Supporting Information

Inter- and Intramolecular Diels-Alder Reaction of Ethenetricarboxylate Derivatives

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I-2. Cartesian coordinates of the optimized geometries. The atom numberings are different from those in eq 1, Figures 1, 2, eq 3, and Figure 4.

Figure 1
1m(cc) (IDA9pcm.log)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.491233	1.065730	0.347940
2	6	0	0.382189	-0.411483	0.058030
3	6	0	-0.780136	-1.070021	-0.053909
4	1	0	-0.768740	-2.142592	-0.216667
5	6	0	1.659020	-1.191636	-0.053956
6	6	0	-2.100114	-0.397113	0.035701
7	8	0	-2.270194	0.790714	0.245595
8	8	0	-3.091896	-1.283498	-0.145872
9	6	0	-4.430888	-0.751464	-0.081646
10	1	0	-4.612830	-0.303309	0.897938
11	1	0	-5.089348	-1.603766	-0.243467
12	8	0	1.717692	-2.393706	-0.219156
13	8	0	0.638570	1.512016	1.465051
14	8	0	0.465462	1.785369	-0.777663
15	6	0	0.565932	3.216150	-0.606826
16	1	0	0.553830	3.628643	-1.614778
17	1	0	1.496168	3.472869	-0.095299
18	1	0	-0.285875	3.583236	-0.029952
19	8	0	2.724363	-0.383449	0.041320
20	6	0	4.015553	-1.021543	-0.057539
21	1	0	4.742942	-0.218048	0.047351
22	1	0	4.118229	-1.512926	-1.027568
23	1	0	4.133084	-1.756916	0.741331
24	1	0	-4.576174	0.001508	-0.859860

SCF Done: E(RB3LYP) = -762.221163575   A.U. after   1 cycles
Sum of electronic and thermal Free Energies=   -762.084267

1m(tc) (IDA7pcm.log)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.280585	1.357611	-0.348362
2	6	0	-0.517810	-0.113595	-0.095689
3	6	0	0.461453	-1.023102	0.017862
4	1	0	0.220259	-2.071146	0.152050
5	6	0	-1.968017	-0.476270	-0.031439
6	6	0	1.900397	-0.657418	-0.032752
7	8	0	2.334055	0.469738	-0.190663
8	8	0	2.667027	-1.749003	0.119816
9	6	0	4.091730	-1.526024	0.089164
10	1	0	4.385055	-1.087890	-0.867588
11	1	0	4.541909	-2.509493	0.216715
12	8	0	-2.854074	0.355493	-0.100045
13	8	0	-0.284732	1.845901	-1.457051
14	8	0	-0.138680	2.030322	0.796385
15	6	0	0.078782	3.452255	0.663135
16	1	0	0.142509	3.831047	1.682300
17	1	0	-0.754786	3.914707	0.130203
18	1	0	1.010489	3.637481	0.123959
19	8	0	-2.171789	-1.791192	0.115176
20	6	0	-3.551126	-2.209485	0.195372
21	1	0	-3.517188	-3.292469	0.304552
22	1	0	-4.083433	-1.929127	-0.716136
23	1	0	-4.035182	-1.748888	1.059438
24	1	0	4.386971	-0.858119	0.901814

SCF Done: E(RB3LYP) = -762.220224318   A.U. after   1 cycles
Sum of electronic and thermal Free Energies=   -762.083318

1m(ct) (IDA11pcm.log)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.177029	0.960150	0.325511
2	6	0	0.418626	-0.500441	0.034340
3	6	0	-0.535409	-1.432334	-0.111679
4	1	0	-0.230041	-2.461489	-0.271153
5	6	0	1.851393	-0.947178	-0.042815
6	6	0	-2.006383	-1.233685	-0.082839
7	8	0	-2.790422	-2.152932	-0.231686
8	8	0	-2.369747	0.042046	0.122139
9	6	0	-3.789047	0.296098	0.169039
10	1	0	-4.252146	0.025759	-0.782640
11	1	0	-3.885357	1.364884	0.354426
12	8	0	2.205535	-2.095923	-0.216234
13	8	0	0.147565	1.418776	1.446800
14	8	0	0.058200	1.666123	-0.803225
15	6	0	-0.145172	3.086534	-0.635059
16	1	0	-0.195104	3.492083	-1.644610
17	1	0	0.688676	3.525425	-0.082878
18	1	0	-1.078891	3.270872	-0.098952
19	8	0	2.685466	0.093288	0.096319
20	6	0	4.095465	-0.211617	0.037166
21	1	0	4.602649	0.742163	0.174057
22	1	0	4.344853	-0.647394	-0.932799
23	1	0	4.362077	-0.909922	0.833390
24	1	0	-4.248508	-0.278561	0.976268

SCF Done: E(RB3LYP) = -762.219169519 A.U. after 1 cycles
Sum of electronic and thermal Free Energies= -762.082332

1m(tt) (IDA3Rpcm.log)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.156231	1.178108	0.339448
2	6	0	0.537787	-0.138969	0.080578
3	6	0	-0.073382	-1.324380	-0.071256
4	1	0	0.526461	-2.216992	-0.207526
5	6	0	2.029732	-0.004821	0.053793
6	6	0	-1.535723	-1.587832	-0.078190
7	8	0	-1.993096	-2.705548	-0.231836
8	8	0	-2.280385	-0.486150	0.100825
9	6	0	-3.709522	-0.683205	0.112500
10	1	0	-4.040842	-1.096751	-0.842669
11	1	0	-4.136291	0.305661	0.273344
12	8	0	2.589808	1.070831	0.160526
13	8	0	-0.357238	1.614383	1.451389
14	8	0	-0.453056	1.801355	-0.803965
15	6	0	-1.081981	3.095084	-0.667632
16	1	0	-1.226745	3.453948	-1.685651
17	1	0	-0.434305	3.772784	-0.107304
18	1	0	-2.040900	2.993654	-0.154395
19	8	0	2.659684	-1.174658	-0.104534
20	6	0	4.101286	-1.113241	-0.150487
21	1	0	4.428739	-2.143802	-0.279309
22	1	0	4.490656	-0.697384	0.781336
23	1	0	4.425388	-0.496491	-0.991656
24	1	0	-3.989694	-1.360787	0.922075

SCF Done: E(RB3LYP) = -762.218171795 A.U. after 1 cycles
Sum of electronic and thermal Free Energies= -762.081514

Figure 2
1m(cc)---2 endo (IDATS10pcm.for.log)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.279178	1.063701	0.703782
2	6	0	0.791849	0.298814	-0.502679
3	6	0	-0.405894	0.485418	-1.076060
4	1	0	-0.692369	-0.132611	-1.919539
5	6	0	1.686197	-0.769328	-1.054444

6	6	0	-1.376130	1.506573	-0.609753
7	8	0	-1.213273	2.249058	0.341927
8	8	0	-2.470366	1.505601	-1.389004
9	6	0	-3.493242	2.458339	-1.035826
10	1	0	-3.863934	2.258533	-0.027626
11	1	0	-4.284996	2.320035	-1.770887
12	6	0	-2.605579	-1.940488	0.040042
13	6	0	-2.539966	-1.442067	1.294642
14	6	0	-1.471589	-2.127333	2.034114
15	1	0	-3.166640	-0.659633	1.710989
16	8	0	1.371015	-1.544359	-1.937461
17	8	0	1.181339	0.650691	1.838874
18	8	0	1.874609	2.206177	0.345026
19	6	0	2.378402	3.014858	1.430155
20	1	0	2.842381	3.878476	0.955476
21	1	0	3.112219	2.453869	2.013104
22	1	0	1.554874	3.326702	2.076487
23	8	0	2.884164	-0.751910	-0.453719
24	6	0	3.834662	-1.741400	-0.902488
25	1	0	4.731836	-1.568796	-0.310063
26	1	0	4.041412	-1.608629	-1.966617
27	1	0	3.442236	-2.745428	-0.726795
28	1	0	-3.096475	3.475188	-1.082955
29	6	0	-0.891885	-3.045146	1.230413
30	1	0	-0.073738	-3.709688	1.484448
31	1	0	-1.204710	-1.911641	3.063587
32	6	0	-1.557990	-3.011842	-0.119935
33	1	0	-0.840990	-2.774600	-0.920791
34	1	0	-1.998304	-3.983810	-0.391057
35	1	0	-3.290784	-1.640632	-0.744688

SCF Done: E(RB3LYP) = -956.325775632 A.U. after 1 cycles
Sum of electronic and thermal Free Energies= -956.106094

2-ester endo TS (IDATS10pcm.log)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.660115	1.127372	0.768021
2	6	0	0.519129	-0.063880	-0.168515
3	6	0	-0.708637	-0.362591	-0.794695
4	1	0	-0.662002	-0.815691	-1.778117
5	6	0	1.750107	-0.366958	-0.950574
6	6	0	-1.927784	0.415098	-0.503968
7	8	0	-2.107700	1.126221	0.472113
8	8	0	-2.862822	0.224127	-1.462118
9	6	0	-4.108431	0.916509	-1.265657
10	1	0	-4.585829	0.592036	-0.337357
11	1	0	-4.726731	0.653972	-2.123927
12	6	0	-1.323105	-2.263234	0.171445
13	6	0	-1.561149	-1.803970	1.477108
14	6	0	-0.333140	-1.560719	2.103673
15	1	0	-2.532493	-1.551950	1.887151
16	8	0	1.797111	-1.044058	-1.965086
17	8	0	0.847270	1.113671	1.965169
18	8	0	0.619058	2.261435	0.038902
19	6	0	0.741484	3.485576	0.786966
20	1	0	0.693953	4.284893	0.047538
21	1	0	1.693438	3.514771	1.322754
22	1	0	-0.081465	3.573790	1.500479
23	8	0	2.844225	0.187289	-0.386066
24	6	0	4.091332	-0.040707	-1.068992
25	1	0	4.845161	0.475396	-0.475208
26	1	0	4.053165	0.369818	-2.080840
27	1	0	4.308613	-1.110317	-1.119046
28	1	0	-3.945812	1.996560	-1.228364
29	6	0	0.702685	-1.880792	1.214630
30	1	0	1.754867	-1.879511	1.476378
31	1	0	-0.203091	-1.089290	3.068655
32	6	0	0.106939	-2.742318	0.130704
33	1	0	0.600846	-2.703114	-0.839817
34	1	0	0.126531	-3.789234	0.474892
35	1	0	-2.093562	-2.627920	-0.499375

SCF Done: E(RB3LYP) = -956.299325396 A.U. after 1 cycles
Sum of electronic and thermal Free Energies= -956.069922

3m-endo (IDATS10pcm.rev.log)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.574080	0.884628	1.014361
2	6	0	0.578366	-0.331210	0.079485
3	6	0	-0.768982	-0.632781	-0.667645
4	1	0	-0.581040	-0.621387	-1.741906
5	6	0	1.708564	-0.097492	-0.941614
6	6	0	-1.939248	0.282987	-0.384020
7	8	0	-2.191340	0.826609	0.674506
8	8	0	-2.736182	0.369332	-1.467203
9	6	0	-3.939667	1.144922	-1.303187
10	1	0	-4.565461	0.717001	-0.516203
11	1	0	-4.449302	1.098300	-2.265120
12	6	0	-1.082254	-2.125737	-0.222319
13	6	0	-1.380563	-2.115638	1.267934
14	6	0	-0.231141	-1.855028	1.905178
15	1	0	-2.370681	-2.199818	1.702422
16	8	0	1.618809	-0.199032	-2.147816
17	8	0	0.720637	0.856307	2.216216
18	8	0	0.447903	2.016152	0.296158
19	6	0	0.392248	3.240544	1.053589
20	1	0	0.308621	4.036712	0.314447
21	1	0	1.299683	3.362380	1.649383
22	1	0	-0.481079	3.232316	1.709779
23	8	0	2.853023	0.201500	-0.304181
24	6	0	4.006050	0.433233	-1.140871
25	1	0	4.818724	0.666919	-0.454310
26	1	0	3.819627	1.270530	-1.817041
27	1	0	4.237900	-0.462201	-1.721795
28	1	0	-3.694330	2.178784	-1.048775
29	6	0	0.852529	-1.695771	0.850425
30	1	0	1.882903	-1.782275	1.195326
31	1	0	-0.084030	-1.681859	2.963626
32	6	0	0.351525	-2.701305	-0.212841
33	1	0	0.860927	-2.631066	-1.179608
34	1	0	0.383413	-3.732955	0.147179
35	1	0	-1.817715	-2.606435	-0.869710

SCF Done: E(RB3LYP) = -956.350303326 A.U. after 1 cycles
Sum of electronic and thermal Free Energies= -956.115803

1m(cc)---2 exo (IDATS9pcm.rev.log)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.288586	1.066440	0.672863
2	6	0	0.788241	0.290599	-0.520252
3	6	0	-0.419595	0.466769	-1.074791
4	1	0	-0.719511	-0.166161	-1.902470
5	6	0	1.680427	-0.777226	-1.078570
6	6	0	-1.379155	1.498675	-0.609493
7	8	0	-1.198282	2.253390	0.329721
8	8	0	-2.481966	1.495576	-1.375127
9	6	0	-3.493441	2.461003	-1.023697
10	1	0	-3.856558	2.275568	-0.009936
11	1	0	-4.293024	2.320950	-1.749879
12	6	0	-2.547193	-1.386616	1.191014
13	6	0	-2.706037	-2.128314	0.072007
14	6	0	-1.654451	-3.153194	0.016799
15	1	0	-3.480496	-2.004257	-0.678492
16	8	0	1.389984	-1.498422	-2.011864
17	8	0	1.180693	0.676200	1.817024
18	8	0	1.908309	2.188981	0.299409
19	6	0	2.426451	3.005568	1.372856
20	1	0	2.902117	3.855132	0.884816
21	1	0	3.152977	2.441310	1.961630
22	1	0	1.608467	3.337951	2.015751
23	8	0	2.847360	-0.821020	-0.418169
24	6	0	3.792904	-1.814309	-0.867944
25	1	0	4.663516	-1.696235	-0.224577
26	1	0	4.056556	-1.636971	-1.912900
27	1	0	3.366236	-2.814126	-0.761670
28	1	0	-3.088609	3.473844	-1.085987
29	6	0	-0.858804	-3.032299	1.101839

30	1	0	0.003752	-3.641742	1.347543
31	1	0	-1.550788	-3.881604	-0.781255
32	6	0	-1.348177	-1.888571	1.950290
33	1	0	-1.605847	-2.206996	2.972276
34	1	0	-0.580226	-1.107540	2.062693
35	1	0	-3.165879	-0.557918	1.516961

SCF Done: E(RB3LYP) = -956.326746054 A.U. after 1 cycles
Sum of electronic and thermal Free Energies= -956.107846

2-ester exo TS (IDATS9pcm.log)
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.488161	1.319290	0.718444
2	6	0	0.452274	0.053531	-0.118791
3	6	0	-0.755668	-0.458417	-0.642434
4	1	0	-0.689226	-0.980608	-1.587874
5	6	0	1.672617	-0.213645	-0.917001
6	6	0	-2.046535	0.219900	-0.388628
7	8	0	-2.284423	0.986473	0.531953
8	8	0	-2.967796	-0.136814	-1.308410
9	6	0	-4.273071	0.449234	-1.146237
10	1	0	-4.703457	0.164320	-0.182917
11	1	0	-4.873198	0.053234	-1.965053
12	6	0	-1.151537	-2.202648	0.583583
13	6	0	-0.125562	-3.047819	0.118671
14	6	0	1.088445	-2.647330	0.688024
15	1	0	-0.240083	-3.807199	-0.647201
16	8	0	1.740832	-0.987859	-1.857334
17	8	0	0.668735	1.406139	1.915333
18	8	0	0.336891	2.390032	-0.085437
19	6	0	0.349784	3.671211	0.573444
20	1	0	0.224279	4.407594	-0.220099
21	1	0	1.298460	3.825185	1.093322
22	1	0	-0.473297	3.734199	1.289402
23	8	0	2.732086	0.493040	-0.461379
24	6	0	3.969760	0.296999	-1.168169
25	1	0	4.688701	0.957935	-0.684527
26	1	0	3.855638	0.561142	-2.222361
27	1	0	4.294860	-0.743547	-1.089297
28	1	0	-4.213648	1.538630	-1.207625
29	6	0	0.854583	-1.546699	1.522148
30	1	0	1.597390	-1.053343	2.135551
31	1	0	2.062525	-3.043300	0.424303
32	6	0	-0.620223	-1.514097	1.817849
33	1	0	-0.810372	-2.169539	2.683858
34	1	0	-1.041075	-0.535554	2.042480
35	1	0	-2.206273	-2.394296	0.414810

SCF Done: E(RB3LYP) = -956.300729214 A.U. after 1 cycles
Sum of electronic and thermal Free Energies= -956.071564

3m-exo (IDATS9pcm.for.log)
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.194416	1.118950	0.981698
2	6	0	0.564407	-0.151532	0.198931
3	6	0	-0.658905	-0.896640	-0.455769
4	1	0	-0.488126	-0.997303	-1.526427
5	6	0	1.588203	0.264517	-0.867788
6	6	0	-2.013828	-0.247431	-0.251484
7	8	0	-2.464463	0.142436	0.810838
8	8	0	-2.705262	-0.209223	-1.404016
9	6	0	-4.040740	0.328284	-1.320283
10	1	0	-4.650285	-0.270153	-0.639080
11	1	0	-4.437441	0.279090	-2.333779
12	6	0	-0.609429	-2.310740	0.265436
13	6	0	0.645648	-2.995830	-0.251130
14	6	0	1.698352	-2.368683	0.292353
15	1	0	0.656218	-3.780121	-1.000815
16	8	0	1.481065	0.108855	-2.065239
17	8	0	0.303714	1.268169	2.178348
18	8	0	-0.234877	2.075727	0.138114

19	6	0	-0.648467	3.316032	0.747967
20	1	0	-0.928353	3.967086	-0.079396
21	1	0	0.173717	3.750877	1.320303
22	1	0	-1.502718	3.139343	1.405441
23	8	0	2.661179	0.821489	-0.278468
24	6	0	3.715114	1.258874	-1.161980
25	1	0	4.486607	1.668931	-0.511416
26	1	0	3.341602	2.024128	-1.846225
27	1	0	4.103322	0.413805	-1.734823
28	1	0	-4.012096	1.362186	-0.968542
29	6	0	1.157879	-1.251198	1.174611
30	1	0	1.836614	-0.828943	1.913649
31	1	0	2.749330	-2.536622	0.081370
32	6	0	-0.148730	-1.900262	1.681404
33	1	0	0.042473	-2.763930	2.324880
34	1	0	-0.824045	-1.201502	2.179147
35	1	0	-1.541185	-2.872554	0.175294

SCF Done: E(RB3LYP) = -956.351539343 A.U. after 1 cycles
Sum of electronic and thermal Free Energies= -956.117453

Figure 3
AlCl3-1m---2 endo (AlDATS2pcm.for.log)
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.309438	-0.848931	0.415016
2	6	0	0.827768	-0.009639	-0.683887
3	6	0	2.054568	-0.155343	-1.231451
4	1	0	2.354578	0.542819	-2.007625
5	6	0	-0.110330	1.019211	-1.198100
6	6	0	3.087049	-1.202486	-0.924791
7	8	0	4.201571	-0.913427	-0.548440
8	8	0	2.642838	-2.426167	-1.205438
9	6	0	3.589324	-3.505121	-1.004786
10	1	0	4.485428	-3.333457	-1.604113
11	1	0	3.069681	-4.404005	-1.331219
12	6	0	3.417060	2.138551	0.992638
13	6	0	2.925383	1.324245	1.953966
14	6	0	1.555803	1.734487	2.280769
15	1	0	3.443430	0.490607	2.415357
16	8	0	-1.315967	1.037857	-0.922784
17	8	0	-0.901698	-0.955069	0.706314
18	8	0	1.218220	-1.479415	1.100457
19	6	0	0.786305	-2.357327	2.185175
20	1	0	1.707425	-2.791558	2.565578
21	1	0	0.117119	-3.120494	1.788323
22	1	0	0.282720	-1.762752	2.947415
23	8	0	0.437271	1.902106	-2.001647
24	6	0	-0.438410	2.901180	-2.599139
25	1	0	0.214399	3.491653	-3.237846
26	1	0	-0.881170	3.513792	-1.813169
27	1	0	-1.216328	2.404128	-3.179317
28	1	0	3.856295	-3.572333	0.051787
29	6	0	1.211897	2.798351	1.515995
30	1	0	0.272142	3.338255	1.540343
31	1	0	0.933287	1.260575	3.033279
32	6	0	2.378640	3.170794	0.640178
33	1	0	2.125678	3.167238	-0.429601
34	1	0	2.730859	4.191653	0.855757
35	1	0	4.399546	2.086572	0.539090
36	13	0	-2.578650	-0.276187	0.057526
37	17	0	-3.388859	1.481344	1.071813
38	17	0	-3.609026	-1.876046	1.230205
39	17	0	-3.249026	-0.857484	-1.946669

SCF Done: E(RB3LYP) = -2579.61549803 A.U. after 1 cycles
Sum of electronic and thermal Free Energies= -2579.396495

2-ester endo TS1 (AlDATS2pcm.log)
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.309866	-0.832043	0.356321

2	6	0	0.850013	0.190693	-0.521916
3	6	0	2.199797	0.287705	-0.822250
4	1	0	2.486166	1.081815	-1.504595
5	6	0	-0.118491	1.125172	-1.096038
6	6	0	3.190393	-0.857360	-0.827094
7	8	0	4.329522	-0.803554	-0.417177
8	8	0	2.660193	-1.902045	-1.473340
9	6	0	3.533386	-3.042363	-1.649200
10	1	0	4.425257	-2.750363	-2.207214
11	1	0	2.945807	-3.767802	-2.209371
12	6	0	3.243892	1.698168	0.831674
13	6	0	3.015134	0.827586	1.874633
14	6	0	1.797238	1.193126	2.553229
15	1	0	3.638868	-0.020059	2.129597
16	8	0	-1.349169	1.044639	-0.937243
17	8	0	-0.914166	-1.041538	0.563585
18	8	0	1.204933	-1.564654	0.975545
19	6	0	0.738561	-2.621010	1.861622
20	1	0	1.648052	-3.091191	2.228876
21	1	0	0.126929	-3.327392	1.299986
22	1	0	0.161847	-2.184835	2.677843
23	8	0	0.405215	2.077418	-1.849507
24	6	0	-0.511132	3.004318	-2.492160
25	1	0	0.128996	3.674170	-3.062533
26	1	0	-1.076502	3.550820	-1.736286
27	1	0	-1.188627	2.455908	-3.147569
28	1	0	3.822471	-3.445101	-0.676101
29	6	0	1.285156	2.315872	1.973672
30	1	0	0.371337	2.825424	2.256723
31	1	0	1.363829	0.647018	3.383236
32	6	0	2.220216	2.802233	0.907206
33	1	0	1.732089	3.054481	-0.039554
34	1	0	2.713367	3.729783	1.240977
35	1	0	4.154347	1.745536	0.249108
36	13	0	-2.563002	-0.264474	0.020115
37	17	0	-3.318001	1.466589	1.147954
38	17	0	-3.627646	-1.868526	1.185550
39	17	0	-3.369155	-0.761284	-1.965134

SCF Done: E(RB3LYP) = -2579.61380845 A.U. after 1 cycles
Sum of electronic and thermal Free Energies= -2579.389783

2-ester endo Int (AlDATS2pcm.rev.log)
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.326924	-0.743169	0.430663
2	6	0	0.853884	0.258500	-0.406714
3	6	0	2.327522	0.459247	-0.548850
4	1	0	2.491810	1.079938	-1.434245
5	6	0	-0.086136	1.021115	-1.164402
6	6	0	3.149273	-0.815757	-0.778659
7	8	0	4.188915	-1.077225	-0.207171
8	8	0	2.605597	-1.565735	-1.741178
9	6	0	3.319934	-2.774894	-2.081628
10	1	0	4.322137	-2.533090	-2.442028
11	1	0	2.730625	-3.245012	-2.867456
12	6	0	3.010127	1.300201	0.646547
13	6	0	2.890451	0.616899	1.944175
14	6	0	1.900122	1.198013	2.733846
15	1	0	3.496540	-0.237164	2.221062
16	8	0	-1.334225	0.879786	-1.123683
17	8	0	-0.901437	-1.028811	0.613356
18	8	0	1.242402	-1.450385	1.098893
19	6	0	0.784373	-2.500468	1.987628
20	1	0	1.694963	-2.926845	2.404996
21	1	0	0.229011	-3.248562	1.420785
22	1	0	0.152599	-2.081189	2.771870
23	8	0	0.440742	1.949796	-1.966964
24	6	0	-0.473535	2.729865	-2.773499
25	1	0	0.163202	3.404003	-3.344229
26	1	0	-1.157977	3.290023	-2.134336
27	1	0	-1.037983	2.074391	-3.438481
28	1	0	3.390298	-3.427755	-1.208968
29	6	0	1.422402	2.319582	2.072662
30	1	0	0.609009	2.947839	2.422645
31	1	0	1.554747	0.831157	3.692231
32	6	0	2.223851	2.609390	0.861394

33	1	0	1.635297	2.961241	0.010875
34	1	0	2.927690	3.421901	1.106738
35	1	0	4.055569	1.418655	0.349710
36	13	0	-2.500265	-0.243531	0.013804
37	17	0	-3.161318	1.622820	1.016595
38	17	0	-3.623176	-1.668376	1.386562
39	17	0	-3.485224	-0.912926	-1.852311

SCF Done: E(RB3LYP) = -2579.63196981 A.U. after 1 cycles
Sum of electronic and thermal Free Energies= -2579.404690

2-ester endo TS2 (AlDATS4pcm.log)
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.361892	-0.873700	-0.178065
2	6	0	-0.889340	0.445678	0.090778
3	6	0	-2.378372	0.690322	0.207547
4	1	0	-2.516654	1.500555	0.928160
5	6	0	0.041223	1.320445	0.801309
6	6	0	-3.227459	-0.464835	0.735359
7	8	0	-4.222930	-0.895893	0.192130
8	8	0	-2.767999	-0.882976	1.922688
9	6	0	-3.513504	-1.948200	2.551927
10	1	0	-4.541746	-1.631045	2.738727
11	1	0	-2.996218	-2.147842	3.489301
12	6	0	-2.955455	1.253043	-1.179066
13	6	0	-2.811517	0.217132	-2.239684
14	6	0	-1.526687	0.226343	-2.707299
15	1	0	-3.585206	-0.493019	-2.504020
16	8	0	1.269488	1.123021	0.896324
17	8	0	0.858415	-1.200854	-0.164805
18	8	0	-1.260213	-1.777765	-0.500571
19	6	0	-0.806255	-3.113357	-0.857418
20	1	0	-1.716128	-3.650458	-1.116238
21	1	0	-0.309146	-3.570441	-0.001349
22	1	0	-0.124133	-3.056785	-1.706103
23	8	0	-0.502983	2.393679	1.352850
24	6	0	0.380719	3.314687	2.045702
25	1	0	-0.271625	4.111632	2.397033
26	1	0	1.132865	3.698402	1.355197
27	1	0	0.861671	2.805280	2.881662
28	1	0	-3.512916	-2.835485	1.914958
29	6	0	-0.832398	1.286737	-2.046342
30	1	0	0.221030	1.512629	-2.182931
31	1	0	-1.073731	-0.497542	-3.374032
32	6	0	-1.864277	2.270909	-1.586351
33	1	0	-1.545967	2.952627	-0.797925
34	1	0	-2.202355	2.861458	-2.447588
35	1	0	-3.965781	1.633018	-1.028846
36	13	0	2.483557	-0.257427	0.079158
37	17	0	3.017685	1.287651	-1.410918
38	17	0	3.560079	-1.974528	-0.906387
39	17	0	3.501109	-0.352615	2.023519

SCF Done: E(RB3LYP) = -2579.62899032 A.U. after 1 cycles
Sum of electronic and thermal Free Energies= -2579.397704

AlCl3-3m-endo (AlDATS4pcm.rev.log)
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.351191	-0.880570	-0.258487
2	6	0	-0.902222	0.526658	-0.165499
3	6	0	-2.441627	0.702846	0.122866
4	1	0	-2.527899	1.458800	0.906897
5	6	0	0.005771	1.329035	0.760210
6	6	0	-3.218948	-0.491681	0.652188
7	8	0	-4.209533	-0.961034	0.134148
8	8	0	-2.711512	-0.899417	1.828920
9	6	0	-3.393597	-2.001689	2.464711
10	1	0	-4.430425	-1.732003	2.677276
11	1	0	-2.847573	-2.186899	3.388780
12	6	0	-3.008516	1.316756	-1.203179
13	6	0	-2.836287	0.306600	-2.323529

14	6	0	-1.528032	0.236005	-2.611428
15	1	0	-3.635426	-0.294297	-2.740036
16	8	0	1.221622	1.131583	0.867249
17	8	0	0.866690	-1.159661	-0.228965
18	8	0	-1.228398	-1.813838	-0.462539
19	6	0	-0.762001	-3.183644	-0.674214
20	1	0	-1.670508	-3.751662	-0.857925
21	1	0	-0.247926	-3.529403	0.222413
22	1	0	-0.093395	-3.206048	-1.534397
23	8	0	-0.583987	2.302999	1.408726
24	6	0	0.246023	3.157067	2.250669
25	1	0	-0.445093	3.887603	2.664607
26	1	0	1.011852	3.635614	1.639924
27	1	0	0.704176	2.555359	3.035816
28	1	0	-3.370594	-2.883634	1.820508
29	6	0	-0.807941	1.193284	-1.684270
30	1	0	0.216977	1.465668	-1.935219
31	1	0	-1.031573	-0.439126	-3.299451
32	6	0	-1.866793	2.302928	-1.538704
33	1	0	-1.656829	3.034411	-0.754069
34	1	0	-2.023154	2.818384	-2.489241
35	1	0	-4.008970	1.729477	-1.072355
36	13	0	2.524526	-0.226683	0.033172
37	17	0	3.105345	1.397535	-1.323363
38	17	0	3.568649	-1.908832	-1.001364
39	17	0	3.419572	-0.400584	2.016899

SCF Done: E(RB3LYP) = -2579.63926393 A.U. after 1 cycles
Sum of electronic and thermal Free Energies= -2579.406185

AlCl3-1m---2 exo (AlDATS1pcm.for.log)
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.332477	-0.989263	-0.308531
2	6	0	-0.873301	-0.044828	0.687602
3	6	0	-2.154615	-0.058035	1.118369
4	1	0	-2.459723	0.695755	1.838211
5	6	0	0.092972	0.934596	1.243710
6	6	0	-3.245653	-1.010341	0.716690
7	8	0	-4.163085	-0.674780	-0.000371
8	8	0	-3.099607	-2.189716	1.312112
9	6	0	-4.136870	-3.168557	1.046874
10	1	0	-5.110813	-2.769269	1.335468
11	1	0	-3.874457	-4.032227	1.654859
12	6	0	-3.112664	2.447983	-1.061612
13	6	0	-2.103182	3.201141	-0.567099
14	6	0	-0.863524	2.874488	-1.279492
15	1	0	-2.176953	3.934205	0.229296
16	8	0	1.308864	0.899767	1.017521
17	8	0	0.881706	-1.121214	-0.573409
18	8	0	-1.228941	-1.704957	-0.927521
19	6	0	-0.780283	-2.681865	-1.916914
20	1	0	-1.693907	-3.167055	-2.251122
21	1	0	-0.100443	-3.390047	-1.443663
22	1	0	-0.284487	-2.159706	-2.735298
23	8	0	-0.443751	1.836441	2.030798
24	6	0	0.449277	2.798598	2.660079
25	1	0	-0.204202	3.430998	3.256650
26	1	0	0.964953	3.376279	1.892420
27	1	0	1.169124	2.271412	3.287113
28	1	0	-4.138987	-3.426021	-0.014128
29	6	0	-1.118229	1.920571	-2.207348
30	1	0	-0.410732	1.494399	-2.909641
31	1	0	0.097792	3.341713	-1.091377
32	6	0	-2.583499	1.577304	-2.169557
33	1	0	-3.071981	1.803036	-3.130437
34	1	0	-2.775498	0.511355	-1.985637
35	1	0	-4.148657	2.456076	-0.744712
36	13	0	2.558347	-0.349262	-0.030425
37	17	0	3.233407	1.446520	-1.082878
38	17	0	3.596955	-1.887810	-1.278607
39	17	0	3.375007	-0.911979	1.923711

SCF Done: E(RB3LYP) = -2579.61646037 A.U. after 1 cycles
Sum of electronic and thermal Free Energies= -2579.398577

2-ester exo TS1 (AlDATS1pcm.log)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.304182	-0.963735	-0.335574
2	6	0	-0.889073	0.106505	0.446553
3	6	0	-2.255074	0.234483	0.690808
4	1	0	-2.539073	0.938824	1.463345
5	6	0	0.050091	1.055931	1.039135
6	6	0	-3.242855	-0.912658	0.546944
7	8	0	-4.167199	-0.989856	-0.230424
8	8	0	-2.967621	-1.809679	1.500928
9	6	0	-3.846946	-2.958588	1.559592
10	1	0	-4.875996	-2.636536	1.730758
11	1	0	-3.482707	-3.553615	2.395435
12	6	0	-3.138521	1.648510	-0.932139
13	6	0	-2.477374	2.803328	-0.554496
14	6	0	-1.257821	2.929861	-1.300354
15	1	0	-2.805115	3.494413	0.214270
16	8	0	1.289189	0.989658	0.935641
17	8	0	0.930090	-1.153763	-0.497278
18	8	0	-1.159807	-1.791596	-0.894260
19	6	0	-0.638269	-2.912380	-1.663512
20	1	0	-1.524102	-3.427305	-2.028455
21	1	0	-0.045634	-3.556567	-1.013428
22	1	0	-0.029182	-2.540387	-2.487496
23	8	0	-0.518778	2.020952	1.739959
24	6	0	0.353589	2.989092	2.380343
25	1	0	-0.319827	3.667023	2.900869
26	1	0	0.937124	3.518371	1.625865
27	1	0	1.016742	2.480629	3.081209
28	1	0	-3.785452	-3.521995	0.626237
29	6	0	-1.179310	1.902596	-2.199555
30	1	0	-0.370207	1.726376	-2.899087
31	1	0	-0.520659	3.711728	-1.159100
32	6	0	-2.432988	1.088654	-2.142987
33	1	0	-3.044485	1.304132	-3.035187
34	1	0	-2.283222	0.006188	-2.147171
35	1	0	-4.154896	1.393319	-0.666257
36	13	0	2.546417	-0.287016	0.017269
37	17	0	3.249693	1.443997	-1.148532
38	17	0	3.668094	-1.874095	-1.122901
39	17	0	3.378018	-0.715120	2.008411

SCF Done: E(RB3LYP) = -2579.61241638 A.U. after 1 cycles
Sum of electronic and thermal Free Energies= -2579.387938

2-ester exo Int (AlDATS1pcm.rev.log)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.272263	-0.928509	-0.391755
2	6	0	-0.872265	0.117010	0.343719
3	6	0	-2.350090	0.277554	0.534075
4	1	0	-2.511599	0.737438	1.513039
5	6	0	0.014796	1.045975	0.960798
6	6	0	-3.156498	-1.029731	0.568889
7	8	0	-4.129146	-1.263758	-0.117409
8	8	0	-2.683878	-1.839888	1.520997
9	6	0	-3.375609	-3.097979	1.680406
10	1	0	-4.422927	-2.924159	1.936675
11	1	0	-2.859766	-3.608922	2.492057
12	6	0	-3.060659	1.259318	-0.529888
13	6	0	-2.582572	2.637127	-0.341486
14	6	0	-1.689846	3.008120	-1.342219
15	1	0	-2.871740	3.262866	0.496211
16	8	0	1.270503	1.018744	0.921153
17	8	0	0.979409	-1.131074	-0.522791
18	8	0	-1.103060	-1.774062	-1.000197
19	6	0	-0.533637	-2.885937	-1.734514
20	1	0	-1.393583	-3.424747	-2.128586
21	1	0	0.048353	-3.518791	-1.063050
22	1	0	0.100089	-2.518405	-2.542703
23	8	0	-0.596110	2.040185	1.618685
24	6	0	0.244221	3.027240	2.263450
25	1	0	-0.449694	3.731171	2.720129

26	1	0	0.876363	3.524986	1.526532
27	1	0	0.864615	2.548362	3.022567
28	1	0	-3.313855	-3.679415	0.757884
29	6	0	-1.629267	1.974411	-2.268161
30	1	0	-0.976744	1.958675	-3.135998
31	1	0	-1.131994	3.934835	-1.387363
32	6	0	-2.630394	0.927775	-1.971252
33	1	0	-3.485473	1.074327	-2.652089
34	1	0	-2.280797	-0.091979	-2.144402
35	1	0	-4.131666	1.155808	-0.336493
36	13	0	2.525314	-0.207706	0.015523
37	17	0	3.177816	1.510146	-1.228668
38	17	0	3.747993	-1.784683	-1.077884
39	17	0	3.460902	-0.540599	1.996429

SCF Done: E(RB3LYP) = -2579.62929972 A.U. after 1 cycles
Sum of electronic and thermal Free Energies= -2579.401851

2-ester exo TS2 (AlDATS3pcm.log)
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.332327	-0.960260	-0.323388
2	6	0	-0.923695	0.283134	0.121092
3	6	0	-2.418987	0.472953	0.279056
4	1	0	-2.588391	1.060385	1.183627
5	6	0	-0.027819	1.112223	0.919993
6	6	0	-3.242358	-0.804813	0.480009
7	8	0	-4.171563	-1.153905	-0.215635
8	8	0	-2.839778	-1.444535	1.587012
9	6	0	-3.553199	-2.658188	1.909076
10	1	0	-4.612690	-2.444579	2.065882
11	1	0	-3.095234	-3.027655	2.825559
12	6	0	-3.001463	1.299804	-0.971410
13	6	0	-2.475164	2.688760	-0.874250
14	6	0	-1.208076	2.731748	-1.384731
15	1	0	-2.983365	3.499286	-0.362760
16	8	0	1.211698	0.978793	0.987426
17	8	0	0.902808	-1.226254	-0.317827
18	8	0	-1.168060	-1.864447	-0.791450
19	6	0	-0.625436	-3.119549	-1.288681
20	1	0	-1.491494	-3.661020	-1.663144
21	1	0	-0.147005	-3.659471	-0.470999
22	1	0	0.093319	-2.922805	-2.084280
23	8	0	-0.628359	2.086033	1.583429
24	6	0	0.206791	2.988572	2.355659
25	1	0	-0.487514	3.705697	2.789100
26	1	0	0.924527	3.483144	1.699921
27	1	0	0.730068	2.431357	3.133641
28	1	0	-3.440897	-3.385470	1.101817
29	6	0	-0.908222	1.432941	-1.899103
30	1	0	0.049737	1.155744	-2.327135
31	1	0	-0.509889	3.557780	-1.326921
32	6	0	-2.208848	0.747542	-2.176842
33	1	0	-2.625927	1.144596	-3.111739
34	1	0	-2.170990	-0.337641	-2.248324
35	1	0	-4.085038	1.198750	-1.001591
36	13	0	2.487175	-0.252028	0.053482
37	17	0	2.940379	1.416065	-1.321648
38	17	0	3.640996	-1.854545	-1.036960
39	17	0	3.534293	-0.433073	1.979758

SCF Done: E(RB3LYP) = -2579.62628353 A.U. after 1 cycles
Sum of electronic and thermal Free Energies= -2579.395351

AlCl3-3m-exo (AlDATS3pcm.rev.log)
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.319693	-0.920827	-0.460713
2	6	0	-0.941061	0.431315	-0.164351
3	6	0	-2.494212	0.481205	0.113821
4	1	0	-2.645929	1.095496	1.002745
5	6	0	-0.087225	1.119829	0.893374
6	6	0	-3.186822	-0.836681	0.440750

7	8	0	-4.139307	-1.292939	-0.153579
8	8	0	-2.649673	-1.381932	1.547100
9	6	0	-3.252212	-2.611737	2.004992
10	1	0	-4.300769	-2.445067	2.261284
11	1	0	-2.683062	-2.902879	2.886799
12	6	0	-3.075888	1.218036	-1.147132
13	6	0	-2.617311	2.662084	-1.024309
14	6	0	-1.299483	2.693584	-1.269758
15	1	0	-3.244482	3.484013	-0.696274
16	8	0	1.137210	0.975041	0.991887
17	8	0	0.907299	-1.147625	-0.421332
18	8	0	-1.138698	-1.848527	-0.857222
19	6	0	-0.592424	-3.148295	-1.249229
20	1	0	-1.457232	-3.710385	-1.592407
21	1	0	-0.130374	-3.616117	-0.380069
22	1	0	0.137768	-3.006735	-2.045230
23	8	0	-0.741686	1.933962	1.680350
24	6	0	0.024599	2.687175	2.665576
25	1	0	-0.718304	3.276137	3.198455
26	1	0	0.744722	3.326334	2.153950
27	1	0	0.536208	1.994599	3.334137
28	1	0	-3.183003	-3.379147	1.230719
29	6	0	-0.865202	1.276054	-1.584137
30	1	0	0.099395	1.151842	-2.075841
31	1	0	-0.620887	3.534693	-1.185787
32	6	0	-2.135206	0.725945	-2.266168
33	1	0	-2.315494	1.230438	-3.218408
34	1	0	-2.150214	-0.354871	-2.418335
35	1	0	-4.143641	1.046849	-1.274375
36	13	0	2.517897	-0.187579	0.018140
37	17	0	3.046371	1.628559	-1.092382
38	17	0	3.656745	-1.667642	-1.209315
39	17	0	3.378902	-0.599543	1.982219

SCF Done: E(RB3LYP) = -2579.63793109 A.U. after 1 cycles
Sum of electronic and thermal Free Energies= -2579.406209

Figure 5
exo10m (DATS4pcm.rev.log)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.573192	0.750626	0.378372
2	6	0	1.534814	-0.310065	0.118071
3	6	0	0.217518	-0.064706	0.053177
4	1	0	-0.443698	-0.915674	-0.072436
5	6	0	1.996137	-1.729132	-0.021031
6	6	0	-0.359824	1.304705	0.227926
7	8	0	0.261024	2.165721	0.861373
8	7	0	-1.594792	1.526545	-0.310333
9	6	0	-2.292712	0.580921	-1.199999
10	1	0	-1.568280	0.020231	-1.793624
11	1	0	-2.865614	1.190122	-1.908582
12	6	0	-3.193640	-0.385775	-0.499974
13	6	0	-3.204745	-1.746318	-0.396246
14	6	0	-4.340545	-2.086932	0.412767
15	1	0	-2.493370	-2.427733	-0.843321
16	8	0	1.252465	-2.686719	-0.118080
17	8	0	3.184391	0.840119	1.421360
18	8	0	2.766281	1.525907	-0.697026
19	6	0	3.709848	2.603358	-0.523853
20	1	0	3.764158	3.099687	-1.492176
21	1	0	4.688053	2.212111	-0.235473
22	1	0	3.349001	3.293377	0.242521
23	8	0	3.334747	-1.807967	-0.052195
24	6	0	3.886409	-3.132973	-0.195786
25	1	0	4.966865	-2.996488	-0.203272
26	1	0	3.546739	-3.584249	-1.130827
27	1	0	3.582537	-3.760614	0.644975
28	6	0	-2.255673	2.808828	-0.076428
29	1	0	-2.299001	3.395565	-1.002332
30	1	0	-1.689956	3.360793	0.671780
31	1	0	-3.275096	2.637052	0.281356
32	6	0	-4.935584	-0.909469	0.742786
33	1	0	-5.803671	-0.648073	1.328611
34	1	0	-4.663092	-3.076257	0.705711
35	8	0	-4.254309	0.139930	0.192160

SCF Done: E(RB3LYP) = -1010.49268313   A.U. after   1 cycles
Sum of electronic and thermal Free Energies=   -1010.272427

