An Unprecedented Stereoselective Base-Induced Trimerization of an α-Bromovinylsulfone.

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Supporting Information

Computational Data

Density functional theory calculations were performed in Gaussian 09.[1] Geometries were optimized with M06-2X/6-31G(d)[2] in implicit tetrahydrofuran as modeled with the SMD[3] solvent model. Vibrational frequency calculations at this level were performed to determine whether stationary points were minima or first-order saddle points and to obtain thermochemical quantities. Single-point energy calculations were subsequently performed with M06-2X/6-311+G(d,p) in SMD implicit tetrahydrofuran. The thermochemical corrections obtained from the M06-2X/6-31G(d) frequencies were added to the solution-phase M06-2X/6-311+G(d,p) potential energies to give Gibbs free energies in solution, which are reported at a standard state of 298.15 K and 1 mol/L. The Cartesian coordinates of optimized structures are given below, along with the following energies (all in Hartree):

E: M06-2X/6-31G(d) potential energy plus solvation energy in SMD tetrahydrofuran
G: M06-2X/6-31G(d) Gibbs free energy in SMD tetrahydrofuran at 298.15 K and 1 mol/L
E_{TZ}: M06-2X/6-311+G(d,p) potential energy plus solvation energy in SMD tetrahydrofuran
G_{soln}: M06-2X/6-311+G(d,p)//M06-2X/6-31G(d) Gibbs free in SMD tetrahydrofuran at 298.15 K and 1 mol/L

-Bromovinyl sulfone 1

C	3.539401	-0.337986	0.431387
C	2.894311	0.624658	1.220192
C	1.649083	1.122431	0.863980
C	1.047002	0.649037	-0.301181
C	1.659404	-0.306824	-1.104441
C	2.908694	-0.792692	-0.729728
S	-0.558218	1.256496	-0.743415
C	-1.667240	0.243490	0.229029
Br	-1.626854	-1.583874	-0.223550
O	-0.791539	0.961273	-2.154851
O	-0.697779	2.625822	-0.247165
C	-2.440943	0.787785	1.164194
C	-3.427882	0.081038	2.028059
C	4.894225	-0.855307	0.832165
H	-2.333750	1.863411	1.297732
H	-3.190571	0.261303	3.081931
H	-4.428866	0.489752	1.851695
H	-3.445191	-0.994140	1.843708
H	1.170513	-0.653571	-2.009232

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2. Zhao, Y.; Truhlar, D. G. *Theor. Chem. Acc.* **2008**, *120*, 215–241.
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H 3.401338 -1.536388 -1.349731
H 3.379445 0.987577 2.122413
H 1.152808 1.872764 1.472164
H 5.212420 -1.677574 0.187020
H 5.645589 -0.060604 0.768231
H 4.885854 -1.211401 1.867132
0 imaginary frequencies
E = -3507.773637
G = -3507.622989
E_{TZ} = -3510.342068
G_{soln} = -3510.191420

Bromovinyl sulfone anion 1a/1a'
C -2.938944 0.622383 -0.990094
C -1.693941 1.171174 -0.696500
C -0.954606 0.668856 0.371598
C -1.448855 -0.389808 1.132934
C -2.692699 -0.932070 0.826489
C -3.453936 -0.438718 -0.239053
S 0.704075 1.288758 0.672046
O 0.928583 1.075923 2.110086
C -4.786449 -1.054624 -0.578956
O 0.706909 2.673738 0.159997
C 1.822039 0.391560 -0.259729
Br 1.880053 -1.462116 0.275180
C 1.866146 0.646984 -1.672094
C 2.220094 -0.176169 -2.680068
H 1.630298 1.684357 -1.915870
H -0.863391 -0.767300 1.965214
H -3.083589 -1.751691 1.425291
H -3.522397 1.024680 -1.814807
H -1.299804 1.998880 -1.278620
H -5.389938 -0.381803 -1.194612
H -4.653099 -1.987213 -1.139628
H -5.354795 -1.296491 0.324450
H 2.470383 -1.217909 -2.504842
H 2.282266 0.193696 -3.698431
0 imaginary frequencies
E = -3507.256211
G = -3507.118168
E_{TZ} = -3509.838937
G_{soln} = -3509.700894

Sulfone isomer 8
C -1.791412 1.168401 -0.851323
C -1.031084 0.684918 0.208810
C -1.542533 -0.242976 1.115179
C -2.845467 -0.689384 0.945211
C -3.636089 -0.226229 -0.115250
C -3.094604 0.705678 -1.005228
S 0.640126 1.244192 0.386486
O 0.755027 2.582909 -0.196070
C -5.047121 -0.723278 -0.275289
C 1.612631 0.166502 -0.741331
C 3.023693 0.668542 -0.751467
C 4.029640 0.149437 -0.056679
Br 1.408903 -1.674291 -0.176776

O 1.078229 0.996612 1.757009
H 3.162944 1.563670 -1.352823
H -0.928025 -0.597322 1.936560
H -3.260959 -1.409653 1.644899
H -3.701353 1.076888 -1.826147
H -1.376257 1.901627 -1.536182
H -5.497079 -0.353312 -1.199558
H -5.074922 -1.817476 -0.290351
H -5.669887 -0.394279 0.563607
H 3.910586 -0.742274 0.551128
H 5.014589 0.603675 -0.092039
H 1.134774 0.255710 -1.719021
0 imaginary frequencies
E = -3507.768122
G = -3507.616881
E_{TZ} = -3510.338398
G_{soln} = -3510.187158

Allyl sulfone cation derived from heterolysis of C–Br bond of 8
C 2.438592 -0.233362 -1.143839
C 1.118970 -0.656839 -1.086927
C 0.400641 -0.433092 0.091141
C 0.966377 0.208700 1.198190
C 2.286380 0.619690 1.115163
C 3.038484 0.405482 -0.050214
S -1.275536 -0.939801 0.169874
O -1.729421 -0.975092 1.552031
C 4.474843 0.838938 -0.106536
O -1.533853 -2.040159 -0.748490
C -2.045001 0.490619 -0.604314
C -2.910433 1.292846 0.093012
C -3.504642 2.329575 -0.607010
H -1.792533 0.654700 -1.653203
H -4.238016 2.978930 -0.135608
H -3.253776 2.512164 -1.649580
H -3.141197 1.098397 1.136329
H 0.384436 0.362585 2.101351
H 2.749520 1.110995 1.965927
H 3.017842 -0.404710 -2.046037
H 0.657982 -1.165955 -1.928017
H 4.859021 0.814920 -1.128424
H 4.593838 1.850018 0.293700
H 5.092380 0.171444 0.505258
0 imaginary frequencies
E = -935.720603
G = -935.568784
E_{TZ} = -935.894313
G_{soln} = -935.742494

Br^-
Br 0.000000 0.000000 0.000000
0 imaginary frequencies
E = -2571.911284
G = -2571.924440
E_{TZ} = -2574.333688
G_{soln} = -2574.346845

TS-S_N2

C	-2.202731	2.449233	1.449740
C	-2.726181	1.540377	0.536381
C	-2.726390	1.800980	-0.832527
C	-2.152304	2.982898	-1.285294
C	-1.591554	3.904145	-0.393339
C	-1.636773	3.628055	0.976748
S	-3.411420	0.010387	1.136489
O	-3.344414	0.001088	2.603027
C	-0.922242	5.152682	-0.902858
C	-2.220959	-1.234707	0.503348
C	-2.283395	-2.565380	1.128766
C	-1.652818	-3.636235	0.644426
O	-4.739692	-0.162825	0.550737
C	-0.575580	-0.581049	2.163459
C	0.468570	-1.209894	1.496679
C	1.077791	-0.765948	0.344556
Br	0.726958	0.958250	-0.358255
S	2.286519	-1.682187	-0.495114
C	3.819322	-0.814459	-0.213022
C	4.220954	0.175109	-1.103855
C	5.395279	0.879392	-0.848073
C	6.167544	0.606040	0.283128
C	5.739141	-0.396564	1.163675
C	4.568691	-1.104607	0.926271
C	7.441090	1.360912	0.558719
O	2.393626	-2.986942	0.172250
O	2.053439	-1.638221	-1.941830
Br	-3.198149	-1.672148	-1.638415
H	3.626856	0.379088	-1.988837
H	5.718611	1.651616	-1.541070
H	6.334537	-0.622306	2.045011
H	4.238082	-1.883427	1.606990
H	7.613693	2.136056	-0.192106
H	7.407008	1.838988	1.543350
H	8.303336	0.685264	0.555716
H	0.756414	-2.217318	1.794362
H	-0.957191	-1.007271	3.083075
H	-0.727971	0.481676	2.019490
H	-1.387948	-0.882887	-0.086409
H	-2.867804	-2.628179	2.045201
H	-1.684622	-4.587514	1.166712
H	-1.096277	-3.589350	-0.287967
H	-1.218801	4.342838	1.680738
H	-2.231722	2.224650	2.511584
H	-0.959246	5.955301	-0.161268
H	-1.391007	5.507067	-1.825038
H	0.133273	4.954786	-1.124350
H	-2.133199	3.193164	-2.351548
H	-3.134316	1.072339	-1.527232

1 imaginary frequency
E = -7015.004226
G = -7014.696071
E_{TZ} = -7020.150127
G_{soln} = -7019.841973

TS-S_N2'

C	-1.918127	2.196306	-1.076830
C	-2.727142	1.879626	0.012318
C	-2.715405	2.645887	1.173039
C	-1.865931	3.746263	1.244009
C	-1.036585	4.084298	0.170629
C	-1.075714	3.296259	-0.986952
S	-3.849294	0.503035	-0.098154
O	-4.830440	0.670126	0.975038
C	-0.104235	5.263705	0.247790
C	-2.827869	-0.963066	0.253415
Br	-4.283622	-2.454818	0.457610
C	-1.854054	-1.270977	-0.773692
C	-0.783779	-2.080965	-0.521281
O	-4.298452	0.408536	-1.489239
C	1.078076	-0.880655	0.041105
Br	1.099059	0.403433	-1.379474
S	2.396827	-2.001574	-0.071379
O	2.446269	-2.569614	-1.425764
C	3.934828	-1.115783	0.148967
C	4.567807	-0.548751	-0.956859
C	5.714858	0.212072	-0.764702
C	6.237310	0.422746	0.517401
C	5.584657	-0.156844	1.609103
C	4.432753	-0.918827	1.433686
C	7.470111	1.267582	0.706464
O	2.268787	-2.917993	1.075986
C	0.762917	-0.375401	1.354421
C	0.155331	0.786434	1.652258
H	-0.131302	1.014953	2.674452
H	-0.039251	1.536740	0.892794
H	0.954067	-1.095267	2.151259
H	3.930481	-1.372356	2.282938
H	5.983330	-0.009577	2.609602
H	6.217477	0.651189	-1.623251
H	4.165941	-0.717305	-1.950873
H	7.257825	2.320583	0.490142
H	7.841551	1.203720	1.732530
H	8.272041	0.953113	0.030871
H	-0.211054	-2.493716	-1.345960
H	-0.712826	-2.621890	0.419061
H	-2.075974	-0.948734	-1.786271
H	-2.455286	-0.892720	1.274443
H	-3.367429	2.386620	2.000777
H	-1.849052	4.353215	2.145065
H	-0.431840	3.548384	-1.825756
H	-1.946294	1.588646	-1.975239
H	0.938732	4.934160	0.186675
H	-0.232741	5.812537	1.184051
H	-0.277364	5.954944	-0.583467

1 imaginary frequency
E = -7015.029254
G = -7014.717526
E_{TZ} = -7020.177751
G_{soln} = -7019.866023

1,5-Diene 12

C	-0.766948	-0.375325	2.089115

C	-0.740459	-1.293824	1.128637
C	-0.759112	-1.047775	-0.351350
C	0.253557	-1.930230	-1.108756
C	1.645296	-1.521535	-0.731217
C	2.371088	-2.153913	0.184251
S	3.919770	-1.518361	0.771052
C	3.846493	0.215901	0.385426
C	4.775868	0.760254	-0.494886
C	4.708191	2.119201	-0.782732
C	3.720014	2.929341	-0.212527
C	2.792970	2.349893	0.661715
C	2.852417	0.996898	0.971945
C	3.669515	4.399243	-0.531394
O	5.030215	-2.112075	0.022219
O	3.883747	-1.679677	2.227653
Br	-0.459355	0.826492	-0.803041
S	-2.434590	-1.506167	-1.014728
C	-3.577061	-0.394649	-0.245086
C	-3.922903	0.786728	-0.901525
C	-4.817397	1.651406	-0.287170
C	-5.366162	1.352400	0.967307
C	-5.001525	0.159320	1.597703
C	-4.106783	-0.722426	0.999573
C	-6.344635	2.299339	1.607271
O	-2.425325	-1.252929	-2.454662
O	-2.671418	-2.861754	-0.511811
H	-0.731177	-2.352998	1.381866
H	-0.772575	-0.675427	3.132155
H	-0.781782	0.688985	1.874885
H	2.072770	-3.071511	0.687245
H	2.015546	-0.604489	-1.183611
H	0.058551	-2.970406	-0.827614
H	0.093047	-1.818033	-2.185234
H	2.126029	0.550936	1.647484
H	2.014421	2.966331	1.102576
H	5.533951	0.125958	-0.943062
H	5.430012	2.558633	-1.466106
H	4.533402	4.916816	-0.100227
H	2.764030	4.861991	-0.131403
H	3.695807	4.567499	-1.612501
H	-3.504212	1.011710	-1.876956
H	-5.100952	2.573095	-0.788159
H	-3.834545	-1.654621	1.484083
H	-5.425778	-0.085533	2.567042
H	-7.274823	2.340839	1.030123
H	-6.590336	1.990067	2.625931
H	-5.939131	3.315395	1.641716

