10.1071/CH15208_AC

Australian Journal of Chemistry 2016, 69(6), 672-682

SUPPLEMENTARY MATERIAL

Study on Pyrrole 4–Pyrazoline Derivatives: Experimental and Quantum Chemical Approaches

Ram N. Singh,[A,B] *Poonam Rawat,*[A] *and Vikas Baboo*[A]

[A]Department of Chemistry, University of Lucknow, Lucknow – 226006, India.

[B]Corresponding author. Email: rnsvk.chemistry@gmail.com

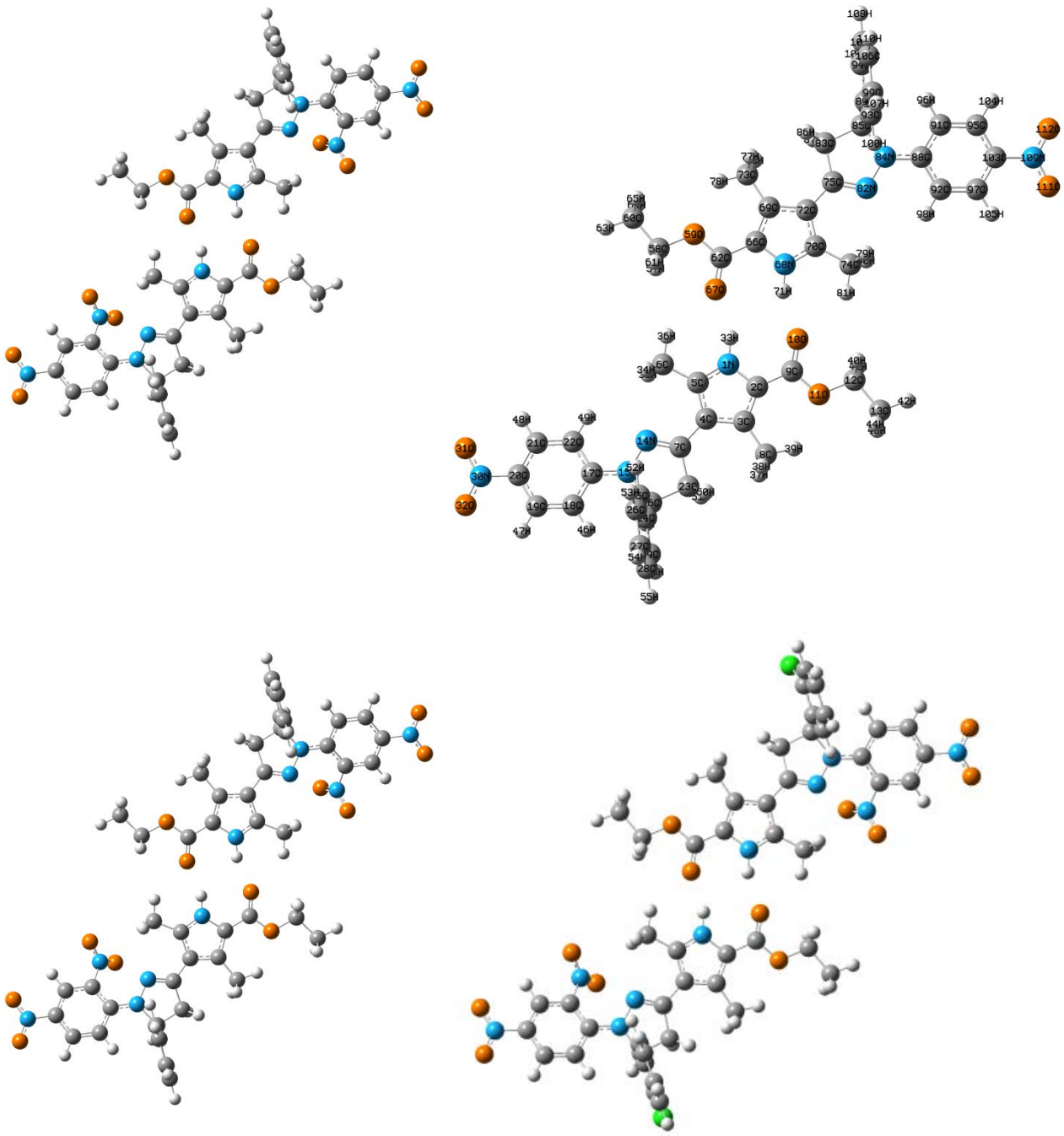
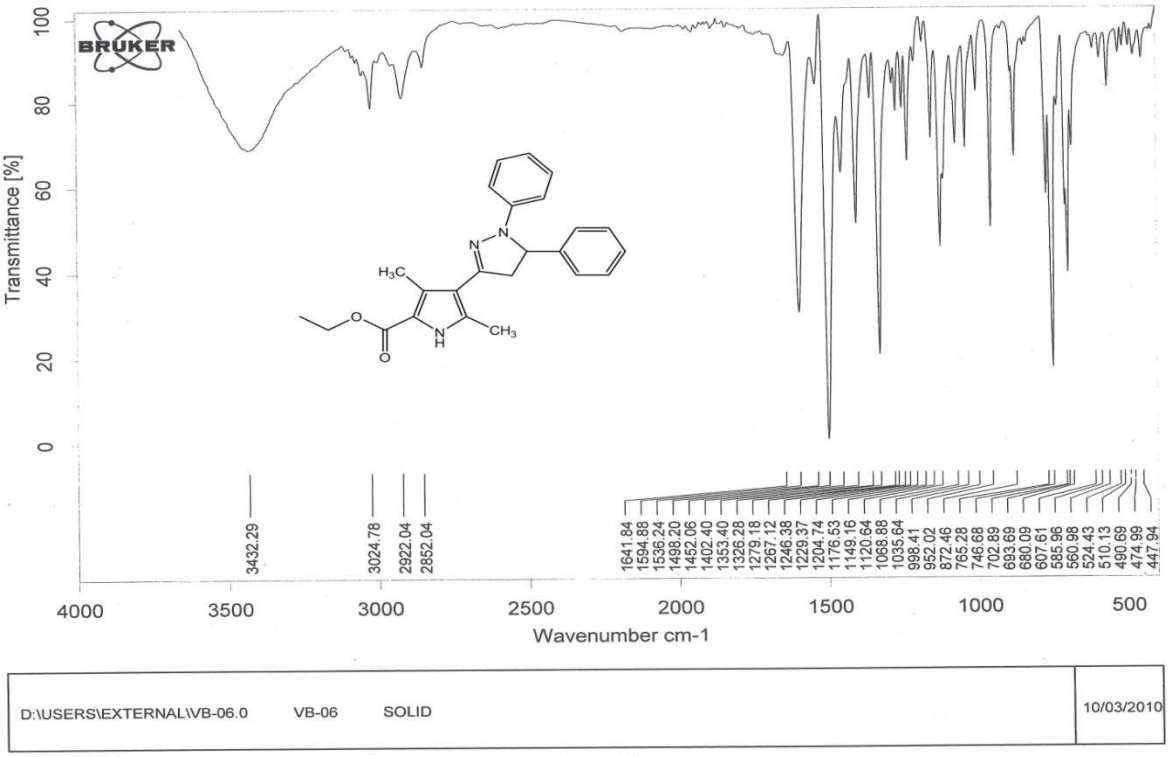
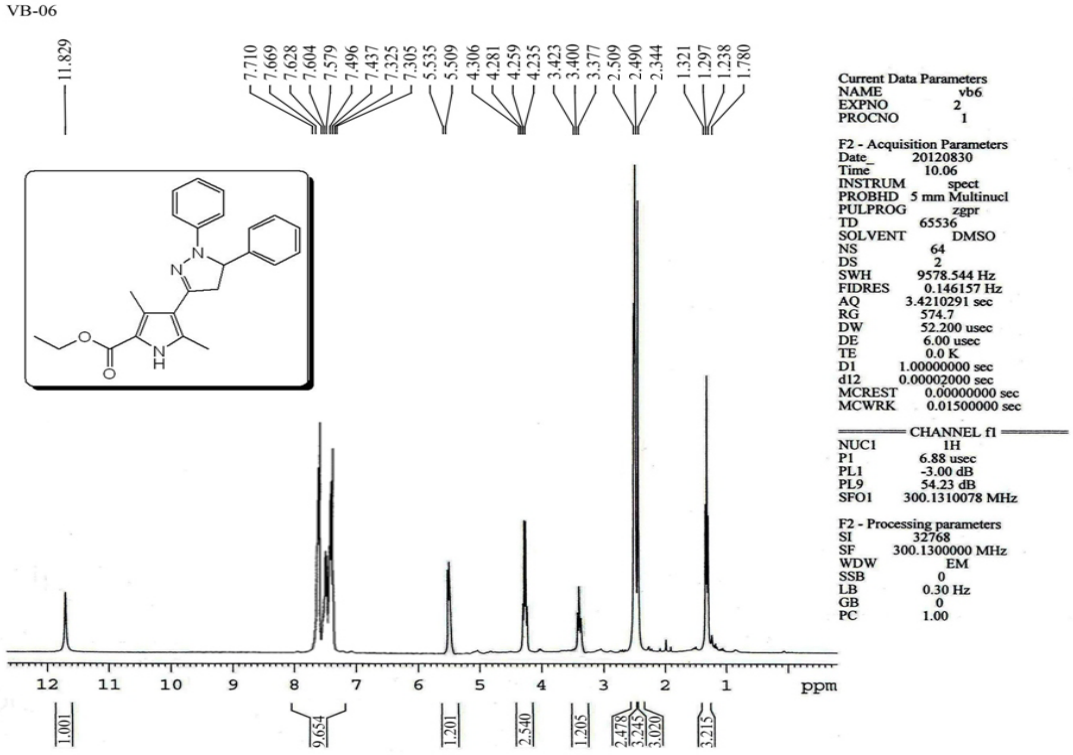


