Supplementary Information

for

Diacetoxyiodobenzene Assisted C-O Bond Formation via Sequential Acylation and Deacylation Process: Synthesis of Benzoxazole Amides and Its Mechanistic Study by DFT

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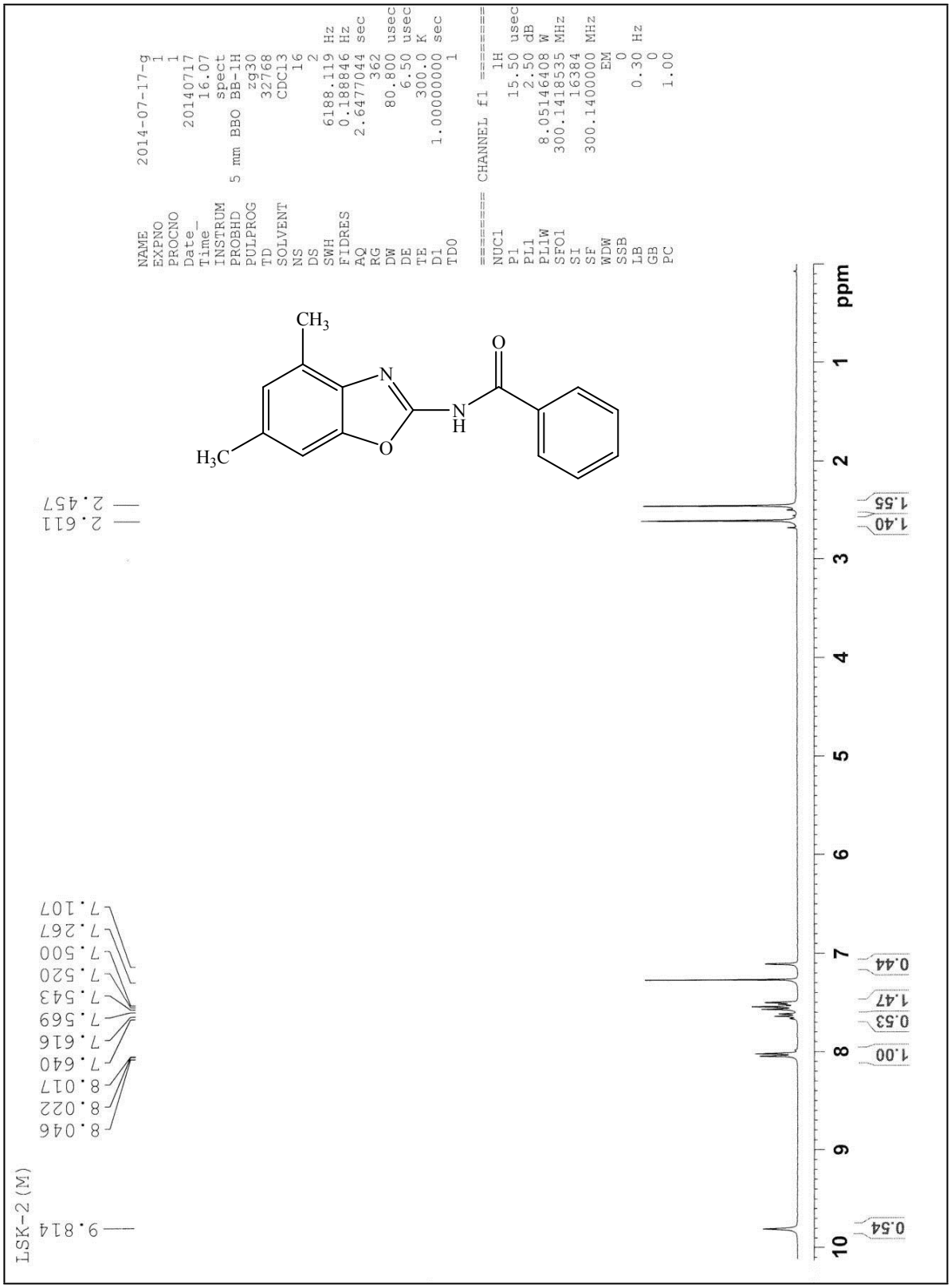
Table of contents

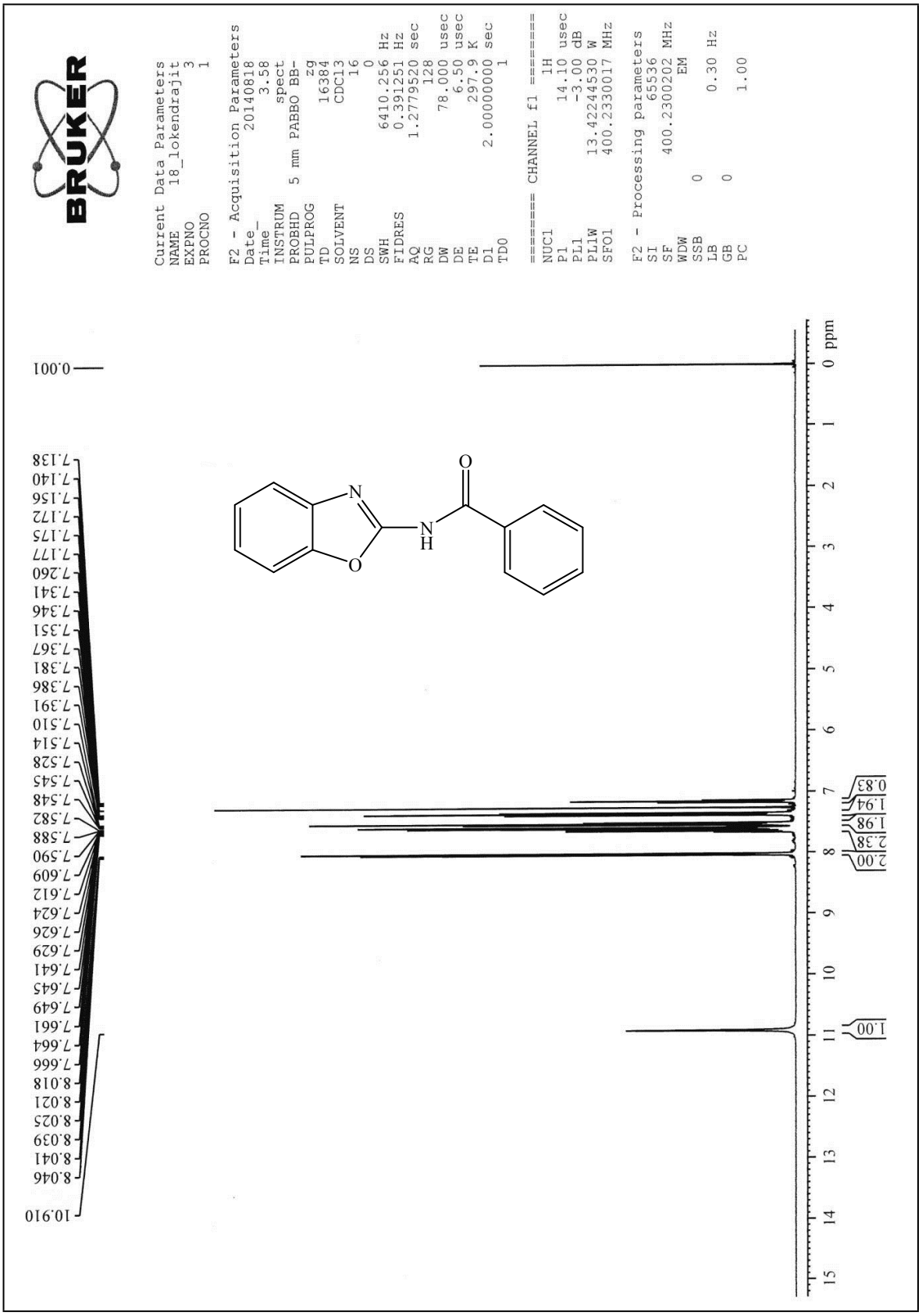
^{1}H NMR and ^{13}C NMR SPECTRA

^{1}H NMR Spectrum of *N*-(4, 6-dimethylbenzo[*d*]oxazol-2-yl) benzamide(2a):

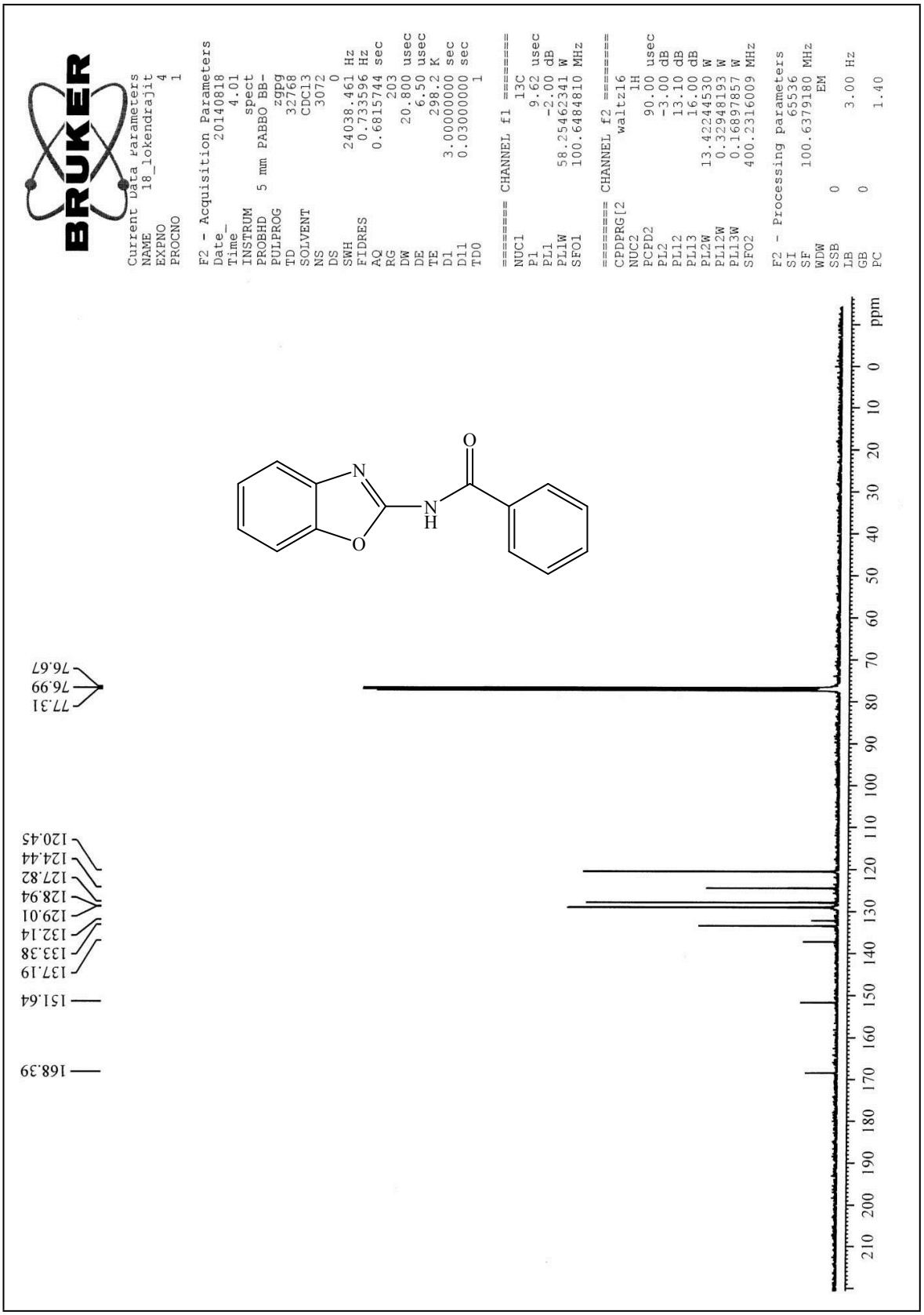


^{13}C NMR Spectrum of *N*-(4, 6-dimethylbenzo[*d*]oxazol-2-yl)benzamide(2a):

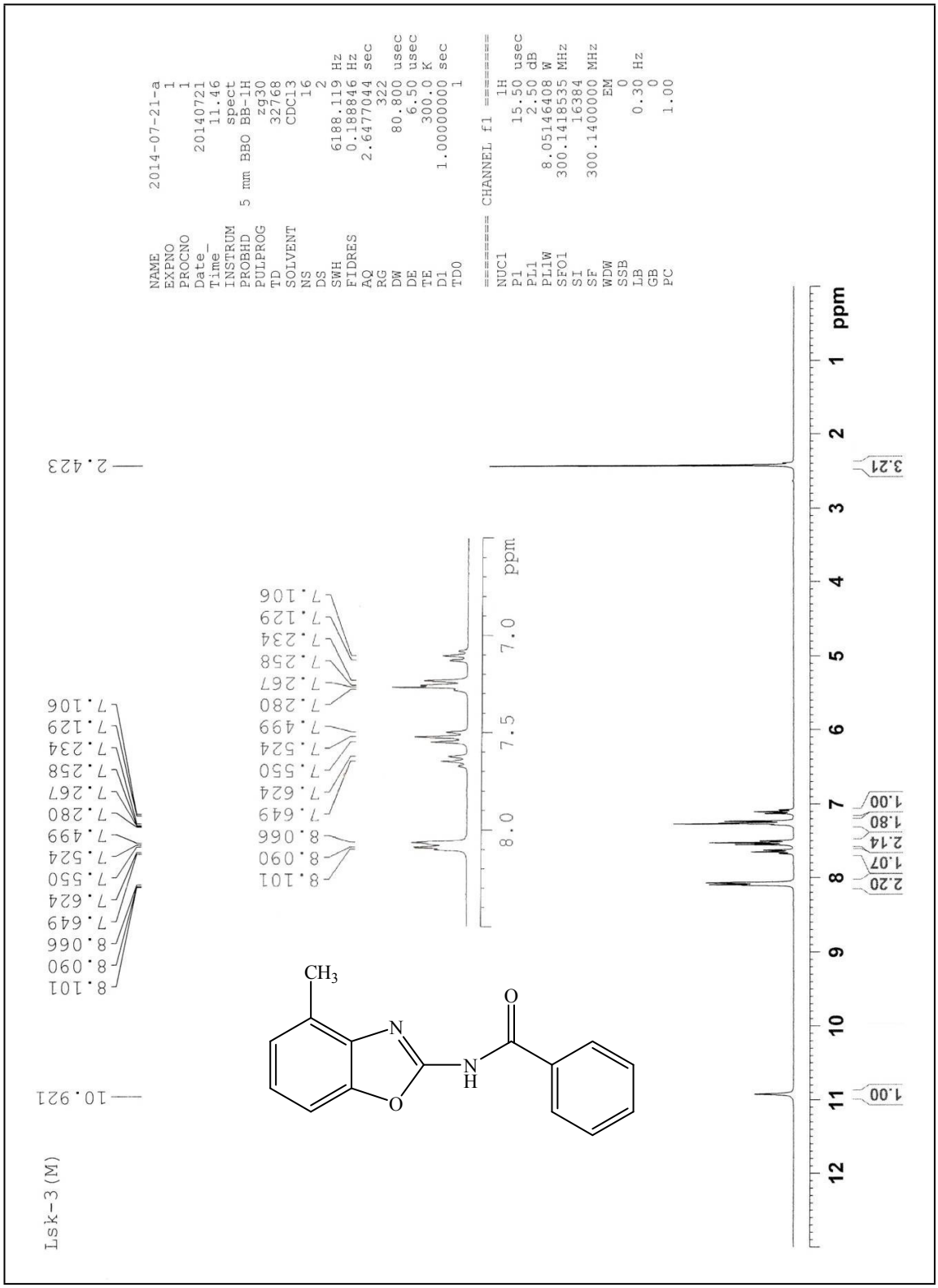
^{1}H NMR Spectrum of *N*-(benzo[*d*]oxazol-2-yl)benzamide (2b):



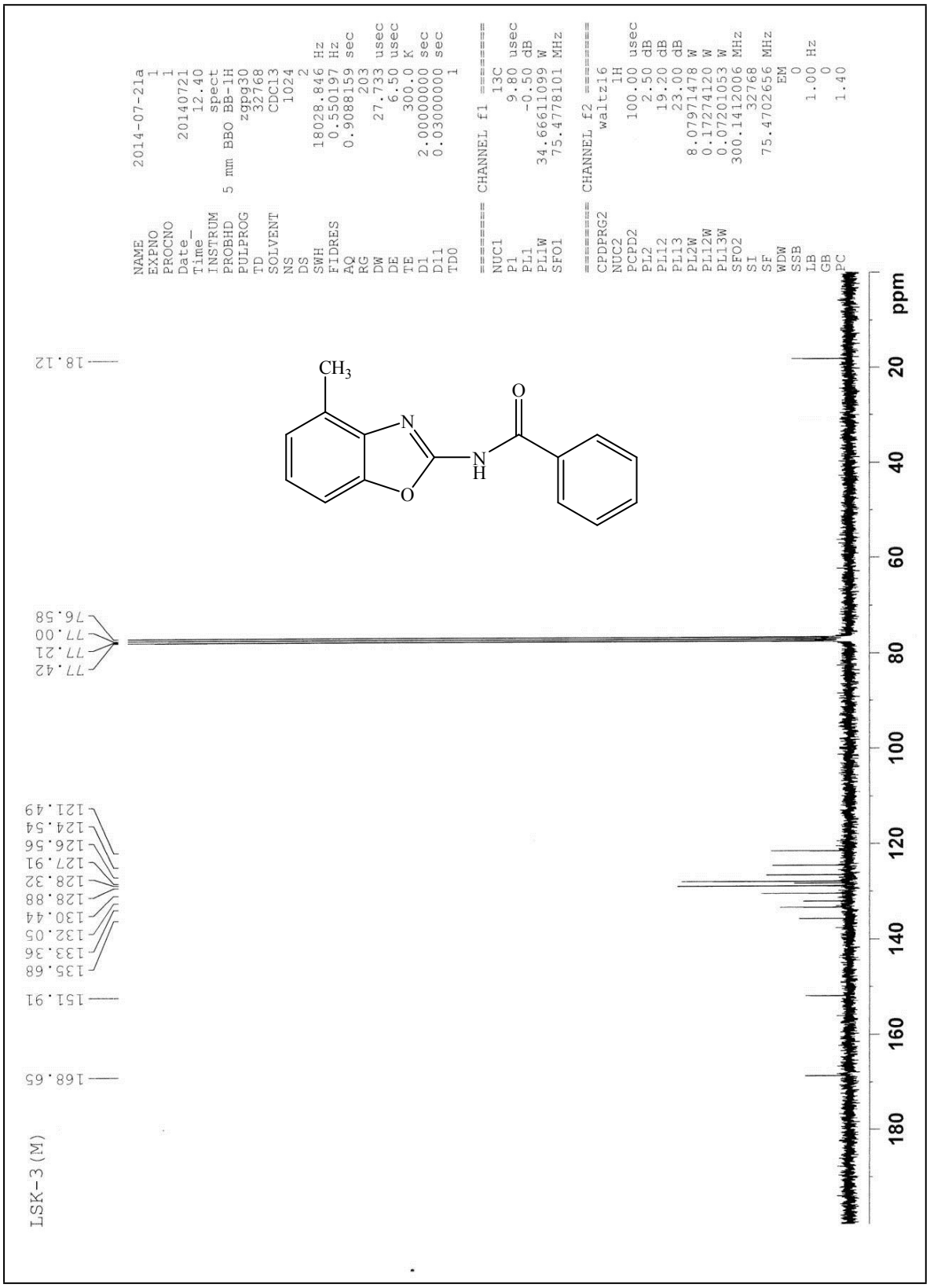
^{13}C NMR Spectrum of *N*-(benzo[*d*]oxazol-2-yl)benzamide (2b):



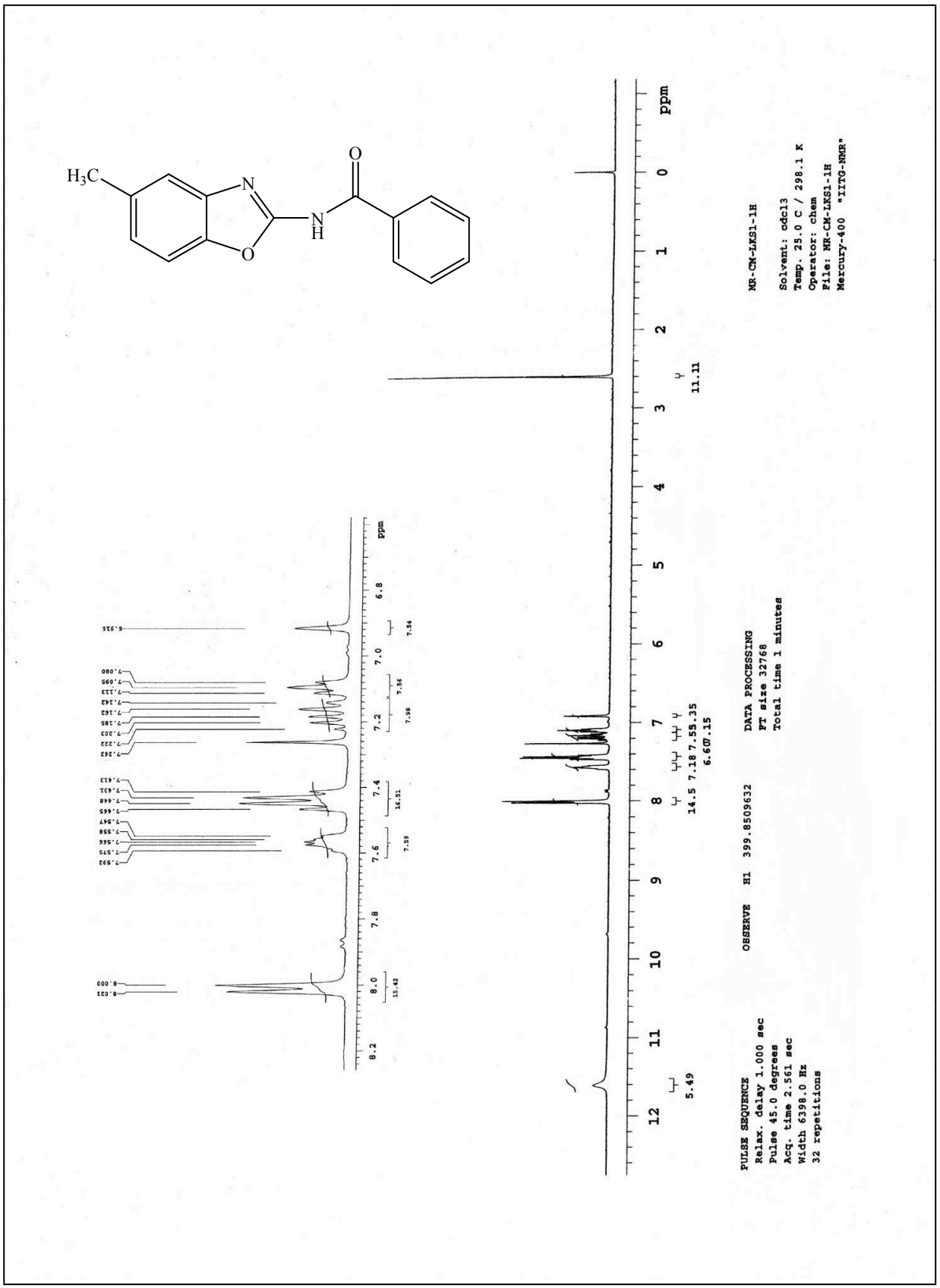
^{1}H NMR Spectrum of *N*-(4-methylbenzo[*d*]oxazol-2-yl)benzamide (2c):



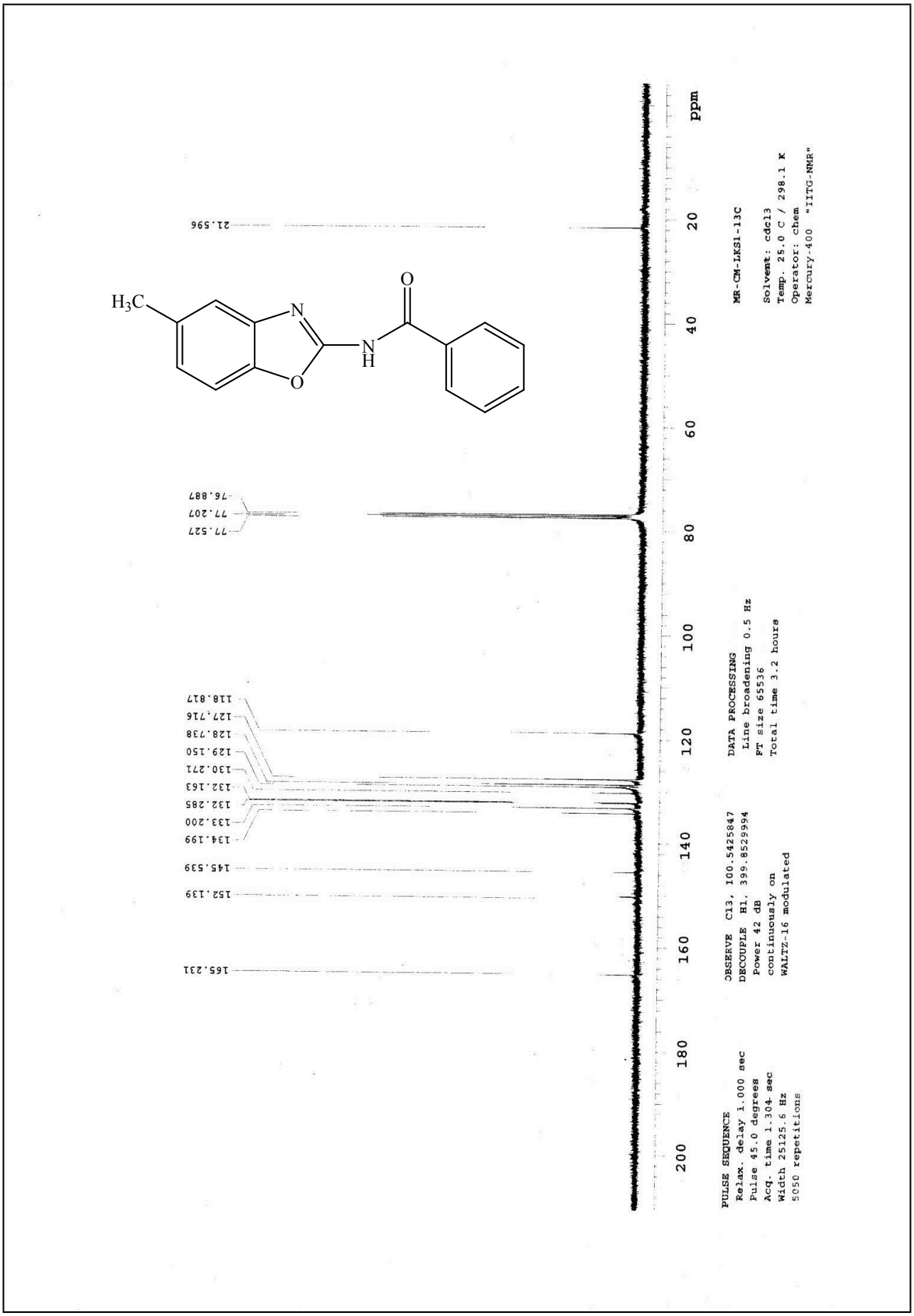
^{13}C NMR Spectrum of *N*-(4-methylbenzo[*d*]oxazol-2-yl)benzamide (2c):



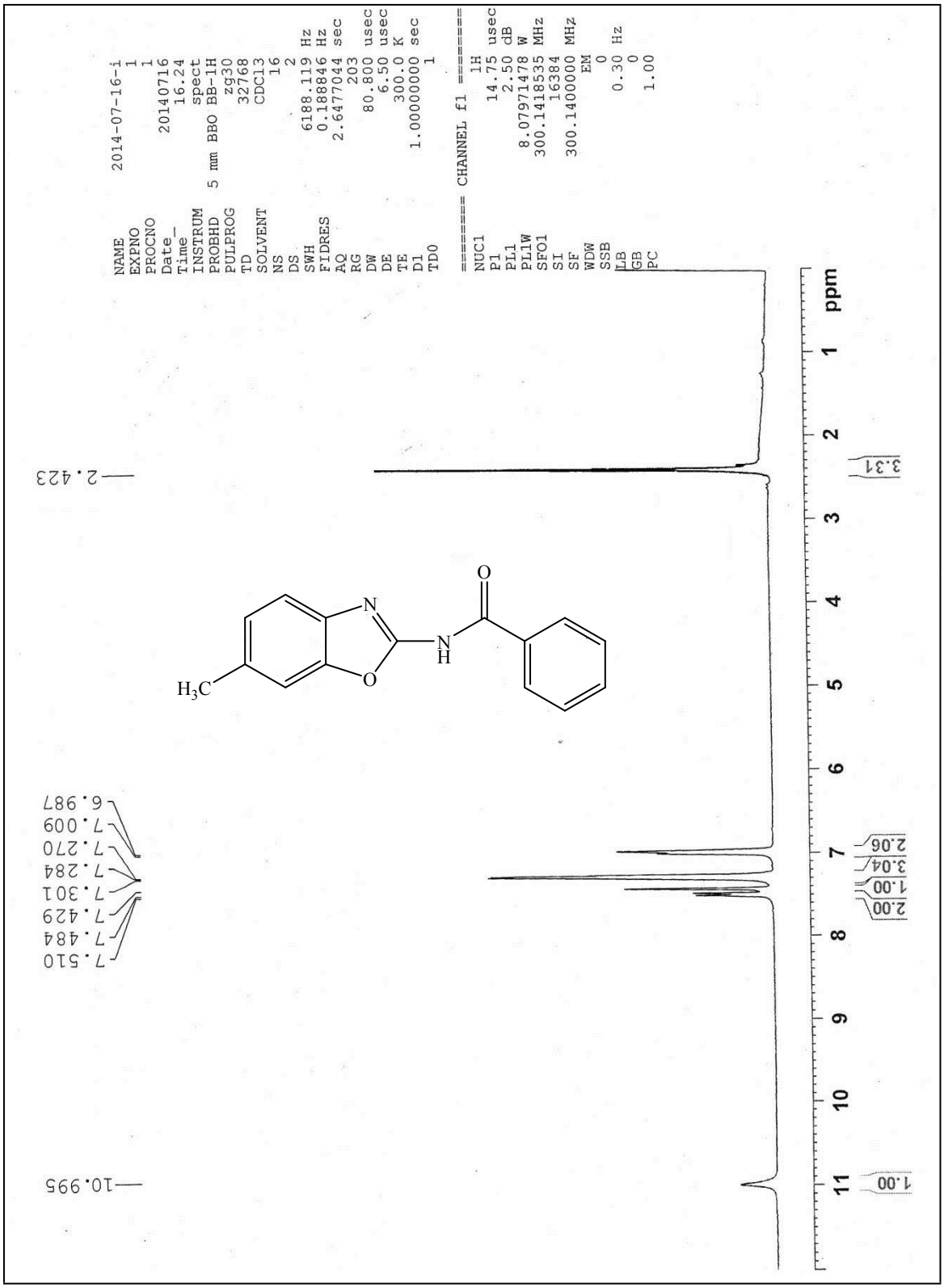
^{1}H NMR Spectrum of *N*-(5-methylbenzo[*d*]oxazol-2-yl)benzamide (2d):



