

Supporting Information for

Regio- and Stereo-selectivity of Spirodienone Formation in 2,14-Dithiacalix[4]arene

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1. SPECTRAL CHARACTERISATION

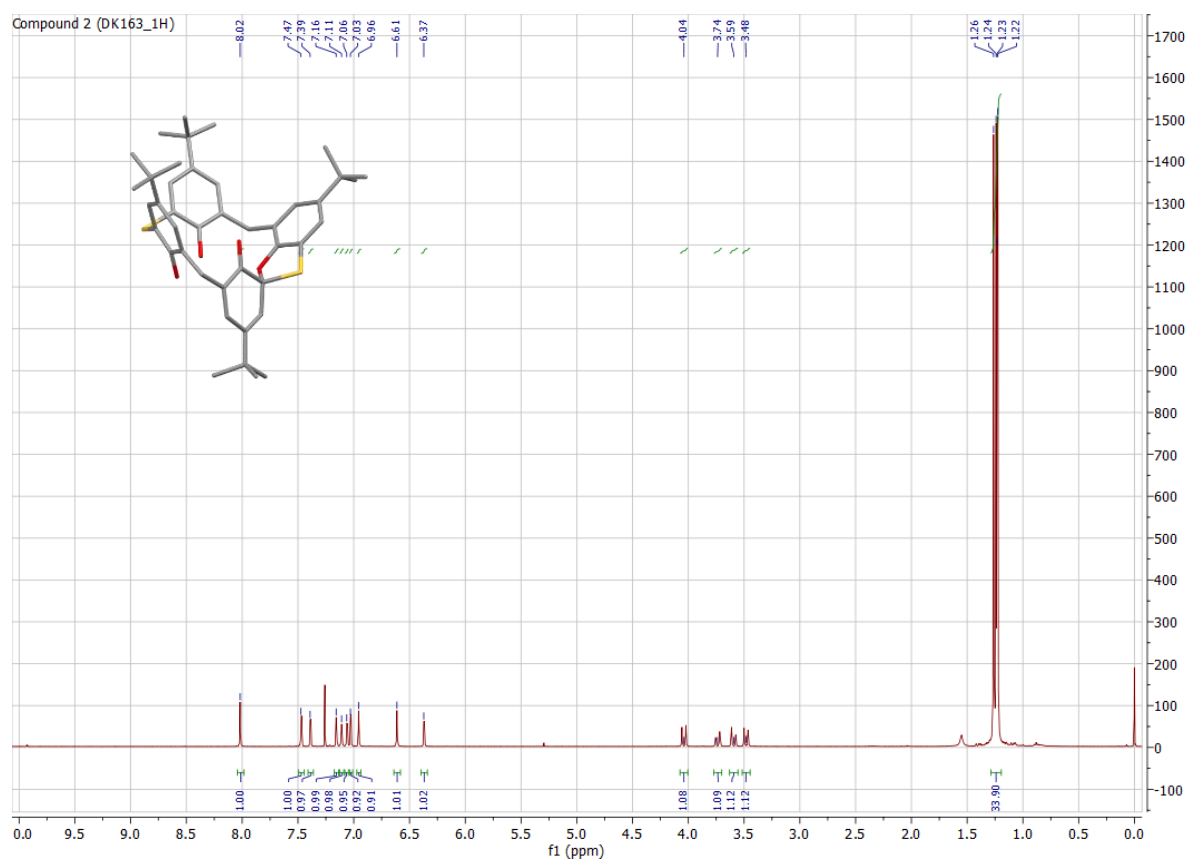


Figure 1. ^1H NMR of compound 5 (CDCl_3 , 400 MHz).

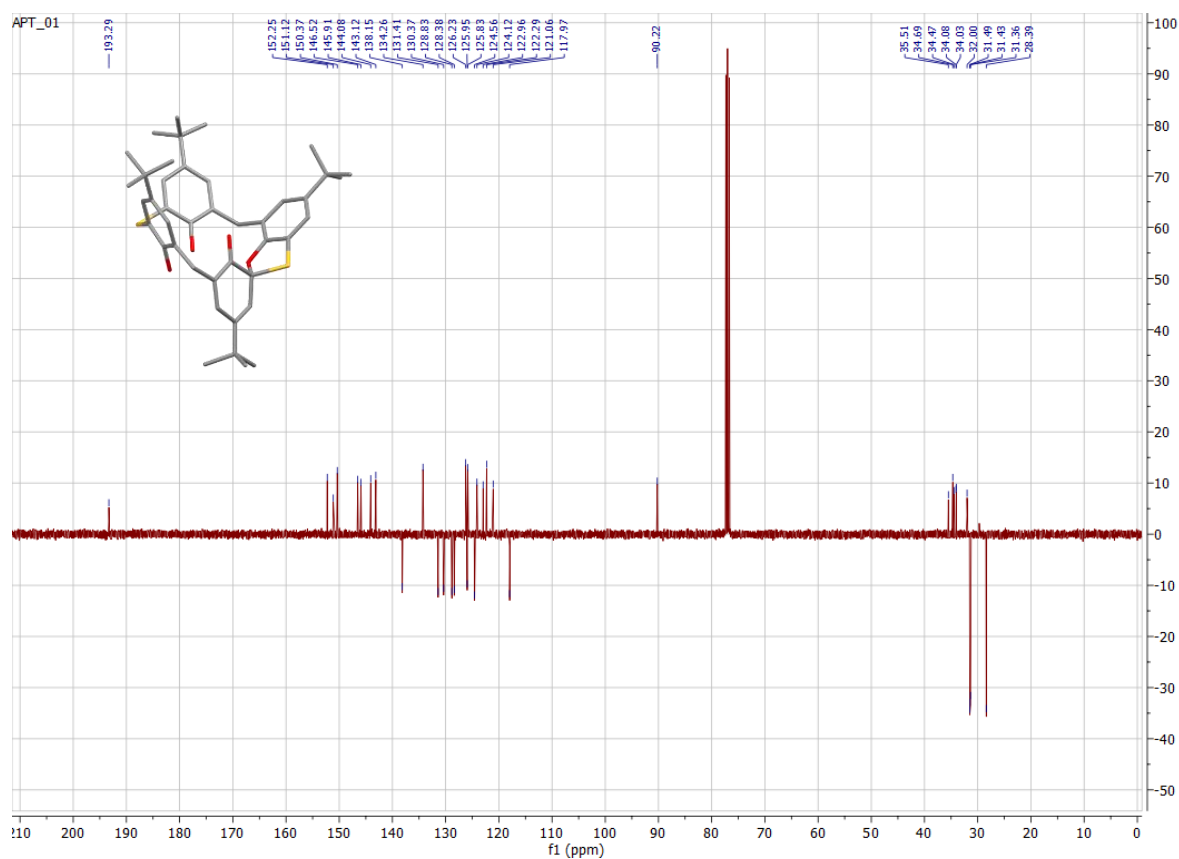


Figure 2. ^{13}C NMR of compound 5 (CDCl_3 , 101 MHz).

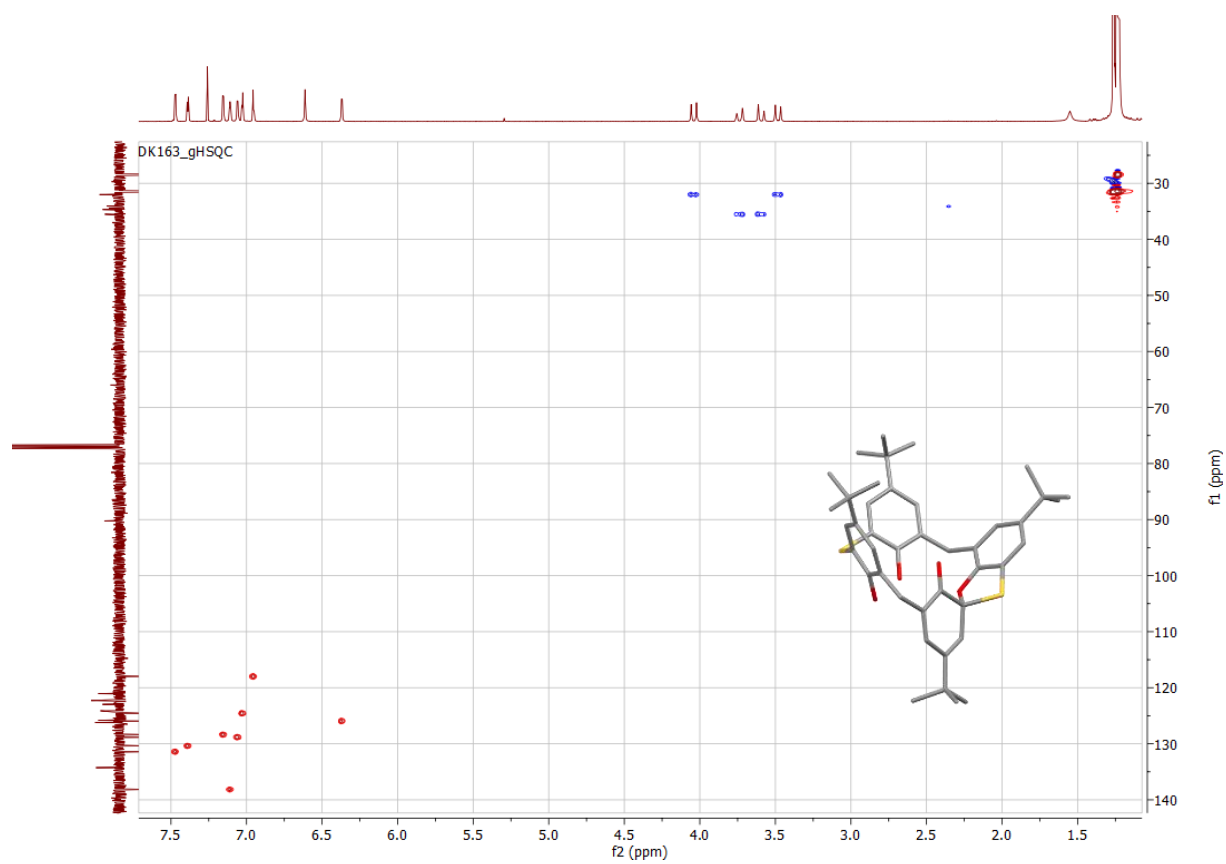


Figure 3. HSQC NMR of compound 5 (CDCl_3).

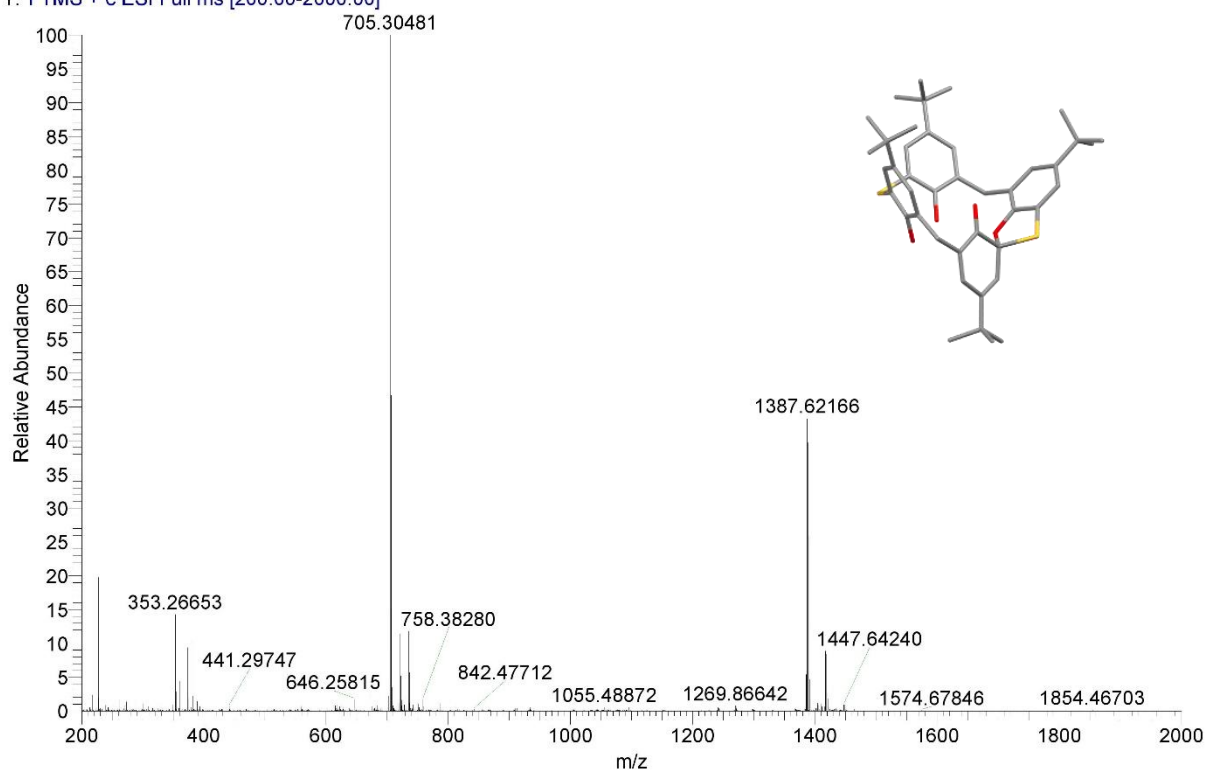


Figure 4. HRMS of compound 5 (ESI⁺).

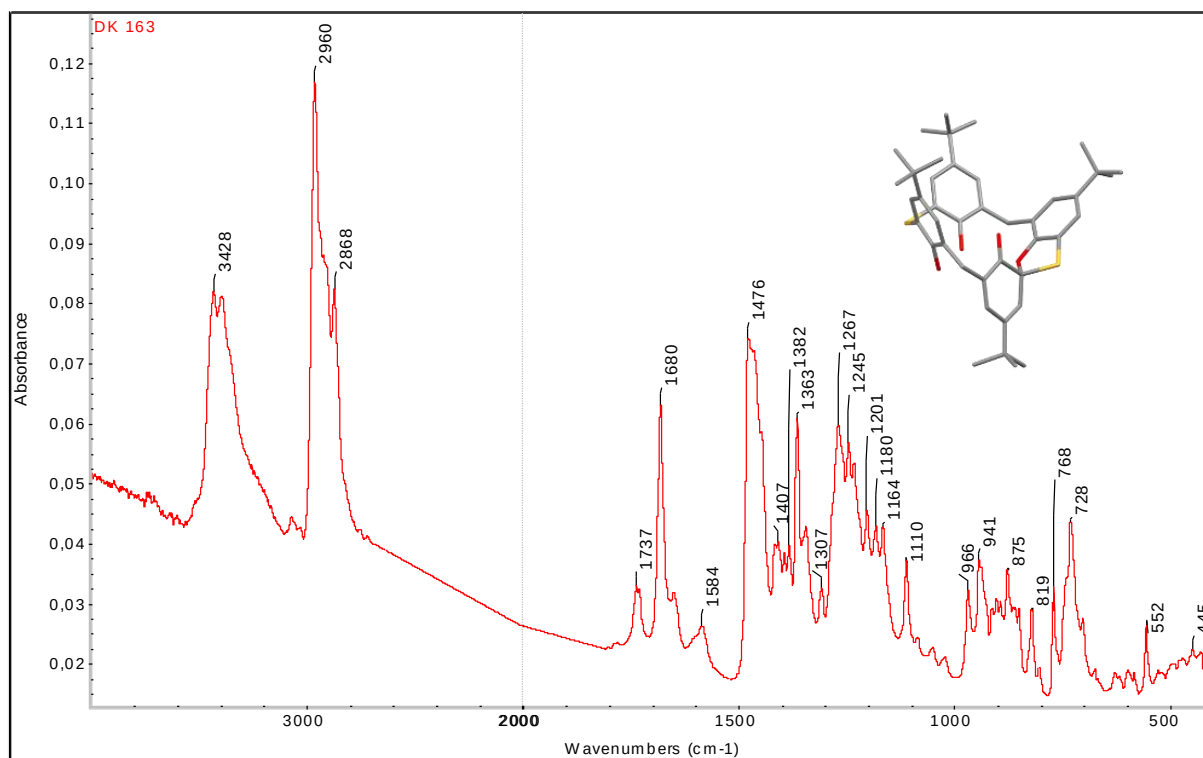


Figure 5. IR of compound 5 (KBr).

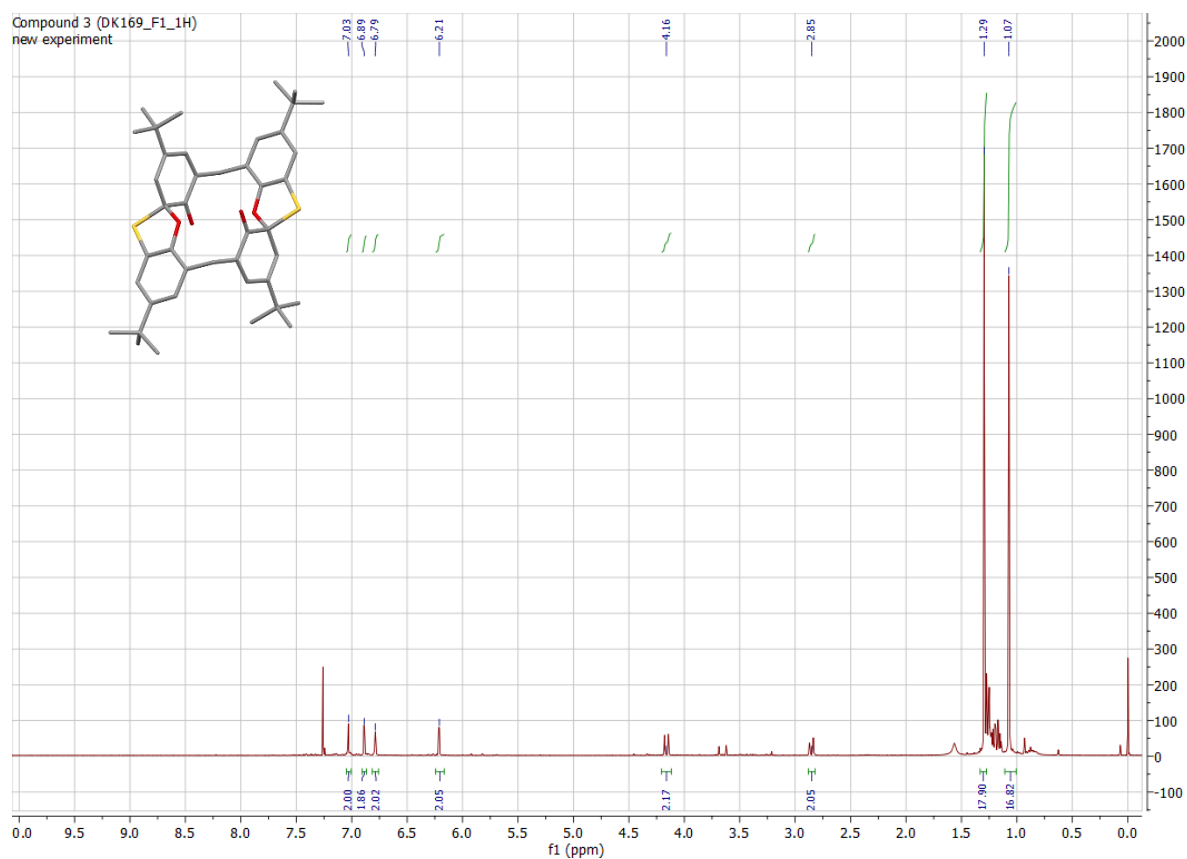


Figure 6. ^1H NMR of compound 7(*meso*) (CDCl_3 , 400 MHz).