0 imaginary frequencies
E = -4443.177830
G = -4442.862675
E_{TZ} = -4445.918696
G_{soln} = -4445.603542

TS-Cope-Z

C	-0.356824	1.531475	0.274231
C	-1.331333	0.573336	0.576557
C	-1.731381	-0.311169	-0.436872

H	-1.887586	0.060590	-1.448748
S	-2.993916	-1.508193	-0.008679
H	-0.372198	1.993227	-0.711223
H	-1.481860	0.269818	1.609921
H	-0.002585	2.185483	1.068408
C	-0.190037	-1.441162	-0.776177
H	-0.545102	-2.048274	-1.604999
H	-0.166421	-1.962013	0.179549
C	0.799036	-0.486903	-1.037826
H	0.941766	-0.134683	-2.057464
C	1.211654	0.388927	-0.024967
Br	1.560902	-0.332474	1.725397
S	2.476210	1.609211	-0.478309
O	2.529744	2.614358	0.580592
O	2.159709	2.004803	-1.852379
C	4.000967	0.705703	-0.473514
C	4.792651	0.714466	0.670019
H	4.488455	1.286462	1.540581
C	5.979368	-0.012332	0.664284
H	6.610384	-0.011855	1.548473
C	6.372824	-0.740614	-0.461522
C	7.654945	-1.527981	-0.468467
H	8.316310	-1.184150	-1.270601
H	8.186691	-1.430771	0.480916
H	7.455658	-2.590370	-0.644101
C	5.552502	-0.726652	-1.598255
H	5.854038	-1.283901	-2.481205
C	4.365026	-0.009380	-1.613832
H	3.735004	0.007690	-2.498018
C	-4.510698	-0.586870	-0.105113
O	-3.018130	-2.527641	-1.060942
O	-2.773950	-1.902032	1.385318
C	-5.242642	-0.608610	-1.286666
C	-6.420550	0.130571	-1.358512
C	-6.865146	0.883520	-0.268960
C	-6.104640	0.883009	0.908957
C	-4.927848	0.153391	1.000648
H	-4.344488	0.146785	1.916548
H	-6.445679	1.460345	1.764316
C	-8.139737	1.680254	-0.341993
H	-7.949353	2.737790	-0.131574
H	-8.600975	1.603537	-1.329443
H	-8.860855	1.325345	0.401909
H	-7.004636	0.118347	-2.274339
H	-4.902672	-1.202897	-2.128842

1 imaginary frequency
E = -4443.124398
G = -4442.809643
E_{TZ} = -4445.867140
G_{soln} = -4445.552385

TS-Cope-*E*

C	3.735607	0.423466	-1.066238
C	3.491966	0.320215	0.302295
C	3.314027	1.450534	1.096412
C	3.357894	2.704571	0.496936
C	3.583233	2.838864	-0.877125

C	3.780183	1.685273	-1.645290
S	3.419057	-1.287967	1.050322
O	4.156535	-2.226574	0.199763
C	3.603164	4.195367	-1.527796
C	1.684399	-1.767509	0.994781
C	0.724541	-0.818094	1.395614
C	-0.617220	-1.234518	1.440060
O	3.788904	-1.158946	2.462086
C	1.300244	-2.129304	-0.804501
C	-0.055139	-2.518255	-0.797258
C	-1.064892	-1.640322	-0.350811
S	-1.184473	-0.026828	-1.225545
C	-2.350022	0.972333	-0.334770
C	-3.707847	0.879217	-0.642205
C	-4.604332	1.680202	0.050520
C	-4.164607	2.573607	1.036594
C	-2.796751	2.655803	1.311109
C	-1.880809	1.861311	0.628240
C	-5.157095	3.435871	1.767581
Br	-2.826892	-2.420302	-0.235563
O	0.131559	0.608253	-1.113009
O	-1.746335	-0.312304	-2.543528
H	0.950791	0.239429	1.296864
H	-1.371863	-0.509956	1.743593
H	-0.820743	-2.232691	1.822098
H	1.554101	-1.152392	-1.206143
H	2.012710	-2.910480	-1.062291
H	-0.291886	-3.578348	-0.779147
H	-0.816185	1.941696	0.828260
H	-2.442533	3.354747	2.063292
H	-5.662204	4.115628	1.073062
H	-5.929855	2.821917	2.241334
H	-4.670556	4.035524	2.540288
H	-5.664752	1.619583	-0.179560
H	-4.048015	0.199130	-1.416077
H	1.620319	-2.777686	1.401795
H	3.904577	-0.469944	-1.659638
H	3.974638	1.779362	-2.710223
H	4.415716	4.270329	-2.256320
H	3.723876	4.990086	-0.787457
H	2.664539	4.374110	-2.064527
H	3.223544	3.594341	1.105685
H	3.157068	1.347689	2.165994

1 imaginary frequency
E = -4443.119082
G = -4442.801915
E_{TZ} = -4445.863363
G_{soln} = -4445.546196

Carbanion 9a

C	-3.824517	-2.041012	0.852227
C	-3.311963	-2.664419	-0.284211
C	-3.892187	-2.482038	-1.534146
C	-4.994453	-1.640773	-1.647818
C	-5.496457	-0.961064	-0.534825
C	-4.908281	-1.184611	0.715823
S	-1.807713	-3.598307	-0.154278

O	-1.874237	-4.374728	1.092083
C	-6.627397	0.021833	-0.670347
C	-0.502529	-2.384775	0.053789
C	-0.446719	-1.734752	1.412549
C	-0.899626	-0.316937	1.597168
C	-1.530312	0.549189	0.807131
Br	-2.092068	0.336460	-0.965223
C	0.380616	-2.301541	-0.944722
C	1.680873	-1.535966	-1.014682
C	1.949532	-0.388201	-0.081432
C	1.755505	0.964041	-0.510561
C	1.105600	1.396621	-1.615649
S	3.056471	-0.661508	1.160582
O	3.125788	0.506988	2.064123
C	4.726168	-0.804389	0.490311
C	5.266617	-2.053028	0.198315
C	6.515633	-2.139224	-0.418025
C	7.236838	-0.991439	-0.748592
C	6.676475	0.257602	-0.444678
C	5.432887	0.355869	0.164161
C	8.589571	-1.077474	-1.406503
O	2.815295	-1.997156	1.757266
O	-1.617351	-4.306454	-1.425795
S	-2.022260	2.132313	1.490704
O	-1.573206	2.172575	2.884701
O	-3.440495	2.329191	1.185842
C	-1.092452	3.328746	0.571193
C	-1.635253	3.866175	-0.591647
C	-0.884661	4.786770	-1.315422
C	0.393111	5.166931	-0.891815
C	0.910873	4.606650	0.282695
C	0.178075	3.683120	1.017797
C	1.216092	6.134406	-1.699384
H	-2.629994	3.574892	-0.912609
H	-1.297758	5.220165	-2.222204
H	1.901856	4.896301	0.622135
H	0.583235	3.239918	1.922584
H	1.800585	6.793763	-1.051425
H	1.922106	5.591052	-2.338162
H	0.585845	6.749842	-2.346587
H	-3.474310	-2.983428	-2.401271
H	-5.457574	-1.490778	-2.619529
H	-5.302346	-0.673504	1.590271
H	-3.379227	-2.216978	1.827132
H	-7.363055	-0.105878	0.129447
H	-6.242814	1.045984	-0.599939
H	-7.136228	-0.083171	-1.632029
H	5.008119	1.327117	0.402293
H	7.229348	1.162067	-0.689262
H	6.937886	-3.116535	-0.639691
H	4.717662	-2.948583	0.472465
H	-0.689371	0.067515	2.595344
H	0.591928	-1.782678	1.758074
H	-1.016059	-2.342535	2.128780
H	0.182736	-2.922131	-1.818740
H	2.457905	-2.313783	-0.922202
H	0.993700	2.459307	-1.812187

H 0.606820 0.717705 -2.300858
H 2.164923 1.722824 0.158067
H 8.858541 -2.114077 -1.626192
H 8.607306 -0.514481 -2.345859
H 9.368064 -0.655141 -0.761384
H 1.776267 -1.182029 -2.053710
0 imaginary frequencies
E = -5378.073172
G = -5377.602917
E_{TZ} = -5381.000234
G_{soln} = -5380.529980

TS-cyc-*trans*
C 4.825226 -2.383907 -0.226815
C 4.458914 -1.180545 0.368430
C 5.292570 -0.064014 0.276929
C 6.493218 -0.162257 -0.413089
C 6.879586 -1.362716 -1.025650
C 6.032695 -2.466966 -0.920037
S 2.865354 -1.027560 1.185310
O 2.478699 -2.414251 1.513005
C 8.183146 -1.445911 -1.775734
C 1.720318 -0.382244 0.070620
C 1.867334 1.024496 -0.211238
C 1.190093 1.705002 -1.156772
C 1.409002 -1.317906 -1.077559
C 0.236446 -2.245020 -0.975068
C -0.600555 -2.373661 0.050665
S -1.838973 -3.651721 -0.098496
O -1.581820 -4.440055 -1.309852
C -0.590482 -1.661407 1.379850
C -0.274802 -0.183345 1.392704
C -1.059079 0.785894 0.847683
S -1.239612 2.346557 1.626129
O -2.676076 2.600775 1.794722
O 3.081164 -0.070049 2.286129
Br -2.260384 0.467257 -0.579568
C -0.648883 3.644579 0.557232
C -1.371497 3.983012 -0.586532
C -0.884585 4.984399 -1.416514
C 0.297374 5.671523 -1.107330
C 0.984186 5.329252 0.060215
C 0.519750 4.315415 0.894719
C 0.795893 6.766861 -2.012769
O -0.374106 2.349016 2.812850
C -3.358872 -2.767164 -0.352073
C -3.718639 -2.410477 -1.648816
C -4.844282 -1.618901 -1.839764
C -5.603596 -1.172105 -0.751198
C -5.230362 -1.564349 0.537427
C -4.108447 -2.359110 0.746502
C -6.781152 -0.259178 -0.962510
O -1.929988 -4.335917 1.197639
H -2.290682 3.459372 -0.828042
H -1.433488 5.248560 -2.317282
H 1.897087 5.859883 0.317938
H 1.058386 4.036304 1.794414

H	0.109000	7.620504	-2.006387
H	1.780660	7.122870	-1.699710
H	0.869849	6.417092	-3.047544
H	-3.120750	-2.746485	-2.490627
H	-5.137279	-1.335581	-2.847446
H	-5.821708	-1.236813	1.388264
H	-3.821219	-2.667859	1.747026
H	-6.460674	0.787941	-0.908625
H	-7.237069	-0.416756	-1.943793
H	-7.544258	-0.409358	-0.193974
H	5.005577	0.864771	0.761278
H	7.149314	0.702834	-0.476552
H	6.322925	-3.408299	-1.379906
H	4.179082	-3.250371	-0.125250
H	0.319278	0.149632	2.240198
H	0.133828	-2.174668	2.018530
H	-1.573788	-1.776636	1.855155
H	0.082860	-2.893351	-1.836301
H	2.274105	-1.962615	-1.314486
H	1.325764	2.774842	-1.281348
H	0.467607	1.224655	-1.812258
H	2.500751	1.592628	0.472213
H	8.178636	-0.776432	-2.642984
H	9.022453	-1.146207	-1.139309
H	8.371311	-2.461622	-2.133088
H	1.271462	-0.720906	-1.989268

1 imaginary frequency
E = -5378.068469
G = -5377.596738
E_{TZ} = -5380.995984
G_{soln} = -5380.524253

TS-cyc-*cis*

C	5.328745	-2.388075	0.604008
C	4.750583	-2.500877	-0.662195
C	3.368333	-2.593861	-0.816553
C	2.557277	-2.578461	0.312225
C	3.109614	-2.467370	1.587470
C	4.488735	-2.378136	1.726551
S	0.772704	-2.585443	0.128583
O	0.509174	-3.199250	-1.174147
C	6.820601	-2.258541	0.769015
C	0.437964	-0.876254	0.165906
Br	1.134244	0.023645	-1.344541
C	-0.177219	-0.287372	1.233761
C	0.113497	1.113904	1.713275
C	-0.151441	2.213814	0.718855
S	1.017595	3.556344	0.743276
C	2.448490	2.866276	-0.057134
C	2.606757	3.051079	-1.428780
C	3.627883	2.376097	-2.084858
C	4.471937	1.497294	-1.393415
C	4.305429	1.348550	-0.015102
C	3.302256	2.034979	0.661850
C	5.520210	0.713102	-2.135275
C	-1.153120	2.271773	-0.156964
C	-2.191388	1.196656	-0.342820

