

"Supporting Information"

Novel 5,6,7,8-tetrahydrobenzo[*b*]pyran Derivatives: Synthesis and Anticancer Activity

Amira E. M. Abdallah,^{1*} Rafat M. Mohareb,² Maher H. E. Helal¹, Mariam M. Abd Elkader¹

¹Department of Chemistry, Faculty of Science, Helwan University, Ain Helwan, Cairo, 11795, A. R. Egypt

²Department of Chemistry, Faculty of Science, Cairo University, Giza 12614, A. R. Egypt

*Correspondence: Amira E. M. Abdallah

Tel: +2 01091769838, Email: amiraelsayed135@yahoo.com

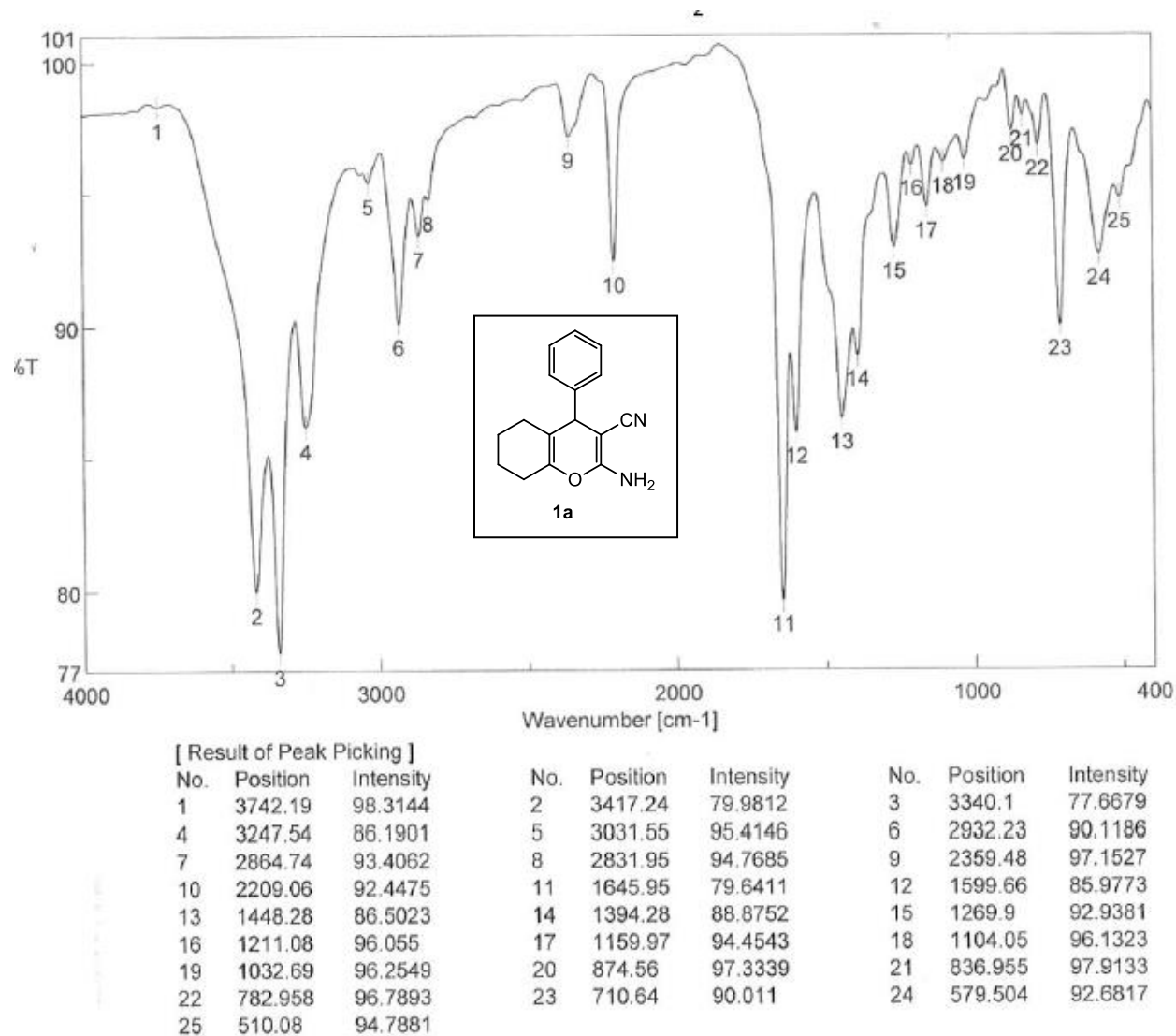


Figure S1: IR spectrum of compound **1a**.

