

Supporting information for

Cr(II)-promoted internal cyclization of acyclic enediynes fused to benzo[*b*]thiophen core: macrocycles *versus* 2-methylenecycloalkan-1-ols formation

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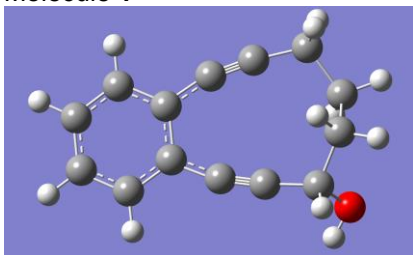
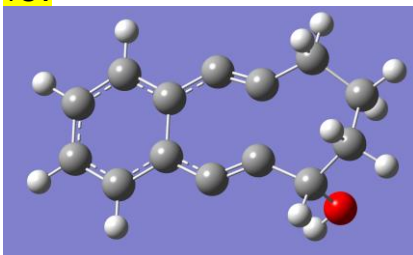
1. Computational details

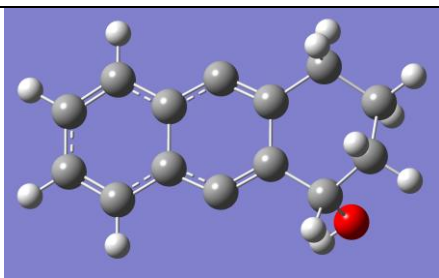
All calculations were performed with the B3LYP density functional method¹⁻³ by using the Gaussian 09 suite of quantum chemical programs⁴ at Resource center "Computer center of Saint Petersburg State University". Geometry optimizations of enediynes **1-5**, **acycl1-5**, the transition states of Bergman cyclization **TS1-5** and the resulting biradicals **birad1-5** were performed using B3LYP with the 6-31++G(d,p) basis set in the gas phase. Because of the open shell nature of the transition-states and the resulting biradicals calculations on these structures were performed using BS-UB3LYP (broken-spin-symmetry, unrestricted) calculations.⁵ Stationary points on the respective potential-energy surfaces were characterized at the same level of theory by evaluating the corresponding Hessian indices. Careful verification of the unique imaginary frequencies for transition states was carried out to check whether the frequency indeed pertains to the desired reaction coordinate.

Values calculated of activation energy (TS) and relative stability of biracial intermediates (BR) of Bergman cyclization for compounds #

compounds #	1	2	3	4a	4c	4d	5
TS, BR, $\Delta G^{(298)}$, kcal/mol	28.0 14.1	27.6 11.4	27.1 11.0	26.0 9.1	26.0 9.1	33.1 15.1	20.4 10.9

Cartesian Coordinates of stationary points (B3LYP/ 6-31G++(d,p)), Absolute Energies (au).

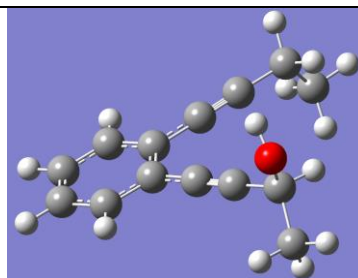
Molecule 1				TS1			
							
E = -615,85350686, H (0K) = -615,635562, H (298K) = -615,621575, G (298K) = -615,674765 au.				E = -615,80827871, H (0K) = -615,592004, H (298K) = -615,579091, G (298K) = -615,630066 au.			
Imaginary frequency = 0.				Imaginary frequency = 1.			
C	-3.9412970	-0.9734370	-0.0331220	C	2.7605770	-1.4215260	-0.2247880
C	-4.1047050	0.4149770	-0.0846300	C	1.5657370	-0.6790090	-0.1693220
C	-2.9914730	1.2557110	-0.0681980	C	1.6613170	0.7733470	0.0765750
C	-1.6947060	0.7235160	-0.0007880	C	2.9418030	1.3383050	0.2299320
C	-1.5291030	-0.6969840	0.0557550	C	4.0923360	0.5614080	0.1627570
C	-2.6618710	-1.5245730	0.0384160	C	4.0024850	-0.8190000	-0.0624410
C	0.6258290	1.9478580	0.0011630	H	2.6912570	-2.4896290	-0.3995020
C	2.4672330	-1.3876180	0.3865420	H	3.0146360	2.4062940	0.4032590
C	1.0100990	-1.3437370	0.2156770	H	5.0637120	1.0305960	0.2868800
C	-0.1944300	-1.1970590	0.1428710	H	4.9035720	-1.4227110	-0.1123990
H	-4.8092990	-1.6255850	-0.0463650	C	0.4493880	1.4779350	0.1265170
H	-5.1009970	0.8436560	-0.1383150	C	-0.7880690	1.1942200	-0.0092300
H	-3.1154340	2.3329900	-0.1095910	C	0.2720940	-1.2080840	-0.3221340
H	-2.5281860	-2.6006980	0.0827190	C	-0.9047870	-0.7012490	-0.2813640
C	2.9492820	1.0754070	-0.3892930	C	-3.3445260	1.0424580	0.2210450
H	2.6009180	0.6158880	-1.3190550	H	-3.3394770	0.7759140	1.2831310
H	3.9487050	1.4706700	-0.6014890	H	-4.2369680	1.6531160	0.0437820
C	2.0456130	2.2931500	-0.0533820	C	-3.4098370	-0.2312370	-0.6218920
H	2.2034270	3.0688760	-0.8141350	H	-4.3691210	-0.7398330	-0.4803010
H	2.3604700	2.7363100	0.9019810	H	-3.3231880	0.0132580	-1.6886850
H	2.6965790	-2.0527820	1.2336370	C	-2.3155120	-1.2294900	-0.2542460
C	3.0635220	-0.0012620	0.7196700	C	-2.1119720	1.8840500	-0.1232550
H	4.1203140	-0.1807700	0.9464830	H	-2.0679980	2.7692770	0.5200640
H	2.5956450	0.3440360	1.6488170	H	-2.2084900	2.2519020	-1.1552120
O	3.1459090	-1.8710870	-0.7846650	O	-2.6409850	-1.7296860	1.0516080
H	2.6785610	-2.6503060	-1.1137610	H	-1.8884870	-2.2454600	1.3721960
C	-0.5136560	1.5251210	0.0037180	H	-2.3377690	-2.0579990	-0.9749920
Molecule birad-1				Molecule acycl-1			



E = -615,83347138, **H (0K)** = -615,614585,
H (298K) = -615,601919, **G (298K)** = -615,652222
 au.

Imaginary frequency = 0.

C	2.7491470	-1.4351010	-0.1976670
C	1.5517390	-0.6719890	-0.1440130
C	1.6488750	0.7741090	0.0591860
C	2.9396900	1.3532700	0.1957520
C	4.0743030	0.5720480	0.1373810
C	3.9793490	-0.8279080	-0.0604050
H	2.6736880	-2.5073400	-0.3487460
H	3.0119000	2.4257390	0.3461370
H	5.0518150	1.0329770	0.2436150
H	4.8844960	-1.4261890	-0.1036840
C	0.4355600	1.4658550	0.0948970
C	-0.8203490	0.9666730	-0.0289160
C	0.2530060	-1.1715890	-0.2654440
C	-0.9157000	-0.4820490	-0.2187310
C	-3.3586700	1.0412710	0.2274550
H	-3.4097300	0.7511700	1.2827030
H	-4.2258100	1.6795590	0.0245760
C	-3.4100550	-0.2208330	-0.6399350
H	-4.3560280	-0.7553740	-0.5047190
H	-3.3331000	0.0472730	-1.7023110
C	-2.2727910	-1.1774380	-0.2884970
C	-2.0720040	1.8301640	-0.0432540
H	-1.9523890	2.6442180	0.6790310
H	-2.1414210	2.3047260	-1.0330850
O	-2.6061380	-1.7595640	0.9849890
H	-1.8353060	-2.2438740	1.3102920
H	-2.2116110	-1.9752790	-1.0405680

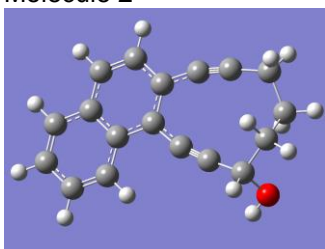


E = -617,07524251, **H (0K)** = -616,838572,
H (298K) = -616,821716, **G (298K)** = -616,886833
 au

Imaginary frequency = 0.

C	-1.7266300	-3.3776060	-0.1498710
C	-2.8932760	-2.6160900	-0.0194860
C	-2.8109110	-1.2318850	0.1094110
C	-1.5656920	-0.5743260	0.1116600
C	-0.3794270	-1.3500380	-0.0222280
C	-0.4845810	-2.7481650	-0.1512880
C	-1.4915700	2.0550780	0.3674500
C	3.3454500	0.3927060	-0.0050800
C	2.0189220	-0.2397390	-0.0332990
C	0.9091180	-0.7342790	-0.0255330
H	-1.7852280	-4.4571470	-0.2502880
H	-3.8651880	-3.1004670	-0.0180850
H	-3.7121570	-0.6361930	0.2112910
H	0.4259560	-3.3298170	-0.2518200
C	-1.4626690	3.5135340	0.4875290
H	-2.0665190	3.8147180	1.3538120
H	-0.4352590	3.8334310	0.7048070
H	3.2034090	1.4802320	-0.1062480
O	4.0347350	0.1215660	1.2275630
H	3.4240710	0.2749390	1.9612140
C	-1.5118060	0.8464390	0.2462620
C	-1.9736040	4.2392640	-0.7731970
H	-1.3650780	3.9811910	-1.6447700
H	-3.0097240	3.9627950	-0.9895250
H	-1.9286440	5.3236220	-0.6285900
C	4.2573780	-0.0910280	-1.1332460
H	4.4100490	-1.1708070	-1.0563630
H	3.8155530	0.1383670	-2.1068590
H	5.2266690	0.4094250	-1.0535880

Molecule 2

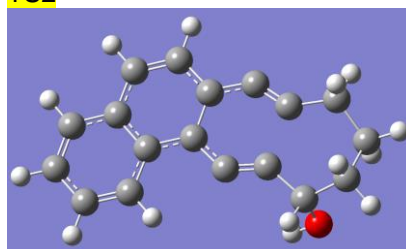


E = -769,50478497, **H (0K)** = -769,240112,
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 au.

Imaginary frequency = 0.

C	-1.4649830	2.4557990	-0.0577480
C	-0.3995040	1.5164290	0.0045210
C	-0.6891570	0.1355700	0.0487170

TS2

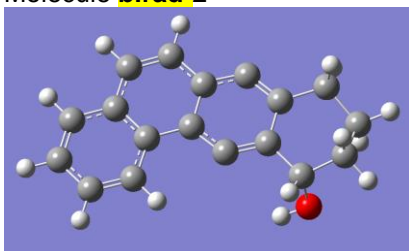


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H (298K) = -769,181578, **G (298K)** = -769,238792
 au.

Imaginary frequency = 1.

C	1.4645960	2.4318880	0.1860640
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C	0.7012900	0.0890330	-0.0765030

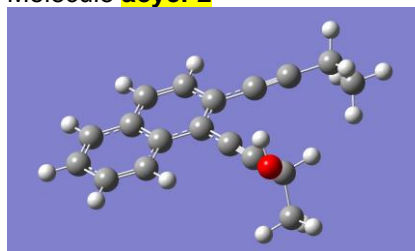
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H	-1.2239090	3.5131690	-0.0892560	H	1.2198280	3.4837490	0.2809760
H	-3.5786560	2.7621360	-0.1292940	H	3.5691120	2.7542050	0.2912960
C	0.4216790	-0.7555520	0.1292880	C	-0.3903560	-0.7827520	-0.2034260
C	1.5195460	-1.2742610	0.1981160	C	-1.6625860	-0.6245100	-0.2164880
C	0.9712540	1.9102620	0.0141280	C	-0.9648500	1.8591690	0.0480910
C	2.1852230	1.9718960	0.0136180	C	-2.0806390	1.2502050	-0.0713950
C	3.8887290	-0.6411500	0.7172860	C	-4.1891910	-0.8731870	-0.6240230
H	3.5472190	-0.1746050	1.6484620	H	-4.1383160	-0.6674570	-1.7012140
H	4.8348750	-1.1444150	0.9452200	H	-4.9775370	-1.6173960	-0.4704690
C	4.1241700	0.4261120	-0.3815770	C	-4.5004700	0.4093670	0.1473790
H	5.1985610	0.4918700	-0.5852920	H	-5.5217720	0.7392660	-0.0735250
H	3.6567510	0.1053350	-1.3173050	H	-4.4499490	0.2079070	1.2225220
C	3.6421580	1.8619830	-0.0381770	C	-3.5398420	1.5416800	-0.2283160
H	4.0761520	2.1798690	0.9204500	H	-3.7127770	1.8234450	-1.2772440
C	2.8909700	-1.7691530	0.3689850	C	-2.8768220	-1.5143860	-0.1816270
H	2.8991210	-2.4808670	1.2092860	H	-2.6508860	-2.3527600	-0.8545460
C	-3.7034880	-2.1014910	0.0468230	C	3.7607030	-2.0840490	-0.1868120
H	-3.9450170	-3.1598610	0.0809760	H	4.0149680	-3.1352890	-0.2865160
C	-4.7474090	-1.1459500	-0.0217110	C	4.7902870	-1.1222270	-0.0501790
H	-5.7815570	-1.4769720	-0.0404180	H	5.8290960	-1.4387920	-0.0438020
C	-4.4498610	0.1993730	-0.0636990	C	4.4713610	0.2137180	0.0728240
H	-5.2459250	0.9376200	-0.1154500	H	5.2553680	0.9592650	0.1771230
C	-2.0476680	-0.3169590	0.0273880	C	2.0774770	-0.3249180	-0.0692700
C	-3.1024080	0.6506080	-0.0401570	C	3.1183280	0.6459620	0.0663380
C	-2.3856050	-1.6965970	0.0710330	C	2.4375490	-1.6942930	-0.1960590
H	-1.5851330	-2.4278070	0.1246890	H	1.6449490	-2.4279230	-0.3039130
H	4.0347810	2.5553840	-0.7934400	H	-3.7544640	2.4320510	0.3724720
O	3.3907910	-2.4285390	-0.8065760	O	-3.0952370	-2.0191430	1.1447710
H	2.7050040	-3.0183120	-1.1467220	H	-2.2405270	-2.2848690	1.5106900

Molecule **birad-2**

E = -769,48906973, **H (0K)** = -769,223421,
H (298K) = -769,208071, **G (298K)** = -769,264541
 au.

Imaginary frequency = 0.

C	1.4579520	2.4457710	0.1590820
C	0.3777060	1.5054430	0.0456560
C	0.6872570	0.0911490	-0.0631250
C	2.7558690	2.0289200	0.1635740
H	1.2123590	3.4996430	0.2409140
H	3.5594510	2.7554160	0.2502680
C	-0.4171940	-0.7455200	-0.1623860
C	-1.7382660	-0.4037940	-0.1724930
C	-0.9716520	1.8424780	0.0271120
C	-2.0479770	1.0113930	-0.0733740
C	-4.1921400	-0.8673980	-0.6403620
H	-4.1624710	-0.6443870	-1.7154410
H	-4.9581620	-1.6343500	-0.4859150
C	-4.5140660	0.4033880	0.1532520
H	-5.5168000	0.7666060	-0.0977940
H	-4.5142780	0.1648950	1.2225890

Molecule **acycl-2**

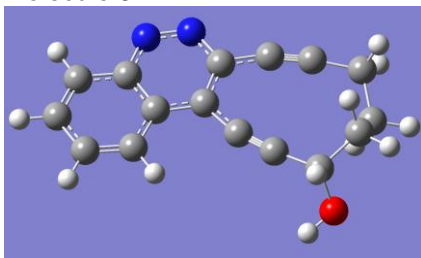
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Imaginary frequency = 1.

C	-2.6921680	-1.3124130	0.0175880
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C	-0.4522550	-0.2574680	-0.0850690
C	-1.8829230	-0.1308380	0.0128170
C	2.7466360	-1.8784570	-0.3693790
C	1.9021170	3.1124510	-0.1259780
C	1.0520110	1.9138960	-0.0884230
C	0.3666240	0.9099700	-0.0904210
C	4.1930880	-2.0845880	-0.4548030
H	4.4051610	-2.8240910	-1.2382880
H	4.6684530	-1.1498300	-0.7795170
H	2.9321010	2.7895580	-0.3449060
O	1.4712210	4.0348200	-1.1412420
H	1.3433740	3.5465250	-1.9658950
C	1.5487990	-1.6963310	-0.2761090
C	-4.6990710	0.0551880	0.2001210

C	-3.4851490	1.5012850	-0.1429840	C	-3.8996010	1.2236590	0.1955050
H	-3.6576120	1.8969960	-1.1546500	C	-2.5260650	1.1331050	0.1044020
C	-2.8453950	-1.4527590	-0.2208390	C	-4.1039270	-1.1851590	0.1128490
H	-2.5449600	-2.2381380	-0.9274210	H	-5.7794200	0.1391590	0.2723390
C	3.7570410	-2.0905610	-0.1634910	H	-4.3719760	2.1992180	0.2644520
H	4.0124120	-3.1427610	-0.2485650	H	-1.9173520	2.0308100	0.1005640
C	4.7798100	-1.1260000	-0.0484080	H	-4.7089700	-2.0881260	0.1155710
H	5.8203900	-1.4366450	-0.0442060	C	1.8999730	3.8827360	1.1954650
C	4.4544800	0.2141860	0.0582720	H	0.8864040	4.2136020	1.4369970
H	5.2375940	0.9627970	0.1465740	H	2.2704250	3.2501740	2.0067540
C	2.0719280	-0.3367430	-0.0603410	H	2.5456120	4.7607120	1.1023780
C	3.1036720	0.6389230	0.0544530	C	4.8220210	-2.5487310	0.8743730
C	2.4290020	-1.7010010	-0.1692760	H	4.6531400	-1.8107510	1.6639280
H	1.6406060	-2.4423420	-0.2599850	H	4.3884530	-3.4987290	1.2003410
H	-3.6079380	2.3473870	0.5411810	H	5.9016010	-2.6853000	0.7533320
O	-3.0403490	-2.0425950	1.0777680	C	-0.6963020	-2.6902530	-0.1662880
H	-2.1750610	-2.2693170	1.4443780	H	-0.2213050	-3.6631190	-0.2357390
				C	-2.0615440	-2.5839420	-0.0732130
				H	-2.6789930	-3.4782260	-0.0684620

Molecule 3

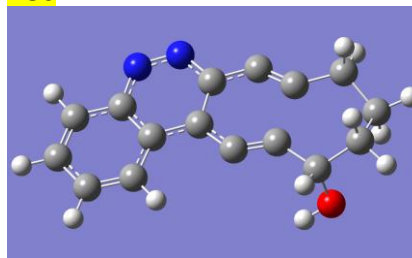


E = -801,54027614, H (OK) = -801,300221,
H (298K) = -801,283783, G (298K) = -801,342856
au.

Imaginary frequency = 0.

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C	0.4420670	-1.4447820	0.0088830
C	0.6870080	-0.0563270	0.0538380
C	2.0412660	0.3642170	0.0283310
C	-2.1223990	-1.9714340	0.0071590
C	-2.9363490	1.7502080	0.3758720
C	-1.5486700	1.2960740	0.2090290
C	-0.4334290	0.8165940	0.1364640
C	-4.1006260	-0.4775330	-0.3908430
H	-3.6400470	-0.1396790	-1.3240010
H	-5.1718740	-0.5715810	-0.5984020
C	-3.5803510	-1.9009230	-0.0520950
H	-3.9466790	-2.6022520	-0.8129040
H	-4.0084360	-2.2373810	0.9025570
H	-2.9657680	2.4555580	1.2209280
C	-3.8988270	0.5894220	0.7151830
H	-4.8591560	1.0634400	0.9454640
H	-3.5446380	0.1277550	1.6440270
O	-3.4456730	2.3957370	-0.7995360
H	-2.8095430	3.0608540	-1.0947490
C	-0.9102970	-1.8929880	0.0137050
C	4.7863760	0.9822970	-0.0338560
C	3.8123250	2.0152930	0.0340860
C	2.4673370	1.7183270	0.0650510
C	4.3990670	-0.3380140	-0.0692360
H	5.8401820	1.2425140	-0.0570350
H	4.1362050	3.0515460	0.0622920

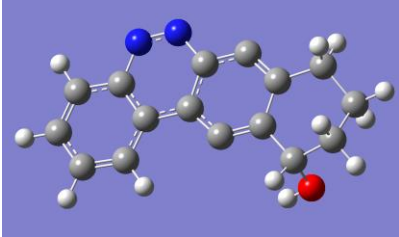
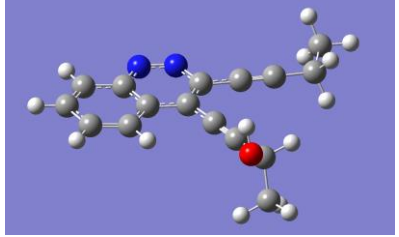
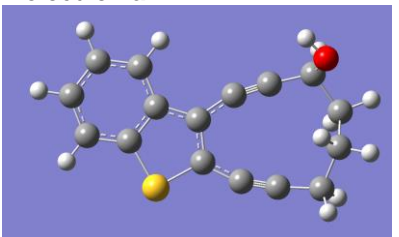
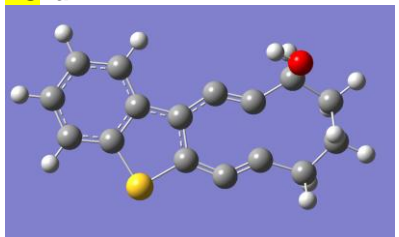
TS3



E = -801,49629195, H (OK) = -801,258156,
H (298K) = 801,242743, G (298K) = -801,299681
au.

Imaginary frequency = 1.

C	0.4324400	1.4383090	0.0566180
C	0.6965880	0.0162800	-0.0830090
C	-0.3993230	-0.8475910	-0.2108240
C	-1.6661260	-0.6416270	-0.2181410
C	-0.9129030	1.8286450	0.0534040
C	-2.0406520	1.2456260	-0.0584310
C	-4.1997690	-0.8136160	-0.6351430
H	-4.1405540	-0.5873000	-1.7077000
H	-5.0069270	-1.5406730	-0.4993050
C	-4.4794870	0.4600330	0.1626570
H	-5.4926280	0.8184460	-0.0498080
H	-4.4331350	0.2365360	1.2335290
C	-3.4939040	1.5767620	-0.1927100
H	-3.6642410	1.8895360	-1.2329140
C	-2.9067250	-1.4987920	-0.2030510
H	-2.7002070	-2.3290000	-0.8922040
C	3.8625000	-1.9910240	-0.1759020
H	4.1954520	-3.0203120	-0.2721630
C	4.8241720	-0.9565730	-0.0321810
H	5.8809740	-1.2049740	-0.0186120
C	4.4188740	0.3541410	0.0880670
H	5.1247170	1.1708070	0.1986810
C	2.0693730	-0.3616330	-0.0723220
C	3.0360140	0.6711380	0.0692360
C	2.5142720	-1.7046550	-0.1958890
H	1.7727130	-2.4893670	-0.3083580
N	1.4511910	2.3542440	0.1843350

H	1.7210450	2.5049570	0.1178430	N	2.6905650	1.9936210	0.1921810
H	5.1161450	-1.1507810	-0.1203080	H	-3.6778820	2.4577200	0.4313060
N	1.4459680	-2.3758190	-0.0504540	O	-3.1355870	-2.0167330	1.1136070
N	2.6910270	-2.0013320	-0.0733370	H	-2.2979360	-2.3551470	1.4588010
Molecule birad-3				Molecule acycl-3			
							
E = -801,52529625, H (0K) = -801,284260, H (298K) = -801,269134, G (298K) = -801,325335 au.				E = -802,76294132, H (0K) = -802,504035, H (298K) = -802,484777, G (298K) = -802,555294 au			
Imaginary frequency = 0.				Imaginary frequency = 0.			
C	0.4151650	1.4226040	0.0494600	C	-2.4001080	-1.5553590	0.0370720
C	0.6838890	0.0062520	-0.0680210	C	0.2908850	-1.3833580	0.0074620
C	-0.4311850	-0.8116860	-0.1718790	C	-0.4144970	-0.1700200	-0.0184030
C	-1.7395680	-0.4226850	-0.1765500	C	-1.8377960	-0.2476520	-0.0010740
C	-0.9206540	1.8101200	0.0375280	C	2.9271100	-1.4999990	-0.0125260
C	-2.0121500	1.0015420	-0.0672150	C	1.5117460	3.4555230	-0.1560290
C	-4.2071980	-0.8136410	-0.6478970	C	0.8167110	2.1606960	-0.0912530
H	-4.1686400	-0.5833780	-1.7210810	C	0.2588350	1.0815960	-0.0595780
H	-4.9937590	-1.5608930	-0.5014800	C	4.3852120	-1.6117090	-0.0222320
C	-4.4955820	0.4589170	0.1554880	H	4.7810650	-1.0428420	-0.8741950
H	-5.4864380	0.8525100	-0.0957150	H	4.7852760	-1.1272330	0.8785960
H	-4.5062760	0.2128120	1.2229150	H	2.5175930	3.2784590	-0.5676170
C	-3.4363540	1.5300780	-0.1300280	O	0.8111950	4.3880430	-0.9920440
H	-3.5949460	1.9407630	-1.1376930	H	0.6709430	3.9849930	-1.8597050
C	-2.8787650	-1.4393610	-0.2298160	C	1.7149290	-1.4336110	-0.0037670
H	-2.5988920	-2.2296550	-0.9390900	C	-4.6306190	-0.6158280	0.0347800
C	3.8769990	-1.9875410	-0.1611970	C	-4.0717220	0.6893620	-0.0020290
H	4.2182520	-3.0150200	-0.2472180	C	-2.7058930	0.8756660	-0.0198000
C	4.8243160	-0.9453900	-0.0366150	C	-3.8100320	-1.7210840	0.0543890
H	5.8843670	-1.1793540	-0.0272920	H	-5.7095660	-0.7361520	0.0480550
C	4.4009760	0.3655730	0.0721150	H	-4.7316770	1.5517930	-0.0155460
H	5.0986160	1.1911800	0.1687000	H	-2.2798990	1.8732180	-0.0465220
C	2.0677820	-0.3791680	-0.0643080	H	-4.2006650	-2.7330310	0.0831980
C	3.0193580	0.6625660	0.0589750	N	-0.3383220	-2.6083060	0.0460150
C	2.5208120	-1.7128820	-0.1750930	N	-1.6328380	-2.6902540	0.0586900
H	1.7912490	-2.5113790	-0.2724250	C	1.6507200	4.1119110	1.2187980
N	1.4358410	2.3600310	0.1661570	H	0.6629880	4.3019320	1.6467610
N	2.6635470	2.0013420	0.1712630	H	2.2141530	3.4650070	1.8964850
H	-3.5329520	2.3728430	0.5618390	H	2.1782950	5.0634670	1.1095730
O	-3.0872260	-2.0214400	1.0678260	C	4.8812150	-3.0689560	-0.0930570
H	-2.2355370	-2.3203010	1.4143010	H	4.5236770	-3.6438410	0.7657790
				H	4.5206040	-3.5592420	-1.0016810
				H	5.9755970	-3.0940180	-0.0962700
Molecule 4a				Molecule TS4a			
							
E = -1090,26160969, H (0K) = -1090,030074,				E = -1090,21931164, H (0K) = -1089,989633,			

H (298K) = -1090,013663, G (298K) = -1090,072652 au.

Imaginary frequency = 0.

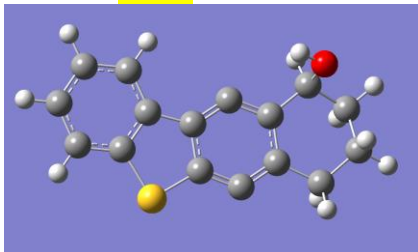
C	3.9581270	1.9992780	0.0279120
C	4.8025850	0.8739770	-0.0374090
C	4.2735090	-0.4138300	-0.0682940
C	2.8827080	-0.5632860	-0.0336920
C	2.0196360	0.5589520	0.0316480
C	2.5772430	1.8506500	0.0627890
S	1.9855980	-2.0769080	-0.0594660
C	-2.0242330	-1.9680410	0.0161530
C	-3.0932600	1.7210800	0.3720570
C	-1.6772380	1.3772770	0.1992600
C	-0.5248910	0.9893440	0.1364620
C	0.6305980	0.1693730	0.0571070
C	0.4592860	-1.2113840	0.0131340
C	-0.8174530	-1.8071620	0.0157390
H	4.3932280	2.9938550	0.0517060
H	5.8795520	1.0096310	-0.0639410
H	4.9259050	-1.2802090	-0.1181930
H	1.9236440	2.7163530	0.1139390
C	-4.0811250	-0.5932310	-0.3872020
H	-3.6274240	-0.2302510	-1.3140710
H	-5.1418830	-0.7510240	-0.6095420
C	-3.4839160	-1.9859700	-0.0409620
H	-3.8105780	-2.7087240	-0.8000220
H	-3.8942690	-2.3403110	0.9151600
H	-3.1791250	2.4251260	1.2143700
C	-3.9572320	0.4860450	0.7194050
H	-4.9520170	0.8784910	0.9570160
H	-3.5589320	0.0546790	1.6448110
O	-3.6675470	2.3223290	-0.8003680
H	-3.0533550	2.9858550	-1.1414730

H (298K) = -1089,974167, G (298K) = -1090,031291 au.

Imaginary frequency = 1.

C	-4.0217920	1.9558370	-0.1615250
C	-4.8430330	0.8216710	-0.0142760
C	-4.2864230	-0.4497940	0.0971100
C	-2.8930250	-0.5733230	0.0610760
C	-2.0537470	0.5560230	-0.0869960
C	-2.6385270	1.8318640	-0.1982960
S	-1.9737850	-2.0691790	0.1827580
C	1.9854790	-1.2023080	-0.0619780
C	4.2946130	0.7130760	-0.6263170
C	3.0459930	1.4795120	-0.2002120
C	1.7541010	0.7075870	-0.2338320
C	0.4992070	0.9778480	-0.2313070
C	-0.6511770	0.2093010	-0.1042560
C	-0.4567250	-1.2069830	0.0397610
C	0.8224210	-1.7306810	0.0520360
H	-4.4758450	2.9383370	-0.2484410
H	-5.9223330	0.9370530	0.0124980
H	-4.9200140	-1.3241390	0.2103210
H	-2.0020970	2.7036000	-0.3142290
H	4.2319390	0.5005430	-1.7014610
H	5.1486210	1.3810220	-0.4740110
C	4.4760330	-0.5835670	0.1621180
H	4.4373820	-0.3655490	1.2344750
H	5.4621720	-1.0130220	-0.0468980
C	3.4148670	-1.6227000	-0.2090670
H	3.5407490	-2.5231520	0.4018400
H	3.5655140	-1.9307390	-1.2541310
O	3.3054670	1.9806770	1.1198690
H	2.4789450	2.3315590	1.4785430
H	2.9021870	2.3257380	-0.8858090

Molecule **birad-4a**

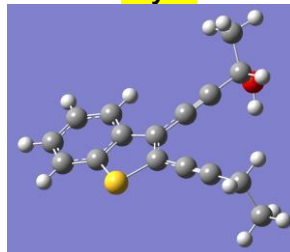


E = -1090,24983962, H (0K) = -1090,017177,
H (298K) = -1090,002099, G (298K) = -1090,058159 au.

Imaginary frequency = 0.

