

Supporting Information for

Unexpected Cleavage of Upper Rim-Bridged Calix[4]arenes Leading to Linear Oligophenolic Derivatives

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Compound 4

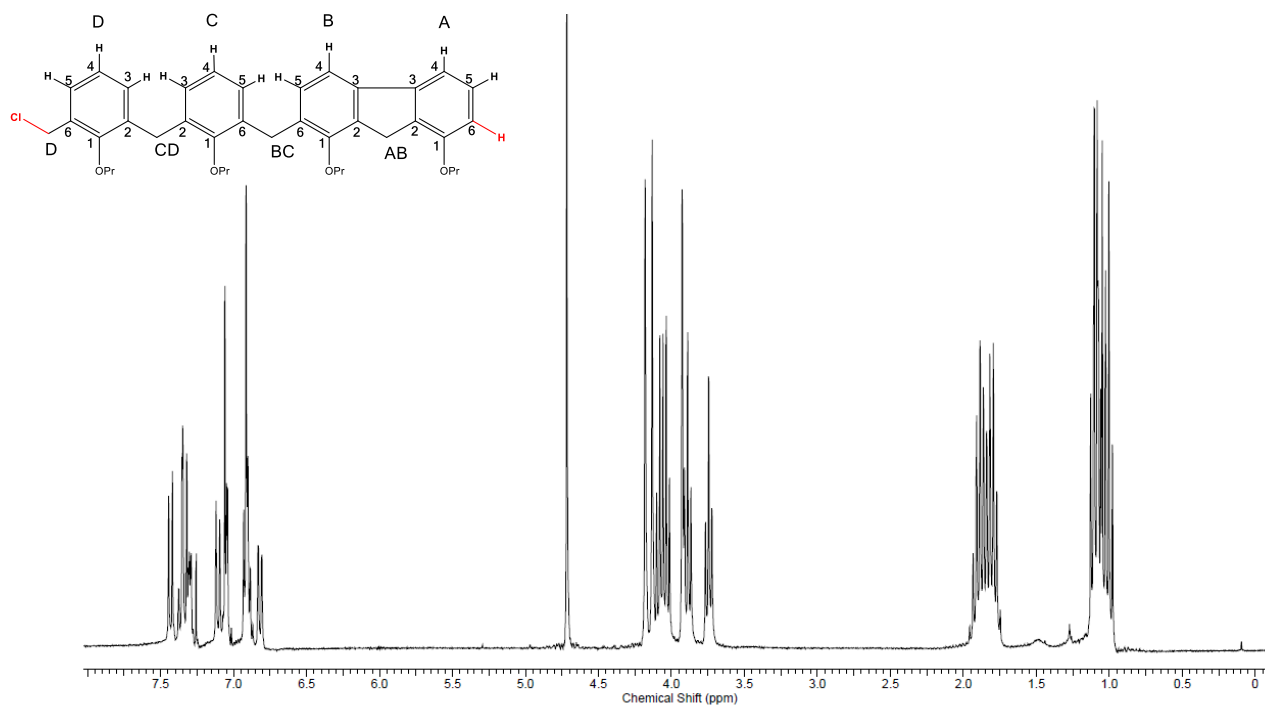


Figure 1. ^1H NMR of compound 4 (CDCl_3 , 600.1 MHz, 293 K).

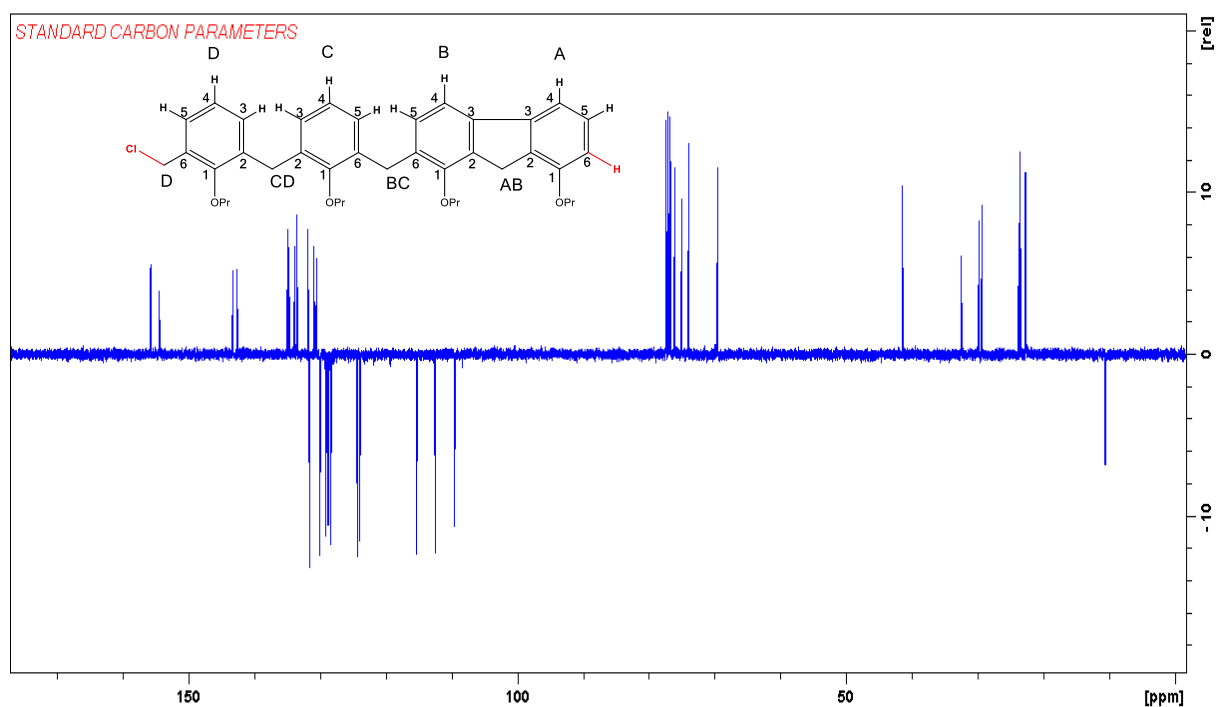


Figure 2. ^{13}C NMR (APT) of compound 4 (CDCl_3 , 150.9 MHz, 293 K).

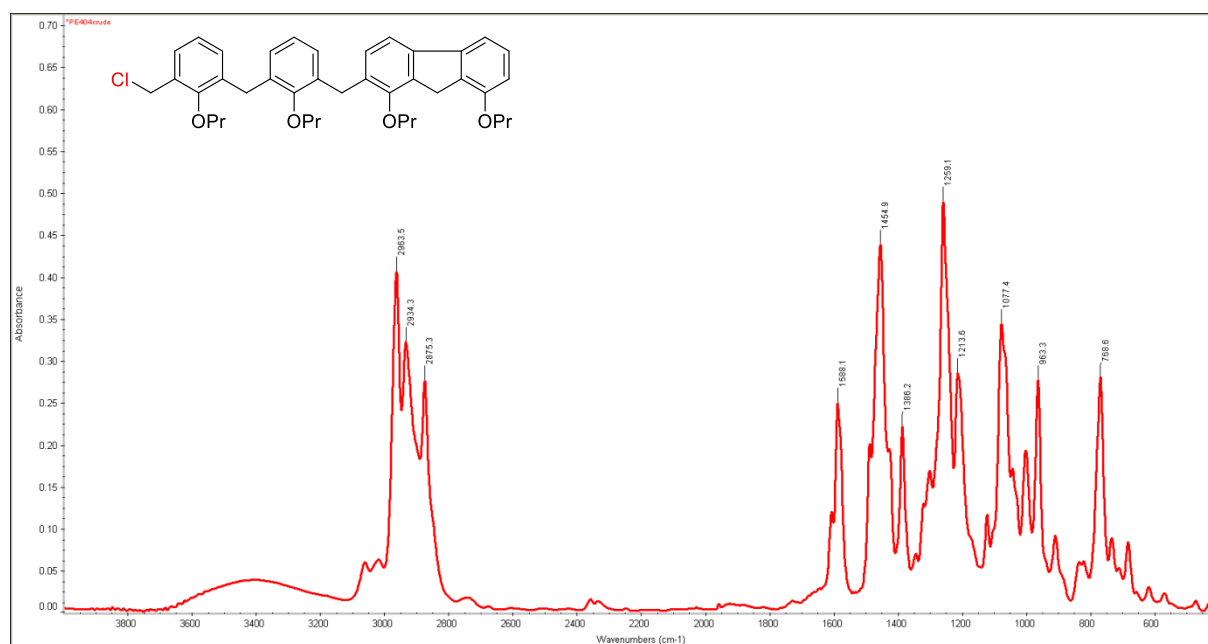


Figure 3. IR of compound **4** (KBr).

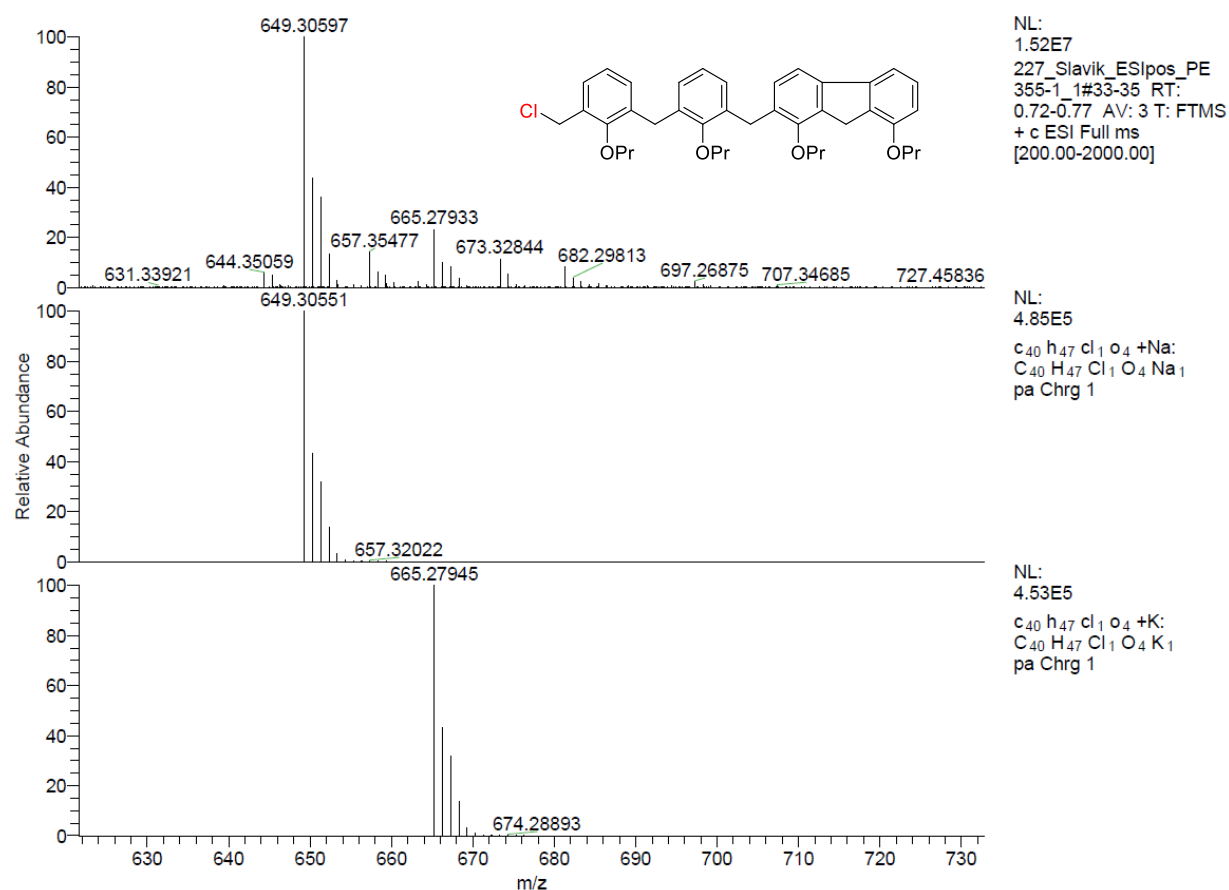


Figure 4. HRMS of compound **4** (ESI⁺).

Compound 5

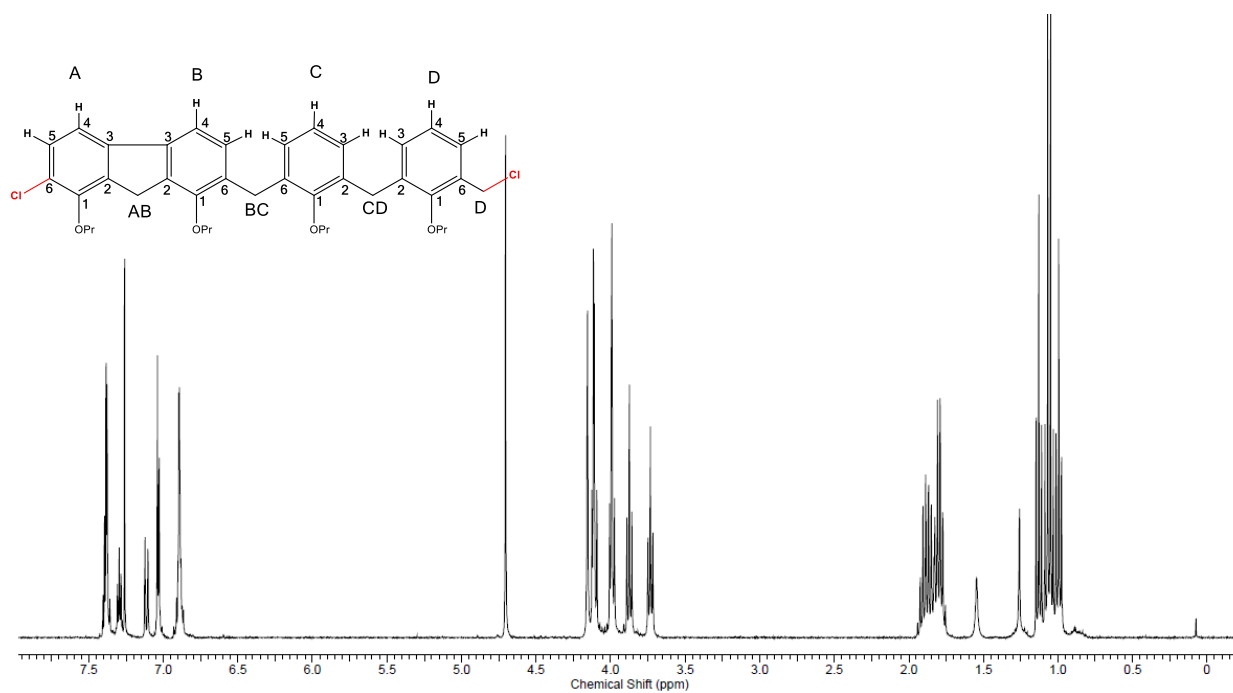


Figure 5. ^1H NMR of compound 5 (CDCl_3 , 600.1 MHz, 293 K).

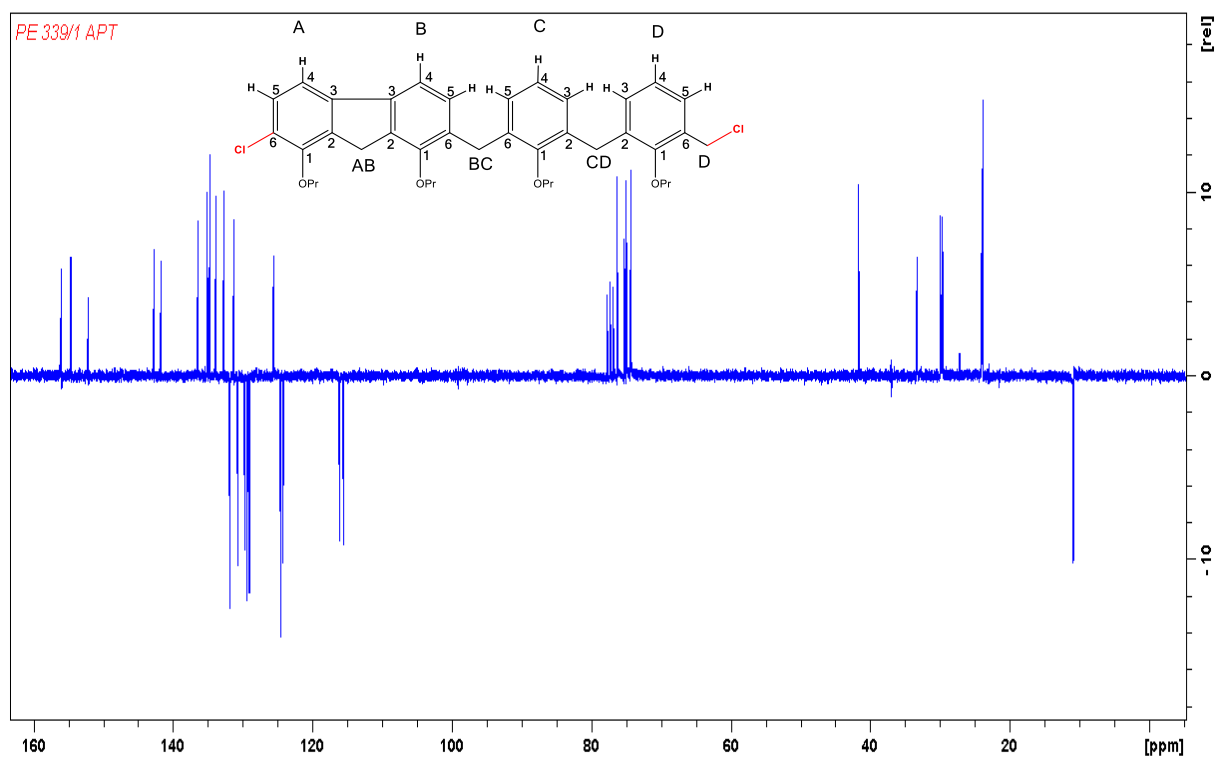


Figure 6. ^{13}C NMR (APT) of compound 5 (CDCl_3 , 150.9 MHz, 293 K).

