Supporting Information

for

Diastereoselective Ruthenium Porphyrin-Catalyzed Tandem Nitrone Formation/1,3-Dipolar Cycloaddition for Isoxazolidines. Synthesis, *in Silico* Docking Study and *in Vitro* Biological Activities

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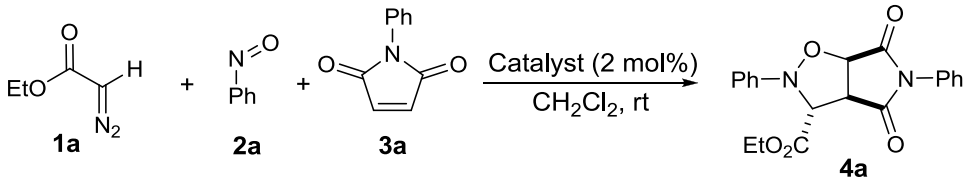
General Experimental Section: Reagents were obtained commercially and used without further purification unless indicated otherwise. All solvents used in the reaction were dried and freshly distilled. Flash chromatography was performed using Merck silica gel 60 and a gradient solvent system (EtOAc/*n*-hexane as eluant). ^{1}H and ^{13}C NMR spectra were measured on either a Bruker DPX-500, DPX-400 or DPX-300 spectrometer. Chemical shifts (δ ppm) were determined with tetramethylsilane (TMS) as internal reference. Mass spectra were determined on a Finnigan MAT 95 mass spectrometer.

General procedure for tandem nitrone formation/1,3-dipolar cycloaddition of EDA, nitrosobenzene and N-phenylmaleimide catalyzed by transition metal complexes

To nitrosobenzene (1.0 mmol), N-phenylmaleimide (1.0 mmol) and catalyst (0.01 mmol) in CH_2Cl_2 (5 mL) was added EDA (0.5 mmol) in CH_2Cl_2 (5 mL) over 4 h via a syringe pump at room temperature. After addition, the resultant solution was stirred for an additional 0.5h. The solvent was removed and the crude residue was purified by silica gel column chromatography to give the corresponding cycloadduct **4a**.

Table S1. Screening of catalyst and reaction condition for the cycloaddition of EDA, nitrosobenzene and N-phenylmaleimide



entry	catalyst	solvent	Conv. (%)	Yield (%)[a]
1	[Ru(TTP)(CO)(MeOH)]	CH_2Cl_2	100	91
2	[Fe(TTP)Cl]	CH_2Cl_2	74	36
3	[Co(TTP)]	CH_2Cl_2	71	47

4	[Ru(*p*-cymene)Cl_2]$_2$	CH_2Cl_2	100	9
5	$Rh_2(OAc)_4$	CH_2Cl_2	100	60
6	$Cu(OTf)_2$	CH_2Cl_2	100	56
7	$[Cu(CH_3CN)_4]PF_6$	CH_2Cl_2	100	53
8	[Ru(TTP)(CO)(MeOH)]	THF	100	65
9	[Ru(TTP)(CO)(MeOH)]	Toluene	100	78
10	[Ru(TTP)(CO)(MeOH)]	CH_2Cl_2	100	90[b]

[a] yield are determined by ^{1}H NMR using 4-iodoanisole as the internal standard; [b] 1 mol% catalyst.

Procedure for scale-up reaction of EDA, nitrosobenzene and N-phenylmaleimide catalyzed by [Ru(TTP)(CO)(MeOH)]

To nitrosobenzene (21.0 mmol), N-phenylmaleimide (21.0 mmol) and [Ru(TTP)(CO)(MeOH)] (0.0175 mmol) in CH_2Cl_2 (40 mL) was added ethyl diazo acetate (17.5 mmol) in CH_2Cl_2 (40 mL) over 20 h via a syringe pump at room temperature. After addition, the resultant solution was stirred for an additional 1 h. The solvent was removed and the crude residue was purified by silica gel column chromatography to give the cycloadduct **4a** in 75% yield (4.8 g, 13.1 mmol).

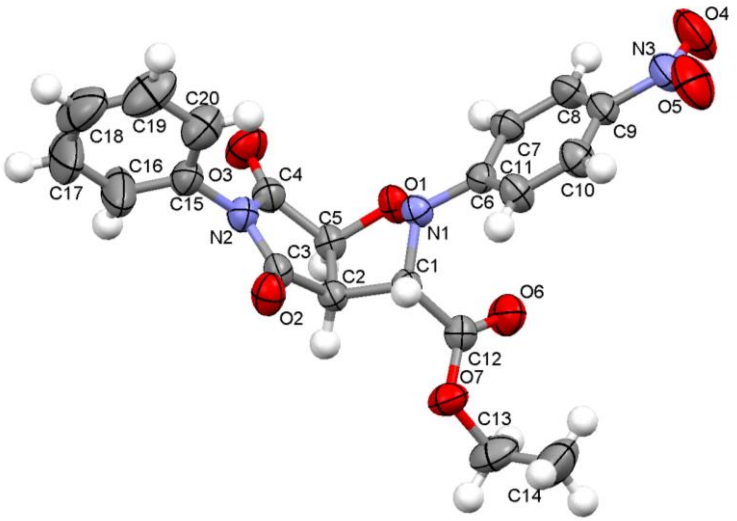


Fig. S1 X-ray crystal structure of **5a** (CCDC 824752 for **5a** contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif)

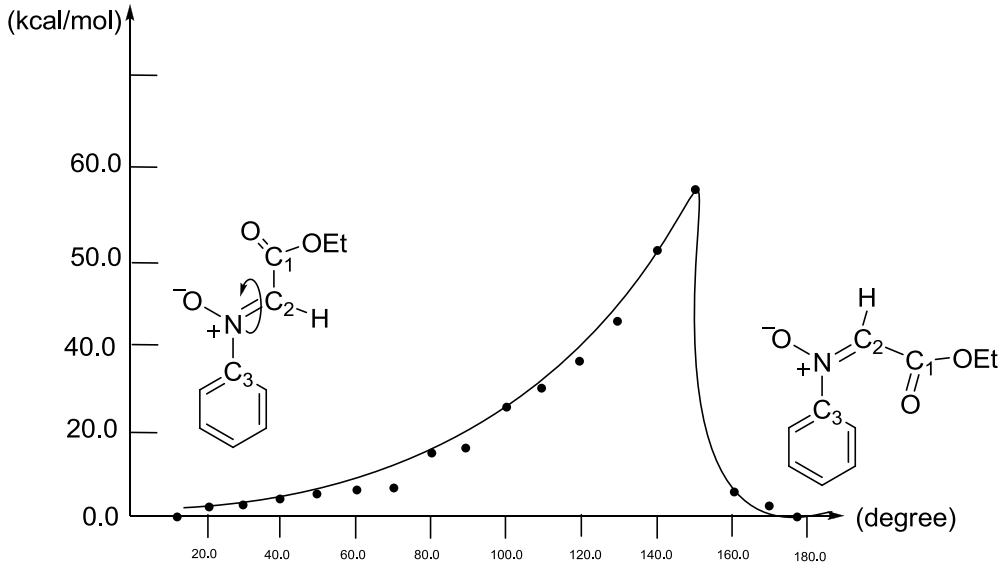


Fig. S2 Potential energy surface of relaxed scan calculation on the C1-C2-N-C3 dihedral angle of *Z*-nitrone for Z/E isomerisation

The Cartesian coordinates, total free energies (Hartree/Particle) of the stationary points found for the cycloaddition of N-phenyl nitrones with ethyl maleate/styrene at the B3LYP/6-31G(d) level.

Z-nitrone

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.994238	-1.451167	0.381852
2	1	0	-4.763148	-1.805515	1.391639
3	1	0	-6.068578	-1.244258	0.326626
4	1	0	-4.761243	-2.252972	-0.326374
5	6	0	-4.209880	-0.193663	0.055954
6	1	0	-4.426090	0.175646	-0.952281
7	1	0	-4.428258	0.619824	0.755798
8	8	0	-2.807762	-0.522000	0.143075
9	6	0	-1.950306	0.511248	-0.102078
10	8	0	-2.310029	1.635824	-0.377666
11	6	0	-0.582915	0.001084	0.021775
12	1	0	-0.426262	-1.036858	0.268931
13	7	0	0.495589	0.760483	-0.129989
14	8	0	0.499720	2.003577	-0.322088
15	6	0	1.816708	0.125779	-0.043746
16	6	0	2.847691	0.888588	0.502938
17	6	0	4.120893	0.332569	0.602383
18	6	0	4.362120	-0.963687	0.139602
19	6	0	3.325402	-1.705373	-0.429178
20	6	0	2.042990	-1.163836	-0.525189
21	1	0	2.634077	1.898123	0.833203
22	1	0	4.927097	0.915303	1.038301
23	1	0	5.358351	-1.390565	0.212035
24	1	0	3.513397	-2.704183	-0.812074
25	1	0	1.245309	-1.726381	-0.998325

Sum of electronic and thermal Free Energies= -667.884505

E-nitrone

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.559761	1.461005	-0.238915
2	8	0	1.039532	2.627919	-0.346730
3	6	0	-0.749906	1.249825	-0.265791
4	6	0	1.563117	0.406073	-0.106663
5	6	0	2.601988	0.635292	0.794069
6	6	0	3.619922	-0.309109	0.902854
7	6	0	3.608681	-1.447845	0.093481
8	6	0	2.575145	-1.645322	-0.824188
9	6	0	1.538980	-0.718463	-0.926976
10	1	0	2.602097	1.543188	1.386198
11	1	0	4.426972	-0.149743	1.611892
12	1	0	4.409514	-2.177689	0.172636
13	1	0	2.572000	-2.522961	-1.463746
14	1	0	0.733055	-0.863368	-1.636131
15	1	0	-1.332093	2.141904	-0.451718
16	6	0	-1.448316	0.007263	0.071594
17	8	0	-0.980337	-1.060592	0.422315
18	8	0	-2.782559	0.235736	-0.044039
19	6	0	-3.638187	-0.879323	0.287999
20	6	0	-5.072635	-0.426118	0.091387
21	1	0	-3.381716	-1.726498	-0.356800
22	1	0	-3.439976	-1.181576	1.321622
23	1	0	-5.757081	-1.246407	0.333511
24	1	0	-5.307581	0.422331	0.741937
25	1	0	-5.249332	-0.124363	-0.945953

Sum of electronic and thermal Free Energies= -667.884373

Z_{exo}-TS(ethyl maleate)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.556085	0.975639	0.147473
2	6	0	-2.813645	-0.063884	-0.420285
3	6	0	-3.399457	-1.313238	-0.655519
4	6	0	-4.724306	-1.528562	-0.280991
5	6	0	-5.467530	-0.503786	0.308953
6	6	0	-4.880364	0.746587	0.514794
7	7	0	-1.451072	0.188274	-0.801533
8	6	0	-0.482203	-0.746236	-0.647766
9	6	0	0.714326	-0.652722	-1.560298
10	8	0	0.742050	-0.016426	-2.586630
11	8	0	-1.045386	1.411962	-0.829588
12	8	0	1.702508	-1.449336	-1.119393
13	6	0	2.952177	-1.337149	-1.851926
14	6	0	3.998690	-2.135953	-1.100542
15	1	0	-2.840047	-2.099937	-1.151142
16	1	0	-5.179476	-2.497342	-0.465675
17	1	0	-6.501601	-0.675217	0.593497
18	1	0	-5.456180	1.551905	0.962031
19	1	0	-3.087709	1.942902	0.280061
20	1	0	-0.806327	-1.748441	-0.390389
21	1	0	2.792495	-1.710919	-2.868569
22	1	0	3.208642	-0.277048	-1.907909

23	1	0	4.958063	-2.068511	-1.625643
24	1	0	4.125384	-1.737761	-0.089803
25	1	0	3.720365	-3.193935	-1.035971
26	6	0	0.146206	1.423041	0.993618
27	6	0	0.134309	0.049869	1.254815
28	1	0	-0.624849	2.050950	1.420841
29	6	0	1.304929	2.136106	0.408503
30	6	0	1.325030	-0.786761	1.602674
31	1	0	-0.750529	-0.307929	1.777218
32	8	0	0.899994	-2.055813	1.852128
33	8	0	2.472965	-0.430968	1.741353
34	6	0	1.918060	-2.973624	2.270978
35	1	0	1.393111	-3.891328	2.540421
36	1	0	2.619908	-3.163343	1.454785
37	1	0	2.466688	-2.578185	3.129815
38	8	0	1.259699	3.450106	0.734230
39	8	0	2.164816	1.649369	-0.296163
40	6	0	2.307299	4.250841	0.168325
41	1	0	2.115149	5.268743	0.509508
42	1	0	3.285110	3.906794	0.516841
43	1	0	2.281521	4.198525	-0.923506

Sum of electronic and thermal Free Energies=-1202.073485

Z_{endo}-TS(ethyl maleate)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.976670	-2.251444	3.491103
2	1	0	1.965891	-1.810485	3.345285
3	1	0	0.427066	-1.671488	4.237069
4	1	0	1.061547	-3.294113	3.798844
5	8	0	0.266074	-2.277351	2.241330
6	6	0	0.028120	-1.069981	1.694598
7	8	0	0.265299	-0.019580	2.250560
8	6	0	-0.664397	-1.241610	0.355046
9	1	0	-1.696507	-1.568525	0.466854
10	6	0	0.019356	-1.731022	-0.760635
11	1	0	-0.538404	-2.135466	-1.595138
12	6	0	1.468463	-1.965481	-0.759701
13	8	0	2.256227	-1.583373	0.092403
14	8	0	1.839881	-2.698183	-1.836659
15	6	0	3.241122	-2.979601	-1.933418
16	1	0	3.595777	-3.499188	-1.038937
17	1	0	3.814340	-2.055562	-2.055043
18	1	0	3.352646	-3.612246	-2.814789
19	7	0	-0.035730	1.003248	-0.876598
20	8	0	0.269289	0.224806	-1.843278
21	6	0	0.958643	1.909992	-0.361574
22	6	0	2.310008	1.649061	-0.596734
23	6	0	3.264065	2.552294	-0.137591
24	6	0	2.878193	3.713250	0.537887
25	6	0	1.523753	3.972251	0.751163
26	6	0	0.557515	3.077118	0.295412
27	1	0	2.595103	0.737599	-1.103924
28	1	0	4.317081	2.343222	-0.303035
29	1	0	3.629213	4.413856	0.891654
30	1	0	1.212781	4.879354	1.261323
31	1	0	-0.496327	3.299127	0.427840
32	6	0	-1.159233	0.694714	-0.171794
33	6	0	-2.429733	0.418605	-0.911473
34	1	0	-1.270563	1.214120	0.771186
35	8	0	-3.444167	0.375471	-0.011067
36	8	0	-2.572135	0.255215	-2.100822
37	6	0	-4.757981	0.113274	-0.559529
38	6	0	-5.729291	0.035140	0.602839

39	1	0	-5.013160	0.918237	-1.256257
40	1	0	-4.721656	-0.819022	-1.132079
41	1	0	-6.739934	-0.160206	0.228277
42	1	0	-5.454592	-0.772052	1.289441
43	1	0	-5.745588	0.974708	1.164284

Sum of electronic and thermal Free Energies=-1202.080805

E_{exo}-TS(ethyl maleate)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.718479	-1.944371	0.659977
2	6	0	2.431751	-0.912724	-0.236538
3	6	0	3.446312	-0.084172	-0.720419
4	6	0	4.750289	-0.266002	-0.266992
5	6	0	5.044399	-1.275898	0.652005
6	6	0	4.026696	-2.114509	1.109679
7	7	0	1.090196	-0.782677	-0.743172
8	6	0	0.310260	0.316571	-0.733049
9	6	0	0.762688	1.676246	-0.329659
10	8	0	-0.063957	2.584216	-0.888333
11	6	0	0.165590	3.960911	-0.504868
12	6	0	-0.817829	4.818991	-1.277365
13	8	0	0.406200	-1.891120	-0.866692
14	8	0	1.677660	1.953620	0.417062
15	1	0	3.219204	0.687925	-1.446386
16	1	0	5.539954	0.378841	-0.641539
17	1	0	6.064097	-1.416119	0.999201
18	1	0	4.249962	-2.910618	1.814300
19	1	0	1.926392	-2.609864	0.981195
20	1	0	-0.547185	0.249317	-1.390670
21	1	0	0.030727	4.043681	0.578191
22	1	0	1.204685	4.219446	-0.731311
23	1	0	-0.675857	5.872667	-1.013590
24	1	0	-0.668431	4.710377	-2.356204
25	1	0	-1.850661	4.540849	-1.044760
26	6	0	-1.011676	-1.756323	0.476846
27	6	0	-0.913039	-0.439355	0.961385
28	1	0	-0.579850	-2.555422	1.068837
29	6	0	-2.131687	-2.176312	-0.431264
30	1	0	-0.194068	-0.257968	1.755327
31	6	0	-2.042699	0.516783	0.955947
32	8	0	-1.717300	1.617478	1.691949
33	8	0	-3.124111	0.384965	0.419532
34	6	0	-2.758153	2.597386	1.799603
35	8	0	-2.815042	-3.205638	0.115300
36	8	0	-2.369965	-1.700891	-1.517144
37	6	0	-3.926228	-3.676798	-0.665693
38	1	0	-2.349493	3.391586	2.426004
39	1	0	-3.029209	2.984151	0.813173
40	1	0	-3.649426	2.165698	2.263447
41	1	0	-4.374648	-4.480602	-0.081004
42	1	0	-4.644202	-2.869048	-0.828820
43	1	0	-3.582146	-4.049748	-1.634152

Sum of electronic and thermal Free Energies=-1202.075815

E_{endo}-TS(ethyl maleate)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-6.203463	-1.680420	-0.605858

2	6	0	-5.231169	-1.625095	-1.107242
3	1	0	-4.808311	-2.633690	-1.151684
4	1	0	-5.391530	-1.271370	-2.130707
5	6	0	-4.315065	-0.687323	-0.344972
6	1	0	-4.134585	-1.027539	0.679379
7	1	0	-4.713629	0.330744	-0.293972
8	8	0	-3.047544	-0.654810	-1.044005
9	8	0	-2.252422	0.810277	0.494245
10	6	0	-2.091672	0.121263	-0.489447
11	6	0	-0.821636	-0.096293	-1.240937
12	1	0	-0.912207	-0.681263	-2.146860
13	7	0	0.217672	0.768189	-1.252337
14	8	0	1.293759	0.237568	-1.780788
15	6	0	0.359221	1.972105	-0.469245
16	6	0	1.391955	2.099621	0.460167
17	6	0	1.531907	3.310282	1.137851
18	6	0	0.663152	4.374742	0.888143
19	6	0	-0.358613	4.232836	-0.052651
20	6	0	-0.508908	3.031518	-0.741619
21	1	0	-1.285402	2.916564	-1.491470
22	1	0	-1.032897	5.058882	-0.260326
23	1	0	0.783074	5.313047	1.422916
24	1	0	2.324628	3.415181	1.873224
25	1	0	2.047322	1.260964	0.663657
26	6	0	1.467210	-1.496620	-0.934639
27	6	0	0.224267	-1.697312	-0.280168
28	1	0	1.558517	-2.026020	-1.876471
29	6	0	2.810674	-1.304465	-0.304421
30	6	0	-0.034036	-1.471503	1.162944
31	1	0	-0.415731	-2.459532	-0.713137
32	8	0	3.706545	-2.061500	-0.992469
33	8	0	3.127644	-0.610673	0.636396
34	6	0	5.062071	-1.966545	-0.530800
35	8	0	-1.158775	-2.153084	1.530422
36	8	0	0.588583	-0.770257	1.929477
37	6	0	-1.573424	-1.927379	2.886577
38	1	0	-2.461079	-2.546009	3.027880
39	1	0	-0.786745	-2.222759	3.585817
40	1	0	-1.809043	-0.870850	3.038875
41	1	0	5.640082	-2.618972	-1.186187
42	1	0	5.419519	-0.935549	-0.600516
43	1	0	5.139852	-2.297895	0.508327

Sum of electronic and thermal Free Energies=-1202.073763

Z_{exo}-TS(styrene)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.175917	-1.426901	0.104189
2	6	0	4.113239	-2.317293	-0.066577
3	6	0	2.818209	-1.844493	-0.265380
4	6	0	2.584311	-0.465650	-0.281846
5	6	0	3.646906	0.435516	-0.139810
6	6	0	4.937228	-0.051656	0.061493
7	1	0	5.760267	0.649237	0.169338
8	1	0	3.477855	1.504689	-0.215760
9	1	0	6.184480	-1.801004	0.254826
10	1	0	4.292284	-3.388783	-0.047304
11	7	0	1.238596	-0.004697	-0.492944
12	8	0	0.366000	-0.859524	-0.890729
13	6	0	0.779088	1.111402	0.128354
14	6	0	-0.293318	1.938222	-0.481842
15	8	0	-0.988935	1.672572	-1.436463
16	8	0	-0.379396	3.103589	0.215645
17	6	0	-1.380566	4.036774	-0.247316

18	1	0	-2.363213	3.555314	-0.200948
19	1	0	-1.182127	4.276784	-1.296819
20	6	0	-1.306585	5.263402	0.642562
21	1	0	-0.318214	5.730567	0.583966
22	1	0	-2.054259	5.998219	0.324818
23	1	0	-1.502839	5.002014	1.687413
24	6	0	-0.712034	-1.148223	1.075967
25	6	0	-0.424993	0.101900	1.619605
26	1	0	0.360443	0.173802	2.366064
27	1	0	-0.027663	-1.959084	1.312297
28	6	0	-2.001373	-1.579366	0.527256
29	1	0	-1.215365	0.839279	1.724755
30	1	0	1.520085	1.677261	0.679805
31	1	0	1.981786	-2.514714	-0.418980
32	6	0	-2.318187	-2.949896	0.543628
33	6	0	-3.543838	-3.413184	0.070466
34	6	0	-4.479918	-2.513580	-0.442100
35	6	0	-4.172570	-1.150627	-0.481498
36	6	0	-2.949912	-0.686934	-0.004517
37	1	0	-1.592399	-3.656370	0.940643
38	1	0	-3.766509	-4.476760	0.099398
39	1	0	-5.435770	-2.870559	-0.816239
40	1	0	-4.886871	-0.444857	-0.897703
41	1	0	-2.713127	0.368265	-0.082382

Sum of electronic and thermal Free Energies=-977.388179

Z_{endo}-TS(styrene)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.144783	3.943011	0.221970
2	6	0	2.638732	2.782040	-0.379655
3	6	0	1.791679	1.715176	-0.665770
4	6	0	0.435584	1.808222	-0.335583
5	6	0	-0.075707	2.978055	0.240088
6	6	0	0.785917	4.036466	0.526141
7	1	0	0.386092	4.942696	0.972550
8	1	0	-1.138341	3.079642	0.435012
9	1	0	2.811390	4.772361	0.440614
10	1	0	3.693797	2.703412	-0.626594
11	7	0	-0.430256	0.708663	-0.665133
12	8	0	0.007277	-0.201240	-1.458173
13	6	0	-1.497553	0.380661	0.109089
14	6	0	-2.704632	-0.225240	-0.523529
15	8	0	-2.812222	-0.675282	-1.640539
16	8	0	-3.719222	-0.197087	0.382358
17	6	0	-4.971061	-0.762965	-0.067523
18	1	0	-4.797273	-1.793962	-0.392405
19	1	0	-5.320124	-0.198756	-0.938527
20	6	0	-5.948707	-0.685454	1.090023
21	1	0	-6.105795	0.352245	1.401587
22	1	0	-6.914929	-1.104548	0.788745
23	1	0	-5.581344	-1.252081	1.951772
24	6	0	0.178318	-1.890691	0.063036
25	6	0	-0.732512	-1.384099	0.991217
26	1	0	-0.374062	-0.956010	1.923818
27	6	0	1.638157	-1.901651	0.205190
28	1	0	-0.213072	-2.524067	-0.726141
29	1	0	-1.703384	-1.861558	1.074466
30	1	0	-1.712596	1.061626	0.924118
31	1	0	2.154910	0.808402	-1.132441
32	6	0	2.417647	-2.491143	-0.810398
33	6	0	3.805136	-2.546643	-0.717042
34	6	0	4.456611	-2.015551	0.399411
35	6	0	3.699926	-1.435482	1.420603

36	6	0	2.311255	-1.383772	1.328816
37	1	0	1.917651	-2.895417	-1.687054
38	1	0	4.380517	-3.004898	-1.517380
39	1	0	5.539634	-2.059638	0.476178
40	1	0	4.193998	-1.027042	2.298604
41	1	0	1.746643	-0.939812	2.143338

Sum of electronic and thermal Free Energies= -977.387465

E_{exo}-TS(styrene)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.033103	-3.073829	0.036968
2	6	0	2.771113	-3.483315	0.472031
3	6	0	1.656446	-2.675337	0.257818
4	6	0	1.813733	-1.439206	-0.375895
5	6	0	3.068144	-1.032387	-0.837712
6	6	0	4.174418	-1.850860	-0.622747
7	1	0	5.149279	-1.533832	-0.982193
8	1	0	3.178073	-0.092610	-1.364862
9	1	0	4.899399	-3.709217	0.198527
10	1	0	2.649879	-4.439398	0.973842
11	7	0	0.636111	-0.654773	-0.639532
12	8	0	-0.470640	-1.302664	-0.810586
13	6	0	0.434940	0.657312	-0.331650
14	1	0	-0.377865	1.087071	-0.903526
15	6	0	-1.552914	-0.645607	1.076661
16	6	0	-0.701849	0.418378	1.383563
17	1	0	0.110960	0.240633	2.082576
18	1	0	-1.307941	-1.627034	1.469748
19	6	0	-2.886643	-0.517966	0.492538
20	1	0	-1.092481	1.432355	1.404919
21	6	0	1.489774	1.617688	0.090613
22	1	0	0.664039	-2.991856	0.554367
23	6	0	-3.716956	-1.652433	0.418223
24	6	0	-4.993067	-1.578628	-0.132542
25	6	0	-5.472727	-0.365220	-0.631387
26	6	0	-4.660908	0.770223	-0.571817
27	6	0	-3.386129	0.696503	-0.016507
28	1	0	-3.345356	-2.602201	0.795566
29	1	0	-5.614195	-2.469542	-0.175769
30	1	0	-6.468118	-0.304746	-1.062987
31	1	0	-5.023742	1.718839	-0.959309
32	1	0	-2.774636	1.593627	0.022225
33	8	0	1.069895	2.871119	-0.207416
34	8	0	2.519284	1.379723	0.688257
35	6	0	1.926476	3.945003	0.246966
36	6	0	1.276638	5.251906	-0.165838
37	1	0	2.044535	3.865948	1.332561
38	1	0	2.916691	3.817578	-0.202159
39	1	0	1.898583	6.093274	0.158418
40	1	0	1.163011	5.306360	-1.253209
41	1	0	0.287267	5.359381	0.290229

Sum of electronic and thermal Free Energies= -977.387314

E_{endo}-TS(styrene)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.599967	4.117320	0.364869
2	6	0	1.592718	3.159479	0.144900

3	6	0	1.263549	1.901170	-0.352852
4	6	0	-0.075537	1.595572	-0.613994
5	6	0	-1.072505	2.557583	-0.427023
6	6	0	-0.730676	3.812278	0.072626
7	1	0	-1.507751	4.557088	0.219663
8	1	0	-2.101973	2.335154	-0.682219
9	1	0	0.862670	5.098629	0.750105
10	1	0	2.632288	3.391192	0.359526
11	7	0	-0.391442	0.327939	-1.213897
12	8	0	0.510118	-0.220131	-1.962297
13	6	0	-1.394078	-0.533144	-0.878327
14	1	0	-1.731348	-1.122850	-1.720452
15	6	0	0.939912	-2.048174	-0.713814
16	6	0	-0.308079	-2.102155	-0.081205
17	1	0	-0.378071	-1.872114	0.978702
18	6	0	2.200611	-1.653665	-0.080809
19	1	0	1.046068	-2.565430	-1.661875
20	1	0	-1.013134	-2.858657	-0.413569
21	6	0	-2.420518	-0.266314	0.166427
22	1	0	2.022744	1.153690	-0.543613
23	8	0	-3.531164	-0.985058	-0.123582
24	8	0	-2.289706	0.392782	1.177262
25	6	0	-4.581846	-0.946230	0.870586
26	6	0	-5.705765	-1.839632	0.381376
27	1	0	-4.172365	-1.282962	1.828471
28	1	0	-4.906253	0.091631	0.997720
29	1	0	-6.525644	-1.834629	1.107782
30	1	0	-6.095046	-1.488947	-0.579747
31	1	0	-5.361032	-2.871295	0.258259
32	6	0	3.401690	-1.798654	-0.804056
33	6	0	4.629677	-1.459340	-0.243150
34	6	0	4.692876	-0.961901	1.060826
35	6	0	3.512537	-0.812550	1.794157
36	6	0	2.284613	-1.157054	1.235427
37	1	0	3.358884	-2.176137	-1.822875
38	1	0	5.539581	-1.581985	-0.825018
39	1	0	5.649968	-0.697185	1.501948
40	1	0	3.548561	-0.428531	2.810421
41	1	0	1.383080	-1.030524	1.827196

Sum of electronic and thermal Free Energies=-977.384641

***In silico* analysis and experimental validation.** A chemical similarity approach (SEA) was recently developed to predict targets for new drugs. [1] With the use of the same approach, [1] the potential target of isoxazolidines was identified to be leukotriene A4 hydrolase (LTA4H). In brief, SEA is a database of a large number of compounds, whose biological targets are known. These reference compounds are classified according to their molecular targets (named as "target set"). Using a statistical model, the chemical similarity between isoxazolidines and all compounds in each target sets were computed and ranked. For more details about the method, please refer to the *Nature* article. [1] Docking was performed using ICM-Pro 3.7-2b program (Molsoft) [2] to evaluate the binding of isoxazolidines with LTA4H. The coordinates of leukotriene A4 hydrolase were taken from the Protein Data Bank (PDB ID: 1HS6). [3] Hydrogen and missing heavy atoms were added to the receptor structure followed by local minimization using the conjugate gradient algorithm and analytical derivatives in the internal coordinate space. The energetically most favorable tautomeric state of His was chosen. Positions of Asn and Gln were optimized to maximize hydrogen bonding. The correct stereochemistry and formal charges were assigned. Each compound was then assigned the MMFF atom types and charges, and subjected to a global energy optimization using the ICM stochastic optimization algorithm. The molecular system is described in terms of internal coordinate variables, using a modified ECEPP/3 force-field with distance-dependent dielectric constant for the energy calculations as implemented in ICM. The biased probability Monte Carlo (BPMC) minimization method consists of the following steps: (1) a random conformation change of the free variables according to a predefined continuous probability distribution, (2) local energy minimization of analytical differentiable terms; (3) calculation of the complete energy including non-differentiable terms such as entropy and salvation energy; (4) acceptance or rejection of the total energy based on the Metropolis criterion and return to step 1.

Aminopeptidase activity of LTA4H was determined as previously described with modification. [4] Recombinant human LTA4H (Cayman, 0.8 μg) was preincubated with the test compounds (2 mM) or vehicle (0.2% DMSO) for 30 min at room temperature in a volume of 90 μL of assay buffer (50 mM Tris-HCl, pH 8.0, 100 mM KCl). Reaction was started with addition of 10 μL of L-alanine-4-nitro-anilide

hydrochloride (Sigma, 5 mM final concentration). The aminopeptidase activity was determined by monitoring absorbance at 405 nm for 2 h.

Reference:

(1) M. J. Keiser, V. Setola, J. J. Irwin, C. Laggner, A. I. Abbas, S. J. Hufeisen, N. H. Jensen, M. B. Kuijer, R. C. Matos, T. B. Tran, R. Whaley, R. A. Glennon, J. Hert, K. L. H. Thomas, D. D. Edwards, B. K. Shoichet and B. L. Roth, *Nature,* 2009, **462**, 175.

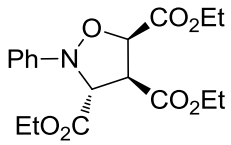
(2) R. A. Abagyan, M. M. Totrov and D. N. Kuznetsov, *J. Comp. Chem.,* 1994, **15**, 488.

(3) M. M. Thunnissen, P. Nordlund and J. Z. Haeggstrom, *Nat. Struct. Biol.,* 2001, **8**, 131.

(4) P. C. Rudberg, F. Tholander, M. M. Thunnissen and J. Z. Haeggström, *J. Biol. Chem.,* 2002, **277**, 1398.

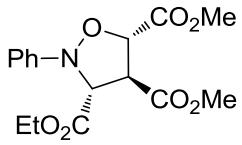
Characterization Data of Isoxazolidines

Triethyl 2-phenylisoxazolidine-3,4,5-tricarboxylate (4b)



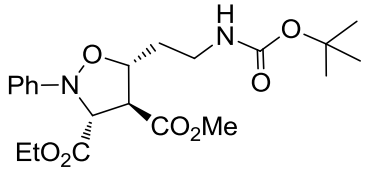
Oil, Yield: 95%; ^{1}H NMR ($CDCl_3$, 400 MHz), δ 1.03 (t, *J* = 7.2 Hz, 3H), 1.18 (t, *J* = 7.2 Hz, 3H), 1.32 (t, *J* = 7.2 Hz, 3H), 3.83-3.97 (m, 2H), 4.10-4.15 (m, 2H), 4.27-4.35 (m, 3H), 4.78 (d, *J* = 7.2 Hz, 1H), 4.97 (d, *J* = 7.6 Hz, 1H), 6.96 (t, *J* = 7.2 Hz, 1H), 7.14 (d, *J* = 8.0 Hz, 2H), 7.23-7.27 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz), δ 13.47, 13.84, 13.99, 53.99, 61.62, 61.68, 62.30, 68.13, 77.86, 114.28, 122.33, 128.61, 150.80, 167.79, 167.83, 169.77; EIMS *m/z* 365.2 (M^+); HRMS (EI) for $C_{18}H_{23}O_7N$, calcd. 365.1475, found 365.1468.

3-Ethyl 4,5-dimethyl 2-phenylisoxazolidine-3,4,5-tricarboxylate (4c)



Oil, Yield: 90%; ^{1}H NMR ($CDCl_3$, 400 MHz), δ 1.30 (t, *J* = 7.2 Hz, 3H), 3.59 (s, 3H), 3.83 (s, 3H), 4.26-4.30 (m, 2H), 4.32-4.34 (m, 1H), 4.81 (d, *J* = 3.6 Hz, 1H), 5.13 (d, *J* = 5.2 Hz, 1H), 7.04 (t, *J* = 7.2 Hz, 1H), 7.11 (d, *J* = 7.6 Hz, 2H), 7.28 (t, *J* = 7.2 Hz, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz), δ 14.05, 52.95, 54.20, 62.41, 70.34, 78.01, 115.35, 123.52, 129.02, 148.92, 168.75, 169.04, 169.86; EIMS *m/z* 337.1 (M^+); HRMS (EI) for $C_{16}H_{19}O_7N$, calcd. 337.1162, found 337.1158.

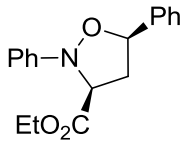
3-Ethyl 4-methyl 5-(2-((tert-butoxycarbonyl)amino)ethyl)-2-phenylisoxazolidine-3,4-dicarboxylate (4d)



Oil, Yield: 55%; ^{1}H NMR ($CDCl_3$, 400 MHz), δ 1.32 (t, *J* = 7.2 Hz, 3H), 1.44 (s, 9H), 1.94-2.03 (m, 1H), 2.17-2.21 (m, 1H), 3.28-3.36 (m, 1H), 3.42-3.46 (m, 1H), 3.65 (s, 3H), 3.74 (dd, *J* = 8.8, 5.2 Hz, 1H), 4.22-4.35 (m, 3H), 4.83 (d, *J* = 5.2 Hz, 1H), 4.93 (brs, 1H), 6.98 (t, *J* = 7.2 Hz, 1H), 7.07 (d, *J* = 8.0 Hz, 2H), 7.29 (t, *J* = 8.4 Hz, 2H);

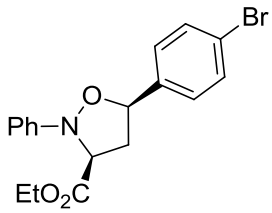
^{13}C NMR ($CDCl_3$, 100 MHz), δ 14.20, 28.50, 32.45, 37.99, 52.84, 56.45, 62.40, 70.40, 79.36, 79.95, 114.32, 122.56, 129.26, 150.07, 155.99, 170.33, 170.43; EIMS *m/z* 422.2 (M^+); HRMS (EI) for $C_{21}H_{30}O_7N_2$, calcd. 422.2053, found 422.2041.