C	-4.0125700	1.9642360	-0.1401860
C	-4.8314900	0.8287610	-0.0157210
C	-4.2742750	-0.4456320	0.0791490
C	-2.8820080	-0.5700250	0.0482540
C	-2.0458740	0.5626300	-0.0760600
C	-2.6271210	1.8375590	-0.1708550
S	-1.9747480	-2.0850160	0.1536180
C	1.9841570	-0.9559640	-0.0671560
C	4.2960390	0.7050310	-0.6453220
C	3.0073330	1.4166970	-0.2399010
C	1.8076110	0.4751120	-0.1807480
C	0.5198730	0.9478710	-0.1828770

Molecule **acycl-4a**



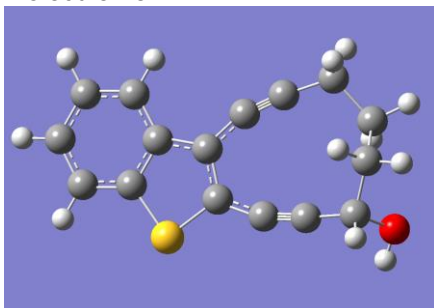
E = -1091,4872861, H (0K) = -1091,236853,
H (298K) = -1091,217644, G (298K) = -1091,287652 au

Imaginary frequency = 0.

C	2.4349670	-1.1847400	-0.0080290
C	-0.0774750	-1.2827210	-0.1764870
C	0.3840690	0.0214910	-0.0774090
C	1.8288430	0.0933150	0.0208120
C	-2.5550210	-2.1234180	-0.3869210
C	-2.0290730	3.3400510	-0.0402510
C	-1.1558860	2.1582830	-0.0730870
C	-0.4602400	1.1608970	-0.0735540
C	-3.9355620	-2.5952330	-0.4844750
H	-4.5503300	-1.8008980	-0.9274420
H	-3.9746250	-3.4394080	-1.1854050
H	-3.0624780	2.9986350	-0.2094740

C	-0.6376870	0.2081160	-0.0865780	O	-1.9577620	4.0176310	1.2258790
C	-0.4443330	-1.2172670	0.0303360	H	-2.0384060	3.3613640	1.9312430
C	0.8366330	-1.7039440	0.0290130	C	-1.4109230	-1.7229040	-0.2860430
H	-4.4651720	2.9483950	-0.2133450	C	4.6096950	-0.1942760	0.1891010
H	-5.9111790	0.9419910	0.0067640	C	4.0212600	1.0848860	0.2200470
H	-4.9093870	-1.3208810	0.1747970	C	2.6424820	1.2350680	0.1370670
H	-1.9915100	2.7124940	-0.2680900	C	3.8237880	-1.3379310	0.0751530
H	4.2496210	0.4702070	-1.7172210	H	5.6890890	-0.2924320	0.2550980
H	5.1284710	1.4007210	-0.4977600	H	4.6536540	1.9629110	0.3101670
C	4.4964750	-0.5777970	0.1677440	H	2.1842850	2.2189810	0.1618900
H	4.5160770	-0.3245130	1.2334670	H	4.2780150	-2.3237180	0.0517230
H	5.4611670	-1.0374530	-0.0739590	C	-1.6716870	4.3725700	-1.1105060
C	3.3704820	-1.5787670	-0.1160180	H	-0.6466690	4.7244120	-0.9667440
H	3.4085100	-2.4184200	0.5858880	H	-1.7617500	3.9353310	-2.1086380
H	3.5098170	-2.0106840	-1.1179550	H	-2.3519980	5.2252100	-1.0303940
O	3.2531700	2.0098760	1.0482120	C	-4.5349500	-3.0202010	0.8714330
H	2.4129250	2.3260610	1.4066170	H	-3.9565480	-3.8355570	1.3153090
H	2.7817880	2.2136480	-0.9612370	H	-4.5380030	-2.1833730	1.5757490
				H	-5.5660480	-3.3619890	0.7355570
				S	1.2386370	-2.4600840	-0.1560490

Molecule 4c

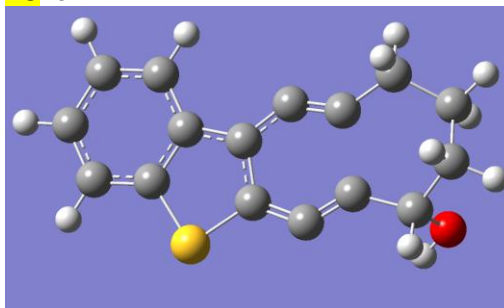


E = -1090,26121601, H (0K) = -1090,029617,
H (298K) = -1090,013225, G (298K) = -
1090,072156 au.

Imaginary frequency = 0.

C	4.3108570	1.6263970	0.0773450
C	4.9602860	0.3760570	0.0815110
C	4.2297190	-0.8085650	0.0458620
C	2.8329190	-0.7283340	0.0047490
C	2.1650950	0.5219200	0.0011310
C	2.9249190	1.7062190	0.0376970
S	1.7030230	-2.0747850	-0.0457230
C	-2.2338270	-1.3033590	-0.1828680
C	-3.7565830	1.3984400	0.3907450
C	-2.7045760	2.4822360	0.0243290
C	-1.3454400	1.9468830	-0.0396380
C	-0.2710120	1.3754440	-0.0436070
C	0.7311380	0.3698660	-0.0395650
C	0.3394590	-0.9650660	-0.0672200
C	-1.0174990	-1.3378120	-0.1310010
H	4.9024220	2.5364580	0.1058010
H	6.0448400	0.3332570	0.1128900
H	4.7328140	-1.7706260	0.0493020
H	2.4193010	2.6671880	0.0351690
H	-3.4511130	0.9032290	1.3171610
H	-4.6886100	1.9255000	0.6212980
C	-4.0407530	0.3394020	-0.7060680
H	-3.5185280	0.5897850	-1.6364230
H	-5.1115550	0.3315160	-0.9371150

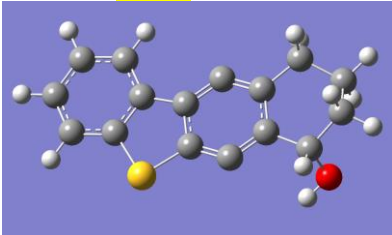
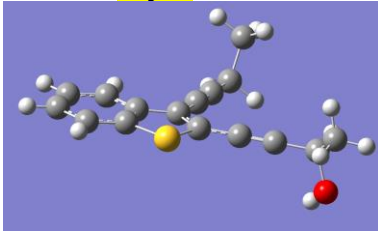
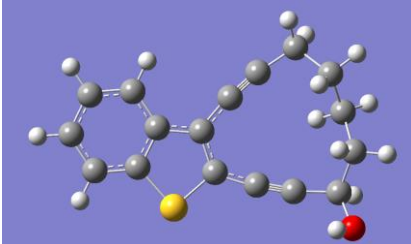
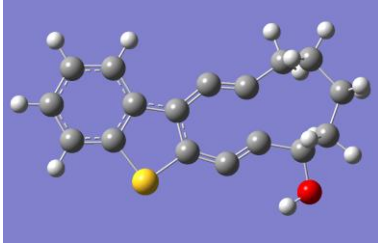
TS4c



E = -1090,21938189, H (0K) = -1089,989660,
H (298K) = -1089,974203, G (298K) = -
1090,031318 au.

Imaginary frequency = 1.

C	4.2459320	1.7611180	0.2062250
C	4.9481100	0.5419870	0.1420370
C	4.2673910	-0.6663640	0.0221720
C	2.8689320	-0.6424730	-0.0345690
C	2.1489670	0.5744520	0.0307220
C	2.8583360	1.7848720	0.1513380
S	1.8058070	-2.0343500	-0.1862170
C	-2.0261860	-0.7002490	-0.2425410
C	-4.1612910	1.4291900	0.2059270
C	-2.8269430	2.0556830	-0.2071090
C	-1.6190620	1.1780780	-0.0956230
C	-0.3463260	1.2651520	-0.0139310
C	0.7201030	0.3782440	-0.0376390
C	0.3813510	-1.0121090	-0.1630180
C	-0.9440270	-1.3987500	-0.2600270
H	4.7964460	2.6922220	0.3005990
H	6.0330120	0.5420510	0.1864160
H	4.8100030	-1.6054030	-0.0273580
H	2.3129690	2.7220920	0.2023160
H	-4.1667730	1.2172400	1.2801850
H	-4.9559820	2.1587930	0.0141640
C	-4.4389900	0.1404500	-0.5672320
H	-4.3395460	0.3141230	-1.6465830
H	-5.4608600	-0.2076300	-0.3847500

C	-3.6802740	-1.1219150	-0.3497640	C	-3.5021780	-0.9930040	-0.1610290
H	-4.0146810	-1.7548560	-1.1864930	H	-3.6662220	-1.8434430	-0.8368700
H	-2.7477410	3.2812360	0.7759940	H	-2.6281680	2.9471960	0.3973540
O	-4.4253270	-1.4680800	0.8282690	O	-3.8707210	-1.3710530	1.1731480
H	-4.1077610	-2.3185520	1.1597630	H	-3.2074550	-1.9915620	1.5053680
H	-2.9716900	2.9501770	-0.9337530	H	-2.8992810	2.3946710	-1.2507580
Molecule birad-4c				Molecule acycl-4c			
							
E = -1090,24968700, H (0K) = -1090,017021, H (298K) = -1090,001940, G (298K) = -1090,058009 au.				E = -1091,48683436, H (0K) = -1091,236373, H (298K) = -1091,217175, G (298K) = -1091,287011 au			
Imaginary frequency = 0.				Imaginary frequency = 0.			
C	4.2487190	1.7640530	0.1762340	C	-2.2526100	-1.4788950	0.0647020
C	4.9434790	0.5433420	0.1201270	C	0.1646060	-0.7813410	0.0129010
C	4.2562660	-0.6649480	0.0159310	C	-0.6867200	0.3075910	-0.1026620
C	2.8590030	-0.6367900	-0.0314580	C	-2.0828160	-0.0808070	-0.0738260
C	2.1471270	0.5829130	0.0239680	C	2.7891200	-0.7939980	0.0323360
C	2.8584390	1.7893730	0.1286470	C	0.5448640	4.1990990	-0.4636810
S	1.7986510	-2.0462730	-0.1611350	C	0.1051180	2.8077320	-0.3511140
C	-2.0099320	-0.4623980	-0.1903470	C	-0.2471640	1.6502210	-0.2331810
C	-4.1742580	1.4356860	0.2133590	C	4.2579390	-0.7752020	0.0117530
C	-2.7866950	1.9975720	-0.1167820	H	4.5827130	0.2479310	0.2586400
C	-1.6893930	0.9442690	-0.0906640	H	1.4941200	4.2286270	-1.0144640
C	-0.3564460	1.2588610	-0.0263430	C	1.5725870	-0.7749190	0.0214960
C	0.7095450	0.3862480	-0.0403550	C	-4.6369410	-1.2256100	0.0212750
C	0.3691940	-1.0122130	-0.1427220	C	-4.4843880	0.1680340	-0.1169370
C	-0.9576030	-1.3455060	-0.2099050	C	-3.2204940	0.7421770	-0.1648440
H	4.8021450	2.6945700	0.2574390	C	-3.5259560	-2.0591790	0.1129980
H	6.0286630	0.5381440	0.1582640	H	-5.6326810	-1.6572950	0.0568570
H	4.7959380	-1.6059470	-0.0269840	H	-5.3656590	0.7984920	-0.1868090
H	2.3174180	2.7297320	0.1718530	H	-3.0965970	1.8154420	-0.2715470
H	-4.2438980	1.2065250	1.2825010	H	-3.6448830	-3.1330260	0.2193040
H	-4.9355370	2.1923860	-0.0062940	C	0.7173140	4.8977870	0.9001100
C	-4.4428000	0.1584450	-0.5887100	H	-0.2264730	4.9128990	1.4529690
H	-4.3527840	0.3617530	-1.6642730	H	1.4601660	4.3786110	1.5125430
H	-5.4559160	-0.2159910	-0.4095560	C	1.0493290	5.9309330	0.7548210
C	-3.4579760	-0.9457350	-0.2115200	C	4.8752400	-1.7453120	1.0203250
H	-3.5328260	-1.7711080	-0.9322290	H	4.5668840	-1.4877490	2.0372370
H	-2.5203880	2.8062030	0.5719210	H	4.5596810	-2.7683700	0.7997210
O	-3.8516350	-1.4228710	1.0876310	H	5.9652530	-1.6892030	0.9517280
H	-3.1638470	-2.0156140	1.4196440	S	-0.7110510	-2.3091940	0.1588710
H	-2.8043110	2.4436520	-1.1219430	H	-0.1789560	4.7557430	-1.0732400
				O	4.7759390	-1.1365990	-1.2792570
				H	4.2982110	-0.6374110	-1.9555530
Molecule 4d				TS4d			
							

E = -1129,58315562, H (0K) = -1129,322598,
H (298K) = -1129,305015, G (298K) = -
1129,366737 au.

Imaginary frequency = 0.

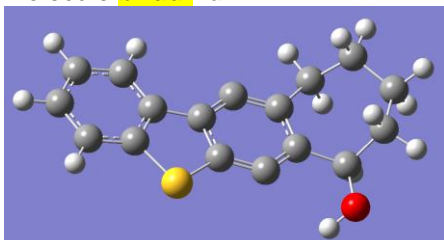
C	2.0846170	-1.5160160	-0.2305840
C	2.0951600	3.1090870	-0.0954190
C	0.8826190	2.2855540	-0.0846400
C	-0.0105070	1.4603430	-0.0656050
C	-0.9192280	0.3693060	-0.0562090
C	-0.4710620	-0.9452860	-0.1102540
C	0.8833630	-1.3282330	-0.1769060
C	4.1050570	-0.1904350	0.2919690
H	3.7844190	-0.1267800	1.3397530
H	5.1978780	-0.2670870	0.2965330
C	3.5566200	-1.5255950	-0.2717270
H	2.2770610	3.4837660	-1.1125210
H	1.9612240	3.9930510	0.5404700
C	3.3194150	2.2909470	0.3972130
H	4.1879800	2.9586900	0.4472410
H	3.1096420	1.9710200	1.4242110
C	3.6183880	1.0555710	-0.4842750
H	2.6961490	0.7895260	-1.0089640
H	4.3474760	1.3190000	-1.2599950
O	4.1181830	-2.6530780	0.4063790
H	3.7378770	-2.6958570	1.2952230
H	3.8866900	-1.6429870	-1.3114830
C	-4.5483130	1.4709060	0.1304770
C	-5.1460110	0.1951990	0.1237700
C	-4.3680180	-0.9575300	0.0589490
C	-2.9763540	-0.8185980	0.0003020
C	-2.3607930	0.4567470	0.0069370
C	-3.1673550	1.6080820	0.0724580
S	-1.7913820	-2.1118700	-0.0888430
H	-5.1759350	2.3554760	0.1813630
H	-6.2273330	0.1072390	0.1692260
H	-4.8307000	-1.9396220	0.0534330
H	-2.7013760	2.5888180	0.0772330

E = -1129,52880999, H (0K) = -1129,270735,
H (298K) = -1129,253871, G (298K) = -
1129,313998 au.

Imaginary frequency = 1.

C	1.7758380	-0.7149450	-0.2954600
C	2.5878460	1.9963450	-0.6439480
C	1.3706890	1.1453430	-0.4753670
C	0.0986860	1.2357820	-0.4004960
C	-0.9626390	0.3661240	-0.2103420
C	-0.6136150	-1.0230360	-0.0643350
C	0.7124490	-1.4142530	-0.1148990
C	4.0641560	-0.4644160	0.8097300
H	3.4738390	-0.5999890	1.7240120
H	4.9310700	-1.1297820	0.8825820
C	3.2556150	-0.9698470	-0.4097840
H	3.1678260	1.6693810	-1.5165650
H	2.2127830	2.9950010	-0.8860470
C	3.5100620	2.0838800	0.5954210
H	4.0301560	3.0489240	0.5529900
H	2.8915240	2.1025910	1.5006590
C	4.5720010	0.9801110	0.6927220
H	5.2284460	1.0479900	-0.1873110
H	5.2103330	1.1895940	1.5599690
O	3.4801880	-2.3655180	-0.6195280
H	2.7468170	-2.8532210	-0.2190620
H	3.6456060	-0.4824140	-1.3122860
C	-4.4831170	1.7721690	-0.0250670
C	-5.1735180	0.5659110	0.2010260
C	-4.4862270	-0.6417630	0.2866060
C	-3.0939320	-0.6294140	0.1445940
C	-2.3859530	0.5742240	-0.0849030
C	-3.1015550	1.7840860	-0.1686660
S	-2.0239370	-2.0225340	0.2188170
H	-5.0380460	2.7032470	-0.0891560
H	-6.2537880	0.5751410	0.3097410
H	-5.0191640	-1.5714530	0.4607730
H	-2.5666410	2.7118660	-0.3461220

Molecule **birad-4d**

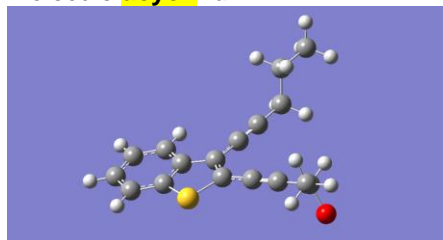


E = -1129,56187712, H (0K) = -1129,300495,
H (298K) = -1129,284295, G (298K) = -
1129,342619 au.

Imaginary frequency = 0.

C	-1.7759080	0.4936840	-0.3110950
C	-2.5310630	-1.9648780	-0.6164870
C	-1.4532200	-0.9111160	-0.4290390
C	-0.1250420	-1.2382580	-0.3442550
C	0.9424470	-0.3799120	-0.1676270
C	0.6002260	1.0115430	-0.0543040
C	-0.7253030	1.3602890	-0.1366110
C	-4.1105650	0.4706010	0.7423360

Molecule **acycl-4d**



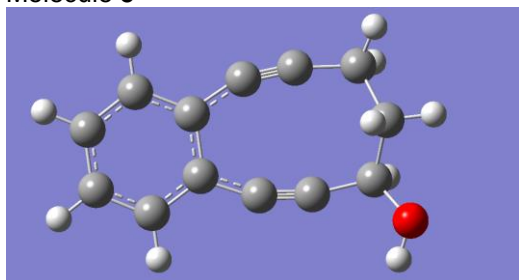
E = -1130,80465465, H (0K) = -1130,525834 ,
H (298K) = -1130,505279, G (298K) = -
1130,578411 au

Imaginary frequency = 0.

C	2.7008580	-1.2139090	-0.1035420
C	0.1869460	-1.1422980	-0.0177670
C	0.7421660	0.1192390	0.1376190
C	2.1905530	0.0918120	0.0896650
C	-2.3521000	-1.8069110	-0.0296160
C	-1.4107800	3.5660560	0.6541840
C	-0.6425190	2.3327010	0.4872970
C	-0.0155520	1.3045190	0.3211730

H	-3.5753590	0.5881560	1.6923740	C	-3.7791640	-2.1546500	-0.0034250
H	-4.9743300	1.1440360	0.7771690	H	-4.3508250	-1.2372220	-0.2150100
C	-3.2173120	0.9813610	-0.3998580	H	-2.3568170	3.3335680	1.1623470
H	-3.0788980	-1.7728580	-1.5505730	C	-1.1784100	-1.4862150	-0.0216840
H	-2.0303150	-2.9287450	-0.7461560	C	4.9477230	-0.3768850	-0.0572500
C	-3.5386580	-2.0678240	0.5485870	C	4.4552100	0.9288450	0.1354250
H	-4.0448400	-3.0386070	0.4732300	C	3.0889530	1.1681220	0.2092820
H	-2.9885820	-2.0767210	1.4985980	C	4.0777920	-1.4567920	-0.1779970
C	-4.6127500	-0.9701000	0.5708490	H	6.0190020	-0.5455230	-0.1124410
H	-5.1989090	-1.0321600	-0.3579120	H	5.1528680	1.7558050	0.2271780
H	-5.3153020	-1.1857190	1.3853040	H	2.7033530	2.1720270	0.3579970
O	-3.2914090	2.4060820	-0.3603460	H	4.4586250	-2.4625750	-0.3262130
H	-2.6051890	2.7736930	-0.9343280	C	-1.7111940	4.2922340	-0.6765970
H	-3.6414550	0.6241190	-1.3544000	H	-0.7631800	4.5214610	-1.1771390
C	4.4724380	-1.7887040	0.0005820	H	-2.2548810	3.6079120	-1.3381610
C	5.1622460	-0.5783640	0.1885930	C	-4.1477790	-3.2156810	-1.0415580
C	4.4742990	0.6322730	0.2536920	H	-3.9249000	-2.8577620	-2.0503990
C	3.0817520	0.6169010	0.1277300	H	-3.5853980	-4.1345210	-0.8562020
C	2.3746130	-0.5924450	-0.0617810	H	-5.2166830	-3.4346130	-0.9673850
C	3.0867720	-1.8013930	-0.1245510	S	1.4130880	-2.3977430	-0.2253520
S	2.0202800	2.0304690	0.1819980	H	-0.8642440	4.2452990	1.3230130
H	5.0262140	-2.7213710	-0.0471740	O	-4.1762190	-2.6737580	1.2766690
H	6.2438380	-0.5831450	0.2846890	H	-3.8287640	-2.0933980	1.9675030
H	5.0098810	1.5653200	0.3992110	C	-2.5195310	5.5760350	-0.4660870
H	2.5502150	-2.7341040	-0.2697970	H	-1.9812620	6.2860620	0.1728870
				H	-2.7207990	6.0741610	-1.4200480
				H	-3.4847770	5.3659310	0.0096170

Molecule 5

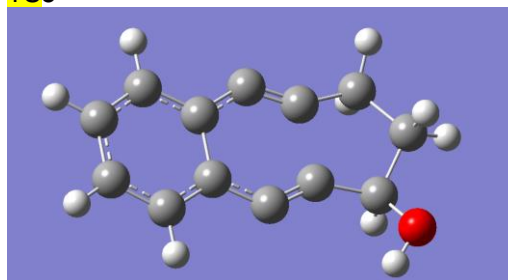


E = -576,52839031, H (0K) = -576,339218,
H (298K) = -576,326539, G (298K) = -576,376579
au.

Imaginary frequency = 0.

C	2.3807830	-1.5465950	0.0477460
C	1.2739580	-0.6870910	0.0694210
C	1.4819500	0.7333750	-0.0046030
C	2.7913610	1.2241100	-0.1016880
C	3.8785140	0.3493390	-0.1248680
C	3.6743120	-1.0323690	-0.0503790
H	2.2181830	-2.6180120	0.1057290
H	2.9474670	2.2964670	-0.1592830
H	4.8862440	0.7465580	-0.2009210
H	4.5225520	-1.7099080	-0.0683710
C	0.3089280	1.5488890	0.0303650
C	-0.8754700	1.8195400	0.0976430
C	-0.0845290	-1.1177880	0.1634240
C	-1.3001090	-1.0806480	0.2034380
C	-2.3359410	1.8809040	0.1832300
C	-3.0208550	0.6183860	-0.4078060
H	-4.1063330	0.7593750	-0.3548790
H	-2.7522450	0.5107700	-1.4629500

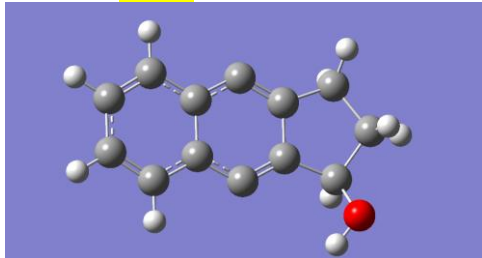
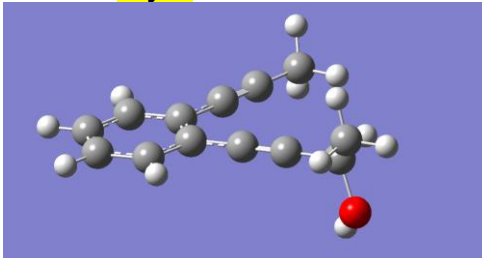
TS5



E = -576,49465282, H (0K) = -576,307479,
H (298K) = -576,295633, G (298K) = -576,344045
au.

Imaginary frequency = 1.

C	-2.4021160	1.4936420	0.0915140
C	-1.2454020	0.6908040	0.0976080
C	-1.4210380	-0.7790490	-0.0276970
C	-2.7323310	-1.2796840	-0.1424920
C	-3.8389950	-0.4398830	-0.1410570
C	-3.6740490	0.9471050	-0.0250200
H	-2.2774200	2.5671950	0.1805140
H	-2.8635460	-2.3522570	-0.2334260
H	-4.8342860	-0.8644850	-0.2313310
H	-4.5411210	1.6007130	-0.0254940
C	-0.2514870	-1.5562390	-0.0222550
C	0.9878360	-1.2788360	0.0782730
C	0.0751190	1.1609580	0.2142820
C	1.1945620	0.5479920	0.2061900
C	2.4008670	-1.7532700	0.1630630
H	2.6210360	-2.0463260	1.1987660
H	2.5390070	-2.6409130	-0.4615260
C	3.3052600	-0.5892390	-0.2738360

C	-2.7225240	-0.7238750	0.2997070	H	4.3399560	-0.7186410	0.0539350
H	-2.9835030	-0.6260020	1.3669510	H	3.2991000	-0.4955310	-1.3649060
O	-3.5945410	-1.6841560	-0.3129850	C	2.6898600	0.6904780	0.2984750
H	-3.3217140	-2.5695830	-0.0375410	H	2.9544480	0.7908760	1.3644390
H	-2.6363640	2.0085800	1.2330930	O	3.1925130	1.8048070	-0.4268750
H	-2.7202340	2.7579320	-0.3517140	H	2.6942060	2.5922280	-0.1682650
Molecule birad-5				Molecule acycl-5			
							
E = -576,51224047, H (0K) = -576,322766, H (298K) = -576,311095, G (298K) = -576,359165 au.				E = -577,75798306, H (0K) = -577,550152, H (298K) = -577,534471, G (298K) = -577,595486 au.			
Imaginary frequency = 0.				Imaginary frequency = 0.			
C	-2.4007300	1.4929730	0.1012900	C	1.2379050	-2.1620190	0.0182030
C	-1.2384460	0.6769560	0.0994940	C	0.7803340	-0.8306890	-0.0076930
C	-1.4077350	-0.7796410	-0.0295100	C	1.7303540	0.2295140	-0.0110610
C	-2.7262620	-1.2948030	-0.1464660	C	3.1021750	-0.0875730	0.0102030
C	-3.8230800	-0.4582500	-0.1388730	C	3.5340920	-1.4112950	0.0357610
C	-3.6599230	0.9417510	-0.0144550	C	2.5994860	-2.4526510	0.0402450
H	-2.2750510	2.5668280	0.1956620	H	0.5051990	-2.9624070	0.0213880
H	-2.8516840	-2.3685270	-0.2422450	H	3.8223690	0.7240770	0.0067930
H	-4.8207750	-0.8773420	-0.2292720	H	4.5974750	-1.6307730	0.0522520
H	-4.5333440	1.5869300	-0.0104720	H	2.9309220	-3.4864110	0.0604160
C	-0.2370320	-1.5480440	-0.0281660	C	1.3169170	1.5963550	-0.0358670
C	1.0207180	-1.0777390	0.0751490	C	0.9943610	2.7666440	-0.0580950
C	0.0785780	1.1380890	0.2118260	C	-0.6227320	-0.5651520	-0.0286670
C	1.1851610	0.3729130	0.1959020	C	-1.8220910	-0.3716040	-0.0479200
C	2.3854010	-1.7376480	0.1140030	C	-3.2658970	-0.0963190	-0.0390950
C	3.3629060	-0.5795390	-0.1872150	H	-3.4085000	0.9681550	-0.2833670
H	4.3489150	-0.7203400	0.2628640	O	-3.8478950	-0.3649110	1.2482630
H	3.4964850	-0.4698010	-1.2689180	H	-3.2872260	0.0328980	1.9280040
C	2.6690020	0.7000700	0.3116440	C	-4.0369240	-0.9410930	-1.0540780
H	2.9087380	0.8844640	1.3717390	H	-3.6803620	-0.7400570	-2.0680780
O	3.1031000	1.8049070	-0.4729160	H	-3.9068690	-2.0040960	-0.8344220
H	2.6199870	2.5950410	-0.1960930	H	-5.1010600	-0.6954850	-0.9939750
H	2.5634840	-2.1574580	1.1130120	C	0.5940780	4.1701150	-0.0869290
H	2.4670920	-2.5615750	-0.6006940	H	0.9441770	4.6615880	-1.0019530
				H	-0.4963610	4.2686570	-0.0492170
				H	1.0110600	4.7177400	0.7660020