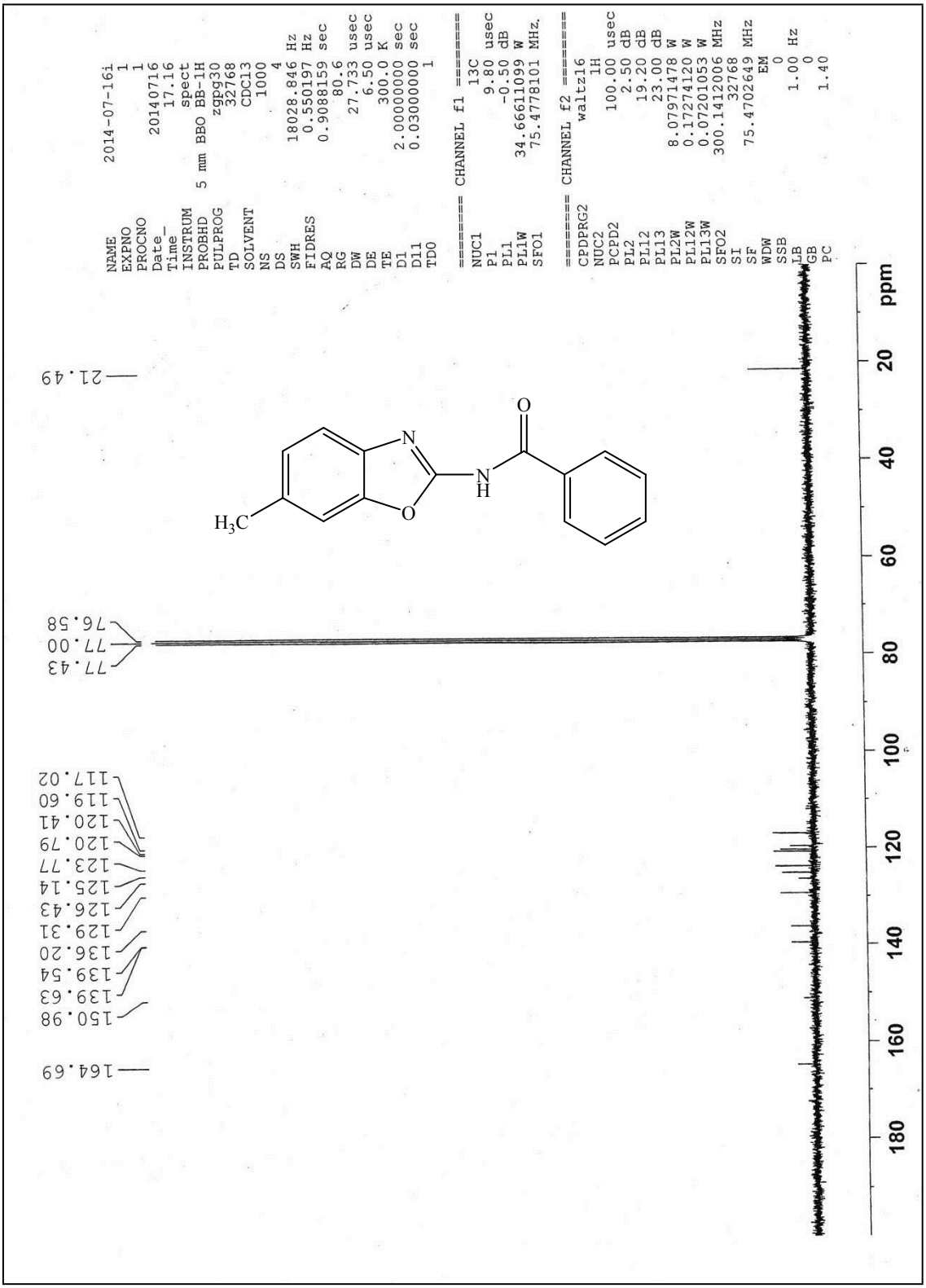
^{13}C NMR Spectrum of *N*-(5-methylbenzo[*d*]oxazol-2-yl)benzamide (2d):



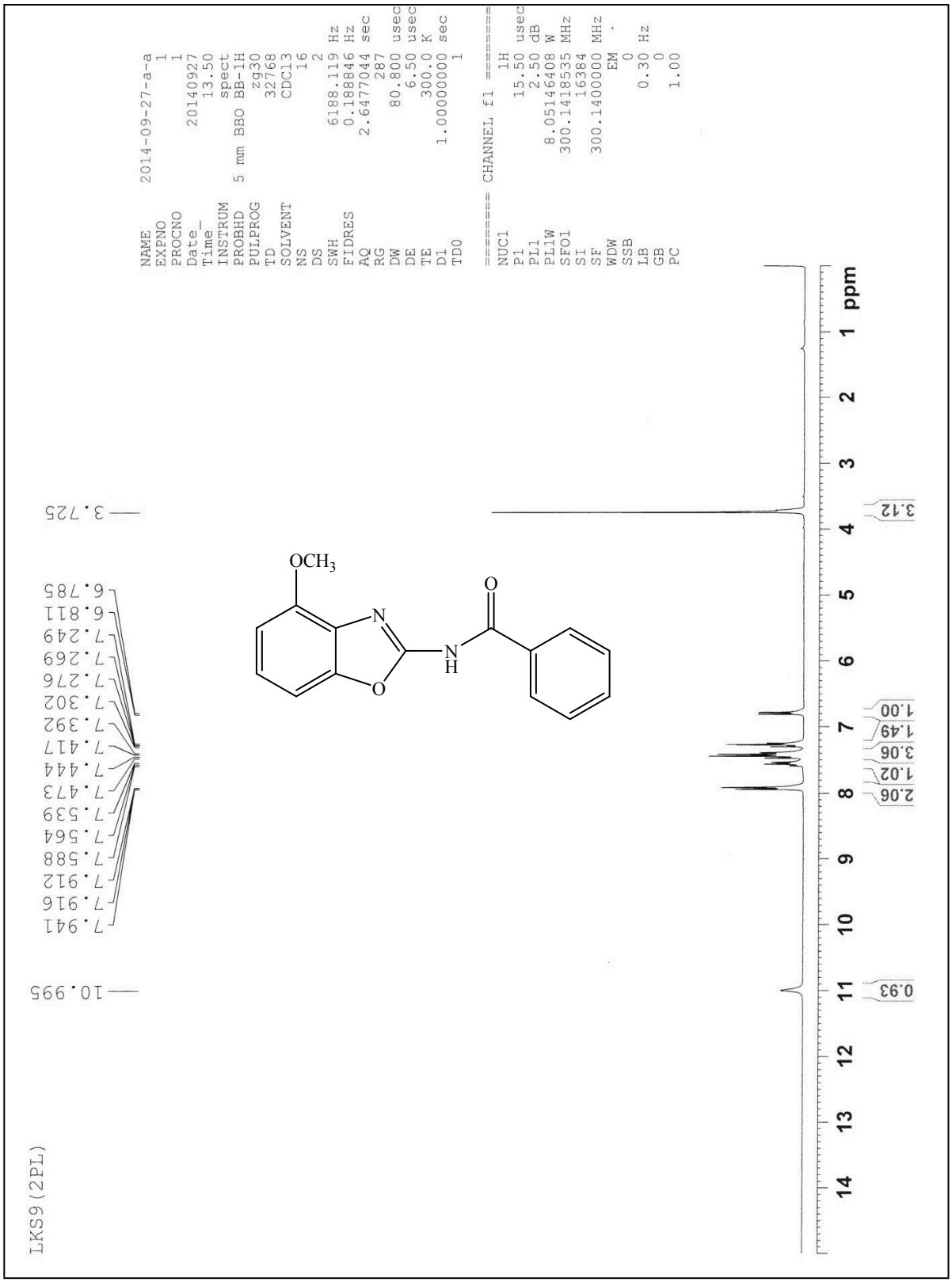
^{1}H NMR Spectrum of *N*-(6-methylbenzo[*d*]oxazol-2-yl)benzamide (2e):



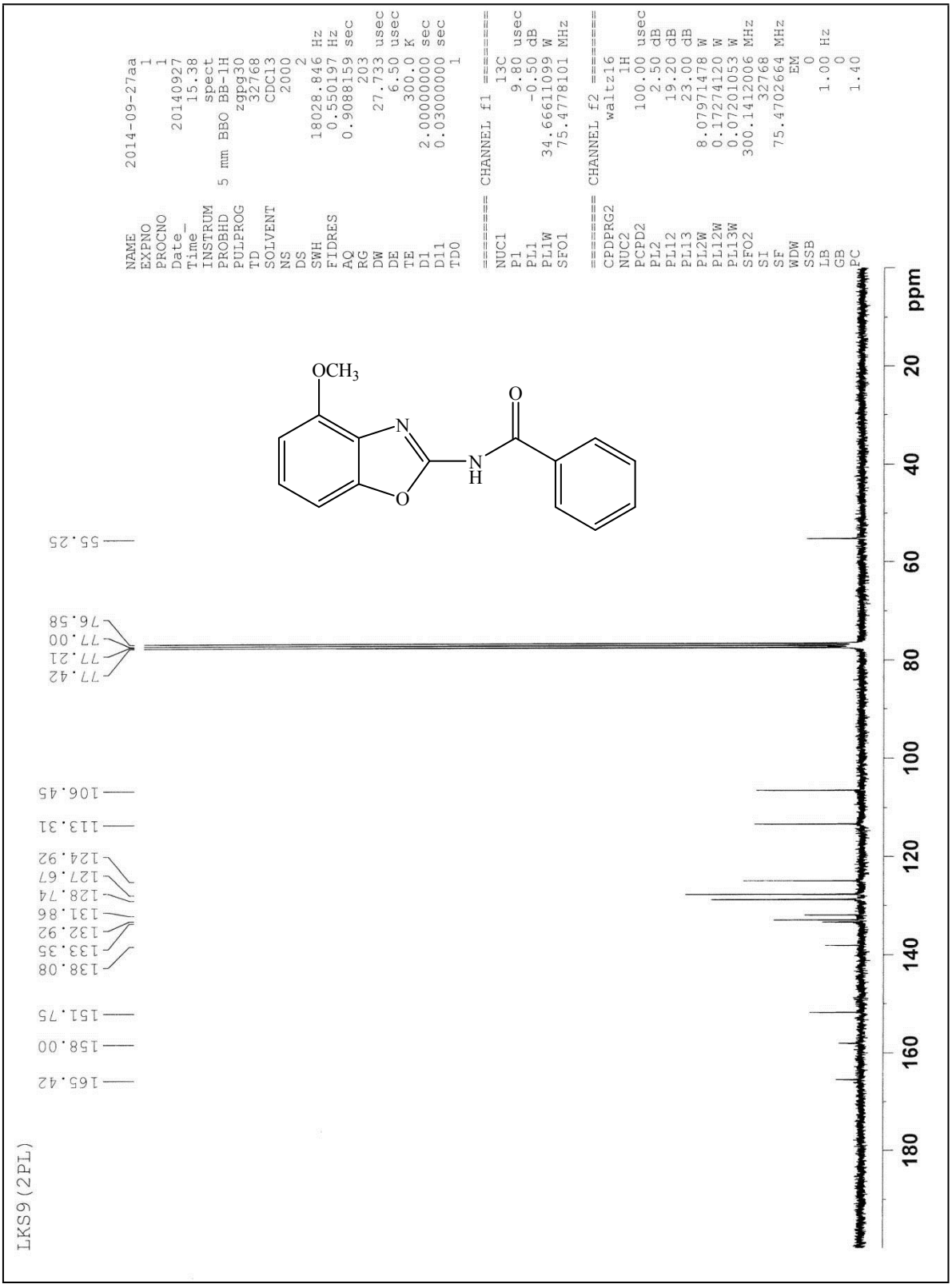
^{13}C NMR Spectrum of *N*-(6-methylbenzo[*d*]oxazol-2-yl)benzamide (2e):



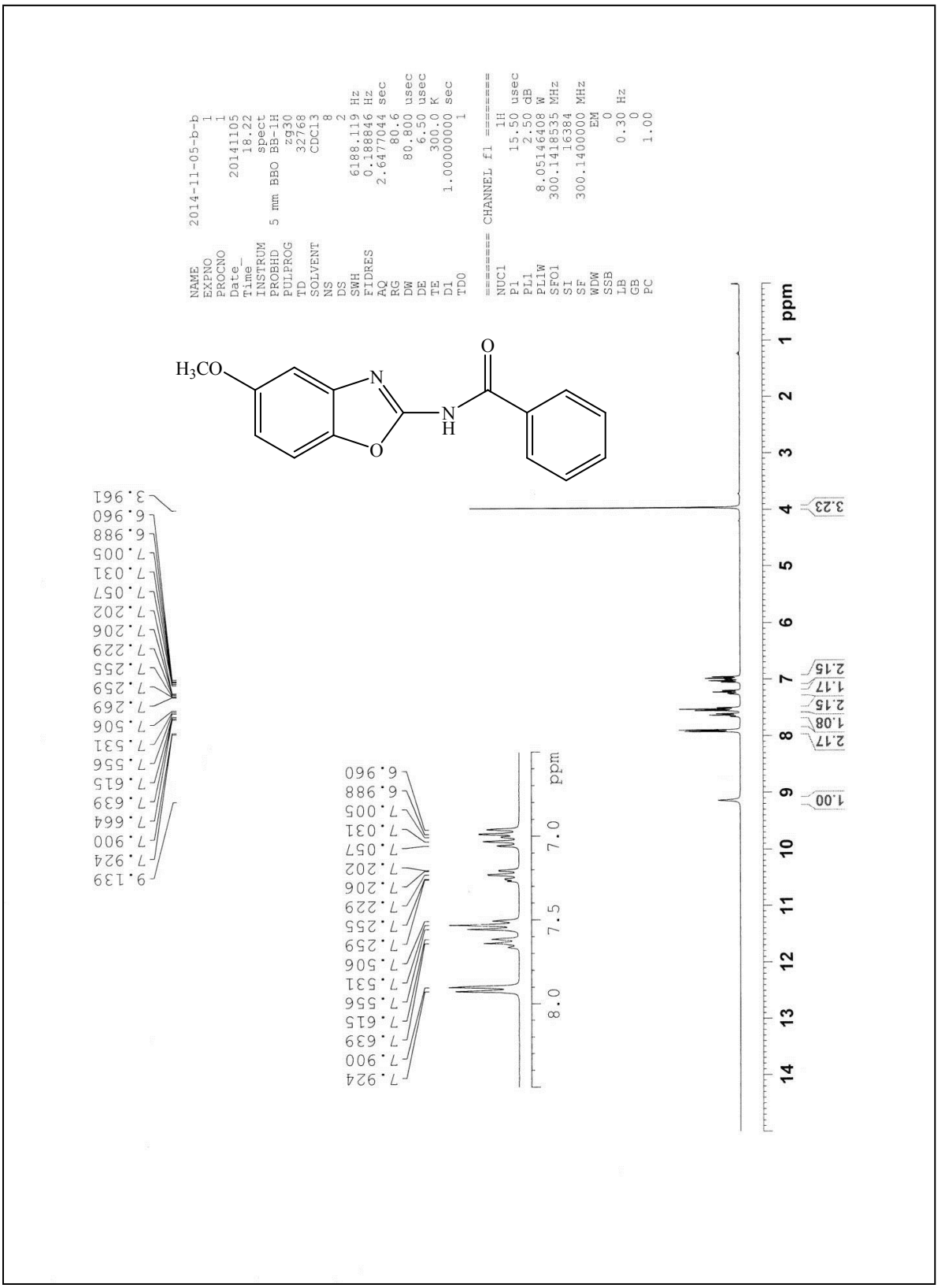
^{1}H NMR Spectrum of *N*-(4-methoxybenzo[*d*]oxazol-2-yl)benzamide (2f):



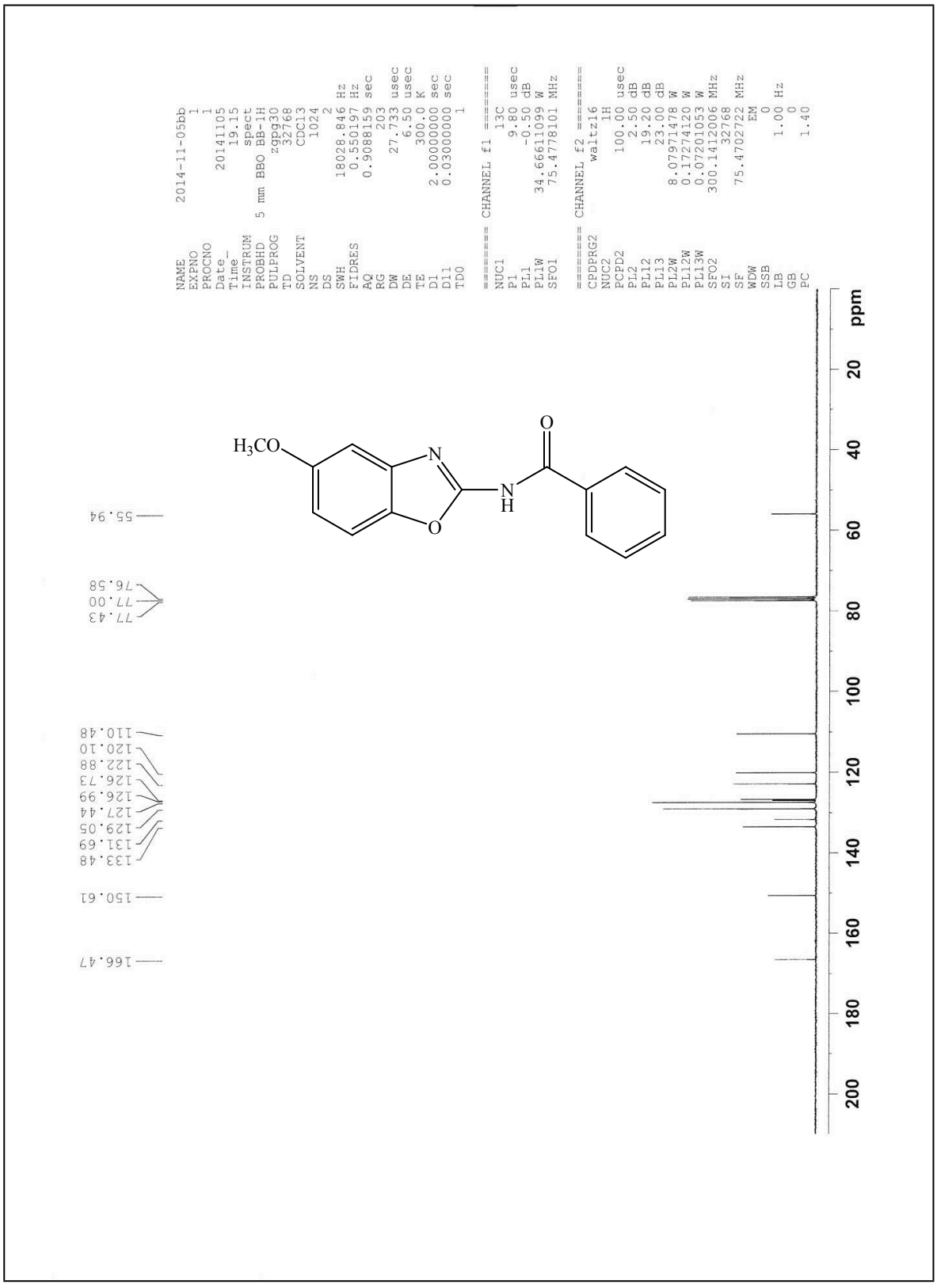
^{13}C NMR Spectrum of *N*-(4-methoxybenzo[*d*]oxazol-2-yl)benzamide (2f):



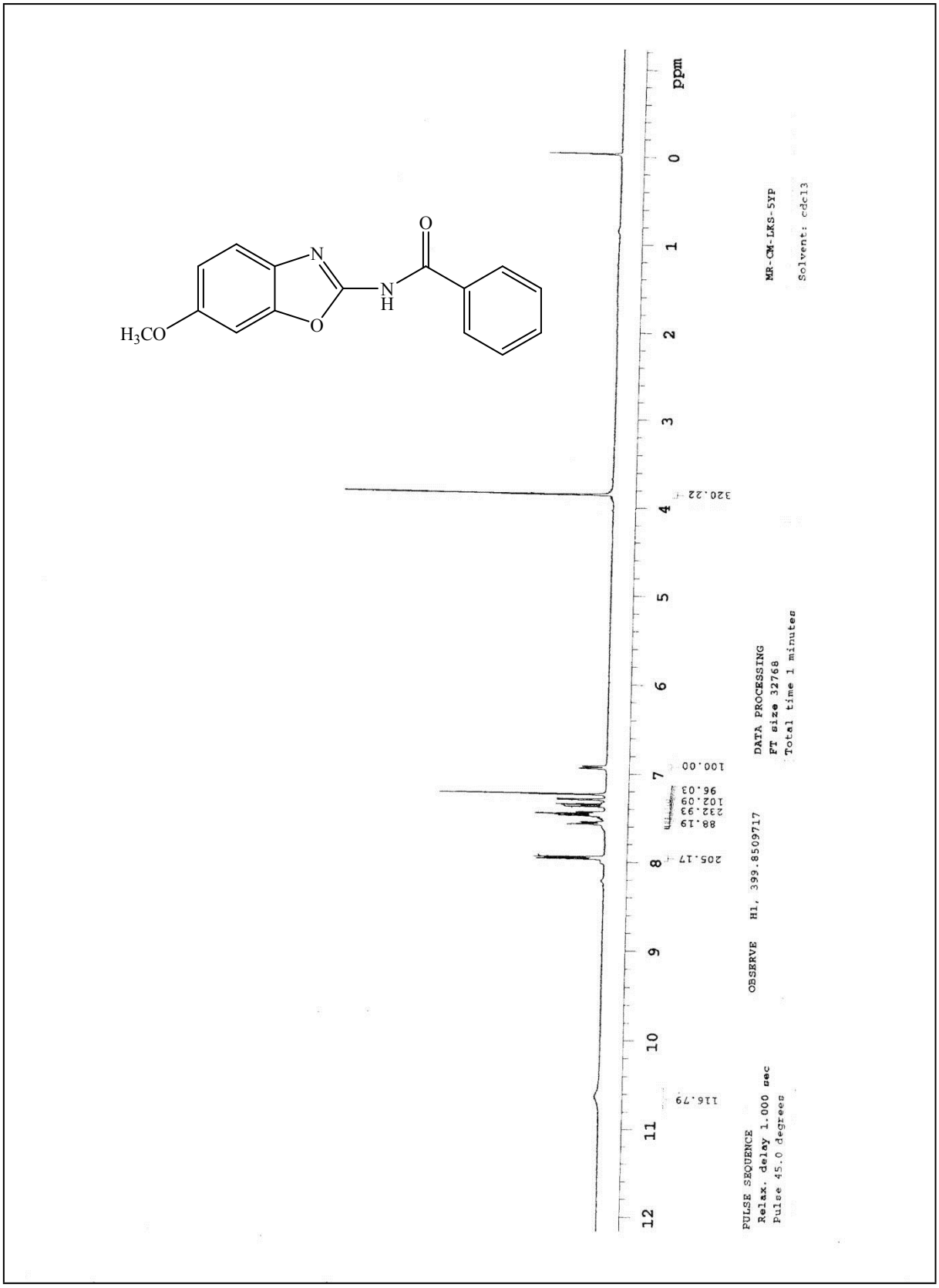
^{1}H NMR Spectrum of *N*-(5-methoxybenzo[*d*]oxazol-2-yl)benzamide (2g):



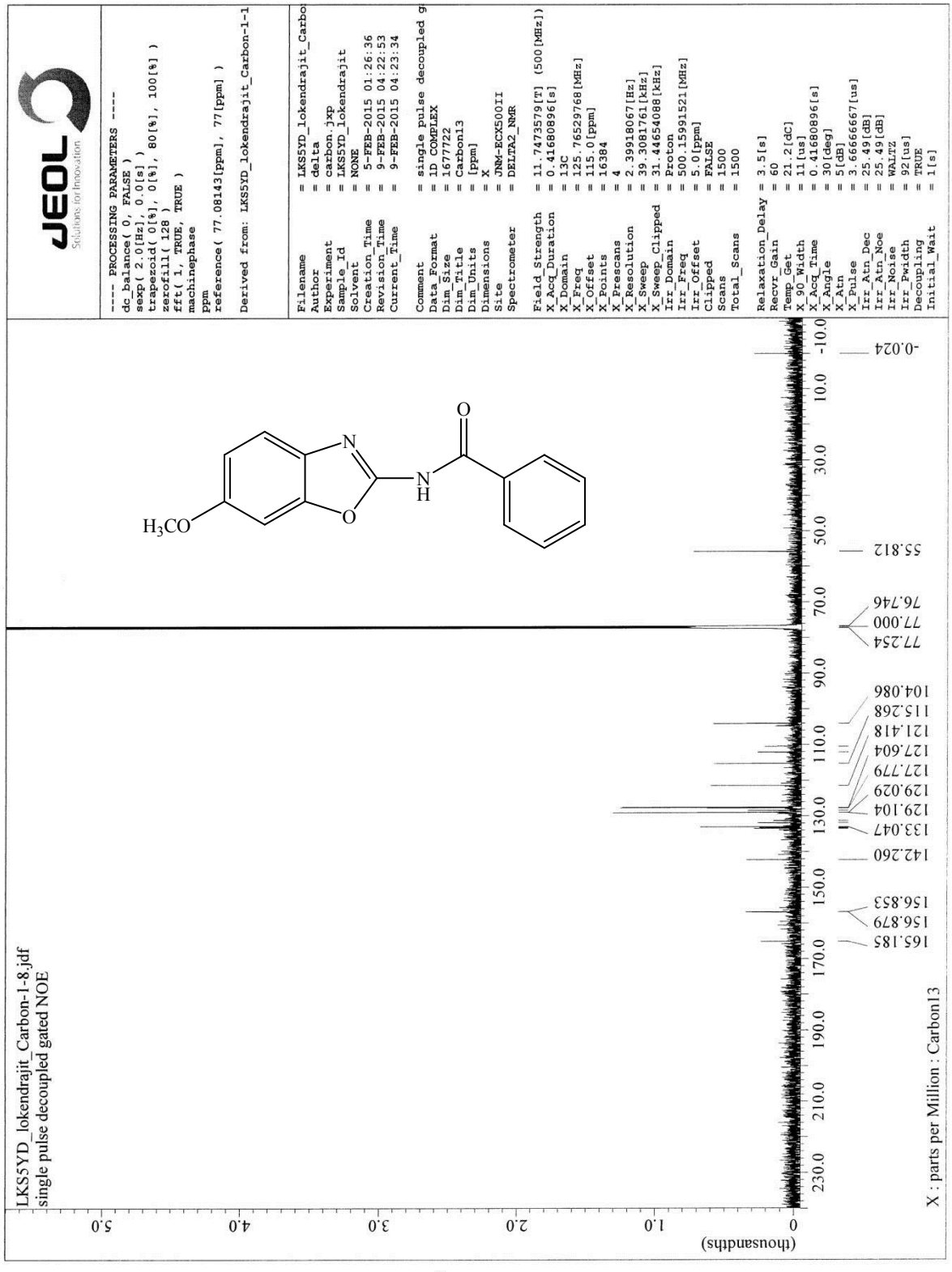
^{13}C NMR Spectrum of *N*-(5-methoxybenzo[*d*]oxazol-2-yl)benzamide (2g):



