

Dimerization Strategies for the Synthesis of High-Order Securinega Alkaloids

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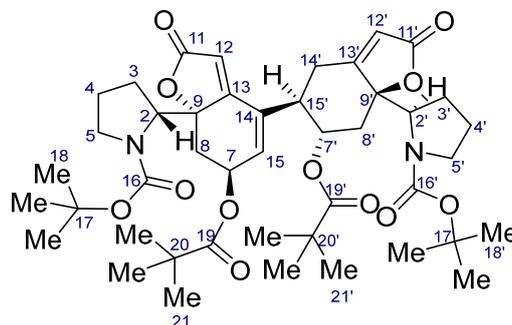
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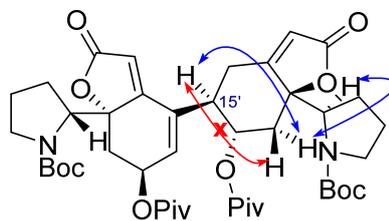
1. NMR Peaks Assignment of Compound 48



48

^1H NMR (400 MHz, CDCl_3): δ 6.26 (s, 1H, H-12), 5.90 (d, $J = 1.9$ Hz, 1H, H-12'), 5.86 (d, $J = 4.5$ Hz, 1H, H-15), 5.44 (dd, $J = 7.1, 4.5$ Hz, 1H, H-7), 4.88 (q, $J = 8.2$ Hz, 1H, H-7'), 4.51 (d, $J = 5.9$ Hz, 1H, H-2), 4.46 (d, $J = 8.2$ Hz, 1H, H-2'), 3.65 (d, $J = 9.3$ Hz, 1H, H-15'), 3.54 (t, $J = 9.4$ Hz, 1H, H-5), 3.47 (dt, $J = 14.6, 6.1$ Hz, 1H, H-5'), 3.36 (m, 3H, H-5, H-5', H-8), 2.99 – 2.88 (m, 1H, H-14'), 2.80 – 2.72 (m, 1H, H-14'), 2.67 (dd, $J = 14.4, 7.9$ Hz, 1H, H-8'), 2.17 (dd, $J = 14.4, 7.2$ Hz, 1H, H-8'), 2.04 – 1.92 (m, 1H, H-3), 1.87 – 1.60 (m, 8H, H-3, H-4, H-3', H-4'), 1.46 (s, 9H, H-18), 1.38 (s, 9H, H-18'), 1.23 (s, 9H, H-21), 1.06 (s, 9H, H-21'); $^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3): δ 178.2 (C-16'), 177.5 (C-16), 172.2 (C-11), 172.0 (C-11'), 168.0 (C-19), 166.7 (C-19'), 156.7 (C-13), 155.1 (C-13'), 135.8 (C-14), 131.3 (C-15), 117.5 (C-12'), 113.3 (C-12), 90.5 (C-9), 88.4 (C-9'), 80.6 (C-17), 79.6 (C-17'), 70.7 (C-7'), 66.6 (C-7), 61.6 (C-2'), 59.7 (C-2), 47.3 (C-5), 47.1 (C-5'), 39.7 (C-15'), 39.2 (C-20), 38.9 (C-20'), 36.3 (C-8'), 34.8 (C-8), 29.9 (C-14'), 28.6 (3) (C-18), 28.6 (3) (C-18'), 28.0 (2) (C-4, C-4'), 27.4 (3) (C-21), 27.2 (3) (C-21'), 25.0 (C-3), 24.3 (C-3').

2. Key NOESY Correlations for the Determination of the Configuration at C15' of 48



48

Key NOESY correlations: blue \longleftrightarrow

Key lack of NOESY correlation: red \longleftrightarrow

3. Computational Details

All calculations were carried out using density functional theory (DFT)¹ calculations implemented in Jaguar 9.1 programs.² For every calculation, B3LYP³⁻⁷ level of theory with Grimme's D3 dispersion correction⁸ was used. Geometry optimizations of all intermediates and transition states were conducted utilizing 6-31G** basis set. Single-point energies of optimized structures were obtained using Dunning's cc-pVTZ(-f) basis set⁹ which includes a double set of polarization functions to gas-phase optimized structure. Vibrational frequency calculations of gas-phase structures were performed using 6-31G** basis set. Standard approximation was used to obtain zero-point vibrational energies and entropy corrections. Solvation energies of gas-phase optimized structures were calculated applying self-consistent reaction field (SCRF) approach¹⁰⁻¹² to solve Poisson-Boltzmann equation with dielectric constant $\epsilon = 7.6$ (THF). As is the case for all continuum models, the solvation energies are subjected to empirical parametrization of the atomic radii that are used to generate the solute surface. The standard set of optimized radii in Jaguar was used for H (1.150 Å), C (1.900 Å), N (1.600 Å), and O (1.600 Å).¹³ The Gibbs free energies in solution phase $G(\text{sol})$ were obtained as follows:

$$G(\text{sol}) = G(\text{gas}) + G^{\text{solv}} \quad (1)$$

$$G(\text{gas}) = H(\text{gas}) - TS(\text{gas}) \quad (2)$$

$$H(\text{gas}) = E(\text{SCF}) + \text{ZPE} \quad (3)$$

$$\Delta G(\text{sol}) = \Sigma G(\text{sol}) \text{ for products} - \Sigma G(\text{sol}) \text{ for reactants} \quad (4)$$

Where $G(\text{gas})$ is Gibbs free energy in gas-phase, G^{solv} is solvation free energy, $H(\text{gas})$ is gas-phase enthalpy, $S(\text{gas})$ is gas-phase entropy, T is temperature (298.15K). $E(\text{SCF})$ is self-consistent field energy which is "raw" electronic energy, ZPE is vibrational zero-point energy. The entropy term we utilized is vibrational / rotational / translational entropy of solute(s), and the entropy of solvent is implicitly included in continuum solvation model.

4. Gas Phase Free Energy Diagram of the Conjugate Addition of 51

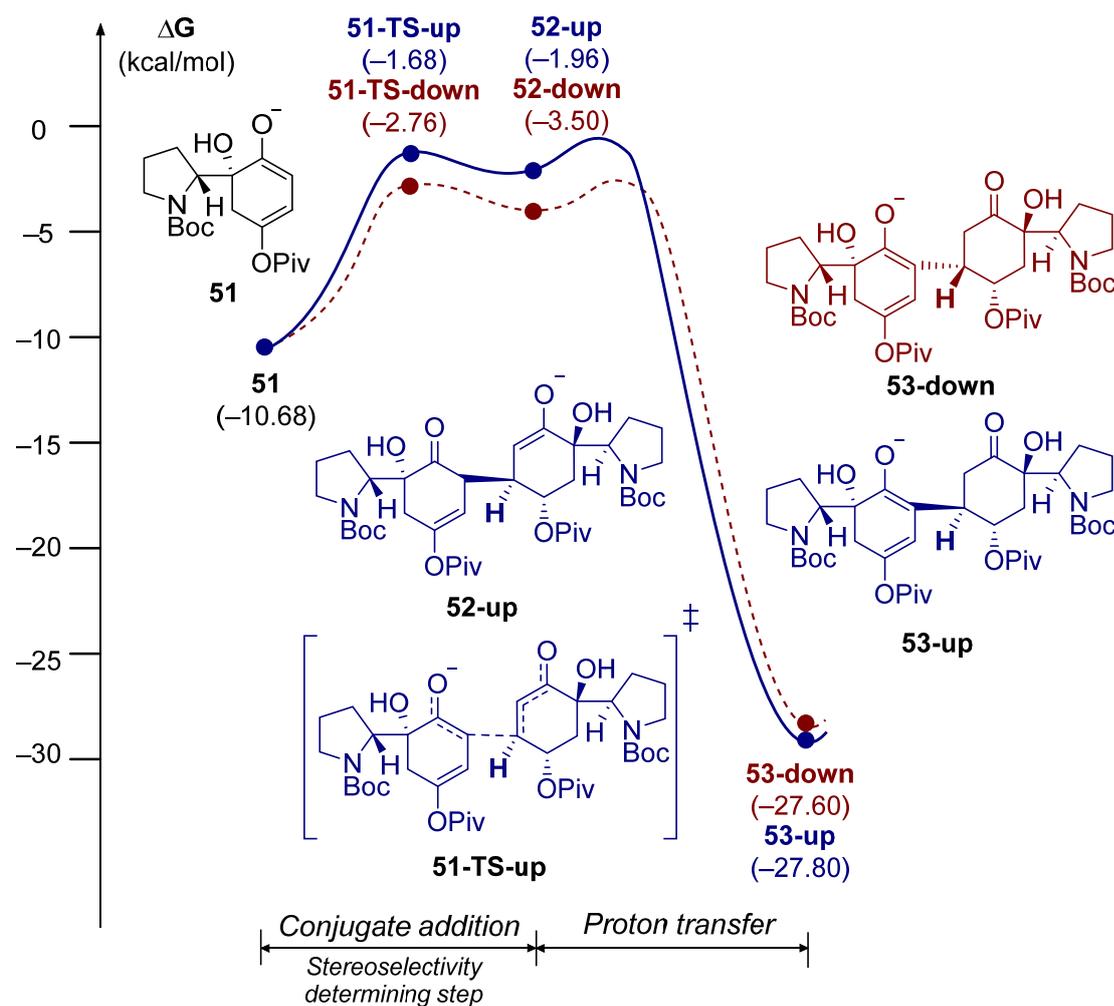


Figure S1. Gas phase free energy diagram for conjugate addition. Gas phase free energy of **54** was employed as reference value.

In gas phase, free energy barrier of **51-TS-down** was 1.08kcal/mol lower than **51-TS-up**, plausibly due to different ring conformation. Cyclohexenone ring conformation which experiences nucleophilic attack adopts “chair-like” conformation in **51-TS-down**, whereas adopts “twisted boat-like” conformation in **51-TS-up** (see below, highlighted).

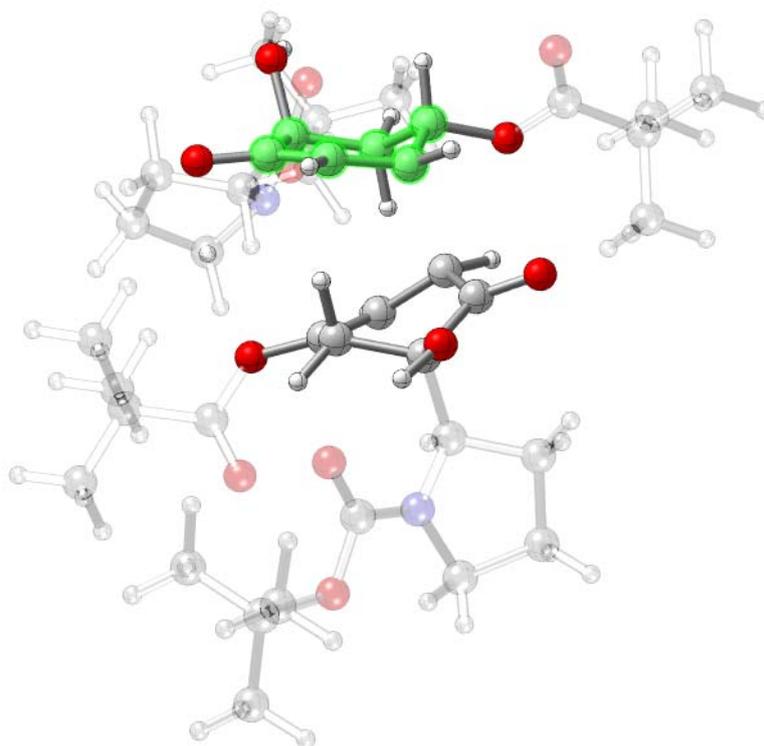


Figure S2. Optimized TS Structure of **51-TS-down**. Carbons of cyclohexenone ring were highlighted.

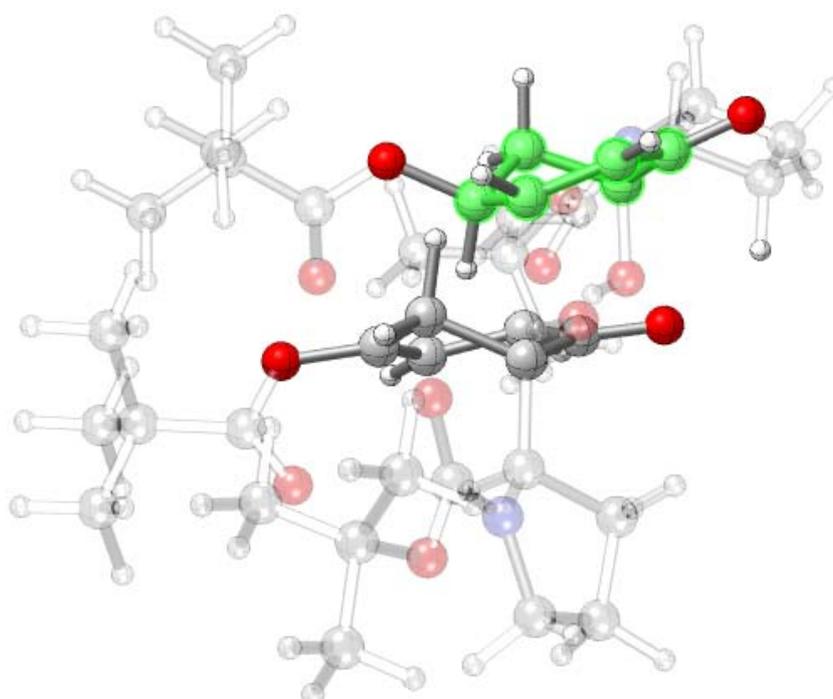


Figure S3. Optimized TS Structure of **51-TS-up**. Carbons of cyclohexenone ring were highlighted.

5. DFT Calculation Data

DFT-optimized structure's energy components.

Table S1. Computed energy components for optimized structures.

	E(SCF)/(eV)	ZPE/(kcal/mol)	S(gas)/(cal/mol·K)	G(solv)/(kcal/mol)
	B3LYP-D3/ cc-pVTZ(-f)	B3LYP-D3/ 6-31G**	B3LYP-D3/ 6-31G**	B3LYP-D3/ 6-31G**
54	-35016.512	302.615	185.799	-48.02
55	-35017.078	303.612	181.688	-45.33
H ₂ O	-2080.542	13.408	46.49	-7.43
54-TS	-35015.867	299.919	181.762	-45.77
55'-TS	-37096.965	318.073	188.186	-51.96
51	-35017.047	303.386	182.813	-52.40
50	-35032.621	312.827	185.336	-11.20
51-TS-up	-70050.000	617.671	317.189	-55.87
51-TS-down	-70050.133	618.19	312.257	-52.75
52-up	-70050.078	618.717	315.603	-59.04
52-down	-70050.188	618.919	312.921	-54.93
53-up	-70051.125	618.689	321.184	-51.31
53-down	-70051.195	619.045	316.296	-48.78

Table S2. Cartesian coordinates of the optimized structures.

The cartesian coordinates of optimized geometries are given below in the standard XYZ format, and units are in Å.

=====	C	-8.738613129	-3.888238907	0.543886185			
54	C	-8.747483253	-2.502605915	-1.593184590			
=====	C	-8.825267792	-0.842625082	0.854627430			
C	-7.853268623	1.498748422	-0.498188525	O	-7.671016693	-1.207501292	0.968472362
C	-6.523141384	1.460714817	0.346167535	H	-6.341800690	2.437799454	0.818084776
C	-5.393182278	1.150233626	-0.618620098	H	-6.567965984	0.693870902	1.116700530
C	-5.314533710	2.148483992	-1.735000253	H	-5.550897121	0.151629582	-1.035651445
C	-6.405862331	2.814476967	-2.132661343	H	-4.357996464	2.263430595	-2.239296675
C	-7.727064610	2.716207743	-1.440671682	H	-6.368567467	3.529537201	-2.953373909
O	-8.615613937	3.515721560	-1.743657947	H	-10.667480469	2.872522831	-0.413068920
C	-9.077740669	1.628291368	0.451356292	H	-10.225602150	1.442752719	-1.350261927
O	-8.003655434	0.480415672	-1.381036758	H	-11.768774033	0.104978539	-0.230977714
C	-10.407898903	1.815687180	-0.341295302	H	-12.389033318	1.528111935	0.624926627
C	-11.479695320	0.965233445	0.380376250	H	-10.843169212	1.204369068	2.447621584
C	-10.750140190	0.466024667	1.637093306	H	-11.107487679	-0.493534267	2.014355183
N	-9.326640129	0.397034913	1.281441212	H	-1.393080473	-0.096372880	2.567957640
O	-4.134231091	1.145414829	0.146522090	H	-3.102463961	0.345796555	2.335894823
C	-3.073796272	0.538494349	-0.397755384	H	-2.485797882	-1.179653645	1.684201121
O	-3.054413319	0.019296670	-1.498627901	H	0.200098142	-0.085477069	0.548317552
C	-1.864030480	0.587642252	0.553971171	H	-0.410042107	0.383731753	-1.056880713
C	-2.237067938	-0.128920317	1.868214369	H	-0.909003317	-1.150236845	-0.348611444
C	-0.671863139	-0.108482942	-0.116039917	H	-2.379470825	2.572717667	1.303364158
C	-1.526906848	2.064774275	0.846703649	H	-0.670671642	2.128565788	1.529006839
H	-8.937151909	2.457620621	1.160684228	H	-1.266004324	2.597631931	-0.074596137
O	-9.830027580	-1.671625853	0.429867804	H	-11.473659515	-2.687530756	-1.216450095
C	-9.510490417	-2.881195307	-0.320401102	H	-10.811896324	-4.338513851	-1.266914487
C	-10.899754524	-3.432554483	-0.657797098	H	-11.450551987	-3.677262783	0.256962627

H	-7.733050346	-3.525198698	0.749463022	C	-8.899616241	-3.005910397	2.651472807
H	-8.680215836	-4.851028442	0.022027003	C	-9.474343300	-4.239443302	1.946716428
H	-9.259035110	-4.043244839	1.495514393	C	-9.442867279	-2.901851416	4.082780361
H	-8.515832901	-3.409817219	-2.164701223	C	-7.365398884	-3.045051813	2.625142097
H	-9.349485397	-1.827690601	-2.206076860	C	-8.982270241	-0.622776568	2.087955952
H	-7.833182812	-1.958008051	-1.357385874	O	-8.393857002	-0.284881234	3.114958525
=====				H	-6.420062065	0.958157480	1.966984272
55				H	-6.787826061	-0.200217128	0.684657633
=====				H	-4.337113857	0.495269418	0.850608289
				H	-3.654230833	2.696073294	0.002427314
C	-7.552032471	1.792274237	0.265626848	H	-5.319033146	4.506340027	0.087369695
C	-6.486195087	0.833139122	0.879276097	H	-10.612215996	3.018764257	0.864099324
C	-5.100185871	1.028797388	0.267524213	H	-9.631130219	2.799771547	-0.605687499
C	-4.708110332	2.479660988	0.143099308	H	-11.360642433	1.287038803	-1.246468544
C	-5.619585037	3.461528063	0.160369083	H	-11.854868889	1.018233418	0.435406327
C	-7.069757938	3.239478827	0.423317105	H	-10.638851166	-1.049748778	0.000271342
O	-7.796330452	4.209232807	0.652016521	H	-9.414932251	-0.163015202	-0.976349235
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O	-7.684840202	1.682981491	-1.084833384	H	-5.835139275	-1.446102381	-3.101416349
C	-10.074180603	2.291803360	0.250171542	H	-6.921067238	-0.108829148	-2.627060413
C	-10.987845421	1.136049509	-0.227724150	H	-6.120482445	2.014258146	-4.565559387
C	-10.095726967	-0.111666106	-0.119596295	H	-4.783075809	2.731322765	-3.637632847
N	-9.308903694	0.198192075	1.075401187	H	-6.288132668	2.227863789	-2.797382832
O	-5.175034046	0.373002738	-1.036704183	H	-3.588197470	-0.805962980	-4.320573807
C	-4.319082737	0.669328392	-2.017439127	H	-4.428294659	0.269757688	-5.454305172
O	-3.176661968	1.064155459	-1.850555182	H	-3.125102282	0.900160611	-4.415789604
C	-5.008385181	0.563841224	-3.382925034	H	-9.107928276	-4.293206692	0.917212725
C	-6.177523136	-0.436495245	-3.359562159	H	-9.180083275	-5.153271198	2.473729610
C	-5.586676598	1.986965179	-3.607064724	H	-10.567114830	-4.186494827	1.919114590
C	-3.973236322	0.211795300	-4.458685875	H	-9.049750328	-2.008855104	4.567524433
H	-8.827775002	1.977464199	2.069008827	H	-9.156288147	-3.789603949	4.658921242
O	-9.394488335	-1.914418340	1.832525253	H	-10.536049843	-2.840865850	4.062419891