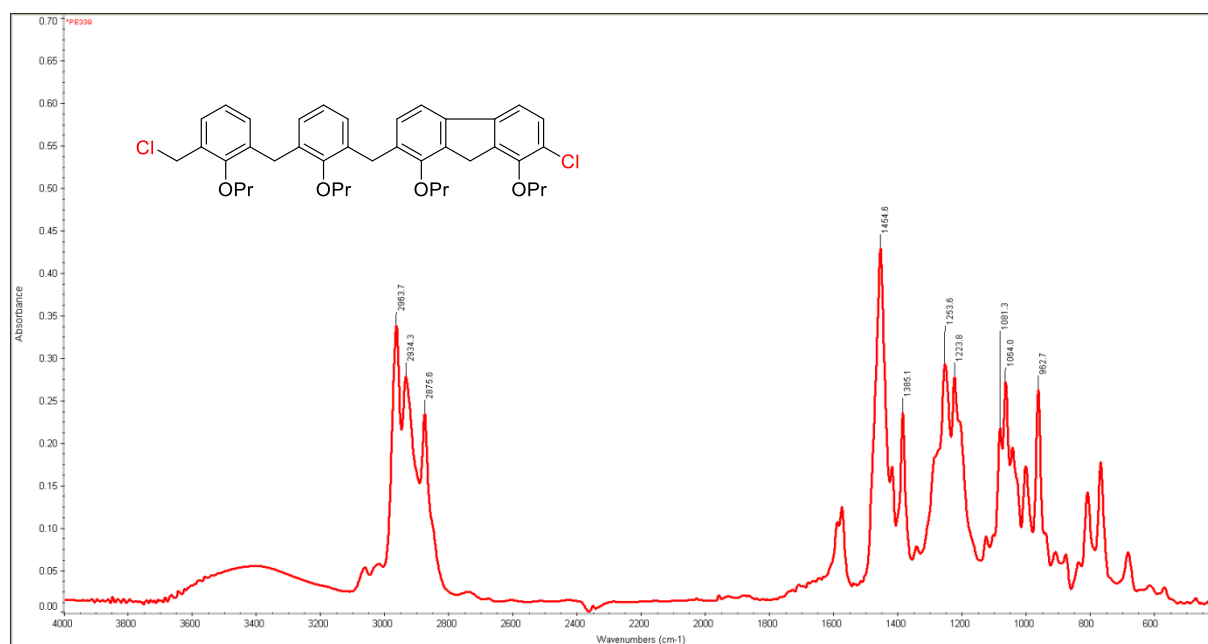


Figure 7. IR of compound 5 (KBr).

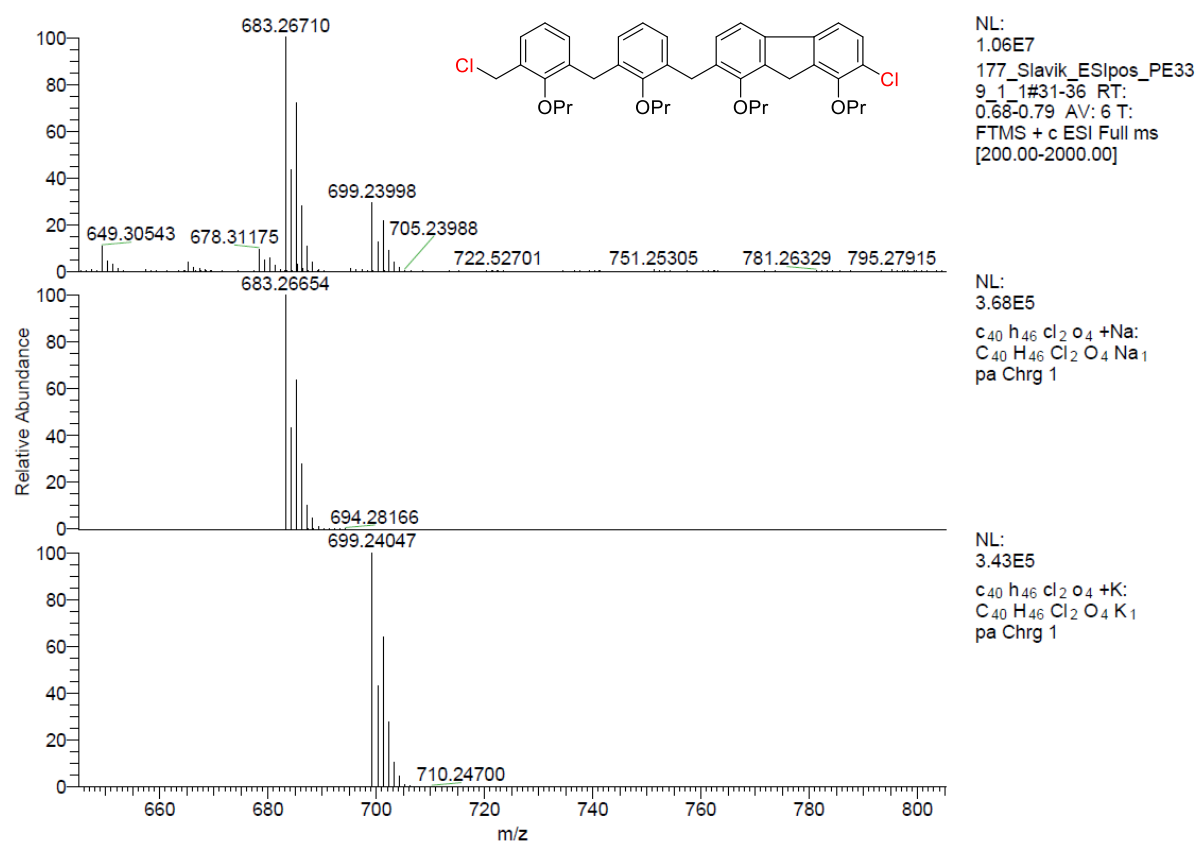


Figure 8. HRMS of compound 5 (ESI⁺).

Compound 6

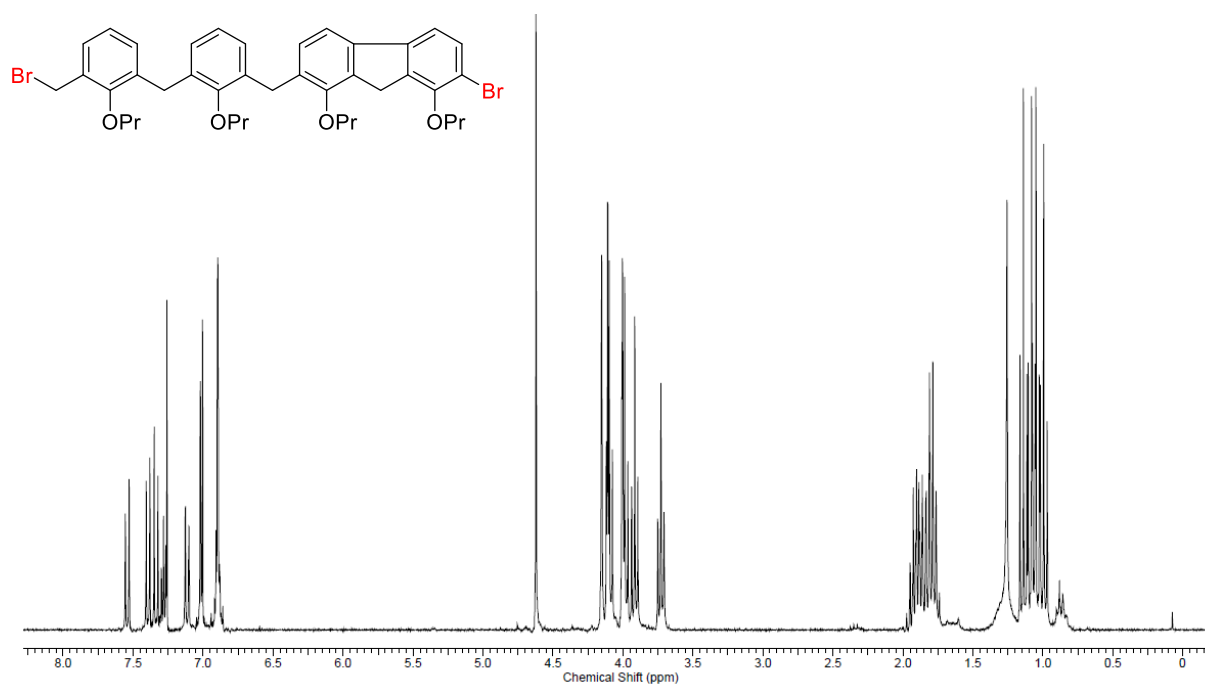


Figure 9. ¹H NMR of compound 6 (CDCl₃, 400 MHz, 293 K).

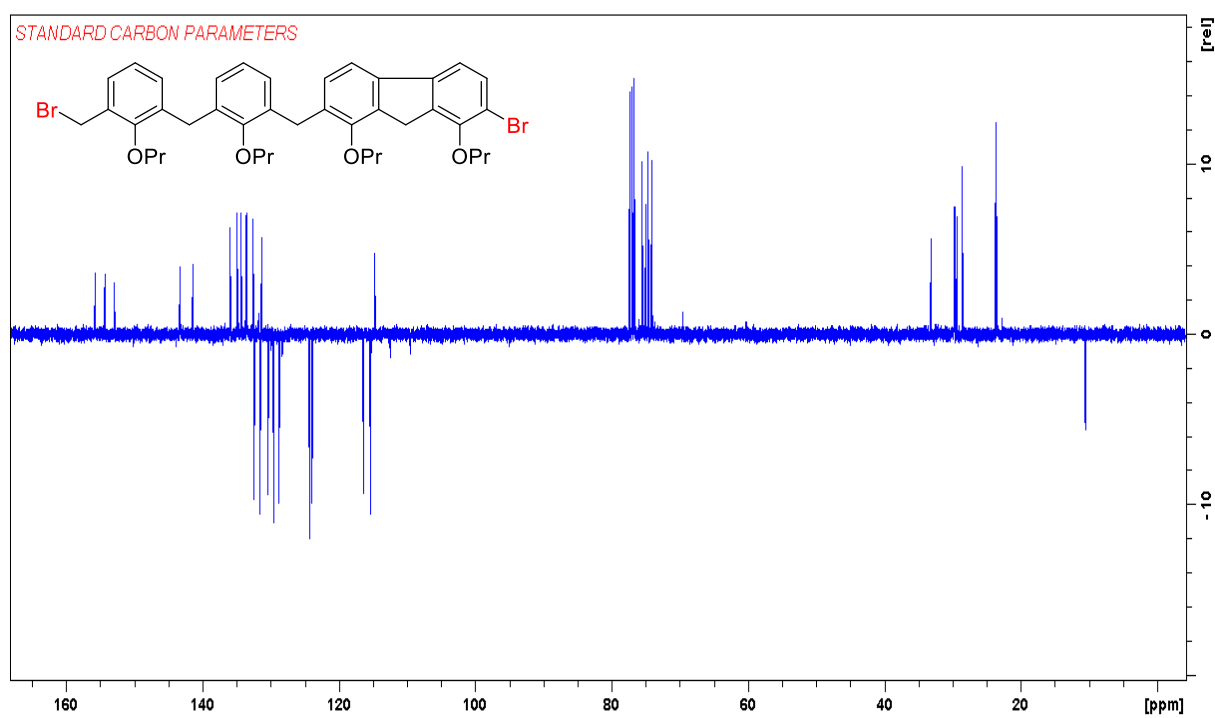


Figure 10. ¹³C NMR (APT) of compound 6 (CDCl₃, 100 MHz, 293 K).

Compound 6

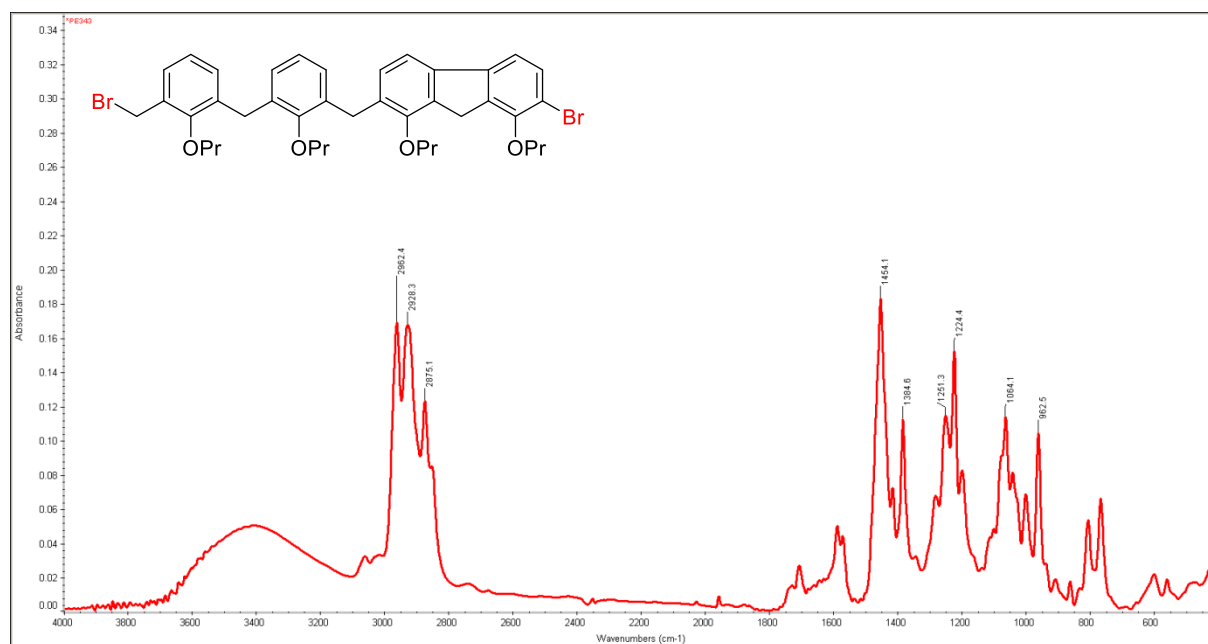


Figure 11. IR of compound 6 (KBr).

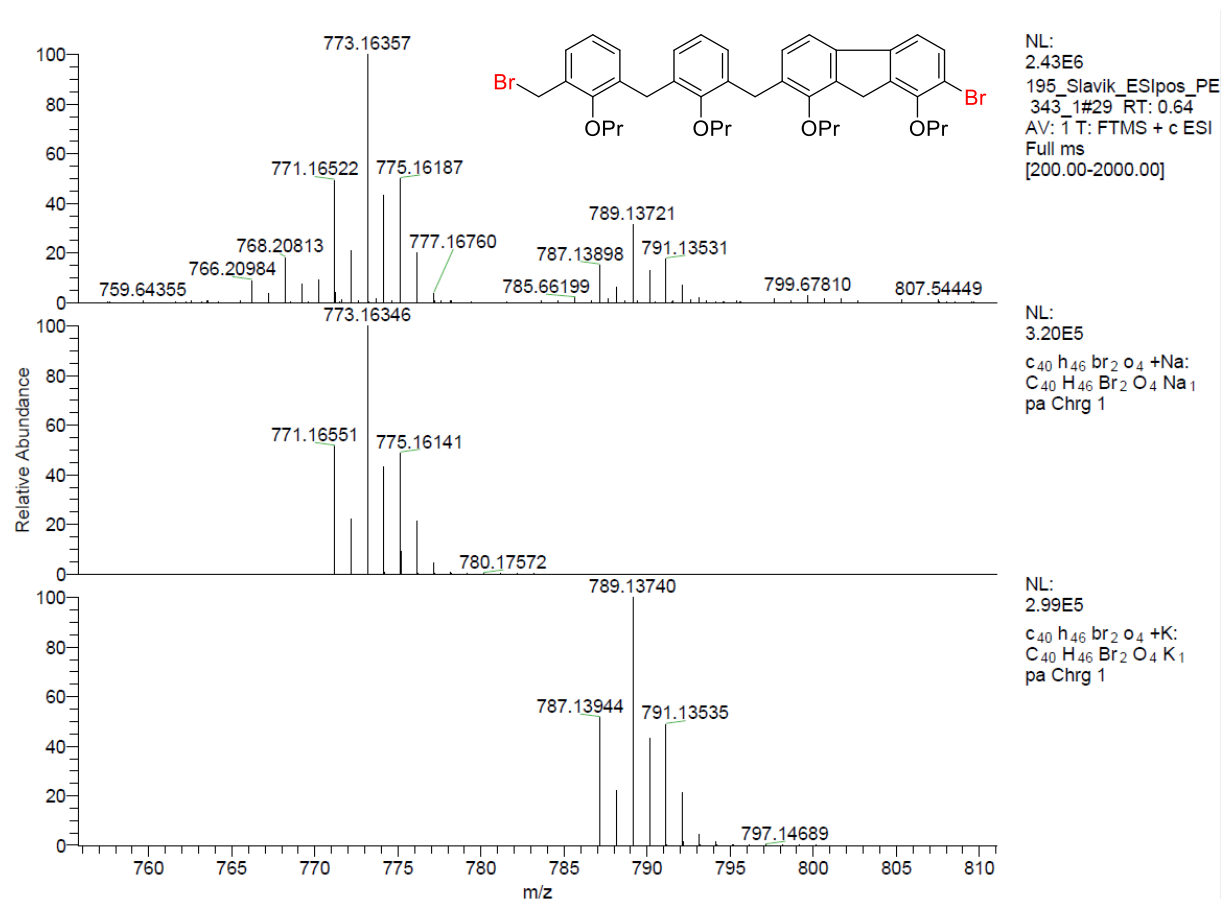


Figure 12. HRMS of compound 6 (ESI⁺).