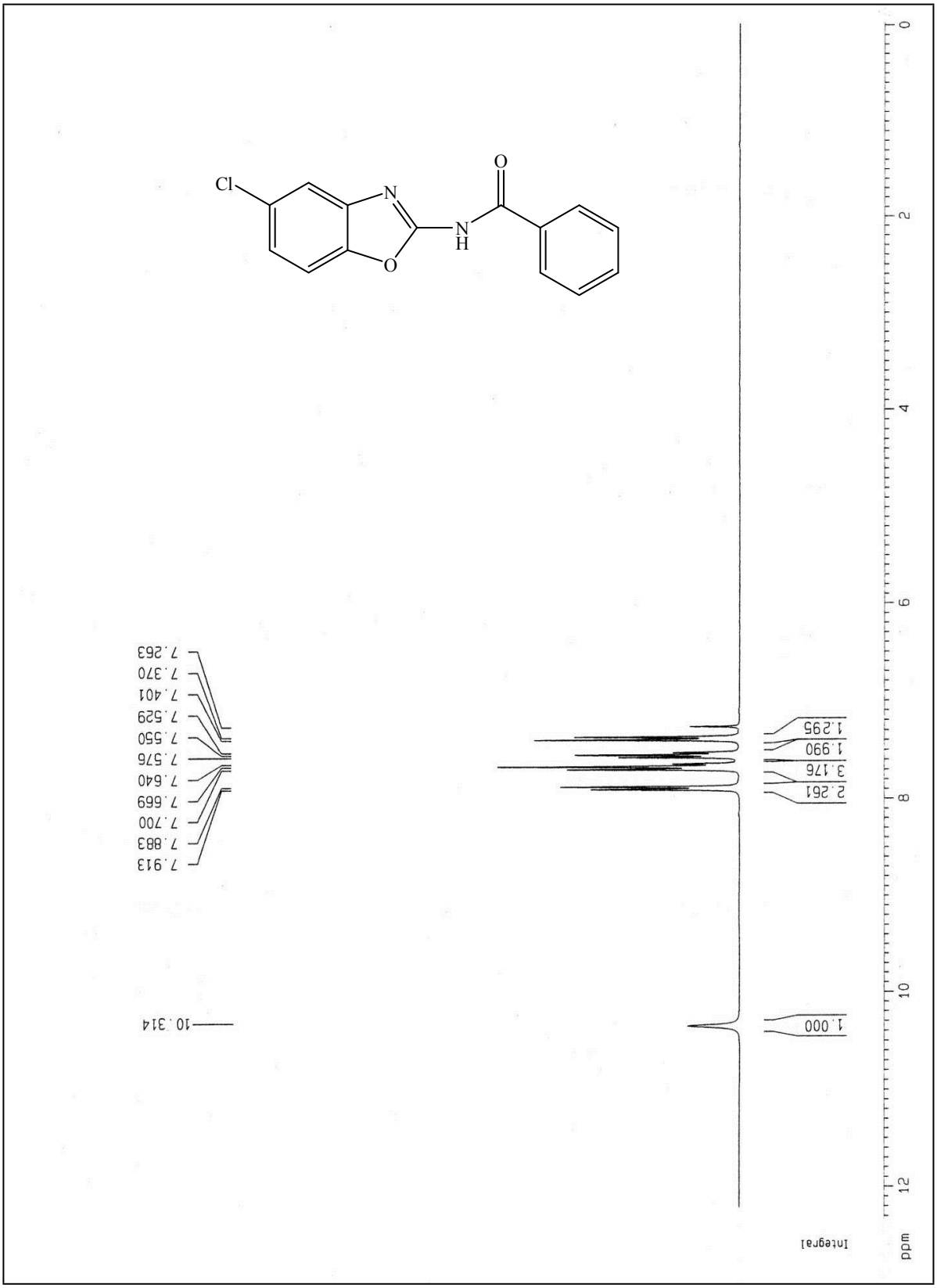
^{1}H NMR Spectrum of *N*-(6-methoxybenzo[*d*]oxazol-2-yl)benzamide (2h):



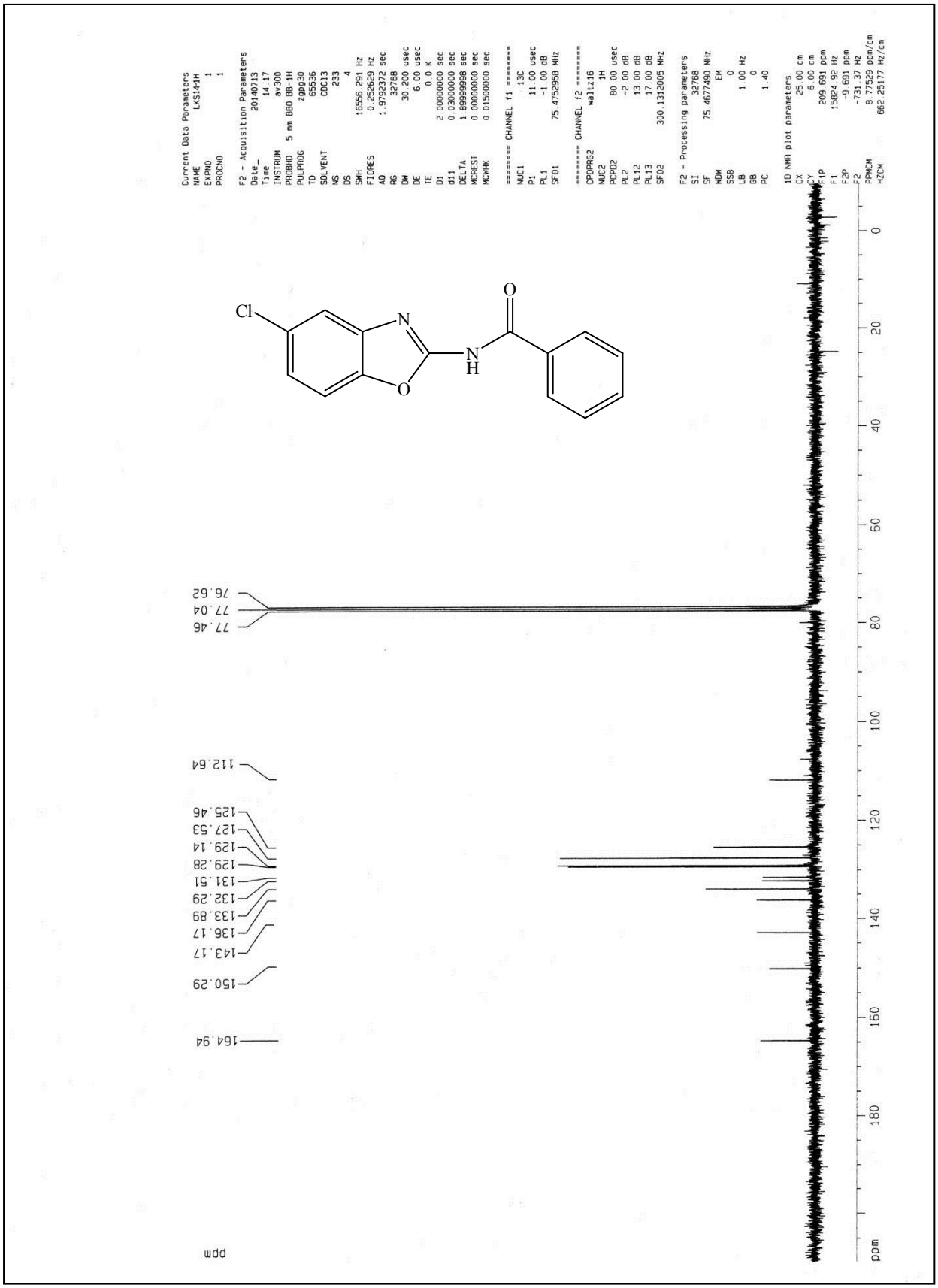
^{13}C NMR Spectrum of *N*-(6-methoxybenzo[*d*]oxazol-2-yl)benzamide (2h):



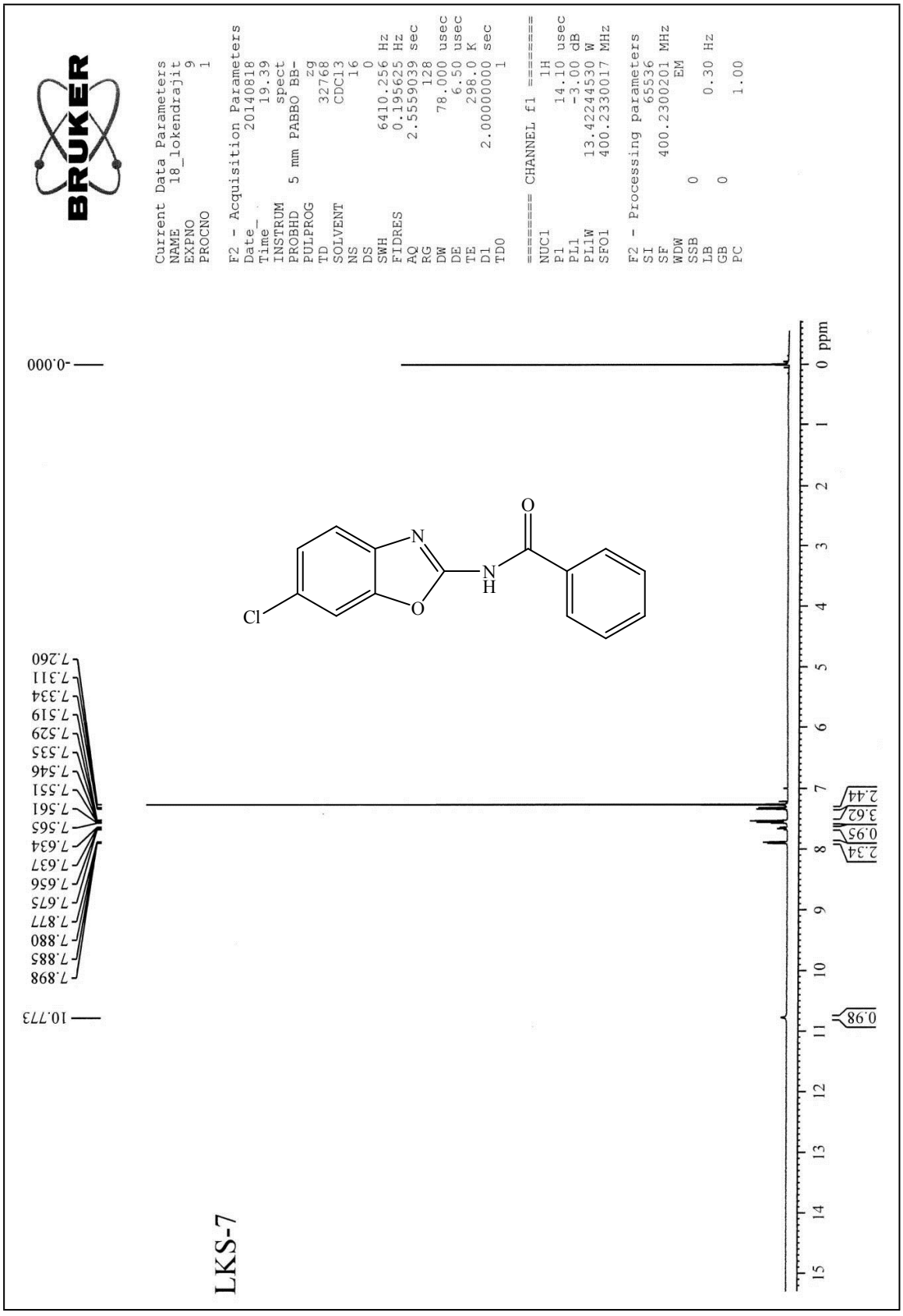
^{1}H NMR Spectrum of *N*-(5-chlorobenzo[*d*]oxazol-2-yl)benzamide (2i):



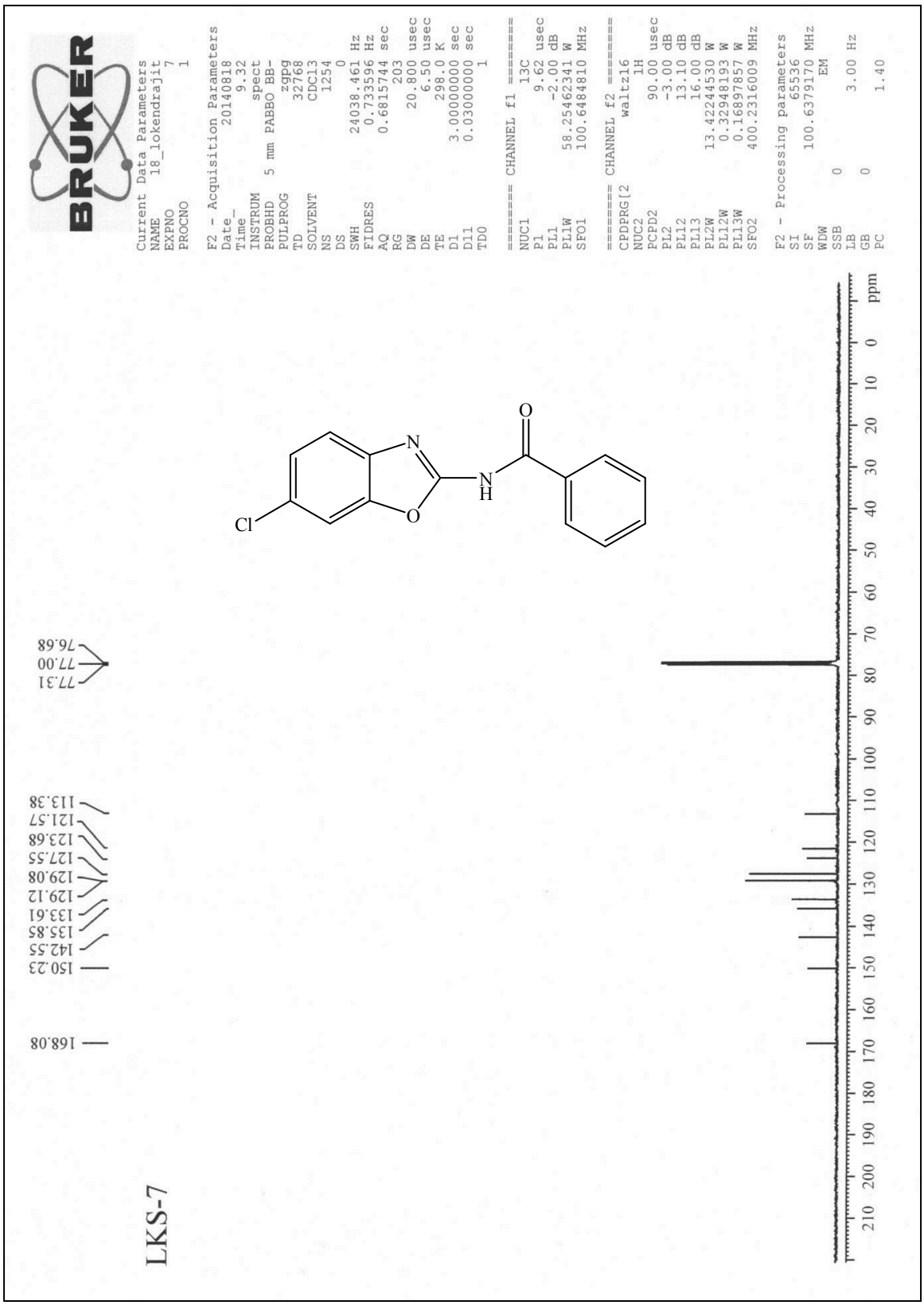
^{13}C NMR Spectrum of *N*-(5-chlorobenzo[*d*]oxazol-2-yl)benzamide (2i):



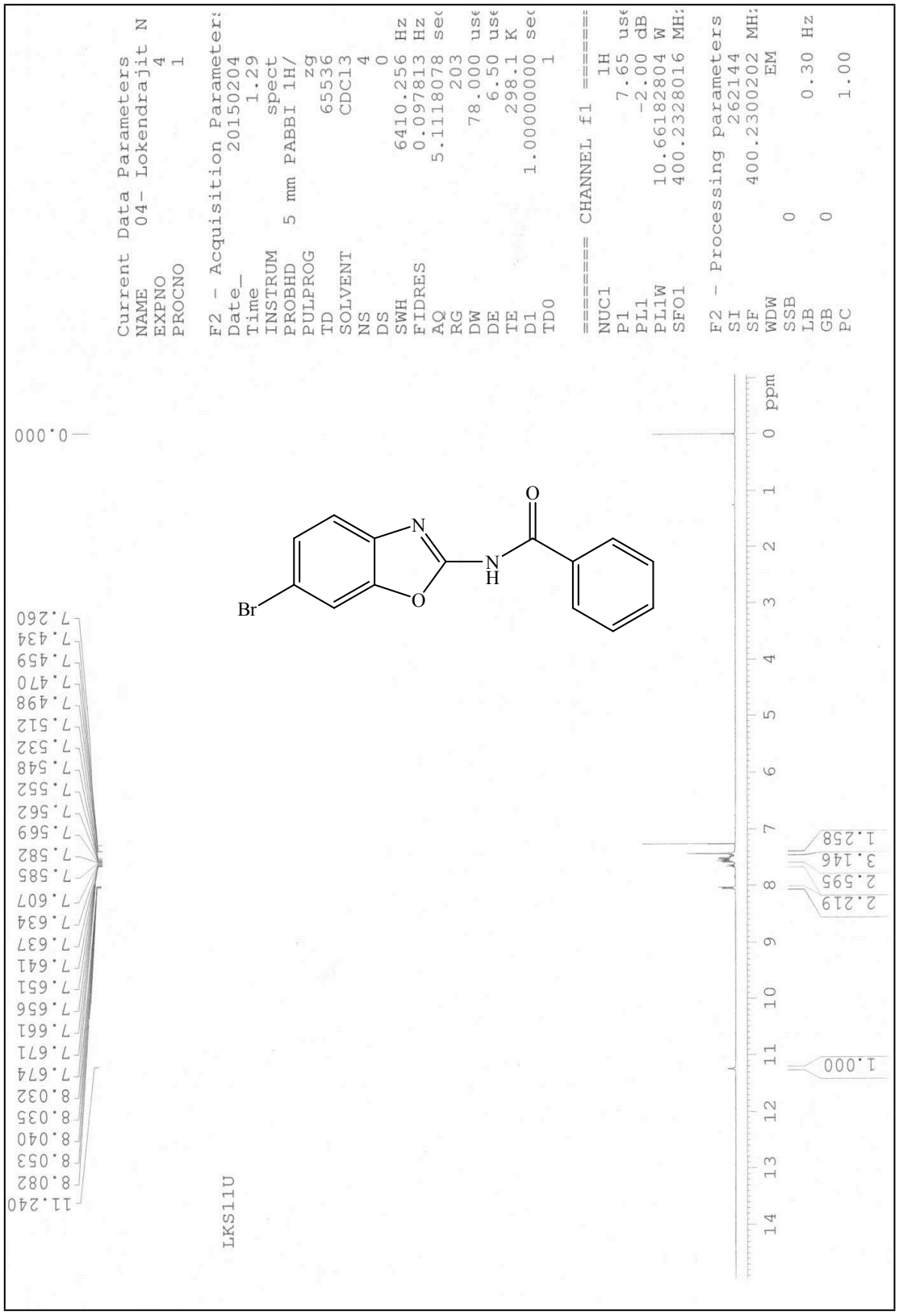
^{1}H NMR Spectrum of *N*-(6-chlorobenzo[*d*]oxazol-2-yl)benzamide (2j):



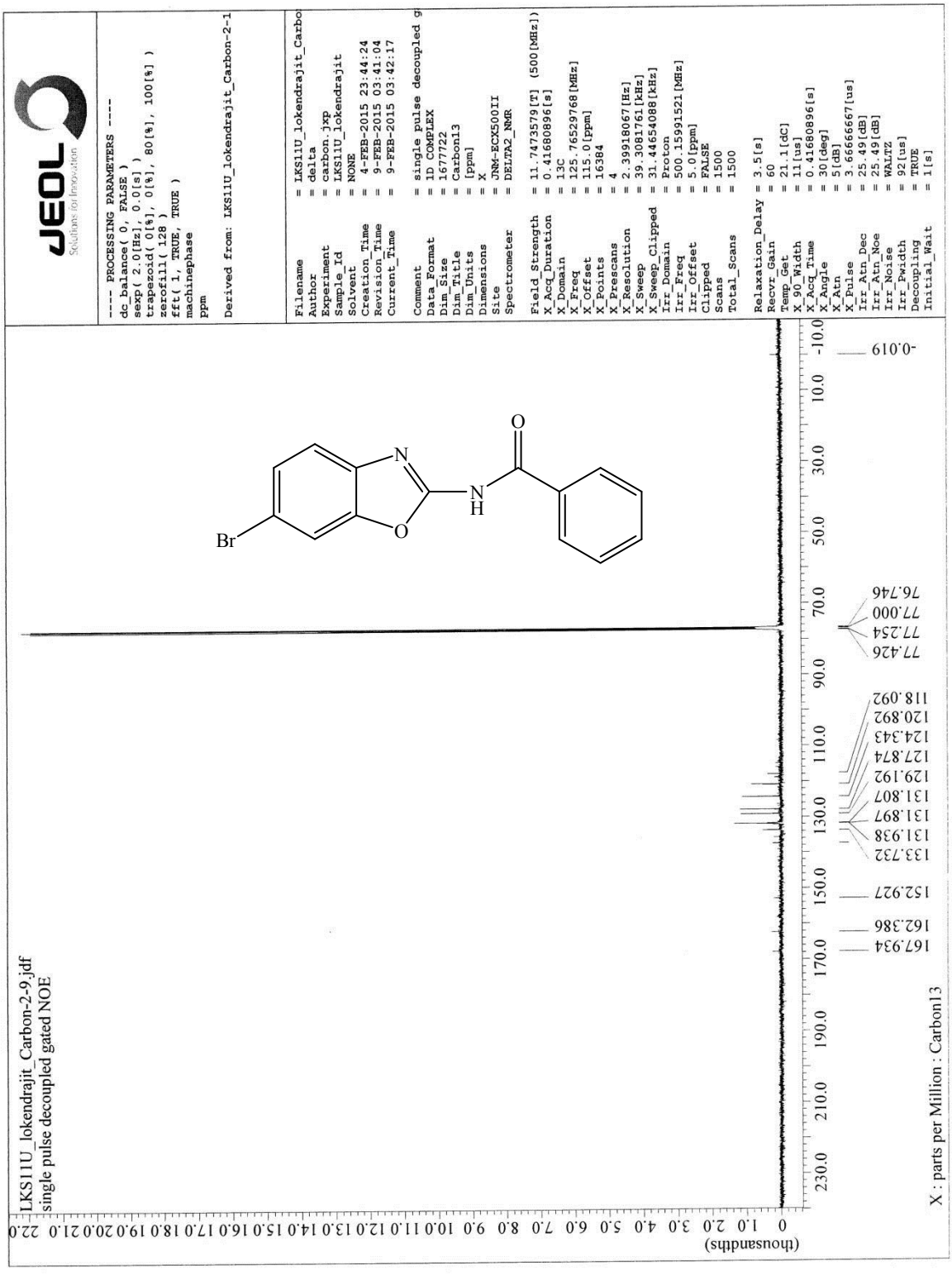
^{13}C NMR Spectrum of *N*-(6-chlorobenzo[*d*]oxazol-2-yl)benzamide (2j):



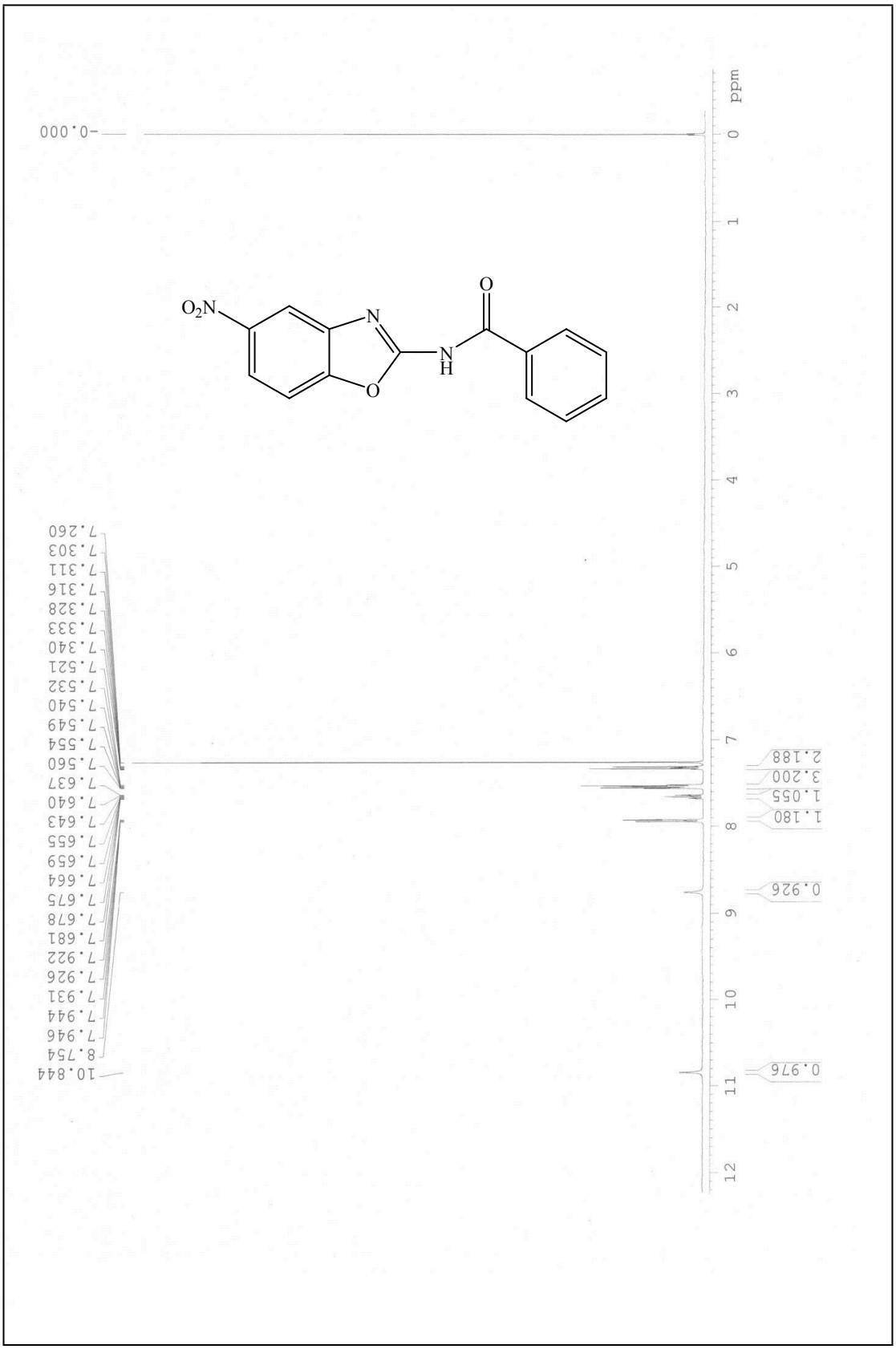
^{1}H NMR Spectrum of *N*-(6-bromobenzo[*d*]oxazol-2-yl)benzamide (2k):



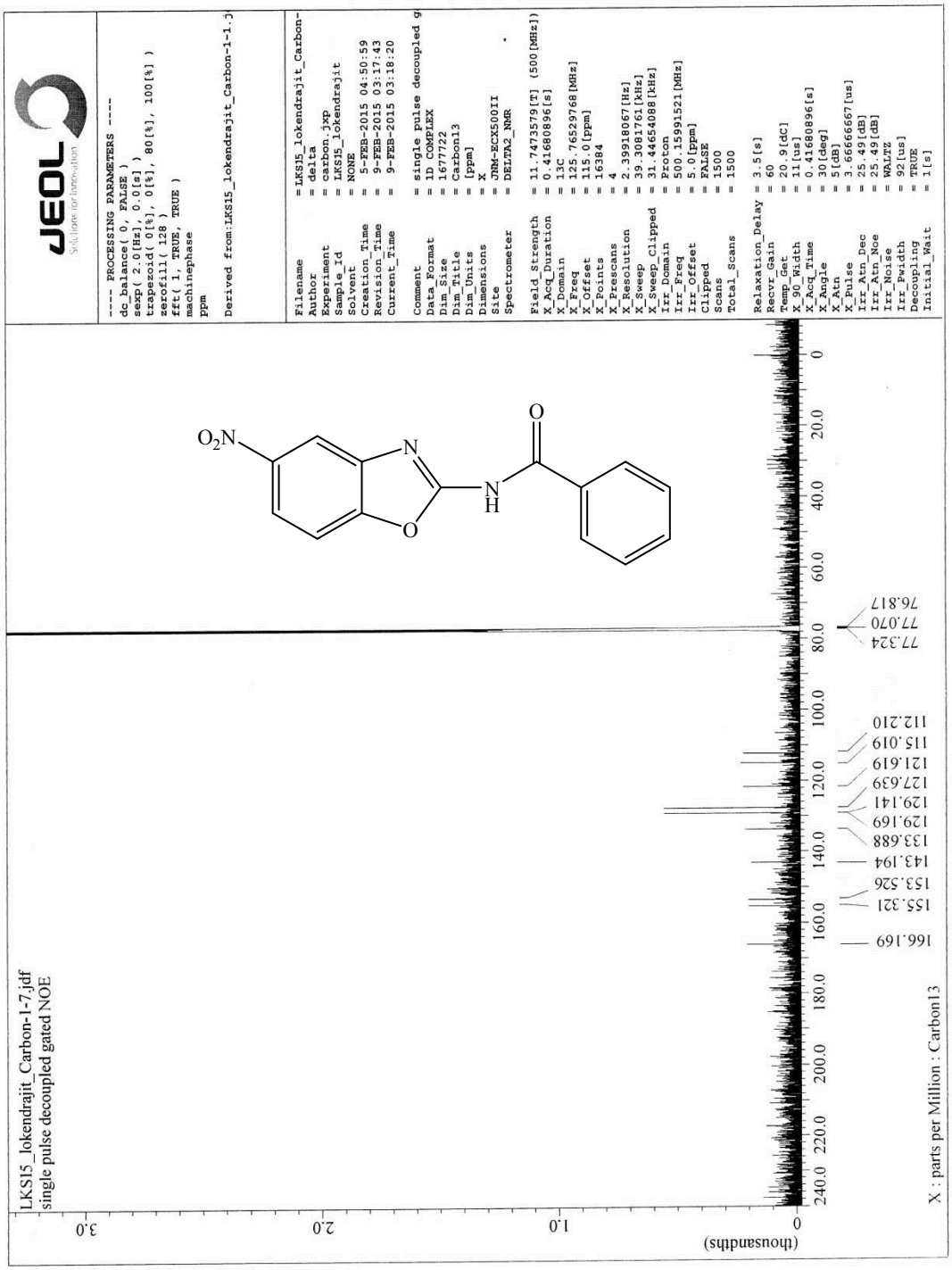
^{13}C NMR Spectrum of *N*-(6-bromobenzo[*d*]oxazol-2-yl)benzamide (2k):