H	-7.005614281	-3.948992729	3.129852772	C	-1.263697028	-0.646481097	-0.492776304			
H	-7.012196064	-3.061351061	1.589197636	C	-1.985798717	0.846280813	1.410808921			
H	-6.951953888	-2.166428804	3.119846106	H	-9.395383835	2.625444651	0.795028687			
=====				O	-9.183974266	-1.519010901	0.484329790			
H ₂ O				C	-8.576266289	-2.776789904	0.055764254			
=====				C	-9.727034569	-3.449459314	-0.698178887			
H				-1.512242436	-0.259922951	-2.434956312	C	-8.168373108	-3.604833364	1.279898286
O	-1.500379086	-0.238467038	-1.470261931	C	-7.398541451	-2.510419846	-0.888777971			
H	-1.950488687	-1.052441359	-1.213115096	C	-8.435756683	-0.558584630	1.087315321			
=====				O	-7.298807144	-0.735932410	1.477987885			
54-TS				H	-6.602375984	3.118233919	0.714903593			
=====				H	-6.597317696	1.397344112	1.220698237			
C	-7.898149967	1.793133497	-0.514674127	H	-6.373469353	0.777451813	-1.140296221			
C	-6.632091522	2.073693275	0.368033886	H	-4.545239449	2.871686935	-2.226166964			
C	-5.546955109	1.741043925	-0.641332686	H	-6.652695656	3.996548176	-2.972397089			
C	-5.486601353	2.700839996	-1.710340858	H	-10.850234985	2.211483479	-1.060724616			
C	-6.643365860	3.300610542	-2.137880325	H	-10.054679871	0.678720176	-1.423771620			
C	-7.936834335	2.983421326	-1.537103176	H	-11.616926193	-0.455270737	-0.108650342			
O	-8.981532097	3.563371658	-1.859096050	H	-12.349049568	1.054838300	0.452143162			
C	-9.204483032	1.677378058	0.273012370	H	-10.921618462	1.188625216	2.331941605			
O	-7.647275925	0.603433132	-1.205002666	H	-10.763659477	-0.562853813	2.133681059			
C	-10.424349785	1.312708735	-0.615543485	H	-2.663094044	-1.815380931	1.633873582			
C	-11.395765305	0.533727467	0.302190483	H	-4.171242714	-0.888099372	1.415546775			
C	-10.616949081	0.397220582	1.633308649	H	-3.600629091	-1.963877916	0.133089527			
N	-9.189289093	0.617904007	1.339652777	H	-0.603829026	-1.219294548	0.169625774			
O	-4.321096420	1.331625104	0.007775633	H	-0.683524966	0.169365853	-0.936524332			
C	-3.414754629	0.628393710	-0.671733618	H	-1.597770691	-1.291245818	-1.309065104			
O	-3.368339062	0.517673433	-1.884638071	H	-2.833753586	1.240903258	1.973961830			
C	-2.462742805	-0.101525880	0.294152170	H	-1.322353482	0.310833186	2.101504326			
C	-3.276807785	-1.263501644	0.910848260	H	-1.428515196	1.694133878	0.996329844			
				H	-10.023715019	-2.834656715	-1.552724600			
				H	-9.420426369	-4.435585499	-1.062115073			

H	-10.595230103	-3.571103573	-0.042188231	O	-5.308043957	-2.625172853	4.337454319
H	-7.378293037	-3.095433950	1.831977129	C	-4.882389545	-3.890482664	3.736973047
H	-7.805767536	-4.588567734	0.960249424	C	-4.569225311	-4.740890026	4.972155571
H	-9.028375626	-3.752503633	1.942764282	C	-3.620911121	-3.678517580	2.893607616
H	-7.112440586	-3.446351767	-1.383413553	C	-6.022985458	-4.519982338	2.928383350
H	-7.683954239	-1.762495160	-1.630857706	C	-5.677391052	-1.573097110	3.553940058
H	-6.542568207	-2.113099813	-0.344129682	O	-5.738946438	-1.649719715	2.329147339
=====				H	-4.230592728	1.866837025	2.639781713
55'-TS				H	-4.371051788	0.206825078	2.076845646
=====				H	-3.385921955	1.865805268	0.452469498
				H	-5.246572971	3.134154320	-0.898055017
C	-6.276472569	1.257013083	2.383184195	H	-6.814679146	4.285068989	0.688370645
C	-4.794378757	1.203248739	1.969797015	H	-6.693832397	-0.341001958	1.416795492
C	-4.550530910	1.660023689	0.536129057	H	-8.372739792	1.725916028	4.441962719
C	-5.416197300	2.763367414	0.110024102	H	-8.494766235	0.161117345	3.623869419
C	-6.311458588	3.354980469	0.942620397	H	-8.530107498	-0.823489428	5.794623852
C	-6.710316658	2.751420498	2.208617449	H	-7.954884529	0.653945982	6.564861298
O	-7.377820015	3.352200270	3.053913832	H	-5.691948414	0.039406363	6.343179226
C	-6.477795124	0.837359250	3.851598024	H	-6.274572372	-1.606598973	6.061367989
O	-7.124104977	0.528042316	1.504536390	H	-2.505822420	-2.622470379	-0.660620689
C	-7.925619602	0.736978710	4.359385490	H	-2.336987495	-1.073914528	0.237697855
C	-7.798295498	-0.013131034	5.710752487	H	-3.931069374	-1.839266300	0.071678698
C	-6.347241402	-0.578088880	5.716643810	H	-3.791888237	-2.539562225	-2.950990915
N	-5.904284477	-0.463904738	4.316418171	H	-4.330608368	-0.962141991	-3.572839737
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51
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H	-4.212346554	2.037350178	-5.860415459	H	-1.363234758	1.422670603	1.016917229
H	-6.555278778	3.075722456	-8.701836586	H	-2.156346321	1.816018820	-0.514293551
H	-8.020170212	2.720717907	-7.761727810	H	-1.248590350	5.544692516	0.008929821
H	-6.997070789	4.104000092	-7.315236092	H	-5.302820683	6.374265194	0.865772605
C	-3.304859877	2.412045717	1.172668815	H	-3.535701036	0.551008224	1.478007793
C	-1.927991867	2.194757462	0.498035520	H	-4.850309372	4.305902958	2.801959753
C	-1.171097517	3.478820562	0.411152750	H	-5.241753578	2.622251987	3.157779694
C	-1.820010900	4.627182484	0.146096855	H	-4.913291931	3.458156586	5.444547653
C	-3.257297277	4.668689251	0.015001374	H	-3.703896523	4.620923042	4.902894020
C	-4.040407658	3.578329086	0.414829612	H	-2.019837379	3.059360027	5.363355637
O	-5.298493385	3.486784697	0.283499002	H	-3.211051941	1.811462283	5.737000942
C	-3.180264950	2.896951914	2.637914658	H	3.974959850	4.233401775	0.693381488
O	-4.092754841	1.241155148	1.074992180	H	2.410622120	4.529437542	-0.100692607
C	-4.480165005	3.397996187	3.277946234	H	2.694754601	5.115268707	1.546203494
C	-4.078053474	3.602604151	4.751932621	H	4.124047756	2.627744436	2.645866871
C	-2.939001799	2.577200890	5.007042408	H	2.705554485	1.692141891	3.163454056

H	2.784485817	3.420705318	3.505539417	H	-2.170233488	-2.152610064	5.320191383
H	2.175040245	2.018047571	-0.547667801	H	-0.672889948	-2.902918339	4.727463245
H	3.732905149	1.713827610	0.257429808	H	-1.778962255	-2.094622850	3.587042809
H	2.271245241	0.861108303	0.792784572	H	0.628160059	-1.472789288	6.431985855
H	0.887789369	0.491641819	3.854535103	H	0.457195401	0.297741801	6.385507107
H	1.352860093	-1.225693941	4.022188663	H	-0.888429105	-0.707154512	6.957427502
H	0.182764456	-0.716997445	2.776887655				

Table S3. Vibrational frequencies (in cm^{-1}) of the optimized structures.

=====	3031.73 3033.88 3033.92 3036.65 3039.15 3042.33
54	3044.21 3091.95 3097.78 3098.28 3099.59 3101.91
=====	3102.37 3112.34 3114.67 3124.03 3127.03 3131.66
14.06 23.55 26.16 40.19 52.32 65.89	3133.06 3138.57 3143.19 3148.54 3154.58 3167.88
78.07 84.73 103.21 108.77 115.17 123.37	3174.49 3180.11 3180.86
168.63 175.76 187.28 204.30 217.02 222.87	=====
233.69 242.67 249.34 270.27 274.53 282.54	55
287.76 288.46 298.71 303.56 313.14 337.38	=====
343.55 363.09 367.13 376.73 392.73 398.72	20.88 29.70 35.53 46.25 59.26 66.97
420.19 443.99 447.10 471.35 499.96 501.90	71.59 83.32 92.73 126.61 133.46 154.52
527.17 544.80 559.03 592.45 616.71 635.67	156.79 163.07 197.92 204.94 227.21 238.58
656.30 690.58 741.18 755.99 769.66 774.03	242.19 247.04 259.57 268.09 273.48 282.90
778.11 796.72 812.14 835.61 863.00 869.89	291.48 293.10 319.13 327.90 339.33 343.05
900.45 910.94 920.43 925.47 932.95 937.06	347.77 362.45 373.44 381.79 394.45 408.06
942.93 950.62 956.19 965.95 974.15 976.14	416.98 438.76 467.08 470.73 492.39 513.11
980.76 993.61 1027.23 1041.13 1058.08 1061.72	528.18 552.29 565.98 592.61 603.52 629.60
1063.30 1064.62 1068.61 1084.51 1111.88 1121.37	690.25 707.90 737.50 746.84 763.74 769.64
1124.36 1138.90 1178.38 1195.54 1220.40 1221.63	798.07 805.90 823.54 851.17 858.04 872.80
1231.94 1239.08 1241.34 1252.89 1262.58 1266.06	903.62 914.34 918.63 929.54 929.80 931.24
1270.36 1281.99 1285.63 1300.99 1305.97 1327.17	934.81 951.38 964.20 973.60 976.37 980.73
1334.31 1353.29 1360.56 1365.01 1371.97 1400.52	999.24 1015.75 1036.70 1052.52 1061.58 1063.37
1405.07 1407.13 1410.34 1416.50 1416.63 1445.64	1064.97 1066.78 1077.70 1088.06 1103.04 1110.30
1446.88 1476.83 1485.95 1487.20 1490.51 1499.60	1156.95 1163.30 1199.38 1214.51 1220.10 1221.89
1499.94 1503.79 1504.53 1505.56 1505.88 1513.07	1232.16 1235.54 1238.33 1271.87 1273.26 1274.18
1513.79 1518.22 1521.24 1537.01 1539.56 1693.77	1287.24 1292.25 1304.41 1314.68 1337.53 1346.91
1724.90 1787.82 1794.56 2993.27 3000.33 3012.44	1355.98 1366.47 1370.68 1387.24 1388.88 1404.73

1409.53	1409.77	1410.01	1417.32	1434.09	1450.52	1061.98	1063.12	1068.27	1077.31	1097.37	1109.61
1470.33	1471.93	1475.07	1480.54	1490.31	1499.79	1127.06	1132.74	1166.74	1179.31	1219.10	1224.56
1502.10	1505.51	1506.76	1507.05	1510.07	1515.71	1229.10	1237.38	1241.32	1249.87	1257.31	1261.74
1523.41	1523.65	1536.84	1547.40	1559.75	1694.51	1264.88	1274.89	1282.15	1288.89	1296.69	1322.98
1729.39	1766.30	1779.81	3002.39	3016.01	3016.62	1333.85	1336.72	1352.16	1360.34	1372.21	1403.96
3027.84	3030.61	3037.98	3041.24	3048.74	3049.96	1406.69	1410.35	1413.87	1415.80	1440.41	1444.09
3060.17	3079.73	3081.73	3085.81	3086.00	3092.98	1445.38	1478.78	1490.03	1494.83	1498.01	1500.11
3100.92	3102.52	3104.95	3105.55	3111.88	3121.17	1501.53	1503.92	1505.11	1505.74	1509.25	1514.89
3126.29	3126.33	3128.72	3144.65	3147.45	3157.84	1517.19	1520.80	1526.48	1539.45	1542.53	1593.37
3169.75	3174.71	3204.06				1704.18	1783.71	1789.63	1827.63	2997.72	3014.18
=====						3020.36	3026.84	3029.53	3037.08	3039.01	3040.92
H ₂ O						3043.69	3048.21	3091.55	3093.51	3098.04	3101.55
=====						3104.36	3105.20	3115.13	3117.19	3128.85	3133.09
1662.03						3135.96	3144.14	3145.43	3163.55	3164.41	3165.42
=====						3169.65	3176.96	3191.58			
54-TS						=====					
=====						55'-TS					
=====						=====					
-1470.10	14.13	30.54	33.35	44.99	49.95	-157.72	24.15	31.01	41.81	43.92	52.82
63.11	72.15	92.50	101.20	121.84	125.81	66.64	71.33	80.88	89.16	104.10	118.46
140.99	173.28	182.84	203.54	217.97	226.54	126.38	146.22	164.78	187.14	202.02	216.80
229.65	230.64	255.29	266.34	270.27	288.62	225.68	230.80	244.40	256.96	260.24	270.39
289.87	291.01	301.21	304.48	332.03	339.25	272.85	285.09	290.94	292.11	302.86	314.47
343.97	361.96	364.71	374.84	392.02	398.03	320.68	332.01	344.94	355.66	364.58	372.40
411.53	445.25	451.70	456.59	476.77	490.89	381.15	399.87	410.61	415.47	447.31	456.88
514.90	550.95	580.14	587.46	599.24	623.51	465.99	475.40	500.48	516.03	532.14	536.49
664.00	686.83	726.11	752.84	762.24	770.15	548.76	578.66	597.30	603.26	621.40	636.51
779.45	793.40	806.40	819.29	819.74	855.37	680.20	699.70	737.40	759.38	765.42	784.36
880.75	904.52	912.11	919.71	925.44	928.95	794.15	806.48	822.68	833.90	857.08	872.87
935.54	938.52	948.81	950.46	958.75	965.70	876.79	908.46	919.69	921.61	932.82	934.23
979.22	980.93	1016.60	1022.43	1054.33	1059.69						

946.56 954.94 957.70 977.77 980.74 989.52
991.39 1009.82 1018.74 1059.08 1062.08 1064.63
1066.63 1073.52 1082.93 1090.43 1118.37 1123.21
1142.86 1163.18 1184.25 1191.44 1213.07 1223.57
1239.05 1246.22 1248.15 1255.80 1267.96 1268.14
1275.94 1279.28 1286.69 1289.78 1319.75 1324.58
1339.72 1363.28 1375.62 1392.84 1394.43 1397.14
1410.84 1414.47 1419.66 1427.50 1439.29 1454.95
1463.30 1481.53 1482.05 1484.17 1502.90 1505.04
1505.39 1506.03 1506.51 1509.77 1512.60 1522.66
1524.46 1531.14 1535.62 1541.55 1545.75 1556.60
1623.97 1721.17 1752.39 1758.52 2056.17 3011.59
3018.04 3021.54 3025.05 3033.51 3040.00 3044.08
3047.03 3053.12 3054.70 3085.29 3090.16 3097.51
3102.39 3106.55 3107.63 3110.26 3117.27 3123.98
3129.85 3136.69 3144.31 3165.06 3172.97 3175.54
3177.21 3177.29 3184.42 3189.70 3681.85 3788.23

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17.72 30.40 36.22 50.83 59.63 69.95
76.99 88.49 97.62 107.61 129.00 139.16
155.44 169.83 177.64 201.89 217.07 231.85
236.36 241.96 254.38 265.89 283.59 286.76
291.01 293.73 303.56 316.38 325.65 346.00
354.88 360.12 366.28 371.57 395.08 403.79
431.47 436.54 442.49 470.97 479.50 490.98
523.04 533.85 565.02 588.10 610.43 615.43
667.18 671.80 715.76 733.78 753.38 768.22
771.99 782.52 793.47 807.26 816.74 841.88

879.88 894.27 897.93 912.31 926.83 933.13
936.12 936.40 949.11 950.92 958.32 979.38
981.66 999.60 1035.29 1040.78 1059.28 1061.74
1062.41 1071.83 1074.46 1078.73 1124.47 1142.57
1151.90 1159.48 1187.27 1209.10 1210.03 1226.94
1232.35 1240.85 1246.30 1255.09 1256.97 1262.86
1274.11 1284.41 1309.31 1318.43 1332.93 1335.94
1344.64 1352.57 1368.46 1399.95 1406.67 1407.75
1413.08 1416.08 1433.04 1437.52 1443.87 1453.06
1470.86 1482.30 1490.30 1490.87 1492.74 1500.35
1502.67 1505.69 1506.31 1506.45 1510.69 1514.05
1517.30 1523.21 1532.37 1539.26 1545.41 1646.27
1689.12 1755.03 1770.91 2941.58 3028.77 3032.22
3032.27 3038.68 3038.95 3041.20 3042.14 3049.02
3049.77 3075.10 3088.34 3096.93 3099.37 3101.70
3105.42 3112.73 3120.46 3123.64 3126.39 3131.75
3134.09 3138.61 3145.61 3150.93 3167.43 3168.77
3171.47 3174.52 3677.41

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21.41 27.29 35.52 42.62 46.82 59.31
65.23 74.31 90.78 102.78 110.86 133.07
147.37 181.44 192.04 209.72 216.30 226.78
230.17 243.83 258.98 266.37 272.24 280.17
286.05 291.58 298.06 304.00 316.64 345.24
359.47 363.45 366.18 382.08 388.65 398.67
413.58 446.42 454.28 465.86 502.48 531.55
534.11 542.70 559.39 596.66 623.48 639.40
704.73 716.40 746.86 764.45 773.92 777.59

783.86	788.34	808.89	816.31	837.97	857.08	262.75	274.79	276.10	286.56	287.62	289.16
869.55	901.42	915.96	921.86	935.48	936.92	292.63	294.05	297.32	297.82	303.49	307.95
944.73	950.23	950.78	960.04	982.21	983.41	314.64	324.68	327.49	343.10	350.80	360.15
994.46	1006.88	1018.25	1022.21	1059.25	1061.76	362.57	363.95	365.26	367.67	369.51	381.24
1064.14	1065.70	1072.51	1077.64	1107.10	1123.04	384.15	390.64	395.00	405.97	408.14	414.73
1140.73	1159.43	1164.30	1188.79	1206.36	1211.48	422.07	431.36	435.00	440.57	449.71	452.45
1230.29	1239.15	1240.56	1250.34	1256.00	1261.97	467.05	470.19	487.33	491.22	506.10	527.66
1275.35	1278.74	1291.59	1297.45	1311.96	1327.07	536.55	541.09	553.70	557.36	566.62	574.53
1333.47	1346.99	1365.86	1367.42	1382.89	1398.95	597.19	600.37	618.09	622.46	626.47	654.58
1413.23	1414.48	1414.74	1417.17	1421.23	1442.42	670.50	695.46	698.62	701.75	716.07	726.91
1449.79	1463.01	1471.97	1483.80	1492.29	1500.10	751.78	760.00	766.37	769.81	771.57	773.34
1502.15	1504.27	1504.83	1505.87	1507.12	1509.07	776.23	781.85	792.05	798.58	807.77	810.36
1515.05	1519.64	1521.75	1523.07	1536.93	1539.61	812.21	821.53	824.97	844.92	852.97	874.96
1545.82	1698.70	1726.89	1782.23	1807.55	3022.39	879.01	890.73	897.95	899.29	911.45	912.15
3042.96	3045.09	3052.39	3053.34	3053.95	3059.44	916.25	932.85	933.90	934.03	934.70	938.63
3060.30	3060.90	3071.41	3083.83	3085.12	3112.21	943.73	948.36	950.84	951.43	952.15	953.45
3113.85	3114.45	3121.26	3123.35	3126.64	3132.92	958.74	959.08	978.65	979.08	980.54	982.19
3135.82	3137.35	3137.78	3140.86	3161.34	3171.07	983.65	991.11	996.43	1001.32	1013.34	1042.13
3174.08	3180.52	3185.64	3191.41	3210.81	3553.65	1054.01	1058.21	1059.47	1060.88	1062.40	1062.72
=====						1063.42	1063.65	1066.42	1068.58	1070.08	1075.27
51-TS-up						1080.84	1090.77	1111.07	1116.74	1134.79	1138.43
=====						1139.76	1151.68	1155.18	1160.01	1177.46	1182.02
-310.17	14.13	15.08	20.73	25.93	28.29	1192.39	1198.59	1207.75	1215.25	1219.15	1219.50
30.55	33.37	37.42	42.51	45.96	49.40	1226.05	1231.12	1231.47	1235.69	1240.01	1241.48
53.72	57.01	64.35	65.01	72.02	75.02	1247.51	1249.65	1261.59	1262.21	1262.91	1265.93
78.54	79.09	81.94	92.53	100.47	105.67	1275.45	1275.80	1280.33	1283.12	1285.69	1287.73
111.99	116.76	127.06	129.96	145.24	152.42	1316.70	1317.74	1321.25	1325.50	1329.97	1333.77
161.35	172.63	176.02	186.68	194.00	196.56	1341.54	1346.11	1350.48	1356.82	1360.83	1371.00
208.33	213.93	219.67	226.01	229.42	231.01	1376.62	1388.66	1392.49	1405.56	1407.03	1409.35
233.19	241.33	243.59	250.50	255.07	261.14	1411.20	1411.33	1412.65	1413.00	1413.33	1415.04