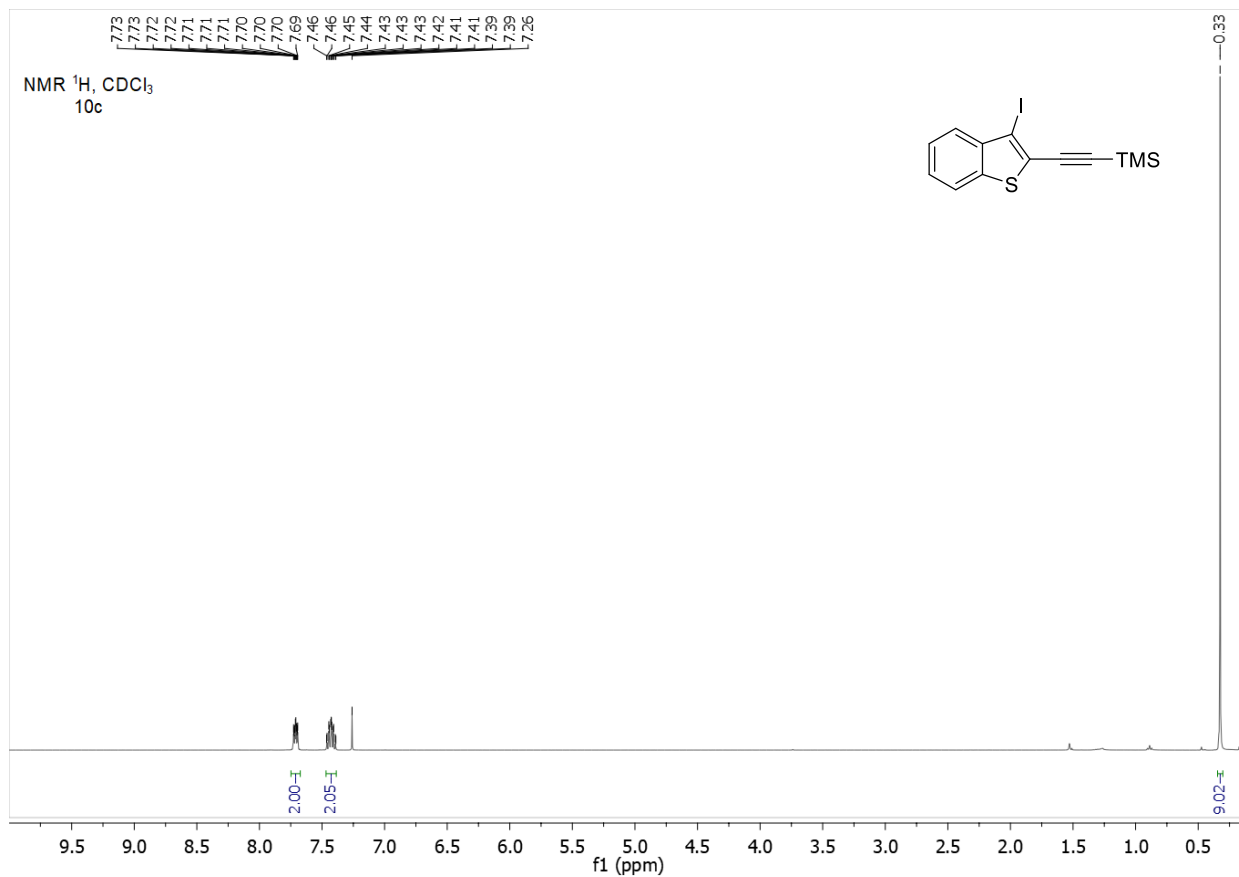
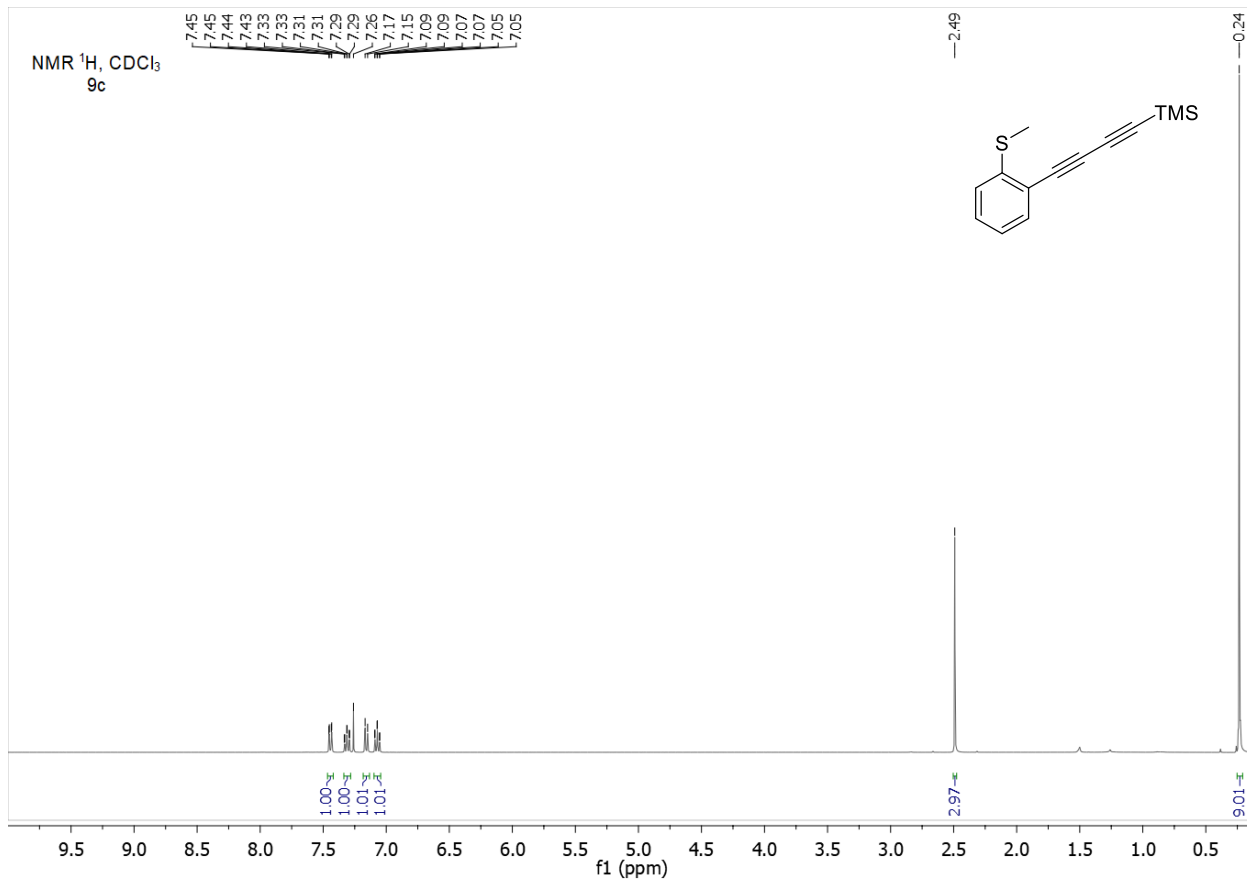
References

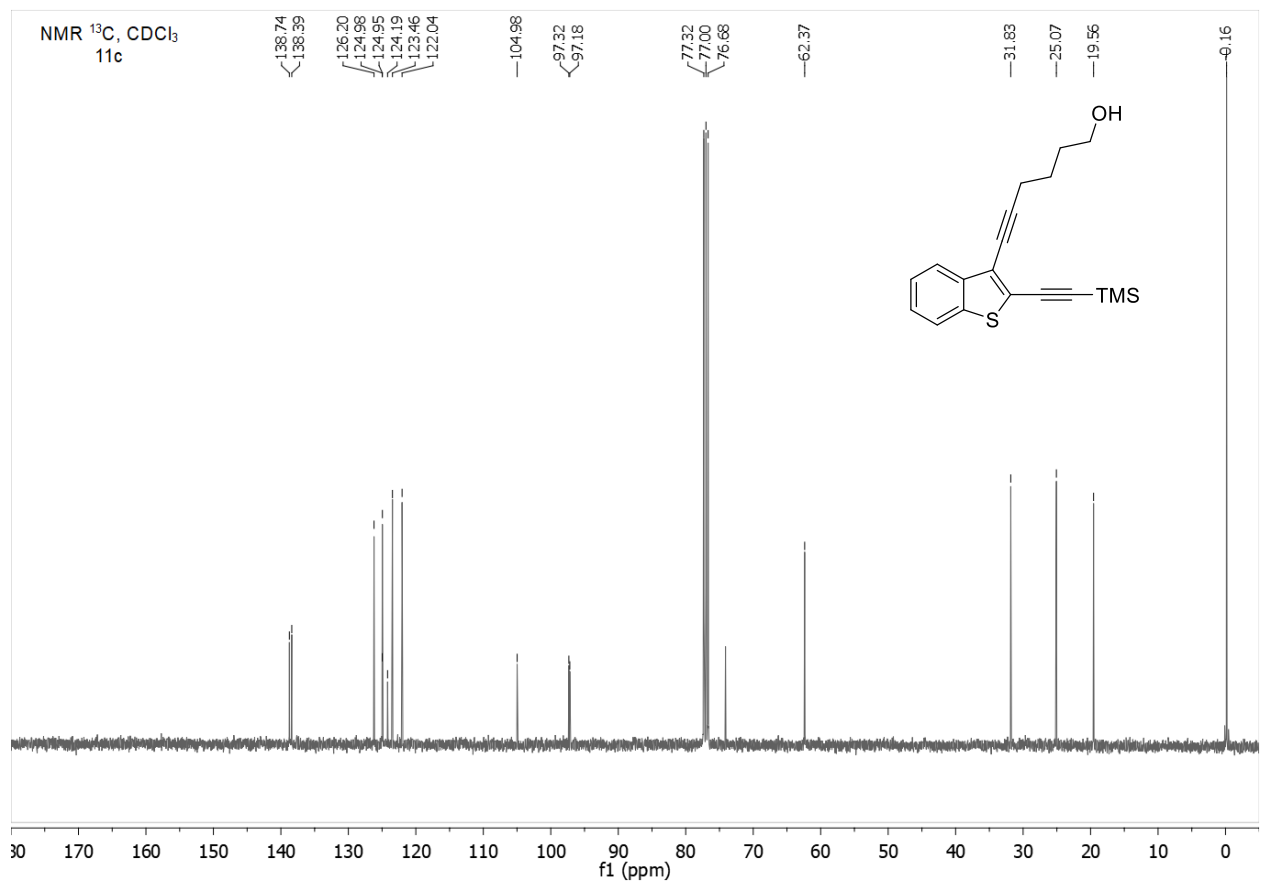
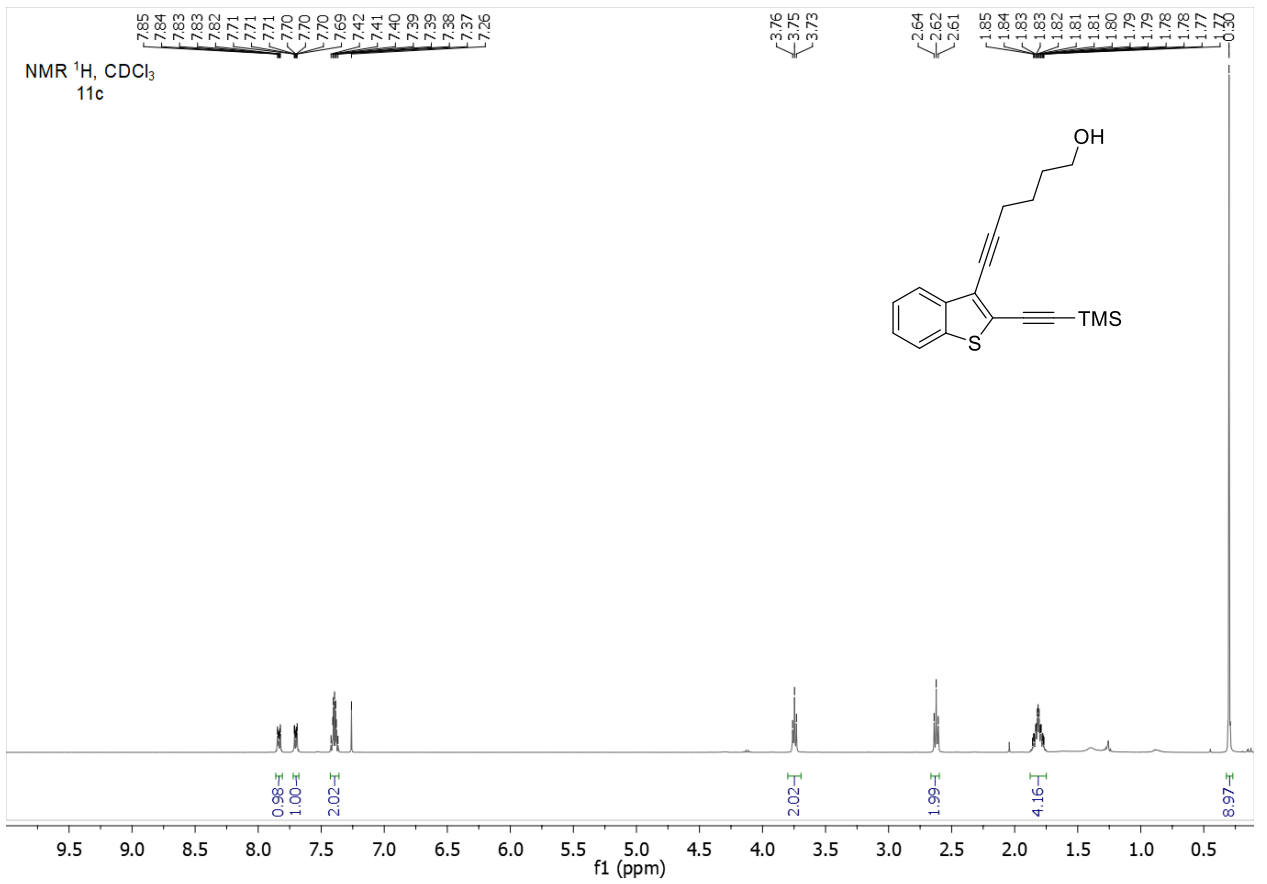
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- (2) Becke, A. D. *Phys. Rev. A* **1988**, *38*, 3098–3100.
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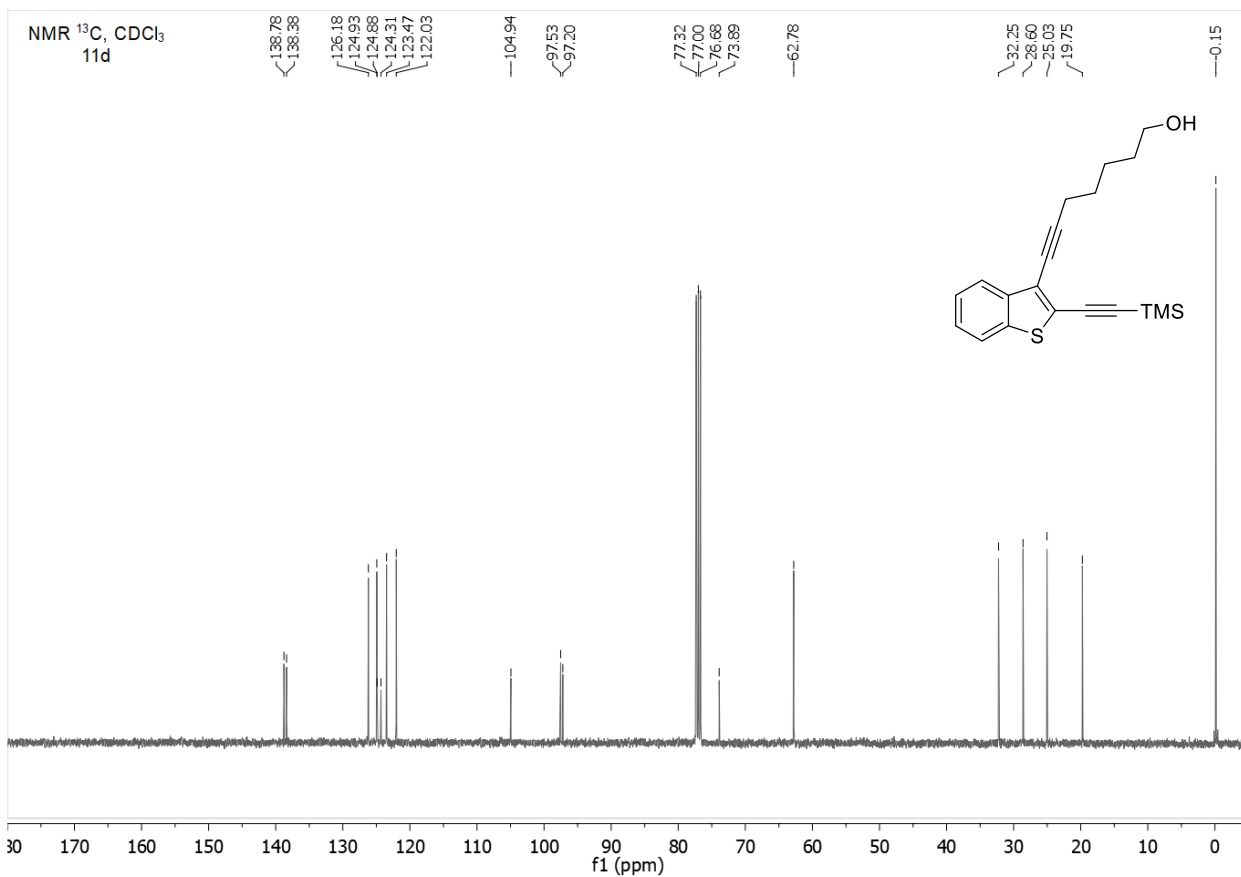
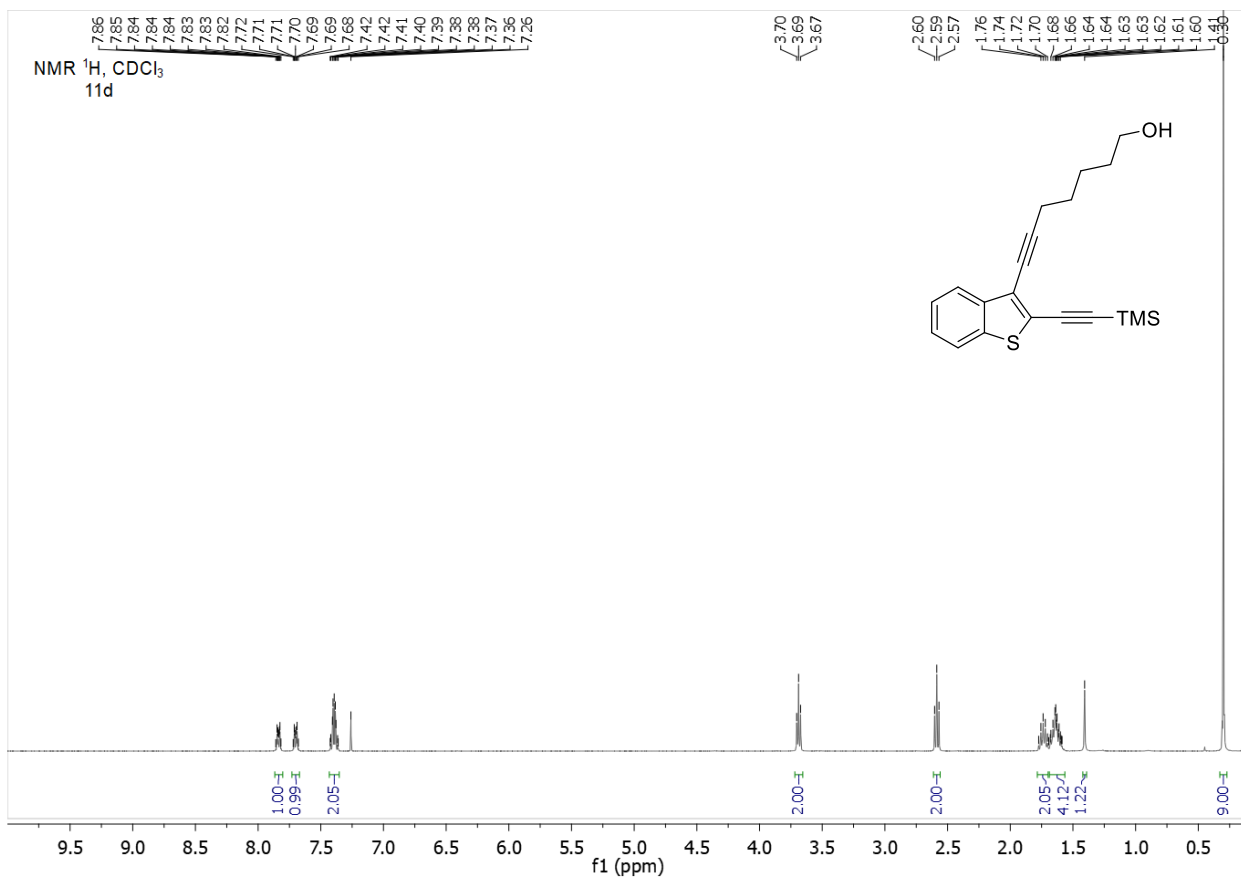
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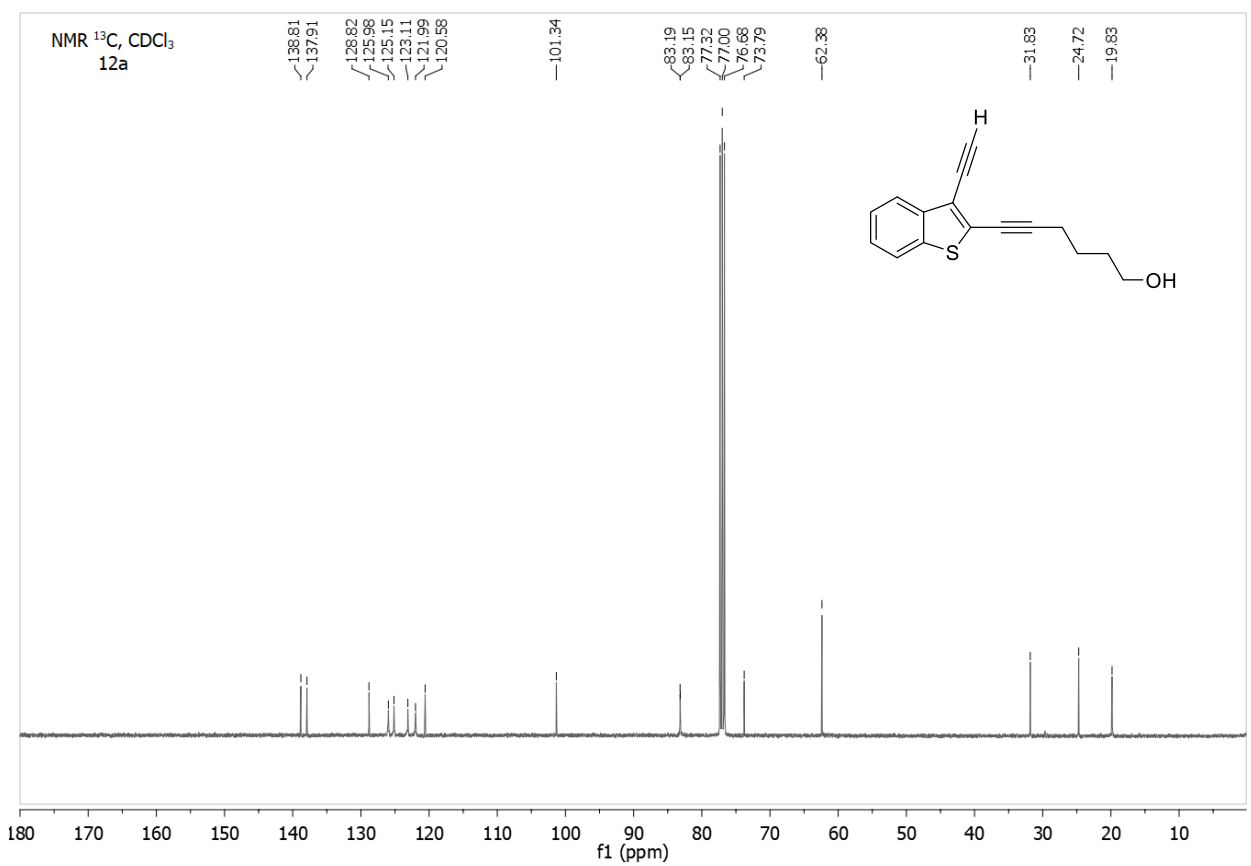
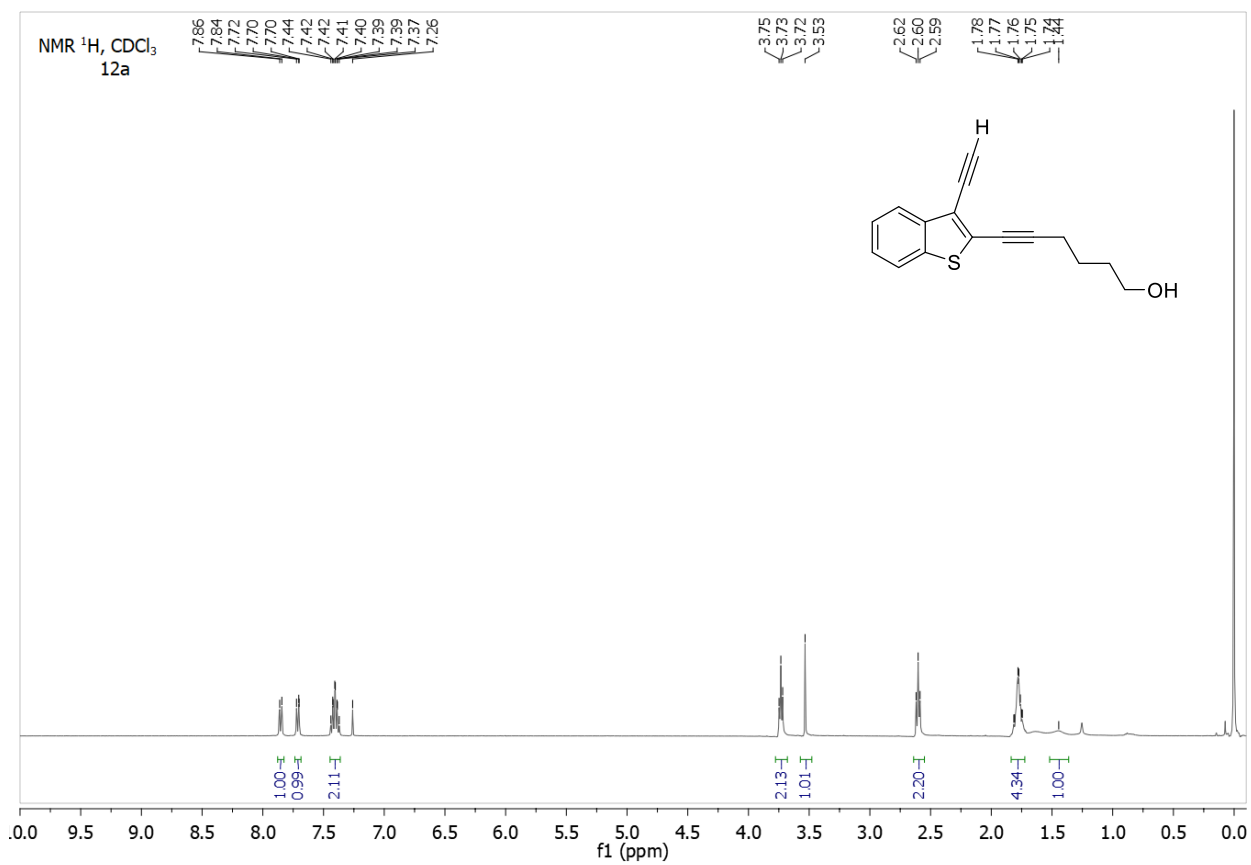
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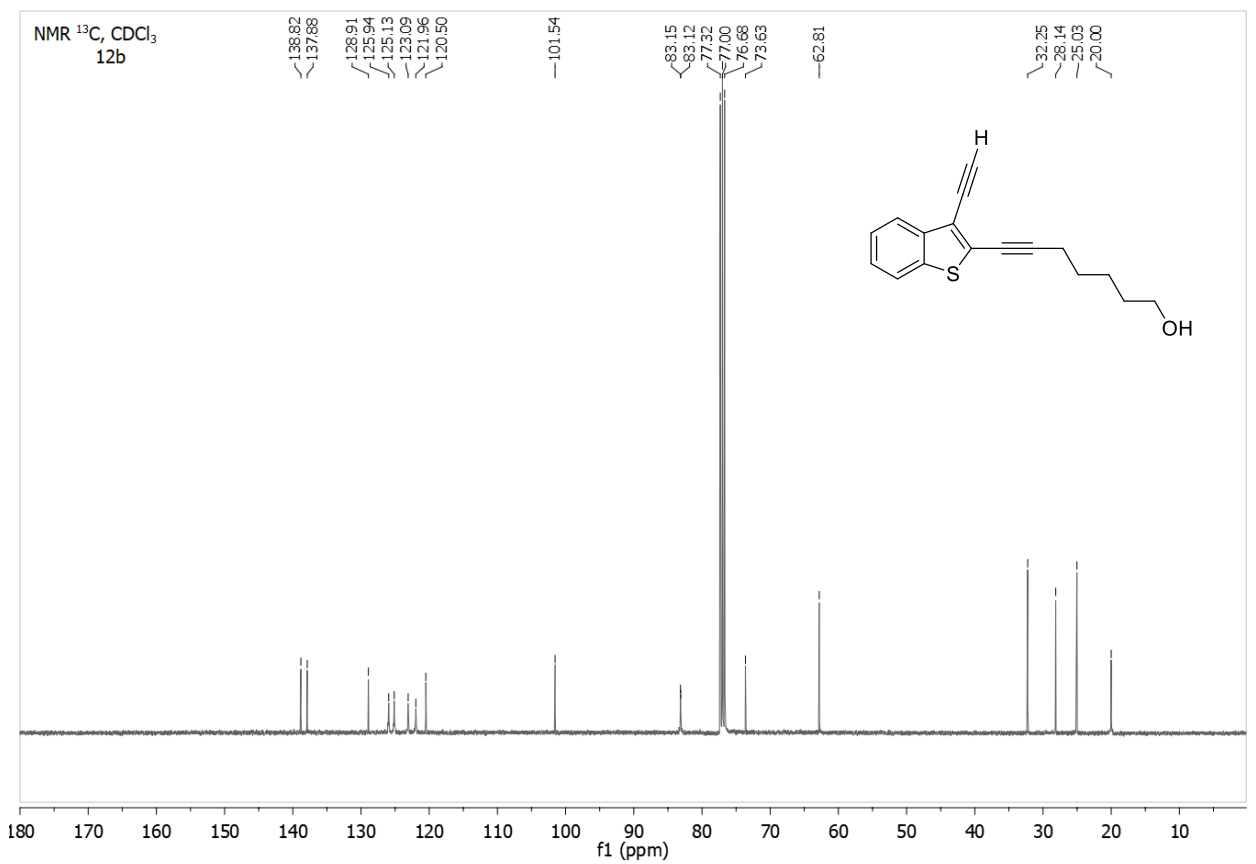
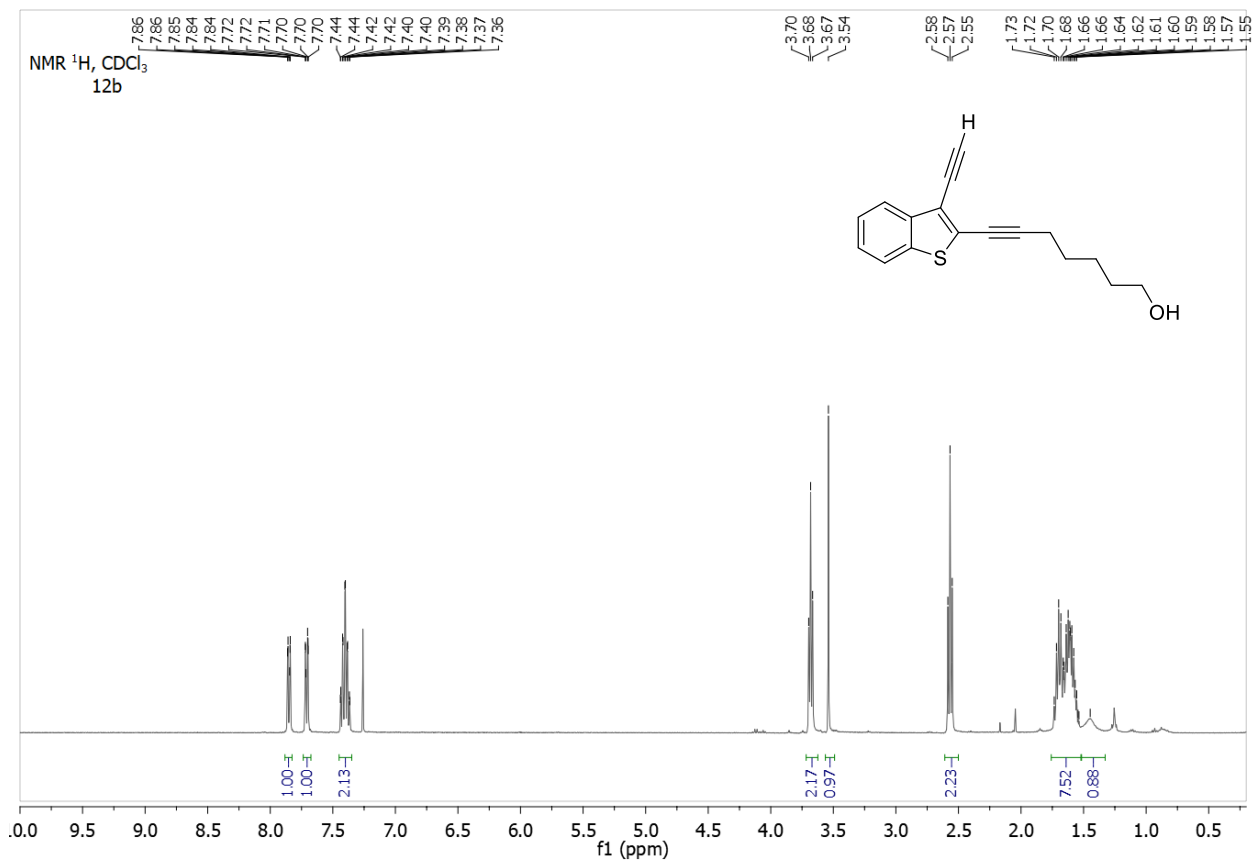
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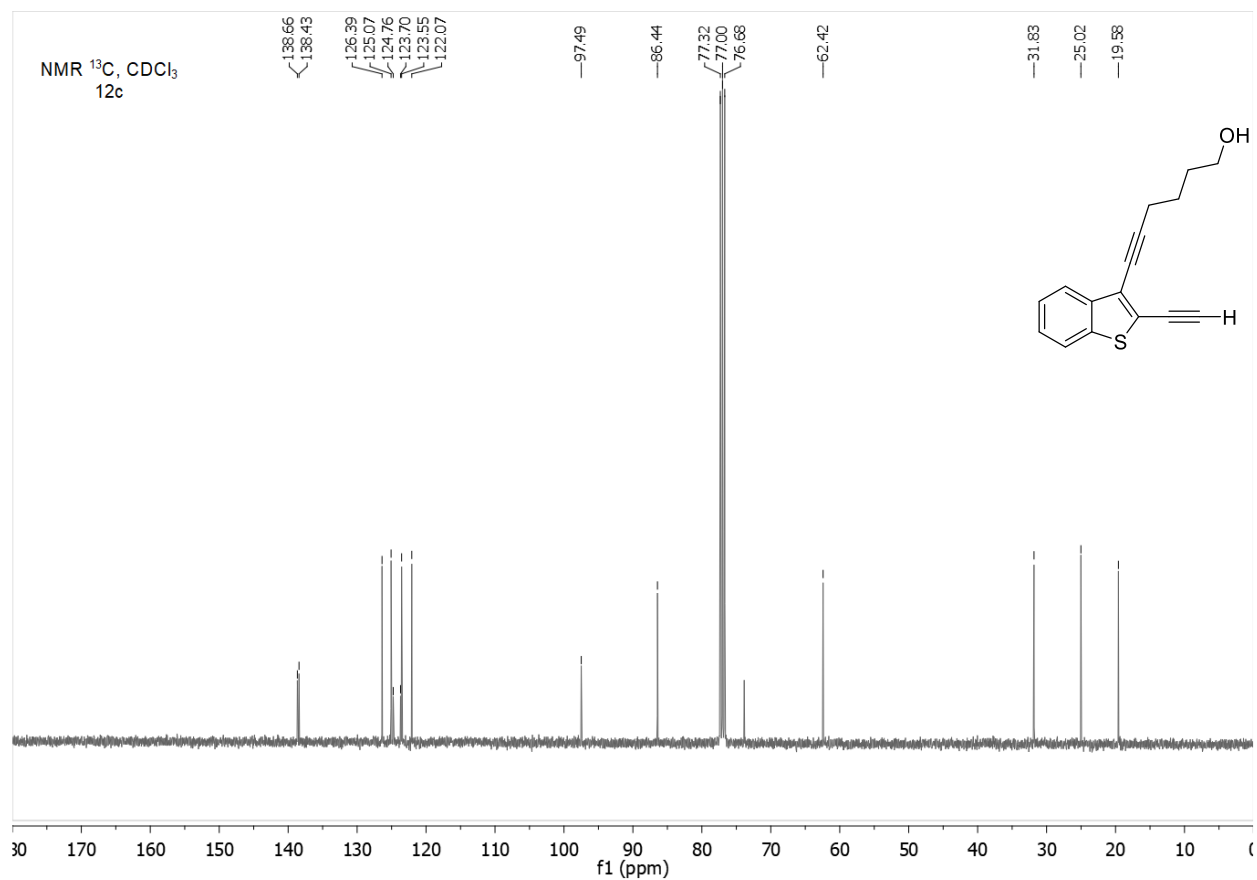
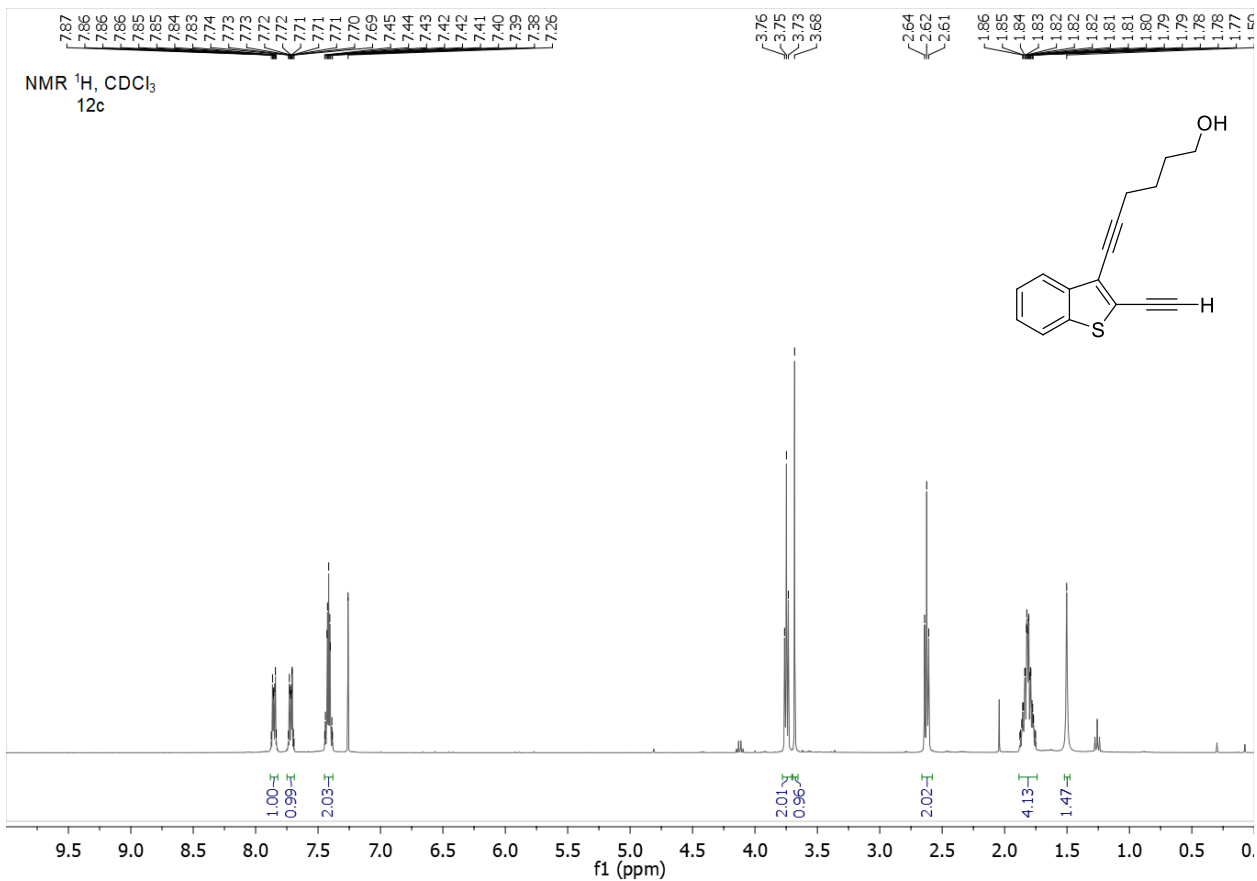