Figure S1. The optimized geometry of dimer (4A-4D

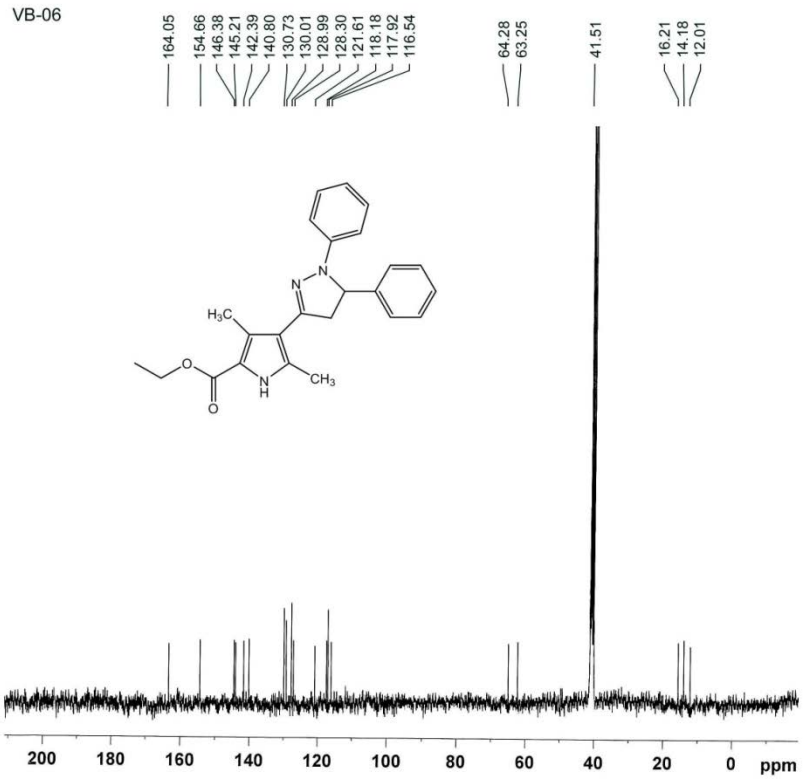

BRUKER
Transmittance [%]
100
80
60
40
20
0
3432.29
3024.78
2922.04
2852.04
1641.84
1594.88
1536.24
1498.20
1452.06
1402.40
1353.40
1326.28
1279.18
1267.12
1246.38
1229.37
1204.74
1176.53
1149.16
1120.64
1068.88
1035.64
998.41
952.02
872.46
765.28
746.68
702.89
693.69
680.09
607.61
585.96
560.98
524.43
510.13
490.69
474.99
447.94
4000
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1
D:\USERS\EXTERNAL\VB-06.0
VB-06
SOLID
10/03/2010