1417.47	1418.62	1437.69	1438.65	1443.14	1444.41	267.45	278.63	283.47	284.90	291.62	291.85
1446.41	1448.34	1461.11	1466.73	1480.33	1480.81	293.45	295.34	303.34	306.35	313.47	318.66
1482.50	1490.60	1491.03	1496.30	1498.70	1500.48	320.53	330.57	336.62	347.05	355.03	361.94
1501.13	1502.25	1503.65	1504.21	1504.88	1505.07	362.64	366.88	367.47	369.88	372.82	381.64
1505.53	1505.92	1506.30	1507.49	1508.60	1512.03	382.04	391.12	396.33	406.53	410.92	420.93
1512.83	1515.13	1518.61	1521.20	1522.20	1523.40	438.80	441.74	444.05	446.99	452.08	467.37
1524.74	1534.18	1535.42	1537.14	1544.10	1544.58	469.64	470.32	481.63	493.57	509.65	527.99
1547.05	1654.93	1701.73	1733.80	1746.69	1749.84	534.12	547.14	552.08	563.34	576.22	580.33
1790.57	1791.06	3018.55	3033.27	3036.21	3036.95	595.93	603.30	615.86	623.03	637.50	652.52
3040.46	3042.84	3043.57	3044.43	3044.80	3044.85	670.18	683.90	694.54	711.63	721.30	736.60
3046.02	3046.33	3047.74	3048.58	3052.27	3053.48	754.21	757.76	759.81	770.49	771.84	777.84
3054.13	3055.25	3064.10	3066.70	3078.48	3083.08	778.98	783.68	790.54	798.26	809.67	810.56
3089.70	3097.26	3099.02	3104.17	3105.73	3106.77	816.85	820.32	825.64	842.04	850.48	873.13
3110.72	3112.01	3114.42	3115.25	3118.15	3119.00	873.62	878.37	900.97	903.28	908.29	913.40
3120.10	3122.36	3124.17	3125.76	3126.84	3128.40	916.85	922.67	932.84	932.99	933.48	936.10
3129.74	3134.56	3137.98	3139.59	3141.18	3147.95	937.37	939.81	942.92	949.29	952.81	953.94
3153.81	3156.60	3166.22	3166.76	3169.44	3172.87	958.34	967.32	969.79	975.25	979.00	983.36
3173.34	3175.76	3175.92	3178.41	3182.07	3193.92	986.68	989.32	994.27	1003.09	1010.47	1029.70
3208.19	3646.68	3676.24				1035.20	1046.03	1060.74	1061.70	1063.71	1063.96
=====						1066.10	1066.85	1069.78	1071.26	1071.74	1083.42
51-TS-down						1085.49	1091.01	1096.91	1118.27	1137.61	1140.54
=====						1145.38	1155.06	1157.36	1160.68	1168.97	1190.45
-344.89	16.71	19.82	24.97	26.61	31.34	1193.48	1200.64	1209.68	1212.05	1215.15	1217.76
31.64	36.97	39.73	44.89	49.90	54.83	1226.20	1234.14	1235.26	1235.97	1239.22	1241.84
55.42	59.84	62.04	65.64	72.28	80.15	1255.43	1257.94	1258.32	1260.77	1261.88	1265.21
84.13	87.69	91.31	95.73	104.99	107.63	1275.38	1276.84	1281.19	1286.68	1288.04	1288.92
111.02	128.69	131.57	136.80	143.58	156.42	1311.72	1318.00	1319.84	1324.42	1333.29	1337.34
159.77	164.98	171.24	187.80	192.37	203.42	1337.71	1345.32	1354.71	1358.84	1359.05	1367.25
208.61	213.63	225.19	227.73	231.28	235.87	1371.87	1382.11	1390.55	1395.67	1405.93	1410.44
243.51	244.47	252.64	252.77	261.78	262.21	1410.62	1411.15	1412.94	1413.08	1416.22	1417.47

1420.77	1421.90	1438.14	1439.96	1441.62	1450.04	273.01	276.45	284.43	288.39	289.32	293.01
1452.88	1458.45	1459.67	1464.71	1480.45	1482.37	295.46	298.14	299.68	304.23	309.33	315.42
1483.34	1492.80	1493.03	1499.14	1501.03	1501.47	327.27	330.96	337.05	351.27	359.74	361.73
1501.51	1503.35	1503.44	1504.75	1505.71	1505.84	364.64	365.75	367.61	369.67	376.85	384.07
1507.07	1507.49	1508.54	1510.28	1514.20	1517.30	391.03	392.60	407.45	409.08	412.76	428.97
1517.52	1517.95	1521.76	1522.84	1522.92	1523.86	433.75	435.19	441.96	448.51	453.79	467.16
1525.10	1534.46	1534.66	1545.44	1545.73	1546.53	469.40	488.99	489.59	495.65	508.05	528.10
1548.13	1628.97	1718.78	1736.76	1744.23	1746.39	538.35	544.28	554.03	564.59	578.58	593.25
1788.00	1801.67	3025.43	3029.48	3030.06	3031.96	597.03	612.58	621.09	632.14	650.37	667.51
3033.94	3035.85	3038.42	3042.82	3043.51	3043.86	677.75	688.28	698.48	705.18	721.12	731.09
3045.35	3046.47	3046.66	3050.52	3053.90	3054.08	744.93	762.84	764.82	768.55	771.45	774.13
3055.84	3058.94	3087.79	3088.80	3092.90	3093.96	774.62	781.14	786.28	791.75	800.44	811.78
3097.40	3097.41	3097.79	3099.13	3099.27	3101.45	815.28	821.22	830.56	843.28	860.29	875.26
3107.14	3109.92	3112.55	3112.73	3116.15	3116.18	877.84	887.11	899.65	901.22	909.69	911.53
3120.41	3124.44	3125.10	3126.60	3128.37	3128.45	913.98	932.38	933.18	933.60	935.13	941.91
3129.33	3130.45	3131.29	3135.68	3136.01	3136.76	943.52	950.30	950.95	951.95	953.11	955.44
3138.87	3150.62	3159.43	3169.07	3172.05	3174.43	958.37	959.47	971.32	978.37	980.44	982.70
3175.15	3176.14	3176.78	3189.08	3189.12	3194.41	984.47	994.57	999.11	1012.32	1030.68	1044.26
3215.78	3631.75	3680.56				1050.43	1057.70	1060.11	1061.67	1063.09	1063.14
=====						1064.20	1066.61	1066.96	1069.04	1074.80	1081.58
52-up						1085.75	1112.31	1123.73	1135.09	1139.03	1148.02
=====						1151.50	1156.87	1169.48	1176.29	1177.99	1188.89
13.80	16.56	21.40	26.65	29.75	32.07	1193.24	1207.56	1209.05	1216.54	1220.29	1223.61
34.27	37.01	43.16	49.40	51.79	54.33	1226.53	1232.43	1233.16	1240.50	1241.34	1246.31
58.40	66.34	68.35	73.76	76.56	79.17	1248.35	1262.67	1262.89	1263.67	1266.17	1274.73
81.33	85.76	92.82	101.02	106.64	114.88	1275.83	1278.05	1282.76	1286.59	1287.11	1298.78
122.47	129.14	133.43	148.57	154.52	175.25	1314.13	1315.79	1320.26	1323.85	1326.96	1328.26
175.44	180.58	192.08	195.40	197.00	210.50	1330.09	1341.13	1351.26	1352.51	1357.25	1360.33
216.16	221.15	225.13	230.42	231.66	236.09	1369.37	1380.00	1389.86	1403.84	1407.50	1410.05
238.22	244.14	251.87	261.24	262.46	263.20	1410.20	1411.03	1411.28	1412.95	1413.05	1414.63

1417.95	1418.42	1433.59	1437.73	1437.95	1440.33	280.39	283.06	284.69	291.40	291.57	293.81
1441.48	1447.06	1448.31	1460.80	1463.73	1481.28	294.63	300.77	304.10	311.08	314.57	321.47
1482.26	1490.66	1491.29	1497.88	1499.05	1499.39	332.09	337.72	347.00	356.34	361.21	363.41
1500.72	1502.18	1503.46	1504.54	1505.17	1505.40	365.70	367.46	369.95	372.47	378.73	383.07
1505.99	1506.45	1507.18	1508.36	1508.66	1512.57	390.00	392.24	405.19	409.16	418.71	435.42
1512.81	1515.39	1518.96	1520.39	1522.30	1523.85	440.41	441.60	443.58	448.41	466.35	467.53
1525.02	1535.01	1535.25	1537.65	1544.17	1545.03	470.26	490.08	493.68	502.79	512.40	529.72
1547.47	1657.53	1733.14	1746.31	1747.42	1777.10	533.64	545.77	553.02	567.46	579.07	590.34
1782.50	1795.80	3004.22	3032.63	3036.18	3037.98	599.84	605.84	617.28	625.89	645.61	651.23
3041.60	3041.98	3042.31	3043.77	3044.24	3044.67	677.40	691.19	696.94	710.17	720.85	741.39
3044.93	3046.62	3046.95	3048.38	3048.59	3051.24	750.80	760.36	761.68	768.82	770.05	777.77
3052.37	3054.20	3054.93	3064.36	3077.77	3079.80	780.82	787.94	794.11	798.24	805.18	812.20
3080.71	3089.51	3094.50	3099.20	3105.81	3107.58	815.36	818.72	820.50	843.26	845.78	869.42
3107.75	3110.65	3110.91	3111.81	3112.54	3112.97	873.32	878.16	899.73	902.83	908.20	911.88
3115.47	3119.16	3120.17	3120.53	3124.96	3127.13	913.66	922.70	932.35	932.57	935.29	936.54
3127.68	3129.23	3133.50	3136.32	3138.11	3139.70	937.75	939.19	948.46	950.26	952.58	953.72
3148.58	3150.22	3156.98	3158.30	3167.83	3168.19	958.06	962.69	967.22	978.58	983.66	984.36
3170.57	3173.10	3175.95	3177.19	3177.95	3189.66	989.15	989.55	1001.62	1007.14	1022.02	1031.41
3206.01	3654.17	3677.70				1036.96	1048.23	1060.48	1060.66	1063.57	1063.81

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15.07	23.48	24.87	27.75	30.87	31.99	1202.01	1205.96	1209.20	1212.64	1213.68	1220.46
36.62	40.62	46.01	49.22	54.24	55.98	1226.15	1233.45	1234.28	1237.09	1240.89	1248.16
57.73	59.58	64.63	70.14	79.24	84.59	1252.67	1254.80	1260.94	1261.61	1262.52	1274.95
85.36	90.20	93.94	102.78	107.23	108.13	1277.29	1277.90	1279.55	1286.93	1287.57	1293.32
128.13	133.08	137.14	145.38	158.91	162.53	1313.37	1316.83	1319.29	1322.41	1331.25	1334.96
165.57	170.14	190.15	197.27	204.17	209.26	1336.37	1342.00	1349.51	1354.24	1359.08	1365.52
215.07	227.33	229.96	232.76	235.35	243.21	1372.96	1381.22	1384.54	1391.13	1406.07	1408.01
245.08	251.61	252.30	261.45	262.38	266.02	1410.17	1411.01	1411.81	1412.36	1414.05	1415.60

1417.74	1419.46	1422.45	1437.90	1441.75	1447.36	274.57	276.26	284.47	285.59	291.85	293.30
1449.14	1453.72	1457.93	1459.92	1480.02	1482.18	294.69	298.41	301.14	303.94	308.34	321.85
1483.24	1492.55	1492.57	1499.01	1499.29	1499.84	326.25	327.65	333.85	336.59	350.80	358.86
1500.99	1503.24	1503.30	1504.20	1505.33	1505.89	361.97	365.49	367.38	368.55	372.33	379.54
1506.82	1507.49	1508.25	1509.29	1514.54	1516.03	383.77	391.51	395.56	407.05	414.38	417.65
1517.15	1520.44	1520.62	1522.54	1522.88	1523.50	435.28	440.34	443.54	448.52	461.65	466.02
1525.02	1534.52	1534.77	1542.52	1545.29	1546.65	467.19	470.58	476.52	491.25	505.62	510.91
1548.42	1633.06	1745.70	1746.10	1752.86	1760.31	542.93	545.87	551.23	561.64	570.81	580.16
1791.48	1801.19	3022.25	3030.25	3031.18	3032.64	594.87	600.60	609.61	636.99	653.58	676.28
3033.11	3037.24	3038.75	3042.66	3044.25	3044.57	680.27	689.44	697.32	712.12	721.18	752.63
3044.78	3045.78	3046.66	3047.38	3053.29	3054.90	754.47	762.23	764.49	772.82	774.23	778.01
3055.74	3060.63	3062.99	3087.26	3088.22	3089.26	779.46	791.15	795.01	802.94	805.96	813.92
3097.90	3097.93	3098.92	3099.00	3100.48	3102.19	821.16	838.16	843.35	861.90	874.31	880.89
3107.45	3110.63	3110.79	3112.05	3112.78	3115.02	889.93	903.68	910.15	912.89	920.84	924.16
3115.76	3123.70	3125.40	3125.86	3126.52	3127.33	926.97	933.31	933.35	934.59	935.52	936.17
3128.39	3128.93	3132.38	3134.09	3135.48	3136.93	943.99	948.58	949.88	951.39	958.24	963.29
3139.78	3148.35	3150.31	3159.41	3167.39	3169.77	966.98	974.62	979.47	980.17	982.15	990.73
3172.17	3174.39	3175.35	3175.48	3190.40	3199.54	1000.41	1006.43	1012.31	1022.25	1032.97	1036.07
3210.12	3618.64	3685.72				1050.95	1059.68	1061.65	1062.63	1062.83	1063.52
=====						1065.05	1066.57	1071.48	1074.67	1079.88	1081.79
53-up						1108.43	1123.99	1128.29	1138.82	1148.48	1150.23
=====						1157.81	1162.41	1178.55	1189.65	1197.27	1205.07
12.93	13.47	15.06	17.73	25.14	27.79	1209.22	1212.22	1222.23	1225.28	1227.86	1229.37
33.53	38.87	42.00	43.35	50.10	52.00	1233.14	1238.38	1238.52	1240.38	1245.82	1256.16
55.46	60.50	66.47	68.04	73.69	74.28	1258.45	1262.33	1264.63	1271.27	1271.66	1275.11
79.82	88.44	90.79	95.68	104.28	111.55	1276.65	1279.75	1285.29	1287.54	1290.47	1306.52
120.45	123.71	130.55	134.62	142.24	154.08	1308.90	1319.67	1324.48	1327.56	1330.55	1337.83
158.75	174.09	181.70	186.28	199.41	204.01	1339.97	1345.23	1347.30	1349.86	1365.86	1368.53
217.60	220.52	223.61	228.05	230.46	232.20	1392.46	1396.53	1403.14	1407.57	1408.69	1409.45
237.38	240.18	247.13	253.68	262.79	266.74	1412.23	1412.57	1413.71	1414.12	1416.45	1417.14

1417.32	1426.47	1437.54	1441.04	1445.64	1449.15	271.31	278.28	284.94	287.02	290.32	291.20
1453.43	1462.82	1470.01	1476.16	1479.39	1482.52	292.62	295.39	299.00	301.11	305.38	308.64
1483.03	1490.23	1490.93	1492.45	1493.56	1499.94	321.46	329.61	333.25	338.80	353.27	361.36
1502.50	1502.85	1502.99	1503.59	1504.77	1505.09	363.47	365.42	366.42	367.02	376.17	383.10
1505.91	1506.14	1506.45	1506.62	1508.86	1511.15	393.61	400.19	406.81	410.94	416.63	426.73
1514.63	1517.73	1518.50	1523.24	1523.31	1523.48	430.42	436.34	444.10	450.89	454.80	468.07
1524.93	1532.18	1535.39	1539.43	1545.61	1545.91	470.00	474.00	487.36	497.77	506.11	517.44
1547.16	1625.95	1690.35	1748.16	1750.83	1778.04	533.21	543.30	561.62	565.29	571.96	593.80
1781.89	1784.72	2974.99	3024.98	3031.71	3032.26	601.04	608.29	615.12	628.16	651.61	653.11
3032.99	3035.46	3037.47	3038.86	3039.99	3040.80	670.51	679.36	699.80	713.54	723.12	749.06
3041.56	3043.88	3043.98	3044.43	3046.06	3047.51	755.37	757.03	767.35	772.39	776.57	778.55
3047.85	3051.81	3053.94	3054.84	3059.97	3068.43	782.87	786.77	797.34	800.89	813.69	816.64
3082.99	3084.99	3089.37	3094.29	3096.24	3100.13	822.09	839.97	842.89	873.23	879.69	880.73
3101.23	3102.69	3102.86	3107.23	3107.38	3112.23	886.97	901.07	904.38	905.32	917.29	927.37
3112.40	3113.97	3116.84	3122.18	3126.02	3126.09	931.85	932.29	933.71	933.92	935.42	936.13
3127.05	3131.47	3132.18	3133.54	3134.20	3138.86	939.99	948.50	949.82	950.24	953.30	959.64
3139.70	3140.64	3147.96	3154.57	3156.97	3157.00	962.40	977.39	980.95	982.31	983.20	985.18
3161.00	3162.45	3167.96	3169.80	3170.97	3171.96	991.34	998.07	1004.07	1028.18	1035.96	1037.64
3178.34	3589.51	3666.79				1045.13	1055.92	1060.04	1060.90	1061.52	1062.86