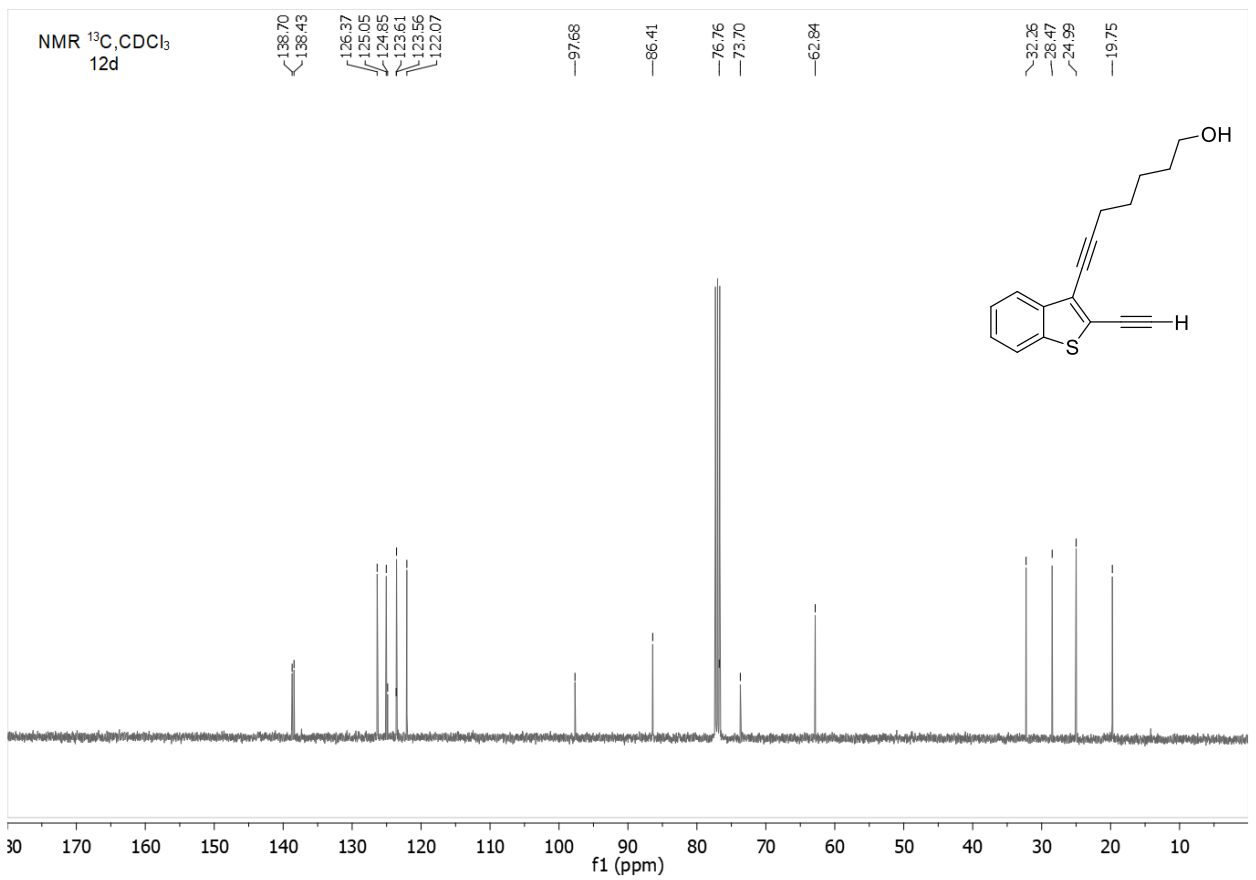
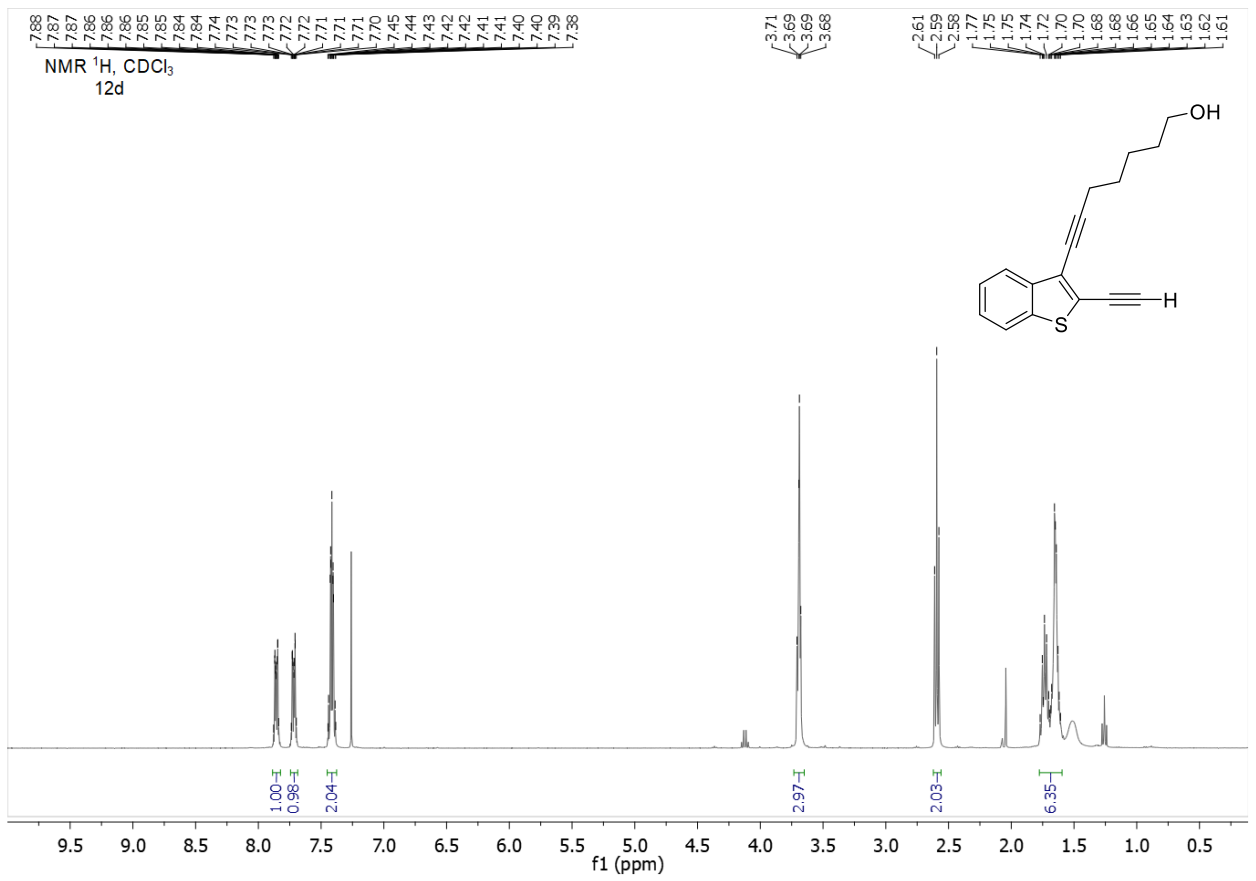


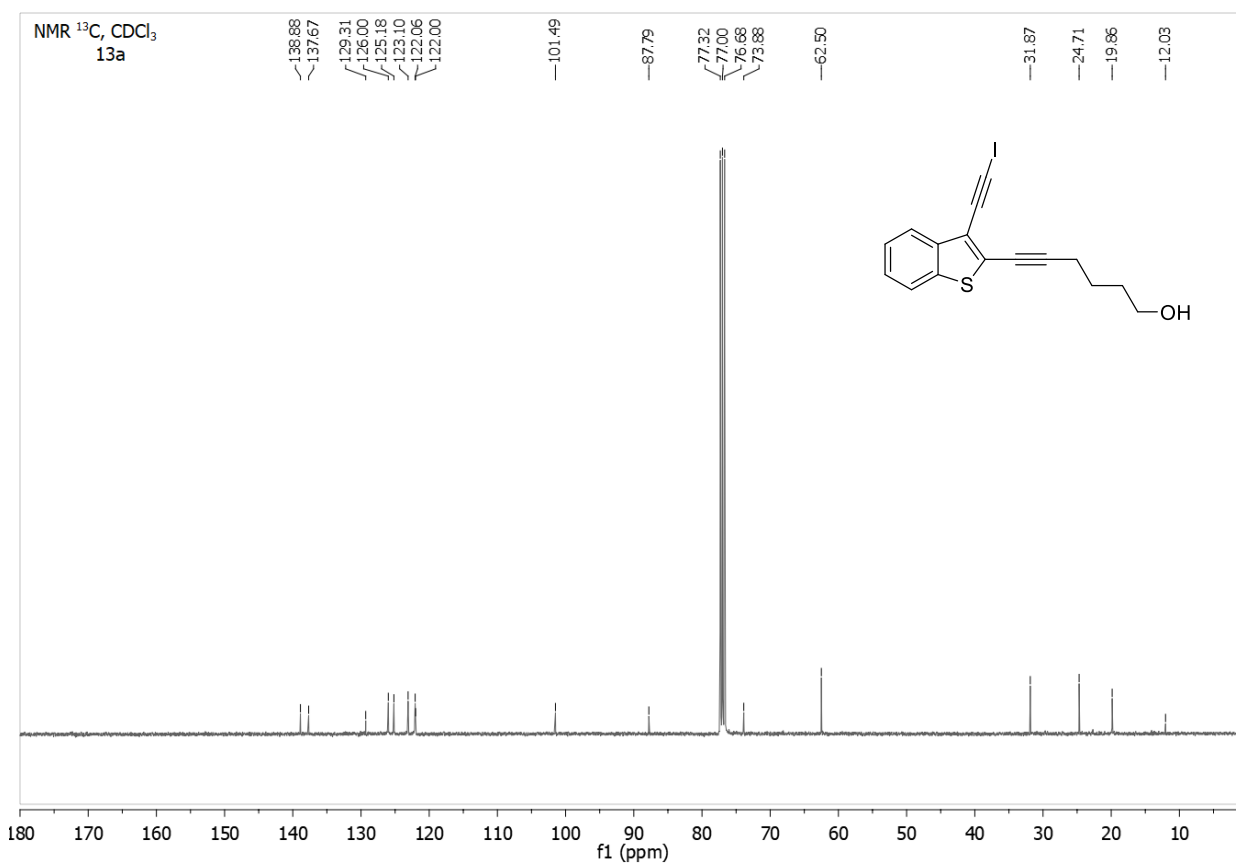
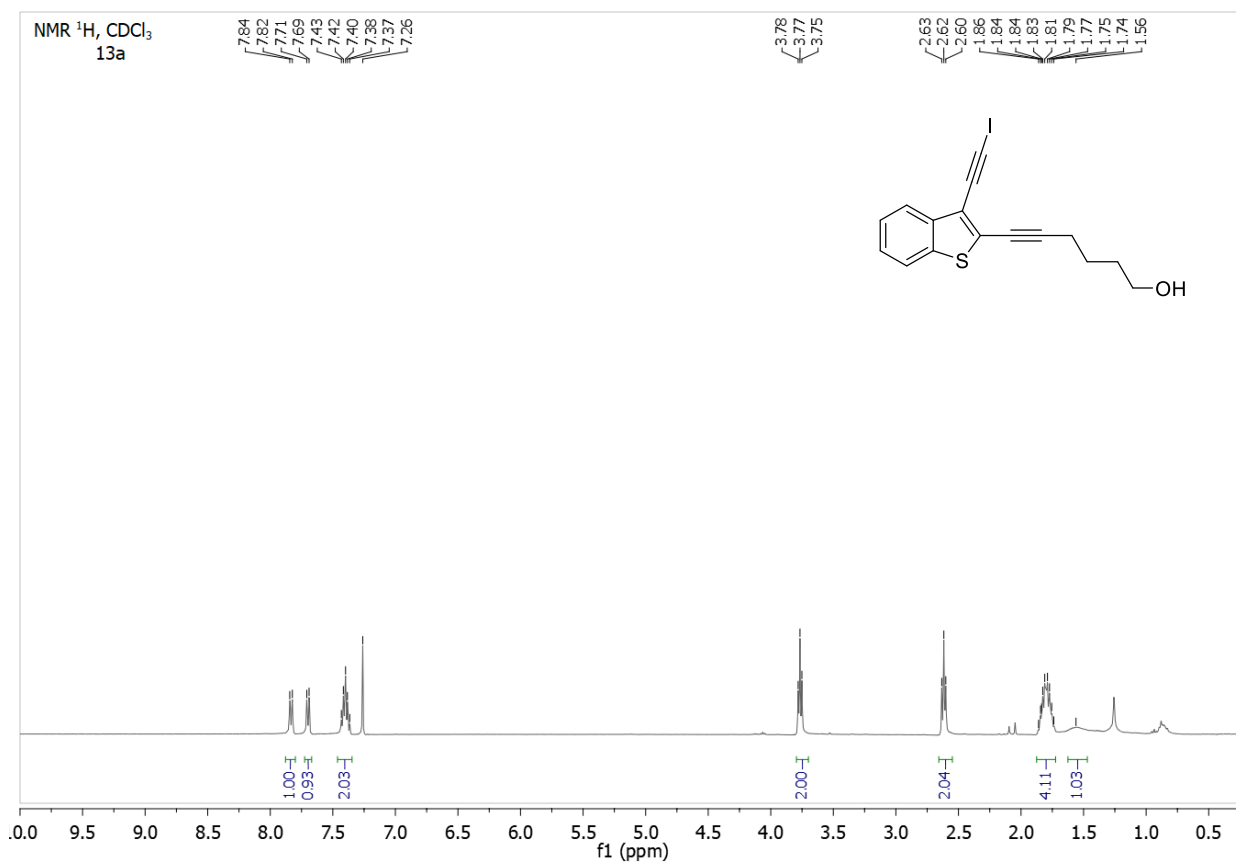


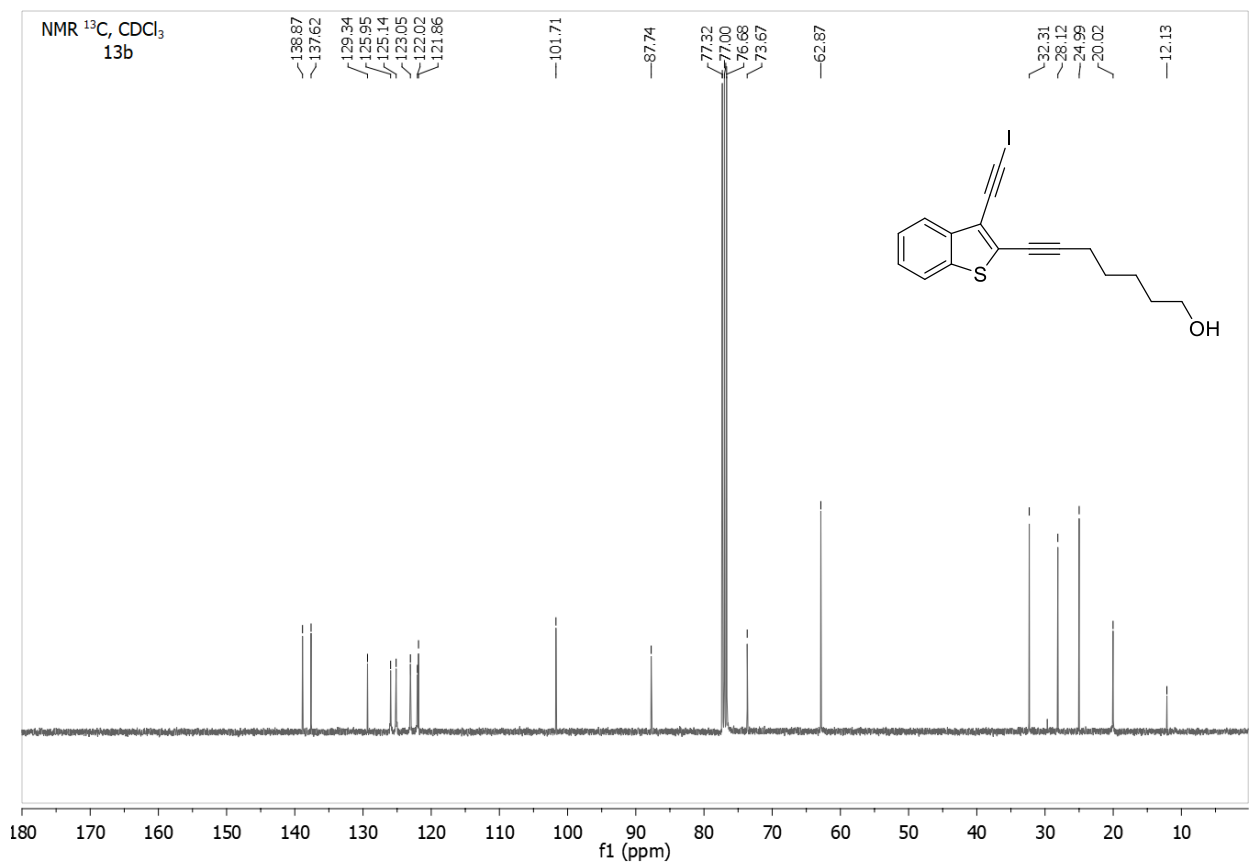
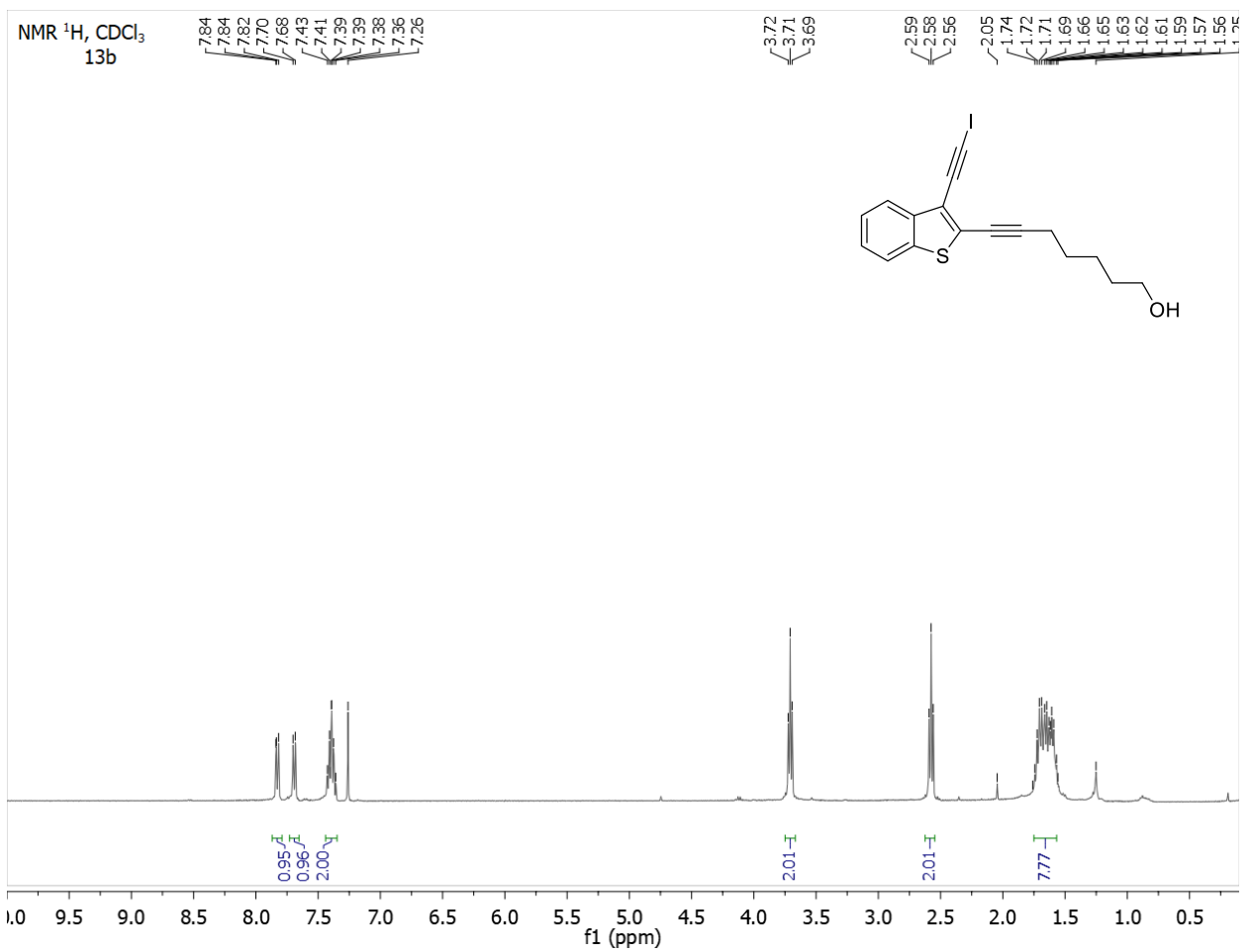


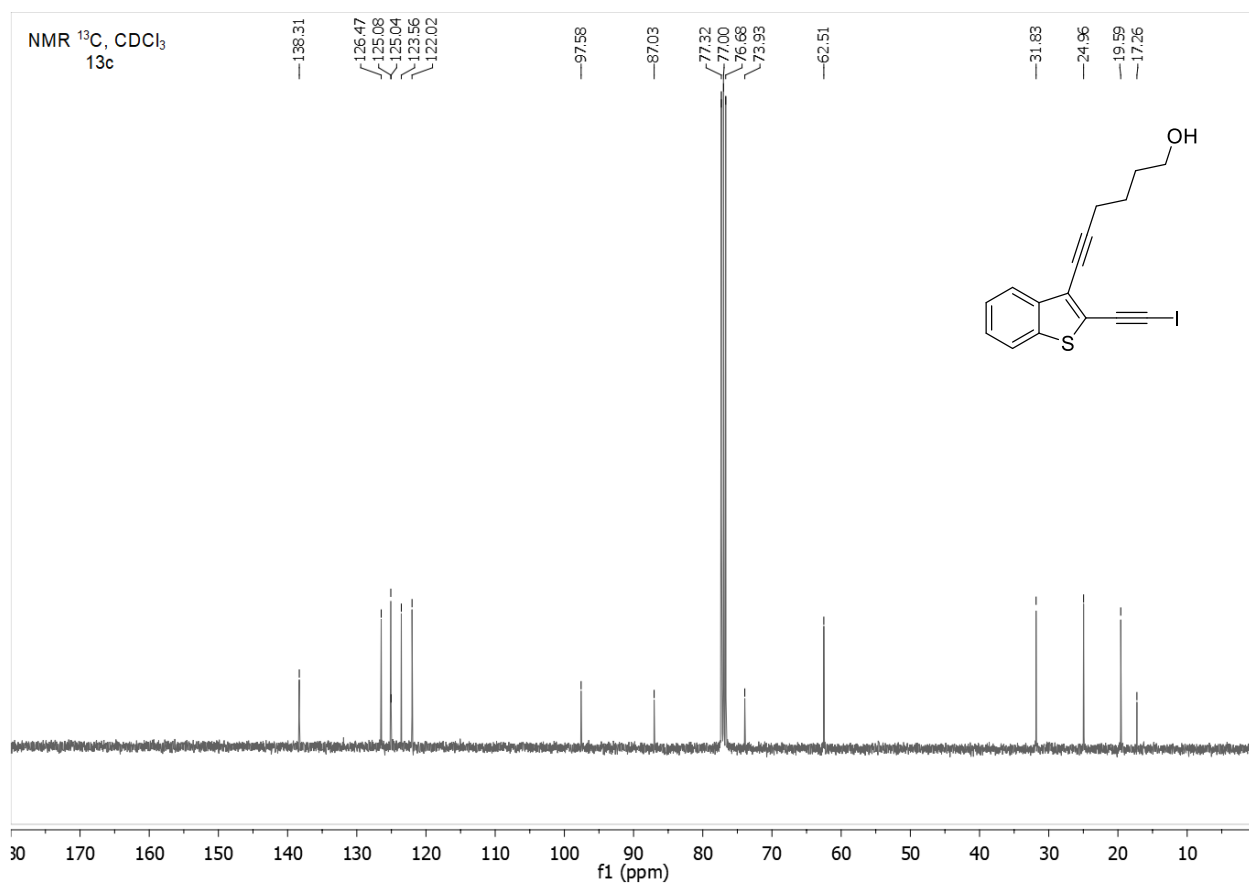
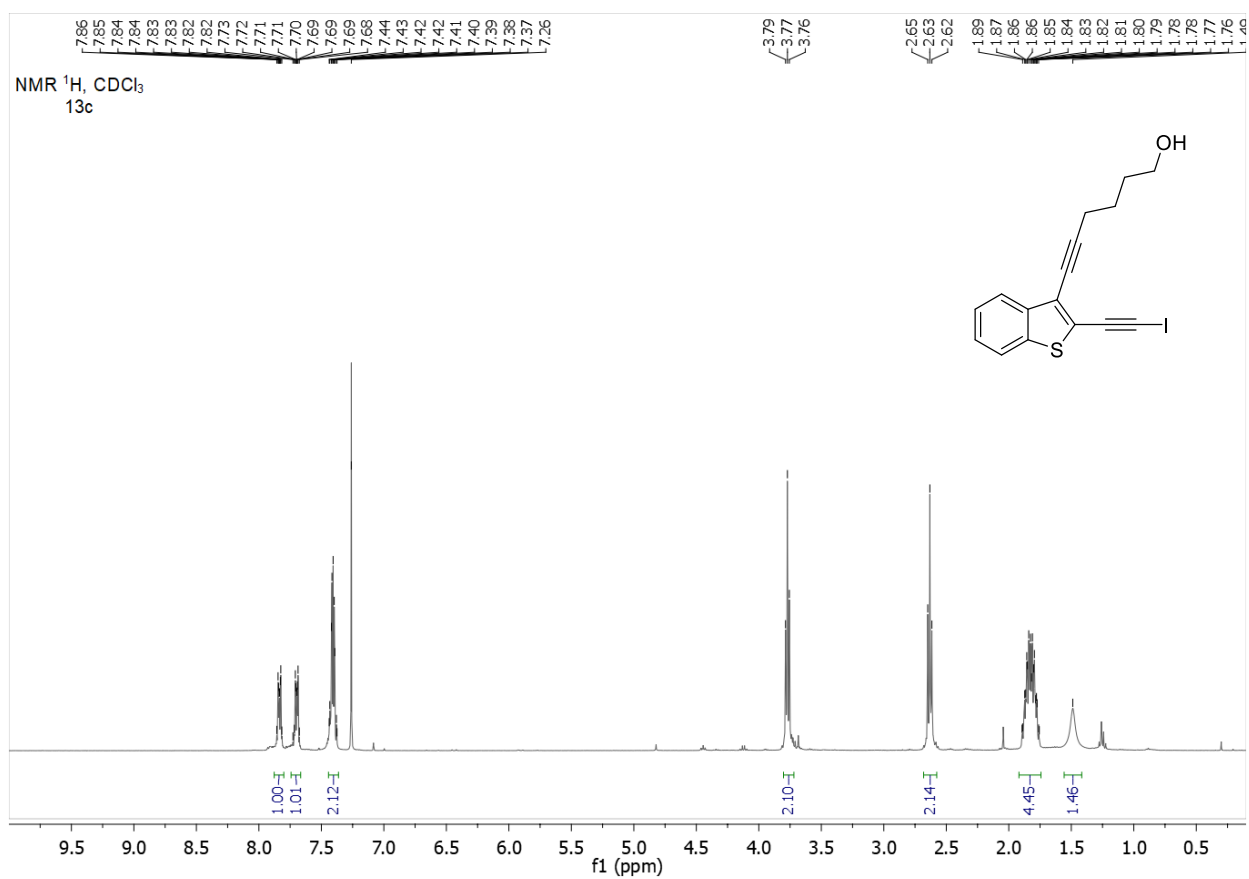