Compound **7**

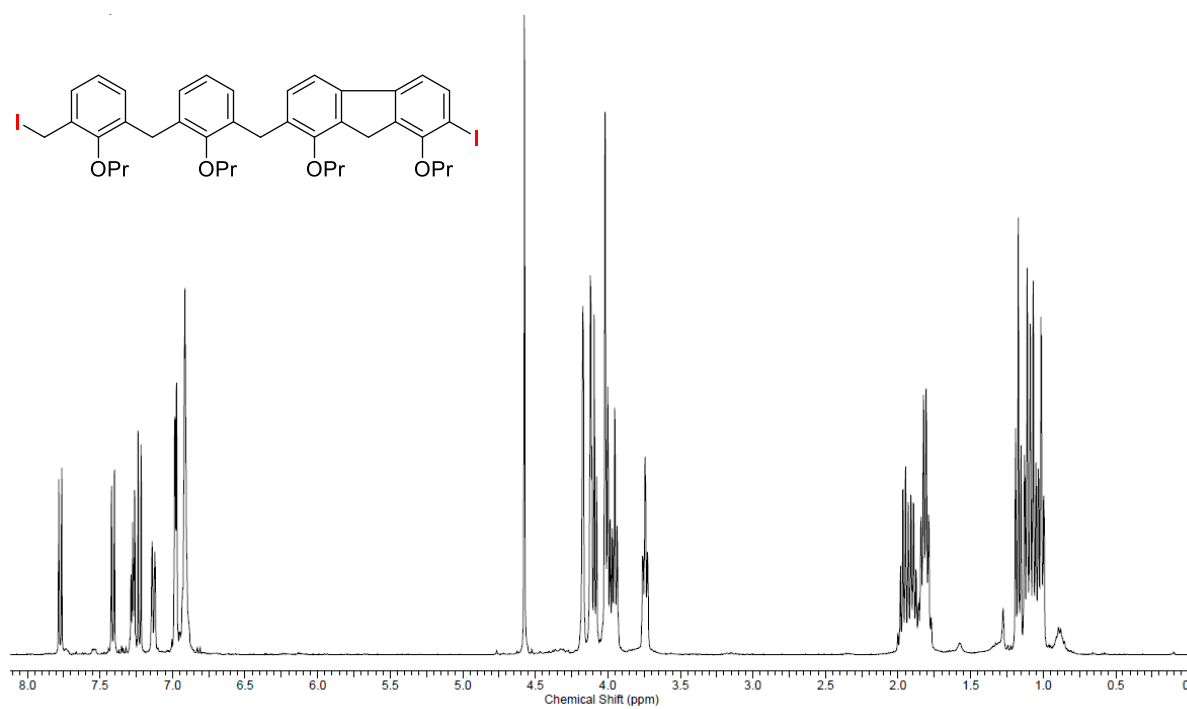


Figure 13. ^1H NMR of compound **7** (CDCl_3 , 400 MHz, 293 K).

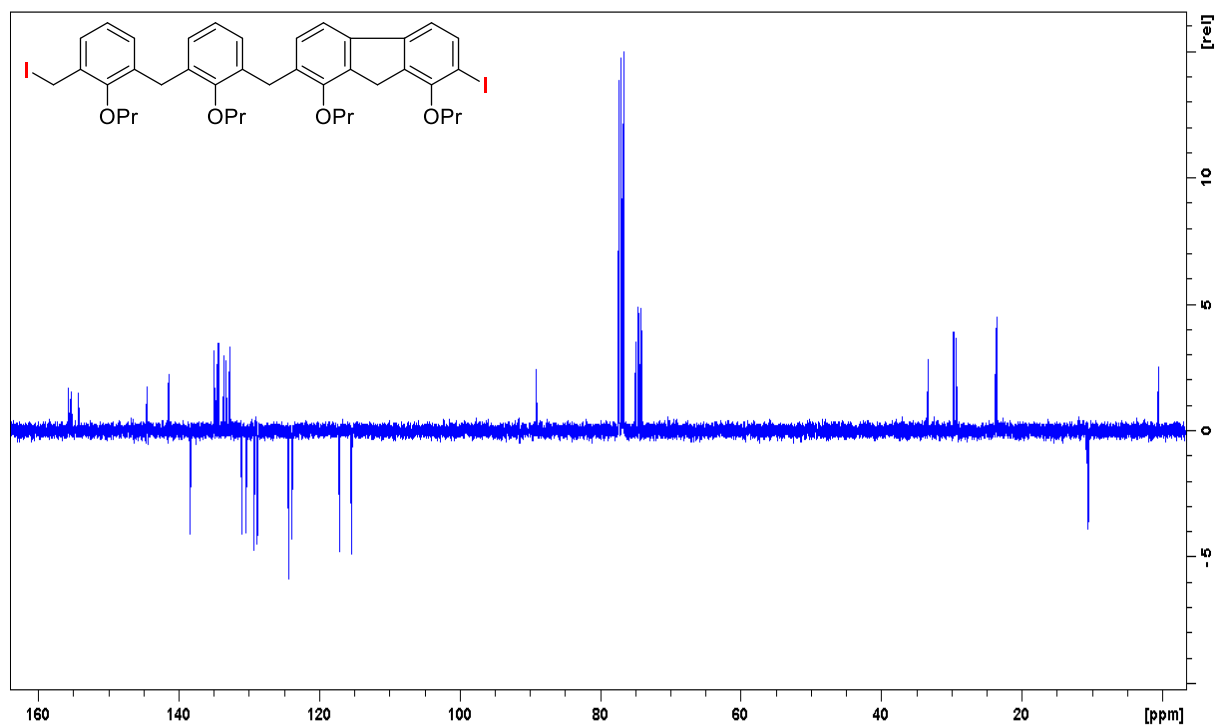


Figure 14. ^{13}C NMR (APT) of compound **7** (CDCl_3 , 100 MHz, 293 K).

Compound 7

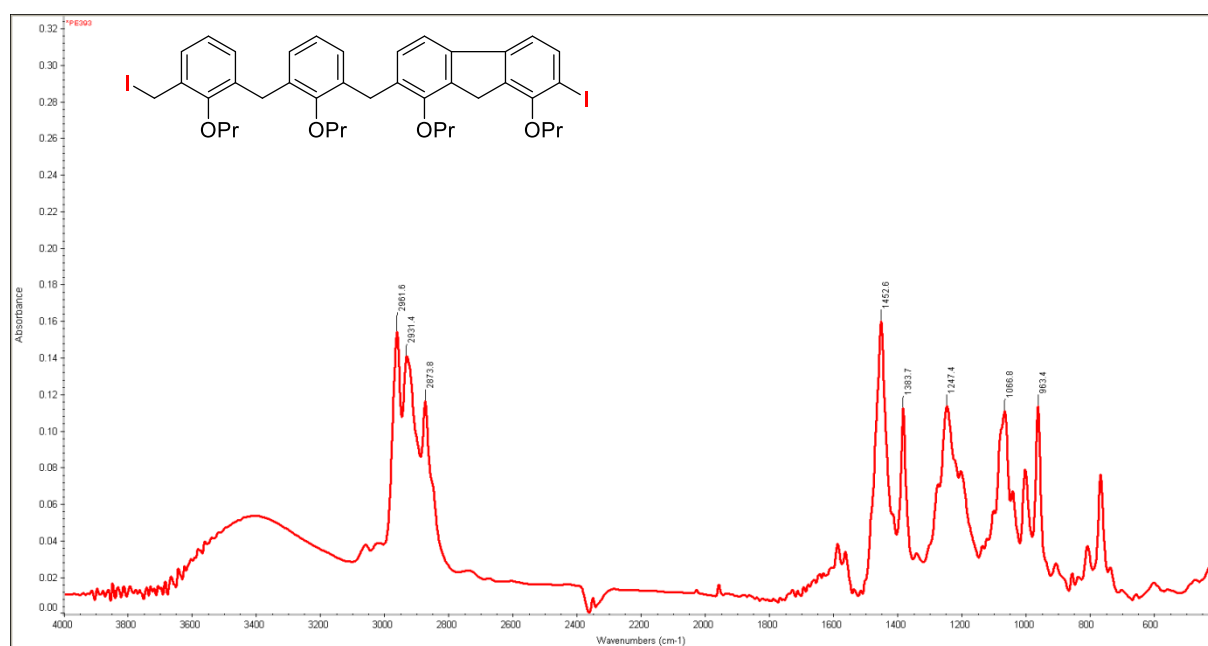


Figure 15. IR of compound **7** (KBr).

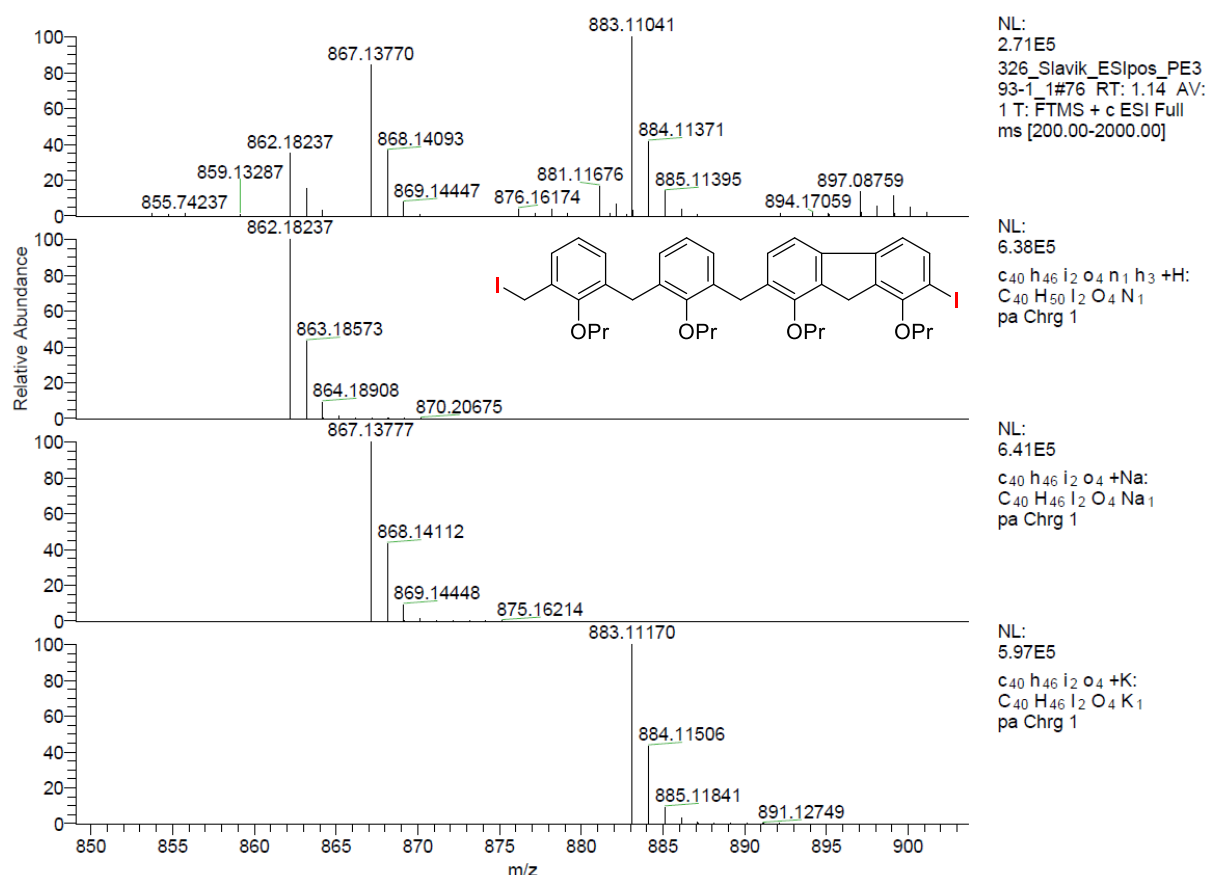


Figure 16. HRMS of compound **7** (ESI⁺).

Compound 9

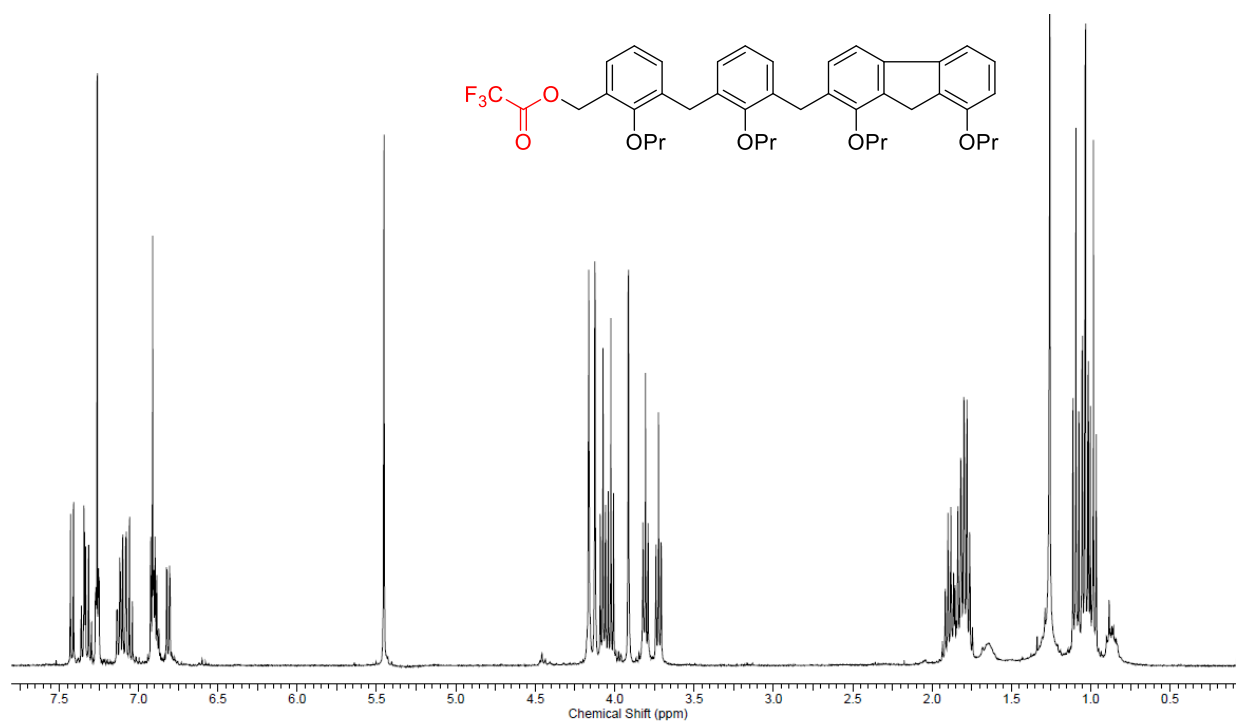


Figure 17. ^1H NMR of compound 9 (CDCl₃, 400 MHz, 293 K).

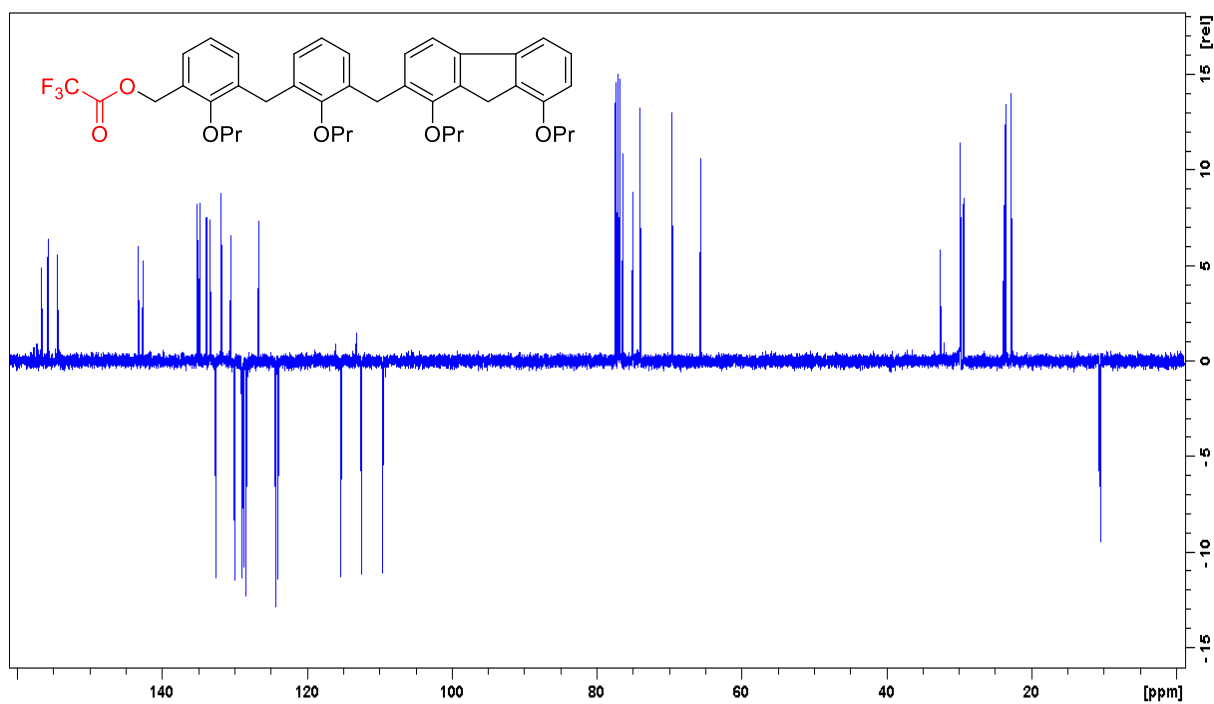


Figure 18. ^{13}C NMR (APT) of compound 9 (CDCl₃, 100 MHz, 293 K).