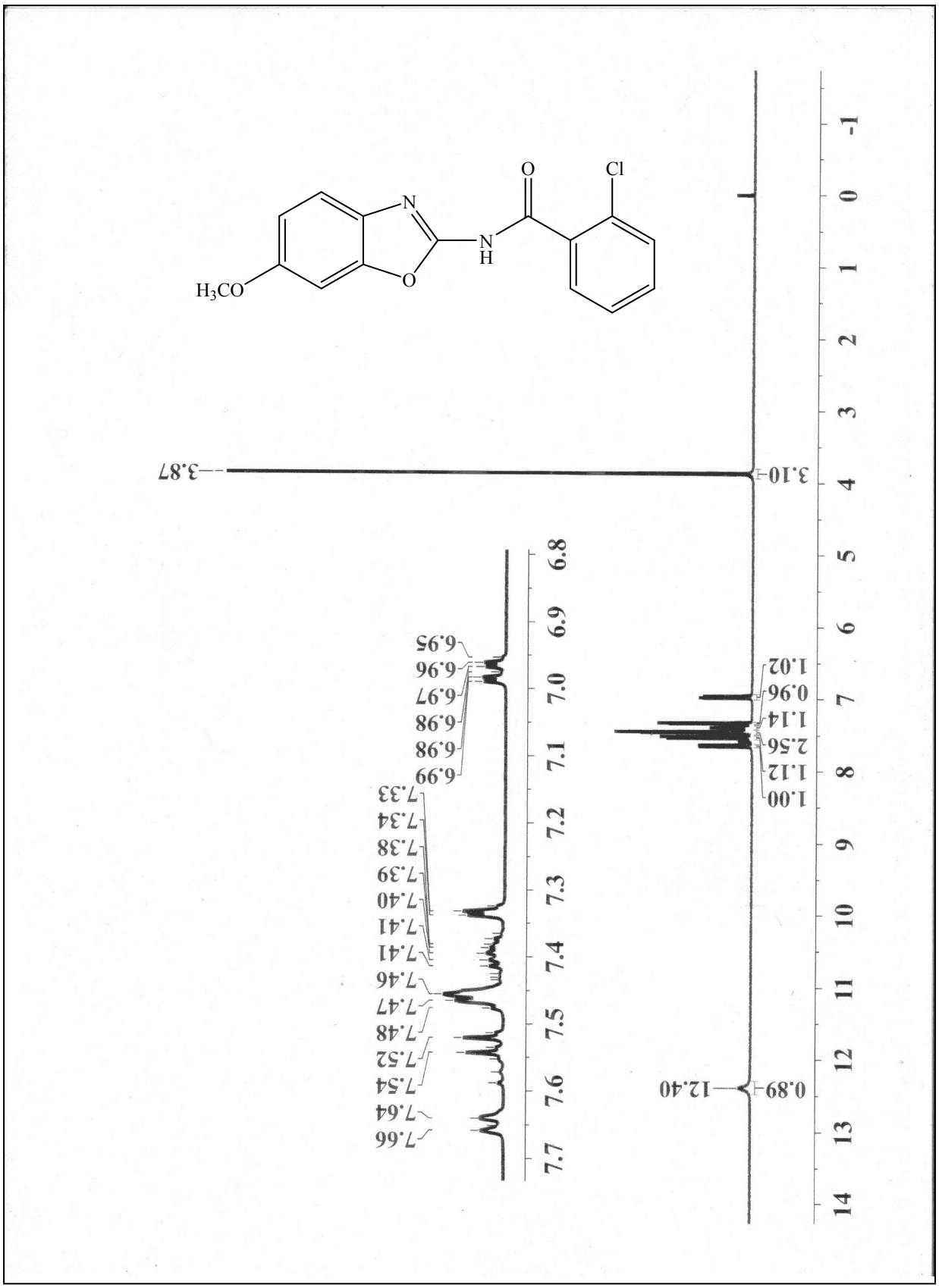
^{1}H NMR Spectrum of *N*-(5-nitrobenzo[*d*]oxazol-2-yl)benzamide (2l):



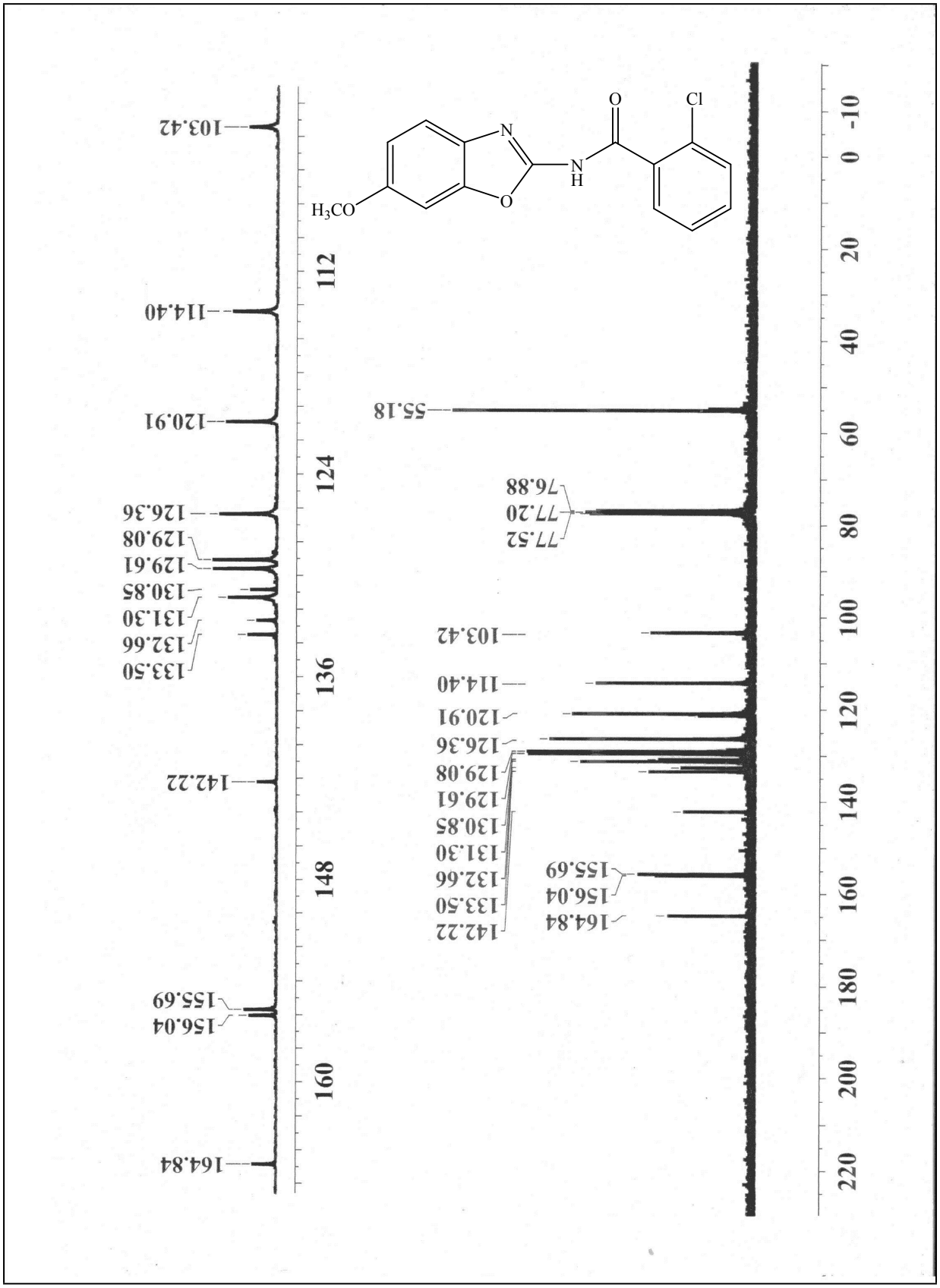
^{13}C NMR Spectrum of *N*-(5-nitrobenzo[*d*]oxazol-2-yl)benzamide (2l):



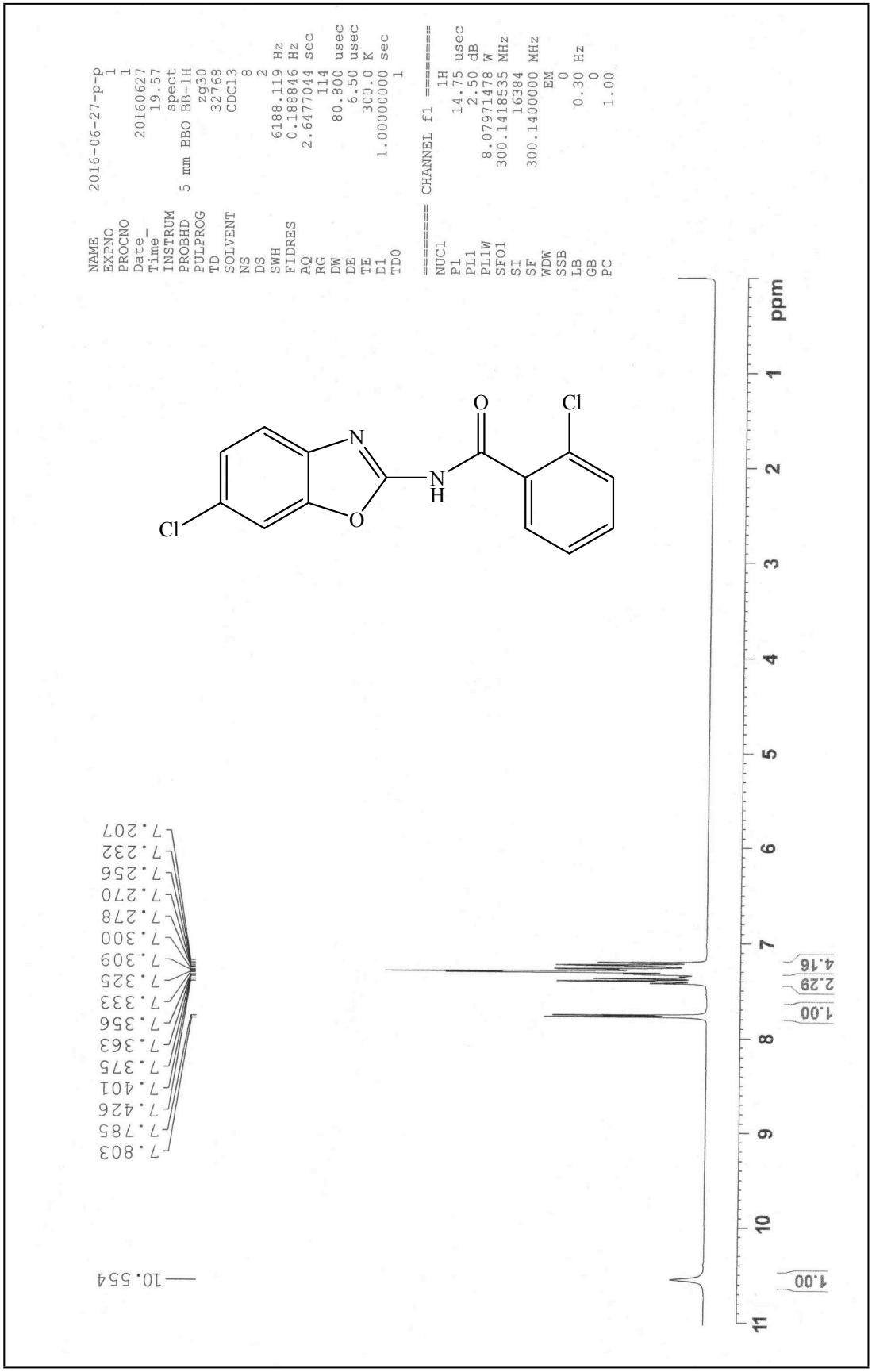
^{1}H NMR Spectrum of 2-Chloro-*N*-(6-methoxybenzo[*d*]oxazol-2-yl) benzamide (2m):



^{13}C NMR Spectrum of 2-Chloro-*N*-(6-methoxybenzo[*d*]oxazol-2-yl) benzamide (2m):



^{1}H NMR Spectrum of 2-Chloro-*N*-(6-chlorobenzo[*d*]oxazol-2-yl) benzamide (2n):



^{13}C NMR Spectrum of 2-Chloro-*N*-(6-chlorobenzo[*d*]oxazol-2-yl) benzamide (2n):

Computational Details:

The geometries of the structures studied, where the multiplicity of all the molecules/species is singlet, were fully optimized by density functional calculation in spin restricted shell wavefunctional manner.[S1,S2] The hybrid functional B3LYP[S3,S4] containing Becke's gradient corrected exchange functional containing 20% of Hartree-Fock exchange[S3] and correlation functional of Lee, Yang and Paar (LYP) was used for the calculations.[S4] The segmented all-electron relativistically contracted Def2-TZVP(-df)[S5] was used as the basis set for the calculations. All the calculations were performed using ORCA version 2.8.[S6] The energies reported are not corrected for zero point energy.

References:

S1. P. Hohenberg, and W. Kohn, *Phys. Rev. B*, 1964, **136**, 864−871.

S2. W. Kohn, and L. J. Sham, *Phys. Rev. A*, 1965, **140**, 1133−1138.

S3. A. D. Becke, *J. Chem. Phys.*, 1993, **98**, 5648−5652.

S4. C. Lee, W. Yang, and R. G. Parr, *Phys. Rev. B*, 1988, **37**, 785−789.

S5. F. Weigend, and R. Ahlrichs, *Phys. Chem. Chem. Phys.*, 2005, **7**, 3297−305.

S6. F. Neese, *WIREs Comput. Mol. Sci.*, 2012, **2**, 73–78.

Table S1. Mulliken atomic charge of the hydrogen atoms attached to N2 and N4 atoms of D

Entry Number	Mulliken Charge of Hydrogen Atom Bonded to	
	N2	N4
1	0.2982	0.2679
2	0.3002	0.2657
3	0.2984	0.2686
4	0.301	0.2654
5	0.3011	0.2653
9	0.3016	0.2675
10	0.3018	0.2671
15	0.3061	0.2658
16	0.3073	0.2671

Optimized Geometries for Intermediates A

Structure: A_1				**Structure: A_2**			
C	0.533755	-2.940788	0.855982	C	0.577920	-2.776537	0.729018
C	1.292938	-2.941221	2.043132	C	1.063309	-3.453365	-0.398528
C	2.515252	-3.607992	2.048276	C	2.314182	-4.059265	-0.361474
C	2.999296	-4.304350	0.937971	C	3.096443	-4.002967	0.789636
C	2.211218	-4.321452	-0.213345	C	2.605172	-3.352090	1.919068
C	0.994464	-3.653229	-0.256625	C	1.348667	-2.761655	1.897974
N	-0.723797	-2.322506	0.868644	N	-0.698652	-2.204547	0.771661
C	-1.199283	-1.514714	0.017324	C	-1.219002	-1.405096	-0.062628
S	-0.389419	-0.741030	-1.422317	S	-0.471548	-0.589761	-1.512064
N	-2.523735	-1.097759	0.240766	N	-2.549384	-1.037053	0.198324
C	-3.453974	-0.702480	-0.708143	C	-3.516150	-0.650751	-0.718687
O	-3.214137	-0.689661	-1.901383	O	-3.308947	-0.609795	-1.916993
C	-4.789966	-0.306432	-0.156517	C	-4.847185	-0.306023	-0.123331
I	1.882026	0.024871	-0.459050	I	1.806343	0.250806	-0.613868
H	-2.873842	-1.417784	1.133996	H	-2.866433	-1.381228	1.094912
O	3.823155	0.816590	0.409770	O	3.721400	1.200503	0.172863
C	4.864654	1.359845	-0.213527	C	4.970518	0.910524	-0.168982
O	5.751091	1.893642	0.420298	O	5.903701	1.457165	0.380771
C	4.904212	1.276143	-1.731552	C	5.177693	-0.123110	-1.266129
C	1.085971	1.977417	0.137088	C	0.957803	2.131476	0.107492
C	-5.892811	-0.395364	-1.010619	C	-5.970411	-0.413762	-0.948240
C	-7.155813	-0.033243	-0.562660	C	-7.230872	-0.100617	-0.458109
C	-7.328269	0.435522	0.737713	C	-7.380716	0.337714	0.855625
C	-6.232495	0.542899	1.588478	C	-6.265119	0.463917	1.677630
C	-4.967763	0.171414	1.145629	C	-5.002534	0.141255	1.192549
C	1.718822	2.632260	1.182134	C	1.581770	2.758576	1.174437
C	1.219984	3.875426	1.568190	C	1.037363	3.958845	1.628841
C	0.124757	4.433622	0.917388	C	-0.090107	4.502597	1.022824
C	-0.483584	3.749614	-0.129638	C	-0.686013	3.848162	-0.049924
C	-0.007017	2.502683	-0.531494	C	-0.164097	2.644901	-0.521513
C	0.808820	-2.201754	3.260499	H	0.457534	-3.507624	-1.293236
C	4.313377	-5.041349	1.001029	H	2.674975	-4.586070	-1.237143
H	3.109423	-3.587408	2.956347	H	4.071846	-4.472592	0.810642
H	2.545950	-4.869895	-1.086860	H	3.198259	-3.314397	2.824985
H	0.391014	-3.684996	-1.154293	H	0.952591	-2.269446	2.777156
H	-5.739934	-0.749922	-2.021620	H	-5.835443	-0.744614	-1.969762
H	-8.007095	-0.113444	-1.227721	H	-8.097889	-0.195601	-1.100418
H	-8.313401	0.723003	1.084746	H	-8.364165	0.586598	1.235708
H	-6.360150	0.923476	2.594384	H	-6.375999	0.821084	2.694020
H	-4.118505	0.290775	1.807971	H	-4.139004	0.275073	1.833259
H	2.589108	2.206999	1.661152	H	2.480958	2.352606	1.612366
H	-0.495485	1.964333	-1.331380	H	-0.640367	2.130176	-1.343792
H	1.701196	4.402043	2.383078	H	1.510536	4.464991	2.461166
H	-1.333147	4.179224	-0.646076	H	-1.559603	4.267729	-0.533197
H	-0.251499	5.401886	1.222894	H	-0.500584	5.437806	1.382436
H	4.807977	0.241933	-2.068542	H	4.742269	-1.084159	-0.978052
H	4.079578	1.843508	-2.170028	H	4.697387	0.196770	-2.194150
H	5.845080	1.686812	-2.090263	H	6.242075	-0.256658	-1.443294

H	-0.223848	-2.470271	3.494695				
H	1.435053	-2.424050	4.125020				
H	0.826831	-1.118466	3.104400				
H	4.206202	-5.995326	1.526758				
H	4.694690	-5.258768	0.002284				
H	5.070128	-4.460799	1.532981				
Structure: A_3				**Structure: A_4**			
C	0.594425	-3.532751	0.160824	C	0.495566	-2.974177	0.934794
C	0.763907	-4.451814	-0.889950	C	1.239301	-2.912627	2.119484
C	1.966667	-5.156441	-0.952454	C	2.478310	-3.537575	2.232695
C	2.975309	-4.976610	-0.011322	C	2.957558	-4.270145	1.141504
C	2.784080	-4.081258	1.034436	C	2.204509	-4.375490	-0.022942
C	1.592457	-3.371343	1.125526	C	0.976308	-3.734046	-0.137613
N	-0.628437	-2.851762	0.327541	N	-0.755121	-2.343973	0.911757
C	-0.937114	-1.762609	-0.237748	C	-1.214531	-1.570494	0.019914
S	0.089464	-0.875710	-1.454476	S	-0.395473	-0.876908	-1.454113
N	-2.153685	-1.180257	0.147832	N	-2.530427	-1.120697	0.225982
C	-3.027785	-0.401222	-0.605327	C	-3.452914	-0.728710	-0.731810
O	-2.838505	-0.114923	-1.770351	O	-3.217868	-0.758816	-1.925519
C	-4.251056	0.046388	0.138635	C	-4.774706	-0.277218	-0.188124
I	1.749532	0.325841	0.101613	I	1.912161	-0.114159	-0.571560
H	-2.543155	-1.635644	0.962615	H	-2.884016	-1.396791	1.132405
O	3.161225	1.404008	1.488108	O	3.879383	0.683151	0.218133
C	4.432740	1.752301	1.284620	C	4.856310	1.308581	-0.433149
O	5.016366	2.424905	2.106479	O	5.759539	1.840322	0.177828
C	5.108366	1.268057	0.012283	C	4.801676	1.318078	-1.952818
C	0.632532	2.234248	0.072492	C	1.122381	1.804148	0.124059
C	-5.388003	0.348153	-0.616543	C	-5.881270	-0.352238	-1.038839
C	-6.551572	0.775289	0.008742	C	-7.131311	0.061294	-0.599183
C	-6.587115	0.921230	1.393621	C	-7.286877	0.567308	0.689308
C	-5.453883	0.640498	2.150646	C	-6.186956	0.660635	1.536369
C	-4.290343	0.201366	1.527946	C	-4.935385	0.238240	1.101875
C	1.006778	3.215957	0.975454	C	1.773263	2.414816	1.184915
C	0.304689	4.421035	0.946610	C	1.279269	3.638567	1.633828
C	-0.733659	4.617516	0.042688	C	0.170823	4.221124	1.028105
C	-1.083500	3.603828	-0.842337	C	-0.455906	3.581568	-0.036207
C	-0.398546	2.388707	-0.836249	C	0.015635	2.354583	-0.500423
C	-0.316631	-4.668170	-1.915688	C	3.272797	-3.454772	3.512087
H	2.111975	-5.864206	-1.761657	H	0.835198	-2.347552	2.951149
H	3.897044	-5.540247	-0.088986	H	3.918898	-4.766455	1.208413
H	3.551275	-3.941556	1.786961	H	2.575817	-4.965373	-0.853031
H	1.418136	-2.695832	1.954217	H	0.392545	-3.821561	-1.043990
H	-5.340461	0.240237	-1.692603	H	-5.741326	-0.736443	-2.040793
H	-7.431330	0.997373	-0.582998	H	-7.985697	-0.007887	-1.261520
H	-7.493877	1.259230	1.880791	H	-8.261856	0.894516	1.029707
H	-5.472306	0.770387	3.225942	H	-6.300860	1.069349	2.532825
H	-3.407538	0.016602	2.128155	H	-4.082133	0.346747	1.760959
H	1.818455	3.056577	1.670632	H	2.653906	1.972749	1.628203
H	-0.688798	1.598634	-1.515730	H	-0.485141	1.849585	-1.314509
H	0.582258	5.203035	1.642993	H	1.774449	4.131285	2.461375

H	-1.893879	3.742291	-1.547429	H	-1.315461	4.031216	-0.517736
H	-1.270350	5.558241	0.029076	H	-0.201315	5.174387	1.381943
H	5.092103	0.176842	-0.042258	H	4.730785	0.302045	-2.346724
H	4.593591	1.650190	-0.871988	H	3.925891	1.869209	-2.304041
H	6.139490	1.612412	0.001483	H	5.698430	1.794359	-2.342127
H	-1.285824	-4.839549	-1.441126	H	3.189430	-4.383555	4.085395
H	-0.428381	-3.799045	-2.570835	H	4.332898	-3.290340	3.308409
H	-0.085067	-5.529154	-2.543556	H	2.921521	-2.640555	4.147468
Structure: A_5				**Structure: A_9**			
C	0.517066	-2.970326	0.885663	C	0.507866	-2.978889	0.965579
C	1.019869	-3.690684	-0.203786	C	1.222562	-2.937821	2.169553
C	2.246467	-4.338117	-0.106470	C	2.427795	-3.613077	2.272587
C	3.008331	-4.293068	1.063269	C	2.936840	-4.363116	1.219433
C	2.483105	-3.590694	2.152813	C	2.200742	-4.430587	0.039615
C	1.251409	-2.958404	2.077344	C	0.996382	-3.751768	-0.096799
N	-0.734719	-2.342644	0.872554	N	-0.729665	-2.331819	0.927095
C	-1.195412	-1.553222	-0.004736	C	-1.183052	-1.570403	0.019179
S	-0.377685	-0.831899	-1.466145	S	-0.356119	-0.904799	-1.458965
N	-2.511080	-1.106097	0.211208	N	-2.497265	-1.118698	0.216132
C	-3.438325	-0.717212	-0.743162	C	-3.417269	-0.720819	-0.744530
O	-3.205015	-0.740191	-1.937494	O	-3.182058	-0.756518	-1.937337
C	-4.762793	-0.279057	-0.195166	C	-4.735073	-0.259693	-0.200623
I	1.916774	-0.057286	-0.557511	I	1.947447	-0.094048	-0.584961
H	-2.861771	-1.393897	1.115151	H	-2.855344	-1.388709	1.122740
O	3.873045	0.749198	0.250777	O	3.889416	0.750849	0.175280
C	4.849327	1.384629	-0.391502	C	4.835896	1.407155	-0.495775
O	5.751667	1.909083	0.227173	O	5.733163	1.961222	0.101337
C	4.795181	1.417237	-1.910957	C	4.752298	1.418463	-2.013569
C	1.105223	1.845105	0.154367	C	1.113474	1.796662	0.126810
C	-5.870308	-0.359095	-1.044193	C	-5.842948	-0.329681	-1.050194
C	-7.123111	0.041022	-0.599965	C	-7.090021	0.091668	-0.609705
C	-7.280661	0.538523	0.691607	C	-7.241164	0.600395	0.678258
C	-6.179956	0.636859	1.537080	C	-6.139842	0.688834	1.524051
C	-4.925530	0.227903	1.097932	C	-4.891240	0.258609	1.088895
C	1.742525	2.447663	1.227999	C	1.738131	2.398788	1.208080
C	1.235044	3.661890	1.687578	C	1.219117	3.608121	1.667448
C	0.127077	4.243029	1.079596	C	0.113247	4.184462	1.051024
C	-0.485835	3.611618	0.002403	C	-0.486224	3.553675	-0.034123
C	-0.000812	2.394049	-0.472629	C	0.010091	2.340647	-0.509049
C	4.333622	-5.004299	1.164949	Cl	3.324650	-3.535404	3.789936
H	0.449166	-3.746871	-1.121224	H	0.829161	-2.375308	3.004564
H	2.615569	-4.894336	-0.961348	H	3.876495	-4.887052	1.324297
H	3.045080	-3.544091	3.079342	H	2.571561	-5.029658	-0.783489
H	0.849309	-2.430258	2.932855	H	0.430166	-3.822466	-1.015181
H	-5.728832	-0.736724	-2.048432	H	-5.706665	-0.716655	-2.051571
H	-7.978118	-0.032114	-1.261076	H	-7.945605	0.026167	-1.270829
H	-8.257831	0.855172	1.035713	H	-8.213929	0.933321	1.019367
H	-6.295545	1.038984	2.536026	H	-6.250378	1.099400	2.520086
H	-4.072028	0.340160	1.756026	H	-4.036937	0.363179	1.747260
H	2.622923	2.007046	1.673204	H	2.617740	1.963155	1.659714

H	-0.490829	1.894590	-1.296564	H	-0.468825	1.841484	-1.339658
H	1.719216	4.148200	2.525326	H	1.692457	4.094319	2.511330
H	-1.345017	4.060309	-0.480689	H	-1.343146	3.999650	-0.523639
H	-0.255540	5.188961	1.441807	H	-0.278204	5.126845	1.412983
H	4.724774	0.407796	-2.321419	H	4.715424	0.401248	-2.409237
H	3.919753	1.973999	-2.254190	H	3.849848	1.935394	-2.348778
H	5.692391	1.899758	-2.291586	H	5.623128	1.930115	-2.416417
H	5.082929	-4.379928	1.656828				
H	4.243866	-5.925730	1.748645				
H	4.715012	-5.275402	0.179607				
Structure: A_10				**Structure: A_15**			
C	0.590956	-2.814343	0.719221	C	0.623908	-2.739649	0.645424
C	1.053962	-3.502770	-0.410601	C	1.484686	-2.674472	1.752421
C	2.284539	-4.147416	-0.389250	C	2.717457	-3.311642	1.751338
C	3.060124	-4.108626	0.763120	C	3.109753	-4.057200	0.644617
C	2.610527	-3.451229	1.902017	C	2.262738	-4.155574	-0.456374
C	1.371534	-2.826258	1.881524	C	1.035401	-3.507774	-0.455018
N	-0.671504	-2.217499	0.775064	N	-0.644962	-2.174930	0.716791
C	-1.189515	-1.418961	-0.063836	C	-1.190231	-1.383304	-0.110572
S	-0.438516	-0.632937	-1.525160	S	-0.470819	-0.569964	-1.570047
N	-2.510965	-1.032006	0.205949	N	-2.518737	-1.039036	0.172341
C	-3.483545	-0.643414	-0.706350	C	-3.503290	-0.636589	-0.720101
O	-3.288536	-0.619230	-1.906646	O	-3.320556	-0.585323	-1.921461
C	-4.803655	-0.277971	-0.099995	C	-4.818333	-0.291684	-0.091612
I	1.817541	0.259259	-0.608162	I	1.801172	0.313656	-0.685485
H	-2.824935	-1.365233	1.107824	H	-2.814734	-1.383483	1.076075
O	3.690973	1.251710	0.200123	O	3.663103	1.349674	0.096752
C	4.954584	0.995658	-0.124008	C	4.921591	0.957903	-0.064910
O	5.859827	1.582531	0.429050	O	5.827882	1.553448	0.477818
C	5.208651	-0.048740	-1.199731	C	5.173008	-0.254185	-0.950607
C	0.919222	2.129565	0.078147	C	0.903069	2.154392	0.039510
C	-5.936860	-0.381264	-0.911838	C	-5.959986	-0.380665	-0.893207
C	-7.188576	-0.051009	-0.410735	C	-7.207124	-0.065807	-0.371209
C	-7.319545	0.399772	0.900816	C	-7.324896	0.355297	0.951459
C	-6.193817	0.521651	1.709631	C	-6.190760	0.462734	1.750484
C	-4.939973	0.182031	1.213693	C	-4.941373	0.138482	1.233478
C	1.502578	2.771673	1.158791	C	1.391529	2.694814	1.218143
C	0.926977	3.965873	1.590060	C	0.817539	3.879431	1.675164
C	-0.190140	4.488887	0.947748	C	-0.206721	4.492423	0.961140
C	-0.744234	3.819863	-0.138300	C	-0.668280	3.924737	-0.221839
C	-0.190921	2.621988	-0.587103	C	-0.112986	2.738995	-0.698283
Cl	4.626468	-4.919552	0.785113	Cl	1.018248	-1.723713	3.158680
H	0.446774	-3.540229	-1.304815	H	3.359835	-3.224481	2.617531
H	2.634174	-4.684888	-1.260606	H	4.068529	-4.559928	0.648774
H	3.216216	-3.439817	2.798285	H	2.553339	-4.745957	-1.316758
H	1.000036	-2.326562	2.766857	H	0.370818	-3.592673	-1.304767
H	-5.816582	-0.722633	-1.931694	H	-5.849794	-0.698708	-1.921724
H	-8.063531	-0.142734	-1.042636	H	-8.088748	-0.146146	-0.995354
H	-8.296263	0.661511	1.289448	H	-8.298072	0.605177	1.356506
H	-6.290044	0.888241	2.724111	H	-6.276795	0.806304	2.773886