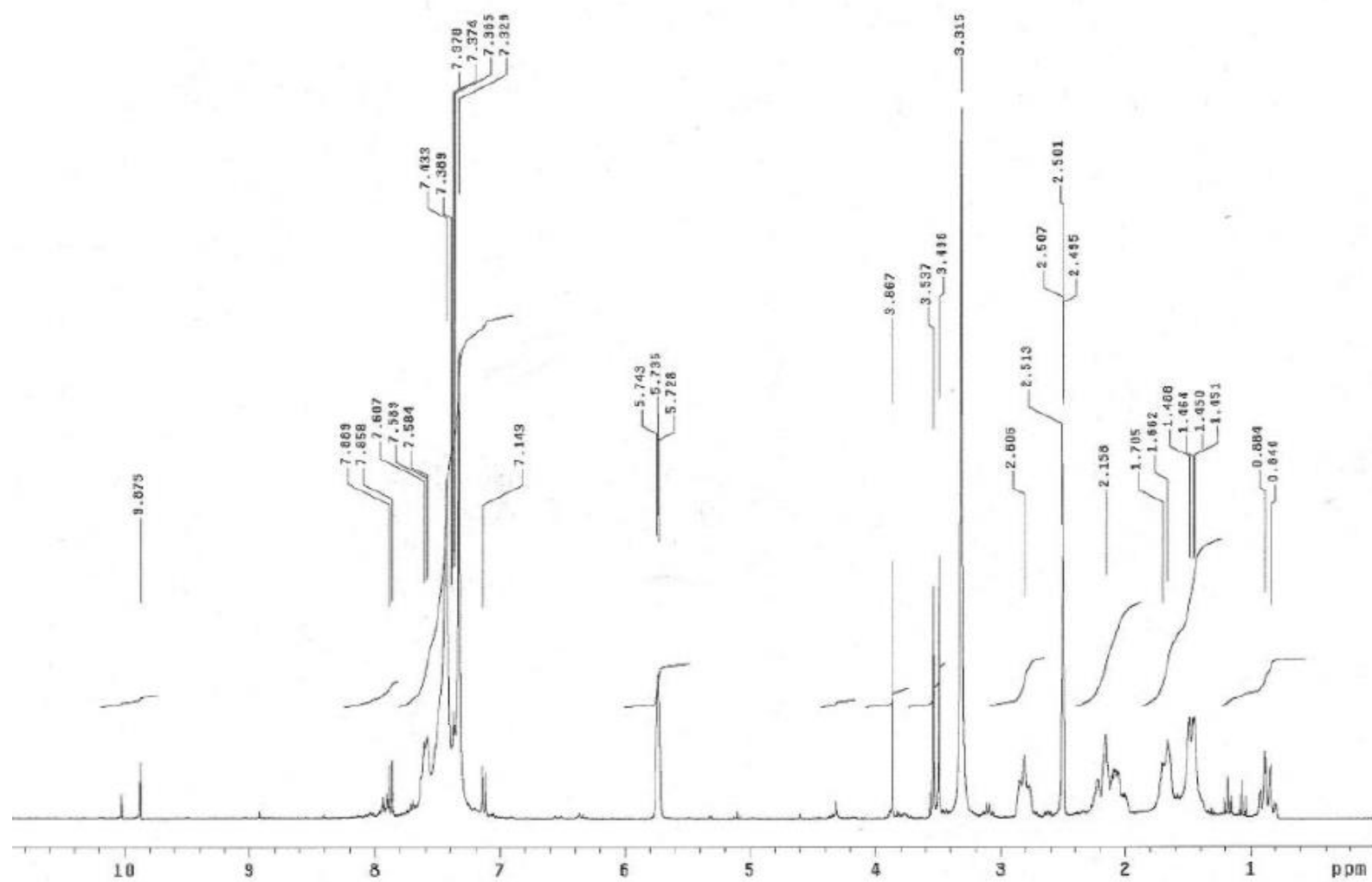


Figure S2: ^1H NMR spectrum of compound **1a**.

Pulse Sequence: s2pu1
Solvent: DMSO
Ambient temperature
Mercury-300SB "NMR300"

Pulse 45.0 degrees
Acq. time 1.707 sec
Width 18761.7 Hz
2015 repetitions
OBSERVE C13, 75.4523914 MHz
DECOUPLE H1, 300.0702830 MHz
Power 34 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 21 hr, 47 min, 2 sec
Date: Feb 17 2020