IM-exo-TS   (DATS4pcm.log)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.753811	1.423267	0.359216
2	6	0	0.661804	0.089840	-0.261803
3	6	0	-0.671779	-0.370530	-0.667786
4	1	0	-0.574452	-1.058553	-1.510391
5	6	0	1.769524	-0.673913	-0.863868
6	6	0	-1.795571	0.612697	-1.015273
7	8	0	-1.691885	1.544569	-1.802669
8	7	0	-2.955666	0.209439	-0.418162
9	6	0	-2.876663	-1.014637	0.364448
10	1	0	-3.330080	-1.861015	-0.169917
11	1	0	-3.392661	-0.903849	1.324426
12	6	0	-1.393534	-1.250001	0.574841
13	6	0	-0.710975	-2.549859	0.595681
14	6	0	0.420008	-2.375665	1.338245
15	1	0	-0.968792	-3.390550	-0.034704
16	8	0	1.589786	-1.636564	-1.606305
17	8	0	-0.216343	2.015883	0.815531
18	8	0	1.996929	1.957433	0.398494
19	6	0	2.083709	3.258542	0.999616
20	1	0	3.136089	3.537119	0.935533
21	1	0	1.761546	3.227678	2.044172
22	1	0	1.465060	3.978844	0.457903
23	8	0	3.009593	-0.294919	-0.486908
24	6	0	4.085829	-1.064330	-1.045548
25	1	0	4.997652	-0.610958	-0.655565
26	1	0	4.073747	-1.015146	-2.137521
27	1	0	4.018702	-2.110791	-0.735347
28	6	0	-4.234174	0.836514	-0.685645
29	1	0	-4.904979	0.150992	-1.219591
30	1	0	-4.052885	1.716392	-1.304133
31	1	0	-4.716584	1.140703	0.250354
32	6	0	0.345741	-1.048686	1.852998
33	1	0	0.984435	-0.554950	2.573509
34	1	0	1.258457	-3.048348	1.453712
35	8	0	-0.899574	-0.574286	1.729852

SCF Done: E(RB3LYP) = -1010.46517273   A.U. after   1 cycles
Sum of electronic and thermal Free Energies=   -1010.238301

exo9m   (DATS4pcm.for.log)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.781724	1.262118	0.735149
2	6	0	0.630517	-0.143207	0.137993
3	6	0	-0.684354	-0.322187	-0.671422
4	1	0	-0.457007	-0.576851	-1.710344
5	6	0	1.869972	-0.480742	-0.692664
6	6	0	-1.749585	0.779770	-0.660837
7	8	0	-1.574062	1.973977	-0.885665
8	7	0	-2.952699	0.184759	-0.411380
9	6	0	-2.884155	-1.244010	-0.108223
10	1	0	-3.258942	-1.850289	-0.943756
11	1	0	-3.471027	-1.483314	0.785418
12	6	0	-1.401422	-1.462498	0.126777
13	6	0	-0.640044	-2.761322	-0.050543
14	6	0	0.479701	-2.606066	0.666569
15	1	0	-0.915193	-3.570021	-0.716770
16	8	0	1.897482	-0.691364	-1.886163
17	8	0	0.392265	1.592084	1.833828
18	8	0	1.406654	2.077314	-0.126803
19	6	0	1.505947	3.459805	0.270780
20	1	0	2.065866	3.950442	-0.524544
21	1	0	2.031963	3.546465	1.223964
22	1	0	0.505090	3.887965	0.357374
23	8	0	2.947696	-0.544412	0.109215
24	6	0	4.201920	-0.848155	-0.537019
25	1	0	4.944138	-0.856410	0.260239

26	1	0	4.439968	-0.080516	-1.276736
27	1	0	4.150039	-1.823745	-1.025579
28	6	0	-4.209497	0.905405	-0.408146
29	1	0	-4.893582	0.499315	-1.163019
30	1	0	-3.998758	1.951335	-0.635641
31	1	0	-4.691546	0.837396	0.574479
32	6	0	0.377146	-1.216871	1.292251
33	1	0	0.916704	-1.017541	2.214940
34	1	0	1.338894	-3.262220	0.731060
35	8	0	-1.033150	-1.079795	1.471162

SCF Done: E(RB3LYP) = -1010.49431313 A.U. after 1 cycles
Sum of electronic and thermal Free Energies= -1010.264583

endo10m (DATS5pcm.for.log)
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.629395	0.688716	0.349807
2	6	0	1.563182	-0.344939	0.089451
3	6	0	0.251510	-0.070446	0.022648
4	1	0	-0.427796	-0.907844	-0.099580
5	6	0	1.994620	-1.774193	-0.044274
6	6	0	-0.287196	1.314908	0.190514
7	8	0	0.387480	2.187784	0.746266
8	7	0	-1.559181	1.545540	-0.253368
9	6	0	-2.320314	0.618500	-1.087411
10	1	0	-1.634585	-0.027121	-1.645443
11	1	0	-2.854044	1.203685	-1.846283
12	6	0	-3.303495	-0.191137	-0.293604
13	6	0	-3.459283	-0.458474	1.034579
14	6	0	-4.593395	-1.334373	1.140171
15	1	0	-2.848606	-0.078594	1.841364
16	8	0	1.232203	-2.717810	-0.126768
17	8	0	3.214647	0.783549	1.407184
18	8	0	2.883498	1.422712	-0.740924
19	6	0	3.868170	2.463604	-0.571977
20	1	0	3.966323	2.931547	-1.550892
21	1	0	4.821595	2.038785	-0.249973
22	1	0	3.519643	3.187956	0.167885
23	8	0	3.331448	-1.877652	-0.086841
24	6	0	3.857572	-3.213465	-0.227221
25	1	0	4.940219	-3.096876	-0.245311
26	1	0	3.501079	-3.663828	-1.156424
27	1	0	3.549764	-3.830354	0.620049
28	6	0	-2.170213	2.849516	-0.003493
29	1	0	-2.086590	3.497862	-0.884584
30	1	0	-1.663452	3.324360	0.835151
31	1	0	-3.228053	2.709178	0.235532
32	6	0	-5.039494	-1.533961	-0.128180
33	1	0	-5.849556	-2.103467	-0.557602
34	1	0	-5.013748	-1.752438	2.044254
35	8	0	-4.264811	-0.840729	-1.018995

SCF Done: E(RB3LYP) = -1010.49235111 A.U. after 1 cycles
Sum of electronic and thermal Free Energies= -1010.272086

IM-endo-TS (DATS5pcm.log)
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.989506	1.343428	-0.027610
2	6	0	0.690240	-0.097643	-0.183158
3	6	0	-0.732186	-0.432702	-0.420180
4	1	0	-0.738569	-1.418287	-0.900995
5	6	0	1.653885	-1.095420	-0.725944
6	6	0	-1.830888	0.343101	-1.138828
7	8	0	-1.742992	1.075824	-2.112742
8	7	0	-3.012863	-0.053969	-0.544730
9	6	0	-2.862497	-1.040482	0.534767
10	1	0	-2.938904	-2.073292	0.165705
11	1	0	-3.624116	-0.883453	1.304050
12	6	0	-1.450498	-0.718508	0.997117
13	6	0	-1.255940	0.394682	1.966480
14	6	0	-0.019487	0.234877	2.487104

15	1	0	-1.940804	1.220860	2.097542
16	8	0	1.318963	-2.091419	-1.353461
17	8	0	0.105317	2.171908	0.148894
18	8	0	2.294343	1.680373	-0.056216
19	6	0	2.570734	3.082832	0.100048
20	1	0	3.654231	3.174057	0.022043
21	1	0	2.227331	3.438218	1.075284
22	1	0	2.079977	3.663470	-0.685154
23	8	0	2.939675	-0.857095	-0.397732
24	6	0	3.892284	-1.815555	-0.889857
25	1	0	4.864305	-1.455111	-0.552678
26	1	0	3.861523	-1.865286	-1.981160
27	1	0	3.689607	-2.808281	-0.479668
28	6	0	-4.314050	0.255221	-1.104272
29	1	0	-4.767283	-0.628143	-1.573125
30	1	0	-4.178242	1.029900	-1.860181
31	1	0	-4.988891	0.623094	-0.323508
32	6	0	0.500147	-0.956308	1.854729
33	1	0	1.418215	-1.481888	2.087820
34	1	0	0.543041	0.905739	3.122527
35	8	0	-0.547667	-1.735709	1.470286

SCF Done: E(RB3LYP) = -1010.44985187 A.U. after 1 cycles
Sum of electronic and thermal Free Energies= -1010.222760

endo9m (DATS5pcm.rev.log)
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.090329	1.300755	0.391819
2	6	0	0.666307	-0.146248	0.116312
3	6	0	-0.768521	-0.292819	-0.433848
4	1	0	-0.699615	-1.029853	-1.242949
5	6	0	1.667006	-0.819994	-0.836334
6	6	0	-1.830249	0.677726	-0.928345
7	8	0	-1.725731	1.734516	-1.533730
8	7	0	-3.019473	0.032126	-0.631212
9	6	0	-2.870041	-1.258283	0.076257
10	1	0	-2.851519	-2.107241	-0.621490
11	1	0	-3.691012	-1.398095	0.786215
12	6	0	-1.515273	-1.009848	0.722895
13	6	0	-1.528884	-0.157956	1.984040
14	6	0	-0.287441	-0.208418	2.467652
15	1	0	-2.378219	0.415611	2.334085
16	8	0	1.520045	-0.893024	-2.039102
17	8	0	0.362922	2.152042	0.853629
18	8	0	2.374500	1.516799	0.058366
19	6	0	2.860191	2.860947	0.260071
20	1	0	3.893390	2.849003	-0.084577
21	1	0	2.809705	3.125391	1.318678
22	1	0	2.265770	3.568081	-0.322398
23	8	0	2.721121	-1.328305	-0.182129
24	6	0	3.737297	-1.937600	-1.004906
25	1	0	4.494260	-2.298958	-0.309850
26	1	0	4.162203	-1.197943	-1.687336
27	1	0	3.314382	-2.764640	-1.579412
28	6	0	-4.304012	0.479956	-1.131398
29	1	0	-4.701245	-0.212700	-1.884615
30	1	0	-4.162286	1.460974	-1.587371
31	1	0	-5.029075	0.561504	-0.313580
32	6	0	0.475920	-1.049493	1.469305
33	1	0	1.385225	-1.552462	1.784619
34	1	0	0.144270	0.319973	3.308015
35	8	0	-0.524818	-2.006512	1.042885

SCF Done: E(RB3LYP) = -1010.46338200 A.U. after 1 cycles
Sum of electronic and thermal Free Energies= -1010.235250

Figure 6
exo10m-H+ (DAHTS2pcm.for.log)
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.400605	1.746038	0.274408

2	6	0	0.757564	0.553695	-0.471443
3	6	0	-0.170378	-0.295055	-1.027761
4	1	0	0.223623	-1.107643	-1.630449
5	6	0	2.211361	0.303968	-0.617008
6	6	0	-1.619294	0.030695	-1.307306
7	8	0	-1.808514	0.874821	-2.183573
8	7	0	-2.580335	-0.661724	-0.661850
9	6	0	-2.290806	-1.758899	0.268664
10	1	0	-2.424590	-2.722420	-0.238166
11	1	0	-3.026813	-1.710036	1.079285
12	6	0	-0.915716	-1.711793	0.844126
13	6	0	0.161310	-2.572768	0.761092
14	6	0	1.129868	-2.109852	1.688420
15	1	0	0.240158	-3.420613	0.094498
16	8	0	3.068387	1.075240	-0.161319
17	8	0	1.289213	2.555889	0.736522
18	8	0	-0.847643	2.007854	0.471160
19	6	0	-1.220950	3.226352	1.188858
20	1	0	-2.307501	3.208403	1.201299
21	1	0	-0.843824	4.092392	0.645068
22	1	0	-0.810480	3.189238	2.197984
23	8	0	2.510854	-0.797150	-1.276822
24	6	0	3.920828	-1.087598	-1.470745
25	1	0	3.939040	-2.019550	-2.031709
26	1	0	4.410387	-1.202891	-0.502647
27	1	0	4.388782	-0.280646	-2.036240
28	6	0	-3.981694	-0.461955	-1.019904
29	1	0	-4.391558	-1.368910	-1.478898
30	1	0	-4.042395	0.361784	-1.729690
31	1	0	-4.563434	-0.222516	-0.123972
32	6	0	0.576100	-1.015169	2.297109
33	1	0	0.917420	-0.348379	3.074986
34	1	0	2.107350	-2.526841	1.883175
35	8	0	-0.677319	-0.784109	1.826045
36	1	0	2.213567	2.164386	0.481278

SCF Done: E(RB3LYP) = -1010.90810456 A.U. after 2 cycles
Sum of electronic and thermal Free Energies= -1010.671717

H+IM-exo-TS1 (DAHTS2pcm.log)
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.478948	1.741740	0.228928
2	6	0	0.776998	0.490892	-0.408882
3	6	0	-0.212545	-0.395857	-0.857304
4	1	0	0.161328	-1.201436	-1.483201
5	6	0	2.205327	0.206495	-0.623113
6	6	0	-1.617324	0.034124	-1.261847
7	8	0	-1.738519	0.898238	-2.124152
8	7	0	-2.621146	-0.656802	-0.679999
9	6	0	-2.303942	-1.743666	0.239209
10	1	0	-2.385252	-2.715496	-0.263848
11	1	0	-3.022779	-1.735935	1.065885
12	6	0	-0.912961	-1.584075	0.778446
13	6	0	0.151273	-2.494507	0.856122
14	6	0	1.028390	-2.025251	1.844815
15	1	0	0.283148	-3.355179	0.214562
16	8	0	3.107796	1.000316	-0.312496
17	8	0	1.397575	2.596831	0.545714
18	8	0	-0.756006	2.037847	0.494558
19	6	0	-1.064515	3.329720	1.097320
20	1	0	-2.146632	3.328017	1.202000
21	1	0	-0.733904	4.128794	0.433388
22	1	0	-0.573806	3.405304	2.068043
23	8	0	2.450276	-0.967017	-1.187044
24	6	0	3.839046	-1.286256	-1.455972
25	1	0	3.816042	-2.268181	-1.924547
26	1	0	4.402744	-1.312345	-0.522045
27	1	0	4.266331	-0.542315	-2.130137
28	6	0	-4.005929	-0.470778	-1.089865
29	1	0	-4.382483	-1.369140	-1.592613
30	1	0	-4.046874	0.373158	-1.777981
31	1	0	-4.630529	-0.265030	-0.214545
32	6	0	0.430517	-0.899728	2.374470
33	1	0	0.724366	-0.220202	3.161580
34	1	0	1.980665	-2.442294	2.138264
35	8	0	-0.763794	-0.666766	1.806106

36	1	0	2.297339	2.177183	0.269741

SCF Done: E(RB3LYP) = -1010.90724029 A.U. after 1 cycles
Sum of electronic and thermal Free Energies= -1010.669311

H+IM-exo-Int (DAHTS2pcm.rev.log)
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.630668	1.733317	0.262107
2	6	0	0.834282	0.473353	-0.315414
3	6	0	-0.278174	-0.441277	-0.659651
4	1	0	0.077644	-1.143692	-1.419852
5	6	0	2.203915	0.118679	-0.623391
6	6	0	-1.580373	0.166097	-1.235657
7	8	0	-1.615720	1.087198	-2.033738
8	7	0	-2.637253	-0.550532	-0.767689
9	6	0	-2.284820	-1.686803	0.061520
10	1	0	-2.306621	-2.627489	-0.504607
11	1	0	-2.954752	-1.784277	0.920587
12	6	0	-0.849994	-1.389716	0.523134
13	6	0	0.089610	-2.468269	0.845076
14	6	0	0.675414	-2.206122	2.053601
15	1	0	0.313690	-3.284916	0.170439
16	8	0	3.183246	0.864481	-0.433966
17	8	0	1.597690	2.588209	0.485624
18	8	0	-0.581952	2.099338	0.615149
19	6	0	-0.786902	3.440106	1.127564
20	1	0	-1.856436	3.501539	1.318695
21	1	0	-0.485160	4.175525	0.380118
22	1	0	-0.219431	3.581853	2.048751
23	8	0	2.349359	-1.115670	-1.128640
24	6	0	3.693069	-1.517164	-1.475554
25	1	0	3.595382	-2.526539	-1.872752
26	1	0	4.330787	-1.510621	-0.589294
27	1	0	4.104710	-0.844202	-2.230123
28	6	0	-3.996797	-0.362927	-1.244450
29	1	0	-4.323324	-1.224205	-1.838848
30	1	0	-4.009905	0.532258	-1.867251
31	1	0	-4.680731	-0.233581	-0.399483
32	6	0	0.044387	-1.041816	2.534809
33	1	0	0.198938	-0.496380	3.459047
34	1	0	1.454067	-2.756323	2.561644
35	8	0	-0.882159	-0.591676	1.739486
36	1	0	2.452484	2.135003	0.163277

SCF Done: E(RB3LYP) = -1010.91463226 A.U. after 1 cycles
Sum of electronic and thermal Free Energies= -1010.675194

H+IM-exo-TS2 (DAHTS4pcm.log)
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.424829	1.713285	0.232105
2	6	0	0.768249	0.302645	0.002895
3	6	0	-0.295253	-0.632402	-0.540100
4	1	0	0.146250	-1.291739	-1.289936
5	6	0	2.168606	0.130241	-0.498203
6	6	0	-1.594324	-0.078478	-1.148066
7	8	0	-1.659845	0.792313	-2.005716
8	7	0	-2.634182	-0.782133	-0.620769
9	6	0	-2.275269	-1.805324	0.358167
10	1	0	-2.363279	-2.813412	-0.066495
11	1	0	-2.916465	-1.747128	1.243724
12	6	0	-0.832705	-1.484862	0.702472
13	6	0	0.233049	-2.467997	1.070051
14	6	0	1.166262	-1.764866	1.741523
15	1	0	0.290064	-3.485602	0.705362
16	8	0	3.028572	1.019909	-0.426367
17	8	0	1.306229	2.650111	0.239704
18	8	0	-0.796547	2.009678	0.510844
19	6	0	-1.156791	3.404104	0.769761
20	1	0	-2.219045	3.368825	0.996244
21	1	0	-0.960564	3.992908	-0.126122
22	1	0	-0.579750	3.775340	1.616441

23	8	0	2.421932	-1.067249	-0.982364
24	6	0	3.774669	-1.319615	-1.453627
25	1	0	3.758417	-2.348016	-1.807750
26	1	0	4.480014	-1.197534	-0.630563
27	1	0	4.014553	-0.629045	-2.263050
28	6	0	-4.005722	-0.618834	-1.067424
29	1	0	-4.372845	-1.538562	-1.537737
30	1	0	-4.028505	0.193589	-1.794542
31	1	0	-4.655218	-0.371367	-0.220642
32	6	0	0.618433	-0.404531	1.860481
33	1	0	0.984812	0.350810	2.548200
34	1	0	2.153140	-2.071150	2.060380
35	8	0	-0.734103	-0.500507	1.756921
36	1	0	2.213579	2.212770	-0.012512

SCF Done: E(RB3LYP) = -1010.89679705 A.U. after 1 cycles
Sum of electronic and thermal Free Energies= -1010.655614

exo9m-H+ (DAHTS4pcm.for.log)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.305792	1.709704	0.326335
2	6	0	0.767612	0.275317	0.166306
3	6	0	-0.250913	-0.653823	-0.553997
4	1	0	0.245437	-1.214887	-1.348108
5	6	0	2.172342	0.238434	-0.434569
6	6	0	-1.538981	-0.062200	-1.133960
7	8	0	-1.602942	0.904857	-1.886382
8	7	0	-2.570205	-0.837101	-0.703931
9	6	0	-2.204076	-1.917081	0.215124
10	1	0	-2.262736	-2.894975	-0.278682
11	1	0	-2.864839	-1.929254	1.088093
12	6	0	-0.775966	-1.578980	0.605162
13	6	0	0.313208	-2.560432	0.970830
14	6	0	1.235737	-1.833965	1.615344
15	1	0	0.366722	-3.591943	0.646246
16	8	0	2.898490	1.235593	-0.530575
17	8	0	1.069626	2.710605	0.117421
18	8	0	-0.883453	1.905964	0.756761
19	6	0	-1.372758	3.279719	0.919461
20	1	0	-2.367183	3.159787	1.340135
21	1	0	-1.407273	3.751632	-0.062061
22	1	0	-0.711139	3.818943	1.596475
23	8	0	2.549327	-0.954072	-0.817960
24	6	0	3.889359	-1.087320	-1.377253
25	1	0	3.981473	-2.142809	-1.622095
26	1	0	4.626474	-0.787970	-0.631612
27	1	0	3.973743	-0.465022	-2.268632
28	6	0	-3.939762	-0.654954	-1.149033
29	1	0	-4.295412	-1.547487	-1.676498
30	1	0	-3.964386	0.200469	-1.825100
31	1	0	-4.597550	-0.464843	-0.293687
32	6	0	0.665024	-0.435144	1.696011
33	1	0	0.995575	0.229809	2.491271
34	1	0	2.220992	-2.124964	1.954152
35	8	0	-0.724535	-0.651197	1.712001
36	1	0	1.999727	2.333568	-0.187074

SCF Done: E(RB3LYP) = -1010.89895776 A.U. after 1 cycles
Sum of electronic and thermal Free Energies= -1010.657524

endo10m-H+ (DAHTS3pcm.for.log)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.578682	1.754622	0.300853
2	6	0	0.832881	0.559381	-0.499815
3	6	0	-0.153893	-0.173082	-1.085370
4	1	0	0.167877	-1.054145	-1.636468
5	6	0	2.265793	0.177859	-0.637637
6	6	0	-1.585517	0.228305	-1.332685
7	8	0	-1.738888	1.182572	-2.097503
8	7	0	-2.570305	-0.534321	-0.814575
9	6	0	-2.317495	-1.748558	-0.013135

10	1	0	-2.147420	-2.611109	-0.669030
11	1	0	-3.240014	-1.941428	0.541732
12	6	0	-1.176673	-1.620953	0.943280
13	6	0	-0.997988	-0.916439	2.103852
14	6	0	0.304484	-1.241663	2.585018
15	1	0	-1.713670	-0.242277	2.553522
16	8	0	3.177767	0.868333	-0.162479
17	8	0	1.534361	2.467458	0.775966
18	8	0	-0.640386	2.086291	0.542657
19	6	0	-0.914523	3.298437	1.320623
20	1	0	-1.999026	3.349230	1.362609
21	1	0	-0.494280	4.157945	0.799005
22	1	0	-0.478935	3.190394	2.313765
23	8	0	2.472102	-0.932521	-1.309892
24	6	0	3.853985	-1.342301	-1.504882
25	1	0	3.792535	-2.254163	-2.094559
26	1	0	4.320023	-1.530551	-0.536701
27	1	0	4.395452	-0.562073	-2.041186
28	6	0	-3.952643	-0.293151	-1.227220
29	1	0	-4.314818	-1.118916	-1.850177
30	1	0	-3.987463	0.632013	-1.800349
31	1	0	-4.592603	-0.205218	-0.344053
32	6	0	0.825057	-2.141299	1.695635
33	1	0	1.756989	-2.683516	1.645713
34	1	0	0.785488	-0.874983	3.480877
35	8	0	-0.061760	-2.392795	0.699865
36	1	0	2.423542	2.007389	0.497305

SCF Done: E(RB3LYP) = -1010.90218060 A.U. after 1 cycles
Sum of electronic and thermal Free Energies= -1010.667349

H+IM-endo-TS1 (DAHTS3pcm.log)
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.814316	1.730352	0.148520
2	6	0	0.880299	0.421298	-0.426783
3	6	0	-0.262002	-0.322152	-0.751643
4	1	0	-0.026937	-1.269352	-1.234838
5	6	0	2.233517	-0.103671	-0.669606
6	6	0	-1.585461	0.244403	-1.244072
7	8	0	-1.616721	1.195453	-2.015934
8	7	0	-2.650987	-0.484683	-0.828121
9	6	0	-2.389675	-1.649668	0.016260
10	1	0	-2.188631	-2.552070	-0.576359
11	1	0	-3.272994	-1.843043	0.632113
12	6	0	-1.192335	-1.323719	0.872298
13	6	0	-1.114921	-0.451890	1.968791
14	6	0	0.004524	-0.827235	2.720732
15	1	0	-1.780296	0.381360	2.145259
16	8	0	3.258870	0.569244	-0.475752
17	8	0	1.862089	2.461552	0.353154
18	8	0	-0.344053	2.193032	0.511211
19	6	0	-0.427780	3.539760	1.068079
20	1	0	-1.486504	3.685141	1.267811
21	1	0	-0.063943	4.257938	0.333006
22	1	0	0.159459	3.592810	1.985299
23	8	0	2.270946	-1.345658	-1.129047
24	6	0	3.579250	-1.895492	-1.425461
25	1	0	3.383436	-2.896455	-1.805014
26	1	0	4.181420	-1.934368	-0.516174
27	1	0	4.078015	-1.283485	-2.178665
28	6	0	-3.982789	-0.271617	-1.377034
29	1	0	-4.262744	-1.089674	-2.051016
30	1	0	-3.972644	0.665000	-1.934227
31	1	0	-4.716085	-0.210577	-0.566941
32	6	0	0.511274	-1.958300	2.105301
33	1	0	1.362355	-2.587493	2.323589
34	1	0	0.400699	-0.354609	3.607864
35	8	0	-0.220861	-2.306348	1.042011
36	1	0	2.670826	1.901038	0.047716

SCF Done: E(RB3LYP) = -1010.89913209 A.U. after 1 cycles
Sum of electronic and thermal Free Energies= -1010.661926

H+IM-endo-Int (DAHTS3pcm.rev.log)
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.966067	1.609236	0.259653
2	6	0	0.983334	0.309669	-0.239253
3	6	0	-0.263149	-0.439799	-0.544281
4	1	0	0.023047	-1.336753	-1.105673
5	6	0	2.287734	-0.250032	-0.525614
6	6	0	-1.341226	0.255645	-1.412275
7	8	0	-1.126002	1.099585	-2.263520
8	7	0	-2.549056	-0.294597	-1.091708
9	6	0	-2.466544	-1.369774	-0.119572
10	1	0	-2.360411	-2.357316	-0.588249
11	1	0	-3.339634	-1.382364	0.537344
12	6	0	-1.157882	-1.020599	0.634609
13	6	0	-1.329681	-0.184100	1.837105
14	6	0	-0.739003	-0.798322	2.903516
15	1	0	-1.850223	0.762909	1.826684
16	8	0	3.360122	0.362415	-0.353926
17	8	0	2.037308	2.335154	0.464808
18	8	0	-0.195996	2.157666	0.578112
19	6	0	-0.214156	3.540326	1.018223
20	1	0	-1.263685	3.757517	1.207776
21	1	0	0.175897	4.184814	0.229080
22	1	0	0.376961	3.654685	1.927970
23	8	0	2.268393	-1.502955	-0.999550
24	6	0	3.545945	-2.087364	-1.331489
25	1	0	3.314205	-3.081420	-1.711575
26	1	0	4.176250	-2.152000	-0.442083
27	1	0	4.048728	-1.490593	-2.095128
28	6	0	-3.769695	-0.037094	-1.838831
29	1	0	-4.039371	-0.899470	-2.459716
30	1	0	-3.590322	0.826263	-2.480491
31	1	0	-4.593880	0.180195	-1.152365
32	6	0	-0.241857	-2.023540	2.408887
33	1	0	0.300430	-2.811930	2.919304
34	1	0	-0.666769	-0.459224	3.926852
35	8	0	-0.499904	-2.215089	1.151469
36	1	0	2.821492	1.747138	0.179021

SCF Done: E(RB3LYP) = -1010.91040111 A.U. after 1 cycles
Sum of electronic and thermal Free Energies= -1010.671936

I-2. Crystallographic data

X-ray Structure Report

for

Compound **9a**
(CCDC 1419386)

Experimental

Data Collection

A colorless unknown crystal of $C_{17}H_{21}NO_6$ having approximate dimensions of 0.500 x 0.400 x 0.200 mm was mounted on a glass fiber. All measurements were made on a Rigaku Mercury70 diffractometer using graphite monochromated Mo-Kα radiation.

The crystal-to-detector distance was 55.05 mm.

Cell constants and an orientation matrix for data collection corresponded to a primitive monoclinic cell with dimensions:

a = 10.6010(7) Å
b = 9.3435(5) Å β = 102.999(3)^o
c = 17.1096(10) Å
V = 1651.3(2) Å^3

For Z = 4 and F.W. = 335.36, the calculated density is 1.349 g/cm^3. Based on the reflection conditions of:

0k0: k = 2n

packing considerations, a statistical analysis of intensity distribution, and the successful solution and refinement of the structure, the space group was determined to be:

$P2_1$ (#4)

The data were collected at a temperature of -119 $\pm$ 1^{o}C to a maximum 2θ value of 54.9^o. A total of 1800 oscillation images were collected. A sweep of data was done using ω oscillations from -65.0 to 115.0^o in 0.3^o steps. The exposure rate was 50.0 [sec./^{o}]. The detector swing angle was 24.98^o. A second sweep was performed using ω oscillations from -65.0 to 115.0^o in 0.3^o steps. The exposure rate was 50.0 [sec./^{o}]. The detector swing angle was 24.98^o. Another sweep was performed using ω oscillations from -65.0 to 115.0^o in 0.3^o steps. The exposure rate was 50.0 [sec./^{o}]. The detector

swing angle was 24.98°. The crystal-to-detector distance was 55.05 mm. Readout was performed in the 0.137 mm pixel mode.

Data Reduction

Of the 16406 reflections that were collected, 7425 were unique (R_{int} = 0.0198); equivalent reflections were merged. Data were collected and processed using CrystalClear (Rigaku).

The linear absorption coefficient, μ, for Mo-Kα radiation is 1.023 cm^{-1}. An empirical absorption correction was applied which resulted in transmission factors ranging from 0.878 to 0.980. The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

The structure was solved by direct methods[2] and expanded using Fourier techniques. The non-hydrogen atoms were refined anisotropically. Some hydrogen atoms were refined isotropically and the rest were refined using the riding model.The final cycle of full-matrix least-squares refinement[3] on F^2 was based on 7425 observed reflections and 561 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R1 = \Sigma \, ||Fo| - |Fc|| \, / \, \Sigma \, |Fo| = 0.0475$$

$$wR2 = [\Sigma \, (w \, (Fo^2 - Fc^2)^2) / \Sigma \, w(Fo^2)^2]^{1/2} = 0.1364$$

The standard deviation of an observation of unit weight[4] was 1.05. Unit weights were used. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.65 and -0.33 $e^-/Å^3$, respectively. The absolute structure was deduced based on Flack parameter, 0.1(7), using 3459 Friedel pairs.[5]

Neutral atom scattering factors were taken from Cromer and Waber[6]. Anomalous dispersion effects were included in Fcalc[7]; the values for Δf' and Δf'' were those of Creagh and McAuley[8]. The values for the mass attenuation coefficients are those of Creagh and Hubbell[9]. All calculations were performed using the CrystalStructure[10] crystallographic software package except for refinement, which was performed using SHELXL-97[11].

References

(1) CrystalClear: Rigaku Corporation, 1999. CrystalClear Software User's Guide, Molecular Structure Corporation, (c) 2000.J.W.Pflugrath (1999) Acta Cryst. D55, 1718-1725.

(2) SHELX97: Sheldrick, G.M. (2008). Acta Cryst. A64, 112-122.

(3) Least Squares function minimized: (SHELXL97)

$\Sigma w(F_o^2-F_c^2)^2$ where w = Least Squares weights.

(4) Standard deviation of an observation of unit weight:

$[\Sigma w(F_o^2-F_c^2)^2/(N_o-N_v)]^{1/2}$

where: N_o = number of observations
N_v = number of variables

(5) Flack, H. D. (1983), Acta Cryst. A39, 876-881.

(6) Cromer, D. T. & Waber, J. T.; "International Tables for X-ray Crystallography", Vol. IV, The Kynoch Press, Birmingham, England, Table 2.2 A (1974).

(7) Ibers, J. A. & Hamilton, W. C.; Acta Crystallogr., 17, 781 (1964).

(8) Creagh, D. C. & McAuley, W.J .; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.6.8, pages 219-222 (1992).

(9) Creagh, D. C. & Hubbell, J.H..; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.4.3, pages 200-206 (1992).

(10) CrystalStructure 4.0: Crystal Structure Analysis Package, Rigaku Corporation (2000-2010). Tokyo 196-8666, Japan.

(11) SHELX97: Sheldrick, G.M. (2008). Acta Cryst. A64, 112-122.

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{17}H_{21}NO_6$
Formula Weight	335.36
Crystal Color, Habit	colorless, unknown
Crystal Dimensions	0.500 X 0.400 X 0.200 mm
Crystal System	monoclinic
Lattice Type	Primitive
Lattice Parameters	a = 10.6010(7) Å b = 9.3435(5) Å c = 17.1096(10) Å β = 102.999(3) ^{o} V = 1651.3(2) $Å^3$
Space Group	$P2_1$ (#4)
Z value	4
D_{calc}	1.349 g/cm^3
F_{000}	712.00
μ(MoKα)	1.023 cm^{-1}

B. Intensity Measurements

Diffractometer	Mercury70
Radiation	MoKα (λ = 0.71070 Å) graphite monochromated
Voltage, Current	50kV, 40mA
Temperature	-119.8^{o}C
Detector Aperture	70 x 70 mm
Data Images	1800 exposures
ω oscillation Range	-65.0 - 115.0^{o}
Exposure Rate	50.0 sec./^{o}
Detector Swing Angle	24.98^{o}
ω oscillation Range	-65.0 - 115.0^{o}
Exposure Rate	50.0 sec./^{o}
Detector Swing Angle	24.98^{o}
ω oscillation Range	-65.0 - 115.0^{o}
Exposure Rate	50.0 sec./^{o}
Detector Swing Angle	24.98^{o}
Detector Position	55.05 mm
Pixel Size	0.137 mm
$2\theta_{max}$	54.9^{o}

No. of Reflections Measured	Total: 16406 Unique: 7425 (R_{int} = 0.0198) Friedel pairs: 3459
Corrections	Lorentz-polarization Absorption (trans. factors: 0.878 - 0.980)

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SHELX97)
Refinement	Full-matrix least-squares on F^2
Function Minimized	Σ w $(Fo^2 - Fc^2)^2$
Least Squares Weights	$w = 1/ [\sigma^2(Fo^2) + (0.0808 \cdot P)^2 + 0.1671 \cdot P]$ where $P = (Max(Fo^2,0) + 2Fc^2)/3$
$2\theta_{max}$ cutoff	54.9^o
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (All reflections)	7425
No. Variables	561
Reflection/Parameter Ratio	13.24
Residuals: R1 (I>2.00σ(I))	0.0475
Residuals: R (All reflections)	0.0526
Residuals: wR2 (All reflections)	0.1364
Goodness of Fit Indicator	1.048
Flack Parameter (Friedel pairs = 3459)	0.1(7)
Max Shift/Error in Final Cycle	0.001
Maximum peak in Final Diff. Map	0.65 $e^-/Å^3$
Minimum peak in Final Diff. Map	-0.33 $e^-/Å^3$

Table 1. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
O1	0.99405(13)	-0.0125(2)	0.53753(8)	2.03(3)
O2	0.69613(13)	0.1422(2)	0.37923(9)	2.90(3)
O3	0.7241(2)	-0.1090(2)	0.51551(10)	2.96(3)
O4	0.59760(13)	0.0709(2)	0.53953(9)	2.61(3)
O5	0.7779(2)	0.3467(2)	0.62119(9)	3.02(3)
O6	0.7904(2)	0.1485(2)	0.69701(8)	3.09(3)
O7	0.50998(12)	0.4628(2)	0.96310(8)	2.01(3)
O8	0.80994(13)	0.6396(2)	1.11743(9)	2.69(3)
O9	0.7783(2)	0.3707(2)	0.99244(10)	2.74(3)
O10	0.90342(13)	0.5331(2)	0.94992(9)	2.70(3)
O11	0.7322(2)	0.8139(2)	0.87511(10)	3.09(3)
O12	0.7123(2)	0.6141(2)	0.79971(8)	2.81(3)
N1	0.9105(2)	0.1213(2)	0.37626(9)	2.18(3)
N2	0.5973(2)	0.6085(2)	1.12272(9)	2.24(3)
C1	1.0105(2)	0.1326(2)	0.51092(11)	2.00(3)
C2	0.8690(2)	0.1878(2)	0.49892(11)	1.84(3)
C3	0.8229(2)	0.1137(2)	0.56846(11)	1.94(3)
C4	0.9504(2)	0.0274(2)	0.60770(11)	2.10(4)
C5	1.0527(2)	0.1363(3)	0.64625(12)	2.43(4)
C6	1.0906(2)	0.1997(3)	0.58576(12)	2.29(4)
C7	0.8107(2)	0.1462(3)	0.41254(11)	2.16(3)
C8	1.0396(2)	0.1324(2)	0.42860(11)	2.13(4)
C9	0.7102(2)	0.0110(2)	0.53804(11)	2.07(4)
C10	0.7920(2)	0.2188(3)	0.62941(12)	2.30(4)
C11	0.8889(3)	0.1103(3)	0.28941(12)	2.73(4)
C12	0.8710(3)	0.2581(3)	0.25051(13)	3.30(5)
C13	0.9268(3)	0.3038(4)	0.1945(2)	3.85(5)
C14	0.4814(2)	-0.0125(3)	0.5033(2)	3.14(5)
C15	0.3755(3)	0.0338(3)	0.5420(2)	3.53(5)
C16	0.7853(3)	0.2358(4)	0.7675(2)	4.47(6)
C17	0.8333(4)	0.1504(4)	0.8373(2)	5.60(7)
C18	0.4936(2)	0.6081(2)	0.98829(11)	1.92(3)
C19	0.6340(2)	0.6658(2)	0.99777(11)	1.82(3)
C20	0.6797(2)	0.5869(2)	0.92961(11)	1.89(3)
C21	0.5517(2)	0.5003(2)	0.89207(11)	2.03(4)
C22	0.4487(2)	0.6081(3)	0.85298(12)	2.26(4)
C23	0.4111(2)	0.6734(3)	0.91316(12)	2.23(4)

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
C24	0.6956(2)	0.6349(2)	1.08491(11)	2.05(3)
C25	0.4674(2)	0.6114(3)	1.07162(11)	2.13(3)
C26	0.7914(2)	0.4838(2)	0.96127(11)	1.93(3)
C27	0.7128(2)	0.6874(2)	0.86707(12)	2.13(4)
C28	0.6207(3)	0.6049(3)	1.21010(12)	2.74(4)
C29	0.6315(3)	0.7535(3)	1.24585(12)	3.01(4)
C30	0.5712(3)	0.8003(4)	1.3007(2)	4.05(6)
C31	1.0177(2)	0.4463(3)	0.9834(2)	3.02(4)
C32	1.1273(2)	0.5052(3)	0.9507(2)	3.18(5)
C33	0.7294(3)	0.6941(4)	0.7299(2)	3.81(5)
C34	0.6112(3)	0.7642(5)	0.6885(2)	6.06(9)

$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$

Table 2. Atomic coordinates and B_{iso} involving hydrogen atoms

atom	x	y	z	B_{iso}
H1	0.864(3)	0.286(3)	0.503(2)	2.6(5)
H2	0.938(3)	-0.062(3)	0.637(2)	3.2(6)
H3	1.076(3)	0.159(3)	0.703(2)	2.3(5)
H4	1.145(3)	0.271(3)	0.587(2)	3.0(6)
H5	1.088(2)	0.058(3)	0.4234(13)	1.5(4)
H6	1.088(3)	0.227(3)	0.419(2)	2.4(5)
H7	0.809(3)	0.050(4)	0.269(2)	4.3(7)
H8	0.951(3)	0.050(3)	0.276(2)	3.2(6)
H9	0.812(4)	0.320(4)	0.271(2)	5.1(8)
H10	0.994(3)	0.227(4)	0.174(2)	4.6(7)
H11	0.912(3)	0.412(4)	0.170(2)	3.8(6)
H12	0.461(4)	0.002(5)	0.443(2)	6.0(9)
H13	0.512(3)	-0.122(4)	0.517(2)	3.8(6)
H14	0.366(4)	0.130(6)	0.533(3)	8.0(11)
H15	0.310(4)	-0.025(4)	0.514(2)	5.2(8)
H16	0.397(4)	0.014(5)	0.594(3)	6.1(10)
H16A	0.8392	0.3226	0.7687	5.36
H16B	0.6952	0.2658	0.7657	5.36
H17A	0.8223	0.2023	0.8851	6.72
H17B	0.9254	0.1303	0.8418	6.72
H17C	0.7852	0.0601	0.8328	6.72
H18	0.634(3)	0.762(3)	0.990(2)	2.0(5)
H19	0.567(3)	0.420(3)	0.861(2)	2.6(5)
H20	0.426(3)	0.635(3)	0.797(2)	3.3(6)
H21	0.361(3)	0.750(4)	0.914(2)	3.9(7)
H22	0.418(3)	0.527(3)	1.082(2)	2.7(5)
H23	0.420(3)	0.693(3)	1.079(2)	2.6(5)
H24	0.549(3)	0.532(3)	1.225(2)	3.0(6)
H25	0.694(3)	0.555(4)	1.232(2)	3.6(6)
H26	0.696(3)	0.814(4)	1.220(2)	4.3(7)
H27	0.507(3)	0.736(4)	1.317(2)	4.1(7)
H28	0.581(3)	0.893(4)	1.326(2)	4.4(7)
H29	0.993(3)	0.344(4)	0.968(2)	5.0(8)
H30	1.034(3)	0.466(4)	1.043(2)	3.5(6)
H31	1.113(3)	0.480(4)	0.891(2)	5.0(8)
H32	1.140(3)	0.606(4)	0.962(2)	3.6(6)
H33A	0.7977	0.7671	0.7471	4.57

Table 2. Atomic coordinates and B_{iso} involving hydrogens/B_{eq} (continued)

atom	x	y	z	B_{eq}
H33B	0.7588	0.6281	0.6924	4.57
H34A	0.5848	0.8342	0.7244	7.27
H34B	0.5427	0.6927	0.6724	7.27
H34C	0.6263	0.8132	0.6408	7.27
H33	1.205(3)	0.446(4)	0.978(2)	3.7(6)

