	6.168510	-0.273165	0.812389
C	7.159344	0.542900	1.380299
H	3.959829	-4.505746	-2.978338
C	6.503023	-1.078716	-0.286579
H	0.908169	-4.615170	-1.561994
H	3.541352	3.090911	-1.565194
H	-3.747590	-4.093389	3.260846
H	-3.046093	-2.486158	2.987905
H	-4.521120	-3.016660	2.098101
H	5.422562	-1.200614	3.260246
H	3.679545	-1.397017	2.990201
H	4.875047	-2.407991	2.097386
C	8.460916	0.548900	0.867661
H	-3.995674	-0.100183	-2.110642
H	2.083495	-3.410420	-2.107772
C	-1.111413	4.737370	2.494488
H	1.910881	3.509654	-2.109654
H	-0.629039	3.881677	2.987812
H	-1.671600	5.291789	3.260808
H	-0.353361	5.424160	2.096919

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[**30a**·Na]$^{+}$ E(gas)=-3269.24411318

C	-2.913187	-0.801108	-0.283676
N	-3.701077	0.200757	0.210005
C	-3.456832	1.530145	-0.352737
C	-2.120914	2.120996	0.166884
C	-3.040119	-2.217002	0.324108
C	2.150658	-2.174575	-0.277716
N	1.678963	-3.350935	0.232143
C	0.405600	-3.811123	-0.325974
C	-0.777798	-2.952049	0.190212
N	-2.056845	-3.134705	-0.265469
O	1.541896	-1.582796	-1.185167

O	-0.548771	-2.077680	1.045230
O	-2.091942	-0.581946	-1.190031
O	-1.486211	1.487143	1.029243
C	2.343612	-4.105224	1.321580
C	-2.634778	-3.985718	-1.350718
C	-4.687021	0.015980	1.300799
C	0.821653	2.893525	-0.270360
N	2.072610	3.077799	0.247998
C	3.115747	2.212127	-0.307321
C	2.953225	0.752017	0.189018
C	-0.354018	3.711438	0.312540
N	3.740196	-0.263789	-0.283804
C	3.450248	-1.575695	0.308921
N	-1.628882	3.311252	-0.296371
O	0.623963	2.076057	-1.185008
O	2.084902	0.507713	1.046150
C	4.764731	-0.319102	-1.369422
C	-2.085953	4.235421	-1.379419
C	2.380223	4.030399	1.340959
H	-4.301343	2.185215	-0.104942
H	-3.405214	1.435414	-1.442425
H	-4.045500	-2.630939	0.158964
H	-2.865791	-2.159728	1.407541
H	0.461797	-3.729927	-1.416287
H	0.261786	-4.867427	-0.066522
H	4.099172	2.611228	-0.028298
H	3.034514	2.235255	-1.398913
H	-0.207334	4.788271	0.142851
H	-0.411385	3.541020	1.396455
H	3.334838	-1.457179	1.395253
H	4.308062	-2.238946	0.125219
Na	0.020200	-0.027136	-0.108124
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H	-1.152734	4.493461	-1.907368
C	-3.013498	3.654947	-2.455587
C	3.318787	3.405886	2.392614
C	2.894544	5.381282	0.828662
H	1.424484	4.214564	1.852913
C	6.173199	-0.466057	-0.791747
H	4.526402	-1.255121	-1.902939
C	4.716573	0.782514	-2.436739
C	1.326467	-4.615236	2.361940
C	3.257075	-5.221902	0.804174
H	2.978944	-3.377694	1.847709
C	-1.664084	-4.619443	-2.355037
C	-3.577852	-5.038768	-0.766520
H	-3.248440	-3.280259	-1.937321
C	-4.565632	1.122371	2.367713
C	-6.123888	-0.144995	0.789303
H	-4.408297	-0.922242	1.802144
C	7.095189	-1.305822	-1.436396