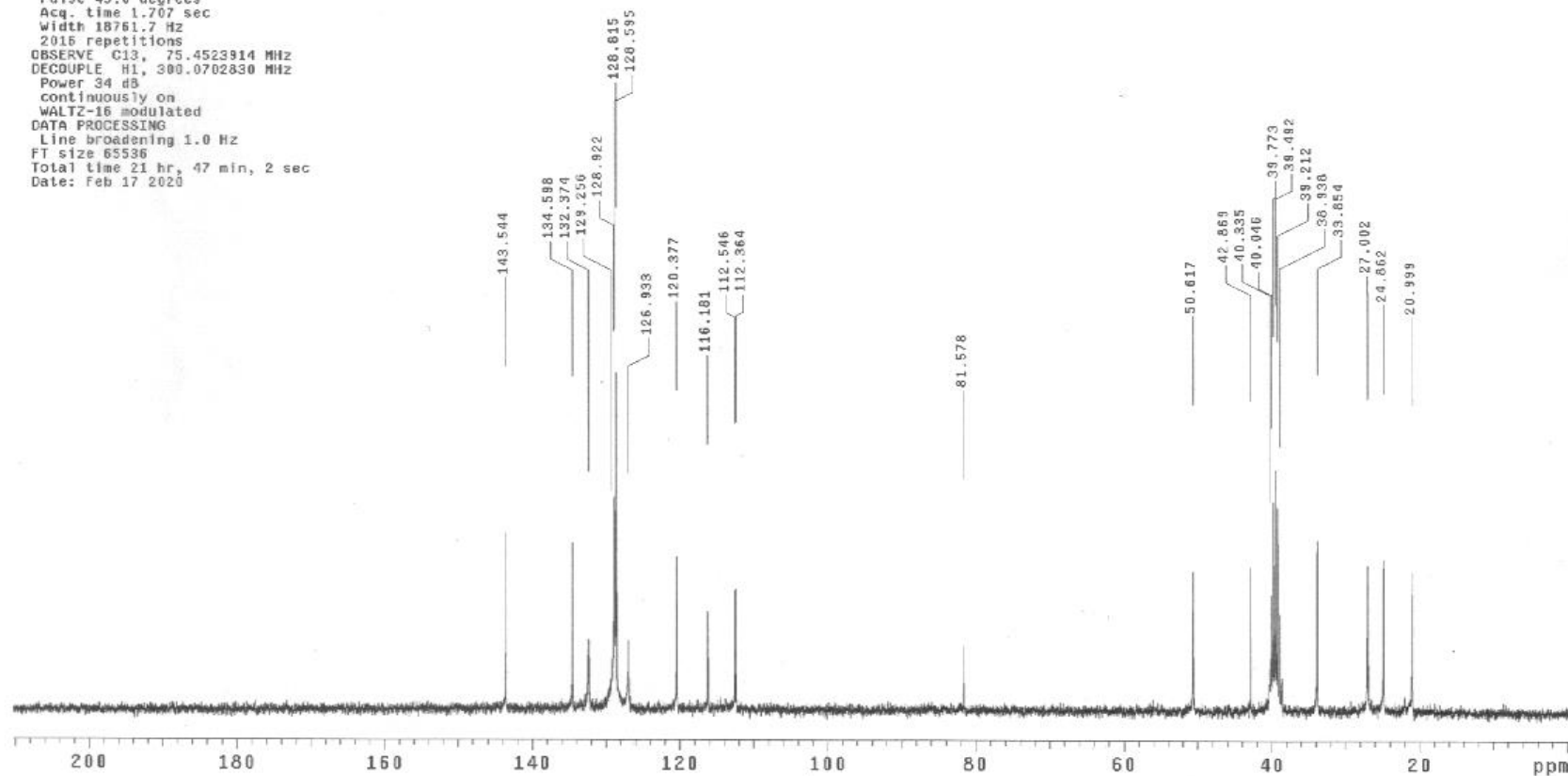
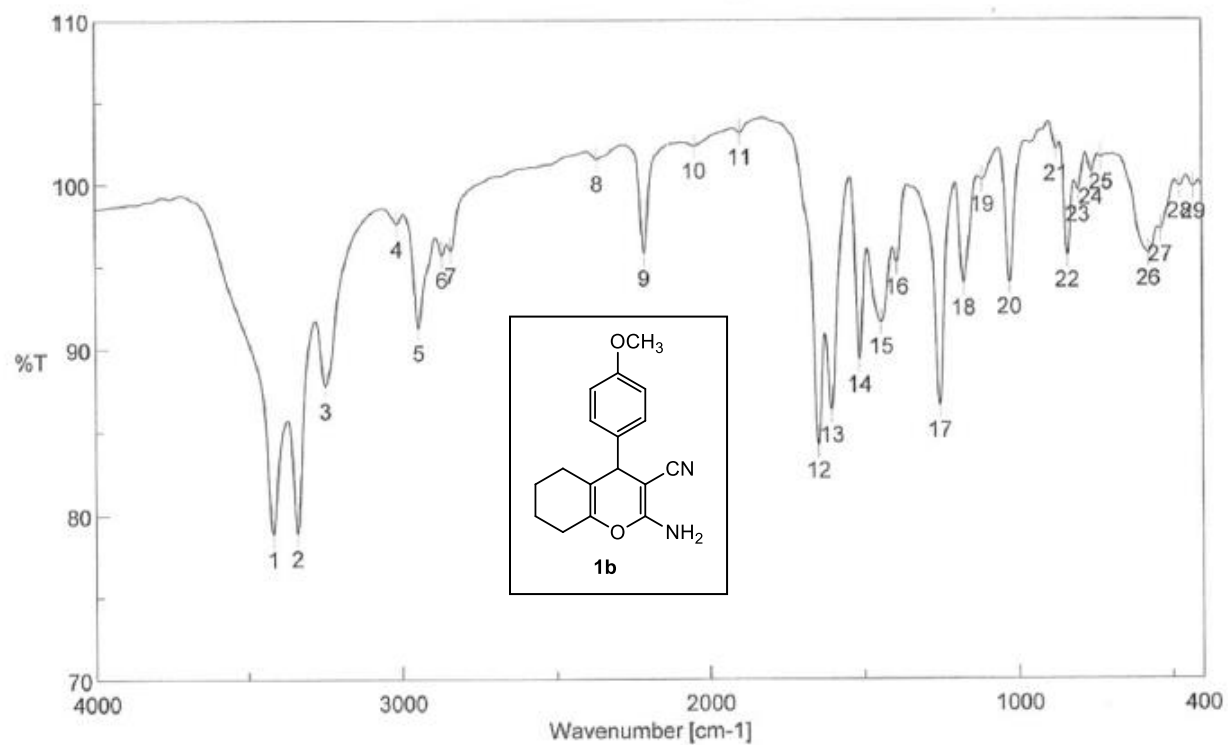


Figure S3: ^{13}C NMR spectrum of compound **1a**.