Ethyl 2,5-diphenylisoxazolidine-3-carboxylate (4e)



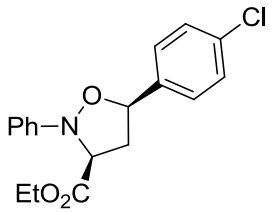
Oil, Yield: 75%; ^{1}H NMR ($CDCl_3$, 400 MHz), δ 1.32 (t, *J* = 7.2 Hz, 3H), 2.70-2.77 (m, 1H), 2.86-2.93 (m, 1H), 4.29 (q, *J* = 7.2 Hz, 2H), 4.51 (dd, *J* = 9.2, 6.0 Hz, 1H), 5.05 (dd, *J* = 9.2, 6.8 Hz, 1H), 6.98 (t, *J* = 7.2 Hz, 1H), 7.14 (d, *J* = 8.0 Hz, 2H), 7.25-7.41 (m, 6H), 7.47-7.49 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz), δ 14.31, 41.31, 61.95, 68.72, 80.29, 114.28, 122.20, 127.21, 128.70, 128.75, 129.27, 137.47, 151.32, 171.62; EIMS *m/z* 297.1 (M^+); HRMS (EI) for $C_{18}H_{19}O_3N$, calcd. 297.1365, found 297.1359.

Ethyl -5-(4-bromophenyl)-2-phenylisoxazolidine-3-carboxylate (4f)



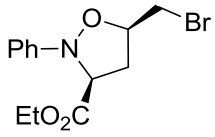
Oil, Yield: 63%; ^{1}H NMR ($CDCl_3$, 400 MHz), δ 1.32 (t, *J* = 7.2 Hz, 3H), 2.65-2.72 (m, 1H), 2.85-2.92 (m, 1H), 4.29 (q, *J* = 7.2 Hz, 2H), 4.51 (dd, *J* = 8.8, 5.2 Hz, 1H), 5.03 (dd, *J* = 9.2, 7.2 Hz, 1H), 7.00 (t, *J* = 7.6 Hz, 1H), 7.13 (d, *J* = 8.0 Hz, 2H), 7.29-7.37 (m, 4H), 7.50-7.52 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz), δ 14.13, 40.92, 61.87, 68.39, 79.37, 114.14, 122.23, 122.45, 128.71, 129.14, 131.71, 136.58, 150.84, 171.28; EIMS *m/z* 375.0 (M^+); HRMS (EI) for $C_{18}H_{18}O_3NBr$, calcd. 375.0470, found 375.0441.

Ethyl 5-(4-chlorophenyl)-2-phenylisoxazolidine-3-carboxylate (4g)



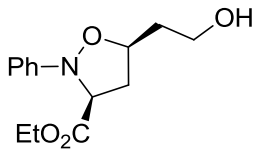
Oil, Yield: 77%; ^{1}H NMR ($CDCl_3$, 400 MHz), δ 1.31 (t, *J* = 7.2 Hz, 3H), 2.65-2.72 (m, 1H), 2.84-2.89 (m, 1H), 4.28 (q, *J* = 7.2 Hz, 2H), 4.50 (dd, *J* = 8.9, 5.2 Hz, 1H), 5.03 (dd, *J* = 9.2, 7.2 Hz, 1H), 6.99 (t, *J* = 7.6 Hz, 1H), 7.12 (d, *J* = 7.6 Hz, 2H), 7.27-7.36 (m, 4H), 7.40-7.43 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz), δ 14.29, 41.09, 62.00, 68.56, 79.51, 114.32, 122.38, 128.59, 128.92, 129.30, 134.45, 136.25, 151.05, 171.44; EIMS *m/z* 331.1 (M^+); HRMS (EI) for $C_{18}H_{18}O_3NCl$, calcd. 331.0975, found 331.0967.

Ethyl 5-(bromomethyl)-2-phenylisoxazolidine-3-carboxylate (4i)



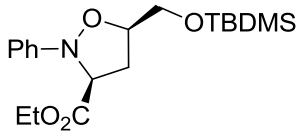
Oil, Yield: 82%; ^{1}H NMR ($CDCl_3$, 400 MHz), δ 1.33 (t, *J* = 7.2 Hz, 3H), 2.54-2.67 (m, 2H), 3.53-3.64 (m, 2H), 4.25-4.31 (m, 2H), 4.41 (dd, *J* = 8.8, 4.4 Hz, Hz, 1H), 4.48 (q, *J* = 6.8 Hz, 1H), 7.00 (t, *J* = 7.6 Hz, 1H), 7.08 (d, *J* = 7.6 Hz, 2H), 7.30 (t, *J* = 7.6 Hz, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz), δ 14.31, 31.52, 37.04, 62.12, 68.10, 77.83, 114.70, 122.80, 129.27, 150.50, 171.16; EIMS *m/z* 313.0 (M^+); HRMS (EI) for $C_{13}H_{16}O_3NBr$, calcd. 313.0314, found 313.0306.

Ethyl 5-(2-hydroxyethyl)-2-phenylisoxazolidine-3-carboxylate (4k)



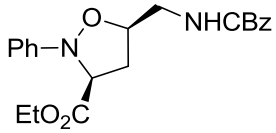
Oil, Yield: 88%; ^{1}H NMR ($CDCl_3$, 400 MHz), δ 1.31 (t, *J* = 7.2 Hz, 3H), 1.98-2.03 (m, 2H), 2.35-2.42 (m, 2H), 2.58-2.64 (m, 1H), 3.81 (t, *J* = 5.6 Hz, 2H), 4.24-4.29 (m, 3H), 4.35 (dd, *J* = 8.8, 5.6 Hz, 1H), 6.95 (t, *J* = 7.6 Hz, 1H), 7.04 (d, *J* = 8.0 Hz, 2H), 7.27 (t, *J* = 8.0 Hz, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz), δ 14.23, 35.35, 38.48, 60.07, 61.90, 68.12, 76.63, 114.24, 122.14, 129.15, 151.13, 171.76; EIMS *m/z* 265.1 (M^+); HRMS (EI) for $C_{14}H_{19}O_4N$, calcd. 265.1314, found 265.1309.

Ethyl 5-(((tert-butyldimethylsilyl)oxy)methyl)-2-phenylisoxazolidine-3-carboxylate (4l)



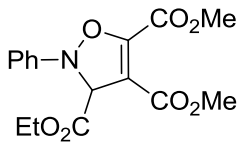
Oil, Yield: 63%; ^{1}H NMR ($CDCl_3$, 400 MHz), δ 0.10 (d, *J* = 3.7 Hz, 6H), 0.91 (s, 9H), 1.31 (t, *J* = 7.2 Hz, 3H), 2.48-2.52 (m, 2H), 3.79-3.89 (m, 2H), 4.23-4.29 (m, 3H), 4.35 (dd, *J* = 8.0, 6.4, Hz, 1H), 6.95 (t, *J* = 7.2 Hz, 1H), 7.07 (d, *J* = 7.6 Hz, 2H), 7.26 (t, *J* = 7.2 Hz, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz), δ -5.21, -5.17, 14.29, 18.42, 25.97, 34.94, 61.79, 63.56, 67.96, 79.02, 114.49, 122.16, 129.09, 151.15, 171.54; EIMS *m/z* 365.2 (M^+); HRMS (EI) for $C_{19}H_{31}O_4NSi$, calcd. 365.2022, found 365.2030.

Ethyl 5-((((benzyloxy)carbonyl)amino)methyl)-2-phenylisoxazolidine-3-carboxylate (4m)



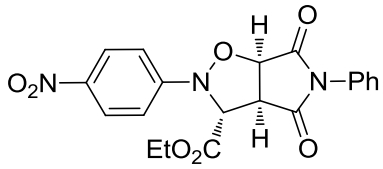
Oil, Yield: 91%; ^{1}H NMR ($CDCl_3$, 400 MHz), δ 1.26 (t, *J* = 7.2 Hz, 3H), 2.37-2.43 (m, 1H), 2.48-2.56 (m, 1H), 3.46-3.53 (m, 1H), 3.58-3.63 (m, 1H), 4.20 (q, *J* = 7.1 Hz, 2H), 4.28-4.39 (m, 2H), 5.12 (dd, *J* = 12.2, 2.8 Hz, 2H), 5.46 (brs, 1H), 6.97 (t, *J* = 7.3 Hz, 1H), 7.02 (d, *J* = 7.8 Hz, 2H), 7.24-7.37 (m, 7H); ^{13}C NMR ($CDCl_3$, 100 MHz), δ 14.16, 34.77, 42.34, 61.88, 66.87, 67.86, 76.88, 114.53, 122.52, 128.08, 128.15, 128.55, 129.13, 136.56, 150.35, 156.77, 171.36; EIMS *m/z* 384.2 (M^+); HRMS (EI) for $C_{21}H_{24}N_2O_5$, calcd. 384.1685, found 384.1680.

3-Ethyl 4,5-dimethyl 2-phenyl-2,3-dihydroisoxazole-3,4,5-tricarboxylate (4n)



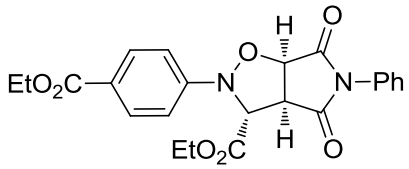
Oil, Yield: 81%; ^{1}H NMR ($CDCl_3$, 400 MHz), δ 1.28 (t, *J* = 6.8 Hz, 3H), 3.61 (s, 3H), 3.89 (s, 1H), 3.93 (s, 3H), 4.23 (q, *J* = 7.2 Hz, 2H), 7.02-7.09 (m, 3H), 7.27 (t, *J* = 8.4 Hz, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz), δ 14.00, 48.33, 53.44, 53.60, 53.98, 62.77, 119.39, 124.53, 129.29, 145.99, 160.22, 163.40, 166.57, 182.37; EIMS *m/z* 335.1 (M^+); HRMS (EI) for $C_{19}H_{17}NO_7$, calcd. 335.1005, found 335.1000.

Ethyl 2-(4-nitrophenyl)-4,6-dioxo-5-phenylhexahydro-2H-pyrrolo[3,4-d]isoxazole-3-carboxylate (5a)



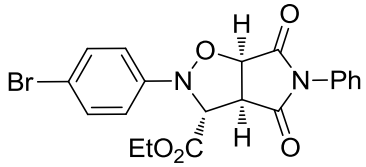
Solid, Yield: 88%; ^{1}H NMR ($CDCl_3$, 400 MHz), δ 1.26 (t, *J* = 7.1 Hz, 3H), 4.24-4.30 (m, 2H), 4.43 (d, *J* = 8.1 Hz, 1H), 5.23 (d, *J* = 7.8 Hz, 2H), 6.77-6.79 (m, 2H), 7.19 (d, *J* = 7.2 Hz, 2H), 7.34-7.36 (m, 3H), 8.16 (d, *J* = 7.2 Hz, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz), δ 14.19, 51.38, 63.23, 67.62, 114.42, 125.50, 125.70, 129.45, 129.52, 130.67, 143.14, 152.53, 166.92, 171.75, 173.08; EIMS *m/z* 411.1 (M^+); HRMS (EI) for $C_{20}H_{17}O_7N_3$, calcd 411.1066, found 411.1056.

Ethyl 2-(4-(ethoxycarbonyl)phenyl)-4,6-dioxo-5-phenylhexahydro-2H-pyrrolo[3,4-d]isoxazole-3-carboxylate (5b)



Oil, Yield: 76%; ^{1}H NMR ($CDCl_3$, 400 MHz), δ 1.28 (t, *J* = 7.2 Hz, 3H), 1.36 (t, *J* = 7.2 Hz, 3H), 4.25-4.37 (m, 4H), 4.41 (d, *J* = 7.6 Hz, 1H), 5.19 (d, *J* = 7.6 Hz, 1H), 5.24 (s, 1H), 6.60-6.63 (m, 2H), 7.16 (d, *J* = 8.8 Hz, 2H), 7.29-7.31 (m, 3H), 7.94-7.96 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz), δ 14.17, 14.47, 51.39, 60.99, 63.02, 68.02, 77.41, 114.02, 125.56, 125.92, 129.23, 129.30, 130.73, 131.25, 151.58, 165.94, 167.57, 172.12, 173.42; EIMS *m/z* 438.2 (M^+); HRMS (EI) for $C_{23}H_{22}O_7N_2$, calcd. 438.1427, found 438.1414.

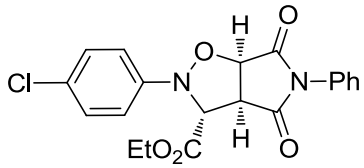
Ethyl 2-(4-bromophenyl)-4,6-dioxo-5-phenylhexahydro-2H-pyrrolo[3,4-d]isoxazole-3-carboxylate (5c)



Oil, Yield: 93%; ^{1}H NMR ($CDCl_3$, 400 MHz), δ 1.26 (t, *J* = 7.2 Hz, 3H), 4.18-4.31 (m, 2H), 4.36 (d, *J* = 8.0 Hz, 1H), 5.13 (d, *J* = 7.6 Hz, 1H), 5.15 (s, 1H), 6.55-6.59 (m,

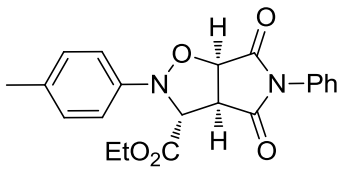
2H), 6.98-7.02 (m, 2H), 7.30-7.37 (m, 5H); ^{13}C NMR ($CDCl_3$, 100 MHz), δ 14.09, 51.38, 62.87, 68.18, 77.42, 116.42, 116.44, 125.94, 129.25, 130.73, 132.31, 147.12, 167.66, 172.31, 173.59; EIMS *m/z* 444.0 (M^+); HRMS (EI) for $C_{20}H_{17}BrO_5N_2$, calcd. 444.0321, found 446.0297.

Ethyl 2-(4-chlorophenyl)-4,6-dioxo-5-phenylhexahydro-2H-pyrrolo[3,4-d]isoxazole-3-carboxylate (5d)



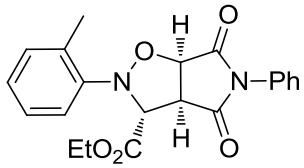
Oil, Yield: 87%; ^{1}H NMR ($CDCl_3$, 400 MHz), δ 1.26 (t, *J* = 7.2 Hz, 3H), 4.19-4.29 (m, 2H), 4.36 (d, *J* = 7.6 Hz, 1H), 5.13 (d, *J* = 7.6 Hz, 1H), 5.15 (s, 1H), 6.58-6.61 (m, 2H), 7.04-7.07 (m, 2H), 7.18-7.21 (m, 2H), 7.31-7.34 (m, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz), δ 14.07, 51.39, 62.83, 68.25, 77.41, 116.09, 125.90, 128.93, 129.21, 129.35, 130.74, 146.56, 167.67, 172.34, 173.61; EIMS *m/z* 400.1 (M^+); HRMS (EI) for $C_{20}H_{17}ClO_5N_2$, calcd. 400.0826, found 400.0818.

Ethyl 4,6-dioxo-5-phenyl-2-(p-tolyl)hexahydro-2H-pyrrolo[3,4-d]isoxazole-3-carboxylate (5e)



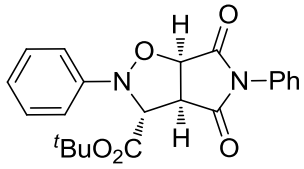
Oil, Yield: 79%; ^{1}H NMR ($CDCl_3$, 400 MHz), δ 1.27 (t, *J* = 7.2 Hz, 3H), 2.24 (s, 3H), 4.21-4.30 (m, 2H), 4.35 (d, *J* = 7.6 Hz, 1H), 5.09 (d, *J* = 7.6 Hz, 1H), 5.21 (s, 1H), 6.47-6.50 (m, 2H), 7.02 (m, 4H), 7.24-7.28 (m, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz), δ 14.04, 20.40, 51.43, 62.67, 68.21, 77.51, 114.55, 126.11, 128.91, 128.98, 129.92, 130.86, 133.27, 145.80, 168.16, 172.55, 173.85; EIMS *m/z* 380.1 (M^+); HRMS (EI) for $C_{21}H_{20}O_5N_2$, calcd. 380.1372, found 380.1365.

Ethyl 4,6-dioxo-5-phenyl-2-(o-tolyl)hexahydro-2H-pyrrolo[3,4-d]isoxazole-3-carboxylate (5f)



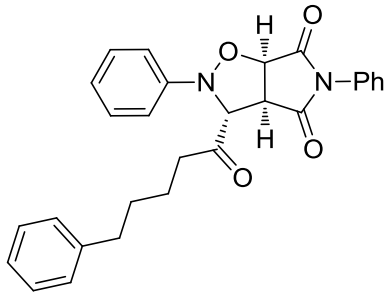
Oil, Yield: 24%; ^{1}H NMR ($CDCl_3$, 400 MHz), δ 0.90 (t, *J* = 7.2 Hz, 3H), 2.25 (s, 3H), 3.87-3.97 (m, 2H), 4.24 (d, *J* = 7.6 Hz, 1H), 4.78 (s, 1H), 5.21 (d, *J* = 7.2 Hz, 1H), 7.04-7.16 (m, 3H), 7.20-7.22 (m, 2H), 7.31 (d, *J* = 7.6 Hz, 1H), 7.39-7.49 (m, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz), δ 13.75, 18.32, 51.61, 61.80, 66.92, 75.44, 117.97, 125.83, 126.42, 126.58, 129.08, 129.29, 129.47, 130.98, 131.33, 143.63, 167.02, 173.21, 174.27; EIMS *m/z* 380.1 (M^+); HRMS (EI) for $C_{21}H_{20}O_5N_2$, calcd. 380.1372, found 380.1365.

Tert-butyl 4,6-dioxo-2,5-diphenylhexahydro-2H-pyrrolo[3,4-d]isoxazole-3-carboxylate (5i)



Oil, Yield: 73%; ^{1}H NMR ($CDCl_3$, 400 MHz), δ 1.44 (s, 9H), 4.30 (d, *J* = 7.6 Hz, 1H), 5.09 (s, 1H), 5.13 (d, *J* = 7.6 Hz, 1H), 6.60-6.63 (m, 2H), 7.01 (t, *J* = 7.2 Hz, 1H), 7.12 (d, *J* = 8.0 Hz, 2H), 7.23-7.27 (m, 2H), 7.29-7.31 (m, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz), δ 27.90, 51.32, 69.13, 77.32, 83.59, 114.81, 123.50, 126.23, 129.13, 129.40, 130.95, 148.10, 166.93, 172.73, 174.12; EIMS *m/z* 394.1 (M^+); HRMS (EI) for $C_{22}H_{22}O_5N_2$, calcd. 394.1529, found 394.1527.

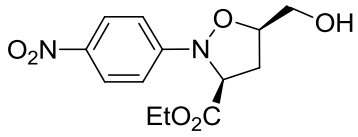
2,5-Diphenyl-3-(5-phenylpentanoyl)dihydro-2H-pyrrolo[3,4-d]isoxazole-4,6(5H,6aH)-dione (5j)



Oil, Yield: 82%; ^{1}H NMR ($CDCl_3$, 400 MHz), δ 1.61-1.70 (m, 4H), 2.60-2.71 (m, 3H), 2.90-2.96 (m, 1H), 4.56 (d, *J* = 7.6 Hz, 1H), 4.91 (d, *J* = 7.6 Hz, 1H), 5.15 (s, 1H),

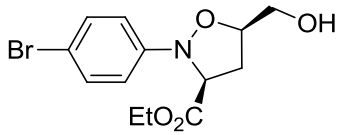
6.35-6.37 (m, 2H), 7.03 (t, *J* = 7.2 Hz, 1H), 7.11 (d, *J* = 8.0 Hz, 2H), 7.15-7.18 (m, 3H), 7.23-7.28 (m, 7H); ^{13}C NMR ($CDCl_3$, 100 MHz), δ 23.34, 30.80, 35.69, 38.54, 49.28, 73.38, 77.91, 113.98, 123.74, 125.94, 126.14, 128.48, 128.52, 129.05, 129.11, 129.88, 130.87, 142.12, 148.66, 172.51, 174.72, 205.26; EIMS *m/z* 454.2 (M^+); HRMS (EI) for $C_{28}H_{26}O_4N_2$, calcd. 454.1893, found 454.1886.

Ethyl 5-(hydroxymethyl)-2-(4-nitrophenyl)isoxazolidine-3-carboxylate (5k)



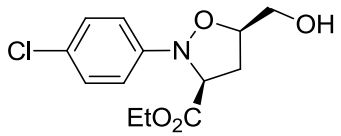
Oil, Yield: 62%; ^{1}H NMR ($CDCl_3$, 400 MHz), δ 1.31 (t, *J* = 7.2 Hz, 3H), 2.39 (brs, 1H), 2.67 (t, *J* = 7.2 Hz, 2H), 3.76-3.79 (m, 1H), 3.97-4.01 (m, 1H), 4.23-4.31 (m, 2H), 4.32-4.38 (m, 1H), 4.52 (t, *J* = 7.0 Hz, 1H), 7.05-7.08 (m, 2H), 8.12-8.16 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz), δ 14.24, 34.05, 61.84, 62.36, 66.08, 79.50, 113.35, 125.55, 142.00, 154.92, 170.59; EIMS *m/z* 296.1 (M^+); HRMS (EI) for $C_{13}H_{16}O_6N_2$, calcd. 296.1008, found 296.1001.

Ethyl 5-(hydroxymethyl)-2-(4-bromophenyl)isoxazolidine-3-carboxylate (5l)



Oil, Yield: 94%; ^{1}H NMR ($CDCl_3$, 400 MHz), δ 1.30 (t, *J* = 7.2 Hz, 3H), 2.48-2.59 (m, 2H), 2.82 (brs, 1H), 3.70-3.73 (m, 1H), 3.92 (d, *J* = 12.4 Hz, 1H), 4.18-4.28 (m, 2H), 4.30-4.37 (m, 2H), 6.93-6.96 (m, 2H), 7.34-7.38 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz), δ 14.17, 33.69, 61.99, 62.09, 67.69, 78.71, 114.90, 116.36, 131.95, 149.53, 171.31; EIMS *m/z* 329.0 (M^+); HRMS (EI) for $C_{13}H_{16}O_4NBr$, calcd. 329.0263, found 329.0251.

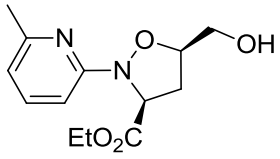
Ethyl 5-(hydroxymethyl)-2-(4-chlorophenyl)isoxazolidine-3-carboxylate (5m)



Oil, Yield: 89%; ^{1}H NMR ($CDCl_3$, 400 MHz), δ 1.30 (t, *J* = 7.2 Hz, 3H), 2.51-2.58 (m, 2H), 2.72 (brs, 1H), 3.72 (dd, *J* = 12.4, 4.8 Hz, 1H), 3.93 (dd, *J* = 12.4, 2.0 Hz,

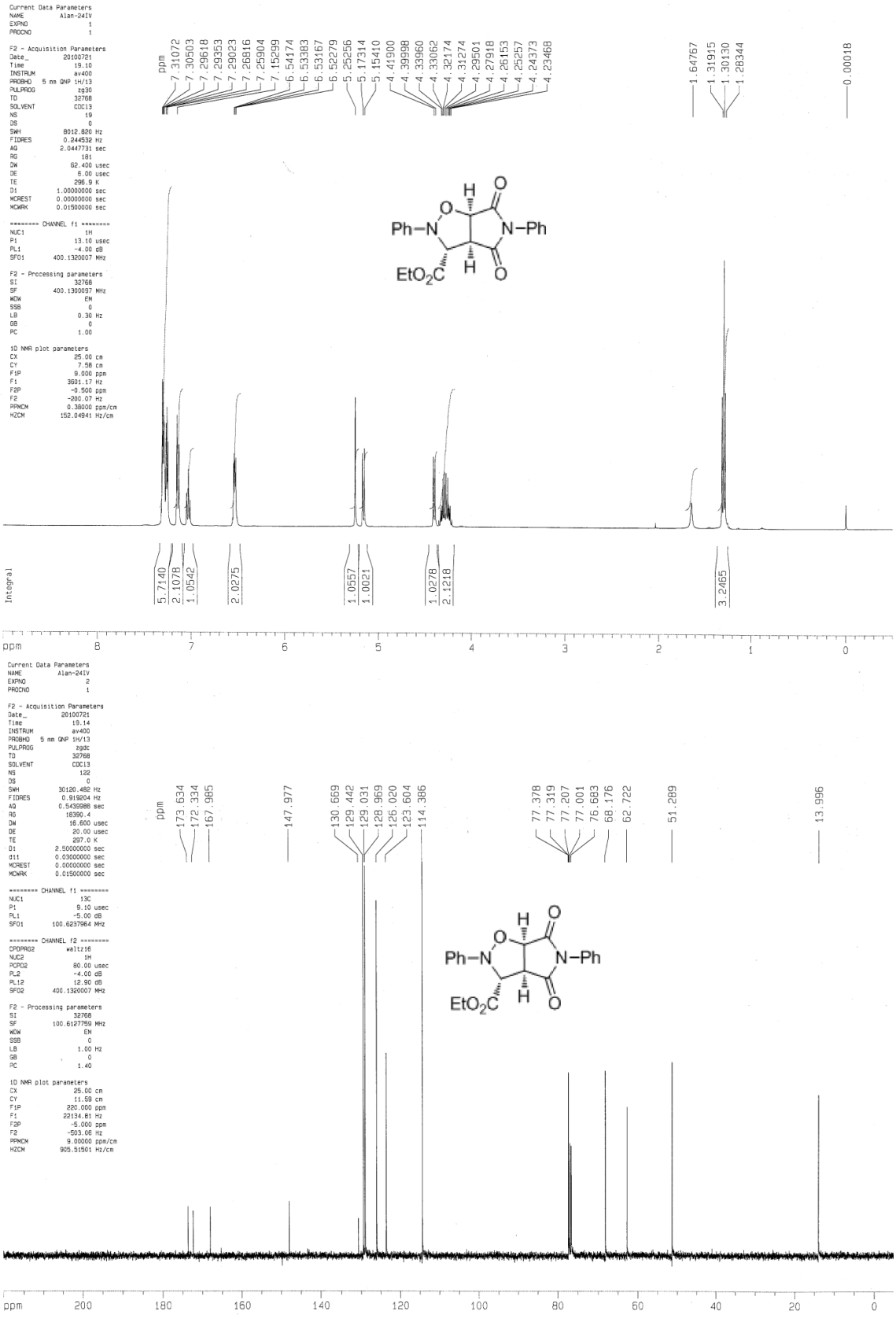
1H), 4.22-4.28 (m, 2H), 4.33-4.38 (m, 2H), 6.98-7.02 (m, 2H), 7.21-7.24 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz), δ 14.19, 33.69, 62.02, 62.17, 67.81, 78.71, 116.04, 129.08, 149.03, 171.36; EIMS *m/z* 285.0 (M^+); HRMS (EI) for $C_{13}H_{16}O_4NCl$, calcd. 285.0768, found 285.0761.

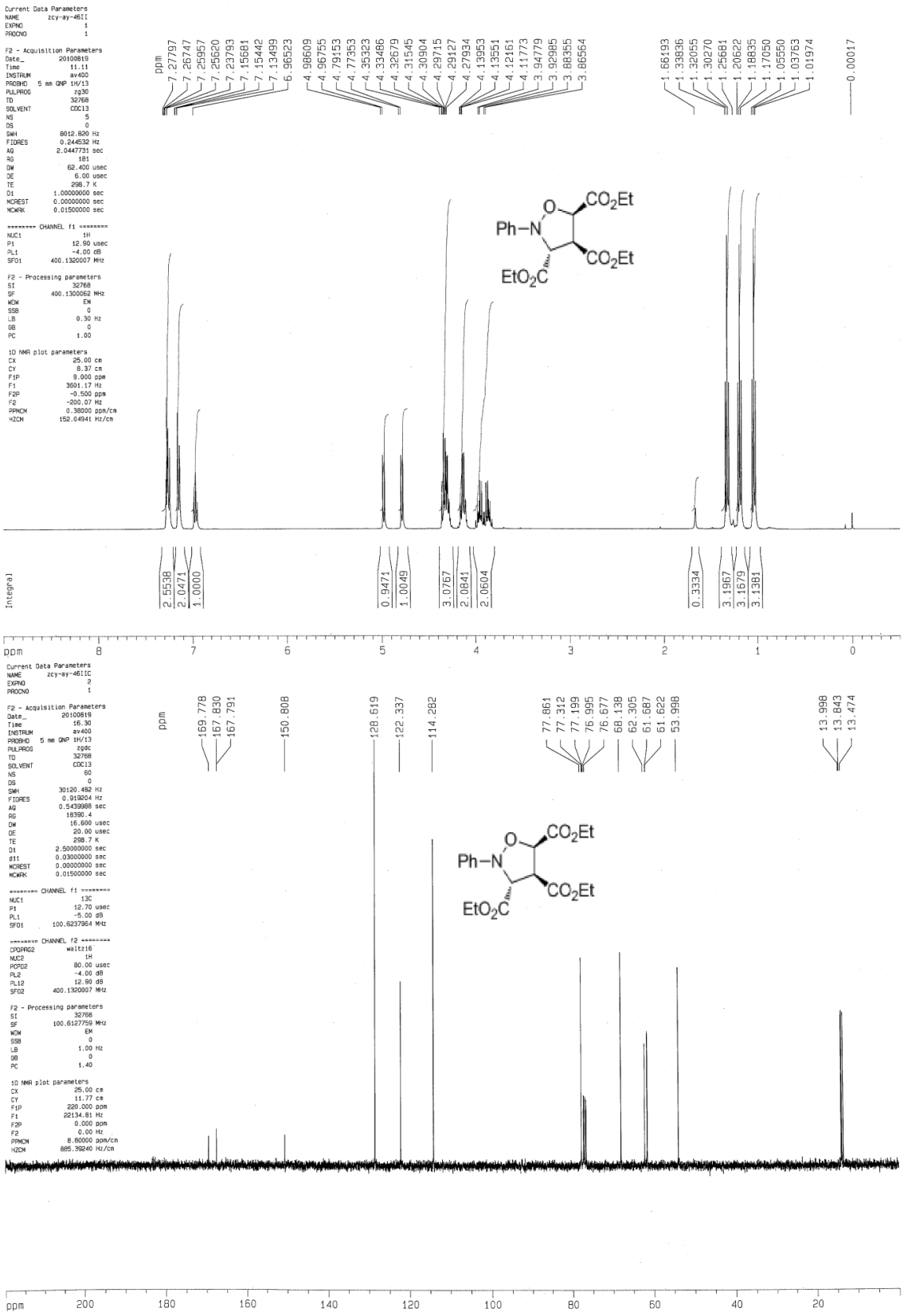
Ethyl 5-(hydroxymethyl)-2-(6-methylpyridin-2-yl)isoxazolidine-3-carboxylate (5n)

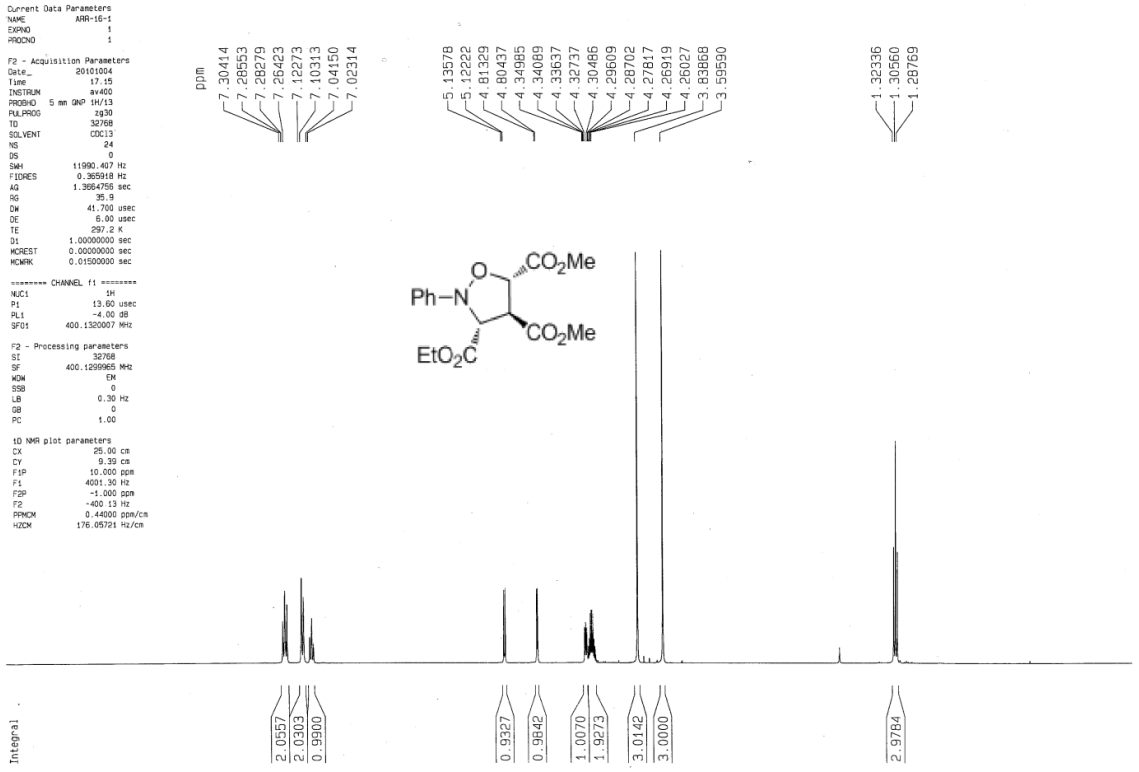


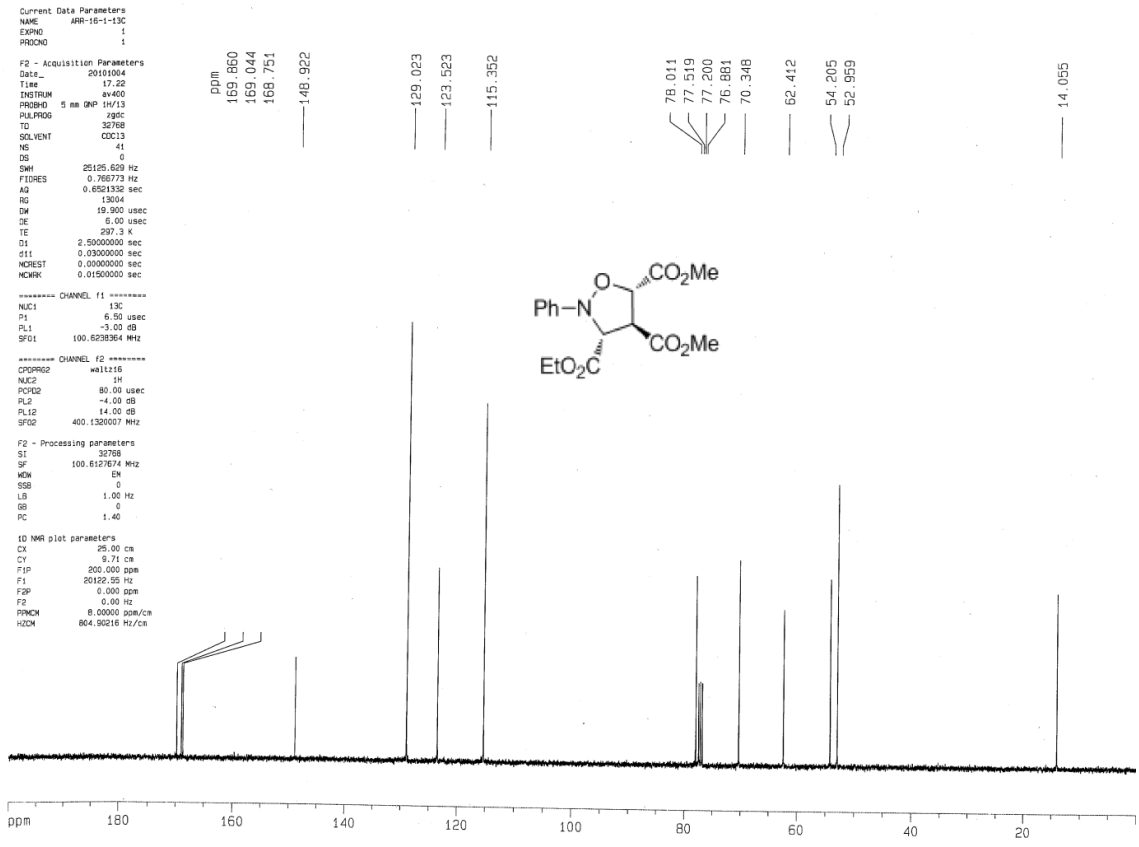
Oil, Yield: 65%; ^{1}H NMR ($CDCl_3$, 400 MHz), δ 1.32 (t, *J* = 7.2 Hz, 3H), 2.43 (s, 3H), 2.46-2.53 (m, 2H), 3.69 (dd, *J* = 12.5, 4.2 Hz, 1H), 3.93 (dd, *J* = 12.5, 2.3 Hz, 1H), 4.22-4.30 (m, 3H), 5.54 (dd, *J* = 9.0, 3.7 Hz, 1H), 6.75 (d, *J* = 7.3 Hz, 1H), 7.07 (d, *J* = 8.2 Hz, 1H), 7.49 (t, *J* = 7.8 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz), δ 14.34, 24.37, 33.16, 61.77, 62.35, 62.80, 79.21, 107.01, 117.51, 138.50, 156.81, 160.62, 172.51; EIMS *m/z* 266.1 (M^+); HRMS (EI) for $C_{13}H_{18}N_2O_4$, calcd. 266.1267, found 266.1257.