C	-2.377208	0.291001	0.852741
C	-2.980661	0.854437	2.047697
C	-3.233911	2.155091	2.296857
S	-3.056698	-1.248220	0.446569
O	-2.335969	-1.833369	-0.694660
C	-4.721925	-0.929230	-0.156451
C	-5.761220	-0.741947	0.752818
C	-7.028835	-0.409774	0.285527
C	-7.274615	-0.250740	-1.082519
C	-6.216776	-0.442173	-1.977513
C	-4.943861	-0.774999	-1.523435
C	-8.639991	0.141644	-1.583715
O	-3.226620	-2.045579	1.674259
O	1.364557	3.819926	2.145606
O	0.519170	4.652542	-0.095216
O	0.215428	-3.187325	1.346111
H	1.929262	3.705908	-1.968143
H	-8.891483	-0.388121	-2.507485
H	-9.413079	-0.074619	-0.841328
H	-8.679870	1.215143	-1.802189
H	-7.843520	-0.274893	0.992657
H	-5.578841	-0.875242	1.815149
H	-4.125900	-0.935755	-2.219286
H	-6.395165	-0.332768	-3.044654
H	2.459722	-2.458390	2.457941
H	4.925903	-2.299268	2.719029
H	2.918430	-2.684028	-1.799855
H	5.390808	-2.520721	-1.540579
H	7.085388	-1.277858	1.180770
H	7.209086	-3.013307	1.460763
H	7.337615	-2.374704	-0.187344
H	-3.214726	0.131339	2.830031
H	-3.032529	2.940561	1.573188
H	-3.634965	2.467579	3.256473
H	-3.134058	1.687767	-0.640908
H	-1.861393	0.595632	-1.204128
H	-1.212206	3.132102	-0.821368
H	1.166012	1.133467	2.020199
H	-0.474089	1.316963	2.614428
H	-0.445464	-0.991177	2.019064
H	3.190588	1.928578	1.736399
H	4.963952	0.681862	0.535751
H	3.762070	2.513482	-3.155073
H	6.099949	1.357862	-2.803493
H	6.210395	0.219316	-1.445333
H	5.049187	-0.060061	-2.753186

1 imaginary frequency
E = -5378.064767
G = -5377.590860
E_{TZ} = -5380.990905
G_{soln} = -5380.516998

Trimer 6

C	2.597146	3.263080	-0.660211
C	2.593399	2.493641	0.502890
C	3.598602	1.572638	0.768423
C	4.626845	1.415769	-0.158894

C	4.646547	2.154595	-1.343616
C	3.626041	3.089688	-1.574594
S	1.170217	2.571764	1.563899
O	0.639791	3.936843	1.516567
C	5.724409	1.944131	-2.372214
C	0.033461	1.484490	0.731346
C	-0.905422	2.027242	-0.036839
C	-1.841969	1.199852	-0.865406
C	-1.902507	-0.272676	-0.456977
C	-0.497140	-0.840969	-0.099489
C	0.252478	0.013057	0.942158
S	-2.939074	-0.451079	1.087456
O	-2.523268	0.545151	2.078142
C	-2.571033	-1.169617	-1.470215
C	-3.246870	-0.755448	-2.539050
C	0.305647	-1.104615	-1.393910
S	1.188993	-2.709881	-1.326088
O	0.128074	-3.697884	-1.110933
C	-4.601471	-0.047606	0.599773
C	-5.445087	-1.056166	0.134848
C	-6.745478	-0.728293	-0.221552
C	-7.212105	0.589988	-0.123050
C	-6.346668	1.577123	0.355384
C	-5.040550	1.267042	0.725069
C	-8.624331	0.921501	-0.523287
O	-2.890965	-1.877226	1.433071
O	1.517909	1.961291	2.850145
Br	1.546495	0.296131	-1.903143
O	2.048001	-2.800979	-2.502962
C	2.191755	-2.619239	0.126201
C	3.430094	-1.980342	0.054741
C	4.168747	-1.839178	1.222829
C	3.687854	-2.317799	2.448894
C	2.448147	-2.964325	2.482631
C	1.691324	-3.119380	1.326512
C	4.486424	-2.113451	3.707072
H	0.731299	-3.626003	1.350795
H	2.071157	-3.351103	3.424941
H	5.139822	-1.351919	1.187182
H	3.801549	-1.604525	-0.893585
H	4.147102	-2.777807	4.505360
H	5.551294	-2.291826	3.532113
H	4.379510	-1.081548	4.061251
H	1.799323	3.976338	-0.845725
H	3.640605	3.680681	-2.486627
H	5.422683	0.701848	0.037089
H	3.574187	0.988703	1.684006
H	6.558101	1.367680	-1.963896
H	5.326366	1.397140	-3.234581
H	6.109826	2.899401	-2.740999
H	-5.087331	-2.078670	0.066010
H	-7.414547	-1.505977	-0.580244
H	-6.700387	2.599851	0.449704
H	-4.377092	2.030140	1.120555
H	-0.682659	-1.829838	0.338700
H	-0.084930	-0.251914	1.949329
H	1.324556	-0.215079	0.903850

H -0.985675 3.108266 -0.117318
H -2.843350 1.644807 -0.870320
H -3.699881 -1.474866 -3.214608
H -3.382969 0.295190 -2.780940
H -2.471703 -2.236378 -1.268696
H -9.340955 0.319982 0.045272
H -8.849386 1.976690 -0.351073
H -8.787730 0.704579 -1.584258
H -1.494984 1.247372 -1.908836
H -0.349366 -1.244657 -2.257773
0 imaginary frequencies
E = -5378.630798
G = -5378.139461
E_{TZ} = -5381.546364
G_{soln} = -5381.055027

Epimer of trimer 6 resulting from protonation of the opposite face of carbanion 10a

C -2.730239 -2.761535 -0.381193
C -2.797710 -2.308643 0.937709
C -3.823662 -1.476311 1.369094
C -4.803451 -1.092704 0.455161
C -4.748904 -1.508307 -0.878165
C -3.702235 -2.350202 -1.282387
S -1.451748 -2.694203 2.038327
O -1.115785 -4.113349 1.903978
C -5.770551 -1.042162 -1.879623
C -0.158884 -1.721901 1.305964
C 0.811202 -2.350121 0.644237
C 1.867626 -1.639997 -0.145392
C 1.687287 -0.112261 -0.242299
C 0.240134 0.374490 0.069873
C -0.302698 -0.227513 1.376826
S 2.730619 0.653859 1.123762
O 2.519912 -0.119261 2.354498
C 2.197517 0.498589 -1.525544
C 3.158571 -0.024806 -2.281633
C -0.828498 0.116255 -1.028886
S -1.425493 1.666757 -1.808283
O -0.276792 2.461056 -2.244928
C 4.434072 0.428041 0.665906
C 5.075095 1.401008 -0.098301
C 6.415138 1.225815 -0.419313
C 7.117882 0.092621 0.008591
C 6.452185 -0.859443 0.787357
C 5.112824 -0.698394 1.125598
C 8.560037 -0.104548 -0.372340
O 2.437976 2.092945 1.109121
O -1.769358 -2.141058 3.357318
Br -0.425670 -1.128039 -2.456884
O -2.466578 1.294624 -2.762160
C -2.181168 2.473879 -0.421120
C -3.469857 2.093697 -0.050048
C -4.042048 2.679558 1.072427
C -3.347193 3.640537 1.817065
C -2.058971 4.008312 1.412566
C -1.465856 3.430924 0.295666
C -3.986835 4.291181 3.012795

H	-0.466951	3.719334	-0.018617
H	-1.512950	4.755769	1.981256
H	-5.045984	2.393072	1.374405
H	-4.015588	1.359694	-0.636266
H	-3.238366	4.564909	3.760965
H	-4.507614	5.208212	2.714049
H	-4.721849	3.629011	3.477633
H	-1.912240	-3.400928	-0.702157
H	-3.648187	-2.676113	-2.317712
H	-5.614267	-0.445917	0.780314
H	-3.847801	-1.132260	2.398556
H	-6.551269	-0.444331	-1.402933
H	-5.295079	-0.431273	-2.654807
H	-6.244935	-1.891606	-2.381405
H	4.533040	2.282918	-0.424130
H	6.927444	1.981769	-1.007883
H	6.992825	-1.731532	1.144551
H	4.607742	-1.422220	1.757471
H	0.317623	1.460061	0.194383
H	0.234080	0.155934	2.247722
H	-1.351117	0.069017	1.496940
H	0.835771	-3.437389	0.628478
H	2.853225	-1.894632	0.263922
H	3.495667	0.488305	-3.177337
H	3.644617	-0.969842	-2.048611
H	1.751982	1.454408	-1.793170
H	9.060991	0.853214	-0.535404
H	9.101909	-0.654909	0.401548
H	8.635117	-0.680518	-1.301947
H	1.862062	-2.059407	-1.155717
H	-1.735342	-0.299990	-0.580201

0 imaginary frequencies
E = -5378.621412
G = -5378.130382
E_{TZ} = -5381.538231
G_{soln} = -5381.047202

-Bromovinyl sulfone 2

C	-3.156289	0.461804	-1.488618
C	-2.014303	1.019017	-0.922483
C	-1.444391	0.390585	0.182328
C	-1.976285	-0.772651	0.732319
C	-3.118748	-1.318544	0.154023
C	-3.703340	-0.703718	-0.952022
S	0.031137	1.081909	0.889349
O	0.169881	0.574249	2.251702
H	-4.594606	-1.134171	-1.398158
O	0.042279	2.522695	0.636477
C	1.338362	0.374023	-0.106114
C	2.111801	1.149884	-0.860681
C	3.253767	0.712819	-1.711723
Br	1.496581	-1.495107	0.058273
H	1.877679	2.213318	-0.838037
H	3.099202	1.054405	-2.740522
H	4.176866	1.182195	-1.354247
H	3.382300	-0.370628	-1.709061
H	-1.509843	-1.228193	1.599837

H -3.553118 -2.221942 0.569594
H -3.620588 0.938672 -2.345686
H -1.577153 1.929670 -1.320483
0 imaginary frequencies
E = -3468.475500
G = -3468.349875
E_{TZ} = -3471.033507
G_{soln} = -3470.907882

Bromovinyl sulfone anion 2a/2a' ($PhSO_2$ analogue of 1a/1a')
C -3.201453 0.317386 -1.251877
C -2.100218 0.946538 -0.677665
C -1.373948 0.289058 0.314094
C -1.727161 -0.995671 0.724423
C -2.828091 -1.620273 0.142479
C -3.564824 -0.966058 -0.843882
S 0.122119 1.049087 0.959876
O 0.267481 0.494590 2.314531
O -0.082551 2.504009 0.816206
C 1.447079 0.611505 -0.026081
Br 1.799710 -1.284522 0.038764
C 1.553264 1.236260 -1.315158
C 2.121248 0.771297 -2.446245
H -4.423753 -1.455372 -1.293727
H 1.157575 2.253458 -1.320095
H -1.146427 -1.485426 1.499183
H -3.113319 -2.618451 0.461912
H -3.778040 0.829542 -2.016624
H -1.807767 1.947820 -0.979401
H 2.537287 -0.229589 -2.506122
H 2.195874 1.401846 -3.326300
0 imaginary frequencies
E = -3467.959038
G = -3467.844858
E_{TZ} = -3470.531546
G_{soln} = -3470.417366

TS-S_N2'-Ph (S_N2' TS for reaction of phenyl sulfone 2)
C 4.658026 -0.455548 1.525441
C 4.206373 -0.692346 0.228577
C 4.838674 -0.121435 -0.874082
C 5.951969 0.690075 -0.670352
C 6.417639 0.928635 0.622007
C 5.772925 0.355324 1.718030
S 2.715527 -1.655061 -0.013739
O 2.628378 -2.591816 1.120471
H 7.286926 1.560978 0.775968
C 1.341231 -0.603391 0.102355
C 0.977907 -0.148300 1.422744
C 0.320086 0.979925 1.741904
Br 1.330248 0.715336 -1.286667
O 2.805668 -2.201562 -1.374690
C -0.434397 -1.885168 -0.535923
C -1.538152 -1.127904 -0.808804
C -2.554775 -0.891667 0.194333
Br -3.942501 -2.452728 0.330960
S -3.634366 0.531328 -0.156241

O	-4.014728	0.467421	-1.569211
C	-2.585751	1.958287	0.055288
C	-1.765884	2.365306	-0.993181
C	-0.989121	3.508810	-0.828184
C	-1.044916	4.225355	0.366653
C	-1.875743	3.805990	1.405536
C	-2.656403	2.663723	1.253904
H	-0.437536	5.117103	0.488902
O	-4.670279	0.614026	0.874098
H	0.004180	1.165614	2.764078
H	0.111518	1.745020	1.001130
H	1.181563	-0.883593	2.202123
H	4.148911	-0.916290	2.366639
H	6.139813	0.538122	2.723473
H	6.457585	1.134908	-1.522130
H	4.464162	-0.325893	-1.871870
H	0.182432	-2.254245	-1.349357
H	-0.365659	-2.439848	0.396663
H	-1.746229	-0.797806	-1.821653
H	-2.214765	-0.824587	1.226914
H	-3.319435	2.324898	2.043015
H	-1.919155	4.370069	2.331851
H	-0.338422	3.838157	-1.632111
H	-1.736022	1.797273	-1.917040

1 imaginary frequency
E = -6936.433811
G = -6936.173755
E_{TZ} = -6941.561982
G_{soln} = -6941.301927

1,5-Diene 12-Ph ($PhSO_2$ analogue of 12)