Compound 9

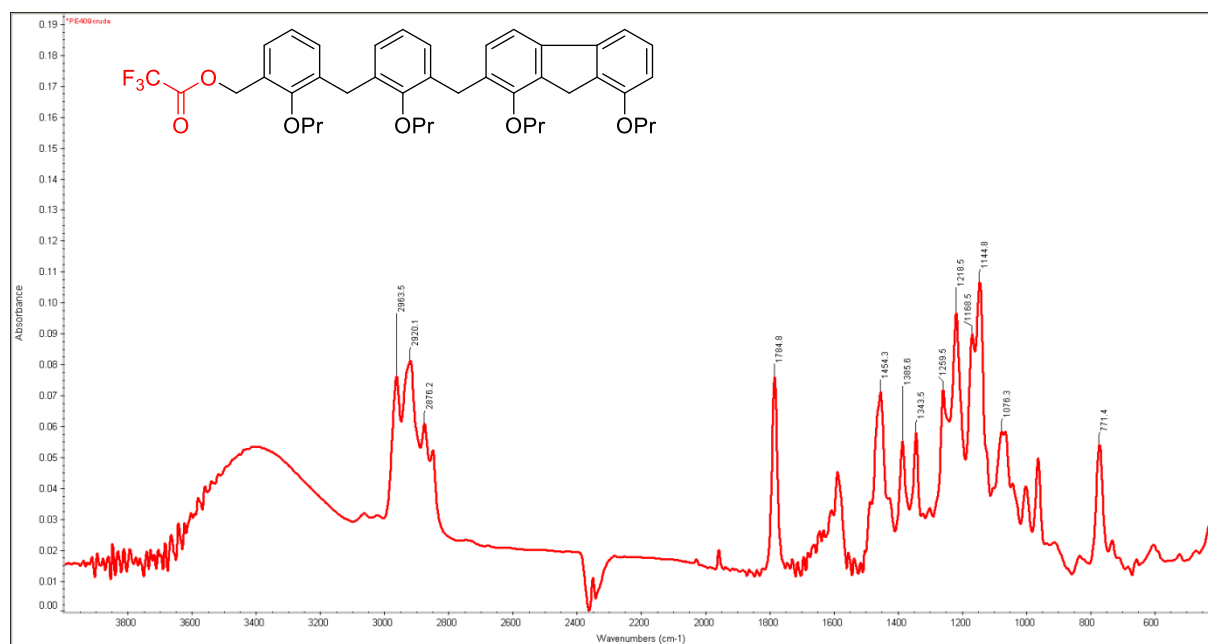


Figure 19. IR of compound 9 (KBr).

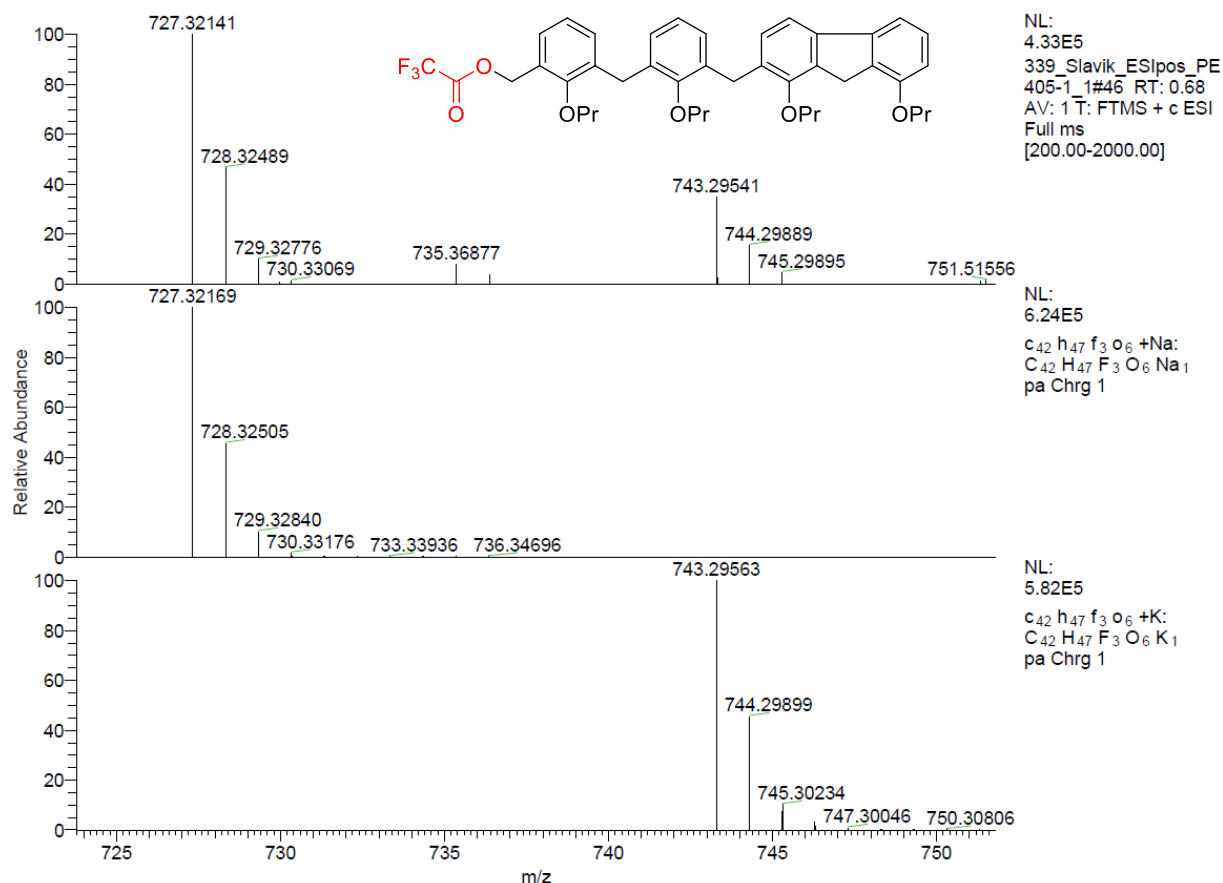


Figure 20. HRMS of compound 9 (ESI⁺).

Compound **10**

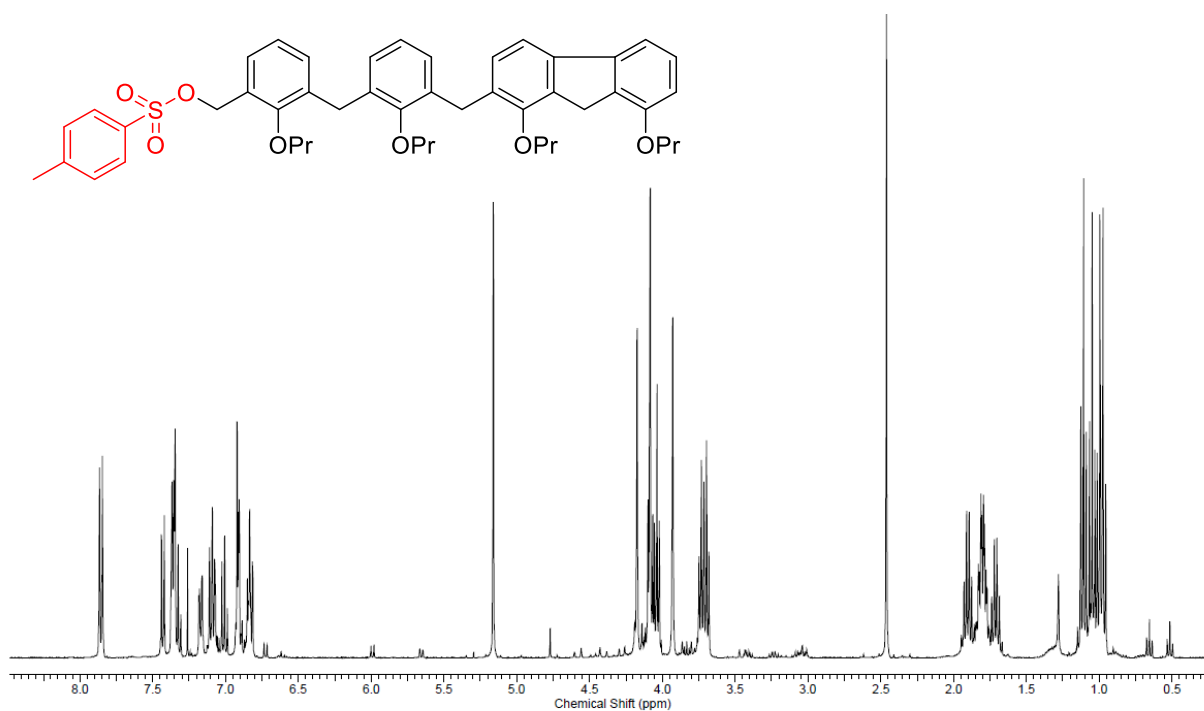


Figure 21. ^1H NMR of compound **10** (CDCl_3 , 400 MHz, 293 K).

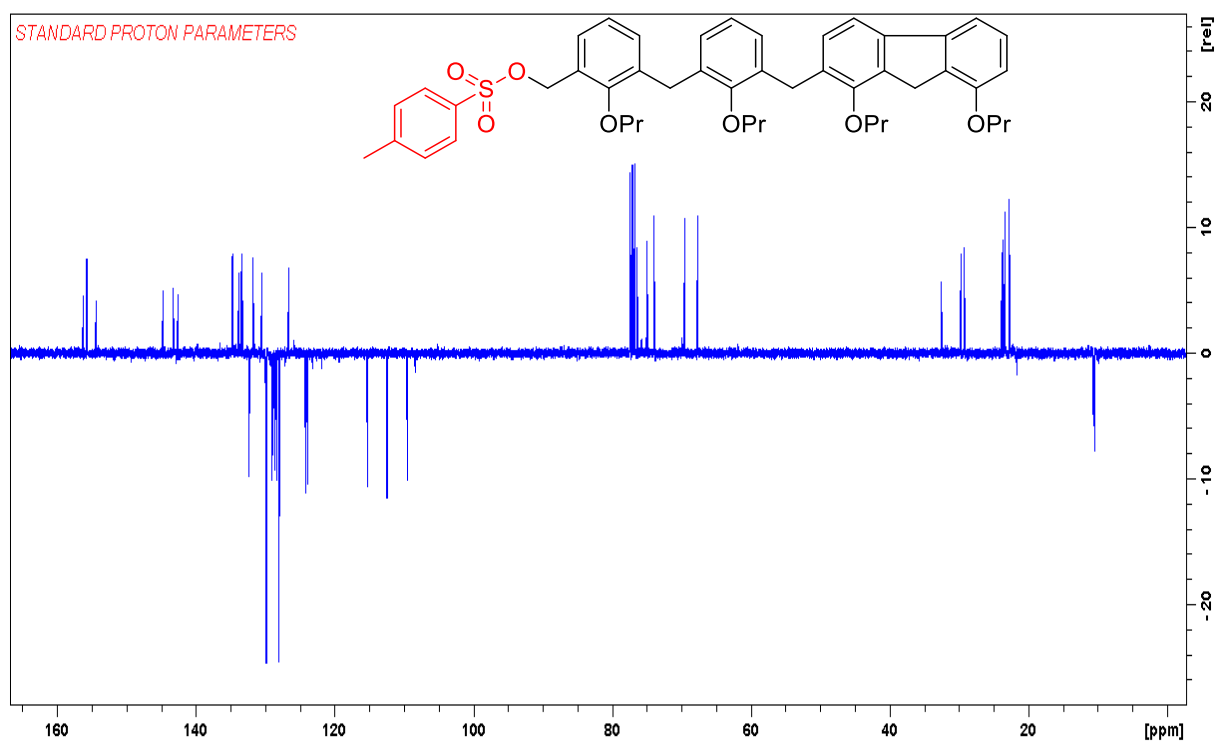


Figure 22. ^{13}C NMR (APT) of compound **10** (CDCl_3 , 100 MHz, 293 K).

Compound 10

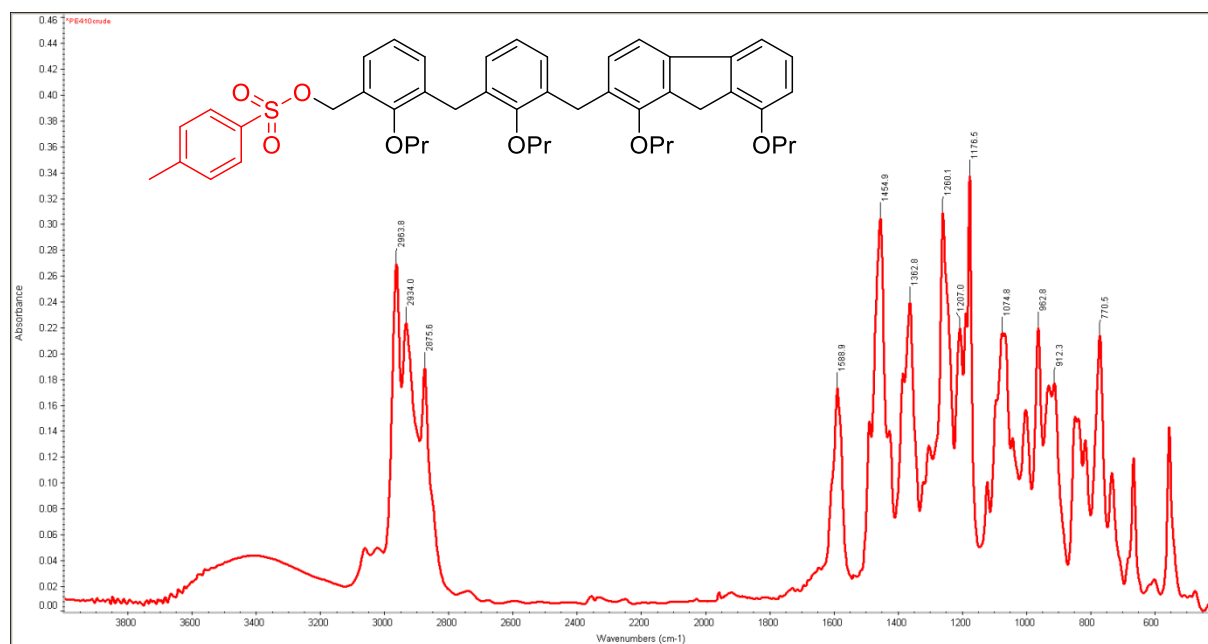


Figure 23. IR of compound 10 (KBr).

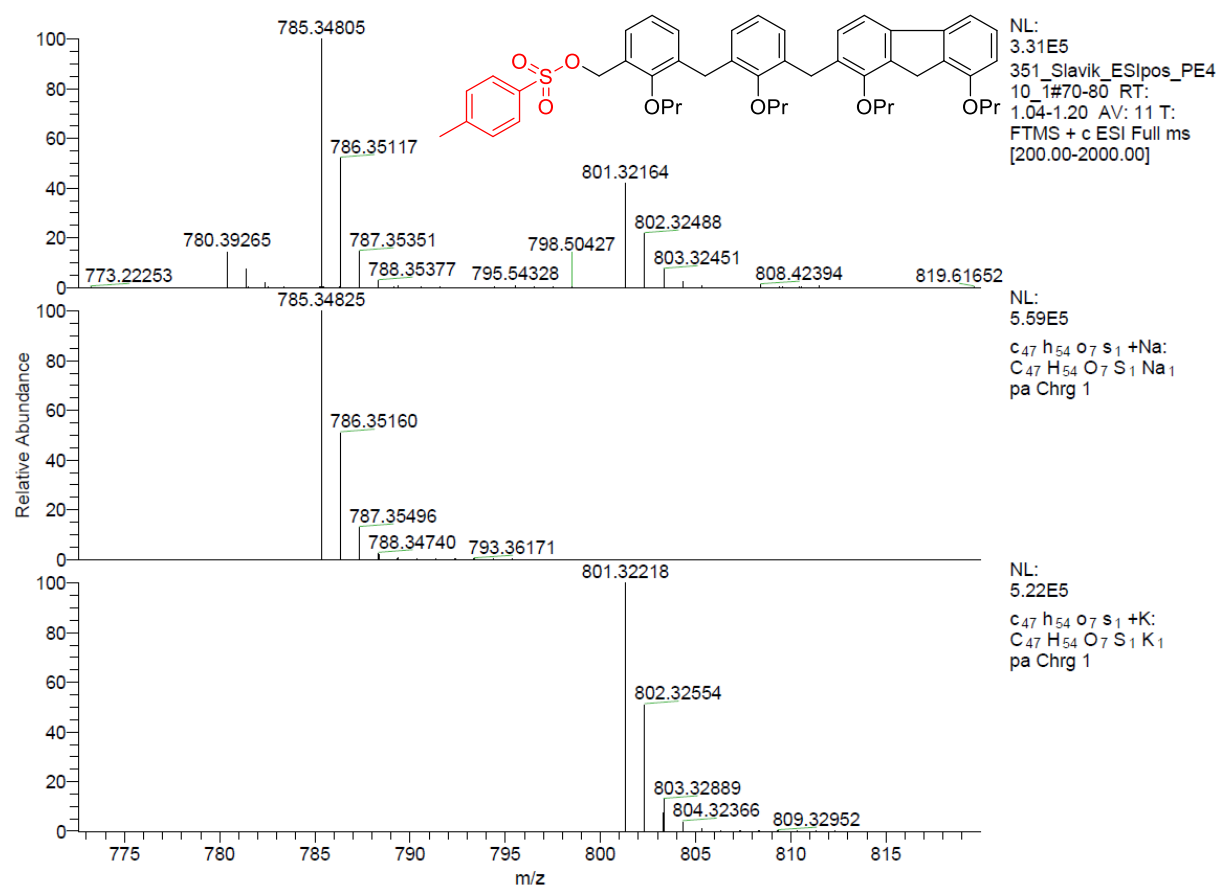


Figure 24. HRMS of compound 10 (ESI⁺).