H	-4.068272	0.312357	1.843947	H	-4.063379	0.257695	1.857110
H	2.395026	2.382528	1.624894	H	2.213173	2.235709	1.746440
H	-0.635089	2.095797	-1.419967	H	-0.485069	2.291414	-1.608581
H	1.367825	4.483798	2.432785	H	1.184685	4.318839	2.594083
H	-1.609096	4.223846	-0.649772	H	-1.460188	4.400477	-0.787101
H	-0.625020	5.419758	1.289518	H	-0.641938	5.415242	1.323674
H	4.813525	-1.021582	-0.894009	H	4.664349	-1.136850	-0.552882
H	4.720427	0.232420	-2.136099	H	4.797761	-0.078953	-1.962192
H	6.278465	-0.142368	-1.369222	H	6.241040	-0.453292	-0.997900
Structure: A_16							
C	0.553314	-2.987387	0.878515				
C	1.375692	-2.935913	2.014823				
C	2.560780	-3.653808	2.093462				
C	2.926062	-4.465994	1.028824				
C	2.127887	-4.562509	-0.104518				
C	0.953365	-3.827941	-0.170953				
N	-0.676096	-2.338480	0.878560				
C	-1.136704	-1.555959	-0.007624				
S	-0.304612	-0.870819	-1.472711				
N	-2.446409	-1.107432	0.206139				
C	-3.373131	-0.703263	-0.747605				
O	-3.145213	-0.739058	-1.941449				
C	-4.684603	-0.239111	-0.193212				
I	1.950683	-0.005874	-0.524005				
H	-2.797449	-1.382721	1.114094				
O	3.834406	0.872702	0.327933				
C	4.801872	1.547359	-0.294689				
O	5.666925	2.101193	0.347783				
C	4.779794	1.581280	-1.814155				
C	1.047535	1.866690	0.140490				
C	-5.798359	-0.300029	-1.035892				
C	-7.040626	0.123953	-0.584653				
C	-7.180796	0.625910	0.707236				
C	-6.073526	0.705102	1.546204				
C	-4.829601	0.272360	1.100401				
C	1.581895	2.463101	1.271517				
C	1.017786	3.663506	1.699773				
C	-0.042341	4.235985	1.004523				
C	-0.550751	3.610575	-0.129151				
C	-0.008138	2.406424	-0.574723				
Cl	0.927892	-1.903633	3.364623				
Cl	4.422183	-5.390294	1.124438				
H	3.183603	-3.579305	2.973148				
H	2.416181	-5.210072	-0.921280				
H	0.320839	-3.906275	-1.044995				
H	-5.670491	-0.682359	-2.040142				
H	-7.900996	0.065559	-1.240191				
H	-8.149930	0.960591	1.056857				
H	-6.175827	1.110149	2.545333				
H	-3.970494	0.369290	1.753590				

H	2.426765	2.029507	1.786818
H	-0.418123	1.911109	-1.443475
H	1.419461	4.145320	2.582351
H	-1.371644	4.053818	-0.679298
H	-0.469492	5.171352	1.343618
H	4.760332	0.570906	-2.227818
H	3.890722	2.103375	-2.176326
H	5.665087	2.100480	-2.173489

Optimized Geometries for Intermediates B

Structure: B_1

C	-1.106737	2.859296	0.580553
C	-1.211339	3.952626	-0.297890
C	-2.462657	4.554968	-0.433470
C	-3.586584	4.139675	0.284123
C	-3.440812	3.075472	1.172696
C	-2.212500	2.443040	1.318580
N	0.151877	2.216773	0.829125
C	0.990917	1.606919	-0.055533
S	0.294585	0.905771	-1.581056
N	2.236614	1.520145	0.253969
C	3.215613	1.057333	-0.610163
O	3.182952	1.232095	-1.820528
C	4.377664	0.383136	0.050574
I	-1.731207	-0.457811	-0.757852
H	0.629116	2.478174	1.683812
O	-3.473112	-1.864503	-0.219136
C	-3.853749	-1.850710	1.033926
O	-3.267619	-1.269344	1.940658
C	-5.122025	-2.652937	1.277534
C	-0.455161	-2.102369	-0.220407
C	5.410565	-0.106525	-0.755178
C	6.500227	-0.750253	-0.184480
C	6.570969	-0.910179	1.198214
C	5.547078	-0.424333	2.006608
C	4.454677	0.220363	1.436475
C	0.261525	-2.747928	-1.217230
C	1.084669	-3.809177	-0.851882
C	1.174273	-4.202074	0.480314
C	0.441445	-3.536320	1.456989
C	-0.386668	-2.468921	1.115689
C	-0.030303	4.487533	-1.063941
C	-4.908074	4.846688	0.117370
H	-2.556366	5.395786	-1.113540
H	-4.289552	2.728002	1.749822
H	-2.114274	1.600558	1.992002
H	5.338518	0.029545	-1.826680
H	7.296972	-1.126479	-0.815248
H	7.423199	-1.410340	1.643726

Structure: B_2

C	-1.062149	2.749787	0.739037
C	-1.279972	3.599486	-0.347600
C	-2.502479	4.248749	-0.480580
C	-3.500095	4.082724	0.476197
C	-3.271993	3.252072	1.569219
C	-2.061553	2.581492	1.698788
N	0.185777	2.096886	0.946027
C	1.065542	1.588138	0.029689
S	0.436340	0.913227	-1.528330
N	2.308874	1.555425	0.362512
C	3.314378	1.143744	-0.500165
O	3.266180	1.299219	-1.712696
C	4.514643	0.547616	0.164849
I	-1.714941	-0.335706	-0.810757
H	0.636293	2.281007	1.833765
O	-3.553377	-1.643529	-0.378737
C	-3.936601	-1.713405	0.872995
O	-3.310996	-1.263953	1.825887
C	-5.265855	-2.431282	1.044298
C	-0.554017	-2.081717	-0.339825
C	5.565804	0.095422	-0.639522
C	6.692426	-0.476935	-0.064851
C	6.782312	-0.602221	1.320287
C	5.740646	-0.153166	2.127216
C	4.611031	0.420013	1.553392
C	0.099534	-2.745736	-1.368034
C	0.850277	-3.873482	-1.049377
C	0.932532	-4.312604	0.268827
C	0.263100	-3.627930	1.277382
C	-0.492381	-2.494564	0.982965
H	-0.499363	3.752218	-1.080512
H	-2.666311	4.902968	-1.328597
H	-4.447446	4.596679	0.370240
H	-4.042648	3.108403	2.316801
H	-1.898780	1.901849	2.526389
H	5.478561	0.203310	-1.713079
H	7.502766	-0.824827	-0.694475
H	7.663086	-1.046978	1.768864

H	5.601814	-0.545232	3.082262	H	5.810348	-0.246900	3.204687
H	3.658458	0.608903	2.056892	H	3.800664	0.779829	2.172654
H	0.197996	-2.435680	-2.250482	H	0.040497	-2.399438	-2.390686
H	-0.980031	-1.959556	1.863079	H	-1.042183	-1.971891	1.753729
H	1.653092	-4.326307	-1.614828	H	1.367804	-4.406048	-1.837492
H	0.509408	-3.840995	2.494196	H	0.323126	-3.970147	2.303307
H	1.817017	-5.028926	0.756689	H	1.517674	-5.191774	0.508883
H	-4.961772	-3.692516	0.985733	H	-5.190170	-3.446178	0.650467
H	-5.397174	-2.600685	2.328925	H	-5.537718	-2.460518	2.097366
H	-5.931147	-2.262742	0.658214	H	-6.039422	-1.917127	0.471724
H	0.860123	4.557225	-0.436258				
H	0.223314	3.842728	-1.909038				
H	-0.249054	5.481120	-1.455369				
H	-4.888491	5.832437	0.591028				
H	-5.148262	4.998718	-0.937290				
H	-5.721255	4.278867	0.571075				
Structure: B_3				**Structure: B_4**			
C	-1.127528	2.861682	0.552056	C	0.644044	-3.007528	1.036940
C	-1.214911	3.955539	-0.327440	C	1.438659	-2.975775	2.185231
C	-2.463922	4.565374	-0.473782	C	2.614708	-3.718352	2.272639
C	-3.577627	4.139334	0.240939	C	2.994723	-4.490112	1.170770
C	-3.464433	3.079463	1.133382	C	2.202297	-4.530384	0.029333
C	-2.238573	2.443678	1.285328	C	1.016935	-3.806284	-0.043537
N	0.125794	2.212396	0.810484	N	-0.565769	-2.261270	1.053107
C	0.974761	1.610879	-0.071939	C	-1.263402	-1.666867	0.039706
S	0.289667	0.911638	-1.603000	S	-0.390554	-1.068352	-1.434451
N	2.217934	1.528446	0.245843	N	-2.527755	-1.500424	0.221540
C	3.204975	1.068633	-0.611950	C	-3.378903	-0.993502	-0.749548
O	3.184551	1.253546	-1.820765	O	-3.193766	-1.136765	-1.950680
C	4.358076	0.386326	0.055398	C	-4.596001	-0.301156	-0.223674
I	-1.730826	-0.466302	-0.787513	I	1.832084	-0.082792	-0.547398
H	0.593136	2.467170	1.672573	H	-1.143692	-2.384472	1.874952
O	-3.463502	-1.880743	-0.249272	O	3.715826	0.877667	0.257518
C	-3.850420	-1.861448	1.002174	C	4.684404	1.514190	-0.396492
O	-3.272165	-1.270436	1.907604	O	5.563652	2.084832	0.213653
C	-5.115913	-2.668191	1.244119	C	4.650305	1.486147	-1.916459
C	-0.443418	-2.096269	-0.232414	C	0.872764	1.781573	0.077628
C	5.397768	-0.100140	-0.743574	C	-5.505720	0.234826	-1.141326
C	6.479530	-0.751556	-0.166706	C	-6.641440	0.898009	-0.697156
C	6.535449	-0.922498	1.215370	C	-6.881593	1.031897	0.669208
C	5.504789	-0.439822	2.017023	C	-5.981711	0.499663	1.588225
C	4.420284	0.212646	1.440744	C	-4.843484	-0.165141	1.145359
C	0.282809	-2.742595	-1.221796	C	1.458923	2.480596	1.120864
C	1.113163	-3.794368	-0.845622	C	0.850558	3.666151	1.530049
C	1.200122	-4.177483	0.489593	C	-0.304302	4.123325	0.904244
C	0.457537	-3.511283	1.458533	C	-0.862578	3.396965	-0.141921
C	-0.377825	-2.453100	1.106422	C	-0.276003	2.206450	-0.567831
C	-0.023097	4.486010	-1.079184	C	3.452344	-3.692836	3.525784
H	-2.554494	5.408043	-1.149889	H	1.139264	-2.343051	3.013790
H	-4.528097	4.641905	0.107327	H	3.914562	-5.062203	1.208627

H	-4.320747	2.740918	1.702920	H	2.499482	-5.145421	-0.811765
H	-2.141720	1.600313	1.957682	H	0.394512	-3.862101	-0.925099
H	5.337254	0.044478	-1.814658	H	-5.303471	0.118117	-2.198328
H	7.281667	-1.125254	-0.792111	H	-7.342244	1.308863	-1.413965
H	7.381585	-1.428679	1.665672	H	-7.769643	1.547126	1.016208
H	5.548138	-0.569193	3.092187	H	-6.169302	0.599761	2.650874
H	3.619078	0.598932	2.056116	H	-4.143852	-0.590023	1.852007
H	0.221197	-2.437903	-2.257421	H	2.373441	2.134336	1.580437
H	-0.978570	-1.943525	1.847783	H	-0.723306	1.634518	-1.368672
H	1.689254	-4.311910	-1.602526	H	1.292712	4.227484	2.343936
H	0.523424	-3.808384	2.498069	H	-1.759826	3.747201	-0.636677
H	1.848565	-4.997019	0.774385	H	-0.767213	5.046527	1.229595
H	-4.948857	-3.708924	0.960310	H	4.634219	0.458783	-2.286641
H	-5.397024	-2.610110	2.293610	H	3.754469	1.985619	-2.293177
H	-5.923494	-2.286172	0.617746	H	5.529399	1.994579	-2.305230
H	0.861094	4.549952	-0.442162	H	3.239763	-4.563528	4.154414
H	0.236195	3.842927	-1.923921	H	4.517791	-3.712781	3.289120
H	-0.233541	5.481737	-1.469778	H	3.255136	-2.799721	4.120336
Structure: B_5				**Structure: B_9**			
C	-1.051874	2.757394	0.736878	C	0.680076	-3.069328	1.051700
C	-1.277743	3.603878	-0.350530	C	1.444504	-3.095135	2.221579
C	-2.505256	4.237798	-0.489820	C	2.569914	-3.902755	2.283605
C	-3.523955	4.076373	0.454607	C	2.971780	-4.672675	1.199761
C	-3.272848	3.243811	1.545975	C	2.201469	-4.637286	0.041912
C	-2.056884	2.584792	1.686497	C	1.052693	-3.858682	-0.038401
N	0.202818	2.117240	0.949486	N	-0.497706	-2.281403	1.066713
C	1.077522	1.592405	0.039793	C	-1.203565	-1.706644	0.039936
S	0.445024	0.905052	-1.511864	S	-0.334728	-1.140098	-1.446003
N	2.322325	1.557685	0.370468	N	-2.462650	-1.534151	0.230553
C	3.323683	1.138227	-0.491435	C	-3.325411	-1.032701	-0.737822
O	3.270804	1.278869	-1.706016	O	-3.176034	-1.229788	-1.934854
C	4.528152	0.551133	0.174891	C	-4.502874	-0.281146	-0.205785
I	-1.711317	-0.328292	-0.786810	I	1.860584	-0.079569	-0.558185
H	0.658489	2.320843	1.830370	H	-1.070026	-2.374863	1.896424
O	-3.560341	-1.625799	-0.352253	O	3.692501	0.944648	0.247973
C	-3.932943	-1.707879	0.901488	C	4.627475	1.635660	-0.405160
O	-3.297024	-1.273076	1.854503	O	5.468503	2.253555	0.210398
C	-5.265048	-2.420295	1.076195	C	4.600874	1.605297	-1.924617
C	-0.564104	-2.089139	-0.338954	C	0.831253	1.748558	0.058029
C	5.577768	0.094369	-0.628830	C	-5.414539	0.259760	-1.118757
C	6.707576	-0.470529	-0.052919	C	-6.514481	0.977157	-0.669163
C	6.802171	-0.583822	1.332911	C	-6.716773	1.160306	0.697732
C	5.762015	-0.130159	2.139250	C	-5.814929	0.623409	1.612010
C	4.629322	0.435623	1.564126	C	-4.712122	-0.095233	1.163923
C	0.070851	-2.754602	-1.377882	C	1.368076	2.450887	1.125208
C	0.813801	-3.891470	-1.073767	C	0.716051	3.614984	1.528405
C	0.907073	-4.338105	0.241173	C	-0.431483	4.047976	0.872747
C	0.256295	-3.651889	1.260852	C	-0.938935	3.319281	-0.197320
C	-0.491032	-2.509488	0.980899	C	-0.308340	2.149632	-0.617731
C	-4.841051	4.793501	0.300459	Cl	3.515137	-3.935612	3.769150

H	-0.498365	3.764330	-1.083426	H	1.166889	-2.482032	3.068839
H	-2.666530	4.886316	-1.344308	H	3.858911	-5.287155	1.264096
H	-4.044031	3.088505	2.291965	H	2.489756	-5.246046	-0.806302
H	-1.898450	1.908674	2.517976	H	0.451185	-3.869380	-0.935264
H	5.486578	0.192680	-1.702992	H	-5.242666	0.103557	-2.176018
H	7.516667	-0.822026	-0.682179	H	-7.217102	1.391968	-1.381850
H	7.685317	-1.022884	1.782454	H	-7.577347	1.717634	1.048958
H	5.835247	-0.214657	3.217273	H	-5.973530	0.761732	2.675027
H	3.819812	0.798680	2.182637	H	-4.011926	-0.523818	1.867721
H	0.003314	-2.402663	-2.398094	H	2.277924	2.124884	1.608388
H	-1.026437	-1.985524	1.760863	H	-0.716129	1.575050	-1.437571
H	1.316709	-4.425084	-1.870586	H	1.118325	4.178648	2.361090
H	0.324886	-3.999848	2.284304	H	-1.830068	3.651399	-0.715079
H	1.486115	-5.224261	0.470025	H	-0.928647	4.954782	1.193780
H	-5.198206	-3.431228	0.670786	H	4.632869	0.578628	-2.295489
H	-5.528664	-2.459571	2.131052	H	3.685422	2.064892	-2.305188
H	-6.040488	-1.895822	0.515589	H	5.457608	2.153523	-2.309024
H	-4.729947	5.866182	0.486147				
H	-5.240756	4.679809	-0.710335				
H	-5.584729	4.411672	1.001141				
Structure: B_10				**Structure: B_15**			
C	-1.076577	2.711314	0.772224	C	0.616954	-3.129496	1.053700
C	-1.263235	3.627053	-0.265006	C	1.400376	-3.181935	2.215488
C	-2.472177	4.299829	-0.394113	C	2.544228	-3.963779	2.284007
C	-3.482580	4.077313	0.533276	C	2.934693	-4.710409	1.179117
C	-3.305332	3.184309	1.581860	C	2.159438	-4.687500	0.023626
C	-2.102783	2.497928	1.693317	C	1.003733	-3.921010	-0.033562
N	0.159640	2.035724	0.966270	N	-0.554891	-2.351015	1.050945
C	1.046147	1.572488	0.028938	C	-1.239083	-1.761242	0.018850
S	0.419016	0.958838	-1.554814	S	-0.346403	-1.210206	-1.460811
N	2.287708	1.533961	0.362033	N	-2.494275	-1.558120	0.198086
C	3.298984	1.161517	-0.514153	C	-3.337083	-1.036903	-0.777226
O	3.257113	1.377443	-1.717027	O	-3.193693	-1.255085	-1.971249
C	4.493040	0.530498	0.128254	C	-4.486438	-0.235597	-0.256529
I	-1.715733	-0.340993	-0.876933	I	1.855140	-0.185542	-0.549463
H	0.607101	2.184323	1.862329	H	-1.098748	-2.372078	1.904860
O	-3.527392	-1.681803	-0.457950	O	3.697416	0.801503	0.278907
C	-3.957916	-1.701588	0.780885	C	4.595693	1.563638	-0.345398
O	-3.381091	-1.188410	1.732442	O	5.469630	2.116325	0.286419
C	-5.272894	-2.447359	0.936900	C	4.485925	1.699669	-1.855651
C	-0.522539	-2.039365	-0.318064	C	0.835144	1.620725	0.130188
C	5.545507	0.109553	-0.691354	C	-5.374442	0.330050	-1.177713
C	6.666506	-0.494006	-0.138119	C	-6.446652	1.094448	-0.738649
C	6.749544	-0.681656	1.240428	C	-6.644541	1.300156	0.625715
C	5.706856	-0.263486	2.062473	C	-5.766073	0.738821	1.548051
C	4.582640	0.340594	1.510191	C	-4.690894	-0.026712	1.110614
C	0.202360	-2.697095	-1.301294	C	1.353445	2.260964	1.244566
C	0.971040	-3.795133	-0.926547	C	0.707585	3.413287	1.688856
C	0.999823	-4.211886	0.401135	C	-0.416751	3.895179	1.026763
C	0.259535	-3.533785	1.363554	C	-0.906949	3.228032	-0.090624

C	-0.515040	-2.429752	1.012839	C	-0.281534	2.071533	-0.552939
Cl	-5.011800	4.939496	0.373608	Cl	0.925400	-2.242927	3.631392
H	-0.466988	3.818166	-0.971534	H	3.125761	-3.973275	3.195905
H	-2.618980	5.007597	-1.198983	H	3.834086	-5.310676	1.227883
H	-4.101676	3.009337	2.292593	H	2.441701	-5.285454	-0.833908
H	-1.974461	1.766345	2.481407	H	0.391870	-3.928666	-0.923953
H	5.463835	0.266210	-1.759259	H	-5.206442	0.155874	-2.232790
H	7.477810	-0.817776	-0.779204	H	-7.131206	1.528387	-1.457527
H	7.626050	-1.150749	1.672224	H	-7.483666	1.894256	0.968660
H	5.771561	-0.405545	3.134876	H	-5.921295	0.894765	2.609102
H	3.771770	0.676964	2.141822	H	-4.009258	-0.474224	1.820851
H	0.184985	-2.367858	-2.331074	H	2.244039	1.896428	1.735971
H	-1.117432	-1.912200	1.747097	H	-0.675453	1.543441	-1.409918
H	1.544306	-4.322519	-1.678820	H	1.094823	3.928367	2.559121
H	0.278408	-3.858343	2.396775	H	-1.780419	3.598556	-0.612341
H	1.599387	-5.068130	0.684710	H	-0.909793	4.792021	1.380378
H	-5.155671	-3.476975	0.594604	H	4.525961	0.720908	-2.338705
H	-5.583836	-2.435049	1.979444	H	3.539045	2.167279	-2.136521
H	-6.037164	-1.981901	0.312571	H	5.306333	2.313355	-2.219977
Structure: B_16							
C	-1.150614	2.802121	0.617615				
C	-1.238442	3.972878	-0.148937				
C	-2.449769	4.633727	-0.312163				
C	-3.577620	4.141242	0.330022				
C	-3.517220	3.005406	1.125576				
C	-2.302592	2.346224	1.260401				
N	0.081279	2.122443	0.845130				
C	0.934957	1.599995	-0.093899				
S	0.236067	1.017627	-1.666664				
N	2.172925	1.492970	0.215942				
C	3.160487	1.072029	-0.667904				
O	3.162462	1.360607	-1.854016				
C	4.275504	0.291457	-0.046871				
I	-1.701257	-0.482369	-0.881373				
H	0.563142	2.350629	1.707071				
O	-3.353660	-1.974878	-0.297122				
C	-3.835231	-1.837144	0.912456				
O	-3.366599	-1.100400	1.775738				
C	-5.057235	-2.702695	1.168217				
C	-0.330410	-1.974442	-0.155722				
C	5.299311	-0.179470	-0.875429				
C	6.344275	-0.923220	-0.344556				
C	6.379422	-1.202135	1.020664				
C	5.365481	-0.734124	1.851665				
C	4.317006	0.009977	1.321437				
C	0.552142	-2.561295	-1.049942				
C	1.431582	-3.525326	-0.565247				
C	1.409768	-3.883683	0.779267				
C	0.510458	-3.278206	1.650494				
C	-0.376032	-2.306924	1.189762				

Cl	0.186603	4.661239	-0.903062
Cl	-5.109178	4.984116	0.128334
H	-2.501938	5.530175	-0.912801
H	-4.401143	2.631829	1.623182
H	-2.252512	1.439986	1.850399
H	5.256095	0.050399	-1.932253
H	7.134087	-1.284674	-0.992362
H	7.197326	-1.780124	1.435262
H	5.393905	-0.946322	2.913950
H	3.529666	0.385257	1.960923
H	0.575120	-2.274023	-2.092112
H	-1.089716	-1.839764	1.855598
H	2.130795	-3.994968	-1.245883
H	0.492868	-3.554862	2.697574
H	2.097275	-4.635058	1.148032
H	-4.797917	-3.754052	1.029111
H	-5.421008	-2.541364	2.180859
H	-5.838959	-2.462283	0.445809

Optimized Geometries for Intermediates C

Structure: C_1			
C	-0.686172	2.997127	0.479172
C	-0.792224	4.312274	-0.014851
C	-1.996055	4.703291	-0.596145
C	-3.094555	3.850092	-0.707013
C	-2.956446	2.556002	-0.209901
C	-1.774169	2.126728	0.380152
N	0.549217	2.622896	1.065494
C	0.910835	1.411064	1.553484
O	0.196394	0.438822	1.682054
N	2.311252	1.339281	1.947150
C	3.334673	1.970496	1.144074
O	3.219443	3.133970	0.815251
C	4.451263	1.120532	0.672005
H	1.293406	3.310540	1.041797
C	2.719436	0.742120	3.167765
O	3.884678	0.803685	3.493236
C	1.674056	0.102479	4.046790
C	5.639225	1.747238	0.280828
C	6.685582	0.994870	-0.231488
C	6.546097	-0.383689	-0.378949
C	5.358653	-1.009009	-0.008658
C	4.315943	-0.262817	0.524123
C	-4.390347	4.321836	-1.317001
C	0.356929	5.286357	0.072889
H	-2.073940	5.715392	-0.979378
H	-3.785882	1.860618	-0.281133
H	-1.689407	1.122451	0.762587
H	5.729528	2.820036	0.392189

Structure: C_2			
C	-0.707988	2.972929	0.501308
C	-1.832059	2.142642	0.469458
C	-3.002206	2.602795	-0.127804
C	-3.075140	3.873362	-0.687119
C	-1.953589	4.697823	-0.649638
C	-0.778440	4.253270	-0.061852
N	0.525147	2.608234	1.088314
C	0.888738	1.399668	1.585181
O	0.168370	0.433257	1.722115
N	2.288491	1.330219	1.970641
C	3.306319	1.989939	1.179189
O	3.180714	3.158935	0.876052
C	4.429317	1.159688	0.688522
H	1.264116	3.303124	1.055557
C	2.709775	0.714900	3.179316
O	3.874388	0.793194	3.502478
C	1.680549	0.036166	4.047455
C	5.611446	1.804759	0.309835
C	6.663746	1.072246	-0.218732
C	6.535947	-0.304060	-0.395119
C	5.354322	-0.947253	-0.037257
C	4.305727	-0.221430	0.511911
H	-1.786070	1.157385	0.904463
H	-3.868343	1.951975	-0.149876
H	-3.992980	4.218215	-1.146621
H	-1.990238	5.690718	-1.080897
H	0.094212	4.897151	-0.039872
H	5.692769	2.875671	0.443657

H	7.609951	1.480732	-0.518985	H	7.583644	1.572031	-0.496489
H	7.362367	-0.969794	-0.784199	H	7.356960	-0.874322	-0.813181
H	5.246246	-2.079143	-0.132654	H	5.250776	-2.015393	-0.183694
H	3.391755	-0.749778	0.807241	H	3.386204	-0.722749	0.785187
H	0.834756	0.773416	4.232927	H	0.832851	0.689152	4.257233
H	1.264949	-0.790815	3.577692	H	1.280870	-0.850309	3.557677
H	2.161476	-0.149944	4.985387	H	2.179018	-0.233644	4.975380
H	-4.883818	3.520364	-1.870905				
H	-5.089449	4.662426	-0.546453				
H	-4.227280	5.155429	-2.002639				
H	0.647904	5.483811	1.109412				
H	1.247671	4.925621	-0.449645				
H	0.080235	6.241012	-0.373562				
Structure: C_3				**Structure: C_4**			
C	-0.748608	2.810399	0.417449	C	-0.706385	2.979130	0.499665
C	-2.011207	2.491657	0.938519	C	-1.829478	2.152530	0.465675
C	-3.130398	2.900000	0.207502	C	-3.015479	2.595521	-0.128765
C	-3.013399	3.613510	-0.978997	C	-3.066271	3.873981	-0.681312
C	-1.753390	3.941933	-1.466862	C	-1.945856	4.700613	-0.644106
C	-0.625075	3.535253	-0.768051	C	-0.769347	4.262044	-0.059788
N	0.453888	2.461619	1.111256	N	0.525718	2.609326	1.088112
C	0.881347	1.186473	1.285478	C	0.888165	1.400168	1.582505
O	0.235647	0.184995	1.067194	O	0.168469	0.432566	1.717196
N	2.243818	1.088144	1.796206	N	2.288013	1.329391	1.969411
C	3.281618	1.934663	1.261548	C	3.306932	1.989415	1.179626
O	3.091329	3.126758	1.120712	O	3.183101	3.159008	0.878512
C	4.528866	1.279371	0.800291	C	4.429316	1.158645	0.687906
H	1.161614	3.180975	1.223675	H	1.264660	3.304125	1.057803
C	2.573410	0.242950	2.888754	C	2.707093	0.715760	3.179168
O	3.680659	0.306975	3.374259	O	3.871772	0.791352	3.503141
C	1.506548	-0.668238	3.441049	C	1.675535	0.041387	4.048095
C	5.689921	2.054610	0.718221	C	5.610857	1.803739	0.307311
C	6.861335	1.501106	0.222461	C	6.662822	1.071143	-0.221797
C	6.876111	0.179313	-0.217925	C	6.535390	-0.305390	-0.396538
C	5.717106	-0.589673	-0.157465	C	5.354437	-0.948706	-0.036619
C	4.547960	-0.046482	0.358020	C	4.306140	-0.222691	0.512809
C	-2.181569	1.759918	2.241612	C	-4.217451	1.684088	-0.161168
H	-4.115616	2.661217	0.591418	H	-1.777580	1.167138	0.902411
H	-3.903603	3.918039	-1.515715	H	-3.982177	4.226238	-1.141383
H	-1.646849	4.502055	-2.387501	H	-1.989668	5.693359	-1.075266
H	0.364836	3.769364	-1.141676	H	0.103392	4.905278	-0.036142
H	5.660735	3.083053	1.052905	H	5.691776	2.874826	0.439954
H	7.763208	2.099139	0.174913	H	7.582211	1.570945	-0.501236
H	7.790083	-0.249696	-0.610903	H	7.356088	-0.875871	-0.814947
H	5.725274	-1.613546	-0.509725	H	5.251445	-2.017087	-0.181799
H	3.646497	-0.644043	0.399822	H	3.386965	-0.723694	0.787699
H	0.597153	-0.120788	3.691749	H	0.828861	0.696628	4.255154
H	1.225893	-1.426511	2.711493	H	1.274694	-0.845493	3.560073
H	1.915963	-1.130394	4.336046	H	2.172193	-0.226910	4.977428
H	-1.952918	0.698677	2.124651	H	-4.009368	0.777917	-0.736280