C	8.410210	-1.412108	-0.972530
C	8.818884	-0.680920	0.147882
C	7.904758	0.151882	0.802393
C	6.590532	0.257444	0.335149
H	6.780725	-1.884207	-2.310415
H	9.114421	-2.072284	-1.483023
H	9.843914	-0.765141	0.514096
H	8.215440	0.719948	1.681892
H	5.880008	0.897425	0.864198
C	-4.805550	-5.289634	-1.398402
C	-5.661357	-6.289642	-0.925059
C	-5.299498	-7.049573	0.191940
C	-4.080397	-6.802010	0.833016
C	-3.225592	-5.802907	0.356204
H	-5.096864	-4.695137	-2.269539
H	-6.614718	-6.470429	-1.425854
H	-5.967175	-7.828377	0.565550
H	-3.794883	-7.388177	1.709195
H	-2.283195	-5.607198	0.874093
C	-2.255571	6.763659	-1.340173
C	-2.796108	7.962599	-0.862361
C	-3.737042	7.942712	0.171465
C	-4.131689	6.719436	0.726126
C	-3.590594	5.523517	0.245183
H	-1.517426	6.786314	-2.147613
H	-2.477701	8.912608	-1.296478
H	-4.158785	8.876654	0.548019
H	-4.861834	6.698132	1.537949
H	-3.894524	4.576384	0.697583
C	4.135884	-5.848859	1.706236
C	4.976746	-6.882111	1.286774
C	4.956047	-7.308445	-0.046752
C	4.095818	-6.685540	-0.953829
C	3.255733	-5.646603	-0.531833
H	4.169652	-5.522976	2.749797
H	5.653464	-7.354011	2.002319
H	5.611817	-8.116953	-0.375619
H	4.077460	-7.004096	-1.998446
H	2.603662	-5.158723	-1.258902
C	-7.127605	-0.522194	1.700289
C	-8.452460	-0.674137	1.285973
C	-8.801498	-0.450389	-0.051372
C	-7.812228	-0.085683	-0.967292
C	-6.482410	0.060983	-0.550761
H	-6.871947	-0.708644	2.747003
H	-9.215209	-0.970481	2.009149
H	-9.837328	-0.566132	-0.376242
H	-8.071557	0.083063	-2.014845
H	-5.719403	0.327436	-1.284555
C	3.009924	6.452067	1.733880
C	3.476096	7.699439	1.312808

C	3.839739	7.900554	-0.024267
C	3.721567	6.847295	-0.933890
C	3.247706	5.598437	-0.510911
H	2.721160	6.315494	2.779766
H	3.553153	8.518936	2.030531
H	4.206979	8.874508	-0.353554
H	3.994832	6.994675	-1.981125
H	3.143099	4.792181	-1.239421
H	5.412964	0.491790	-3.236161
H	3.715340	0.872145	-2.881674
H	5.055912	1.756795	-2.061445
H	3.363417	4.059263	3.274211
H	2.944364	2.421791	2.706069
H	4.347673	3.307763	2.017336
H	-3.102165	4.410785	-3.249043
H	-2.592505	2.744842	-2.906771
H	-4.029390	3.462117	-2.087938
H	-5.171850	0.852999	3.242844
H	-3.520331	1.233755	2.686749
H	-4.944316	2.088265	2.003463
H	-2.274442	-5.111456	-3.125832
H	-1.040346	-3.864938	-2.855185
H	-1.032419	-5.398817	-1.909554
H	1.865608	-5.003510	3.236364
H	0.670339	-3.797160	2.689530
H	0.717289	-5.442918	1.970966