Page 1/1

4A

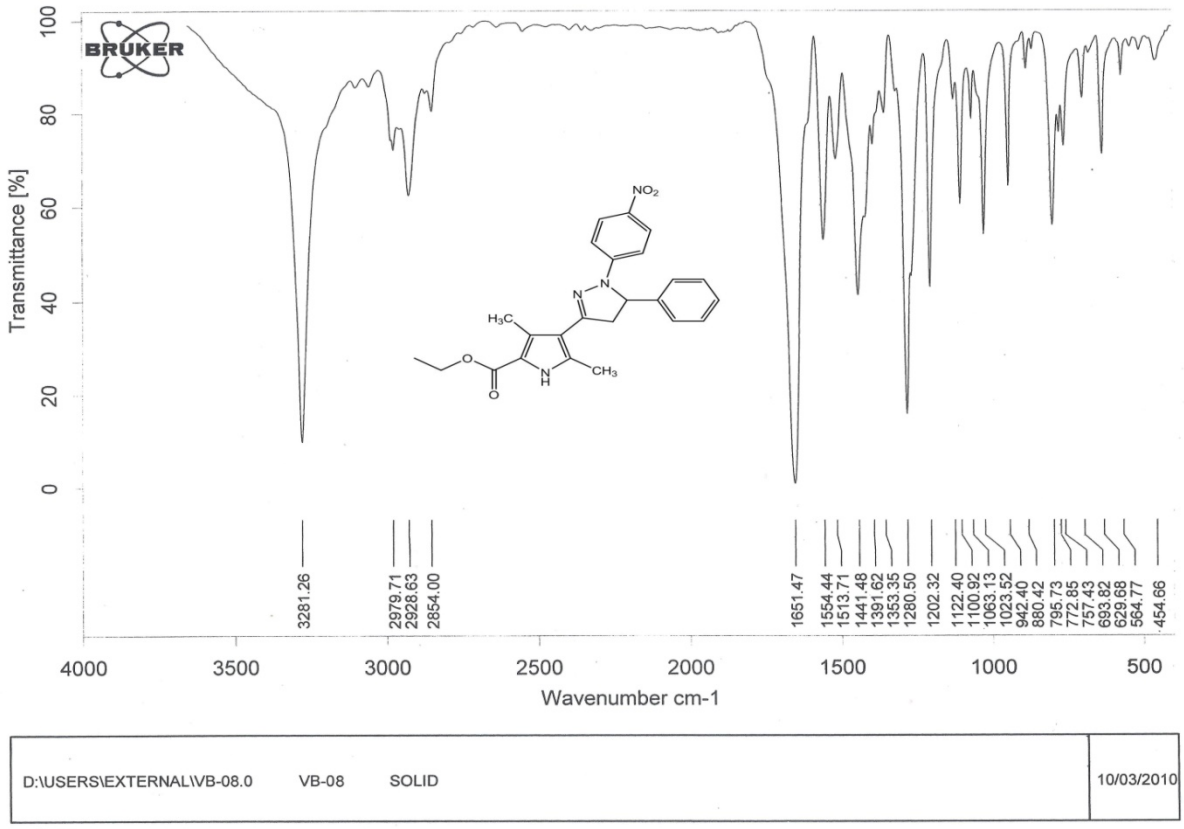

VB-06
11.829
7.710
7.669
7.628
7.604
7.579
7.496
7.437
7.325
7.305
5.535
5.509
4.306
4.281
4.259
4.235
3.423
3.400
3.377
2.509
2.490
2.344
1.321
1.297
1.238
1.780
Current Data Parameters
NAME vb6
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120830
Time 10.06
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpr
TD 65536
SOLVENT DMSO
NS 64
DS 2
SWH 9578.544 Hz
FIDRES 0.146157 Hz
AQ 3.4210291 sec
RG 574.7
DW 52.200 usec
DE 6.00 usec
TE 0.0 K
D1 1.00000000 sec
d12 0.00002000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
CHANNEL f1
NUC1 1H
P1 6.88 usec
PL1 -3.00 dB
PL9 54.23 dB
SFO1 300.1310078 MHz
F2 - Processing parameters
SI 32768
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
12
11
10
9
8
7
6
5
4
3
2
1
ppm
1.001
9.654
1.201
2.540
1.205
2.478
3.245
3.020
3.215

4A

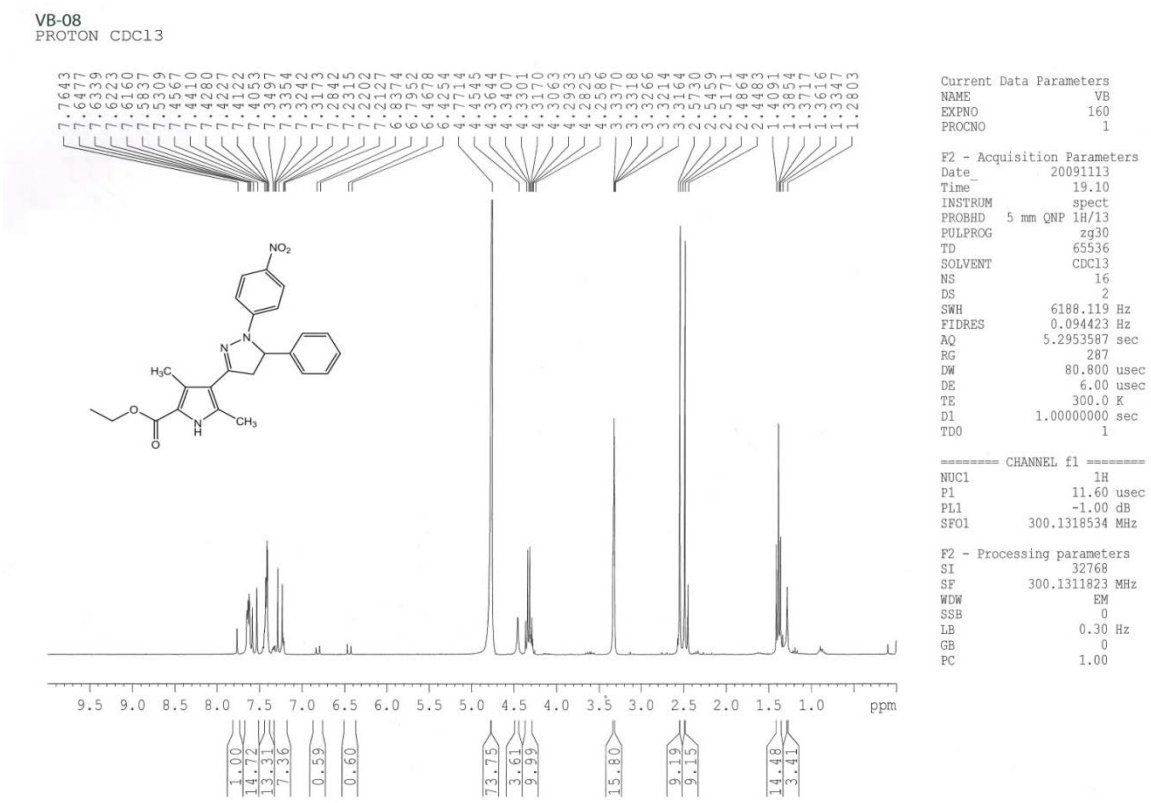



```
Current Data Parameters
NAME                  SAIF.06
EXPNO                     100
PROCNO                      1

F2 - Acquisition Parameters
Date_                20120525
Time                    16.20
INSTRUM                  spect
PROBHD    5 mm QNP 1H/13
PULPROG                zgpg30
TD                      65536
SOLVENT                  DMSO
NS                        4096
DS                           4
SWH                18028.846 Hz
FIDRES                 0.275098 Hz
AQ                     1.8175818 sec
RG                          11.3
DW                        27.733 usec
DE                         6.00 usec
TE                        673.2 K
D1                    2.00000000 sec
d11                   0.03000000 sec
DELTA                 1.89999998 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                       13C
P1                        8.70 usec
PL1                      -3.00 dB
SFO1                75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                    80.00 usec
PL2                      -1.00 dB
PL12                     17.00 dB
PL13                     21.00 dB
SFO2               300.1312005 MHz

F2 - Processing parameters
SI                        32768
SF                 75.4677324 MHz
WDW                          EM
SSB                           0
LB                         3.00 Hz
GB                            0
PC                         1.40
```

4A


BRUKER
Transmittance [%]
100
80
60
40
20
0
4000
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1
3281.26
2979.71
2928.63
2854.00
1651.47
1554.44
1513.71
1441.48
1391.62
1353.35
1280.50
1202.32
1122.40
1100.92
1063.13
1023.52
942.40
880.42
795.73
772.85
757.43
693.82
629.68
564.77
454.66
NO2
H3C
CH3
N
H
O
D:\USERS\EXTERNAL\VB-08.0
VB-08
SOLID
10/03/2010
Page 1/1

4B



Current Data Parameters

NAME	VB
EXPNO	160
PROCNO	1

F2 - Acquisition Parameters

Date_	20091113
Time	19.10
INSTRUM	spect
PROBHD	5 mm QNP 1H/13
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	6188.119 Hz
FIDRES	0.094423 Hz
AQ	5.2953587 sec
RG	287
DW	80.800 usec
DE	6.00 usec
TE	300.0 K
D1	1.00000000 sec
TD0	1