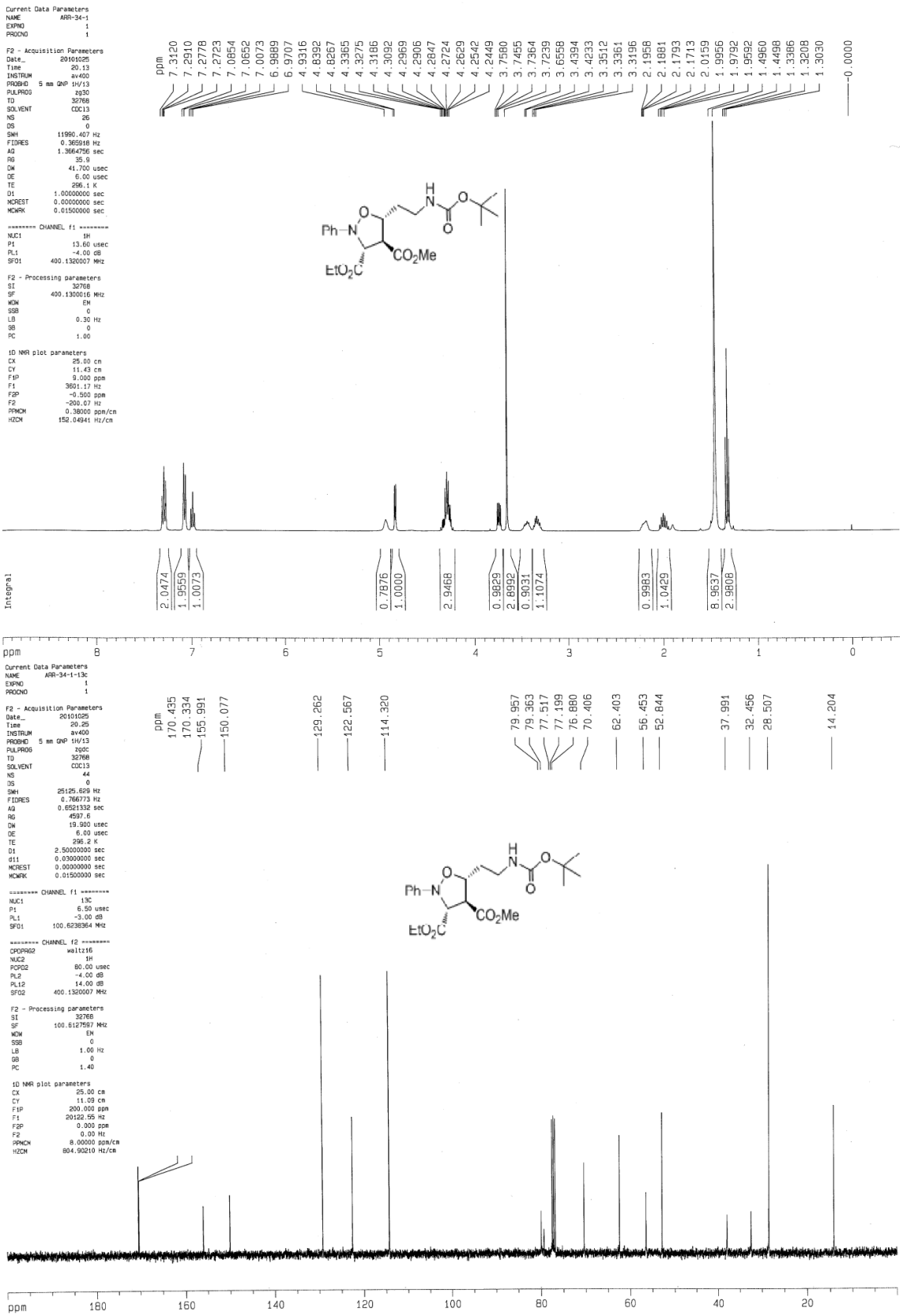
^{1}H and ^{13}C NMR Spectra

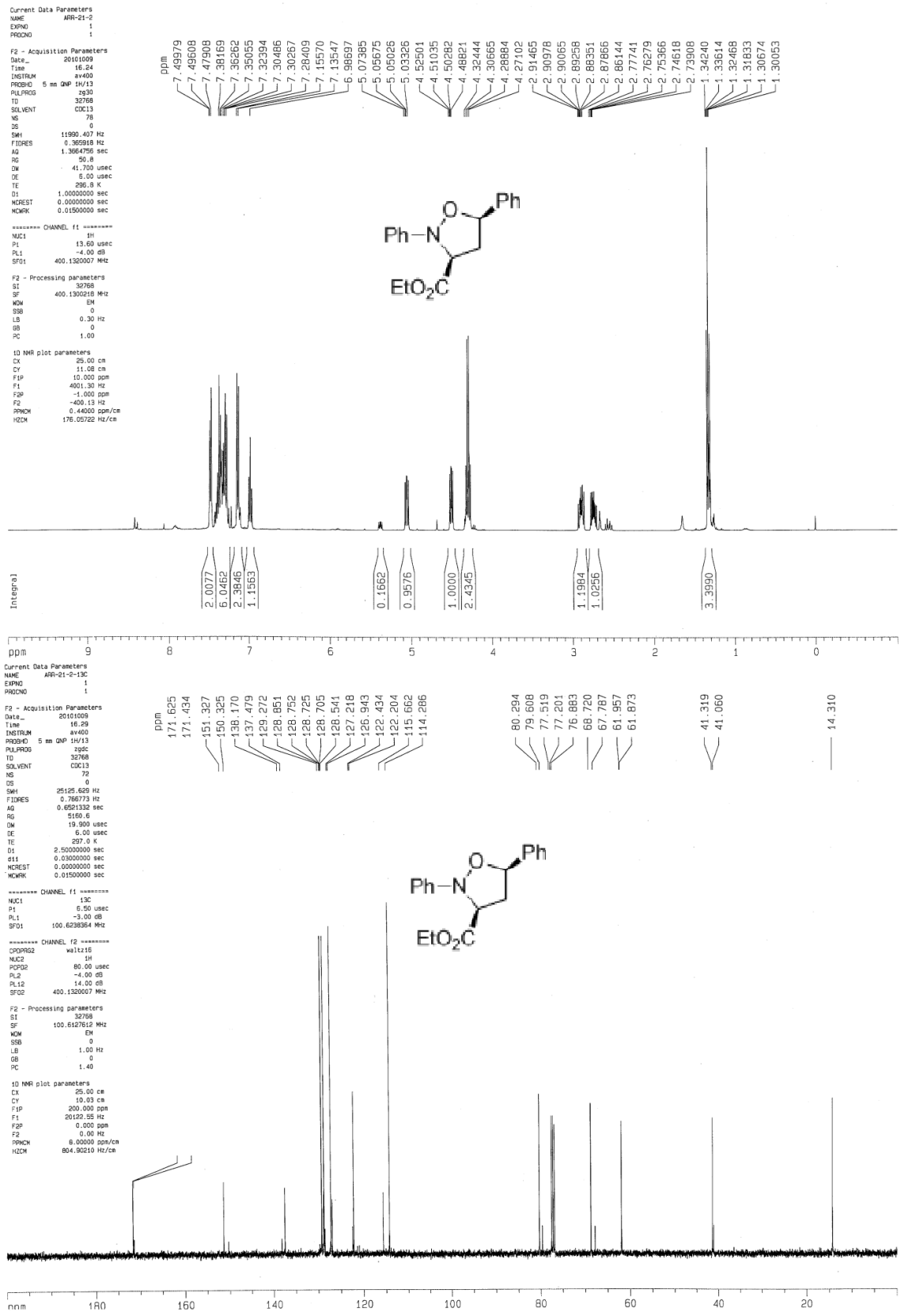


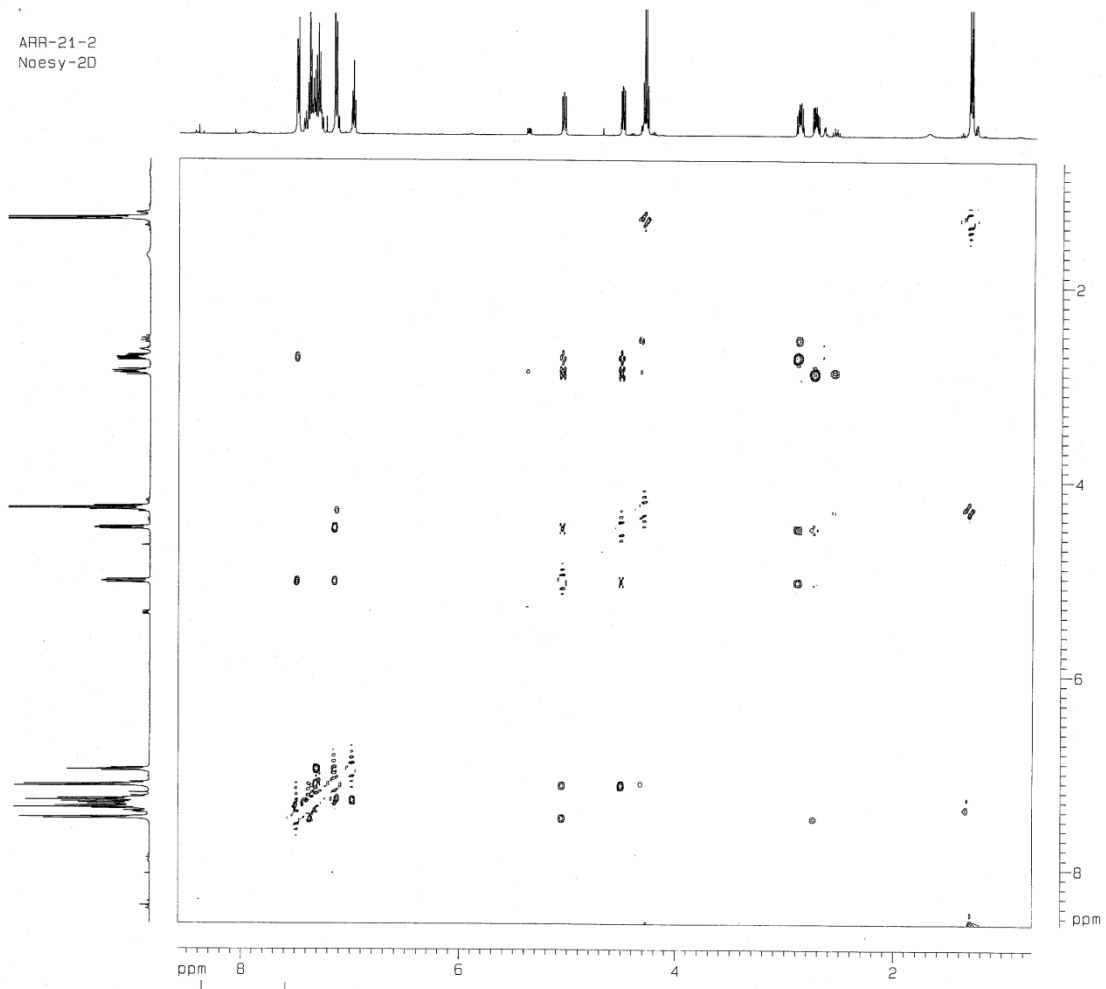


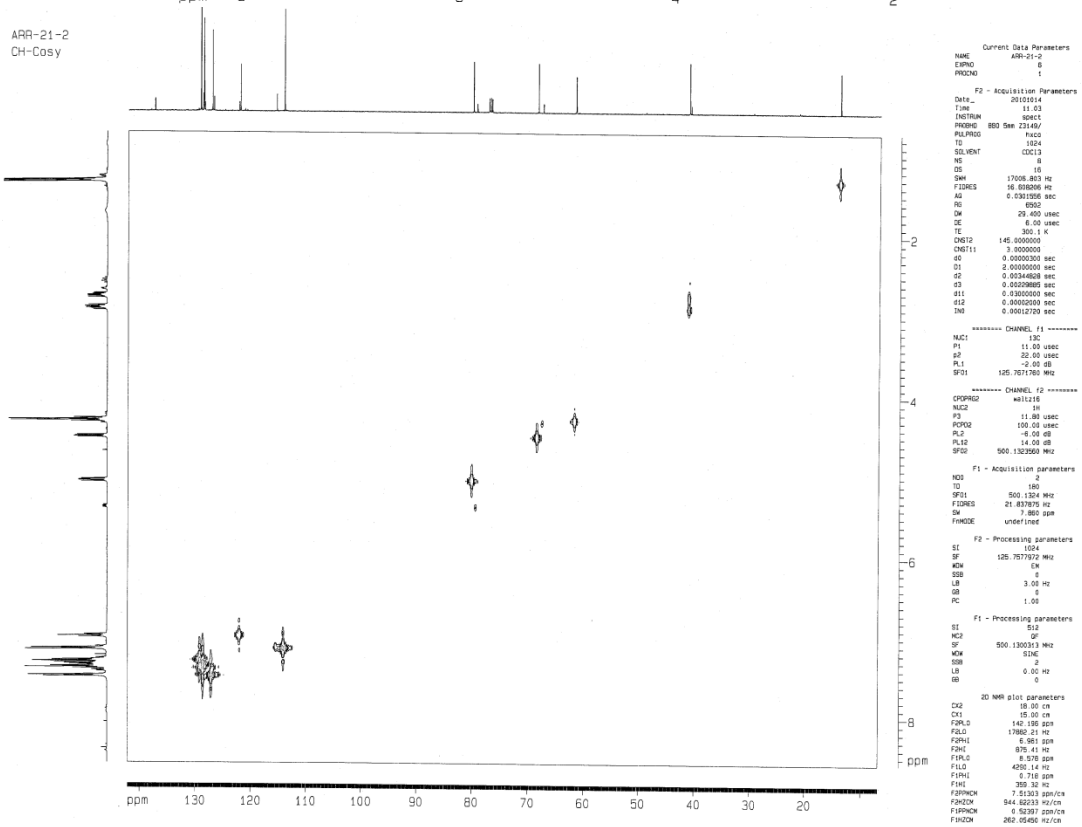


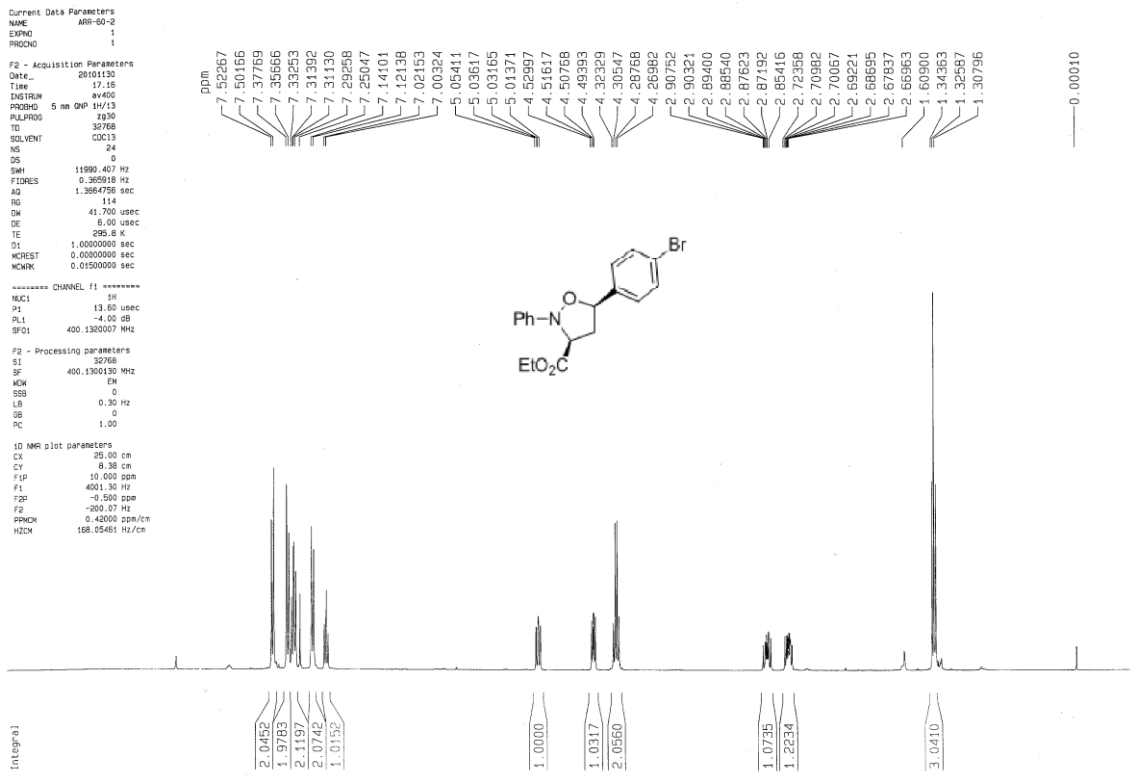


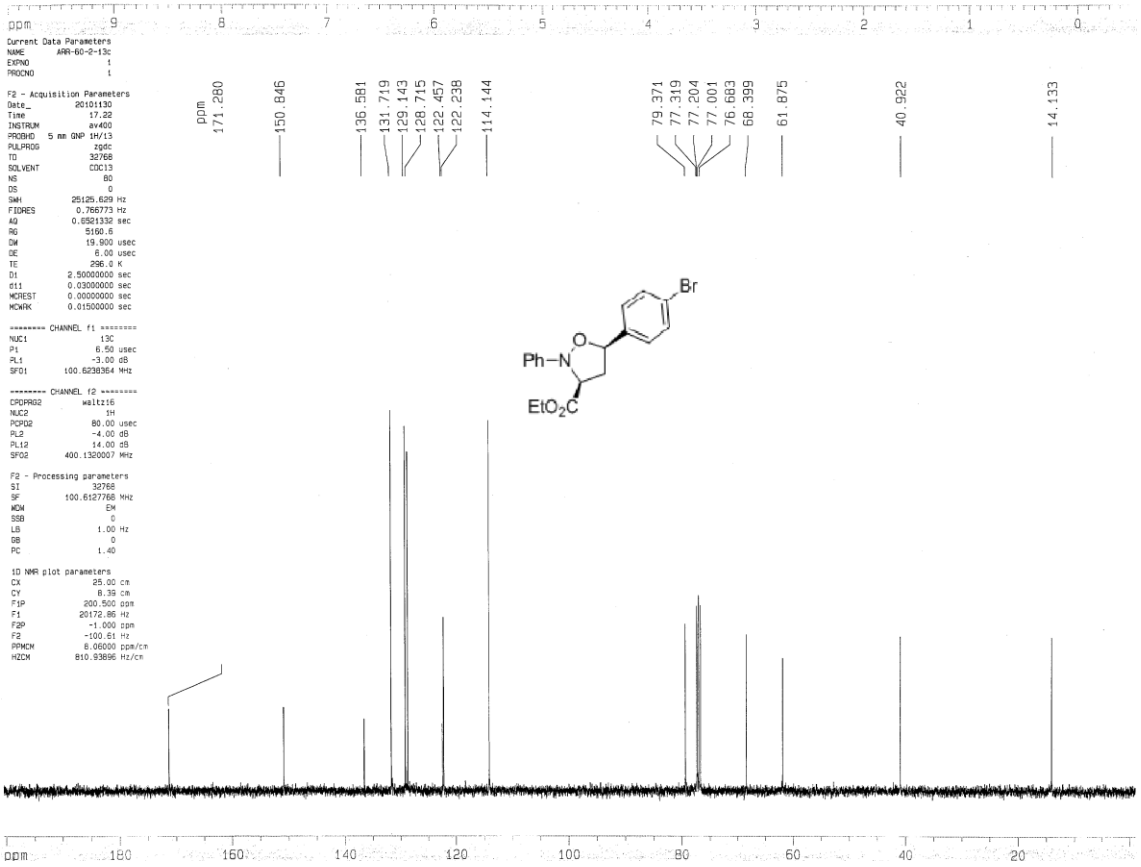

Current Data Parameters
NAME ARR-34-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20101025
Time 20.13
INSTRUM av400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 26
DS 0
SWH 11990.407 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 35.9
DW 41.700 usec
DE 6.00 usec
TE 296.1 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 13.60 usec
PL1 -4.00 dB
SFO1 400.1320007 MHz
F2 - Processing parameters
SI 32768
SF 400.1300016 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 25.00 cm
CY 11.43 cm
F1P 9.000 ppm
F1 3601.17 Hz
F2P -0.500 ppm
F2 -200.07 Hz
PPMCM 0.38000 ppm/cm
HZCM 152.04941 Hz/cm
ppm
7.3120
7.2910
7.2778
7.2723
7.0854
7.0652
7.0073
6.9889
6.9707
4.9316
4.8392
4.8267
4.3365
4.3275
4.3186
4.3092
4.2969
4.2906
4.2847
4.2724
4.2629
4.2542
4.2449
3.7580
3.7455
3.7364
3.7239
3.6558
3.4394
3.4233
3.3512
3.3361
3.3196
2.1958
2.1881
2.1793
2.1713
2.0159
1.9956
1.9792
1.9592
1.4960
1.4498
1.3386
1.3208
1.3030
0.0000
Ph–N
O
H
N
O
O
CO2Me
EtO2C
Integral
2.0474
1.9559
1.0073
0.7876
1.0000
2.9468
0.9829
2.8992
0.9031
1.1074
0.9983
1.0429
8.9637
2.9808
ppm
8
7
6
5
4
3
2
1
0
Current Data Parameters
NAME ARR-34-1-13c
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20101025
Time 20.25
INSTRUM av400
PROBHD 5 mm QNP 1H/13
PULPROG zgdc
TD 32768
SOLVENT CDCl3
NS 44
DS 0
SWH 25125.629 Hz
FIDRES 0.766773 Hz
AQ 0.6521332 sec
RG 4597.6
DW 19.900 usec
DE 6.00 usec
TE 296.2 K
D1 2.50000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 6.50 usec
PL1 -3.00 dB
SFO1 100.6238364 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -4.00 dB
PL12 14.00 dB
SFO2 400.1320007 MHz
F2 - Processing parameters
SI 32768
SF 100.6127597 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 25.00 cm
CY 11.09 cm
F1P 200.000 ppm
F1 20122.55 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 8.00000 ppm/cm
HZCM 804.90210 Hz/cm
ppm
170.435
170.334
155.991
150.077
129.262
122.567
114.320
79.957
79.363
77.517
77.199
76.880
70.406
62.403
56.453
52.844
37.991
32.456
28.507
14.204
Ph–N
O
H
N
O
O
CO2Me
EtO2C
ppm
180
160
140
120
100
80
60
40
20