H	-1.509477	2.155709	3.006794	H	-4.501395	1.368840	0.845849
H	-3.205281	1.856939	2.604865	H	-5.077763	2.178015	-0.614218
Structure: C_5				**Structure: C_9**			
C	-0.703471	2.972707	0.501249	C	-0.700579	2.978894	0.496686
C	-1.824834	2.140779	0.453188	C	-1.827896	2.152376	0.494301
C	-2.991629	2.600368	-0.148109	C	-2.990160	2.620498	-0.104262
C	-3.089975	3.876378	-0.704404	C	-3.075258	3.873622	-0.692893
C	-1.958401	4.692960	-0.645632	C	-1.943744	4.683985	-0.677547
C	-0.782999	4.253438	-0.054714	C	-0.765487	4.248118	-0.091987
N	0.529978	2.608249	1.090090	N	0.529377	2.613740	1.082211
C	0.893862	1.398814	1.581149	C	0.884891	1.405749	1.593524
O	0.175142	0.429682	1.711615	O	0.152127	0.451251	1.741924
N	2.293510	1.329093	1.969798	N	2.282535	1.326165	1.972721
C	3.312033	1.987542	1.178927	C	3.302510	1.990194	1.185785
O	3.187491	3.156366	0.874806	O	3.176767	3.160736	0.887604
C	4.434985	1.156105	0.689391	C	4.425877	1.163073	0.693120
H	1.267374	3.304681	1.060583	H	1.273305	3.303513	1.040514
C	2.711196	0.717095	3.180481	C	2.705139	0.701694	3.179537
O	3.875856	0.791112	3.505160	O	3.868961	0.783397	3.501939
C	1.677767	0.045244	4.049188	C	1.679444	0.011618	4.042145
C	5.616745	1.800407	0.308192	C	5.607560	1.811596	0.318270
C	6.668958	1.066765	-0.219019	C	6.661112	1.082817	-0.212650
C	6.541551	-0.310083	-0.391289	C	6.535069	-0.292830	-0.395283
C	5.360357	-0.952640	-0.030829	C	5.354078	-0.939393	-0.041266
C	4.311827	-0.225544	0.516728	C	4.304166	-0.217569	0.510297
C	-4.376454	4.363215	-1.321695	Cl	-4.413202	1.575930	-0.105213
H	-1.779553	1.150352	0.876749	H	-1.793504	1.175549	0.946850
H	-3.850550	1.938427	-0.181136	H	-3.997643	4.206001	-1.148190
H	-1.991792	5.688964	-1.072630	H	-1.983747	5.666548	-1.130749
H	0.084158	4.904833	-0.029806	H	0.110331	4.886723	-0.091183
H	5.697668	2.871743	0.438879	H	5.687568	2.881931	0.457213
H	7.588537	1.565978	-0.498909	H	7.580645	1.584871	-0.487386
H	7.362431	-0.881397	-0.808209	H	7.357024	-0.860204	-0.815346
H	5.257329	-2.021281	-0.174104	H	5.252314	-2.006936	-0.192899
H	3.392432	-0.725931	0.791986	H	3.385071	-0.721435	0.780232
H	0.831836	0.702067	4.254409	H	0.829735	0.659137	4.260185
H	1.276073	-0.841571	3.561740	H	1.281791	-0.871389	3.544436
H	2.172870	-0.222645	4.979462	H	2.180373	-0.265828	4.966463
H	-4.894079	3.559293	-1.849285				
H	-5.061964	4.745112	-0.558300				
H	-4.195112	5.171290	-2.032596				
Structure: C_10				**Structure: C_15**			
C	-0.701231	2.976431	0.501138	C	-0.728028	2.841057	0.399533
C	-1.827205	2.148517	0.474102	C	-1.964729	2.649458	1.022111
C	-3.001135	2.597179	-0.122220	C	-3.144710	3.006035	0.380121
C	-3.058358	3.864386	-0.682742	C	-3.098139	3.583176	-0.883011
C	-1.948572	4.699570	-0.660032	C	-1.873948	3.800945	-1.506459
C	-0.776233	4.252341	-0.070198	C	-0.700107	3.424211	-0.867654
N	0.530393	2.614498	1.087634	N	0.495519	2.497584	1.038082
C	0.888445	1.405679	1.592166	C	0.903189	1.209979	1.186487

O	0.158620	0.447137	1.734385	O	0.245041	0.231464	0.921747
N	2.286151	1.328067	1.973186	N	2.250732	1.077857	1.722328
C	3.305445	1.989836	1.183614	C	3.308348	1.927346	1.240698
O	3.179818	3.159929	0.883840	O	3.126381	3.122424	1.107059
C	4.427239	1.160722	0.690596	C	4.572106	1.276972	0.818602
H	1.272763	3.306058	1.050386	H	1.196558	3.217162	1.185521
C	2.707687	0.708233	3.181774	C	2.532490	0.201712	2.808521
O	3.872074	0.786164	3.503479	O	3.625190	0.236002	3.327075
C	1.679088	0.026989	4.048243	C	1.430273	-0.696845	3.307686
C	5.608202	1.807280	0.310128	C	5.736821	2.050590	0.797312
C	6.659920	1.076049	-0.221120	C	6.925924	1.503476	0.337790
C	6.532772	-0.300204	-0.398325	C	6.955655	0.190315	-0.126927
C	5.352465	-0.944903	-0.038645	C	5.793711	-0.576683	-0.126978
C	4.304431	-0.220526	0.513108	C	4.606254	-0.040263	0.352188
Cl	-4.554516	4.424309	-1.431903	Cl	-2.060226	1.987126	2.646746
H	-1.784852	1.165210	0.913772	H	-4.090092	2.841868	0.879293
H	-3.871724	1.955250	-0.144360	H	-4.021130	3.863569	-1.374863
H	-1.997019	5.686438	-1.099523	H	-1.832237	4.251756	-2.489603
H	0.092767	4.900760	-0.056498	H	0.259932	3.569721	-1.347581
H	5.689087	2.878098	0.444833	H	5.696391	3.072531	1.150174
H	7.578886	1.576653	-0.500345	H	7.830168	2.099790	0.337838
H	7.353299	-0.869507	-0.818577	H	7.883659	-0.233611	-0.491417
H	5.249844	-2.012987	-0.185957	H	5.813918	-1.593855	-0.497660
H	3.385850	-0.722854	0.787544	H	3.702811	-0.636339	0.347583
H	0.832145	0.679549	4.262290	H	0.520158	-0.137652	3.527710
H	1.278151	-0.857240	3.555414	H	1.166289	-1.441449	2.557938
H	2.178505	-0.247095	4.974369	H	1.797852	-1.177574	4.211106

Structure: C_16

C	-0.652131	2.992286	0.485180
C	-0.829310	4.304488	0.015295
C	-2.010253	4.716371	-0.582062
C	-2.909865	2.503772	-0.261745
C	-1.722969	2.101825	0.336163
C	-3.048016	3.805912	-0.717180
N	0.577082	2.646993	1.071694
C	0.919731	1.446843	1.619519
O	0.173923	0.503424	1.781107
N	2.304073	1.362033	2.015043
C	3.343058	2.015456	1.232726
O	3.254922	3.196828	0.980638
C	4.425158	1.158664	0.700415
H	1.302861	3.359123	1.061881
C	2.716989	0.737998	3.223626
O	3.885010	0.794999	3.536797
C	1.680833	0.081740	4.100018
C	5.613540	1.775855	0.294003
C	6.630751	1.020553	-0.269459
C	6.462226	-0.350707	-0.451554
C	5.274889	-0.966170	-0.064974
C	4.261023	-0.217610	0.517613

Cl	0.473528	5.482792	0.173673
Cl	-4.553274	4.320531	-1.473232
H	-2.111884	5.732710	-0.933661
H	-3.724178	1.800103	-0.368543
H	-1.618003	1.093013	0.700611
H	5.726237	2.843161	0.433418
H	7.555188	1.498352	-0.569649
H	7.256177	-0.938942	-0.896116
H	5.140311	-2.030306	-0.215044
H	3.337430	-0.697737	0.813592
H	0.841126	0.746392	4.304637
H	1.270857	-0.805493	3.620088
H	2.177675	-0.185318	5.029618

Optimized Geometries for Intermediates D

Structure: D_1			
C	-0.885423	3.033425	0.404093
C	-2.063546	2.270428	0.436699
C	-3.278560	2.956332	0.428251
C	-3.365872	4.348029	0.365313
C	-2.178011	5.074915	0.309656
C	-0.952105	4.422702	0.334207
N	0.405877	2.424901	0.377829
C	0.908222	1.662986	1.379364
O	0.330426	1.310449	2.389200
N	2.255274	1.230976	1.188756
C	3.154466	1.544758	0.194588
O	2.893305	2.326753	-0.711882
C	4.492526	0.878744	0.291483
H	1.078087	2.720691	-0.326828
H	2.573698	0.680593	1.971922
C	-2.042885	0.766648	0.461951
C	-4.709132	5.033617	0.338644
C	5.574561	1.513439	-0.324709
C	6.840019	0.944814	-0.275913
C	7.034384	-0.272357	0.372504
C	5.958256	-0.919845	0.971363
C	4.692327	-0.346133	0.935660
H	-4.194822	2.374730	0.457610
H	-2.207056	6.157694	0.256739
H	-0.030870	4.992967	0.309905
H	5.404660	2.451379	-0.836702
H	7.675489	1.448444	-0.746337
H	8.020956	-0.718964	0.404725
H	6.101749	-1.875535	1.459841
H	3.861182	-0.881068	1.379806
H	-1.321236	0.369474	-0.256143
H	-1.751240	0.398090	1.447583
H	-3.026059	0.364736	0.215004

Structure: D_2			
C	-0.882212	3.004279	0.287876
C	-2.053930	2.390037	0.740672
C	-3.269972	3.051888	0.598162
C	-3.342024	4.312455	0.015997
C	-2.172405	4.920351	-0.432789
C	-0.952367	4.274170	-0.299361
N	0.398553	2.421685	0.383485
C	0.724832	1.211117	0.899871
O	-0.022343	0.389810	1.396092
N	2.116086	0.898412	0.838449
C	3.169988	1.619605	0.325316
O	3.035204	2.748776	-0.133223
C	4.507315	0.949367	0.372263
H	1.188785	2.961490	0.034014
H	2.304995	0.010767	1.279109
C	5.638905	1.769757	0.353645
C	6.909298	1.211307	0.390951
C	7.062961	-0.172236	0.430600
C	5.941677	-0.996086	0.429514
C	4.668001	-0.439537	0.403915
H	-2.005886	1.412819	1.193521
H	-4.172565	2.567623	0.951452
H	-4.295491	4.815419	-0.087638
H	-2.207183	5.902403	-0.888420
H	-0.044338	4.751107	-0.651294
H	5.502559	2.842501	0.308204
H	7.780841	1.854276	0.385806
H	8.054536	-0.608034	0.454787
H	6.057843	-2.073090	0.442427
H	3.809455	-1.099940	0.370435

H	-5.248203	4.813342	-0.587962				
H	-5.340991	4.703231	1.167276				
H	-4.601638	6.117083	0.410082				
Structure: D_3				**Structure: D_4**			
C	-0.890405	3.032259	0.404217	C	-0.881154	3.012001	0.283840
C	-2.065233	2.264860	0.442221	C	-2.051806	2.399588	0.732728
C	-3.283141	2.950531	0.430710	C	-3.284532	3.046980	0.602276
C	-3.347640	4.336611	0.358338	C	-3.333488	4.312481	0.020061
C	-2.174003	5.079419	0.295147	C	-2.165251	4.924259	-0.427914
C	-0.950527	4.423988	0.323591	C	-0.943756	4.284359	-0.300134
N	0.401147	2.425356	0.380072	N	0.398431	2.424475	0.379135
C	0.901613	1.658043	1.379261	C	0.724287	1.216095	0.899703
O	0.321547	1.300894	2.385893	O	-0.022198	0.396223	1.400068
N	2.249235	1.229326	1.189583	N	2.115448	0.901824	0.837960
C	3.150199	1.550092	0.198822	C	3.169600	1.619613	0.321195
O	2.890087	2.339007	-0.701909	O	3.036120	2.747477	-0.140662
C	4.487857	0.883516	0.293168	C	4.506799	0.948682	0.370867
H	1.076332	2.728171	-0.319075	H	1.188726	2.961901	0.026675
H	2.566617	0.674023	1.969728	H	2.303415	0.015280	1.281052
C	-2.041934	0.761517	0.471231	C	-4.538719	2.365650	1.091691
C	5.571224	1.523108	-0.315595	C	5.638936	1.768191	0.348013
C	6.836419	0.953758	-0.268887	C	6.908990	1.209221	0.387434
C	7.029098	-0.268805	0.369789	C	7.061957	-0.174233	0.433370
C	5.951632	-0.921015	0.961097	C	5.940237	-0.997386	0.436367
C	4.685958	-0.346723	0.927633	C	4.666826	-0.440165	0.408652
H	-4.201849	2.375454	0.462918	H	-1.997398	1.419939	1.182050
H	-4.310614	4.833047	0.344012	H	-4.284637	4.821573	-0.083949
H	-2.208024	6.160441	0.232679	H	-2.207037	5.908079	-0.879339
H	-0.025728	4.987987	0.293578	H	-0.035635	4.761941	-0.650084
H	5.402696	2.465275	-0.820208	H	5.503102	2.840784	0.297579
H	7.672994	1.460997	-0.733408	H	7.780867	1.851711	0.379054
H	8.015488	-0.715914	0.400304	H	8.053288	-0.610496	0.459200
H	6.093921	-1.880771	1.441858	H	6.055798	-2.074393	0.454050
H	3.853721	-0.885142	1.365498	H	3.807980	-1.100289	0.378634
H	-1.320113	0.362975	-0.245962	H	-4.698819	1.416147	0.575114
H	-1.750205	0.395770	1.457870	H	-4.477027	2.144084	2.160153
H	-3.024961	0.358468	0.225676	H	-5.418227	2.989668	0.927786
Structure: D_5				**Structure: D_9**			
C	-0.879008	3.001284	0.276421	C	-0.876766	3.007356	0.282108
C	-2.052924	2.387421	0.721664	C	-2.043658	2.383091	0.734473
C	-3.267751	3.048898	0.578760	C	-3.251033	3.053638	0.592574
C	-3.362654	4.317139	0.004258	C	-3.344035	4.315153	0.022671
C	-2.179309	4.911903	-0.438682	C	-2.172352	4.921025	-0.421916
C	-0.956676	4.270341	-0.306774	C	-0.949448	4.280949	-0.296945
N	0.402986	2.418617	0.370880	N	0.400122	2.423696	0.374258
C	0.729076	1.211862	0.893356	C	0.724466	1.211245	0.894156
O	-0.018179	0.392143	1.393293	O	-0.028300	0.396045	1.389887
N	2.120755	0.898301	0.834675	N	2.112669	0.896301	0.834164
C	3.174924	1.616447	0.319470	C	3.168120	1.616813	0.319988
O	3.041080	2.743320	-0.145090	O	3.031860	2.745275	-0.139625

C	4.512794	0.946905	0.372581	C	4.505064	0.948202	0.370570
H	1.192443	2.957563	0.018958	H	1.192206	2.961483	0.024242
H	2.308407	0.012573	1.279491	H	2.300475	0.008828	1.275769
C	-4.687199	5.028646	-0.107059	Cl	-4.723712	2.262083	1.163618
C	5.644277	1.767314	0.351032	C	5.636146	1.769328	0.346235
C	6.914736	1.209485	0.394034	C	6.906709	1.211839	0.387182
C	7.068812	-0.173771	0.442292	C	7.061043	-0.171352	0.436235
C	5.947777	-0.997855	0.443933	C	5.940402	-0.996026	0.440829
C	4.673962	-0.441741	0.412601	C	4.666414	-0.440544	0.411571
H	-2.009163	1.407098	1.168437	H	-2.001689	1.404068	1.182246
H	-4.168307	2.554731	0.927382	H	-4.301847	4.807712	-0.071166
H	-2.210792	5.894407	-0.896327	H	-2.216779	5.905714	-0.870177
H	-0.052727	4.753097	-0.661646	H	-0.044465	4.762954	-0.647435
H	5.507611	2.839717	0.298821	H	5.499389	2.841697	0.294055
H	7.786088	1.852715	0.386714	H	7.777864	1.855218	0.377756
H	8.060455	-0.609155	0.471004	H	8.052836	-0.606391	0.463426
H	6.064175	-2.074745	0.463434	H	6.057325	-2.072787	0.461061
H	3.815703	-1.102576	0.381677	H	3.808676	-1.102164	0.382656
H	-5.500020	4.328197	-0.309248				
H	-4.933931	5.553929	0.821433				
H	-4.674424	5.770622	-0.907923				
Structure: D_10				**Structure: D_15**			
C	-0.877353	3.005787	0.283935	C	-0.861315	3.031022	0.270426
C	-2.049007	2.389957	0.734839	C	-0.994942	4.311457	-0.293701
C	-3.269797	3.043136	0.600973	C	-2.229430	4.930155	-0.411815
C	-3.327532	4.302522	0.022922	C	-3.374118	4.281009	0.034698
C	-2.172247	4.926965	-0.429355	C	-3.263107	3.014461	0.595498
C	-0.954351	4.277429	-0.297156	C	-2.027098	2.392471	0.715438
N	0.401923	2.424803	0.375696	N	0.419985	2.462928	0.357369
C	0.726024	1.213167	0.894820	C	0.742721	1.248666	0.880076
O	-0.026791	0.397078	1.390747	O	-0.013116	0.435317	1.376800
N	2.114458	0.897618	0.835183	N	2.125408	0.922631	0.825138
C	3.169965	1.618043	0.321542	C	3.192957	1.630244	0.313930
O	3.034135	2.746703	-0.137934	O	3.070835	2.756818	-0.147172
C	4.506610	0.948691	0.371234	C	4.521254	0.942995	0.372093
H	1.194058	2.962659	0.026049	H	1.207169	3.009154	0.004564
H	2.302033	0.009987	1.276477	H	2.300792	0.034130	1.269585
Cl	-4.883110	5.122047	-0.141988	Cl	0.434979	5.174078	-0.872206
C	5.638229	1.769123	0.349591	C	5.662602	1.749548	0.343761
C	6.908408	1.210667	0.389699	C	6.926069	1.176531	0.390489
C	7.061819	-0.172756	0.435043	C	7.063192	-0.208073	0.449897
C	5.940620	-0.996684	0.436860	C	5.932271	-1.018528	0.458659
C	4.667018	-0.440248	0.408563	C	4.665349	-0.447212	0.423226
H	-2.002884	1.411090	1.184335	H	-2.284546	5.916587	-0.851714
H	-4.175325	2.565292	0.950133	H	-4.338440	4.764493	-0.057394
H	-2.221382	5.909355	-0.878587	H	-4.146402	2.496519	0.947972
H	-0.051498	4.762716	-0.649857	H	-1.944679	1.410626	1.151987
H	5.502215	2.841722	0.300105	H	5.538765	2.823081	0.283070
H	7.779991	1.853493	0.382431	H	7.805188	1.808962	0.377381
H	8.053315	-0.608522	0.461439	H	8.049470	-0.655266	0.481730

H	6.056827	-2.073584	0.454037	H	6.035634	-2.096537	0.487039
H	3.808723	-1.101055	0.377357	H	3.799520	-1.098347	0.397834
Structure: D_16							
C	-0.856185	3.032750	0.266168				
C	-0.992641	4.312163	-0.299014				
C	-2.225547	4.935137	-0.415310				
C	-3.357650	4.276322	0.040325				
C	-3.261481	3.013189	0.603670				
C	-2.021943	2.398249	0.715422				
N	0.423016	2.463942	0.350566				
C	0.742122	1.247164	0.872513				
O	-0.019441	0.437489	1.366210				
N	2.122493	0.918578	0.819424				
C	3.191507	1.627810	0.311366				
O	3.067988	2.755096	-0.148043				
C	4.519526	0.942167	0.371614				
H	1.212804	3.008006	-0.000853				
H	2.296892	0.029309	1.262880				
Cl	0.429392	5.175582	-0.884091				
Cl	-4.928886	5.061914	-0.103983				
C	5.660286	1.749775	0.346143				
C	6.923948	1.177567	0.395696				
C	7.061755	-0.206968	0.455017				
C	5.931466	-1.018383	0.460877				
C	4.664281	-0.448074	0.422704				
H	-2.293807	5.919771	-0.854048				
H	-4.148044	2.505022	0.957213				
H	-1.942730	1.416673	1.153412				
H	5.536095	2.823277	0.285900				
H	7.802660	1.810549	0.384987				
H	8.048246	-0.653458	0.489121				
H	6.035620	-2.096285	0.489120				
H	3.799121	-1.100011	0.394884				

Optimized Geometries for Intermediates E

Structure: E_1				**Structure: E_2**			
C	-2.728726	-0.796277	-0.442779	C	-2.694888	-0.733220	-0.104376
C	-1.254399	-0.615128	-0.564023	C	-1.235254	-0.721897	-0.402791
N	-0.728842	0.690743	-0.322662	N	-0.587337	0.556212	-0.442880
C	0.564720	0.742012	0.244082	C	0.736411	0.605153	0.023802
N	1.575056	1.271539	-0.314916	N	1.719915	1.096601	-0.614301
O	0.679821	0.178224	1.456960	O	0.926302	0.102110	1.260562
O	-0.501857	-1.535141	-0.785256	O	-0.588079	-1.732246	-0.542351
C	-1.325498	1.942460	-0.669389	C	-1.131501	1.763495	-1.000759
O	-1.001694	2.943864	-0.081888	O	-0.758093	2.834833	-0.599976
C	-2.279292	1.973738	-1.840908	C	-2.078095	1.619740	-2.166639
C	-3.328989	-1.820607	-1.182349	C	-3.450722	-1.819995	-0.557189
C	-4.687384	-2.070256	-1.049874	C	-4.800659	-1.905501	-0.249168
C	-5.452153	-1.318032	-0.159746	C	-5.401762	-0.921112	0.533857

C	-4.854564	-0.315037	0.597538	C	-4.649178	0.149591	1.006448
C	-3.497579	-0.048452	0.454010	C	-3.300107	0.249363	0.685419
C	2.069806	0.482892	1.887726	C	2.365203	0.256263	1.530165
C	2.682457	1.103065	0.601630	C	2.858318	1.007939	0.263635
C	2.761267	-0.709789	2.444151	C	3.030375	-1.057759	1.796453
C	3.867938	-1.211047	1.877841	C	4.134843	-1.421046	1.138406
C	4.388179	-0.647863	0.631209	C	4.682744	-0.627723	0.042653
C	3.837394	0.397012	-0.012207	C	4.070414	0.479919	-0.395810
I	3.287599	3.377375	1.005477	I	3.255269	3.321647	0.694467
O	3.883654	5.608725	1.617841	O	3.662404	5.589452	1.315453
C	4.721470	6.199628	0.820078	C	4.734924	6.107924	0.793723
C	4.918218	7.679635	1.130255	C	4.893605	7.596802	1.082444
O	5.330561	5.657672	-0.102804	O	5.571276	5.494173	0.131913
C	4.300149	0.835540	-1.370721	C	4.770474	2.901246	2.139065
C	4.608954	-2.380071	2.463738	C	4.396751	2.692139	3.462173
C	5.129671	2.855530	1.969053	C	5.386247	2.412843	4.401143
C	5.092169	2.304210	3.243943	C	6.721113	2.351970	4.013359
C	6.292959	1.954372	3.855758	C	7.073624	2.582001	2.686800
C	7.500662	2.160602	3.196223	C	6.098197	2.861346	1.733485
C	7.513276	2.724341	1.924190	H	2.411776	0.867174	2.433002
C	6.322503	3.078384	1.293977	H	-2.528981	0.637522	-2.267525
H	1.927097	1.230811	2.669573	H	-2.852081	2.382214	-2.095929
H	-2.446581	1.011294	-2.314943	H	-1.486987	1.821418	-3.064869
H	-3.232889	2.394735	-1.522512	H	-2.964779	-2.588691	-1.144725
H	-1.843109	2.660586	-2.569552	H	-5.384691	-2.742574	-0.611650
H	-2.717638	-2.413012	-1.851078	H	-6.453818	-0.994018	0.781988
H	-5.150980	-2.856603	-1.632927	H	-5.110184	0.905450	1.630557
H	-6.510901	-1.520692	-0.050344	H	-2.715816	1.073478	1.074324
H	-5.442758	0.256538	1.305001	H	2.605778	-1.670028	2.583039
H	-3.033548	0.718061	1.062075	H	4.630533	-2.351029	1.391456
H	2.352275	-1.134708	3.353464	H	5.566848	-0.994127	-0.464619
H	5.235046	-1.152120	0.177966	H	4.409968	0.999439	-1.283217
H	3.953311	8.187950	1.156375	H	4.002444	8.136633	0.757478
H	5.369304	7.785898	2.119376	H	4.993116	7.751221	2.158934
H	5.563892	8.136472	0.382397	H	5.772935	7.985474	0.572290
H	4.592936	1.888434	-1.383739	H	3.362806	2.772702	3.769895
H	5.150221	0.237342	-1.698768	H	5.108503	2.252696	5.435883
H	3.491172	0.727353	-2.097222	H	7.488303	2.139846	4.748153
H	4.128648	-2.747257	3.370312	H	8.114234	2.557132	2.386854
H	4.661506	-3.202657	1.743946	H	6.369560	3.096058	0.714795
H	5.639007	-2.102580	2.706670				
H	4.156429	2.159697	3.766037				
H	6.278524	1.529811	4.851971				
H	8.432752	1.891988	3.678334				
H	8.452873	2.900544	1.414830				
H	6.324391	3.568962	0.330481				
Structure: E_3				**Structure: E_4**			
C	-2.727339	-0.743877	-0.309492	C	-2.709895	-0.729335	-0.113293
C	-1.253855	-0.650377	-0.502316	C	-1.245582	-0.715025	-0.388334
N	-0.660781	0.651086	-0.408590	N	-0.599994	0.563344	-0.417627

C	0.630102	0.702333	0.153996	C	0.722092	0.611974	0.055156
N	1.659493	1.175525	-0.419971	N	1.708027	1.103825	-0.577916
O	0.723764	0.201516	1.399842	O	0.906862	0.107377	1.292522
O	-0.552363	-1.621020	-0.661364	O	-0.594994	-1.724661	-0.519178
C	-1.194608	1.869333	-0.933939	C	-1.140866	1.772468	-0.975497
O	-0.808480	2.928737	-0.509673	O	-0.772371	2.842389	-0.566685
C	-2.187385	1.772414	-2.069723	C	-2.080188	1.633297	-2.147968
C	-3.403577	-1.814823	-0.903302	C	-3.456491	-1.816242	-0.580852
C	-4.764583	-1.981554	-0.692241	C	-4.811282	-1.904405	-0.295693
C	-5.456220	-1.096866	0.133779	C	-5.426930	-0.922426	0.478999
C	-4.783092	-0.044479	0.747088	C	-4.683914	0.148354	0.966301
C	-3.423231	0.138038	0.522728	C	-3.329746	0.250684	0.668220
C	2.126168	0.428730	1.805266	C	2.344545	0.259797	1.565306
C	2.748243	1.053209	0.519712	C	2.844285	1.012104	0.304264
C	2.775079	-0.813462	2.313513	C	3.008350	-1.055328	1.822098
C	3.902700	-1.267992	1.758885	C	4.110758	-1.415876	1.162154
C	4.492260	-0.662724	0.573587	C	4.682516	-0.626156	0.064006
C	3.948199	0.392312	-0.061535	C	4.059002	0.487908	-0.350405
I	3.255266	3.362319	0.920343	I	3.234119	3.326723	0.743146
O	3.744580	5.614285	1.552497	O	3.668260	5.599311	1.371546
C	4.658854	6.198469	0.837619	C	4.714201	6.121301	0.805182
C	4.821368	7.682112	1.150351	C	4.893574	7.606286	1.104191
O	5.360249	5.646924	-0.010839	O	5.517215	5.514481	0.095586
C	4.454579	0.874352	-1.389426	C	5.916960	-1.157267	-0.608113
C	5.012710	2.898672	2.051709	C	4.790766	2.904494	2.142926
C	4.874706	2.435257	3.354708	C	4.452025	2.640422	3.465585
C	6.021955	2.117629	4.076820	C	5.468103	2.353250	4.373486
C	7.277575	2.268744	3.497276	C	6.795202	2.338879	3.956081
C	7.391823	2.747612	2.195911	C	7.112670	2.624265	2.631406
C	6.255974	3.068462	1.456604	C	6.110118	2.911877	1.708872
H	2.045348	1.154175	2.616404	H	2.390479	0.865183	2.471616
H	-2.268221	0.780892	-2.507662	H	-2.513866	0.645541	-2.268260
H	-3.171922	2.091655	-1.726147	H	-2.867576	2.381033	-2.067952
H	-1.857719	2.481239	-2.830180	H	-1.488476	1.861555	-3.039328
H	-2.847688	-2.508834	-1.520967	H	-2.959504	-2.583035	-1.161589
H	-5.286769	-2.805413	-1.163026	H	-5.387858	-2.741667	-0.669505
H	-6.517056	-1.234149	0.306275	H	-6.482943	-0.997311	0.709222
H	-5.315166	0.632053	1.404737	H	-5.156454	0.902373	1.583977
H	-2.899820	0.945817	1.018497	H	-2.753334	1.074873	1.068567
H	2.324370	-1.292528	3.173984	H	2.584606	-1.673390	2.604835
H	4.390626	-2.142384	2.173919	H	4.600282	-2.351174	1.412750
H	5.367609	-1.139435	0.148265	H	4.400121	1.020221	-1.230567
H	3.855118	8.185612	1.095663	H	3.987676	8.153049	0.836416
H	5.191339	7.797802	2.171646	H	5.052437	7.745468	2.175722
H	5.523494	8.136900	0.454072	H	5.745058	7.999833	0.552229
H	4.749128	1.926271	-1.361137	H	6.747714	-1.226680	0.101570
H	5.314176	0.285239	-1.708957	H	5.746247	-2.164888	-0.999079
H	3.669650	0.789548	-2.145049	H	6.228362	-0.518232	-1.434593
H	3.901451	2.340540	3.816297	H	3.423525	2.684623	3.798131
H	5.928111	1.759970	5.094786	H	5.216769	2.150866	5.407596