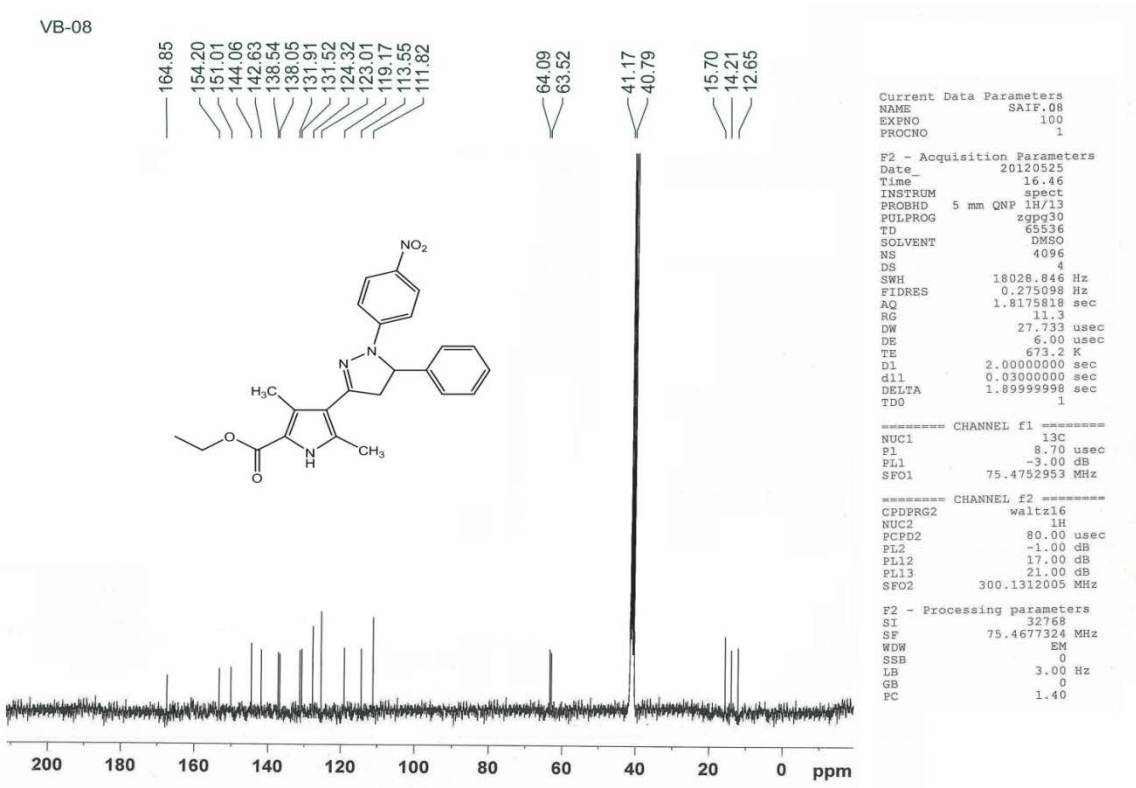
======== CHANNEL f1 ========

NUC1	1H
P1	11.60 usec
PL1	-1.00 dB
SFO1	300.1318534 MHz

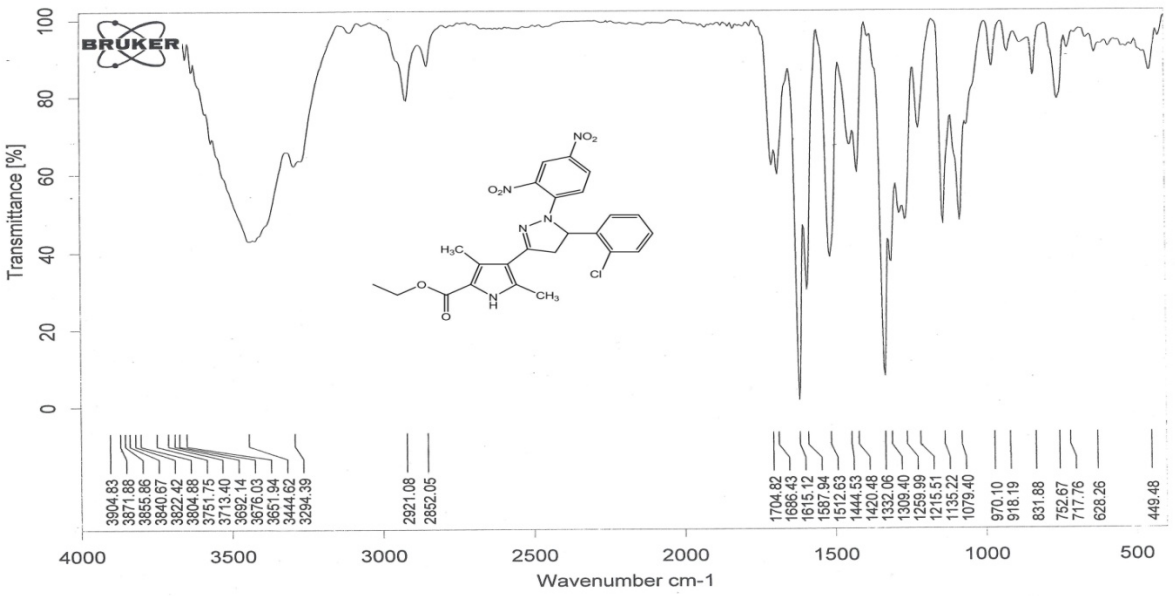
F2 - Processing parameters

SI	32768
SF	300.1311823 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

4B

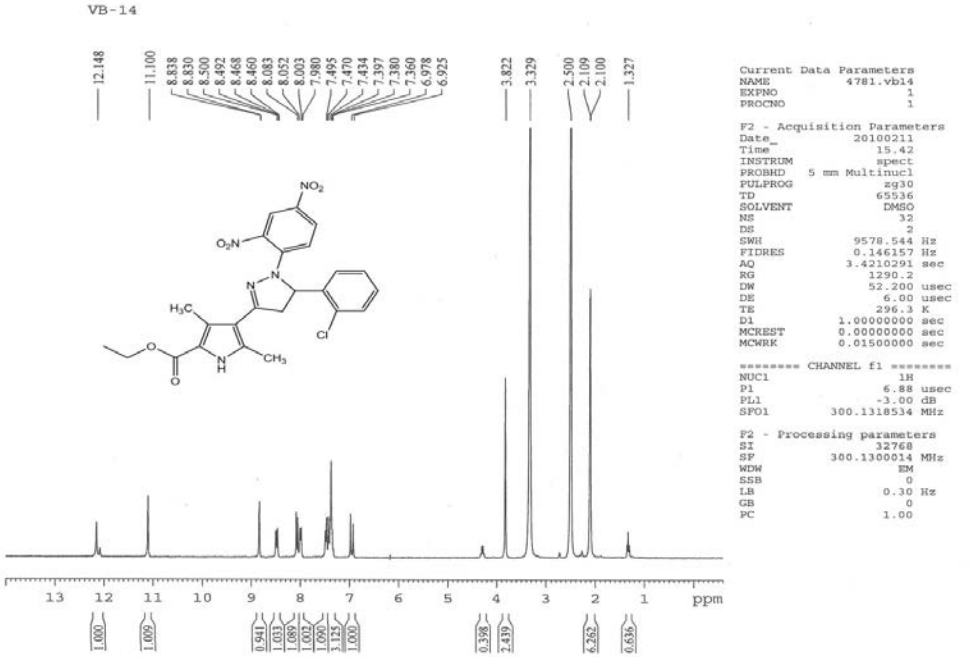

VB-08
164.85
154.20
151.01
144.06
142.63
138.54
138.05
131.91
131.52
124.32
123.01
119.17
113.55
111.82
64.09
63.52
41.17
40.79
15.70
14.21
12.65
NO2
H3C
CH3
N
H
O
200
180
160
140
120
100
80
60
40
20
0
ppm
Current Data Parameters
NAME SAIF.08
EXPNO 100
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120525
Time 16.46
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 4096
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175818 sec
RG 11.3
DW 27.733 usec
DE 6.00 usec
TE 673.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.70 usec
PL1 -3.00 dB
SFO1 75.4752953 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -1.00 dB
PL12 17.00 dB
PL13 21.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677324 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40

4B

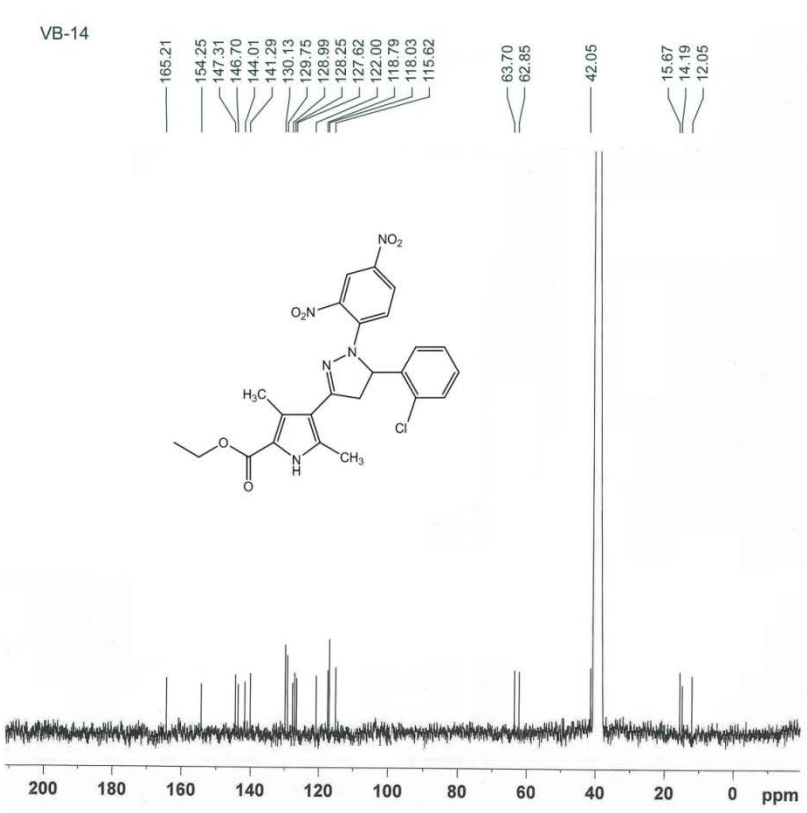

BRUKER
Transmittance [%]
100
80
60
40
20
0
3904.83