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53-down

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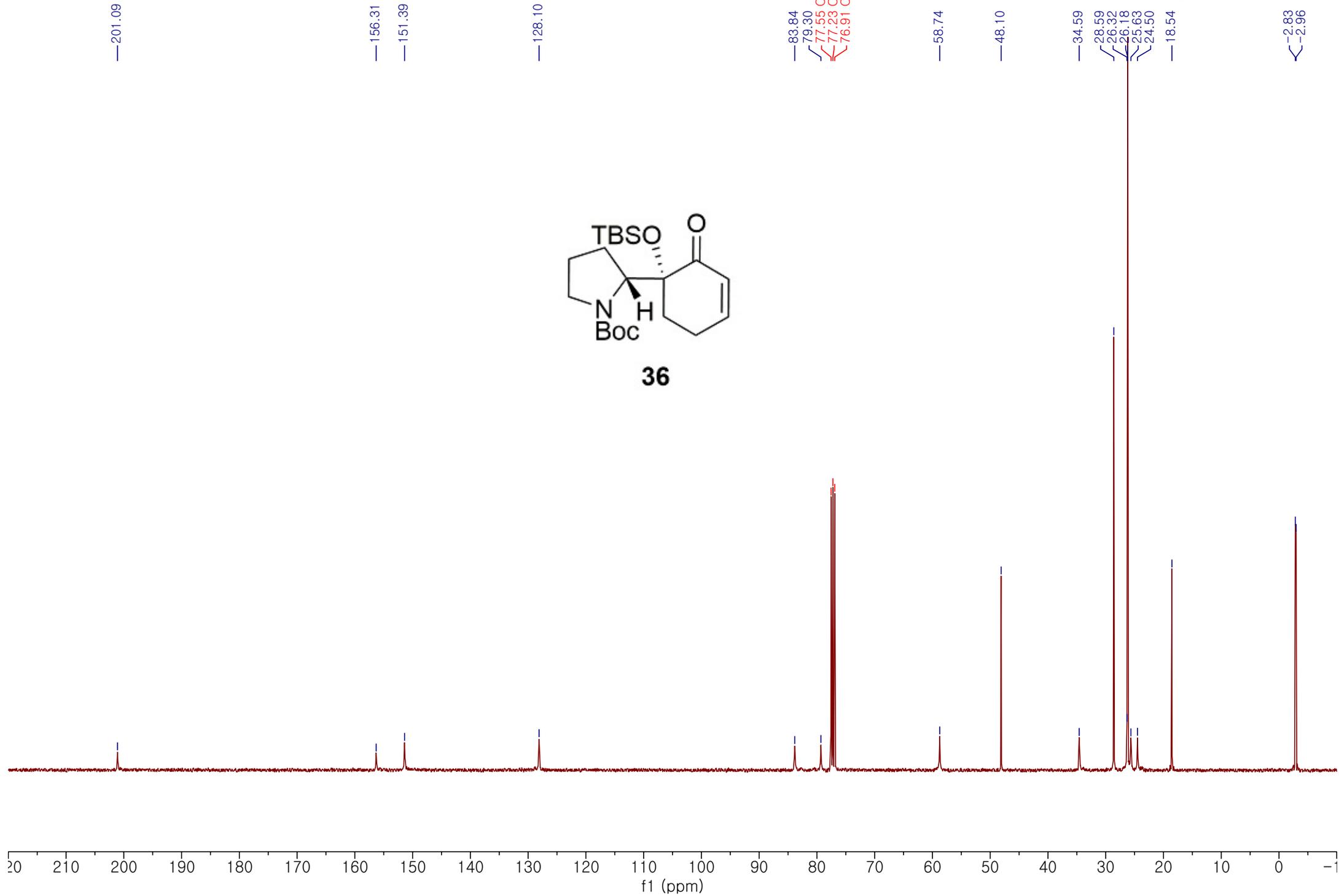
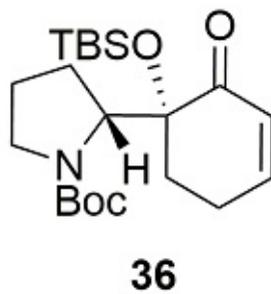
12.39	15.78	18.80	25.00	28.98	33.12	1108.36	1123.94	1130.11	1137.50	1140.41	1151.13
33.87	36.13	41.94	45.78	48.56	49.43	1161.48	1163.93	1171.34	1191.60	1197.88	1204.39
51.42	60.86	70.61	73.26	78.91	84.07	1205.81	1213.34	1218.52	1222.37	1226.68	1227.01
87.89	88.44	97.87	102.92	109.72	114.66	1234.38	1236.94	1238.25	1240.41	1241.76	1255.99
124.36	125.08	131.96	147.59	159.09	163.29	1256.64	1261.37	1265.20	1265.55	1266.43	1274.61
178.90	185.73	192.66	196.77	203.04	217.08	1275.42	1285.23	1285.67	1287.80	1292.55	1309.73
218.42	224.91	229.41	230.75	234.07	236.47	1317.57	1319.25	1320.35	1327.76	1333.12	1345.98
238.51	242.30	250.95	258.07	263.99	264.97	1348.18	1350.82	1362.03	1368.88	1369.10	1374.19
						1391.41	1397.75	1400.42	1408.39	1409.57	1409.84
						1410.88	1413.62	1413.74	1415.41	1416.80	1417.51

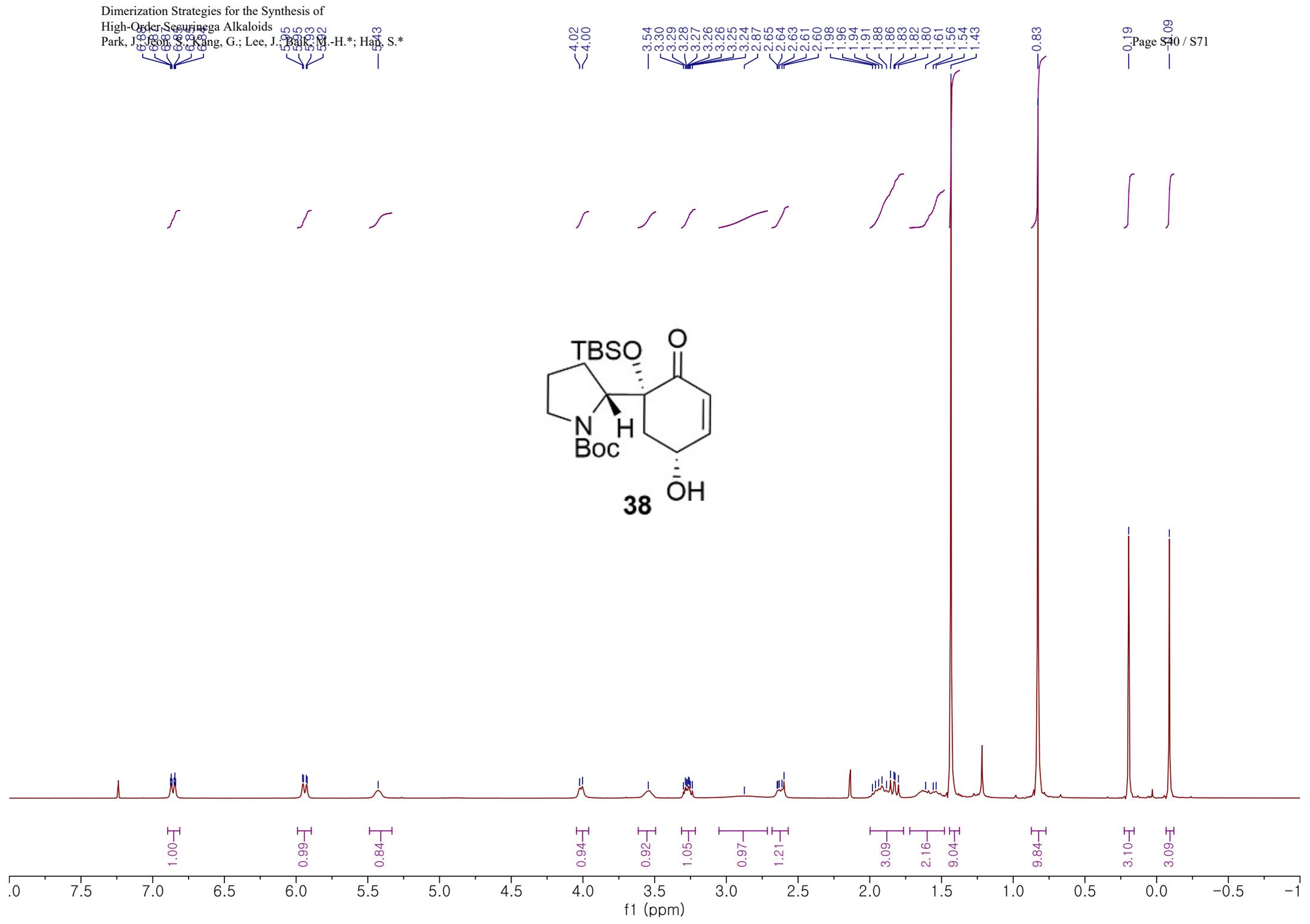
1418.93	1422.83	1438.21	1438.65	1445.73	1447.42	3042.67	3043.24	3044.60	3044.66	3045.49	3051.89
1458.97	1465.91	1470.34	1474.03	1477.51	1481.80	3052.28	3052.51	3054.98	3055.94	3061.14	3068.81
1482.47	1490.38	1491.00	1491.26	1493.91	1500.55	3077.77	3084.99	3093.51	3095.34	3099.23	3101.23
1501.24	1502.03	1502.89	1503.18	1504.17	1505.34	3102.40	3103.32	3108.40	3108.93	3110.28	3111.84
1505.78	1506.12	1506.54	1507.51	1511.47	1514.13	3112.22	3115.15	3115.29	3123.98	3124.81	3125.19
1514.62	1515.50	1517.87	1519.00	1522.72	1522.91	3127.95	3129.52	3131.39	3132.02	3134.91	3137.49
1526.01	1532.80	1534.49	1539.68	1540.25	1545.08	3138.67	3142.67	3145.42	3151.11	3160.69	3161.76
1548.17	1591.65	1699.91	1743.71	1749.99	1782.01	3162.51	3167.61	3168.41	3172.38	3179.36	3179.51
1783.63	1785.86	2956.41	2990.01	3012.78	3031.03	3189.56	3622.85	3661.53			
3032.79	3033.47	3034.32	3036.33	3041.52	3041.96						

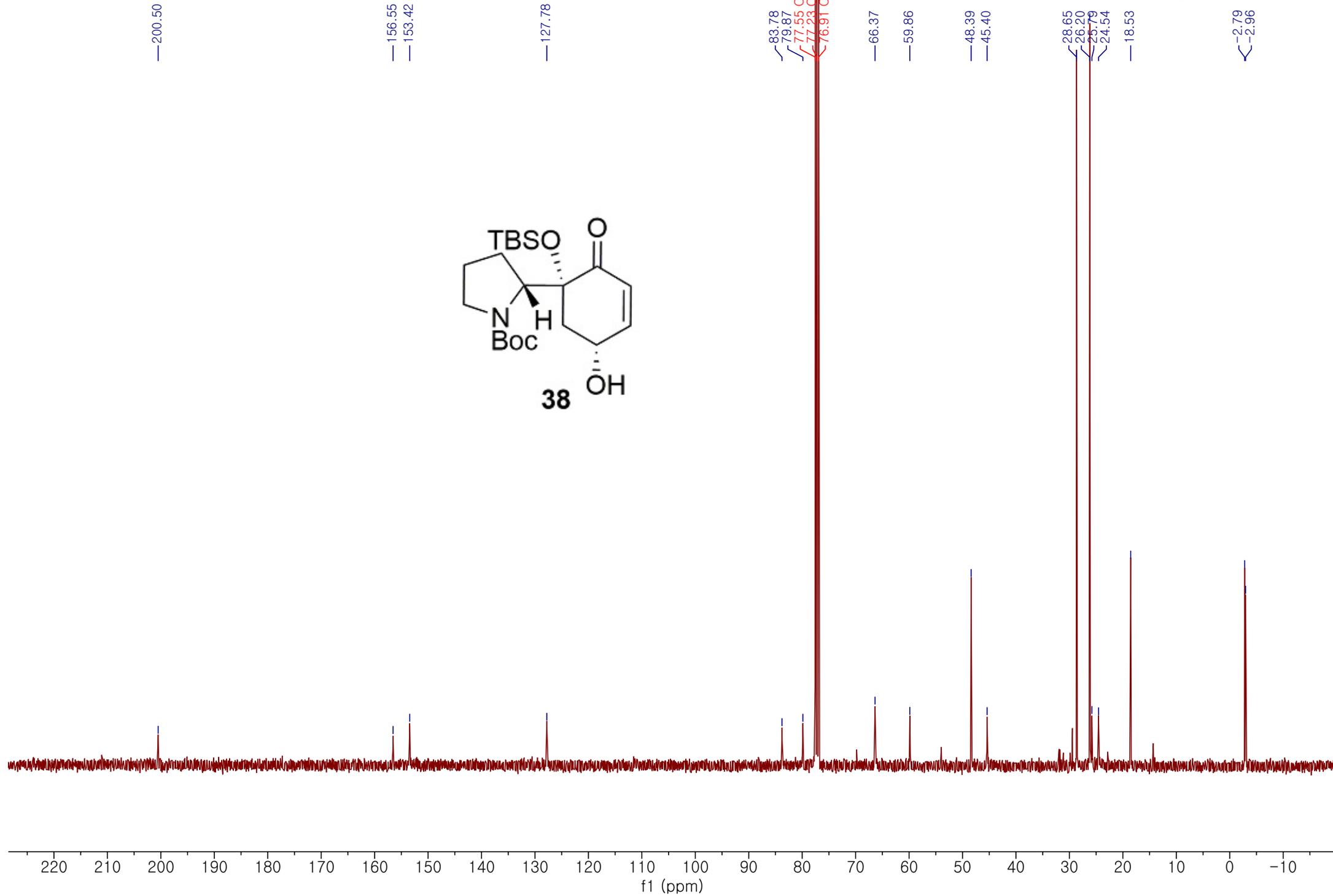
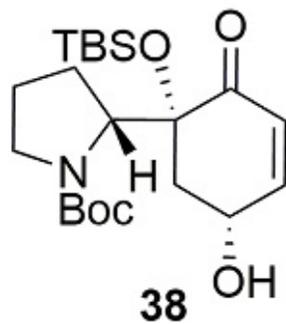
6. References

- (1) Parr, R. G.; Yang, W. *Density Functional Theory of Atoms and Molecules*. Oxford University Press: New York, **1989**
- (2) Bochevarov, A. D.; Harder, E.; Hughes, T. F.; Greenwood, J. R.; Braden, D. A.; Philipp, D. M.; Rinaldo, D.; Halls, M. D.; Zhang, J.; Friesner, R. Jaguar: a high-performance quantum chemistry software program with strengths in life and materials sciences. *Int. J. Quantum Chem.* **2013**, *113*, 2110–2142.
- (3) Slater, J. C. *Quantum Theory of Molecules and Solids, Vol. 4: The Self-Consistent Field for Molecules and Solids*. McGraw-Hill: New York, 1974.
- (4) Vosko, S. H.; Wilk, L.; Nusair, M. Accurate spin-dependent electron liquid correlation energies for local spin density calculations: a critical analysis. *Can. J. Phys.* **1980**, *58*, 1200–1211.
- (5) Becke, A. D. Density-functional exchange-energy approximation with correct asymptotic behavior. *Phys. Rev. A* **1988**, *38*, 3098–3100.
- (6) Becke, A. D. Density-functional thermochemistry. III. The role of exact exchange. *J. Chem. Phys.* **1993**, *98*, 5648–5652.
- (7) Lee, C.; Yang, W.; Parr, R. G. Development of the Colle-Salvetti correlation-energy formula into a functional of the electron density. *Phys. Rev. B* **1988**, *37*, 785.
- (8) Grimme, S.; Antony, J.; Ehrlich, S.; Krieg, H. A consistent and accurate *ab initio* parametrization of density functional dispersion correction (DFT-D) for the 94 elements H-Pu. *J. Chem. Phys.* **2010**, *132*, 154104.
- (9) Dunning, T. H., Jr. Gaussian basis sets for use in correlated molecular calculations. I. The atoms boron through neon and hydrogen. *J. Phys. Chem.* **1989**, *90*, 1007.
- (10) Marten, B.; Kim, K.; Cortis, C.; Friesner, R. A.; Murphy, R. B.; Ringnalda, M. N.; Sitkoff, D.; Honig, B. New model for calculation of solvation free energies: correction of self-consistent reaction field continuum dielectric theory for short-range hydrogen-bonding effects. *J. Phys. Chem.* **1996**, *100*, 11775–11788.
- (11) Edinger, S. R.; Cortis, C.; Shenkin, P. S.; Friesner, R. A. Solvation free energies of peptides: Comparison of approximate continuum solvation models with accurate solution of the Poisson–Boltzmann equation. *J. Phys. Chem. B* **1997**, *101*, 1190–1197.
- (12) Friedrichs, M.; Zhou, R.; Edinger, S. R.; Friesner, R. A. Poisson– Boltzmann analytical gradients for molecular modeling calculations. *J. Phys. Chem. B* **1999**, *103*, 3057–3061.
- (13) Rashin, A. A.; Honig, B. Reevaluation of the Born model of ion hydration. *J. Phys. Chem.* **1985**, *89*, 5588–5593.

7. Copies of NMR and IR Spectra



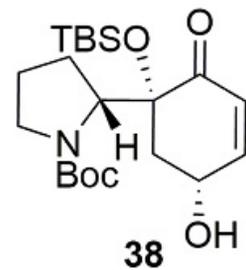




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Transmittance [%]

100
95
90
85
80
75
70
65



3500

3000

2500

2000

1500

1000

500

Wavenumber cm-1

3421.58

2955.28

2929.14

2894.78

2855.84

1690.21

1668.83

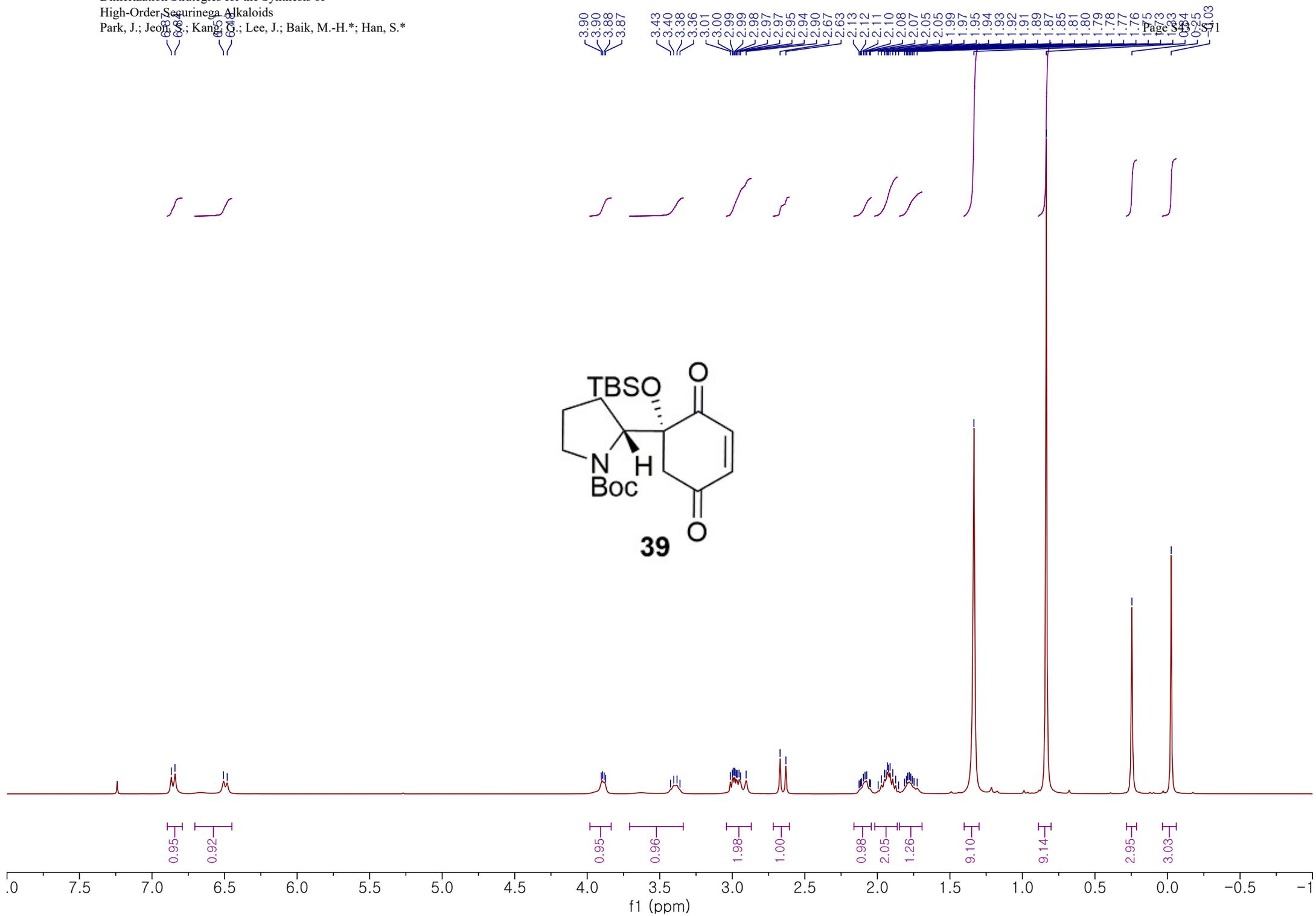
1390.39

D:\USERS\PJNDMDO.0

Sample description

Instrument type and / or accessory

12/12/2018



— 198.88
— 195.06

— 155.47

— 142.24
— 138.47

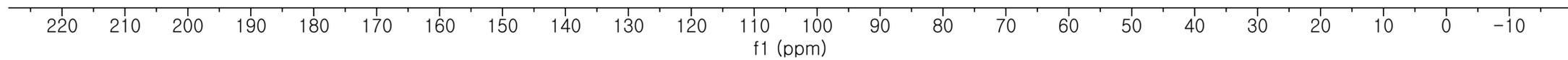
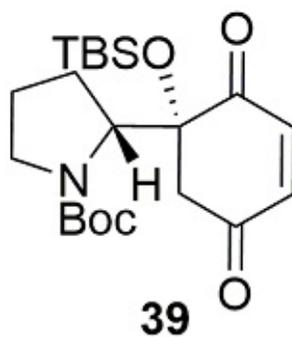
83.48
80.52
77.55 CDCl₃
77.23 CDCl₃
76.91 CDCl₃