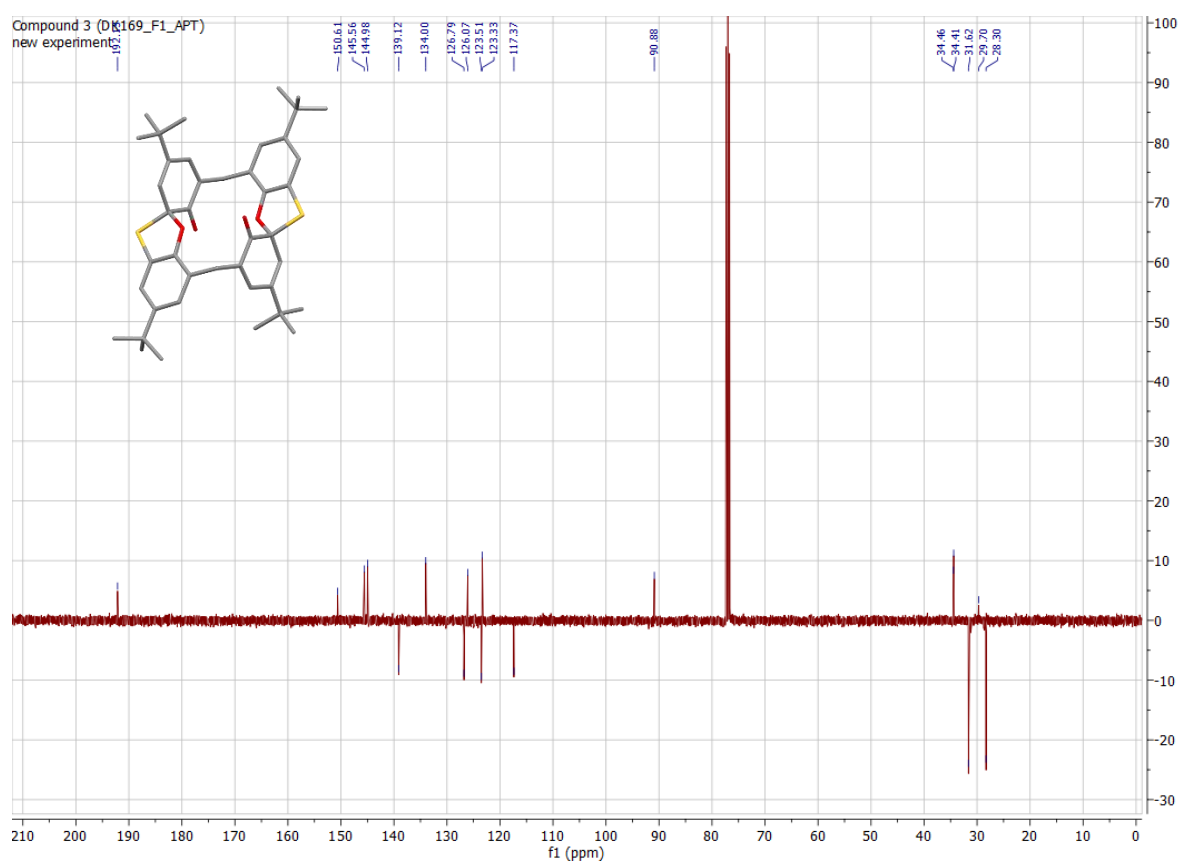


Figure 7. ^{13}C NMR of compound 7(*meso*) (CDCl_3 , 101 MHz).

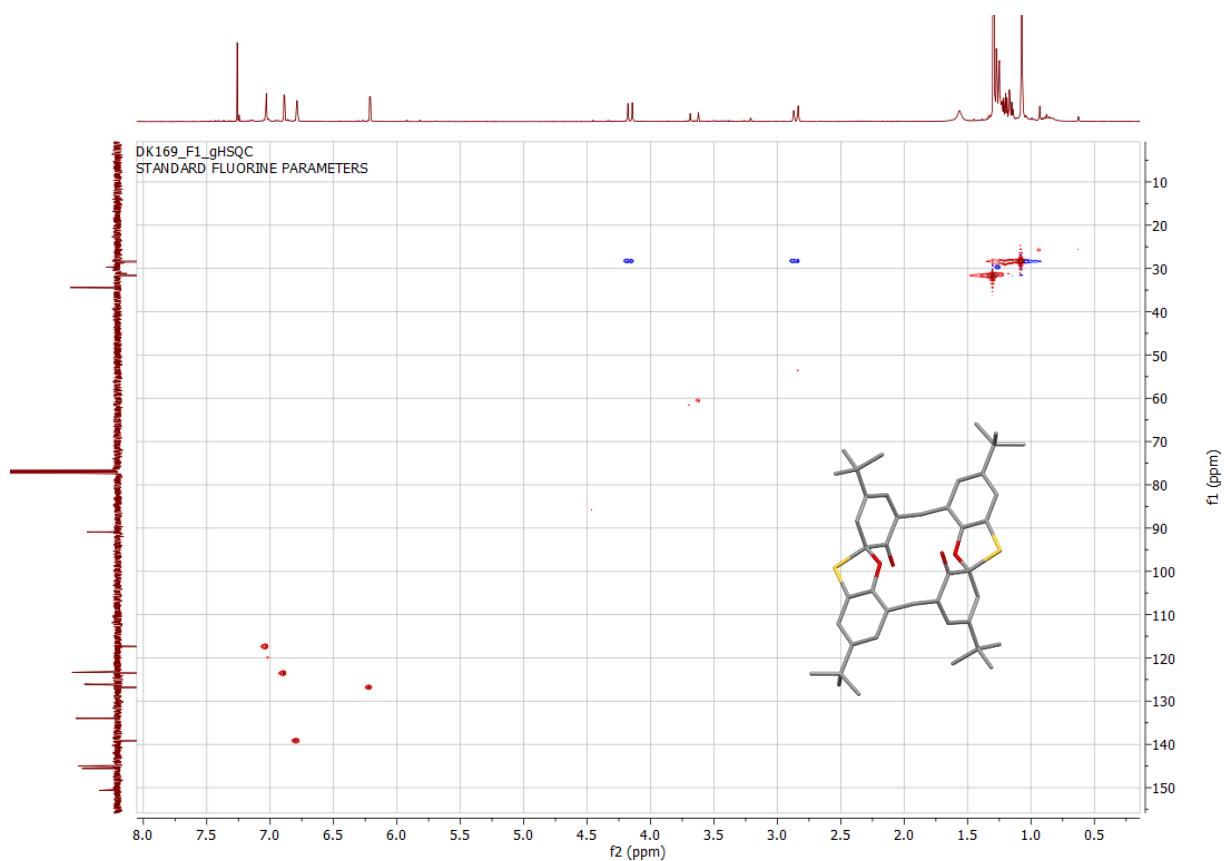


Figure 8. HSQC NMR of compound **7(meso)** (CDCl_3).

106_Kortus_ESIpos_DK167-F1_1
MeOH

6/10/2020 10:18:08 AM

106_Kortus_ESIpos_DK167-F1_1 #59-65 RT: 0.85-0.94 AV: 7 NL: 4.89E6
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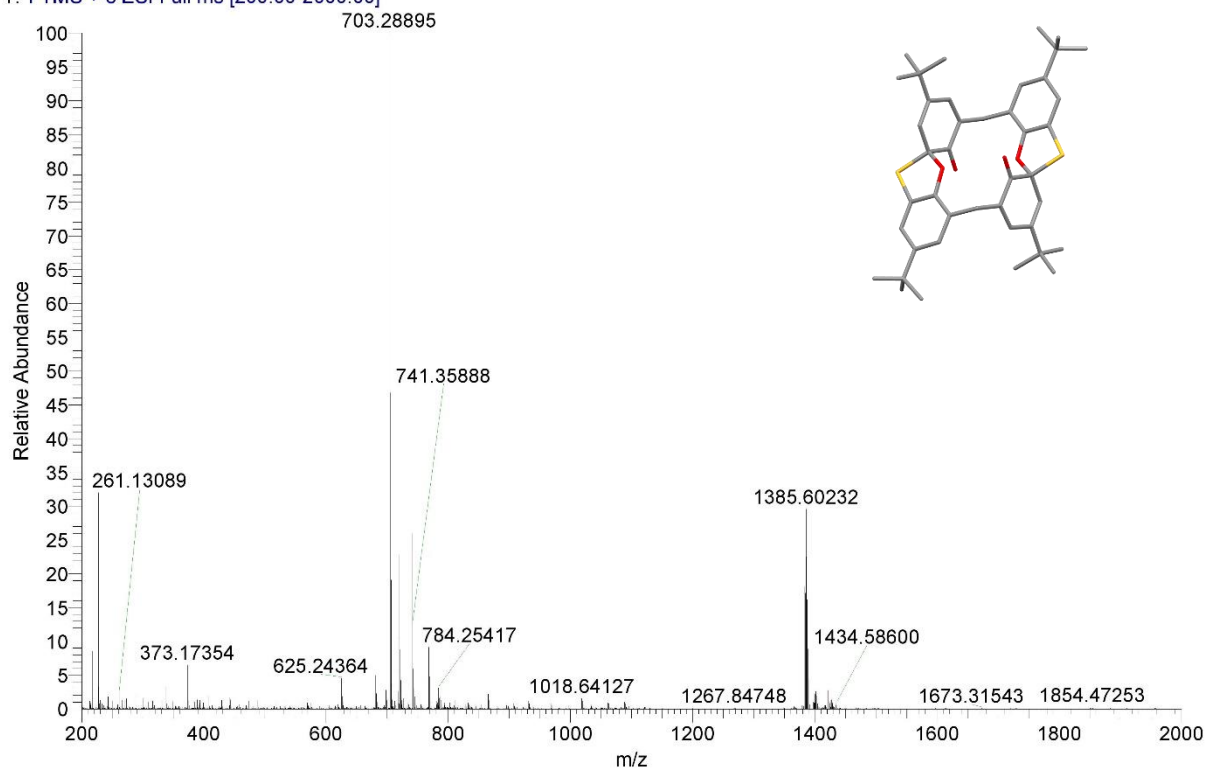


Figure 9. HRMS of compound **7(meso)** (ESI^+).

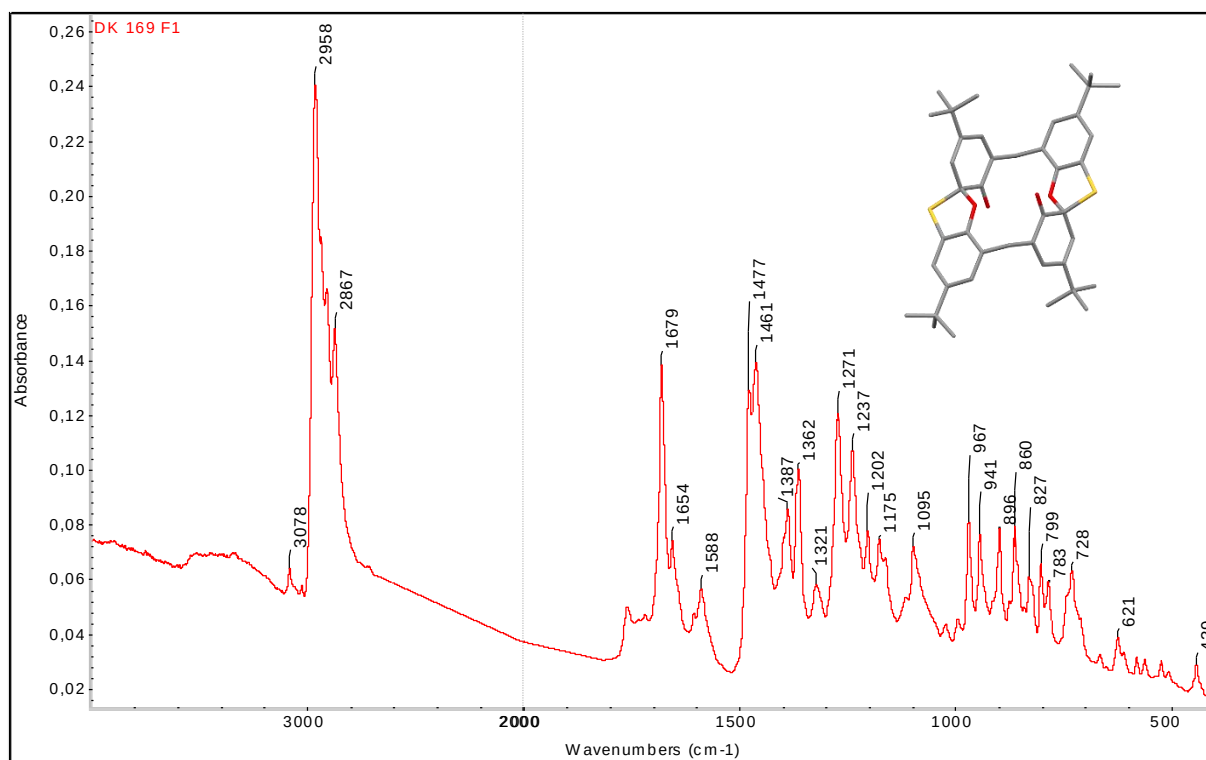


Figure 10. IR of compound 7(*meso*) (KBr).

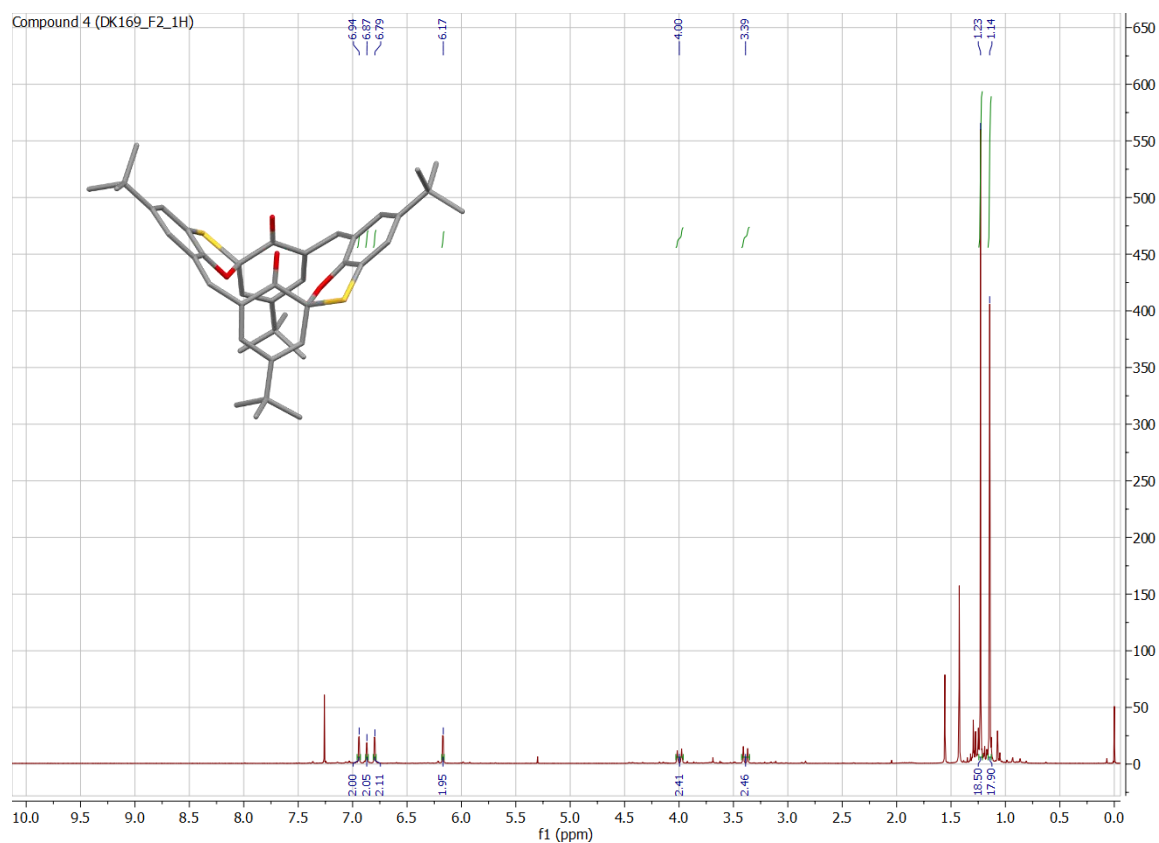


Figure 11. ^1H NMR of compound 7(*chiral*) (CDCl_3 , 400 MHz).

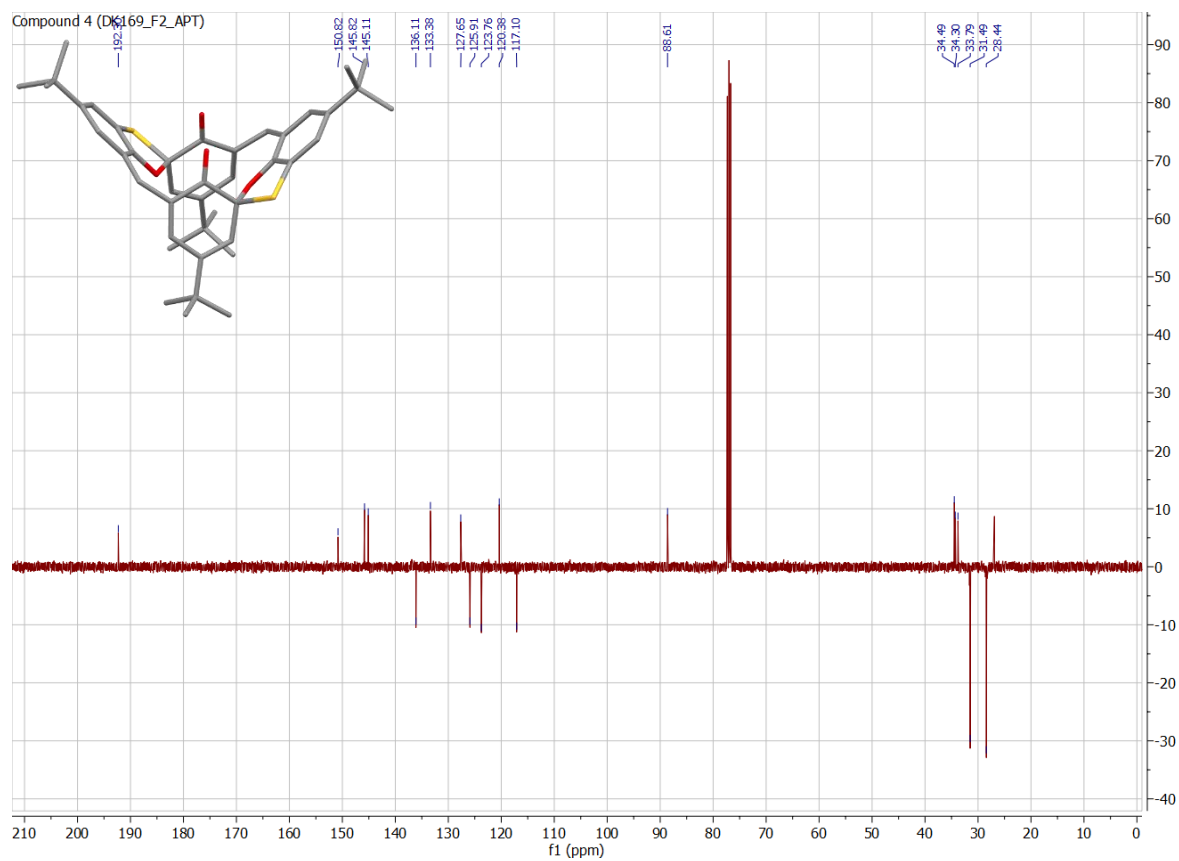


Figure 12. ^{13}C NMR of compound 7(*chiral*) (CDCl_3 , 101 MHz).