C	-0.762068	-0.299552	2.154424
C	-0.789085	-1.140463	1.125358
C	-0.872240	-0.779939	-0.328950
C	0.101291	-1.603893	-1.196683
C	1.510199	-1.221437	-0.855568
C	2.261639	-1.895978	0.007789
Br	-0.583159	1.123010	-0.647881
H	-0.722766	-0.680400	3.170044
H	-0.776013	0.778260	2.024510
H	-0.778801	-2.216368	1.294214
H	1.872135	-0.289705	-1.283899
H	1.973213	-2.830768	0.484265
H	-0.082313	-2.661985	-0.982917
H	-0.108254	-1.414522	-2.253675
S	-2.577612	-1.180844	-0.951440
O	-2.797784	-2.574627	-0.557968
O	-2.637068	-0.800915	-2.361537
S	3.835034	-1.295028	0.564024
O	4.913251	-1.852503	-0.255596
O	3.855954	-1.522504	2.011795
C	-3.678933	-0.139285	-0.029583
C	-4.143765	-0.583725	1.206541
H	-3.679705	1.398830	-1.538264
C	-4.049591	1.092678	-0.565211
H	-5.379544	-0.089270	2.891637
C	-5.002714	0.239190	1.928593

C	-5.379379	1.477888	1.411674
C	-4.909425	1.902792	0.169197
H	-6.050271	2.115594	1.979058
H	-5.216112	2.863861	-0.230410
H	-3.848485	-1.556866	1.585158
C	3.751658	0.459244	0.262898
C	4.647911	1.035921	-0.629298
C	2.782480	1.208958	0.929719
H	5.266849	2.879402	-1.545318
C	4.573756	2.409462	-0.855073
C	2.711759	2.575181	0.685473
C	3.608185	3.172495	-0.202914
H	2.086766	0.727884	1.613219
H	5.383568	0.417787	-1.133708
H	1.957062	3.173605	1.186069
H	3.549603	4.240417	-0.389356

0 imaginary frequencies
E = -4364.581348
G = -4364.315521
E_{TZ} = -4367.301636
G_{soln} = -4367.035809

TS-Cope-*Z*-Ph ($PhSO_2$ analogue of TS-Cope-*Z*)

C	4.943381	0.290225	-1.079523
C	4.557921	-0.199703	0.166007
C	5.249530	0.113325	1.332861
C	6.361085	0.947191	1.244559
C	6.760783	1.448607	0.006946
C	6.057141	1.120751	-1.152093
S	3.118057	-1.242446	0.271630
O	2.928835	-1.905971	-1.020535
H	7.629113	2.097122	-0.056118
C	1.768094	-0.086451	0.493188
C	1.302192	0.568823	-0.656722
C	0.258229	1.490580	-0.517102
O	3.227475	-2.040246	1.495287
C	0.315815	-1.252545	1.050294
C	-0.741948	-0.342557	1.150491
C	-1.219628	0.303982	0.002949
S	-2.572531	1.488280	0.246897
C	-4.025740	0.482218	0.425838
C	-4.804834	0.215513	-0.697007
C	-5.931959	-0.586936	-0.545709
C	-6.258345	-1.103985	0.706989
C	-5.466762	-0.822321	1.820444
C	-4.336098	-0.023472	1.685965
H	-7.139328	-1.728489	0.818226
Br	-1.512107	-0.742460	-1.586104
O	-2.704255	2.278381	-0.974539
O	-2.290439	2.147266	1.523468
H	1.894114	0.471677	1.420131
H	0.239608	2.121083	0.369988
H	1.476126	0.098285	-1.621553
H	-0.144483	1.963861	-1.410146
H	0.715762	-1.673434	1.969240
H	0.332528	-1.935979	0.202938
H	-0.911503	0.174134	2.093060

H -4.535623 0.635976 -1.660340
H -6.555413 -0.805945 -1.406408
H -5.731430 -1.221522 2.794079
H -3.712316 0.214400 2.542138
H 4.387717 0.015892 -1.970999
H 6.378520 1.507949 -2.113524
H 6.916804 1.200167 2.141696
H 4.929057 -0.297328 2.285098
1 imaginary frequency
E = -4364.528190
G = -4364.262800
E_{TZ} = -4367.250206
G_{soln} = -4366.984817

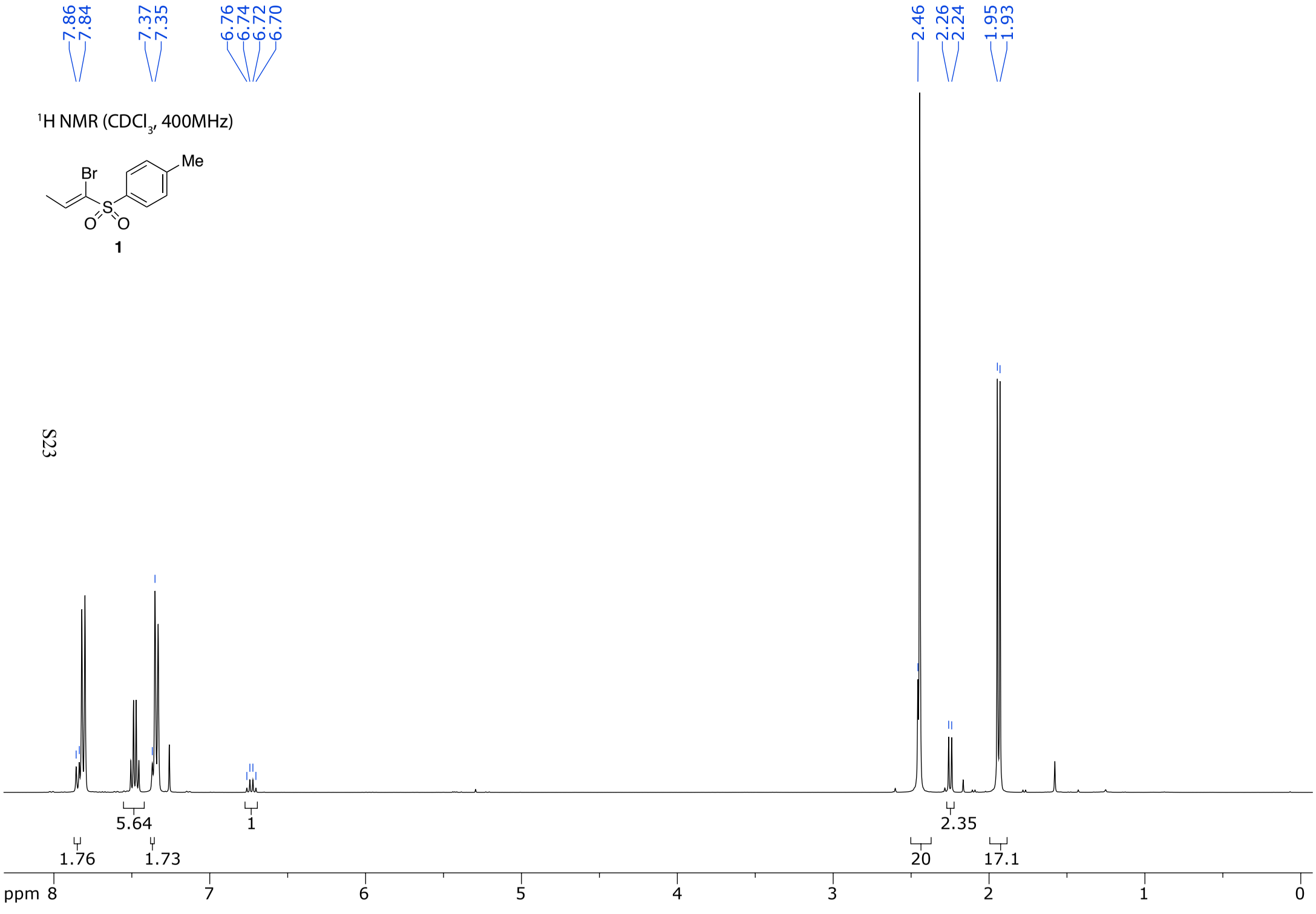
α-Bromovinyl sulfone 3-*p*-Cl (*p*-Cl-C_6H_4 analogue of 1)
C 3.251450 -0.111518 0.223912
C 2.653045 0.819802 1.069086
C 1.365298 1.255649 0.781436
C 0.716241 0.752679 -0.342803
C 1.316989 -0.175615 -1.188411
C 2.604515 -0.614366 -0.901298
S -0.939823 1.294864 -0.690538
C -1.951908 0.183180 0.277401
Br -1.840933 -1.616886 -0.263026
O -1.209517 1.047797 -2.103856
O -1.118115 2.631811 -0.126230
C -2.712908 0.646723 1.265404
C -3.629672 -0.147226 2.130357
Cl 4.866298 -0.661988 0.583953
H -2.652875 1.719161 1.445762
H -3.354309 -0.009294 3.181354
H -4.653610 0.224742 2.015763
H -3.608176 -1.211313 1.890841
H 0.791565 -0.540577 -2.064860
H 3.099871 -1.333973 -1.543641
H 3.186214 1.199160 1.933845
H 0.876830 1.986363 1.418455
0 imaginary frequencies
E = -3928.044964
G = -3927.931058
E_{TZ} = -3930.633772
G_{soln} = -3930.519867

Bromovinyl sulfone anion 3a/3a'-*p*-Cl (*p*-Cl-C_6H_4 analogue of 2a/2a')
C 3.152873 -0.153075 0.078734
C 2.628598 0.807118 0.938934
C 1.340925 1.280382 0.709197
C 0.606970 0.803856 -0.375264
C 1.142828 -0.161716 -1.225550
C 2.428585 -0.645473 -1.001685
S -1.102426 1.323847 -0.582416
C -2.112793 0.285068 0.318405
C -2.129447 0.444990 1.746763
C -2.377636 -0.470632 2.704430
O -1.353754 1.191926 -2.024961
O -1.176547 2.666636 0.024848
Br -2.055937 -1.527218 -0.339031

Cl 4.774019 -0.754567 0.361607
H -1.970598 1.480025 2.053867
H 0.558109 -0.519955 -2.066372
H 2.864101 -1.391734 -1.657835
H 3.217538 1.177936 1.771176
H 0.909380 2.033170 1.361688
H -2.549477 -1.515238 2.464356
H -2.433762 -0.177090 3.747651
0 imaginary frequencies
E = -3927.531143
G = -3927.429647
E_{TZ} = -3930.133993
G_{soln} = -3930.032497

TS-S_N2'-*p*-Cl (S_N2' TS for reaction of *p*-chlorophenyl sulfone 1-*p*-Cl)
C 2.814850 2.557362 -1.151200
C 2.868673 1.778844 0.001172
C 2.075029 2.054809 1.110308
C 1.194325 3.129683 1.062491
C 1.137659 3.901136 -0.094623
C 1.936251 3.633890 -1.203215
S 4.045948 0.440624 0.077694
O 5.002398 0.665172 -1.006042
C 3.071667 -1.054335 -0.279951
Br 4.581570 -2.484632 -0.511931
C 2.118201 -1.402897 0.751747
C 1.067415 -2.238262 0.494655
O 4.512999 0.352100 1.462130
C -0.821342 -1.087065 -0.028322
Br -0.878223 0.168325 1.416538
S -2.095541 -2.256982 0.079340
O -2.110944 -2.850552 1.422384
C -3.668226 -1.417908 -0.098813
C -4.198703 -1.225741 -1.372169
C -5.380500 -0.508078 -1.523886
C -5.999066 0.012186 -0.391014
C -5.473311 -0.168529 0.884524
C -4.292796 -0.889789 1.029141
O -1.960030 -3.143231 -1.089105
C -0.542581 -0.546935 -1.337617
C -0.000886 0.649412 -1.622249
Cl -7.486509 0.914877 -0.574577
Cl 0.029652 5.249225 -0.155942
H 0.264890 0.908520 -2.642594
H 0.153374 1.399148 -0.853252
H -0.701303 -1.264549 -2.143395
H -3.698274 -1.648789 -2.237634
H -5.816261 -0.356302 -2.505571
H -5.979929 0.245449 1.749636
H -3.863307 -1.054488 2.011869
H 0.518593 -2.684372 1.318237
H 1.005997 -2.767670 -0.452955
H 2.343069 -1.094753 1.768039
H 2.687385 -0.984662 -1.296911
H 3.458199 2.328333 -1.994191
H 1.874076 4.257116 -2.088495
H 0.559408 3.364745 1.909672