H	8.167682	2.024338	4.064088	H	7.583157	2.120509	4.666695
H	8.368945	2.883525	1.748411	H	8.146909	2.637260	2.309256
H	6.337918	3.494997	0.467052	H	6.353078	3.192573	0.694481
Structure: E_5				**Structure: E_9**			
C	-2.705305	-0.725116	-0.175688	C	-2.687245	-0.730013	-0.073864
C	-1.236423	-0.670701	-0.415535	C	-1.225602	-0.720326	-0.360186
N	-0.617926	0.621721	-0.396451	N	-0.582224	0.558663	-0.430729
C	0.691502	0.677393	0.116906	C	0.744671	0.618630	0.021849
N	1.700018	1.144912	-0.498413	N	1.722956	1.097248	-0.633147
O	0.831253	0.198663	1.367996	O	0.948265	0.139993	1.268442
O	-0.559533	-1.661807	-0.553838	O	-0.572163	-1.730957	-0.465234
C	-1.156901	1.825501	-0.954311	C	-1.129268	1.752846	-1.017301
O	-0.760588	2.896921	-0.573306	O	-0.759504	2.832858	-0.637771
C	-2.168076	1.692261	-2.069975	C	-2.070296	1.580590	-2.183376
C	-3.421384	-1.803134	-0.706532	C	-3.434193	-1.831616	-0.505135
C	-4.778830	-1.930843	-0.450253	C	-4.786483	-1.914976	-0.207186
C	-5.426923	-0.999191	0.359313	C	-5.398840	-0.913116	0.544320
C	-4.713801	0.061093	0.910458	C	-4.655152	0.172858	0.995805
C	-3.357543	0.204223	0.640125	C	-3.303658	0.270184	0.684588
C	2.262508	0.363309	1.693677	C	2.388932	0.278127	1.510822
C	2.809726	1.056790	0.417561	C	2.867786	1.027225	0.237879
C	2.906191	-0.935912	2.052167	C	3.040152	-1.047618	1.754542
C	4.017754	-1.376872	1.448745	C	4.138006	-1.417706	1.092627
C	4.590430	-0.635536	0.317993	C	4.678785	-0.599862	0.012130
C	4.018816	0.463751	-0.186923	C	4.080118	0.509569	-0.430174
I	3.262561	3.365938	0.776976	I	3.248296	3.345274	0.667419
O	3.731478	5.639354	1.336570	O	3.641747	5.593430	1.309401
C	4.767124	6.145670	0.735833	C	4.733270	6.109379	0.819286
C	4.953237	7.636918	0.994609	C	4.899882	7.590203	1.139473
O	5.555532	5.519148	0.028098	O	5.574402	5.496364	0.165801
C	4.707079	-2.646792	1.860606	Cl	6.136144	-1.209466	-0.770152
C	4.850814	2.950486	2.144685	C	4.750353	2.907159	2.119909
C	4.544067	2.700326	3.477483	C	4.373680	2.767455	3.451387
C	5.582126	2.420005	4.362305	C	5.354180	2.476164	4.396185
C	6.898412	2.398932	3.911999	C	6.681964	2.332931	4.005152
C	7.183293	2.669291	2.576958	C	7.037943	2.492800	2.669254
C	6.158491	2.949134	1.676845	C	6.071902	2.786054	1.710680
H	2.262386	1.019223	2.565492	H	2.467147	0.881955	2.416326
H	-2.275048	0.682289	-2.456634	H	-2.518585	0.595327	-2.263456
H	-3.140349	2.050128	-1.729843	H	-2.846022	2.342975	-2.133855
H	-1.834635	2.354377	-2.870104	H	-1.475422	1.762747	-3.083349
H	-2.899103	-2.532915	-1.312295	H	-2.939830	-2.613032	-1.068282
H	-5.332082	-2.760389	-0.873205	H	-5.363655	-2.763698	-0.553135
H	-6.484844	-1.105762	0.567446	H	-6.452855	-0.984114	0.784512
H	-5.211713	0.774897	1.555395	H	-5.125078	0.942666	1.595698
H	-2.803057	1.019352	1.087697	H	-2.726571	1.106857	1.057232
H	2.454529	-1.486697	2.869685	H	2.610996	-1.672373	2.528552
H	5.474973	-1.045610	-0.156240	H	4.634042	-2.353042	1.316575
H	4.394681	0.930894	-1.088652	H	4.426379	1.026370	-1.314973
H	4.033384	8.175940	0.762022	H	4.022549	8.145399	0.803104

H	5.165095	7.797204	2.054081	H	4.975318	7.723931	2.220660
H	5.776121	8.021291	0.394908	H	5.795181	7.977972	0.657314
H	4.188410	-3.135692	2.685079	H	3.346340	2.910054	3.758584
H	4.758272	-3.348023	1.021765	H	5.075501	2.370060	5.437637
H	5.736847	-2.446324	2.171805	H	7.441892	2.110113	4.744245
H	3.524334	2.748254	3.835229	H	8.073506	2.401274	2.365509
H	5.356328	2.227820	5.404257	H	6.350460	2.962247	0.682138
H	7.703501	2.186075	4.604852				
H	8.208959	2.674952	2.228377				
H	6.375889	3.215758	0.652796				
Structure: E_10				**Structure: E_15**			
C	-2.692178	-0.742693	-0.106413	C	-2.731891	-0.692726	-0.131151
C	-1.232997	-0.715789	-0.403561	C	-1.256161	-0.717118	-0.333906
N	-0.597165	0.569263	-0.439918	N	-0.585173	0.545598	-0.403268
C	0.726379	0.626421	0.023863	C	0.724056	0.589643	0.102589
N	1.706919	1.122169	-0.615211	N	1.736080	1.021436	-0.532558
O	0.922035	0.124839	1.261455	O	0.865646	0.151918	1.370532
O	-0.574307	-1.718212	-0.545191	O	-0.618963	-1.742845	-0.376799
C	-1.150430	1.774628	-0.994123	C	-1.079231	1.739057	-1.037269
O	-0.778650	2.846820	-0.594173	O	-0.705780	2.818244	-0.659078
C	-2.101539	1.627737	-2.155655	C	-1.967485	1.564008	-2.243538
C	-3.435306	-1.838272	-0.559230	C	-3.474721	-1.789770	-0.580595
C	-4.784257	-1.939019	-0.251674	C	-4.843233	-1.841377	-0.359100
C	-5.396850	-0.961181	0.530622	C	-5.477567	-0.811536	0.334048
C	-4.656834	0.118368	1.003005	C	-4.739400	0.270317	0.804112
C	-3.308897	0.233382	0.682597	C	-3.370606	0.335431	0.569019
C	2.357813	0.290904	1.531099	C	2.296822	0.279537	1.674162
C	2.847495	1.037604	0.260374	C	2.847073	0.963504	0.381321
C	3.026424	-1.018173	1.814766	C	2.909215	-1.034197	2.037914
C	4.124039	-1.369505	1.144936	C	4.024604	-1.460973	1.440814
C	4.671580	-0.602677	0.031942	C	4.637385	-0.746569	0.328678
C	4.050538	0.499010	-0.405337	C	4.065626	0.347136	-0.192043
I	3.262484	3.346759	0.680612	I	3.214940	3.290641	0.798153
O	3.682308	5.595043	1.298114	O	3.518037	5.518379	1.504209
C	4.765962	6.103803	0.784162	C	4.498938	6.154815	0.925611
C	4.941709	7.586779	1.087560	C	4.572900	7.626885	1.312745
O	5.594576	5.482505	0.121883	O	5.308035	5.653224	0.150616
Cl	4.977192	-2.859266	1.547153	Cl	4.710114	1.061374	-1.661063
C	4.767921	2.905686	2.130276	C	4.900571	2.885982	2.046256
C	4.388187	2.719138	3.455196	C	4.695106	2.610991	3.393677
C	5.370569	2.425042	4.397070	C	5.799846	2.339467	4.196652
C	6.703639	2.327751	4.010426	C	7.080049	2.352517	3.651924
C	7.062407	2.536488	2.682061	C	7.262860	2.647273	2.304431
C	6.094319	2.830687	1.725665	C	6.170494	2.919900	1.485259
H	2.399583	0.907446	2.430196	H	2.335463	0.941514	2.540529
H	-2.539389	0.640317	-2.262259	H	-2.419151	0.581304	-2.335650
H	-2.885645	2.378716	-2.074254	H	-2.738811	2.332510	-2.236873
H	-1.518548	1.845689	-3.055377	H	-1.329685	1.734272	-3.115917
H	-2.940283	-2.601810	-1.145881	H	-2.964370	-2.592853	-1.096968
H	-5.358416	-2.783057	-0.613696	H	-5.416364	-2.687035	-0.719058

H	-6.448045	-1.046132	0.778503	H	-6.544882	-0.857508	0.514734
H	-5.126758	0.869113	1.626609	H	-5.227352	1.062072	1.359401
H	-2.734338	1.064228	1.071702	H	-2.799291	1.169392	0.956419
H	2.621259	-1.625621	2.612931	H	2.439749	-1.589073	2.840775
H	5.549985	-0.986197	-0.468945	H	4.491605	-2.385422	1.758597
H	4.386130	1.007264	-1.300658	H	5.530635	-1.154485	-0.124707
H	4.058469	8.140794	0.765043	H	3.617524	8.114378	1.110742
H	5.039923	7.729452	2.165752	H	4.762584	7.713779	2.384735
H	5.827510	7.968698	0.583726	H	5.368899	8.118289	0.756944
H	3.356335	2.827619	3.761209	H	3.702731	2.633214	3.823903
H	5.088938	2.280900	5.433058	H	5.654328	2.126766	5.248854
H	7.464917	2.102547	4.747345	H	7.937104	2.145154	4.281041
H	8.102005	2.482043	2.382859	H	8.260239	2.677481	1.882820
H	6.372610	3.047445	0.704807	H	6.308674	3.191628	0.449069
Structure: E_16							
C	-2.739408	-0.725212	-0.176647				
C	-1.263088	-0.707554	-0.370636				
N	-0.621414	0.573726	-0.401648				
C	0.678813	0.632190	0.125283				
N	1.693974	1.087960	-0.487106				
O	0.807743	0.173130	1.387418				
O	-0.598586	-1.714368	-0.433428				
C	-1.130772	1.769952	-1.015119				
O	-0.773929	2.847653	-0.616172				
C	-2.016433	1.605646	-2.225094				
C	-3.450055	-1.833280	-0.650710				
C	-4.817794	-1.925670	-0.438128				
C	-5.483188	-0.926197	0.270052				
C	-4.776958	0.166180	0.764361				
C	-3.409220	0.272226	0.538791				
C	2.224870	0.353019	1.730066				
C	2.796618	1.018418	0.436313				
C	2.855777	-0.929865	2.162265				
C	3.970596	-1.357028	1.569801				
C	4.582041	-0.701520	0.423212				
C	4.002844	0.372772	-0.128324				
I	3.225610	3.335280	0.838470				
O	3.586899	5.544607	1.526008				
C	4.561029	6.168286	0.919041				
C	4.666774	7.637169	1.307527				
O	5.337986	5.655222	0.120336				
Cl	4.642527	1.033425	-1.619959				
Cl	4.784116	-2.813858	2.134760				
C	4.937732	2.885796	2.036343				
C	4.760930	2.564992	3.377546				
C	5.882207	2.258329	4.144002				
C	7.149294	2.281994	3.569772				
C	7.302990	2.622719	2.229645				
C	6.193915	2.930768	1.445977				
H	2.212523	1.043904	2.574441				

H	-2.431206	0.610874	-2.352896
H	-2.816716	2.343064	-2.187820
H	-1.389471	1.833666	-3.091974
H	-2.915390	-2.612818	-1.178408
H	-5.365904	-2.779820	-0.816441
H	-6.549800	-1.004212	0.443762
H	-5.289144	0.934037	1.331220
H	-2.862638	1.113619	0.945247
H	2.408504	-1.456579	2.994037
H	5.470320	-1.137060	-0.010058
H	3.711577	8.137797	1.140375
H	4.894558	7.717369	2.372554
H	5.449881	8.119629	0.726295
H	3.779225	2.576777	3.831776
H	5.759885	2.008435	5.190811
H	8.018916	2.045048	4.170389
H	8.290348	2.659382	1.785627
H	6.308990	3.238082	0.416953

Optimized Geometries for Intermediates D'

Structure: D'_1				**Structure: D'_2**			
C	-2.723422	-0.567614	-0.782115	C	-2.934140	-0.669359	0.106436
C	-1.406179	-0.569021	-0.058496	C	-1.598335	-0.858075	0.762487
N	-0.364975	0.047855	-0.759356	N	-0.601899	0.002734	0.283740
C	0.938936	0.260842	-0.374215	C	0.700626	0.137226	0.702712
N	1.785668	0.815550	-1.171892	N	1.550144	0.840702	0.041926
O	1.326066	-0.135697	0.837659	O	1.075387	-0.473287	1.831639
O	-1.264505	-1.079357	1.028337	O	-1.401104	-1.692220	1.615119
H	-0.533537	0.332116	-1.712028	H	-0.790369	0.523232	-0.559993
C	-3.661043	-1.527351	-0.388776	C	-3.806472	-1.761575	0.107660
C	-4.905437	-1.586438	-1.000934	C	-5.063696	-1.654471	-0.470573
C	-5.234016	-0.679114	-2.005358	C	-5.470376	-0.450684	-1.041764
C	-4.313803	0.290481	-2.391258	C	-4.615510	0.646882	-1.029440
C	-3.063333	0.346040	-1.784840	C	-3.350722	0.538831	-0.461482
C	2.716678	0.389555	0.970068	C	2.478964	-0.051279	2.051490
C	3.038638	0.814477	-0.478108	C	2.786832	0.767748	0.770073
C	3.637009	-0.598340	1.590345	C	3.367410	-1.225666	2.302327
C	4.682416	-1.106059	0.921043	C	4.430517	-1.470117	1.528700
C	4.897964	-0.771727	-0.487658	C	4.732050	-0.674054	0.344766
C	4.121473	0.078744	-1.183553	C	3.945368	0.342864	-0.034572
I	3.986669	3.039549	-0.372732	I	3.113016	3.084107	1.274764
O	4.757531	5.331983	-0.251130	O	3.389324	5.364253	1.966576
C	5.237018	5.701774	0.894689	C	4.080815	6.106154	1.155174
C	5.904415	7.074252	0.866753	C	4.090907	7.582892	1.537013
O	5.175574	5.051325	1.940543	O	4.694982	5.701130	0.167859
C	4.264599	0.276932	-2.664666	C	5.088951	2.831807	2.060995
C	5.656810	-2.056597	1.558194	C	5.249019	2.290150	3.330455
C	2.196311	3.801145	0.512124	C	6.539655	2.109500	3.820819
C	1.054573	3.902611	-0.274262	C	7.638686	2.469695	3.047513

C	-0.113453	4.382311	0.313599	C	7.452700	3.020419	1.783350
C	-0.125445	4.747104	1.656405	C	6.169768	3.207094	1.274193
C	1.033405	4.642748	2.419378	H	2.428599	0.572050	2.945955
C	2.213301	4.165112	1.853152	H	-3.481819	-2.685097	0.568672
H	-3.395149	-2.216828	0.401868	H	-5.729586	-2.508954	-0.472902
H	-5.621673	-2.338576	-0.693178	H	-6.453650	-0.366356	-1.488254
H	-6.206313	-0.722646	-2.480846	H	-4.934073	1.589919	-1.456036
H	2.593114	1.250613	1.628450	H	-2.713637	1.415313	-0.431780
H	-4.570299	1.008590	-3.160642	H	3.129701	-1.846531	3.157526
H	-2.378154	1.132250	-2.079916	H	5.081301	-2.305713	1.759556
H	3.449606	-0.863124	2.624150	H	5.581652	-0.958792	-0.264064
H	5.698421	-1.293234	-1.002914	H	4.111017	0.870690	-0.965633
H	6.665387	7.104198	0.084932	H	3.068811	7.947300	1.650803
H	5.158957	7.834911	0.625122	H	4.588805	7.704715	2.501456
H	6.351741	7.294454	1.834292	H	4.614272	8.162767	0.779053
H	4.397709	1.329560	-2.928656	H	4.395305	2.031010	3.941661
H	5.114501	-0.286297	-3.050700	H	6.679783	1.694026	4.811137
H	3.359667	-0.056629	-3.178398	H	8.640618	2.331029	3.435409
H	5.700208	-2.997392	1.001264	H	8.306337	3.316465	1.186028
H	6.667015	-1.635657	1.553953	H	6.012454	3.684285	0.317144
H	5.384230	-2.280581	2.589207				
H	1.071476	3.619103	-1.316846				
H	-1.011225	4.477612	-0.285348				
H	-1.037223	5.121353	2.105920				
H	1.029859	4.938992	3.461069				
H	3.136881	4.133802	2.417080				
Structure: D'_3				**Structure: D'_4**			
C	-2.946396	-0.636226	0.033195	C	-2.915260	-0.658418	0.144011
C	-1.627883	-0.841584	0.718738	C	-1.564441	-0.859141	0.764475
N	-0.611124	0.009088	0.265959	N	-0.576063	-0.000809	0.265531
C	0.677759	0.141404	0.725234	C	0.736236	0.126380	0.654788
N	1.535581	0.877333	0.110118	N	1.582656	0.803676	-0.035383
O	1.033588	-0.511498	1.834429	O	1.123537	-0.457519	1.794743
O	-1.459391	-1.681705	1.571510	O	-1.349741	-1.699880	1.606545
H	-0.779803	0.548391	-0.570010	H	-0.780915	0.520328	-0.573988
C	-3.829555	-1.719470	0.010926	C	-3.793825	-1.745487	0.158204
C	-5.072587	-1.597528	-0.594266	C	-5.064017	-1.626521	-0.388464
C	-5.454538	-0.387552	-1.169404	C	-5.477135	-0.415984	-0.940483
C	-4.589197	0.701203	-1.134043	C	-4.615822	0.676559	-0.940242
C	-3.338273	0.578144	-0.538996	C	-3.338342	0.556746	-0.403856
C	2.402339	-0.016736	2.137576	C	2.542954	-0.080813	1.960820
C	2.766016	0.766157	0.848762	C	2.825022	0.750125	0.683058
C	3.318656	-1.127501	2.515833	C	3.409275	-1.283879	2.143837
C	4.401009	-1.396832	1.777602	C	4.462128	-1.507565	1.353127
C	4.697773	-0.698003	0.538092	C	4.787162	-0.671149	0.192034
C	3.922613	0.289864	0.049701	C	3.988824	0.359429	-0.131117
I	3.139724	3.074723	1.409402	I	3.100746	3.075303	1.201511
O	3.447858	5.337478	2.157087	O	3.359445	5.374126	1.888147
C	3.993697	6.138373	1.293763	C	4.092746	6.098868	1.100790
C	3.976584	7.602206	1.722587	C	4.104683	7.580381	1.466208

O	4.499813	5.797109	0.223558	O	4.744807	5.677532	0.143854
C	4.142111	0.886689	-1.308075	C	5.982048	-1.056143	-0.633875
C	5.187644	2.829997	1.996601	C	5.036716	2.834639	2.080586
C	5.479357	2.137438	3.164628	C	5.137420	2.320237	3.367754
C	6.813942	1.971159	3.524956	C	6.403574	2.142174	3.919416
C	7.825760	2.492856	2.725188	C	7.538359	2.478909	3.188340
C	7.507625	3.189719	1.563548	C	7.412227	3.004730	1.906094
C	6.178678	3.365667	1.184727	C	6.154626	3.188275	1.336310
H	2.248736	0.649468	2.988238	H	2.555622	0.519860	2.871475
H	-3.524486	-2.647860	0.475583	H	-3.463625	-2.674513	0.604042
H	-5.746876	-2.445183	-0.614485	H	-5.734898	-2.477051	-0.381266
H	-6.426991	-0.291608	-1.636804	H	-6.470242	-0.322619	-1.362755
H	-4.888899	1.649031	-1.563655	H	-4.939022	1.624726	-1.351736
H	-2.693740	1.448479	-0.491787	H	-2.695416	1.429131	-0.382684
H	3.088246	-1.678768	3.418972	H	3.169457	-1.939421	2.972423
H	5.078077	-2.185531	2.086629	H	5.099220	-2.364778	1.544622
H	5.550953	-1.035818	-0.039357	H	4.150063	0.925249	-1.041143
H	2.958517	7.907889	1.968479	H	3.083135	7.959285	1.525877
H	4.579352	7.722911	2.625209	H	4.556100	7.707442	2.452649
H	4.375930	8.230488	0.928436	H	4.671717	8.144887	0.728324
H	4.279076	1.970467	-1.261668	H	6.901393	-0.986336	-0.042758
H	5.018833	0.448066	-1.784604	H	5.903497	-2.090930	-0.981557
H	3.270399	0.711062	-1.943674	H	6.090052	-0.410200	-1.505088
H	4.695212	1.742737	3.795599	H	4.255361	2.083510	3.947185
H	7.056702	1.439473	4.436904	H	6.496330	1.748064	4.923925
H	8.862236	2.364216	3.013140	H	8.521183	2.343475	3.623432
H	8.292430	3.608666	0.945769	H	8.293742	3.285462	1.342777
H	5.916960	3.953569	0.315099	H	6.042678	3.648607	0.364834
Structure: D'_5				**Structure: D'_9**			
C	-2.948250	-0.640782	0.032972	C	-2.676994	-0.509762	-0.771993
C	-1.630126	-0.842980	0.720491	C	-1.359864	-0.516205	-0.050008
N	-0.612346	0.003511	0.262561	N	-0.307084	0.063652	-0.767186
C	0.675682	0.140582	0.723028	C	0.996589	0.270304	-0.383627
N	1.530383	0.881424	0.109369	N	1.857613	0.792630	-1.183844
O	1.034377	-0.514191	1.830051	O	1.369489	-0.097254	0.847728
O	-1.462914	-1.678048	1.578483	O	-1.224385	-0.998683	1.050198
H	-0.781826	0.541382	-0.574137	H	-0.469049	0.323901	-1.727912
C	-3.832109	-1.723556	0.016644	C	-3.637342	-1.429845	-0.340206
C	-5.074837	-1.604350	-0.589740	C	-4.884181	-1.481680	-0.947866
C	-5.455809	-0.397492	-1.172051	C	-5.192080	-0.606981	-1.987075
C	-4.589808	0.690908	-1.142624	C	-4.248708	0.322969	-2.412599
C	-3.339197	0.570513	-0.546358	C	-2.996247	0.371598	-1.809972
C	2.401407	-0.013836	2.134453	C	2.774611	0.345008	0.965812
C	2.762272	0.771214	0.846366	C	3.099800	0.816568	-0.472787
C	3.321467	-1.121410	2.512558	C	3.642417	-0.745322	1.504473
C	4.403192	-1.388716	1.772616	C	4.676530	-1.229440	0.811216
C	4.695722	-0.690175	0.531889	C	4.952474	-0.779936	-0.548207
C	3.918086	0.296368	0.044837	C	4.201672	0.130250	-1.177943
I	3.136729	3.078144	1.408824	I	3.974271	3.060022	-0.392638
O	3.451470	5.337290	2.162711	O	4.651811	5.356863	-0.322486

C	4.006025	6.137218	1.303889	C	5.126939	5.766583	0.814430
C	3.995484	7.600061	1.736309	C	5.721893	7.169741	0.757586
O	4.515170	5.795721	0.235287	O	5.109793	5.126635	1.866771
C	4.134970	0.894664	-1.312679	Cl	6.294424	-1.569503	-1.372844
C	5.184060	2.829413	1.995050	C	2.177653	3.761792	0.531404
C	5.474087	2.154512	3.173805	C	1.025951	3.863909	-0.240449
C	6.808324	1.988820	3.535590	C	-0.144502	4.305191	0.371942
C	7.821423	2.493779	2.726711	C	-0.149422	4.631796	1.724651
C	7.505092	3.173244	1.554343	C	1.018865	4.528483	2.473046
C	6.176486	3.348172	1.173968	C	2.201571	4.089317	1.881933
H	2.244220	0.651248	2.985284	H	-3.386981	-2.094481	0.476283
H	-3.527770	-2.649420	0.486782	H	-5.618308	-2.202840	-0.609827
H	-5.749644	-2.451692	-0.605305	H	-6.166067	-0.645172	-2.459564
H	-6.428022	-0.303641	-1.640367	H	2.736509	1.171937	1.676965
H	-4.888736	1.636450	-1.577787	H	-4.488398	1.015310	-3.210391
H	-2.694307	1.440837	-0.503955	H	-2.292815	1.127954	-2.138165
H	3.094256	-1.672456	3.416625	H	3.414658	-1.112453	2.497325
H	5.082953	-2.175297	2.081074	H	5.317783	-1.993071	1.232015
H	5.548017	-1.027038	-0.047497	H	4.356586	0.374100	-2.220769
H	2.978323	7.910791	1.979585	H	1.038069	3.612623	-1.291476
H	4.595974	7.715266	2.641182	H	-1.049987	4.400881	-0.215107
H	4.401020	8.227962	0.945009	H	-1.063199	4.976365	2.193280
H	4.282399	1.977040	-1.263667	H	1.020698	4.796428	3.522372
H	5.005036	0.449529	-1.795308	H	3.130467	4.063682	2.436263
H	3.257993	0.729114	-1.943622	H	6.460106	7.231563	-0.043761
H	4.688794	1.773485	3.811739	H	4.932225	7.888907	0.529814
H	7.049901	1.470775	4.455643	H	6.180863	7.421102	1.711918
H	8.857618	2.365968	3.016019				
H	8.290935	3.579387	0.929385				
H	5.916405	3.922411	0.294917				
Structure: D'_10				**Structure: D'_15**			
C	-2.689793	-0.534541	-0.787518	C	-2.710604	-0.525762	-0.851395
C	-1.375930	-0.531459	-0.059309	C	-1.411141	-0.499216	-0.098204
N	-0.325803	0.061861	-0.769153	N	-0.343770	0.055789	-0.812449
C	0.975753	0.275119	-0.380969	C	0.951181	0.280384	-0.408598
N	1.830114	0.821562	-1.173100	N	1.819052	0.790928	-1.209311
O	1.353777	-0.113315	0.841180	O	1.306779	-0.057750	0.834036
O	-1.241105	-1.017705	1.039187	O	-1.301525	-0.935548	1.024077
H	-0.488541	0.331692	-1.727057	H	-0.483803	0.280389	-1.785714
C	-3.640997	-1.469774	-0.368378	C	-3.677657	-1.433928	-0.409712
C	-4.884170	-1.531270	-0.982658	C	-4.908906	-1.513839	-1.045492
C	-5.197663	-0.651085	-2.015549	C	-5.194601	-0.678958	-2.123061
C	-4.263660	0.294041	-2.428058	C	-4.244705	0.239314	-2.559117
C	-3.014650	0.352235	-1.819073	C	-3.007525	0.315717	-1.928328
C	2.752912	0.359445	0.971123	C	2.702814	0.419455	0.969201
C	3.075284	0.834982	-0.465134	C	3.052615	0.834248	-0.486702
C	3.638633	-0.705407	1.529095	C	3.571328	-0.616126	1.598312
C	4.658405	-1.180563	0.810749	C	4.612413	-1.139176	0.942648
C	4.936704	-0.776469	-0.561963	C	4.920942	-0.793932	-0.436822
C	4.165776	0.134552	-1.170501	C	4.166924	0.084954	-1.111250

I	3.977948	3.062249	-0.383932	I	3.934801	3.089983	-0.471125
O	4.671937	5.348857	-0.323396	O	4.595029	5.386736	-0.418182
C	5.156931	5.758525	0.810256	C	5.159535	5.789515	0.680584
C	5.756166	7.159116	0.747326	C	5.732603	7.199577	0.588306
O	5.144495	5.119114	1.862463	O	5.234249	5.140009	1.723864
Cl	5.738418	-2.395241	1.488849	Cl	4.475032	0.399943	-2.813203
C	2.190912	3.776458	0.549318	C	2.210722	3.754064	0.599517
C	1.035805	3.884431	-0.216399	C	0.997849	3.829646	-0.076052
C	-0.127987	4.334597	0.402244	C	-0.127287	4.251431	0.628036
C	-0.122656	4.663900	1.754248	C	-0.027747	4.588567	1.974273
C	1.049191	4.554292	2.496114	C	1.199909	4.514319	2.624873
C	2.225444	4.106241	1.898921	C	2.338292	4.093095	1.941560
H	-3.386564	-2.138478	0.443537	H	-3.444917	-2.067113	0.436399
H	-5.611095	-2.264253	-0.654575	H	-5.648326	-2.225835	-0.699593
H	-6.168841	-0.696820	-2.493109	H	-6.156422	-0.739242	-2.617716
H	2.684294	1.187991	1.677876	H	2.620356	1.287051	1.625446
H	-4.508036	0.990787	-3.220604	H	-4.467016	0.900683	-3.387555
H	-2.318845	1.120121	-2.136707	H	-2.298798	1.062353	-2.267339
H	3.437180	-1.054707	2.532394	H	3.335704	-0.906411	2.614099
H	5.743476	-1.270509	-1.086178	H	5.251777	-1.865135	1.431083
H	4.305376	0.374469	-2.217975	H	5.744152	-1.292076	-0.931053
H	1.039761	3.629953	-1.266632	H	0.929424	3.572972	-1.123753
H	-1.036316	4.434578	-0.179679	H	-1.079724	4.323303	0.116779
H	-1.031441	5.015141	2.227605	H	-0.907019	4.917959	2.514279
H	1.058960	4.823952	3.544940	H	1.282459	4.790401	3.668843
H	3.157485	4.073979	2.447757	H	3.310201	4.086230	2.417956
H	6.490087	7.217092	-0.058228	H	6.422190	7.267770	-0.254881
H	4.967748	7.880566	0.522554	H	4.923600	7.909774	0.405435
H	6.221366	7.410260	1.698662	H	6.244778	7.456492	1.513735
Structure: D'_16							
C	-2.712967	-0.531899	-0.852618				
C	-1.416143	-0.493352	-0.096368				
N	-0.349509	0.064668	-0.811425				
C	0.943729	0.292673	-0.406846				
N	1.809898	0.813153	-1.203195				
O	1.302580	-0.054527	0.833024				
O	-1.305715	-0.921420	1.028698				
H	-0.490180	0.288386	-1.784834				
C	-3.675109	-1.444314	-0.408884				
C	-4.903623	-1.536194	-1.048245				
C	-5.191505	-0.709198	-2.131259				
C	-4.246664	0.213345	-2.569320				
C	-3.012099	0.301663	-1.935119				
C	2.695454	0.430216	0.971580				
C	3.044838	0.851040	-0.481442				
C	3.563023	-0.600467	1.608788				
C	4.588241	-1.124596	0.934560				
C	4.901289	-0.795044	-0.446929				
C	4.148655	0.091730	-1.111771				
I	3.941296	3.099516	-0.465294				