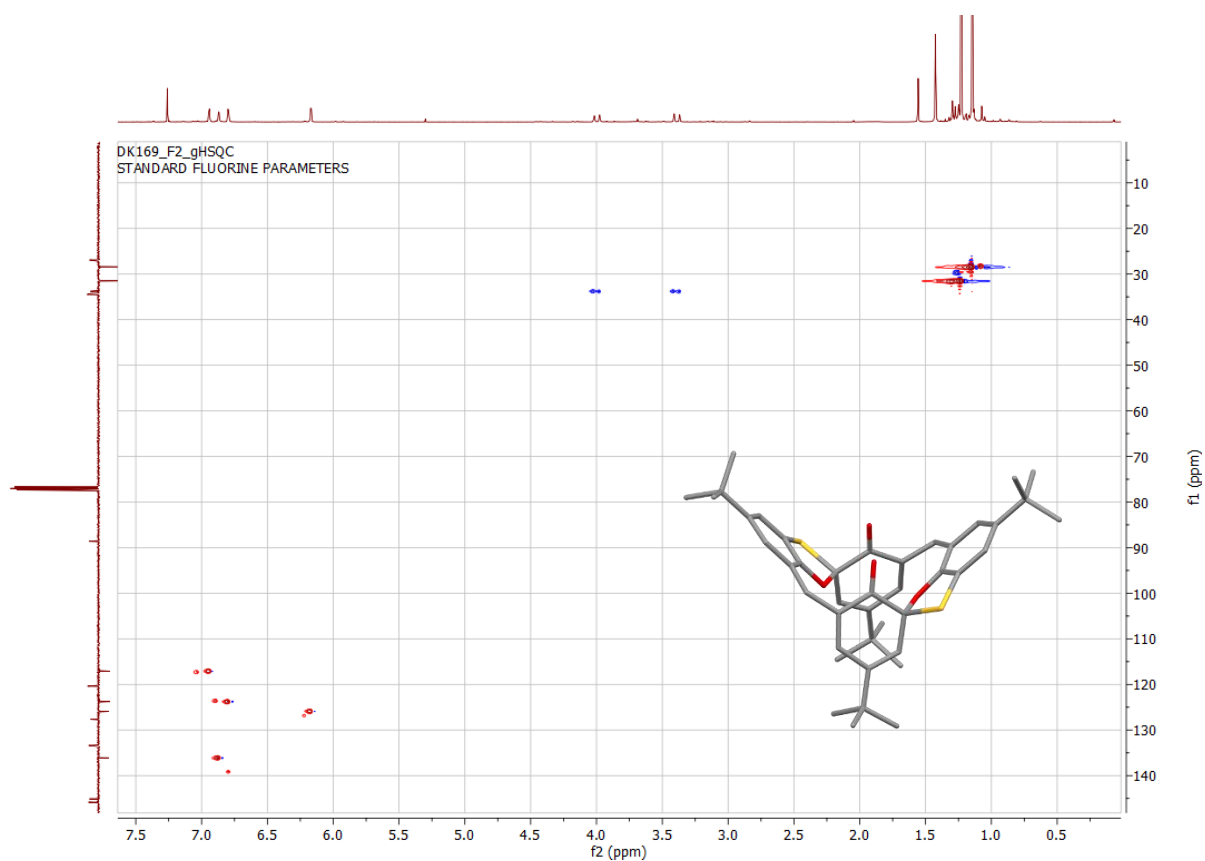


Figure 13. HSQC NMR of compound **7(chiral)** (CDCl_3).

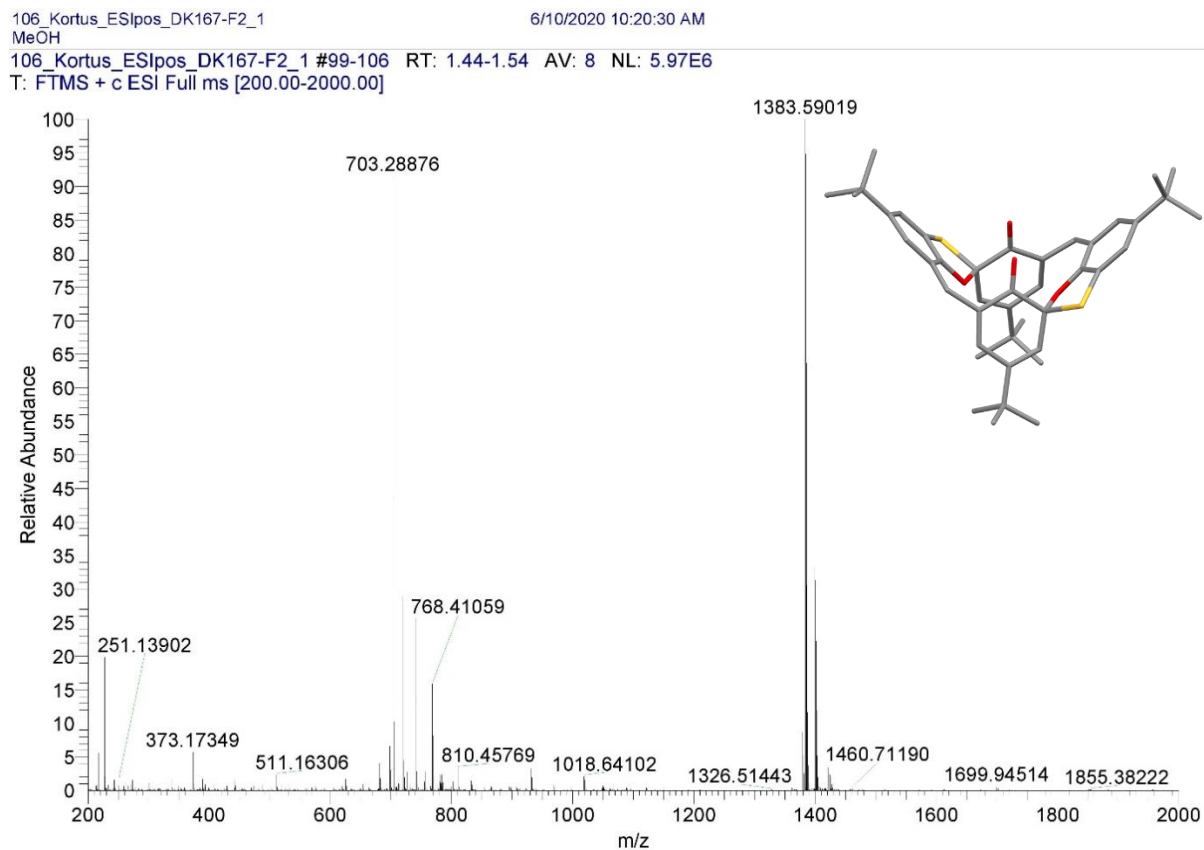


Figure 14. HRMS of compound **7(chiral)** (ESI^+).

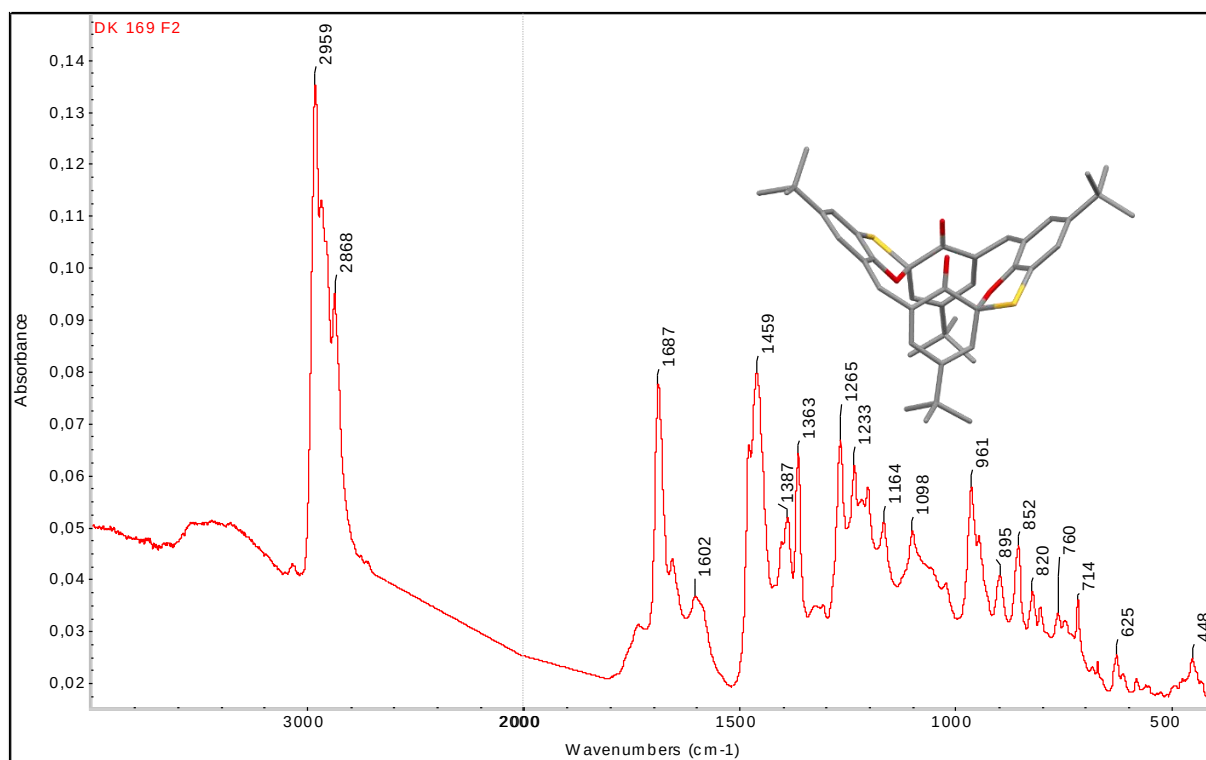


Figure 15. IR of compound 7(*chiral*) (KBr).

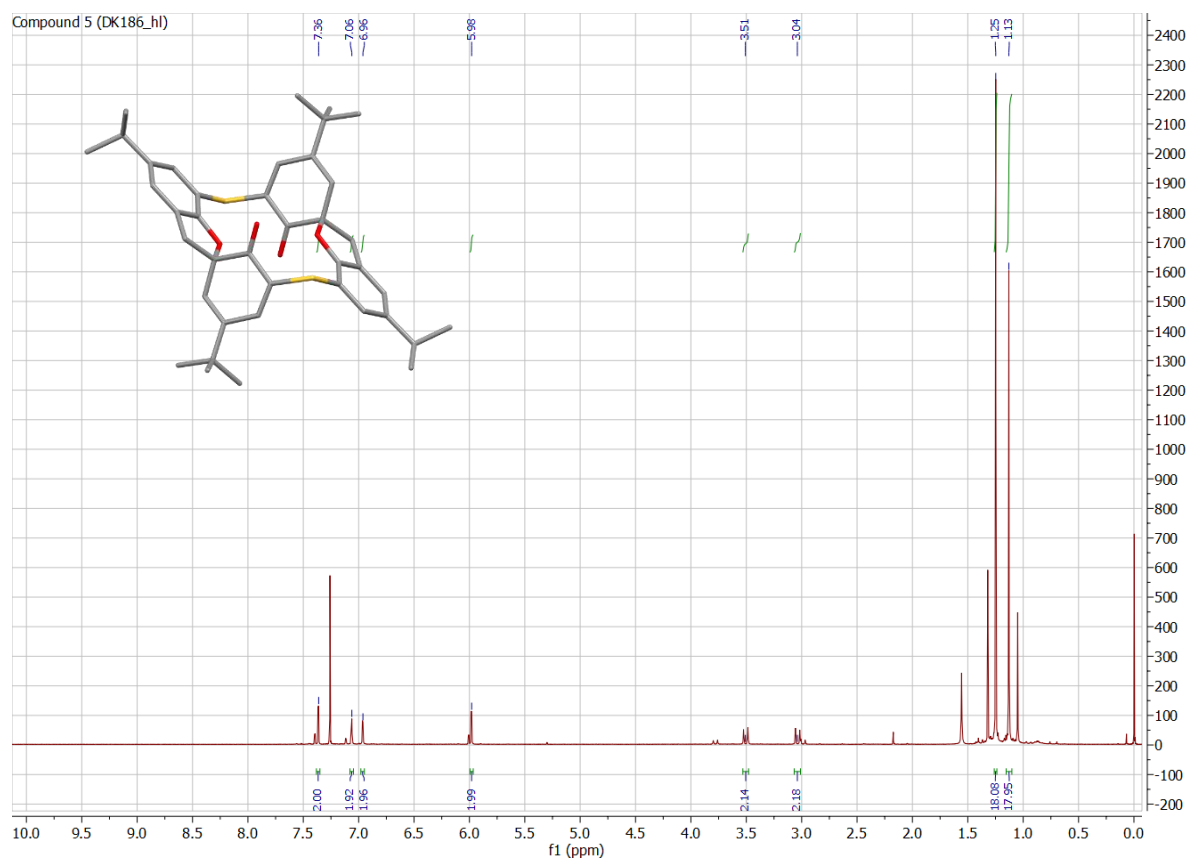


Figure 16. ^1H NMR of compound **7B** (CDCl_3 , 400 MHz).

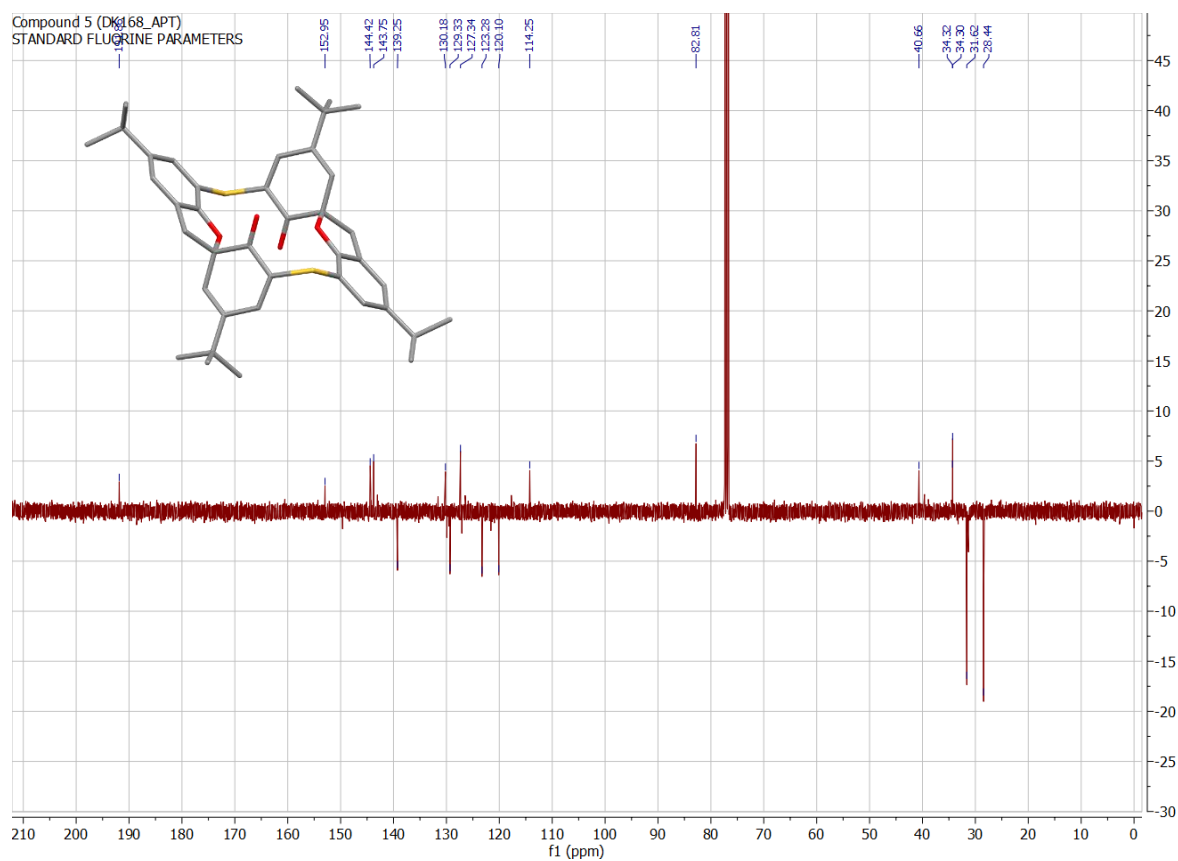


Figure 17. ^{13}C NMR of compound **7B** (CDCl_3 , 101 MHz).

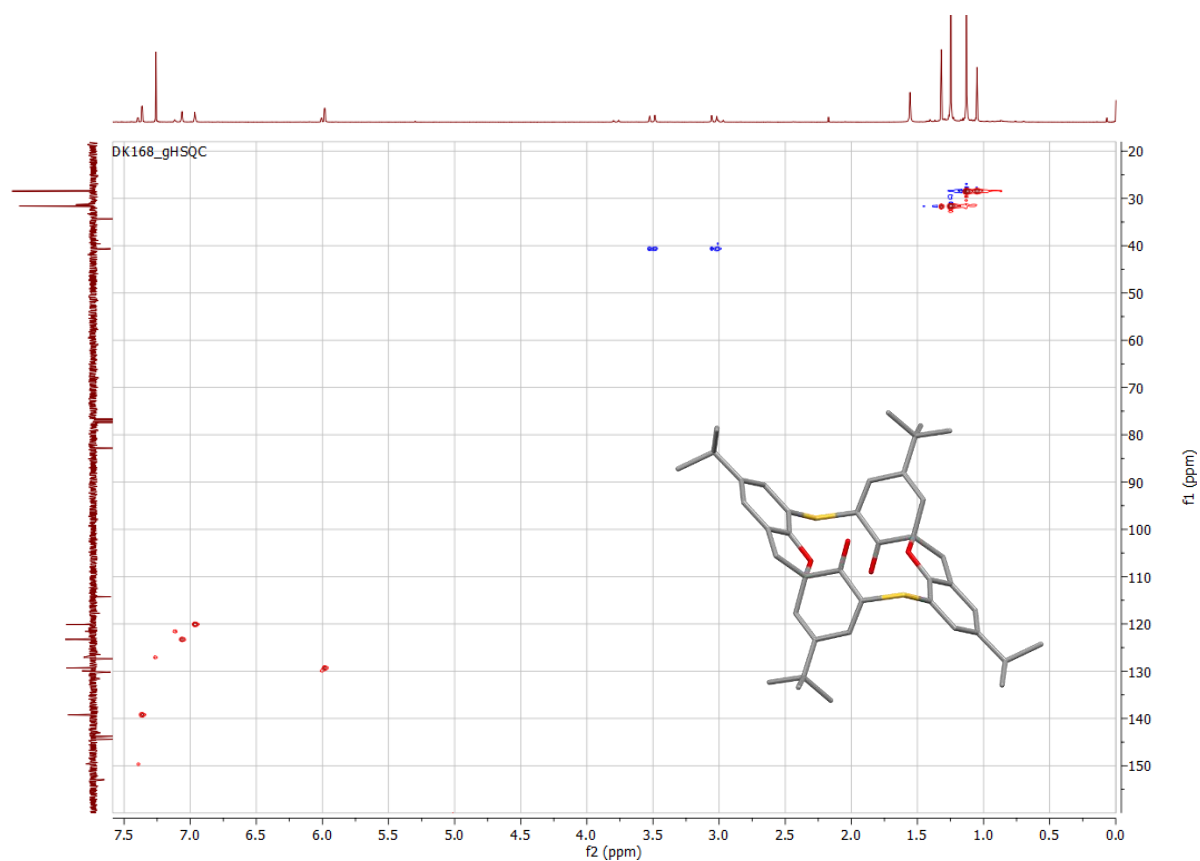


Figure 18. HSQC NMR of compound **7B** (CDCl_3).