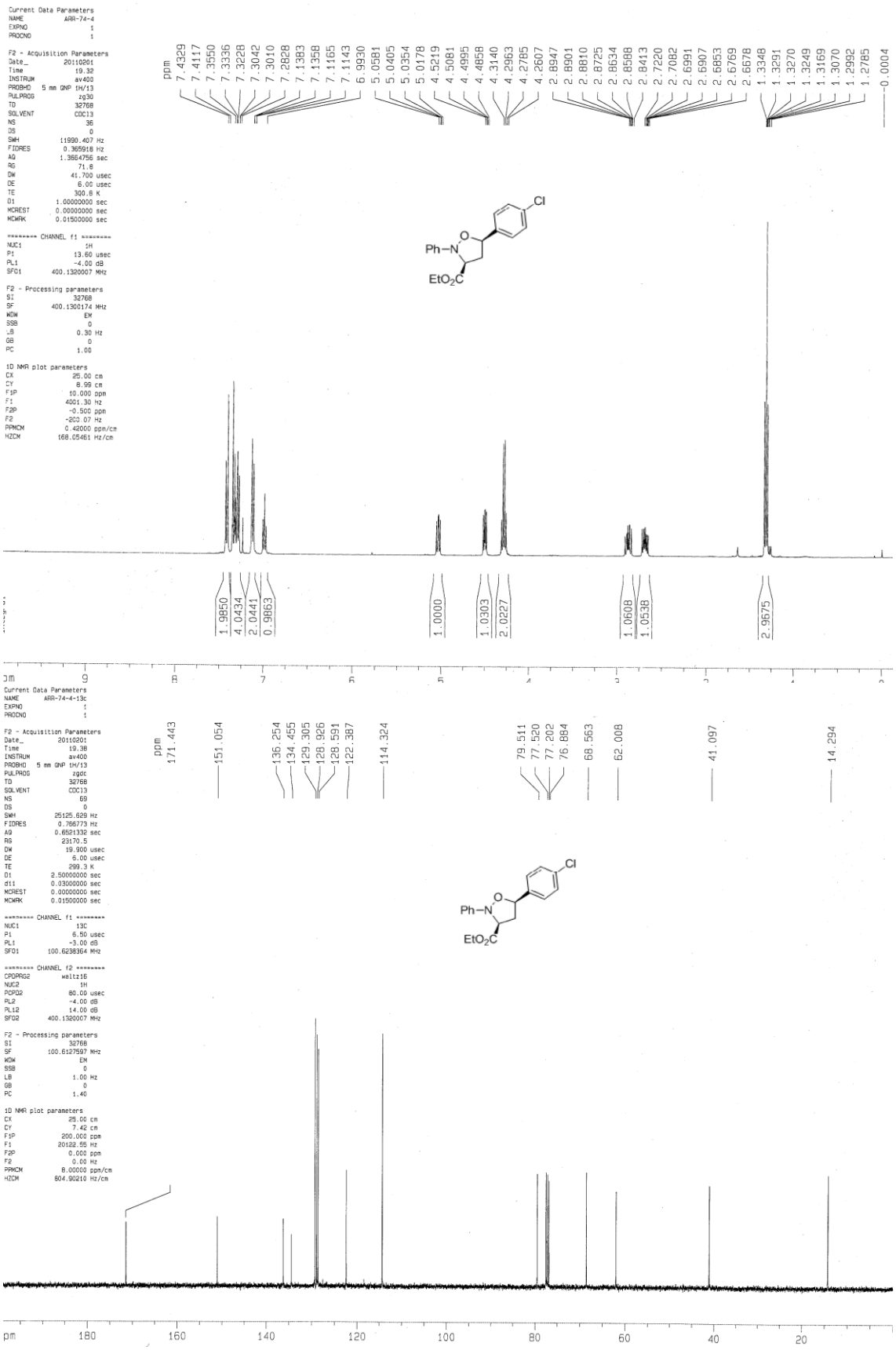


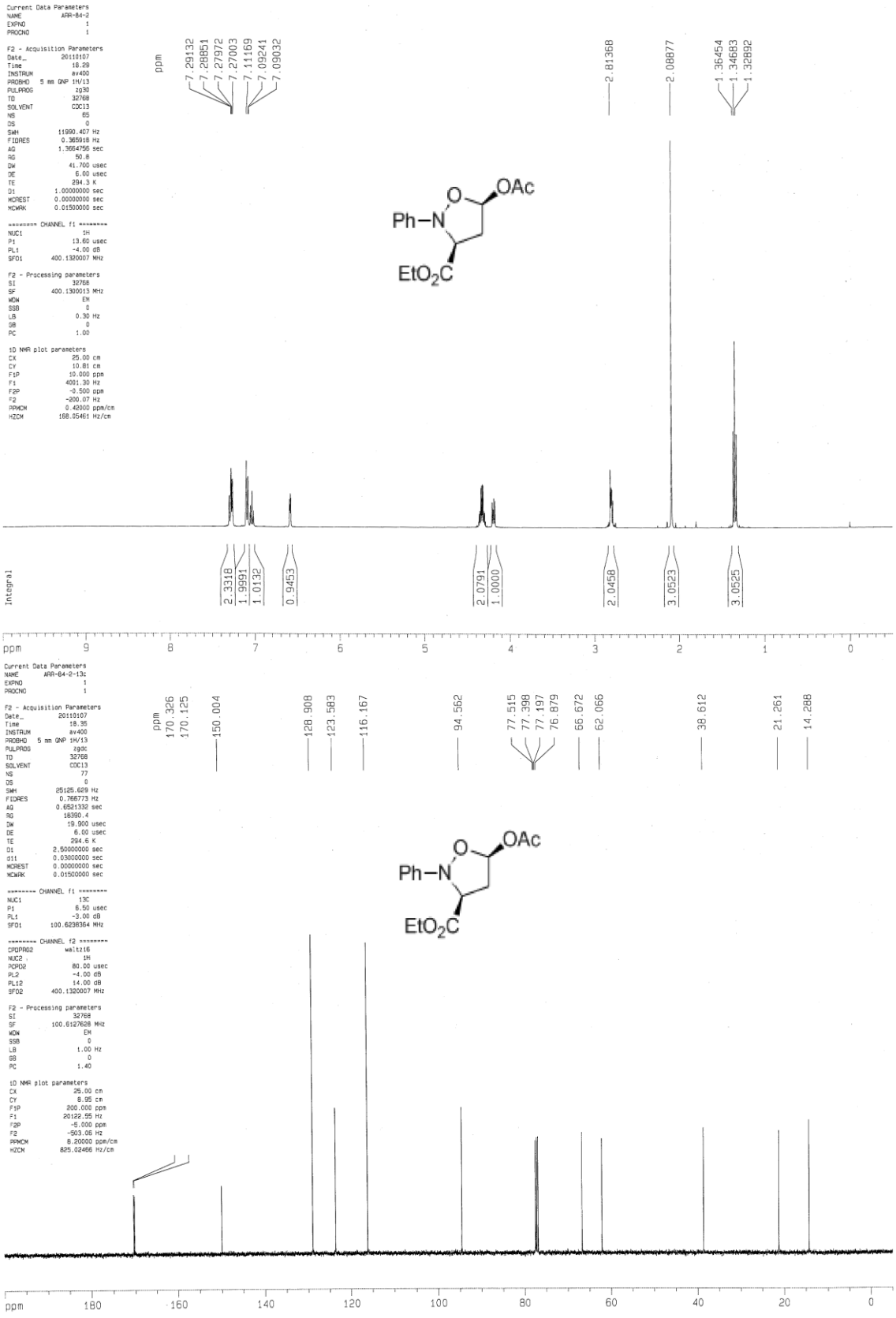

ARR-21-2
Noesy-2D
ppm
8
6
4
2

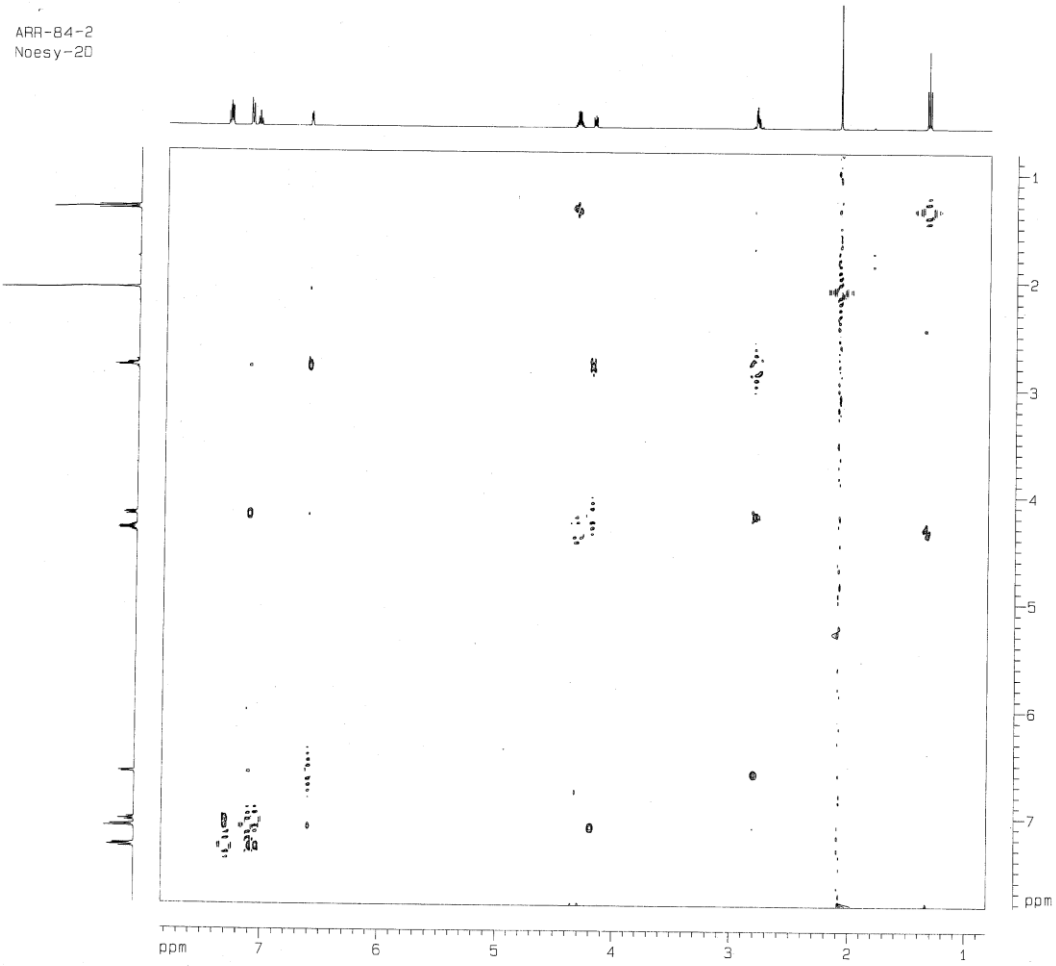

ARR-21-2
CH-Cosy
ppm
130
120
110
100
90
80
70
60
50
40
30
20

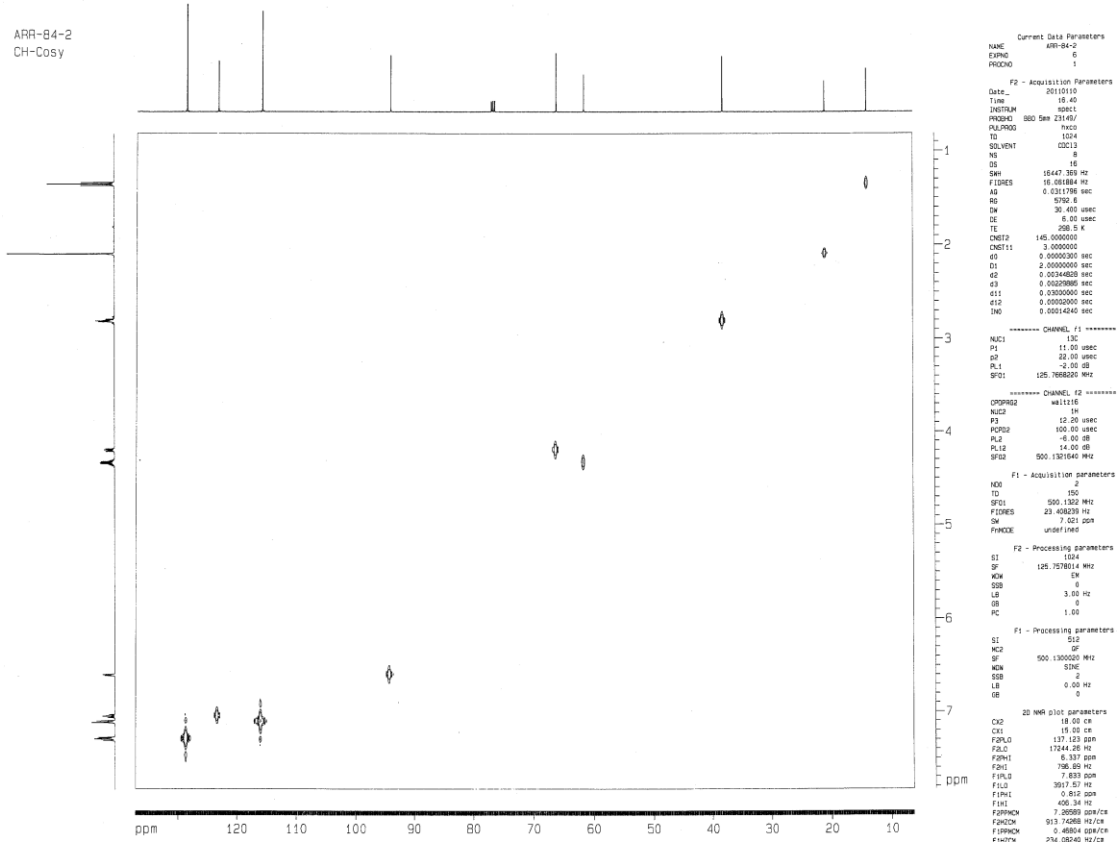


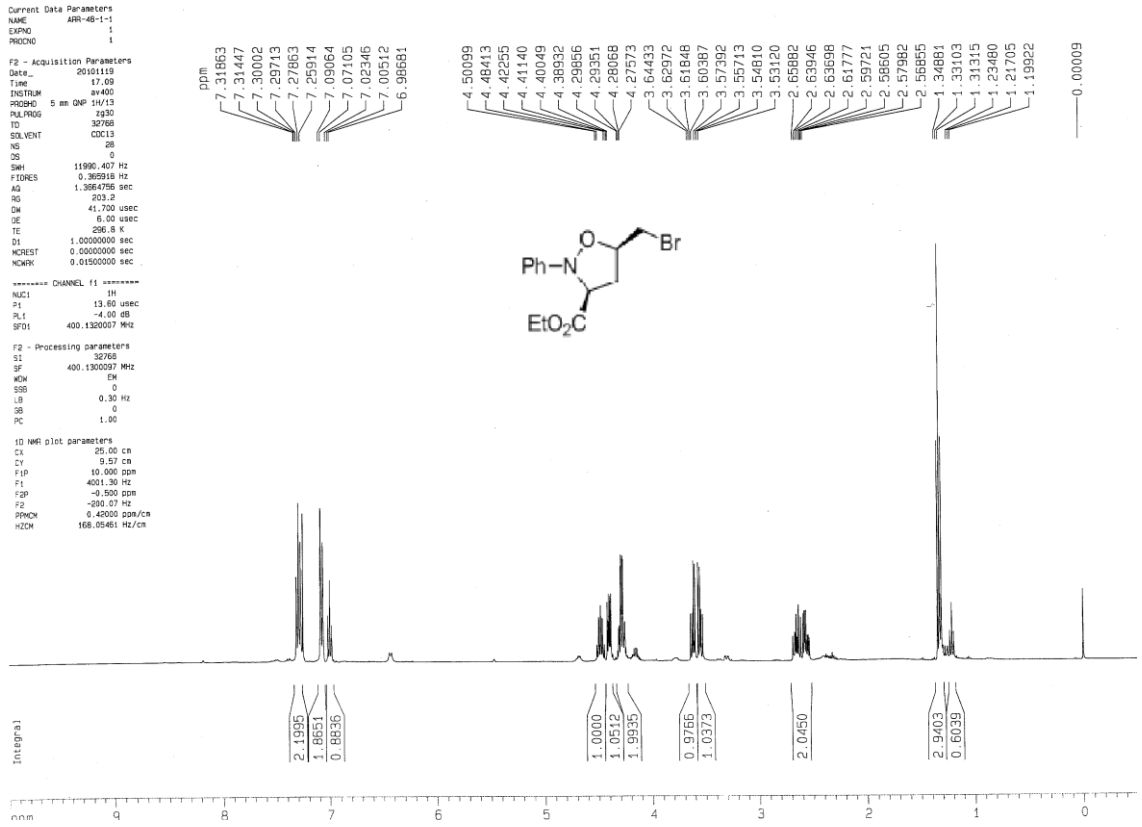


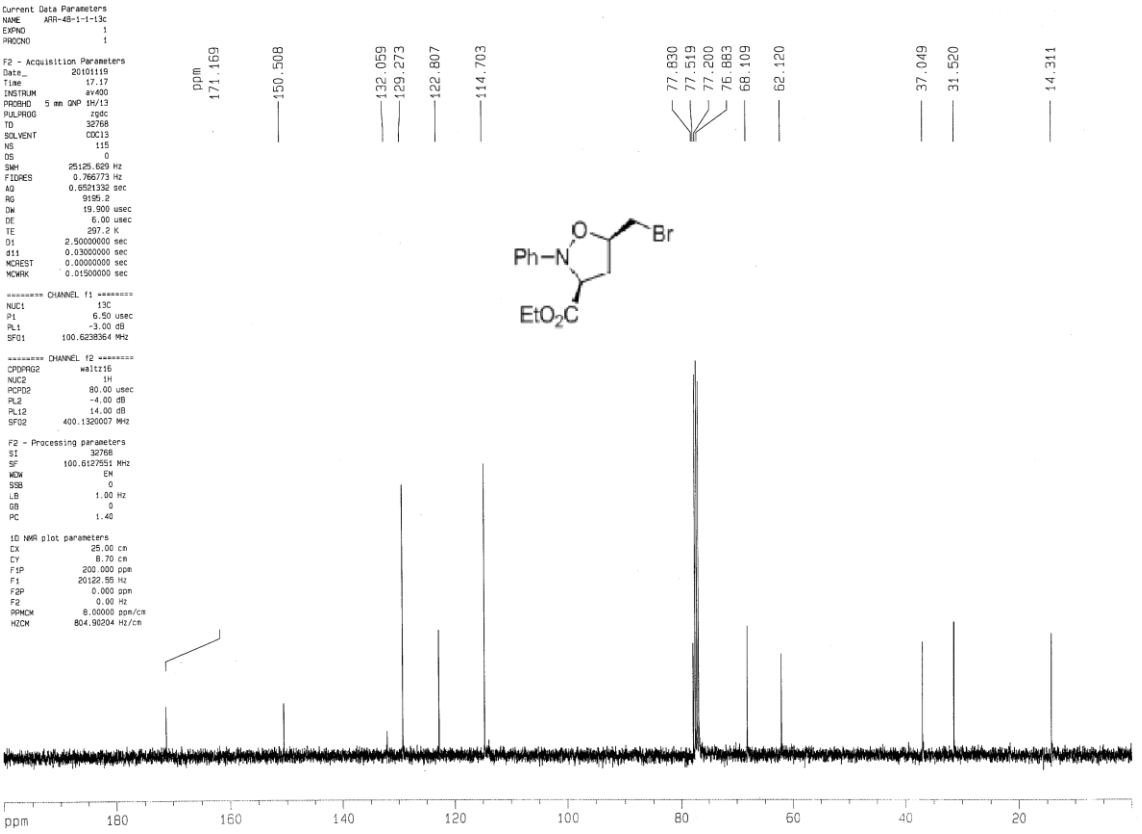


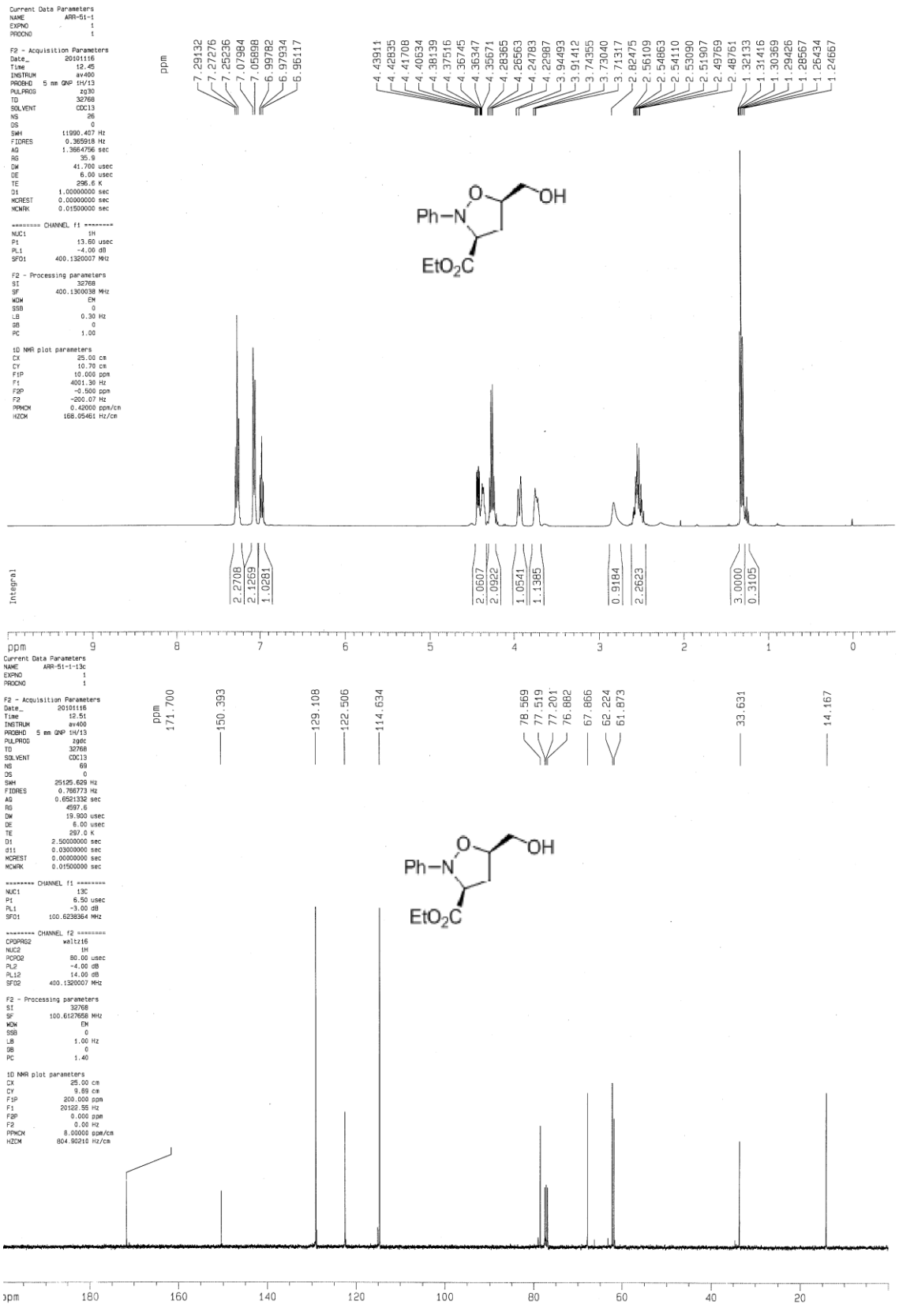


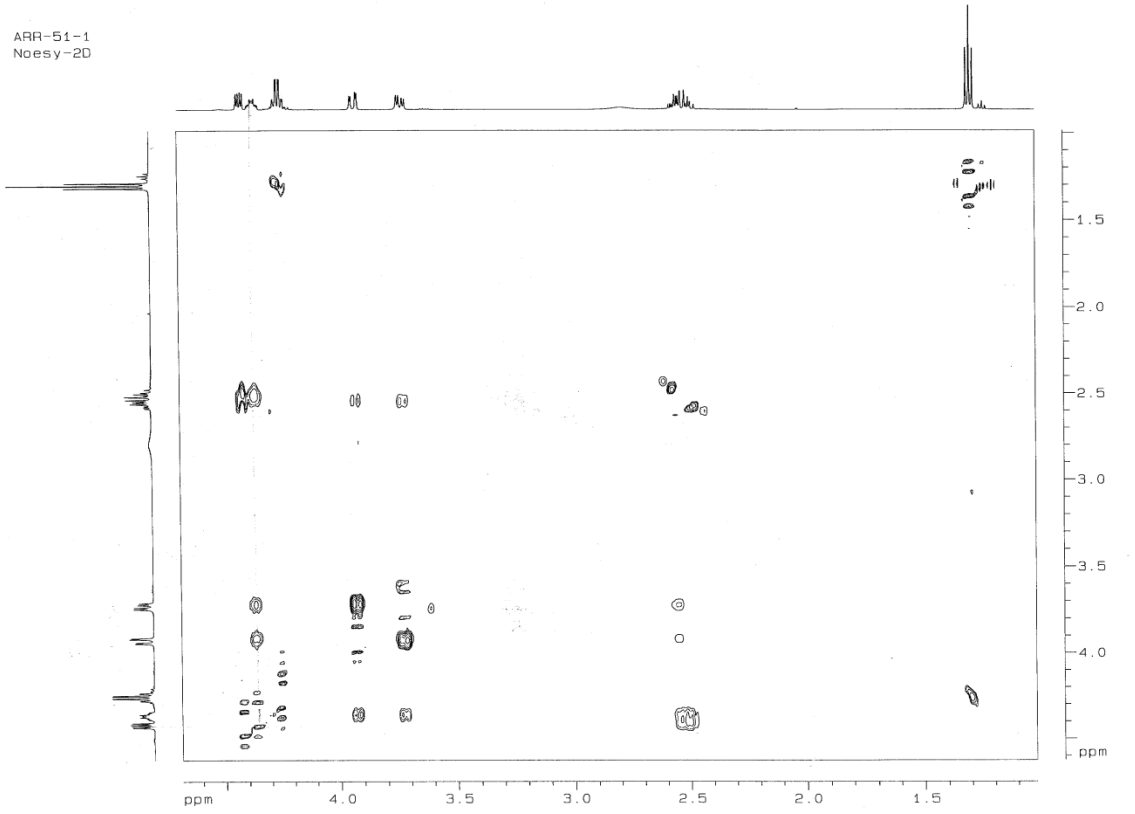


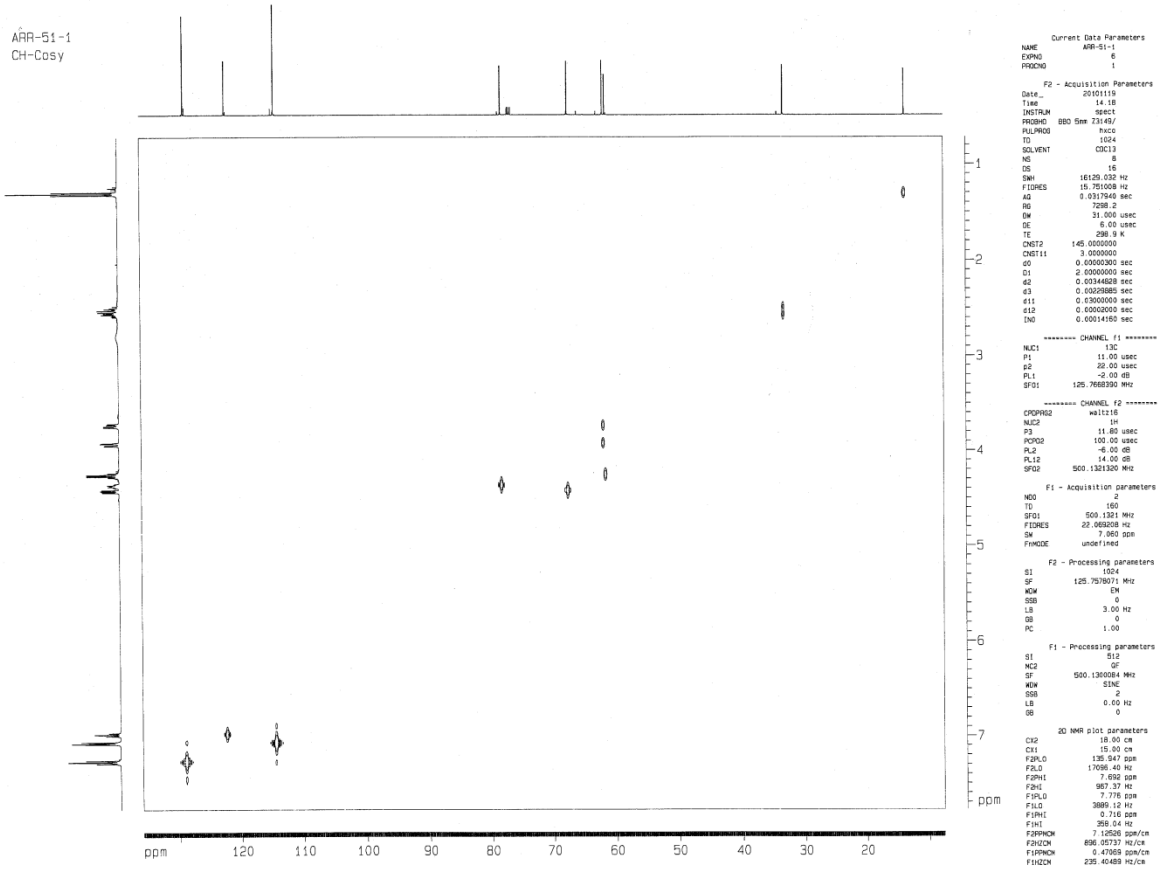



Current Data Parameters
NAME ARR-48-1-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20101119
Time 17.09
INSTRUM av400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 28
DS 0
SWH 11990.407 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 203.2
DW 41.700 usec
DE 6.00 usec
TE 296.8 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 13.60 usec
PL1 -4.00 dB
SFO1 400.1320007 MHz
F2 - Processing parameters
SI 32768
SF 400.1300097 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 25.00 cm
CY 9.57 cm
F1P 10.000 ppm
F1 4001.30 Hz
F2P -0.500 ppm
F2 -200.07 Hz
PPMCM 0.42000 ppm/cm
HZCM 168.05461 Hz/cm
ppm
7.31863
7.31447
7.30002
7.29713
7.27863
7.25914
7.09064
7.07105
7.02346
7.00512
6.98681
4.50099
4.48413
4.42255
4.41140
4.40049
4.38932
4.29856
4.29351
4.28068
4.27573
3.64433
3.62972
3.61848
3.60387
3.57392
3.55713
3.54610
3.53120
2.65882
2.63946
2.63698
2.61777
2.59721
2.58605
2.57982
2.56855
1.34881
1.33103
1.31315
1.23480
1.21705
1.19922
0.00009
Ph–N
O
Br
EtO2C
Integral
2.1995
1.8651
0.8836
1.0000
1.0512
1.9935
0.9766
1.0373
2.0450
2.9403
0.6039
ppm
9
8
7
6
5
4
3
2
1
0


Current Data Parameters
NAME ARR-48-1-1-13c
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20101119
Time 17.17
INSTRUM av400
PROBHD 5 mm QNP 1H/13
PULPROG zgdc
TD 32768
SOLVENT CDCl3
NS 115
DS 0
SWH 25125.629 Hz
FIDRES 0.766773 Hz
AQ 0.6521332 sec
RG 9195.2
DW 19.900 usec
DE 6.00 usec
TE 297.2 K
D1 2.50000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 6.50 usec
PL1 -3.00 dB
SFO1 100.6238364 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -4.00 dB
PL12 14.00 dB
SFO2 400.1320007 MHz
F2 - Processing parameters
SI 32768
SF 100.6127551 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 25.00 cm
CY 8.70 cm
F1P 200.000 ppm
F1 20122.55 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 8.00000 ppm/cm
HZCM 804.90204 Hz/cm
ppm
171.169
150.508
132.059
129.273
122.807
114.703
77.830
77.519
77.200
76.883
68.109
62.120
37.049
31.520
14.311
Ph–N
O
Br
EtO2C
ppm
180
160
140
120
100
80
60
40
20







Current Data Parameters

NAME	ARR-51-1
EXPNO	6
PROCNO	1

F2 - Acquisition Parameters

Date_	20101119
Time	14.18
INSTRUM	spect
PROBHD	BBO 5mm 23149/
PULPROG	hxco
TD	1024
SOLVENT	CDCl3
NS	8
DS	16
SWH	16129.032 Hz
FIDRES	15.751008 Hz
AQ	0.0317940 sec
RG	7298.2
DW	31.000 usec
DE	6.00 usec
TE	298.9 K
CNST2	145.0000000
CNST11	3.0000000
d0	0.00000300 sec
D1	2.00000000 sec
d2	0.00344828 sec
d3	0.00229885 sec
d11	0.03000000 sec
d12	0.00002000 sec
IN0	0.00014160 sec

======== CHANNEL f1 ========

NUC1	13C
P1	11.00 usec
p2	22.00 usec
PL1	-2.00 dB
SFO1	125.7668390 MHz

======== CHANNEL f2 ========

CPDPRG2	waltz16
NUC2	1H
P3	11.80 usec
PCPD2	100.00 usec
PL2	-6.00 dB
PL12	14.00 dB
SFO2	500.1321320 MHz

F1 - Acquisition parameters

ND0	2
TD	160
SFO1	509.1321 MHz
FIDRES	22.069208 Hz
SW	7.060 ppm
FnMODE	undefined

F2 - Processing parameters

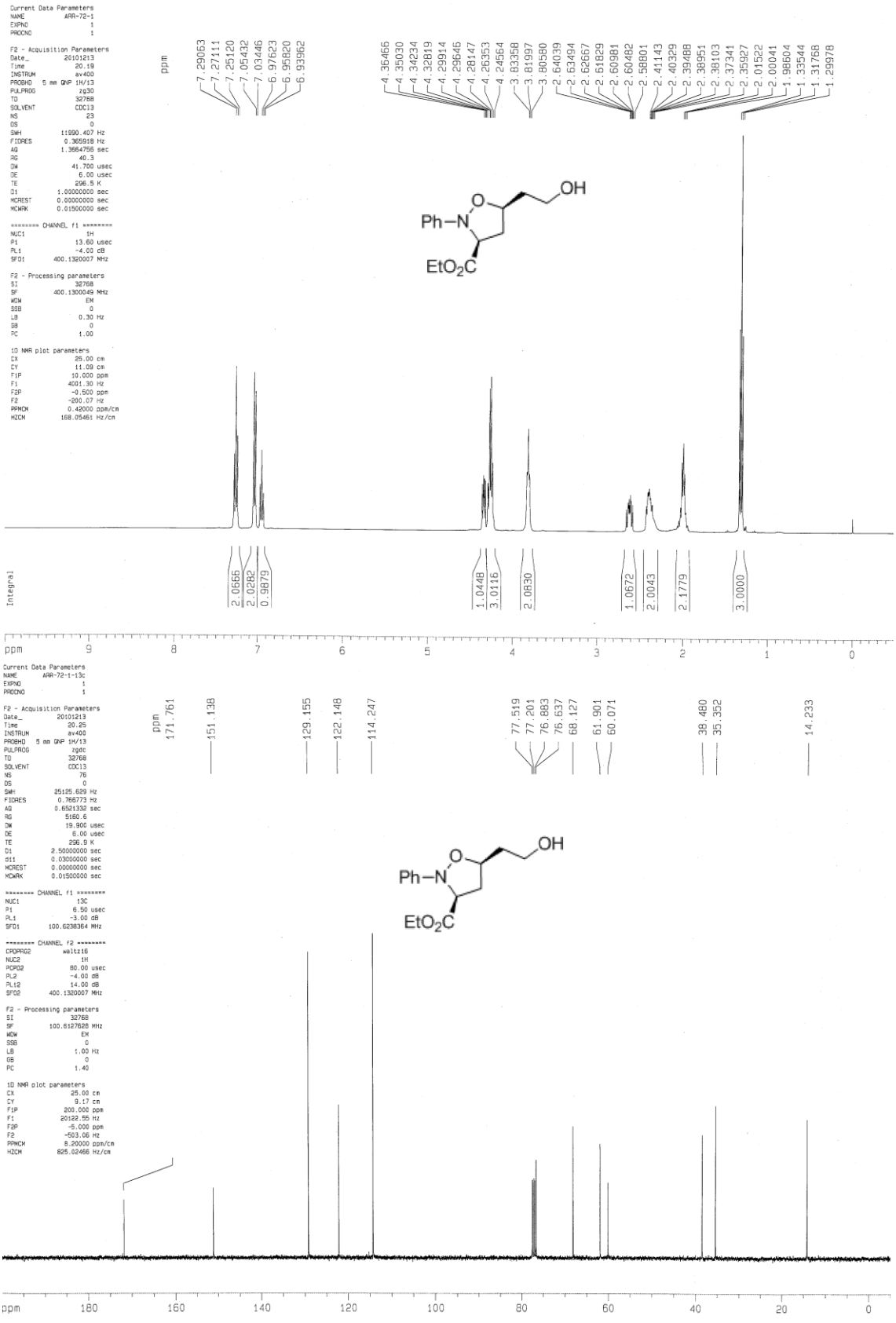
SI	1024
SF	125.7578071 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.00

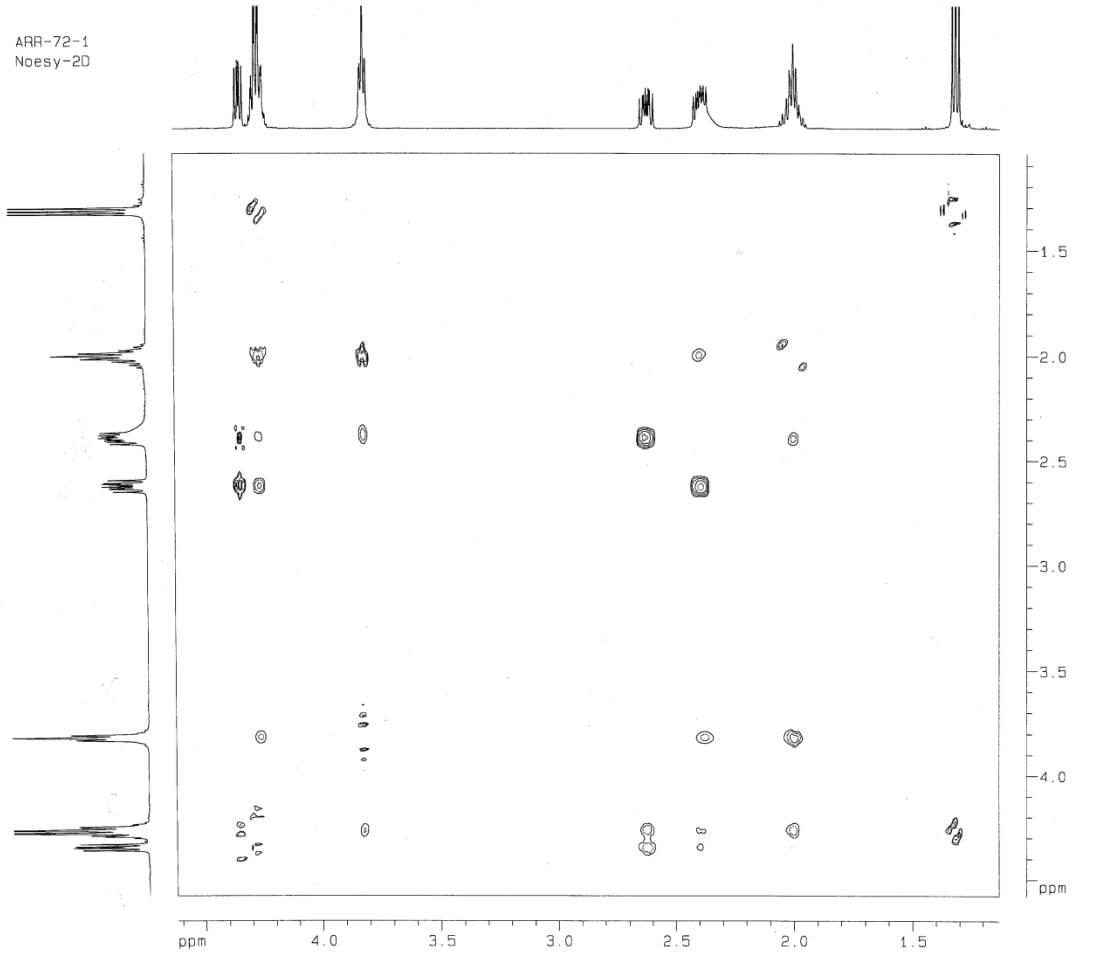
F1 - Processing parameters

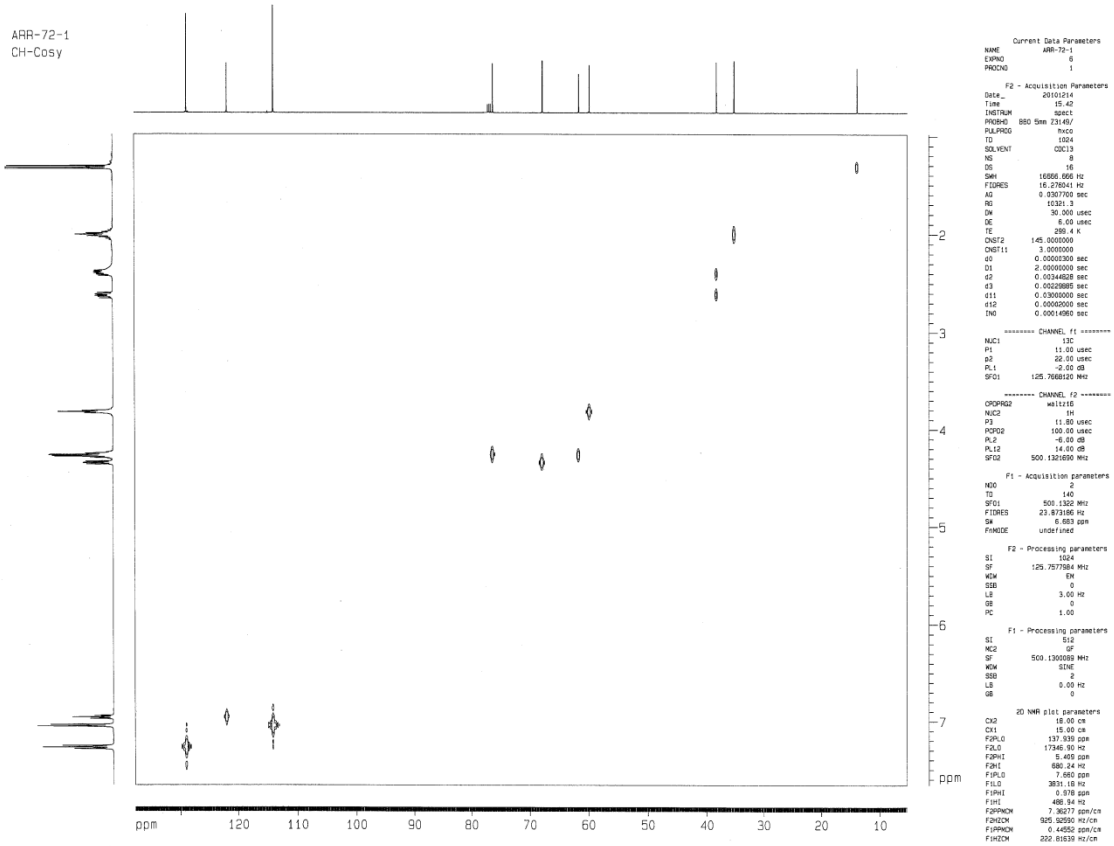
SI	512
MC2	QF
SF	500.1300084 MHz
WDW	SINE
SSB	2
LB	0.00 Hz
GB	0

2D NMR plot parameters

CX2	18.00 cm
CX1	15.00 cm
F2PLO	135.947 ppm
F2LO	17096.40 Hz
F2PHI	7.692 ppm
F2HI	967.37 Hz
F1PLO	7.776 ppm
F1LO	3889.12 Hz
F1PHI	0.716 ppm
F1HI	358.04 Hz
F2PPMCM	7.12526 ppm/cm
F2HZCM	896.05737 Hz/cm
F1PPMCM	0.47969 ppm/cm
F1HZCM	235.40489 Hz/cm


Current Data Parameters
NAME ARR-72-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20101213
Time 20.19
INSTRUM av400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 23
DS 0
SWH 11990.407 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 40.3
DW 41.700 usec
DE 6.00 usec
TE 296.5 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 13.60 usec
PL1 -4.00 dB
SFO1 400.1320007 MHz
F2 - Processing parameters
SI 32768
SF 400.1300049 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 25.00 cm
CY 11.09 cm
F1P 10.000 ppm
F1 4001.30 Hz
F2P -0.500 ppm
F2 -200.07 Hz
PPMCM 0.42000 ppm/cm
HZCM 168.05461 Hz/cm
ppm
7.29063
7.27111
7.25120
7.05432
7.03446
6.97623
6.95820
6.93962
4.36465
4.35030
4.34234
4.32819
4.29914
4.29646
4.28147
4.26353
4.24564
3.83358
3.81997
3.80580
2.64039
2.63494
2.62667
2.61829
2.60981
2.60482
2.58801
2.41143
2.40329
2.39488
2.38951
2.38103
2.37341
2.35927
2.01522
2.00041
1.98604
1.33544
1.31768
1.29978
OH
Ph–N
O
EtO2C
Integral
2.0666
2.0282
0.9879
1.0448
3.0116
2.0830
1.0672
2.0043
2.1779
3.0000
ppm
9
8
7
6
5
4
3
2
1
0
Current Data Parameters
NAME ARR-72-1-13c
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20101213
Time 20.25
INSTRUM av400
PROBHD 5 mm QNP 1H/13
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 76
DS 0
SWH 25125.629 Hz
FIDRES 0.766773 Hz
AQ 0.6521332 sec
RG 5160.6
DW 19.900 usec
DE 6.00 usec
TE 296.9 K
D1 2.50000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 6.50 usec
PL1 -3.00 dB
SFO1 100.6238364 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -4.00 dB
PL12 14.00 dB
SFO2 400.1320007 MHz
F2 - Processing parameters
SI 32768
SF 100.6127628 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 25.00 cm
CY 9.17 cm
F1P 200.000 ppm
F1 20122.55 Hz
F2P -5.000 ppm
F2 -503.06 Hz
PPMCM 8.20000 ppm/cm
HZCM 825.02466 Hz/cm
ppm
171.761
151.138
129.155
122.148
114.247
77.519
77.201
76.883
76.637
68.127
61.901
60.071
38.480
35.352
14.233
OH
Ph–N
O
EtO2C
ppm
180
160
140
120
100
80
60
40
20
0





Current Data Parameters
NAME ARR-72-1
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20101214
Time 15.42
INSTRUM spect
PROBHD 5mm Z3149/
PULPROG fxco
TD 1024
SOLVENT CDCl3
NS 8
DS 16
SWH 16666.666 Hz
FIDRES 16.276041 Hz
AQ 0.0307700 sec
RG 16331.3
DW 30.000 usec
DE 6.00 usec
TE 299.4 K
CNST2 145.0000000
CNST11 3.0000000
d0 0.00001300 sec
D1 2.00000000 sec
d2 0.00344828 sec
d3 0.00229885 sec
d11 0.03000000 sec
d12 0.00002000 sec
IN0 0.00014960 sec

======== CHANNEL f1 ========
NUC1 13C
P1 11.00 usec
p2 22.00 usec
PL1 -2.00 dB
SFO1 125.7668120 MHz