[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1	3419.17	78.8189	2	3340.1	78.8761	3	3247.54	87.772
4	3013.23	97.5753	5	2943.8	91.2651	6	2865.7	95.7085
7	2836.77	95.972	8	2363.34	101.507	9	2211.95	95.7955
10	2046.1	102.291	11	1897.61	103.115	12	1645.95	84.2014
13	1602.56	86.3206	14	1512.88	89.3356	15	1443.46	91.6305
16	1392.35	95.2445	17	1255.43	86.5854	18	1176.36	93.9617
19	1116.58	100.218	20	1027.87	94.0254	21	874.56	102.089
22	837.919	95.6636	23	803.206	99.5747	24	758.852	100.65
25	726.068	101.557	26	572.755	95.7446	27	534.185	97.1781
28	472.474	99.7905	29	428.12	99.755			

Figure S4: IR spectrum of compound **1b**.

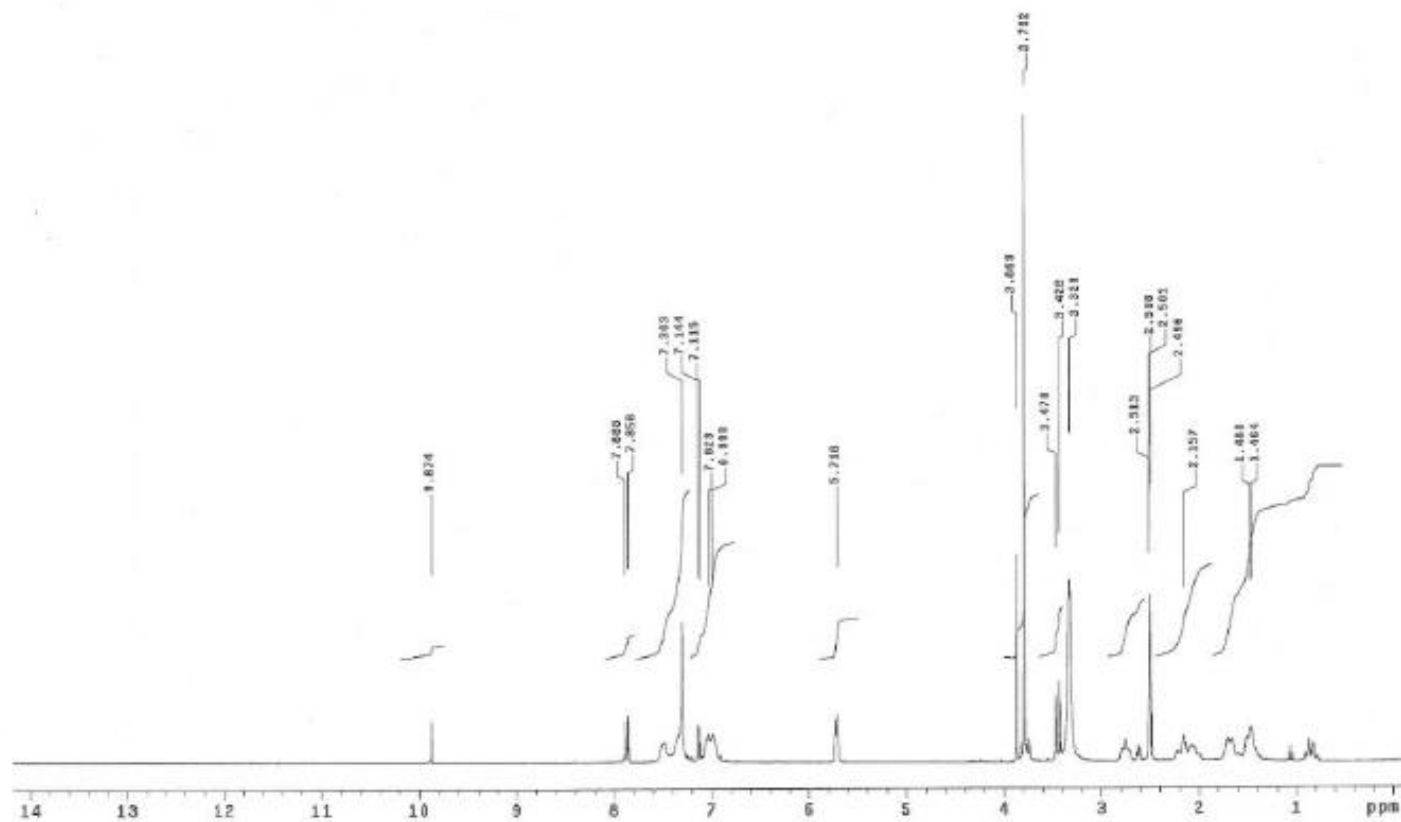


Figure S5: ^1H NMR spectrum of compound **1b**.