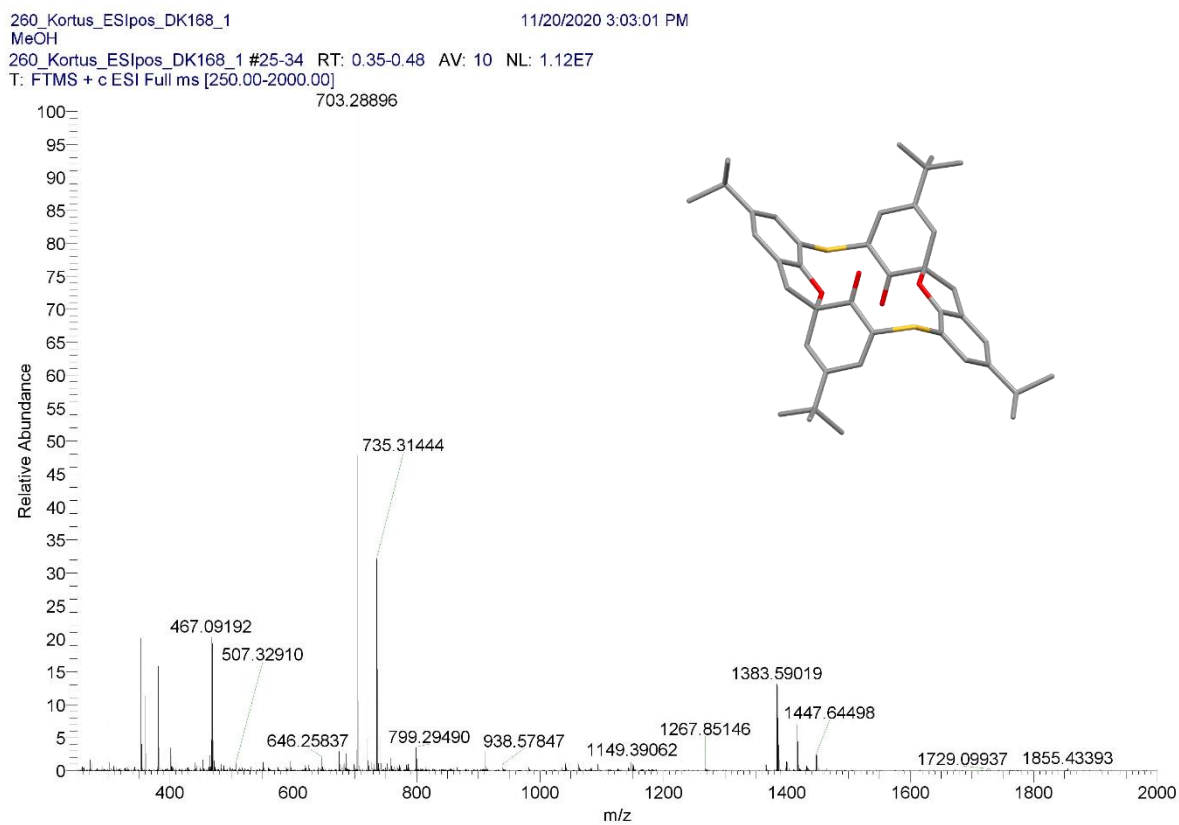


Figure 19. HRMS of compound **7B** (ESI^+).

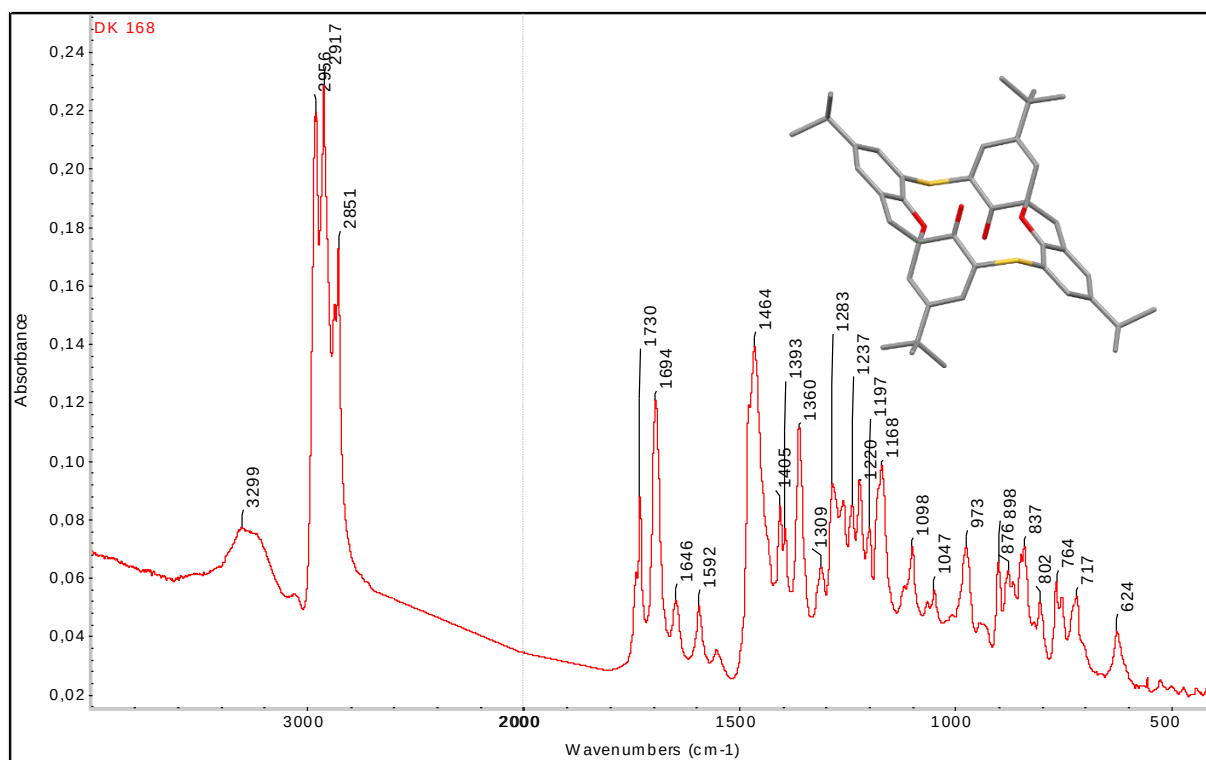


Figure 20. IR of compound **7B** (KBr).

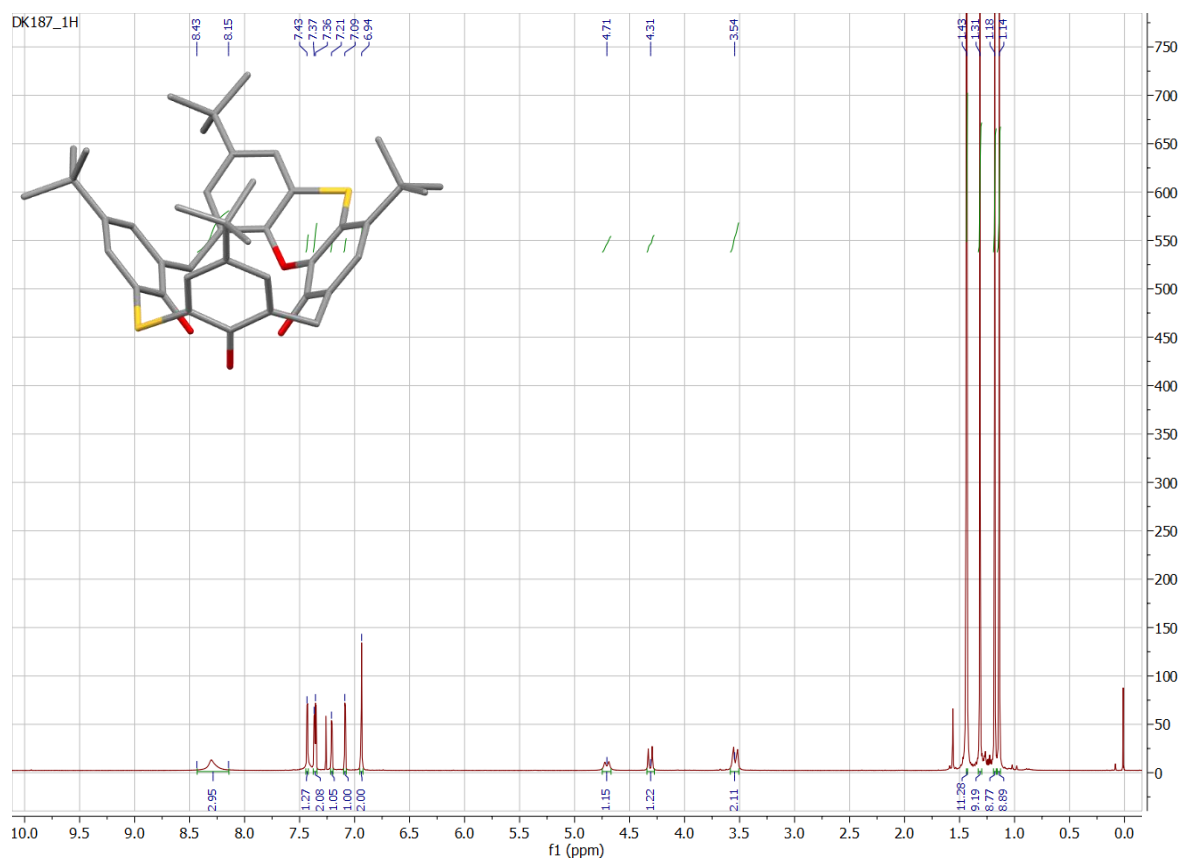


Figure 21. ^1H NMR of compound **8** (CDCl_3 , 400 MHz).

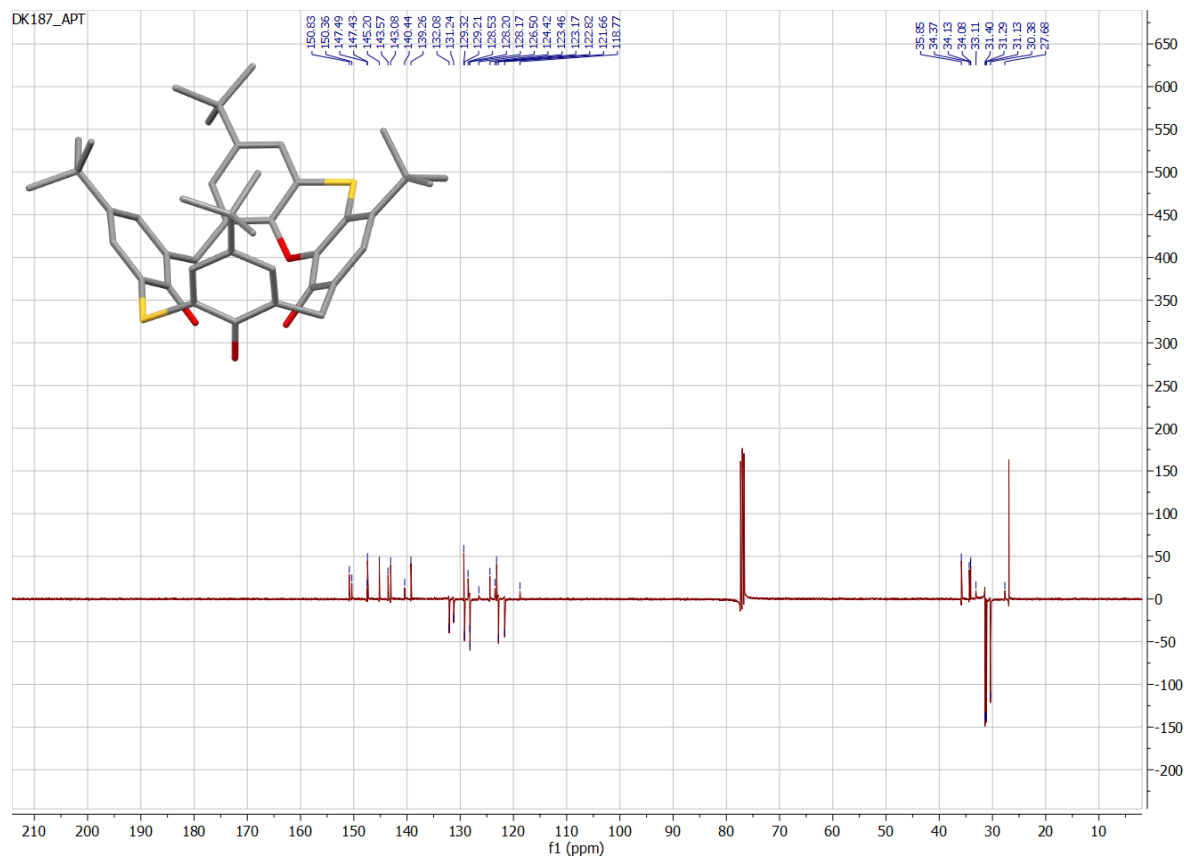


Figure 22. ^{13}C NMR of compound **8** (CDCl_3 , 101 MHz).

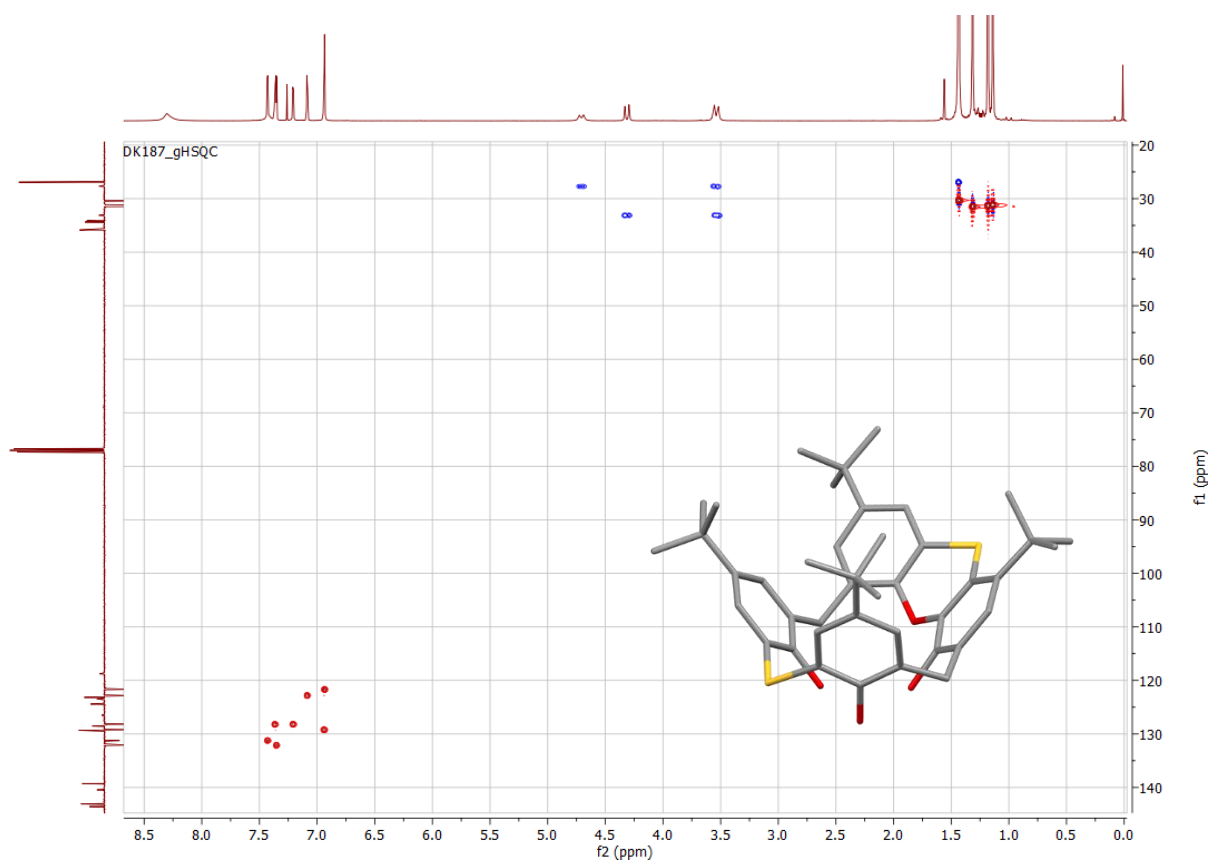


Figure 23. HSQC NMR of compound **8** (CDCl_3).

279_Kortus_ESIpos_DK187_1

12/15/2020 7:02:11 AM

MeOH

279_Kortus_ESIpos_DK187_1 #22-28 RT: 0.31-0.40 AV: 7 NL: 4.15E6

T: FTMS + c ESI Full ms [200.00-2000.00]

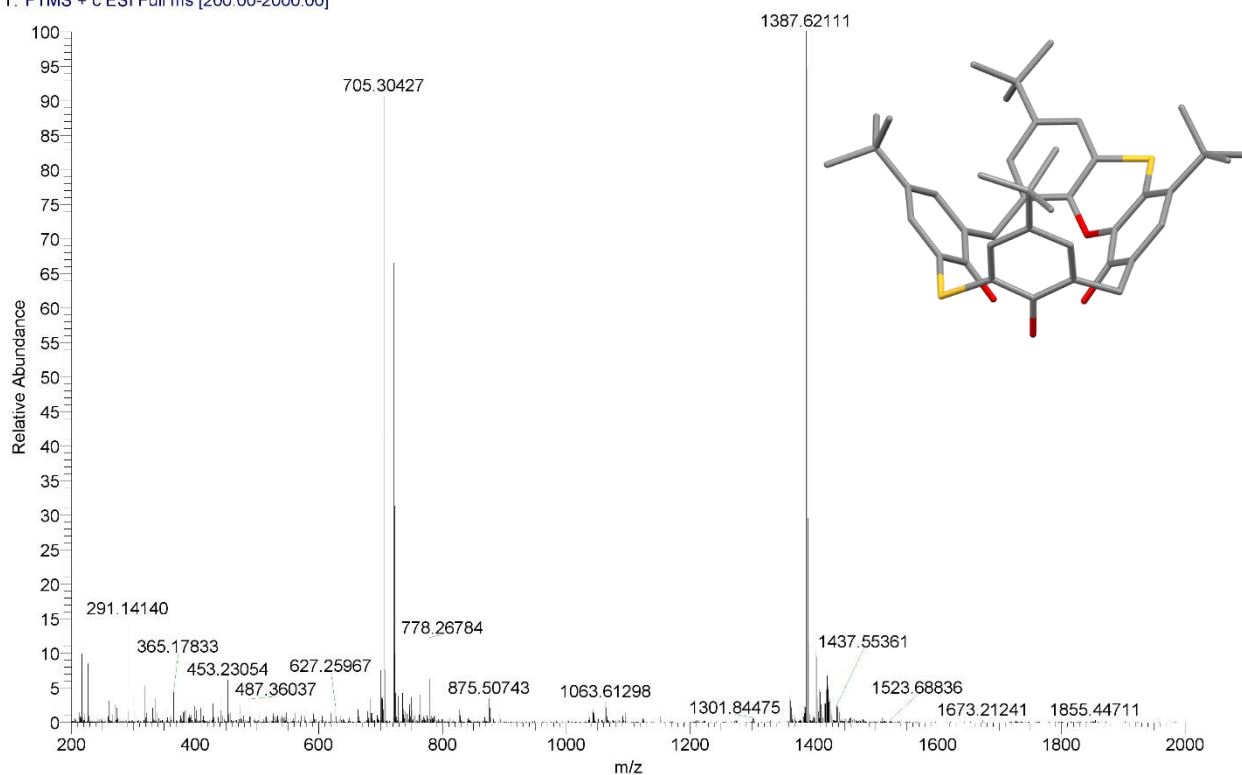


Figure 24. HRMS of compound **8** (ESI^+).

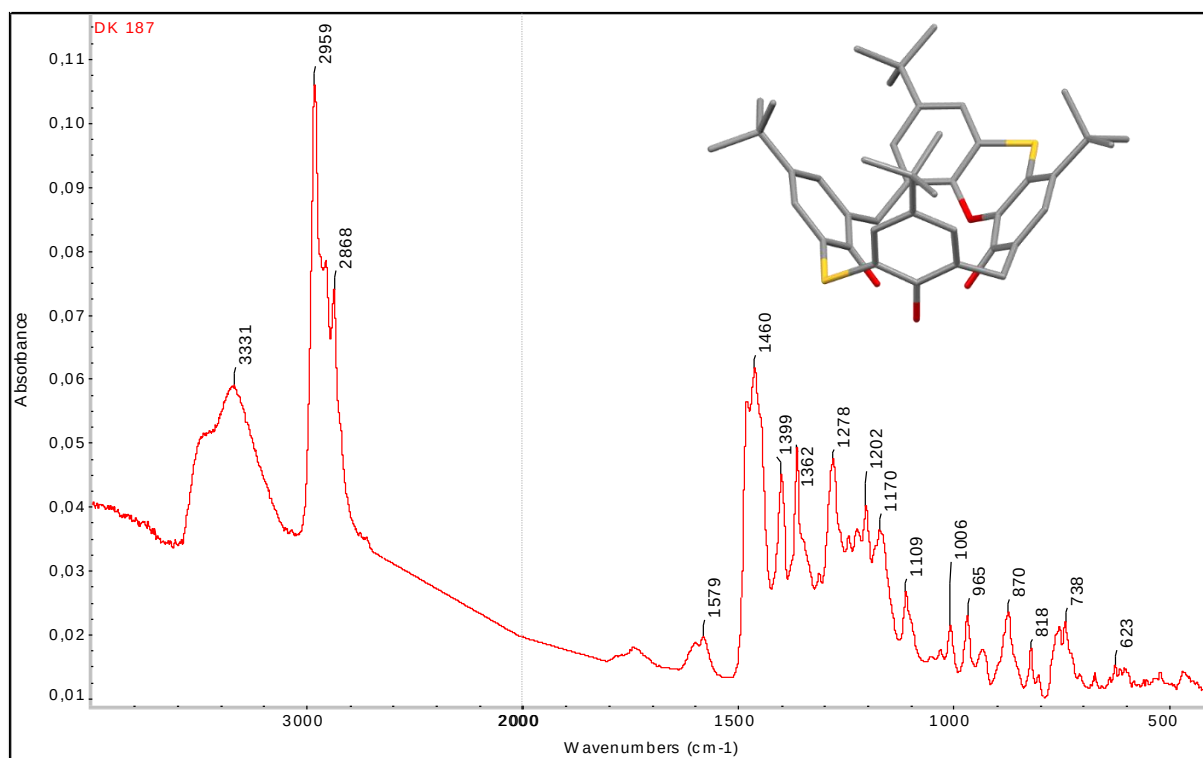


Figure 25. IR of compound 8 (KBr).