Compound **11**

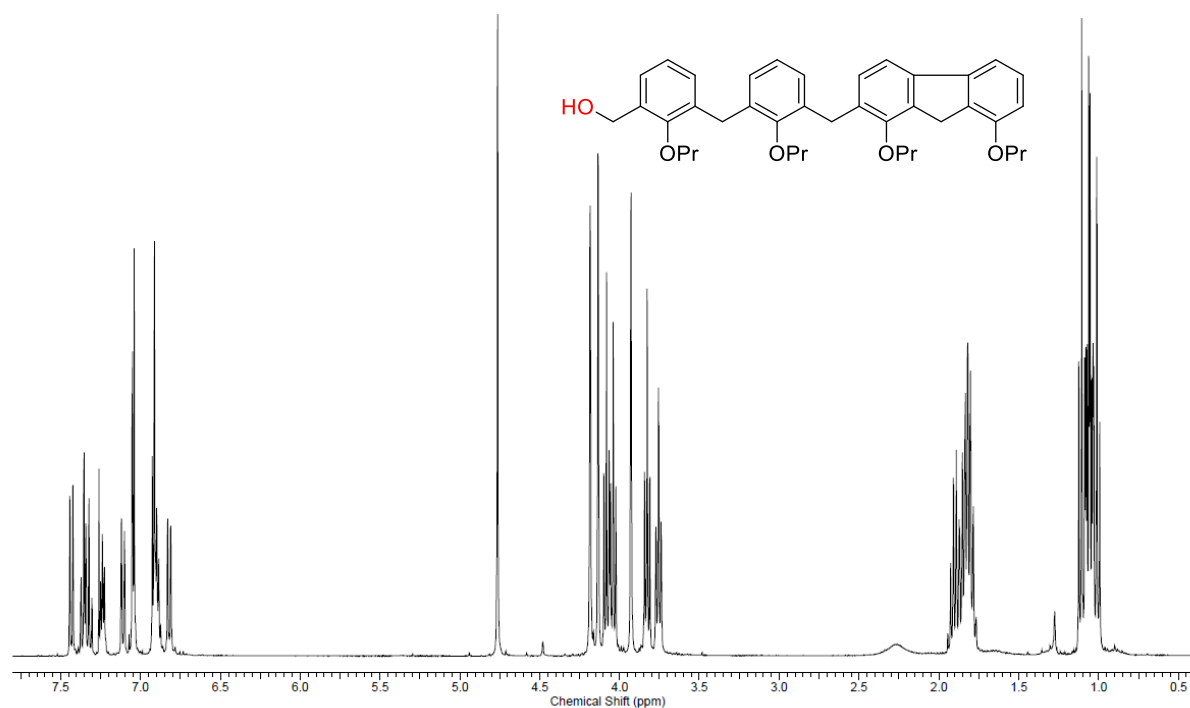


Figure 25. ¹H NMR of compound **11** (CDCl₃, 400 MHz, 293 K).

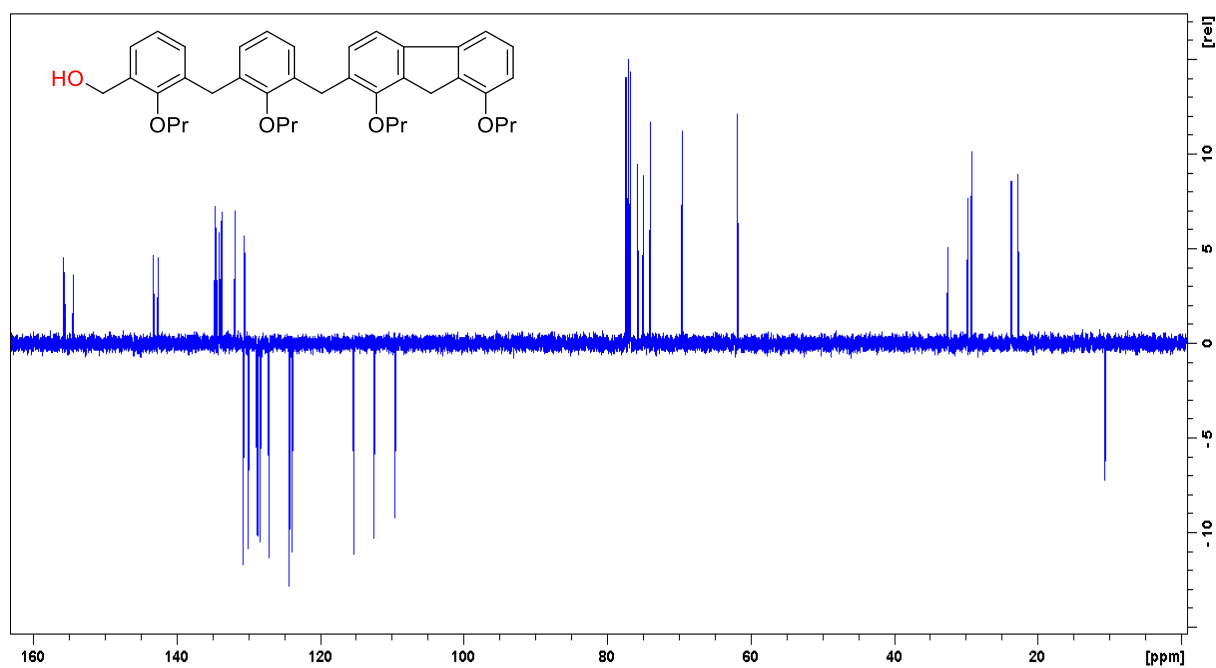


Figure 26. ¹³C NMR (APT) of compound **11** (CDCl₃, 100 MHz, 293 K).

Figure 1. IR spectrum of compound 1. The chemical structure of compound 1 is shown above the IR spectrum. The IR spectrum displays absorbance versus wavenumber (cm⁻¹). Key peaks are labeled with their wavenumbers: 3603.5, 2934.4, 2875.4, 1587.8, 1462.3, 1386.5, 1259.0, 1203.7, 1084.7, 984.2, and 770.4.

Relative Abundance

628.39075 631.33942 632.34277 633.34601 638.60864 640.40045 644.49329 647.31317 648.31647 649.31769 654.41406

647.31333

648.31669 649.32004 651.31816

631.33940 632.34275 633.34611 635.35281 638.36042

630 635 640 645 650 655

Oc1ccc(cc1)C2=CC(OC)C=C2Cc3ccc(cc3)C4=CC(OC)C=C4Cc5c6ccccc6c5C7=CC(OC)C=C7

NL: 2.87E5
339_Slavik_ESIpos_PE
405-1_1#23 RT: 0.33
AV: 1 T: FTMS + c ESI
Full ms
[200.00-2000.00]

NL: 5.96E5
C₄₀ H₄₈ O₅ +K:
C₄₀ H₄₈ O₅ K₁
pa Chrg 1

NL: 6.39E5
C₄₀ H₄₈ O₅ +Na:
C₄₀ H₄₈ O₅ Na₁
pa Chrg 1

15

Compound **14**

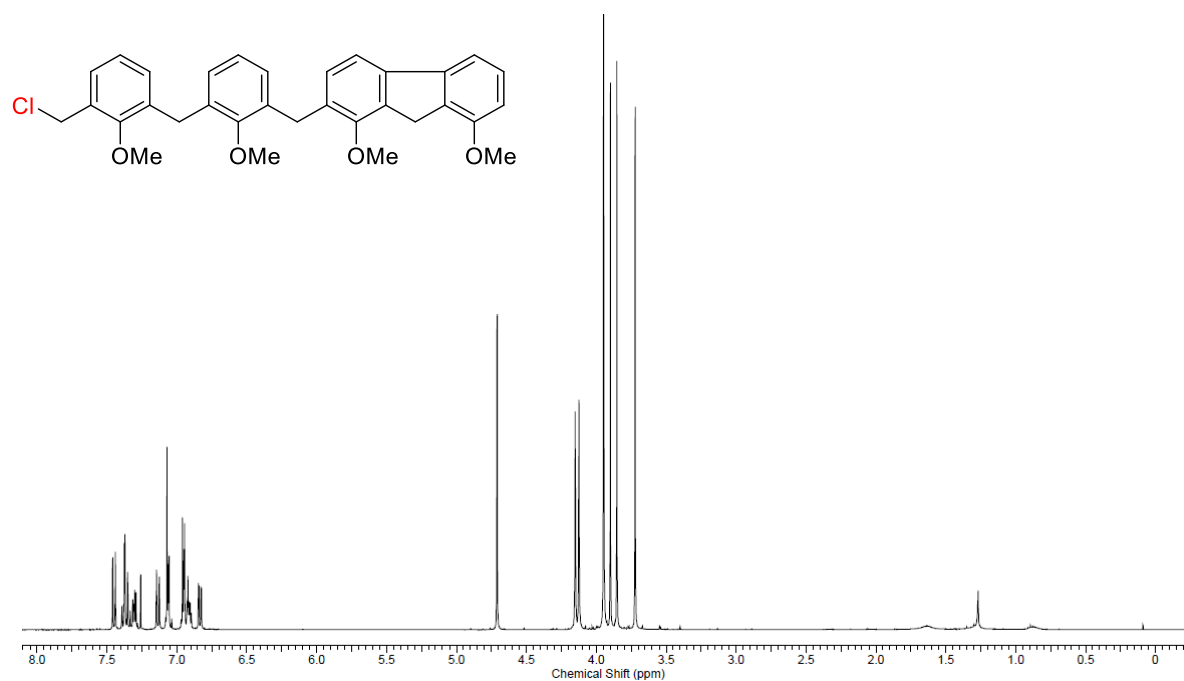


Figure 29. ¹H NMR of compound **14** (CDCl₃, 400 MHz, 293 K).

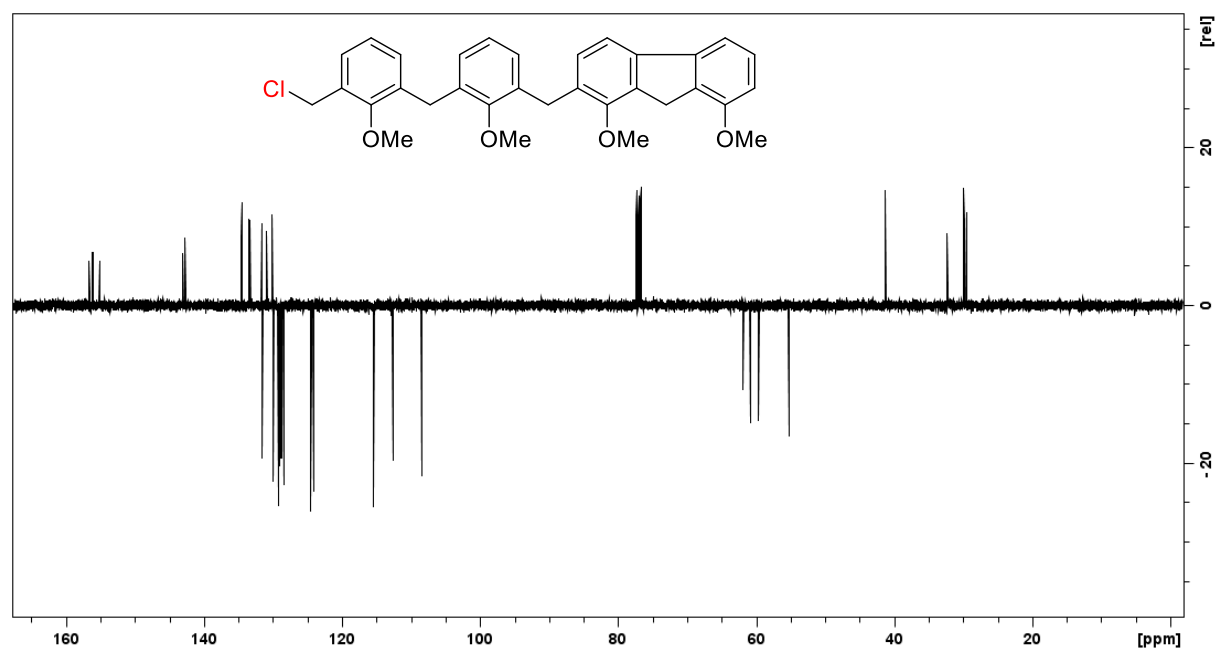


Figure 30. ¹³C NMR (APT) of compound **14** (CDCl₃, 100 MHz, 293 K).

Compound 14

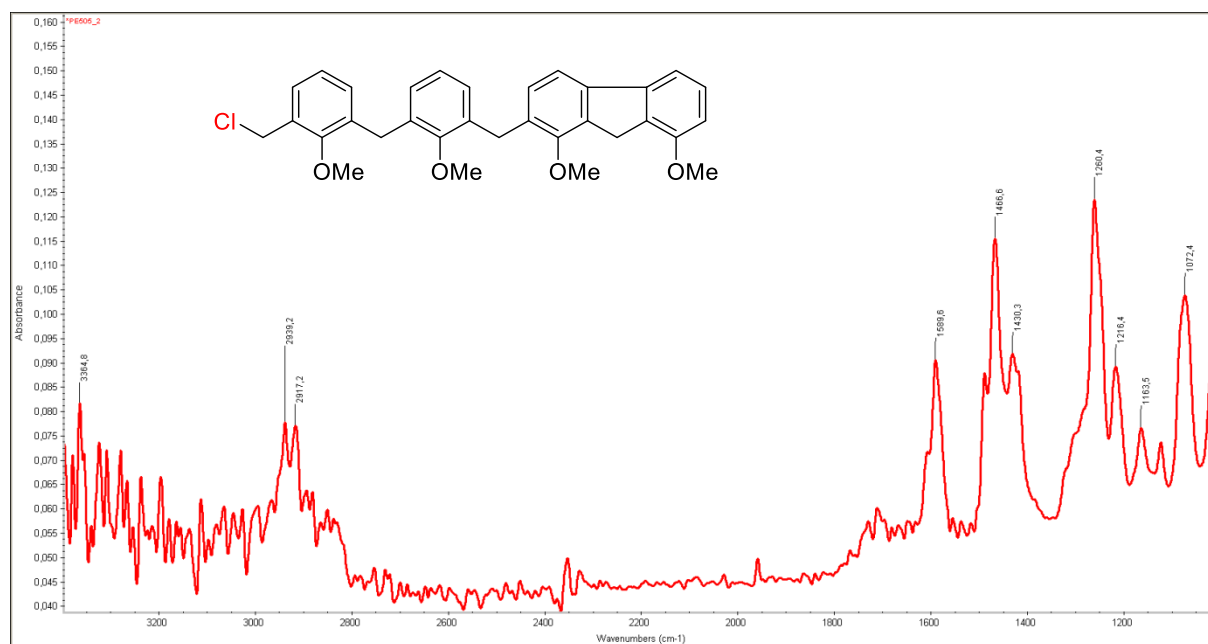


Figure 31. IR of compound 14 (KBr).