Table 3. Anisotropic displacement parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O1	0.0269(7)	0.0225(8)	0.0280(7)	0.0052(6)	0.0069(6)	0.0031(5)
O2	0.0211(7)	0.0535(10)	0.0329(8)	-0.0032(7)	0.0001(6)	0.0035(7)
O3	0.0311(8)	0.0305(9)	0.0523(10)	-0.0050(6)	0.0123(7)	-0.0062(7)
O4	0.0208(7)	0.0370(9)	0.0410(8)	-0.0022(6)	0.0062(6)	-0.0076(7)
O5	0.0442(9)	0.0287(9)	0.0432(9)	0.0077(7)	0.0123(7)	-0.0047(7)
O6	0.0490(9)	0.0416(10)	0.0284(8)	0.0110(8)	0.0116(7)	0.0006(7)
O7	0.0252(7)	0.0217(8)	0.0296(7)	-0.0041(5)	0.0063(6)	-0.0026(5)
O8	0.0234(7)	0.0394(9)	0.0355(8)	0.0019(6)	-0.0017(6)	-0.0022(7)
O9	0.0297(8)	0.0244(8)	0.0517(9)	0.0029(6)	0.0131(7)	0.0069(7)
O10	0.0197(7)	0.0350(9)	0.0479(9)	0.0028(6)	0.0072(6)	0.0116(7)
O11	0.0448(9)	0.0290(9)	0.0443(9)	-0.0100(7)	0.0116(7)	0.0044(7)
O12	0.0364(8)	0.0427(10)	0.0289(7)	0.0008(7)	0.0100(6)	0.0024(7)
N1	0.0240(8)	0.0324(9)	0.0254(8)	-0.0007(7)	0.0032(6)	-0.0006(7)
N2	0.0265(9)	0.0315(9)	0.0261(8)	-0.0010(7)	0.0034(7)	0.0009(7)
C1	0.0204(9)	0.0247(10)	0.0303(10)	0.0009(7)	0.0046(7)	0.0017(7)
C2	0.0186(8)	0.0215(10)	0.0290(9)	-0.0003(7)	0.0043(7)	0.0010(7)
C3	0.0216(9)	0.0241(10)	0.0279(9)	0.0014(7)	0.0057(7)	0.0011(7)
C4	0.0243(10)	0.0287(11)	0.0260(9)	0.0036(7)	0.0037(7)	0.0015(7)
C5	0.0235(9)	0.0362(12)	0.0296(10)	0.0038(8)	-0.0002(8)	-0.0025(8)
C6	0.0195(9)	0.0314(11)	0.0344(11)	-0.0004(8)	0.0021(8)	-0.0023(8)
C7	0.0248(9)	0.0280(10)	0.0283(9)	0.0013(8)	0.0040(7)	0.0049(8)
C8	0.0220(9)	0.0277(10)	0.0311(10)	0.0036(8)	0.0056(7)	0.0019(8)
C9	0.0222(9)	0.0305(10)	0.0262(9)	-0.0027(8)	0.0058(7)	0.0008(8)
C10	0.0245(9)	0.0344(12)	0.0277(9)	0.0004(8)	0.0041(8)	-0.0021(8)
C11	0.0332(11)	0.0418(12)	0.0276(10)	-0.0033(10)	0.0043(9)	-0.0030(9)
C12	0.0353(13)	0.060(2)	0.0272(10)	-0.0012(11)	0.0010(9)	0.0024(10)
C13	0.049(2)	0.054(2)	0.0394(13)	-0.0124(12)	0.0004(11)	0.0040(11)
C14	0.0257(11)	0.050(2)	0.0420(13)	-0.0084(10)	0.0044(9)	-0.0101(11)
C15	0.0255(11)	0.050(2)	0.058(2)	-0.0062(10)	0.0075(11)	-0.0131(13)
C16	0.075(2)	0.063(2)	0.0331(12)	0.027(2)	0.0141(12)	-0.0074(12)
C17	0.109(3)	0.059(2)	0.045(2)	0.007(2)	0.018(2)	-0.008(2)
C18	0.0194(8)	0.0214(9)	0.0319(10)	0.0003(7)	0.0054(7)	-0.0018(7)
C19	0.0187(8)	0.0190(9)	0.0308(10)	-0.0017(7)	0.0046(7)	-0.0001(7)
C20	0.0202(9)	0.0224(10)	0.0288(9)	-0.0006(7)	0.0049(7)	0.0008(7)
C21	0.0244(9)	0.0244(10)	0.0279(10)	-0.0037(7)	0.0053(8)	-0.0033(7)
C22	0.0193(9)	0.0325(11)	0.0314(10)	-0.0028(8)	0.0004(8)	0.0002(8)
C23	0.0202(9)	0.0303(11)	0.0332(10)	0.0001(8)	0.0037(8)	0.0010(8)

Table 3. Anisotropic displacement parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C24	0.0243(9)	0.0219(9)	0.0300(9)	-0.0001(7)	0.0030(7)	-0.0032(7)
C25	0.0240(10)	0.0259(10)	0.0307(10)	-0.0020(8)	0.0057(8)	-0.0012(8)
C26	0.0207(9)	0.0247(10)	0.0272(9)	0.0010(7)	0.0038(7)	-0.0015(7)
C27	0.0214(9)	0.0290(10)	0.0307(10)	-0.0011(7)	0.0057(7)	0.0029(8)
C28	0.0391(12)	0.0376(11)	0.0263(10)	0.0043(10)	0.0048(9)	0.0062(9)
C29	0.0385(13)	0.0464(13)	0.0265(10)	0.0069(10)	0.0014(9)	0.0005(9)
C30	0.060(2)	0.058(2)	0.0328(12)	0.025(2)	0.0046(12)	-0.0001(12)
C31	0.0226(10)	0.0362(12)	0.054(2)	0.0040(9)	0.0036(9)	0.0136(10)
C32	0.0225(10)	0.0429(13)	0.056(2)	0.0065(9)	0.0100(10)	0.0094(11)
C33	0.0409(13)	0.070(2)	0.0367(12)	-0.0077(12)	0.0152(10)	0.0085(11)
C34	0.068(2)	0.110(3)	0.049(2)	-0.013(2)	0.007(2)	0.038(2)

The general temperature factor expression: $\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

Table 4. Fragment Analysis

fragment: 1

O(1)	O(2)	O(3)	O(4)	O(5)
O(6)	N(1)	C(1)	C(2)	C(3)
C(4)	C(5)	C(6)	C(7)	C(8)
C(9)	C(10)	C(11)	C(12)	C(13)
C(14)	C(15)	C(16)	C(17)	

fragment: 2

O(7)	O(8)	O(9)	O(10)	O(11)
O(12)	N(2)	C(18)	C(19)	C(20)
C(21)	C(22)	C(23)	C(24)	C(25)
C(26)	C(27)	C(28)	C(29)	C(30)
C(31)	C(32)	C(33)	C(34)	

Table 5. Bond lengths (Å)

atom	atom	distance	atom	atom	distance
O1	C1	1.453(3)	O1	C4	1.430(3)
O2	C7	1.221(3)	O3	C9	1.206(3)
O4	C9	1.324(3)	O4	C14	1.472(3)
O5	C10	1.208(3)	O6	C10	1.334(3)
O6	C16	1.467(4)	O7	C18	1.447(3)
O7	C21	1.427(3)	O8	C24	1.215(3)
O9	C26	1.205(3)	O10	C26	1.329(3)
O10	C31	1.463(3)	O11	C27	1.202(3)
O12	C27	1.340(3)	O12	C33	1.454(4)
N1	C7	1.361(3)	N1	C8	1.461(3)
N1	C11	1.455(3)	N2	C24	1.367(3)
N2	C25	1.456(3)	N2	C28	1.460(3)
C1	C2	1.556(3)	C1	C6	1.505(3)
C1	C8	1.508(3)	C2	C3	1.548(3)
C2	C7	1.518(3)	C3	C4	1.587(3)
C3	C9	1.529(3)	C3	C10	1.521(3)
C4	C5	1.524(3)	C5	C6	1.331(3)
C11	C12	1.526(4)	C12	C13	1.306(4)
C14	C15	1.490(4)	C16	C17	1.430(4)
C18	C19	1.557(3)	C18	C23	1.511(3)
C18	C25	1.513(3)	C19	C20	1.547(3)
C19	C24	1.515(3)	C20	C21	1.586(3)
C20	C26	1.528(3)	C20	C27	1.523(3)
C21	C22	1.525(3)	C22	C23	1.333(3)
C28	C29	1.511(4)	C29	C30	1.322(4)
C31	C32	1.502(4)	C33	C34	1.450(4)

Table 6. Bond lengths involving hydrogens (Å)

atom	atom	distance	atom	atom	distance
C2	H1	0.92(3)	C4	H2	1.01(3)
C5	H3	0.97(3)	C6	H4	0.88(3)
C8	H5	0.88(3)	C8	H6	1.05(3)
C11	H7	1.01(4)	C11	H8	0.93(3)
C12	H9	0.98(4)	C13	H10	1.12(4)
C13	H11	1.09(3)	C14	H12	1.01(4)
C14	H13	1.09(3)	C15	H14	0.91(5)
C15	H15	0.92(4)	C15	H16	0.89(4)
C16	H16A	0.990	C16	H16B	0.990
C17	H17A	0.980	C17	H17B	0.980
C17	H17C	0.980	C19	H18	0.90(3)
C21	H19	0.96(3)	C22	H20	0.96(3)
C23	H21	0.90(4)	C25	H22	0.99(3)
C25	H23	0.94(3)	C28	H24	1.09(3)
C28	H25	0.91(3)	C29	H26	1.06(4)
C30	H27	1.00(4)	C30	H28	0.96(4)
C31	H29	1.01(4)	C31	H30	1.01(3)
C32	H31	1.02(4)	C32	H32	0.96(4)
C32	H33	1.01(3)	C33	H33A	0.990
C33	H33B	0.990	C34	H34A	0.980
C34	H34B	0.980	C34	H34C	0.980

Table 7. Bond angles (^{o})

atom	atom	atom	angle	atom	atom	atom	angle
C1	O1	C4	95.96(14)	C9	O4	C14	116.16(18)
C10	O6	C16	116.69(19)	C18	O7	C21	95.96(14)
C26	O10	C31	116.06(17)	C27	O12	C33	117.81(19)
C7	N1	C8	115.16(15)	C7	N1	C11	121.21(16)
C8	N1	C11	122.74(17)	C24	N2	C25	115.56(15)
C24	N2	C28	121.13(16)	C25	N2	C28	122.35(18)
O1	C1	C2	99.84(15)	O1	C1	C6	101.94(15)
O1	C1	C8	110.85(16)	C2	C1	C6	108.47(16)
C2	C1	C8	105.72(14)	C6	C1	C8	126.86(17)
C1	C2	C3	102.24(14)	C1	C2	C7	102.28(16)
C3	C2	C7	120.28(16)	C2	C3	C4	99.56(15)
C2	C3	C9	112.12(15)	C2	C3	C10	113.06(16)
C4	C3	C9	110.58(15)	C4	C3	C10	109.39(14)
C9	C3	C10	111.51(17)	O1	C4	C3	100.55(14)
O1	C4	C5	101.79(16)	C3	C4	C5	107.44(16)
C4	C5	C6	105.70(17)	C1	C6	C5	105.34(17)
O2	C7	N1	125.12(18)	O2	C7	C2	127.33(19)
N1	C7	C2	107.46(15)	N1	C8	C1	102.24(16)
O3	C9	O4	125.11(18)	O3	C9	C3	123.35(18)
O4	C9	C3	111.54(17)	O5	C10	O6	124.3(2)
O5	C10	C3	126.8(2)	O6	C10	C3	108.83(18)
N1	C11	C12	110.89(19)	C11	C12	C13	125.7(3)
O4	C14	C15	107.6(2)	O6	C16	C17	107.7(3)
O7	C18	C19	100.39(14)	O7	C18	C23	102.16(14)
O7	C18	C25	111.06(16)	C19	C18	C23	107.80(16)
C19	C18	C25	105.61(14)	C23	C18	C25	126.83(17)
C18	C19	C20	102.13(14)	C18	C19	C24	103.09(16)
C20	C19	C24	120.82(15)	C19	C20	C21	99.46(15)
C19	C20	C26	112.48(15)	C19	C20	C27	113.35(15)
C21	C20	C26	110.25(15)	C21	C20	C27	109.97(14)
C26	C20	C27	110.79(16)	O7	C21	C20	100.44(14)
O7	C21	C22	101.98(16)	C20	C21	C22	107.68(16)
C21	C22	C23	105.81(17)	C18	C23	C22	104.84(17)
O8	C24	N2	125.30(18)	O8	C24	C19	127.44(19)
N2	C24	C19	107.14(15)	N2	C25	C18	102.45(16)
O9	C26	O10	124.33(17)	O9	C26	C20	123.56(18)
O10	C26	C20	112.11(16)	O11	C27	O12	124.7(2)

Table 7. Bond angles (°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
O11	C27	C20	125.9(2)	O12	C27	C20	109.41(17)
N2	C28	C29	111.95(19)	C28	C29	C30	125.9(3)
O10	C31	C32	107.0(2)	O12	C33	C34	112.3(3)

Table 8. Bond angles involving hydrogens (°)

atom	atom	atom	angle	atom	atom	atom	angle
C1	C2	H1	113.1(16)	C3	C2	H1	110.9(17)
C7	C2	H1	107.7(14)	O1	C4	H2	108.0(17)
C3	C4	H2	116.3(15)	C5	C4	H2	120.0(14)
C4	C5	H3	125.5(16)	C6	C5	H3	128.5(16)
C1	C6	H4	125.4(17)	C5	C6	H4	129.1(17)
N1	C8	H5	111.7(13)	N1	C8	H6	112.7(12)
C1	C8	H5	109.9(15)	C1	C8	H6	110.3(14)
H5	C8	H6	110(2)	N1	C11	H7	108.9(19)
N1	C11	H8	109.4(16)	C12	C11	H7	109.8(19)
C12	C11	H8	117.9(18)	H7	C11	H8	99(3)
C11	C12	H9	114(3)	C13	C12	H9	121(3)
C12	C13	H10	116.5(18)	C12	C13	H11	122.5(17)
H10	C13	H11	121(3)	O4	C14	H12	109(2)
O4	C14	H13	103.2(15)	C15	C14	H12	114(2)
C15	C14	H13	113.5(17)	H12	C14	H13	109(3)
C14	C15	H14	106(3)	C14	C15	H15	99(3)
C14	C15	H16	109(3)	H14	C15	H15	117(4)
H14	C15	H16	112(4)	H15	C15	H16	113(4)
O6	C16	H16A	110.2	O6	C16	H16B	110.2
C17	C16	H16A	110.2	C17	C16	H16B	110.2
H16A	C16	H16B	108.5	C16	C17	H17A	109.5
C16	C17	H17B	109.5	C16	C17	H17C	109.5
H17A	C17	H17B	109.5	H17A	C17	H17C	109.5
H17B	C17	H17C	109.5	C18	C19	H18	111.0(15)
C20	C19	H18	110.7(16)	C24	C19	H18	108.5(14)
O7	C21	H19	114.1(16)	C20	C21	H19	113.0(15)
C22	C21	H19	117.7(14)	C21	C22	H20	127.1(17)
C23	C22	H20	126.3(18)	C18	C23	H21	122.3(18)
C22	C23	H21	131.9(19)	N2	C25	H22	110.4(13)
N2	C25	H23	113.6(14)	C18	C25	H22	111.7(15)
C18	C25	H23	110.8(16)	H22	C25	H23	108(3)
N2	C28	H24	106.5(13)	N2	C28	H25	112(2)
C29	C28	H24	118.2(15)	C29	C28	H25	108.9(19)
H24	C28	H25	99(3)	C28	C29	H26	108.8(18)
C30	C29	H26	125.3(18)	C29	C30	H27	118.3(19)
C29	C30	H28	127(2)	H27	C30	H28	115(3)
O10	C31	H29	106.3(17)	O10	C31	H30	103.2(16)

Table 8. Bond angles involving hydrogens (°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C32	C31	H29	116(2)	C32	C31	H30	109.8(17)
H29	C31	H30	114(3)	C31	C32	H31	109.5(19)
C31	C32	H32	112(2)	C31	C32	H33	104.4(18)
H31	C32	H32	114(3)	H31	C32	H33	105(3)
H32	C32	H33	112(3)	O12	C33	H33A	109.1
O12	C33	H33B	109.1	C34	C33	H33A	109.1
C34	C33	H33B	109.1	H33A	C33	H33B	107.9
C33	C34	H34A	109.5	C33	C34	H34B	109.5
C33	C34	H34C	109.5	H34A	C34	H34B	109.5
H34A	C34	H34C	109.5	H34B	C34	H34C	109.5

Table 9. Torsion Angles(O)
(Those having bond angles > 160 or < 20 degrees are excluded.)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C1	O1	C4	C3	60.97(13)	C1	O1	C4	C5	-49.53(13)
C4	O1	C1	C2	-60.79(13)	C4	O1	C1	C6	50.64(14)
C4	O1	C1	C8	-171.91(12)	C9	O4	C14	C15	154.29(16)
C14	O4	C9	O3	-6.3(3)	C14	O4	C9	C3	173.51(16)
C10	O6	C16	C17	-158.18(18)	C16	O6	C10	O5	-6.9(3)
C16	O6	C10	C3	169.36(18)	C18	O7	C21	C20	61.34(13)
C18	O7	C21	C22	-49.44(13)	C21	O7	C18	C19	-60.14(13)
C21	O7	C18	C23	50.80(14)	C21	O7	C18	C25	-171.47(12)
C26	O10	C31	C32	169.47(15)	C31	O10	C26	O9	-4.5(3)
C31	O10	C26	C20	175.83(16)	C27	O12	C33	C34	-79.3(3)
C33	O12	C27	O11	-3.5(3)	C33	O12	C27	C20	174.14(15)
C7	N1	C8	C1	13.7(2)	C8	N1	C7	O2	179.96(18)
C8	N1	C7	C2	3.3(3)	C7	N1	C11	C12	77.4(3)
C11	N1	C7	O2	10.4(4)	C11	N1	C7	C2	-166.24(17)
C8	N1	C11	C12	-91.3(3)	C11	N1	C8	C1	-176.95(17)
C24	N2	C25	C18	13.5(2)	C25	N2	C24	O8	178.59(17)
C25	N2	C24	C19	2.2(3)	C24	N2	C28	C29	78.1(3)
C28	N2	C24	O8	9.6(3)	C28	N2	C24	C19	-166.77(17)
C25	N2	C28	C29	-90.1(3)	C28	N2	C25	C18	-177.71(17)
O1	C1	C2	C3	36.36(15)	O1	C1	C2	C7	-88.76(14)
O1	C1	C6	C5	-32.89(18)	O1	C1	C8	N1	83.01(16)
C2	C1	C6	C5	71.87(18)	C6	C1	C2	C3	-69.86(17)
C6	C1	C2	C7	165.02(14)	C2	C1	C8	N1	-24.28(17)
C8	C1	C2	C3	151.45(13)	C8	C1	C2	C7	26.33(17)
C6	C1	C8	N1	-152.78(17)	C8	C1	C6	C5	-160.72(17)
C1	C2	C3	C4	-0.21(15)	C1	C2	C3	C9	-117.16(14)
C1	C2	C3	C10	115.74(14)	C1	C2	C7	O2	165.18(19)
C1	C2	C7	N1	-18.24(19)	C3	C2	C7	O2	53.0(3)
C3	C2	C7	N1	-130.47(17)	C7	C2	C3	C4	112.04(16)
C7	C2	C3	C9	-4.9(3)	C7	C2	C3	C10	-132.01(16)
C2	C3	C4	O1	-36.74(15)	C2	C3	C4	C5	69.30(16)
C2	C3	C9	O3	81.1(2)	C2	C3	C9	O4	-98.64(18)
C2	C3	C10	O5	14.1(3)	C2	C3	C10	O6	-162.07(13)
C4	C3	C9	O3	-29.0(3)	C4	C3	C9	O4	151.23(15)
C9	C3	C4	O1	81.36(18)	C9	C3	C4	C5	-172.60(14)
C4	C3	C10	O5	124.08(19)	C4	C3	C10	O6	-52.11(19)
C10	C3	C4	O1	-155.46(15)	C10	C3	C4	C5	-49.4(2)

Table 9. Torsion angles (°) (continued)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C9	C3	C10	O5	-113.3(2)	C9	C3	C10	O6	70.52(18)
C10	C3	C9	O3	-150.93(17)	C10	C3	C9	O4	29.3(2)
O1	C4	C5	C6	31.50(18)	C3	C4	C5	C6	-73.66(19)
C4	C5	C6	C1	1.1(2)	N1	C11	C12	C13	133.8(2)
O7	C18	C19	C20	34.88(15)	O7	C18	C19	C24	-91.14(14)
O7	C18	C23	C22	-33.24(18)	O7	C18	C25	N2	85.19(16)
C19	C18	C23	C22	72.00(18)	C23	C18	C19	C20	-71.60(16)
C23	C18	C19	C24	162.38(14)	C19	C18	C25	N2	-22.76(17)
C25	C18	C19	C20	150.38(13)	C25	C18	C19	C24	24.36(17)
C23	C18	C25	N2	-150.04(17)	C25	C18	C23	C22	-161.59(16)
C18	C19	C20	C21	1.46(15)	C18	C19	C20	C26	-115.20(14)
C18	C19	C20	C27	118.15(14)	C18	C19	C24	O8	167.27(17)
C18	C19	C24	N2	-16.46(18)	C20	C19	C24	O8	54.3(3)
C20	C19	C24	N2	-129.41(16)	C24	C19	C20	C21	114.92(16)
C24	C19	C20	C26	-1.7(3)	C24	C19	C20	C27	-128.40(16)
C19	C20	C21	O7	-38.05(15)	C19	C20	C21	C22	68.22(16)
C19	C20	C26	O9	73.9(2)	C19	C20	C26	O10	-106.45(17)
C19	C20	C27	O11	16.5(3)	C19	C20	C27	O12	-161.13(13)
C21	C20	C26	O9	-36.1(3)	C21	C20	C26	O10	143.54(15)
C26	C20	C21	O7	80.28(17)	C26	C20	C21	C22	-173.45(14)
C21	C20	C27	O11	126.78(18)	C21	C20	C27	O12	-50.81(19)
C27	C20	C21	O7	-157.26(14)	C27	C20	C21	C22	-50.99(19)
C26	C20	C27	O11	-111.08(19)	C26	C20	C27	O12	71.33(17)
C27	C20	C26	O9	-158.05(16)	C27	C20	C26	O10	21.6(2)
O7	C21	C22	C23	31.13(18)	C20	C21	C22	C23	-74.06(19)
C21	C22	C23	C18	1.5(2)	N2	C28	C29	C30	131.9(2)

Table 10. Intramolecular contacts less than 3.60 Å

atom	atom	distance	atom	atom	distance
O1	O3	2.942(2)	O1	N1	2.977(2)
O1	C7	2.946(3)	O1	C9	3.019(3)
O2	O3	3.275(3)	O2	O4	3.217(3)
O2	C1	3.579(2)	O2	C3	3.225(3)
O2	C8	3.549(3)	O2	C9	2.954(3)
O2	C11	2.836(3)	O2	C12	3.361(3)
O3	C2	3.213(3)	O3	C4	2.857(3)
O3	C7	3.219(3)	O3	C14	2.690(3)
O4	O5	3.323(2)	O4	O6	3.0796(19)
O4	C2	3.294(3)	O4	C7	3.540(3)
O4	C10	2.664(3)	O5	C2	2.902(3)
O5	C4	3.533(3)	O5	C5	3.460(3)
O5	C9	3.452(3)	O5	C16	2.695(3)
O6	C4	2.767(3)	O6	C5	3.096(3)
O6	C9	2.955(3)	O7	O9	2.906(2)
O7	N2	3.005(2)	O7	C24	2.993(3)
O7	C26	2.997(3)	O8	O9	3.268(3)
O8	O10	3.386(3)	O8	C18	3.589(2)
O8	C20	3.237(3)	O8	C25	3.549(3)
O8	C26	3.010(3)	O8	C28	2.842(3)
O8	C29	3.378(3)	O9	C19	3.165(3)
O9	C21	2.887(3)	O9	C24	3.161(3)
O9	C31	2.672(3)	O10	O11	3.282(3)
O10	O12	2.9900(19)	O10	C19	3.379(3)
O10	C27	2.623(3)	O11	C19	2.896(3)
O11	C21	3.547(3)	O11	C22	3.516(3)
O11	C26	3.416(3)	O11	C33	2.719(4)
O11	C34	3.195(4)	O12	C21	2.782(3)
O12	C22	3.128(3)	O12	C26	2.964(3)
N1	C13	3.585(4)	N2	C30	3.597(4)
C1	C9	3.507(3)	C1	C10	3.498(3)
C2	C5	2.858(3)	C3	C6	2.900(3)
C4	C7	3.514(3)	C4	C8	3.543(3)
C5	C10	2.821(3)	C6	C10	3.417(3)
C7	C9	2.893(3)	C7	C12	3.160(4)
C8	C12	3.378(3)	C9	C15	3.570(4)
C10	C17	3.543(4)	C18	C26	3.490(3)

Table 10. Intramolecular contacts less than 3.60 Å (continued)

atom	atom	distance	atom	atom	distance
C18	C27	3.524(3)	C19	C22	2.846(3)
C20	C23	2.912(3)	C21	C24	3.540(3)
C21	C25	3.542(3)	C22	C27	2.853(3)
C23	C27	3.465(3)	C24	C26	2.910(3)
C24	C29	3.180(3)	C25	C29	3.368(3)
C27	C34	3.087(4)			

Table 11. Intramolecular contacts less than 3.60 Å involving hydrogens

atom	atom	distance	atom	atom	distance
O1	H1	3.11(3)	O1	H3	3.20(3)
O1	H4	3.11(3)	O1	H5	2.47(3)
O1	H6	3.32(3)	O2	H1	2.78(3)
O2	H7	2.60(4)	O2	H9	2.94(4)
O2	H12	3.22(4)	O3	H2	2.75(3)
O3	H12	2.97(4)	O3	H13	2.26(3)
O4	H14	2.49(5)	O4	H15	3.11(4)
O4	H16	2.56(4)	O5	H1	2.47(3)
O5	H16A	2.471	O5	H16B	2.903
O6	H2	2.84(3)	O6	H3	3.01(3)
O6	H17A	3.199	O6	H17B	2.573
O6	H17C	2.478	O7	H18	3.08(3)
O7	H20	3.21(3)	O7	H21	3.13(3)
O7	H22	2.52(3)	O7	H23	3.21(3)
O8	H18	2.77(2)	O8	H25	2.66(4)
O8	H26	2.86(4)	O8	H30	3.35(3)
O9	H19	2.84(3)	O9	H29	2.41(4)
O9	H30	2.80(3)	O10	H31	2.68(4)
O10	H32	2.56(3)	O10	H33	3.23(3)
O11	H18	2.47(3)	O11	H33A	2.480
O11	H34A	2.705	O12	H19	2.74(3)
O12	H20	3.03(3)	O12	H34A	2.634
O12	H34B	2.599	O12	H34C	3.251
N1	H1	2.79(3)	N1	H9	2.63(4)
N2	H18	2.78(3)	N2	H26	2.60(3)
C1	H2	3.06(3)	C1	H3	3.21(3)
C2	H2	3.29(3)	C2	H4	3.08(3)
C2	H5	3.15(3)	C2	H6	2.96(3)
C3	H3	3.15(3)	C4	H1	3.03(3)
C4	H4	3.15(3)	C5	H1	3.13(3)
C6	H1	2.63(3)	C6	H2	3.17(3)
C6	H5	3.07(3)	C6	H6	2.85(3)
C7	H5	3.02(3)	C7	H6	3.01(3)
C7	H7	2.62(4)	C7	H8	3.16(3)
C7	H9	2.91(4)	C8	H1	2.86(3)
C8	H4	2.99(3)	C8	H7	3.32(3)
C8	H8	2.68(3)	C9	H1	3.17(3)

Table 11. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C9	H2	2.71(3)	C9	H12	2.77(3)
C9	H13	2.40(3)	C10	H1	2.53(3)
C10	H2	3.04(3)	C10	H3	3.05(3)
C10	H16A	2.517	C10	H16B	2.786
C11	H5	2.79(2)	C11	H6	2.91(3)
C11	H10	2.71(4)	C11	H11	3.53(3)
C12	H6	3.27(2)	C13	H7	3.08(4)
C13	H8	2.74(3)	C16	H3	3.58(3)
C18	H19	3.04(3)	C18	H20	3.19(3)
C19	H19	3.25(3)	C19	H21	3.03(3)
C19	H22	3.24(3)	C19	H23	2.92(3)
C20	H20	3.13(3)	C21	H18	2.98(3)
C21	H21	3.17(4)	C22	H18	3.06(3)
C22	H34A	3.579	C22	H34B	3.542
C23	H18	2.57(3)	C23	H19	3.13(3)
C23	H22	3.18(3)	C23	H23	2.82(3)
C24	H22	3.10(3)	C24	H23	2.95(3)
C24	H24	3.28(3)	C24	H25	2.63(3)
C24	H26	2.86(4)	C25	H18	2.85(3)
C25	H21	2.97(3)	C25	H24	2.67(3)
C25	H25	3.26(3)	C26	H18	3.18(3)
C26	H19	2.67(3)	C26	H29	2.48(4)
C26	H30	2.64(3)	C27	H18	2.53(3)
C27	H19	2.93(3)	C27	H20	3.05(3)
C27	H33A	2.531	C27	H33B	3.183
C27	H34A	2.862	C27	H34B	3.413
C28	H22	2.80(3)	C28	H23	2.85(3)
C28	H27	2.70(4)	C28	H28	3.42(4)
C29	H23	3.26(3)	C30	H24	2.81(3)
C30	H25	3.00(4)	C34	H20	3.23(3)
H1	H4	3.01(4)	H1	H6	3.08(4)
H2	H3	2.64(4)	H3	H4	2.49(4)
H3	H16A	3.344	H3	H17B	3.160
H4	H5	3.38(4)	H4	H6	2.83(4)
H5	H7	3.50(4)	H5	H8	2.61(3)
H6	H8	3.04(4)	H6	H9	3.52(4)
H7	H9	2.52(5)	H7	H10	3.26(5)

Table 11. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H8	H9	2.91(5)	H8	H10	2.52(5)
H9	H10	2.95(6)	H9	H11	2.40(5)
H12	H14	2.34(6)	H12	H15	2.23(6)
H12	H16	2.81(6)	H13	H14	2.86(6)
H13	H15	2.32(5)	H13	H16	2.36(6)
H16A	H17A	2.328	H16A	H17B	2.261
H16A	H17C	2.798	H16B	H17A	2.259
H16B	H17B	2.798	H16B	H17C	2.330
H18	H21	2.90(4)	H18	H23	3.06(4)
H19	H20	2.59(4)	H20	H21	2.50(5)
H20	H34A	2.967	H20	H34B	2.755
H21	H22	3.49(4)	H21	H23	2.79(4)
H22	H24	2.53(4)	H22	H25	3.44(4)
H23	H24	2.97(4)	H23	H26	3.54(4)
H24	H26	3.07(5)	H24	H27	2.58(5)
H25	H26	2.43(5)	H25	H27	3.20(5)
H26	H27	2.97(5)	H26	H28	2.51(5)
H29	H31	2.39(5)	H29	H32	2.91(5)
H29	H33	2.41(5)	H30	H31	2.91(5)
H30	H32	2.37(5)	H30	H33	2.34(5)
H33A	H34A	2.291	H33A	H34B	2.806
H33A	H34C	2.305	H33B	H34A	2.805
H33B	H34B	2.318	H33B	H34C	2.277

Table 12. Intermolecular contacts less than 3.60 Å

atom	atom	distance	atom	atom	distance
O1	C1[1]	3.416(3)	O1	C2[1]	3.278(3)
O1	C6[1]	3.411(3)	O1	C8[1]	3.401(3)
O2	C34[2]	3.400(4)	O3	C6[1]	3.404(3)
O3	C8[1]	3.457(3)	O3	C15[2]	3.572(4)
O5	C8[3]	3.512(3)	O5	C14[4]	3.345(3)
O5	C15[4]	3.384(4)	O7	C18[5]	3.419(3)
O7	C19[5]	3.307(3)	O7	C23[5]	3.420(3)
O7	C25[5]	3.355(3)	O8	C13[6]	3.519(4)
O9	C13[6]	3.516(3)	O9	C17	3.509(4)
O9	C23[5]	3.391(3)	O9	C25[5]	3.546(3)
O11	C17[7]	3.430(4)	O11	C31[8]	3.396(3)
O11	C32[8]	3.507(3)	C1	O1[3]	3.416(3)
C2	O1[3]	3.278(3)	C6	O1[3]	3.411(3)
C6	O3[3]	3.404(3)	C8	O1[3]	3.401(3)
C8	O3[3]	3.457(3)	C8	O5[1]	3.512(3)
C13	O8[9]	3.519(4)	C13	O9[9]	3.516(3)
C14	O5[2]	3.345(3)	C15	O3[4]	3.572(4)
C15	O5[2]	3.384(4)	C17	O9	3.509(4)
C17	O11[10]	3.430(4)	C18	O7[11]	3.419(3)
C19	O7[11]	3.307(3)	C21	C29[5]	3.549(3)
C23	O7[11]	3.420(3)	C23	O9[11]	3.391(3)
C23	C32[12]	3.579(4)	C25	O7[11]	3.355(3)
C25	O9[11]	3.546(3)	C29	C21[11]	3.549(3)
C31	O11[13]	3.396(3)	C32	O11[13]	3.507(3)
C32	C23[14]	3.579(4)	C34	O2[4]	3.400(4)

Symmetry Operators:

(1) -X+2,Y+1/2-1,-Z+1
(2) -X+1,Y+1/2-1,-Z+1
(3) -X+2,Y+1/2,-Z+1
(4) -X+1,Y+1/2,-Z+1
(5) -X+1,Y+1/2-1,-Z+2
(6) X,Y,Z+1
(7) X,Y+1,Z
(8) -X+2,Y+1/2,-Z+2
(9) X,Y,Z-1
(10) X,Y-1,Z
(11) -X+1,Y+1/2,-Z+2
(12) X-1,Y,Z
(13) -X+2,Y+1/2-1,-Z+2
(14) X+1,Y,Z

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens

atom	atom	distance	atom	atom	distance
O1	H1[1]	2.60(3)	O1	H4[1]	3.06(3)
O1	H6[1]	2.74(3)	O1	H15[2]	3.47(4)
O2	H20[3]	3.01(3)	O2	H28[4]	2.69(4)
O2	H34A[3]	3.585	O2	H34B[3]	2.531
O3	H4[1]	2.71(3)	O3	H6[1]	2.56(3)
O3	H14[3]	2.69(5)	O3	H28[4]	3.25(3)
O3	H34C[5]	2.684	O4	H13[6]	3.16(3)
O4	H27[7]	3.29(4)	O4	H34C[5]	2.942
O5	H5[8]	2.64(3)	O5	H8[8]	3.56(3)
O5	H12[6]	2.91(4)	O5	H13[6]	3.44(3)
O5	H15[6]	2.59(4)	O5	H27[7]	3.57(4)
O5	H33B	2.923	O6	H27[7]	3.21(4)
O7	H18[7]	2.66(3)	O7	H21[7]	2.99(3)
O7	H23[7]	2.77(3)	O7	H33[9]	3.30(3)
O8	H3[10]	3.04(3)	O8	H11[11]	2.46(3)
O8	H17B[10]	2.736	O8	H29[10]	3.40(4)
O8	H31[10]	3.30(4)	O8	H33[10]	3.28(3)
O9	H11[11]	3.07(3)	O9	H17A	2.540
O9	H21[7]	2.65(4)	O9	H23[7]	2.74(3)
O9	H32[12]	2.68(4)	O10	H10[8]	3.16(4)
O10	H17A	3.331	O10	H29[10]	3.30(4)
O11	H10[8]	3.30(4)	O11	H17C[13]	2.513
O11	H22[14]	2.75(3)	O11	H29[10]	3.50(3)
O11	H30[10]	2.93(3)	O11	H33[10]	2.75(3)
O12	H10[8]	3.22(4)	O12	H16A	3.135
O12	H16B	3.303	N1	H2[8]	3.40(3)
N1	H4[1]	3.41(3)	N2	H19[14]	3.43(3)
N2	H21[7]	3.45(4)	C1	H1[1]	3.53(3)
C1	H15[2]	3.49(4)	C2	H15[6]	3.27(4)
C4	H6[1]	2.86(3)	C4	H9[1]	3.47(4)
C5	H9[1]	3.45(4)	C5	H25[12]	3.10(3)
C5	H26[12]	3.51(3)	C6	H14[2]	3.32(5)
C6	H15[2]	3.55(4)	C7	H4[1]	3.53(3)
C7	H28[4]	3.48(4)	C8	H1[1]	3.52(3)
C8	H2[8]	3.10(3)	C8	H14[2]	3.52(4)
C8	H15[2]	3.26(4)	C8	H33B[1]	3.293
C9	H6[1]	3.38(3)	C9	H34C[5]	2.829

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C10	H15[6]	3.43(4)	C10	H27[7]	3.49(4)
C11	H20[3]	3.34(3)	C11	H26[4]	3.49(4)
C11	H31[1]	3.32(4)	C12	H2[8]	2.97(3)
C12	H20[3]	3.28(3)	C12	H21[3]	3.30(3)
C12	H25[15]	3.32(4)	C12	H31[1]	3.58(4)
C12	H33A[1]	3.504	C13	H2[8]	3.17(3)
C13	H17B[8]	3.548	C13	H21[3]	3.23(3)
C13	H25[15]	3.57(4)	C13	H30[15]	3.41(3)
C13	H31[1]	3.34(4)	C13	H32[1]	3.19(3)
C13	H33A[1]	2.887	C14	H28[4]	3.54(4)
C14	H34B[3]	3.525	C14	H34C[5]	2.987
C15	H1[3]	3.39(3)	C15	H4[9]	3.51(3)
C15	H5[9]	3.27(2)	C15	H27[7]	3.10(3)
C15	H34C[5]	3.486	C16	H19	3.54(3)
C16	H27[7]	3.11(3)	C17	H11[1]	3.52(3)
C17	H22[7]	3.46(3)	C17	H23[7]	3.34(3)
C17	H29	3.08(3)	C17	H30[12]	2.80(3)
C17	H32[12]	3.41(3)	C18	H18[7]	3.56(3)
C18	H33[9]	3.38(3)	C19	H33[10]	3.10(3)
C21	H23[7]	2.92(3)	C21	H26[7]	3.37(3)
C22	H7[6]	3.09(3)	C22	H26[7]	3.25(4)
C23	H31[9]	3.58(4)	C23	H32[9]	3.23(3)
C23	H33[9]	3.40(4)	C24	H11[11]	3.19(3)
C24	H33[10]	3.35(3)	C25	H17A[14]	3.423
C25	H17C[14]	3.470	C25	H18[7]	3.53(3)
C25	H19[14]	3.16(3)	C25	H32[9]	3.56(3)
C25	H33[9]	3.27(3)	C26	H11[11]	3.57(3)
C26	H17A	2.985	C26	H23[7]	3.49(3)
C27	H10[8]	3.36(4)	C27	H33[10]	3.55(3)
C28	H3[10]	3.26(3)	C28	H9[11]	3.37(4)
C28	H16[14]	3.51(4)	C29	H3[10]	3.15(3)
C29	H4[10]	3.28(3)	C29	H7[16]	3.33(4)
C29	H16B[14]	3.426	C29	H19[14]	2.90(3)
C30	H4[10]	3.20(3)	C30	H7[16]	3.57(4)
C30	H12[16]	3.48(4)	C30	H14[14]	3.20(5)
C30	H16[14]	3.20(4)	C30	H16B[14]	2.815
C30	H19[14]	3.03(3)	C30	H20[14]	3.55(3)

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C31	H17A	3.279	C31	H17A[10]	3.456
C31	H17B[10]	3.384	C31	H17C[10]	3.526
C32	H10[8]	3.05(4)	C32	H17A[10]	3.300
C32	H18[12]	3.39(3)	C32	H21[2]	3.53(4)
C32	H22[2]	3.38(3)	C33	H6[8]	3.55(3)
C33	H10[8]	3.04(3)	C34	H12[6]	3.30(4)
C34	H13[13]	3.08(3)	C34	H16[13]	3.40(4)
C34	H24[14]	3.53(3)	H1	O1[8]	2.60(3)
H1	C1[8]	3.53(3)	H1	C8[8]	3.52(3)
H1	C15[6]	3.39(3)	H1	H5[8]	2.83(4)
H1	H15[6]	2.53(5)	H1	H16[6]	3.59(5)
H2	N1[1]	3.40(3)	H2	C8[1]	3.10(3)
H2	C12[1]	2.97(3)	H2	C13[1]	3.17(3)
H2	H6[1]	2.18(4)	H2	H9[1]	2.97(4)
H2	H11[1]	3.34(4)	H2	H33A[5]	3.087
H2	H34C[5]	3.516	H3	O8[12]	3.04(3)
H3	C28[12]	3.26(3)	H3	C29[12]	3.15(3)
H3	H9[1]	3.38(5)	H3	H11[1]	3.16(4)
H3	H25[12]	2.63(4)	H3	H26[12]	2.87(4)
H4	O1[8]	3.06(3)	H4	O3[8]	2.71(3)
H4	N1[8]	3.41(3)	H4	C7[8]	3.53(3)
H4	C15[2]	3.51(3)	H4	C29[12]	3.28(3)
H4	C30[12]	3.20(3)	H4	H7[8]	3.55(5)
H4	H14[2]	3.02(6)	H4	H16[2]	3.58(5)
H4	H26[12]	3.37(4)	H4	H28[12]	3.16(4)
H5	O5[1]	2.64(3)	H5	C15[2]	3.27(2)
H5	H1[1]	2.83(4)	H5	H14[2]	3.19(5)
H5	H15[2]	2.63(4)	H5	H33B[1]	2.905
H6	O1[8]	2.74(3)	H6	O3[8]	2.56(3)
H6	C4[8]	2.86(3)	H6	C9[8]	3.38(3)
H6	C33[1]	3.55(3)	H6	H2[8]	2.18(4)
H6	H14[2]	3.28(5)	H6	H15[2]	3.47(5)
H6	H33A[1]	3.360	H6	H33B[1]	2.928
H6	H34C[1]	3.509	H7	C22[3]	3.09(3)
H7	C29[4]	3.33(4)	H7	C30[4]	3.57(4)
H7	H4[1]	3.55(5)	H7	H20[3]	2.62(4)
H7	H26[4]	2.56(5)	H7	H28[4]	3.17(5)

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H7	H31[1]	3.10(5)	H8	O5[1]	3.56(3)
H8	H16A[1]	3.290	H8	H26[4]	3.45(5)
H8	H31[1]	2.87(5)	H8	H33A[1]	3.442
H8	H33B[1]	3.089	H9	C4[8]	3.47(4)
H9	C5[8]	3.45(4)	H9	C28[15]	3.37(4)
H9	H2[8]	2.97(4)	H9	H3[8]	3.38(5)
H9	H20[3]	3.06(5)	H9	H21[3]	3.36(4)
H9	H24[15]	3.37(5)	H9	H25[15]	2.54(5)
H10	O10[1]	3.16(4)	H10	O11[1]	3.30(4)
H10	O12[1]	3.22(4)	H10	C27[1]	3.36(4)
H10	C32[1]	3.05(4)	H10	C33[1]	3.04(3)
H10	H30[15]	3.26(5)	H10	H31[1]	2.70(5)
H10	H32[1]	2.68(4)	H10	H33A[1]	2.343
H10	H33B[1]	3.202	H11	O8[15]	2.46(3)
H11	O9[15]	3.07(3)	H11	C17[8]	3.52(3)
H11	C24[15]	3.19(3)	H11	C26[15]	3.57(3)
H11	H2[8]	3.34(4)	H11	H3[8]	3.16(4)
H11	H17B[8]	2.706	H11	H17C[8]	3.506
H11	H21[3]	3.29(4)	H11	H25[15]	3.07(5)
H11	H30[15]	2.81(5)	H11	H33A[1]	3.371
H12	O5[3]	2.91(4)	H12	C30[4]	3.48(4)
H12	C34[3]	3.30(4)	H12	H13[6]	3.58(5)
H12	H27[4]	3.39(5)	H12	H28[4]	2.80(5)
H12	H33B[3]	3.124	H12	H34B[3]	2.656
H12	H34C[3]	3.284	H13	O4[3]	3.16(3)
H13	O5[3]	3.44(3)	H13	C34[5]	3.08(3)
H13	H12[3]	3.58(5)	H13	H14[3]	2.87(6)
H13	H28[4]	3.50(5)	H13	H34A[5]	3.485
H13	H34B[5]	3.129	H13	H34C[5]	2.274
H14	O3[6]	2.69(5)	H14	C6[9]	3.32(5)
H14	C8[9]	3.52(4)	H14	C30[7]	3.20(5)
H14	H4[9]	3.02(6)	H14	H5[9]	3.19(5)
H14	H6[9]	3.28(5)	H14	H13[6]	2.87(6)
H14	H27[7]	2.80(5)	H14	H28[7]	3.40(6)
H14	H34C[3]	3.443	H15	O1[9]	3.47(4)
H15	O5[3]	2.59(4)	H15	C1[9]	3.49(4)
H15	C2[3]	3.27(4)	H15	C6[9]	3.55(4)