— 64.33

< 48.56
< 48.29

< 28.43
< 26.79
< 26.12
< 24.82
— 18.79

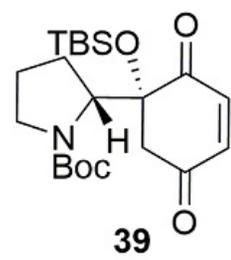
< -2.48
< -2.78





Transmittance [%]

95
90
85
80
75
70
65



3500 3000 2500 2000 1500 1000 500

Wavenumber cm-1

2979.35
2957.51
2928.41
2890.69
2853.39

1698.33
1681.09

1383.12

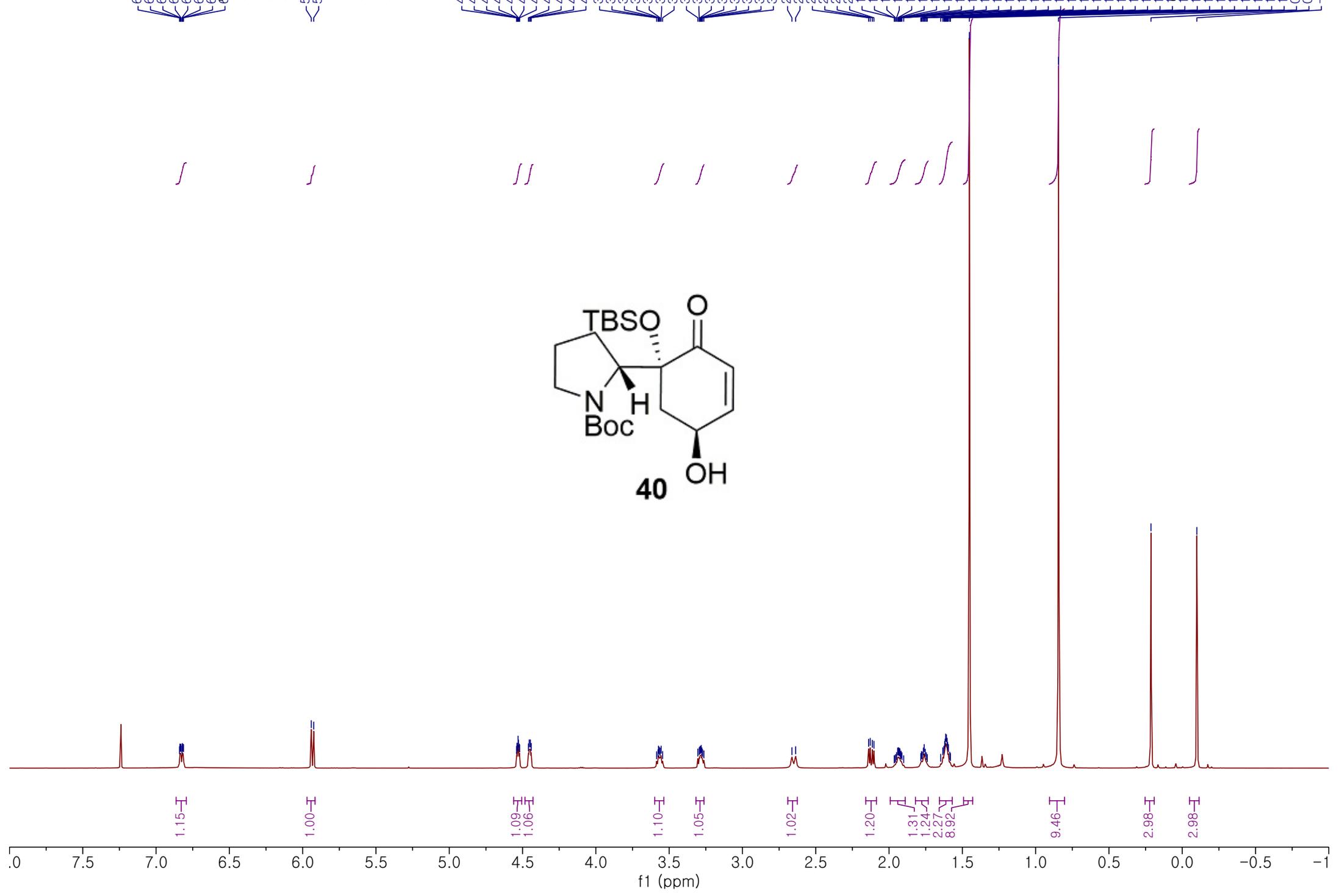
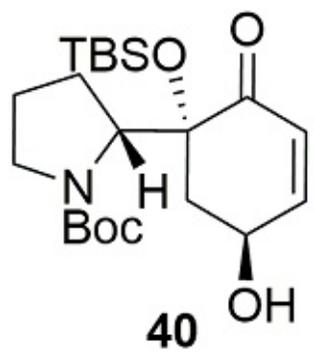
1143.94

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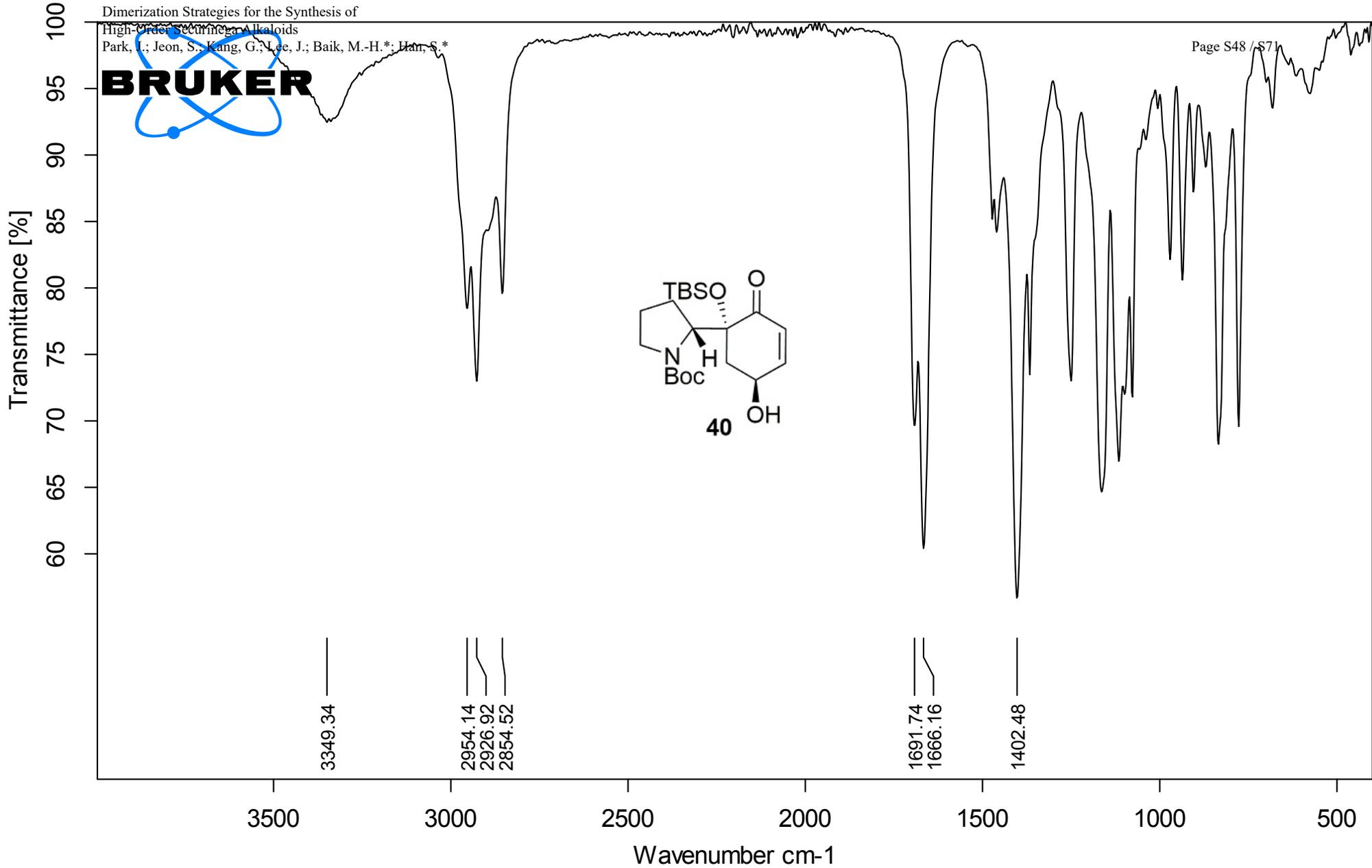
Sample description

Instrument type and / or accessory

12/12/2018



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D:\USERS\PJNLuche.0	Sample description	Instrument type and / or accessory	12/12/2018
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211.95

206.57

158.32

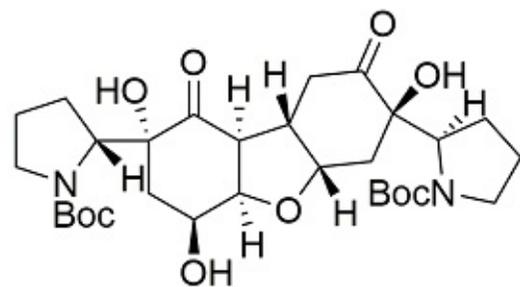
156.84

81.30
80.82
79.46
78.66
77.78
77.44
77.26
77.02
74.42
65.99
64.35
63.80

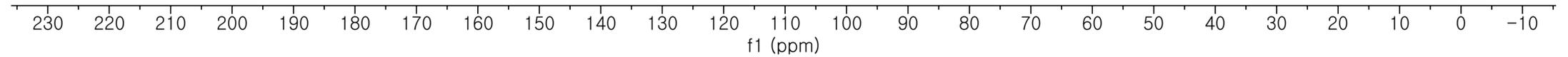
52.56
48.76
48.42

41.16
40.06
39.15
35.93

28.83
28.61
28.56
28.03
24.52
22.86



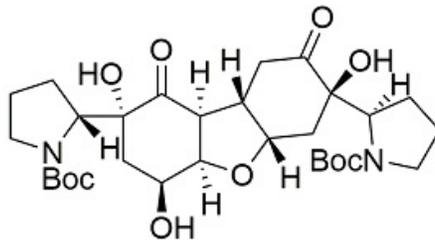
41



BRUKER

Transmittance [%]

100
98
96
94
92
90
88
86



41

3500 3000 2500 2000 1500 1000 500

Wavenumber cm-1

3437.57

3194.02

2959.73

2924.23

2853.83

1723.49

1690.45

1651.35

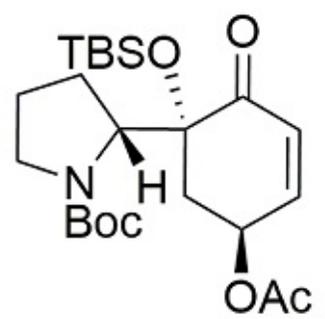
1410.52

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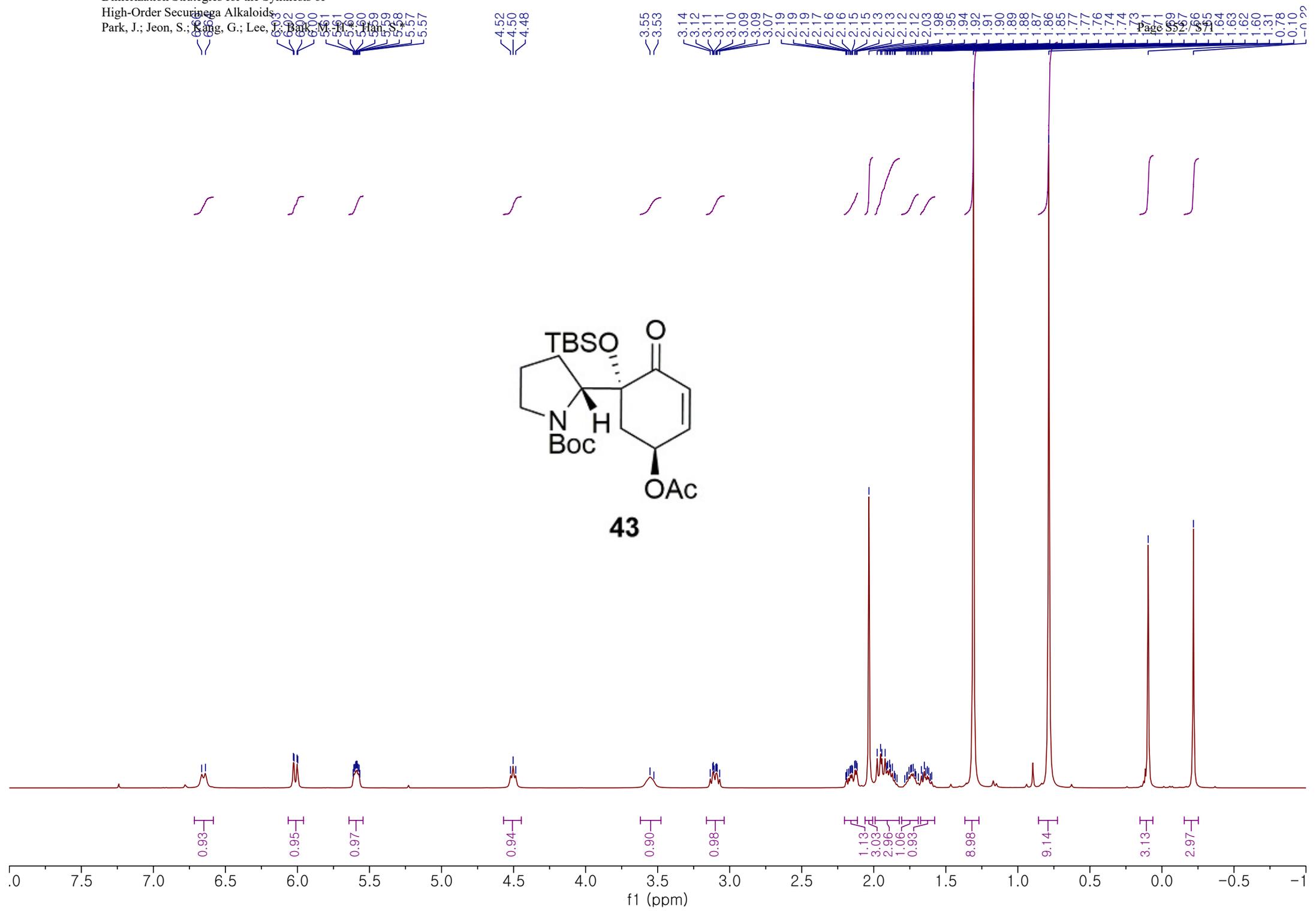
Sample description

Instrument type and / or accessory

12/12/2018

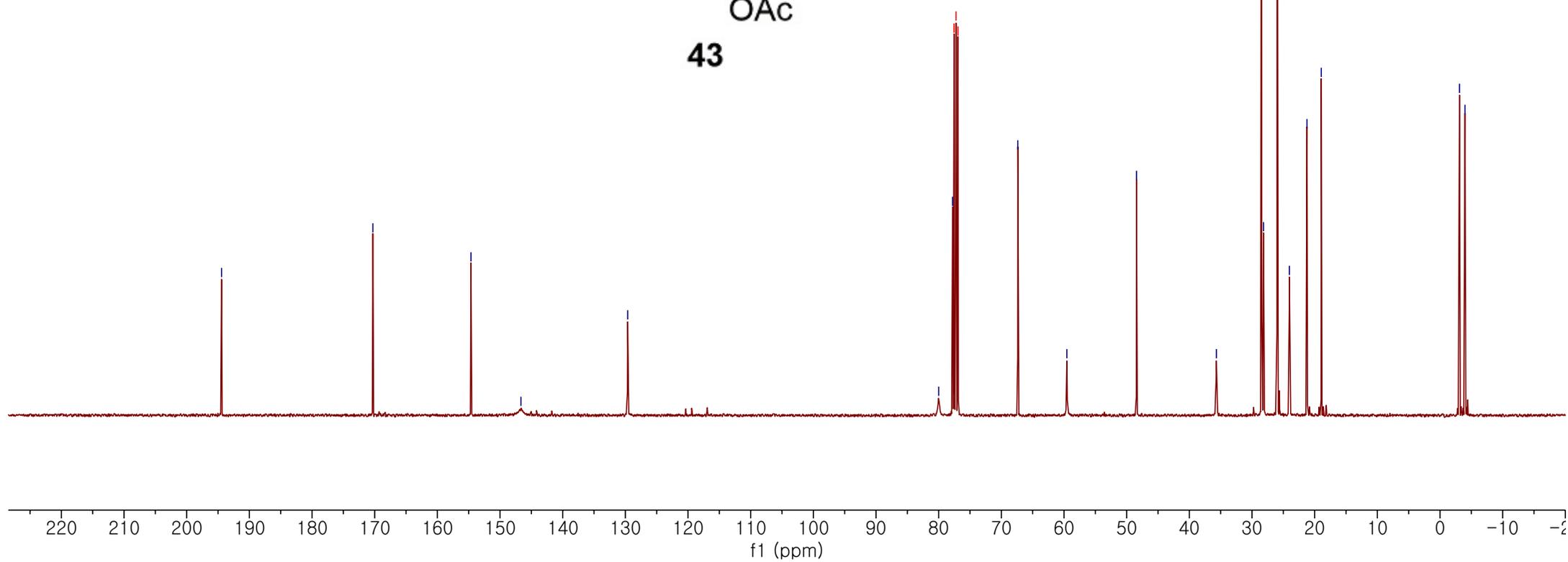
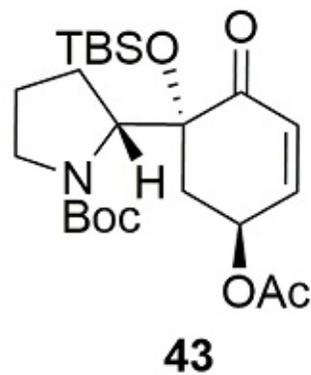


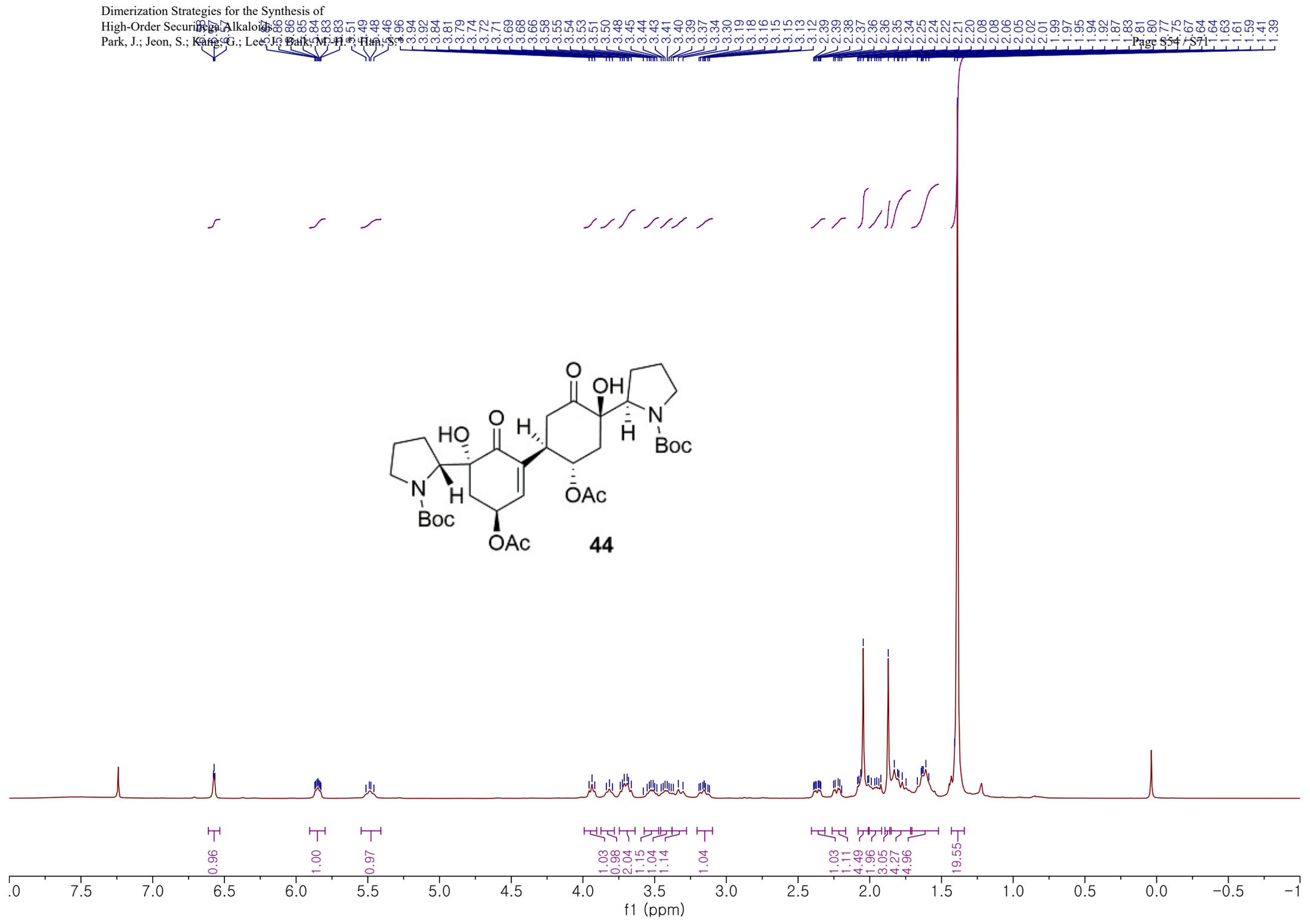
43



— 194.44 — 170.29 — 154.63 — 146.66 — 129.62

80.00 77.78 77.55 CDC13 77.23 CDC13 76.91 CDC13 — 67.37 — 59.54 — 48.43 — 35.68 — 28.46 — 28.17 — 26.00 — 24.03 — 21.23 — 18.95 — 3.11 — 3.99