H 2.141689 1.440366 2.001806
1 imaginary frequency
E = -7855.575849
G = -7855.339199
E_{TZ} = -7860.765040
G_{soln} = -7860.528390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1.93
^{1}H NMR ($CDCl_3$, 400MHz)
Br
Me
S
O
O
1
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1.76
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20
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7
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5
4
3
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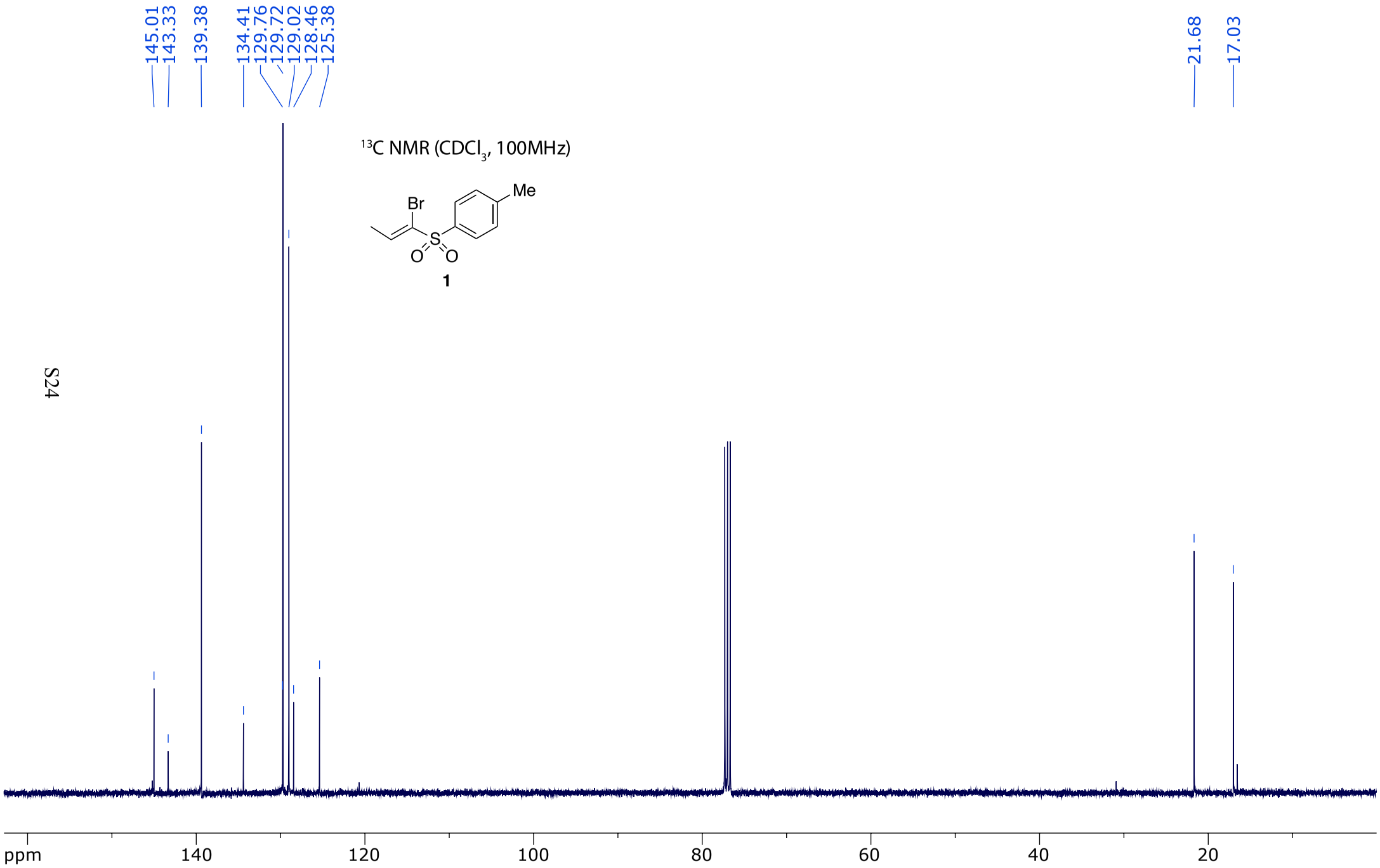
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128.46
125.38
21.68
17.03
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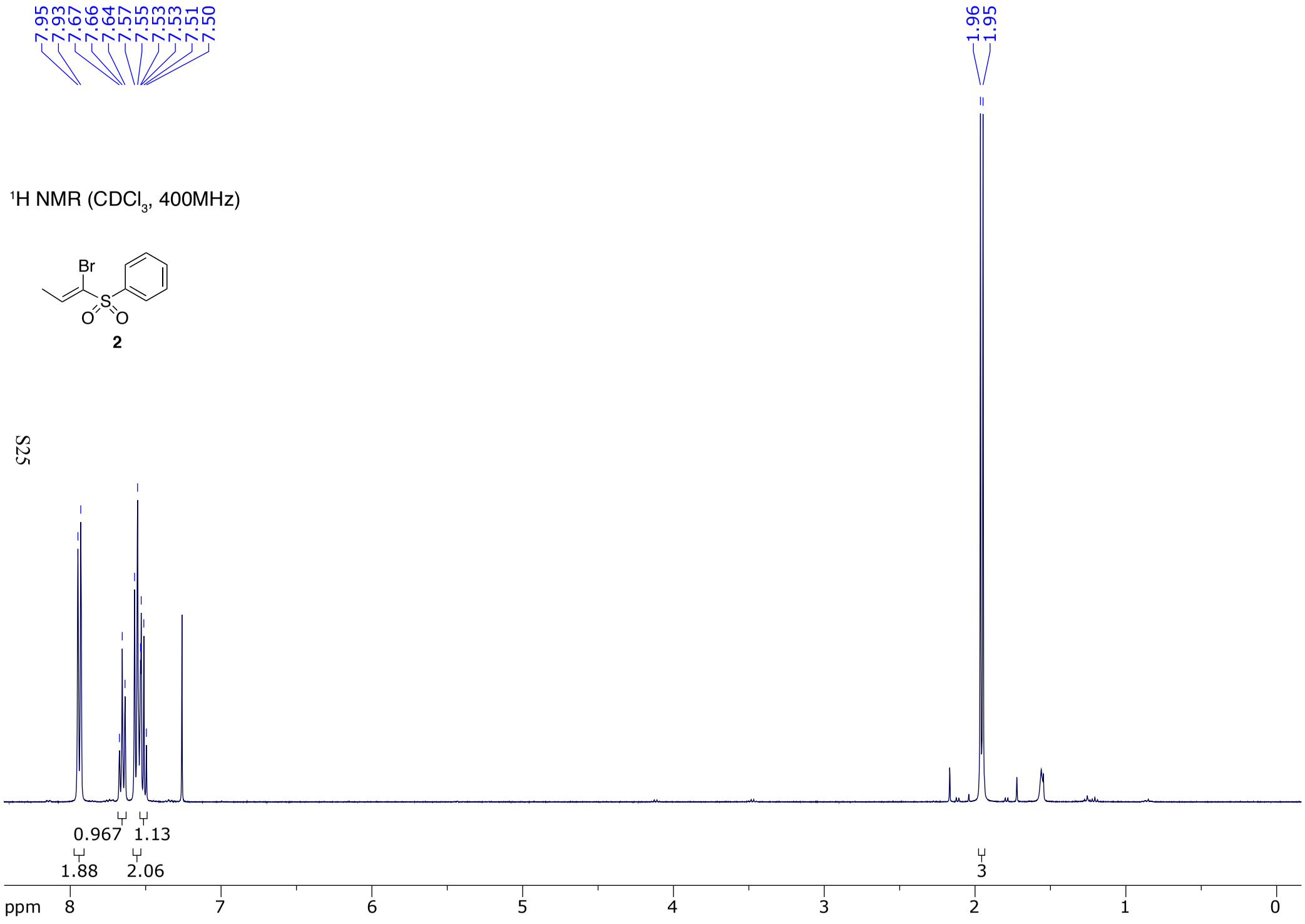
Br
Me
S
O
O
1
ppm
140
120
100
80
60
40
20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7.93
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7.57
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7.51
7.50
1.96
1.95
^{1}H NMR ($CDCl_3$, 400MHz)
Br
S
O
O
2
S25
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1.13
1.88
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ppm