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H15	C8[9]	3.26(4)	H15	C10[3]	3.43(4)
H15	H1[3]	2.53(5)	H15	H5[9]	2.63(4)
H15	H6[9]	3.47(5)	H16	C28[7]	3.51(4)
H16	C30[7]	3.20(4)	H16	C34[5]	3.40(4)
H16	H1[3]	3.59(5)	H16	H4[9]	3.58(5)
H16	H24[7]	3.03(5)	H16	H25[7]	3.35(6)
H16	H27[7]	2.64(5)	H16	H34A[5]	3.122
H16	H34B[5]	3.500	H16	H34C[5]	3.028
H16A	O12	3.135	H16A	H8[8]	3.290
H16A	H29	3.445	H16A	H31	3.500
H16A	H33B	3.175	H16B	O12	3.303
H16B	C29[7]	3.426	H16B	C30[7]	2.815
H16B	H19	2.749	H16B	H23[7]	3.242
H16B	H24[7]	3.419	H16B	H27[7]	2.301
H16B	H28[7]	3.222	H17A	O9	2.540
H17A	O10	3.331	H17A	C25[7]	3.423
H17A	C26	2.985	H17A	C31	3.279
H17A	C31[12]	3.456	H17A	C32[12]	3.300
H17A	H19	3.336	H17A	H22[7]	3.182
H17A	H23[7]	2.777	H17A	H29	2.431
H17A	H30[12]	2.804	H17A	H32[12]	2.718
H17A	H33[12]	3.408	H17B	O8[12]	2.736
H17B	C13[1]	3.548	H17B	C31[12]	3.384
H17B	H11[1]	2.706	H17B	H29	2.917
H17B	H30[12]	2.457	H17B	H32[12]	3.590
H17C	O11[5]	2.513	H17C	C25[7]	3.470
H17C	C31[12]	3.526	H17C	H11[1]	3.506
H17C	H22[7]	2.874	H17C	H23[7]	3.170
H17C	H24[7]	3.468	H17C	H30[12]	2.671
H17C	H32[12]	3.454	H17C	H33A[5]	3.123
H17C	H34A[5]	3.261	H17C	H33[12]	3.390
H18	O7[14]	2.66(3)	H18	C18[14]	3.56(3)
H18	C25[14]	3.53(3)	H18	C32[10]	3.39(3)
H18	H22[14]	2.77(4)	H18	H33[10]	2.40(4)
H19	N2[7]	3.43(3)	H19	C16	3.54(3)
H19	C25[7]	3.16(3)	H19	C29[7]	2.90(3)
H19	C30[7]	3.03(3)	H19	H16B	2.749

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H19	H17A	3.336	H19	H23^{7}	2.35(4)
H19	H26^{7}	2.98(4)	H19	H27^{7}	3.42(4)
H19	H28^{7}	3.24(4)	H20	O2^{6}	3.01(3)
H20	C11^{6}	3.34(3)	H20	C12^{6}	3.28(3)
H20	C30^{7}	3.55(3)	H20	H7^{6}	2.62(4)
H20	H9^{6}	3.06(5)	H20	H26^{7}	3.25(5)
H20	H28^{7}	3.09(5)	H21	O7^{14}	2.99(3)
H21	O9^{14}	2.65(4)	H21	N2^{14}	3.45(4)
H21	C12^{6}	3.30(3)	H21	C13^{6}	3.23(3)
H21	C32^{9}	3.53(4)	H21	H9^{6}	3.36(4)
H21	H11^{6}	3.29(4)	H21	H22^{14}	3.48(4)
H21	H31^{9}	3.60(5)	H21	H32^{9}	2.97(5)
H21	H33^{9}	3.57(5)	H22	O11^{7}	2.75(3)
H22	C17^{14}	3.46(3)	H22	C32^{9}	3.38(3)
H22	H17A^{14}	3.182	H22	H17C^{14}	2.874
H22	H18^{7}	2.77(4)	H22	H21^{7}	3.48(4)
H22	H32^{9}	3.28(4)	H22	H33^{9}	2.65(4)
H23	O7^{14}	2.77(3)	H23	O9^{14}	2.74(3)
H23	C17^{14}	3.34(3)	H23	C21^{14}	2.92(3)
H23	C26^{14}	3.49(3)	H23	H16B^{14}	3.242
H23	H17A^{14}	2.777	H23	H17C^{14}	3.170
H23	H19^{14}	2.35(4)	H23	H32^{9}	3.29(4)
H23	H33^{9}	3.42(4)	H24	C34^{7}	3.53(3)
H24	H9^{11}	3.37(5)	H24	H16^{14}	3.03(5)
H24	H16B^{14}	3.419	H24	H17C^{14}	3.468
H24	H34A^{7}	2.598	H25	C5^{10}	3.10(3)
H25	C12^{11}	3.32(4)	H25	C13^{11}	3.57(4)
H25	H3^{10}	2.63(4)	H25	H9^{11}	2.54(5)
H25	H11^{11}	3.07(5)	H25	H16^{14}	3.35(6)
H26	C5^{10}	3.51(3)	H26	C11^{16}	3.49(4)
H26	C21^{14}	3.37(3)	H26	C22^{14}	3.25(4)
H26	H3^{10}	2.87(4)	H26	H4^{10}	3.37(4)
H26	H7^{16}	2.56(5)	H26	H8^{16}	3.45(5)
H26	H19^{14}	2.98(4)	H26	H20^{14}	3.25(5)
H26	H31^{10}	3.45(5)	H27	O4^{14}	3.29(4)
H27	O5^{14}	3.57(4)	H27	O6^{14}	3.21(4)
H27	C10^{14}	3.49(4)	H27	C15^{14}	3.10(3)

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H27	C16[14]	3.11(3)	H27	H12[16]	3.39(5)
H27	H14[14]	2.80(5)	H27	H16[14]	2.64(5)
H27	H16B[14]	2.301	H27	H19[14]	3.42(4)
H28	O2[16]	2.69(4)	H28	O3[16]	3.25(3)
H28	C7[16]	3.48(4)	H28	C14[16]	3.54(4)
H28	H4[10]	3.16(4)	H28	H7[16]	3.17(5)
H28	H12[16]	2.80(5)	H28	H13[16]	3.50(5)
H28	H14[14]	3.40(6)	H28	H16B[14]	3.222
H28	H19[14]	3.24(4)	H28	H20[14]	3.09(5)
H28	H34B[14]	3.099	H29	O8[12]	3.40(4)
H29	O10[12]	3.30(4)	H29	O11[12]	3.50(3)
H29	C17	3.08(3)	H29	H16A	3.445
H29	H17A	2.431	H29	H17B	2.917
H29	H30[12]	3.55(5)	H29	H32[12]	3.02(5)
H30	O11[12]	2.93(3)	H30	C13[11]	3.41(3)
H30	C17[10]	2.80(3)	H30	H10[11]	3.26(5)
H30	H11[11]	2.81(5)	H30	H17A[10]	2.804
H30	H17B[10]	2.457	H30	H17C[10]	2.671
H30	H29[10]	3.55(5)	H31	O8[12]	3.30(4)
H31	C11[8]	3.32(4)	H31	C12[8]	3.58(4)
H31	C13[8]	3.34(4)	H31	C23[2]	3.58(4)
H31	H7[8]	3.10(5)	H31	H8[8]	2.87(5)
H31	H10[8]	2.70(5)	H31	H16A	3.500
H31	H21[2]	3.60(5)	H31	H26[12]	3.45(5)
H32	O9[10]	2.68(4)	H32	C13[8]	3.19(3)
H32	C17[10]	3.41(3)	H32	C23[2]	3.23(3)
H32	C25[2]	3.56(3)	H32	H10[8]	2.68(4)
H32	H17A[10]	2.718	H32	H17B[10]	3.590
H32	H17C[10]	3.454	H32	H21[2]	2.97(5)
H32	H22[2]	3.28(4)	H32	H23[2]	3.29(4)
H32	H29[10]	3.02(5)	H33A	C12[8]	3.504
H33A	C13[8]	2.887	H33A	H2[13]	3.087
H33A	H6[8]	3.360	H33A	H8[8]	3.442
H33A	H10[8]	2.343	H33A	H11[8]	3.371
H33A	H17C[13]	3.123	H33B	O5	2.923
H33B	C8[8]	3.293	H33B	H5[8]	2.905
H33B	H6[8]	2.928	H33B	H8[8]	3.089

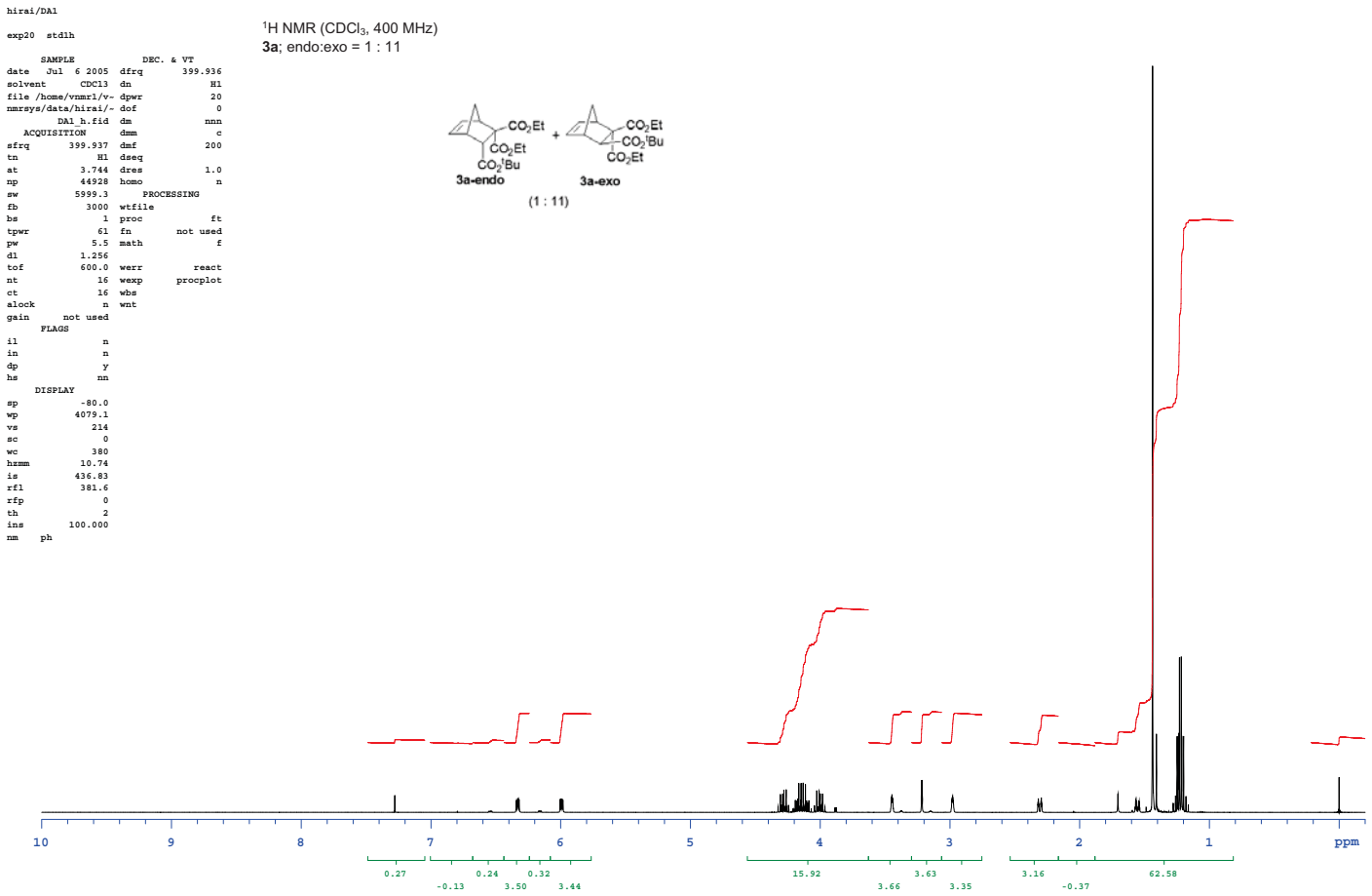
Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

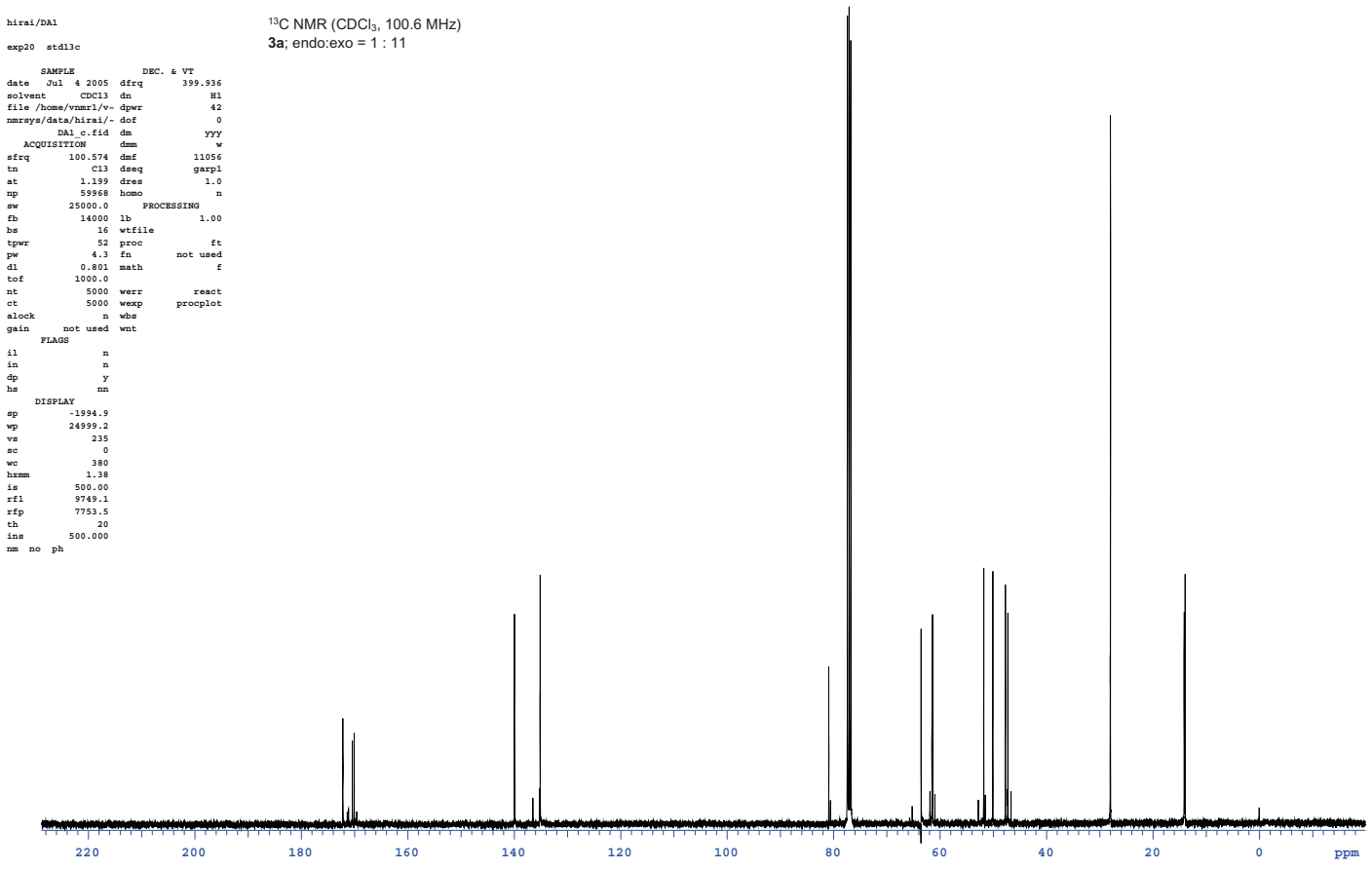
atom	atom	distance	atom	atom	distance
H33B	H10[8]	3.202	H33B	H12[6]	3.124
H33B	H16A	3.175	H34A	O2[6]	3.585
H34A	H13[13]	3.485	H34A	H16[13]	3.122
H34A	H17C[13]	3.261	H34A	H24[14]	2.598
H34B	O2[6]	2.531	H34B	C14[6]	3.525
H34B	H12[6]	2.656	H34B	H13[13]	3.129
H34B	H16[13]	3.500	H34B	H28[7]	3.099
H34C	O3[13]	2.684	H34C	O4[13]	2.942
H34C	C9[13]	2.829	H34C	C14[13]	2.987
H34C	C15[13]	3.486	H34C	H2[13]	3.516
H34C	H6[8]	3.509	H34C	H12[6]	3.284
H34C	H13[13]	2.274	H34C	H14[6]	3.443
H34C	H16[13]	3.028	H33	O7[2]	3.30(3)
H33	O8[12]	3.28(3)	H33	O11[12]	2.75(3)
H33	C18[2]	3.38(3)	H33	C19[12]	3.10(3)
H33	C23[2]	3.40(4)	H33	C24[12]	3.35(3)
H33	C25[2]	3.27(3)	H33	C27[12]	3.55(3)
H33	H17A[10]	3.408	H33	H17C[10]	3.390
H33	H18[12]	2.40(4)	H33	H21[2]	3.57(5)
H33	H22[2]	2.65(4)	H33	H23[2]	3.42(4)

Symmetry Operators:

(1) -X+2,Y+1/2-1,-Z+1
(2) X+1,Y,Z
(3) -X+1,Y+1/2-1,-Z+1
(4) X,Y-1,Z-1
(5) X,Y-1,Z
(6) -X+1,Y+1/2,-Z+1
(7) -X+1,Y+1/2-1,-Z+2
(8) -X+2,Y+1/2,-Z+1
(9) X-1,Y,Z
(10) -X+2,Y+1/2,-Z+2
(11) X,Y,Z+1
(12) -X+2,Y+1/2-1,-Z+2
(13) X,Y+1,Z
(14) -X+1,Y+1/2,-Z+2
(15) X,Y,Z-1
(16) X,Y+1,Z+1

II. Copies of the ^{1}H and ^{13}C NMR spectra





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ACQUISITION		dmm	c
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tn	H1	dseq	
at	3.744	dres	1.0
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nt	16	wexp	procplot
ct	16	wbs	
alock	n	wnt	
gain	not used		
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il	n		
in	n		
dp	y		
hs	nn		
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wc	380		
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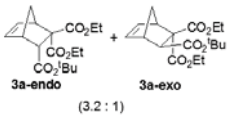

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(3.2 : 1)

hirai/DA2

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bs	16	wtfile	
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tof	1000.0		
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ct	2048	wexp	procplot
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gain	not used	wnt	
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in	n		
dp	y		
hs	nn		
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wc	380		
hzmm	1.21		
is	500.00		
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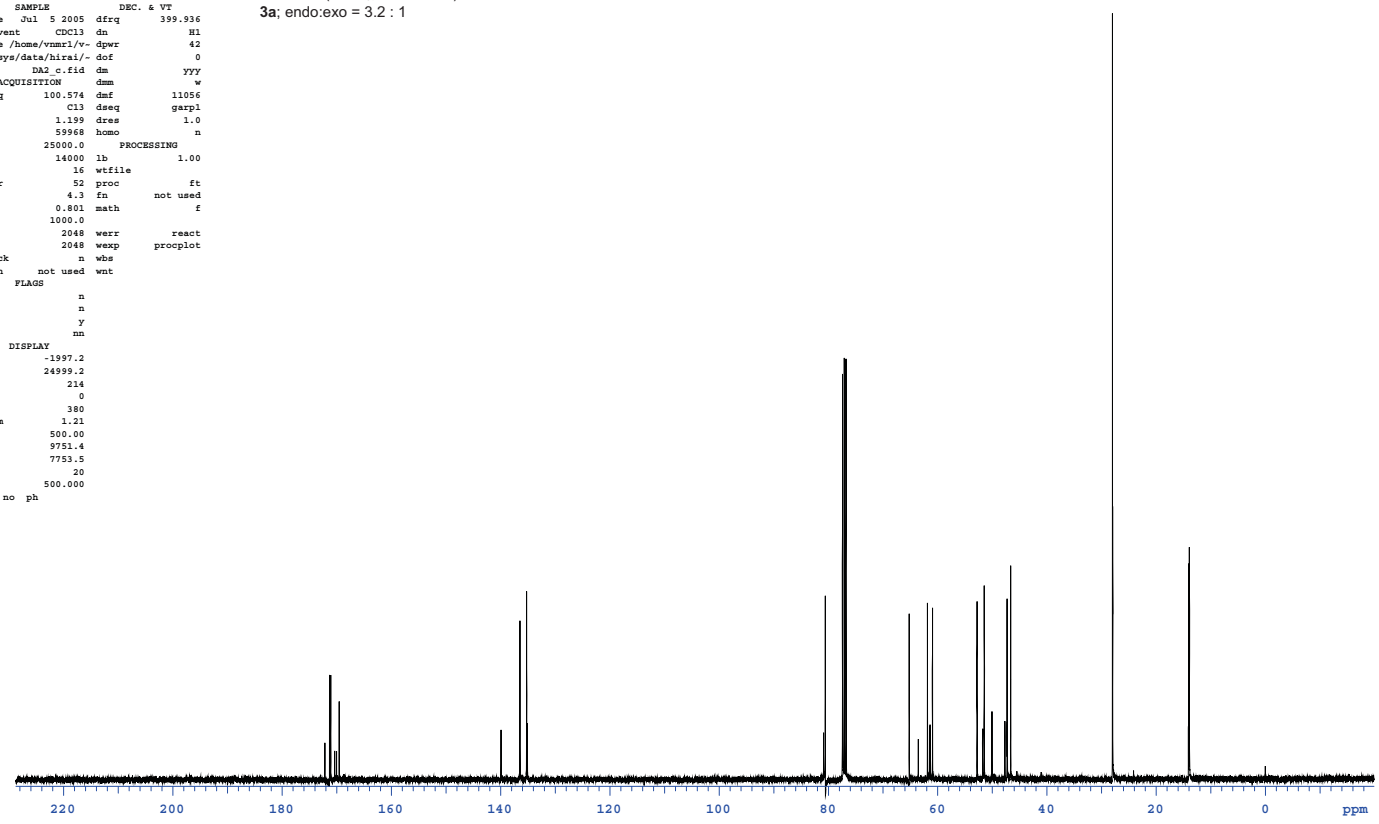
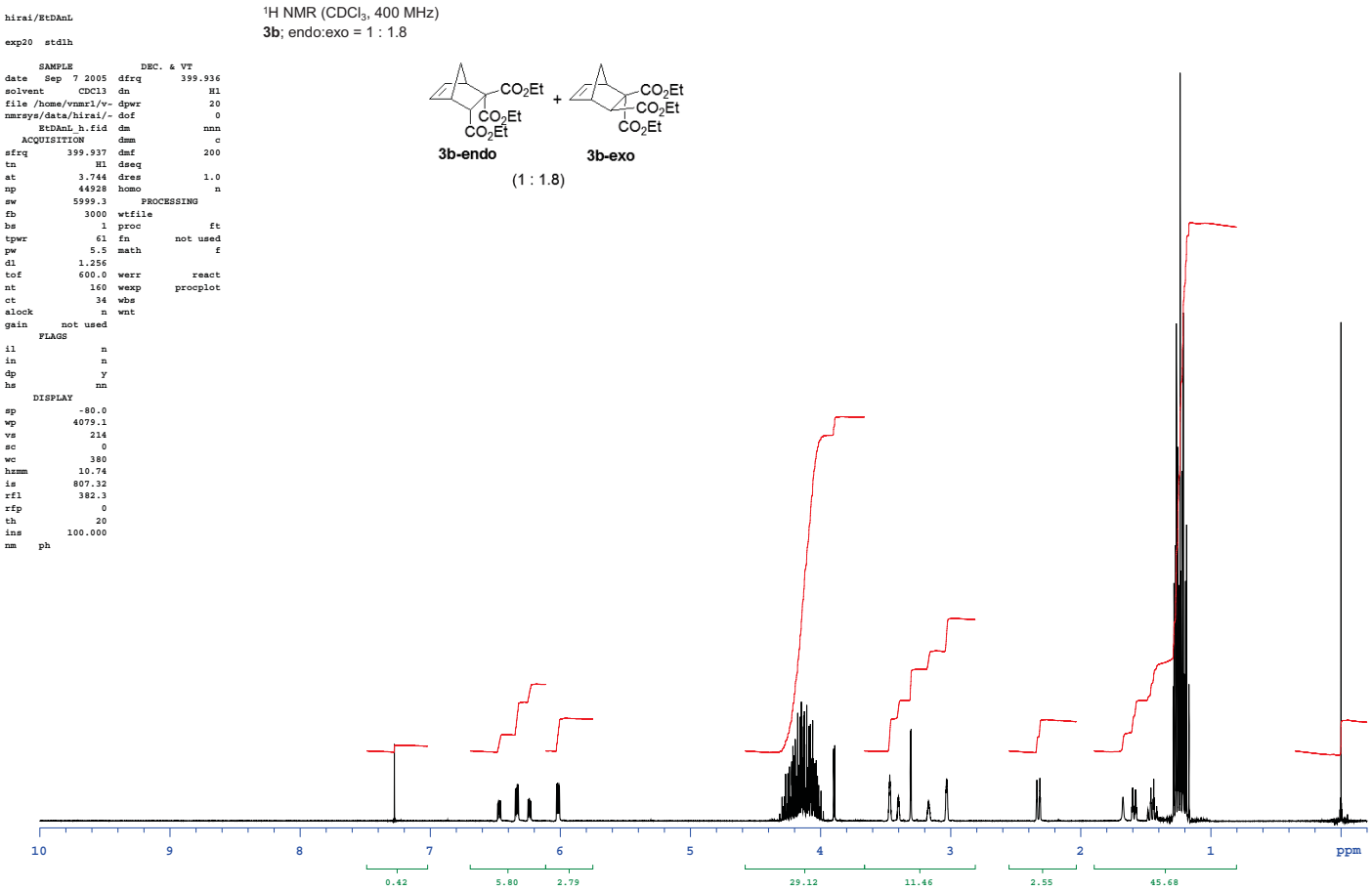
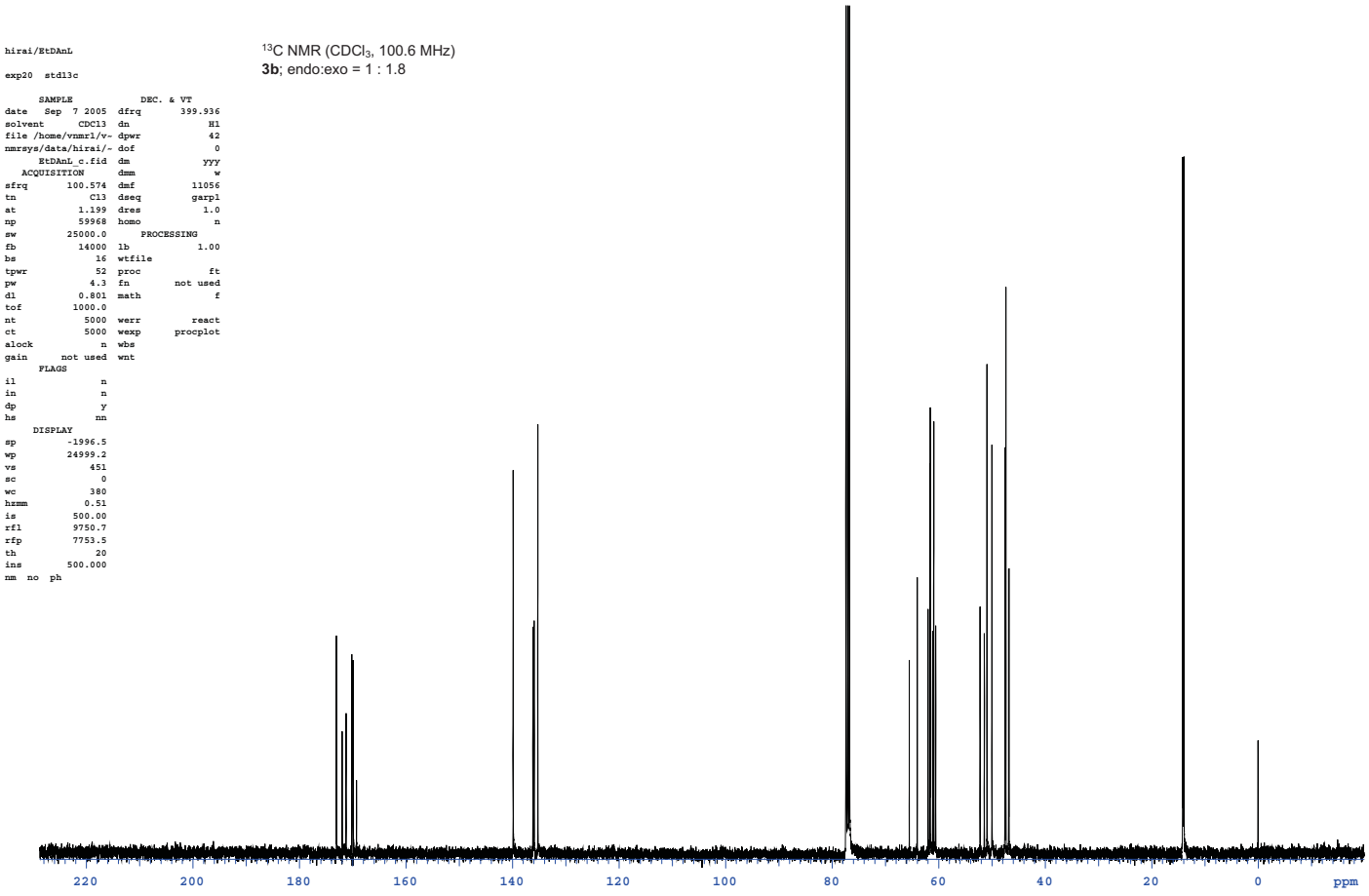



hirai/EtDAnL
exp20 stdlh
SAMPLE
date Sep 7 2005
solvent CDCl3
file /home/vnmrl/v~
nmrsys/data/hirai/~
EtDAnL_h.fid
ACQUISITION
sfrq 399.937
tn H1
at 3.744
np 44928
sw 5999.3
fb 3000
bs 1
tpwr 61
pw 5.5
dl 1.256
tof 600.0
nt 160
ct 34
alock n
gain not used
FLAGS
il n
in n
dp y
hs nn
DISPLAY
sp -80.0
wp 4079.1
vs 214
sc 0
wc 380
hzmm 10.74
is 807.32
rfl 382.3
rfp 0
th 20
ins 100.000
nm ph
DEC. & VT
dfrq 399.936
dn H1
dpwr 20
dof 0
dm nnn
dmm c
dmf 200
dseq
dres 1.0
homo n
PROCESSING
wtfile
proc ft
fn not used
math f
werr react
wexp procplot
wbs
wnt
1H NMR (CDCl3, 400 MHz)
3b; endo:exo = 1 : 1.8
CO2Et
CO2Et
CO2Et
3b-endo
+
3b-exo
(1 : 1.8)
10
9
8
7
6
5
4
3
2
1
ppm
0.42
5.80
2.79
29.12
11.46
2.55
45.68

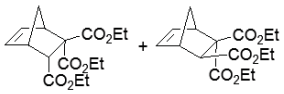

hirai/EtDAnL
exp20 stdl3c
SAMPLE
date Sep 7 2005
solvent CDCl3
file /home/vnmrl/v~
nmrsys/data/hirai/~
EtDAnL_c.fid
ACQUISITION
sfrq 100.574
tn C13
at 1.199
np 59968
sw 25000.0
fb 14000
bs 16
tpwr 52
pw 4.3
dl 0.801
tof 1000.0
nt 5000
ct 5000
alock n
gain not used
FLAGS
il n
in n
dp y
hs nn
DISPLAY
sp -1996.5
wp 24999.2
vs 451
sc 0
wc 380
hzmm 0.51
is 500.00
rfl 9750.7
rfp 7753.5
th 20
ins 500.000
nm no ph
DEC. & VT
dfrq 399.936
dn H1
dpwr 42
dof 0
dm yyy
dmm w
dmf 11056
dseq garp1
dres 1.0
homo n
PROCESSING
lb 1.00
wtfile
proc ft
fn not used
math f
werr react
wexp procplot
wbs
wnt
13C NMR (CDCl3, 100.6 MHz)
3b; endo:exo = 1 : 1.8
220
200
180
160
140
120
100
80
60
40
20
0
ppm

hirai/EtDALA

exp20 stdlh

SAMPLE		DEC. & VT	
date	Sep 6 2005	dfrq	399.936
solvent	CDCl3	dn	H1
file	/home/vnmrl/v~	dpwr	20
nmrsys/data/hirai/~		dof	0
	EtDALA_h.fid	dm	nnn
ACQUISITION		dmm	c
sfrq	399.937	dmf	200
tn	H1	dseq	
at	3.744	dres	1.0
np	44928	homo	n
sw	5999.3	PROCESSING	
fb	3000	wtfile	
bs	1	proc	ft
tpwr	61	fn	not used
pw	5.5	math	f
d1	1.256		
tof	600.0	werr	react
nt	160	wexp	procplot
ct	19	wbs	
alock	n	wnt	
gain	not used		
FLAGS			
il	n		
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-80.0		
wp	4079.1		
vs	214		
sc	0		
wc	380		
hzmm	10.74		
is	905.77		
rfl	382.8		
rfp	0		
th	20		
ins	100.000		
nm	ph		

^{1}H NMR ($CDCl_3$, 400 MHz)
3b; endo:exo = 3.3 : 1



3b-endo **3b-exo**

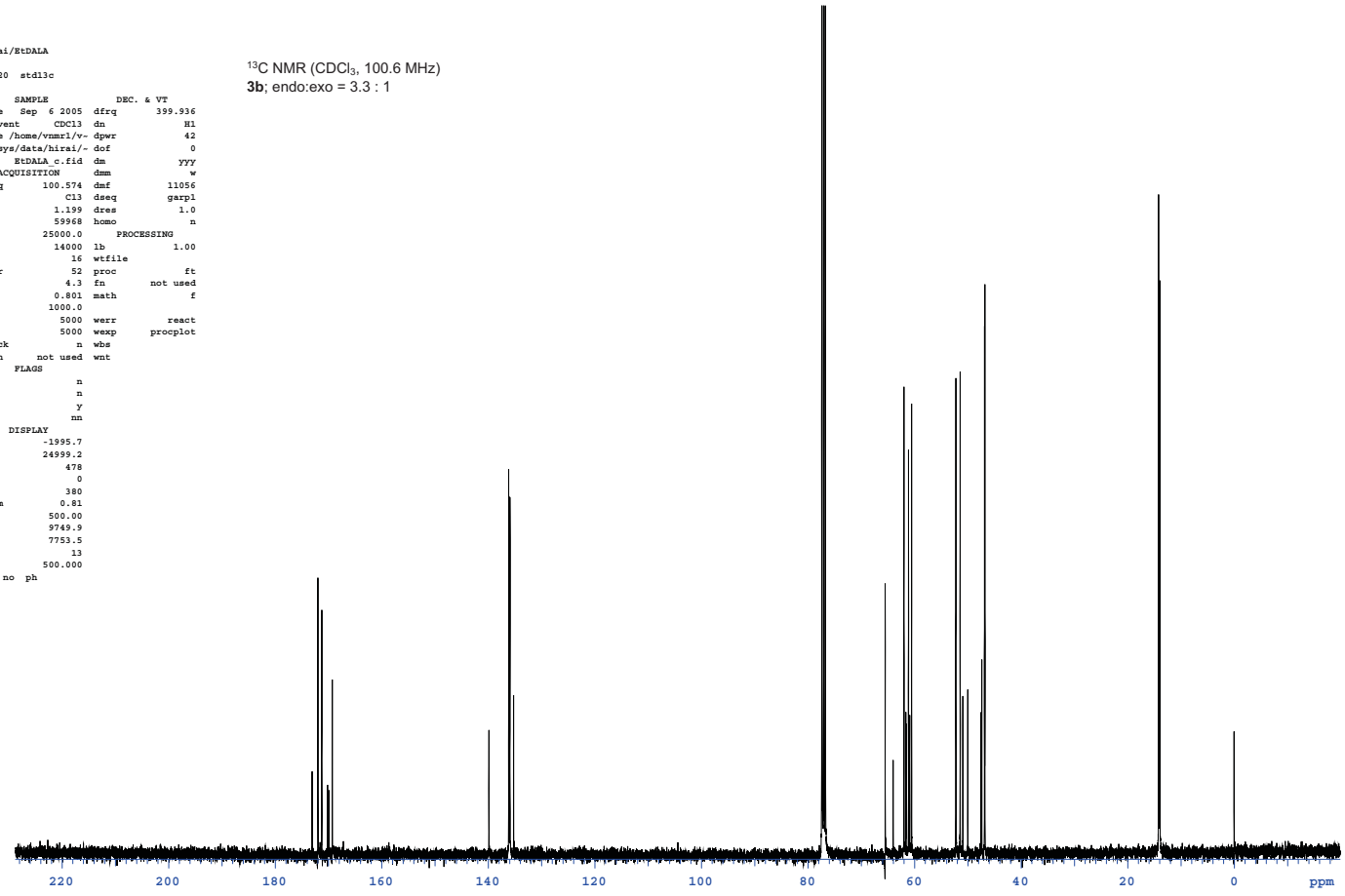
(3.3 : 1)

hirai/EtDALA

exp20 stdl3c

SAMPLE		DEC. & VT	
date	Sep 6 2005	dfrq	399.936
solvent	CDCl3	dn	H1
file	/home/vnmrl/v~	dpwr	42
nmrsys/data/hirai/~		dof	0
	EtDALA_c.fid	dm	yyy
ACQUISITION		dmm	w
sfrq	100.574	dmf	11056
tn	C13	dseq	garp1
at	1.199	dres	1.0
np	59968	homo	n
sw	25000.0	PROCESSING	
fb	14000	lb	1.00
bs	16	wtfile	
tpwr	52	proc	ft
pw	4.3	fn	not used
d1	0.801	math	f
tof	1000.0		
nt	5000	werr	react
ct	5000	wexp	procplot
alock	n	wbs	
gain	not used	wnt	
FLAGS			
il	n		
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-1995.7		
wp	24999.2		
vs	478		
sc	0		
wc	380		
hzmm	0.81		
is	500.00		
rfl	9749.9		
rfp	7753.5		
th	13		
ins	500.000		
nm	no ph		

^{13}C NMR ($CDCl_3$, 100.6 MHz)
3b; endo:exo = 3.3 : 1



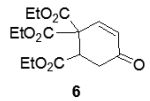
miyake/DA

exp20 stdlh

SAMPLE		DEC. & VT	
date	Jun 8 2012	dfrq	399.956
solvent	CDCl3	dn	H1
file	/home/vnmrl/v~	dpwr	20
nmrsys/data/miyake~		dof	0
	/DA_h.fid	dm	nnn
ACQUISITION		dmm	c
sfrq	399.956	dmf	200
tn	H1	dseq	
at	3.744	dres	1.0
np	44928	homo	n
sw	6000.6	PROCESSING	
fb	not used	wtfile	
bs	1	proc	ft
tpwr	61	fn	not used
pw	5.5	math	f
d1	1.256		
tof	600.0	werr	react
nt	16	wexp	procplot
ct	16	wbs	
alock	n	wnt	
gain	not used		
FLAGS			
il	n		
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-80.0		
wp	4079.4		
vs	214		
sc	0		
wc	380		
hzmm	10.74		
is	1743.09		
rfl	377.8		
rfp	0		
th	20		
ins	100.000		
nm	ph		

^{1}H NMR ($CDCl_3$, 400 MHz)

6



6

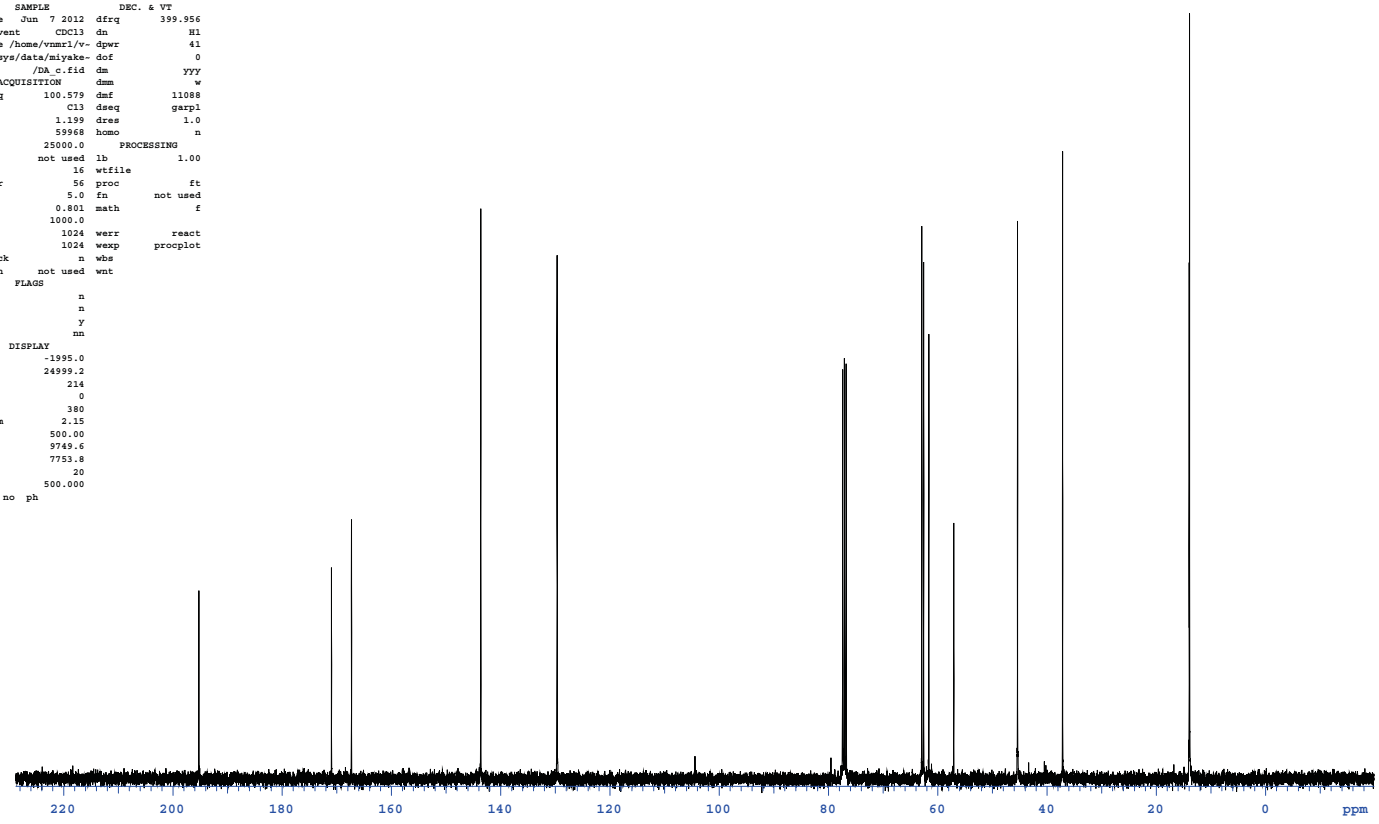
miyake/DA

exp20 stdl3c

SAMPLE		DEC. & VT	
date	Jun 7 2012	dfrq	399.956
solvent	CDCl3	dn	H1
file	/home/vnmrl/v~	dpwr	41
nmrsys/data/miyake~		dof	0
	/DA_c.fid	dm	yyy
ACQUISITION		dmm	w
sfrq	100.579	dmf	11088
tn	C13	dseq	garp1
at	1.199	dres	1.0
np	59968	homo	n
sw	25000.0	PROCESSING	
fb	not used	lb	1.00
bs	16	wtfile	
tpwr	56	proc	ft
pw	5.0	fn	not used
d1	0.801	math	f
tof	1000.0		
nt	1024	werr	react
ct	1024	wexp	procplot
alock	n	wbs	
gain	not used	wnt	
FLAGS			
il	n		
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-1995.0		
wp	24999.2		
vs	214		
sc	0		
wc	380		
hzmm	2.15		
is	500.00		
rfl	9749.6		
rfp	7753.8		
th	20		
ins	500.000		
nm	no ph		

^{13}C NMR ($CDCl_3$, 100.6 MHz)

6



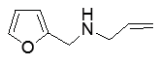
^{1}H NMR ($CDCl_3$, 400 MHz)

8a

```
niina/furanN

exp20  stdlh

      SAMPLE           DEC. & VT
date   Nov 15 2013  dfrq       399.956
solvent      CDCl3  dn              H1
file /home/vnmrl/v~ dpwr            20
nmrsys/data/niina/~ dof              0
      furanN_h.fid  dm             nnn
   ACQUISITION      dmm              c
sfrq       399.956  dmf            200
tn              H1  dseq
at           3.744  dres           1.0
np           44928  homo             n
sw          6000.6      PROCESSING
fb         not used  wtfile
bs                1  proc            ft
tpwr             61  fn         not used
pw              5.5  math             f
d1            1.256
tof           600.0  werr         react
nt               16  wexp      procplot
ct               16  wbs
alock             n  wnt
gain       not used
      FLAGS
il                n
in                n
dp                y
hs               nn
     DISPLAY
sp            -80.0
wp           4079.4
vs              214
sc                0
wc              380
hzmm          10.74
is          1844.61
rfl           381.3
rfp               0
th               20
ins          100.000
nm    ph
```