Dimerization Strategies for the Synthesis of High-Order Securinega Alkaloids

Park, J.; Jeon, S.; Kang, G.; Lee, J.; Baik, M.-H.*; Han, S.*

— 208.35

— 194.75

< 170.31
< 170.07

< 158.19
< 158.08

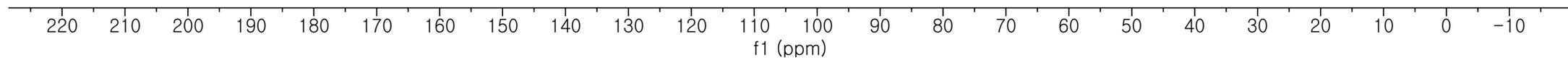
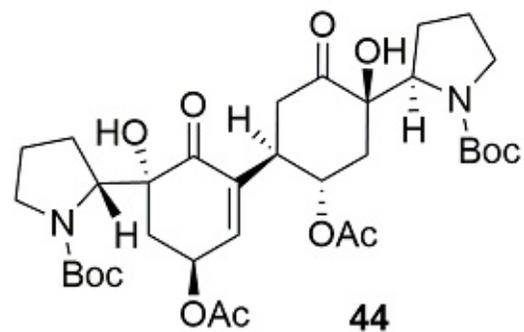
— 143.02

— 138.63

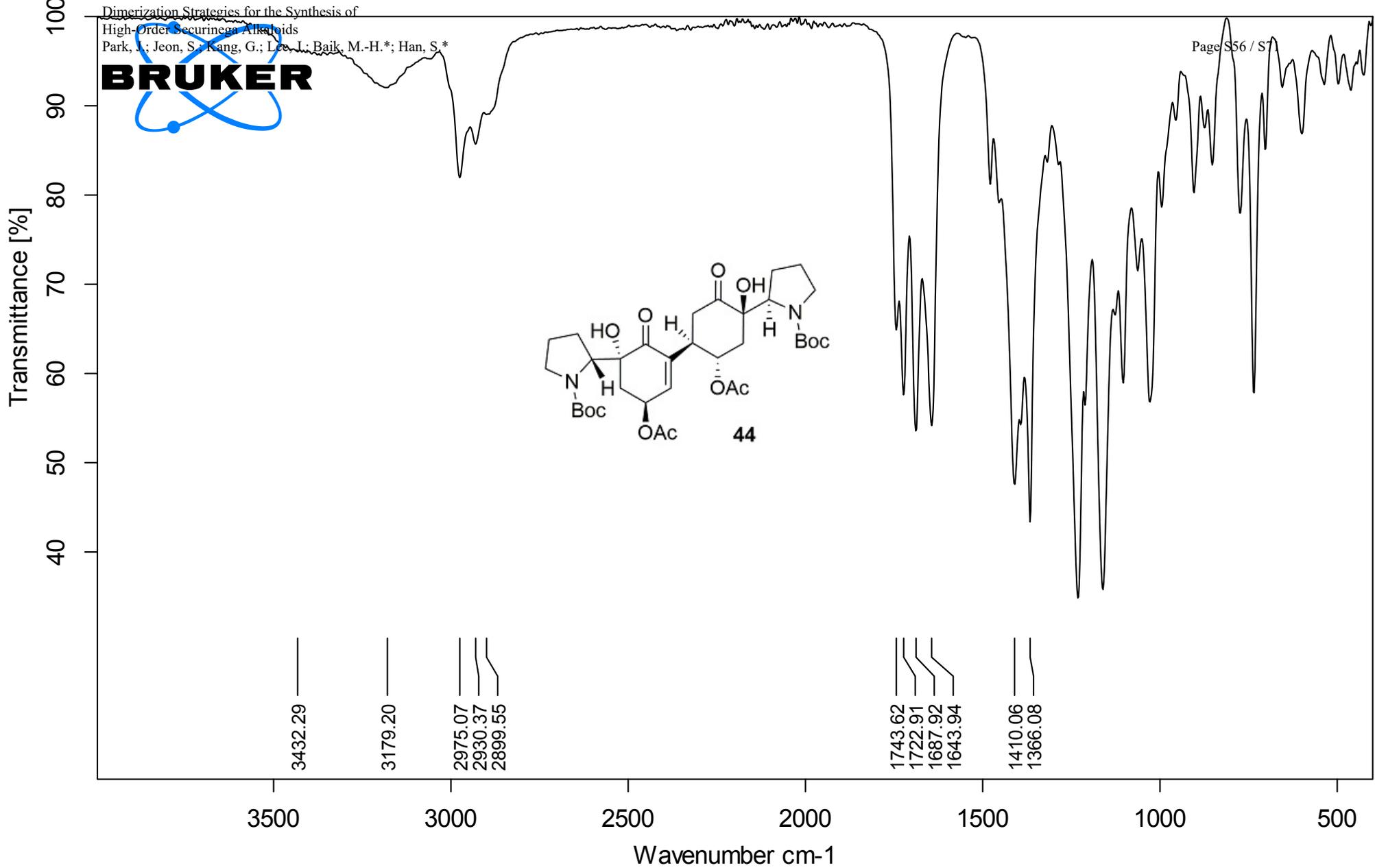
81.07
81.04
79.20
77.55 CDC13
77.23 CDC13
76.91 CDC13
72.18
68.17
64.18
63.92

< 48.52
< 48.29
< 42.09
< 41.31
< 40.91
< 40.77

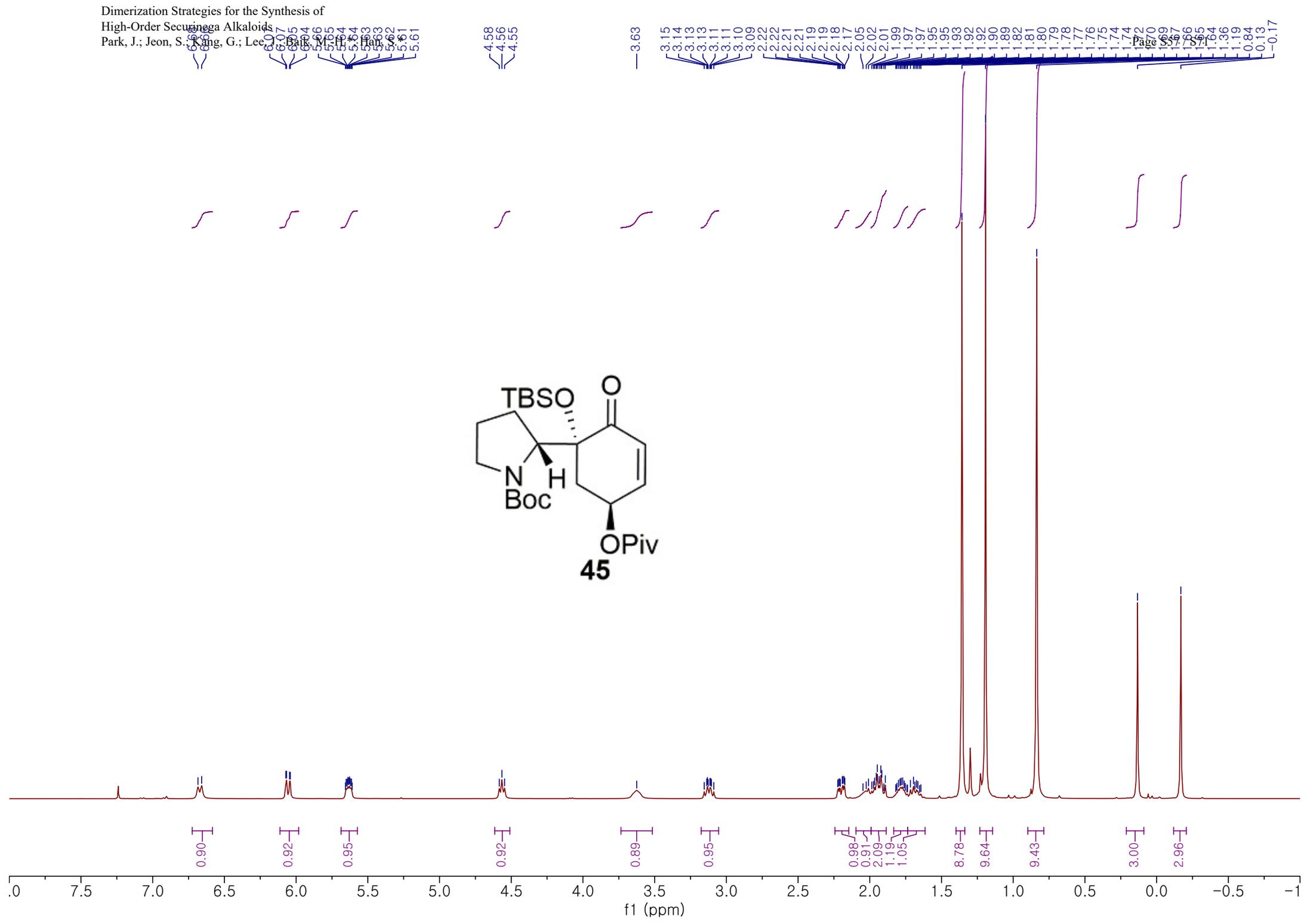
< 29.00
< 28.85
< 28.55
< 24.64
< 21.29
< 21.17

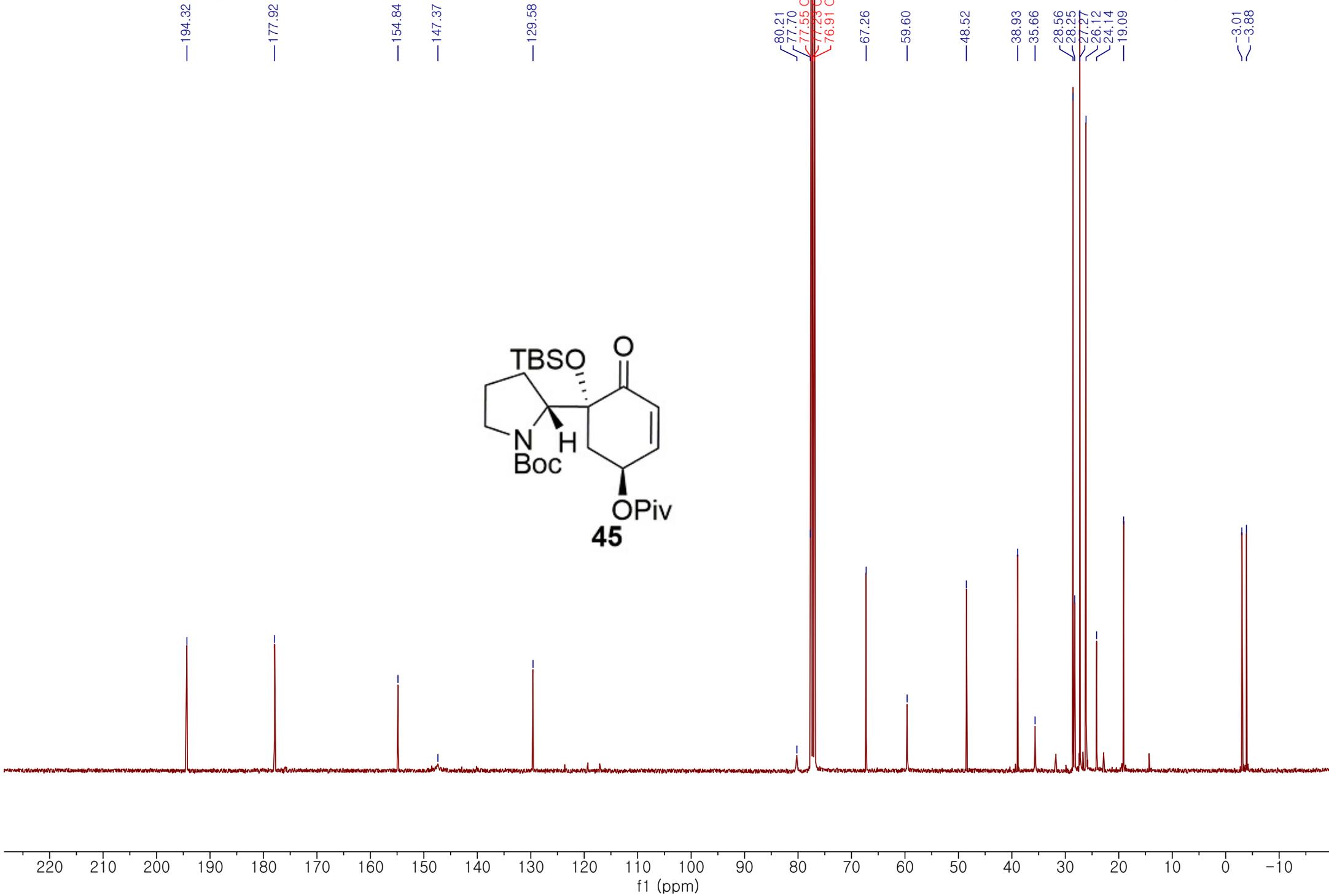


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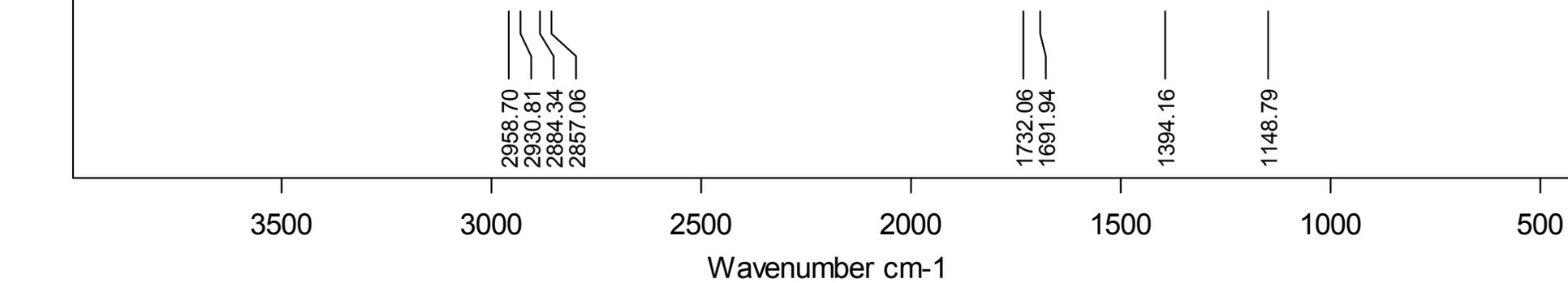
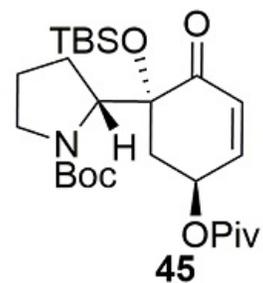
D:\USERS\PJNTBAF-OAc.0	Sample description	Instrument type and / or accessory	12/12/2018
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Transmittance [%]