nmrdat15ayed-MS19G-DMSU-C13

Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: D05mm_test_12Mar2014-21:34:40
File: PROTON

Pulse Sequence: s2pu1

Solvent: DMSO

Ambient temperature
Mercury-300BB "NMR300"

Pulse 45.0 degrees
Acq. time 1.707 sec
Width 18761.7 Hz
4536 repetitions
OBSERVE C13, 75.4523891 MHz
DECOUPLE H1, 300.0702830 MHz
Power 34 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 21 hr, 47 min, 2 sec
Date: Jan 5 2020

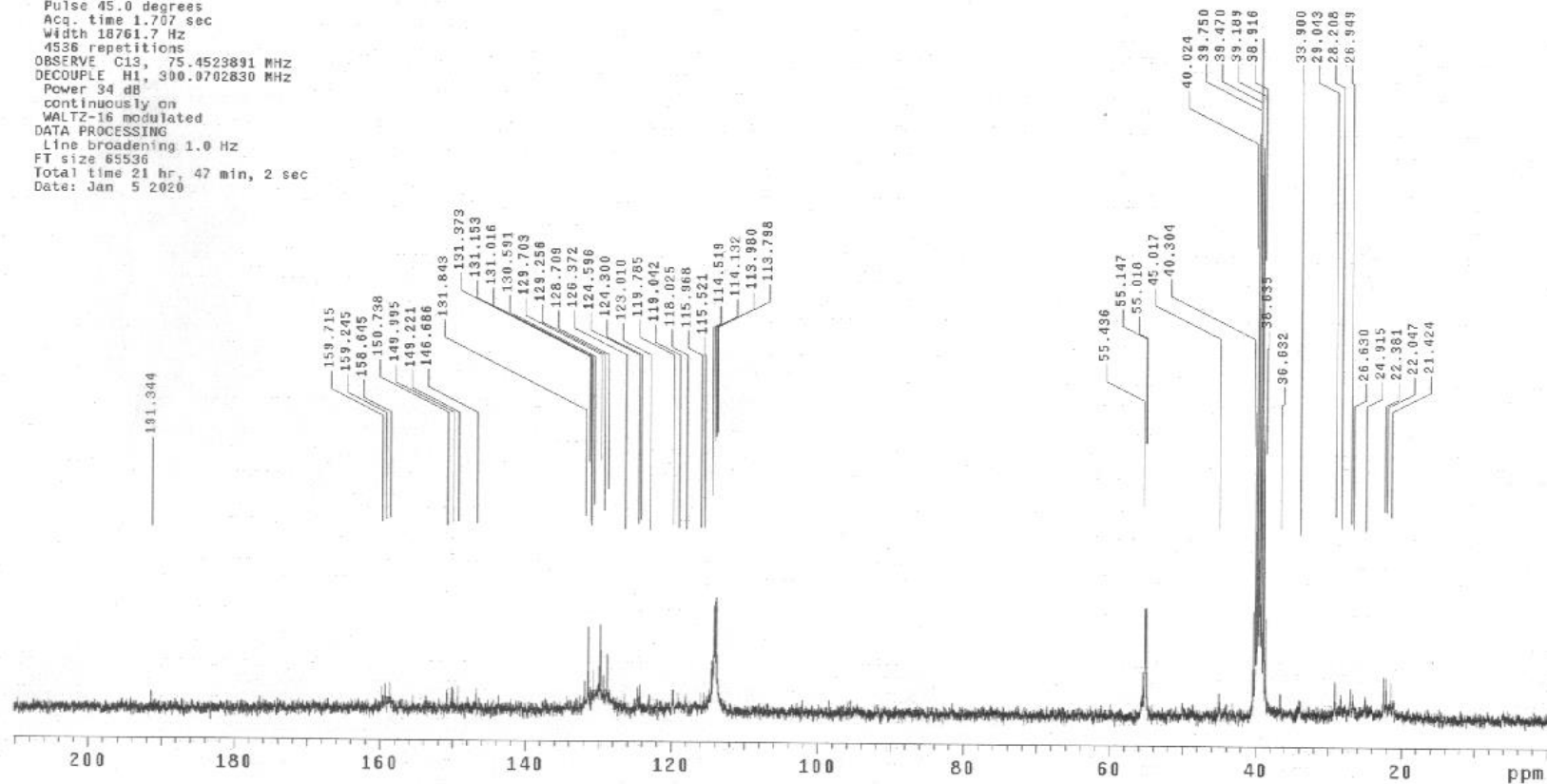
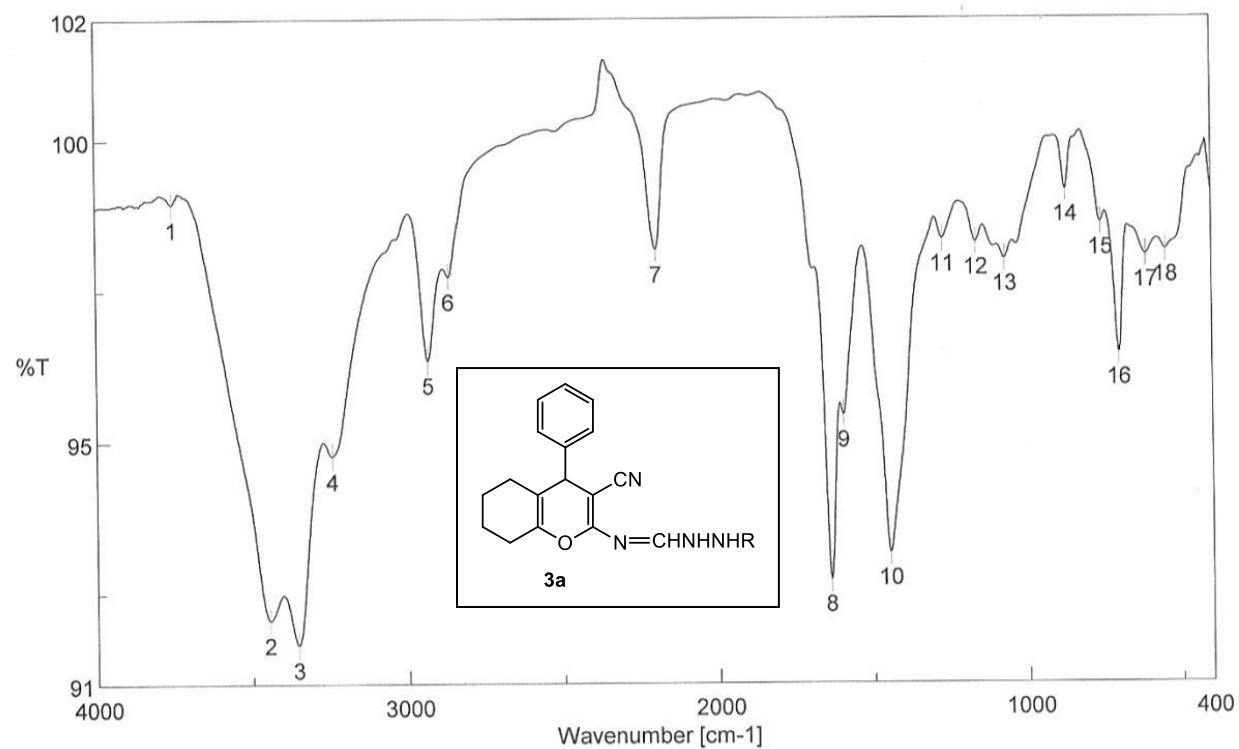