8a

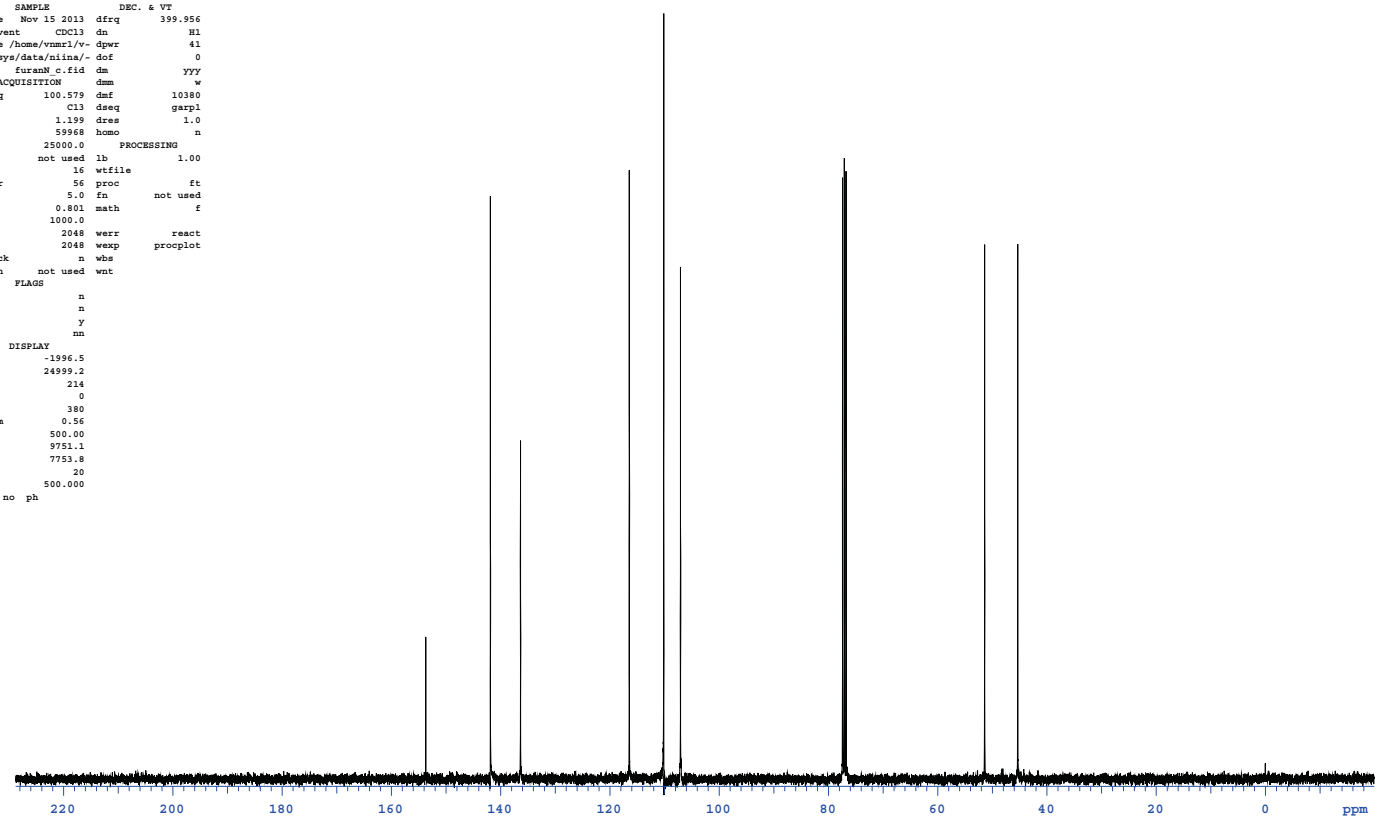
^{13}C NMR ($CDCl_3$, 100.6 MHz)

8a

```
niina/furanN

exp20  stdl3c

      SAMPLE           DEC. & VT
date   Nov 15 2013  dfrq       399.956
solvent      CDCl3  dn              H1
file /home/vnmrl/v~ dpwr            41
nmrsys/data/niina/~ dof              0
      furanN_c.fid  dm             yyy
   ACQUISITION      dmm              w
sfrq       100.579  dmf          10380
tn              C13  dseq         garp1
at           1.199  dres           1.0
np           59968  homo             n
sw       25000.0      PROCESSING
fb         not used  lb            1.00
bs               16  wtfile
tpwr             56  proc            ft
pw              5.0  fn         not used
d1            0.801  math             f
tof          1000.0
nt               2048  werr         react
ct               2048  wexp      procplot
alock             n  wbs
gain       not used  wnt
      FLAGS
il                n
in                n
dp                y
hs               nn
     DISPLAY
sp          -1996.5
wp          24999.2
vs              214
sc                0
wc              380
hzmm           0.56
is           500.00
rfl          9751.1
rfp          7753.8
th               20
ins          500.000
nm  no  ph
```



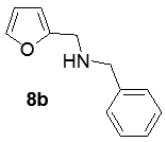
niina/BzNFur

exp20 stdlh

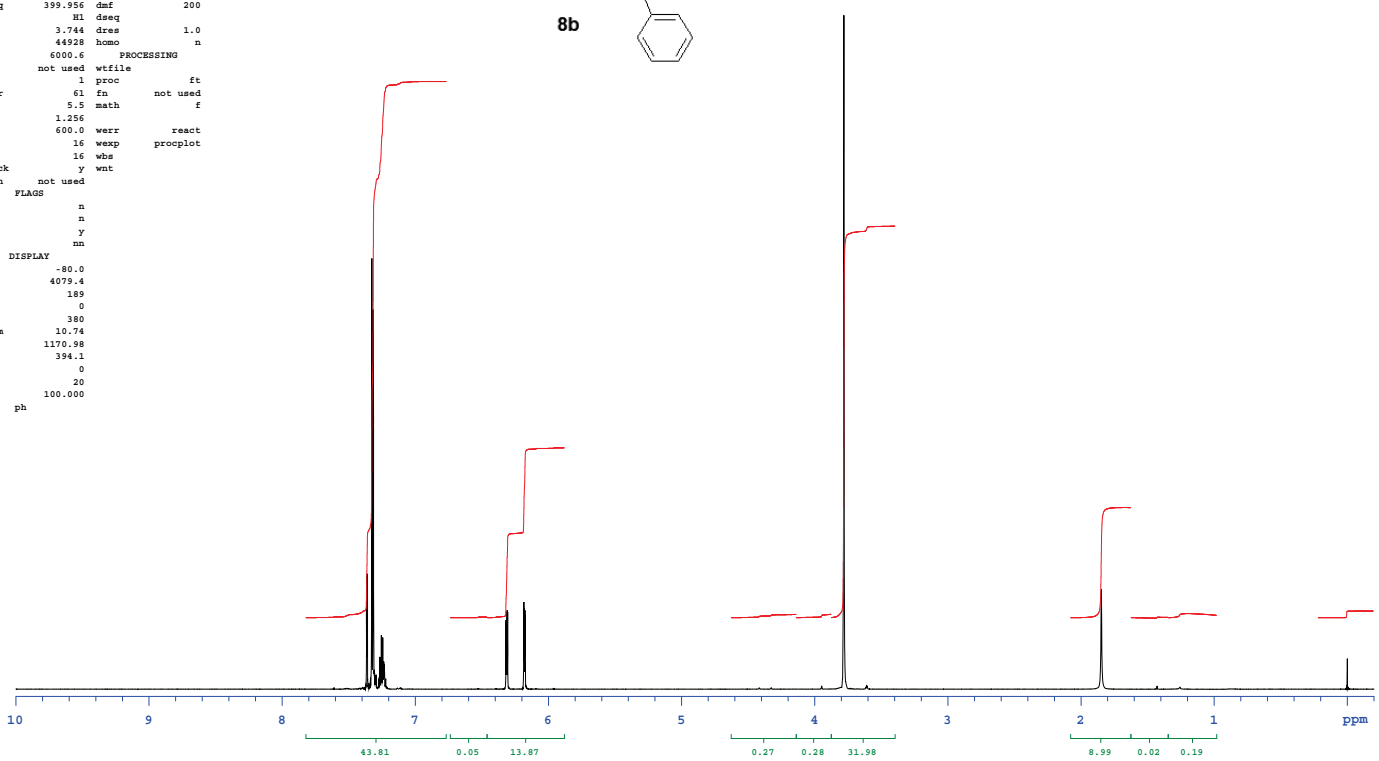
SAMPLE		DEC. & VT	
date	Nov 26 2013	dfrq	399.956
solvent	CDCl3	dn	H1
file	/home/vnmrl/v~	dpwr	20
nmrsys/data/niina/~		dof	0
	BzNFur_h.fid	dm	nnn
ACQUISITION		dmm	c
sfrq	399.956	dmf	200
tn	H1	dseq	
at	3.744	dres	1.0
np	44928	homo	n
sw	6000.6	PROCESSING	
fb	not used	wtfile	
bs	1	proc	ft
tpwr	61	fn	not used
pw	5.5	math	f
d1	1.256		
tof	600.0	werr	react
nt	16	wexp	procplot
ct	16	wbs	
alock	y	wnt	
gain	not used		
FLAGS			
il	n		
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-80.0		
wp	4079.4		
vs	189		
sc	0		
wc	380		
hzmm	10.74		
is	1170.98		
rfl	394.1		
rfp	0		
th	20		
ins	100.000		
nm	ph		

^{1}H NMR ($CDCl_3$, 400 MHz)

8b



8b



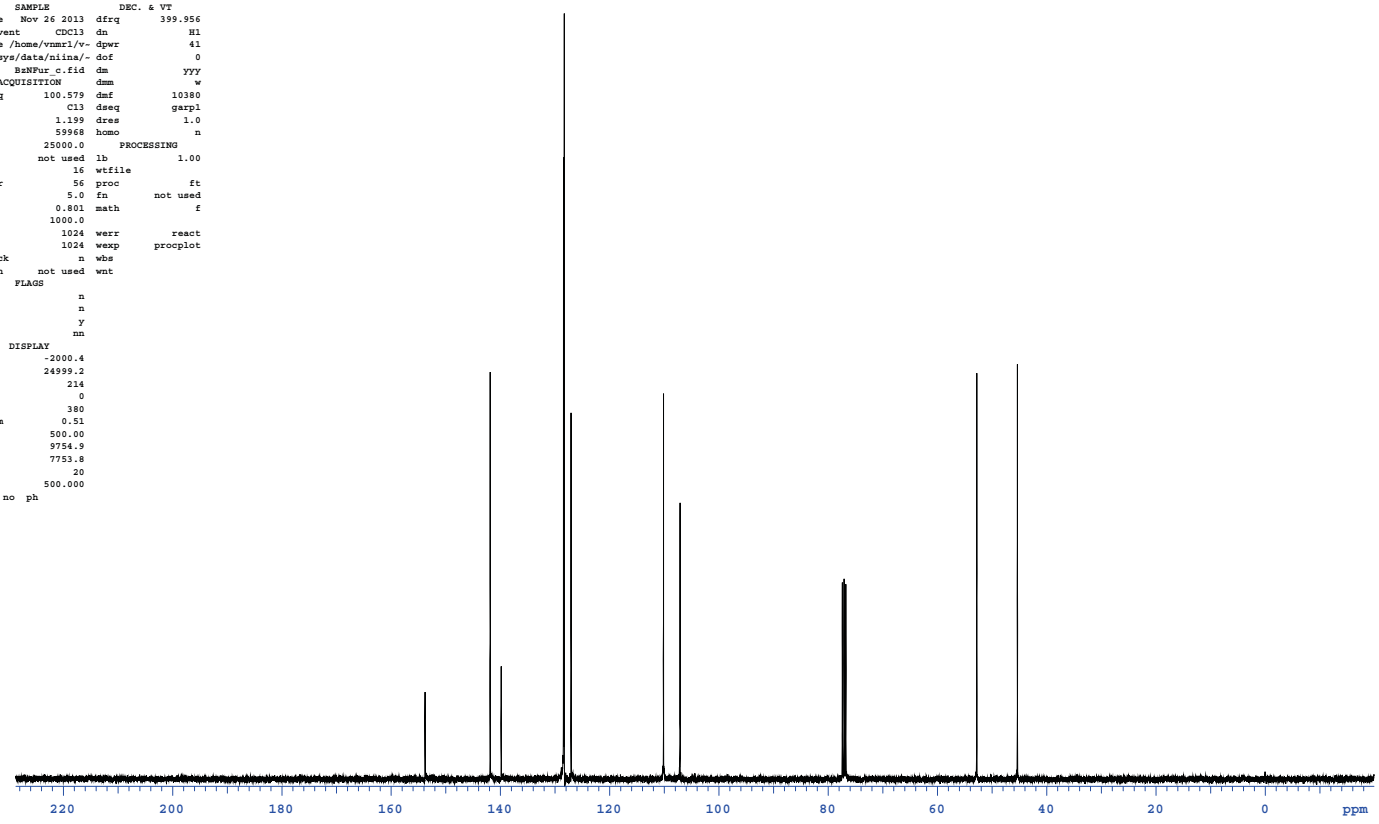
niina/BzNFur

exp20 stdl3c

SAMPLE		DEC. & VT	
date	Nov 26 2013	dfrq	399.956
solvent	CDCl3	dn	H1
file	/home/vnmrl/v~	dpwr	41
nmrsys/data/niina/~		dof	0
	BzNFur_c.fid	dm	yyy
ACQUISITION		dmm	w
sfrq	100.579	dmf	10380
tn	C13	dseq	garp1
at	1.199	dres	1.0
np	59968	homo	n
sw	25000.0	PROCESSING	
fb	not used	lb	1.00
bs	16	wtfile	
tpwr	56	proc	ft
pw	5.0	fn	not used
d1	0.801	math	f
tof	1000.0		
nt	1024	werr	react
ct	1024	wexp	procplot
alock	n	wbs	
gain	not used	wnt	
FLAGS			
il	n		
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-2000.4		
wp	24999.2		
vs	214		
sc	0		
wc	380		
hzmm	0.51		
is	500.00		
rfl	9754.9		
rfp	7753.8		
th	20		
ins	500.000		
nm	no ph		

^{13}C NMR ($CDCl_3$, 100.6 MHz)

8b



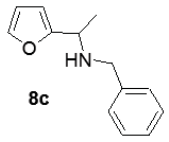
^{1}H NMR ($CDCl_3$, 400 MHz)

8c

```
miyake3/EtFuranN

exp20  PROTON

      SAMPLE          PRESATURATION
date   Jun 25 2014  satmode          n
solvent      cdcl3  wet              n
file /home/vnmrl/v-     SPECIAL
nmrsys/data/miyake- temp       not used
  3/EtfuranN_h.fid  gain       not used
   ACQUISITION      spin            20
sw          6402.0  hst           0.008
at           3.500  pw90         11.000
np           44814  alfa         10.000
fb       not used        FLAGS
bs                4  il               n
dl            1.500  in               n
nt               16  dp               y
ct               16  hs              nn
   TRANSMITTER           PROCESSING
tn               H1  lb            0.20
sfrq       399.956  fn        not used
tof          400.0       DISPLAY
tpwr            61  sp           -80.1
pw           5.500  wp          4079.4
     DECOUPLER      rfl          790.9
dn              C13  rfp             0
dof               0  rp           141.5
dm              nnn  lp           -43.9
decwave W40_HCN5mm        PLOT
dpwr             33  wc             382
dmf           29412  sc               0
                     vs              60
                     th               0
                     ai    ph
```



8c

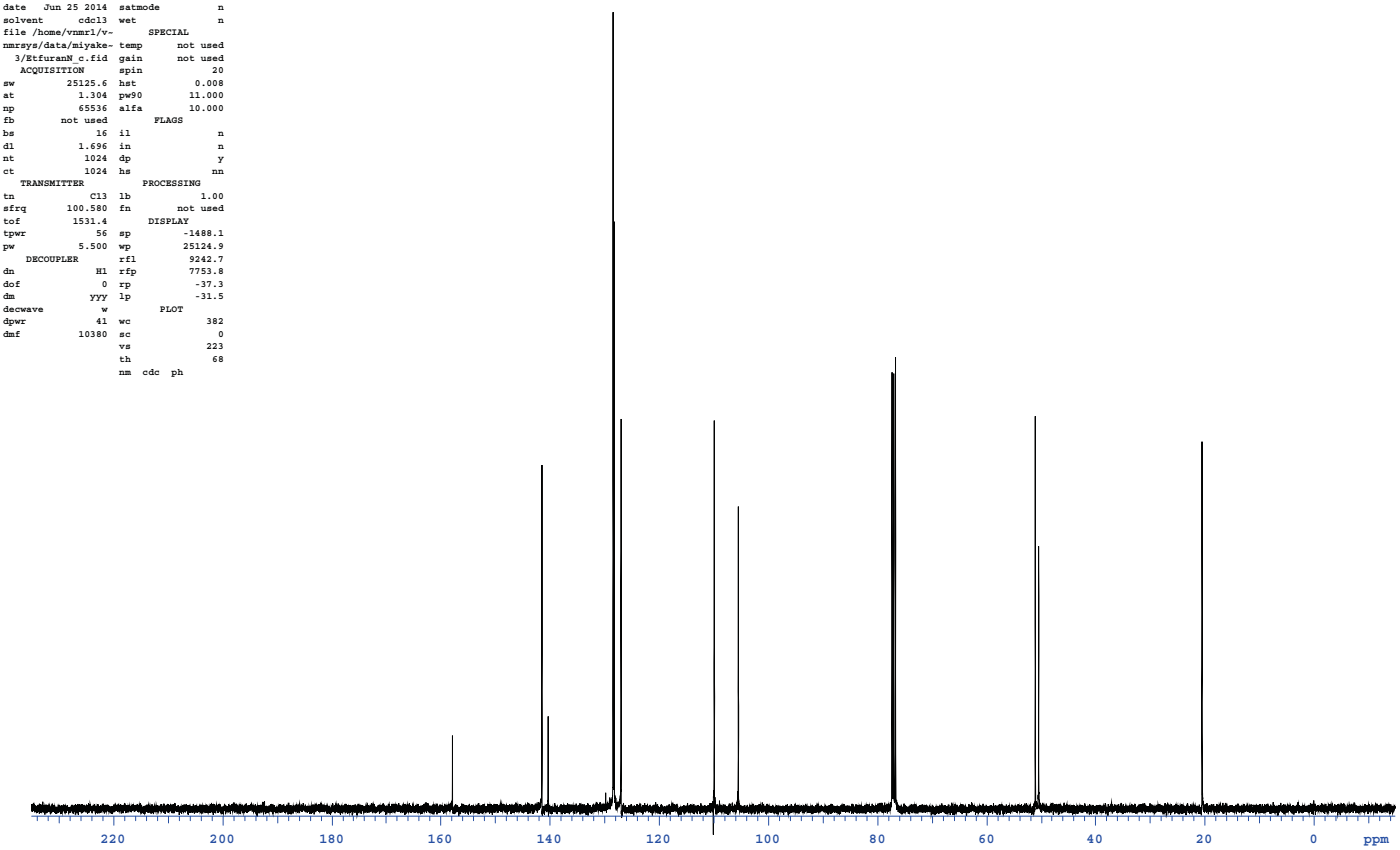
^{13}C NMR ($CDCl_3$, 100.6 MHz)

8c

```
miyake3/EtFuranN

exp20  CARBON

      SAMPLE          PRESATURATION
date   Jun 25 2014  satmode          n
solvent      cdcl3  wet              n
file /home/vnmrl/v-     SPECIAL
nmrsys/data/miyake- temp       not used
  3/EtfuranN_c.fid  gain       not used
   ACQUISITION      spin            20
sw         25125.6  hst           0.008
at           1.304  pw90         11.000
np           65536  alfa         10.000
fb       not used        FLAGS
bs                16  il               n
dl            1.696  in               n
nt             1024  dp               y
ct             1024  hs              nn
   TRANSMITTER           PROCESSING
tn               C13  lb            1.00
sfrq       100.580  fn        not used
tof         1531.4       DISPLAY
tpwr            56  sp          -1488.1
pw           5.500  wp         25124.9
     DECOUPLER      rfl          9242.7
dn               H1  rfp          7753.8
dof               0  rp            -37.3
dm              yyy  lp            -31.5
decwave           w        PLOT
dpwr             41  wc             382
dmf           10380  sc               0
                     vs             223
                     th              68
                     nm  cdc  ph
```



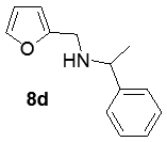
^{1}H NMR ($CDCl_3$, 400 MHz)

8d

```
miyake3/FurNEtPh

exp20  PROTON

      SAMPLE          PRESATURATION
date   Aug 23 2014  satmode          n
solvent       c6d6  wet              n
file /home/vnmr1/v-     SPECIAL
nmrsys/data/miyake- temp       not used
  3/FurNEtPh_h.fid  gain       not used
   ACQUISITION      spin            20
sw          6402.0  hst           0.008
at           3.500  pw90         11.000
np           44814  alfa         10.000
fb       not used        FLAGS
bs                4  il               n
d1            1.500  in               n
nt               16  dp               y
ct               16  hs              nn
   TRANSMITTER          PROCESSING
tn               H1  lb            0.20
sfrq        399.956  fn       not used
tof           400.0      DISPLAY
tpwr             61  sp           -80.1
pw            5.500  wp          4079.4
   DECOUPLER         rfl           753.2
dn               C13  rfp             0
dof                0  rp            140.9
dm               nnn  lp            -43.2
decwave W40_HCN5mm       PLOT
dpwr              33  wc             382
dmf            29412  sc               0
                      vs              64
                      th               0
                      ai    ph
```



8d

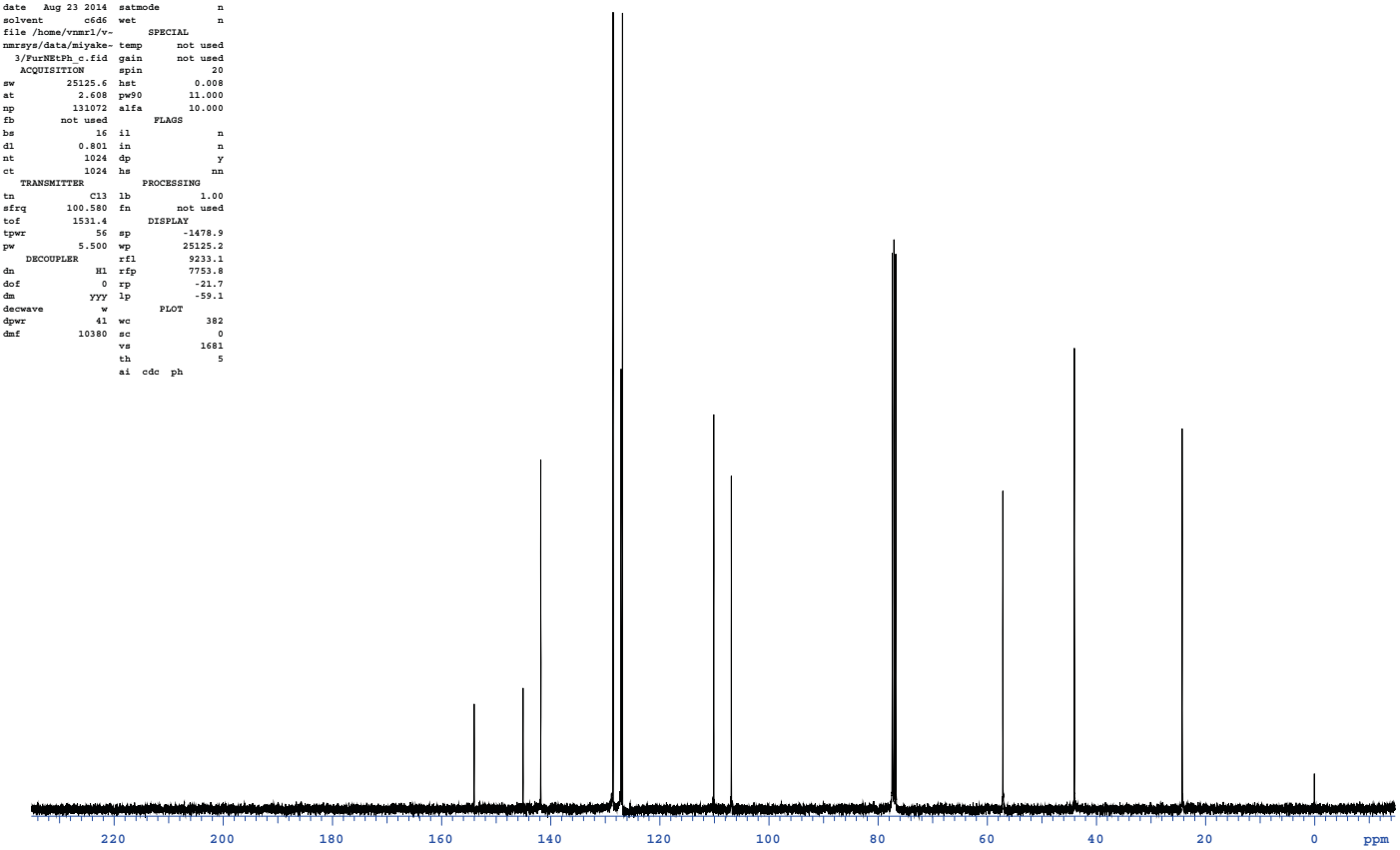

```
miyake3/FurNEtPh

exp20  CARBON

      SAMPLE          PRESATURATION
date   Aug 23 2014  satmode          n
solvent       c6d6  wet              n
file /home/vnmr1/v-     SPECIAL
nmrsys/data/miyake- temp       not used
  3/FurNEtPh_c.fid  gain       not used
   ACQUISITION      spin            20
sw         25125.6  hst           0.008
at           2.608  pw90         11.000
np          131072  alfa         10.000
fb       not used        FLAGS
bs                16  il               n
d1             0.801  in               n
nt              1024  dp               y
ct              1024  hs              nn
   TRANSMITTER          PROCESSING
tn               C13  lb            1.00
sfrq        100.580  fn       not used
tof          1531.4      DISPLAY
tpwr             56  sp         -1478.9
pw            5.500  wp         25125.2
   DECOUPLER         rfl          9233.1
dn               H1  rfp          7753.8
dof                0  rp           -21.7
dm               yyy  lp           -59.1
decwave            w       PLOT
dpwr              41  wc             382
dmf            10380  sc               0
                      vs            1681
                      th               5
                      ai  cdc  ph
```

^{13}C NMR ($CDCl_3$, 100.6 MHz)

8d



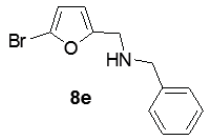
^{1}H NMR ($CDCl_3$, 400 MHz)

8e

```
nakai/BrFur

exp20  PROTON

      SAMPLE           PRESATURATION
date   Nov 21 2014  satmode          n
solvent      cdcl3  wet              n
file /home/vnmrl/v-      SPECIAL
nmrsys/data/nakai/- temp       not used
       BrFur_h.fid  gain       not used
   ACQUISITION      spin            20
sw          6402.0  hst           0.008
at           3.500  pw90         11.000
np           44814  alfa         10.000
fb       not used        FLAGS
bs                4  il               n
dl            1.500  in               n
nt               16  dp               y
ct               16  hs              nn
   TRANSMITTER           PROCESSING
tn               H1  lb            0.20
sfrq       399.956  fn        not used
tof          400.0       DISPLAY
tpwr            61  sp           -80.1
pw           5.500  wp          4079.4
      DECOUPLER      rfl          806.7
dn              C13  rfp             0
dof               0  rp           -41.6
dm              nnn  lp           -49.9
decwave W40_HCN5mm        PLOT
dpwr             33  wc             382
dmf           29412  sc               0
                     vs              63
                     th               0
                     ai    ph
```



8e

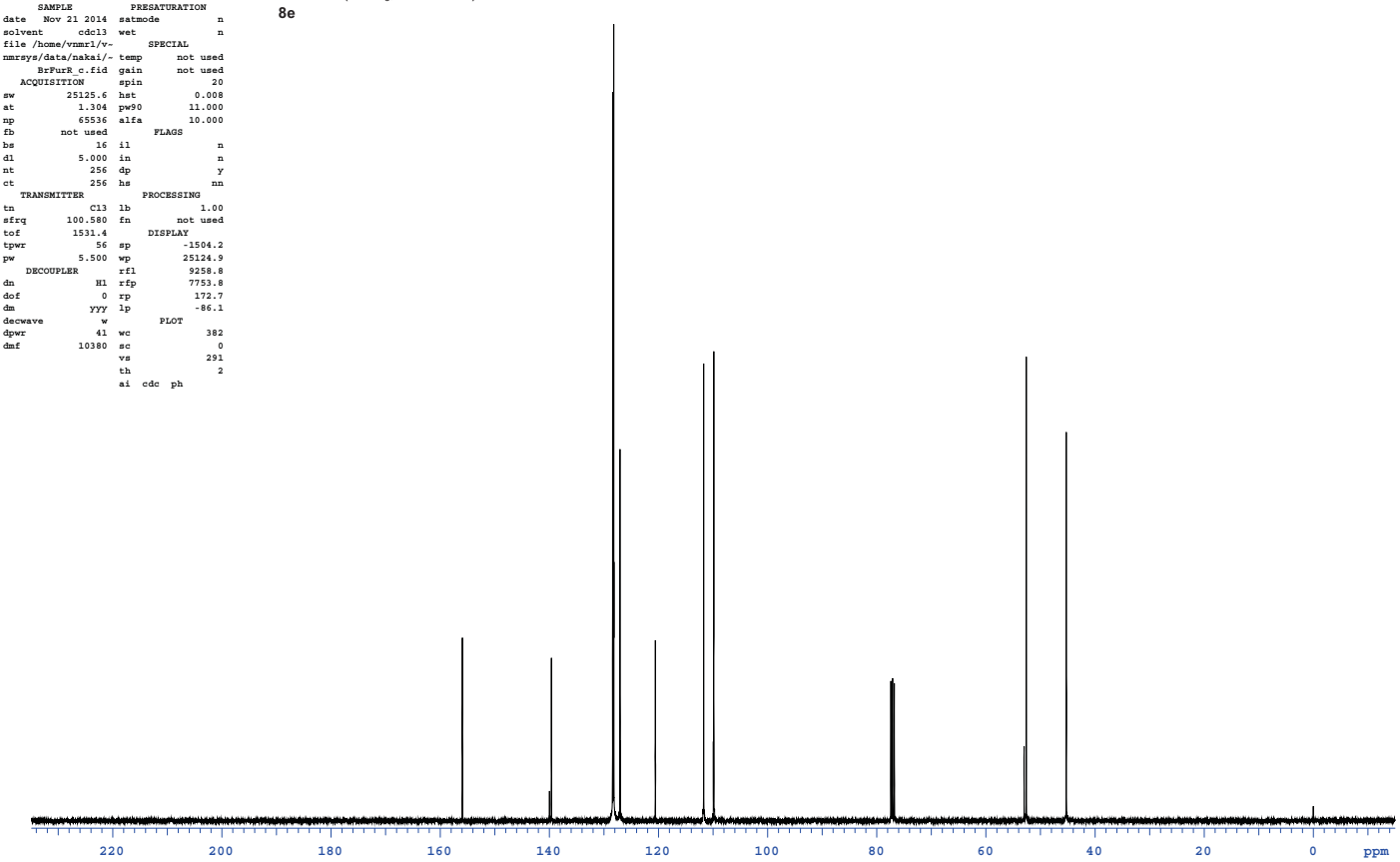

```
nakai/BrFur

exp20  CARBON

      SAMPLE           PRESATURATION
date   Nov 21 2014  satmode          n
solvent      cdcl3  wet              n
file /home/vnmrl/v-      SPECIAL
nmrsys/data/nakai/- temp       not used
       BrFurR_c.fid  gain       not used
   ACQUISITION      spin            20
sw         25125.6  hst           0.008
at           1.304  pw90         11.000
np           65536  alfa         10.000
fb       not used        FLAGS
bs               16  il               n
dl            5.000  in               n
nt              256  dp               y
ct              256  hs              nn
   TRANSMITTER           PROCESSING
tn              C13  lb            1.00
sfrq       100.580  fn        not used
tof         1531.4       DISPLAY
tpwr            56  sp         -1504.2
pw           5.500  wp         25124.9
      DECOUPLER      rfl         9258.8
dn               H1  rfp         7753.8
dof               0  rp          172.7
dm              yyy  lp          -86.1
decwave           w        PLOT
dpwr             41  wc             382
dmf           10380  sc               0
                     vs             291
                     th               2
                     ai  cdc  ph
```

^{13}C NMR ($CDCl_3$, 100.6 MHz)

8e



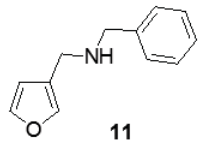
ueda/3FuranN

exp20 PROTON

SAMPLE		PRESATURATION	
date	Jul 2 2014	satmode	n
solvent	cdcl3	wet	n
file	/home/vnmrl/v-	SPECIAL	
nmrsys/data/ueda/3-		temp	not used
	FuranN_h.fid	gain	not used
ACQUISITION		spin	20
sw	6402.0	hst	0.008
at	3.500	pw90	11.000
np	44814	alfa	10.000
fb	not used	FLAGS	
bs	4	il	n
dl	1.500	in	n
nt	16	dp	y
ct	16	hs	nn
TRANSMITTER		PROCESSING	
tn	H1	lb	0.20
sfrq	399.956	fn	not used
tof	400.0	DISPLAY	
tpwr	61	sp	-80.1
pw	5.500	wp	4079.4
DECOUPLER		rfl	795.0
dn	C13	rfp	0
dof	0	rp	141.1
dm	nnn	lp	-41.3
decwave	W40_HCN5mm	PLOT	
dpwr	33	wc	382
dmf	29412	sc	0
		vs	68
		th	68
		ai ph	

^{1}H NMR ($CDCl_3$, 400 MHz)

11



11

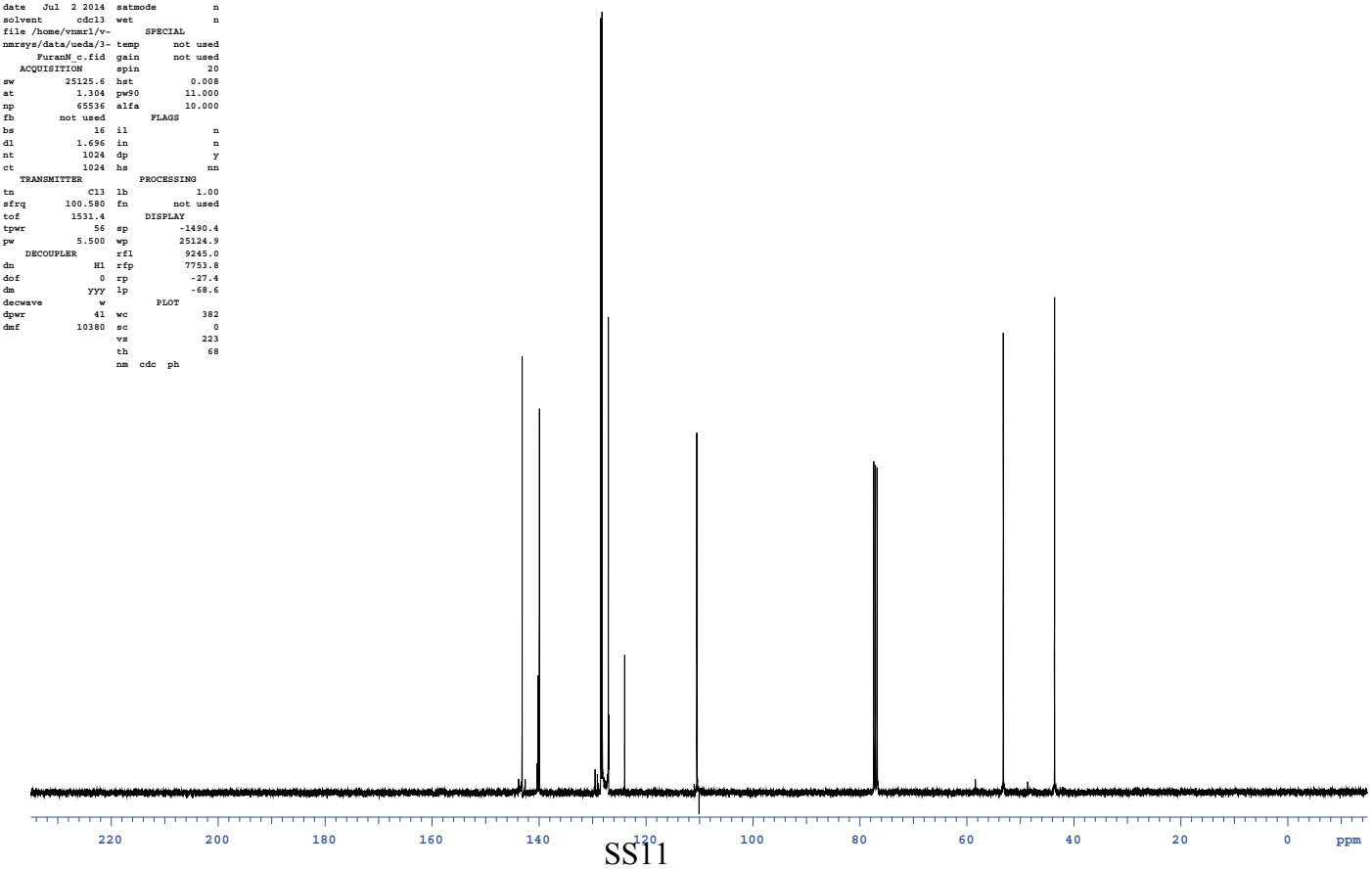
ueda/3FuranN

exp20 CARBON

SAMPLE		PRESATURATION	
date	Jul 2 2014	satmode	n
solvent	cdcl3	wet	n
file	/home/vnmrl/v-	SPECIAL	
nmrsys/data/ueda/3-		temp	not used
	FuranN_c.fid	gain	not used
ACQUISITION		spin	20
sw	25125.6	hst	0.008
at	1.304	pw90	11.000
np	65536	alfa	10.000
fb	not used	FLAGS	
bs	16	il	n
dl	1.696	in	n
nt	1024	dp	y
ct	1024	hs	nn
TRANSMITTER		PROCESSING	
tn	C13	lb	1.00
sfrq	100.580	fn	not used
tof	1531.4	DISPLAY	
tpwr	56	sp	-1490.4
pw	5.500	wp	25124.9
DECOUPLER		rfl	9245.0
dn	H1	rfp	7753.8
dof	0	rp	-27.4
dm	yyy	lp	-68.6
decwave	w	PLOT	
dpwr	41	wc	382
dmf	10380	sc	0
		vs	223
		th	68
		nm cdc ph	

^{13}C NMR ($CDCl_3$, 100.6 MHz)

11



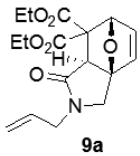
niia/furanC=Cr

exp20 stdlh

SAMPLE		DEC. & VT	
date	Nov 11 2013	dfrq	399.956
solvent	CDCl3	dn	H1
file	/home/vnmrl/v~	dpwr	20
nmrsys/data/niina/~		dof	0
furanC=Cr_h.fid		dm	nnn
ACQUISITION		dmm	c
sfrq	399.956	dmf	200
tn	H1	dseq	
at	3.744	dres	1.0
np	44928	homo	n
sw	6000.6	PROCESSING	
fb	not used	wtfile	
bs	1	proc	ft
tpwr	61	fn	not used
pw	5.5	math	f
d1	1.256		
tof	600.0	werr	react
nt	16	wexp	procplot
ct	16	wbs	
alock	y	wnt	
gain	not used		
FLAGS			
il	n		
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-80.0		
wp	4079.4		
vs	189		
sc	0		
wc	380		
hzmm	10.74		
is	1186.19		
rfl	373.8		
rfp	0		
th	20		
ins	100.000		
nm	ph		

^{1}H NMR ($CDCl_3$, 400 MHz)

9a



9a

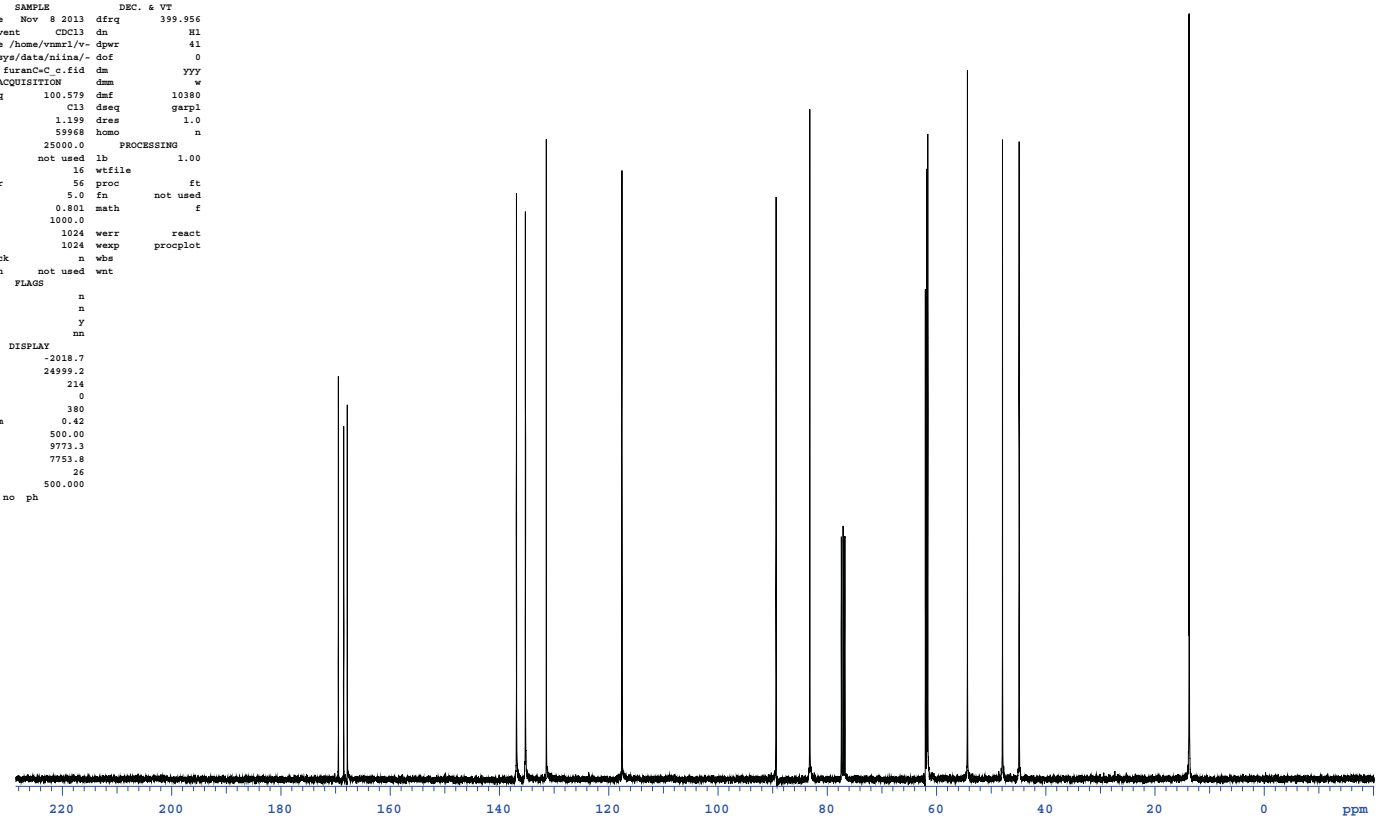
niina/furanC=C

exp20 stdl3c

SAMPLE		DEC. & VT	
date	Nov 8 2013	dfrq	399.956
solvent	CDCl3	dn	H1
file	/home/vnmrl/v~	dpwr	41
nmrsys/data/niina/~		dof	0
furanC=C_c.fid		dm	yyy
ACQUISITION		dmm	w
sfrq	100.579	dmf	10380
tn	C13	dseq	garp1
at	1.199	dres	1.0
np	59968	homo	n
sw	25000.0	PROCESSING	
fb	not used	lb	1.00
bs	16	wtfile	
tpwr	56	proc	ft
pw	5.0	fn	not used
d1	0.801	math	f
tof	1000.0		
nt	1024	werr	react
ct	1024	wexp	procplot
alock	n	wbs	
gain	not used	wnt	
FLAGS			
il	n		
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-2018.7		
wp	24999.2		
vs	214		
sc	0		
wc	380		
hzmm	0.42		
is	500.00		
rfl	9773.3		
rfp	7753.8		
th	26		
ins	500.000		
nm	no ph		