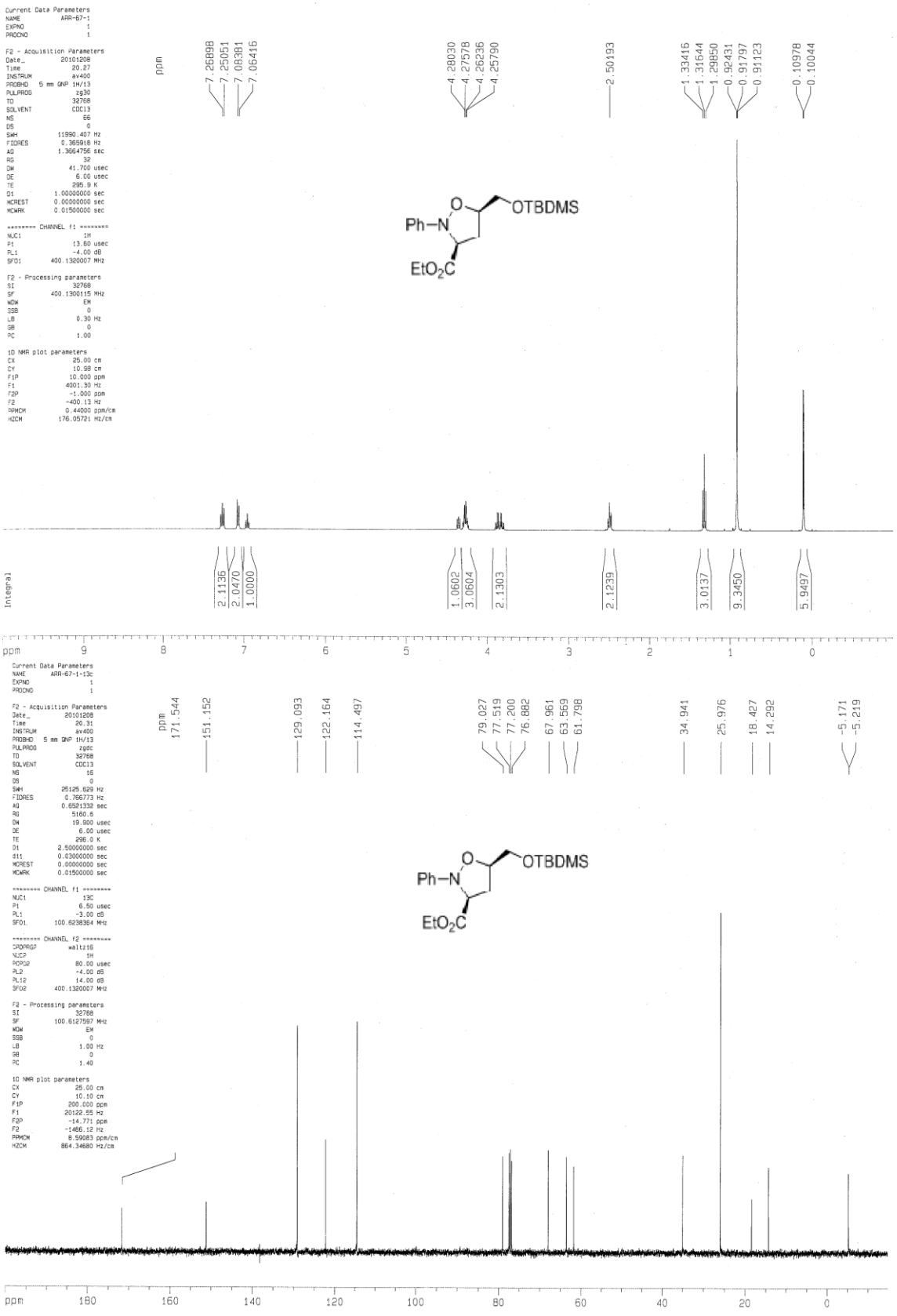
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
P3 11.80 usec
PCPD2 100.00 usec
PL2 -6.00 dB
PL12 14.00 dB
SFO2 500.1321690 MHz

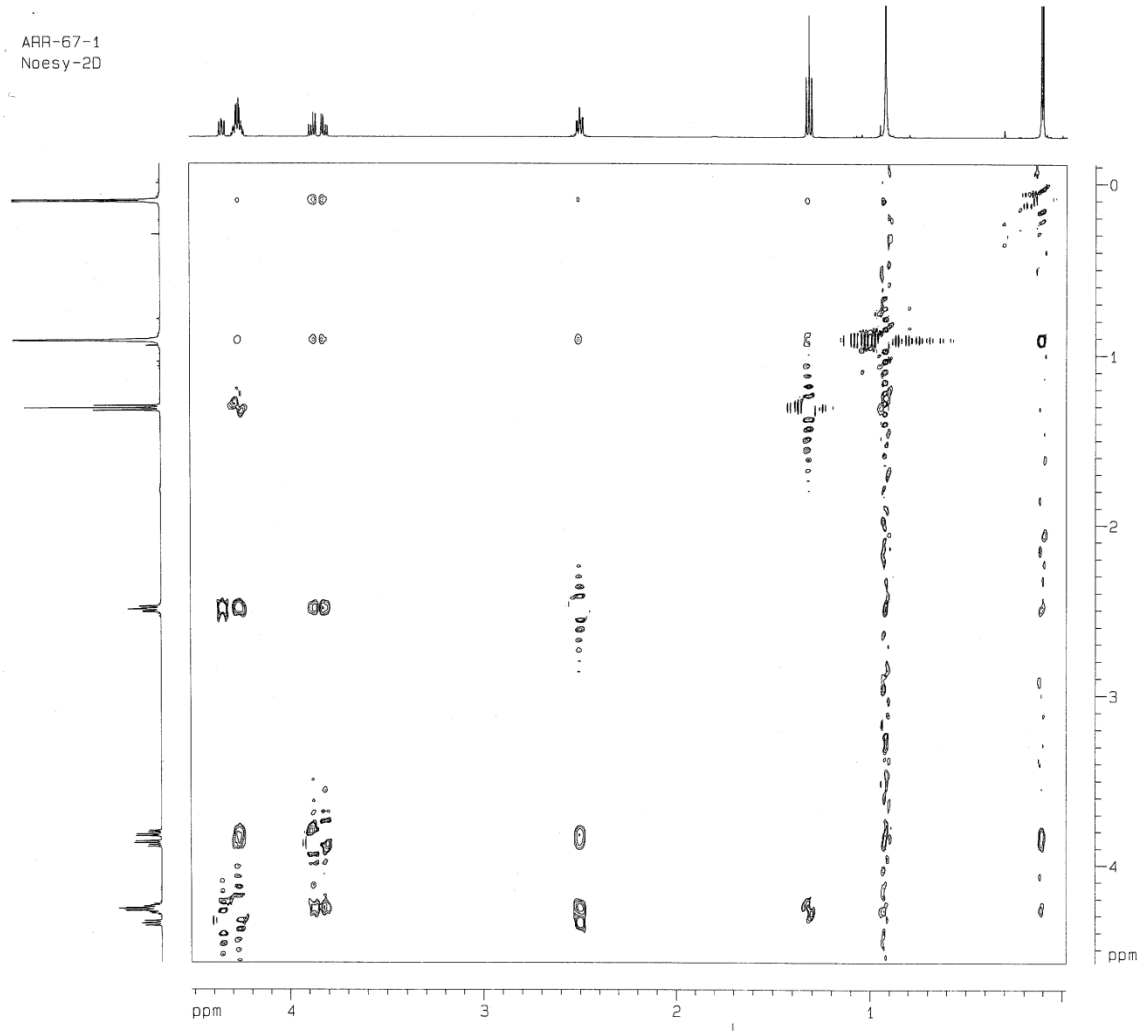
F1 - Acquisition parameters
ND0 2
TD 140
SFO1 500.1322 MHz
FIDRES 23.873186 Hz
SW 6.683 ppm
FnMODE undefined

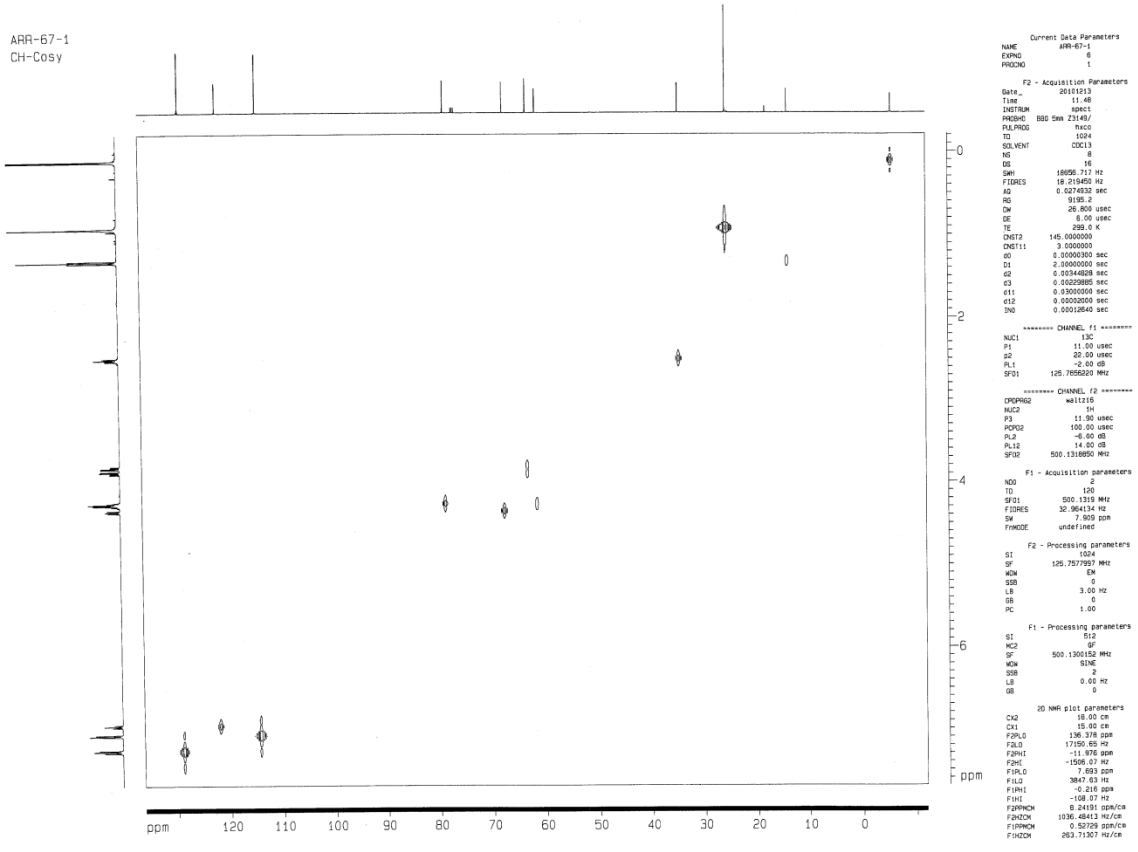
F2 - Processing parameters
SI 1024
SF 125.7577884 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 512
MC2 SF
SF 500.1300089 MHz
WDW SINE
SSB 2
LB 0.00 Hz
GB 0

2D NMR plot parameters
CX2 18.00 cm
CX1 15.00 cm
F2PLO 137.939 ppm
F2LO 17346.90 Hz
F2PHI 5.469 ppm
F2HI 680.24 Hz
F1PLO 7.680 ppm
F1LO 3831.18 Hz
F1PHI 0.978 ppm
F1HI 488.94 Hz
F2PPMCM 7.36277 ppm/cm
F2HZCM 925.92590 Hz/cm
F1PPMCM 0.44552 ppm/cm
F1HZCM 222.81539 Hz/cm


Current Data Parameters
NAME ARR-67-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20101208
Time 20.27
INSTRUM av400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 66
DS 0
SWH 11990.407 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 32
DW 41.700 usec
DE 6.00 usec
TE 295.9 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 13.60 usec
PL1 -4.00 dB
SFO1 400.1320007 MHz
F2 - Processing parameters
SI 32768
SF 400.1300115 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 25.00 cm
CY 10.98 cm
F1P 10.000 ppm
F1 4001.30 Hz
F2P -1.000 ppm
F2 -400.13 Hz
PPMCM 0.44000 ppm/cm
HZCM 176.05721 Hz/cm
ppm
7.26898
7.25051
7.08381
7.06416
4.28030
4.27578
4.26236
4.25790
2.50193
1.33415
1.31644
1.29850
0.92431
0.91797
0.91123
0.10978
0.10044
Ph–N
O
OTBDMS
EtO2C
Integral
2.1136
2.0470
1.0000
1.0602
3.0604
2.1303
2.1239
3.0137
9.3450
5.9497
ppm
Current Data Parameters
NAME ARR-67-1-13c
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20101208
Time 20.31
INSTRUM av400
PROBHD 5 mm QNP 1H/13
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 25125.629 Hz
FIDRES 0.766773 Hz
AQ 0.6521332 sec
RG 5160.6
DW 19.900 usec
DE 6.00 usec
TE 296.0 K
D1 2.50000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 6.50 usec
PL1 -3.00 dB
SFO1 100.6238364 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -4.00 dB
PL12 14.00 dB
SFO2 400.1320007 MHz
F2 - Processing parameters
SI 32768
SF 100.6127597 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 25.00 cm
CY 10.10 cm
F1P 200.000 ppm
F1 20122.55 Hz
F2P -14.771 ppm
F2 -1486.12 Hz
PPMCM 8.59083 ppm/cm
HZCM 864.34680 Hz/cm
ppm
171.544
151.152
129.093
122.164
114.497
79.027
77.519
77.200
76.882
67.961
63.569
61.798
34.941
25.976
18.427
14.292
-5.171
-5.219
Ph–N
O
OTBDMS
EtO2C
ppm





Current Data Parameters
NAME ARR-67-1
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20101213
Time 11.48
INSTRUM spect
PROBHD BBS Sma Z3140/
PULPROG hsco
TD 1024
SOLVENT CDCl3
NS 8
DS 16
SWH 18656.717 Hz
FIDRES 18.219450 Hz
AQ 0.0274932 sec
RG 9195.2
DW 26.800 usec
DE 6.00 usec
TE 298.0 K
CNST2 145.0000000
CNST11 3.0000000
d0 0.00000300 sec
D1 2.00000000 sec
d2 0.00344828 sec
d3 0.00229885 sec
d11 0.03000000 sec
d12 0.00002000 sec
IN0 0.00012640 sec

======== CHANNEL f1 ========
NUC1 13C
P1 11.00 usec
p2 22.00 usec
PL1 -2.00 dB
SFO1 125.7656220 MHz

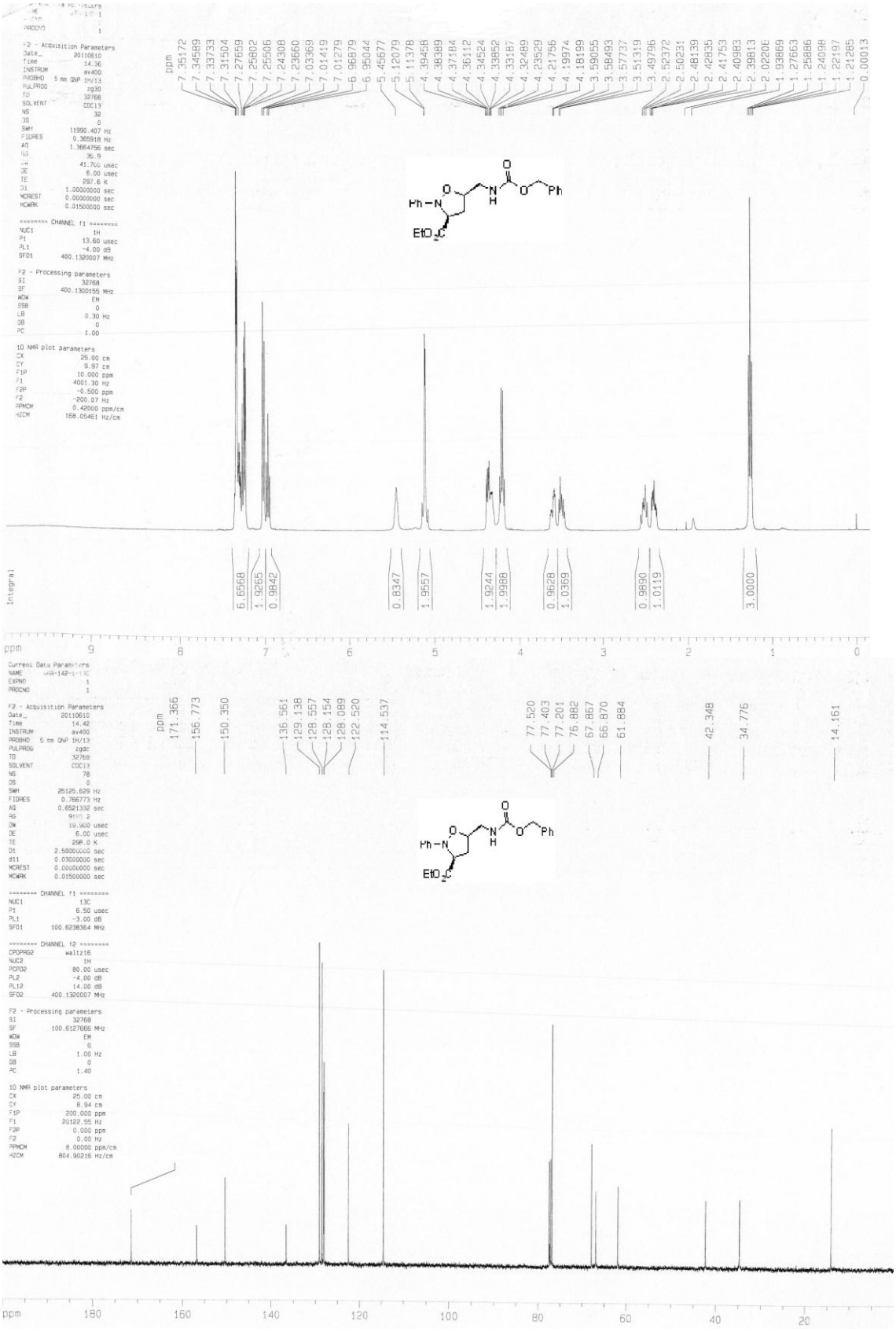
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
P3 11.90 usec
PCPD2 100.00 usec
PL2 -6.00 dB
PL12 14.00 dB
SFO2 500.1318850 MHz

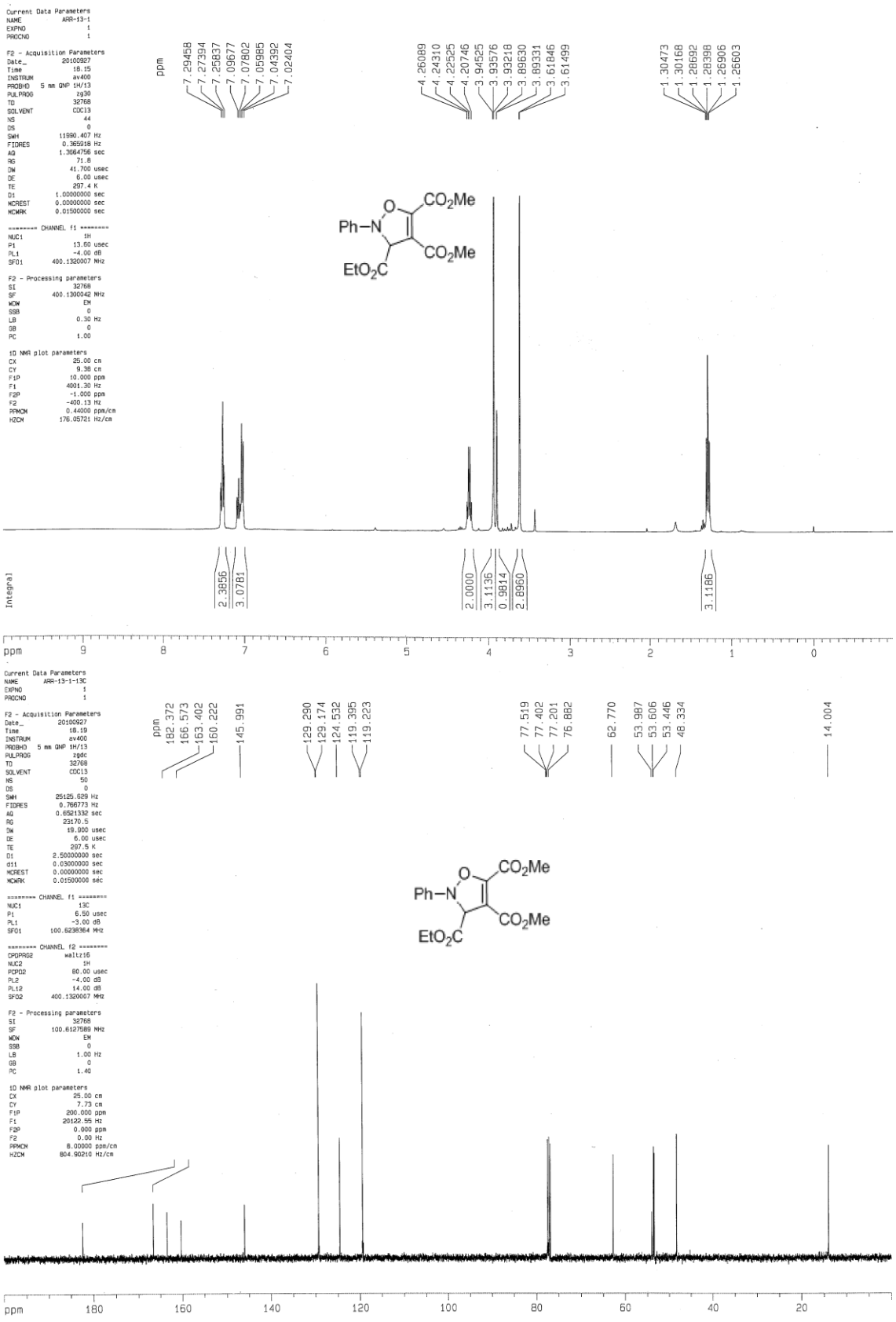
F1 - Acquisition parameters
ND0 2
TD 120
SFO1 500.1319 MHz
FIDRES 32.964134 Hz
SW 7.909 ppm
FnMODE undefined

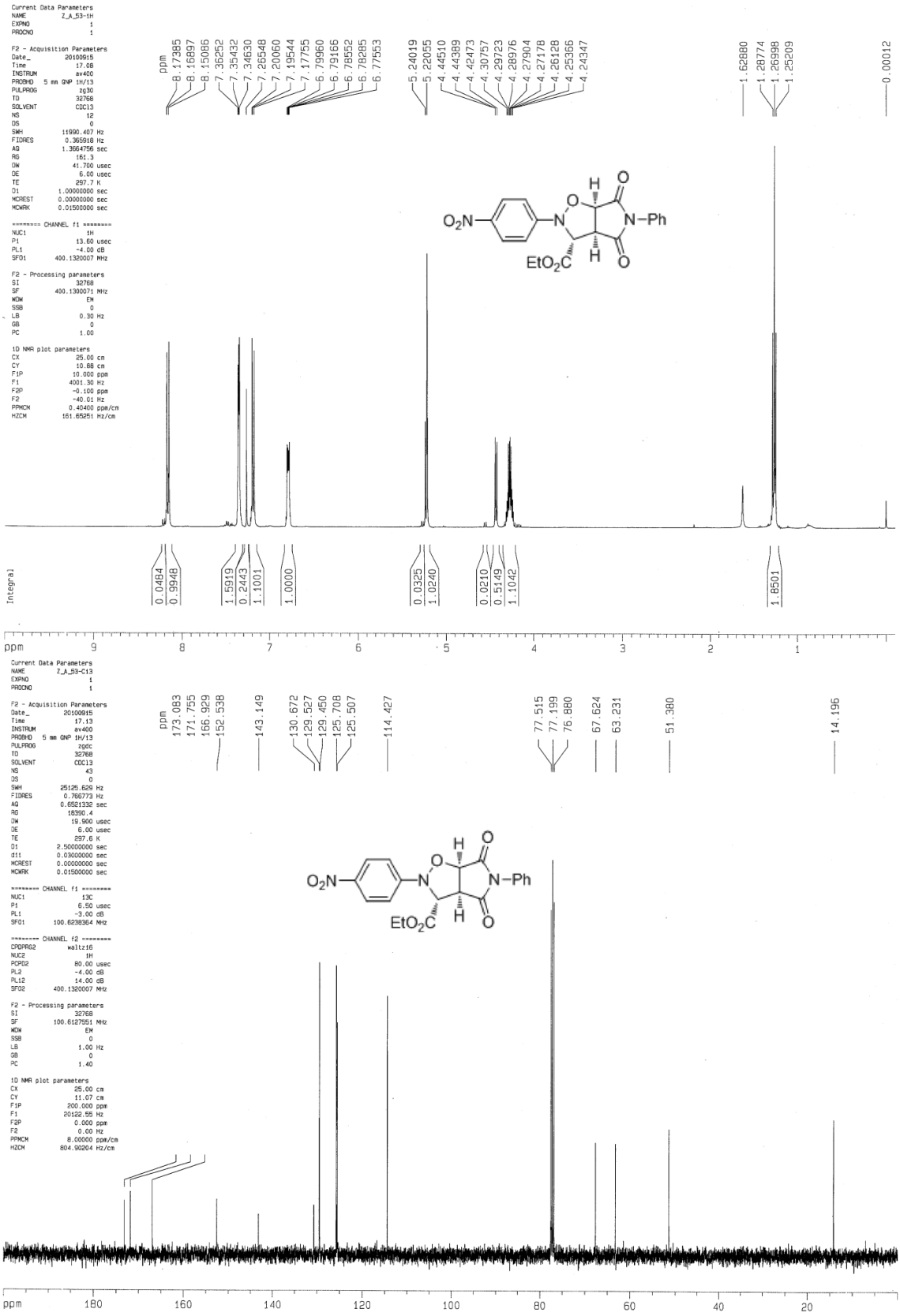
F2 - Processing parameters
SI 1024
SF 125.7577897 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00

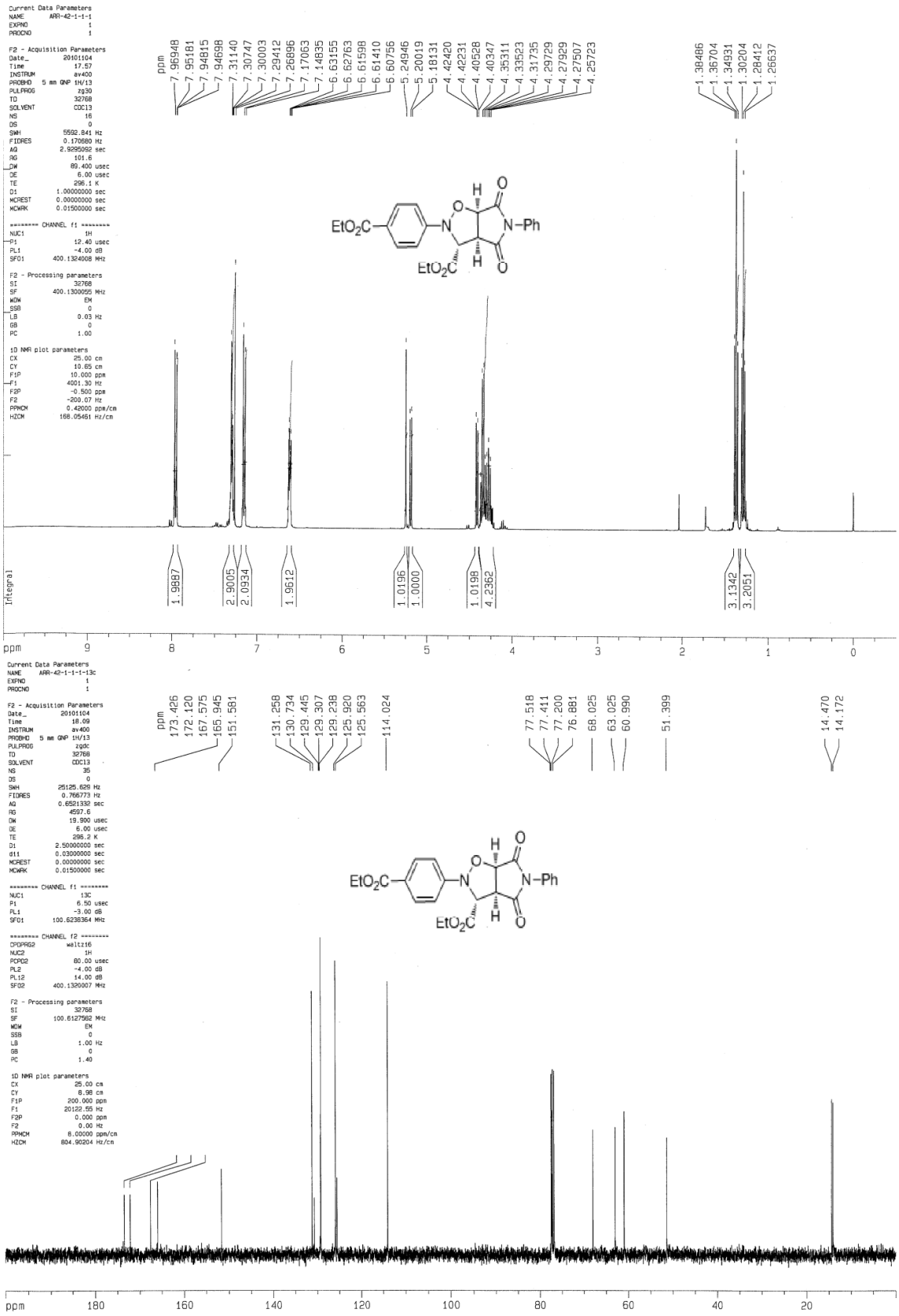
F1 - Processing parameters
SI 512
MC2 QF
SF 500.1300152 MHz
WDW SINE
SSB 2
LB 0.00 Hz
GB 0

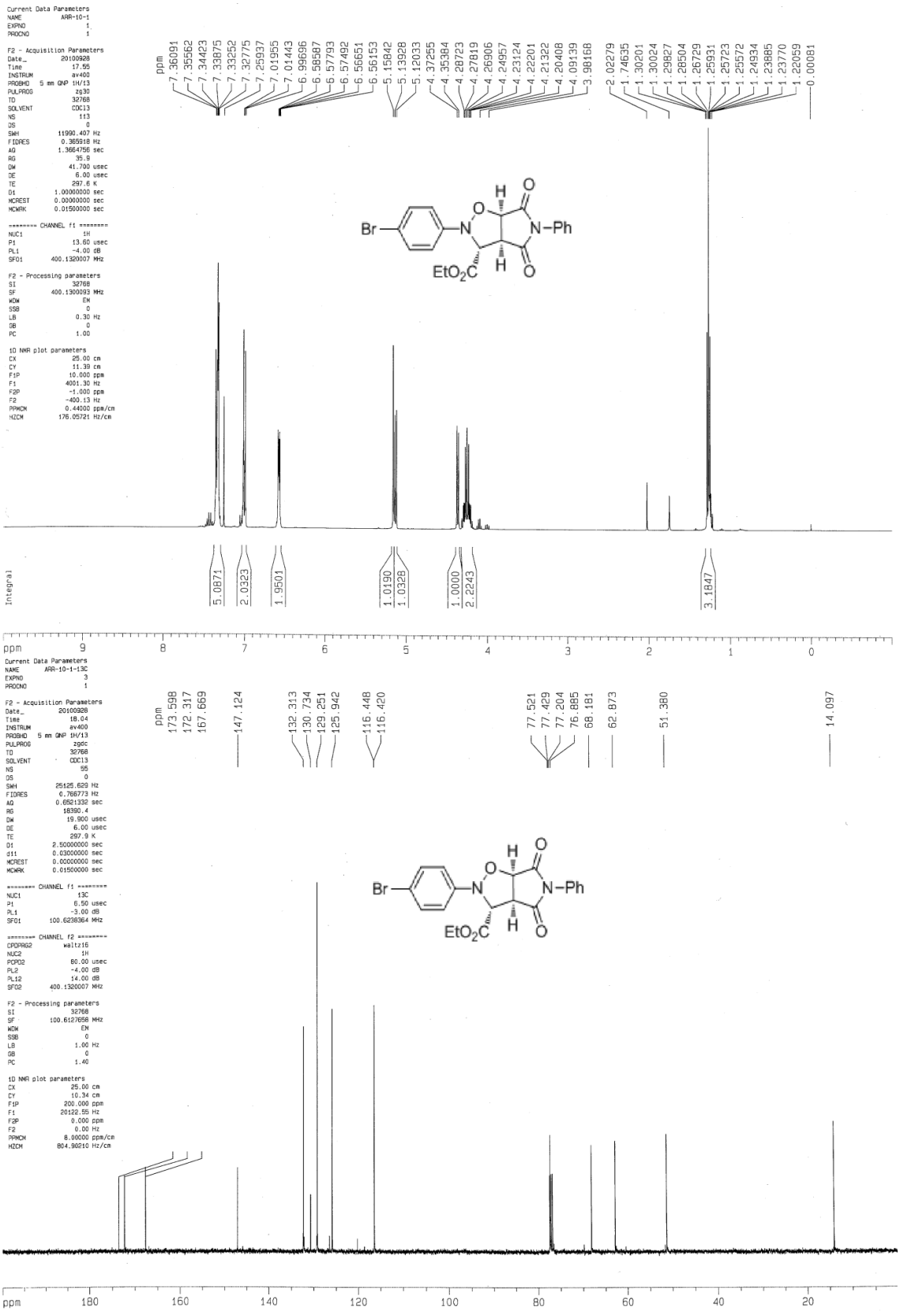
2D NMR plot parameters
CX2 18.00 cm
CX1 15.00 cm
F2PLO 136.378 ppm
F2LO 17150.65 Hz
F2PHI -11.976 ppm
F2HI -1506.07 Hz
F1PLO 7.693 ppm
F1LO 3847.63 Hz
F1PHI -0.216 ppm
F1HI -108.07 Hz
F2PPMCM 6.24191 ppm/cm
F2HZCM 1036.48413 Hz/cm
F1PPMCM 0.52729 ppm/cm
F1HZCM 263.71307 Hz/cm