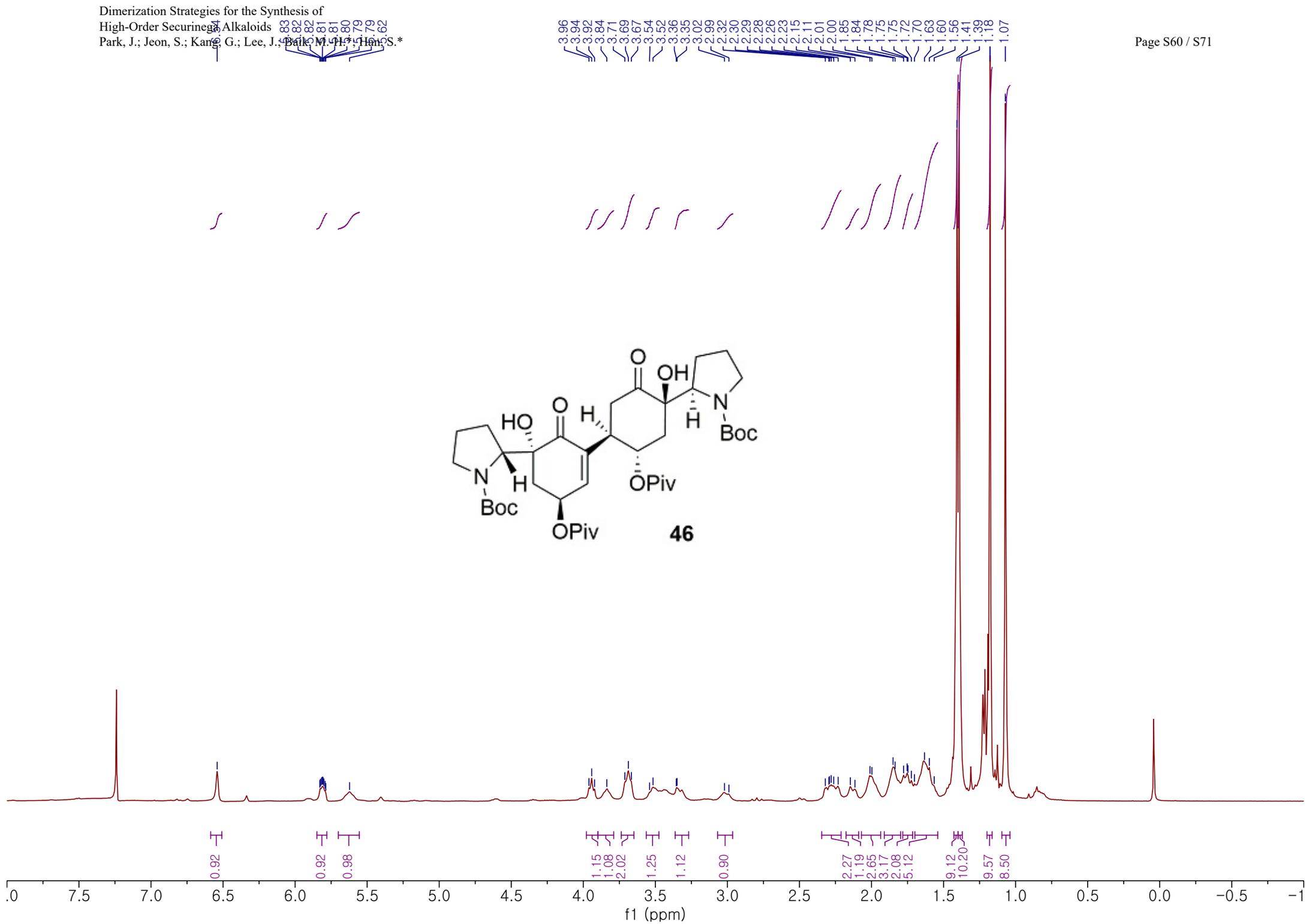


D:\USERS\PJN\pival-monomer.0

Sample description

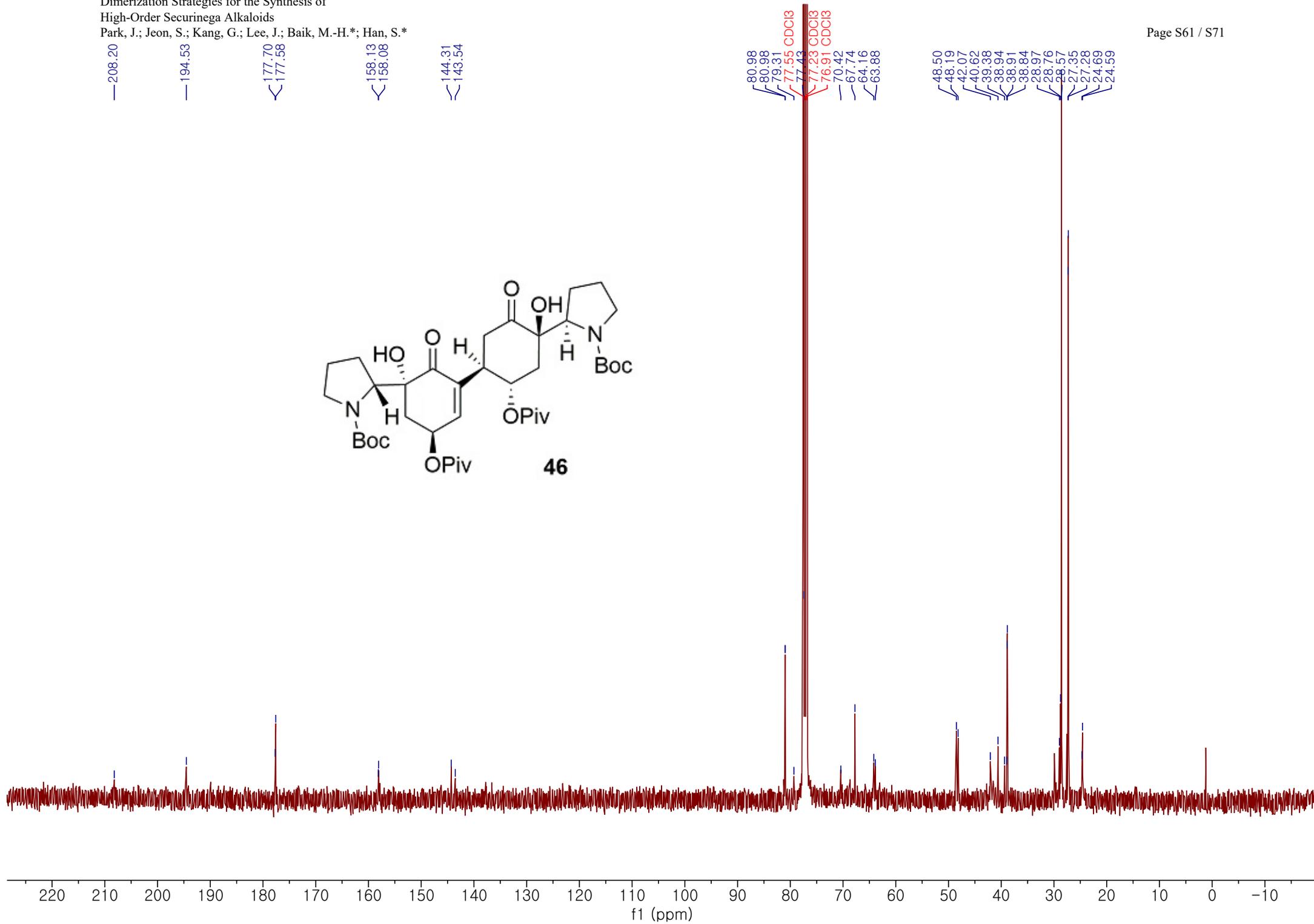
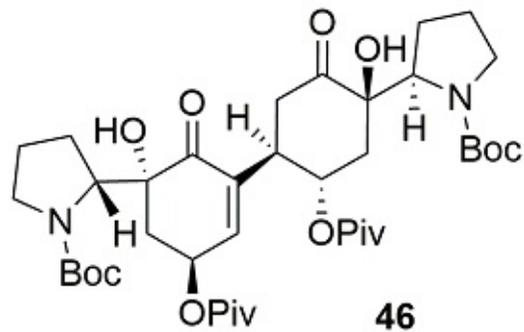
Instrument type and / or accessory

12/12/2018



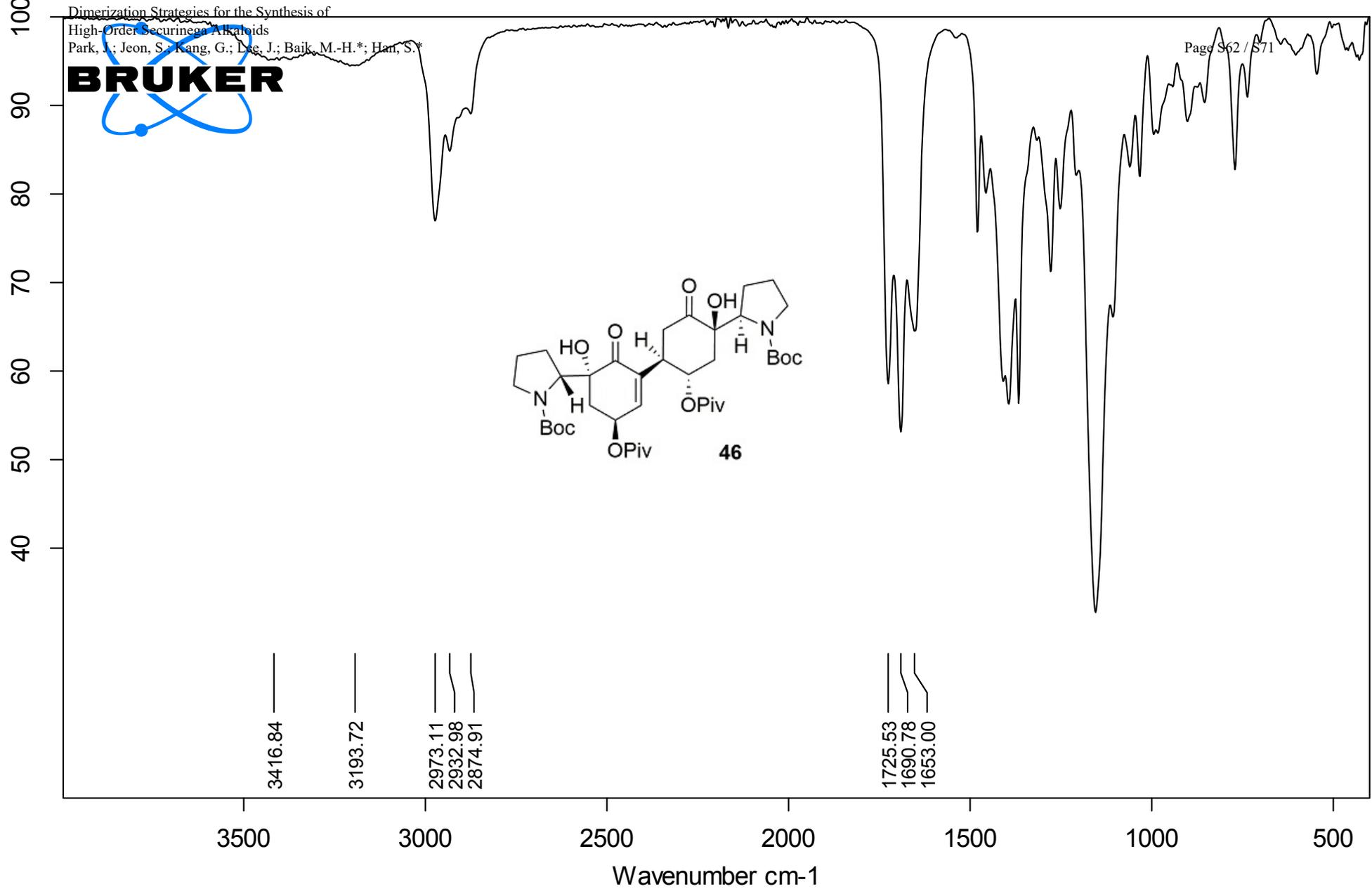
— 208.20
— 194.53
∠ 177.70
∠ 177.58
∠ 158.13
∠ 158.08
∠ 144.31
∠ 143.54

80.98
80.98
79.31
77.55 CDCl3
77.43
77.23 CDCl3
76.91 CDCl3
70.42
67.74
64.16
63.88
48.50
48.19
42.07
40.62
39.38
38.94
38.91
38.84
28.97
28.76
28.57
27.35
27.28
24.69
24.59

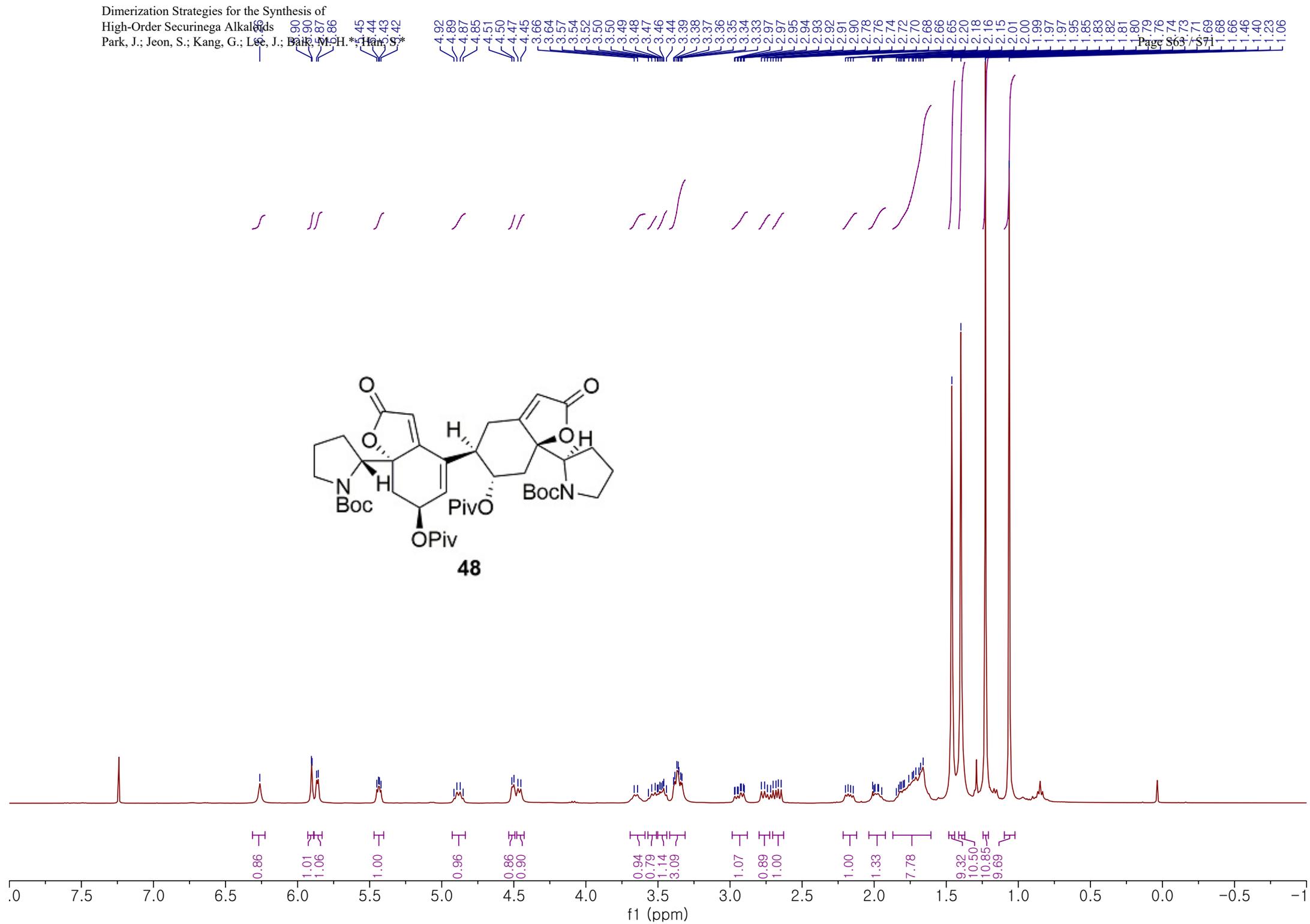


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Transmittance [%]



D:\Users\PJN\Pival-dimer.0	Sample description	Instrument type and / or accessory	12/17/2018
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178.15
177.50
172.23
171.98
168.01
166.73

156.68
155.06

135.75
131.29

117.45
113.32

90.50
88.39

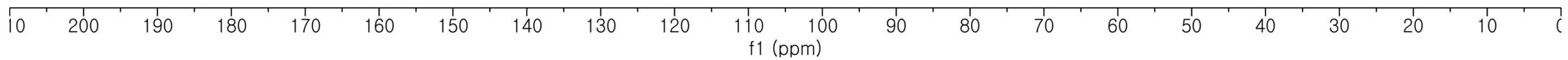
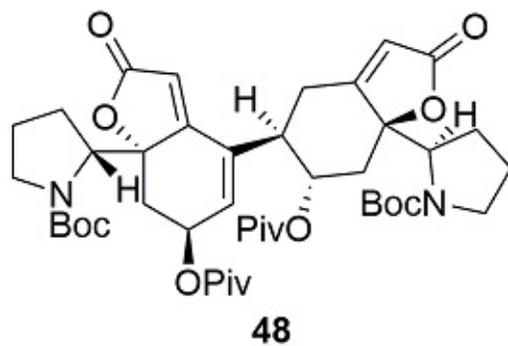
80.63
79.60
77.55 CDCl3
77.26 CDCl3
76.91 CDCl3