^{13}C NMR ($CDCl_3$, 100.6 MHz)

9a



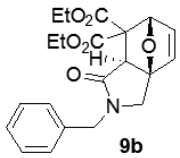
niina/BzfuranDA

exp20 stdh

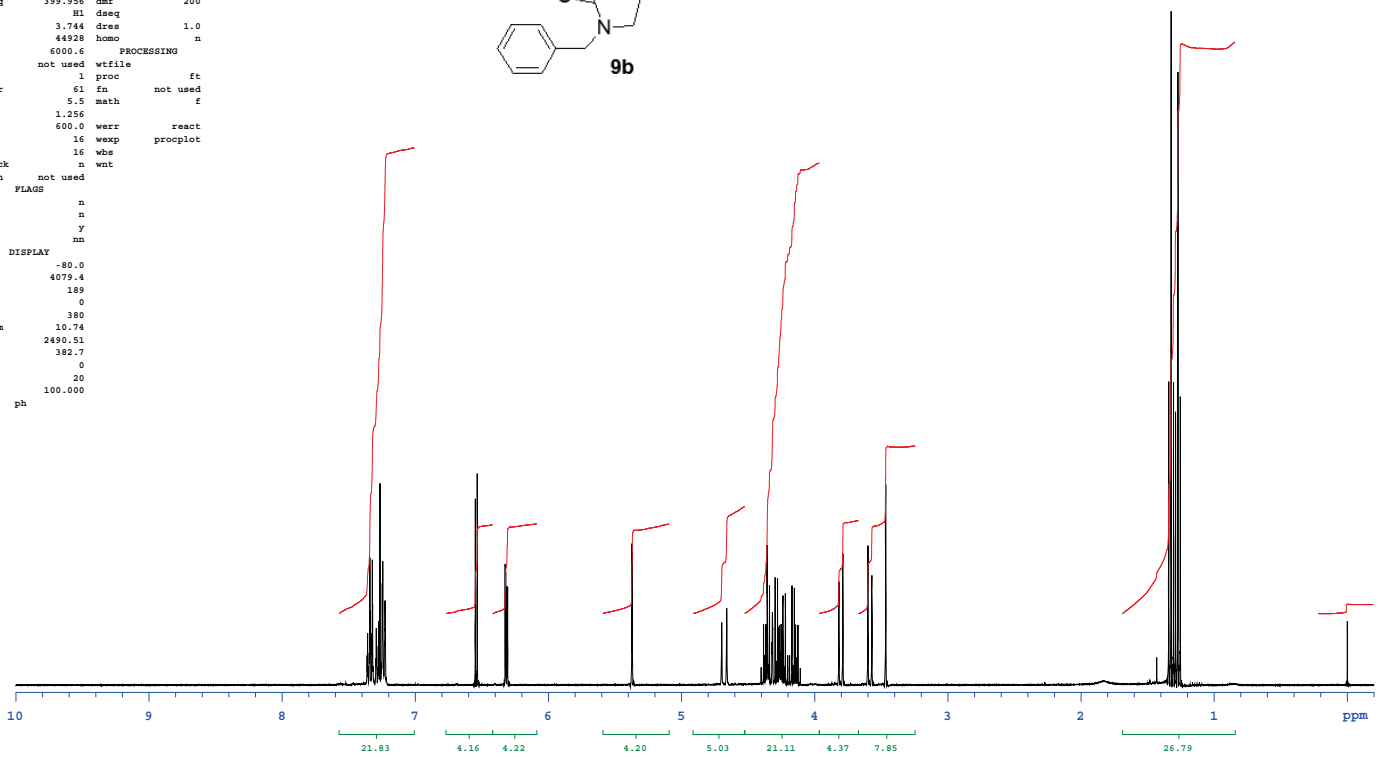
SAMPLE		DEC. & VT	
date	Dec 9 2013	dfrq	399.956
solvent	CDCl3	dn	H1
file	/home/vnmrl/v~	dpwr	20
nmrsys/data/niina/~		dof	0
BzfuranDA_h.fid		dm	nnn
ACQUISITION		dmm	c
sfrq	399.956	dmf	200
tn	H1	dseq	
at	3.744	dres	1.0
np	44928	homo	n
sw	6000.6	PROCESSING	
fb	not used	wtfile	
bs	1	proc	ft
tpwr	61	fn	not used
pw	5.5	math	f
d1	1.256		
tof	600.0	werr	react
nt	16	wexp	procplot
ct	16	wbs	
alock	n	wnt	
gain	not used		
FLAGS			
il	n		
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-80.0		
wp	4079.4		
vs	189		
sc	0		
wc	380		
hzmm	10.74		
is	2490.51		
rfl	382.7		
rfp	0		
th	20		
ins	100.000		
nm	ph		

^{1}H NMR ($CDCl_3$, 400 MHz)

9b



9b



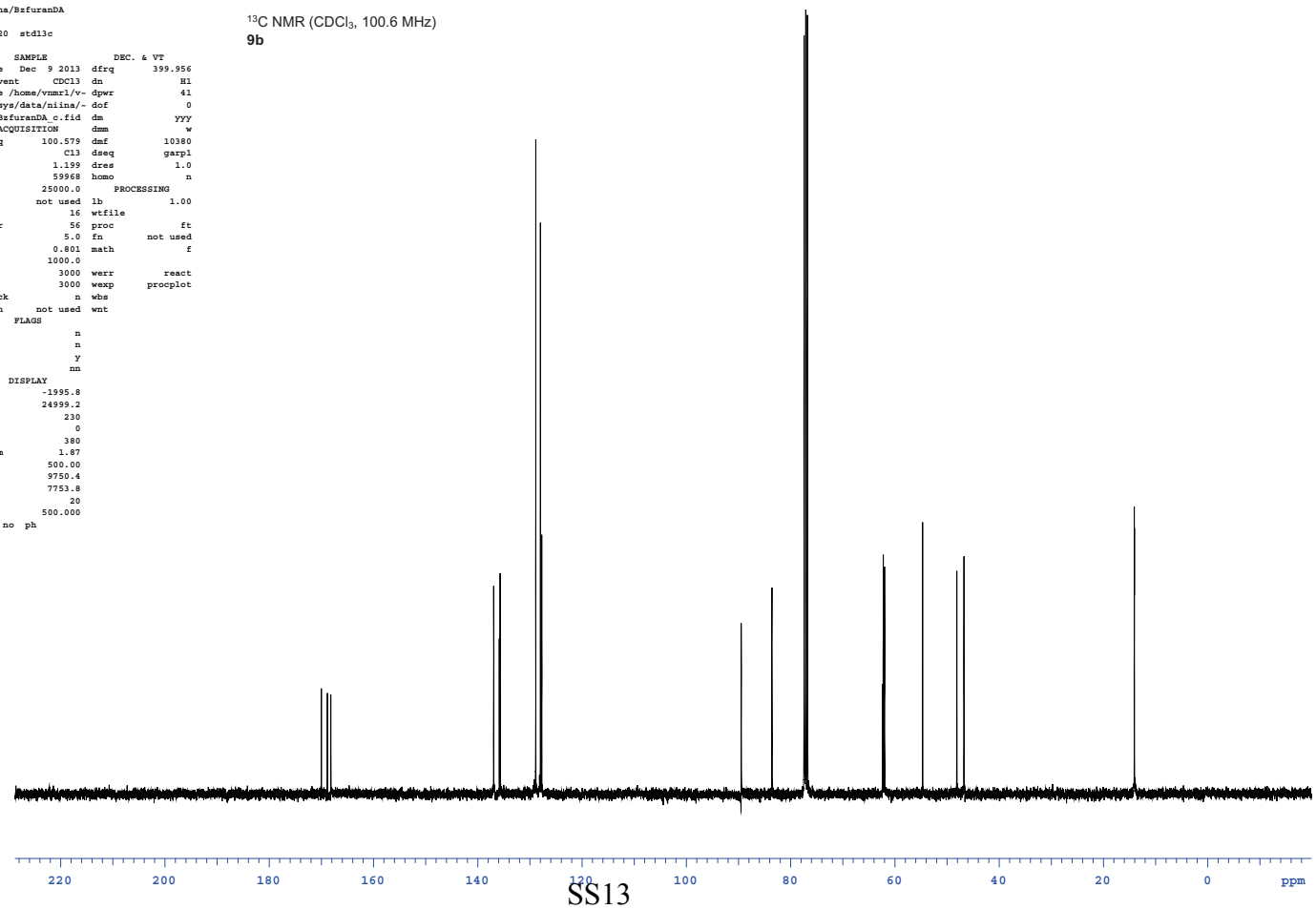
niina/BzfuranDA

exp20 stdl3c

SAMPLE		DEC. & VT	
date	Dec 9 2013	dfrq	399.956
solvent	CDCl3	dn	H1
file	/home/vnmrl/v~	dpwr	41
nmrsys/data/niina/~		dof	0
BzfuranDA_c.fid		dm	yyy
ACQUISITION		dmm	w
sfrq	100.579	dmf	10380
tn	C13	dseq	garp1
at	1.199	dres	1.0
np	59968	homo	n
sw	25000.0	PROCESSING	
fb	not used	lb	1.00
bs	16	wtfile	
tpwr	56	proc	ft
pw	5.0	fn	not used
d1	0.801	math	f
tof	1000.0		
nt	3000	werr	react
ct	3000	wexp	procplot
alock	n	wbs	
gain	not used	wnt	
FLAGS			
il	n		
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-1995.8		
wp	24999.2		
vs	230		
sc	0		
wc	380		
hzmm	1.87		
is	500.00		
rfl	9750.4		
rfp	7753.8		
th	20		
ins	500.000		
nm	no ph		

^{13}C NMR ($CDCl_3$, 100.6 MHz)

9b



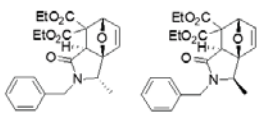
miyake3/MeFurMixR

exp20 PROTON

SAMPLE		PRESATURATION	
date	Jul 23 2014	satmode	n
solvent	cdcl3	wet	n
file	/home/vnmrl/v-	SPECIAL	
nmrsys/data/miyake-		temp	not used
3/MeFurMixR_h.fid		gain	not used
ACQUISITION		spin	20
sw	6402.0	hst	0.008
at	3.500	pw90	11.000
np	44814	alfa	10.000
fb	not used	FLAGS	
bs	4	il	n
dl	1.500	in	n
nt	16	dp	y
ct	16	hs	nn
TRANSMITTER		PROCESSING	
tn	H1	lb	0.20
sfrq	399.956	fn	not used
tof	400.0	DISPLAY	
tpwr	61	sp	-80.1
pw	5.500	wp	4079.4
DECOUPLER		rfl	784.0
dn	C13	rfp	0
dof	0	rp	144.6
dm	nnn	lp	-45.7
decwave	W40_HCN5mm	PLOT	
dpwr	33	wc	382
dmf	29412	sc	0
		vs	185
		th	3
		ai ph	

^{1}H NMR ($CDCl_3$, 400 MHz)

9c



(2 : 1)

9c

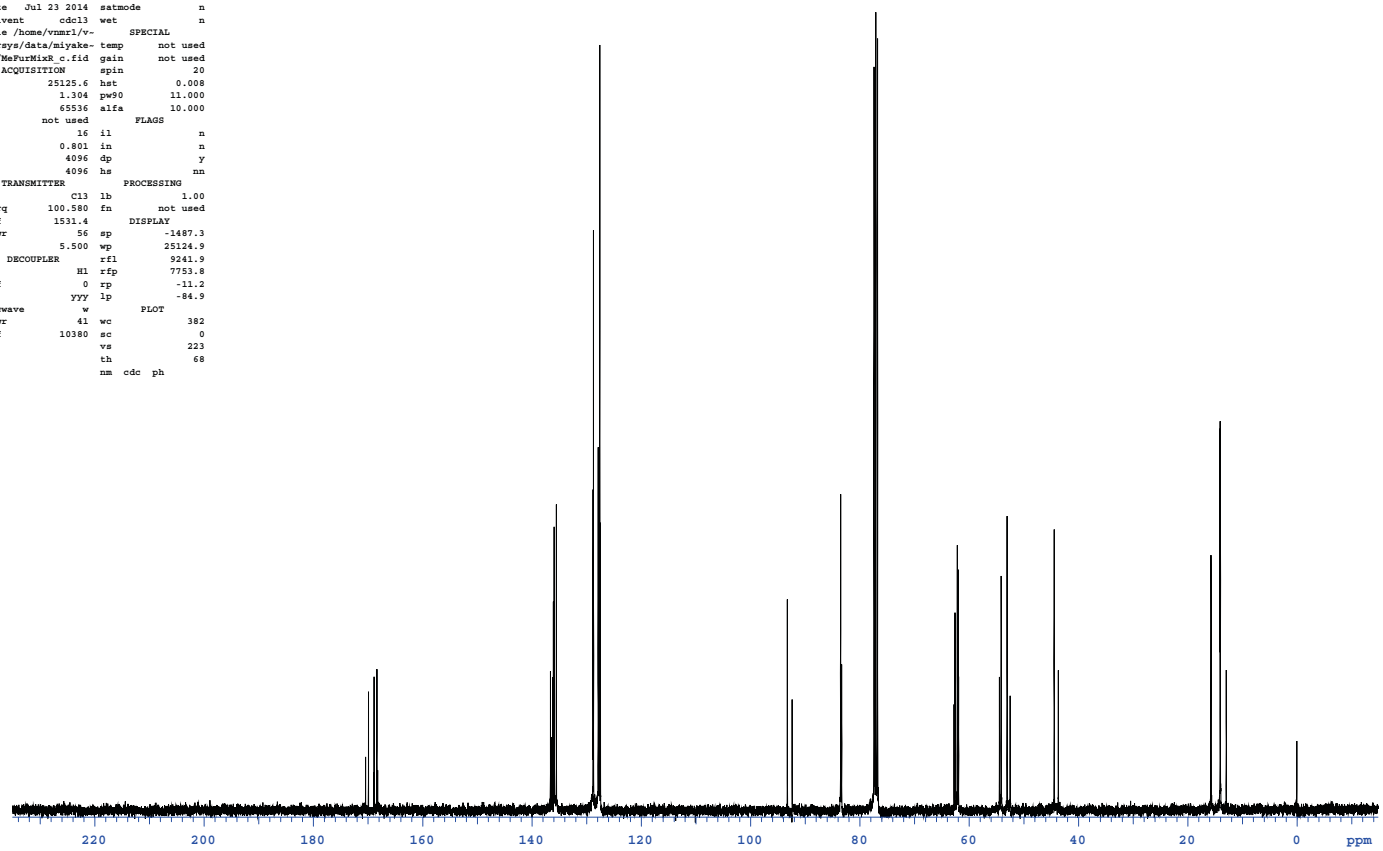
miyake3/MeFurMixR

exp20 CARBON

SAMPLE		PRESATURATION	
date	Jul 23 2014	satmode	n
solvent	cdcl3	wet	n
file	/home/vnmrl/v-	SPECIAL	
nmrsys/data/miyake-		temp	not used
3/MeFurMixR_c.fid		gain	not used
ACQUISITION		spin	20
sw	25125.6	hst	0.008
at	1.304	pw90	11.000
np	65536	alfa	10.000
fb	not used	FLAGS	
bs	16	il	n
dl	0.801	in	n
nt	4096	dp	y
ct	4096	hs	nn
TRANSMITTER		PROCESSING	
tn	C13	lb	1.00
sfrq	100.580	fn	not used
tof	1531.4	DISPLAY	
tpwr	56	sp	-1487.3
pw	5.500	wp	25124.9
DECOUPLER		rfl	9241.9
dn	H1	rfp	7753.8
dof	0	rp	-11.2
dm	yyy	lp	-84.9
decwave	w	PLOT	
dpwr	41	wc	382
dmf	10380	sc	0
		vs	223
		th	68
		nm cdc ph	

^{13}C NMR ($CDCl_3$, 100.6 MHz)

9c



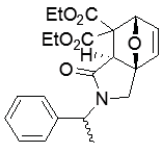
miyake3/NEtPhR

exp20 PROTON

SAMPLE		PRESATURATION	
date	Sep 10 2014	satmode	n
solvent	cdcl3	wet	n
file	/home/vnmr1/v-	SPECIAL	
nmrsys/data/miyake-		temp	not used
3/NEtPhR_h.fid		gain	not used
ACQUISITION		spin	20
sw	6402.0	hst	0.008
at	3.500	pw90	11.000
np	44814	alfa	10.000
fb	not used	FLAGS	
bs	4	il	n
d1	1.500	in	n
nt	16	dp	y
ct	16	hs	nn
TRANSMITTER		PROCESSING	
tn	H1	lb	0.20
sfrq	399.956	fn	not used
tof	400.0	DISPLAY	
tpwr	61	sp	-80.1
pw	5.500	wp	4079.4
DECOUPLER		rfl	781.3
dn	C13	rfp	0
dof	0	rp	139.4
dm	nnn	lp	-48.5
decwave	W40_HCN5mm	PLOT	
dpwr	33	wc	382
dmf	29412	sc	0
		vs	243
		th	17
		ai	ph

^{1}H NMR ($CDCl_3$, 400 MHz)

9d



(dr = 1:1)

9d

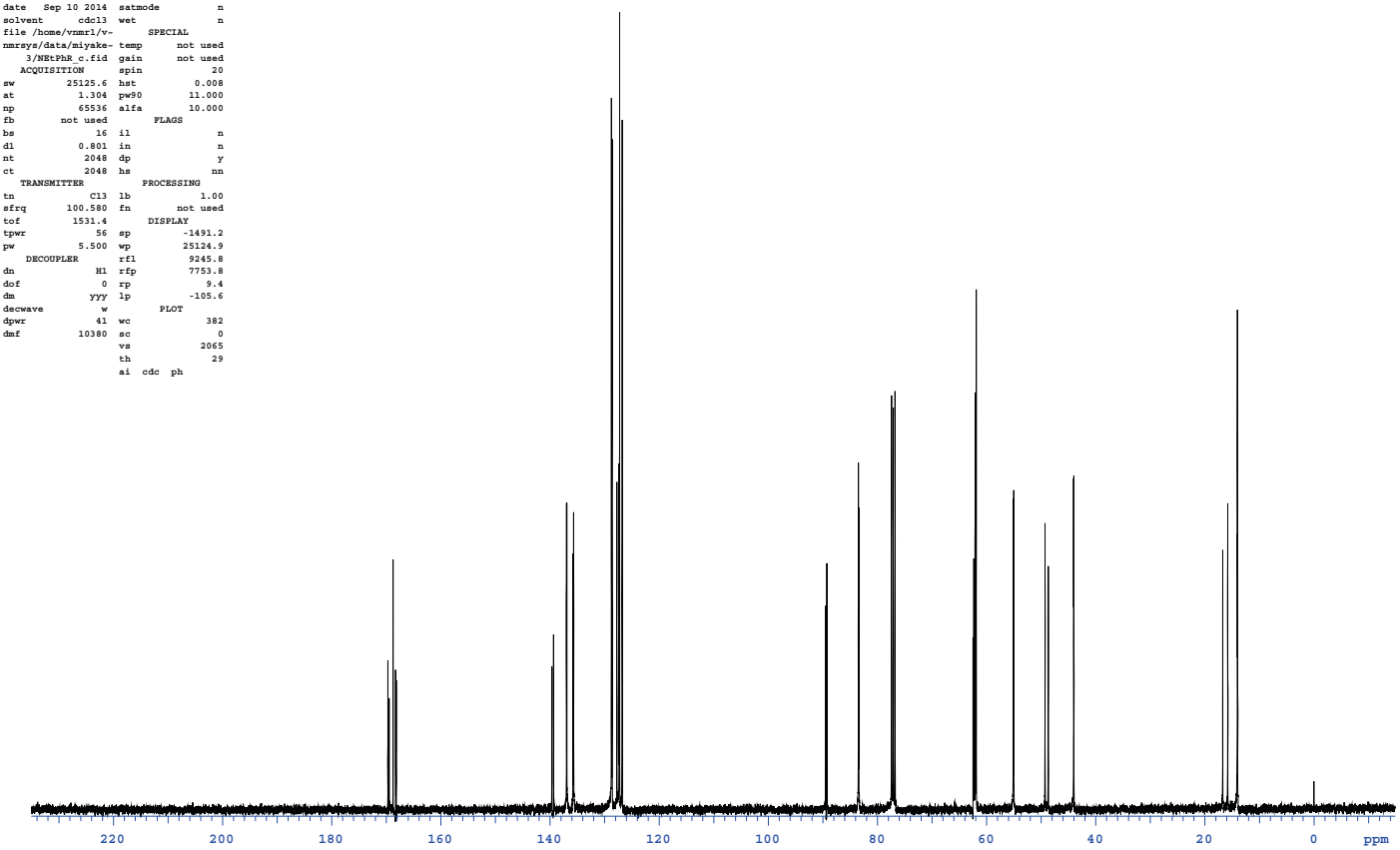
miyake3/NEtPhR

exp20 CARBON

SAMPLE		PRESATURATION	
date	Sep 10 2014	satmode	n
solvent	cdcl3	wet	n
file	/home/vnmr1/v-	SPECIAL	
nmrsys/data/miyake-		temp	not used
3/NEtPhR_c.fid		gain	not used
ACQUISITION		spin	20
sw	25125.6	hst	0.008
at	1.304	pw90	11.000
np	65536	alfa	10.000
fb	not used	FLAGS	
bs	16	il	n
d1	0.801	in	n
nt	2048	dp	y
ct	2048	hs	nn
TRANSMITTER		PROCESSING	
tn	C13	lb	1.00
sfrq	100.580	fn	not used
tof	1531.4	DISPLAY	
tpwr	56	sp	-1491.2
pw	5.500	wp	25124.9
DECOUPLER		rfl	9245.8
dn	H1	rfp	7753.8
dof	0	rp	9.4
dm	yyy	lp	-105.6
decwave	w	PLOT	
dpwr	41	wc	382
dmf	10380	sc	0
		vs	2065
		th	29
		ai	cdc ph

^{13}C NMR ($CDCl_3$, 100.6 MHz)

9d



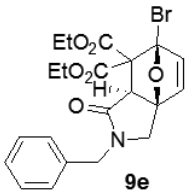
sugiura/BrFuranDAr

exp20 PROTON

SAMPLE		PRESATURATION	
date	Dec 17 2014	satmode	n
solvent	cdcl3	wet	n
file	/home/vnmrl/v-	SPECIAL	
nmrsys/data/sugiur-		temp	not used
a/BrFuranDAr_h.fid		gain	not used
ACQUISITION		spin	20
sw	6402.0	hst	0.008
at	3.500	pw90	11.000
np	44814	alfa	10.000
fb	not used	FLAGS	
bs	4	il	n
dl	1.500	in	n
nt	16	dp	y
ct	16	hs	nn
TRANSMITTER		PROCESSING	
tn	H1	lb	0.20
sfrq	399.956	fn	not used
tof	400.0	DISPLAY	
tpwr	61	sp	-80.1
pw	5.500	wp	4079.4
DECOUPLER		rfl	781.7
dn	C13	rfp	0
dof	0	rp	-45.6
dm	nnn	lp	-47.4
decwave	W40_HCN5mm	PLOT	
dpwr	33	wc	382
dmf	29412	sc	0
		vs	136
		th	2
		ai ph	

^{1}H NMR ($CDCl_3$, 400 MHz)

9e



9e

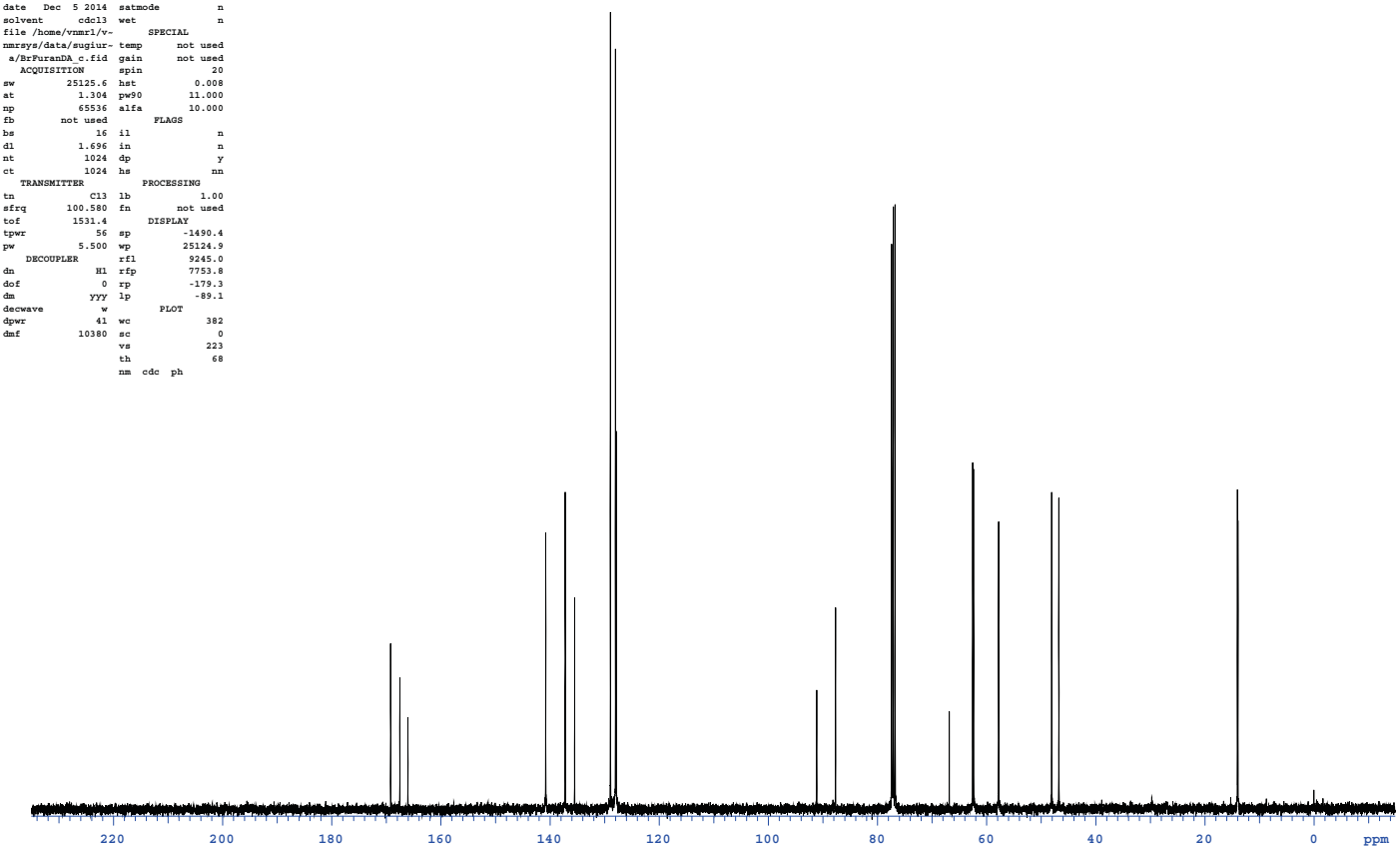
sugiura/BrFuranDA

exp20 CARBON

SAMPLE		PRESATURATION	
date	Dec 5 2014	satmode	n
solvent	cdcl3	wet	n
file	/home/vnmrl/v-	SPECIAL	
nmrsys/data/sugiur-		temp	not used
a/BrFuranDA_c.fid		gain	not used
ACQUISITION		spin	20
sw	25125.6	hst	0.008
at	1.304	pw90	11.000
np	65536	alfa	10.000
fb	not used	FLAGS	
bs	16	il	n
dl	1.696	in	n
nt	1024	dp	y
ct	1024	hs	nn
TRANSMITTER		PROCESSING	
tn	C13	lb	1.00
sfrq	100.580	fn	not used
tof	1531.4	DISPLAY	
tpwr	56	sp	-1490.4
pw	5.500	wp	25124.9
DECOUPLER		rfl	9245.0
dn	H1	rfp	7753.8
dof	0	rp	-179.3
dm	yyy	lp	-89.1
decwave	w	PLOT	
dpwr	41	wc	382
dmf	10380	sc	0
		vs	223
		th	68
		nm cdc ph	

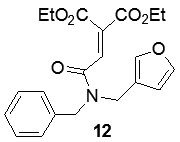
^{13}C NMR ($CDCl_3$, 100.6 MHz)

9e

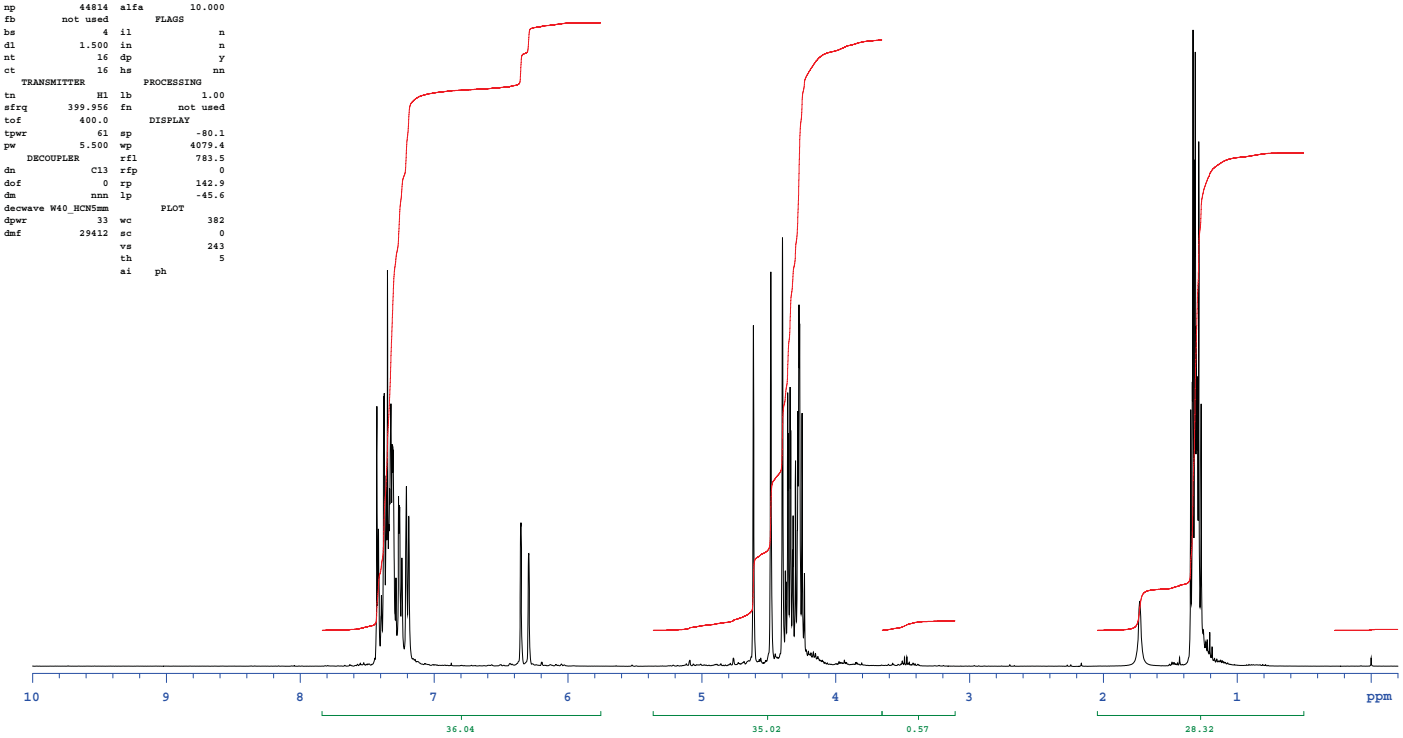


^{1}H NMR ($CDCl_3$, 400 MHz)

12



12



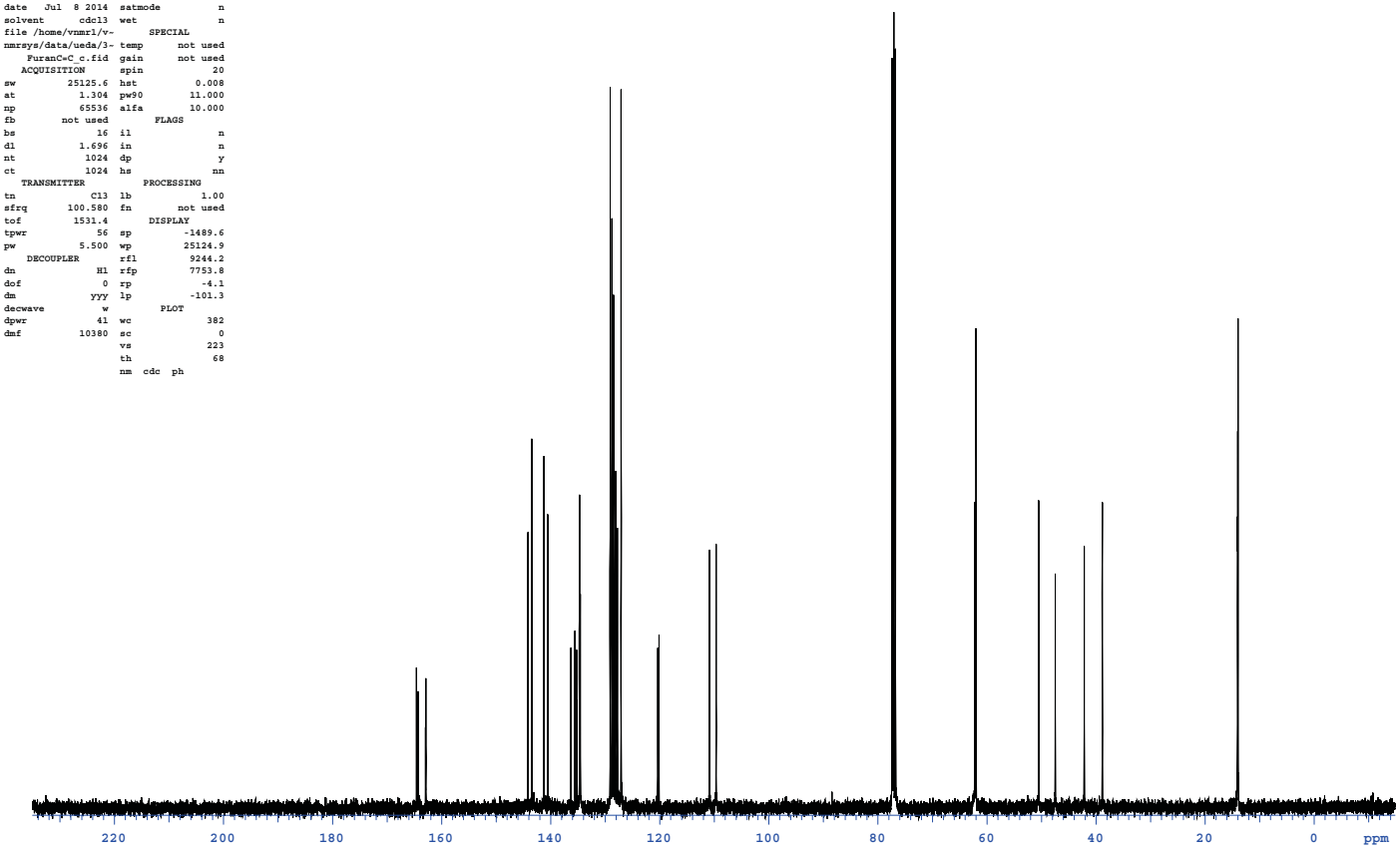

```
ueda/3FuranC=C

exp20  PROTON

      SAMPLE          PRESATURATION
date   Jul  8 2014  satmode          n
solvent      cdcl3  wet              n
file /home/vnmrl/v-      SPECIAL
nmrsys/data/ueda/3- temp       not used
    FuranC=C_h.fid  gain       not used
   ACQUISITION      spin             20
sw          6402.0  hst           0.008
at           3.500  pw90         11.000
np           44814  alfa         10.000
fb        not used        FLAGS
bs                4  il               n
dl            1.500  in               n
nt               16  dp               y
ct               16  hs              nn
   TRANSMITTER          PROCESSING
tn               H1  lb            1.00
sfrq       399.956  fn        not used
tof          400.0       DISPLAY
tpwr             61  sp           -80.1
pw            5.500  wp          4079.4
    DECOUPLER        rfl          783.5
dn               C13 rfp              0
dof                0 rp           142.9
dm               nnn lp           -45.6
decwave W40_HCN5mm         PLOT
dpwr              33 wc             382
dmf            29412 sc               0
                     vs             243
                     th               5
                     ai    ph
```

^{13}C NMR ($CDCl_3$, 100.6 MHz)

12




```
ueda/3FuranC=C

exp20  CARBON

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solvent      cdcl3  wet              n
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nmrsys/data/ueda/3- temp       not used
    FuranC=C_c.fid  gain       not used
   ACQUISITION      spin             20
sw         25125.6  hst           0.008
at           1.304  pw90         11.000
np           65536  alfa         10.000
fb        not used        FLAGS
bs                16  il               n
dl            1.696  in               n
nt             1024  dp               y
ct             1024  hs              nn
   TRANSMITTER          PROCESSING
tn               C13 lb            1.00
sfrq       100.580  fn        not used
tof         1531.4       DISPLAY
tpwr             56  sp         -1489.6
pw            5.500  wp         25124.9
    DECOUPLER        rfl          9244.2
dn               H1  rfp          7753.8
dof                0 rp            -4.1
dm               yyy lp          -101.3
decwave            w         PLOT
dpwr              41  wc             382
dmf            10380 sc               0
                     vs             223
                     th              68
                     nm  cdc  ph
```

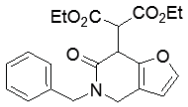
ueda/3FuranCyc

exp20 PROTON

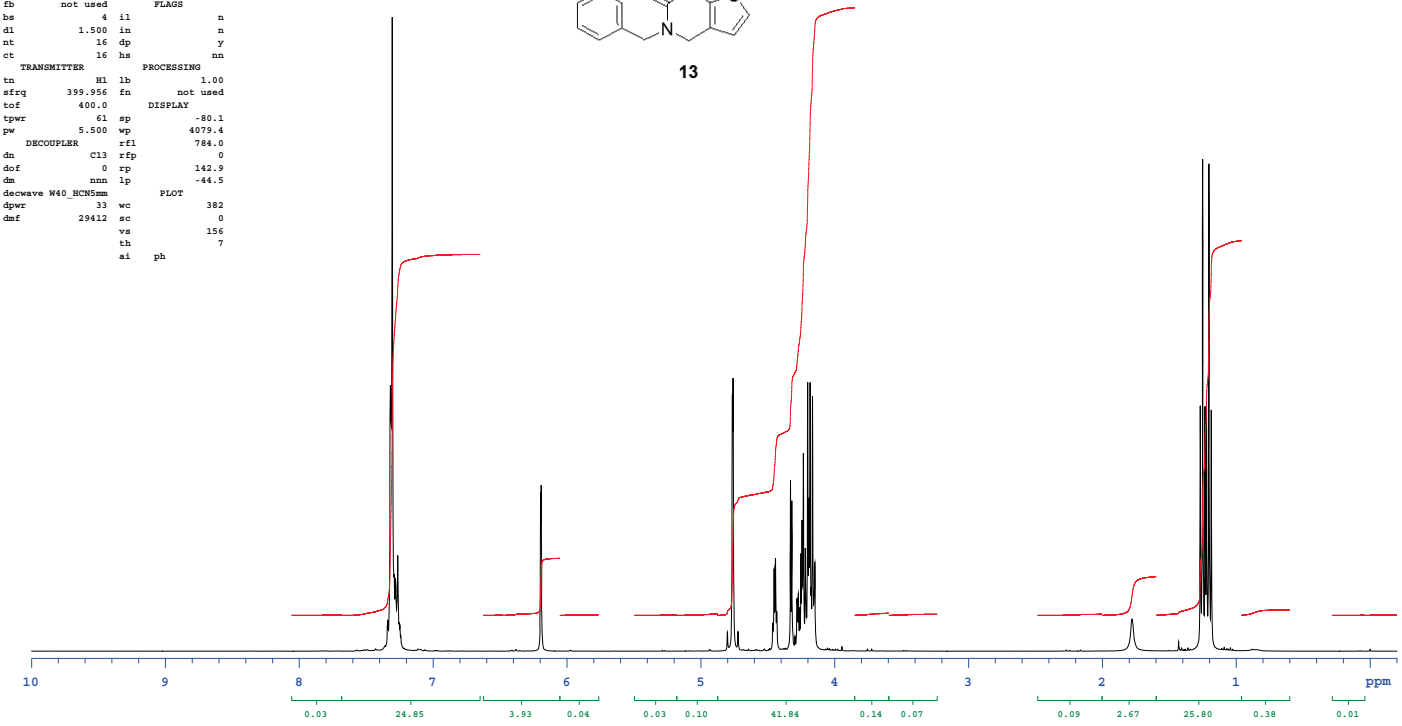
SAMPLE		PRESATURATION	
date	Jul 11 2014	satmode	n
solvent	cdcl3	wet	n
file	/home/vnmrl/v-	SPECIAL	
nmrsys/data/ueda/3-		temp	not used
FuranCyc_h.fid		gain	not used
ACQUISITION		spin	20
sw	6402.0	hst	0.008
at	3.500	pw90	11.000
np	44814	alfa	10.000
fb	not used	FLAGS	
bs	4	il	n
dl	1.500	in	n
nt	16	dp	y
ct	16	hs	nn
TRANSMITTER		PROCESSING	
tn	H1	lb	1.00
sfrq	399.956	fn	not used
tof	400.0	DISPLAY	
tpwr	61	sp	-80.1
pw	5.500	wp	4079.4
DECOUPLER		rfl	784.0
dn	C13	rfp	0
dof	0	rp	142.9
dm	nnn	lp	-44.5
decwave	W40_HCN5mm	PLOT	
dpwr	33	wc	382
dmf	29412	sc	0
		vs	156
		th	7
		ai	ph

^{1}H NMR ($CDCl_3$, 400 MHz)