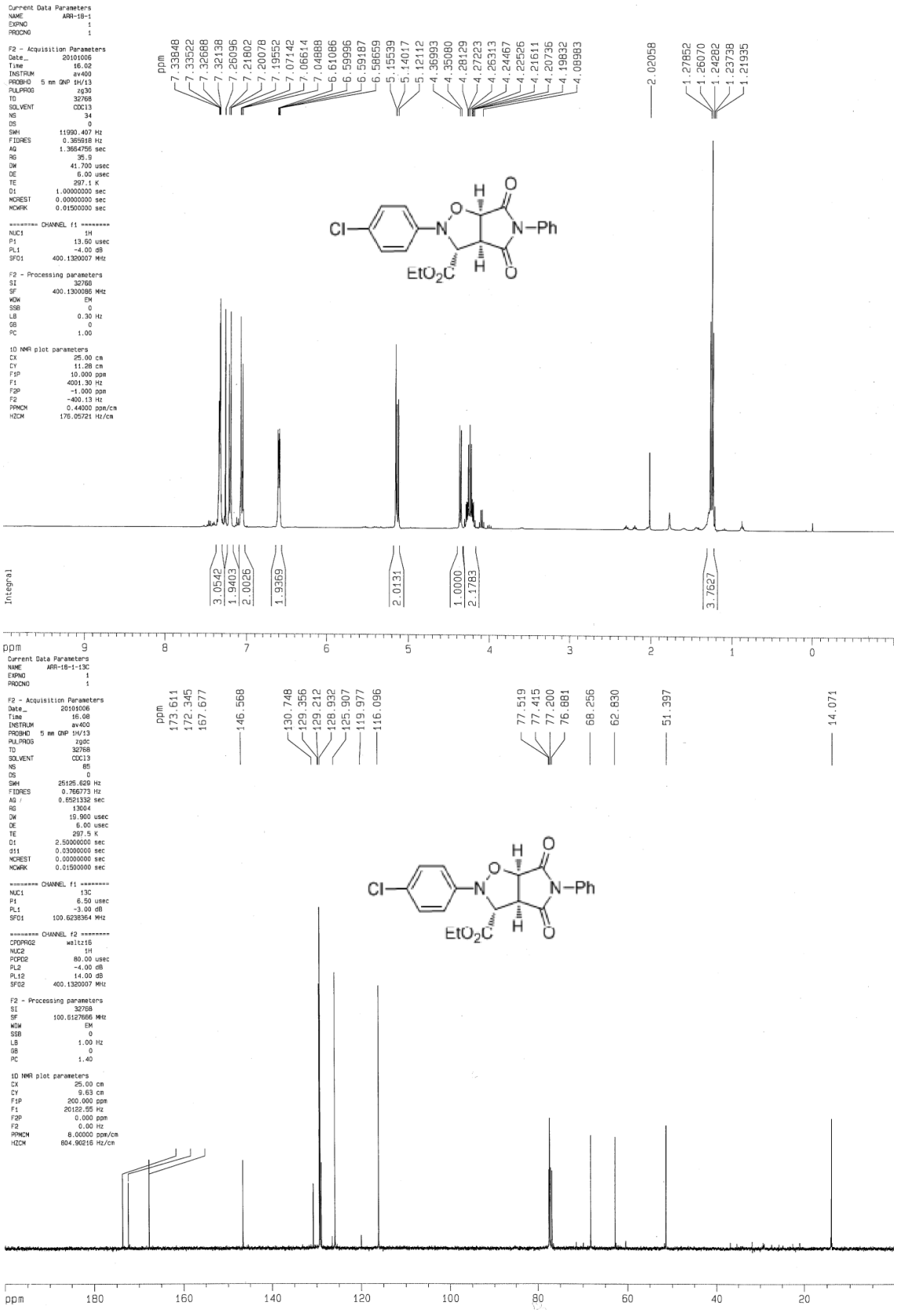


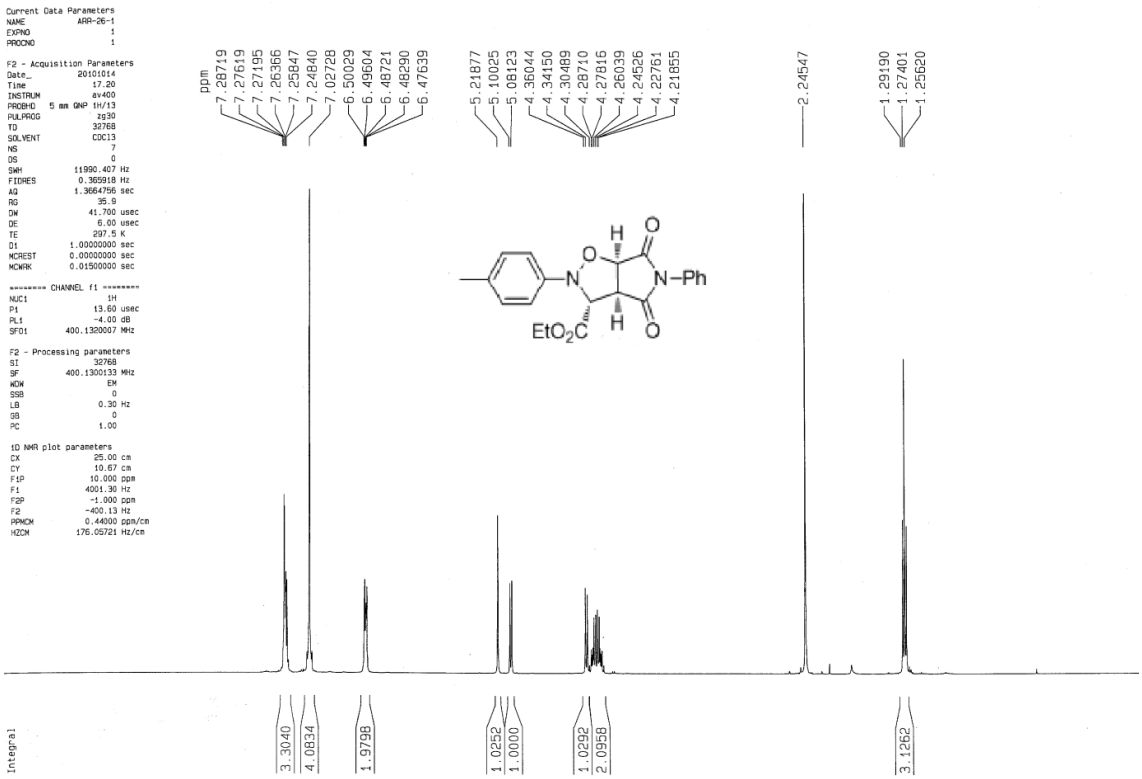

Current Data Parameters
NAME ARR-13-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100927
Time 18.15
INSTRUM av400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 44
DS 0
SWH 11990.407 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 71.8
DW 41.700 usec
DE 6.00 usec
TE 297.4 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 13.50 usec
PL1 -4.00 dB
SFO1 400.1320007 MHz
F2 - Processing parameters
SI 32768
SF 400.1300042 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 25.00 cm
CY 9.36 cm
F1P 10.000 ppm
F1 4001.30 Hz
F2P -1.000 ppm
F2 -400.13 Hz
PPMCM 0.44000 ppm/cm
HZCM 176.05721 Hz/cm
ppm
7.29458
7.27394
7.25837
7.09677
7.07802
7.05985
7.04392
7.02404
4.26089
4.24310
4.22525
4.20746
3.94525
3.93576
3.93218
3.89630
3.89331
3.61846
3.61499
1.30473
1.30168
1.28692
1.28398
1.26906
1.26603
CO2Me
Ph–N
O
CO2Me
EtO2C
Integral
2.3856
3.0781
2.0000
3.1136
0.9814
2.8960
3.1186
ppm
9
8
7
6
5
4
3
2
1
0
Current Data Parameters
NAME ARR-13-1-13C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100927
Time 18.19
INSTRUM av400
PROBHD 5 mm QNP 1H/13
PULPROG zgdc
TD 32768
SOLVENT CDCl3
NS 50
DS 0
SWH 25125.629 Hz
FIDRES 0.766773 Hz
AQ 0.6521332 sec
RG 23170.5
DW 19.900 usec
DE 6.00 usec
TE 297.5 K
D1 2.50000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 6.50 usec
PL1 -3.00 dB
SFO1 100.6238364 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -4.00 dB
PL12 14.00 dB
SFO2 400.1320007 MHz
F2 - Processing parameters
SI 32768
SF 100.6127589 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 25.00 cm
CY 7.73 cm
F1P 200.000 ppm
F1 20122.55 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 8.00000 ppm/cm
HZCM 804.90210 Hz/cm
ppm
182.372
166.573
163.402
160.222
145.991
129.290
129.174
124.532
119.395
119.223
77.519
77.402
77.201
76.882
62.770
53.987
53.606
53.446
48.334
14.004
CO2Me
Ph–N
O
CO2Me
EtO2C
ppm
180
160
140
120
100
80
60
40
20

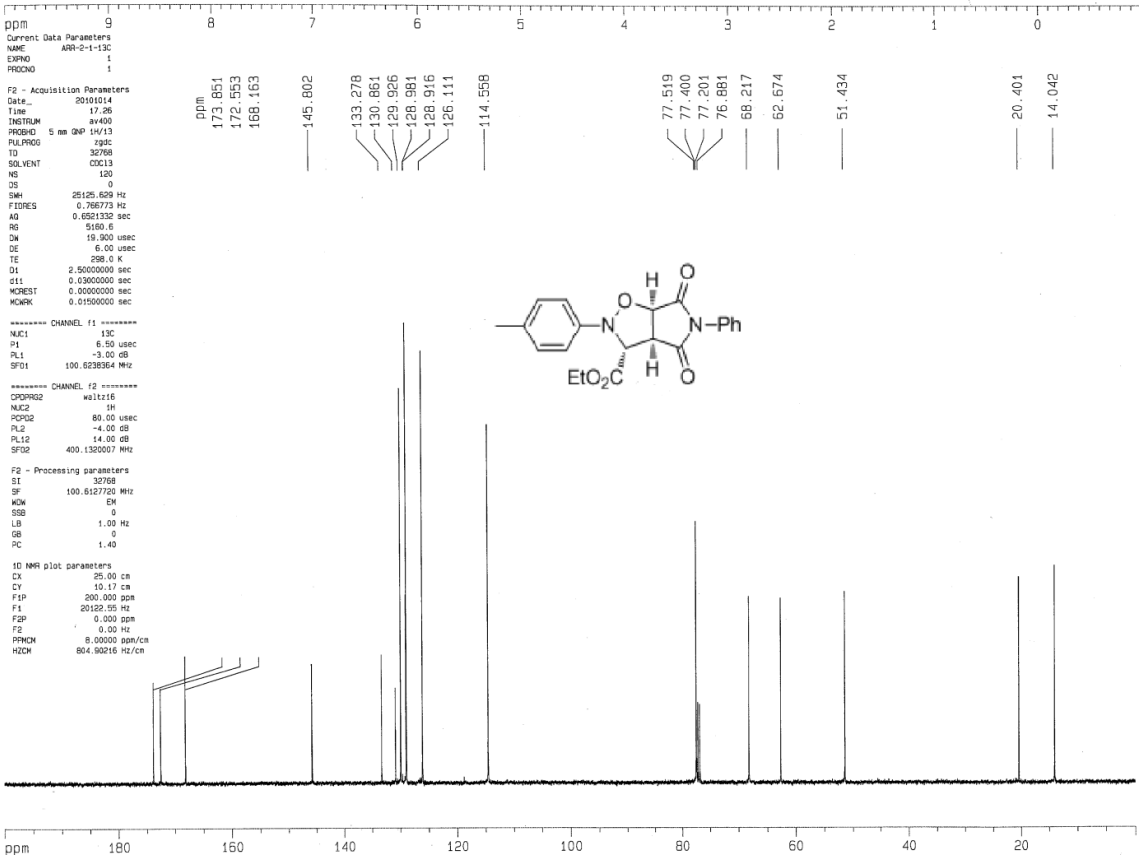

Current Data Parameters
NAME Z_A_53-1H
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100915
Time 17.08
INSTRUM av400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 12
DS 0
SWH 11990.407 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 161.3
DW 41.700 usec
DE 6.00 usec
TE 297.7 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 13.60 usec
PL1 -4.00 dB
SFO1 400.1320007 MHz
F2 - Processing parameters
SI 32768
SF 400.1300071 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 25.00 cm
CY 10.88 cm
F1P 10.000 ppm
F1 4001.30 Hz
F2P -0.100 ppm
F2 -40.01 Hz
PPMCM 0.40400 ppm/cm
HZCM 161.65251 Hz/cm
ppm
8.17385
8.16897
8.15086
7.36252
7.35432
7.34630
7.26548
7.20060
7.19544
7.17755
6.79960
6.79166
6.78552
6.78285
6.77553
5.24019
5.22055
4.44510
4.44389
4.42473
4.30757
4.29723
4.28976
4.27904
4.27178
4.26128
4.25366
4.24347
1.62880
1.28774
1.25998
1.25209
0.00012
Integral
0.0484
0.9948
1.5919
0.2443
1.1001
1.0000
0.0325
1.0240
0.0210
0.5149
1.1042
1.8501
ppm
9
8
7
6
5
4
3
2
1
Current Data Parameters
NAME Z_A_53-C13
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100915
Time 17.13
INSTRUM av400
PROBHD 5 mm QNP 1H/13
PULPROG zgdc
TD 32768
SOLVENT CDCl3
NS 43
DS 0
SWH 25125.629 Hz
FIDRES 0.766773 Hz
AQ 0.6521332 sec
RG 18390.4
DW 19.900 usec
DE 6.00 usec
TE 297.6 K
D1 2.50000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 6.50 usec
PL1 -3.00 dB
SFO1 100.6238364 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -4.00 dB
PL12 14.00 dB
SFO2 400.1320007 MHz
F2 - Processing parameters
SI 32768
SF 100.6127551 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 25.00 cm
CY 11.07 cm
F1P 200.000 ppm
F1 20122.55 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 8.00000 ppm/cm
HZCM 804.90204 Hz/cm
ppm
173.083
171.755
166.929
152.538
143.149
130.672
129.527
129.450
125.708
125.507
114.427
77.515
77.199
76.880
67.624
63.231
51.380
14.196
ppm
180
160
140
120
100
80
60
40
20

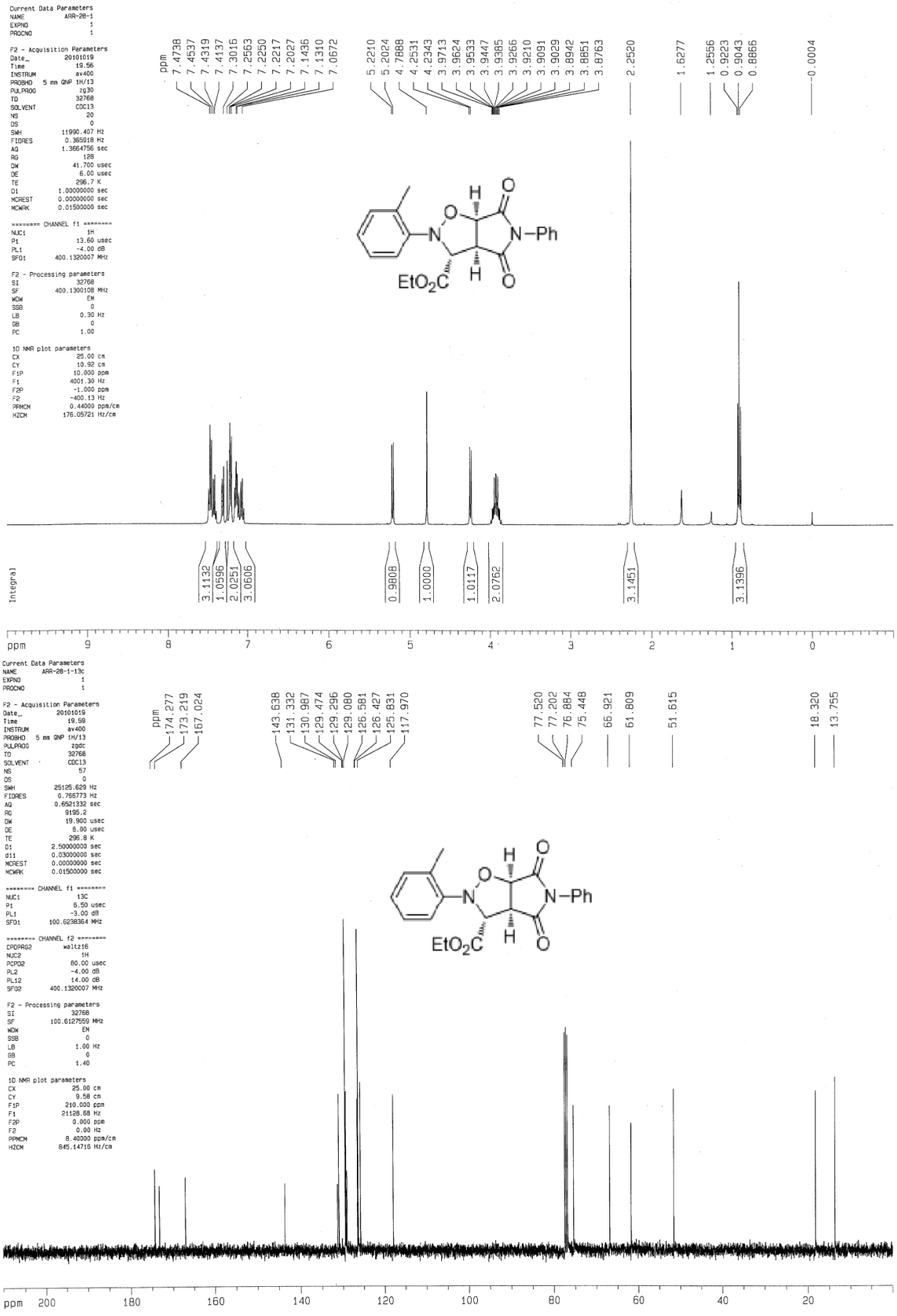

Current Data Parameters
NAME ARR-42-1-1-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20101104
Time 17.57
INSTRUM av400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 5592.841 Hz
FIDRES 0.170680 Hz
AQ 2.9295092 sec
RG 101.6
DW 89.400 usec
DE 6.00 usec
TE 296.1 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 12.40 usec
PL1 -4.00 dB
SFO1 400.1324008 MHz
F2 - Processing parameters
SI 32768
SF 400.1300055 MHz
WDW EM
SSB 0
LB 0.03 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 25.00 cm
CY 10.65 cm
F1P 10.000 ppm
F1 4001.30 Hz
F2P -0.500 ppm
F2 -200.07 Hz
PPMCM 0.42000 ppm/cm
HZCM 168.05461 Hz/cm
ppm
7.96948
7.95181
7.94815
7.94698
7.31140
7.30747
7.30003
7.29412
7.26896
7.17063
7.14835
6.63155
6.62763
6.61598
6.61410
6.60756
5.24946
5.20019
5.18131
4.42420
4.42231
4.40528
4.40347
4.35311
4.33523
4.31735
4.29729
4.27929
4.27507
4.25723
1.38486
1.36704
1.34931
1.30204
1.28412
1.26637
EtO2C
N
O
H
O
N–Ph
EtO2C
H
O
Integral
1.9887
2.9005
2.0934
1.9612
1.0196
1.0000
1.0198
4.2362
3.1342
3.2051
ppm
9
8
7
6
5
4
3
2
1
0
Current Data Parameters
NAME ARR-42-1-1-1-13C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20101104
Time 18.09
INSTRUM av400
PROBHD 5 mm QNP 1H/13
PULPROG zgdc
TD 32768
SOLVENT CDCl3
NS 35
DS 0
SWH 25125.629 Hz
FIDRES 0.766773 Hz
AQ 0.6521332 sec
RG 4597.6
DW 19.900 usec
DE 6.00 usec
TE 296.2 K
D1 2.50000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 6.50 usec
PL1 -3.00 dB
SFO1 100.6238364 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -4.00 dB
PL12 14.00 dB
SFO2 400.1320007 MHz
F2 - Processing parameters
SI 32768
SF 100.6127582 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 25.00 cm
CY 8.98 cm
F1P 200.000 ppm
F1 20122.55 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 8.00000 ppm/cm
HZCM 804.90204 Hz/cm
ppm
173.426
172.120
167.575
165.945
151.581
131.258
130.734
129.445
129.307
129.238
125.920
125.563
114.024
77.518
77.411
77.200
76.881
68.025
63.025
60.990
51.399
14.470
14.172
EtO2C
N
O
H
O
N–Ph
EtO2C
H
O
ppm
180
160
140
120
100
80
60
40
20

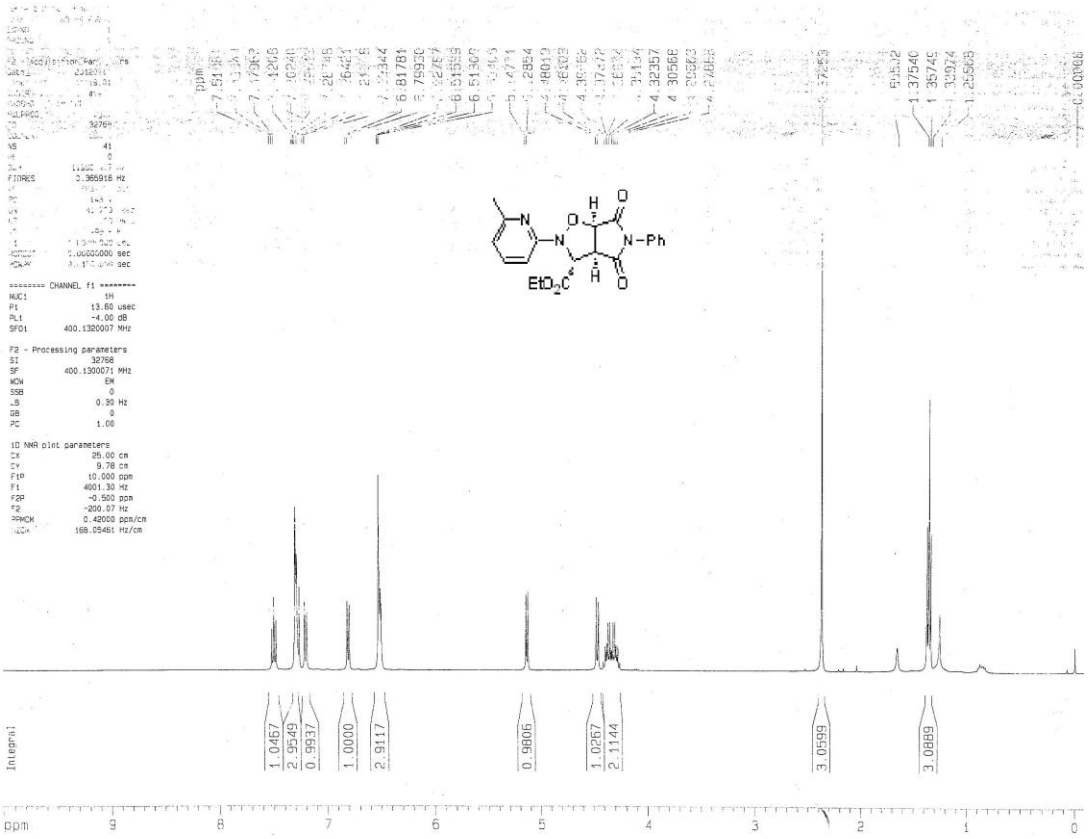

Current Data Parameters
NAME ARR-10-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100928
Time 17.55
INSTRUM av400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 113
DS 0
SWH 11990.407 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 35.9
DW 41.700 usec
DE 6.00 usec
TE 297.6 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 13.60 usec
PL1 -4.00 dB
SFO1 400.1320007 MHz
F2 - Processing parameters
SI 32768
SF 400.1300093 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 25.00 cm
CY 11.39 cm
F1P 10.000 ppm
F1 4001.30 Hz
F2P -1.000 ppm
F2 -400.13 Hz
PPMCM 0.44000 ppm/cm
HZCM 176.05721 Hz/cm
ppm
7.36091
7.35562
7.34423
7.33875
7.33252
7.32775
7.25937
7.01955
7.01443
6.99696
6.58587
6.57793
6.57492
6.56651
6.56153
5.15842
5.13928
5.12033
4.37255
4.35384
4.28723
4.27819
4.26906
4.24957
4.23124
4.22201
4.21322
4.20408
4.09139
3.98168
2.02279
1.74635
1.30201
1.30024
1.29827
1.28504
1.26729
1.25931
1.25723
1.25572
1.24934
1.23885
1.23770
1.22059
0.00081
Br
N
O
H
O
N–Ph
H
O
EtO2C
Integral
5.0871
2.0323
1.9501
1.0190
1.0328
1.0000
2.2243
3.1847
ppm
9
8
7
6
5
4
3
2
1
0
Current Data Parameters
NAME ARR-10-1-13C
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100928
Time 18.04
INSTRUM av400
PROBHD 5 mm QNP 1H/13
PULPROG zgdc
TD 32768
SOLVENT CDCl3
NS 55
DS 0
SWH 25125.629 Hz
FIDRES 0.766773 Hz
AQ 0.6521332 sec
RG 18390.4
DW 19.900 usec
DE 6.00 usec
TE 297.9 K
D1 2.50000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 6.50 usec
PL1 -3.00 dB
SFO1 100.6238364 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -4.00 dB
PL12 14.00 dB
SFO2 400.1320007 MHz
F2 - Processing parameters
SI 32768
SF 100.6127658 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 25.00 cm
CY 10.34 cm
F1P 200.000 ppm
F1 20122.56 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 8.00000 ppm/cm
HZCM 804.90210 Hz/cm
ppm
173.598
172.317
167.669
147.124
132.313
130.734
129.251
125.942
116.448
116.420
77.521
77.429
77.204
76.885
68.181
62.873
51.380
14.097
Br
N
O
H
O
N–Ph
H
O
EtO2C
ppm
180
160
140
120
100
80
60
40
20

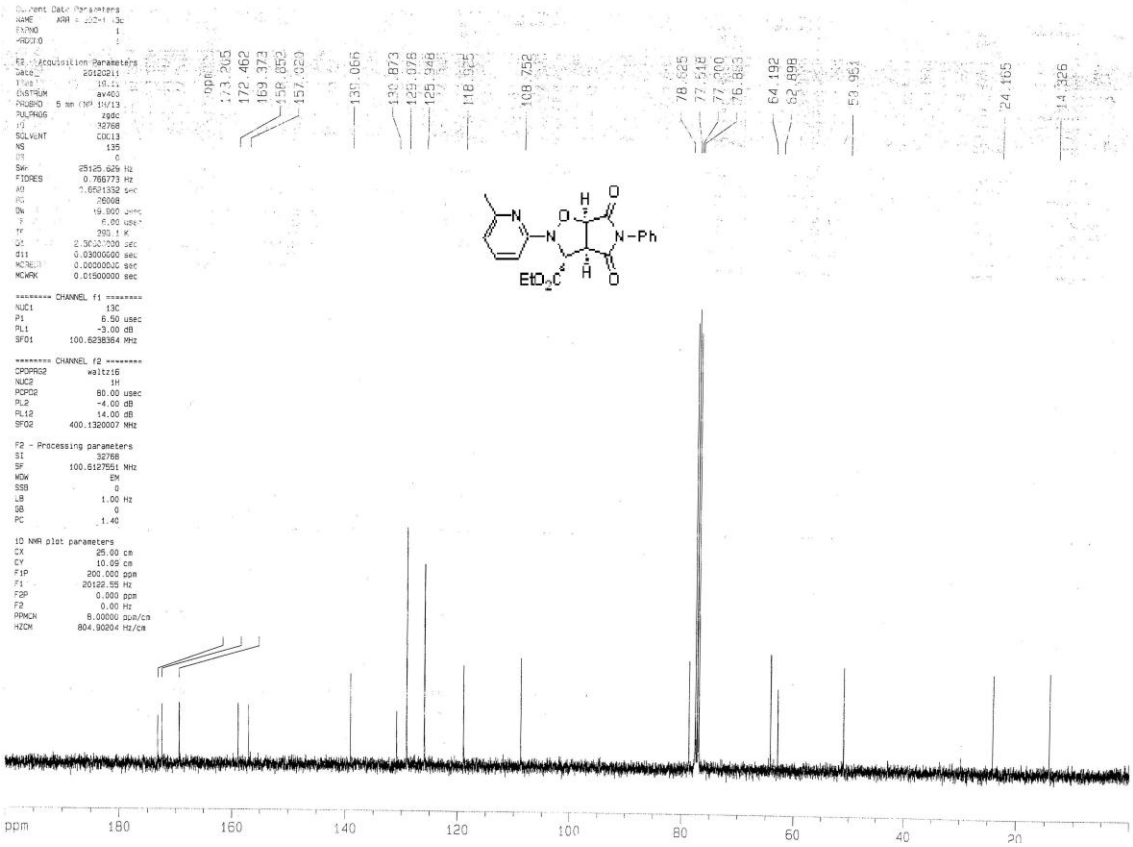


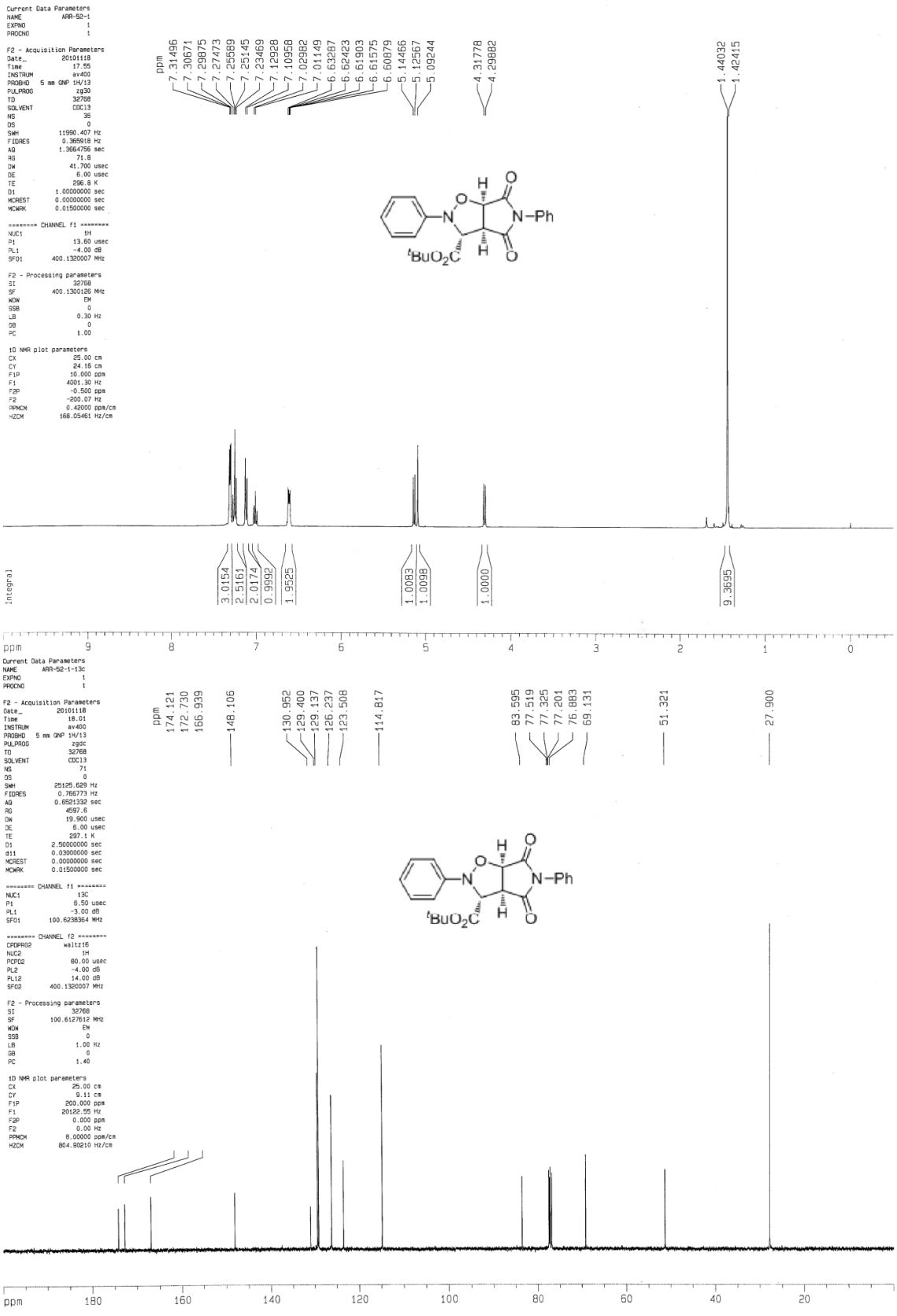


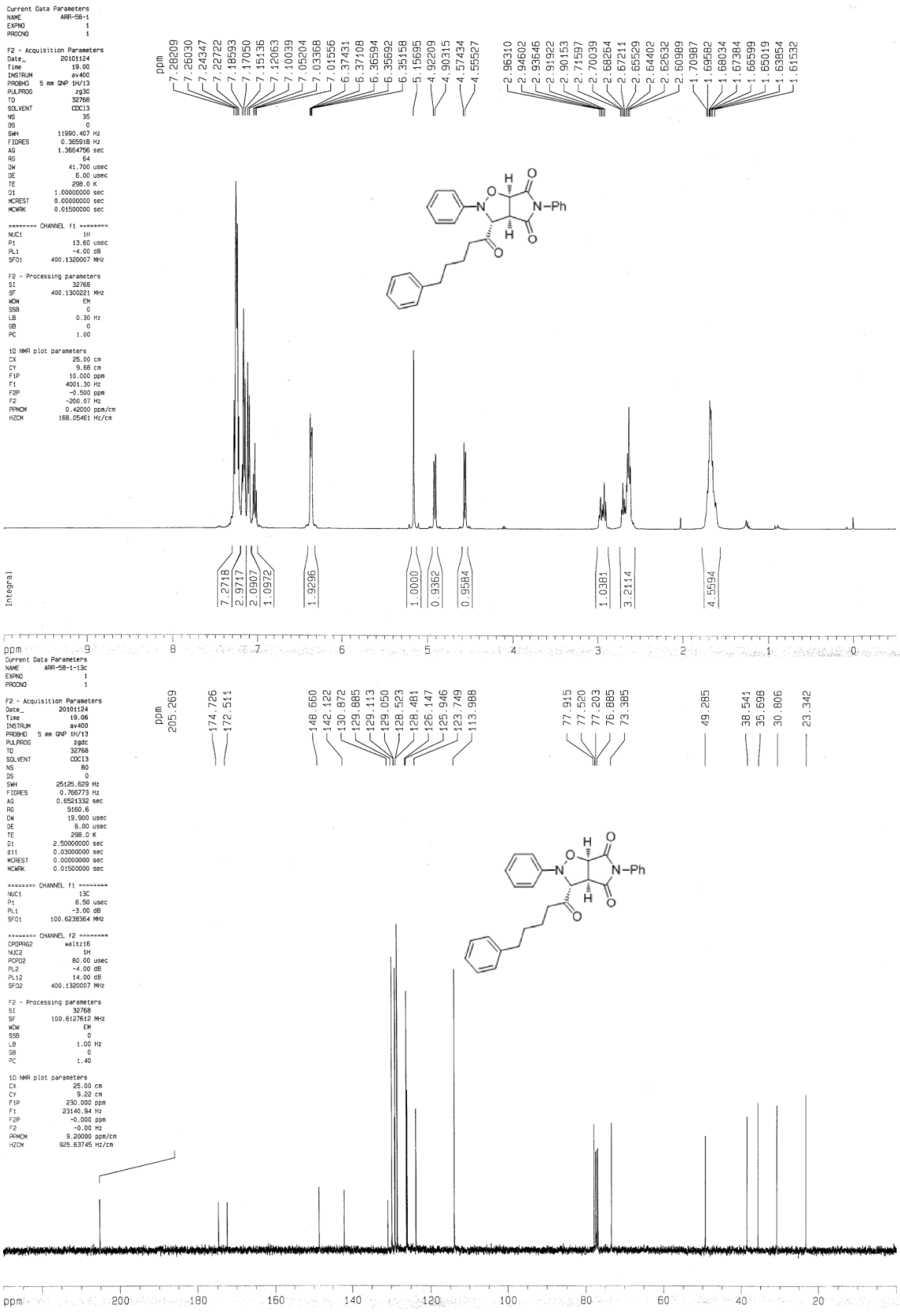


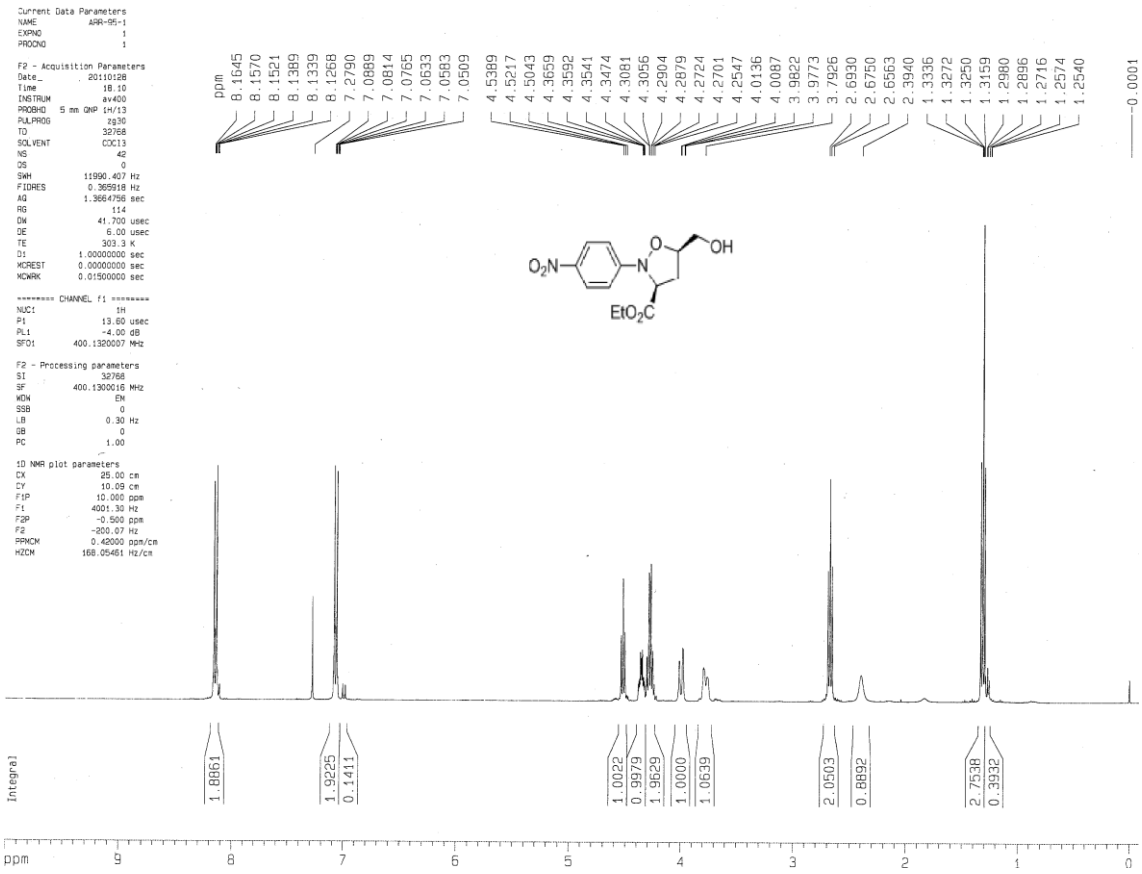


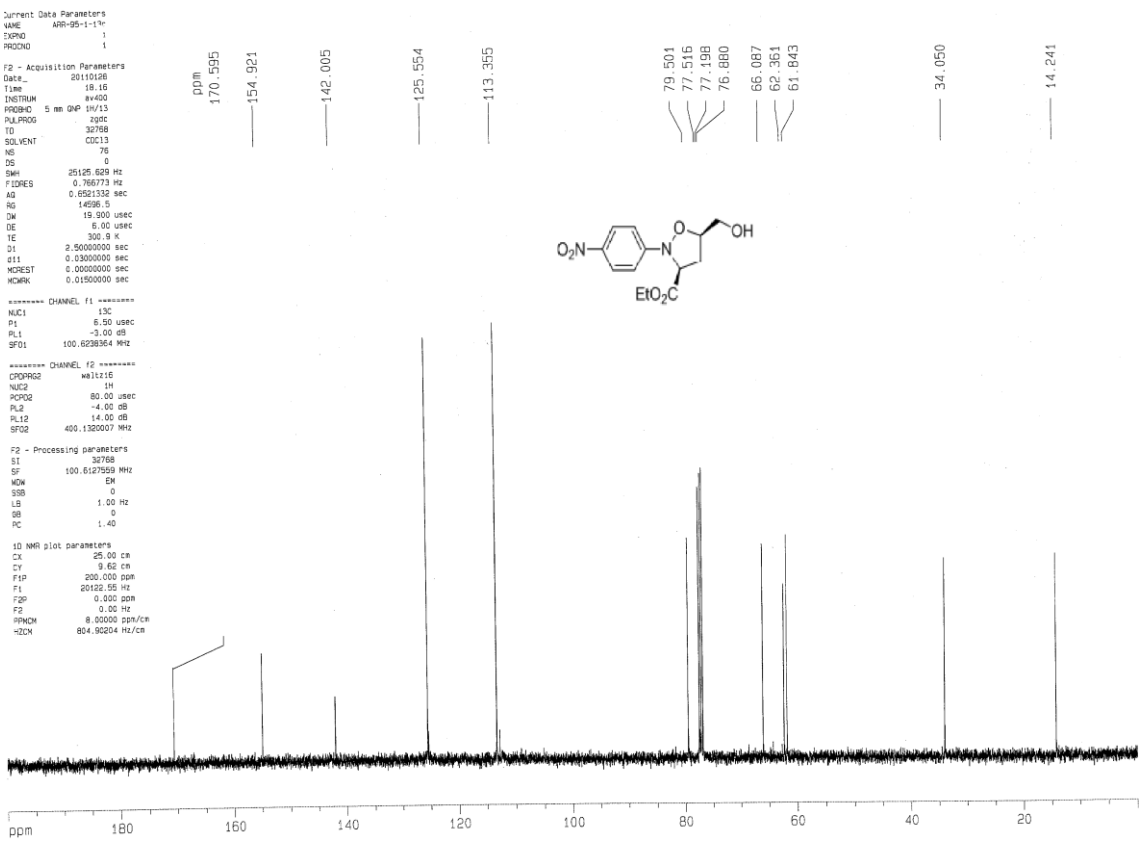

N-Ph
EtO2C
Integral
1.0467
2.9549
0.9937
1.0000
2.9117
0.9806
1.0267
2.1144
3.0599
3.0889
ppm