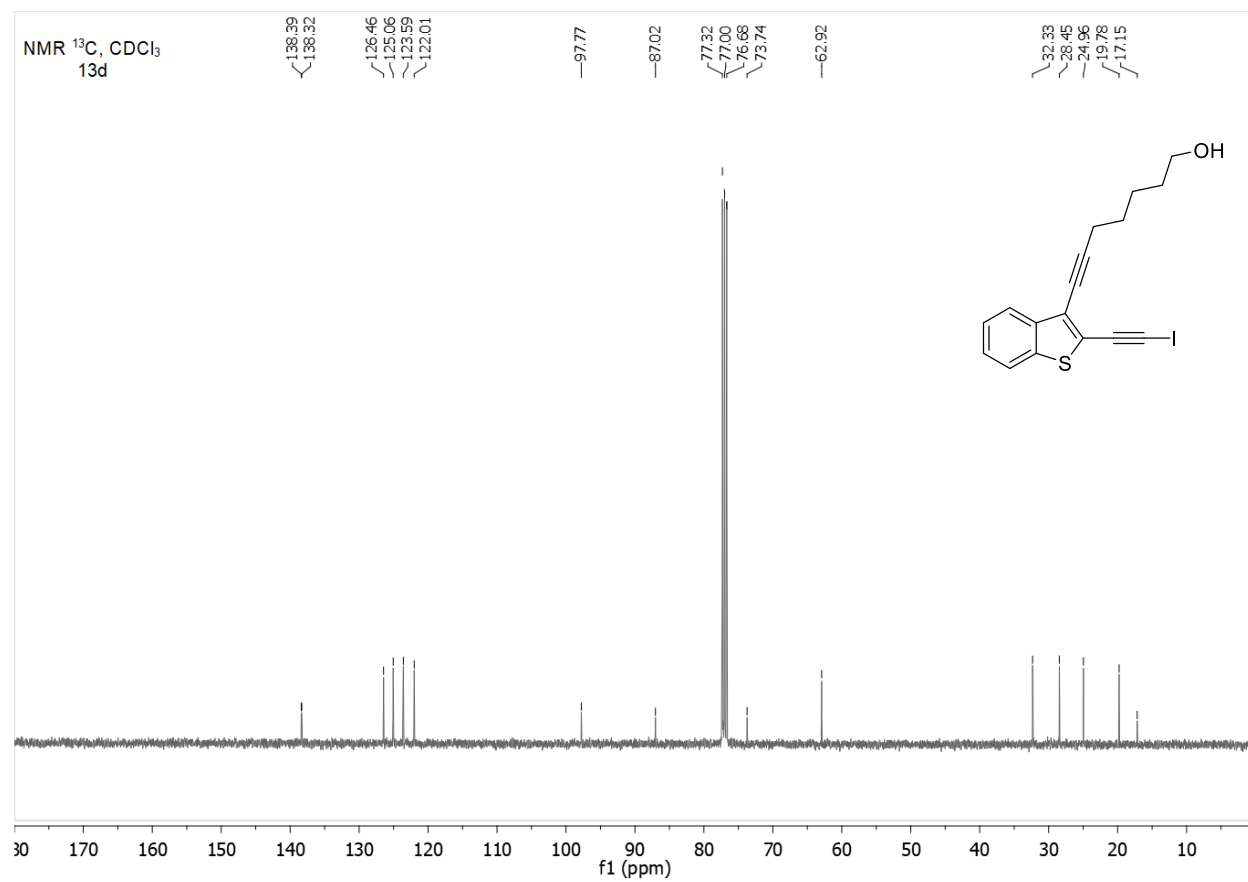
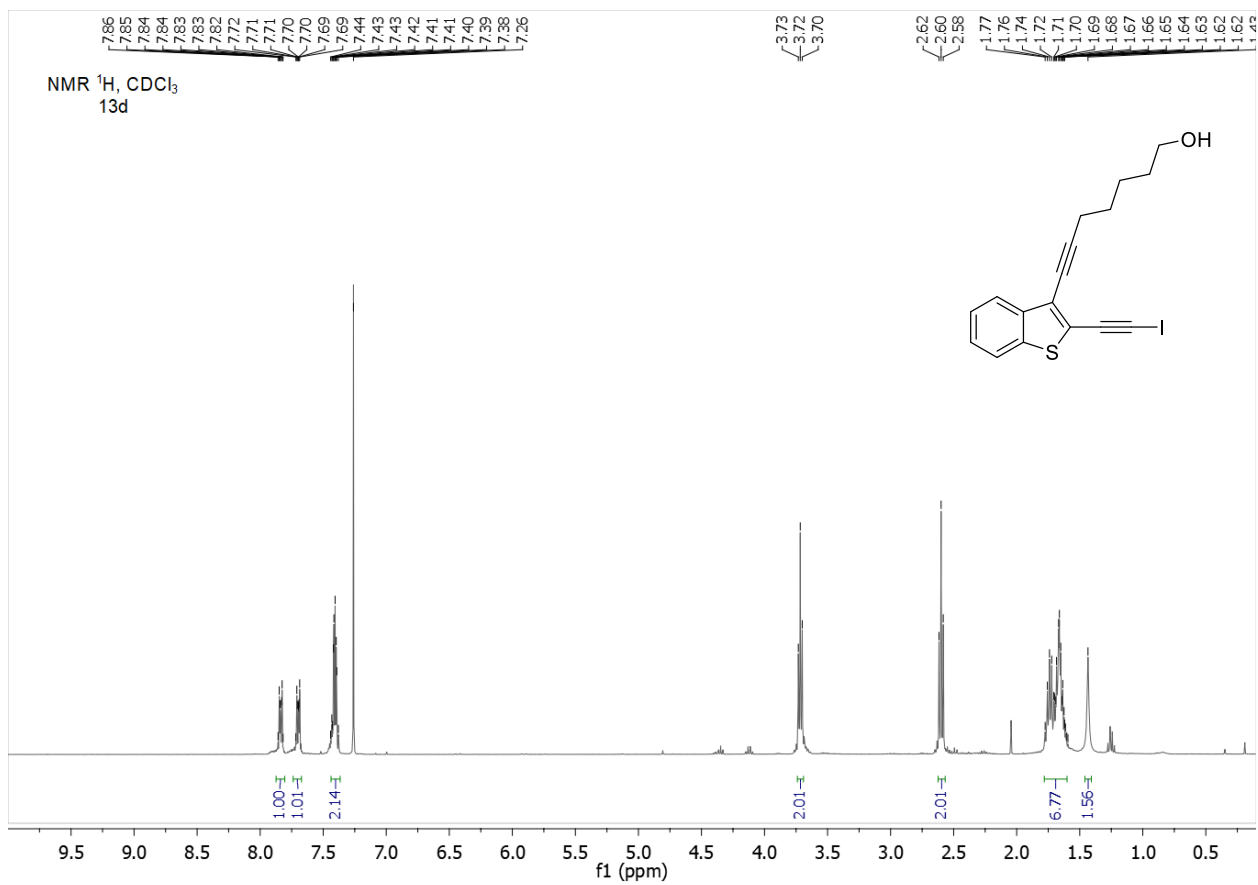


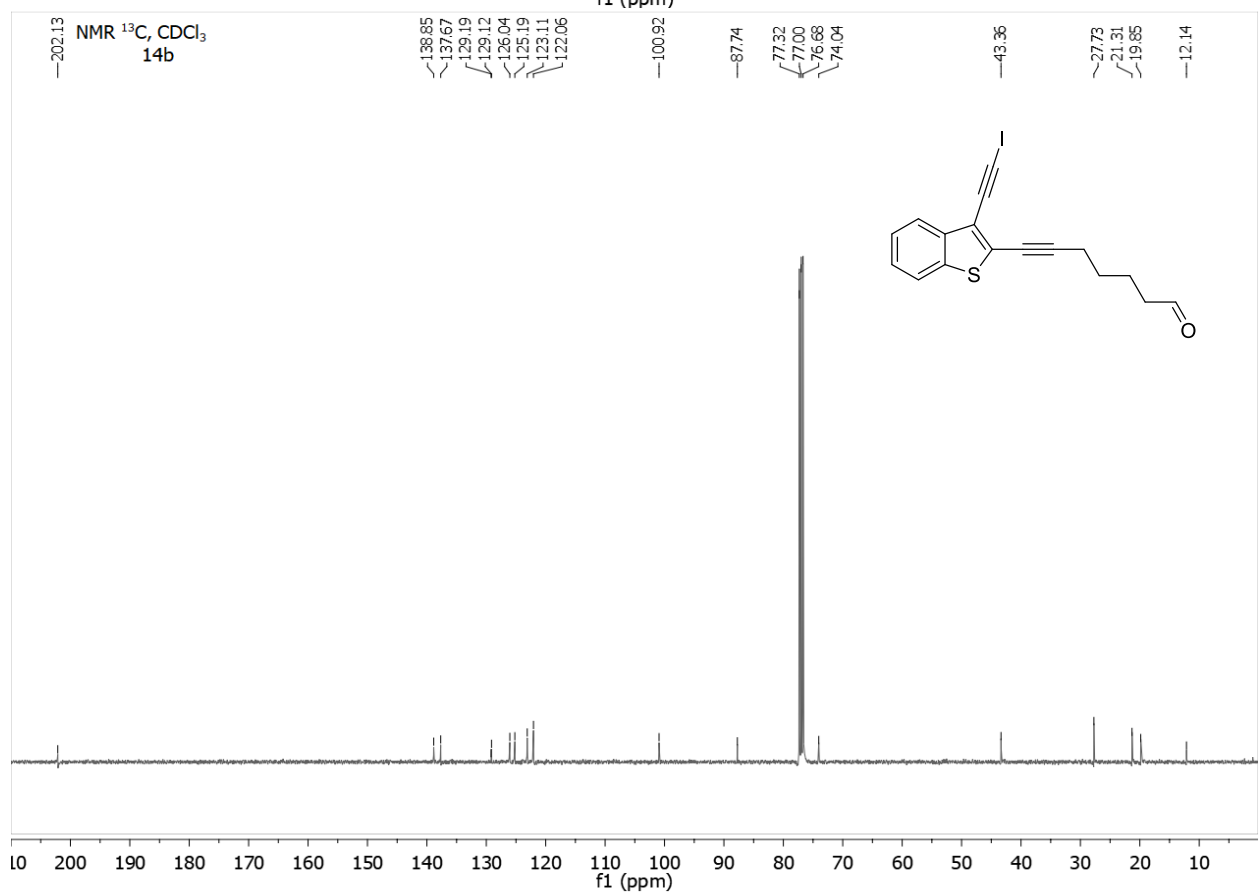
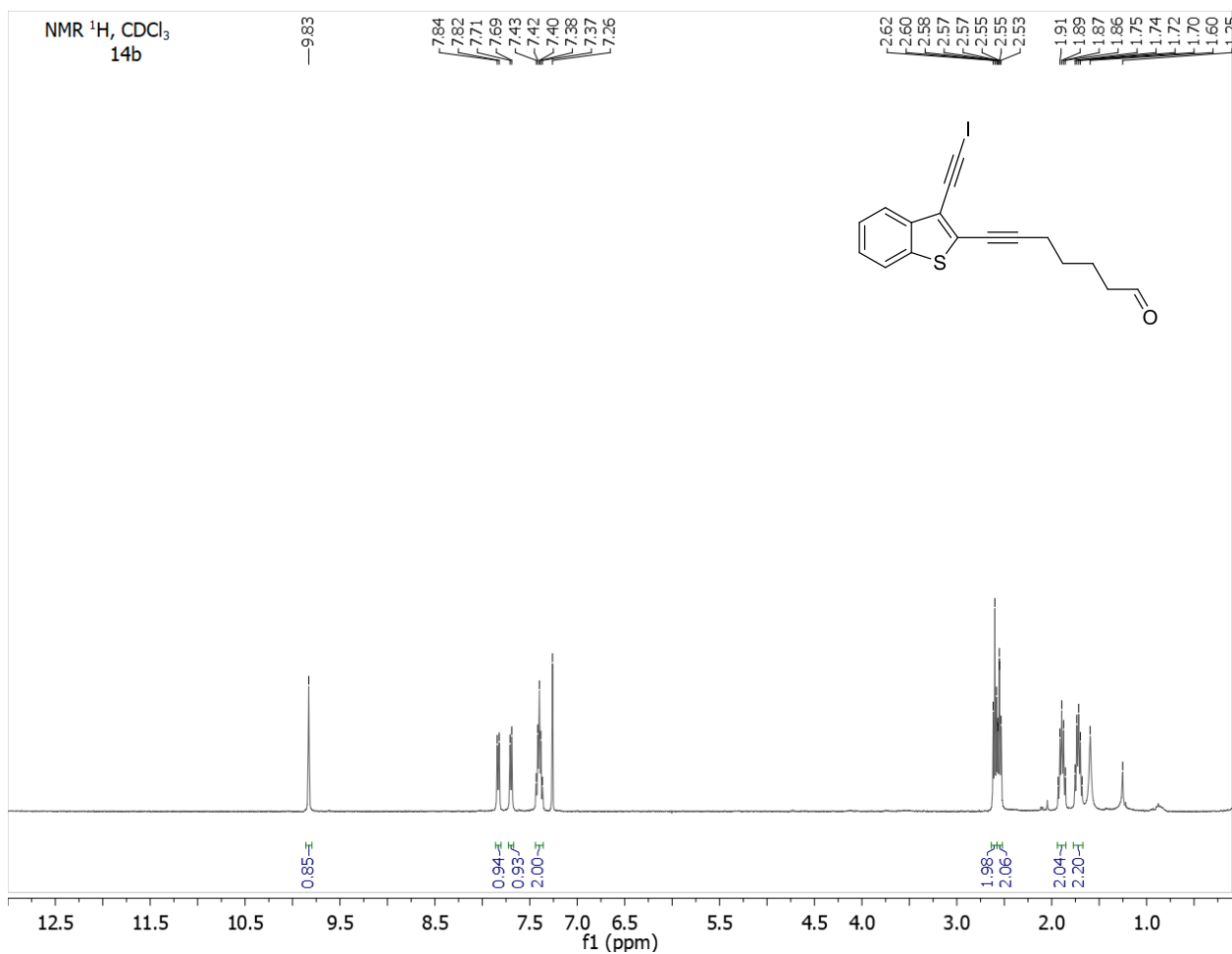


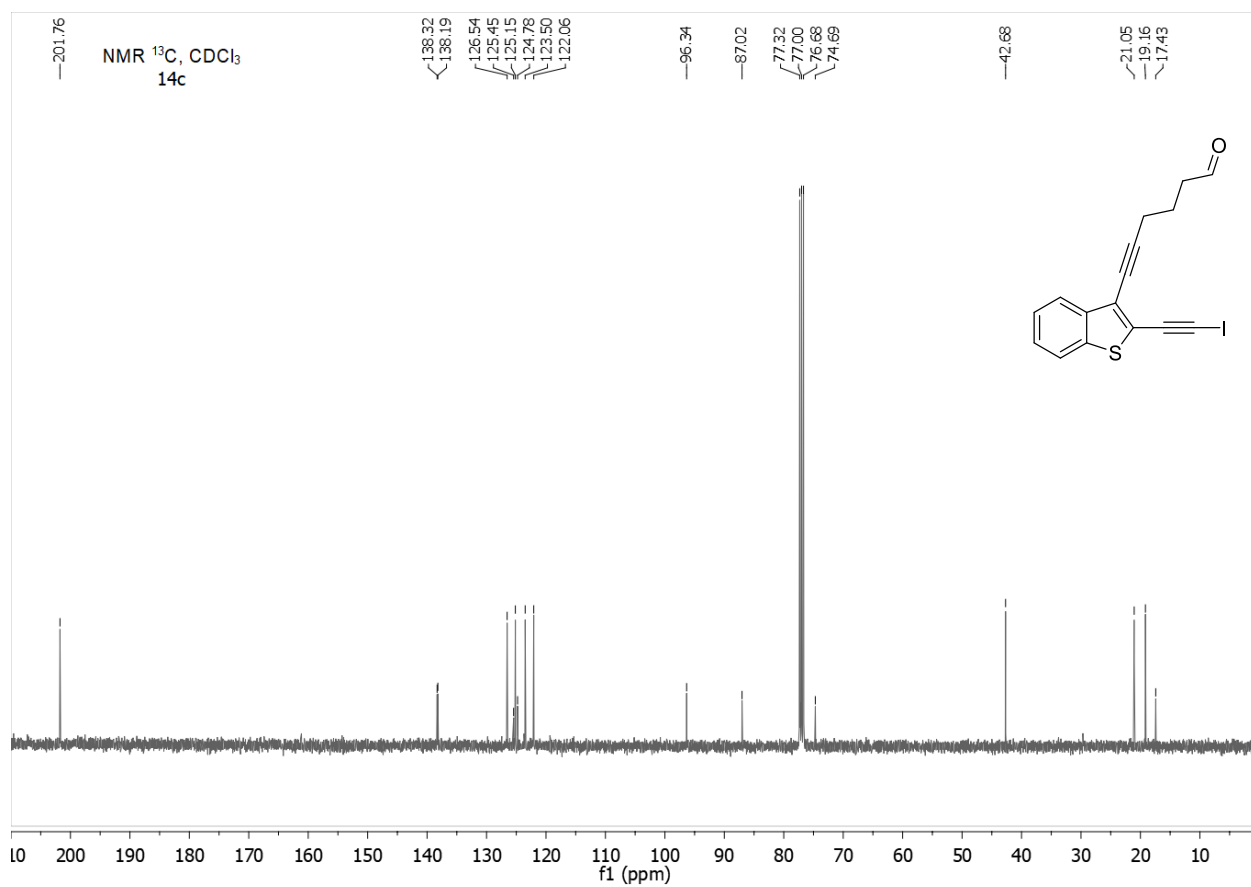
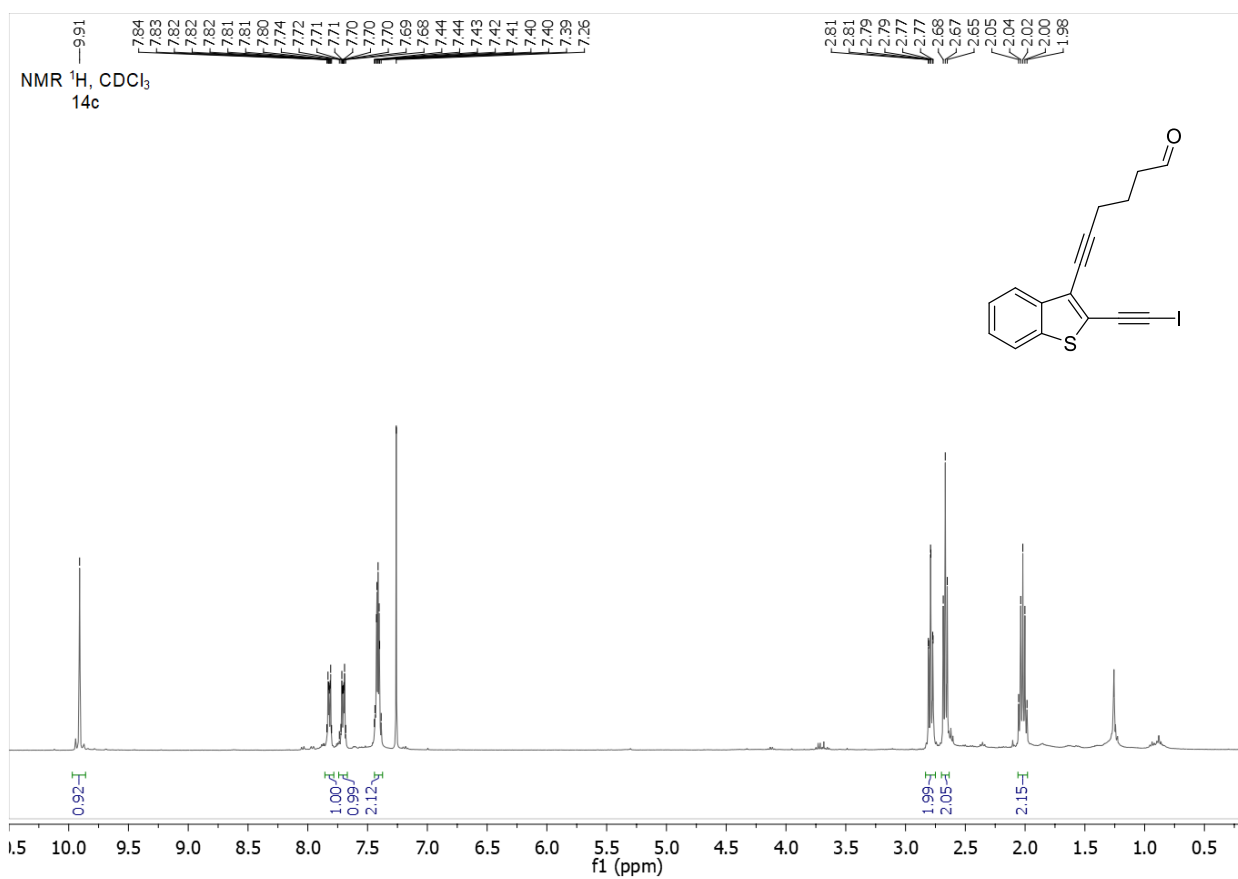


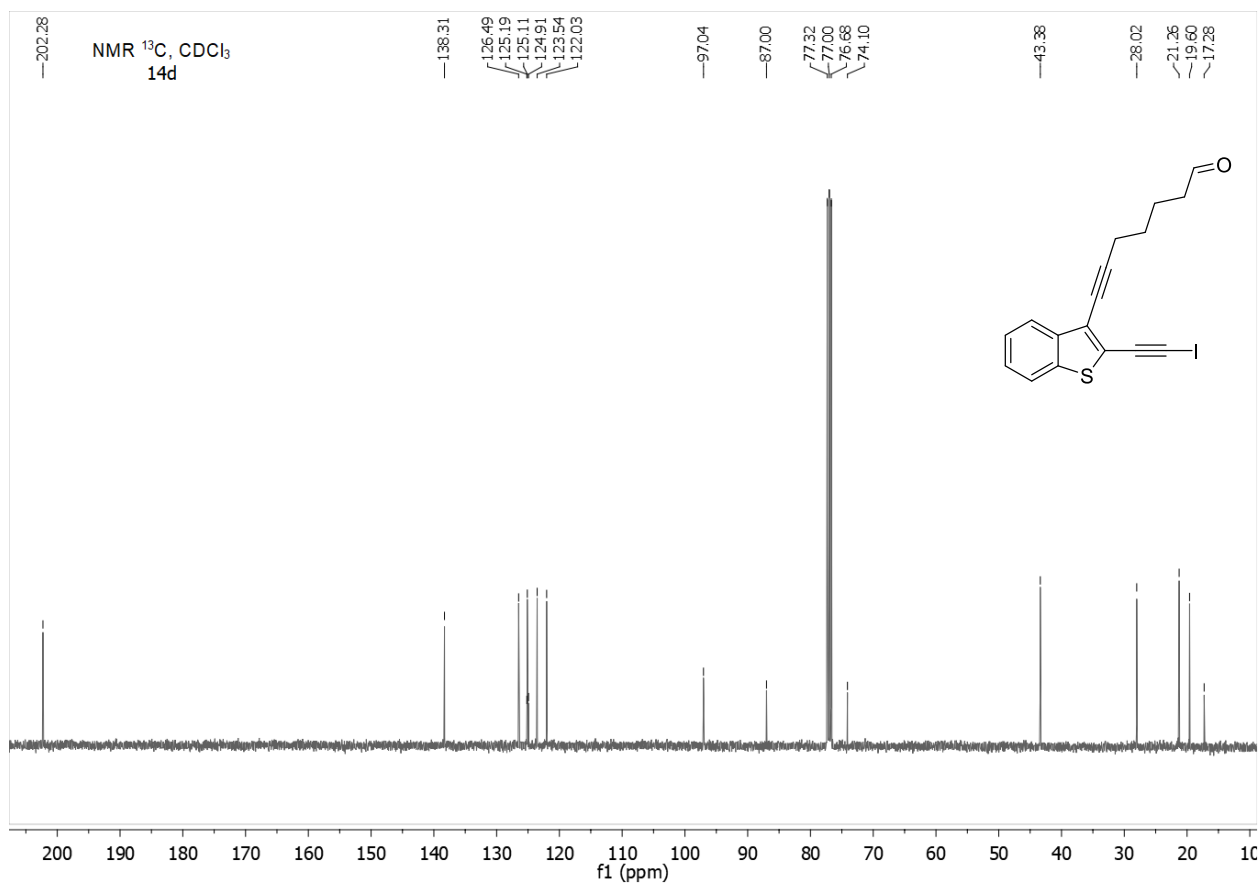
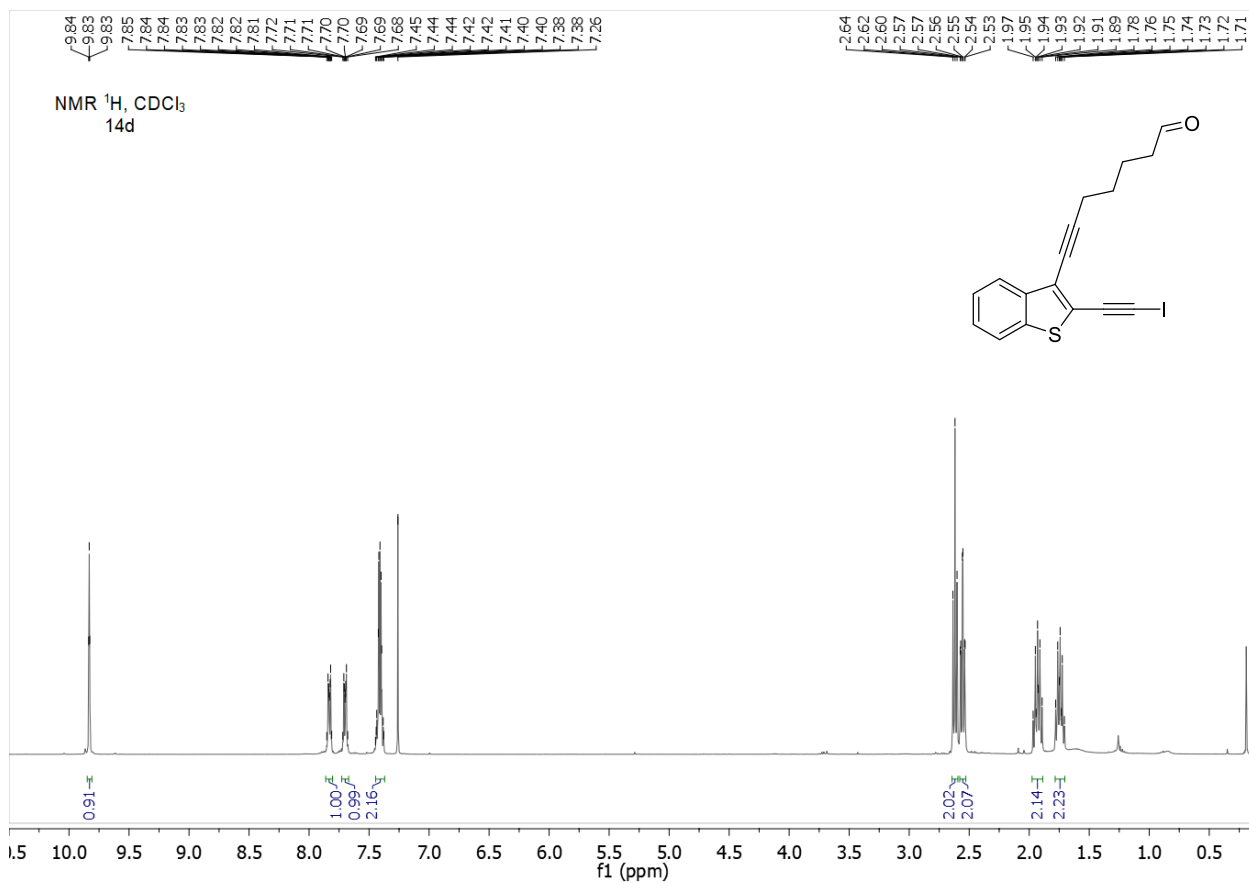