13



13



ueda/3FuranCyc

exp20 CARBON

SAMPLE		PRESATURATION	
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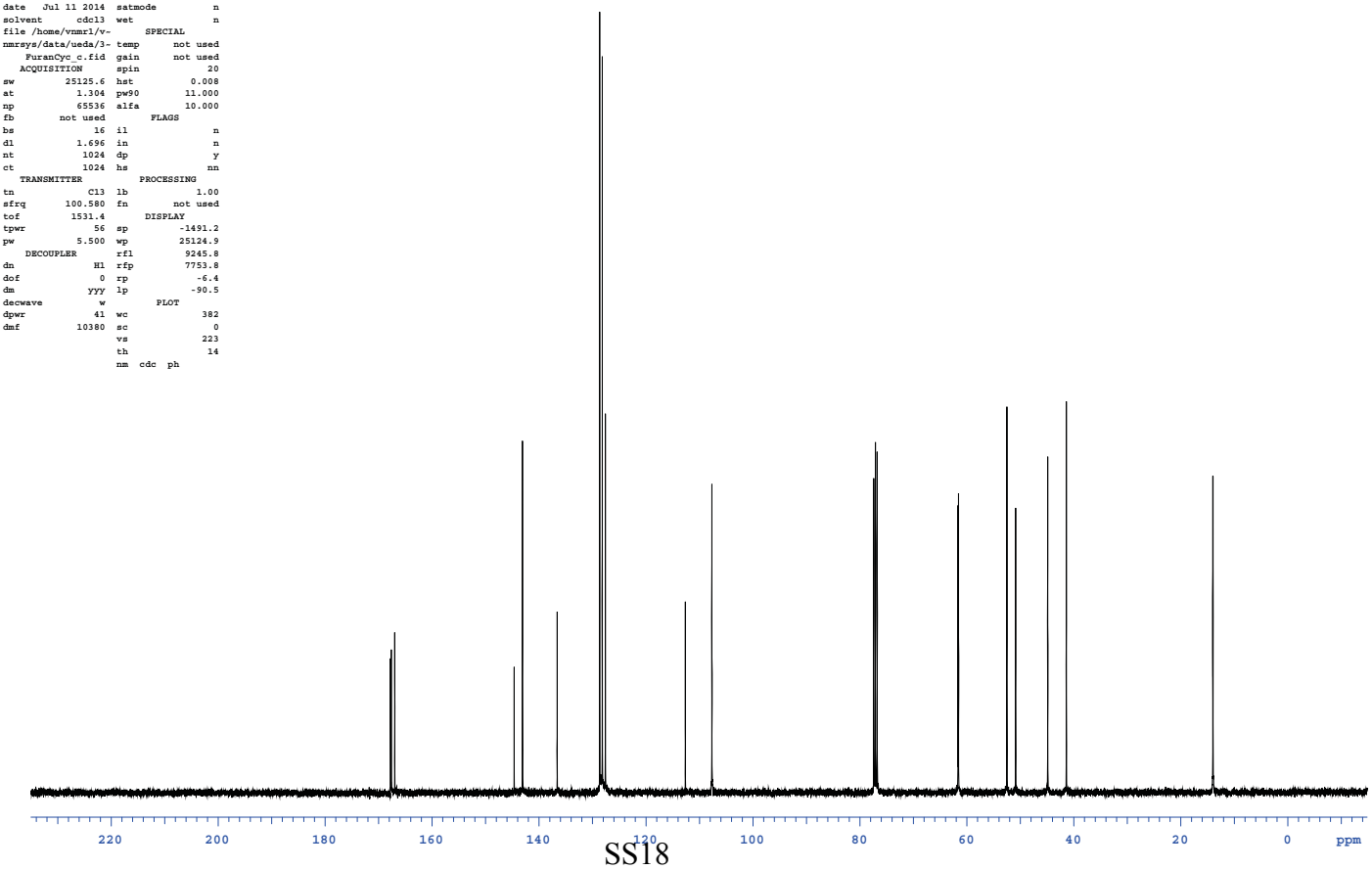
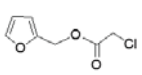
solvent	cdcl3	wet	n
file	/home/vnmrl/v-	SPECIAL	
nmrsys/data/ueda/3-		temp	not used
FuranCyc_c.fid		gain	not used
ACQUISITION		spin	20
sw	25125.6	hst	0.008
at	1.304	pw90	11.000
np	65536	alfa	10.000
fb	not used	FLAGS	
bs	16	il	n
dl	1.696	in	n
nt	1024	dp	y
ct	1024	hs	nn
TRANSMITTER		PROCESSING	
tn	C13	lb	1.00
sfrq	100.580	fn	not used
tof	1531.4	DISPLAY	
tpwr	56	sp	-1491.2
pw	5.500	wp	25124.9
DECOUPLER		rfl	9245.8
dn	H1	rfp	7753.8
dof	0	rp	-6.4
dm	yyy	lp	-90.5
decwave	w	PLOT	
dpwr	41	wc	382
dmf	10380	sc	0
		vs	223
		th	14
		nm	cdc ph

^{13}C NMR ($CDCl_3$, 100.6 MHz)

13



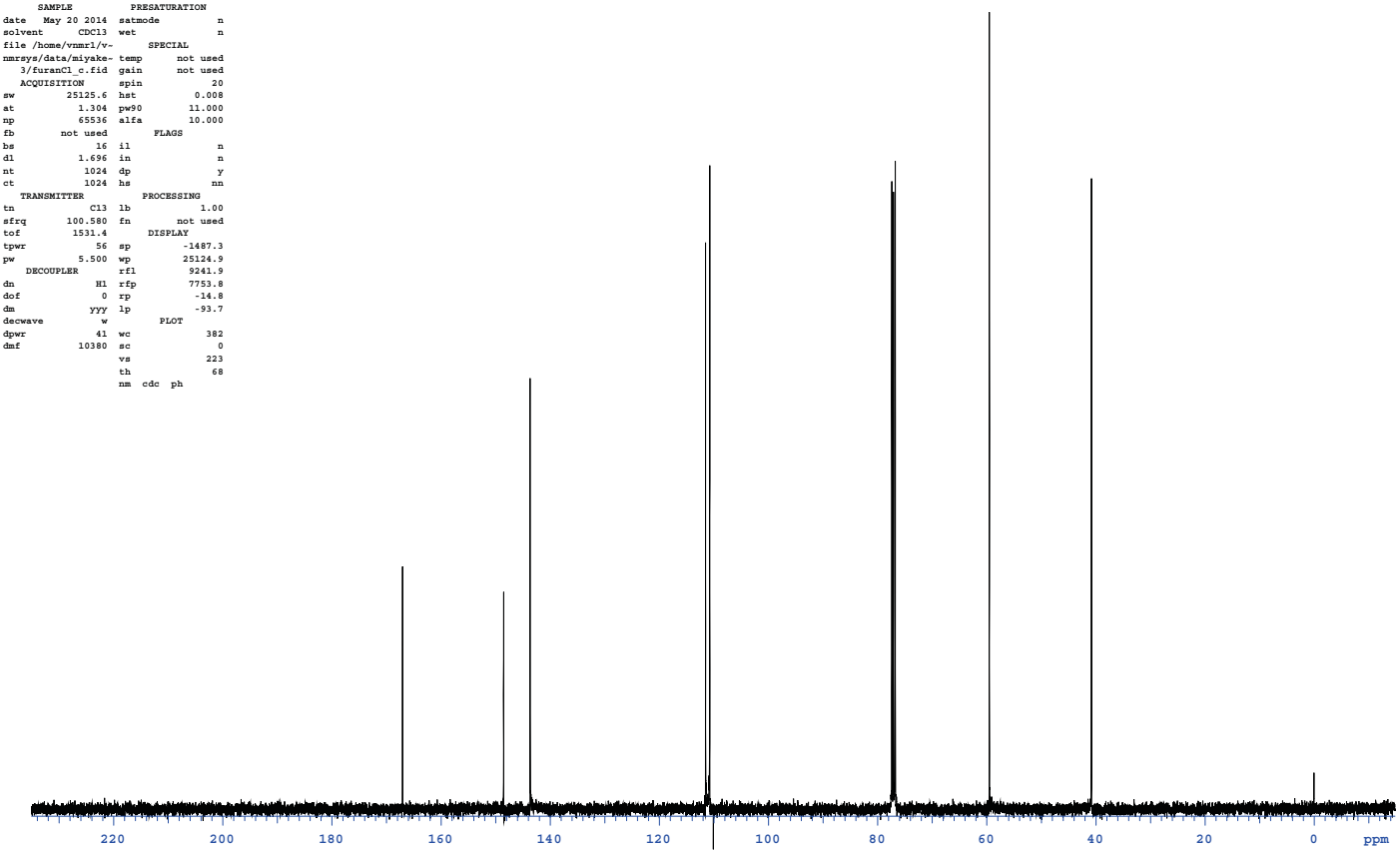
^{1}H NMR ($CDCl_3$, 400 MHz)
(Furan-2-yl)methyl 2-chloroacetate



(Furan-2-yl)methyl 2-chloroacetate


```
miyake3/furanCl

exp20  PROTON

      SAMPLE          PRESATURATION
date   May 20 2014  satmode          n
solvent      cdcl3  wet              n
file /home/vnmrl/v~     SPECIAL
nmrsys/data/miyake~ temp       not used
   3/furanCl_h.fid  gain       not used
   ACQUISITION      spin            20
sw          6402.0  hst          0.008
at           3.500  pw90        11.000
np           44814  alfa        10.000
fb        not used       FLAGS
bs                4  il               n
dl            1.500  in               n
nt               16  dp               y
ct               16  hs              nn
   TRANSMITTER          PROCESSING
tn               H1  lb            0.20
sfrq       399.956  fn        not used
tof          400.0      DISPLAY
tpwr            61  sp           -80.1
pw           5.500  wp          4079.4
   DECOUPLER        rfl          784.6
dn              C13  rfp              0
dof               0  rp           141.7
dm              nnn  lp           -44.0
decwave W40_HCN5mm       PLOT
dpwr             33  wc             382
dmf           29412  sc               0
                     vs              23
                     th               0
                     ai    ph
```

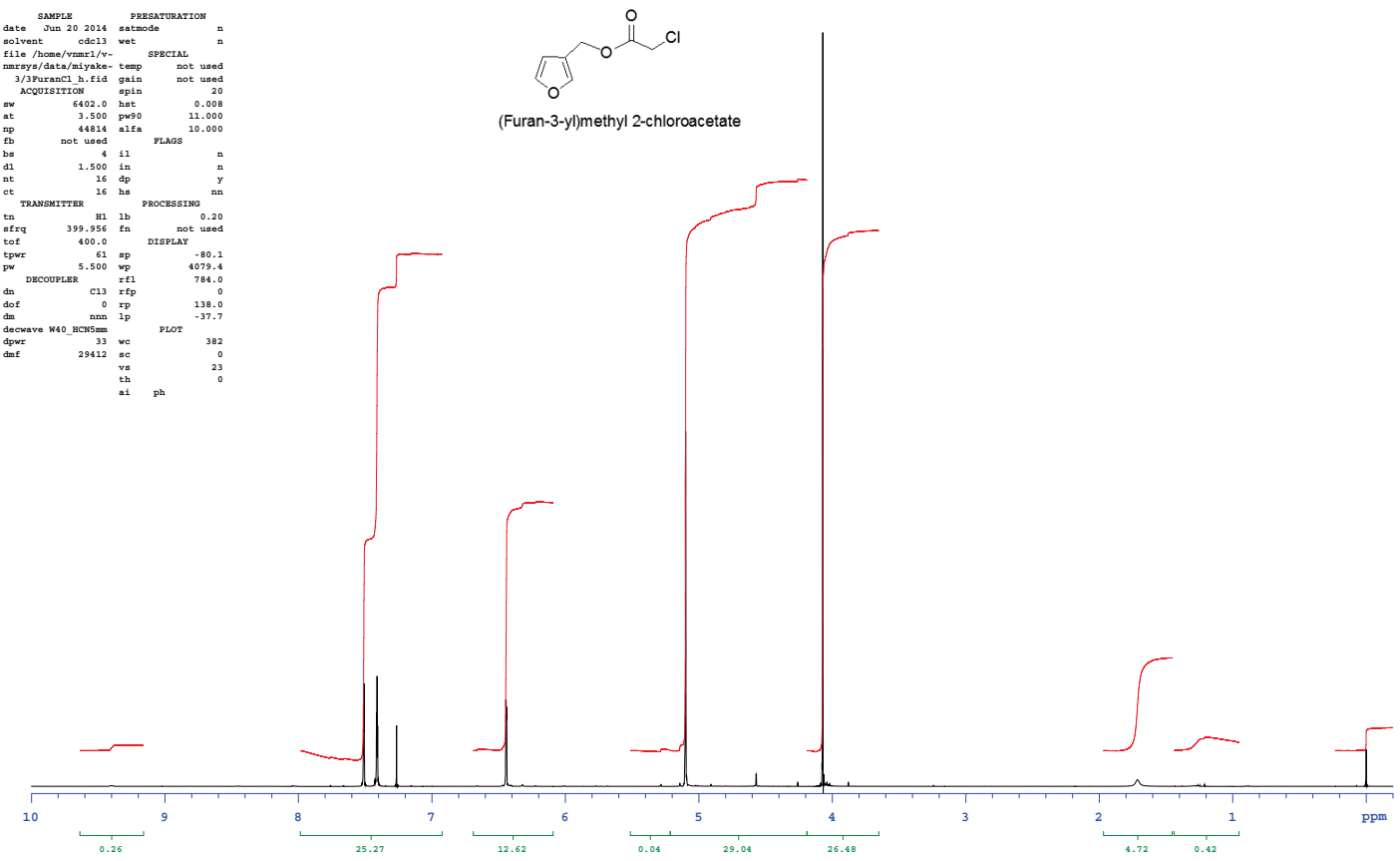
^{13}C NMR ($CDCl_3$, 100.6 MHz)
(Furan-2-yl)methyl 2-chloroacetate




```
miyake3/furanCl

exp20  CARBON

      SAMPLE          PRESATURATION
date   May 20 2014  satmode          n
solvent      CDCl3  wet              n
file /home/vnmrl/v~     SPECIAL
nmrsys/data/miyake~ temp       not used
   3/furanCl_c.fid  gain       not used
   ACQUISITION      spin            20
sw         25125.6  hst          0.008
at           1.304  pw90        11.000
np           65536  alfa        10.000
fb        not used       FLAGS
bs               16  il               n
dl            1.696  in               n
nt            1024  dp               y
ct            1024  hs              nn
   TRANSMITTER          PROCESSING
tn              C13  lb            1.00
sfrq       100.580  fn        not used
tof         1531.4      DISPLAY
tpwr            56  sp         -1487.3
pw           5.500  wp         25124.9
   DECOUPLER        rfl         9241.9
dn               H1  rfp         7753.8
dof               0  rp           -14.8
dm              yyy  lp           -93.7
decwave           w       PLOT
dpwr             41  wc             382
dmf           10380  sc               0
                     vs             223
                     th              68
                     nm  cdc  ph
```

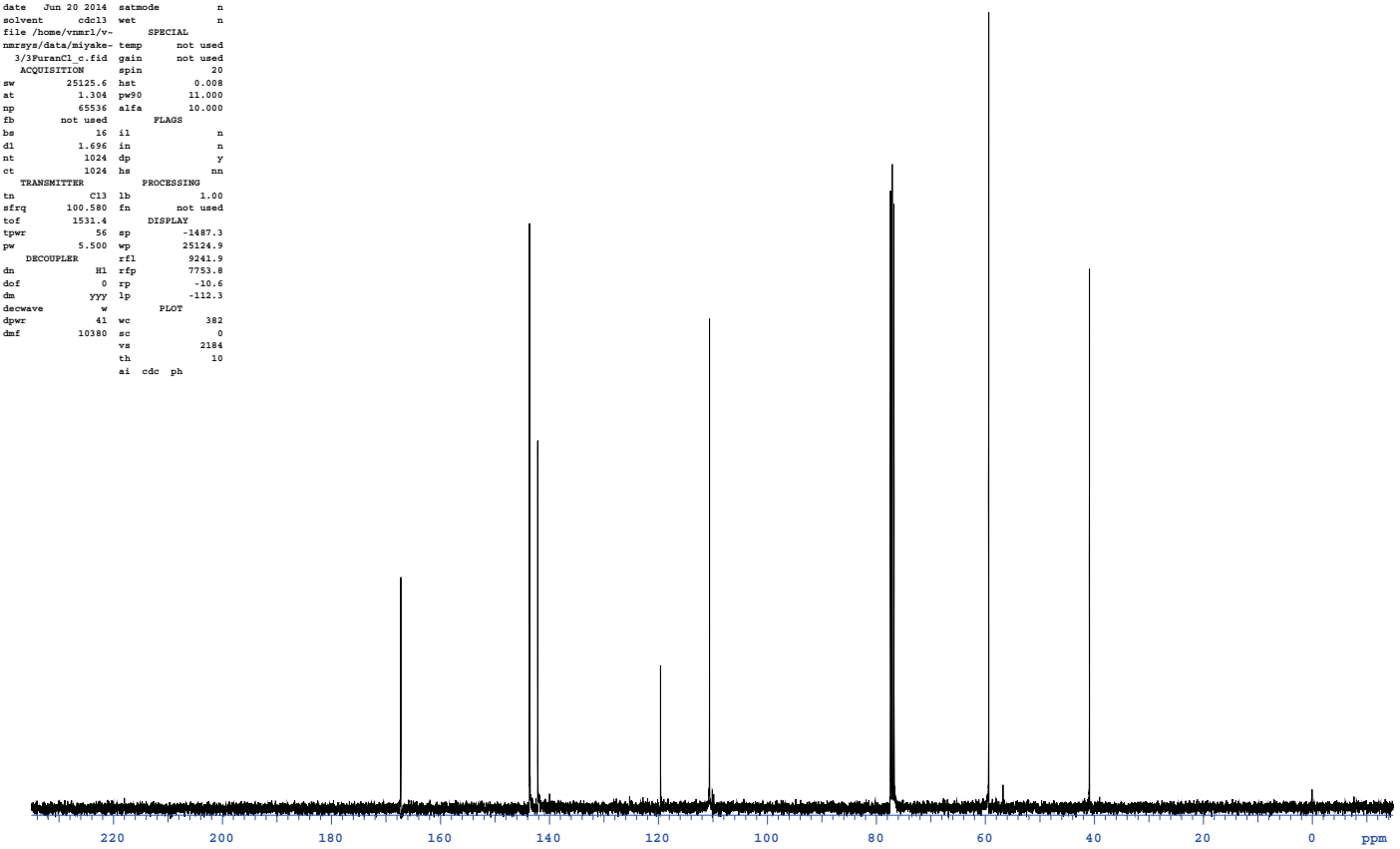
^{1}H NMR ($CDCl_3$, 400 MHz)
(Furan-3-yl)methyl 2-chloroacetate

```
miyake3/3FuranCl

exp20  PROTON

      SAMPLE          PRESATURATION
date   Jun 20 2014  satmode          n
solvent      cdcl3  wet              n
file /home/vnmrl/v-      SPECIAL
nmrsys/data/miyake- temp       not used
  3/3FuranCl_h.fid  gain       not used
   ACQUISITION      spin             20
sw          6402.0  hst           0.008
at           3.500  pw90         11.000
np           44814  alfa         10.000
fb       not used        FLAGS
bs                4  il               n
dl            1.500  in               n
nt               16  dp               y
ct               16  hs              nn
   TRANSMITTER          PROCESSING
tn               H1  lb            0.20
sfrq        399.956  fn       not used
tof           400.0       DISPLAY
tpwr             61  sp           -80.1
pw            5.500  wp          4079.4
    DECOUPLER       rfl           784.0
dn               C13  rfp             0
dof                0  rp           138.0
dm               nnn  lp           -37.7
decwave W40_HCN5mm        PLOT
dpwr              33  wc             382
dmf            29412  sc               0
                      vs              23
                      th               0
                      ai    ph
```



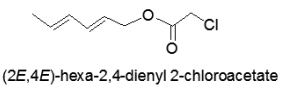
^{13}C NMR ($CDCl_3$, 100.6 MHz)
(Furan-3-yl)methyl 2-chloroacetate

```
miyake3/3FuranCl

exp20  CARBON

      SAMPLE          PRESATURATION
date   Jun 20 2014  satmode          n
solvent      cdcl3  wet              n
file /home/vnmrl/v-      SPECIAL
nmrsys/data/miyake- temp       not used
  3/3FuranCl_c.fid  gain       not used
   ACQUISITION      spin             20
sw         25125.6  hst           0.008
at           1.304  pw90         11.000
np           65536  alfa         10.000
fb       not used        FLAGS
bs                16  il               n
dl            1.696  in               n
nt             1024  dp               y
ct             1024  hs              nn
   TRANSMITTER          PROCESSING
tn               C13  lb            1.00
sfrq        100.580  fn       not used
tof          1531.4       DISPLAY
tpwr             56  sp          -1487.3
pw            5.500  wp         25124.9
    DECOUPLER       rfl          9241.9
dn               H1  rfp          7753.8
dof                0  rp           -10.6
dm               yyy  lp          -112.3
decwave            w        PLOT
dpwr              41  wc             382
dmf            10380  sc               0
                      vs            2184
                      th              10
                      ai  cdc  ph
```



^{1}H NMR ($CDCl_3$, 400 MHz)
(2*E*,4*E*)-hexa-2,4-dienyl 2-chloroacetate

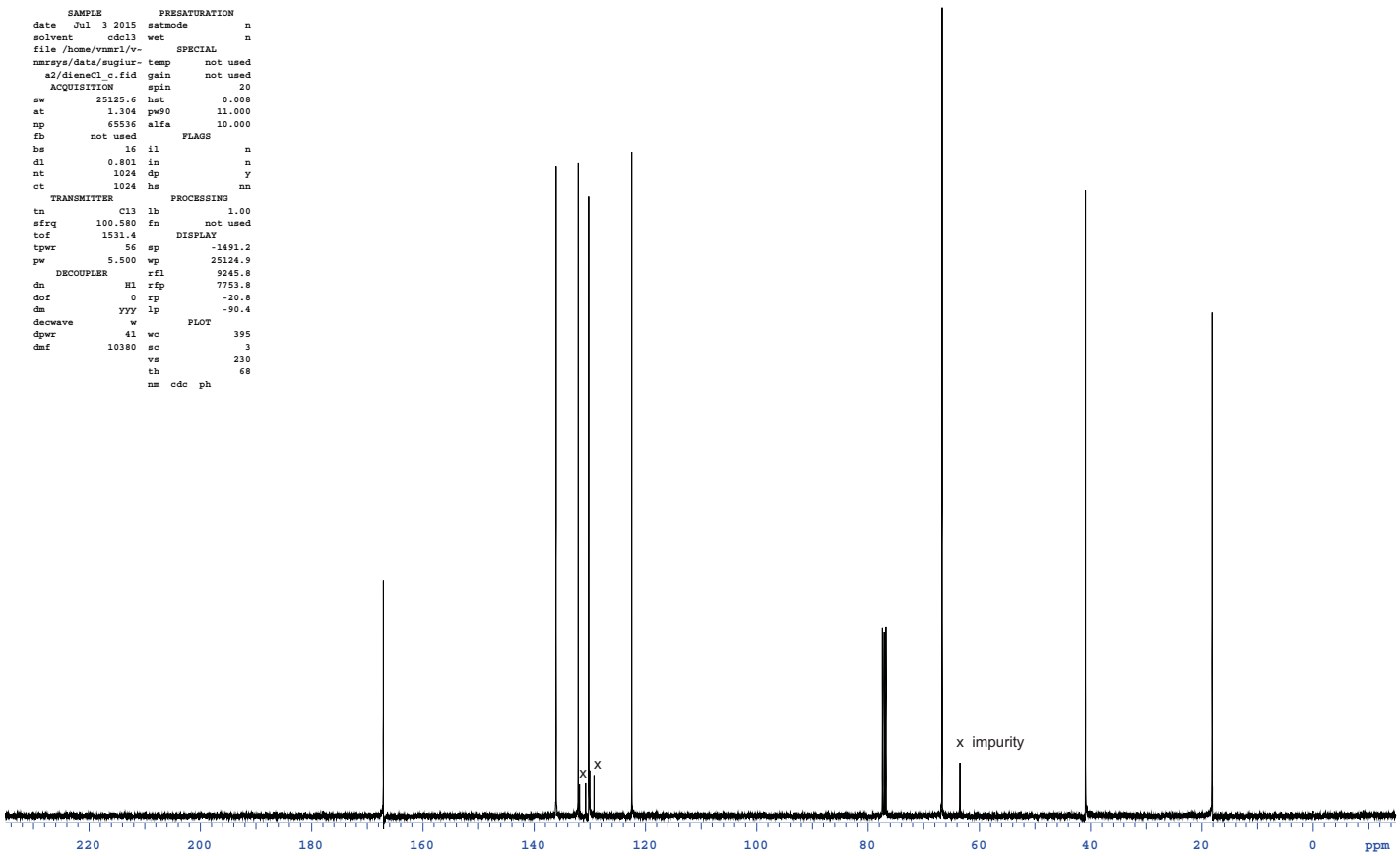
```
sugiura2/dieneCl

exp20  PROTON

      SAMPLE          PRESATURATION
date   Jul  3 2015  satmode          n
solvent      cdcl3  wet              n
file /home/vnmrl/v-            SPECIAL
nmrsys/data/sugiur- temp       not used
  a2/dieneCl_h.fid  gain       not used
   ACQUISITION      spin            20
sw          6402.0  hst           0.008
at           3.500  pw90         11.000
np           44814  alfa         10.000
fb       not used         FLAGS
bs                4  il               n
dl            1.500  in               n
nt               16  dp               y
ct               16  hs              nn
   TRANSMITTER           PROCESSING
tn               H1  lb            0.20
sfrq        399.956  fn       not used
tof            400.0      DISPLAY
tpwr              61  sp           -80.1
pw            5.500  wp          4079.4
    DECOUPLER        rfl           779.0
dn               C13  rfp             0
dof                0  rp           116.4
dm               nnn  lp           -47.3
decwave W40_HCN5mm         PLOT
dpwr              33  wc             382
dmf            29412  sc               8
                      vs              63
                      th               2
                      ai    ph
```



(2*E*,4*E*)-hexa-2,4-dienyl 2-chloroacetate

^{13}C NMR ($CDCl_3$, 100.6 MHz)
(2*E*,4*E*)-hexa-2,4-dienyl 2-chloroacetate

```
sugiura2/dieneCl

exp20  CARBON

      SAMPLE          PRESATURATION
date   Jul  3 2015  satmode          n
solvent      cdcl3  wet              n
file /home/vnmrl/v-            SPECIAL
nmrsys/data/sugiur- temp       not used
  a2/dieneCl_c.fid  gain       not used
   ACQUISITION      spin            20
sw         25125.6  hst           0.008
at           1.304  pw90         11.000
np           65536  alfa         10.000
fb       not used         FLAGS
bs                16  il               n
dl             0.801  in               n
nt              1024  dp               y
ct              1024  hs              nn
   TRANSMITTER           PROCESSING
tn               C13  lb            1.00
sfrq        100.580  fn       not used
tof          1531.4      DISPLAY
tpwr             56  sp          -1491.2
pw            5.500  wp         25124.9
    DECOUPLER        rfl          9245.8
dn               H1  rfp          7753.8
dof                0  rp           -20.8
dm               yyy  lp           -90.4
decwave            w         PLOT
dpwr              41  wc             395
dmf            10380  sc               3
                      vs             230
                      th              68
                      nm  cdc  ph
```



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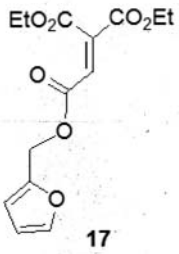
Gee

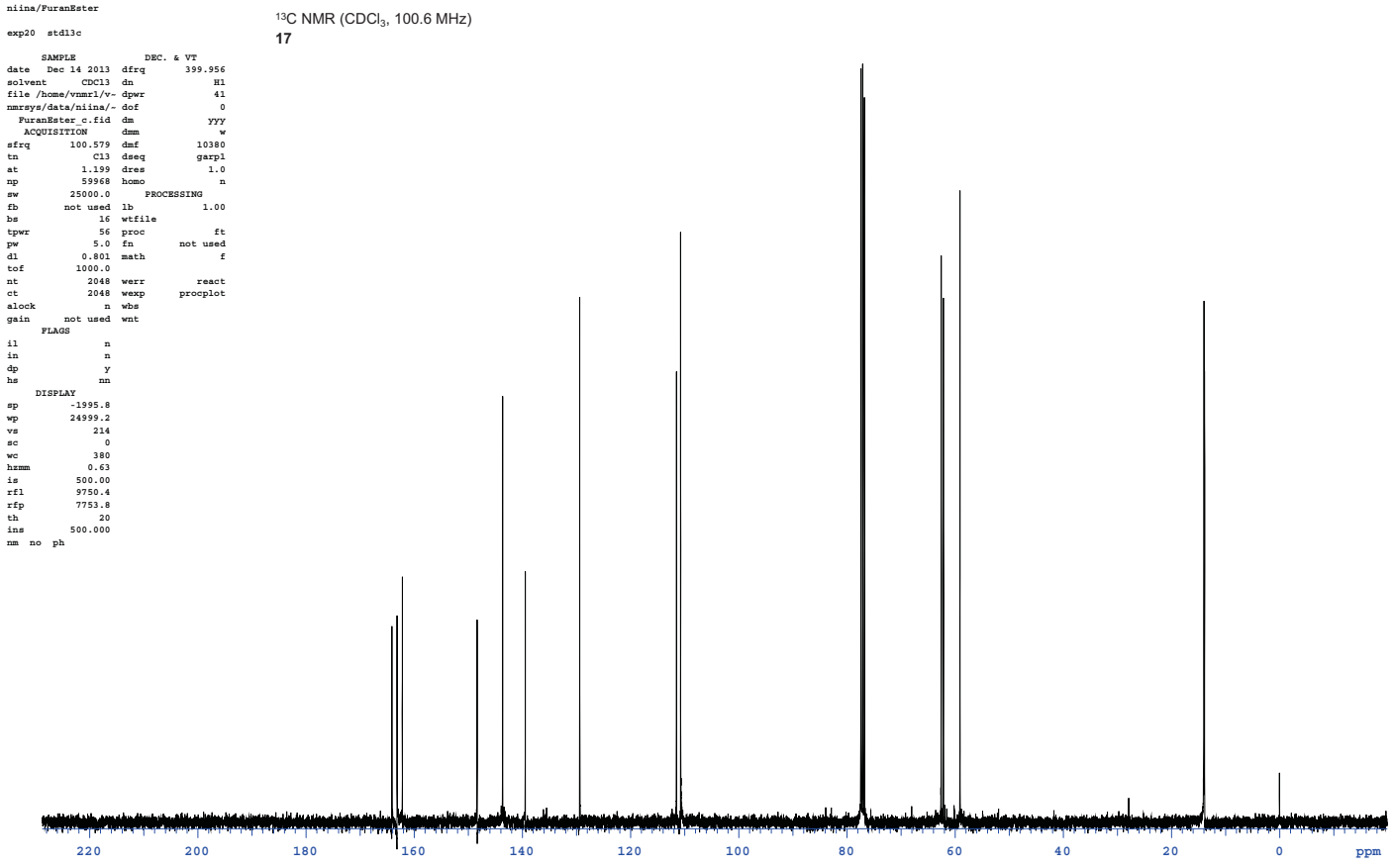
^{1}H NMR ($CDCl_3$, 400 MHz)

17



^{13}C NMR ($CDCl_3$, 100.6 MHz)

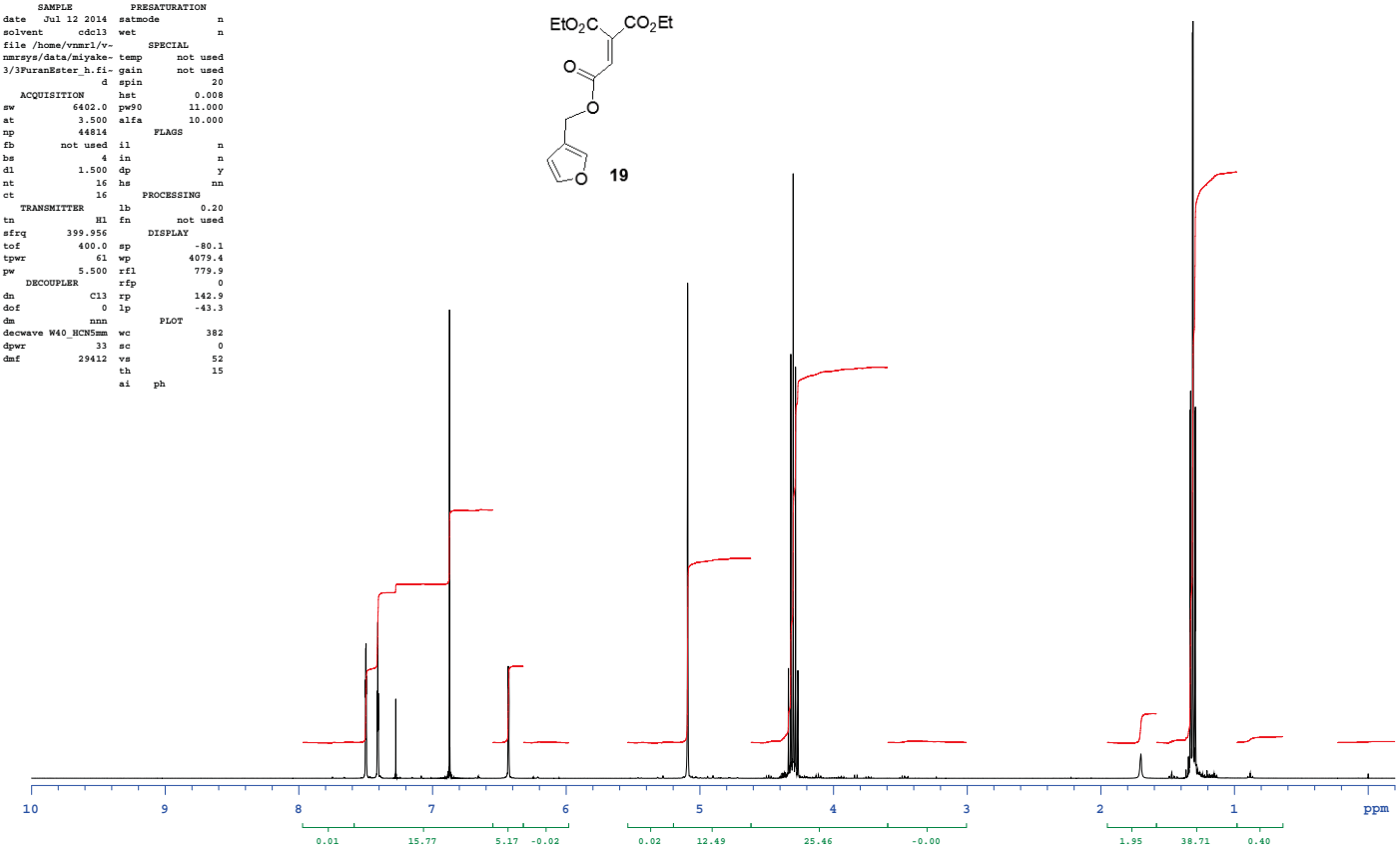
17



^{1}H NMR ($CDCl_3$, 400 MHz)

19

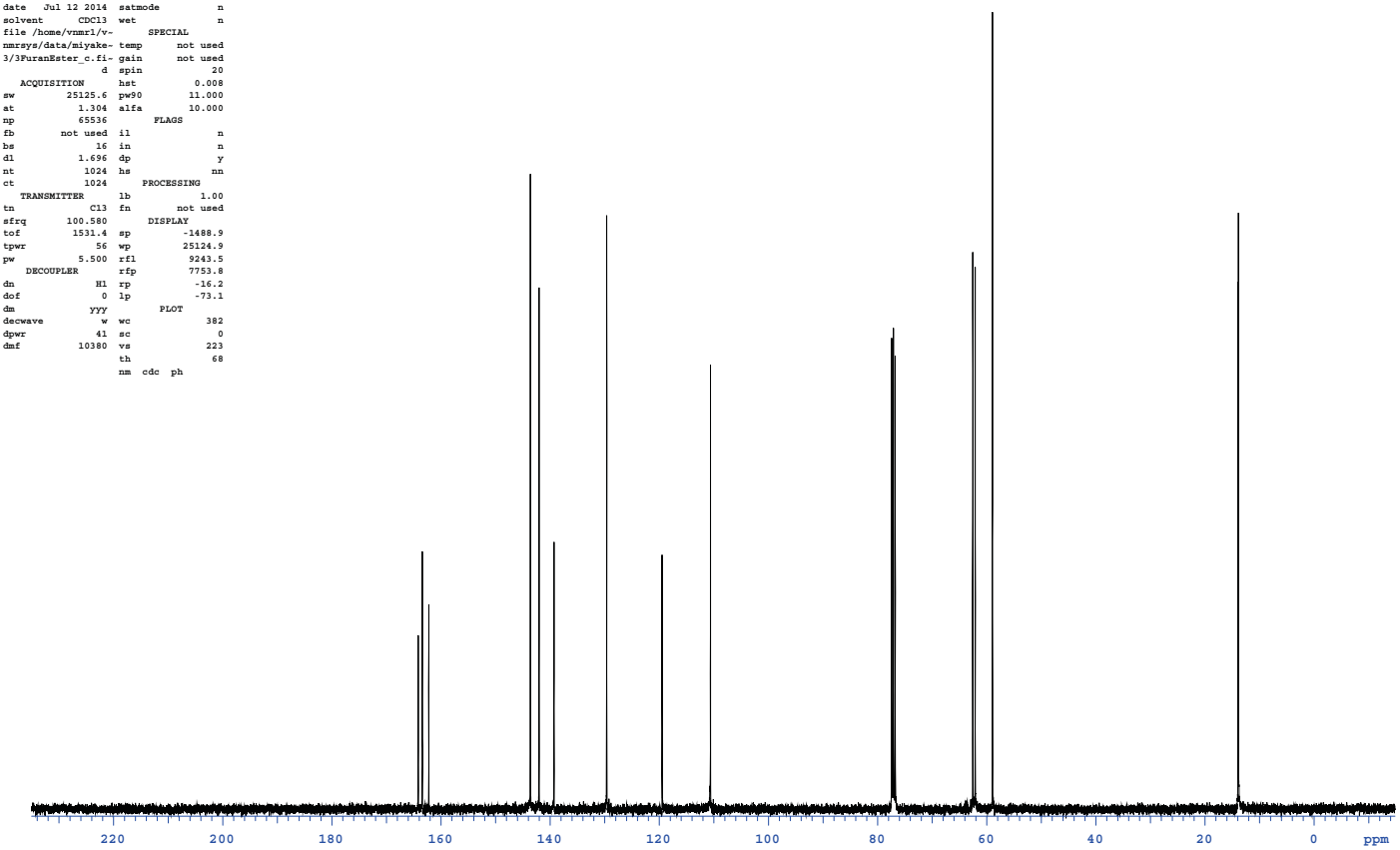
```
miyake3/3FuranEster

exp20  PROTON

      SAMPLE          PRESATURATION
date   Jul 12 2014  satmode          n
solvent      cdcl3  wet              n
file /home/vnmrl/v-      SPECIAL
nmrsys/data/miyake- temp       not used
3/3FuranEster_h.fi- gain       not used
                 d  spin           20
   ACQUISITION      hst         0.008
sw          6402.0  pw90       11.000
at             3.5  alfa       10.000
np           44814        FLAGS
fb       not used  il               n
bs              4  in               n
dl          1.500  dp               y
nt             16  hs              nn
ct             16      PROCESSING
   TRANSMITTER      lb           0.20
tn              H1  fn       not used
sfrq       399.956      DISPLAY
tof          400.0  sp          -80.1
tpwr            61  wp         4079.4
pw           5.500  rfl         779.9
   DECOUPLER        rfp            0
dn             C13  rp          142.9
dof              0  lp          -43.3
dm             nnn        PLOT
decwave W40_HCN5mm  wc           382
dpwr            33  sc             0
dmf          29412  vs            52
                    th            15
                    ai    ph
```



^{13}C NMR ($CDCl_3$, 100.6 MHz)

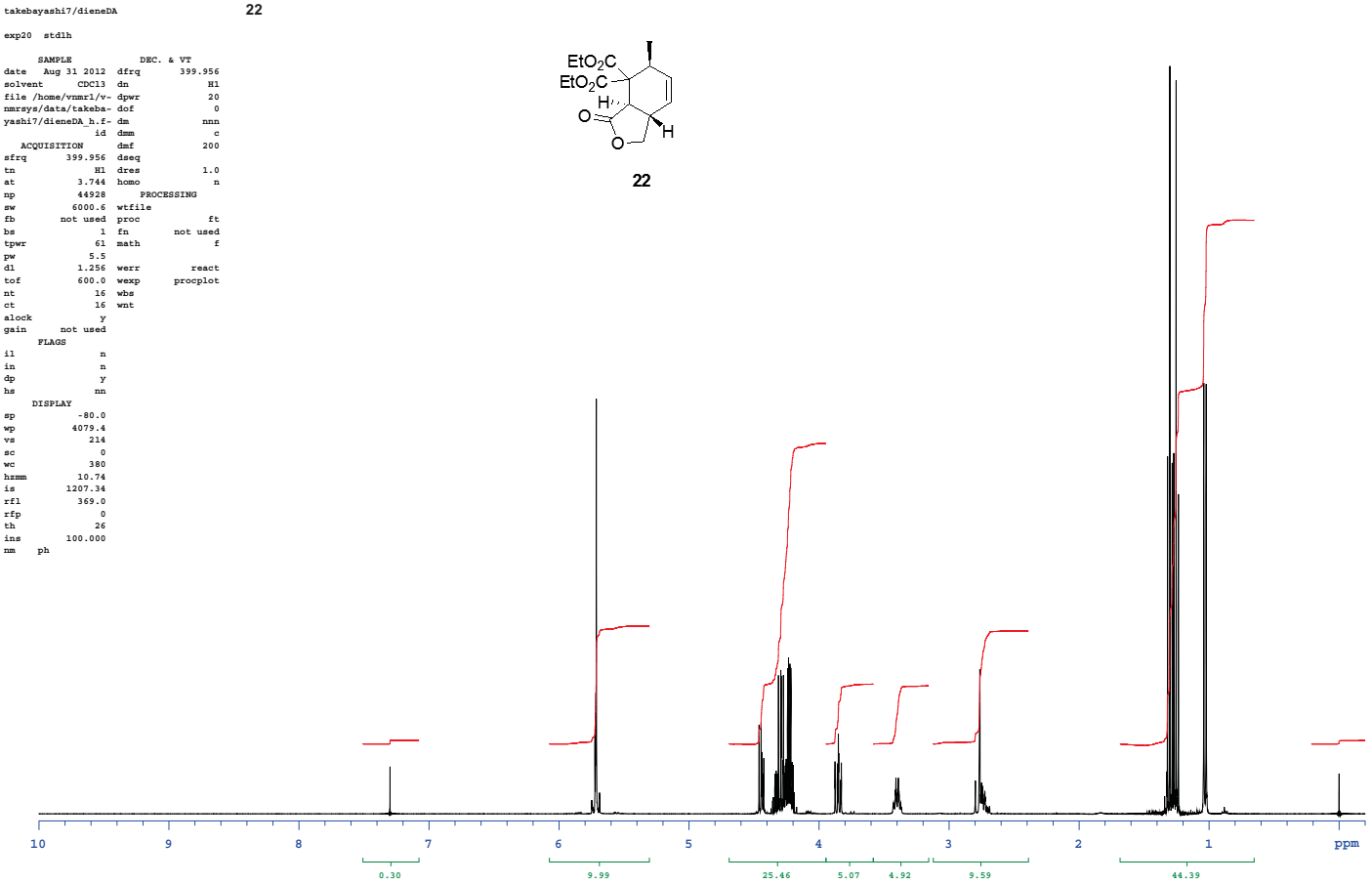
19

```
miyake3/3FuranEster

exp20  CARBON

      SAMPLE          PRESATURATION
date   Jul 12 2014  satmode          n
solvent      CDCl3  wet              n
file /home/vnmrl/v-      SPECIAL
nmrsys/data/miyake- temp       not used
3/3FuranEster_c.fi- gain       not used
                 d  spin           20
   ACQUISITION      hst         0.008
sw         25125.6  pw90       11.000
at           1.304  alfa       10.000
np           65536        FLAGS
fb       not used  il               n
bs             16  in               n
dl          1.696  dp               y
nt          1024  hs              nn
ct          1024      PROCESSING
   TRANSMITTER      lb           1.00
tn             C13  fn       not used
sfrq       100.580      DISPLAY
tof         1531.4  sp         -1488.9
tpwr            56  wp        25124.9
pw           5.500  rfl         9243.5
   DECOUPLER        rfp         7753.8
dn              H1  rp           -16.2
dof              0  lp           -73.1
dm             yyy        PLOT
decwave          w  wc           382
dpwr            41  sc             0
dmf          10380  vs           223
                    th            68
                    nm   cdc   ph
```