5.0 Single crystal X-ray crystallography

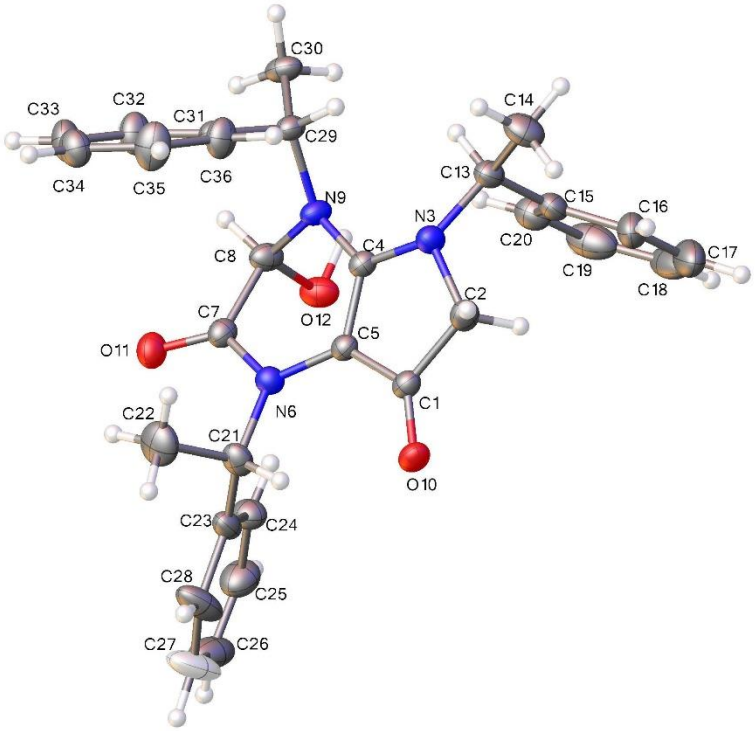

Figure S33. ORTEP drawing of bicyclic compound **15**. Ellipsoids are drawn at 20% probability level.