3871.88
3855.86
3840.67
3822.42
3804.88
3751.75
3713.40
3692.14
3676.03
3651.94
3444.62
3294.39
2921.08
2852.05
1704.82
1686.43
1615.12
1587.94
1512.63
1444.53
1420.48
1332.06
1309.40
1259.99
1215.51
1135.22
1079.40
970.10
918.19
831.88
752.67
717.76
628.26
449.48
4000
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1
D:\USERS\EXTERNAL\VB-14.0
VB-14
SOLID
02/02/2010

Page 1/1

4C

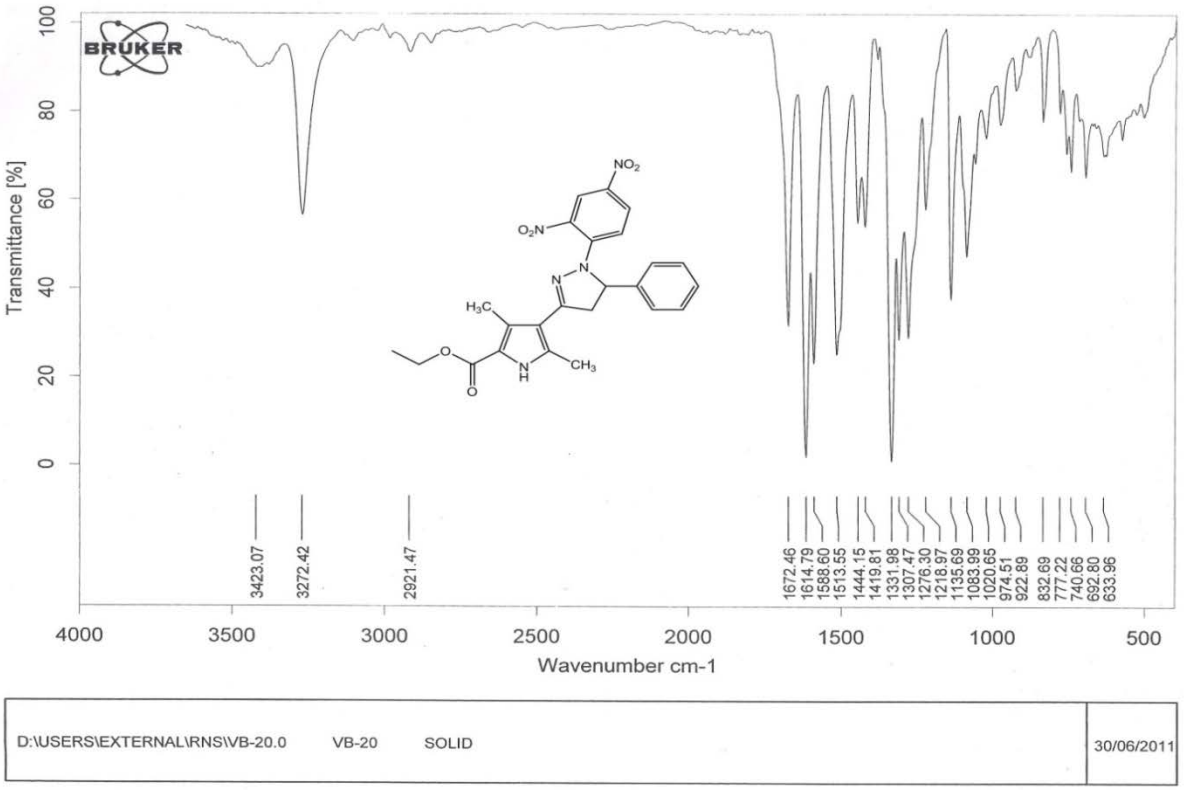

VB-14
12.148
11.100
8.838
8.830
8.500
8.492
8.468
8.460
8.083
8.052
8.003
7.980
7.495
7.470
7.434
7.397
7.380
7.360
6.978
6.925
3.822
3.329
2.500
2.109
2.100
1.327
NO2
O2N
N
N
H3C
Cl
O
O
CH3
H
13 12 11 10 9 8 7 6 5 4 3 2 1 ppm
1.000
1.009
0.941
1.033
1.087
1.003
1.090
3.125
1.000
0.398
2.439
6.262
0.636
Current Data Parameters
NAME 4781.vb14
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100211
Time 15.42
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 9578.544 Hz
FIDRES 0.146157 Hz
AQ 3.4210291 sec
RG 1290.2
DW 52.200 usec
DE 6.00 usec
TE 296.3 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 6.88 usec
PL1 -3.00 dB
SFO1 300.1318534 MHz
F2 - Processing parameters
SI 32768
SF 300.1300014 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