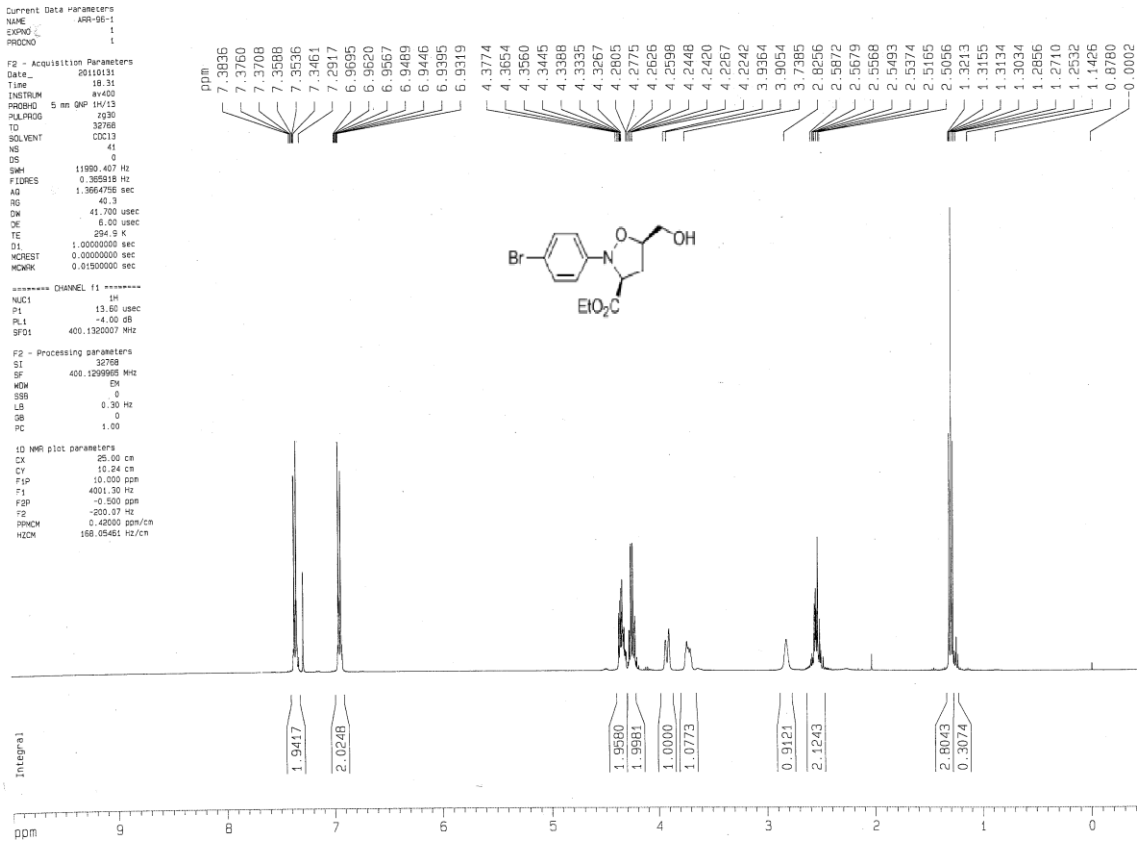

N-Ph
EtO2C
ppm

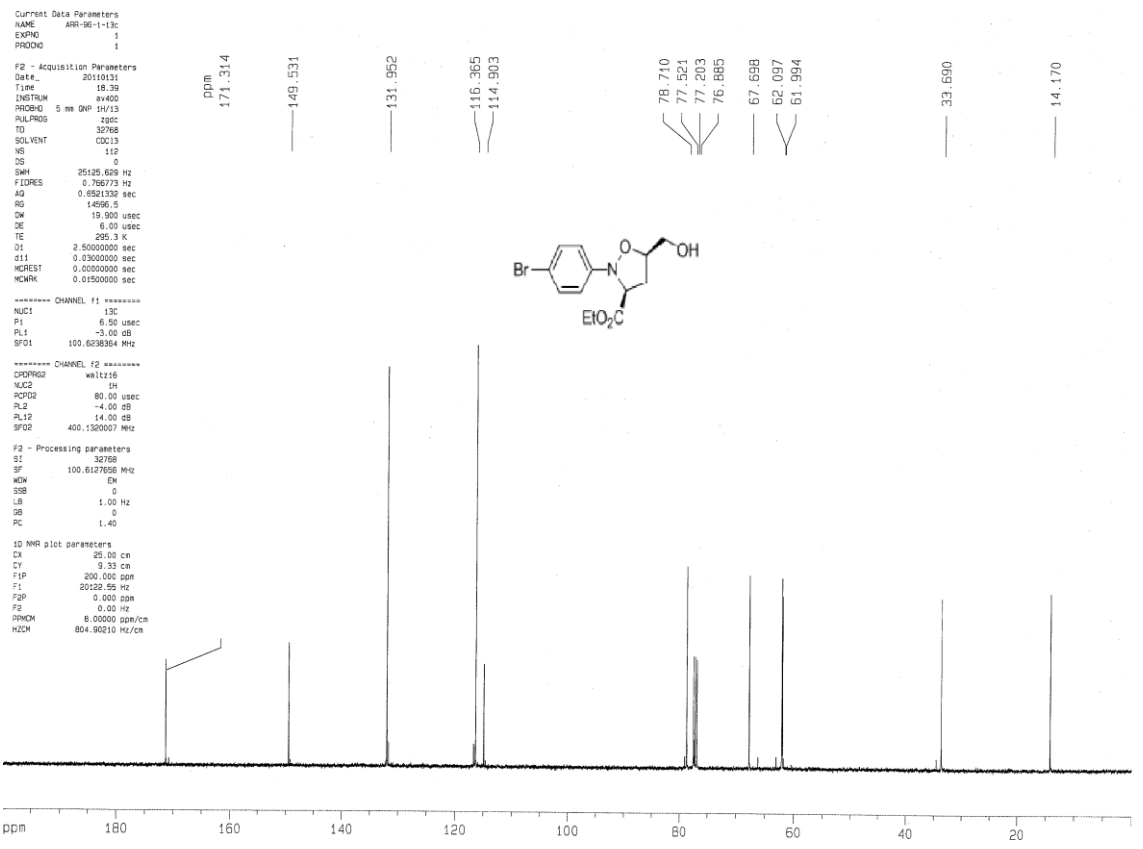


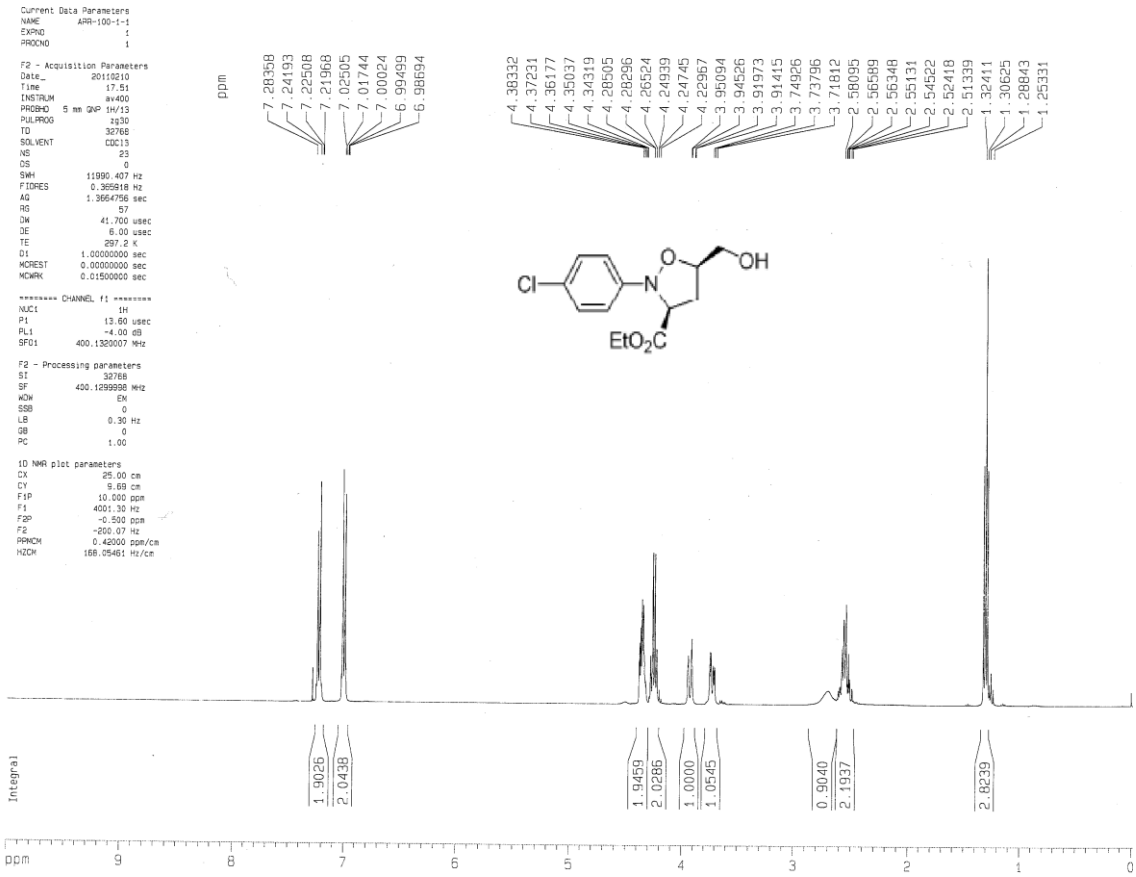


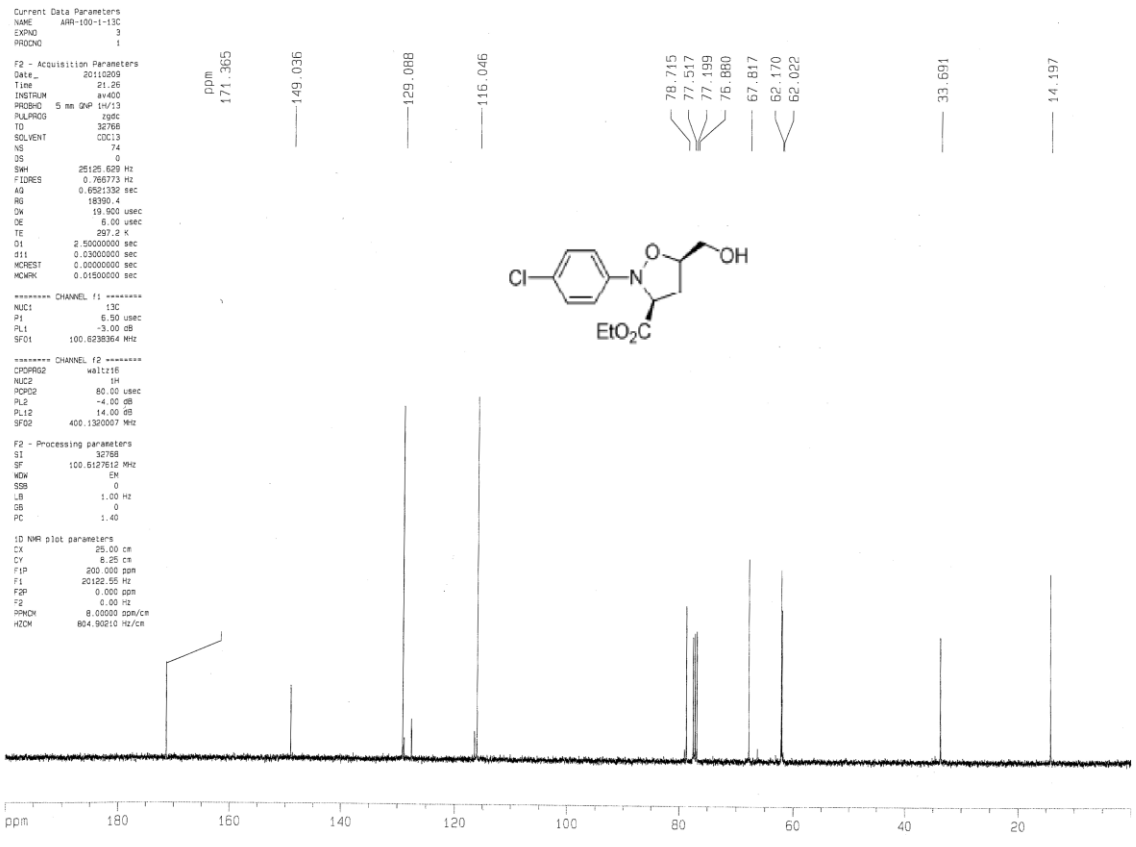


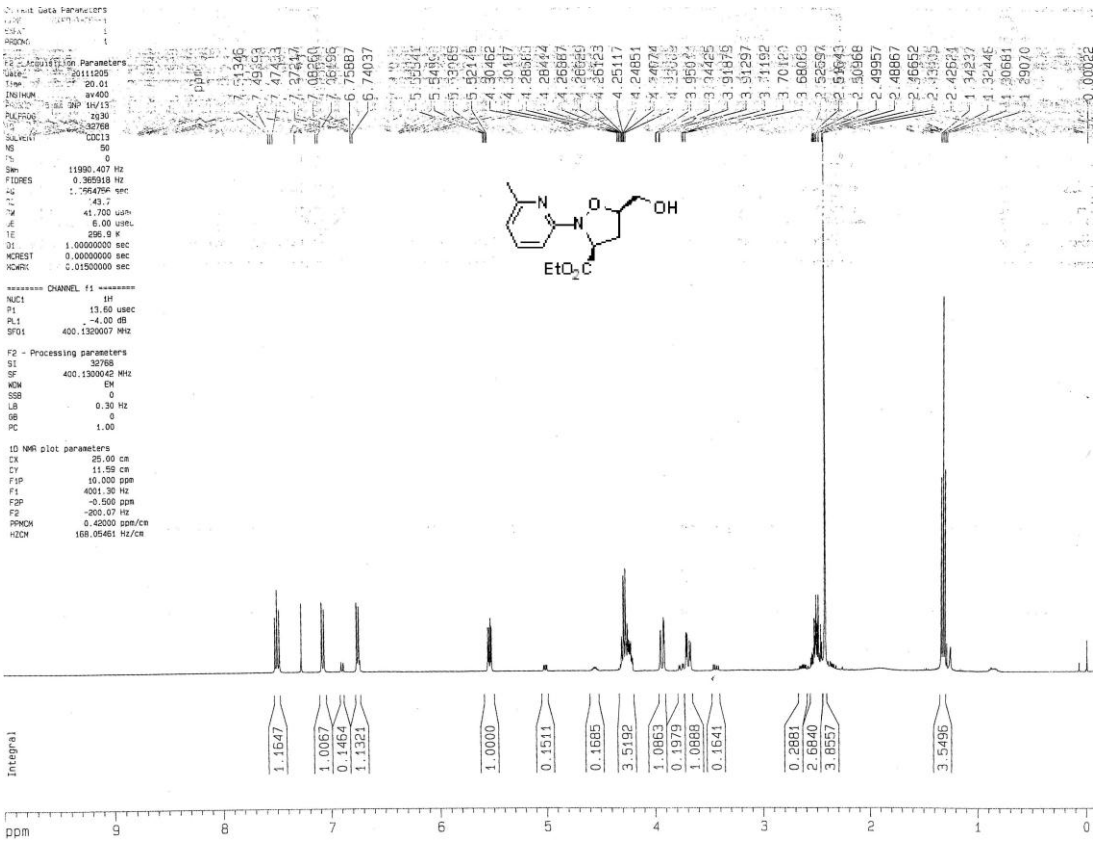


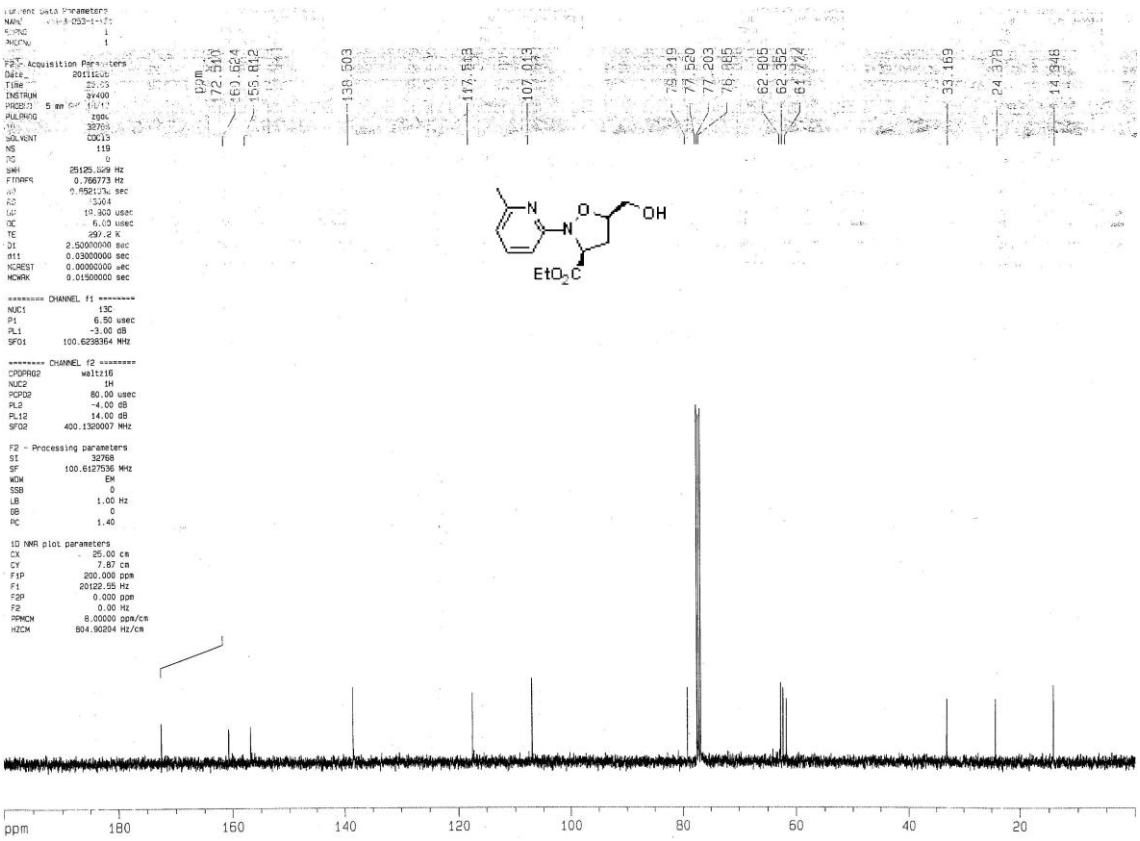


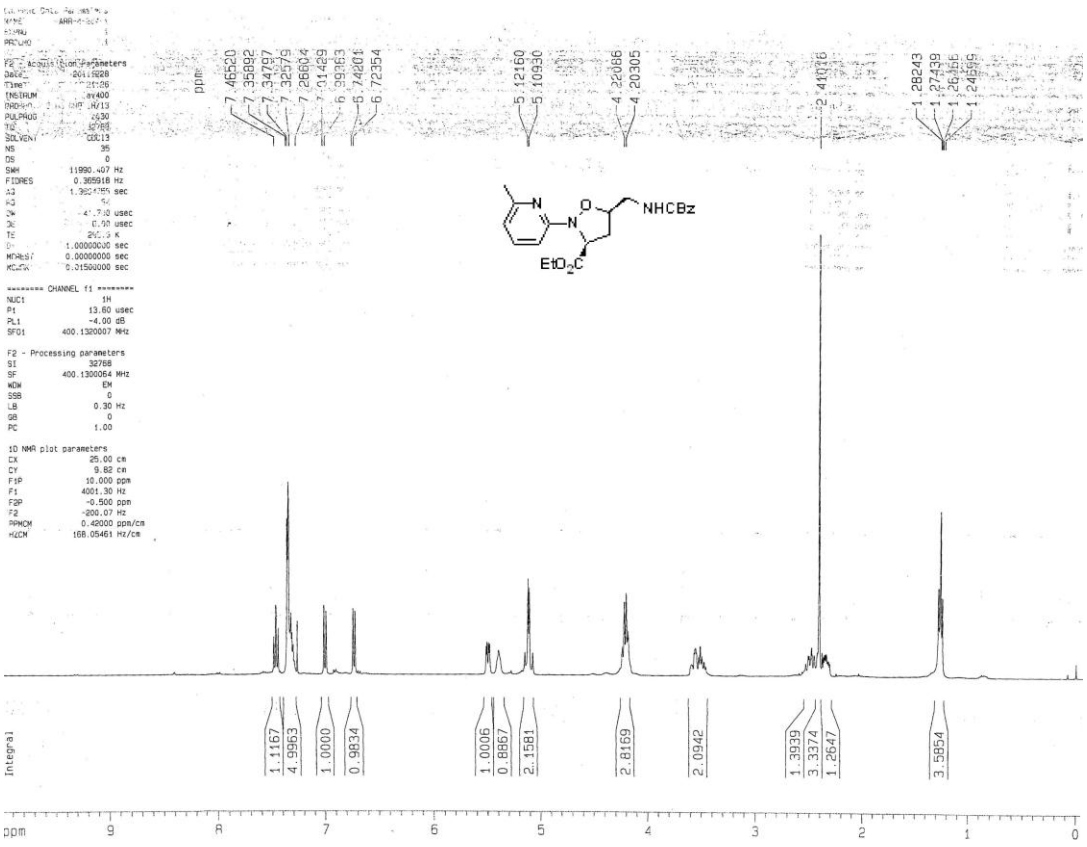


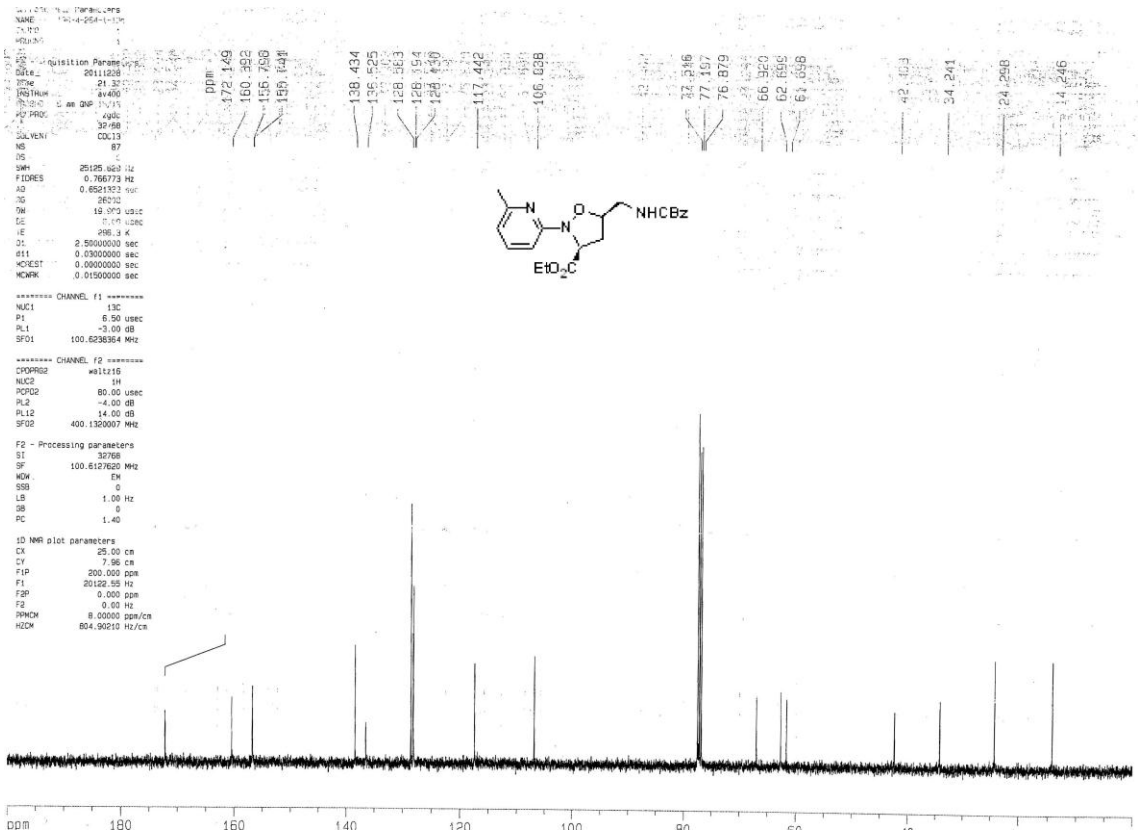


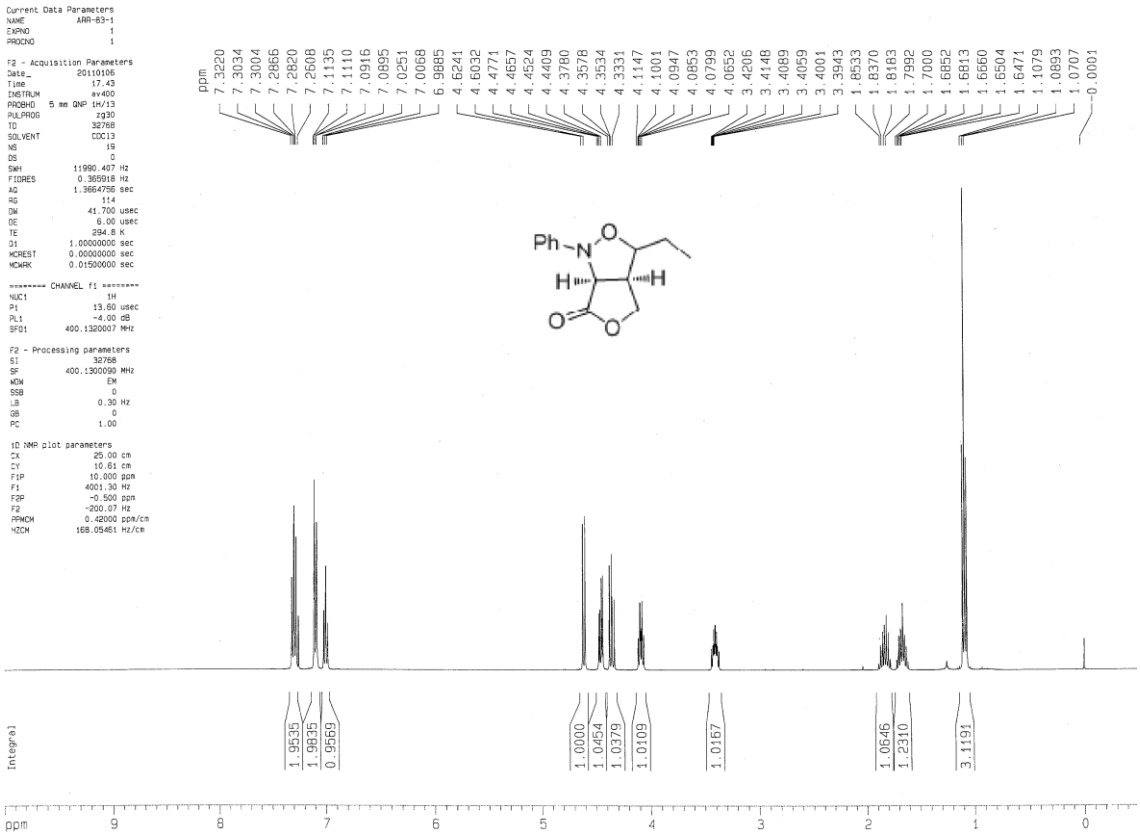


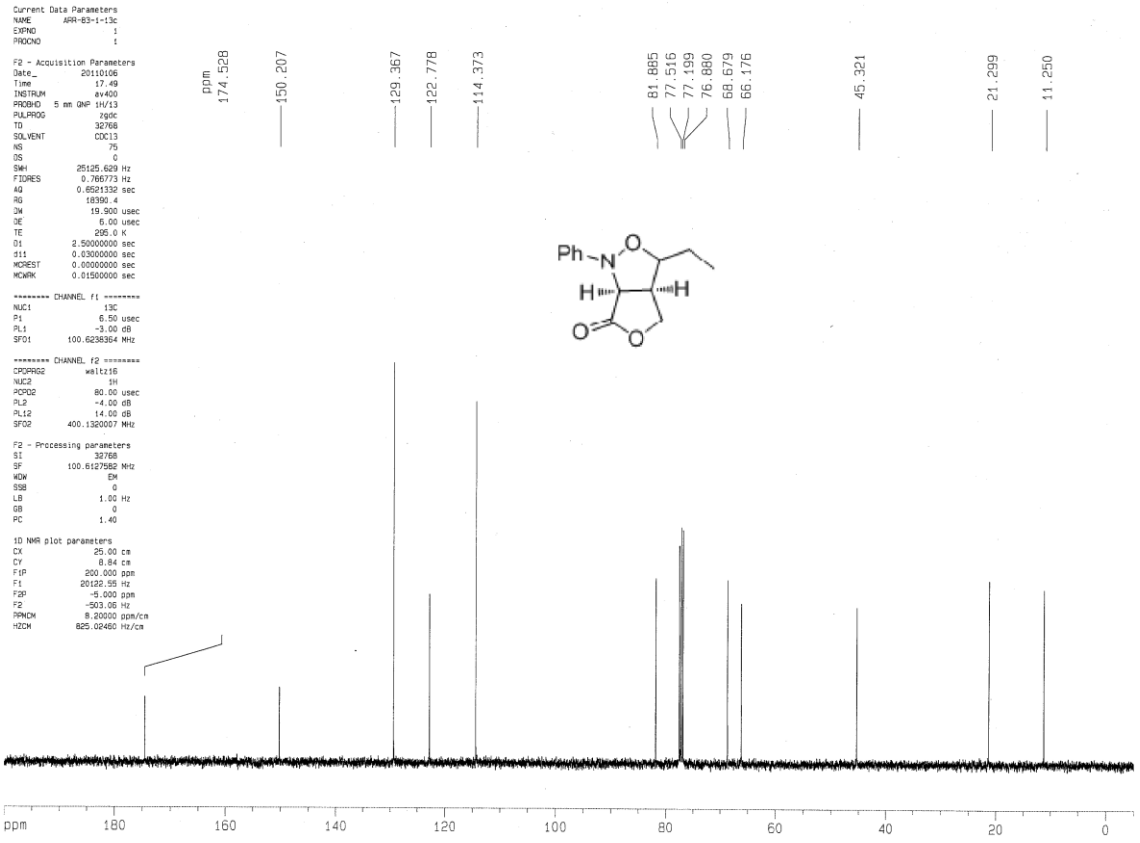

OH
EtO2C
Integral
1.1647
1.0067
0.1464
1.1321
1.0000
0.1511
0.1685
3.5192
1.0863
0.1979
1.0888
0.1641
0.2881
2.6840
3.8557
3.5496
ppm