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3
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1
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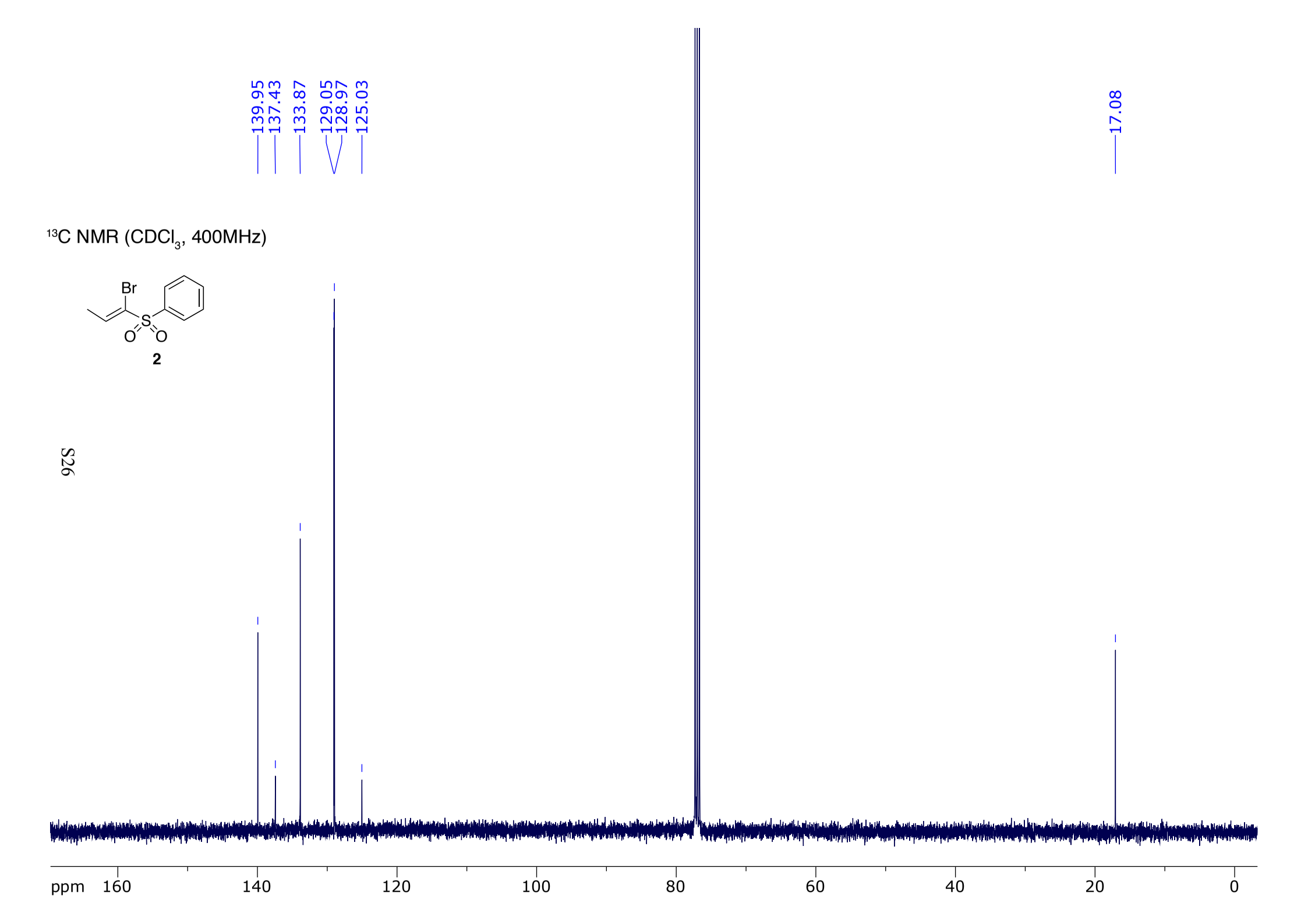
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20
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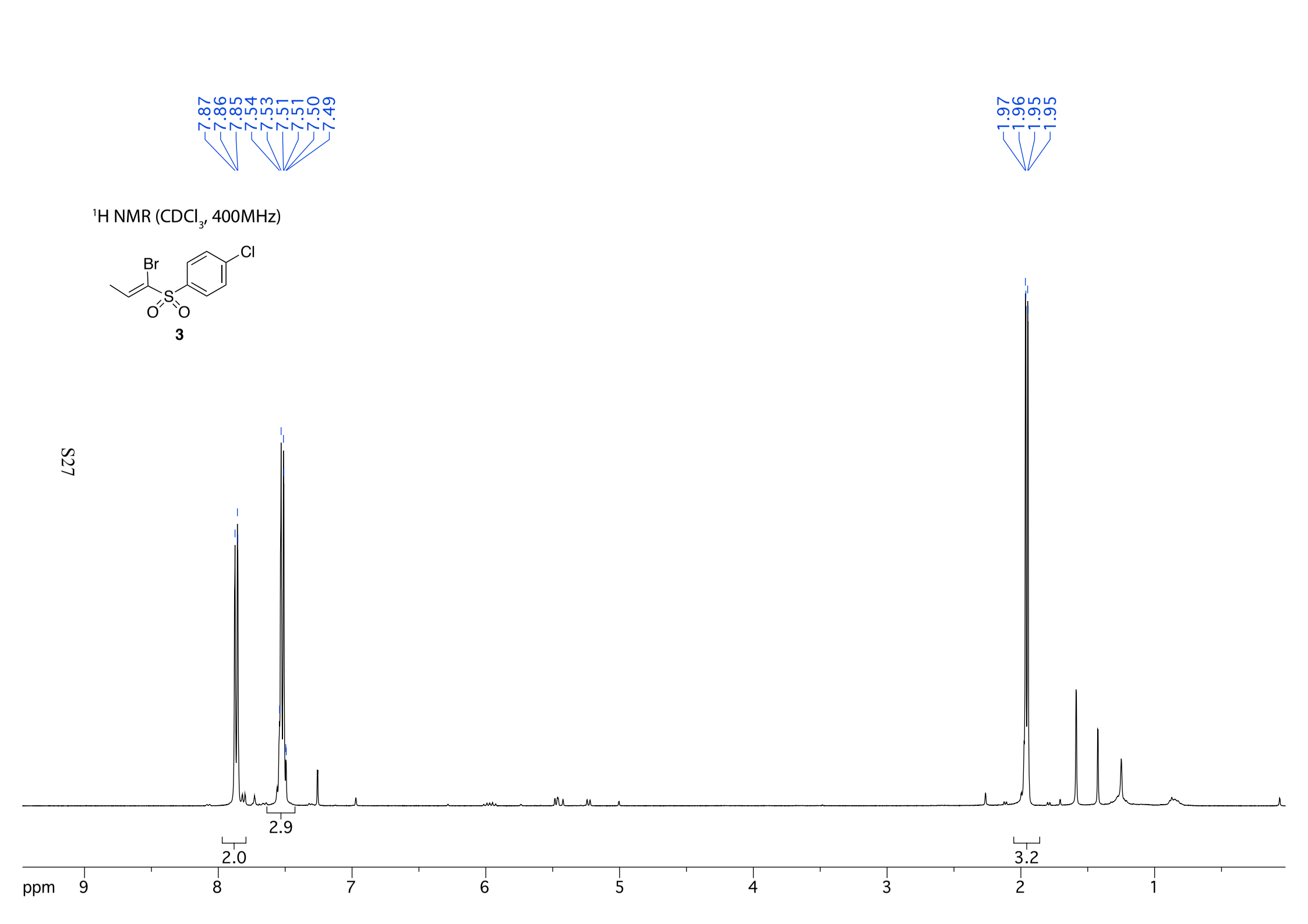
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7.51
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1.97
1.96
1.95
1.95
^{1}H NMR ($CDCl_3$, 400MHz)
Br
Cl
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O
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ppm
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8
7
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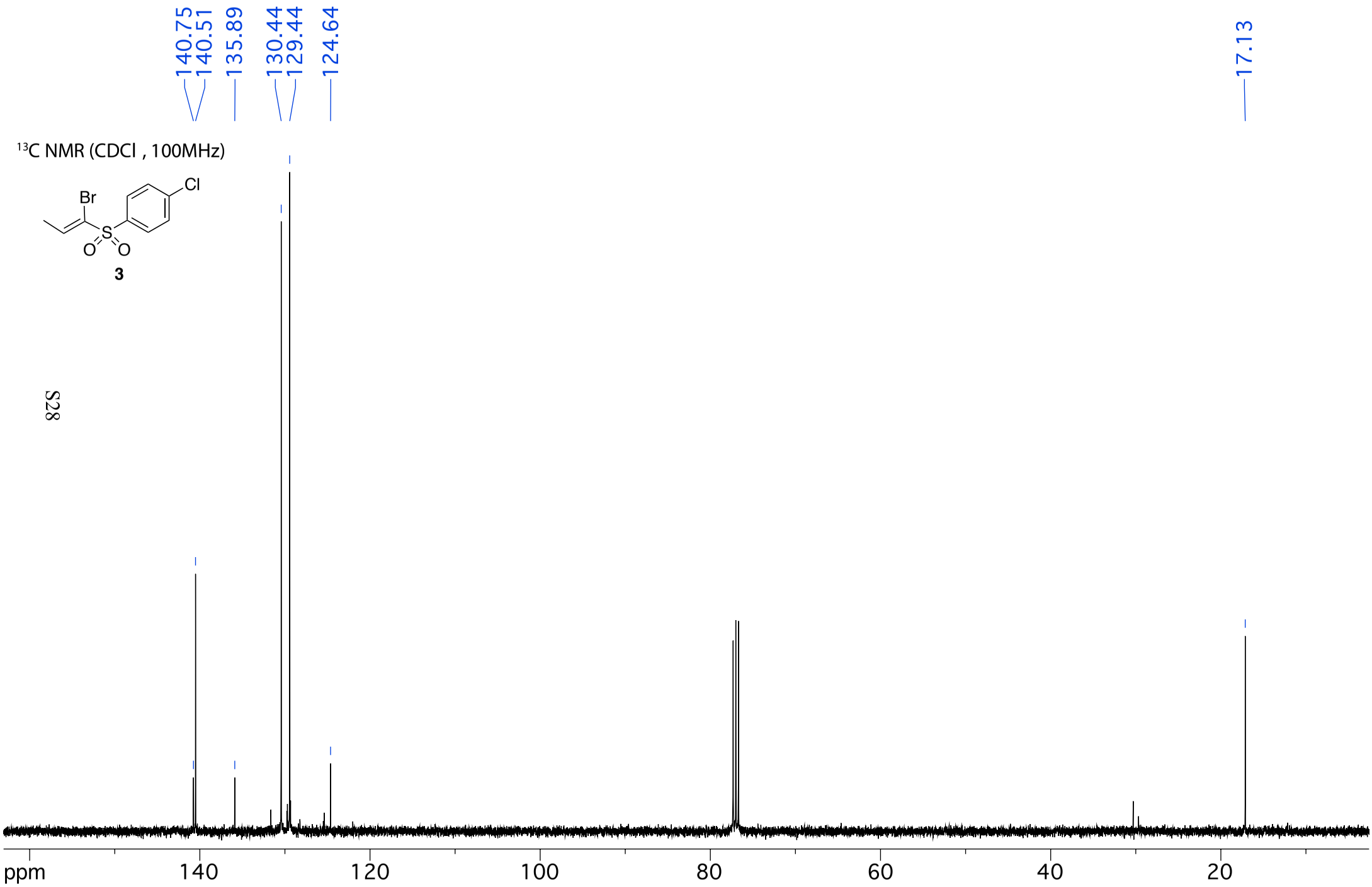
5
4
3
2
1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140.51
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17.13
13C NMR (CDCl , 100MHz)
Br
Cl
S
O
O
3
ppm
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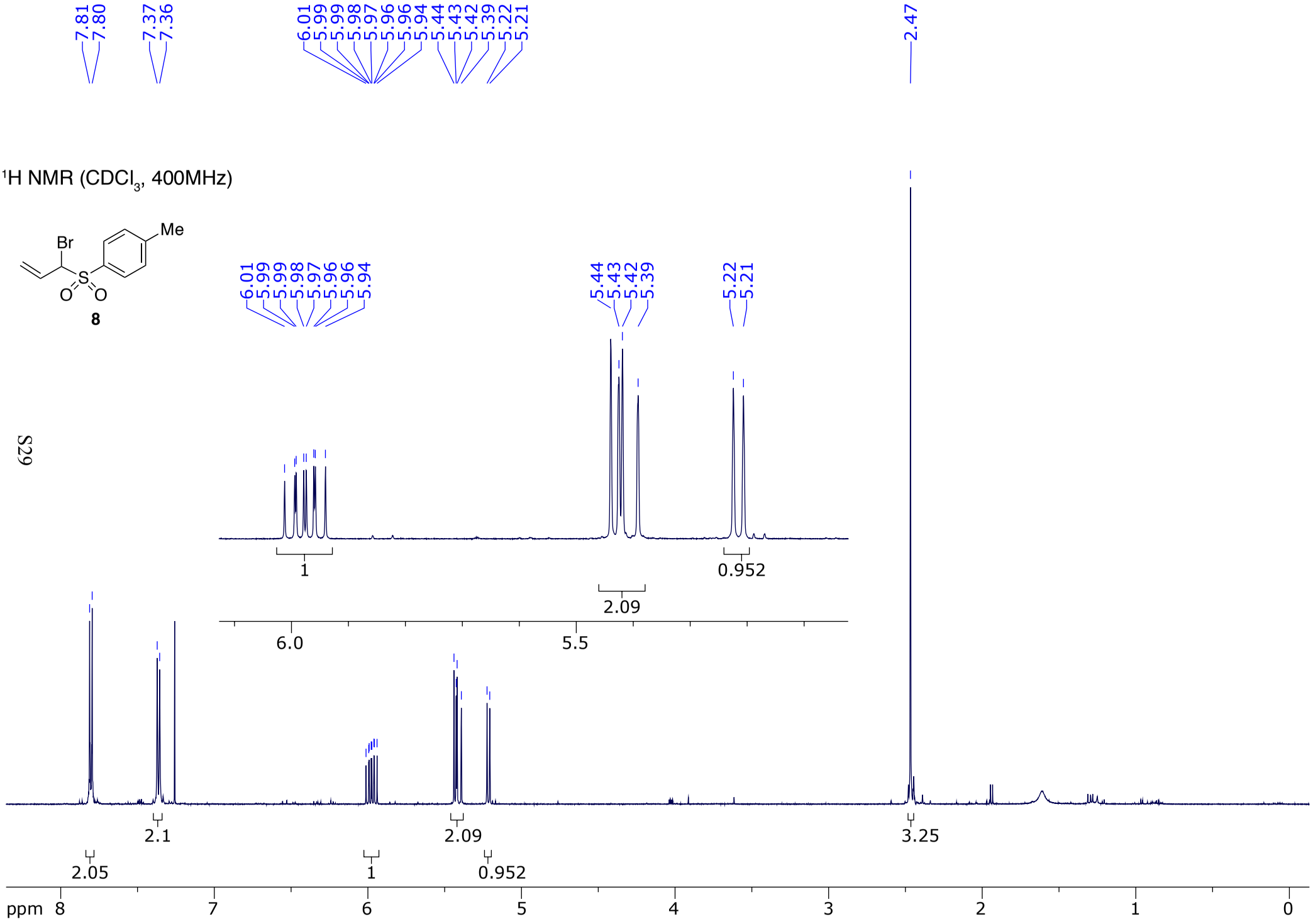
100
80
60
40
20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5.96