4c




```
Current Data Parameters
NAME                  SAIF.14
EXPNO                     100
PROCNO                      1

F2 - Acquisition Parameters
Date_                20120528
Time                    13.17
INSTRUM                 spect
PROBHD   5 mm QNP 1H/13
PULPROG                 zgpg30
TD                       65536
SOLVENT                   DMSO
NS                        4096
DS                           4
SWH                  18028.846 Hz
FIDRES                0.275098 Hz
AQ                    1.8175818 sec
RG                         11.3
DW                       27.733 usec
DE                         6.00 usec
TE                        673.2 K
D1                   2.00000000 sec
d11                  0.03000000 sec
DELTA                1.89999998 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                       13C
P1                        8.70 usec
PL1                      -3.00 dB
SFO1                75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                        1H
PCPD2                     80.00 usec
PL2                       -1.00 dB
PL12                      17.00 dB
PL13                      21.00 dB
SFO2                300.1312005 MHz

F2 - Processing parameters
SI                         32768
SF                  75.4677324 MHz
WDW                           EM
SSB                            0
LB                          3.00 Hz
GB                             0
PC                          1.40
```

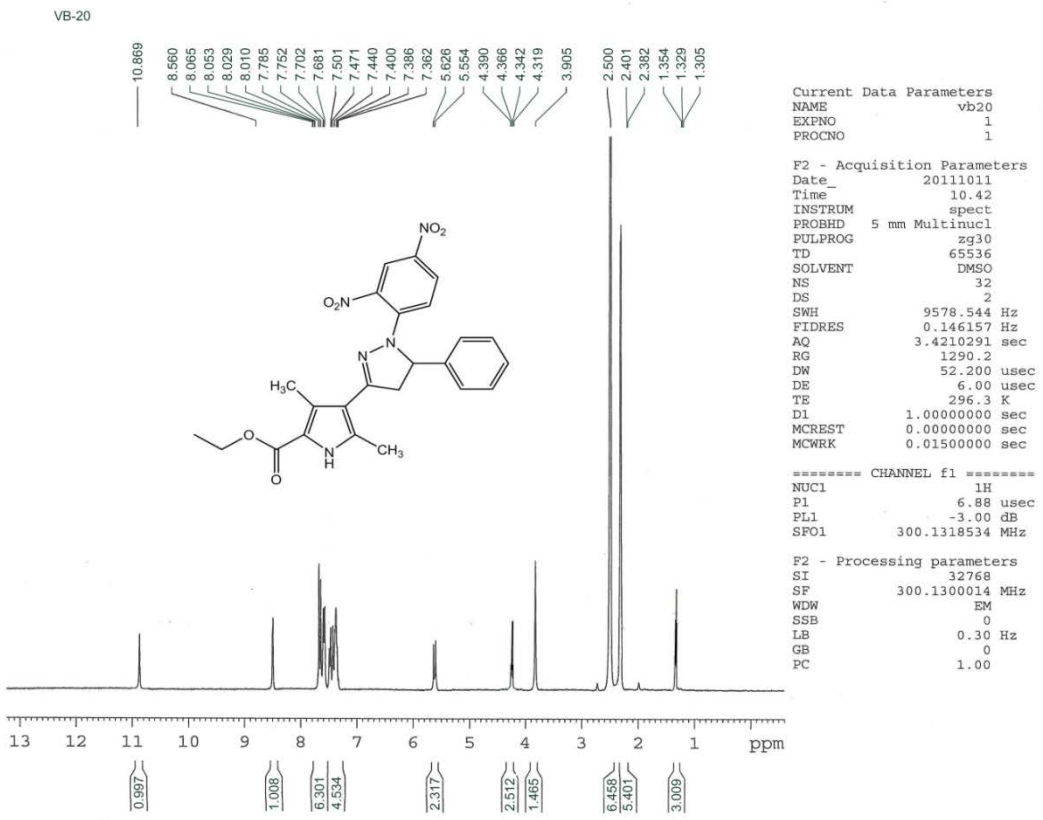
4C



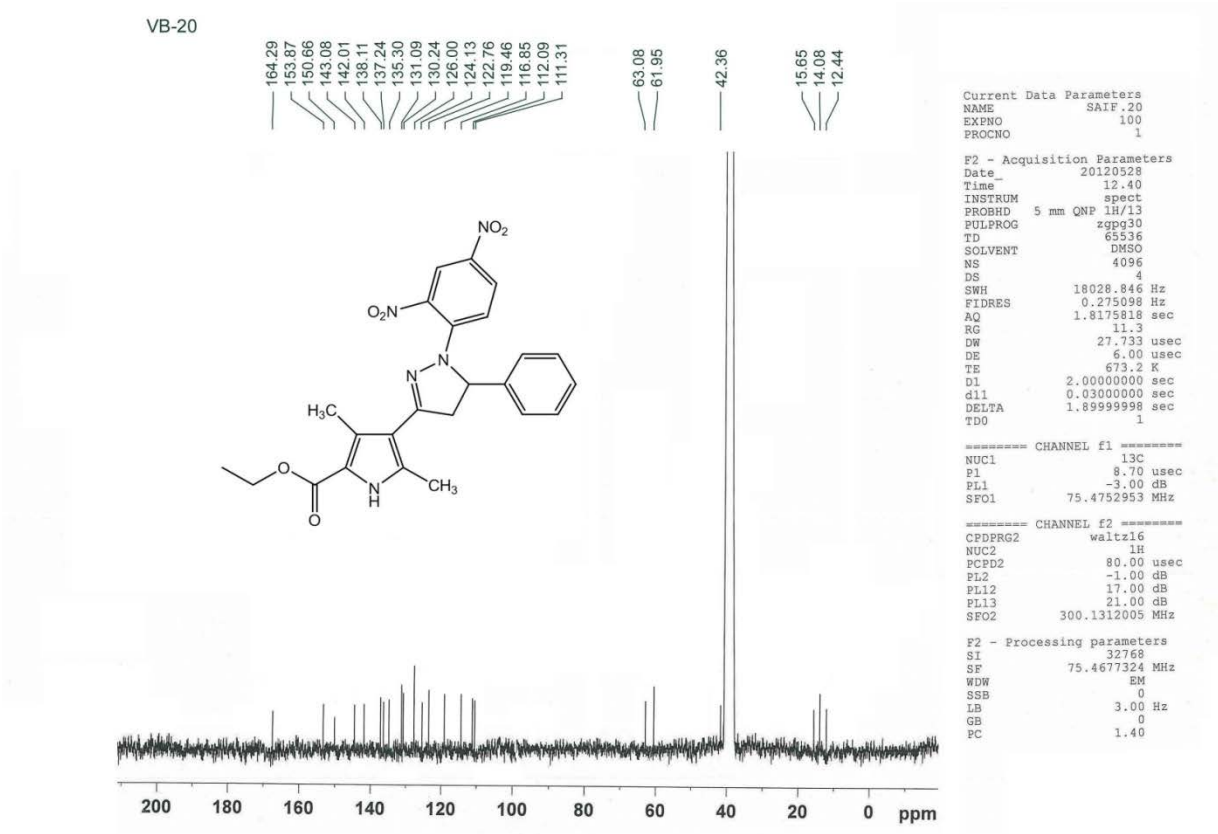
D:\USERS\EXTERNAL\RNS\VB-20.0	VB-20	SOLID	30/06/2011