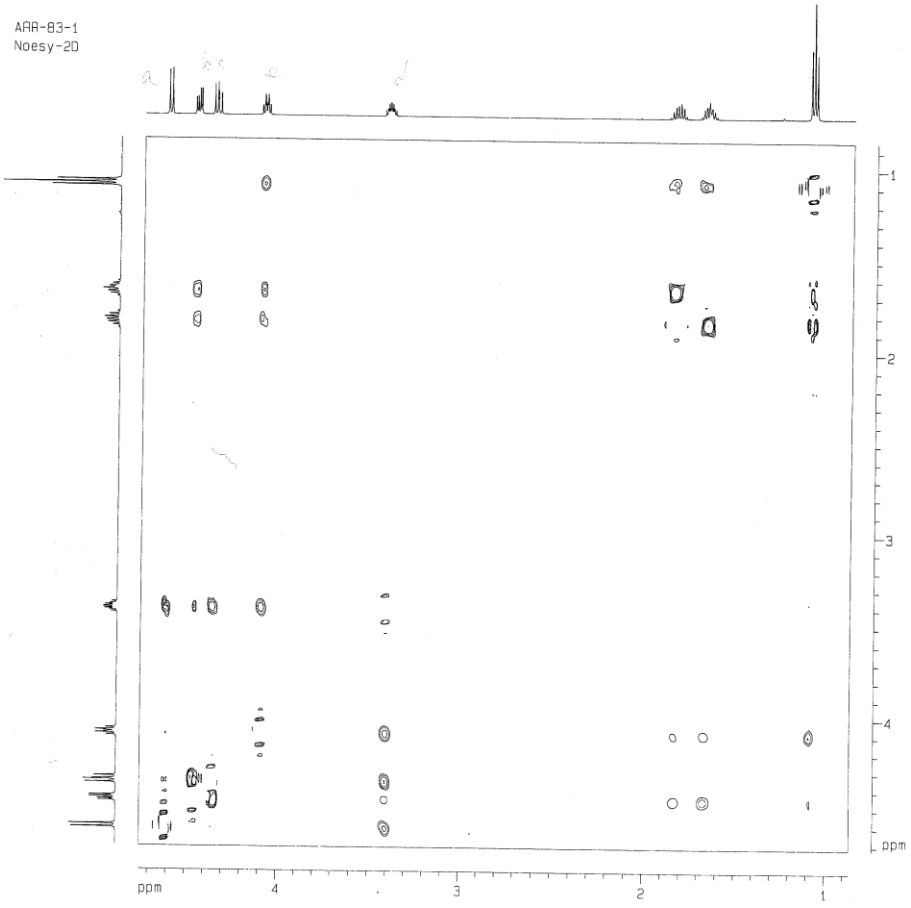

OH
EtO2C
ppm

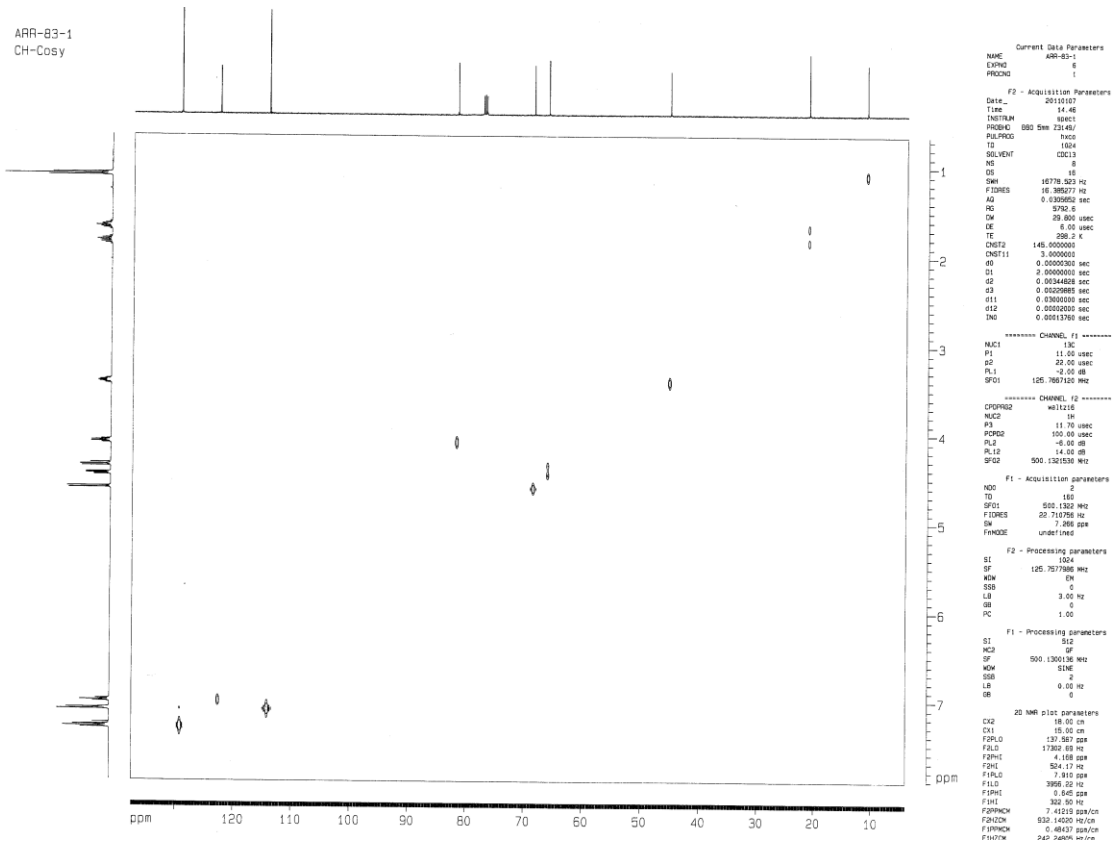

NHCBz
EtO2C


NHCBz
EtO2C


Current Data Parameters
NAME ARR-83-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110106
Time 17.43
INSTRUM av400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 11990.407 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 114
DW 41.700 usec
DE 6.00 usec
TE 294.8 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 13.60 usec
PL1 -4.00 dB
SFO1 400.1320007 MHz
F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 25.00 cm
CY 10.61 cm
F1P 10.000 ppm
F1 4001.30 Hz
F2P -0.500 ppm
F2 -200.07 Hz
PPMCM 0.42000 ppm/cm
HZCM 168.05461 Hz/cm
ppm
7.3220
7.3034
7.3004
7.2866
7.2820
7.2608
7.1135
7.1110
7.0916
7.0895
7.0251
7.0068
6.9885
4.6241
4.6032
4.4771
4.4657
4.4524
4.4409
4.3780
4.3578
4.3534
4.3331
4.1147
4.1001
4.0947
4.0853
4.0799
4.0652
3.4206
3.4148
3.4089
3.4059
3.4001
3.3943
1.8533
1.8370
1.8183
1.7992
1.7000
1.6852
1.6813
1.6660
1.6504
1.6471
1.1079
1.0893
1.0707
0.0001
Ph
N
O
H
H
O
O
Integral
1.9535
1.9835
0.9569
1.0000
1.0454
1.0379
1.0109
1.0167
1.0646
1.2310
3.1191
ppm


Current Data Parameters
NAME ARR-83-1-13c
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110106
Time 17.49
INSTRUM av400
PROBHD 5 mm QNP 1H/13
PULPROG zgpc
TD 32768
SOLVENT CDCl3
NS 75
DS 0
SWH 25125.629 Hz
FIDRES 0.766773 Hz
AQ 0.6521332 sec
RG 18390.4
DW 19.900 usec
DE 6.00 usec
TE 295.0 K
D1 2.50000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 6.50 usec
PL1 -3.00 dB
SFO1 100.6238364 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -4.00 dB
PL12 14.00 dB
SFO2 400.1320007 MHz
F2 - Processing parameters
SI 32768
SF 100.6127582 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 25.00 cm
CY 8.84 cm
F1P 200.000 ppm
F1 20122.55 Hz
F2P -5.000 ppm
F2 -503.06 Hz
PPMCM 8.20000 ppm/cm
HZCM 825.02460 Hz/cm
ppm
174.528
150.207
129.367
122.778
114.373
81.885
77.516
77.199
76.880
68.679
66.176
45.321
21.299
11.250
Ph
N
O
H
H
O
O
ppm





Current Data Parameters
NAME ARR-83-1
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110107
Time 14.46
INSTRUM spect
PROBHD BBO 5mm Z3145/
PULPROG hxco
TD 1024
SOLVENT CDCl3
NS 8
DS 16
SWH 16778.523 Hz
FIDRES 16.385277 Hz
AQ 0.0305852 sec
RG 5792.6
DW 29.800 usec
DE 6.00 usec
TE 298.2 K
CNST2 145.0000000
CNST11 3.0000000
d0 0.00000300 sec
D1 2.00000000 sec
d2 0.00344828 sec
d3 0.00229885 sec
d11 0.03000000 sec
d12 0.00002000 sec
IN0 0.00013760 sec

======== CHANNEL f1 ========
NUC1 13C
P1 11.00 usec
p2 22.00 usec
PL1 -2.00 dB
SFO1 125.7667120 MHz

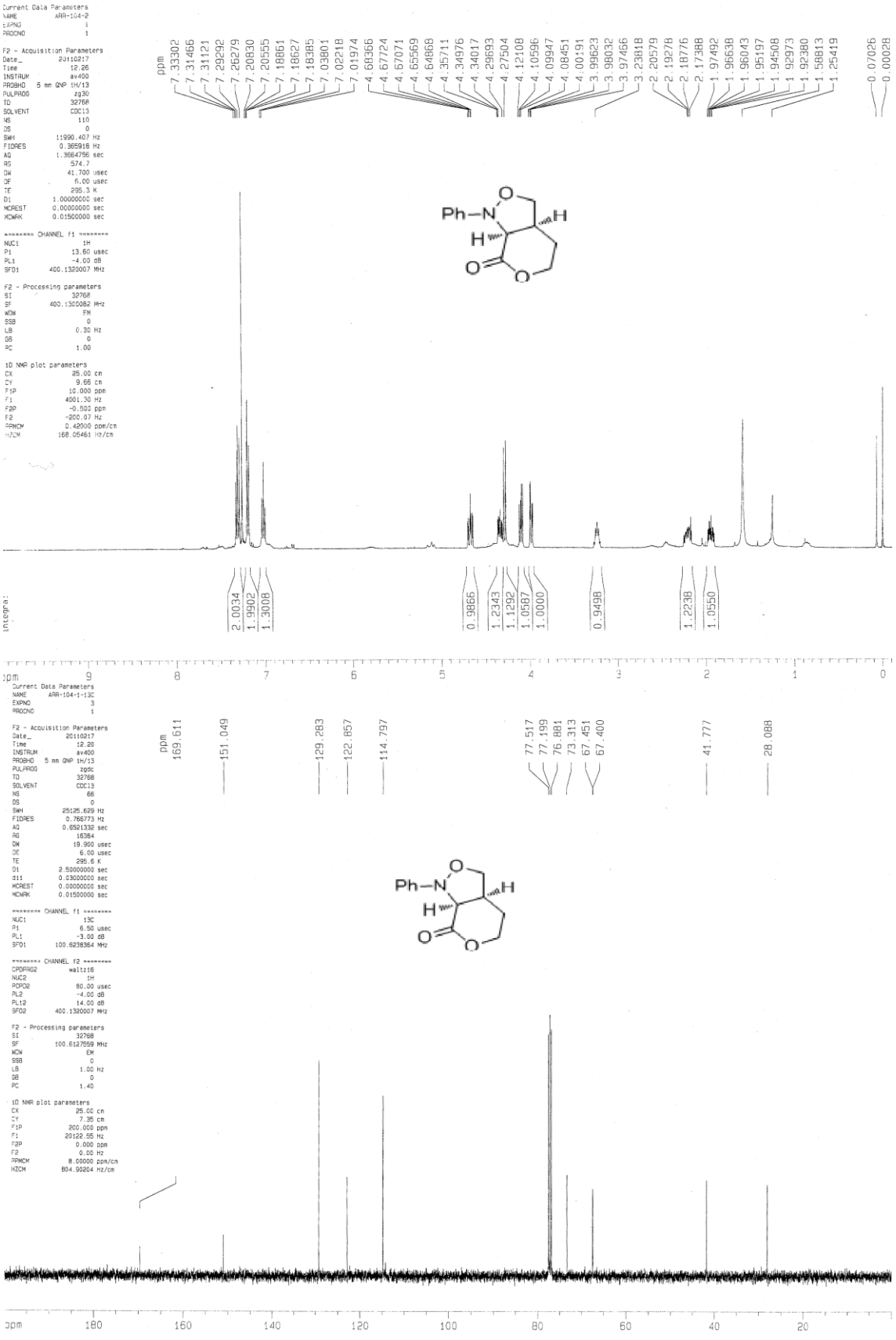
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
P3 11.70 usec
PCPD2 100.00 usec
PL2 -6.00 dB
PL12 14.00 dB
SFO2 500.1321530 MHz

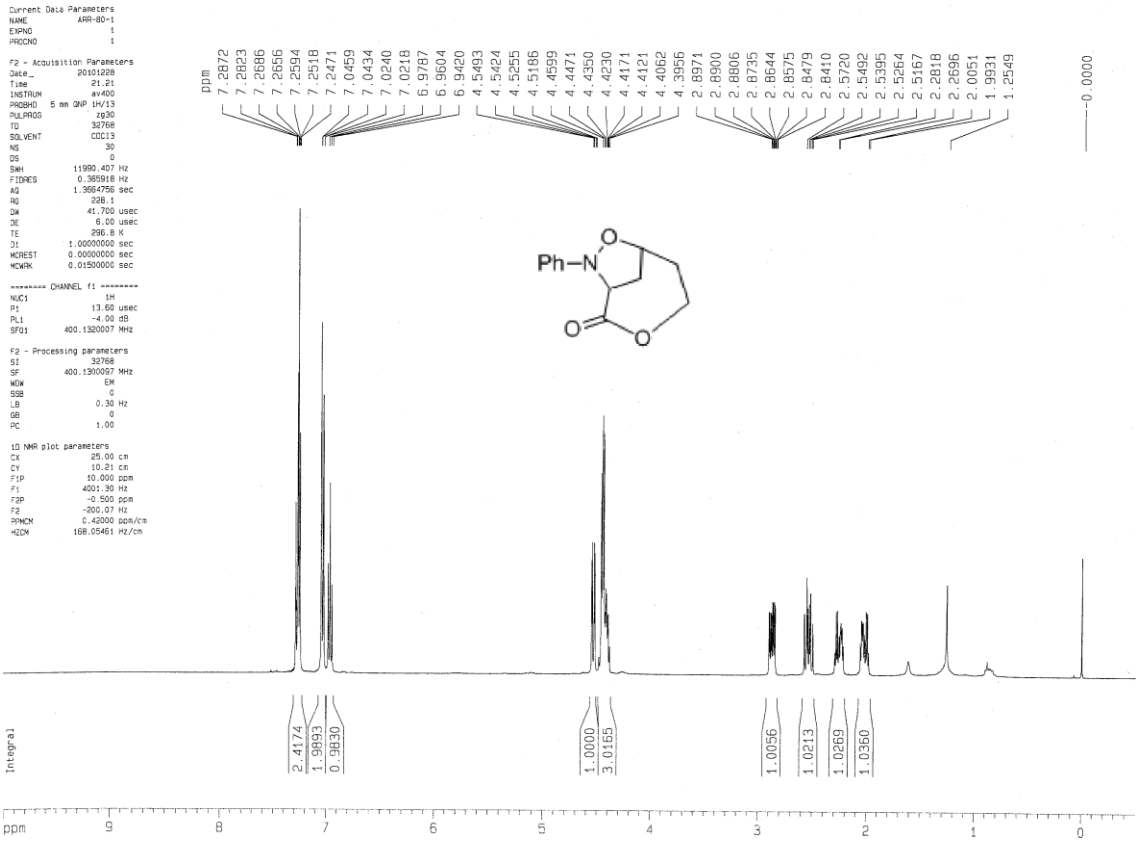
F1 - Acquisition parameters
NDO 2
TD 160
SFO1 500.1302 MHz
FIDRES 22.710756 Hz
SW 7.366 ppm
FnMODE undefined

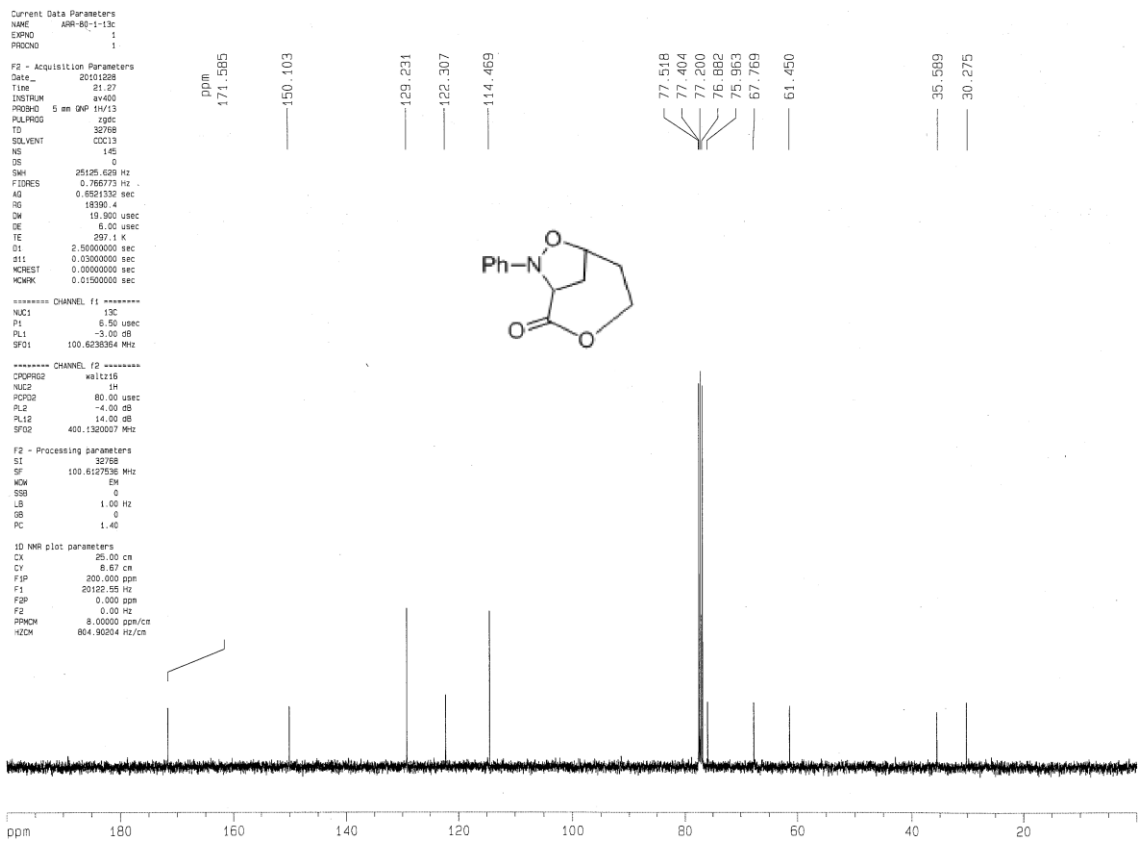
F2 - Processing parameters
SI 1024
SF 125.7577886 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00

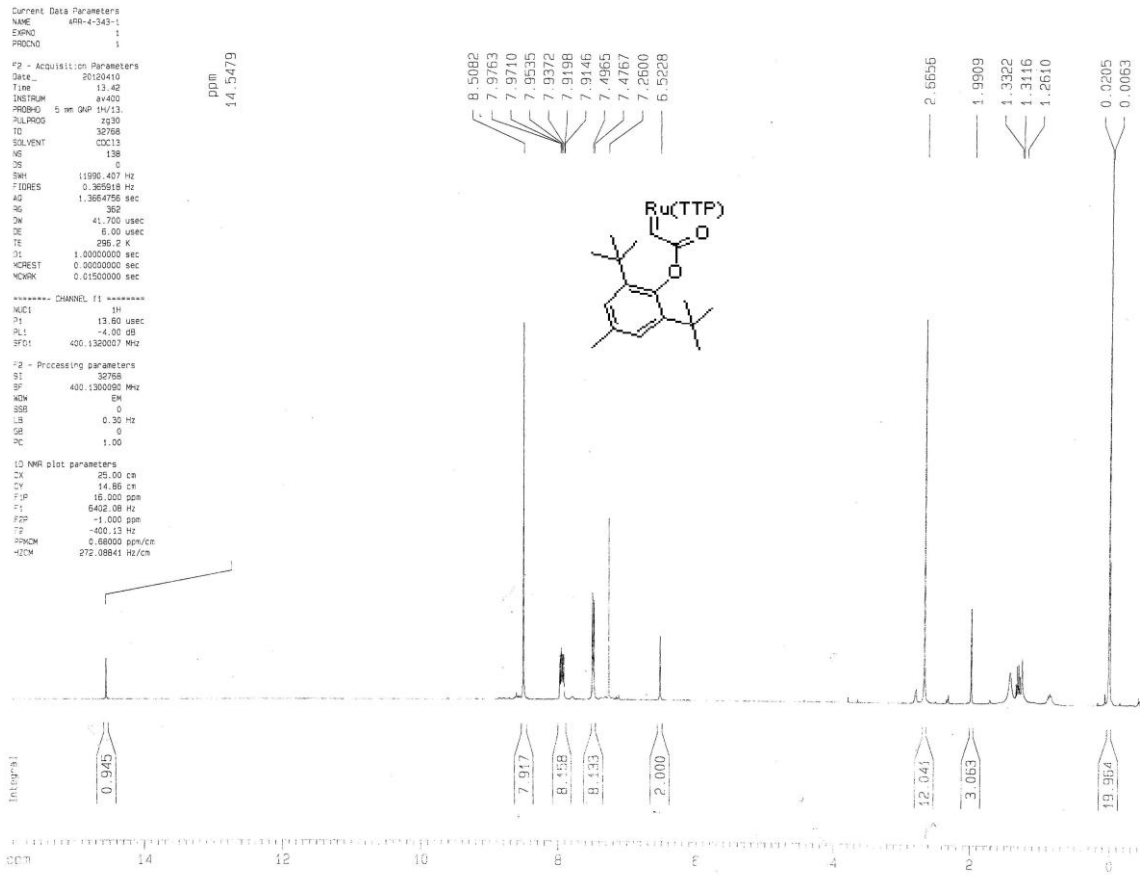
F1 - Processing parameters
SI 512
MC2 QF
SF 500.1300136 MHz
WDW SINE
SSB 2
LB 0.00 Hz
GB 0

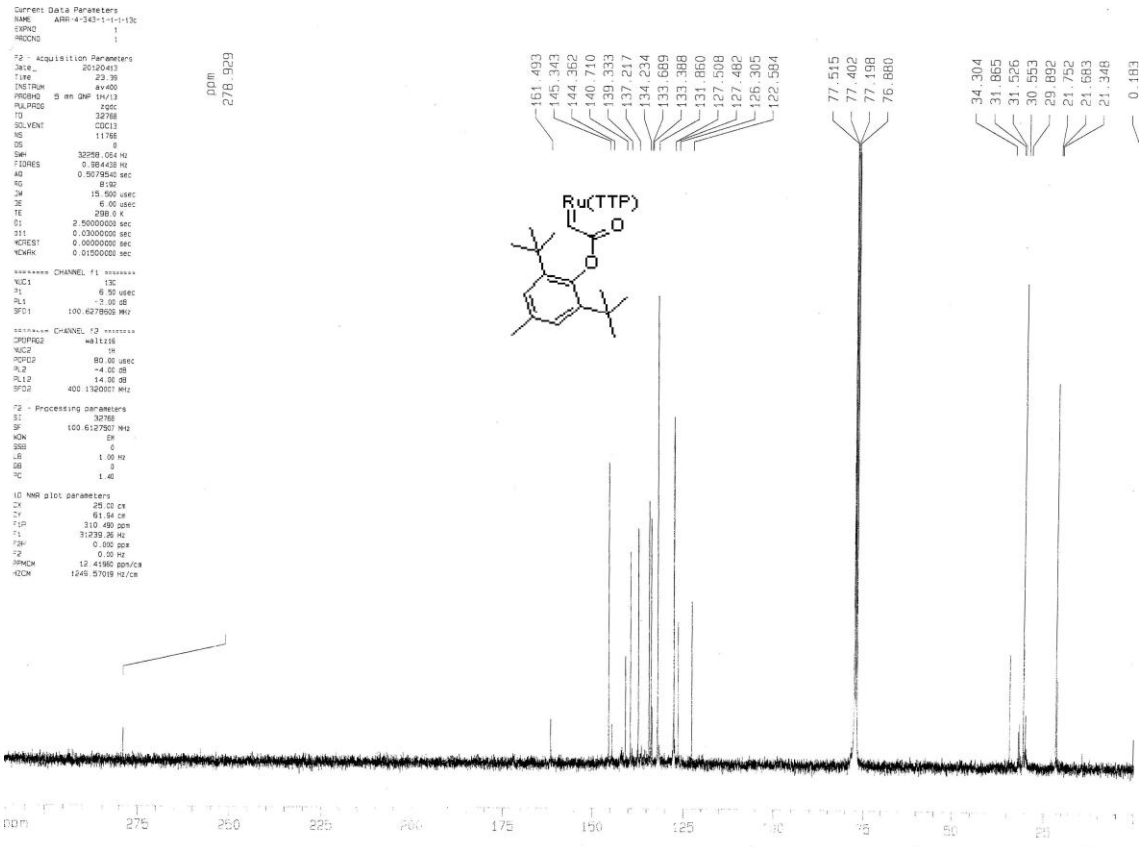
2D NMR plot parameters
CX2 18.00 cm
CX1 15.00 cm
F2PLO 137.567 ppm
F2LO 17302.69 Hz
F2PHI 4.168 ppm
F2HI 524.17 Hz
F1PLO 7.910 ppm
F1LO 3956.02 Hz
F1PHI 0.645 ppm
F1HI 322.90 Hz
F2PPMCM 7.41219 ppm/cm
F2HZCM 932.14020 Hz/cm
F1PPMCM 0.48437 ppm/cm
F1HZCM 242.24855 Hz/cm

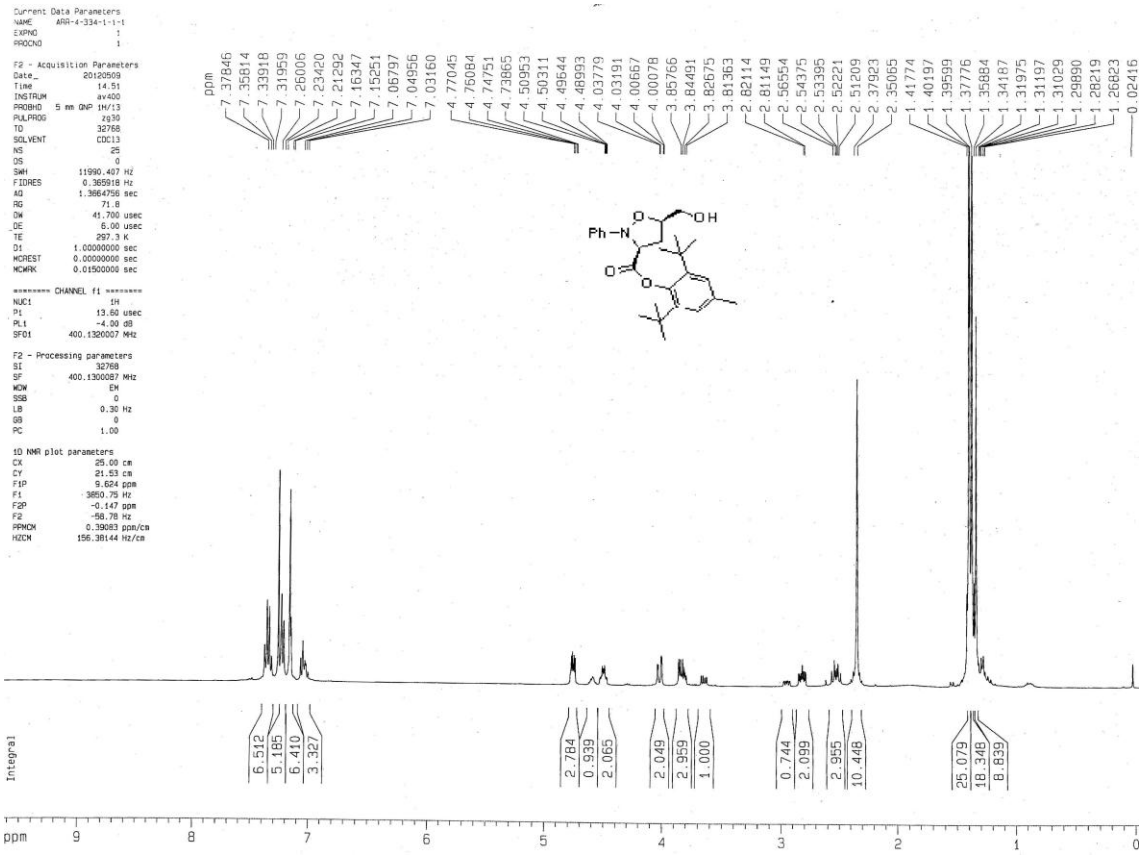


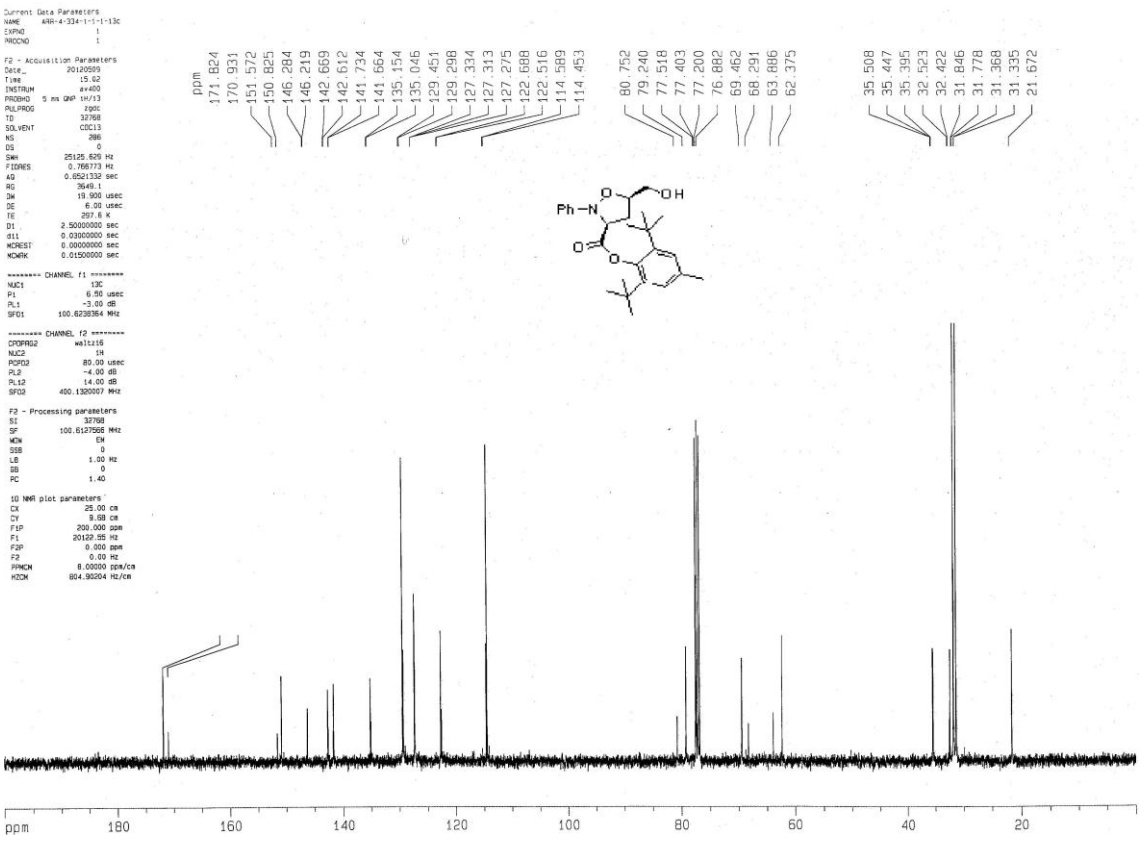

Current Data Parameters
NAME ARR-80-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20101228
Time 21.21
INSTRUM av400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 30
DS 0
SWH 11990.407 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 228.1
DW 41.700 usec
DE 6.00 usec
TE 296.8 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 13.60 usec
PL1 -4.00 dB
SFO1 400.1320007 MHz
F2 - Processing parameters
SI 32768
SF 400.1300097 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 25.00 cm
CY 10.21 cm
F1P 10.000 ppm
F1 4001.30 Hz
F2P -0.500 ppm
F2 -200.07 Hz
PPMCM 0.42000 ppm/cm
HZCM 168.05461 Hz/cm
ppm
7.2872
7.2823
7.2686
7.2656
7.2594
7.2518
7.2471
7.0459
7.0434
7.0240
7.0218
6.9787
6.9604
6.9420
4.5493
4.5424
4.5255
4.5186
4.4599
4.4471
4.4350
4.4230
4.4171
4.4121
4.4062
4.3956
2.8971
2.8900
2.8806
2.8735
2.8644
2.8575
2.8479
2.8410
2.5720
2.5492
2.5395
2.5264
2.5167
2.2818
2.2696
2.0051
1.9931
1.2549
0.0000
Ph–N
O
O
O
Integral
2.4174
1.9893
0.9830
1.0000
3.0165
1.0056
1.0213
1.0269
1.0360
ppm
9
8
7
6
5
4
3
2
1
0


Current Data Parameters
NAME ARR-80-1-13c
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20101228
Time 21.27
INSTRUM av400
PROBHD 5 mm QNP 1H/13
PULPROG zgdc
TD 32768
SOLVENT CDCl3
NS 145
DS 0
SWH 25125.629 Hz
FIDRES 0.766773 Hz
AQ 0.6521332 sec
RG 18390.4
DW 19.900 usec
DE 6.00 usec
TE 297.1 K
D1 2.50000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 6.50 usec
PL1 -3.00 dB
SFO1 100.6238364 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -4.00 dB
PL12 14.00 dB
SFO2 400.1320007 MHz
F2 - Processing parameters
SI 32768
SF 100.6127536 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 25.00 cm
CY 8.67 cm
F1P 200.000 ppm
F1 20122.55 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 8.00000 ppm/cm
HZCM 804.90204 Hz/cm
ppm
171.585
150.103
129.231
122.307
114.469
77.518
77.404
77.200
76.882
75.963
67.769
61.450
35.589
30.275
Ph–N
O
O
O
ppm
180
160
140
120
100
80
60
40
20


Ru(TTP)
O
O
8.5082
7.9763
7.9710
7.9535
7.9372
7.9198
7.9146
7.4965
7.4767
7.2600
6.5228
2.6656
1.9909
1.3322
1.3116
1.2610
0.0205
0.0063
0.945
7.917
8.158
8.133
2.000
12.041
3.063
19.964


Ru(TTP)
O
O
161.493
145.343
144.362
140.710
139.333
137.217
134.234
133.689
133.388
131.860
127.508
127.482
126.305
122.584
77.515
77.402
77.198
76.880
34.304
31.865
31.526
30.553
29.892
21.752
21.683
21.348
0.183


Current Data Parameters
NAME ARR-4-334-1-1-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120509
Time 14.51
INSTRUM av400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 25
DS 0
SWH 11990.407 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 71.8
DW 41.700 usec
DE 6.00 usec
TE 297.3 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 13.60 usec
PL1 -4.00 dB
SFO1 400.1320007 MHz
F2 - Processing parameters
SI 32768
SF 400.1300087 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 25.00 cm
CY 21.53 cm
F1P 9.624 ppm
F1 3850.75 Hz
F2P -0.147 ppm
F2 -58.78 Hz
PPMCM 0.39083 ppm/cm
HZCM 156.38144 Hz/cm
ppm
7.37846
7.35814
7.33918
7.31959
7.26006
7.23420
7.21292
7.16347
7.15251
7.05797
7.04956
7.03160
4.77045
4.76084
4.74751
4.73865
4.50953
4.50311
4.49644
4.48993
4.03779
4.03191
4.00667
4.00078
3.85766
3.84491
3.82675
3.81363
2.82114
2.81149
2.56554
2.54375
2.53395
2.52221
2.51209
2.37923
2.35065
1.41774
1.40197
1.39599
1.37776
1.35884
1.34187
1.31975
1.31197
1.31029
1.29890
1.28219
1.26823
0.02416
Ph–N
OH
O
Integral
6.512
5.185
6.410
3.327
2.784
0.939
2.065
2.049
2.959
1.000
0.744
2.099
2.955
10.448
25.079
18.348
8.839
ppm


Current Data Parameters
NAME ARR-4-334-1-1-1-13C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120509
Time 15.62
INSTRUM av400
PROBHD 5 mm QNP 1H/13
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 286
DS 0
SWH 25125.629 Hz
FIDRES 0.766773 Hz
AQ 0.6521332 sec
RG 3649.1
DW 19.900 usec
DE 6.00 usec
TE 297.6 K
D1 2.50000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 6.50 usec
PL1 -3.00 dB
SFO1 100.6238364 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -4.00 dB
PL12 14.00 dB
SFO2 400.1320007 MHz
F2 - Processing parameters
SI 32768
SF 100.6127568 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 25.00 cm
CY 9.68 cm
F1P 200.000 ppm
F1 20122.55 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 8.00000 ppm/cm
HZCM 804.90204 Hz/cm
ppm
171.824
170.931
151.572
150.825
146.284
146.219
142.669
142.612
141.734
141.664
135.154
135.046
129.451
129.298
127.334
127.313
127.275
122.688
122.516
114.589
114.453
80.752
79.240
77.518
77.403
77.200
76.882
69.462
68.291
63.886
62.375
35.508
35.447
35.395
32.523
32.422
31.846
31.778
31.368
31.335
21.672
Ph–N
OH
O
ppm

[Ru(TTP)(CO)(MeOH)]-catalyzed reaction of EDA with nitrosobenzene

To nitrosobenzene (2.2 mmol) and [Ru(TTP)(CO)(MeOH)] (0.02 mmol) in CH_2Cl_2 (10 mL) was added EDA (2.0 mmol) in CH_2Cl_2 (10 mL) over 3 h via a syringe pump at room temperature. After addition, the resultant solution was stirred for an additional 0.5 h. The ^1H NMR of reaction mixture indicated that the intermediate nitrone was formed.