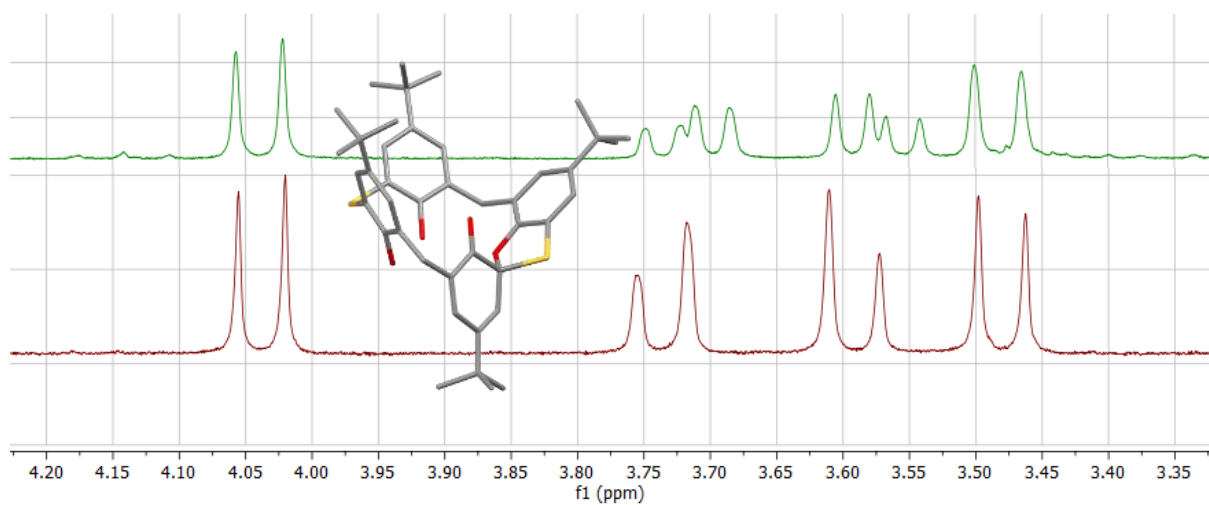


Figure 26. Methylene bridges splitting of compound 5 before (lower) and after (upper) adding 10 equivalents of Pirkle's alcohol.

2. CRYSTALLOGRAPHIC STRUCTURES

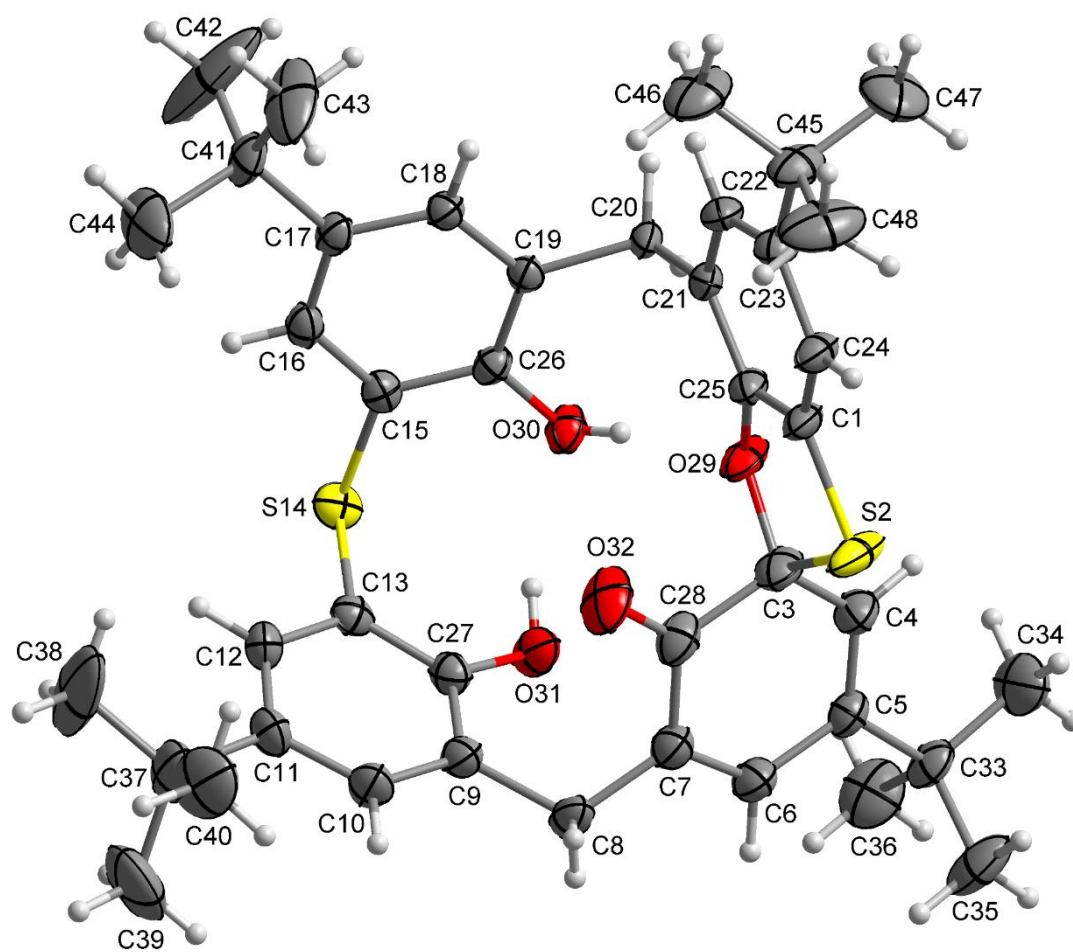


Figure 27. Crystallographic structure of compound 5.

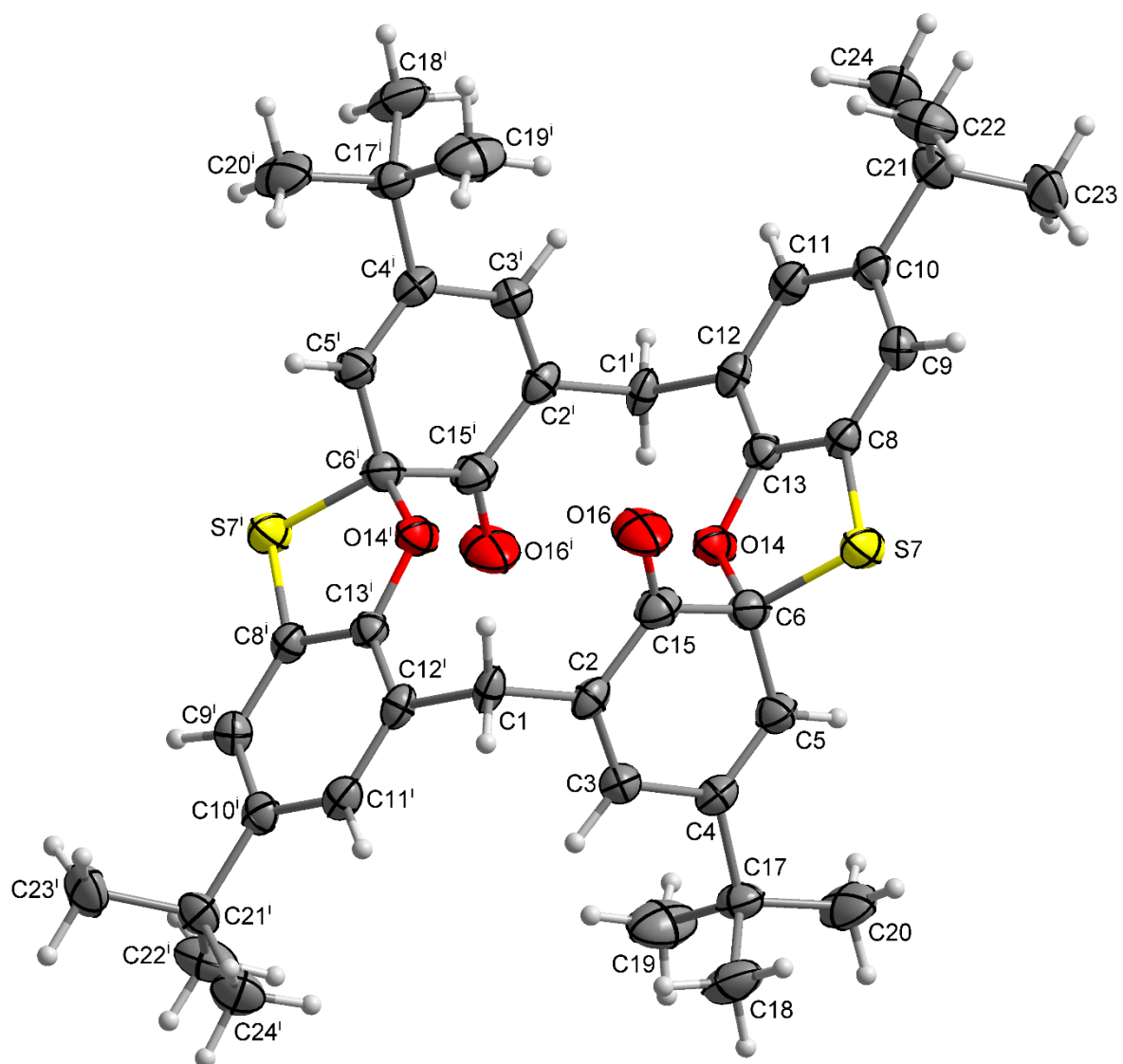


Figure 28. Crystallographic structure of compound **7A** (*meso*).

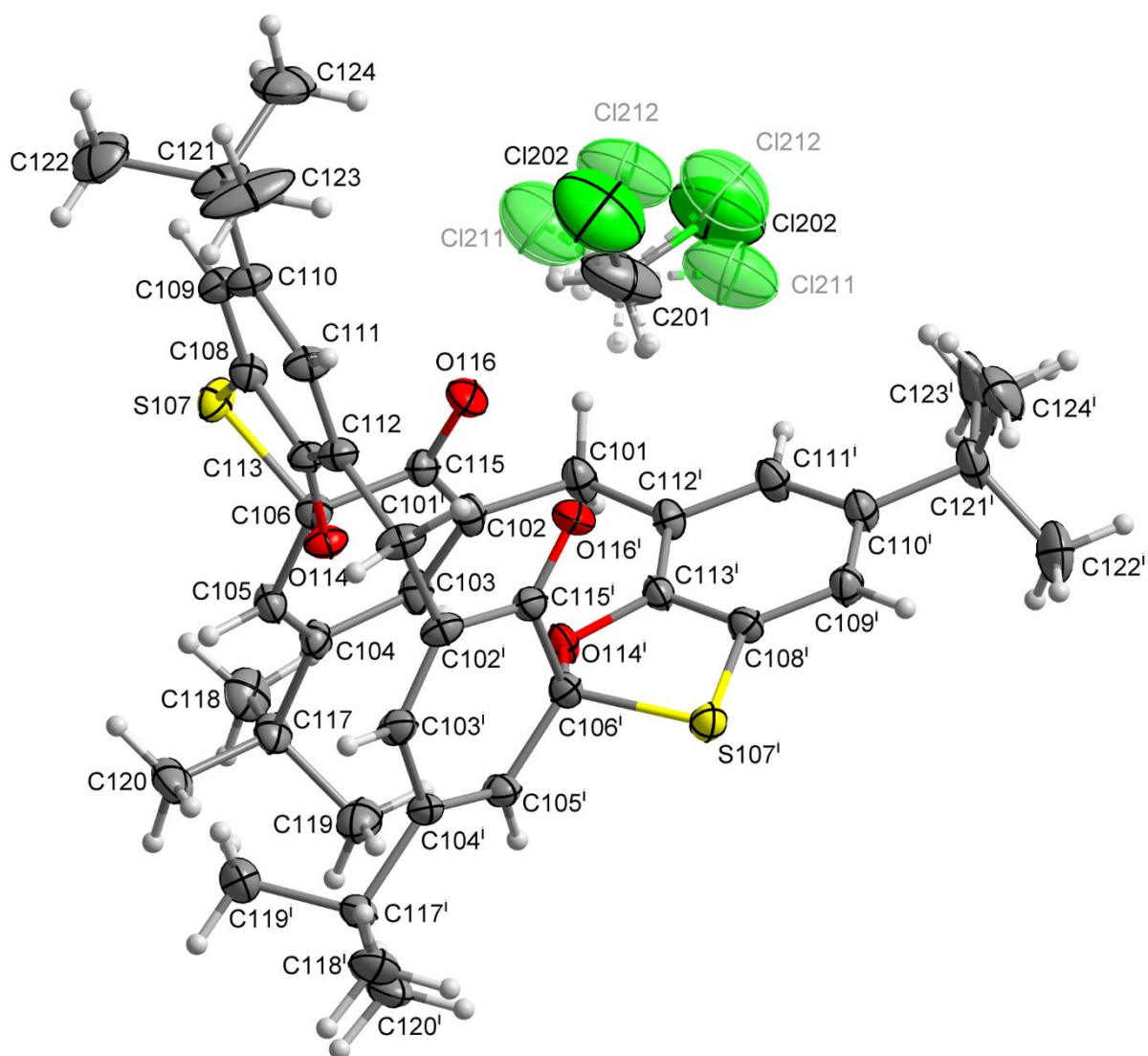


Figure 29. Crystallographic structure of compound 7A (*chiral*).

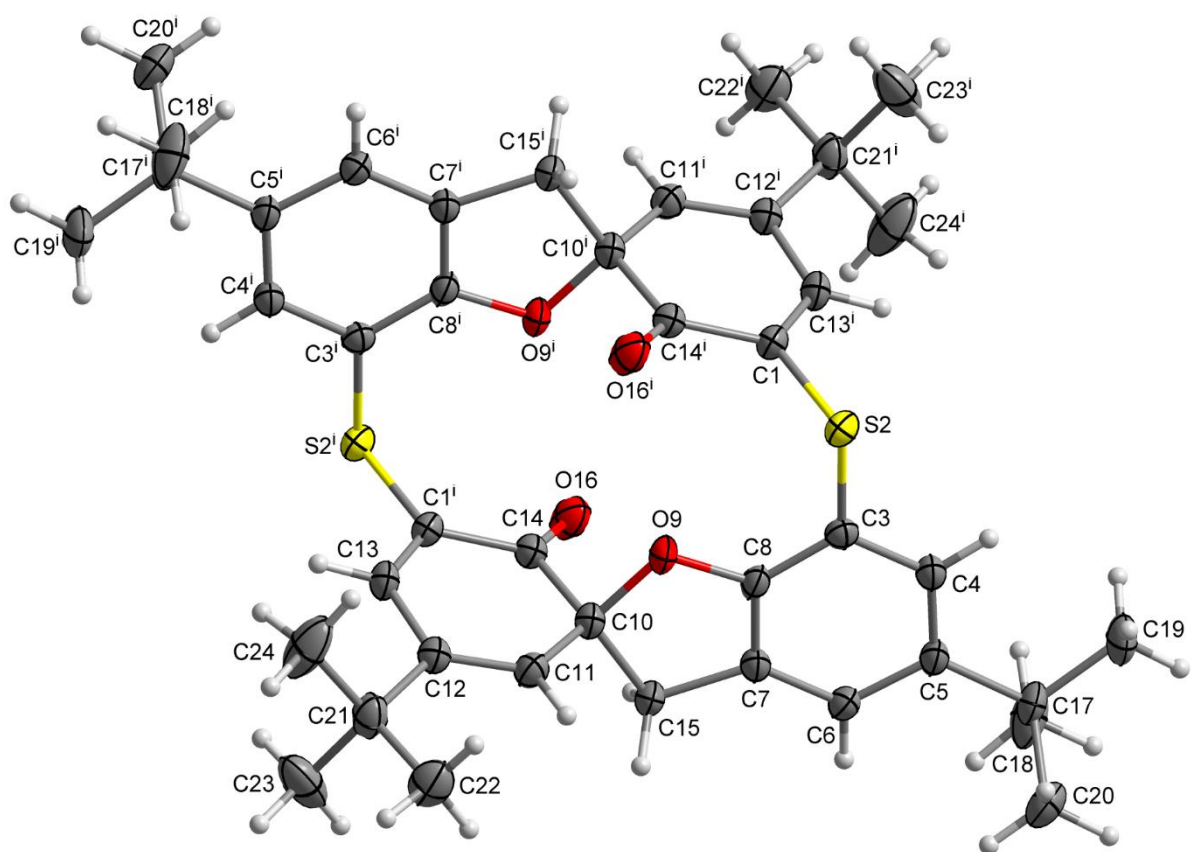


Figure 30. Crystallographic structure of compound **7B**.

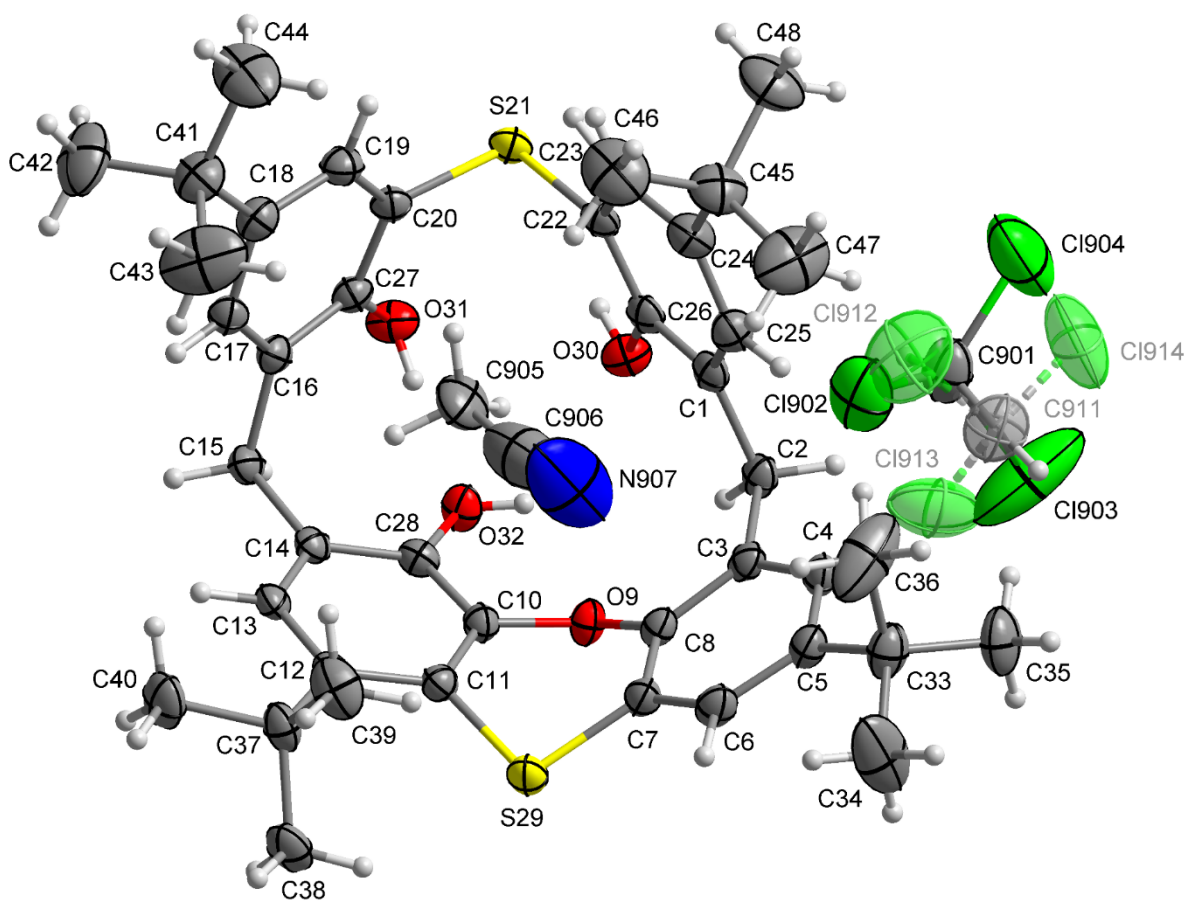


Figure 31. Crystallographic structure of compound **8**.