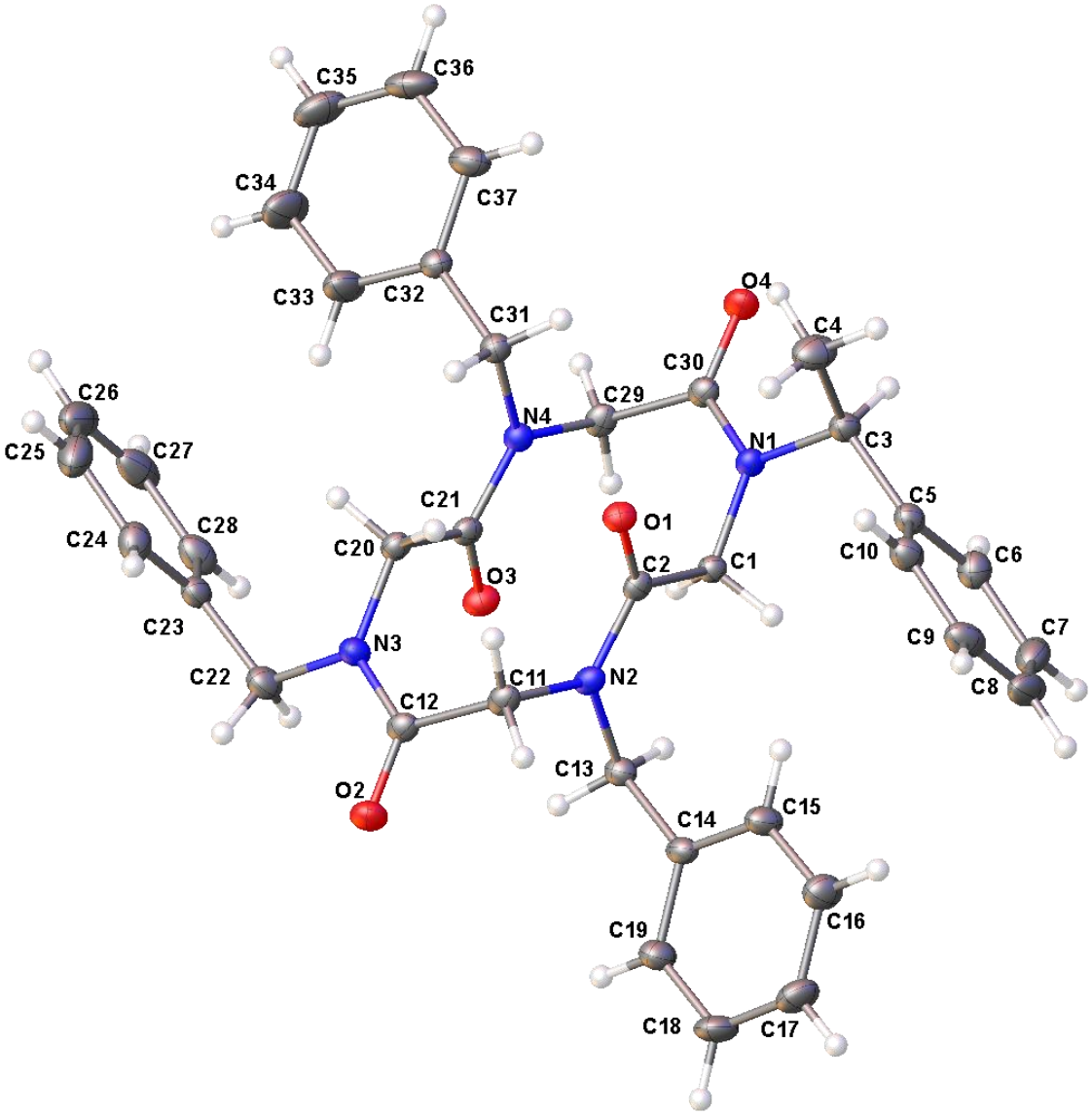

Figure S34. ORTEP drawing of compound **16**. Ellipsoids are drawn at 20% probability level.