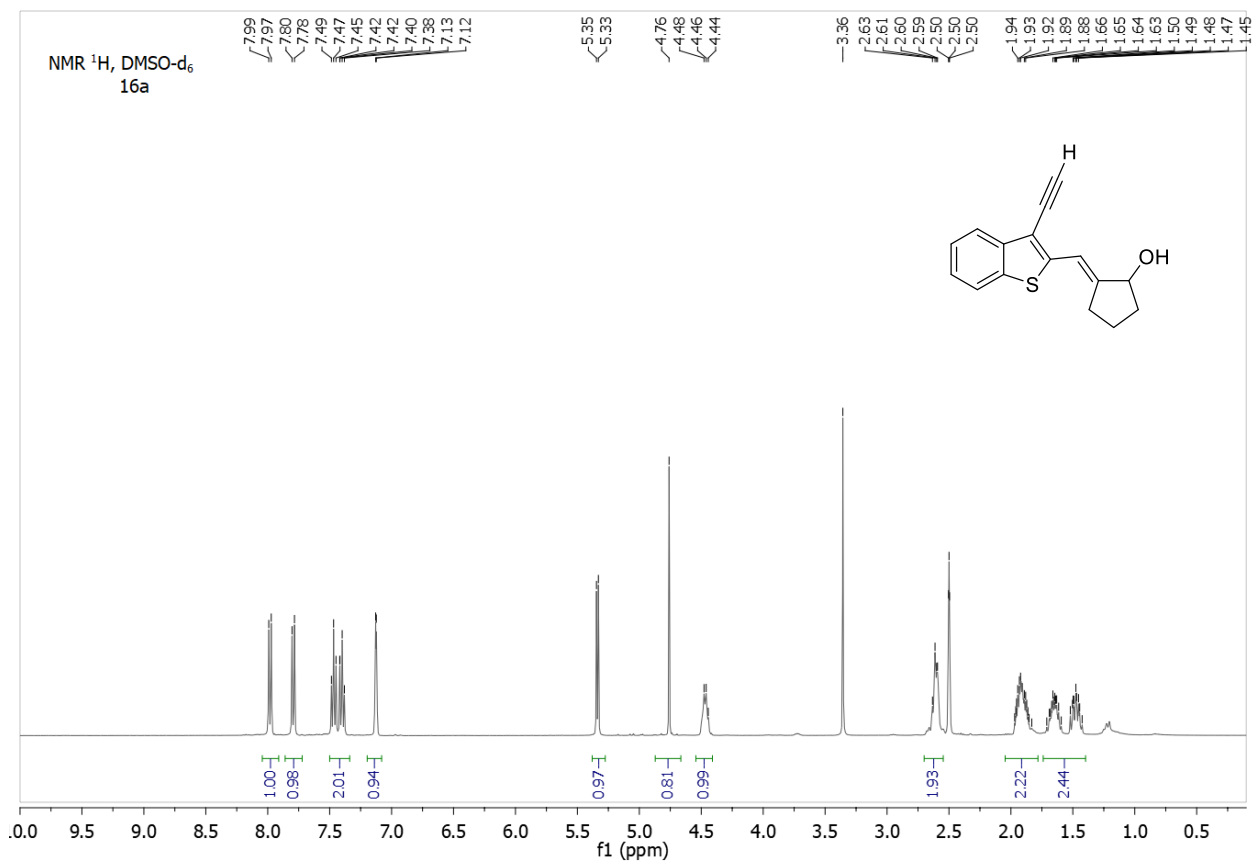
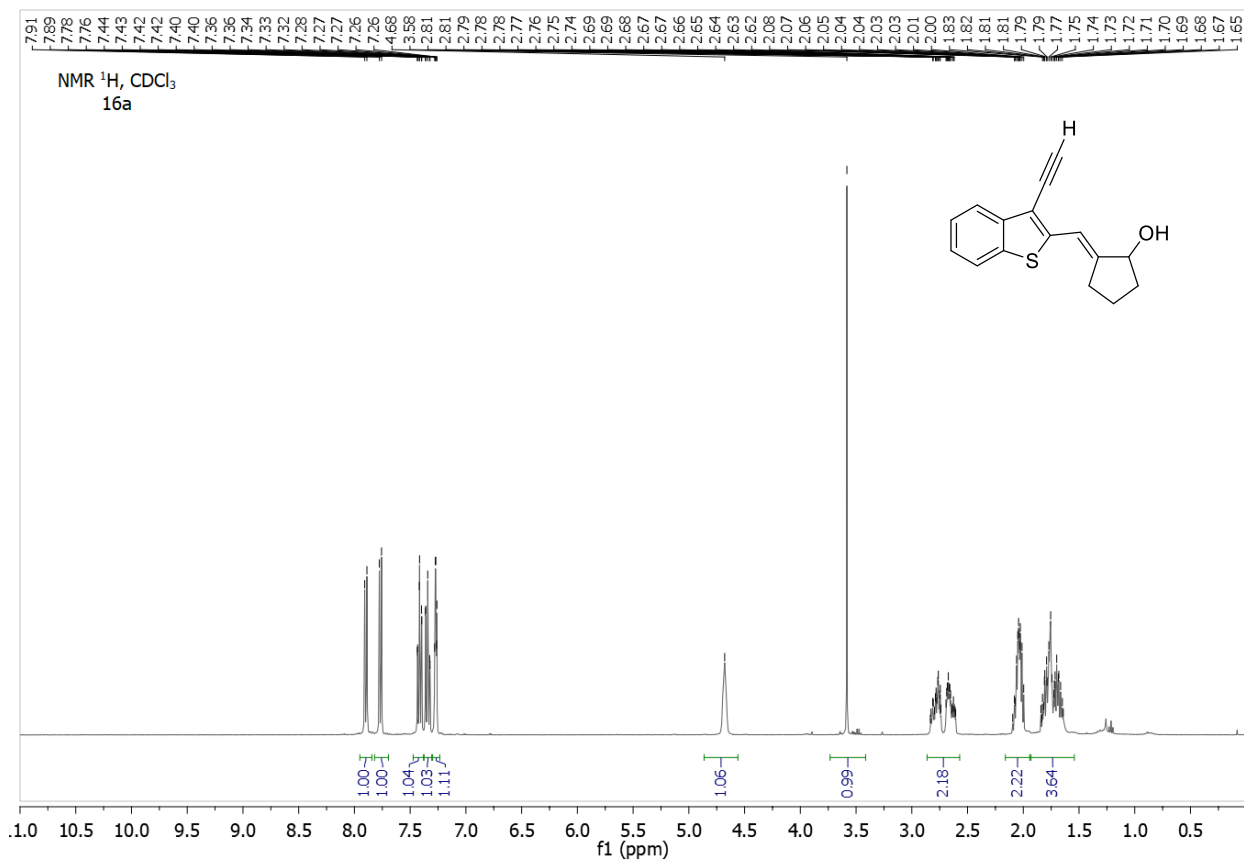


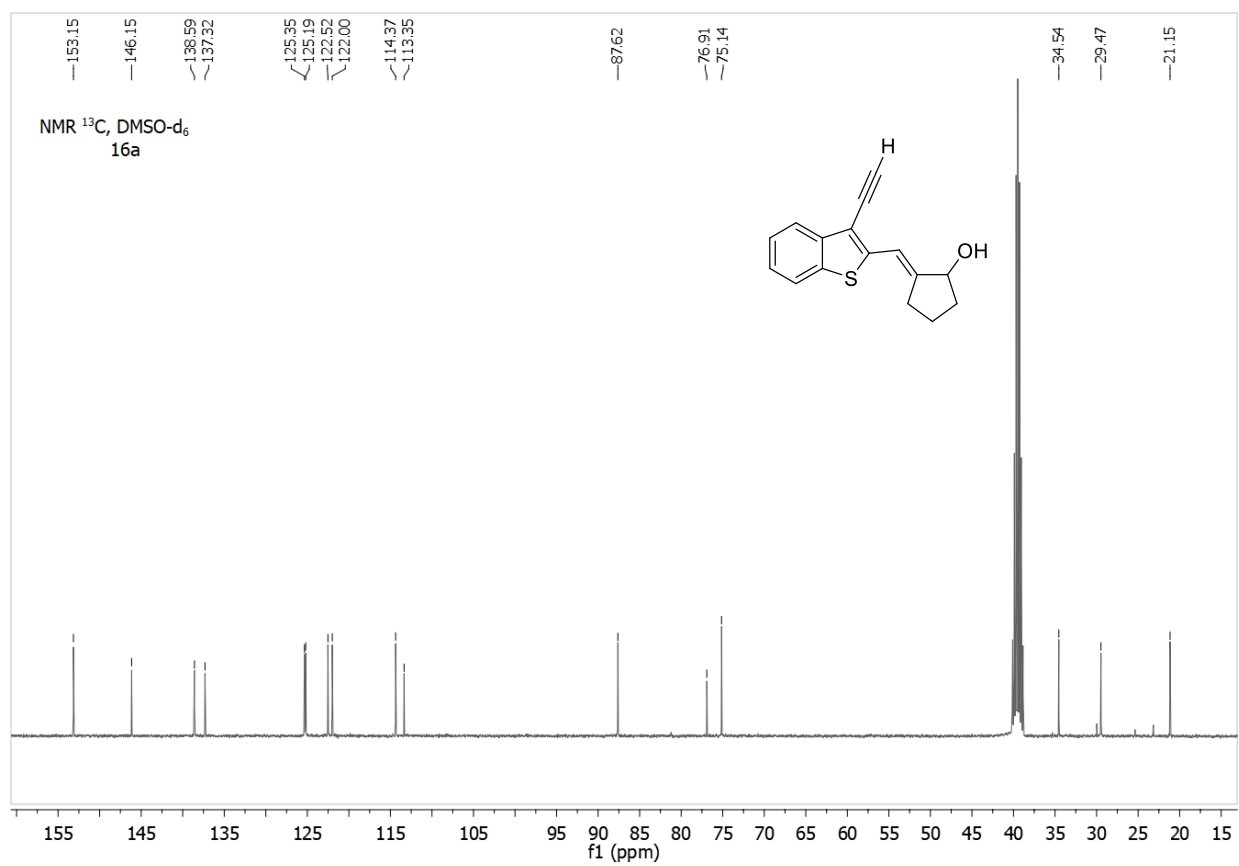
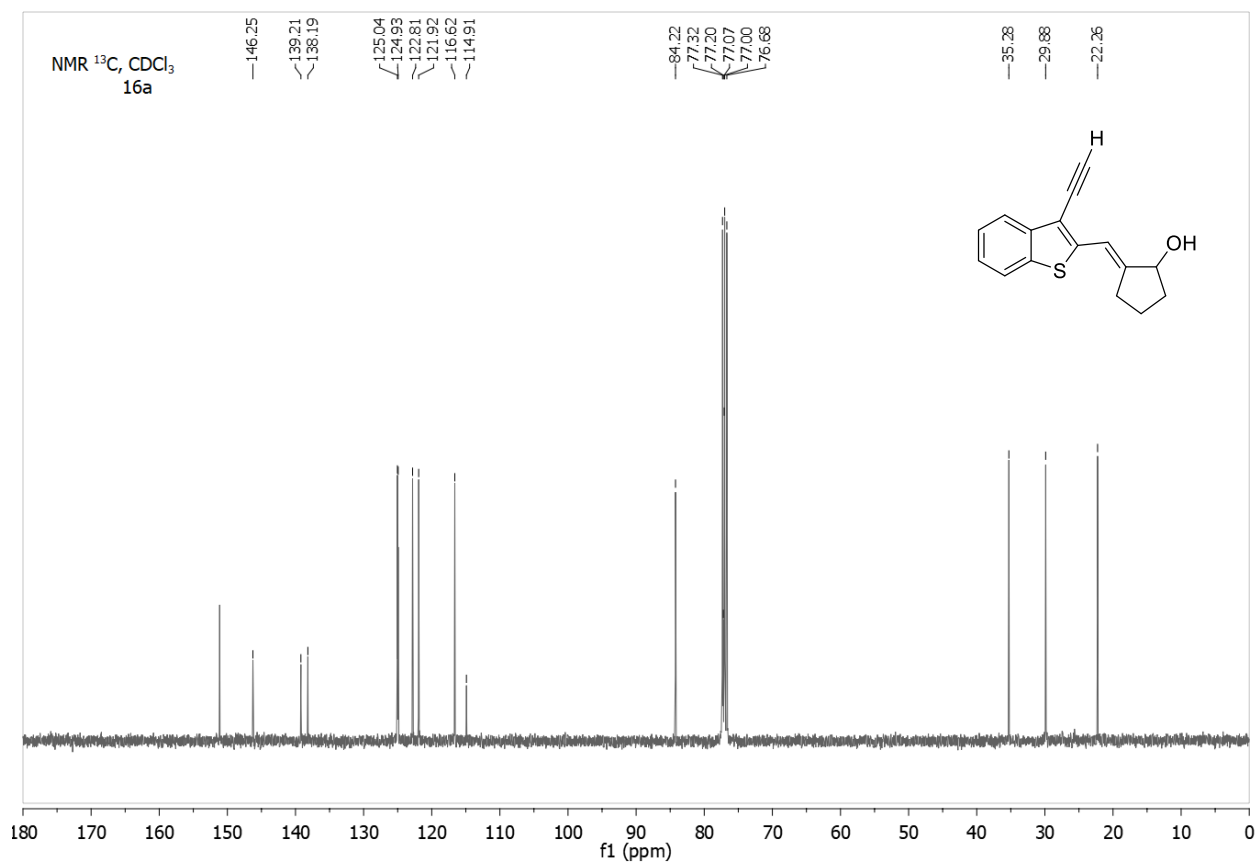


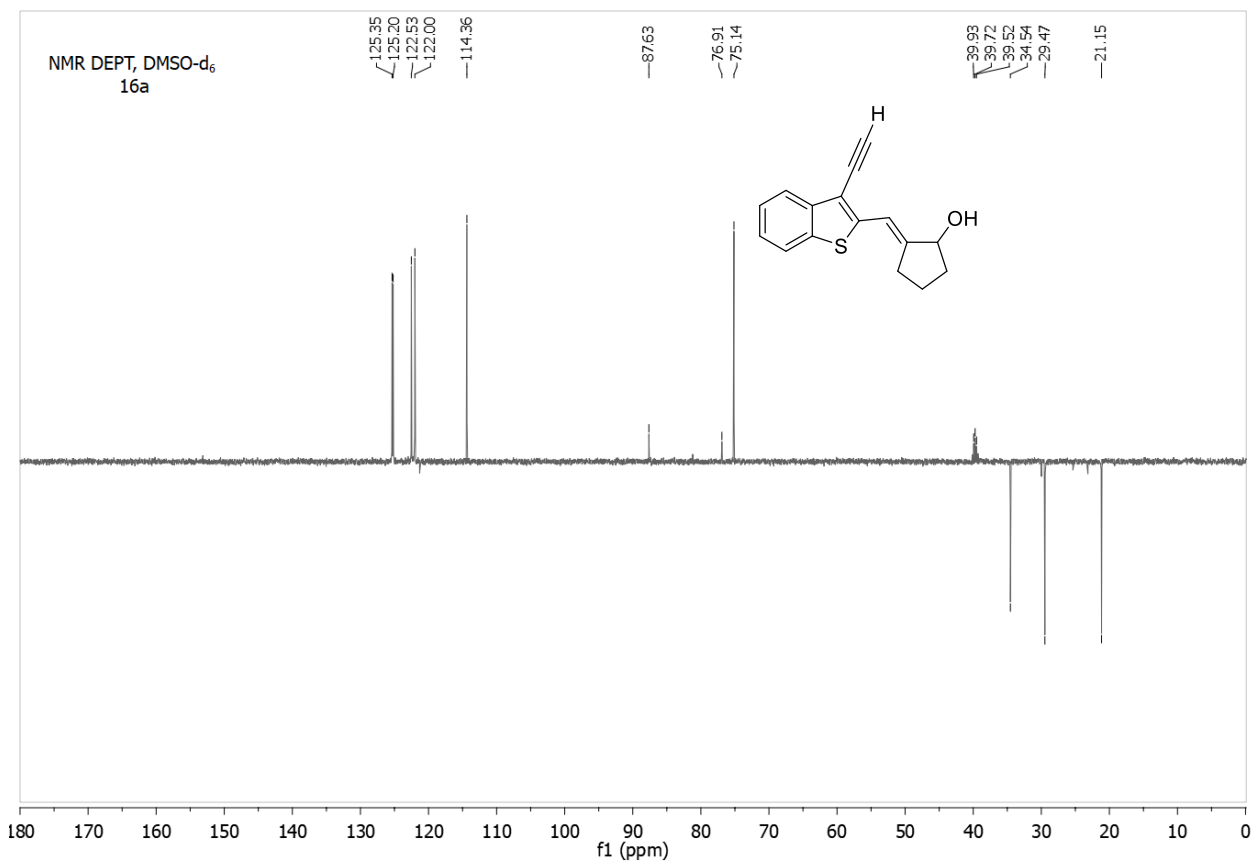
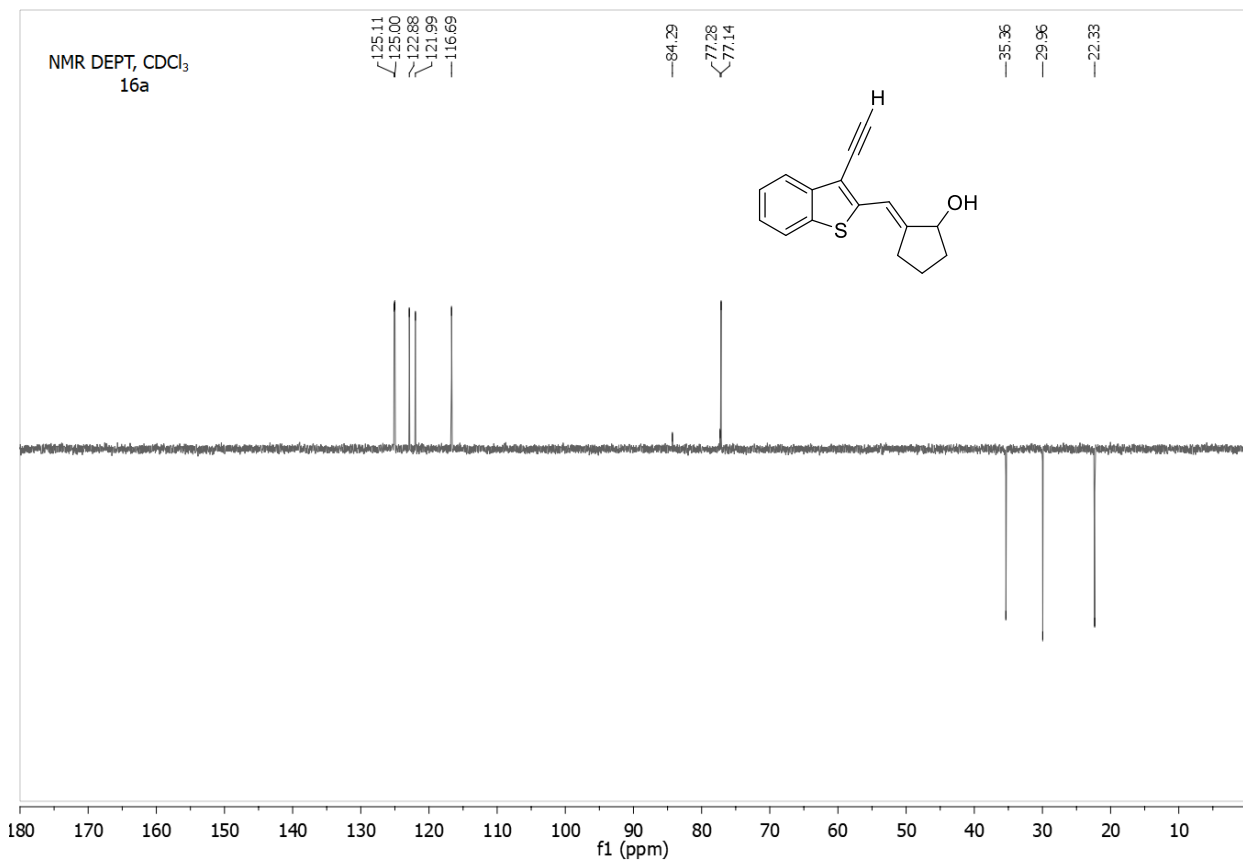