3. HPLC MEASUREMENTS

Compound 5 was subjected to HPLC on a chiral column Chiralpak IA (250×4.6 mm ID, 10 μm) using heptane: CH_2Cl_2 = 90:10 as a mobile phase. Flow rate was 0.7 mL min^{-1} , column temperature 298 K and detection wavelength 254 nm. These conditions have led to a base-line separation of two peaks.

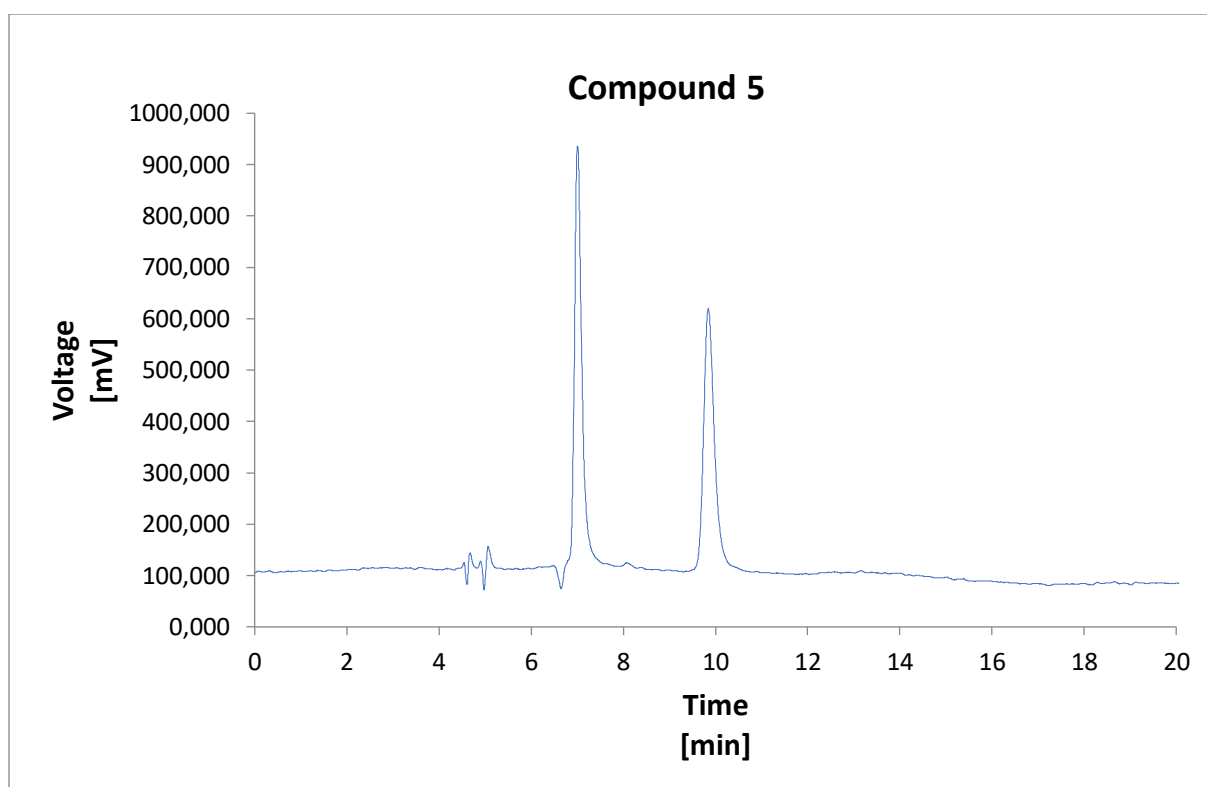


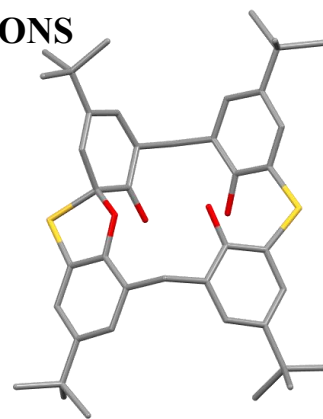
Figure 32. HPLC measurement of compound 5, retention times: 7.01 and 9.85 min.

4. RESULTS OF QUATUM CHEMICAL CALCULATIONS

Mono S-spiro (1,2-alt)

Final single point energy = -2725.21869041749

C	-2.54590733472459	6.73483936057760	9.28052604682473
C	1.62673899386302	3.14301797032570	11.70917283034912
C	2.10674282602490	3.75092890093132	10.39979692214686
C	3.47960857553402	3.90736826008940	10.12628956032907
C	3.96860903707423	4.49291559391327	8.95416280477022
C	3.03147301656103	4.94728493481074	8.00204393052950
C	1.67578277972051	4.79601451580295	8.24671939126277
S	0.31834344528656	5.24529256864298	7.19106683549280
C	-0.87225987220566	4.87698684531247	8.62049786178574
C	-2.04715639811249	4.14956786863737	8.05959412988890
C	-3.26651451907906	4.71864545177166	7.96875092221534
C	-3.48088670495090	6.03370771955767	8.58981797451231
C	-1.18228381625167	6.20454683281989	9.34680241120161
C	1.22812447003586	4.19782358591469	9.42516616641497
O	-0.14780674041674	4.04184933280516	9.53524073597193
O	-0.27243359005895	6.75460223963711	9.96432905803300
C	5.47350508010004	4.66248869552799	8.66961176603754
C	6.35075265427311	4.11934472554909	9.81411175282722
C	5.84206773109928	3.89576055583743	7.37631908286822
C	5.79805107388589	6.16503860983778	8.48661983500026
C	-4.46626975746967	4.04413205179113	7.28747138054052
C	-4.09971120458674	2.66859848154917	6.70049924314592
C	-4.96539035225862	4.94943772870659	6.13435141647138
C	-5.60423475240900	3.84413622864613	8.31941798424119
C	1.45164270657951	4.13950605515219	12.85426122680332
C	-2.87814537798389	7.93716372085572	10.14877741349773
C	-3.23681609488092	7.45015795387276	11.54926867638306
C	-4.56974902368811	7.11150257609668	11.82483413316427
C	-4.96656297712710	6.52825444141262	13.03080427320829
C	-3.94836824286913	6.22787452578958	13.94993517982051
C	-2.61407055893589	6.55605003302060	13.71321782957144
S	-1.45301723488643	6.14261265407376	15.00383908709883
C	0.07595831452364	5.53875074412650	14.28755685295569
C	1.21717744727438	5.85471511302502	15.03756912296233
C	2.47891044814752	5.33073362402313	14.74080415960261
C	2.55850859357434	4.46681363950416	13.64175281990073
C	0.19426911170656	4.69512071068988	13.16628196500483
C	-2.24952150739790	7.22655903805678	12.52693987224525
C	-6.42882993304795	6.17670928653481	13.36081573317503
C	-7.39776444093080	6.59618529096524	12.23862746553610
C	-6.85327525638051	6.90680822793004	14.65801474835741
C	-6.56272553263702	4.64859324076551	13.56645478356758
C	3.73911866089339	5.66276630336677	15.56144457092585
C	3.43889633856297	6.61370524550498	16.73618545987777
C	4.33765863005106	4.35846702868668	16.14230382708541
C	4.78574554613880	6.34407782619355	14.64783853185677
O	-0.96307299554912	7.63662125565399	12.40453581122426
O	-0.93019216051479	4.40314888425734	12.44646905178832
H	2.36490772765382	2.39727728275285	12.02570188494355
H	0.69543725519851	2.58839508100848	11.54409458399400

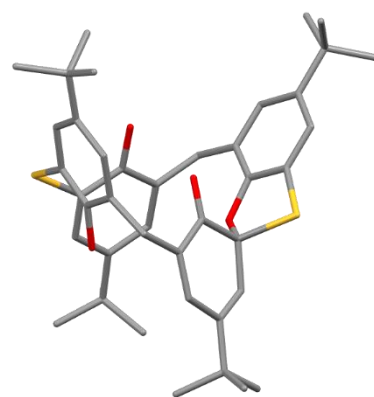


H 4.17512176803605	3.55328455497268	10.87886729986207
H 3.36244488440496	5.41545889636395	7.08052970660339
H -1.82706787912596	3.16513572819333	7.66472211877123
H -4.48763172656827	6.44245659127455	8.55180081298317
H 7.40888019912900	4.25921914366927	9.56407011248783
H 6.18986630059984	3.04736559192173	9.97951343987115
H 6.16299462419593	4.64563180834360	10.75725081885445
H 5.28531841167697	4.26644002337795	6.50888665625952
H 5.62641057182051	2.82563275305867	7.47986652620887
H 6.91140206325574	4.00759277686645	7.15696197068445
H 5.24102510693279	6.60570388769071	7.65278546872038
H 6.86725438091954	6.30190045779256	8.28090514409667
H 5.55006584819991	6.73297280770274	9.39085521717563
H -3.30709145830020	2.74611072915322	5.94707397429152
H -4.97829974452964	2.23138907326833	6.21356540630420
H -3.77115427402227	1.96914049207204	7.47764246428405
H -4.18581470825935	5.08950976891920	5.37624089779934
H -5.27326600043996	5.93989805703733	6.48643798740890
H -5.83417140137164	4.48955545215743	5.64824789197629
H -6.46777493376969	3.37103191427248	7.83688166805004
H -5.94803730132590	4.79036235730583	8.75059974692507
H -5.27782038403406	3.19842778638875	9.14224186308763
H -3.73089521424663	8.47194531319029	9.71651239729924
H -2.03270492490352	8.63283508517964	10.17081183470238
H -5.30801411999419	7.32072358158995	11.05587278368964
H -4.18495964843000	5.70512191109074	14.87217949256042
H 1.09005102392977	6.53344273731754	15.87363294082700
H 3.51284646467444	4.01355324310088	13.38384722029350
H -7.18068643954045	6.07772467426013	11.29677934991732
H -7.36216412559650	7.67615608951425	12.05198702662584
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H -6.77574124141052	7.99409122101049	14.53836832937257
H -6.22600706572048	6.61975152773467	15.50858094264179
H -7.89290107859125	6.66452006908129	14.91292315189412
H -6.27246520179151	4.10532745373512	12.65918102265566
H -7.60021340764198	4.38193369895570	13.80572066299633
H -5.93019228316828	4.28984501754471	14.38542845020860
H 3.03387081486163	7.57188989177800	16.39197909336784
H 4.36332354919185	6.82390567501929	17.28712195900705
H 2.72497597017415	6.17430807377017	17.44347198392280
H 4.61737455562069	3.65118311908933	15.35361959769337
H 3.61682458077561	3.85797371013907	16.79980503151271
H 5.23877089890598	4.57801675067082	16.72935481302140
H 5.07089486781768	5.70195235733408	13.80664489476771
H 5.69678112429060	6.57776165201136	15.21333558359111
H 4.39240744223911	7.27941288330794	14.23366540260114
H -0.65856889799877	7.55759629859808	11.47506626172264
H -0.68380458137763	4.13152819154521	11.54450684329037

Mono S-spiro (1,3-alt)

Final single point energy = -2726.45471106038

C	8.05543627890159	10.54888667217084	12.63531513299695
C	9.17877409595389	11.37873207898922	12.04042811610596
C	9.00528717710181	12.74585406624499	11.83372015089279
C	9.95630080711587	13.56145189621729	11.19712224623850
C	11.12466945710115	12.93499265475967	10.75880072676562
C	11.34236812178824	11.55791095044812	10.94568587462235
S	12.84098611463513	10.84456321988029	10.23678906546751
C	13.64383414842394	10.09054709437045	11.66198648824193
C	14.04944831350306	8.75262943552425	11.57411179587742
C	14.68972654511581	8.10376529537858	12.63844403219525
C	14.84333909966953	8.83600841902705	13.82356994553223
C	14.43303476677024	10.16460532504942	13.95551603765469
C	13.89139069841302	10.81997100368294	12.83998371642616
C	10.36832249152927	10.77135681229726	11.59048170248976
C	9.68915344583178	15.06612885065081	11.00960584161655
C	8.40861660041783	15.26433188659717	10.16253530942531
C	9.49395848305401	15.73222902211063	12.39337633169998
C	10.85173286977758	15.78001581308909	10.29270509927098
C	15.14258687993643	6.63927200992931	12.48682219936395
C	16.17034105580084	6.53571696442493	11.33466999456271
C	15.80156734666102	6.09769814373550	13.77043176267871
C	13.91988140634370	5.74751962887161	12.16313901975624
C	14.51887982723984	10.87397856836009	15.29919059160711
C	13.24524308487652	11.57573804037611	15.74522779648984
C	13.24913112839393	12.82978203047901	16.25435614537164
C	12.05096934624544	13.60338531385606	16.61544406308730
C	10.83715473841293	13.04153208056808	16.44830237198283
C	10.66635754507050	11.62512832442773	16.01713506062474
S	9.96513547266026	10.61906759418102	17.47069412633840
C	8.98234556981066	9.71739588959186	16.29198530710453
C	8.27279168510035	8.54768871328033	16.50123050053688
C	7.52315671556658	7.98890946076219	15.44422800916880
C	7.52764871387170	8.66063171526054	14.21977416652974
C	8.23271980391634	9.85989665807352	13.98391991681358
C	8.96489717023320	10.36591335702933	15.04949450099874
O	9.68050859677386	11.54401455824368	14.99134922136681
C	11.95211470230587	10.88996204394989	15.54868799281564
O	11.85423361377672	9.78927451906827	15.03093935598858
C	12.25518744245279	15.03787742912473	17.12671214047407
C	13.10554444038556	15.00045598288448	18.42082494013556
C	12.99205066411523	15.87035044322966	16.04781985106208
C	10.92025740597802	15.73618346299276	17.44451964706809
C	6.75285175719313	6.67465297609126	15.67611540989731
C	5.72448350984714	6.87351388068049	16.81557540294720
C	5.99011190686801	6.21239334204808	14.41957397330678
C	7.74575696293304	5.55590232165287	16.07414691851410
O	10.48667237368737	9.43438449220900	11.78060275732389
O	13.59088195121667	12.14011276559396	12.97802153869817
H	7.78858536541294	9.76650489040880	11.91325395519704
H	7.17437106225076	11.20271354082029	12.70697247281258
H	8.07861259944459	13.18822629351210	12.19050768594212

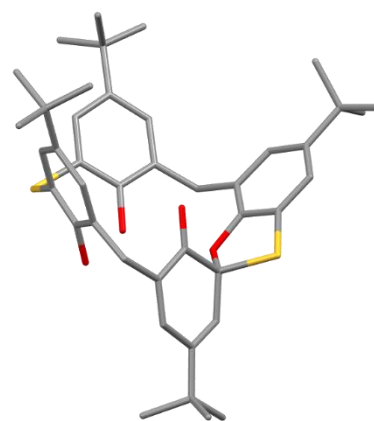


H	11.89703744748268	13.49907327198509	10.24643969326032
H	13.85265078560425	8.22258997108814	10.64600483085906
H	15.26368960051059	8.35612651997093	14.70155971209514
H	8.51874857115725	14.80750739620846	9.17233677653810
H	8.20364234784230	16.33332332139468	10.02363995749963
H	7.53043793499300	14.81724909794148	10.64058518794808
H	9.29443214071007	16.80531914610107	12.27789696447271
H	10.39093609469397	15.61523249380719	13.01295579116183
H	8.65268137529483	15.29296911534609	12.94039693586265
H	11.02737534179422	15.36986148582370	9.29138195777994
H	11.78718081418664	15.70925869680130	10.86072145944471
H	10.61694223642779	16.84431792588179	10.17655436838149
H	15.74599095499939	6.86687183363553	10.38042437287142
H	16.50213060693529	5.49755234862223	11.20862295349981
H	17.05310421587322	7.15281211742862	11.53860056039844
H	16.11510052386597	5.05938524369097	13.61358614699046
H	15.10787212038538	6.10878705969098	14.61928177305516
H	16.69208623511598	6.67412514143432	14.04759655221626
H	13.43279203929076	6.04819759510249	11.22875182470625
H	13.17235305242741	5.80205685809874	12.96355033400251
H	14.22783921918664	4.69998153718929	12.05354793807112
H	15.32469826106291	11.62054482702185	15.28765576913321
H	14.79706098702367	10.12302152149720	16.05084608670281
H	14.20967056344183	13.32924529497596	16.35509949553921
H	9.91261439239553	13.56746137451569	16.65653425064725
H	8.30862007802953	8.06355476023728	17.47213923413505
H	6.96838274843546	8.25327422938789	13.38427849480623
H	14.08628913162730	14.53922407796160	18.26049517353328
H	12.59380211414137	14.43681017516855	19.20934753429439
H	13.27754795527466	16.01955593984420	18.78714143508750
H	12.40099896325414	15.92410390086627	15.12626558249744
H	13.97133079299739	15.45125673088016	15.79328874665330
H	13.15497603520636	16.89259448683643	16.40924519106400
H	10.28619542318064	15.82228755492326	16.55483846045231
H	11.11253437140444	16.75056933763467	17.81228889506396
H	10.35668506317105	15.20281927400542	18.21833425085813
H	4.99888876433917	7.65310829872322	16.55564423147511
H	6.20695412941178	7.16642601240774	17.75441845282316
H	5.17372226416791	5.94241991550482	17.00147231456418
H	6.66726886586621	6.02530194797160	13.57843470002515
H	5.24435574985681	6.95056040080881	14.10201157086764
H	5.45945491468476	5.27690011600024	14.63239603105749
H	8.48606204500605	5.38923490244368	15.28312724028080
H	7.21086461135430	4.61311479940589	16.24591310840184
H	8.29049942110514	5.80086452080161	16.99263318491001
H	11.40750259654534	9.15841937930430	11.63172836214621
H	13.04478473835160	12.43179011142179	12.22815970177780

Mono S-spiro Compound 5 (*partical cone*)

Final single point energy = -2726.46562097766

C	4.97289875396543	19.05799969395245	9.23683917407655
S	6.27093574165512	17.89655045555414	8.89210993250751
C	6.75493497154180	18.91412856233298	7.36778172241038
C	8.23915639940306	19.04162028484372	7.33581577195616
C	8.99015898984766	18.41628732027773	6.40724779396403
C	8.31963566690293	17.70309662415464	5.30950550381688
C	6.98040170951164	17.62947926402601	5.12786567381682
C	6.36426195662069	16.99362653170267	3.89506695461359
C	5.28768911518239	17.80435451820693	3.18147916894230
C	4.16758625400251	17.16385106425058	2.65781106947655
C	3.10542181046422	17.84762025634248	2.03939939865186
C	3.19290762748435	19.24097927927621	1.99933586787965
C	4.30327223021549	19.92302886660405	2.51583255652274
S	4.36169489422695	21.72427081224556	2.46082155148255
C	3.57133320918423	22.18455351657567	4.01814714374687
C	2.24776350533490	22.62663280305155	3.99987783822161
C	1.57693411283958	23.02696657975237	5.16626558712759
C	2.30170788391260	22.96684029955554	6.36037121752716
C	3.63485004230931	22.53949879459591	6.42402541797946
C	4.36953993160711	22.55080683625220	7.76116822983178
C	4.22987782609625	21.28373678078589	8.59475597973639
C	3.22628111259796	21.15647194657784	9.56715715171113
C	3.06201959758758	20.01488240705502	10.36666886306333
C	3.96503044984016	18.95213638945843	10.18969504742002
C	5.08869105166626	20.19912083526121	8.44936682638141
C	4.27380499237806	22.14307185184652	5.23903821992240
C	5.37930775773467	19.20508303788063	3.06417242073861
C	6.09018832281863	18.24540324570240	6.13032142640912
O	6.15310121177760	20.21254373930560	7.56106302568525
O	5.58891517535961	21.75793150419505	5.22355608114650
O	6.50700490484850	19.80536380120160	3.52195945638989
O	4.87447717313169	18.26138553358367	6.03732573651651
C	10.52585859675386	18.44176045211408	6.40904878602790
C	11.09172015960066	19.24316055761129	7.59615014011667
C	11.05078778395118	16.98800232946785	6.50734267558094
C	11.03849089232481	19.09286780223630	5.10048572723866
C	1.90844071967467	17.06272423642327	1.47191130590655
C	0.84825190023582	17.98904930001875	0.84599668634091
C	2.40399513898030	16.09193066768177	0.37290075745272
C	1.23117794488225	16.25261788349304	2.60308847151210
C	0.11103326920129	23.49502960137799	5.09316829248149
C	-0.00871220376489	24.68579245981379	4.11220142153337
C	-0.42383246066950	23.95110160112171	6.46526952728604
C	-0.77505587477616	22.32902138971212	4.59280600976560
C	1.91840761191808	19.96035332046410	11.39858758308916
C	0.56003658318282	20.10222585762127	10.67049314872201
C	2.08038966281662	21.11850871471107	12.41203642310462
C	1.90213409022051	18.63602792565797	12.18590818584898
H	7.18299398222099	16.75899343755388	3.20092758841996
H	5.91344297801881	16.03264391689333	4.17778606799437
H	3.97815450452952	23.38455955981002	8.35511208357600