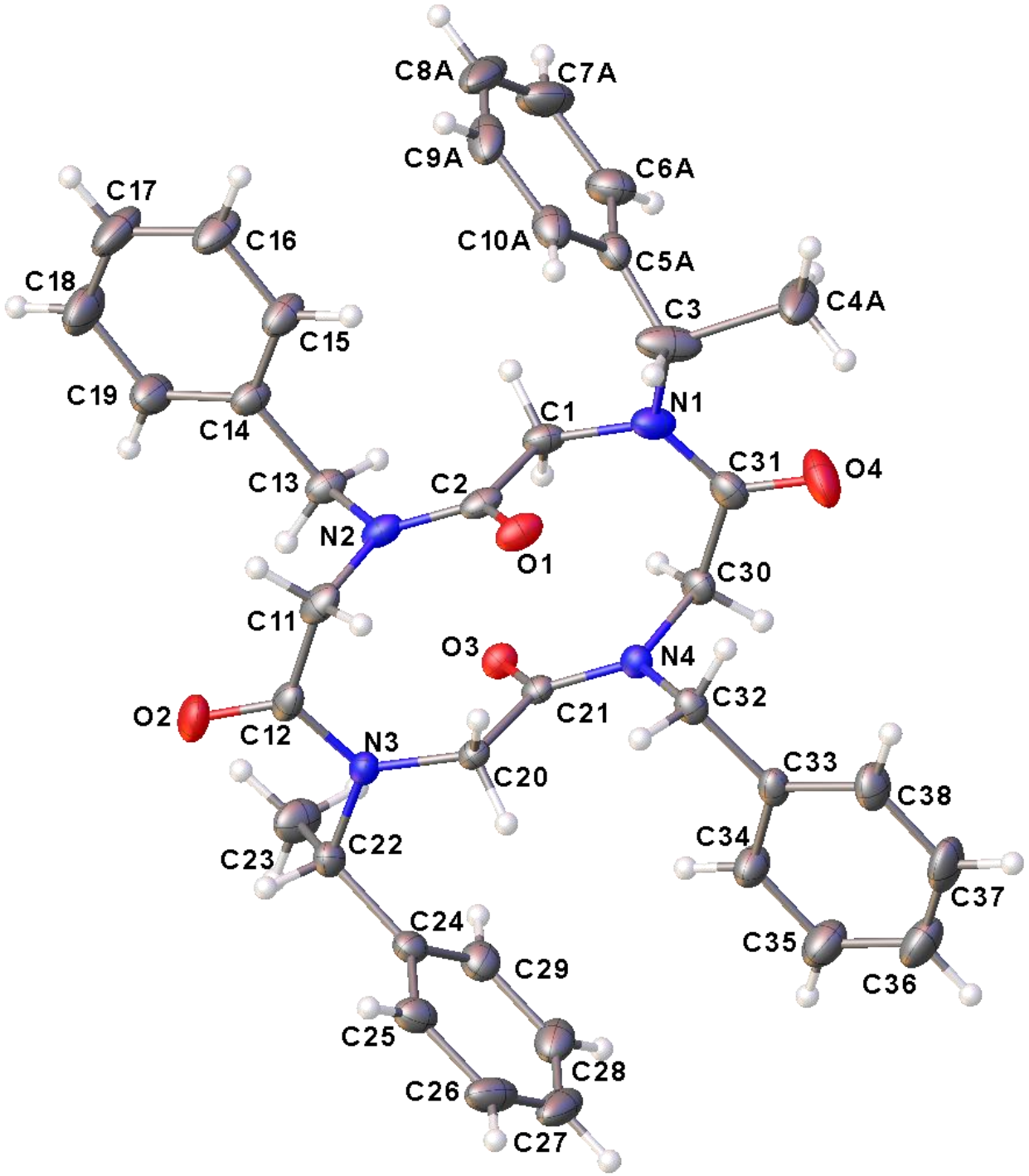

Figure S35. ORTEP drawing of compound **19**. Ellipsoids are drawn at 20% probability level. For clarity only one possible position for C4>>C10 atoms is displayed.