Page 1/1

4D


VB-20
10.869
8.560
8.065
8.053
8.029
8.010
7.785
7.752
7.702
7.681
7.501
7.471
7.440
7.400
7.386
7.362
5.626
5.554
4.390
4.366
4.342
4.319
3.905
2.500
2.401
2.382
1.354
1.329
1.305
NO2
O2N
N
N
H3C
O
O
N
H
CH3
13
12
11
10
9
8
7
6
5
4
3
2
1
ppm
0.997
1.008
6.301
4.534
2.317
2.512
1.465
6.458
5.401
3.009
Current Data Parameters
NAME vb20
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20111011
Time 10.42
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 9578.544 Hz
FIDRES 0.146157 Hz
AQ 3.4210291 sec
RG 1290.2
DW 52.200 usec
DE 6.00 usec
TE 296.3 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 6.88 usec
PL1 -3.00 dB
SFO1 300.1318534 MHz
F2 - Processing parameters
SI 32768
SF 300.1300014 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

4D



4D

Figure S2. FT-IR, 1H and 13C NMR spectra of compounds 3A-4D

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-3.205699	-1.877442	0.706098
2	6	0	-3.701437	-0.690453	0.200918
3	6	0	-2.614246	0.085240	-0.200800
4	6	0	-1.436564	-0.684601	0.083514
5	6	0	-1.855898	-1.904799	0.650382
6	6	0	-1.076861	-3.081644	1.134930
7	6	0	-0.045485	-0.325593	-0.150404
8	6	0	-2.694702	1.452176	-0.819524
9	6	0	-5.153361	-0.557976	0.218692
10	8	0	-5.887783	-1.437038	0.651135
11	8	0	-5.615016	0.611725	-0.280042
12	6	0	-7.052755	0.767995	-0.270771
13	6	0	-7.366320	2.138094	-0.839625
14	7	0	0.924905	-1.142929	0.109857
15	7	0	2.139845	-0.535780	-0.139449
16	6	0	1.986240	0.802130	-0.748408
17	6	0	3.267072	-1.345177	-0.324085
18	6	0	4.462045	-0.804182	-0.833693
19	6	0	5.585179	-1.614565	-0.996405
20	6	0	5.551285	-2.966529	-0.658851
21	6	0	4.365174	-3.501831	-0.149490
22	6	0	3.233509	-2.711171	0.018684
23	6	0	0.449599	1.015574	-0.664595
24	6	0	2.775347	1.895307	-0.044257
25	6	0	2.956938	1.877841	1.343803
26	6	0	3.629015	2.920343	1.981126
27	6	0	4.125905	3.995187	1.240741
28	6	0	3.951131	4.018532	-0.143292
29	6	0	3.281469	2.972760	-0.780431
30	1	0	-3.818714	-2.597212	1.062524
31	1	0	-0.332412	-2.779126	1.876847
32	1	0	-0.519798	-3.549321	0.316880
33	1	0	-1.740339	-3.829302	1.580719
34	1	0	-2.304105	1.452927	-1.843647
35	1	0	-2.116010	2.188496	-0.252311
36	1	0	-3.728009	1.793050	-0.857820
37	1	0	-7.414382	0.656410	0.755959
38	1	0	-7.499479	-0.035439	-0.864662
39	1	0	-8.449330	2.294924	-0.851101
40	1	0	-6.995337	2.231957	-1.864302
41	1	0	-6.911850	2.927417	-0.233990
42	1	0	2.306944	0.758980	-1.799255
43	1	0	4.525110	0.246980	-1.086897
44	1	0	6.496419	-1.174297	-1.391999
45	1	0	6.429706	-3.591030	-0.787437

46	1	0	4.315971	-4.553748	0.119169
47	1	0	2.315494	-3.132406	0.406696
48	1	0	0.200805	1.823444	0.031086
49	1	0	0.017351	1.278212	-1.632987
50	1	0	2.582978	1.034299	1.916115
51	1	0	3.769277	2.891072	3.057893
52	1	0	4.651142	4.804983	1.738532
53	1	0	4.340207	4.846623	-0.728767
54	1	0	3.153703	2.991710	-1.860480

3B

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-3.518946	-2.139214	0.726557
2	6	0	-4.222255	-1.079064	0.185407
3	6	0	-3.296129	-0.158051	-0.298431
4	6	0	-1.996704	-0.707222	-0.024681
5	6	0	-2.187215	-1.948616	0.617106
6	6	0	-1.207955	-2.953841	1.124153
7	6	0	-0.696263	-0.135937	-0.327308
8	6	0	-3.626587	1.146966	-0.965358
9	6	0	-5.676644	-1.189074	0.255975
10	8	0	-6.234420	-2.156824	0.755629
11	8	0	-6.342652	-0.138819	-0.271633
12	6	0	-7.786835	-0.223393	-0.214769
13	6	0	-8.342287	1.039736	-0.842800
14	7	0	0.408590	-0.739713	-0.013526
15	7	0	1.484105	0.033610	-0.399552
16	6	0	1.087626	1.347919	-0.945540
17	6	0	2.763264	-0.470057	-0.343716
18	6	0	3.863904	0.314212	-0.764014
19	6	0	5.149474	-0.199120	-0.717676
20	6	0	5.361556	-1.497368	-0.249831
21	6	0	4.288328	-2.287670	0.174858
22	6	0	3.001751	-1.783686	0.129317
23	6	0	-0.453115	1.182247	-1.044410
24	6	0	1.509282	2.521237	-0.071398
25	6	0	1.489396	2.426917	1.325418
26	6	0	1.825234	3.529027	2.110896
27	6	0	2.183113	4.738221	1.510958
28	6	0	2.206712	4.839063	0.119706
29	6	0	1.872686	3.734858	-0.665911
30	7	0	6.711082	-2.031269	-0.201725
31	8	0	6.865122	-3.181871	0.222430
32	8	0	7.635906	-1.307728	-0.587639
33	1	0	-3.992465	-2.932391	1.136851