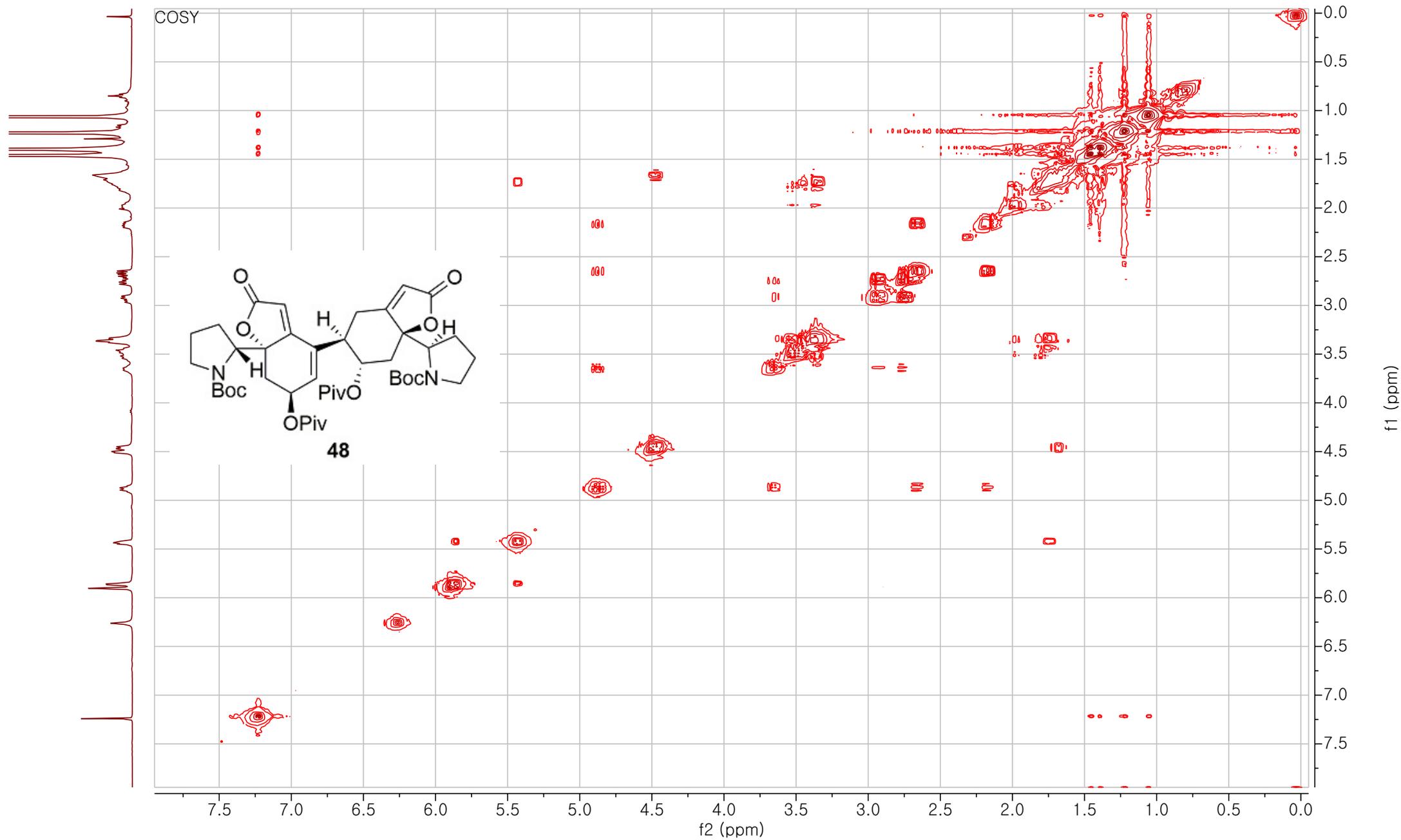
70.70
66.61

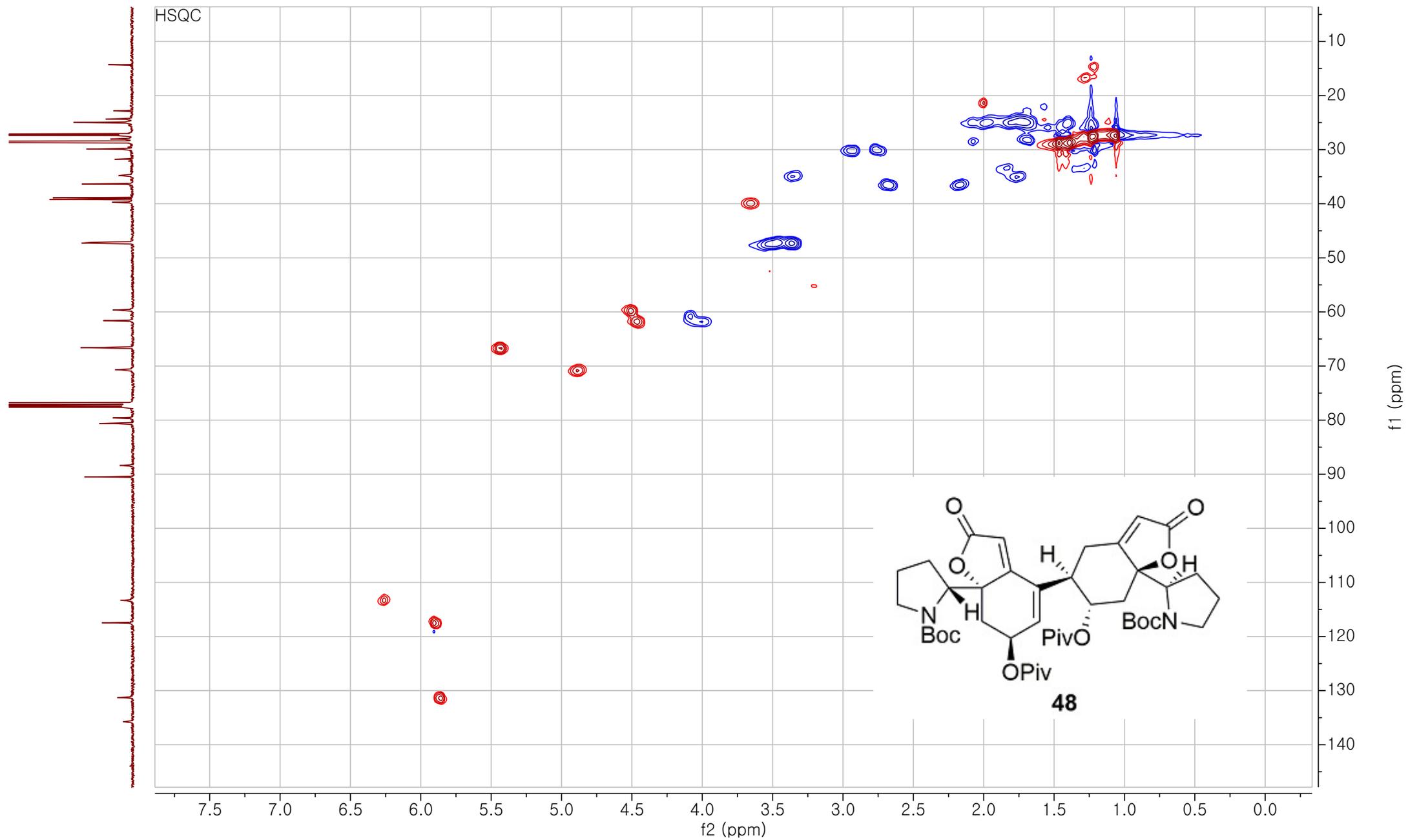
61.62
59.65

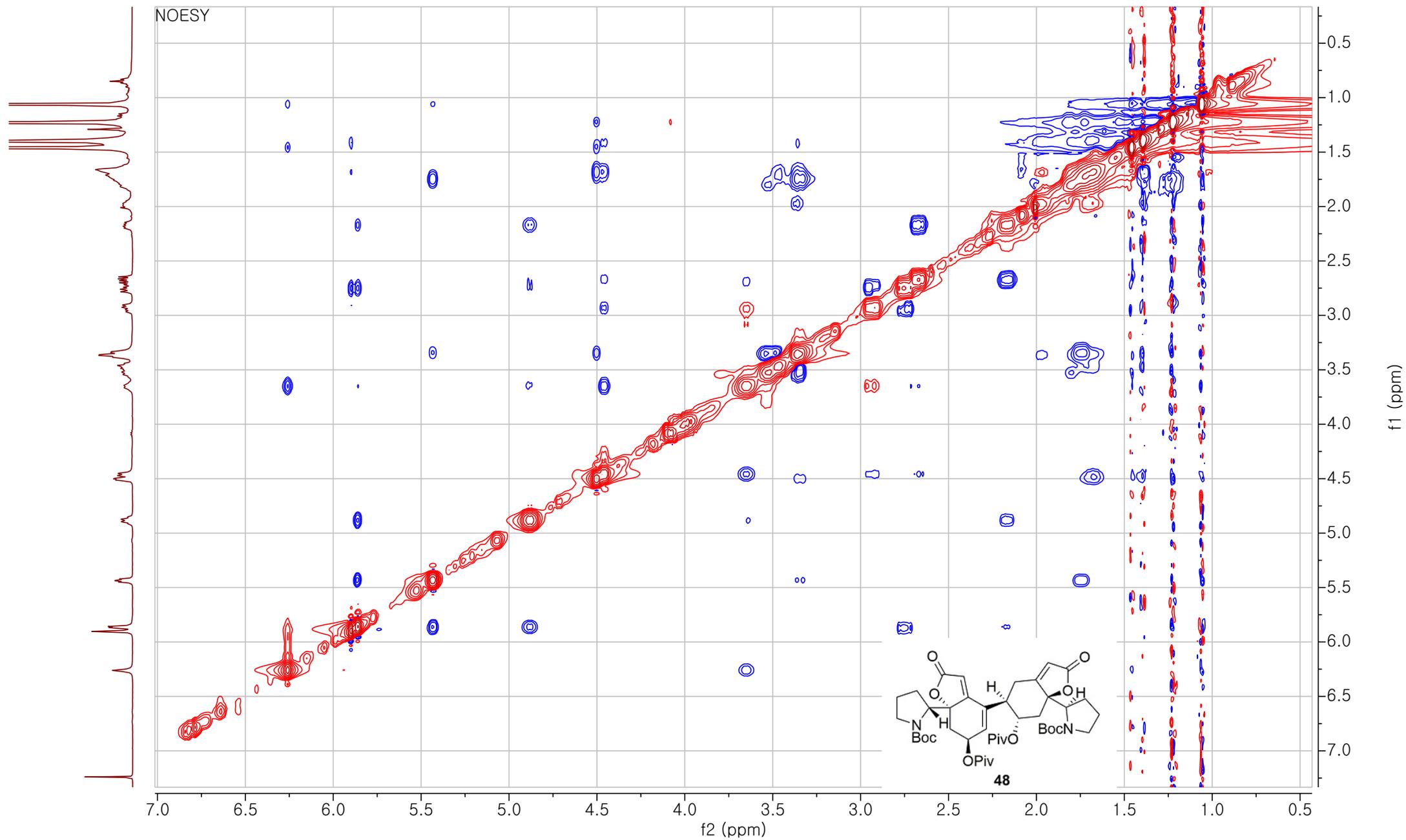
47.26
47.13

39.74
39.20
38.92
36.34
34.77
29.88
28.55
28.03
27.36
27.17
24.97
24.34

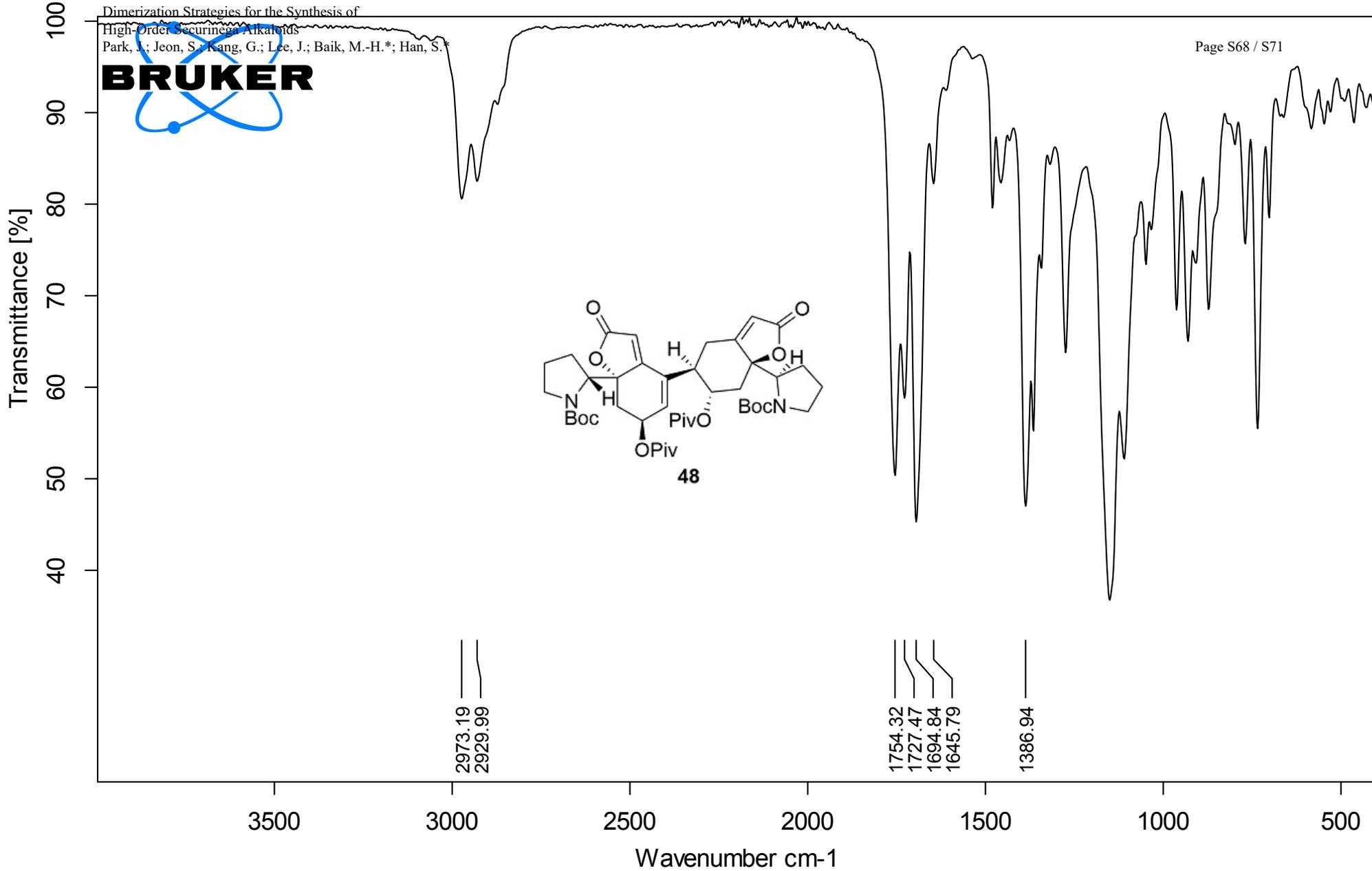




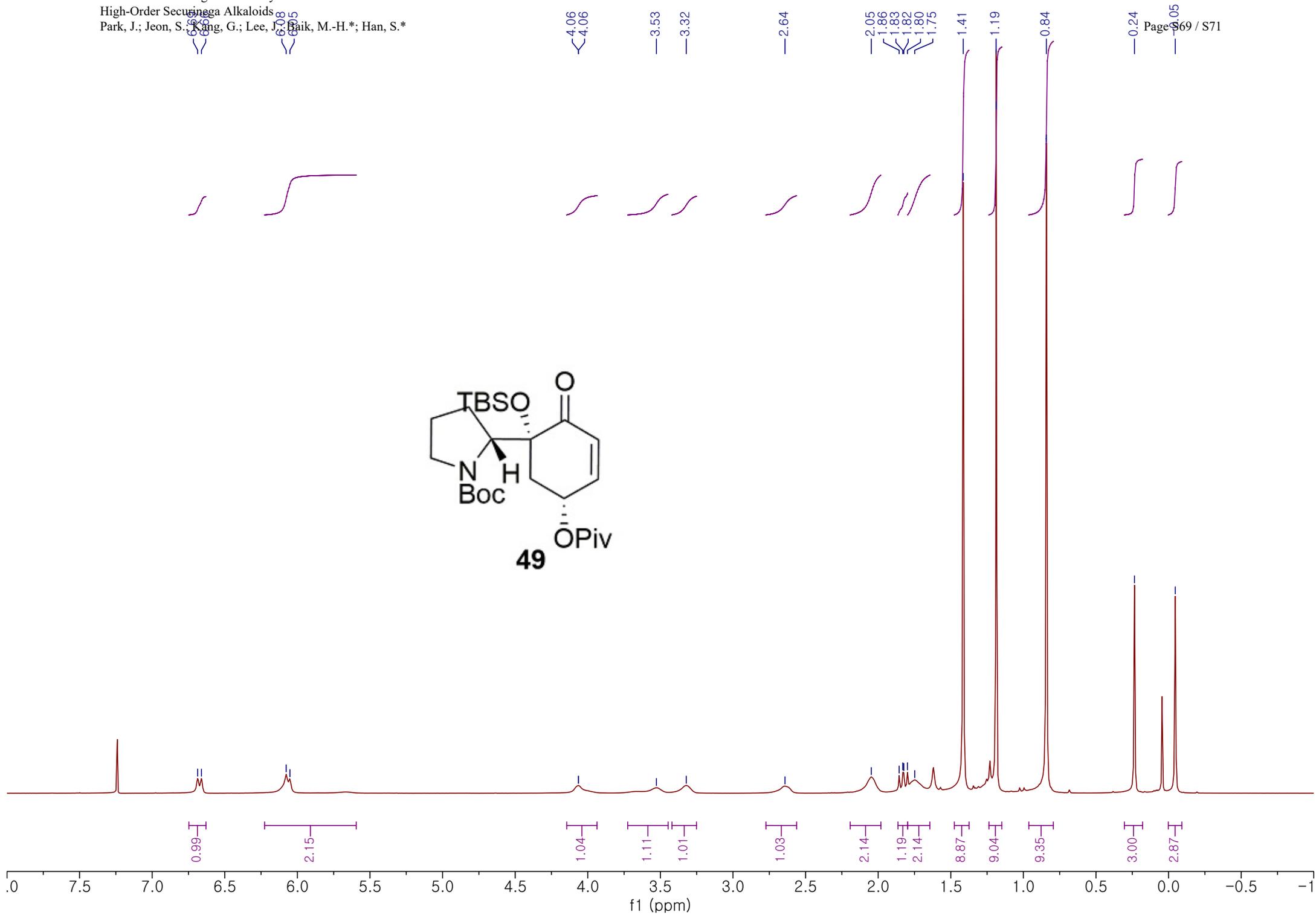


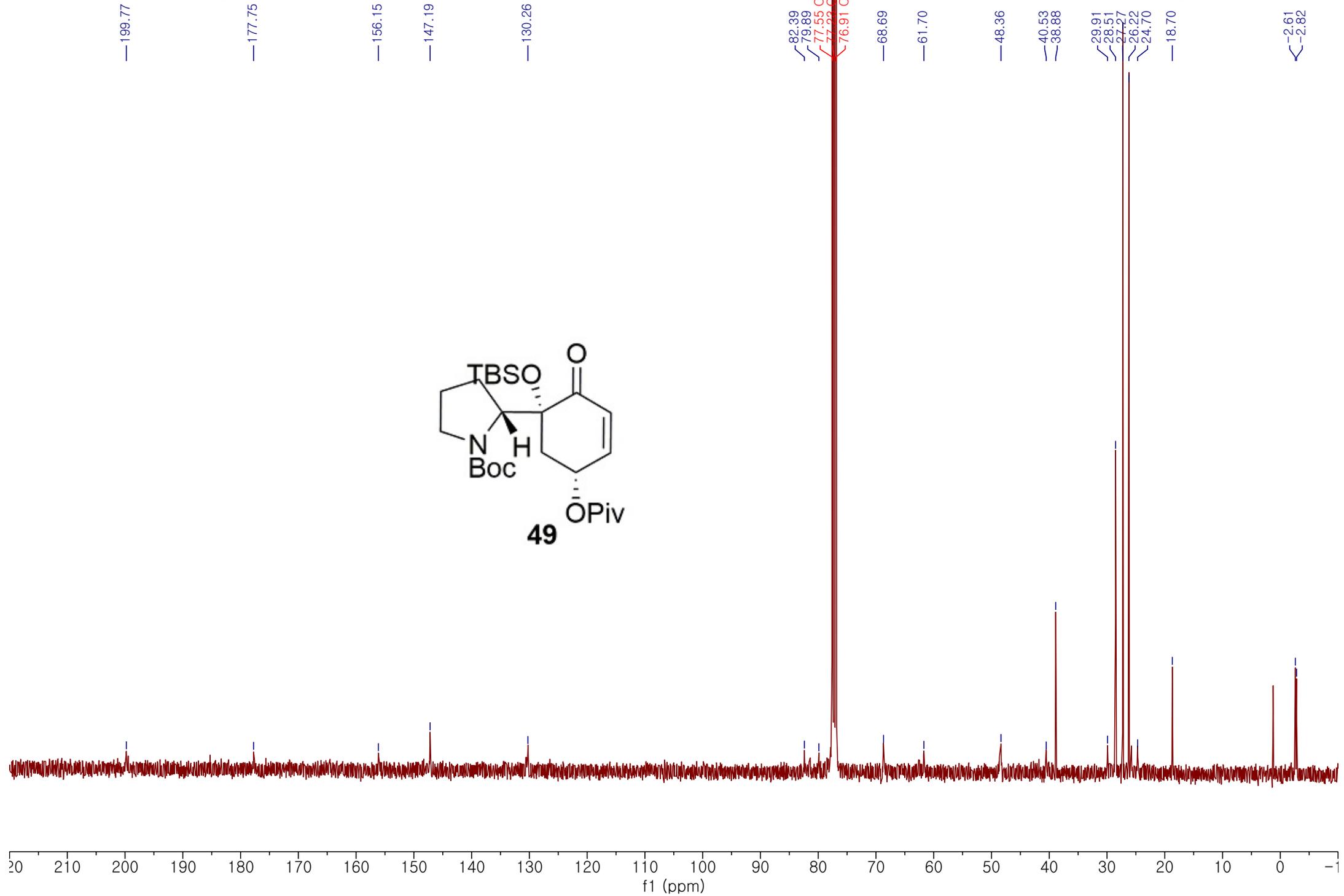
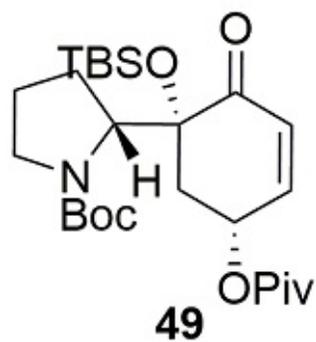


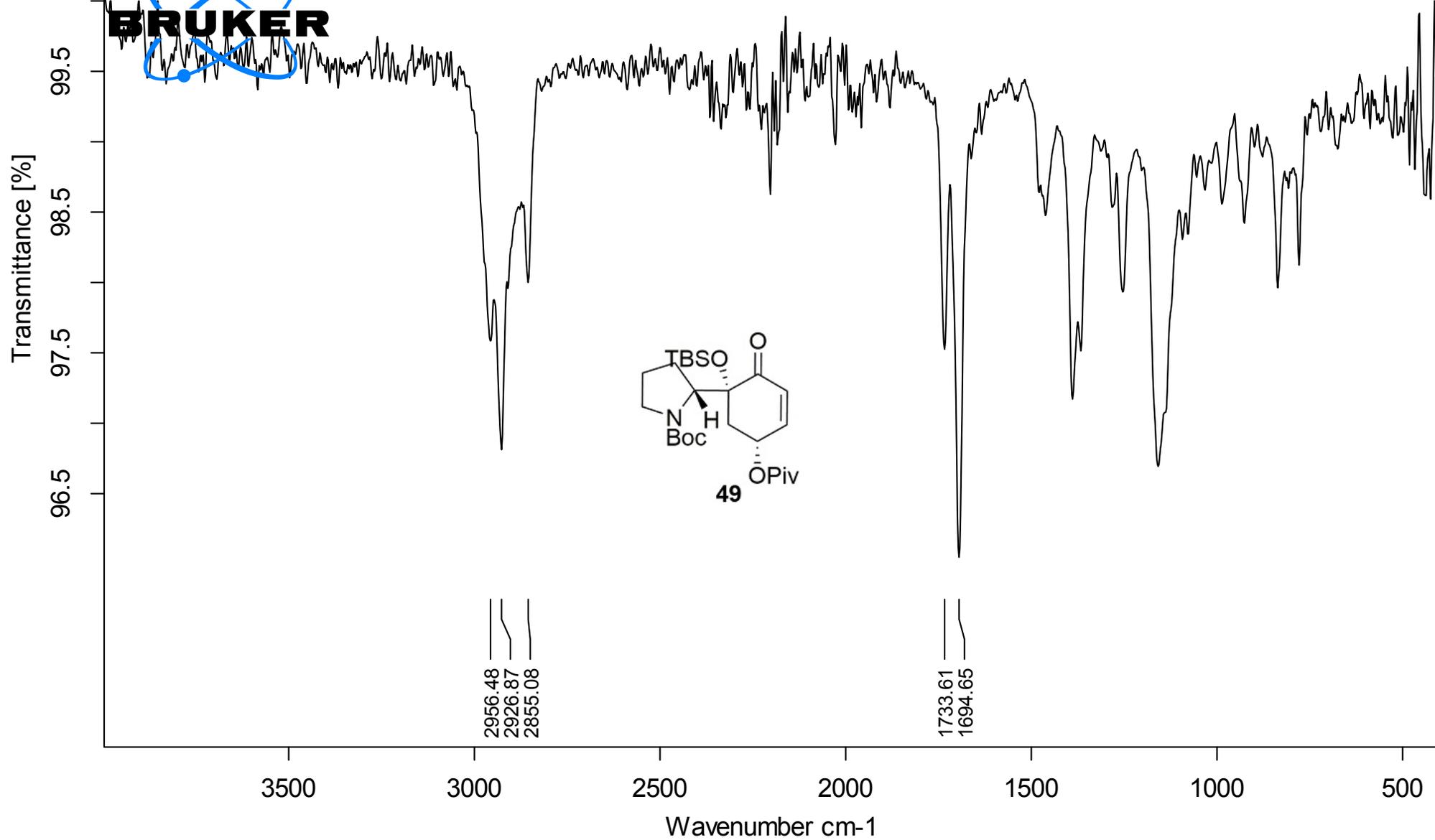
BRUKER



D:\USERS\PJ\NDBU.0	Sample description	Instrument type and / or accessory	12/12/2018
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D:\USERS\PJN\normal-monomer-pival.1

Sample description

Instrument type and / or accessory

12/12/2018