5.96
5.94
5.44
5.43
5.42
5.39
5.22
5.21
2.47
^{1}H NMR ($CDCl_3$, 400MHz)
Br
Me
S
O
O
8
S29
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2.09
6.0
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1
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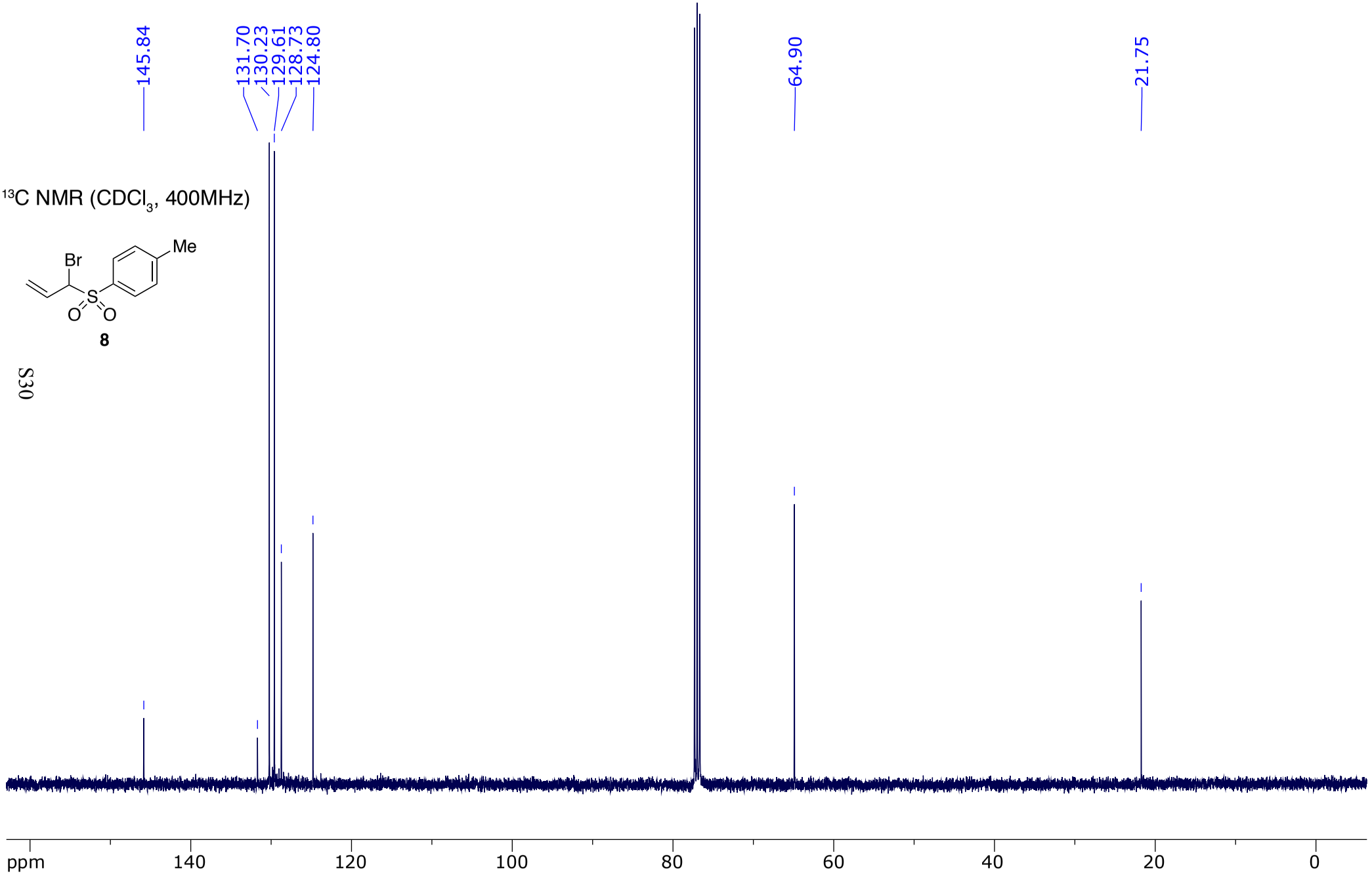
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Br
Me
S
O
O
8
ppm
140
120
100
80
60
40
20
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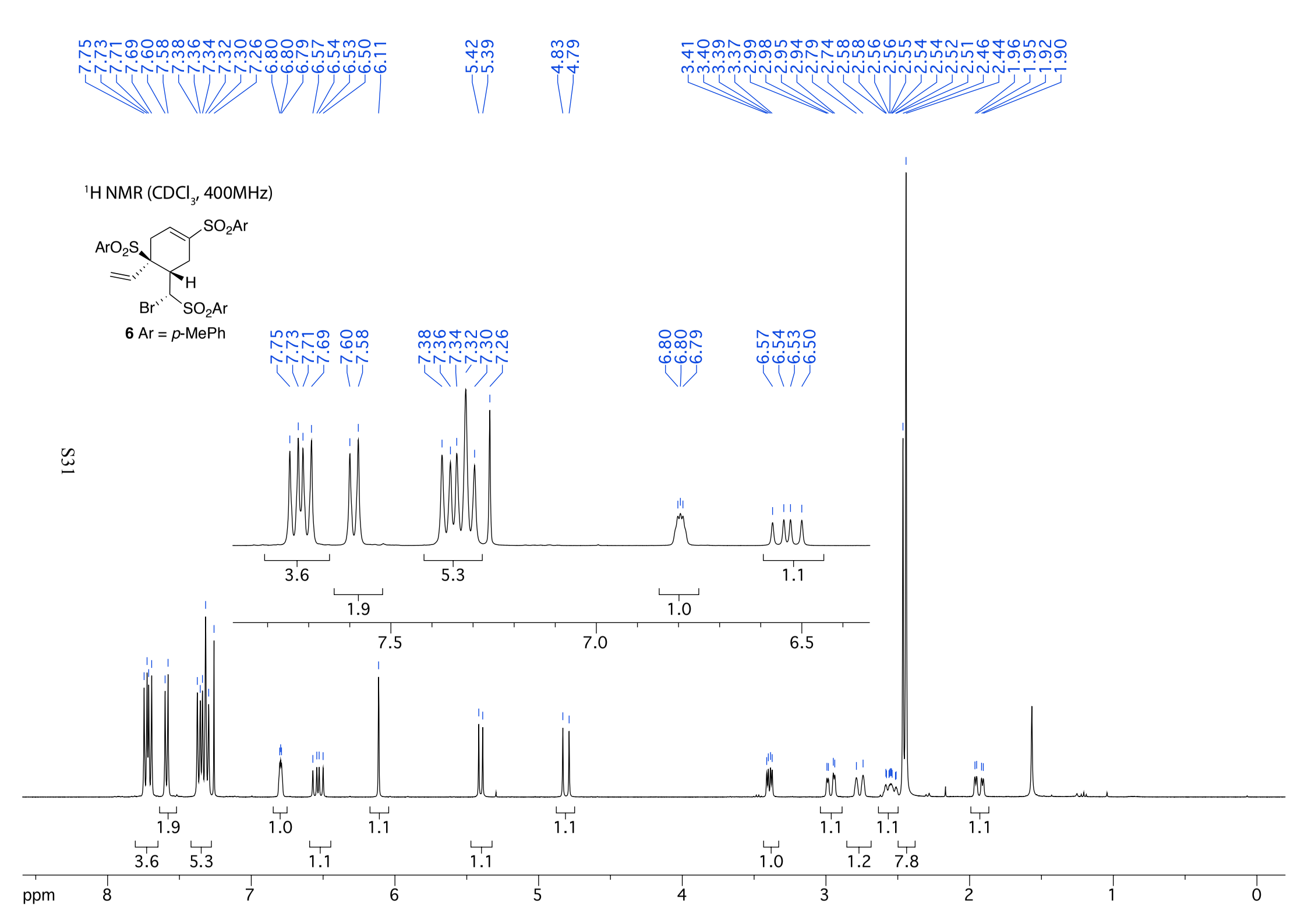
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7.30
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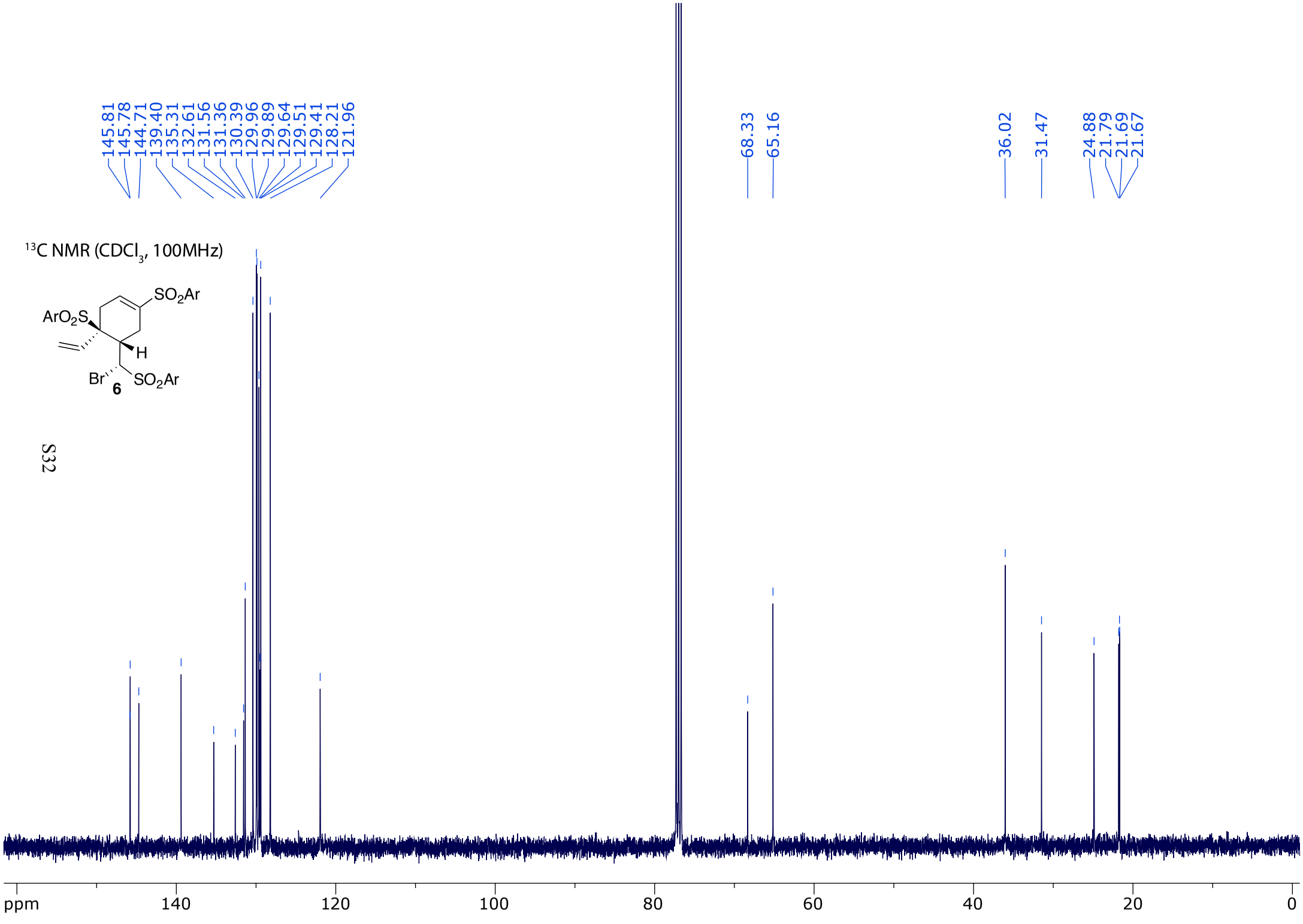
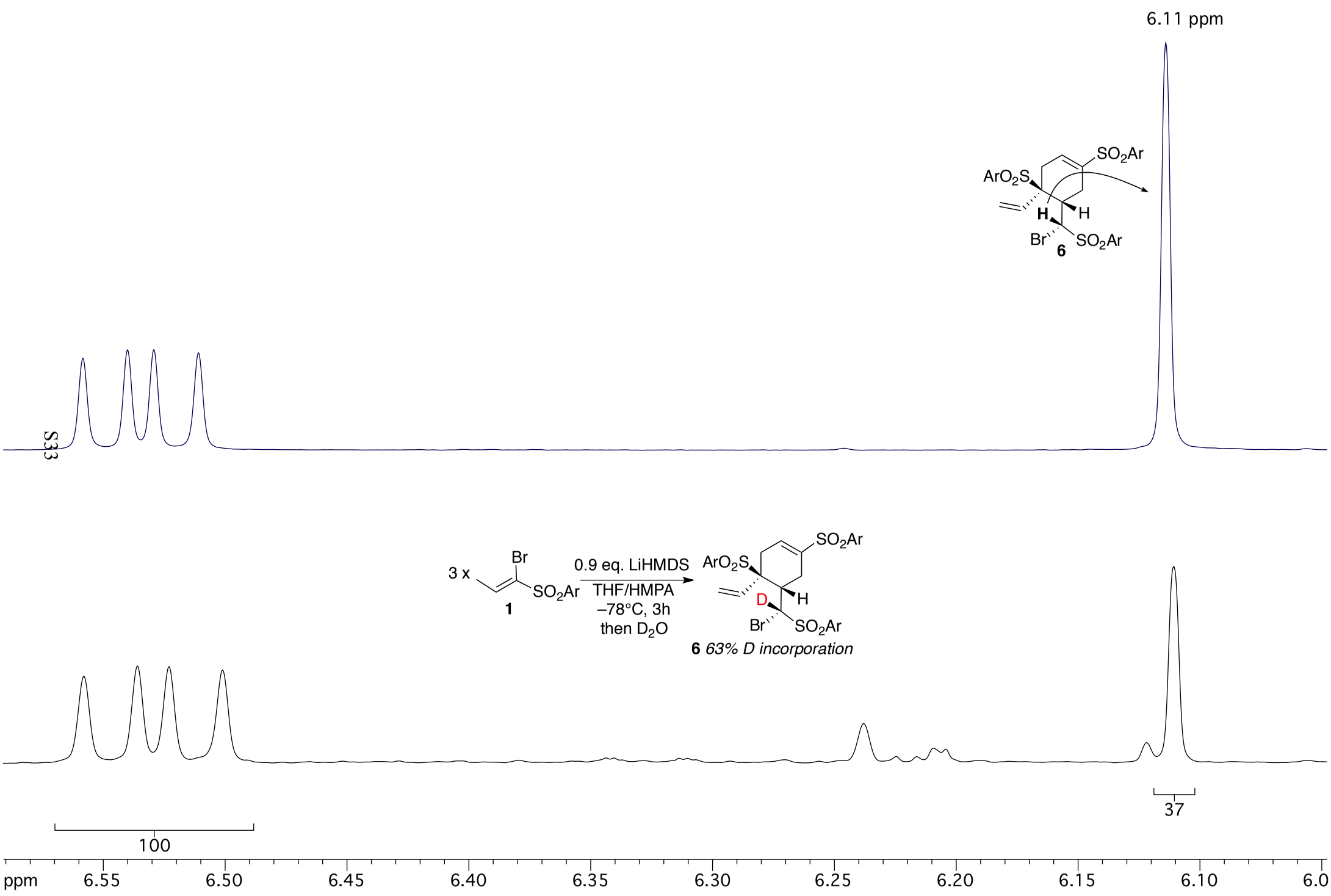
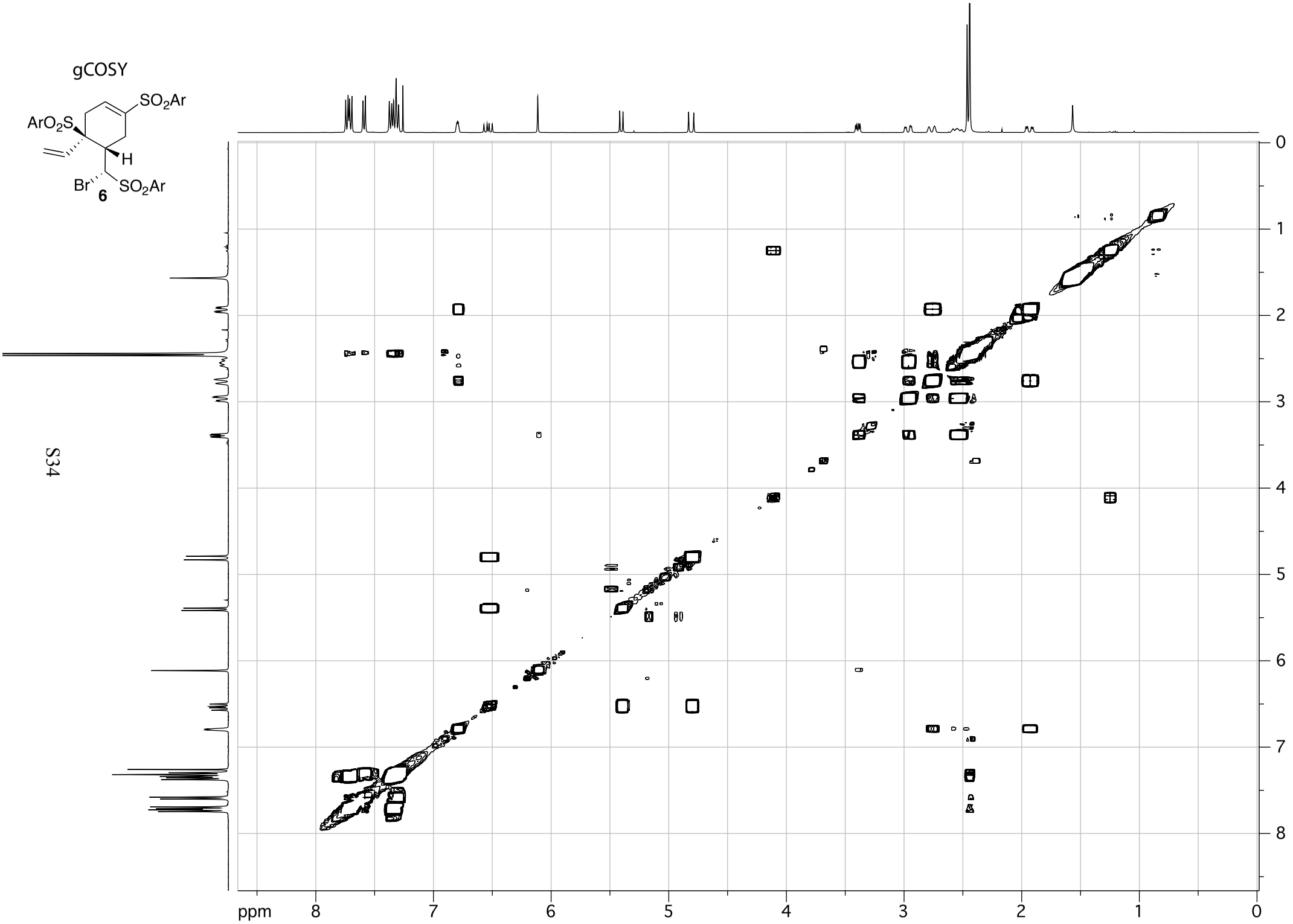
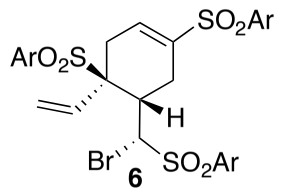
6.57
6.54
6.53
6.50
6.11
5.42
5.39
4.83
4.79
3.41
3.40
3.39
3.37
2.99
2.98
2.95
2.94
2.79
2.74
2.58
2.58
2.56
2.56
2.55
2.54
2.54
2.52
2.51
2.46
2.44
1.96
1.95
1.92
1.90
^{1}H NMR ($CDCl_3$, 400MHz)
SO_2Ar
ArO_2S
H
Br
SO_2Ar
6 Ar = p-MePh
3.6
5.3
1.1
1.9
1.0
7.5
7.0
6.5
1.9
1.0
1.1
1.1
1.1
1.1
1.1
3.6
5.3
1.1
1.1
1.0
1.2
7.8
ppm
8
7
6
5
4
3
2
1
0