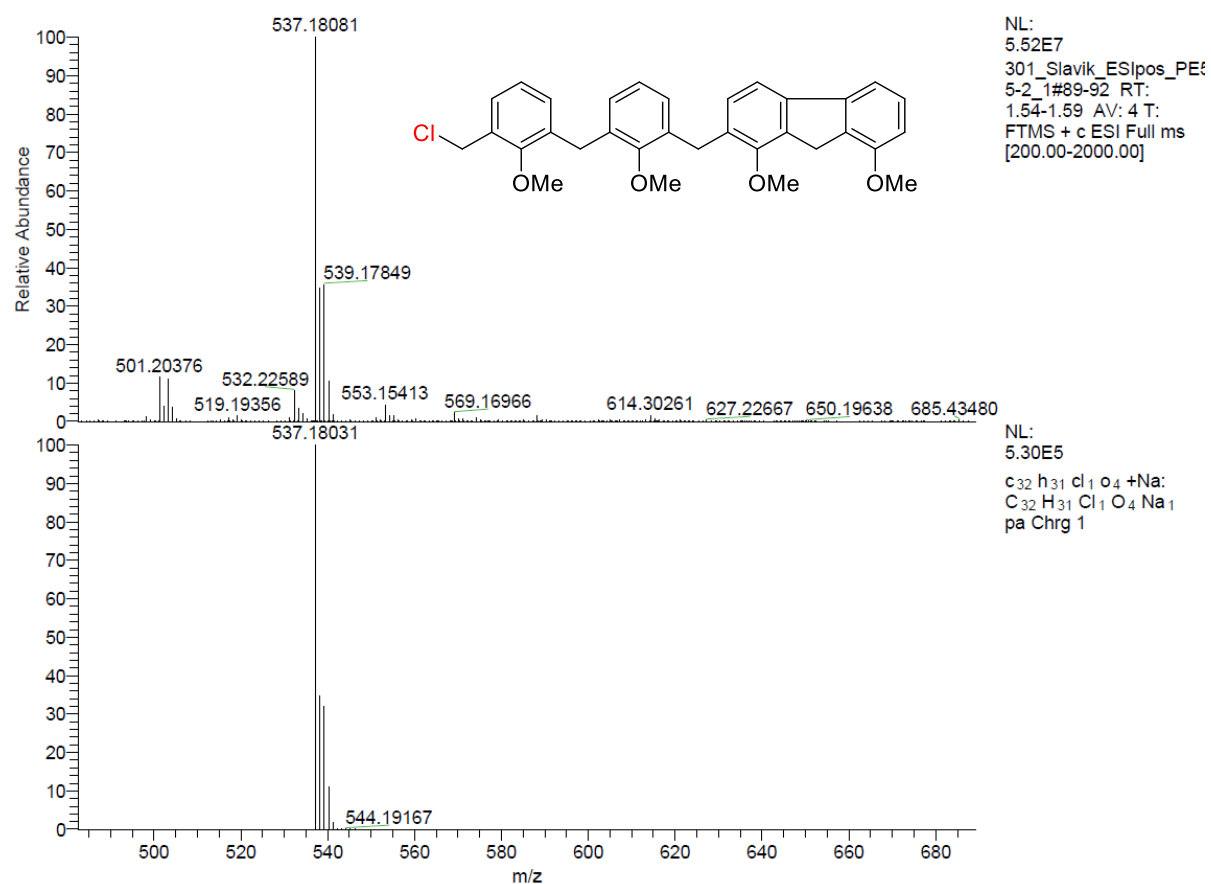


Figure 32. HRMS of compound 14 (ESI⁺).

NOE Experiments

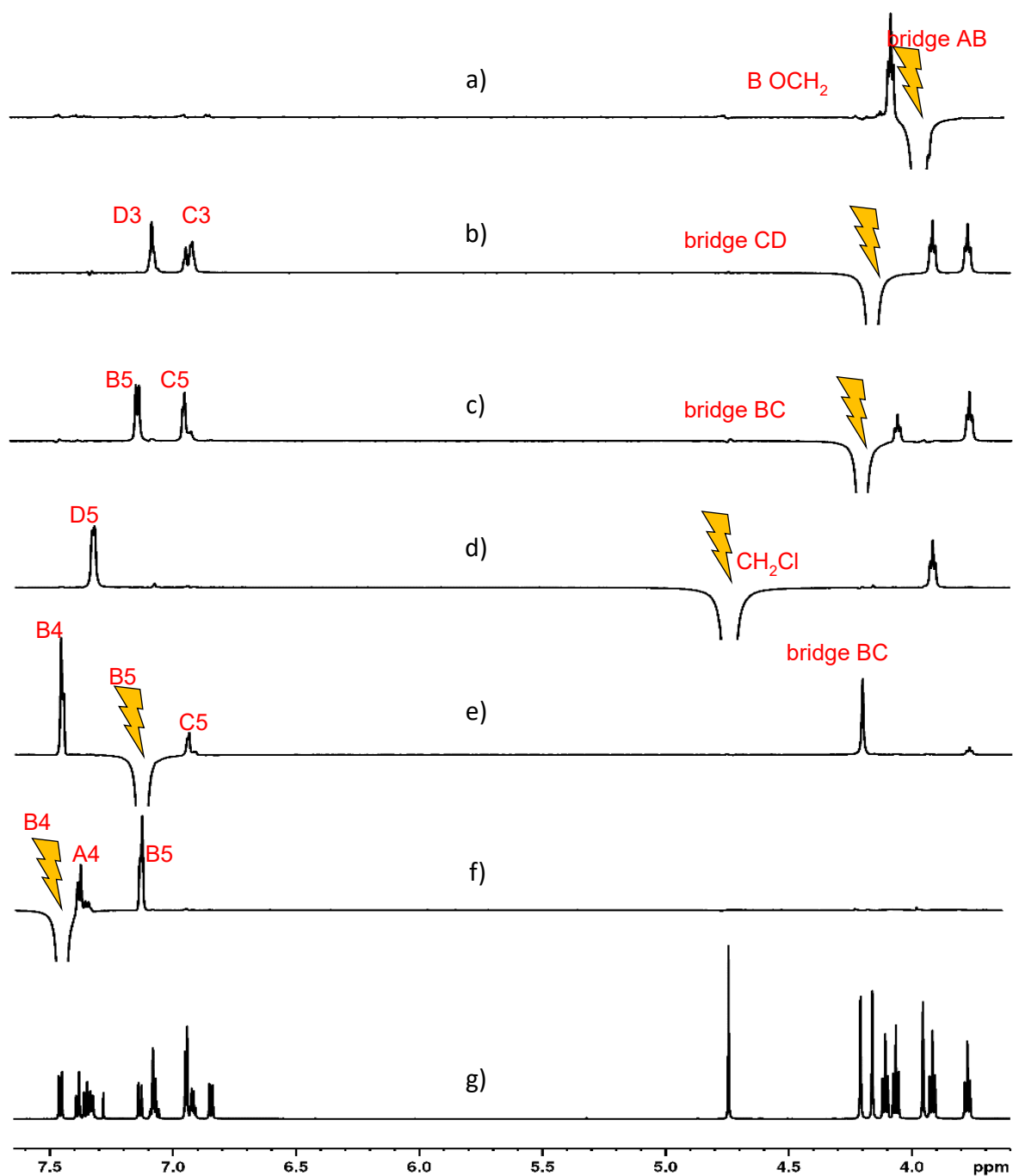
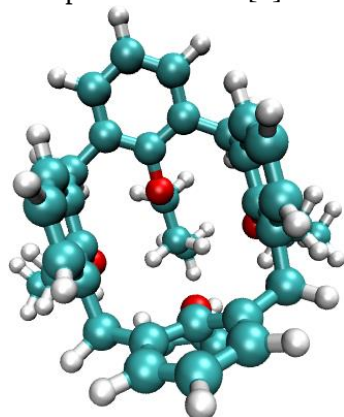


Figure 33. Partial NOE spectra of compound **4A** with a) **bridge AB** irradiated, b) with **bridge CD** irradiated, c) with **bridge BC** irradiated, d) with **CH₂Cl** irradiated, e) with **B5** irradiated, f) with **B4** irradiated, g) partial ¹H NMR spectrum of compound **4A** in CDCl₃.

Computational results – coordinates of stationary points

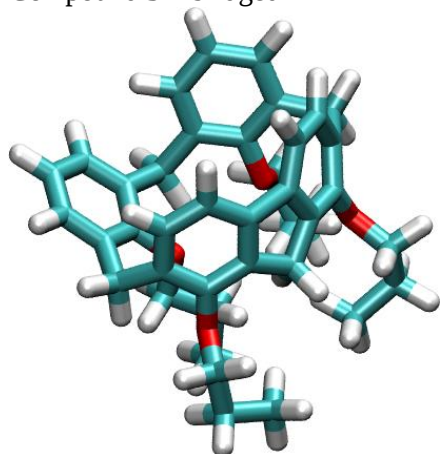
Compound 1 – calix[4]arene



C	3.89957745846149	9.25533292050903	4.09869168445039
C	3.68149108907781	10.35479237078169	4.93551790756702
C	4.53104893117089	11.45373055060493	4.80850662543585
C	5.51432794650072	11.48931923831386	3.82942852331583
C	5.60843361534797	10.44836280072773	2.91608121425713
C	4.79107264641735	9.32439397458043	3.02242062145765
C	2.45296425157384	10.41521614747316	5.81553004896216
C	1.27683596930051	10.94393081509088	4.99983946258309
C	1.39646181565903	12.16124658238748	4.32907079959624
C	0.09029973126422	10.21784854302495	4.84311051253867
C	-0.92202891418944	10.65687501617690	3.97741705122430
C	-0.75960019167396	11.87593247400299	3.32633095821713
C	0.38186528158473	12.63862243673678	3.51576651249978
C	-2.14611461772676	9.81445500179881	3.66264574409059
C	-2.14349843645984	9.41710000991454	2.20224828873432
C	-2.96946938868733	10.03267201970518	1.26439150226850
C	-2.85354966039752	9.73520564615195	-0.08884197710831
C	-1.87544005415750	8.84795636414370	-0.52298417228710
C	-1.02550929793328	8.22386882232321	0.38713476733991
C	-1.20669117762228	8.48593637966407	1.74667143663653
C	0.15044525151968	7.38694318005723	-0.06169171849503
C	1.43842427788657	8.19247940057410	0.00235797506122
C	1.55023899746098	9.37575566941575	-0.72436048417906
C	2.69936858418578	10.14915212274035	-0.66051012575374
C	3.73956558162199	9.76208271934583	0.16876864613023
C	3.65734019355924	8.60001671517847	0.93353573871006
C	2.51018601102704	7.80479125569142	0.81898828446080
C	4.76491496375204	8.28062956009062	1.92498262373443
O	2.39764129103712	6.64527733090894	1.55917273611125
C	2.96305446860773	5.47344134104403	0.97145419751571
C	2.37046617696531	4.25752522634370	1.65687365105663
C	2.92161891079388	2.94186260350927	1.11595162562513
O	-0.39227280407376	7.86469919790192	2.65743203457273
C	-0.87430022856036	6.59441216540322	3.10862884261565
C	0.17259970383230	6.00989812340615	4.02535726132943
C	-0.12613664932528	4.57324959960221	4.43928270639578
O	-0.08117191450678	9.03495911548088	5.53343152380080
C	-0.84056504861987	9.16038200278859	6.73819241643071

C	-1.34961744966255	7.79301218469798	7.14622244009628
C	-2.17371737400693	7.86418137832179	8.42910985538779
O	3.21817669510616	8.08324804934308	4.35573718729838
C	4.06986383369561	7.12262284226475	5.00362037737353
C	3.25193064019685	6.01516514730210	5.63052529923283
C	2.36274961307173	6.50140334507674	6.76867043232665
H	-3.70571040823332	10.75477241766193	1.59806939328447
H	-3.05071974238044	10.38917040055872	3.87475634241572
H	-2.15873678035003	8.93098723126937	4.29614591938091
H	6.17692480147471	12.34196207425287	3.75203070563783
H	4.61903747409897	10.38720501437232	0.25356351587093
H	4.60671293851664	7.28870862826401	2.33423003835908
H	5.72641499450011	8.28258238250590	1.40657065335635
H	-2.52499898313217	6.87584131148800	8.72877753506241
H	-1.58432755409368	8.27329511404562	9.25357060876246
H	-3.05049135007047	8.50251946570311	8.29888777238597
H	-3.50935874354571	10.21181170343991	-0.80597449353231
H	2.20458150158353	9.43432857097454	6.20776746151533
H	2.64279317323659	11.08304537983599	6.65944520551765
H	0.25991675581795	6.50755722132920	0.56563064172625
H	-0.02095893489912	7.04541296016839	-1.08559281501680
H	0.71480053605933	9.70273809665626	-1.33032391541914
H	0.49446859370724	13.58667301761743	3.00631988045790
H	2.77523637567647	11.06185156276412	-1.23721854290764
H	2.45152621971415	2.09337239865141	1.61423448768726
H	2.73067027215558	2.84175685256572	0.04395198226756
H	3.99983767264849	2.86361363728468	1.27963999184518
H	-0.50058700559193	7.11917098178016	7.27748209568540
H	-1.95028355622066	7.38417823843088	6.32962785753002
H	-1.52967575526955	12.21339918014754	2.64346485803274
H	4.65762007402949	7.63755182029418	5.77243561892362
H	4.77557254844191	6.70960635221165	4.27445365286724
H	6.32492300655160	10.50542669508708	2.10526789543454
H	2.65203712561609	5.53484013157635	4.85755196553706
H	3.95872986170321	5.26292681696367	5.99641078872726
H	-1.75911726067870	8.64063803594737	-1.58064802601122
H	0.25905877267669	6.65603691689776	4.89553867284506
H	1.12212302685688	6.07351582482405	3.49798419992639
H	-1.67946556330433	9.84658775253606	6.57613443494317
H	-0.20986265655004	9.59472909935542	7.52496458807893
H	1.77874968458537	5.68104962978601	7.19150212218808
H	2.96200573393507	6.93637730098449	7.57283546416290
H	1.67207108922772	7.26332202605621	6.41092051760488
H	0.65810267942567	4.18756075453654	5.09341082885669
H	-1.07153727115765	4.49166259072015	4.98242623194989
H	-0.18467972405115	3.91010461321929	3.57260031412601
H	1.28515900659627	4.28801477144379	1.53050333410745
H	2.56892132379559	4.33109426840863	2.72876430949293
H	4.05504043879480	5.48870777795450	1.09204084198531
H	2.74155722258835	5.45752967530742	-0.10259178379148
H	-1.05508616132276	5.94189961454094	2.24510803589337
H	-1.83519684027279	6.72539416012299	3.62268271838810
H	2.30947740268813	12.73082099951451	4.43199216305882
H	4.40717626134681	12.29563213934155	5.47905989218153

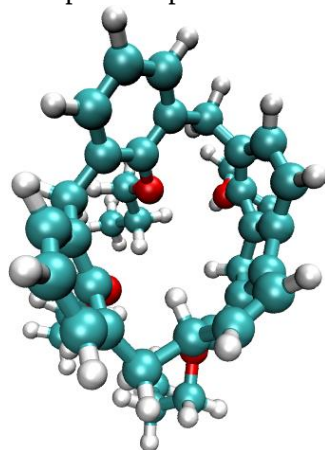
Compound 3 – bridged



O	2.71232598586232	7.01506466874381	1.78237712987591
O	-1.05816835325159	8.96124236182130	5.57968332127326
O	-0.61349003356357	8.21886080725546	2.81187460154909
O	4.14006934989828	7.62535353221149	4.34755101642210
C	-2.79462892132686	10.50837509539717	0.96885234414399
C	-2.55547639107807	10.26991440943436	3.47963193774763
C	2.82070408024009	11.04941306349821	4.09417889717302
C	3.70616958734687	11.62846269858348	3.18868362956064
C	4.24753011696312	9.53867665145391	-0.36316256255704
C	1.41519096333202	11.38160464916084	4.35355753693033
C	5.17522658315822	8.50127195009647	1.74692384568742
C	-2.20587996617591	9.85827406943005	2.05174267133967
C	4.09622385039681	8.62040817547815	0.67154714443201
C	-0.60978899776064	7.04124797927797	7.88861797007264
C	-2.41244986461572	10.22141981462774	-0.33619771322652
C	1.88029486846435	9.27647108029925	5.39395392336476
C	0.38412988707797	7.68559858326529	0.22552317737106
C	1.93088137745004	9.31612759846702	-0.95700662762150
C	0.60474672371645	12.31414757848846	3.70862265265734
C	1.74392817852052	8.34819282768025	0.03155564336532
C	3.17659475023194	9.88127133850235	-1.17824674580953
C	3.05154431868688	9.74885995155623	4.56551325292309
C	3.25645679005757	3.29378521258213	1.98372530921963
C	-1.85039232947224	7.86493758861458	7.55967805450194
C	-0.74349407096609	12.01956566662483	3.56788183014286
C	2.84758837106079	7.99048629006939	0.81648346399153
C	0.83376570298123	10.30177046217433	5.03301382098888
C	4.60222320592070	7.41077563647400	5.68822333856719
C	-1.31173673699722	10.86233911149765	4.11191326834595
C	4.62875398903110	10.79989218519854	2.57467127661452
C	4.31839654473535	5.97342640846244	6.08327087298156
C	-1.40095152199559	9.30306919450462	-0.57512871051348
C	-0.76176415803080	8.64787207229862	0.47766217414852
C	-1.20808979885829	8.90552837123226	1.78025766004844
C	4.71333078595144	9.43069519512630	2.85837713998248
C	-0.53040314309195	10.08066167881872	4.96840989776058
C	4.01910541932528	8.94333440934543	3.97418020772973
C	-0.36579144033888	6.20223238613123	4.06424314642869
C	-1.54413841764027	9.19753077169199	6.90622067905633
C	2.82900522122977	5.66861966530781	6.21748292939237