34	1	0	-0.529573	-2.505906	1.856076
35	1	0	-0.578360	-3.332295	0.312911
36	1	0	-1.724881	-3.797984	1.590354
37	1	0	-3.167039	1.223260	-1.956249
38	1	0	-3.274115	2.001730	-0.376694
39	1	0	-4.703645	1.249310	-1.086231
40	1	0	-8.092231	-0.332507	0.830202
41	1	0	-8.108396	-1.123802	-0.746927
42	1	0	-9.435976	1.014556	-0.817486
43	1	0	-8.025735	1.131696	-1.885716
44	1	0	-8.006981	1.927899	-0.299676
45	1	0	1.527378	1.472289	-1.941510
46	1	0	3.713629	1.329857	-1.107070
47	1	0	5.998856	0.392399	-1.035363
48	1	0	4.483460	-3.291080	0.532283
49	1	0	2.162257	-2.385820	0.448637
50	1	0	-0.974674	2.019469	-0.577440
51	1	0	-0.791686	1.123234	-2.084332
52	1	0	1.223071	1.484529	1.794981
53	1	0	1.811875	3.442130	3.193362
54	1	0	2.448302	5.594006	2.124441
55	1	0	2.491589	5.773221	-0.355329
56	1	0	1.897859	3.816433	-1.750344

3C

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-3.566874	-2.028213	0.719642
2	6	0	-4.317107	-0.969832	0.236815
3	6	0	-3.434441	-0.021213	-0.269825
4	6	0	-2.112613	-0.551202	-0.069365
5	6	0	-2.247154	-1.813530	0.551777
6	6	0	-0.842999	0.044529	-0.431798
7	6	0	-5.764404	-1.110828	0.372755
8	6	0	-1.230159	-2.819513	0.972407
9	6	0	-3.821751	1.292730	-0.886347
10	7	0	0.290058	-0.488773	-0.087040
11	7	0	1.325004	0.284459	-0.584160
12	6	0	0.855398	1.588275	-1.106946
13	6	0	-0.656376	1.295610	-1.276202
14	6	0	1.130173	2.759549	-0.171871
15	6	0	2.621645	-0.129536	-0.505427
16	6	0	1.392921	4.023888	-0.712562
17	6	0	1.592814	5.125290	0.121082
18	6	0	1.533835	4.971587	1.506461
19	6	0	1.275854	3.712516	2.052358

20	6	0	1.074339	2.612069	1.219646
21	6	0	3.678163	0.806818	-0.669389
22	6	0	4.996731	0.454046	-0.464901
23	6	0	5.315816	-0.852060	-0.075589
24	6	0	4.323117	-1.815477	0.049625
25	6	0	3.004546	-1.471266	-0.210490
26	7	0	2.073057	-2.598383	-0.308490
27	8	0	1.346395	-2.644006	-1.300897
28	8	0	2.123459	-3.462747	0.566771
29	7	0	6.702191	-1.216090	0.172433
30	8	0	6.941618	-2.375806	0.517727
31	8	0	7.558989	-0.339959	0.023609
32	8	0	-6.278884	-2.098881	0.878226
33	8	0	-6.474792	-0.065142	-0.103916
34	6	0	-7.912974	-0.181989	0.016042
35	6	0	-8.523136	1.072958	-0.576602
36	1	0	-4.003663	-2.843198	1.128361
37	1	0	-1.715216	-3.703504	1.396681
38	1	0	-0.546465	-2.403486	1.717311
39	1	0	-0.608921	-3.129982	0.126718
40	1	0	-4.905235	1.375843	-0.951504
41	1	0	-3.413672	1.402442	-1.896459
42	1	0	-3.457460	2.139257	-0.292290
43	1	0	1.331223	1.776880	-2.073693
44	1	0	-0.916213	1.082163	-2.319836
45	1	0	-1.264319	2.136662	-0.945004
46	1	0	1.444435	4.148312	-1.791927
47	1	0	1.800474	6.099169	-0.312187
48	1	0	1.694169	5.825724	2.157309
49	1	0	1.235197	3.584850	3.129984
50	1	0	0.883142	1.633729	1.650049
51	1	0	3.441099	1.834874	-0.908923
52	1	0	5.791875	1.180550	-0.574721
53	1	0	4.577892	-2.835967	0.303650
54	1	0	-8.169182	-0.304929	1.072679
55	1	0	-8.238049	-1.085552	-0.508396
56	1	0	-9.613780	1.023537	-0.502553
57	1	0	-8.255842	1.178800	-1.631909
58	1	0	-8.183260	1.964637	-0.042110

3D

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-3.649603	-2.296054	0.617464
2	6	0	-4.380511	-1.191365	0.214927

3	6	0	-3.479992	-0.213690	-0.194988
4	6	0	-2.167176	-0.774968	-0.020228
5	6	0	-2.325312	-2.084203	0.488305
6	6	0	-0.885799	-0.166727	-0.311059
7	6	0	-5.831495	-1.326573	0.316154
8	6	0	-1.326419	-3.135962	0.833838
9	6	0	-3.843422	1.152098	-0.703976
10	7	0	0.235751	-0.745489	-0.001821
11	7	0	1.285731	0.059235	-0.415912
12	6	0	0.835212	1.412252	-0.797339
13	6	0	-0.670614	1.149872	-1.042463
14	6	0	1.074405	2.453008	0.293081
15	6	0	2.575455	-0.383947	-0.401628
16	6	0	1.128791	3.821875	-0.005995
17	6	0	1.315248	4.786592	0.983197
18	6	0	1.443049	4.387353	2.312193
19	6	0	1.383648	3.032811	2.639687
20	6	0	1.202500	2.081369	1.638161
21	6	0	3.646023	0.547897	-0.474638
22	6	0	4.960805	0.153353	-0.330503
23	6	0	5.260748	-1.192895	-0.092506
24	6	0	4.252742	-2.147810	-0.058930
25	6	0	2.937128	-1.755444	-0.259705
26	7	0	1.982862	-2.849467	-0.463136
27	8	0	1.244471	-2.777140	-1.444865
28	8	0	2.026416	-3.800962	0.316796
29	7	0	6.643786	-1.605161	0.094463
30	8	0	6.866002	-2.799904	0.304842
31	8	0	7.513753	-0.731850	0.033210
32	8	0	-6.363417	-2.346335	0.732665
33	8	0	-6.523244	-0.238584	-0.086439
34	6	0	-7.964596	-0.348025	0.001207
35	6	0	-8.552333	0.952157	-0.511104
36	1	0	-4.102005	-3.137161	0.949136
37	1	0	-1.827775	-4.043576	1.182494
38	1	0	-0.642195	-2.791387	1.613920
39	1	0	-0.703738	-3.387337	-0.030315
40	1	0	-4.925009	1.255897	-0.770679
41	1	0	-3.424506	1.339080	-1.698203
42	1	0	-3.473391	1.941556	-0.039191
43	1	0	1.340134	1.716451	-1.715643
44	1	0	-0.890254	1.023027	-2.109107
45	1	0	-1.288456	1.964736	-0.668614
46	1	0	1.358552	5.834213	0.707350
47	1	0	1.589321	5.135458	3.084901
48	1	0	1.481669	2.714480	3.672581
49	1	0	1.163876	1.027495	1.893456
50	1	0	3.424733	1.599600	-0.601585
51	1	0	5.767524	0.874141	-0.372780
52	1	0	4.492416	-3.193984	0.078646
53	1	0	-8.239816	-0.542222	1.042302
54	1	0	-8.289107	-1.208789	-0.591033

55	1	0	-9.644466	0.909728	-0.457595
56	1	0	-8.266918	1.128617	-1.552092
57	1	0	-8.212374	1.800424	0.089866
58	17	0	0.951868	4.376597	-1.674647