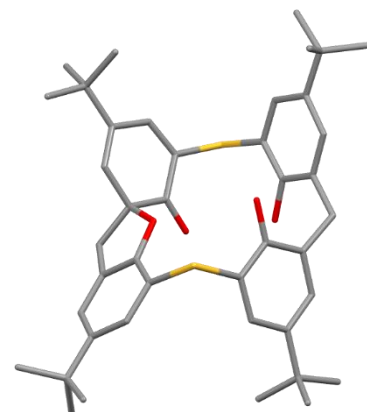


H 5.43142587400697	22.76750102947466	7.59561041031955
H 1.73977430202038	22.64625048724868	3.04057977954147
H 1.83425856303962	23.27601743522049	7.28984484345897
H -1.05004201858051	25.02605569908640	4.04954389086319
H 0.60610306135794	25.53046950534157	4.44409316834748
H 0.31262367188189	24.41519939138586	3.10070130101846
H -1.46306119870741	24.28436164934538	6.36461415362264
H 0.15644378730526	24.78954254895452	6.86849428385592
H -0.40838461879789	23.13721851396757	7.19996501814029
H -1.82428151928869	22.64431659531089	4.52962083587429
H -0.46940122880330	21.98567683159152	3.59849592733023
H -0.71667745010273	21.47144698501804	5.27354274211106
H 2.55005157600264	21.99750915159365	9.69767484505654
H 3.88962901300284	18.05021810900789	10.78502650892238
H 1.07242933579200	18.64424717102588	12.90259167294062
H 2.82713294842301	18.48657813244328	12.75527706906593
H 1.75981744123517	17.77102289767694	11.52731011138737
H -0.26568898847158	20.06749720205256	11.39294634936045
H 0.48643658778620	21.04942525457412	10.12559550998530
H 0.41511114943472	19.29062490648058	9.94785566937819
H 1.26967860442781	21.09554590736642	13.15170921785423
H 2.05456129790254	22.09770600614665	11.92131184570329
H 3.03289401769255	21.03884689674971	12.94939372604020
H 8.66774598090914	19.61494174154201	8.14944102953279
H 8.95591751776458	17.26267688805688	4.54639814764758
H 12.18728822252198	19.22881141719849	7.56052880414039
H 10.77394148262736	20.29160633073180	7.56602761808397
H 10.78516148900112	18.81846134132464	8.55925089534716
H 12.13518069746196	19.11355272094394	5.09949995724141
H 10.67799669533402	20.12360135889836	5.00822004336893
H 10.71847350771550	18.54686065442738	4.20701696673805
H 12.14800448274675	16.98239546359268	6.49990657180687
H 10.71509034041725	16.51316094352117	7.43677050761701
H 10.71229870813023	16.36590983370884	5.67098601764277
H 4.11284000503807	16.08189752356277	2.76085062947807
H 2.39601450795449	19.83601576276859	1.56871815095488
H 0.37816492247377	15.68492781694203	2.20968991203703
H 0.86379090052791	16.91667275922481	3.39392162215652
H 1.92101179097416	15.53681923312083	3.06452225707513
H 1.56509709416045	15.51381495411707	-0.03527297382164
H 2.87209995111825	16.64130158280330	-0.45234869890622
H 3.14239235660088	15.37979939236069	0.75938527584812
H 0.01984811077029	17.38956951786186	0.45089912015763
H 1.25842276418451	18.57395229964926	0.01397974477815
H 0.42936454267126	18.68674736638448	1.58093277345617
H 5.82313084353763	21.29151230861013	6.05148222584544
H 6.29878521544795	20.74296203139152	3.72396482992437

Mono C-spiro (1,2-alt)

Final single point energy = -2726.46254157057

C	-2.60707746395938	7.15091141331589	9.48363106027794
S	1.16253139290278	2.80458257969372	11.99346001454620
C	1.85891773104950	3.57167861955065	10.52880940973977
C	3.18666524969027	3.29792950798869	10.15228510781329
C	3.79433552605598	3.87648313436760	9.02936327974136
C	3.03317791983019	4.79191601073164	8.27204855894087
C	1.72073620847012	5.07025868470859	8.62120151744393
C	0.71929592357415	6.03996876254863	8.03945532790422
C	-0.58915059019270	5.67835274060805	8.81929536060325
C	-1.56555946370777	4.94407429917676	7.94756700434157
C	-2.86001968328944	5.29482971377333	7.81984809370468
C	-3.36220801298476	6.41267218691826	8.63134476301578
C	-1.15928848054290	6.90394629841400	9.56987784399069
C	1.13369141651560	4.44249189687665	9.71871261878175
O	-0.17962264313737	4.76651588192038	9.89988781464795
O	-0.38808042997519	7.59629444970761	10.22202093270135
C	5.24536009202983	3.56304053540368	8.61541911520751
C	5.91231255069439	2.53326308464469	9.54828662979754
C	5.25770933622570	2.98694377267811	7.17828585686590
C	6.08827429603086	4.86124751127386	8.65321159032904
C	-3.85935503547950	4.57366063457974	6.90289629754367
C	-3.19130657267558	3.44362758610304	6.09898508086404
C	-4.46073733359004	5.59109819566735	5.90350904531000
C	-4.99186300329497	3.95574434149265	7.75916685878899
C	1.08607781810470	4.19488770918901	13.14223195226730
S	-3.32474706186150	8.43560454758124	10.51839770877269
C	-3.55870172690720	7.48508506738437	12.03153318892632
C	-4.80754181539756	6.89051075079025	12.27021522794070
C	-5.04215619625370	6.11358092638767	13.40404546416076
C	-3.95286937325519	5.92651122971953	14.27539410744574
C	-2.69955387643065	6.49474396466391	14.07266164421248
C	-1.56710626098522	6.22662885898523	15.04964701424729
C	-0.24423118939893	5.71699220515862	14.49043197236355
C	0.95088550386801	6.29323656575164	14.92969420014555
C	2.21916260977421	5.85924879902390	14.51796375429233
C	2.25659022636619	4.78775273645685	13.61936239796517
C	-0.17469070194580	4.65046307130371	13.57603618073812
C	-2.50297032734980	7.32554325910497	12.94812620350159
C	-6.40071213179549	5.45829833057539	13.71044480564262
C	-7.45856233236489	5.77963443306896	12.63737063283342
C	-6.92695502087239	5.97194549615923	15.07296819256625
C	-6.23472080669399	3.92099164269571	13.77488833401951
C	3.53136632932138	6.49734842052069	15.01240924896937
C	3.28396341910057	7.68600589721790	15.96136954224004
C	4.36412045668595	5.43811871390132	15.77457395712735
C	4.34644455006020	7.01297820182027	13.80191103507335
O	-1.29564116388691	7.92022972024208	12.82568571161381
O	-1.33278373670188	4.08295924726839	13.14613824438261
H	3.74065914777509	2.60788965880038	10.77821010690531
H	3.47320672403088	5.28715942200268	7.41047445548880
H	-1.14913045587965	4.09587128559660	7.41315848987673

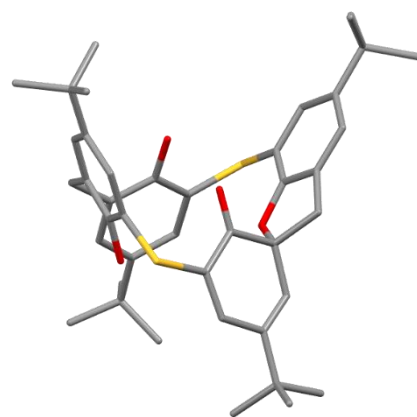


H -4.42032216246859	6.64958193610080	8.56831763480583
H 6.93510510636434	2.33569929132960	9.20744430705123
H 5.37548440427599	1.57764856051754	9.55299521457486
H 5.97419067625546	2.89739156990554	10.58028523606746
H 4.83759934346581	3.69206527411291	6.45237517377391
H 4.67304769301938	2.06152354853331	7.12307559486889
H 6.28467860230427	2.76130743983917	6.86593055703112
H 5.69112975132567	5.62748302647579	7.97803542504620
H 7.12192579971854	4.65384899278197	8.34891976176656
H 6.10902893010255	5.28490589316014	9.66406610829488
H -2.38520086575458	3.82088891853021	5.45858040508630
H -3.93316549229897	2.96542804314267	5.44913126544897
H -2.77739072761972	2.66747067959229	6.75278789064273
H -3.67933342673555	6.03204189600353	5.27322817372443
H -4.98751121753573	6.40966746843122	6.40645594986795
H -5.18265534110174	5.09023780421058	5.24710874325622
H -5.71810623709859	3.44981268176572	7.11145959419374
H -5.53831750063511	4.70919342071137	8.33720576271394
H -4.59348494794641	3.21748320340840	8.46479192089745
H -5.58984625081203	7.06014447783415	11.53897756056794
H -4.07791163593263	5.29254309671342	15.15026205812406
H 0.86888961049858	7.12538407567998	15.62189653830642
H 3.20697573120126	4.39910162066544	13.26523526186464
H -7.16366369676841	5.40490630922669	11.64999185680143
H -7.64092213169385	6.85740633047280	12.55346175367572
H -8.40949810490843	5.30152902764083	12.90011448673611
H -7.06732251390880	7.05897571254572	15.05289178112145
H -6.23389511320201	5.73955765125336	15.88927407580871
H -7.89163934185115	5.50711029589430	15.31257058159268
H -5.87786460513730	3.52530678870935	12.81668473299719
H -7.19466714210109	3.44114222636870	14.00514727204762
H -5.51736651770606	3.62020354933184	14.54603123944151
H 2.71466082302689	8.48588271928608	15.47324553091255
H 4.24380648291331	8.10859325333760	16.28101755797762
H 2.74249501767045	7.38172454619692	16.86471495346231
H 4.60396708199786	4.57813862129137	15.13985438101764
H 3.81693251324529	5.06521672697949	16.64830628382372
H 5.31032903297441	5.87003535717893	16.12384215625038
H 4.59895841347854	6.20480921641409	13.10669068521629
H 5.28570427254393	7.46917904193003	14.13947302813862
H 3.78101199619587	7.76803015205492	13.24352331986407
H -1.14145135776044	8.20817922780043	11.90097195255609
H -1.10406516805720	3.47307942316721	12.41645311438749
H -1.93914491185743	5.50429095406914	15.78984146407502
H -1.34792687503389	7.14763602228919	15.60632256187147
H 0.57956324855353	5.93432359265670	6.95763073869885
H 1.00628721744770	7.07654833094381	8.24929539692824

Mono C-spiro (1,3-*alt*)

Final single point energy = -2726.45105307391

S	7.71860845872920	10.88658599036617	12.70354061071362
C	9.18911649949349	11.60442114388965	11.98472303233355
C	9.07385301416315	12.93057789247299	11.55904466561453
C	10.07773314801242	13.58073912771709	10.82727620013093
C	11.22489271491337	12.83439389776909	10.53925112989788
C	11.38741879286367	11.50076846128789	10.95417463138690
C	12.63467633644715	10.72905294000701	10.53645723137360
C	13.45333476775549	10.10365332703463	11.66041061428025
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C	14.53642549140980	10.22143456392221	13.82961275472078
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C	10.36142256495513	10.87891937032213	11.69380707559023
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C	15.22996329392266	6.73291990243532	12.29649363493639
C	16.10203739033915	6.67641635214332	11.01883440886362
C	16.08102095060932	6.23054685469505	13.47875877472578
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C	13.30690696891359	11.68573580442676	15.88597439483856
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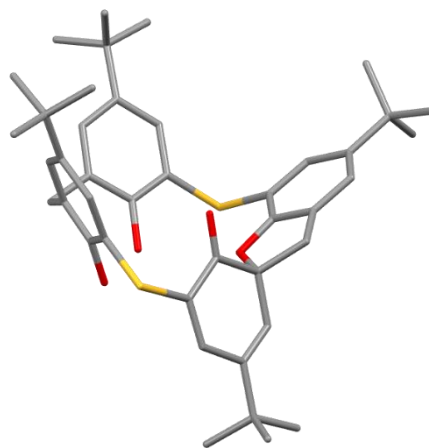


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H 9.52253284309064	16.98188578113237	11.32690907128478
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H 11.29129727282713	15.01368685731508	8.69260899055979
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Mono C-spiro (*partial cone*)

Final single point energy = -2726,46683649266

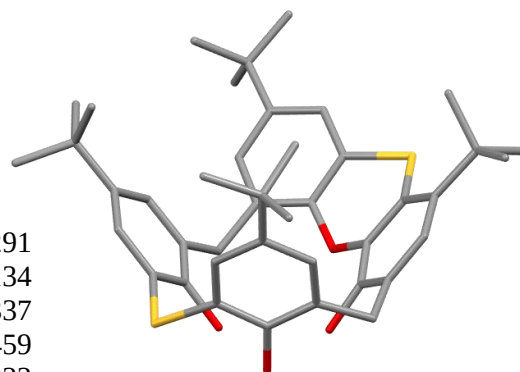
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C	8.82062484227123	18.31516678694861	6.59981903444648
C	8.36257006346504	17.78220350306919	5.30921408133614
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S	6.65497675177968	16.90484548093307	3.37611841863495
C	5.28593239862369	17.90142173430388	2.78779854266241
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C	3.08424005897689	17.96501321469868	1.73164693843957
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C	3.51524428793116	22.06890115926142	3.81926167665823
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C	1.49303822444984	22.85298876804766	4.99591917379970
C	2.24425729167890	22.93206894912791	6.17058056299080
C	3.60418399821157	22.59401647910880	6.19647500418520
S	4.56672773010419	22.82268076532387	7.70292541108076
C	4.32198485040703	21.29661669940314	8.61879076484626
C	3.50398783141408	21.27380662405443	9.75707078332687
C	3.35166414180464	20.13575043934586	10.56786844623487
C	4.05812137445407	18.97556625389926	10.20319812819388
C	5.00521899170067	20.12020961444914	8.30220641137337
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C	5.31961451092391	19.30764399343883	2.85947773901195
C	5.99833370652832	17.95202720408670	5.92788770733527
O	5.86045839470232	19.97537480948848	7.24406774385290
O	5.57325048340466	21.85142104125854	4.99907484767134
O	6.44530563695173	19.89290707420098	3.35094946498642
O	4.81439743642009	17.72964324134680	5.74521120300888
C	10.33741133349951	18.41067381261965	6.82795992444977
C	10.67963582979754	18.98748267260766	8.21453200318012
C	10.96101024795185	16.99714723266278	6.72403142580852
C	10.96028667525624	19.33317362842062	5.75100682242474
C	1.89377350342022	17.20366528293821	1.11922864674260
C	0.79199133892901	18.15209338798308	0.60843461699305
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C	2.43189784301336	20.19965172980821	11.80349433326635
C	0.99002418782253	20.54364278752936	11.35782379906892
C	2.94209964223077	21.29318559036708	12.77257190330288
C	2.39023699016116	18.86333479104145	12.57030277932827
H	1.61806240292877	22.35028710957965	2.90185875835900
H	1.79425651912759	23.26921309592304	7.09658055399468
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H	-0.44361115941495	22.95304772138831	7.07238624263055
H	-1.88565295118254	22.19738338740041	4.47423579922194
H	-0.50895761067995	21.57577557663936	3.54962782079052
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H	2.97847122481679	22.19033746832520	10.00735166023921
H	3.97215184342379	18.06959856715883	10.79381089457272
H	1.73080476443836	18.95837455741617	13.44070377613186
H	3.38101126565066	18.57259345240653	12.93855975674897
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H	0.59551642749069	19.77714257909935	10.68034098143029
H	2.29155509939680	21.35662197379872	13.65372828214840
H	2.95997993147063	22.28120588389529	12.30000746385031
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H	9.11898123197277	17.53282798594353	4.57098292930117
H	11.76771135827724	19.03126336316567	8.33717114559987
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H	10.79519120403775	18.95821177296903	4.73514442109459
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H	10.54328175079933	16.32697233537500	7.48457179865823
H	10.79226502039262	16.53775183301640	5.74361036783007
H	4.18972531082566	16.16648196066142	2.20955307289812
H	2.28391553926975	19.95257294805177	1.50516335791294
H	0.42203788187525	15.71966541001889	1.76794620343248
H	0.90481010161179	16.85691206705841	3.04450402090593
H	1.99255852181371	15.54651864928526	2.56917868719011
H	1.54677800311843	15.79418129839023	-0.51738785258143
H	2.82177802736733	16.98318975178204	-0.85575093219337
H	3.14415879122812	15.62233860463810	0.22877712345954
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H	0.36882673546828	18.75814822656771	1.41796108642597
H	5.86656003264227	21.62905421890611	5.90731302558430
H	6.20549411728262	20.71505967884941	3.82973850923234
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H	6.43955383017906	17.45197755564839	9.16013746182929
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Phenoxathiin-based Compound 8 (cone)