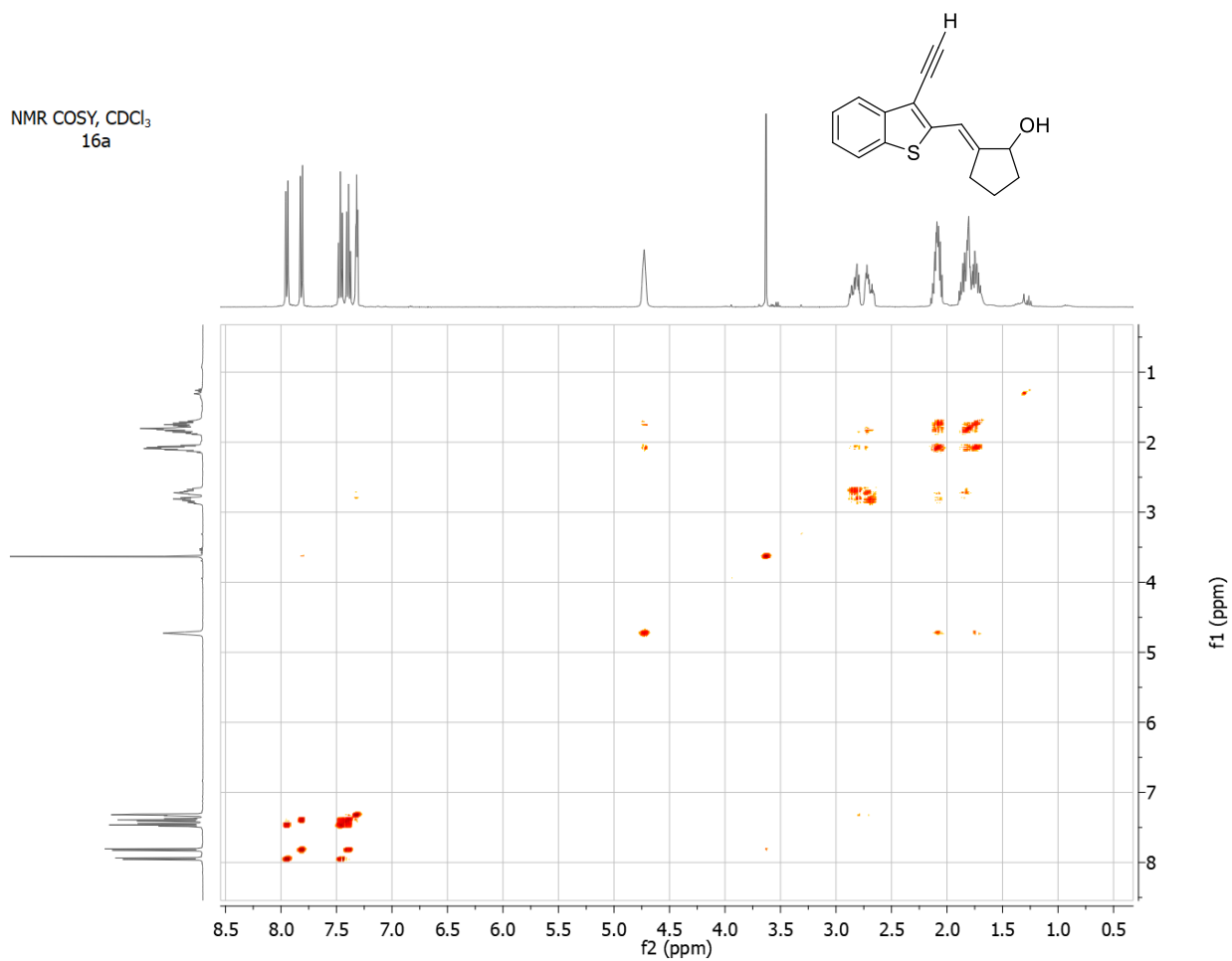




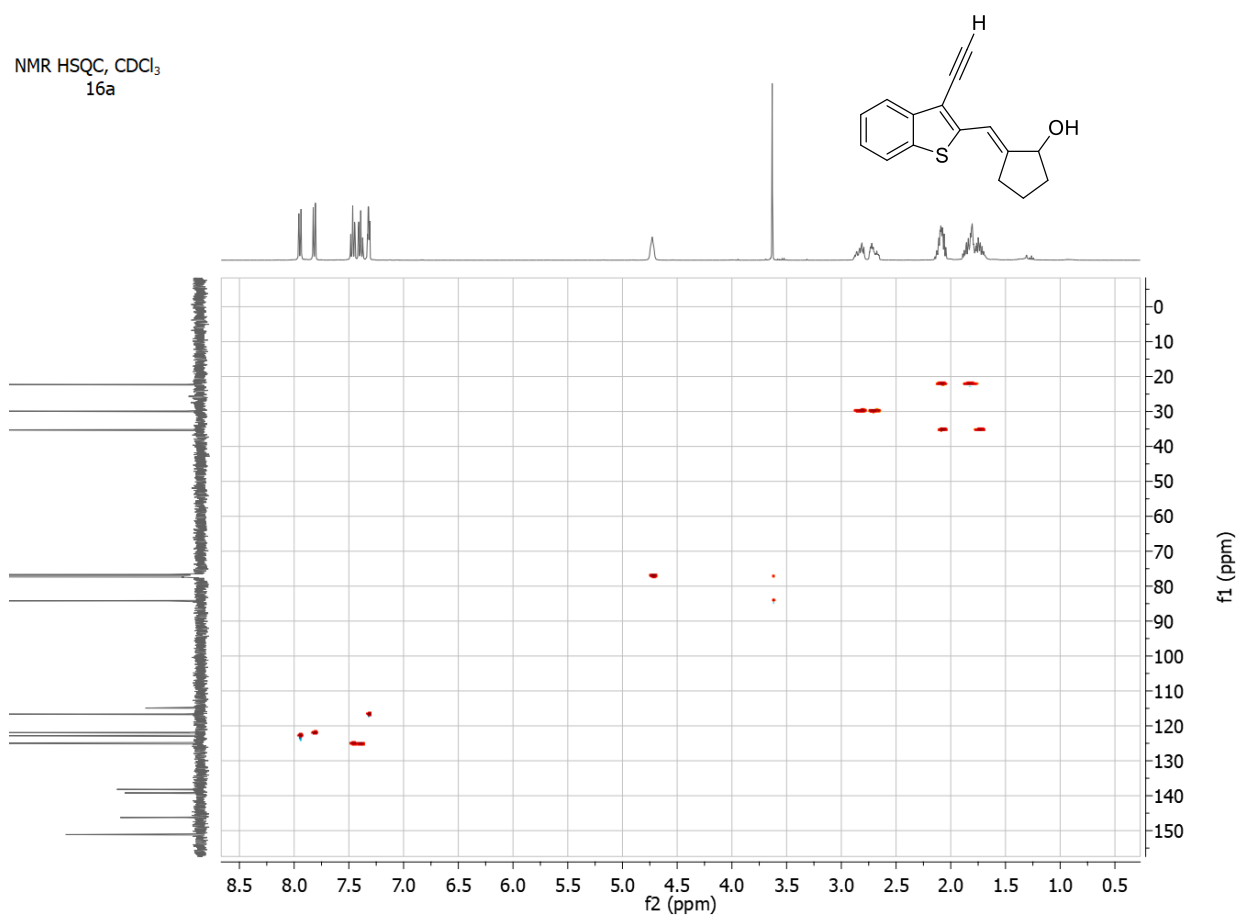




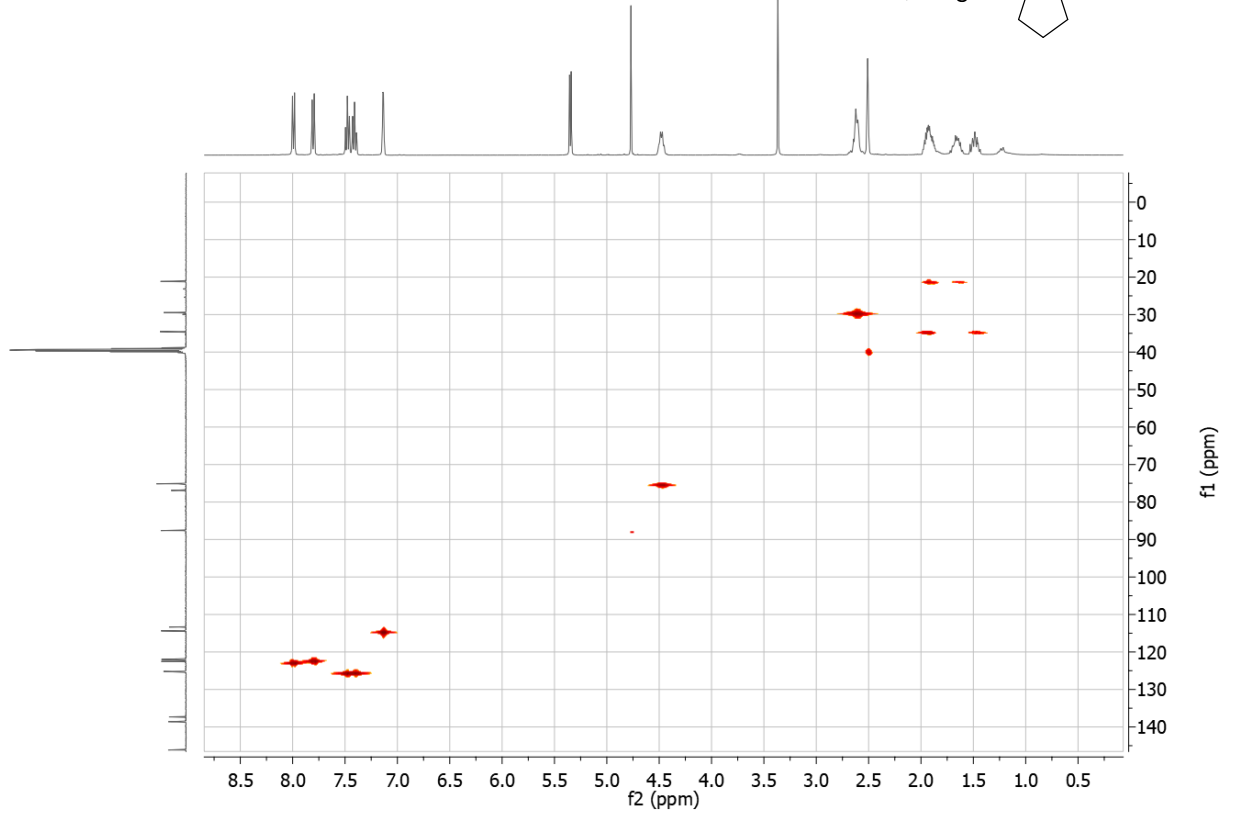
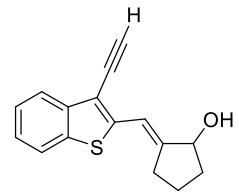
NMR COSY, CDCl₃
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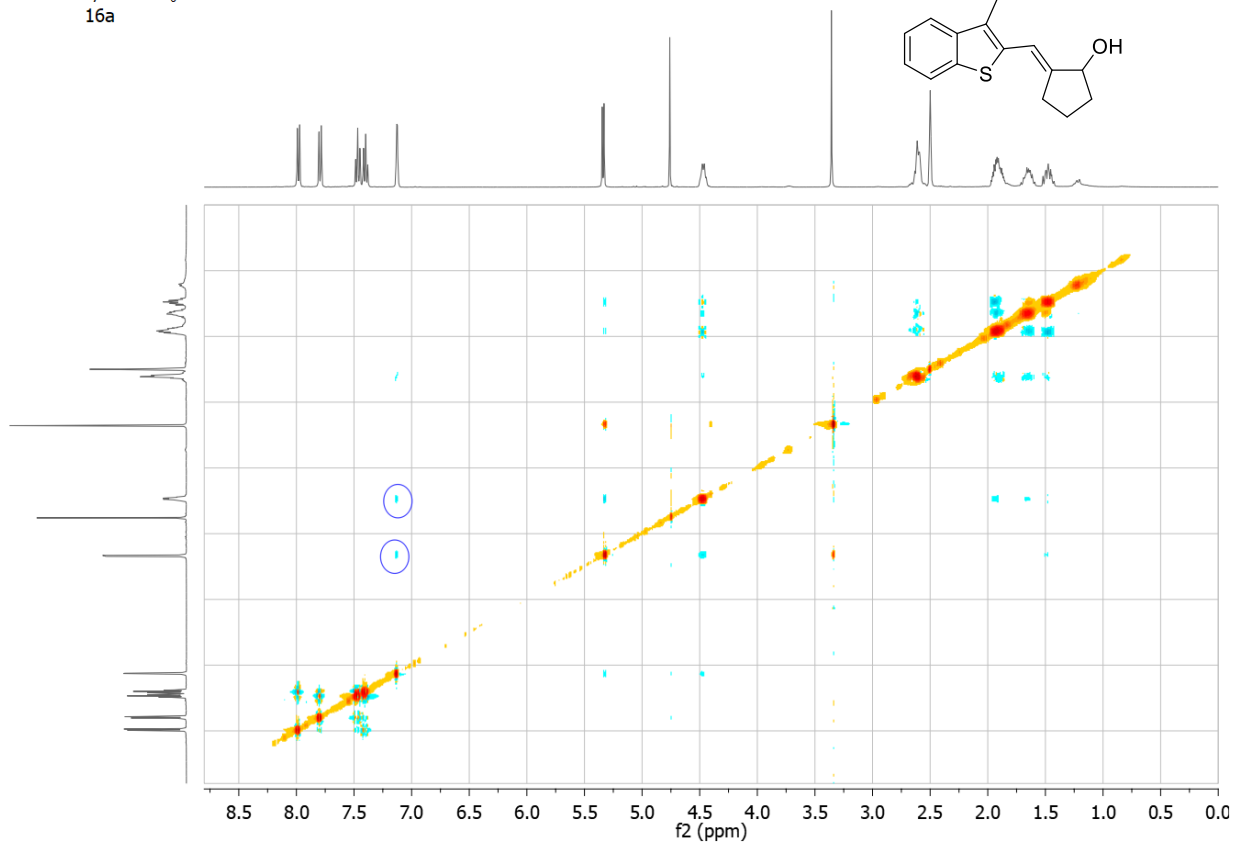
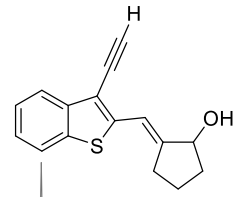
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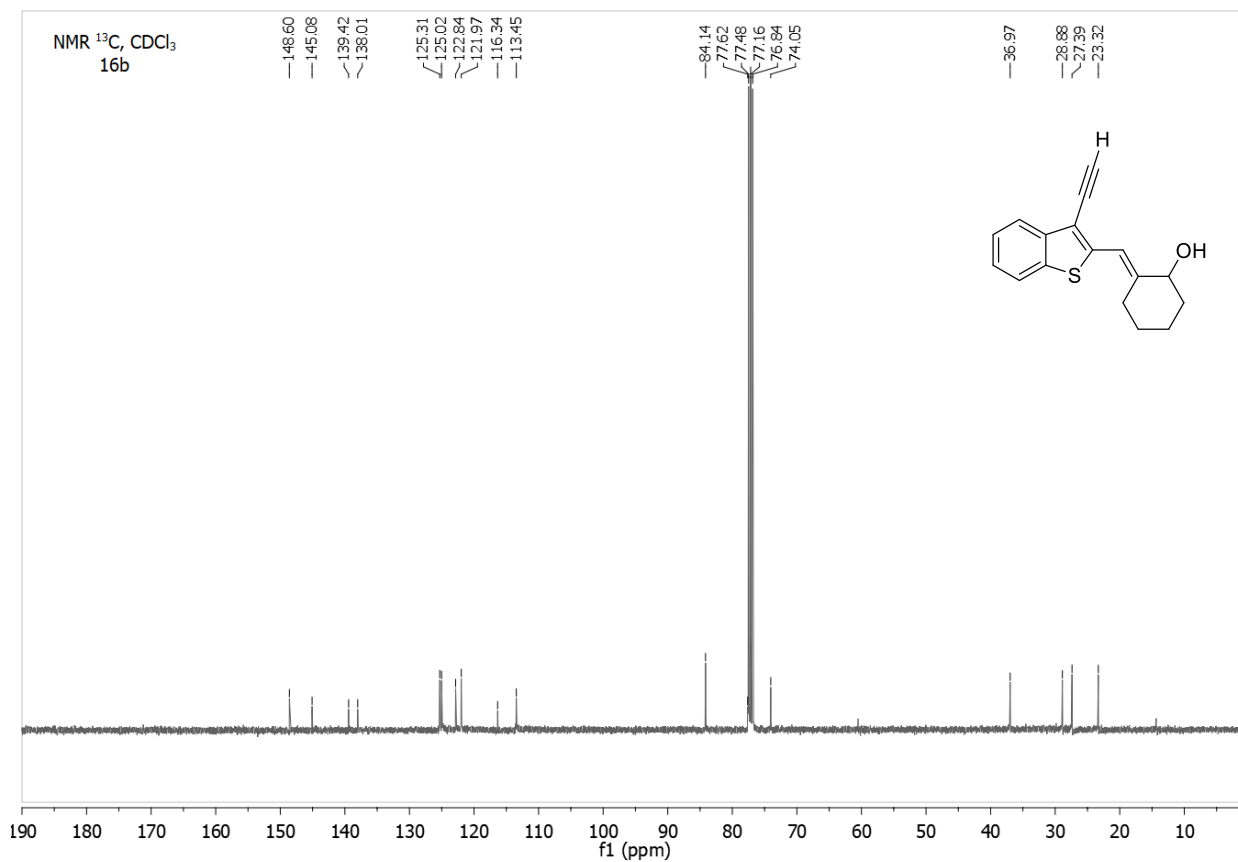
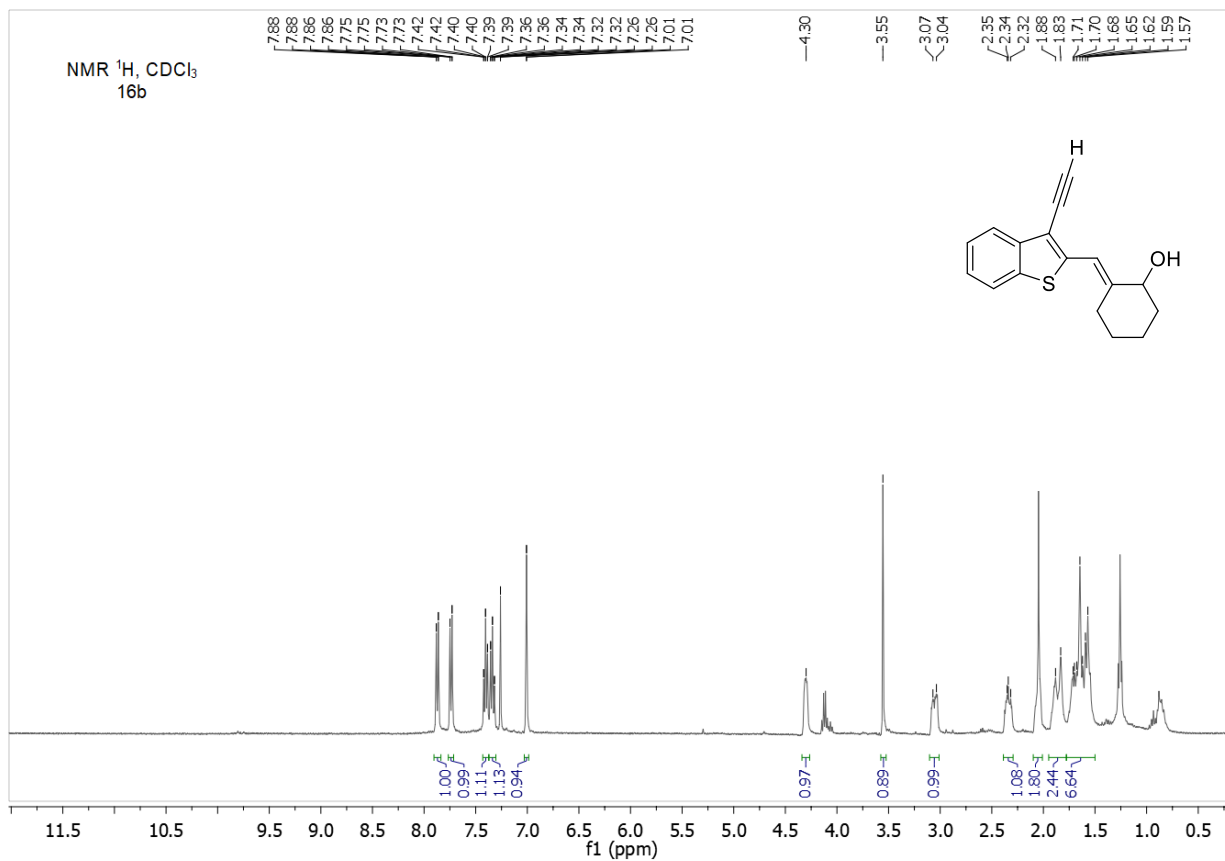


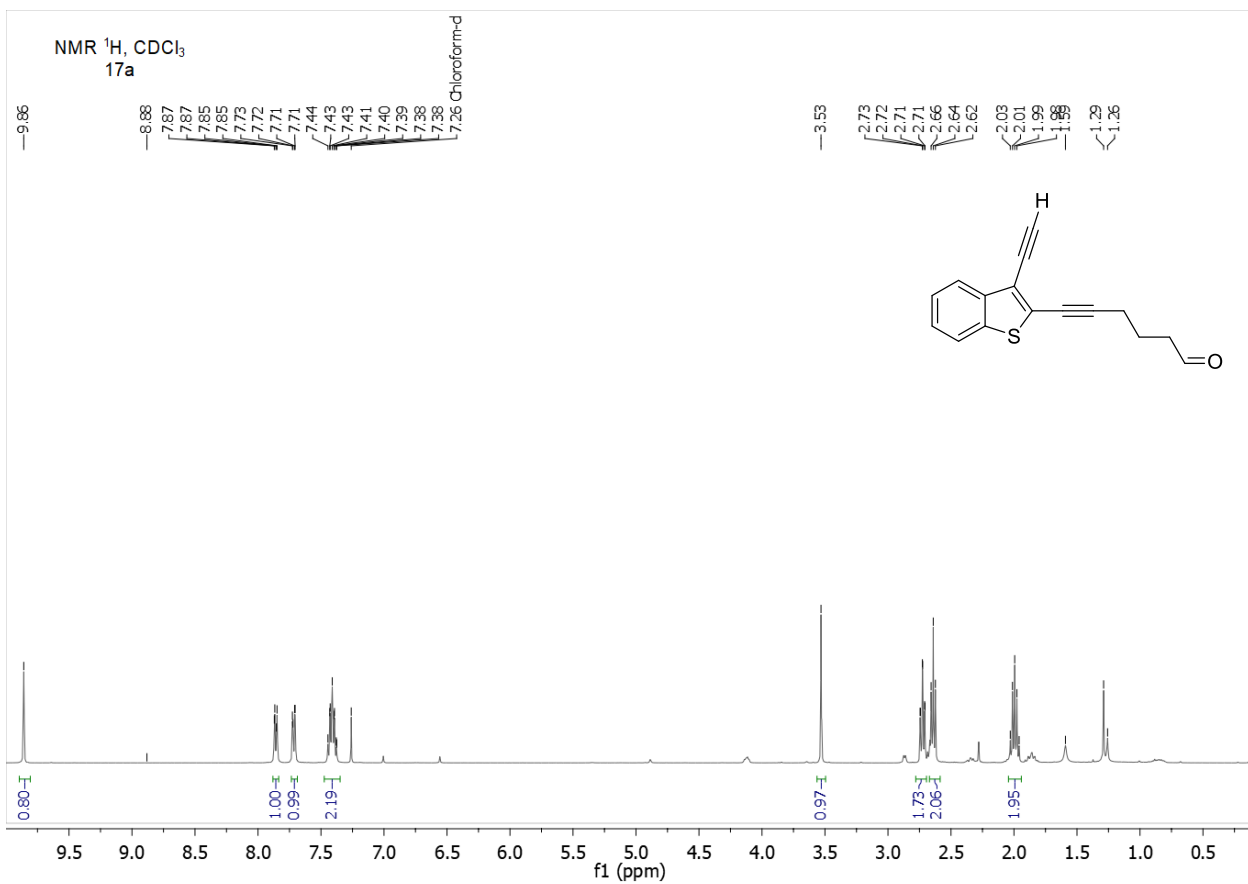
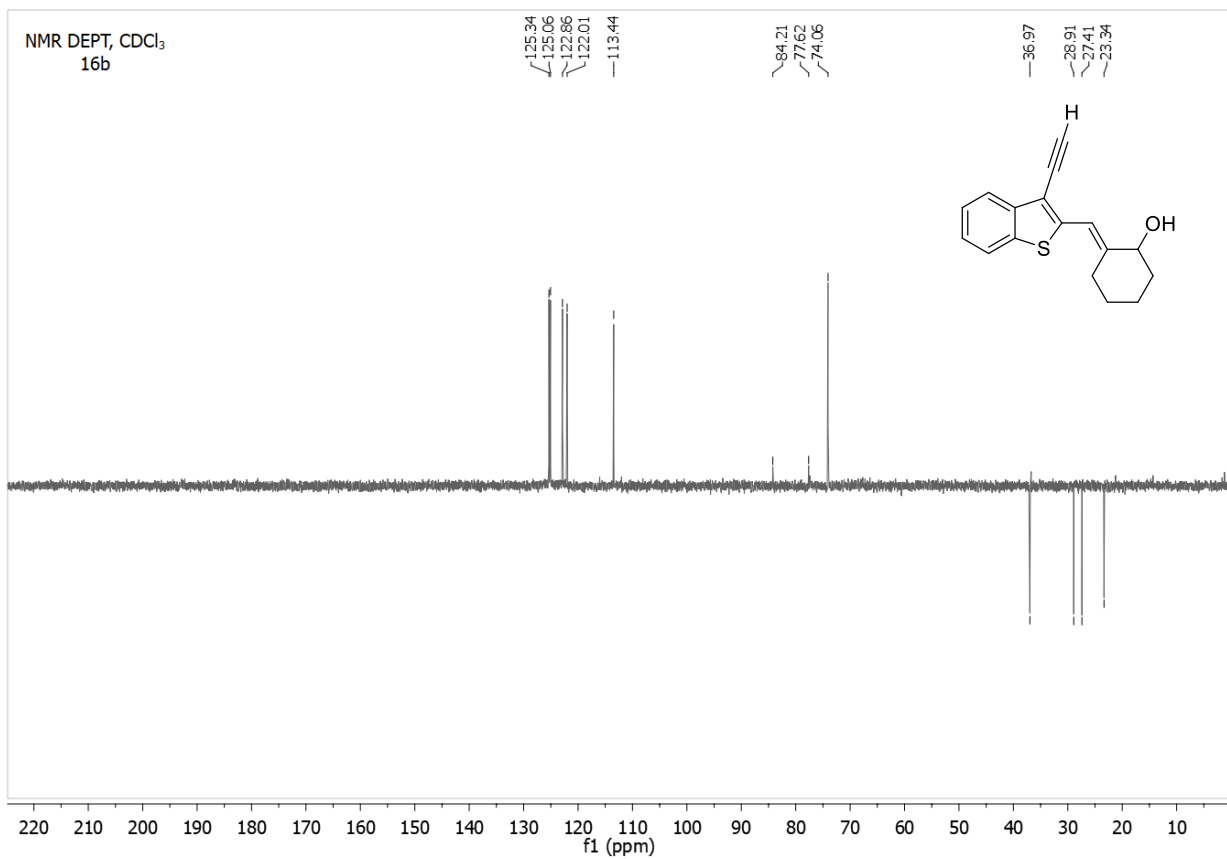
NMR HSQC, DMSO-d₆
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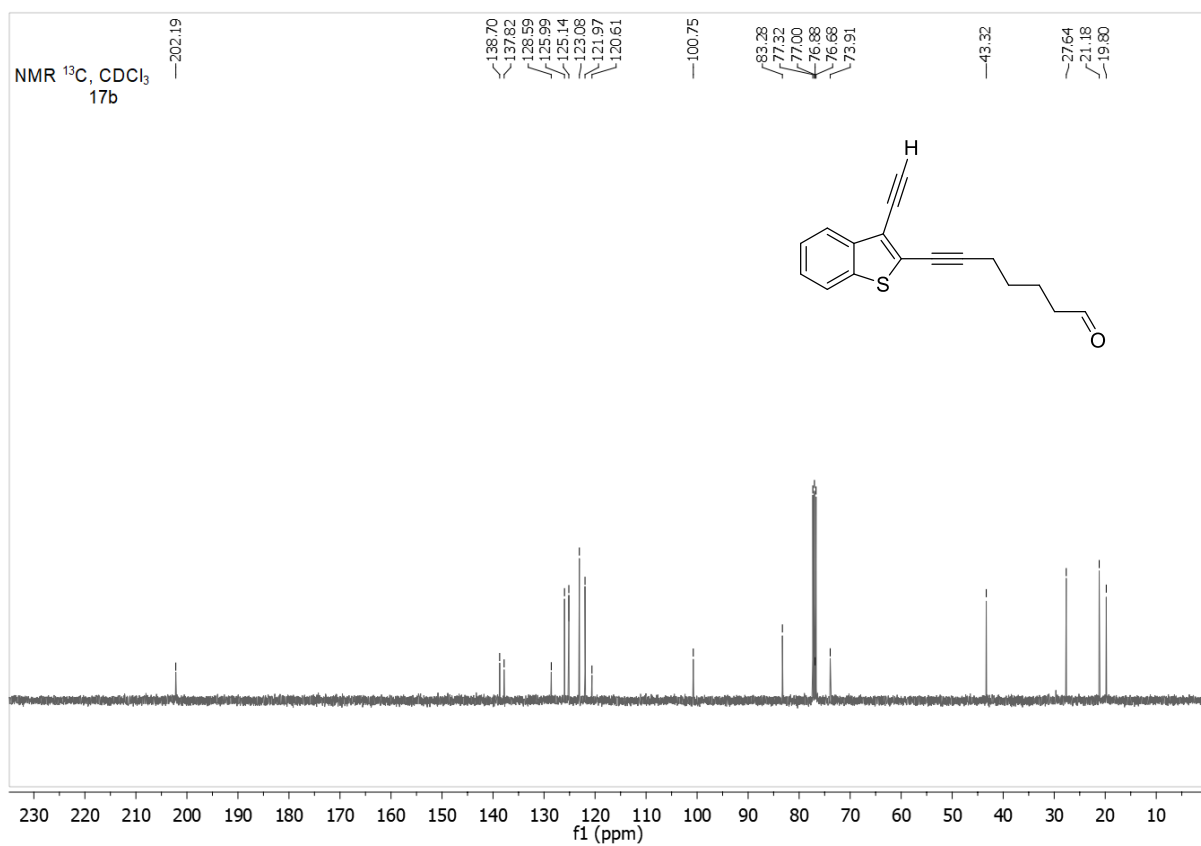
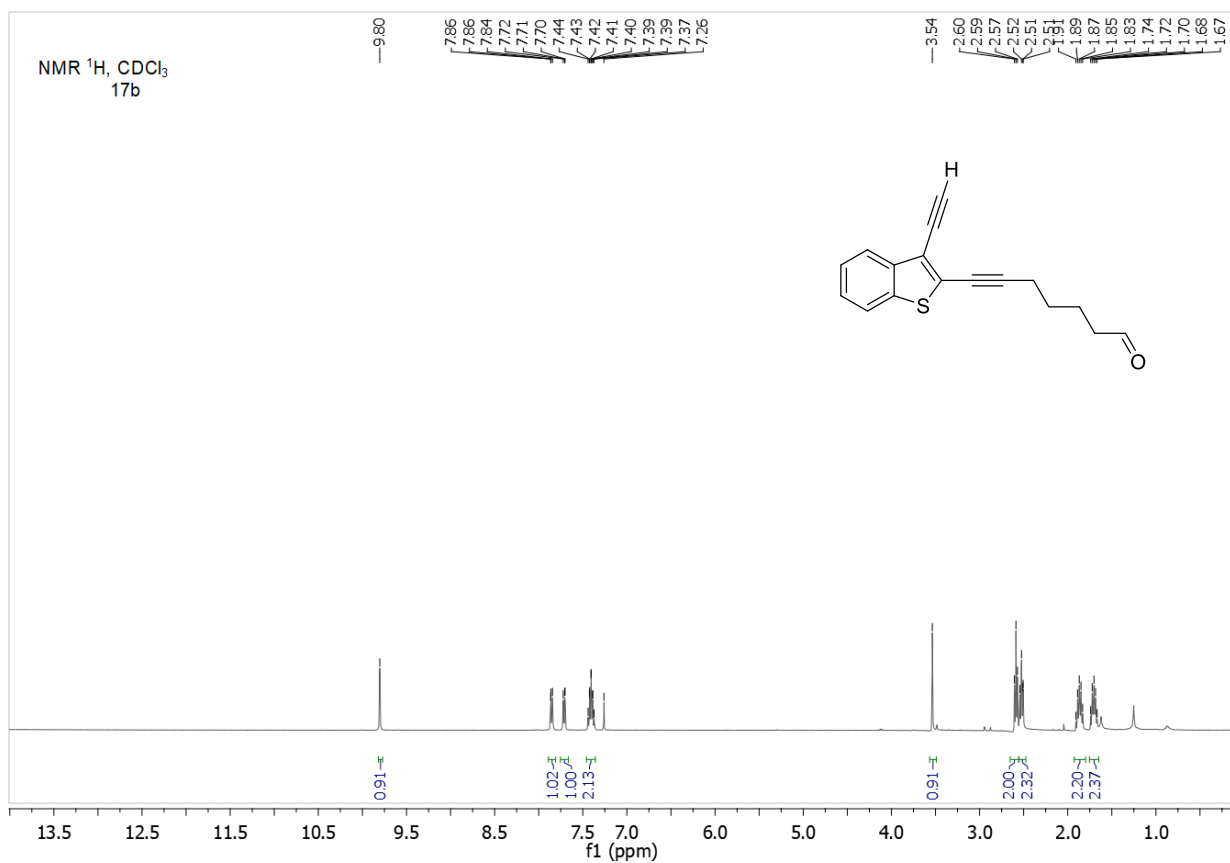


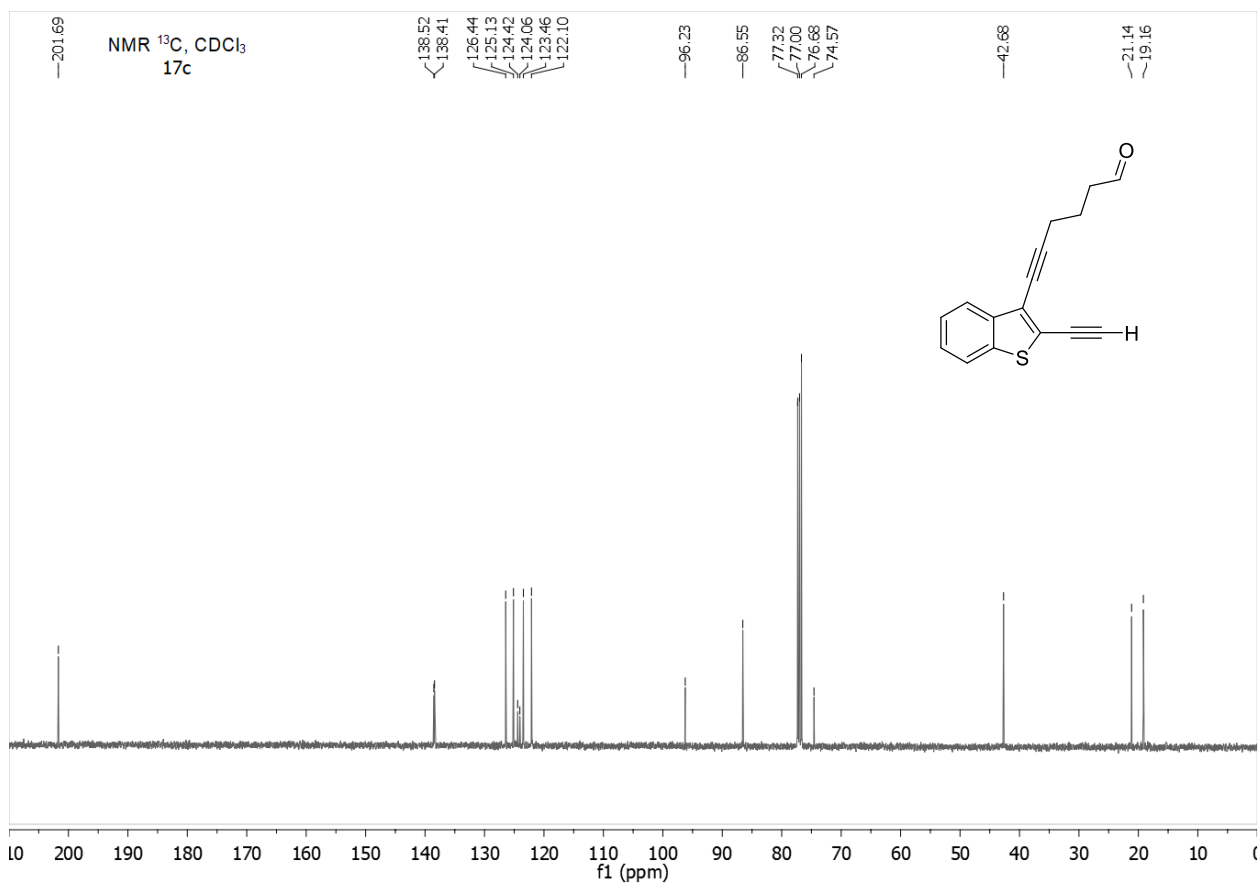
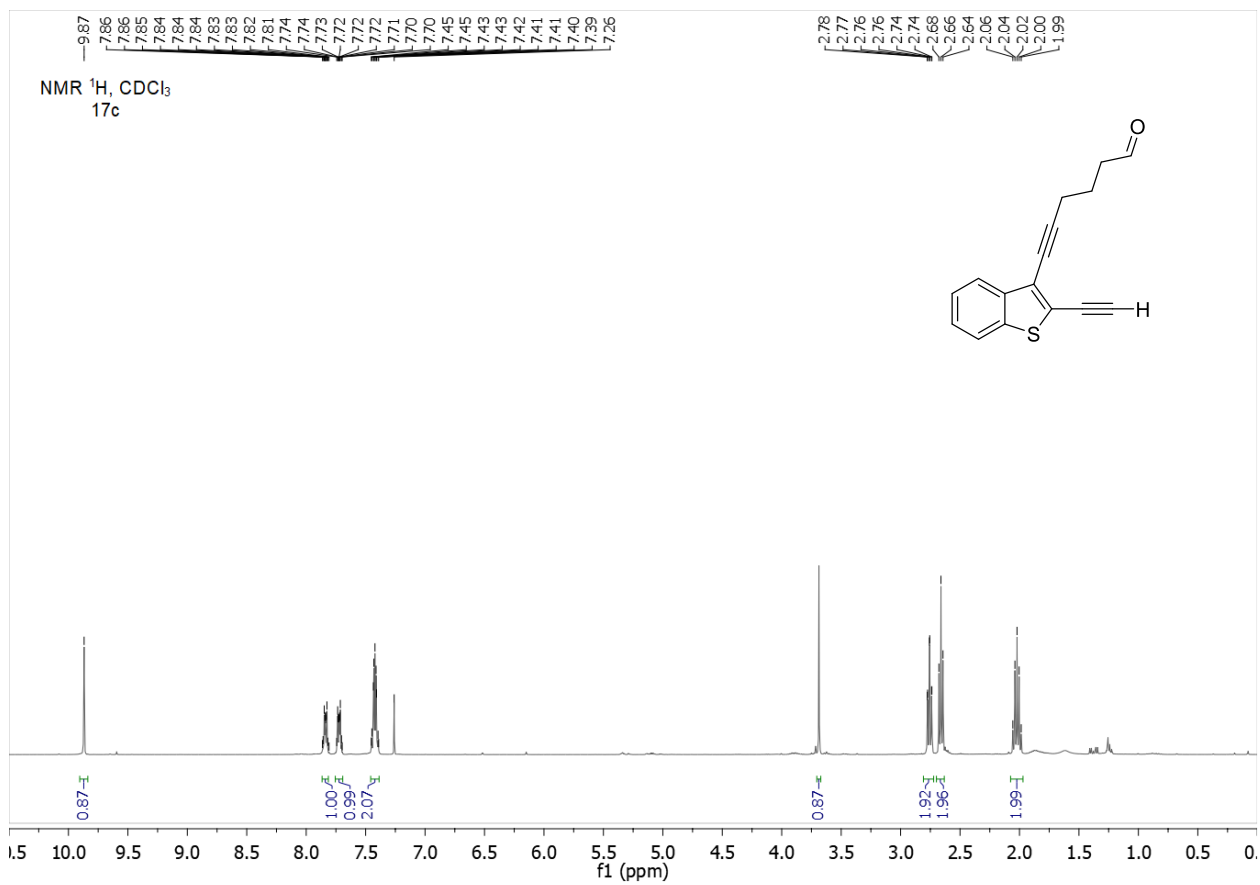
NMR NOESY, DMSO-d₆
16a