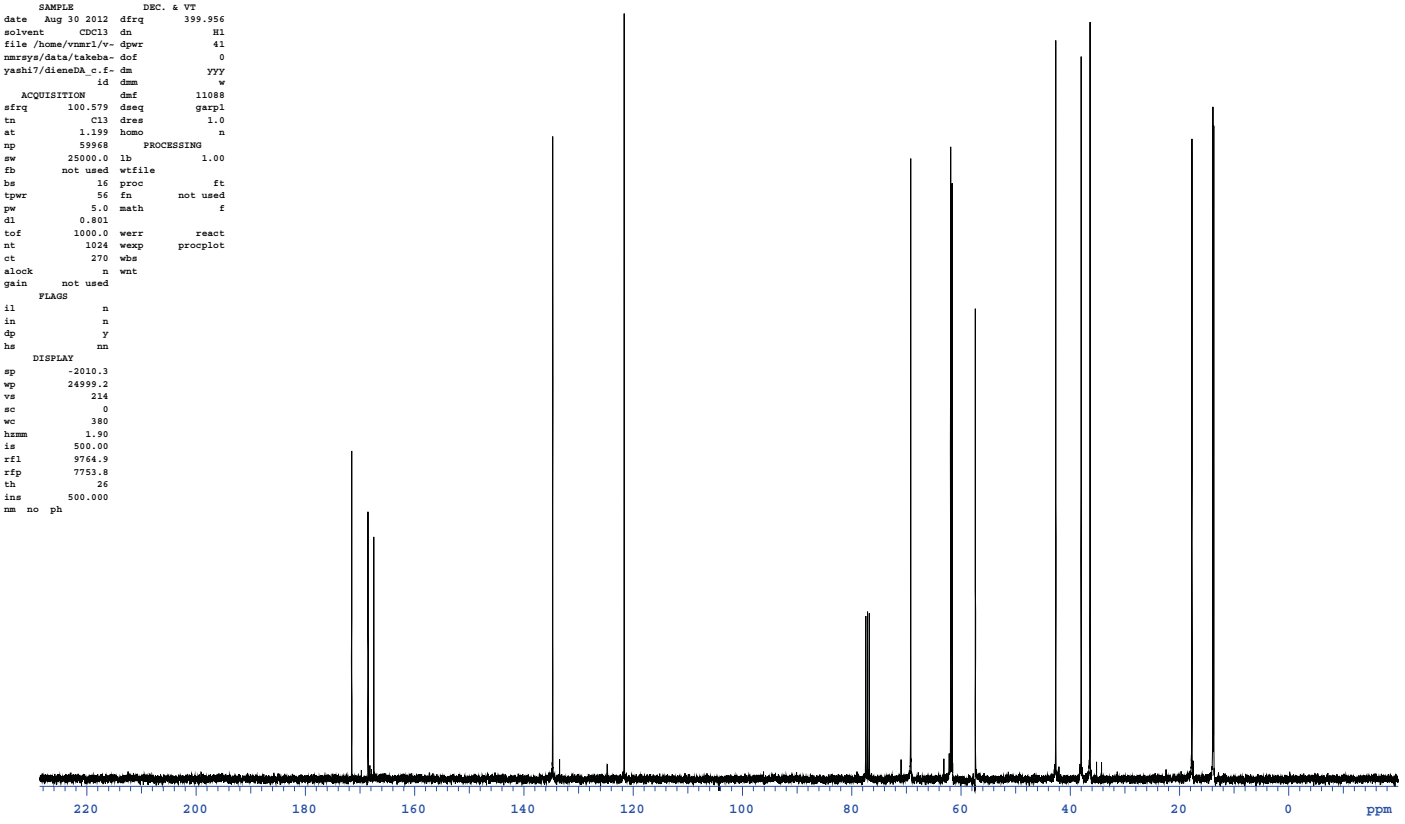
^{1}H NMR ($CDCl_3$, 400 MHz)

22

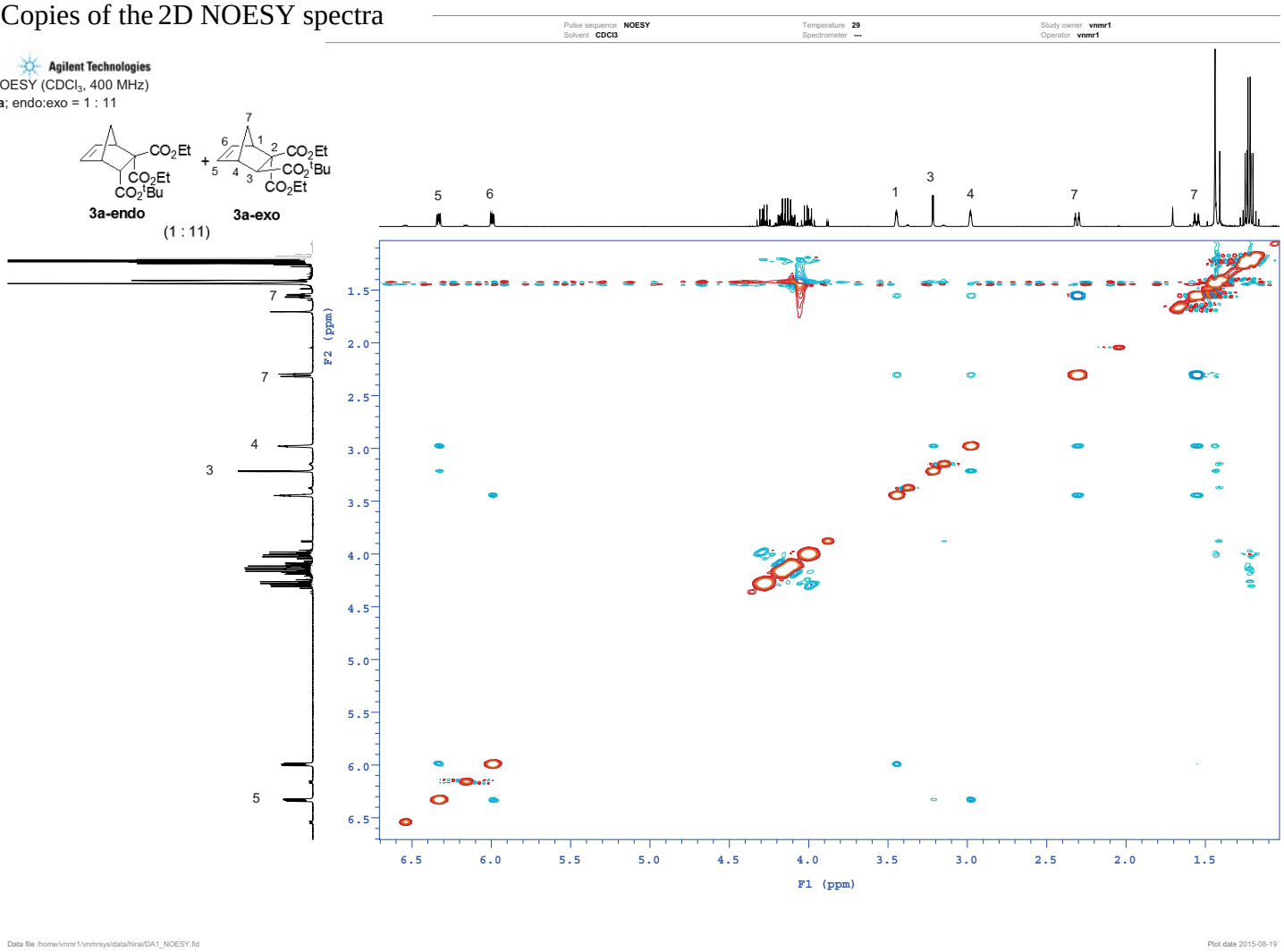


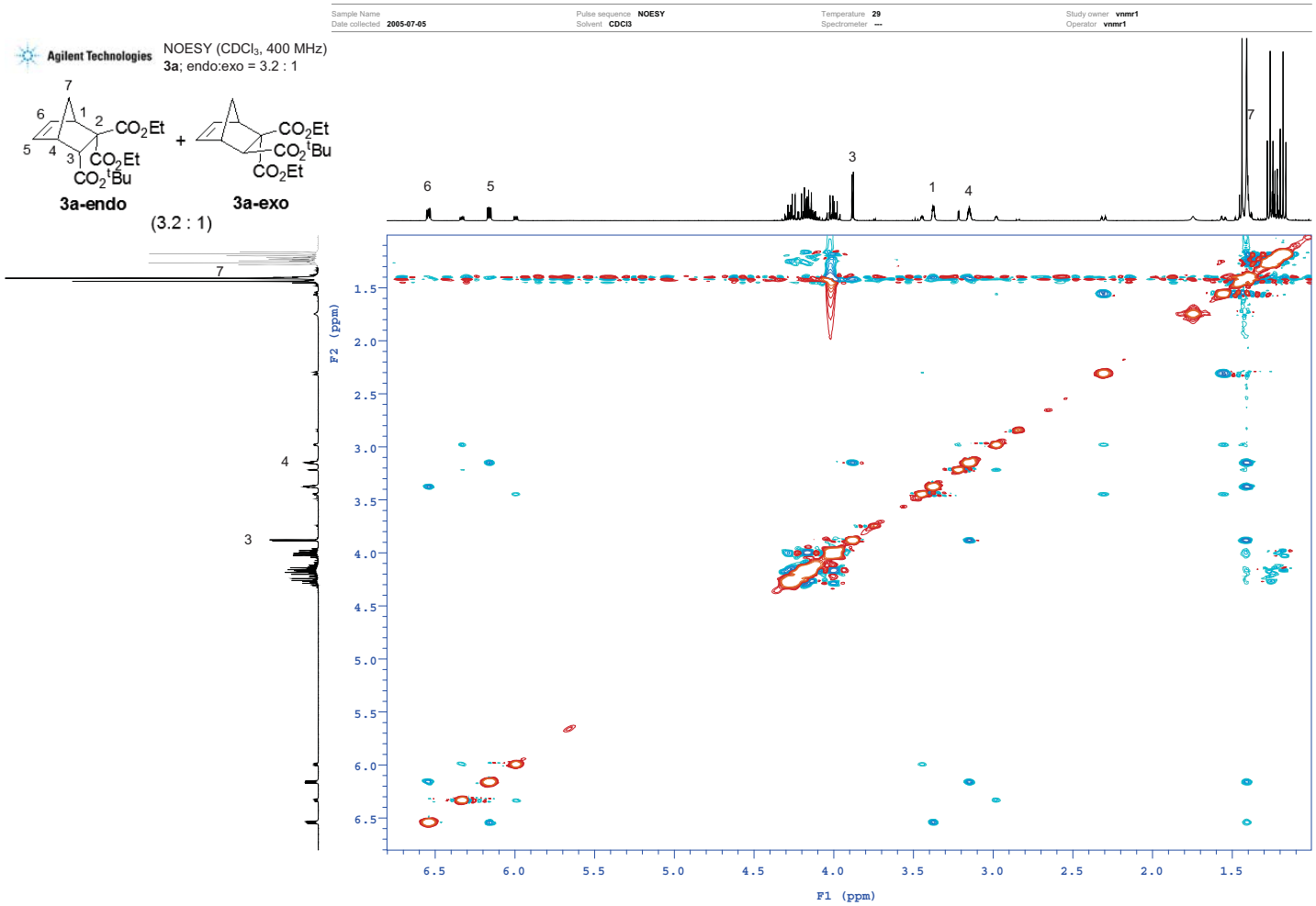
^{13}C NMR ($CDCl_3$, 100.6 MHz)

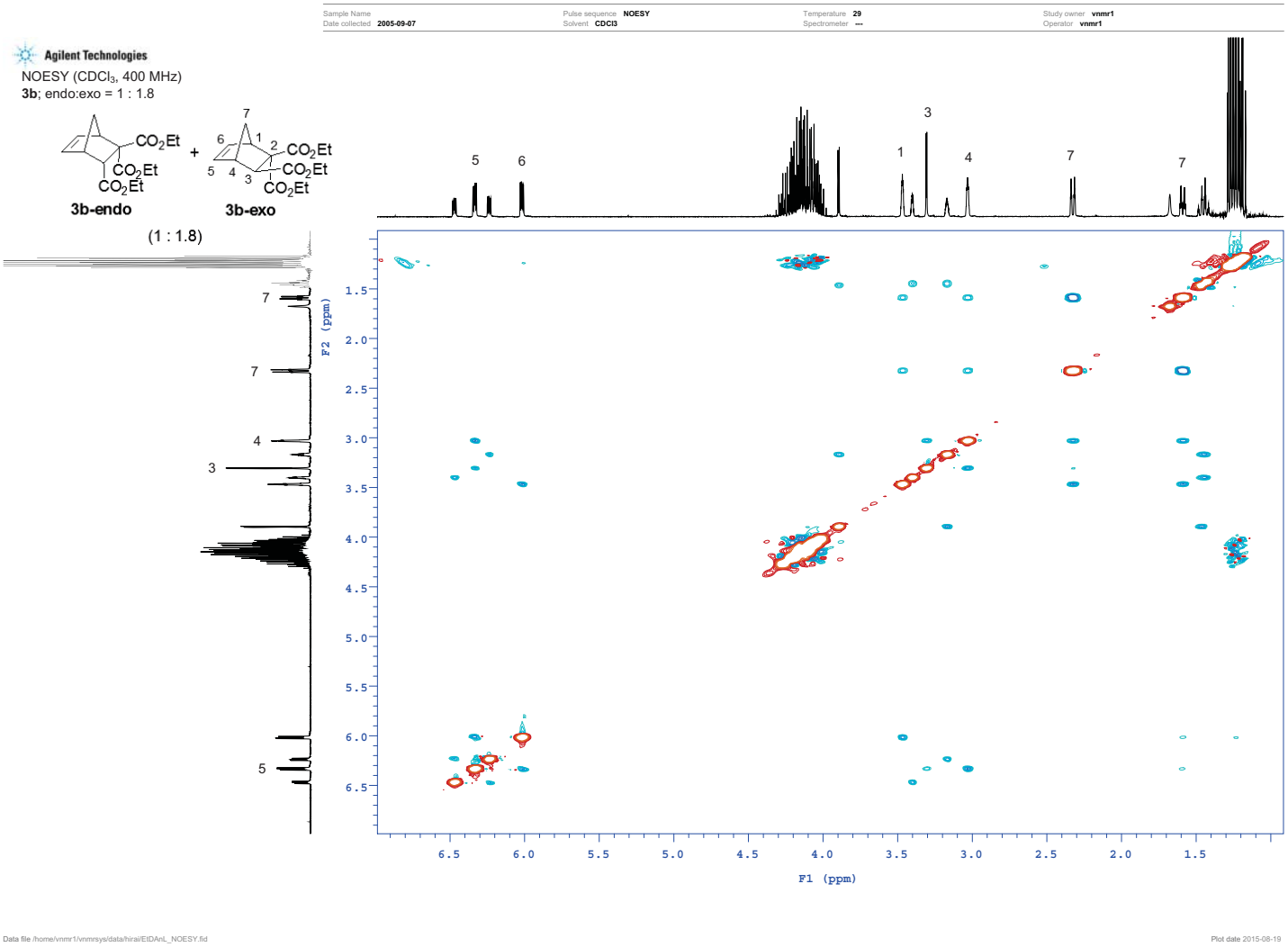
22

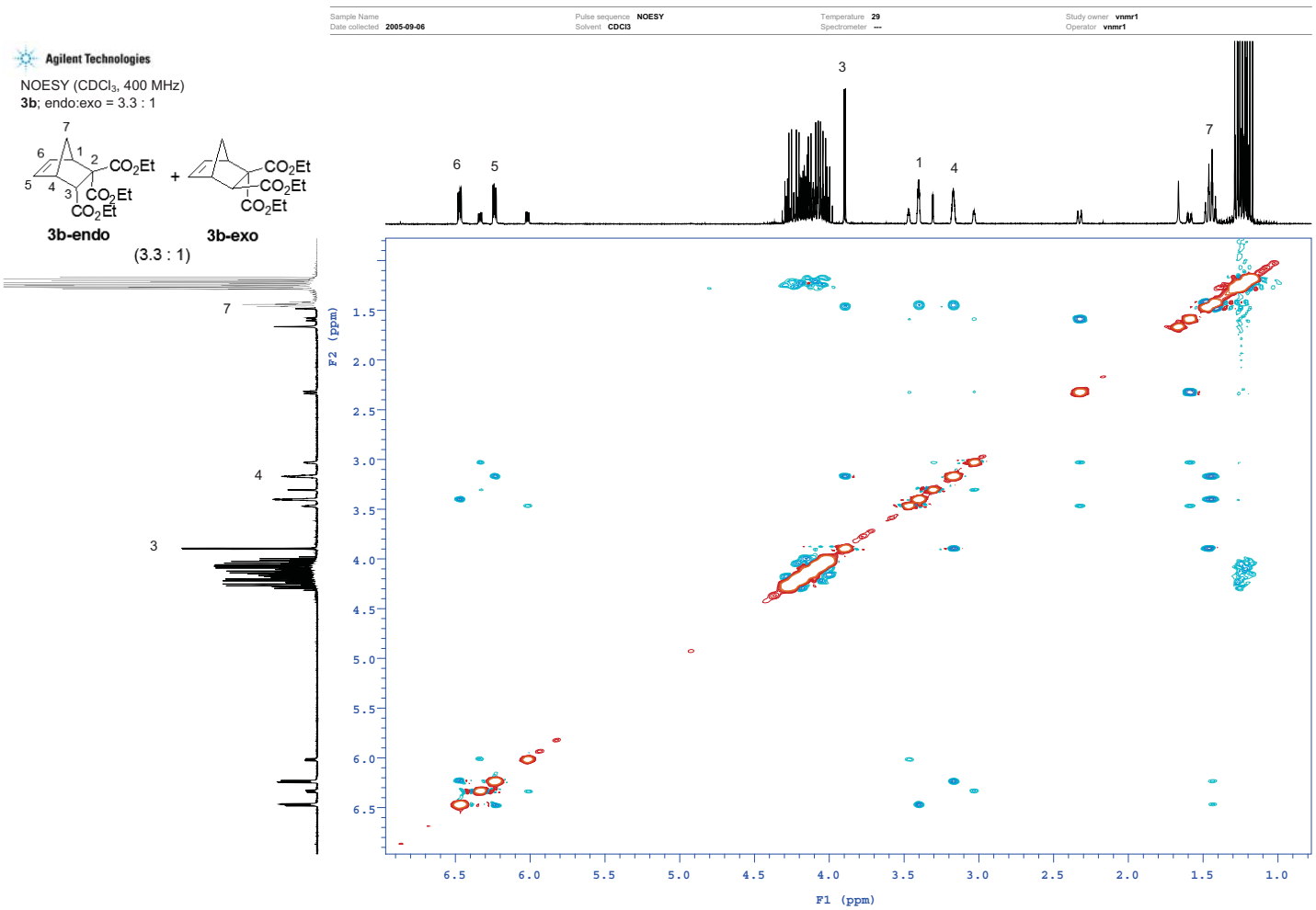


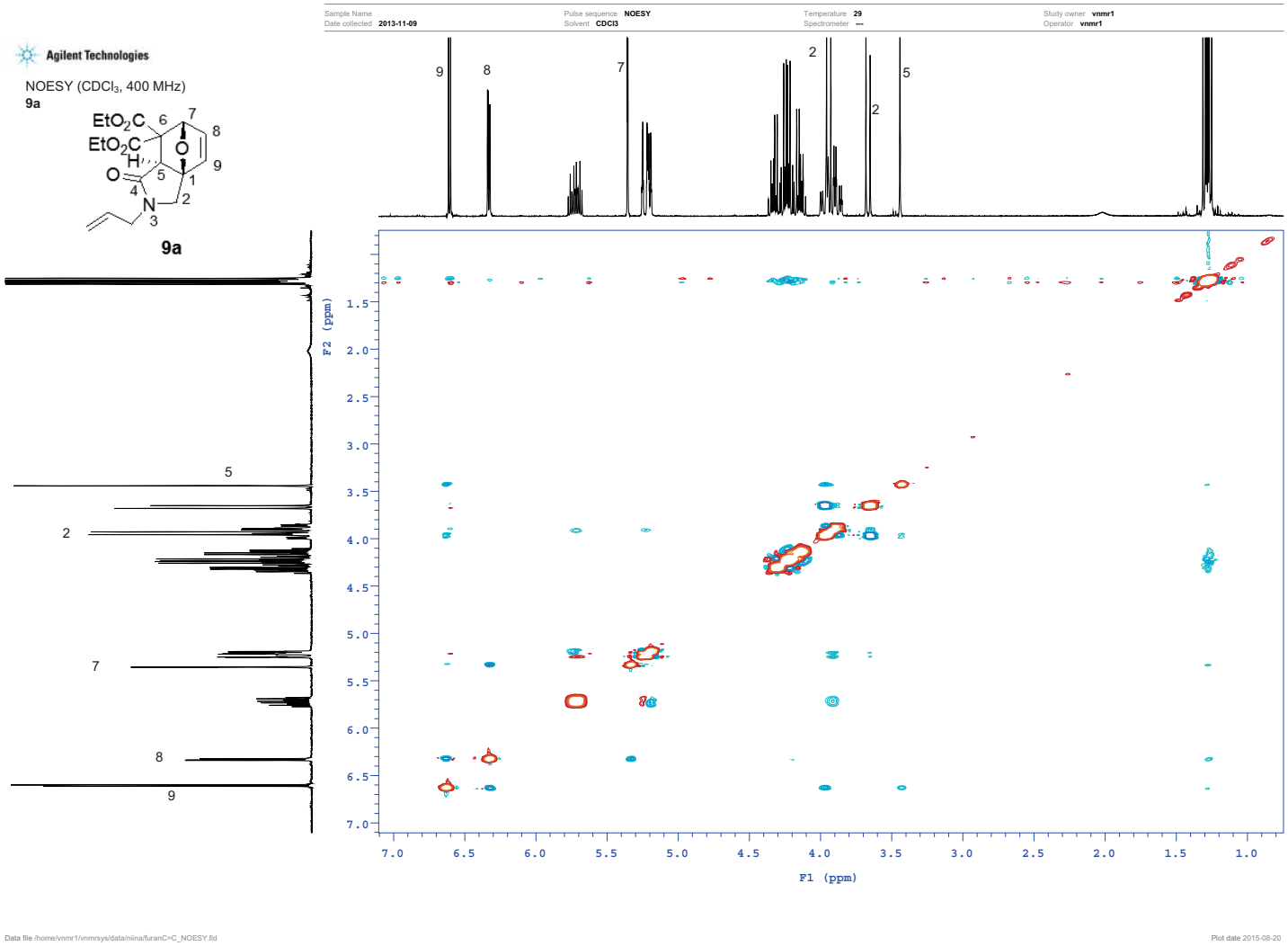
III. Copies of the 2D NOESY spectra

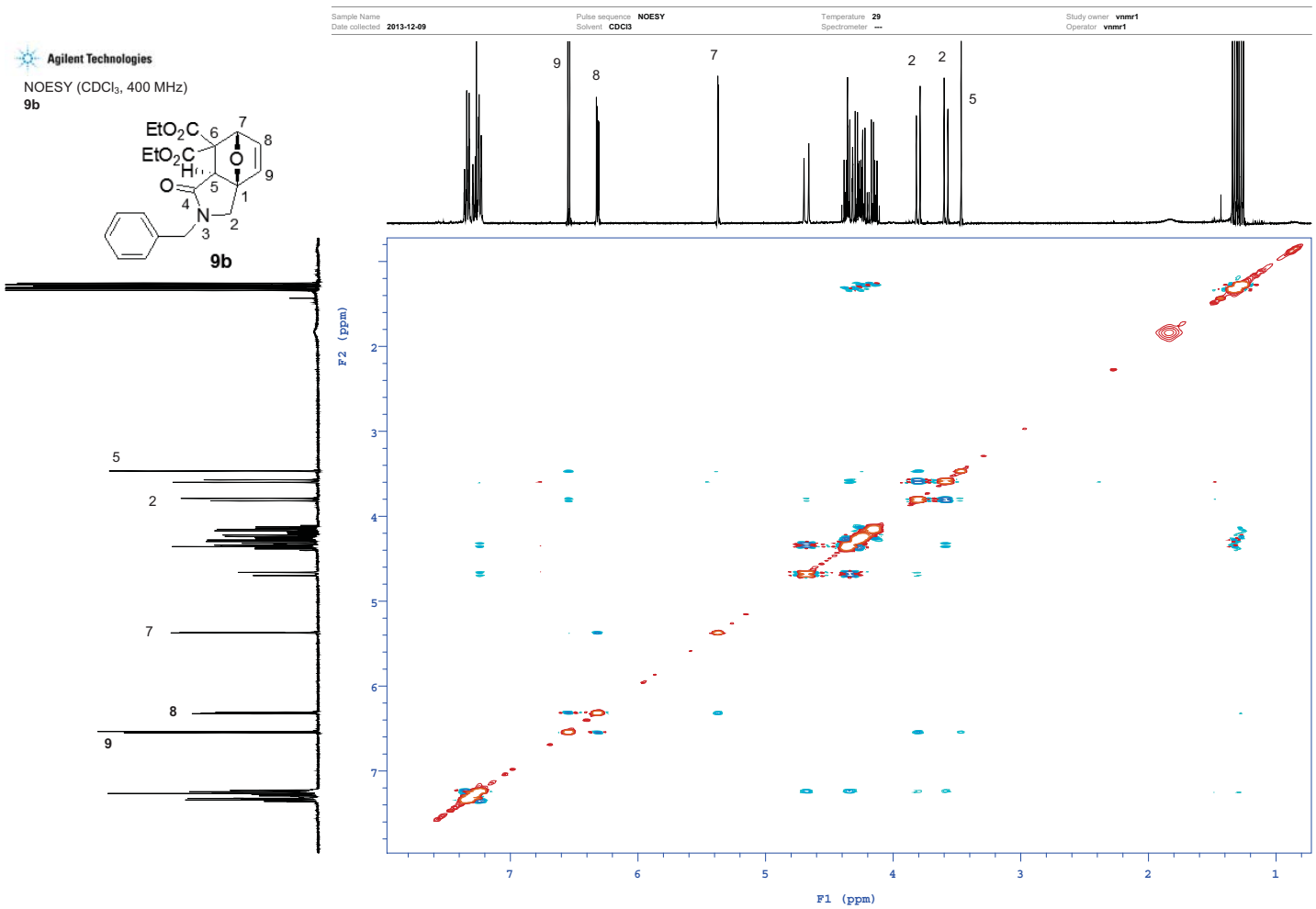


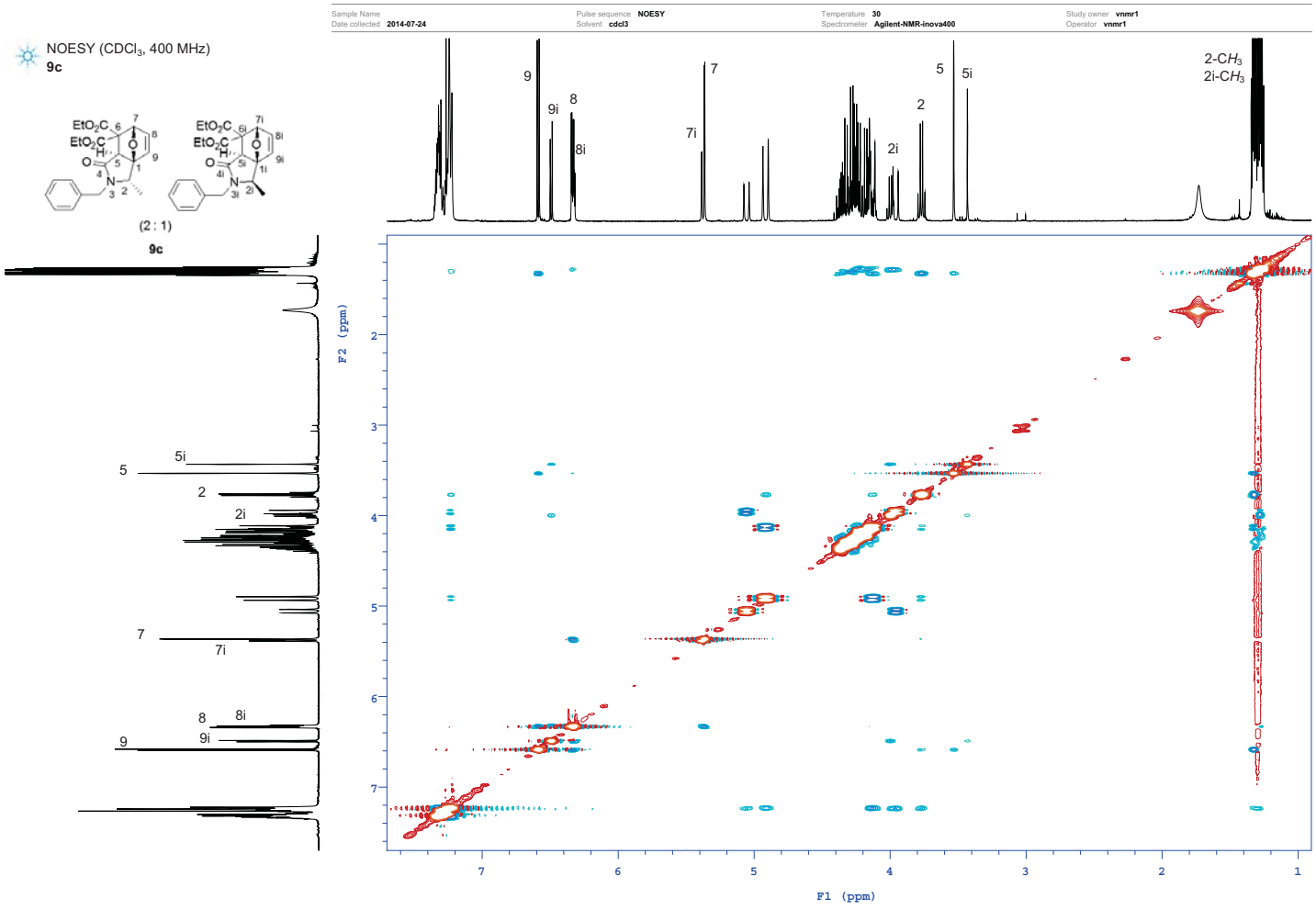


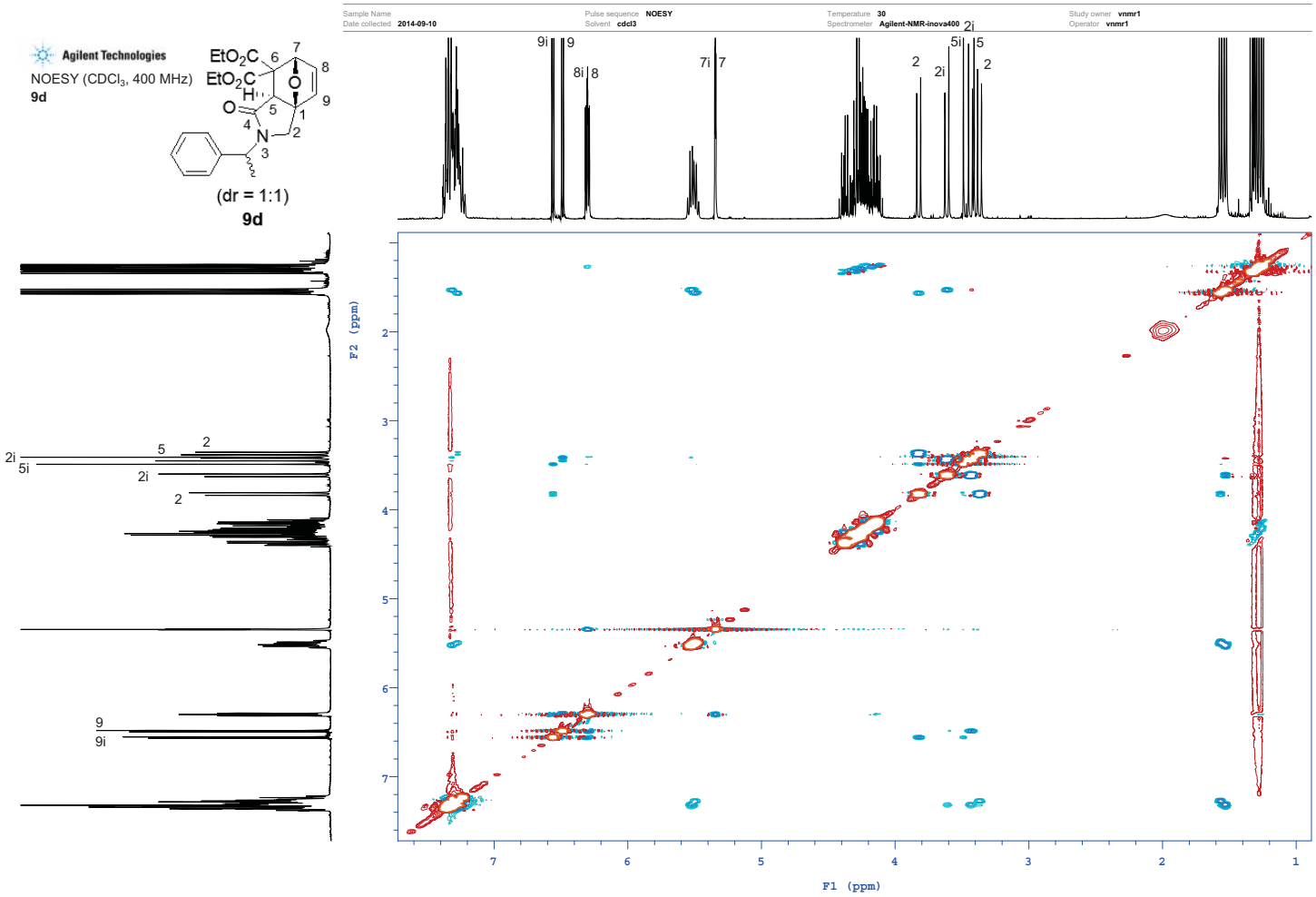

Sample Name
Date collected 2005-09-07
Pulse sequence NOESY
Solvent CDCl3
Temperature 29
Spectrometer ---
Study owner vnmr1
Operator vnmr1
Agilent Technologies
NOESY (CDCl3, 400 MHz)
3b; endo:exo = 1 : 1.8
3b-endo
3b-exo
(1 : 1.8)
F2 (ppm)
F1 (ppm)
Data file /home/vnmr1/vnmrsys/data/hirai/EtDAnL_NOESY.fid
Plot date 2015-08-19

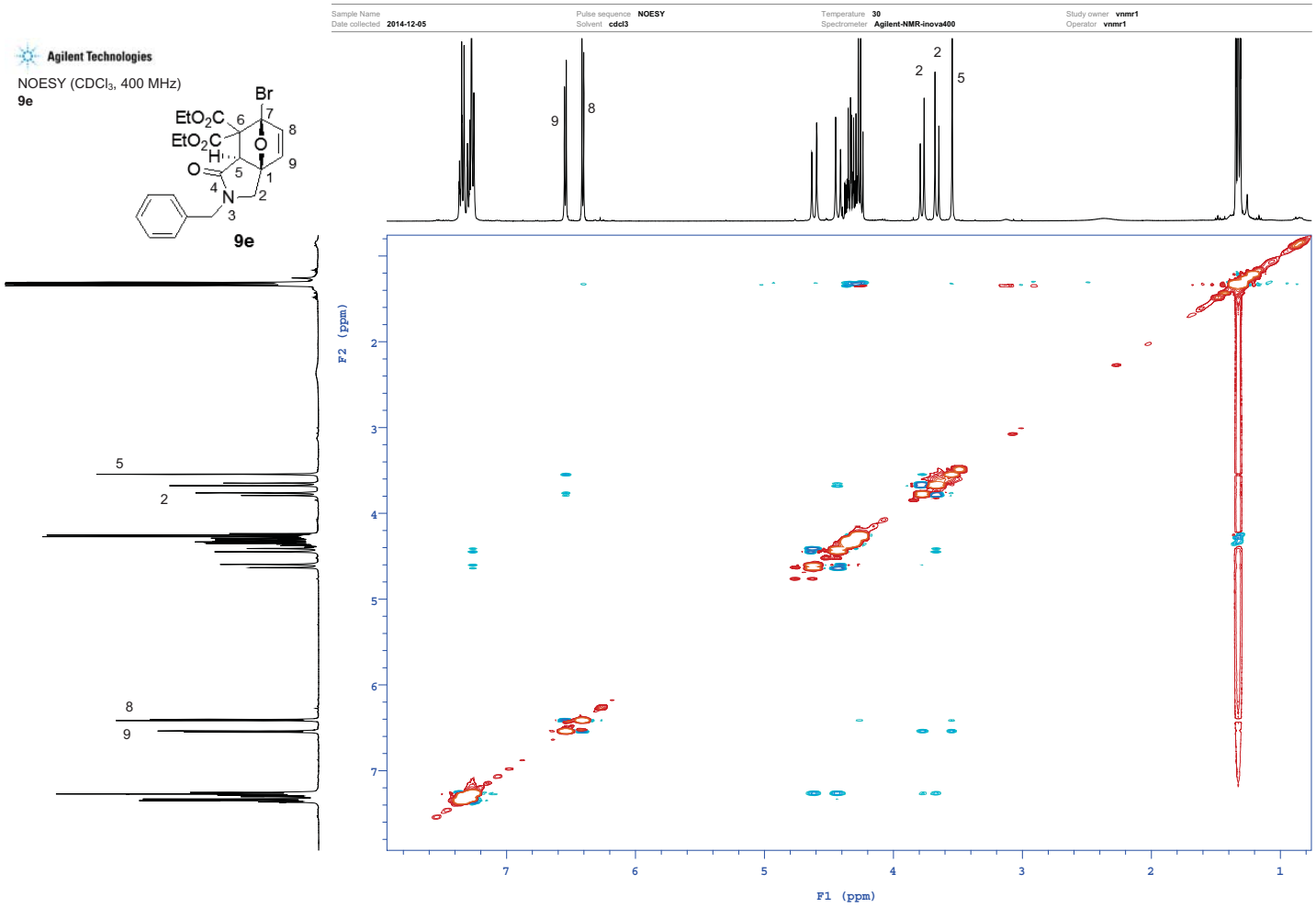

Sample Name
Date collected 2005-09-06
Pulse sequence NOESY
Solvent CDCl3
Temperature 29
Spectrometer ---
Study owner vnmr1
Operator vnmr1
Agilent Technologies
NOESY (CDCl3, 400 MHz)
3b; endo:exo = 3.3 : 1
3b-endo
3b-exo
(3.3 : 1)
F2 (ppm)
F1 (ppm)
Data file /home/vnmr1/vnmrsys/data/hirai/EtDALA_NOESY.fid
Plot date 2015-08-19

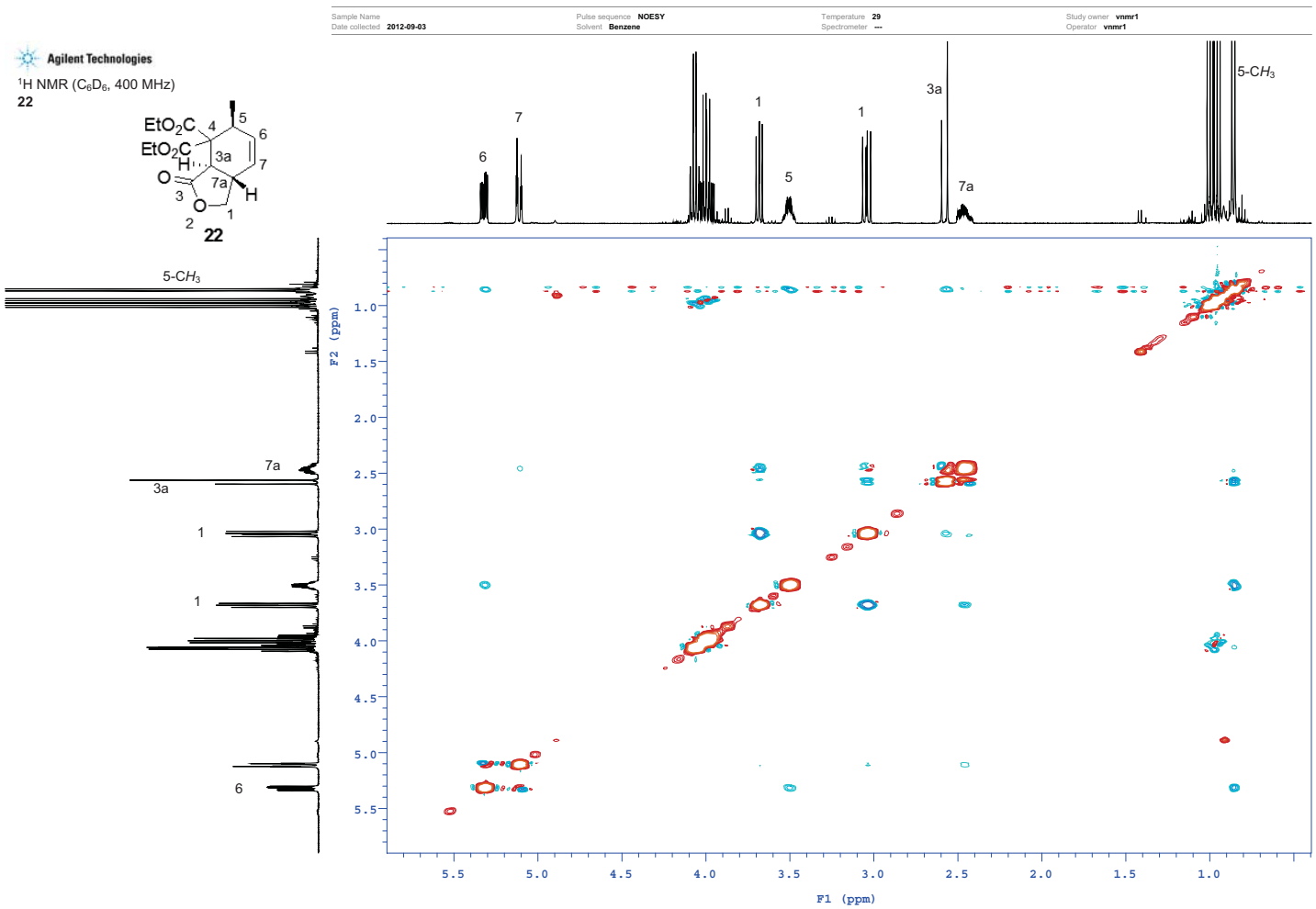

Agilent Technologies
NOESY (CDCl3, 400 MHz)
9a
9a
Sample Name
Date collected 2013-11-09
Pulse sequence NOESY
Solvent CDCl3
Temperature 29
Spectrometer ---
Study owner vnmr1
Operator vnmr1
F2 (ppm)
F1 (ppm)
Data file /home/vnmr1/vnmrsys/data/niina/furanC=C_NOESY.fid
Plot date 2015-08-20


Agilent Technologies
NOESY (CDCl3, 400 MHz)
9b
9b
Sample Name
Date collected 2013-12-09
Pulse sequence NOESY
Solvent CDCl3
Temperature 29
Spectrometer ---
Study owner vnmr1
Operator vnmr1
F2 (ppm)
F1 (ppm)
Data file /home/vnmr1/vnmrsys/data/niina/BzfuranDA_NOESY.fid
Plot date 2015-08-20


Sample Name
Date collected 2014-07-24
Pulse sequence NOESY
Solvent cdcl3
Temperature 30
Spectrometer Agilent-NMR-inova400
Study owner vnmr1
Operator vnmr1
NOESY (CDCl3, 400 MHz)
9c
(2 : 1)
9c
2-CH3
2i-CH3
F2 (ppm)
F1 (ppm)
Data file /home/vnmr1/vnmrsys/data/miyake3/MeFurMixR_NOESY.fid
Plot date 2015-08-20


Agilent Technologies
NOESY (CDCl3, 400 MHz)
9d
(dr = 1:1)
9d
Sample Name
Date collected 2014-09-10
Pulse sequence NOESY
Solvent cdcl3
Temperature 30
Spectrometer Agilent-NMR-inova400
Study owner vnmr1
Operator vnmr1
F2 (ppm)
F1 (ppm)
Data file /home/vnmr1/vnmrsys/data/miyake3/NEtPhR_NOESY.fid
Plot date 2015-08-20


Agilent Technologies
NOESY ($CDCl_3$, 400 MHz)
9e
9e
Sample Name
Date collected 2014-12-05
Pulse sequence NOESY
Solvent cdcl3
Temperature 30
Spectrometer Agilent-NMR-inova400
Study owner vnmr1
Operator vnmr1
F2 (ppm)
F1 (ppm)
Data file /home/vnmr1/vnmrsys/data/sugiura/BrFuranDA_NOESY.fid
Plot date 2015-09-03


Agilent Technologies
^{1}H NMR (C_6D_6, 400 MHz)
22
22
Sample Name
Date collected 2012-09-03
Pulse sequence NOESY
Solvent Benzene
Temperature 29
Spectrometer ---
Study owner vnmr1
Operator vnmr1
5-CH_3
F2 (ppm)
F1 (ppm)
Data file /home/vnmr1/vnmrsys/data/takebayashi7/dieneDAC6D6_NOESY.fid
Plot date 2015-08-20