Figure S6: ^{13}C NMR spectrum of compound **2b**.



[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1	3750.87	98.9376	2	3444.24	92.0593	3	3355.53	91.6538
4	3243.68	94.7668	5	2934.16	96.3443	6	2865.7	97.7284
7	2197.49	98.1685	8	1639.2	92.7186	9	1596.77	95.4366
10	1448.28	93.1574	11	1273.75	98.3352	12	1165.76	98.28
13	1073.19	98.0053	14	875.524	99.1494	15	761.744	98.5954
16	704.855	96.4521	17	615.181	98.0655	18	550.577	98.1468

Figure S7: IR spectrum of compound **3a**.

AmerAETsayed-MS17C-DMSO-C13

Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: DD5mm_test_12Mar2014-21:34:40
File: PROTON

Pulse Sequence: s2pu1

Solvent: DMSO

Ambient temperature

Mercury-300BB "NMR300"

Pulse 45.0 degrees
Acq. time 1.707 sec
Width 18761.7 Hz
3392 repetitions
OBSERVE C13, 75.4523914 MHz
DECOUPLE H1, 300.0702630 MHz
Power 34 dB
Continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 21 hr, 47 min, 2 sec
Date: Feb 18 2020

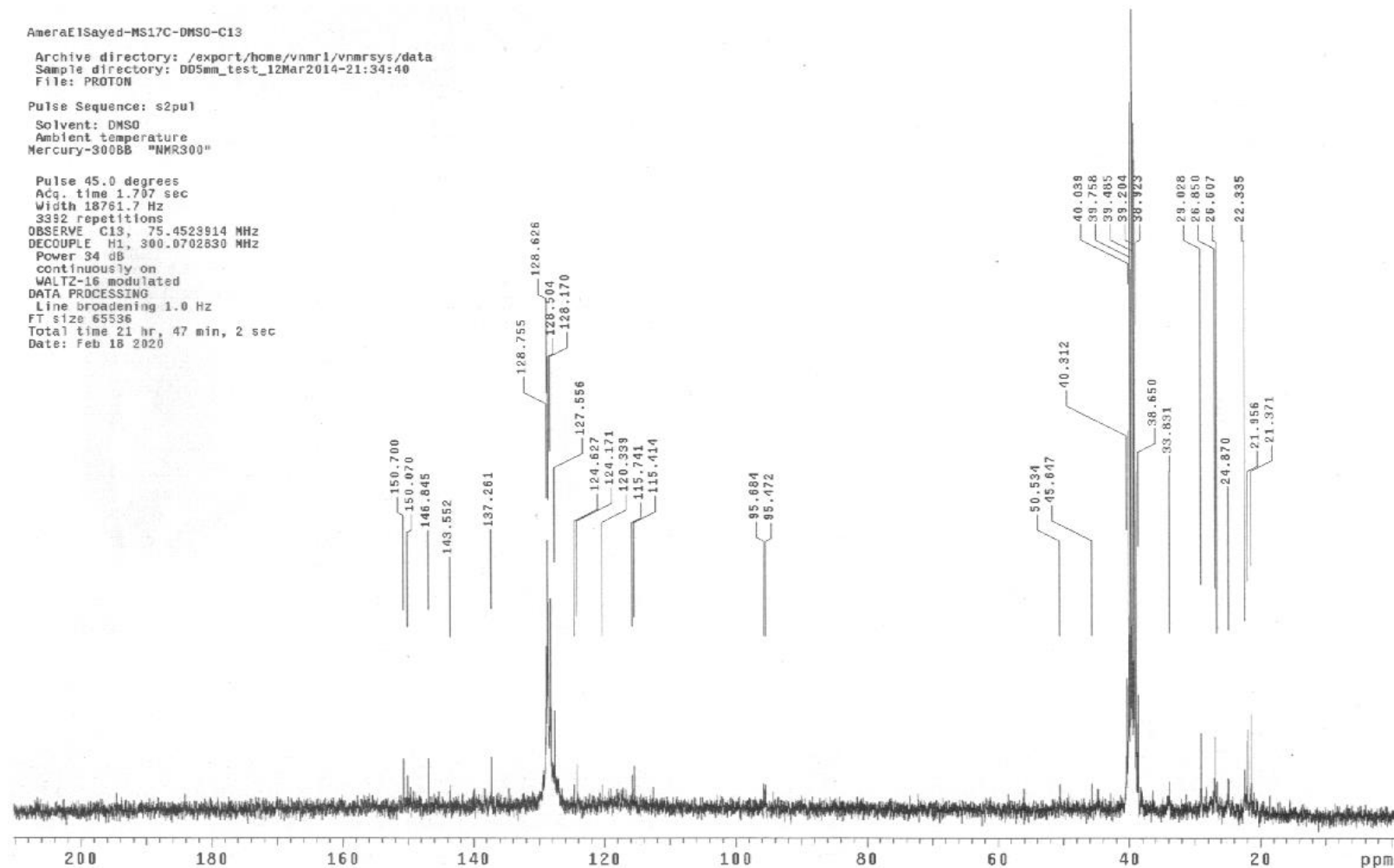


Figure S8: ^{13}C NMR spectrum of compound 3a.