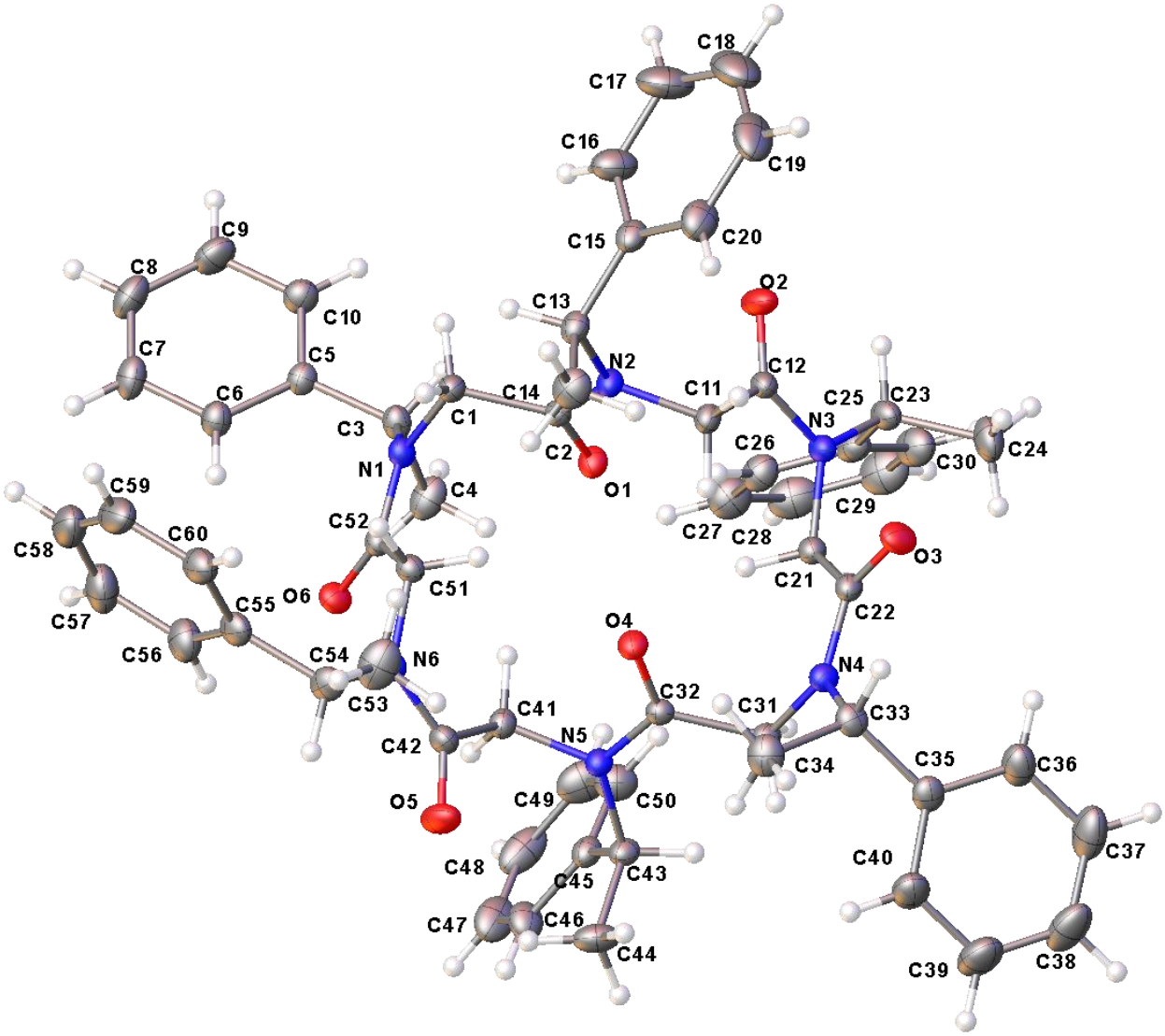

Figure S36. ORTEP drawing of conformational isomer **30**. Ellipsoids are drawn at 20% probability level.