145.81
145.78
144.71
139.40
135.31
132.61
131.56
131.36
130.39
129.96
129.89
129.64
129.51
129.41
128.21
121.96
68.33
65.16
36.02
31.47
24.88
21.79
21.69
21.67
13C NMR (CDCl3, 100MHz)
SO2Ar
ArO2S
H
Br
SO2Ar
6
ppm
140
120
100
80
60
40
20
0


6.11 ppm
SO2Ar
ArO2S
H
H
Br
SO2Ar
6
3 x
Br
SO2Ar
1
0.9 eq. LiHMDS
THF/HMPA
–78°C, 3h
then D2O
SO2Ar
ArO2S
D
H
Br
SO2Ar
6 63% D incorporation
37
100
ppm
6.55
6.50
6.45
6.40
6.35
6.30
6.25
6.20
6.15
6.10
6.0

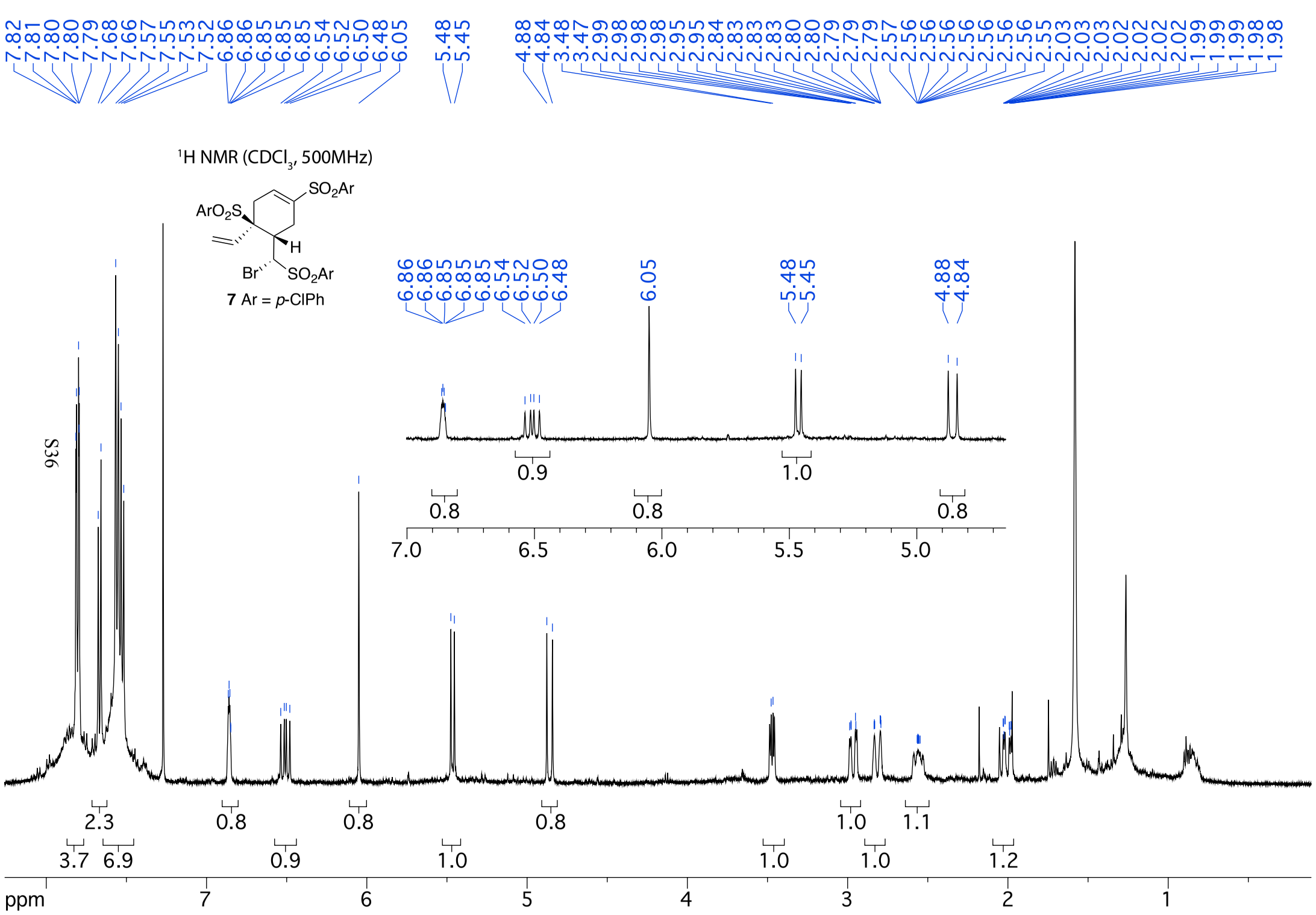

gCOSY
SO_2Ar
ArO_2S
H
Br
SO_2Ar
6
ppm
8
7
6
5
4
3
2
1
0

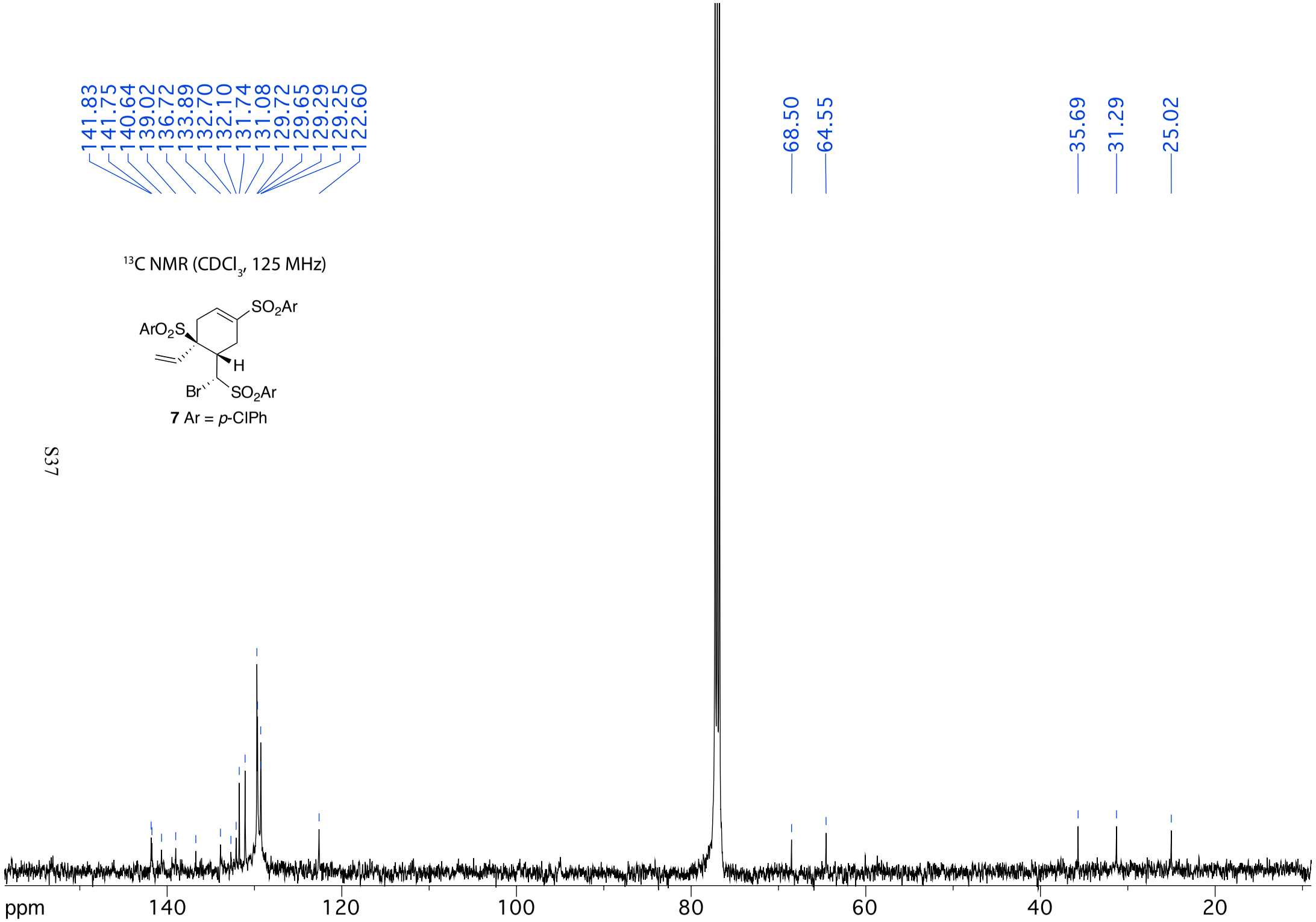
gHSQC


SO2Ar
ArO2S
H
Br
SO2Ar

6

2.0
2.5
3.0
3.5
4.0
4.5
5.0
5.5
6.0
6.5
7.0
7.5
8.0
ppm
150
100
50


7.82 7.81 7.80 7.80 7.79 7.68 7.66 7.57 7.55 7.53 7.52 6.86 6.86 6.85 6.85 6.85 6.54 6.52 6.50 6.48 6.05 5.48 5.45 4.88 4.84 3.48 3.47 2.99 2.98 2.98 2.98 2.95 2.95 2.84 2.83 2.83 2.83 2.80 2.80 2.79 2.79 2.79 2.57 2.56 2.56 2.56 2.56 2.56 2.56 2.56 2.55 2.03 2.03 2.03 2.02 2.02 2.02 2.02 1.99 1.99 1.99 1.98 1.98
^{1}H NMR ($CDCl_3$, 500MHz)
SO_2Ar
ArO_2S
H
Br
SO_2Ar
7 Ar = p-ClPh
S36
6.86 6.86 6.85 6.85 6.85 6.54 6.52 6.50 6.48 6.05 5.48 5.45 4.88 4.84
0.9 1.0
0.8 0.8 0.8
7.0 6.5 6.0 5.5 5.0
2.3 0.8 0.8 0.8 1.0 1.1
3.7 6.9 0.9 1.0 1.0 1.0 1.2
ppm 7 6 5 4 3 2 1



^{13}C NMR ($CDCl_3$, 125 MHz)

7 Ar = *p*-ClPh