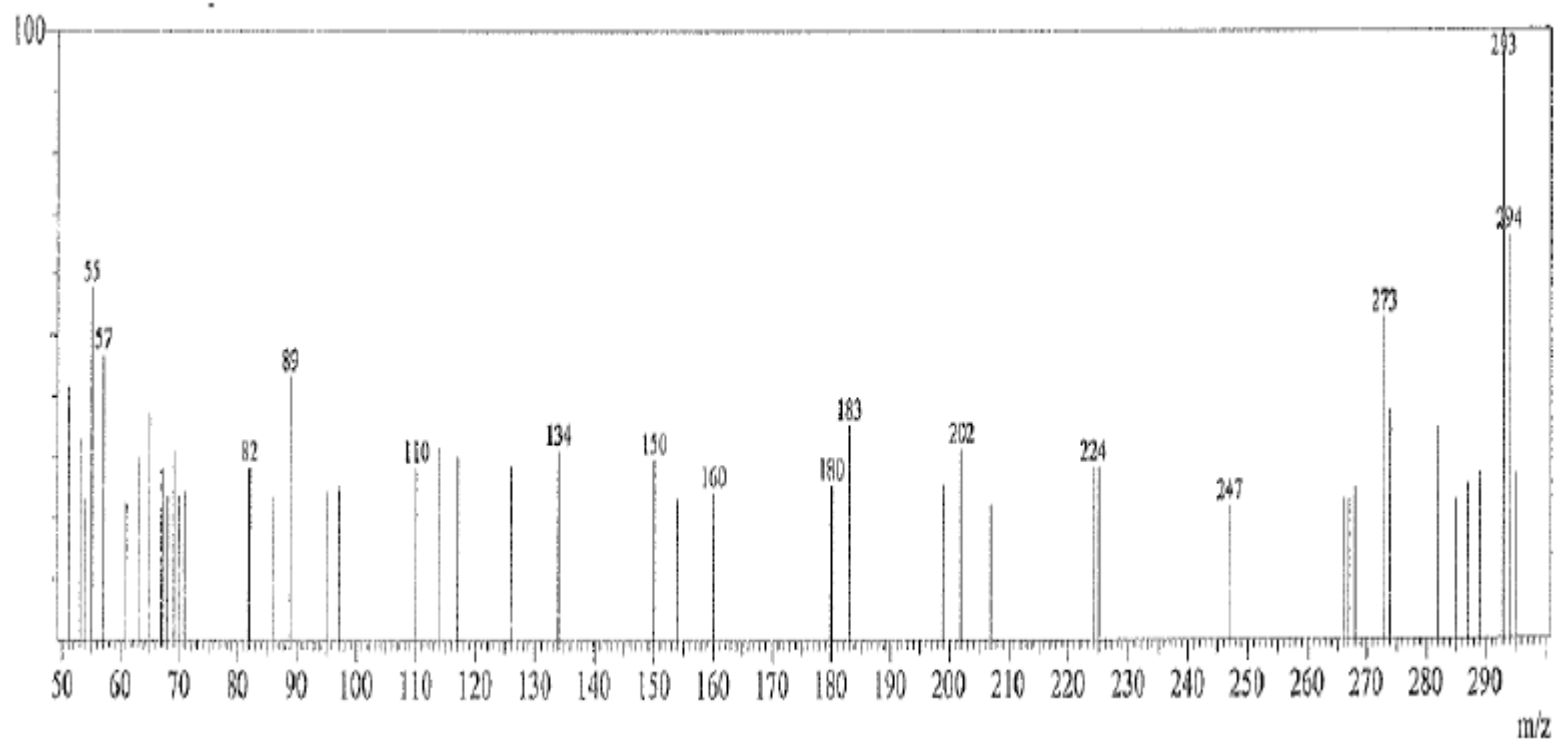


Figure S9: Mass spectrum of compound **3a**.