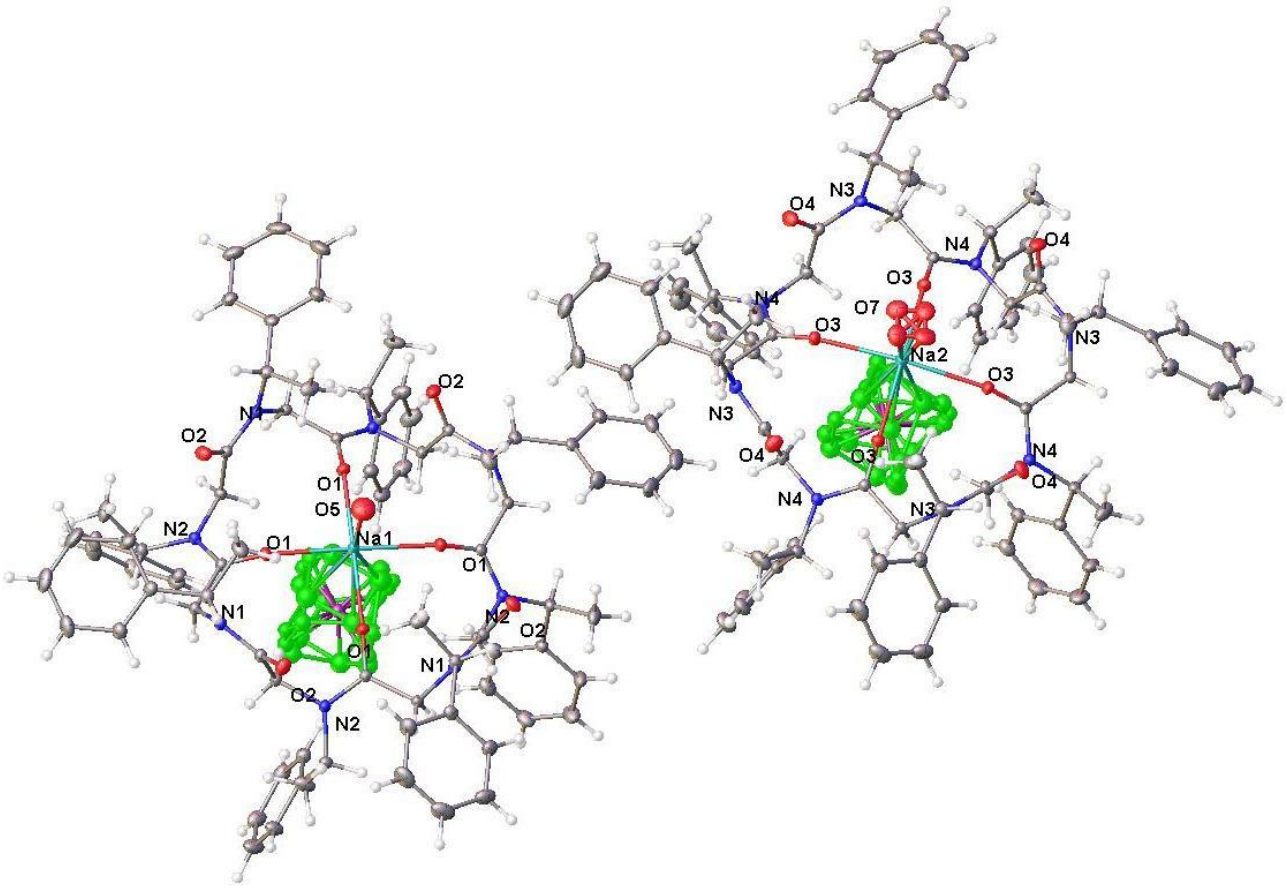

Figure S37. ORTEP drawing of the two independent moieties in compound [**36b**·Na(H_2O)]$^+$[PF_6]$^-$·0.25(CH_3CN). Ellipsoids are drawn at 10% probability level.

	15	**16**	**19**	**30**	[**36b**·Na(H_2O)]$^+$[PF_6]$^-$ ·0.25(CH_3CN)
T (K)	296	296	296	296	295
Crystal size (mm x mm x mm)	0.41x0.27x0.12	0.22x0.19x0.15	0.46x0.12x0.06	0.37x0.25x0.21	0.55x0.31x0.28
Formula	$C_{30}H_{31}N_3O_3$	$C_{37}H_{38}N_4O_4$	$C_{38}H_{40}N_4O_4$	$C_{60}H_{66}N_6O_6$	[($C_{80}H_{88}N_8O_8$)(H_2O)Na]$^+PF_6^-$ 0.25 (CH_3CN)
Formula weight	481.58	602.71	616.74	967.19	2966.10
System	Orthorhombic	Monoclinic	Monoclinic	Monoclinic	Tetragonal
Space group	$P2_12_12_1$	$P2_1$	$P2_1$	$P2_1$	$P4$
***a* (Å)**	12.8492(7)	8.8020(5)	8.9528(11)	10.962(4)	20.141(3)
***b* (Å)**	23.7824(12)	11.2590(6)	11.419(3)	19.047(5)	20.141(3)
***c* (Å)**	8.4063(4)	15.7919(8)	15.863(2)	12.850(4)	10.316(3)
***α* (°)**	90	90	90	90	90
***β* (°)**	90	95.669(2)	93.945(12)	97.523(17)	90
***γ* (°)**	90	90	90	90	90
***V* (Å^3)**	2568.8(2)	1557.35(14)	1617.8(5)	967.19	4184.8(17)
Z	4	2	2	2	1
***Dx* (g cm^{-3})**	1.245	1.285	1.266	1.208	1.179
λ (Å)	1.54178	1.54178	1.54178	1.54178	1.54178
***μ* (mm^{-1})**	0.646	0.675	0.661	0.624	0.931
***F*$_{000}$**	1024.0	640.0	656.0	1032.0	1564
R1 (I > 2σI)	0.0510 (4422)	0.0449 (4405)	0.0420 (5364)	0.0347 (9465)	0.0556(7536)
$_wR_2$	0.1439 (4896)	0.1164 (6045)	0.1116 (6225)	0.0919(10023)	0.1707(7930)
N. of param.	333	408	470	656	489
GooF	1.070	1.030	1.015	1.024	1.052
ρ_{min}, ρ_{max} (eÅ^{-3})	-0.155, 0.480	-0.144, 0.155	-0.163, 0.174	-0.118, 0.149	-0.516, 0.528

Table S1. Crystallographic data and refinement details for compounds **15**, **16**, **19**, **30,** [**36b**·Na(H_2O)]$^+$[PF_6]$^-$ ·0.25(CH_3CN).