Final single point energy = -2726,49419552178



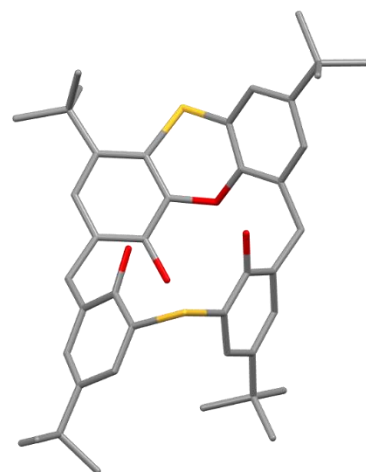
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C	2.63634699683718	8.41116210514613	4.05463629625322
C	1.39801665454019	7.78519855442953	4.23273057726623
C	1.29515827697184	6.59935988918902	4.96622090051605
C	2.43273441839658	5.99742218544125	5.49811752521387
O	2.30982884978696	4.87899053712656	6.31115711766396
C	1.40477229504437	3.89083871631389	5.94927077407904
C	0.16012936391907	4.14699481627371	5.36328118482198
C	-0.66836127296608	3.06453005504131	4.96669778224057
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C	1.07616904844698	1.50301717344785	5.78663838362481
C	1.66322813282023	0.09428437142918	5.83010830003613
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C	4.58136774710645	-0.02961483632478	2.63885092310935
C	4.99634409648813	0.31286435607574	3.93121540438619
S	6.65730761063062	0.97699965492904	4.19482211351265
C	6.36824574287212	2.73742642128334	3.89703172516986
C	6.73723041346510	3.29423424386540	2.67257161378525
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C	5.81341814733648	3.56351508252178	4.90009741585216
C	4.09854230551086	0.22275994696450	5.00712573824256
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C	2.78960167055787	9.75514418722514	3.31734943563137
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C	3.38502668300273	10.80375565012959	4.28779902755530
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C	6.99325554113720	5.22542248452967	1.02790305547703
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H	5.72312506363887	6.62337526969032	5.95835710254386
H	4.81484238539719	5.28208530534598	6.62611505932542
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H	5.80450714157610	6.49226223256198	3.21829579509109
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H	0.97502667463426	9.60435186324408	2.08388728498504
H	3.50313799405252	11.76963168840349	3.78117850642491
H	2.72868121327431	10.95137706766094	5.15296329735733
H	4.36858646101379	10.50113581282330	4.66218996995898
H	3.85507968336800	10.53678744759854	1.57598860057297
H	4.73119054519370	9.24331019431616	2.40295086682706
H	3.32998348464238	8.85048119399343	1.39392358551481
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H	-2.67458822729448	5.03661262732566	5.47067580864487
H	-3.12113852859590	3.49739478286089	6.21945381267511
H	-2.93040006713936	4.07162861465945	2.49539130244151
H	-1.50173643640669	4.96009256830872	3.04591095217161
H	-1.31228318049977	3.38041223343695	2.26688427864466
H	-3.73695774644571	2.06524270251167	3.60209177058355
H	-2.89577356228312	1.29746152611972	4.95289807148021
H	-2.18476839200959	1.27374896876240	3.32220115860907
H	1.90320967234922	-2.58491095526179	0.01473266320683
H	3.06558730557224	-2.96768288805483	1.30053924317451
H	1.43941964625468	-2.40280279393777	1.71464074020963
H	1.26490156478138	-0.16528542011171	-0.47167810550553
H	1.95519881662800	1.15896893105646	0.48910176891947
H	0.76719487184784	0.06342607556193	1.21072405386643
H	3.50098152846267	-1.02365674098607	-1.06810729609284
H	4.73348321849186	-1.39007576434149	0.14500103780804
H	4.27959163719163	0.29528121055231	-0.18557342159985
H	6.50363462198093	4.90842692774323	-1.07993197357570
H	6.36869148290412	3.43950491438792	-0.10117938616586
H	5.12181249814933	4.69264159003660	0.01546372558962
H	7.06543054800942	7.09907090730092	-0.06548590684347
H	7.30111468951733	7.30401626805297	1.67419421268380
H	5.67779840368686	6.98916936396792	1.02430886948586
H	8.82897047378402	5.36902637362516	-0.15280623759908
H	9.09639570600163	5.47121860432571	1.59896100633137
H	8.75131941356595	3.90814127768712	0.84338106781898
H	3.64304909545356	3.07024269590648	6.76333053714064
H	3.88383947664063	0.91694424639210	6.78100071992470
H	5.62427527068719	2.09896877898384	6.14744006153471

Phenoxathiin-based derivative (1,2-*alt*)

Final single point energy = -2726.47530210572

C	-4.68408761155431	-1.03710378354099	1.55070467945899
C	-4.48759156945539	-1.70104870494452	0.33018325914486
C	-3.38911858016759	-1.51671237974150	-0.51257508318987
C	-2.42981592871030	-0.56851634148158	-0.14012245277251
C	-2.55153487360246	0.06362091232126	1.10213797261132
C	-3.65258101208538	-0.14838386690336	1.93956827933669
C	1.55179855240842	0.31808813020088	0.64588787901323
C	1.66090272287594	-1.08391550593675	0.67997029046700
C	1.66184862557667	0.96553672971734	-0.59231114428978
C	1.84365699634149	-1.79068382297725	-0.52267617578583
C	1.87649849929490	0.28847790250946	-1.80166602179070
H	1.57764669557452	2.04816546347493	-0.59101348608403
C	1.97041062279842	-1.10485477719339	-1.73153223157327
H	2.09533723517216	-1.68917864813977	-2.63706502999403
C	-1.87599082458189	0.65767819184077	3.80592843361208
C	-0.98641055149910	0.78312918444659	2.73881223291113
C	-1.40938293171537	0.51610848715748	5.11553164256112
C	0.39609787353188	0.83151056419915	2.97280833909579
C	-0.03842926654353	0.53586528454540	5.38950222998493
C	0.82776018684785	0.70690141616388	4.29900469084399
C	-1.94484749970098	-3.04760409102823	-2.09738113882285
C	-1.71537582061595	-3.42162292464880	-3.42878554721325
C	-0.93437492973654	-3.31205007949139	-1.15943410871955
C	-0.52675458813309	-4.00599043702363	-3.88526748742701
H	-2.51749706501144	-3.22776097555719	-4.13509183510252
C	0.32585882503399	-3.75018751111043	-1.61987624432084
C	0.51373675973818	-4.11752237609237	-2.95148296162034
H	1.49547600827822	-4.46971105686147	-3.25375101093036
O	1.56741531111928	-1.70732434994798	1.88926799575318
O	-1.16999348163917	-3.09317027010459	0.15785550532132
C	-3.26752534743982	-2.34856761823006	-1.77619870346775
H	-4.06840393205549	-3.10076066921029	-1.74980980615511
H	-3.49046173559782	-1.71260052394537	-2.64513417261771
C	1.42853307114931	1.16081379929388	1.90443501058155
H	1.26008795619717	2.19644990993669	1.57961235713946
H	2.40634947137872	1.16356310195721	2.40472151181872
S	1.75259523164956	-3.60281555658548	-0.52351937986083
O	-1.38438595571484	-0.30185545409815	-0.96611339629185
H	-5.22585203153991	-2.42533611633456	0.00842871982912
H	1.89950101541668	0.74419317544480	4.47513606806400
H	-2.13864432889854	0.39534117645661	5.90828123175938
O	-1.48751567903268	0.90854272717438	1.44799244384401
C	-0.31584411868893	-4.47058064827592	-5.33893039960884
C	0.02383911810573	-5.98034387269112	-5.34398637397482
H	0.17956717888231	-6.33578888296769	-6.37034819450965
H	0.93660157462735	-6.19218712332008	-4.77605951585163
H	-0.78899452010678	-6.56706411322928	-4.90005859824171
C	-1.57089196864906	-4.25792801369306	-6.20809160165432
H	-2.43680262343625	-4.80061338521126	-5.81202479974787
H	-1.83893552688496	-3.19800068536413	-6.28749875196245
H	-1.38369284514984	-4.62702838652125	-7.22297228036603

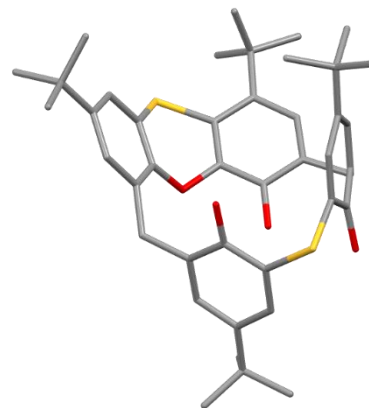


C	0.85240972579316	-3.68437299908561	-5.98161405781164
H	1.01789490666590	-4.01856663204244	-7.01372323299857
H	0.63733829007791	-2.60938991378658	-6.00213980623445
H	1.79111407270246	-3.82911384682115	-5.43504855207450
C	1.95627515234154	0.99850598103638	-3.16531465202065
C	1.85578769741037	2.53024348643549	-3.03172056010578
H	2.66583450045526	2.94128533635075	-2.41680173060933
H	1.92648583378025	2.99308156709029	-4.02259435157206
H	0.89996733334366	2.84102464951377	-2.59381648403797
C	3.30166981678281	0.66273941412701	-3.85212130698914
H	3.42704958362716	-0.41508387404327	-4.00269578504775
H	3.35697759015887	1.14404781227501	-4.83583317337661
H	4.14850340095906	1.01688266919247	-3.25220432577618
C	0.78458191170011	0.51135366873024	-4.05363910821616
H	-0.17947862206857	0.70716909083462	-3.57050714054134
H	0.79993381536850	1.02635782904256	-5.02200431617313
H	0.84039554925785	-0.56626160438336	-4.24378996064966
C	-5.95826020967196	-1.31242828795620	2.38823393312397
C	-6.95316739330825	-2.22897111039051	1.63977725778561
H	-6.53991762698665	-3.22623457365588	1.45148469276317
H	-7.84873858600625	-2.36072605492313	2.25718784143421
H	-7.27048203275181	-1.79940437494556	0.68272430483050
C	-6.71812064988664	0.00607599834359	2.67890274742157
H	-6.14403783206617	0.70561218991473	3.29217719642579
H	-6.98058285599912	0.51587230027781	1.74457571777177
H	-7.64818070082708	-0.20918636572648	3.21980678399447
C	-5.59432891303947	-2.03290582874188	3.71086017213255
H	-5.10376747927024	-2.99089787250305	3.50133940247786
H	-4.92393223662864	-1.43774094377403	4.33470730982722
H	-6.50423596046574	-2.23822220951612	4.28933634463586
C	0.53118963735357	0.38149964742557	6.81205017922688
C	-0.57667546933217	0.19287549158239	7.86590354881838
H	-1.25164791633632	1.05628822333191	7.90827684447218
H	-1.17766866699211	-0.70305699601709	7.67032057059390
H	-0.12604085206500	0.07880608932023	8.85853158093558
C	1.46062765524569	-0.85503300950547	6.86279431409185
H	0.91173895008362	-1.76827129007552	6.60492284061324
H	2.30056529482188	-0.76302841459162	6.16607018897781
H	1.87478451930122	-0.98002747095060	7.87101455861687
C	1.34122999794188	1.64717776663953	7.18386284090978
H	0.70523530325011	2.54008757825398	7.16188157820594
H	1.75856138921448	1.55155208893609	8.19406945334704
H	2.17477503708296	1.81354279557929	6.49329210088642
H	-0.35189204959509	-3.29280449892994	0.64861590741934
H	-0.73667402796509	0.24333440012748	-0.48120168707205
H	1.68141459570430	-2.66543230765944	1.74646965730656
S	-3.62239386321338	0.77416120122606	3.48130752305607

Phenoxathiin-based derivative (*partical cone 1*)

Final single point energy = -2726.47758807556

C	-3.96061016410150	0.27381478229923	0.46961738131214
C	-3.26573873478607	-0.05666389762080	-0.70643445125797
C	-2.18104693830970	0.67589799802965	-1.19699844959121
C	-1.75064123873549	1.80423353293599	-0.46816467633984
C	-2.40308899651959	2.14178734906962	0.73211681747980
C	-3.50475098876470	1.39289068940541	1.16774175544069
C	1.22109699284860	-1.39519741578563	2.44794743901010
C	0.38335096925542	-1.36433912887432	1.32562670610257
C	2.46714604217621	-2.01382597690986	2.31551582774929
C	0.87196500734538	-1.82637897333881	0.10111487957392
C	2.97545819250874	-2.53667060876774	1.11372719584549
H	3.08267578715297	-2.05819197031116	3.20670476478392
C	2.14899817897281	-2.38075298429709	-0.02657944927826
H	0.94759087636303	4.31316376915278	1.49552122501473
C	0.95670211608756	3.37235142529730	2.03959825859999
C	2.17383183068307	2.76485776825148	2.38194450222553
C	-0.26909151236706	2.79264356861529	2.37536608417796
C	2.09537479422049	1.49761994337615	2.97528686828464
C	-0.30695993068340	1.59426526167893	3.11782746450911
C	0.88599876147040	0.88275276513683	3.31566883434194
H	3.00397058433620	0.93132320929085	3.15149367567288
C	-0.13155676884221	0.00246153438750	-2.77304536707722
C	0.52213329181496	0.61750931016694	-3.85566975993696
C	0.57150091296290	-0.99515581253790	-2.08739006754294
C	1.81030579361203	0.27699831183988	-4.28112747306456
H	-0.02306885620438	1.39534071623264	-4.37815361708724
C	1.84374282838013	-1.39169251828493	-2.51572630889513
C	2.46145306947438	-0.75547189943212	-3.58928755641501
H	3.45651979846180	-1.07748979065876	-3.87932140254731
O	-1.46001371980557	1.07313177082116	3.60859630059878
O	-0.86322379873567	-0.84436520578855	1.42979827334911
O	0.01250929008494	-1.64456123476816	-0.99125452796537
C	-1.60656806860193	0.33170972248124	-2.56102013284518
H	-2.18815766645847	-0.51844967377597	-2.94265697002485
H	-1.83314944894003	1.16949355727669	-3.23334754459137
S	-1.80909556801130	3.51013240222992	1.75686045520535
C	0.84984724517273	-0.59808753675013	3.69114092941700
H	1.57020957197249	-0.81551030845809	4.48843036810928
H	-0.14540075978991	-0.86282642491953	4.05571354135592
O	-0.71807061295510	2.52246708623371	-0.97572767226005
H	-3.58198920598483	-0.92094943055924	-1.28569690082270
H	-3.99845288773442	1.70375111684792	2.08181994053340
C	4.37328979196361	-3.20371153217250	1.08323430697234
C	4.95108149118321	-3.39563386917899	2.50411208141578
H	5.90958535058280	-3.92251368870892	2.43135214691319
H	5.14513077792960	-2.44256813325211	3.00802956783863
H	4.28889057583163	-3.99585608864281	3.13900873563290
C	4.29026388909855	-4.61764275717329	0.45426112476034
H	3.58430336890205	-5.24661229011018	1.00898207366820
H	3.97631243111879	-4.60338981939133	-0.59267167019238
H	5.27481736260447	-5.10039317917834	0.49001404254650

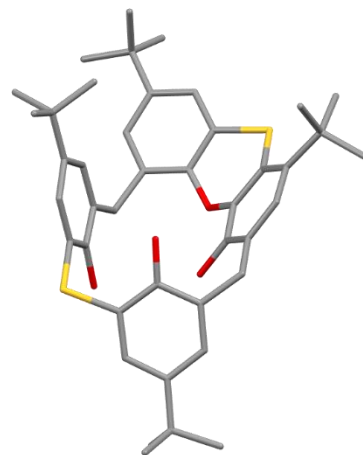


C	5.37780365284445	-2.32150193363637	0.30037748984022
H	5.06507086581920	-2.15810525859401	-0.73322964728510
H	5.48385381555468	-1.34220391683072	0.78253411419771
H	6.36602231892495	-2.79888899854583	0.28502547378120
C	2.51480510812124	0.96981601952943	-5.46325986037167
C	3.85870569162227	1.57056785431402	-4.98388236108910
H	3.69672592614888	2.31087528617753	-4.19175098760027
H	4.53225749524107	0.80133330178064	-4.59093562066732
H	4.37184709313181	2.06729850563887	-5.81697923664342
C	2.78715267976818	-0.06993375551217	-6.57759480968785
H	1.84971979853408	-0.50417223226623	-6.94428990501113
H	3.29820578903516	0.40304890056755	-7.42570580115475
H	3.41980417066797	-0.89043821906634	-6.22219392378135
C	1.66887496122685	2.10934129441356	-6.06462220589114
H	2.21783863535492	2.57864390847605	-6.88938490178368
H	0.71843354380719	1.74417017400847	-6.47024738248436
H	1.45134860999226	2.88877253479379	-5.32493446926301
C	3.50707152542986	3.45483420584177	2.03652564600703
C	3.57316441793738	4.82674497243840	2.74926765211884
H	4.51021091633379	5.34369923464347	2.50420852074184
H	2.74528028619047	5.47982338199865	2.45074952063925
H	3.52634021794424	4.70452709117146	3.83789004700864
C	3.60503980700595	3.66552126727622	0.50637385594022
H	2.79897910535589	4.30473733937204	0.12984779275482
H	4.55690332127058	4.14591930600649	0.24572823152770
H	3.54907305164218	2.70843340920705	-0.02413022592038
C	4.72427437551749	2.62093795132074	2.48221906747492
H	4.71904558445019	2.43932486226207	3.56341856406101
H	4.76358399385969	1.65230580679482	1.97112303738004
H	5.64877728170686	3.15798985622678	2.23955103810815
C	-5.13330281945266	-0.59867964000100	0.95034801654998
C	-6.25711488522400	-0.59226758889334	-0.11314279479627
H	-7.09155322567460	-1.22716356857593	0.20915084132931
H	-6.64314431510322	0.42160771333676	-0.27137361319688
H	-5.90544716033097	-0.96976324074389	-1.07932462583886
C	-5.72355463423546	-0.09334323232022	2.28113343970102
H	-4.98112013685277	-0.11542201555424	3.08809197885808
H	-6.11259791988579	0.92836163328791	2.19578135201997
H	-6.55746221426535	-0.73713495934530	2.58363884207704
C	-4.63213750181520	-2.04797652986172	1.16635664379643
H	-5.43939710751580	-2.67619898454385	1.56390123885302
H	-4.29118136406613	-2.50509865165165	0.23116238442937
H	-3.79559284730778	-2.06988505095238	1.87463030232597
H	-1.26080699267037	-0.80629726964940	0.53958958366057
H	-2.18420703254112	1.68656591145107	3.39726025857304
H	-0.54816190984593	3.27337270718486	-0.37758000228087
S	2.61307691810676	-2.78853482438572	-1.71533212971385

Phenoxathiin-based derivative (*partical cone 2*)

Final single point energy = -2726,47290230754

C	-4.90341991108579	0.89772129839256	0.13891802116469
C	-4.43611733057820	0.27907330155665	-1.02897172608902
C	-3.17466675247514	0.55294019151322	-1.56996235784784
C	-2.33527782570627	1.49442939080539	-0.93906456629235
C	-2.73253321843353	2.04931000431091	0.29453977070315
C	-4.01184313547072	1.76079453627728	0.79087028624818
C	3.61734223344998	-0.89507677400244	1.79425342253991
C	2.38461810195457	-1.41623239814228	1.40559202205575
C	4.79753584633809	-1.48107309493156	1.33744540066407
C	2.30521512951834	-2.46236361015679	0.48090303581314
C	4.76529851932145	-2.61188108951411	0.50427082106575
H	5.74560741814828	-1.05111121480864	1.64790042157590
C	3.50740551809469	-3.06758167575806	0.08201852267575
H	3.43852501608263	-3.90891258655138	-0.60091426531991
H	0.42981133603024	4.20281503412313	1.74526291158783
C	0.62240735303108	3.13795166149537	1.84012592842463
C	1.89575483479392	2.73681610761523	2.28137226319879
C	-0.43885754685576	2.28807697379150	1.51707802399777
C	2.11578149620316	1.33662075752567	2.32666000141797
C	-0.20961450416642	0.90948012784278	1.62664428531949
C	1.07518505015308	0.46841296733933	1.96989132070387
C	-1.01205358108984	-0.83208164243704	-2.72955651472260
C	0.01358763235922	-0.35429206649864	-3.56581167644008
C	-0.71328022654033	-1.69967342867287	-1.66036075287946
C	1.34854329690702	-0.69295082523963	-3.33921516237869
H	-0.26879939845412	0.28866511061731	-4.39266815811005
C	0.63332549300672	-1.99815728065445	-1.36565587421723
C	1.61782557892213	-1.49575021868026	-2.21577046678387
H	2.64938768125144	-1.73357606950014	-1.97732169944683
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C	6.89952796387831	-3.69059156376221	1.30784155878600
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H	5.32839924795762	-4.28698225627037	-1.73705766735061
H	6.82078678118542	-4.96445726958938	-1.07927392783282
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H	7.15082633074490	-1.35479167793574	-0.19190379956609
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H	3.68488734095336	4.05886484387336	0.61419238005325
C	4.22466346186172	3.47448776835954	3.26144660142292
H	4.09756926633102	2.88263844133812	4.17476390804766
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H	4.77413946458306	4.38265351288021	3.53887314720949
C	-6.31590383593290	0.58429227670806	0.66699583133586
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H	-8.37595561764680	0.77604366859958	-0.03933573128993
H	-7.30422041146913	2.07468135871129	-0.60381163676625
H	-7.21671812644814	0.46743572160996	-1.34102653646372
C	-6.62866580894146	1.34113066371571	1.97227720770077
H	-5.94609849071887	1.05938084341398	2.78256535761245
H	-6.57343706918751	2.42778405214282	1.83719434419842
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H	-2.54475083413002	-1.97736098229480	-1.21916962341493
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H	-2.30189695568948	3.27376776894463	1.98112154957623
H	-1.52538312158465	3.81372207989286	0.50230754889925
H	1.00104347470539	-3.90974055927163	-0.42852818096019
H	0.17059141902339	-2.73981044322251	0.59098348759936
S	3.63102148437686	0.51536908364416	2.88137400518790