C	-1.05342743448591	4.98558150624233	4.67434143301015
C	3.03863793493044	4.72785025297997	2.46175372876610
C	3.07531110190609	5.71327758169222	1.31229653552844
C	-1.30358633540205	7.02852725626324	3.21390629895178
H	-3.56172397503656	11.25096243797720	1.15439513911174
H	-3.37157700355778	10.99361277336170	3.44298659520321
H	-2.89507702499269	9.41655951462076	4.06418692218555
H	3.57851609129603	12.64675972879037	2.84492443520918
H	5.20625930334876	10.02299952734314	-0.50498519094579
H	5.28087064704058	7.48525123651165	2.11723674493242
H	6.13134994687523	8.82379907404341	1.33167051812626
H	-0.88272098764215	6.09276247811808	8.35450355926809
H	-0.03470625737022	6.81856953592313	6.99197701201338
H	0.04272178598272	7.57980629684122	8.58077019922643
H	-2.89757357581059	10.72083848114462	-1.16474524387050
H	1.56823592195287	8.27401311161457	5.10513396682934
H	2.09818264213644	9.25427925534729	6.46721888581632
H	0.46071816052532	6.99097762018807	1.05552089221338
H	0.15573988809060	7.10462390397820	-0.67301696624658
H	1.09018610076287	9.62845429704148	-1.56052634356289
H	1.03065327130419	13.16080793061505	3.18634075346871
H	3.30902584305021	10.61050933160686	-1.96730913916919
H	3.19902164703409	2.59204661974628	2.81699949290582
H	2.49727667338409	3.00358680818804	1.25367567234079
H	4.23233015017408	3.17062605495041	1.50663241369558
H	-2.51485544574121	7.30085408121480	6.89861291213535
H	-2.41661414198308	8.06571911755558	8.47406497164234
H	-1.35076891872844	12.63452944467809	2.91404632080094
H	4.09535356685548	8.09638732246736	6.37234427617057
H	5.67542628453485	7.63017424333565	5.73389438602318
H	5.20480969805235	11.18785043391269	1.74419020792360
H	4.77496619429442	5.30940285775105	5.34442911300505
H	4.82995877962009	5.77970858948969	7.03120523990154
H	-1.10428905056936	9.08145909230774	-1.59288594354558
H	0.01598584528347	6.84866113887312	4.85235406768076
H	0.48829031928437	5.90633995203569	3.45465544693133
H	-2.44260650245747	9.82360617945998	6.85495220022289
H	-0.78698501077589	9.74687099882656	7.47787874103723
H	2.66301992623231	4.63693752979267	6.53406052064952
H	2.36160190091852	6.32090522299151	6.95808926541878
H	2.32019548871056	5.81906748720891	5.26699572040114
H	-0.35045275505607	4.39638674265858	5.26628053237123
H	-1.86881551121651	5.28686673864540	5.33590129209849
H	-1.47334395584583	4.33195064820139	3.90496635603956
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H	3.78986157815465	5.01600865388346	3.19866912379360
H	4.07711974824988	5.75153933529397	0.86758369475022
H	2.37989324255623	5.40879631761244	0.51982340541911
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H	-2.19903663506752	7.29760608107360	3.78304778594124

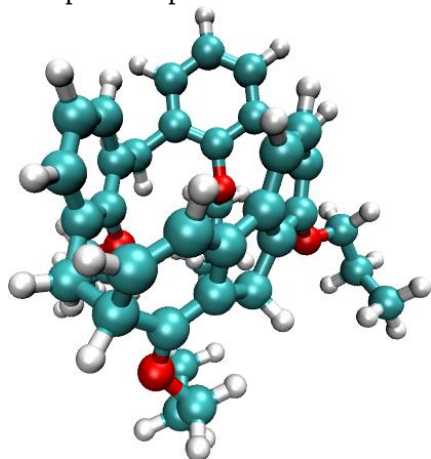
Compound 3 protonated – A-endo



O	2.50306097493158	7.48707983334562	2.05308317691235
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O	-0.94245119593931	7.82827012824673	2.66145096325785
O	4.50484373555704	7.64867398524336	4.54314777965666
C	-2.61240328874287	10.72633920989817	1.18377144467930
C	-2.39469083571585	10.01874879520678	3.62236358461088
C	2.93731302000765	10.92707493718648	4.29098813318359
C	3.69901868523356	11.57454250898497	3.30594841688619
C	4.33592450853694	9.26878484547948	-0.55762400353232
C	1.57190203125844	11.16570253945459	4.63833264004767
C	5.14939839017269	8.52625066911780	1.71550327749138
C	-2.18530688311740	9.80902134745662	2.13276737480192
C	4.06664958142933	8.61854570695679	0.64250170275937
C	-2.06568032745532	6.43882748799739	7.27568527589480
C	-2.14140274699760	10.64712028255900	-0.12528556890269
C	2.20918707800651	9.10280804425592	5.66451161235096
C	0.34128593966482	7.73492573021718	0.11785520264633
C	2.07075213352456	8.93855692771624	-1.28195361651347
C	0.70717789303151	12.19025886544442	4.13226694497584
C	1.74851519130023	8.28690584222277	-0.09043061854475
C	3.34850015291730	9.41968101921504	-1.52073319391406
C	3.27292243242825	9.62951527436382	4.73416536851133
C	2.11455525062212	3.97277787943882	3.30234233576534
C	-2.81777685196053	7.59901688239060	6.62828529271930
C	-0.57033287104399	11.83813141430973	3.89249762064950
C	2.76744872174703	8.12596393716966	0.86081735060170
C	1.07118078485025	10.04788714145368	5.33864871429575
C	5.84432723718875	7.11312119960105	4.48529669623339
C	-1.00233837944165	10.43825778711773	4.14834694283314
C	4.57330236402830	10.78883747297904	2.59290887505416
C	6.11347736288460	6.32040690775799	5.74908439385974
C	-1.18738786446354	9.70108500367931	-0.46825472719555
C	-0.72928764423716	8.75893575418477	0.45916560962088
C	-1.30259297666594	8.78638717026853	1.73042671147748
C	4.74602487088554	9.41822572375848	2.87089029312980
C	-0.27851490868117	9.76673174072164	5.29158132324203
C	4.25305109763543	8.89394394465672	4.07967324837721
C	-1.33296648810954	5.66136293198946	3.63926821903551
C	-2.05428550469242	8.90139136753159	6.63498324533308
C	6.17775394569049	7.16196778243844	7.01939566101914
C	-2.38506494646472	4.63207092426185	4.04606188264794

C	2.34836033390377	5.47885808989285	3.36295002521685
C	2.63198906804491	6.05684170883723	1.99237857060441
C	-1.89889648107086	6.75245215248620	2.75800192712963
H	-3.29574353682556	11.51747911579542	1.46802215925347
H	-3.14940802050964	10.78112790037830	3.81255425988478
H	-2.71375433846659	9.09983196970220	4.10340276486509
H	3.50330497617396	12.59526698864928	3.00897334752899
H	5.33142028717046	9.65319517465477	-0.74288850480310
H	5.28114098045778	7.49945454363757	2.03907747325458
H	6.09437836168405	8.85620418185313	1.28144674674019
H	-2.68084826161328	5.53968150592740	7.27892813418795
H	-1.14561407790411	6.21368373964301	6.73743908554425
H	-1.79907697363998	6.66937565829032	8.30903031520304
H	-2.49484842156920	11.34894816171146	-0.86876528177573
H	1.95547870456484	8.06412702114528	5.45451892658368
H	2.52146660595006	9.16460029648004	6.71231641711811
H	0.36012517878677	7.00219638338073	0.91663321529772
H	0.04795789997081	7.21571775599236	-0.79827520080358
H	1.31259070695020	9.05051390918006	-2.04623957687093
H	1.09828180762796	13.15469343635982	3.84069756882698
H	3.57830833248525	9.91056967675898	-2.45678404541569
H	1.86283535554271	3.57281975810403	4.28531315758702
H	1.29395950677758	3.72509281404689	2.62516364085367
H	2.99971947322321	3.44329754973612	2.94247423364559
H	-3.09679231994742	7.34688591809979	5.60267874881625
H	-3.75261017114463	7.78679883977846	7.16460516766484
H	-1.25302579156358	12.50028995205949	3.37669211988352
H	6.55184440335329	7.93886379176935	4.37061880941220
H	5.92808578028500	6.46064299120812	3.61458418529189
H	5.04280949045979	11.19086613749029	1.70431652597046
H	5.34587566892644	5.54742453159792	5.84464047069989
H	7.06133690121608	5.79436871895073	5.60057560528551
H	-0.79519158194464	9.68769048900745	-1.47608471512654
H	-0.90115981637568	6.12881585931043	4.52650449418183
H	-0.51454662014112	5.16617068461964	3.11479841356302
H	-2.61425072254599	9.70766325564573	6.16383350649398
H	-1.79479509567067	9.20655777688026	7.65112711031423
H	6.39580183784343	6.53583382582641	7.88541765293728
H	6.96099218910047	7.92106751864330	6.95406760777326
H	5.23246620256326	7.67501371592969	7.20295678215392
H	-1.93486621979665	3.84751157824687	4.65529762504692
H	-3.18859142804457	5.08892137797096	4.62850184425744
H	-2.84017604684994	4.15511534536576	3.17535263887437
H	1.46651897712002	5.98457794549464	3.76086061490215
H	3.17081212519256	5.71838548430979	4.03550963588120
H	3.63835574083013	5.79670533822734	1.64511623113826
H	1.92701453967806	5.66239206372780	1.25285709644629
H	-2.11693684174656	6.37893986421427	1.75278611630152
H	-2.83620891050432	7.14068734384470	3.17167023924006
H	-0.36340101628036	9.92466015080829	3.40542865333980

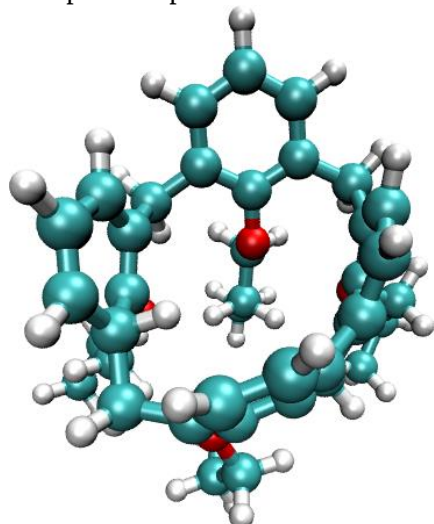
Compound 3 protonated – A-exo



O	2.50314725878977	7.39598323344561	2.11058697038678
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O	-1.05931295025123	7.78556534342047	2.70599524972929
O	4.09704637282055	7.82724786543333	4.64658709204150
C	-1.74579063290775	11.15911264415397	1.45244038480622
C	-2.53051882739431	10.12774060420682	3.58564794183193
C	2.24091292987801	10.86348835950209	3.89953481220216
C	3.00761745530682	11.48530963593534	2.90227850039621
C	4.48028777248278	8.78562054975022	-0.62541372979590
C	0.92238598211601	11.15337042400256	4.35723959885878
C	5.07806588107109	8.55166305732263	1.83937205930426
C	-1.75062372557298	10.04976642422455	2.29958651394337
C	4.13588660541280	8.36877162224514	0.65737621950560
C	-0.65065696458889	6.29817370312260	6.54539779605550
C	-1.02690096940889	11.15847651588450	0.27090417500227
C	1.61434479547013	9.13439215098248	5.42614047953130
C	0.42156874387830	7.63426300899237	0.22125157656662
C	2.25225441561535	8.32043255749118	-1.40654111856401
C	0.09560352767494	12.27139075369366	4.01515646537872
C	1.86442986311482	7.92308345318471	-0.12800128869551
C	3.55592920243167	8.72683785823628	-1.66138498419547
C	2.65093569800754	9.64284105412372	4.46787826087843
C	1.70767349015086	4.02194696469623	3.54197464266821
C	-1.22839637973298	7.17975379947941	7.64540016356402
C	-1.22024152115809	12.17788574392477	4.25395613054793
C	2.83958826525445	7.88558198391562	0.86996462459968
C	0.47511622283289	10.10613400357166	5.20034927838703
C	5.46915548660514	7.39511209770602	4.74702586435391
C	-1.82498582037315	10.93313902784414	4.79032503992446
C	4.04710464686761	10.75810372977485	2.37389461682032
C	5.67031522639171	6.67872848666872	6.06731221489761
C	-0.30891078247185	10.02825970796553	-0.09010200260282
C	-0.31801369056551	8.87942034122733	0.69623785172611
C	-1.04372523861478	8.90430546546778	1.90086529682576
C	4.37383053745706	9.46162377002233	2.82843698333488
C	-0.86384175868420	10.04036392288838	5.50589281361832
C	3.77965326245169	8.97921699685721	4.00916306701707
C	-1.56042844257536	5.43026754861027	2.75312647003247
C	-0.84798949295822	8.63728766907018	7.51203621725216

C	5.61279842980846	7.57964739774928	7.29560212764650
C	-2.61529633401160	4.33731418360399	2.62402543578858
C	1.97922733541354	5.52349307954642	3.51749844493770
C	2.55978588717218	5.96272624478835	2.18983748022686
C	-2.06980574058986	6.80564833213099	2.37797576777067
H	-2.32260993063043	12.03416347488778	1.72285656988266
H	-3.46753797007440	10.65267557375682	3.40135070494151
H	-2.77148260188368	9.14350034825303	3.97710676223646
H	2.73513478078527	12.44661030914482	2.49116772755731
H	5.47906440882643	9.15963140609953	-0.81468892513749
H	5.32728463672218	7.59321868776631	2.28026547446933
H	6.00711051233499	9.00271199630321	1.48812325682616
H	-1.01424221678106	5.27447328537773	6.63962129822341
H	-0.93929547866578	6.66762793606517	5.56119062393595
H	0.44044319390979	6.26982946499743	6.59207204906896
H	-1.03309175980118	12.02811283233182	-0.37293930785068
H	1.33213942351292	8.10408131292988	5.20402564266176
H	1.99693670396889	9.15814585310262	6.45129180761153
H	0.36479198423175	6.88084894084968	0.99898612531771
H	-0.08968487569033	7.23516416283847	-0.65876169424887
H	1.52341461555911	8.31555161656523	-2.20843820613438
H	0.52576926805305	13.13558210331825	3.52929074151371
H	3.84681096986542	9.02583960400878	-2.65956013491257
H	1.30779106187400	3.71028649846539	4.50822508793054
H	0.98071924201349	3.73871115829567	2.77883167698619
H	2.61674851687894	3.44618358044186	3.35423149318087
H	-2.31830464873970	7.10200319783930	7.66772800473171
H	-0.87315573549410	6.84711173583196	8.62500483079795
H	-1.89851692325449	12.96682604473167	3.95667335411769
H	6.12411850275530	8.26630564129239	4.65831478847405
H	5.68977745355055	6.70884989909105	3.92810088217571
H	4.56976147211729	11.13170524300509	1.50254613982302
H	4.92752319270964	5.87966115277411	6.14412554725793
H	6.64542628826896	6.18564054522689	6.01466524867641
H	0.26083568056085	10.03510181497798	-1.00879898494049
H	-1.19261009592886	5.46600823092940	3.77890122929267
H	-0.70101738805162	5.19186862622547	2.12385089319120
H	-1.24689371356451	9.22602463746022	8.33922388970834
H	0.22810013255532	8.78002869370756	7.46747462681441
H	5.79562184491307	7.00395944191339	8.20395738841292
H	6.36915156877468	8.36643207996118	7.24477974264366
H	4.63862890460279	8.06228075168499	7.39062225093032
H	-2.19715794101818	3.37329758681602	2.91734907427156
H	-3.47645364706398	4.53415677372519	3.26555185233164
H	-2.97822318632938	4.24413901702972	1.59854278313091
H	1.05251814780269	6.07871226803564	3.67091984953800
H	2.65763034236501	5.81051047004091	4.32176971966499
H	3.59895843656577	5.63411161344033	2.06859592195856
H	1.98903173635481	5.53242150691165	1.36039755306218
H	-2.29528395299264	6.86220230427692	1.30967812867873
H	-2.98826166201064	7.04782262371402	2.92476600338075
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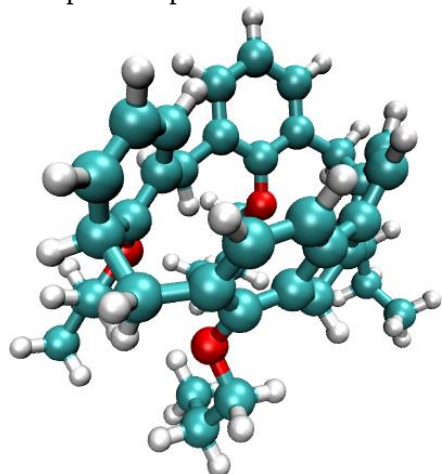
Compound 3 protonated – B-endo



O	2.43107182674416	7.64319853937299	1.99621853512584
O	-0.86485053237048	8.68748809042725	5.57787127623033
O	-1.02284040658264	7.49465720449684	2.35331102444521
O	4.37803072354998	7.93937449679475	4.36414983134986
C	-2.31922507349743	10.73545385037165	1.11675499524327
C	-2.43977190754798	10.03018760317552	3.60028769025812
C	2.73487807488795	11.20577464823383	4.11179181776455
C	3.437404444859371	11.80180750503224	3.06483289832183
C	4.49149451960904	8.97359416820007	-0.72800637933363
C	1.34638915722192	11.43771298501365	4.52946870096720
C	5.15345325347363	8.72310703652651	1.69232210395077
C	-1.83627497290527	9.82386990054428	2.17033602309339
C	4.14610940539127	8.56304353459757	0.55823092966473
C	-0.43089879846530	5.89854598010164	6.53969687368277
C	-1.79765296241998	10.67303503331943	-0.12895768186403
C	2.07013948575341	9.38069098986310	5.50758387737583
C	0.48560440427746	7.57090049371821	-0.02402104616841
C	2.29047181726316	8.48152666380920	-1.54988478201858
C	0.42505445219153	12.36501670728651	4.04473607161150
C	1.90035038496601	8.06232176829934	-0.27905152995010
C	3.58468226793053	8.92526627466183	-1.77817541766248
C	3.11576974781013	9.94083841539721	4.57857805010294
C	2.23015003803450	4.40760202329711	3.91240104250532
C	-1.15818841960923	7.01404646427026	7.28529327669733
C	-0.90181537512862	11.97148580769394	3.96517824764234
C	2.83996931466078	8.08454714794200	0.75921612373180
C	0.89956815516885	10.28183887646266	5.19406712352584
C	5.51332685539355	7.87284475086229	5.25045144675106
C	-1.32509868795963	10.70015617100571	4.38232149304297
C	4.34163505409366	11.01875959824514	2.36203721686273
C	5.47671837723444	6.54545260749043	5.98085910322543
C	-0.82914455671400	9.68214537388496	-0.43168408232833
C	-0.47383861701578	8.66396660190327	0.42522532455442
C	-1.16450035536440	8.58620488905626	1.67099108301080
C	4.60636379118440	9.69118262347325	2.71805391831926
C	-0.43808905923644	9.91173313670028	5.13231395312130
C	4.08985893699380	9.20808188498216	3.92295304051061