O	4.605090	5.378646	-0.419323
C	5.169212	5.783881	0.681176
C	5.745667	7.191239	0.583904
O	5.242540	5.134533	1.723321
Cl	4.455576	0.402565	-2.811271
Cl	5.649892	-2.306300	1.692026
C	2.217319	3.762999	0.606883
C	1.007751	3.854217	-0.072584
C	-0.116722	4.276766	0.632082
C	-0.019527	4.598886	1.982149
C	1.205038	4.508745	2.636545
C	2.342899	4.086587	1.952946
H	-3.440759	-2.071581	0.441166
H	-5.639118	-2.251581	-0.701036
H	-6.151172	-0.779015	-2.628808
H	2.607104	1.295428	1.629864
H	-4.470860	0.868524	-3.402124
H	-2.307565	1.051430	-2.276147
H	3.343184	-0.887495	2.627445
H	5.718521	-1.307420	-0.933267
H	0.941049	3.608764	-1.123054
H	-1.066766	4.360732	0.118322
H	-0.898326	4.928894	2.522483
H	1.285673	4.772837	3.683738
H	3.312483	4.066875	2.433387
H	6.436359	7.254403	-0.258714
H	4.938827	7.902938	0.397751
H	6.257550	7.449466	1.509021

Optimized Geometries for Intermediates E'

Structure: E'_1				**Structure: E'_2**			
C	-2.462155	-3.358119	2.279884	C	-2.382333	-3.393538	2.305637
C	-2.322544	-3.816145	0.872540	C	-2.352254	-3.853084	0.893300
N	-3.325903	-3.315778	-0.070827	N	-3.414080	-3.332403	0.022325
C	-3.530484	-1.950896	-0.146604	C	-3.579442	-1.965371	-0.062023
N	-4.634783	-1.306581	-0.313332	N	-4.670376	-1.290193	-0.196916
O	-2.401322	-1.175460	-0.028392	O	-2.423099	-1.225038	0.007811
O	-1.457931	-4.555078	0.490611	O	-1.533547	-4.607486	0.447826
C	-4.000740	-4.256765	-0.910470	C	-4.187385	-4.269112	-0.735525
O	-4.012699	-5.421354	-0.605712	O	-4.205107	-5.425067	-0.400312
C	-4.667277	-3.716360	-2.151468	C	-4.938373	-3.737783	-1.930359
C	-1.336339	-3.430680	3.108154	C	-1.206156	-3.505080	3.056416
C	-1.428564	-3.063067	4.442061	C	-1.195892	-3.134438	4.392454
C	-2.647935	-2.634226	4.964823	C	-2.361769	-2.663234	4.994827
C	-3.774022	-2.575232	4.149724	C	-3.537472	-2.564679	4.257200
C	-3.683711	-2.929624	2.808526	C	-3.549995	-2.922800	2.914139
C	-4.251537	0.036756	-0.331912	C	-4.249230	0.039378	-0.245653
C	-2.874815	0.113698	-0.130879	C	-2.860590	0.076763	-0.093620
C	-2.162515	1.294977	-0.063469	C	-2.118370	1.239895	-0.061706

C	-2.903129	2.468171	-0.217782	C	-2.844484	2.421596	-0.204222
C	-4.294898	2.397482	-0.426821	C	-4.237619	2.412875	-0.362302
C	-5.008639	1.202543	-0.488757	H	-5.263082	-4.595286	-2.515009
C	-6.493932	1.151301	-0.709033	H	-5.805970	-3.160639	-1.610789
C	-2.224587	3.813382	-0.134364	H	-4.314445	-3.080901	-2.538311
H	-5.575362	-3.172714	-1.891116	C	-4.963247	1.226081	-0.384696
H	-4.014910	-3.027663	-2.690843	H	-0.313639	-3.885700	2.577030
H	-4.917899	-4.566980	-2.780969	H	-0.281825	-3.215277	4.968093
H	-6.738194	0.600022	-1.620892	H	-2.353404	-2.377421	6.039776
H	-6.995911	0.636116	0.113871	H	-4.446491	-2.210345	4.727254
H	-6.912080	2.154502	-0.792830	H	-4.470133	-2.855398	2.348657
H	-2.640724	4.514581	-0.860579	H	-1.043542	1.233593	0.061064
H	-2.353827	4.257275	0.858140	H	-2.318492	3.367992	-0.193824
H	-1.152650	3.731058	-0.320429	H	-4.759462	3.355811	-0.468643
H	-0.401248	-3.779647	2.689869	H	-6.039079	1.217339	-0.502552
H	-0.552897	-3.113497	5.077675				
H	-2.719847	-2.350735	6.008048				
H	-4.724425	-2.254142	4.557847				
H	-4.564920	-2.892219	2.181796				
H	-1.091836	1.308712	0.094336				
H	-4.840361	3.327729	-0.546606				
Structure: E'_3				**Structure: E'_4**			
C	-2.451728	-3.358989	2.274129	C	-2.446693	-3.366700	2.274506
C	-2.350582	-3.843450	0.873103	C	-2.347620	-3.846440	0.871922
N	-3.366768	-3.339445	-0.058417	N	-3.364495	-3.338178	-0.057150
C	-3.527628	-1.972739	-0.172604	C	-3.521464	-1.971678	-0.171276
N	-4.611778	-1.298035	-0.354418	N	-4.603751	-1.297331	-0.367045
O	-2.374320	-1.232462	-0.078432	O	-2.367449	-1.234203	-0.060217
O	-1.509636	-4.604615	0.483494	O	-1.508672	-4.607689	0.478273
C	-4.096451	-4.287285	-0.842437	C	-4.103685	-4.284951	-0.834842
O	-4.128150	-5.440125	-0.496752	O	-4.138589	-5.436226	-0.484199
C	-4.790214	-3.771681	-2.078560	C	-4.800884	-3.771083	-2.069531
C	-1.314214	-3.452578	3.084414	C	-1.310137	-3.469704	3.085013
C	-1.371538	-3.058506	4.412649	C	-1.365847	-3.079506	4.414431
C	-2.567368	-2.581380	4.947873	C	-2.559058	-2.596782	4.950503
C	-3.705182	-2.500785	4.151033	C	-3.695937	-2.506658	4.153346
C	-3.649721	-2.882246	2.815461	C	-3.642134	-2.884514	2.816652
C	-4.186521	0.031292	-0.412483	C	-4.177245	0.031406	-0.418581
C	-2.805199	0.068574	-0.216586	C	-2.797708	0.067693	-0.203442
C	-2.057991	1.229148	-0.179960	C	-2.065871	1.234202	-0.158768
C	-2.783367	2.403019	-0.366409	C	-2.789602	2.410492	-0.355370
C	-4.171195	2.388938	-0.567788	C	-4.177887	2.419089	-0.579559
C	-4.916828	1.210335	-0.596476	C	-4.882853	1.213158	-0.610430
C	-6.404442	1.188785	-0.804017	C	-4.908070	3.724904	-0.786021
H	-5.674704	-3.195406	-1.807410	H	-5.680323	-3.188273	-1.796012
H	-4.139657	-3.118935	-2.662702	H	-4.150428	-3.123959	-2.659800
H	-5.083373	-4.636439	-2.669202	H	-5.101446	-4.637154	-2.654430
H	-0.397897	-3.838086	2.656802	H	-0.395907	-3.859274	2.656598
H	-0.486993	-3.125569	5.034270	H	-0.482042	-3.153926	5.036289
H	-2.611946	-2.277024	5.986664	H	-2.602325	-2.295413	5.990234

H	-4.637533	-2.141893	4.569143	H	-4.626306	-2.143219	4.571916
H	-4.540369	-2.828210	2.203469	H	-4.532321	-2.822878	2.204670
H	-0.987995	1.224605	-0.022942	H	-0.997819	1.239684	0.013139
H	-2.263041	3.352743	-0.356605	H	-2.259723	3.355402	-0.335399
H	-4.685482	3.333083	-0.705638	H	-5.953190	1.191897	-0.776888
H	-6.669839	0.615047	-1.695784	H	-5.392704	3.757313	-1.765303
H	-6.912601	0.713392	0.038856	H	-5.687356	3.867327	-0.032875
H	-6.797868	2.199095	-0.917001	H	-4.226662	4.574072	-0.724457
Structure: E'_5				**Structure: E'_9**			
C	-2.385585	-3.388346	2.305179	C	-2.391448	-3.378864	2.270595
C	-2.332876	-3.835029	0.888577	C	-2.366663	-3.786340	0.844320
N	-3.386773	-3.320739	0.009198	N	-3.462312	-3.266097	0.004507
C	-3.595454	-1.956686	-0.039297	C	-3.622580	-1.902379	-0.083737
N	-4.707060	-1.313568	-0.154892	N	-4.709487	-1.221019	-0.234632
O	-2.462168	-1.181106	0.046158	O	-2.464713	-1.167026	0.008191
O	-1.498001	-4.575995	0.449181	O	-1.534013	-4.495446	0.354803
C	-4.120836	-4.253842	-0.791090	C	-4.271022	-4.215026	-0.698042
O	-4.124167	-5.418522	-0.487211	O	-4.259810	-5.365872	-0.343970
C	-4.851920	-3.706468	-1.991599	C	-5.087970	-3.708457	-1.858733
C	-1.212560	-3.473973	3.063863	C	-1.211833	-3.515702	3.012347
C	-1.222732	-3.116571	4.403640	C	-1.195603	-3.187556	4.359211
C	-2.406086	-2.685375	5.001811	C	-2.358095	-2.733096	4.980880
C	-3.578611	-2.613428	4.256130	C	-3.536829	-2.608793	4.251979
C	-3.570780	-2.957569	2.909271	C	-3.555780	-2.925418	2.898771
C	-4.327393	0.029730	-0.170004	C	-4.280714	0.104460	-0.271704
C	-2.941954	0.107947	-0.020174	C	-2.895245	0.136029	-0.096850
C	-2.234052	1.291082	0.035067	C	-2.154906	1.298478	-0.049278
C	-2.975878	2.471541	-0.075107	C	-2.869151	2.485967	-0.198574
C	-4.373445	2.405068	-0.233730	C	-4.256870	2.464795	-0.378127
C	-5.068229	1.201869	-0.281752	C	-4.995351	1.289521	-0.418646
C	-2.285335	3.810901	0.004987	Cl	-5.102741	4.004281	-0.558584
H	-5.754857	-3.181548	-1.679645	H	-5.938889	-3.127797	-1.503075
H	-4.238582	-2.999905	-2.552375	H	-4.501468	-3.060580	-2.511634
H	-5.120889	-4.552848	-2.619345	H	-5.440179	-4.577826	-2.408732
H	-0.306058	-3.824481	2.587790	H	-0.321654	-3.881507	2.517333
H	-0.310921	-3.176894	4.985357	H	-0.279468	-3.288186	4.928316
H	-2.413718	-2.410065	6.049624	H	-2.344664	-2.480001	6.034205
H	-4.501038	-2.290441	4.722656	H	-4.442890	-2.267226	4.736865
H	-4.488155	-2.910480	2.337250	H	-4.478584	-2.839160	2.340247
H	-1.157702	1.303914	0.152137	H	-1.082401	1.295795	0.090638
H	-4.926755	3.332843	-0.322748	H	-2.351642	3.434866	-0.177391
H	-6.143439	1.172862	-0.403343	H	-6.067572	1.294113	-0.554415
H	-2.805343	4.561684	-0.592392				
H	-2.255985	4.175911	1.036449				
H	-1.255364	3.751167	-0.350302				
Structure: E'_10				**Structure: E'_15**			
C	-2.393884	-3.377904	2.271600	C	-2.391495	-3.377604	2.269830
C	-2.371053	-3.789767	0.846491	C	-2.364298	-3.787527	0.843922
N	-3.465473	-3.269898	0.005589	N	-3.457485	-3.268558	0.001739
C	-3.630022	-1.906160	-0.079634	C	-3.621894	-1.905330	-0.082583

N	-4.716677	-1.225479	-0.224130	N	-4.711501	-1.227320	-0.225016
O	-2.470241	-1.167257	0.005406	O	-2.466512	-1.164772	0.000807
O	-1.539926	-4.502101	0.358922	O	-1.530943	-4.498606	0.358289
C	-4.268786	-4.217593	-0.704260	C	-4.266433	-4.217584	-0.702133
O	-4.259166	-5.369684	-0.354162	O	-4.251332	-5.369357	-0.352067
C	-5.080244	-3.707479	-1.867502	C	-5.087297	-3.707050	-1.857948
C	-1.212732	-3.510828	3.011582	C	-1.212616	-3.511867	3.013216
C	-1.194548	-3.178932	4.357506	C	-1.198624	-3.183074	4.359959
C	-2.356627	-2.724680	4.980039	C	-2.362811	-2.730503	4.979909
C	-3.536892	-2.604349	4.252937	C	-3.540764	-2.608606	4.249371
C	-3.557789	-2.924551	2.900595	C	-3.557467	-2.925781	2.896255
C	-4.289772	0.101290	-0.264905	C	-4.287691	0.095081	-0.265819
C	-2.903133	0.132895	-0.097857	C	-2.899255	0.137459	-0.100782
C	-2.150211	1.288342	-0.052412	C	-2.151059	1.295574	-0.057199
C	-2.878441	2.465498	-0.199463	C	-2.872034	2.479286	-0.202559
C	-4.266758	2.479956	-0.373323	C	-4.261789	2.483276	-0.373682
C	-4.991848	1.293599	-0.407457	C	-4.980888	1.294934	-0.406069
Cl	-2.011596	4.000976	-0.166681	Cl	-6.720099	1.299738	-0.613597
H	-5.933166	-3.128255	-1.514299	H	-5.932011	-3.118740	-1.499941
H	-4.490383	-3.057466	-2.515298	H	-4.498652	-3.064905	-2.514925
H	-5.429376	-4.575115	-2.422160	H	-5.448535	-4.574299	-2.405476
H	-0.322837	-3.876454	2.515933	H	-0.321264	-3.876603	2.519531
H	-0.277139	-3.276257	4.925122	H	-0.283088	-3.281889	4.930357
H	-2.341615	-2.468520	6.032597	H	-2.351305	-2.477137	6.033202
H	-4.442607	-2.262946	4.738601	H	-4.448183	-2.268550	4.732768
H	-4.481658	-2.841330	2.343369	H	-4.479835	-2.841245	2.336731
H	-1.078021	1.285538	0.081297	H	-1.077984	1.283737	0.075417
H	-4.773039	3.429238	-0.481302	H	-2.347189	3.425875	-0.184674
H	-6.066021	1.298497	-0.537507	H	-4.788935	3.421481	-0.482023
Structure: E'_16							
C	-2.390424	-3.375845	2.266495				
C	-2.363655	-3.767399	0.836407				
N	-3.469534	-3.250737	0.004607				
C	-3.637653	-1.890267	-0.080904				
N	-4.726195	-1.211991	-0.229842				
O	-2.481671	-1.145574	0.009504				
O	-1.527557	-4.464269	0.336109				
C	-4.286207	-4.206094	-0.683979				
O	-4.260055	-5.355328	-0.326875				
C	-5.123224	-3.705966	-1.832380				
C	-1.209372	-3.511859	3.006259				
C	-1.195106	-3.197277	4.356332				
C	-2.360670	-2.757647	4.982962				
C	-3.540714	-2.634381	4.255957				
C	-3.557924	-2.937246	2.899627				
C	-4.302957	0.109641	-0.268447				
C	-2.916037	0.152658	-0.095176				
C	-2.161935	1.306463	-0.044932				
C	-2.890100	2.482854	-0.194386				
C	-4.276514	2.501611	-0.374314				

C	-4.991910	1.310871	-0.411687
Cl	-6.726683	1.324050	-0.629335
Cl	-2.030323	4.018940	-0.157598
H	-5.961715	-3.112791	-1.468139
H	-4.543213	-3.071257	-2.504032
H	-5.492718	-4.578377	-2.365811
H	-0.316670	-3.866098	2.507397
H	-0.278055	-3.296871	4.924082
H	-2.348593	-2.515226	6.038804
H	-4.449047	-2.304611	4.744665
H	-4.481990	-2.852545	2.342860
H	-1.090754	1.303151	0.093560
H	-4.792588	3.444246	-0.484291

Optimized Geometries for Products (2)

Structure: 2a			
C	-2.529078	-3.477564	2.427721
C	-3.001965	-4.031264	1.125476
N	-3.816074	-3.243421	0.303181
C	-3.919059	-1.880002	0.155868
N	-4.862886	-1.269433	-0.477780
O	-2.912467	-1.097662	0.645786
O	-2.756458	-5.169830	0.777612
H	-4.286875	-3.770611	-0.420899
C	-1.286993	-3.901948	2.906019
C	-0.836290	-3.478298	4.149104
C	-1.636031	-2.653735	4.936528
C	-2.886251	-2.250961	4.475463
C	-3.329557	-2.652982	3.221495
C	-3.288357	0.182537	0.277801
C	-4.483883	0.076150	-0.429199
C	-2.632336	1.368895	0.530676
C	-3.235338	2.523918	0.024343
C	-4.440784	2.424824	-0.694707
C	-5.099360	1.220062	-0.943203
C	-6.386912	1.139290	-1.713472
C	-2.612392	3.876099	0.272357
H	-0.688089	-4.565265	2.295154
H	0.133982	-3.798350	4.508040
H	-1.289785	-2.332757	5.911406
H	-3.517688	-1.624551	5.093935
H	-4.308475	-2.345593	2.875914
H	-1.701182	1.402006	1.081243
H	-4.882118	3.337918	-1.080189
H	-6.281566	0.494613	-2.589532
H	-7.184284	0.709840	-1.101324
H	-6.705122	2.126615	-2.048694
H	-2.819664	4.565547	-0.548219
H	-3.006922	4.329444	1.187340

Structure: 2b			
C	-2.526367	-3.478117	2.424797
C	-2.992638	-4.031390	1.120542
N	-3.809582	-3.243002	0.298209
C	-3.911370	-1.881109	0.153063
N	-4.855349	-1.269713	-0.481091
O	-2.904930	-1.100439	0.646449
O	-2.745220	-5.168027	0.770320
H	-4.284589	-3.769362	-0.423838
C	-1.285075	-3.899196	2.908074
C	-0.840835	-3.473903	4.152888
C	-1.646195	-2.651327	4.936745
C	-2.895723	-2.252222	4.470699
C	-3.332732	-2.655731	3.214986
C	-3.279286	0.179361	0.278860
C	-4.477996	0.073951	-0.431184
C	-2.631924	1.368915	0.536154
C	-3.248942	2.512349	0.026862
C	-4.450581	2.437368	-0.689472
C	-5.084911	1.221404	-0.931070
H	-0.681716	-4.560897	2.299854
H	0.128851	-3.791047	4.515881
H	-1.304722	-2.328984	5.912833
H	-3.531771	-1.627922	5.086525
H	-4.311598	-2.351822	2.866014
H	-1.703890	1.411898	1.089916
H	-2.787337	3.477969	0.190182
H	-4.895582	3.350485	-1.064687
H	-6.015204	1.163389	-1.480544

H	-1.529332	3.800752	0.385303				
Structure: 2c				**Structure: 2d**			
C	-2.529035	-3.477030	2.425943	C	-2.524366	-3.483503	2.427233
C	-3.002382	-4.027988	1.123106	C	-2.995755	-4.031739	1.122498
N	-3.816258	-3.236747	0.302008	N	-3.811787	-3.239783	0.304092
C	-3.915334	-1.873798	0.156629	C	-3.911514	-1.876868	0.161751
N	-4.854206	-1.260686	-0.483143	N	-4.853533	-1.264560	-0.475162
O	-2.913051	-1.094358	0.656609	O	-2.906743	-1.098658	0.659641
O	-2.760914	-5.166419	0.773253	O	-2.751395	-5.168414	0.769259
H	-4.289478	-3.761858	-0.422056	H	-4.286884	-3.763451	-0.419832
C	-1.288384	-3.905081	2.904798	C	-1.282401	-3.908754	2.905102
C	-0.837198	-3.482588	4.148075	C	-0.833430	-3.489222	4.150192
C	-1.634958	-2.655514	4.934890	C	-1.634726	-2.668173	4.939728
C	-2.883716	-2.248957	4.473148	C	-2.884778	-2.264578	4.478881
C	-3.327515	-2.649821	3.219022	C	-3.326394	-2.662273	3.222976
C	-3.283778	0.187214	0.288298	C	-3.280122	0.182475	0.290100
C	-4.475384	0.084016	-0.429599	C	-4.474576	0.079168	-0.423548
C	-2.633788	1.374570	0.553104	C	-2.645063	1.376834	0.550010
C	-3.252477	2.512219	0.037867	C	-3.267155	2.515673	0.038843
C	-4.449037	2.433647	-0.687171	C	-4.468398	2.458395	-0.690703
C	-5.098448	1.224668	-0.944438	C	-5.082899	1.225415	-0.922596
C	-6.383528	1.134404	-1.717434	C	-5.073496	3.725503	-1.246047
H	-0.690865	-4.569932	2.294246	H	-0.682113	-4.569118	2.292391
H	0.131971	-3.805298	4.507546	H	0.136727	-3.809703	4.509007
H	-1.288178	-2.335234	5.909794	H	-1.289744	-2.350485	5.916123
H	-3.513486	-1.620384	5.091090	H	-3.517392	-1.641002	5.098983
H	-4.305254	-2.339305	2.872774	H	-4.305246	-2.354452	2.877480
H	-1.709466	1.417582	1.112441	H	-1.722180	1.429997	1.111609
H	-2.796997	3.481014	0.200643	H	-2.807423	3.481583	0.212285
H	-4.888720	3.349416	-1.064996	H	-6.013645	1.156778	-1.472032
H	-6.271639	0.490052	-2.592856	H	-4.840670	4.586610	-0.617277
H	-7.179595	0.700396	-1.106837	H	-4.688517	3.938229	-2.247870
H	-6.706797	2.119630	-2.053880	H	-6.159384	3.647019	-1.323578
Structure: 2e				**Structure: 2i**			
C	-2.526914	-3.477369	2.424828	C	-2.527592	-3.477519	2.424420
C	-2.993870	-4.034578	1.122116	C	-2.994988	-4.032642	1.122030
N	-3.810701	-3.249934	0.298355	N	-3.817167	-3.244767	0.300628
C	-3.916726	-1.887583	0.151824	C	-3.917139	-1.885487	0.153261
N	-4.865872	-1.278455	-0.475254	N	-4.858678	-1.273942	-0.486395
O	-2.906026	-1.104563	0.636102	O	-2.914475	-1.102378	0.650318
O	-2.744631	-5.172504	0.776015	O	-2.746227	-5.167344	0.769422
H	-4.283491	-3.778708	-0.423340	H	-4.298779	-3.772439	-0.416406
C	-1.285481	-3.897274	2.908648	C	-1.281639	-3.890712	2.902674
C	-0.840739	-3.469500	4.152453	C	-0.835650	-3.462659	4.145874
C	-1.645711	-2.645260	4.934916	C	-1.643556	-2.645618	4.932892
C	-2.895225	-2.246798	4.468194	C	-2.897550	-2.254532	4.471841
C	-3.332683	-2.652971	3.213514	C	-3.336588	-2.660564	3.217758
C	-3.285616	0.174425	0.270229	C	-3.285343	0.176210	0.281357
C	-4.488372	0.066222	-0.429625	C	-4.481203	0.063012	-0.435296
C	-2.632748	1.362279	0.516923	C	-2.635116	1.362482	0.544536

C	-3.234535	2.524112	0.017455	C	-3.247830	2.505895	0.032901
C	-4.444288	2.428883	-0.692811	C	-4.443890	2.440930	-0.690496
C	-5.087769	1.216791	-0.927383	C	-5.070439	1.222951	-0.930552
C	-2.599524	3.870091	0.266553	Cl	-6.569635	1.146251	-1.833397
H	-0.682422	-4.560317	2.301595	H	-0.675924	-4.548016	2.292016
H	0.128950	-3.786186	4.515897	H	0.137312	-3.773610	4.505349
H	-1.304063	-2.321268	5.910411	H	-1.300693	-2.321648	5.907924
H	-3.530837	-1.620911	5.082900	H	-3.535453	-1.635156	5.090669
H	-4.311348	-2.349407	2.863685	H	-4.319206	-2.363956	2.872792
H	-1.698027	1.394569	1.062204	H	-1.710515	1.401787	1.103261
H	-4.891262	3.339693	-1.074219	H	-2.789191	3.472573	0.196468
H	-6.019484	1.166970	-1.475434	H	-4.892827	3.347750	-1.072138
H	-2.932391	4.606677	-0.466072				
H	-2.861122	4.252418	1.258474				
H	-1.510027	3.813341	0.216684				
Structure: 2j				**Structure: Product_15**			
C	-2.527994	-3.477139	2.423969	C	-2.527593	-3.478161	2.424623
C	-2.994746	-4.032323	1.121475	C	-2.995414	-4.030991	1.121514
N	-3.815941	-3.244744	0.299110	N	-3.816382	-3.240869	0.300851
C	-3.918073	-1.885057	0.152133	C	-3.913533	-1.881139	0.154509
N	-4.858156	-1.271366	-0.485953	N	-4.853845	-1.266637	-0.485096
O	-2.912021	-1.102306	0.650809	O	-2.909022	-1.101957	0.654049
O	-2.745320	-5.166994	0.768693	O	-2.747891	-5.165409	0.767122
H	-4.292344	-3.772913	-0.420885	H	-4.296912	-3.767254	-0.417750
C	-1.282895	-3.891476	2.903495	C	-1.283565	-3.895715	2.904135
C	-0.837103	-3.462598	4.146478	C	-0.837703	-3.469814	4.148124
C	-1.644234	-2.643393	4.932005	C	-1.643770	-2.650393	4.934552
C	-2.897364	-2.251002	4.469702	C	-2.895766	-2.254592	4.472058
C	-3.336223	-2.658029	3.215896	C	-3.334614	-2.658554	3.217253
C	-3.284193	0.173698	0.281710	C	-3.279207	0.177075	0.285022
C	-4.479122	0.070161	-0.434276	C	-4.473586	0.073454	-0.431806
C	-2.631806	1.358699	0.547712	C	-2.636525	1.368155	0.542425
C	-3.252380	2.494076	0.032171	C	-3.244891	2.514571	0.031702
C	-4.447475	2.438577	-0.691627	C	-4.440479	2.422993	-0.688009
C	-5.077353	1.221345	-0.934319	C	-5.082753	1.216607	-0.938828
Cl	-2.495600	4.064244	0.305792	Cl	-5.164335	3.911859	-1.304401
H	-0.677546	-4.550054	2.293861	H	-0.679251	-4.554687	2.293891
H	0.135330	-3.774212	4.506777	H	0.133753	-3.784215	4.508644
H	-1.301277	-2.318281	5.906600	H	-1.301013	-2.328060	5.910156
H	-3.534418	-1.629466	5.087226	H	-3.532195	-1.633152	5.090331
H	-4.318082	-2.360124	2.869845	H	-4.315668	-2.358169	2.871098
H	-1.707532	1.408305	1.104644	H	-1.711613	1.417999	1.100358
H	-4.879787	3.357173	-1.063605	H	-2.793059	3.483603	0.190764
H	-6.004608	1.172456	-1.489294	H	-6.008451	1.167659	-1.493922
Structure: Product_16							
C	-2.528614	-3.476586	2.423939				
C	-2.997359	-4.033153	1.123412				
N	-3.824992	-3.245973	0.303235				
C	-3.924903	-1.888748	0.153117				
N	-4.861565	-1.275858	-0.492636				

O	-2.924021	-1.102990	0.656820	
O	-2.746669	-5.165688	0.767409	
H	-4.307974	-3.775132	-0.411952	
C	-1.279048	-3.883851	2.898062	
C	-0.830866	-3.452495	4.139290	
C	-1.639827	-2.638394	4.928273	
C	-2.897336	-2.253489	4.471479	
C	-3.338847	-2.662688	3.219359	
C	-3.292466	0.171761	0.284629	
C	-4.483131	0.059595	-0.439714	
C	-2.637377	1.353110	0.557295	
C	-3.252020	2.489600	0.038497	
C	-4.440780	2.441385	-0.693909	
C	-5.064422	1.222186	-0.936892	
Cl	-6.554439	1.156447	-1.848985	
Cl	-2.499027	4.057877	0.314891	
H	-0.672119	-4.538587	2.285848	
H	0.144786	-3.758415	4.495655	
H	-1.294929	-2.311688	5.901627	
H	-3.535859	-1.636747	5.092241	
H	-4.324429	-2.371612	2.877923	
H	-1.717344	1.398532	1.120812	
H	-4.877283	3.353625	-1.073619	