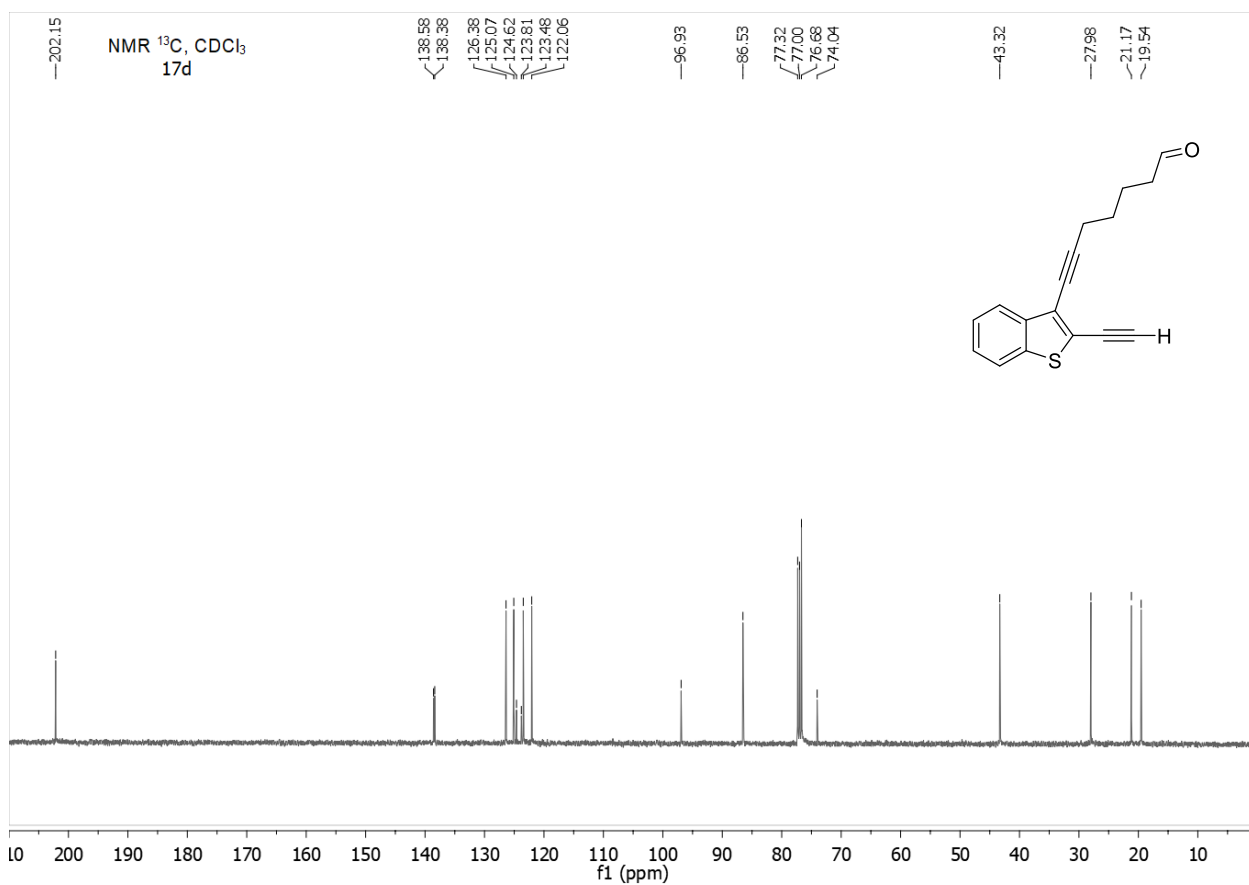
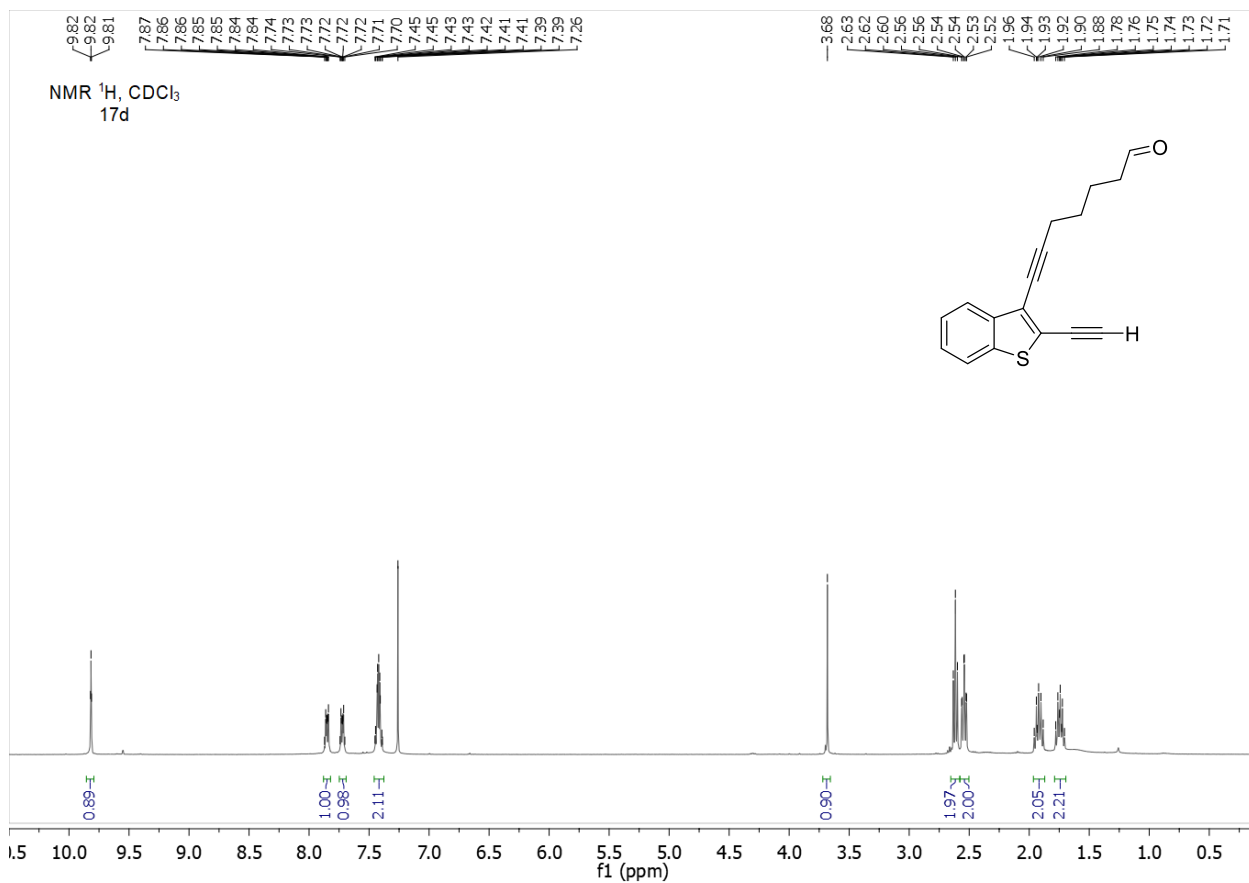


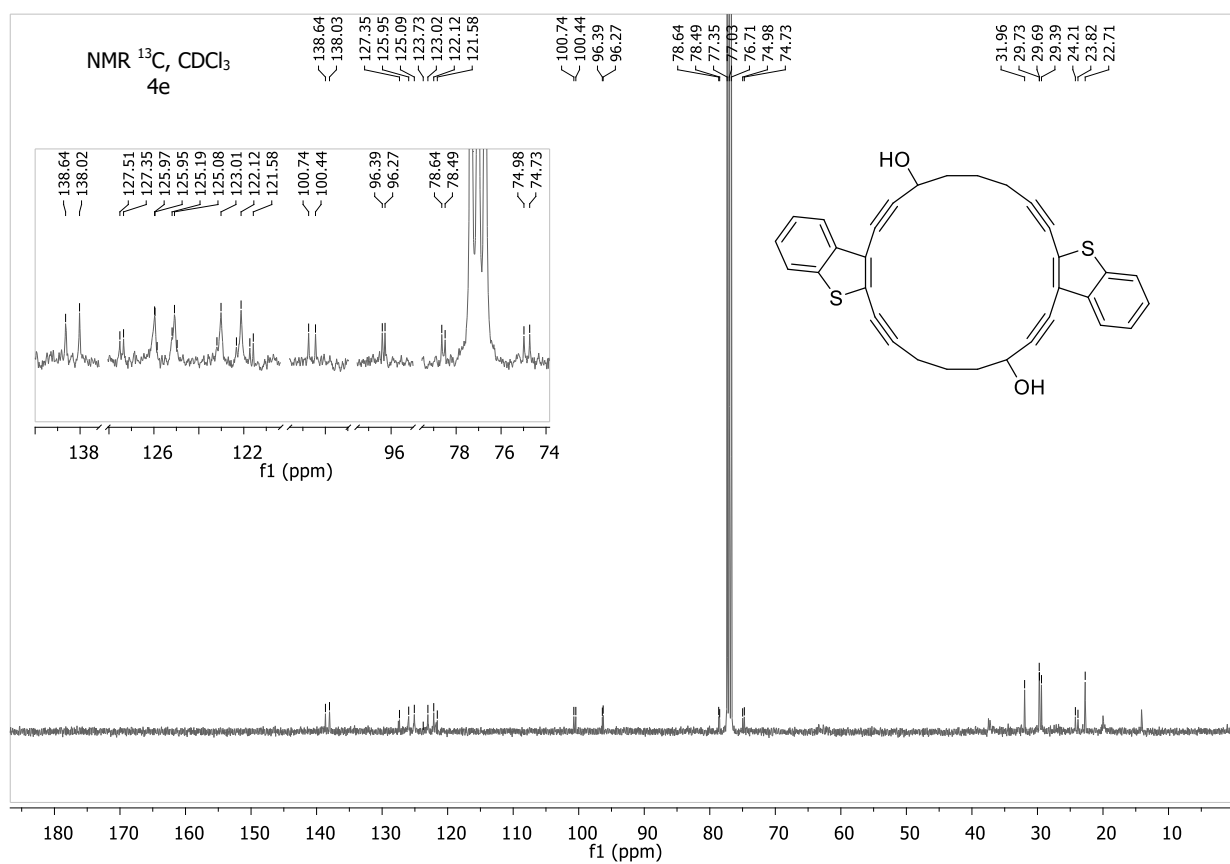
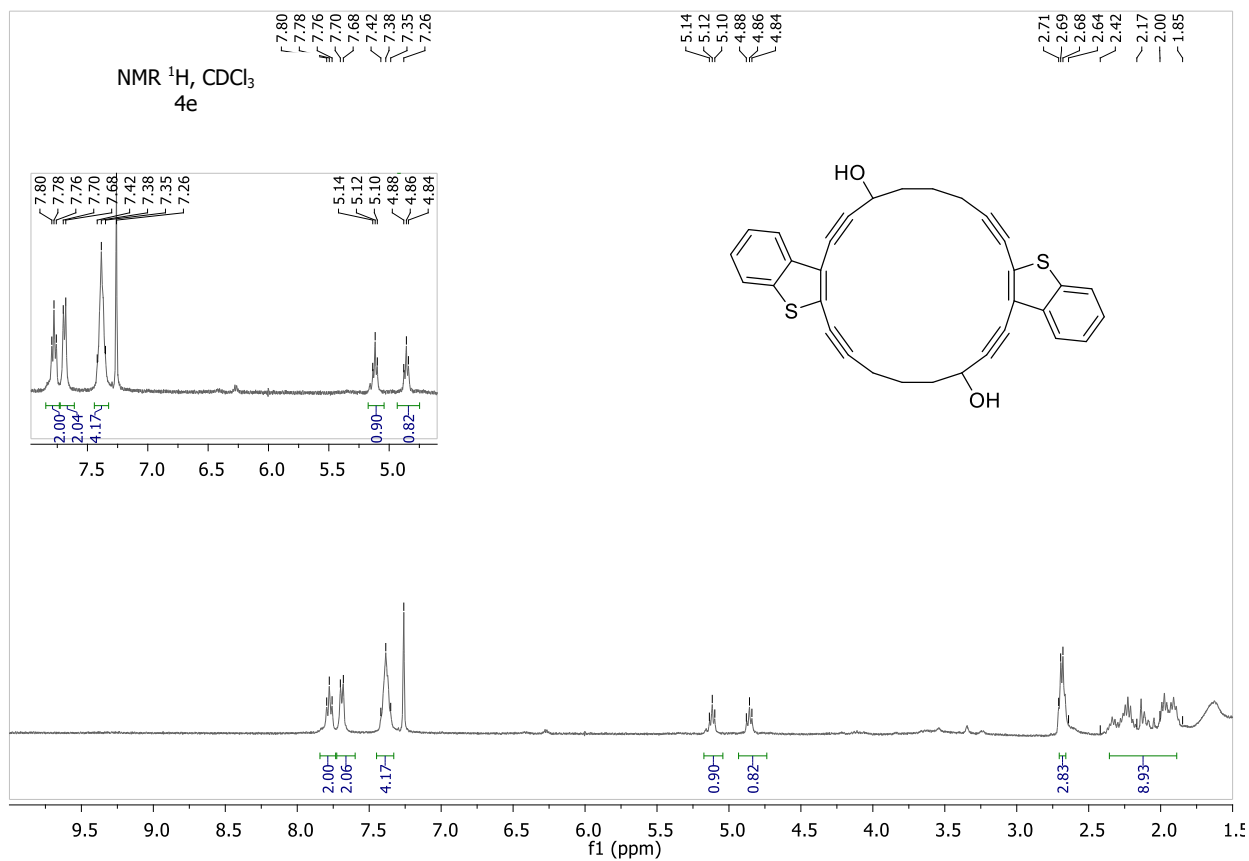


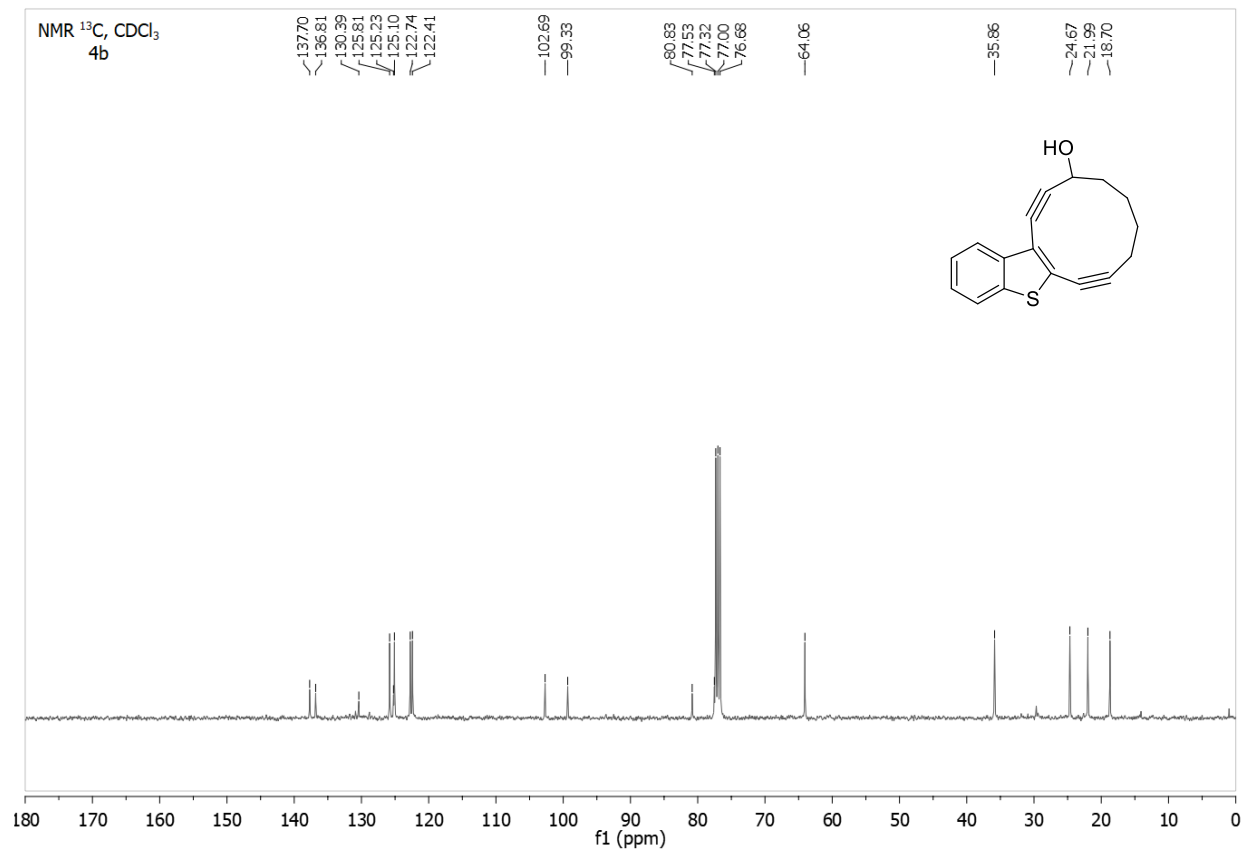
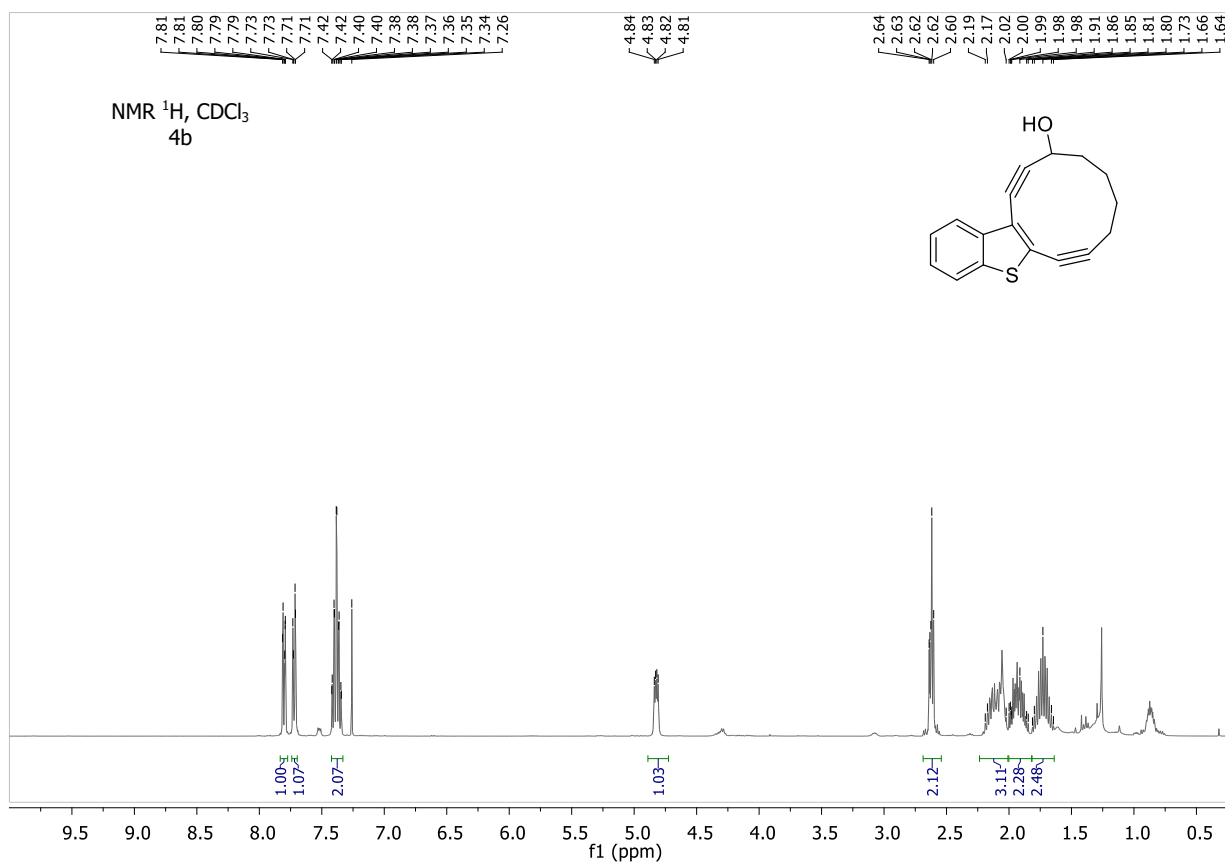


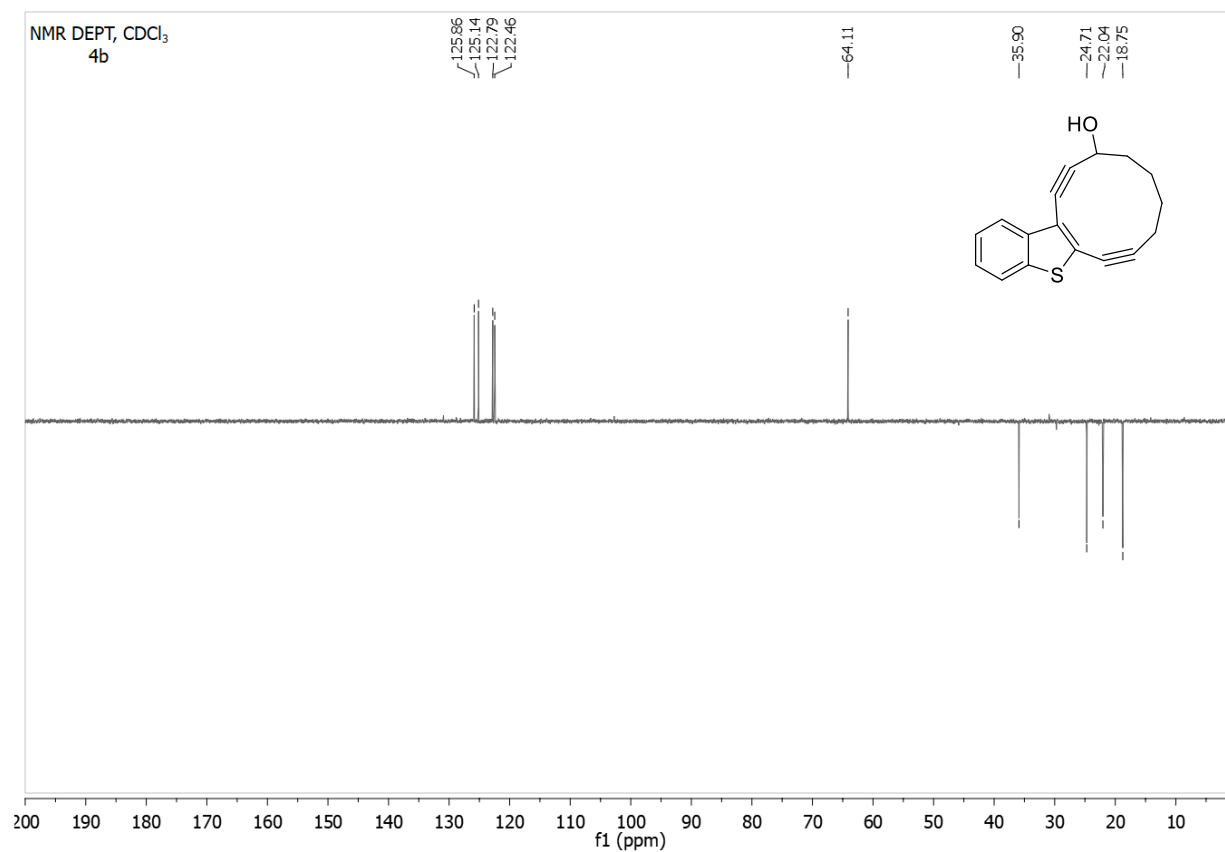






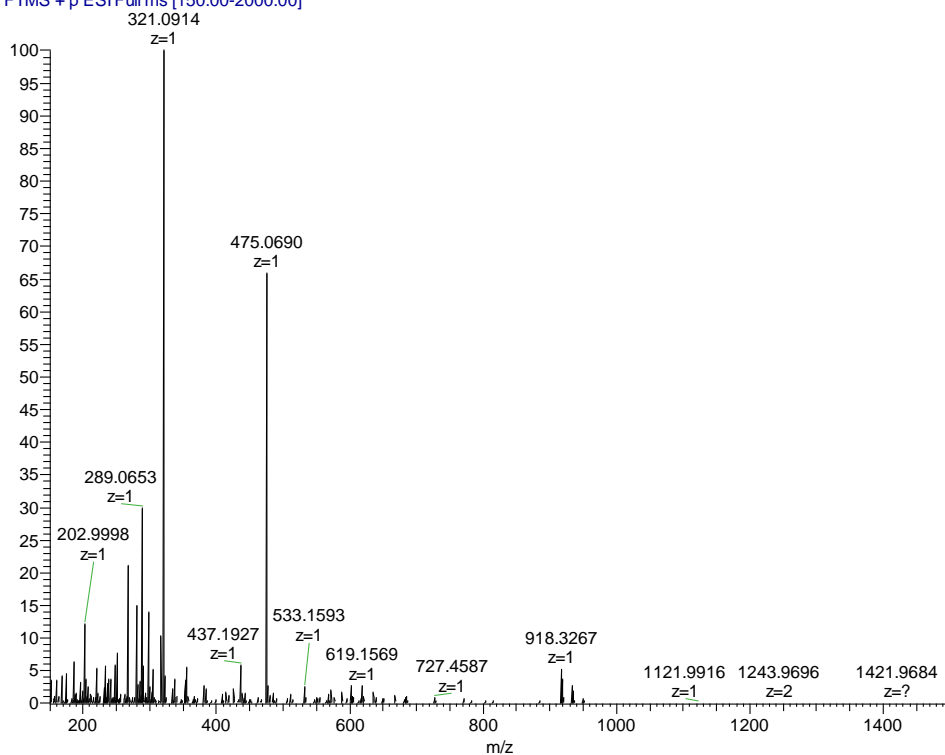


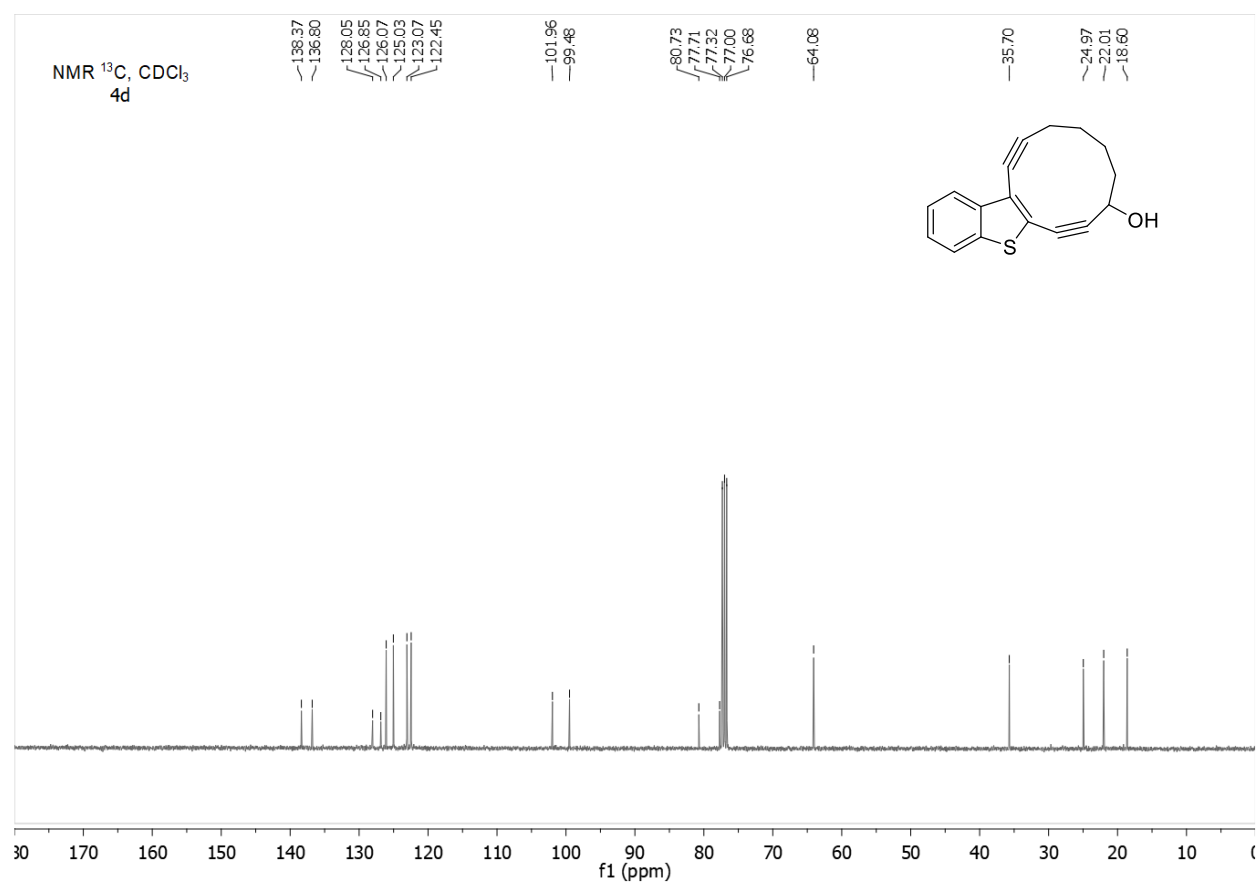
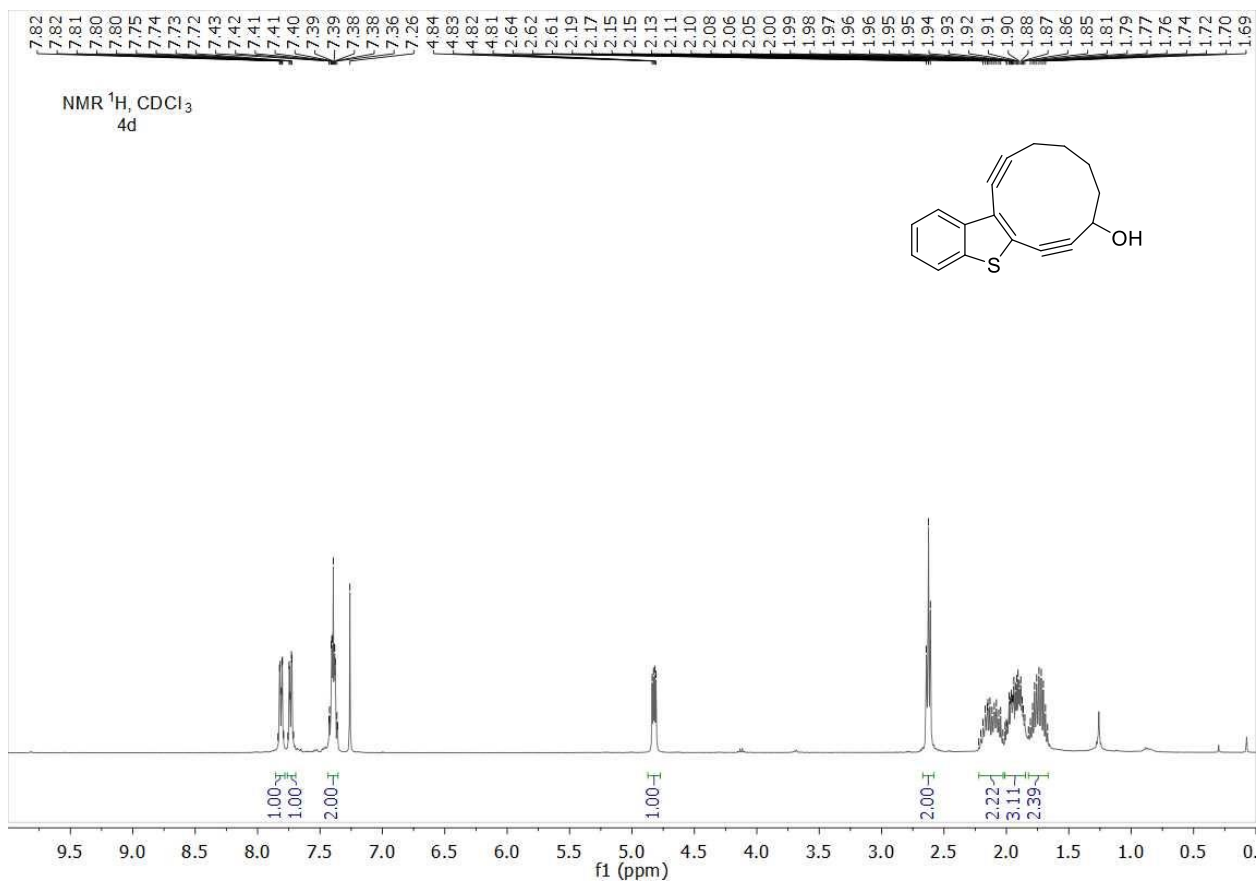




Mass ESI, 4b

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Mass ESI, 4d

Display Report

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Comment	MeOH		

Acquisition Parameter					
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Scan End	1200 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source