C	-2.08478649738087	5.41182933596609	2.88069919277644
C	-0.66166203535011	8.41305595949922	6.97943332429512
C	4.31509540694032	6.43943770064028	6.96450042534022
C	-3.20852053665602	4.70789984295762	3.63698842676969
C	2.01947791424290	5.87542049222825	3.55442324695591
C	2.67910212311775	6.24757459940211	2.24511083681158
C	-2.08878265786872	6.89691283575954	3.16960432724380
H	-3.00598508184137	11.51886311084576	1.40800253766989
H	-3.31966383697060	10.66672053170676	3.50691133327983
H	-2.75023663160200	9.10811241016057	4.07080803056567
H	3.18561596759082	12.79056080150276	2.70532348380356
H	5.49467820999558	9.34055540995606	-0.90674082280722
H	5.36234763816197	7.76705126582628	2.16907432598861
H	6.08841386205501	9.08777757795536	1.26544089722170
H	-0.83088154652360	4.92474199311099	6.82740087494427
H	-0.53756200816811	5.99599635300064	5.45915154520281
H	0.63807378862808	5.89980393391234	6.76522372676927
H	-2.09494058897931	11.37858415004417	-0.89233369689086
H	1.85679448325020	8.33541195784843	5.29271665877542
H	2.37082912473582	9.44742425928358	6.55925446387233
H	0.49046248730595	6.78527862391276	0.72346555617830
H	0.09679555666996	7.13560782949294	-0.94695798013109
H	1.58585108609746	8.42957134950964	-2.37206412982574
H	0.74222082431005	13.29903610828334	3.60143657764686
H	3.88965417110798	9.23575641441978	-2.76854372358904
H	1.71046075400537	4.15349601512208	4.83686869966294
H	1.85767032618935	3.74035130933412	3.13129586386346
H	3.28936966510050	4.18608243073070	4.05999363236685
H	-2.23236116915144	6.96526538393152	7.08192992810386
H	-1.03811249561905	6.86769479478987	8.36298232616108
H	-1.60931758758086	12.60999281132577	3.44839655772424
H	5.45956303326177	8.70597911182085	5.96040887005235
H	6.42915955894176	7.98879588509396	4.66164500727406
H	4.77910195584206	11.40836135038697	1.45072458316374
H	5.42781226946680	5.74032681878692	5.24156771441351
H	6.42486957295826	6.42506405573451	6.51251329848387
H	-0.36635258341719	9.70258781467574	-1.41060885848154
H	-1.11577979186133	4.99469625995391	3.16232650534242
H	-2.20357983965736	5.25743168997062	1.80518093414648
H	-1.21484426822772	9.15786010962949	7.55730160383576
H	0.39754286014142	8.50810269341379	7.22570597338969
H	4.31592550401351	5.47519685183489	7.47453218945217
H	4.38313716978652	7.21800393890264	7.72881451631220
H	3.35807946415403	6.55100510312822	6.45299682847394
H	-3.21812314898279	3.64558711212954	3.39368239383551
H	-3.08759571349813	4.80558881430013	4.71805500901077
H	-4.18385651092589	5.11721590590007	3.36413614769768
H	0.95491005510941	6.10822945947597	3.48486223193132
H	2.43802974196025	6.51242683453387	4.33035963212545
H	3.75769105027813	6.07256878734396	2.28519014376120
H	2.27313188393614	5.65527129818357	1.41617752924659
H	-3.03615911646896	7.34980363128211	2.88101249774624
H	-1.85792696667767	7.12779573181248	4.20614992121820
H	-0.82075663355669	10.30839363273319	2.29831790745470

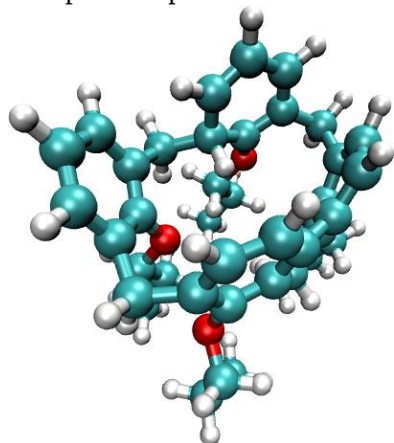
Compound 3 protonated – B-exo



O	2.79352885599468	7.55756341981327	2.34088224108958
O	-1.06402589893115	8.56027689517678	5.19163778900553
O	-1.57584535381542	7.37675898551803	2.16168670752218
O	4.49457251649256	7.87905371081119	4.67890143209697
C	-2.72866811264496	10.70843874057330	1.05492079524155
C	-2.73026688329306	10.05695663651083	3.48241472705307
C	2.75516184655225	10.99664967678104	3.96414332648645
C	3.62701514571797	11.65265042230603	3.09410879885632
C	4.54422318679130	9.13485705128299	-0.44707603257346
C	1.31345601223219	11.17575106879559	4.13160597307702
C	5.42500199146170	8.64844892459614	1.88501242556350
C	-2.72595237787954	9.52335021576642	1.94021909139381
C	4.32927773648837	8.60497619940258	0.82204764791797
C	-0.92975289262602	5.90872474020528	6.50983981198460
C	-1.65673265679317	11.03230474694822	0.31305652365459
C	1.93954782694943	9.17395025993421	5.27431014875943
C	0.58448066347962	7.88206112187262	0.67096188908628
C	2.22668415208664	8.84184093990176	-1.02516709305006
C	0.45627490377840	12.09731195469221	3.53998019517410
C	1.96247497565851	8.32584168685564	0.24363160975779
C	3.51295055503648	9.22669789059416	-1.37473448077943
C	3.10867355812218	9.76586764203150	4.52665788920260
C	1.73035838399357	4.13322933710123	3.43375720934951
C	-1.61581888448163	7.15202974155770	7.07207702393438
C	-0.88572402100249	11.76779119782365	3.42988574553923
C	3.03500042992099	8.15737020648666	1.12837424113099
C	0.80078524398101	10.03313232140621	4.77569246277415
C	5.84636268158237	7.39533743577824	4.75796534416278
C	-1.39181628151898	10.55724812993006	3.91408347247546
C	4.68355396916462	10.91727680369300	2.59065812902364
C	6.04243789235679	6.64895456880131	6.06332590692181
C	-0.52190745335422	10.16358238675414	0.27807050775243
C	-0.49049649459045	8.93183537560381	0.88164970003804
C	-1.60926480248753	8.57805806731385	1.67690870255298
C	4.91457123619834	9.58493509918313	2.97121457260413
C	-0.54531743168929	9.72523793847080	4.67088716432085
C	4.24589785671228	9.08603222237488	4.10146563910849
C	-2.36060310124258	5.22703857149915	2.79616410889712
C	-1.00257609860248	8.46431620131000	6.63043949593405

C	6.00465087315631	7.53159800190213	7.30583252262209
C	-3.34412808405517	4.39067733714593	3.60486153299004
C	2.09376110872975	5.61083422658402	3.55229358001101
C	2.78520478837190	6.12260533667713	2.30342249172005
C	-2.61505166410515	6.71252538800986	2.93613688590649
H	-3.59767894393277	11.35186576395748	1.09974523626166
H	-3.49641778494391	10.83081693050122	3.50937811724140
H	-3.05838113157229	9.23246224372097	4.10656868448247
H	3.40828220975491	12.63670792960805	2.70248651917026
H	5.53466640629634	9.48448218682054	-0.71147916900220
H	5.63398276783626	7.65293109217422	2.26364890733645
H	6.34102806306218	9.02277461918634	1.42663611238014
H	-1.40802644594341	5.00430484386172	6.88831614529006
H	-0.97454667227729	5.88345144272866	5.42030180279248
H	0.12321030488294	5.87459218098627	6.79906663215486
H	-1.63557227347426	11.94315831190171	-0.26890586898934
H	1.80023023749949	8.11688408543852	5.05082242796428
H	2.07013719336007	9.26791265559137	6.35823728504451
H	0.67214054438922	7.33268650594107	1.60000078504276
H	0.18319552672106	7.16909104364677	-0.05931892218174
H	1.42661794828310	8.92070208936577	-1.75229523862934
H	0.83389734231125	13.00349051181402	3.08644384271450
H	3.71215349433444	9.61430215956305	-2.36474752191603
H	1.29916087155843	3.75897603613292	4.36332537837604
H	0.99820111378476	3.97054164550084	2.63822531131235
H	2.60362608976818	3.51946681358217	3.20174978552958
H	-2.67845382015523	7.14732007389124	6.81000756450830
H	-1.56519203663914	7.13426922732868	8.16494160123018
H	-1.55153103059513	12.43888500412058	2.90367605383515
H	6.53328088073650	8.24237505637728	4.67721282394684
H	6.03892253264506	6.71738240878673	3.92287791641145
H	5.25744480964958	11.31871013935759	1.76367390803630
H	5.28637443098759	5.86138740400686	6.13272889097133
H	7.00906782189949	6.14022581229485	5.99736394783022
H	0.34099193886021	10.47101153730489	-0.29901698900731
H	-1.33799975655880	5.02086528014769	3.12170351494512
H	-2.42403886088288	4.95619439852568	1.73927030871119
H	-1.54728600187214	9.31166890596292	7.05682458839759
H	0.03806743095537	8.53367522853219	6.95396870436326
H	6.17920540392393	6.93954358544413	8.20551901211795
H	6.77500981023299	8.30536822603613	7.26345996406407
H	5.04040818410007	8.03147158231268	7.40773743516620
H	-3.12163136961400	3.33115439330096	3.47548995770790
H	-3.28188484563508	4.61757509864205	4.67134014993468
H	-4.37384545957040	4.55452135887131	3.27878536651978
H	1.18702371721315	6.20358090302689	3.70736475380358
H	2.73352964758134	5.79480531491725	4.41701637192071
H	3.81441565067751	5.75432926444066	2.22806892929498
H	2.25442620470856	5.78375730173141	1.40702598839881
H	-3.59189114860251	6.99952204345676	2.54142221588369
H	-2.50443476478822	7.05627627696794	3.96293837373301
H	-3.67496531885352	8.98640357641429	1.84586415860968

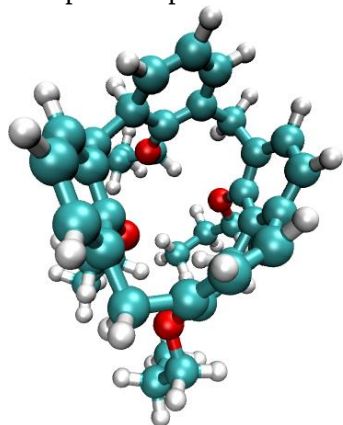
Compound 3 protonated – C-endo



O	3.38597674120471	6.90610634773342	1.46281199458807
O	-0.95116772462271	8.81132445299149	5.37680719058373
O	-0.65505303000275	7.94123095841714	2.62418423061962
O	4.35723360249020	7.63107816697287	4.16332106149328
C	-2.79847605895015	10.29572605270522	0.80229226793934
C	-2.53018964156086	10.11111810214055	3.31614027186664
C	2.89850629603433	10.99179916704033	3.90195975214648
C	3.83754111946886	11.65632112890287	3.11500219122708
C	4.27154492060649	9.83046108866619	-0.23975252597199
C	1.47114434371410	11.25676020054977	4.10122183326978
C	5.50596376187918	8.68093890455815	1.64400514061330
C	-2.21358149197863	9.65419157478171	1.89403838421138
C	4.33492109352369	8.80584892235313	0.66740860641953
C	-0.45807032713862	6.87745136090160	7.66677590484310
C	-2.39296764865805	10.03136033654994	-0.50076613650682
C	1.98640102683620	9.16441191683073	5.14524478518724
C	0.56134884572842	7.71237495345792	0.15223790863811
C	1.89245646425310	9.74950477328903	-0.43441525034488
C	0.64042440689223	12.17061576548933	3.45440436036725
C	1.81356751453785	8.59607491721263	0.50438818933213
C	3.05832890507937	10.28171505305089	-0.83476898900532
C	3.16477978617810	9.69111270524681	4.35926583602648
C	2.40933682614786	3.68541604424327	3.12541699656992
C	-1.67244592338595	7.76720118501557	7.42334166096765
C	-0.70374508505002	11.85107643802820	3.32779774626315
C	3.15798861131801	8.02132408772263	0.85520962128839
C	0.91580423801429	10.15661277784613	4.76918954159270
C	4.85716853641784	7.41020938261133	5.50649573543110
C	-1.25100565445499	10.69060598515562	3.88877245966537
C	4.86964949670987	10.90726363129601	2.57618106004786
C	4.56101890592815	5.98692841835071	5.93770684137080
C	-1.32866989965878	9.17114130766415	-0.73086383595143
C	-0.70313639579219	8.52288625775862	0.33245272625773
C	-1.21353547785939	8.70467691115064	1.62454056453119
C	4.99500064885521	9.52930487174405	2.80515190476486
C	-0.44683234173565	9.91437826237281	4.73058854510373
C	4.21802856138629	8.95631842532426	3.82659527218438
C	-0.72582780207705	5.87354799760594	3.86970567854451
C	-1.34713040606300	9.07637539063791	6.73829061701524
C	3.07620611403541	5.71083358025007	6.15811589409855

C	-1.62045133933950	4.89258022874956	4.61963271798346
C	3.28033472322165	4.80037701358524	2.55418544248096
C	2.44792505643424	5.88393663027358	1.91197989784108
C	-1.53773821140418	6.91150865269538	3.13017547702411
H	-3.57958421359735	11.02457737813586	0.98082836678311
H	-3.32118220077355	10.86030153273823	3.27313210962299
H	-2.88582517767100	9.29453806944740	3.94048144303548
H	3.70131595692586	12.68804937961495	2.81925517004113
H	5.18279363924849	10.37363856941617	-0.46033537659981
H	5.69942117042662	7.65374066130597	1.93516314230428
H	6.40475416641836	9.10285156696462	1.19532620988211
H	-0.75049250305870	5.94385982678326	8.14891416947675
H	0.04379508000219	6.62737334847194	6.73310518981870
H	0.26617451181382	7.37592913896191	8.31591075732775
H	-2.88463193723444	10.52064911666502	-1.33040166704747
H	1.70706305302383	8.15107398261435	4.85741726775707
H	2.18723306462050	9.14290438824419	6.22109160132024
H	0.51772941010771	6.85786852594706	0.80952271542312
H	0.65853474892272	7.35904073536825	-0.87395647427135
H	0.94867769994409	10.15281573287339	-0.76866265221376
H	1.04228346521752	13.04050851098111	2.95219238269608
H	3.08435476463199	11.10155960035874	-1.53909776035349
H	3.03298657390328	2.91835909651577	3.58410038470458
H	1.73322904284635	4.06246452884421	3.89256105557356
H	1.80877994448196	3.20404360186514	2.34978346790384
H	-2.41927241029315	7.23710634306735	6.82586838316636
H	-2.15427488393029	8.00792872034430	8.37499562762853
H	-1.33447458434408	12.46782663751869	2.69875803027638
H	4.38153002254631	8.12033374731290	6.18693595844010
H	5.93232690131245	7.61126924128677	5.50770354217237
H	5.51942115357990	11.36805469106146	1.84130385719753
H	4.97946293001810	5.29556134624551	5.20217145853332
H	5.11198263930383	5.80592775086034	6.86471603455663
H	-0.97510258046676	8.99950797833872	-1.74080949677356
H	-0.06182833723816	6.39179698245535	4.56324888800065
H	-0.10193872177750	5.32350866416833	3.16293302841346
H	-2.21640862201326	9.74186329319030	6.72952982493422
H	-0.53113758960752	9.59614277129456	7.25183131659527
H	2.90744000141156	4.67749147200323	6.46442828700141
H	2.67067223282215	6.35726646248029	6.93809232027153
H	2.50349884863504	5.88648603770634	5.24743222520888
H	-1.02585008749664	4.15389031629384	5.15795341178667
H	-2.24521074494978	5.41264700351869	5.34782239807150
H	-2.28035051250014	4.35377321288466	3.93517434053521
H	3.88677724221515	5.25678704876934	3.33302192826632
H	3.96525725184573	4.39574461218407	1.80480938730362
H	1.90986407511633	5.50588732383069	1.04538234778466
H	1.75703778587520	6.35854817746663	2.60724715150451
H	-2.07190123325018	6.46352174272853	2.28650628130118
H	-2.26517141878983	7.36313030065482	3.80406808034526
H	1.56804502461204	9.06088026029321	1.48712525167415

Compound 3 protonated –C-exo



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