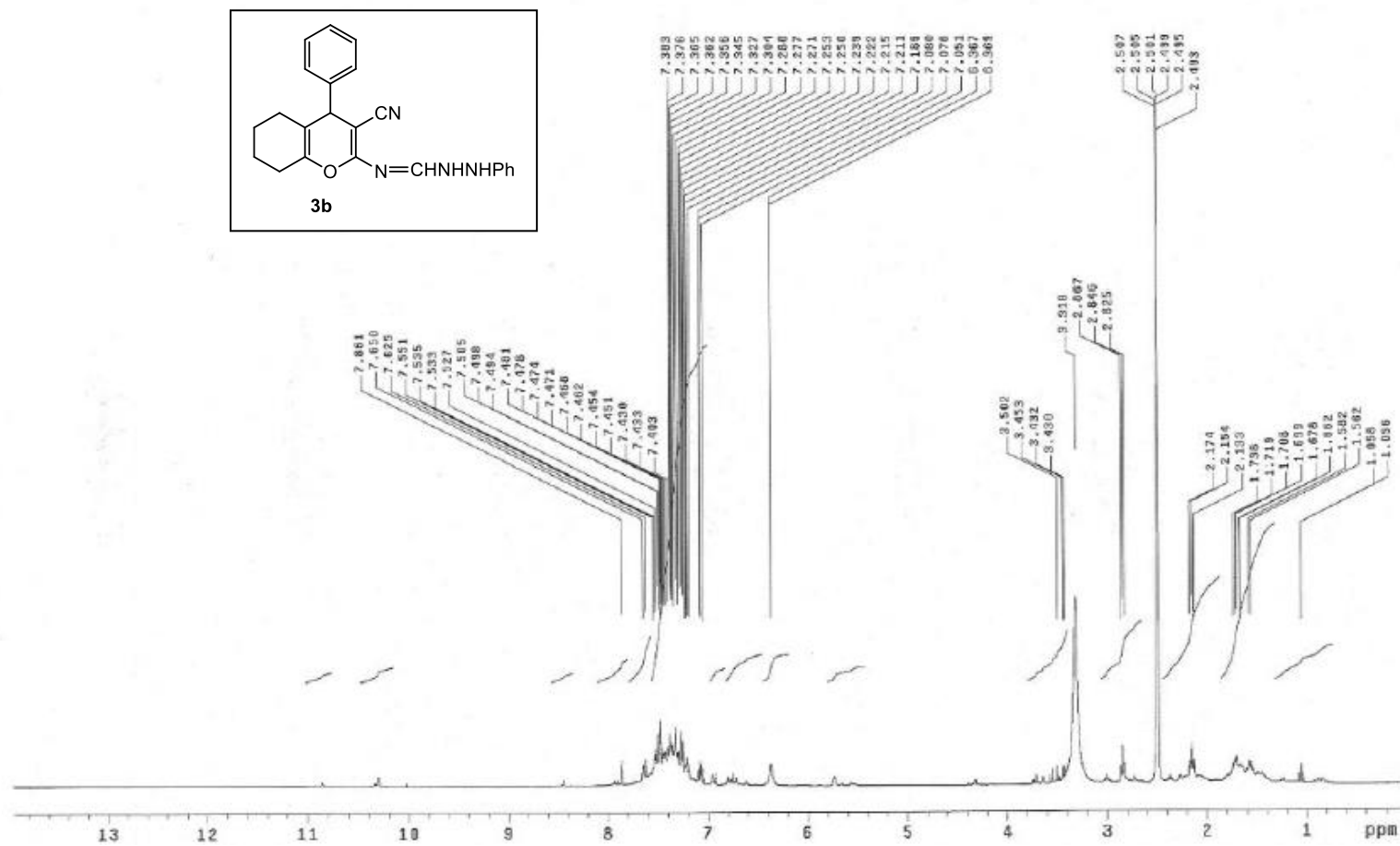


Figure S10: ¹H NMR spectrum of compound **3b**.

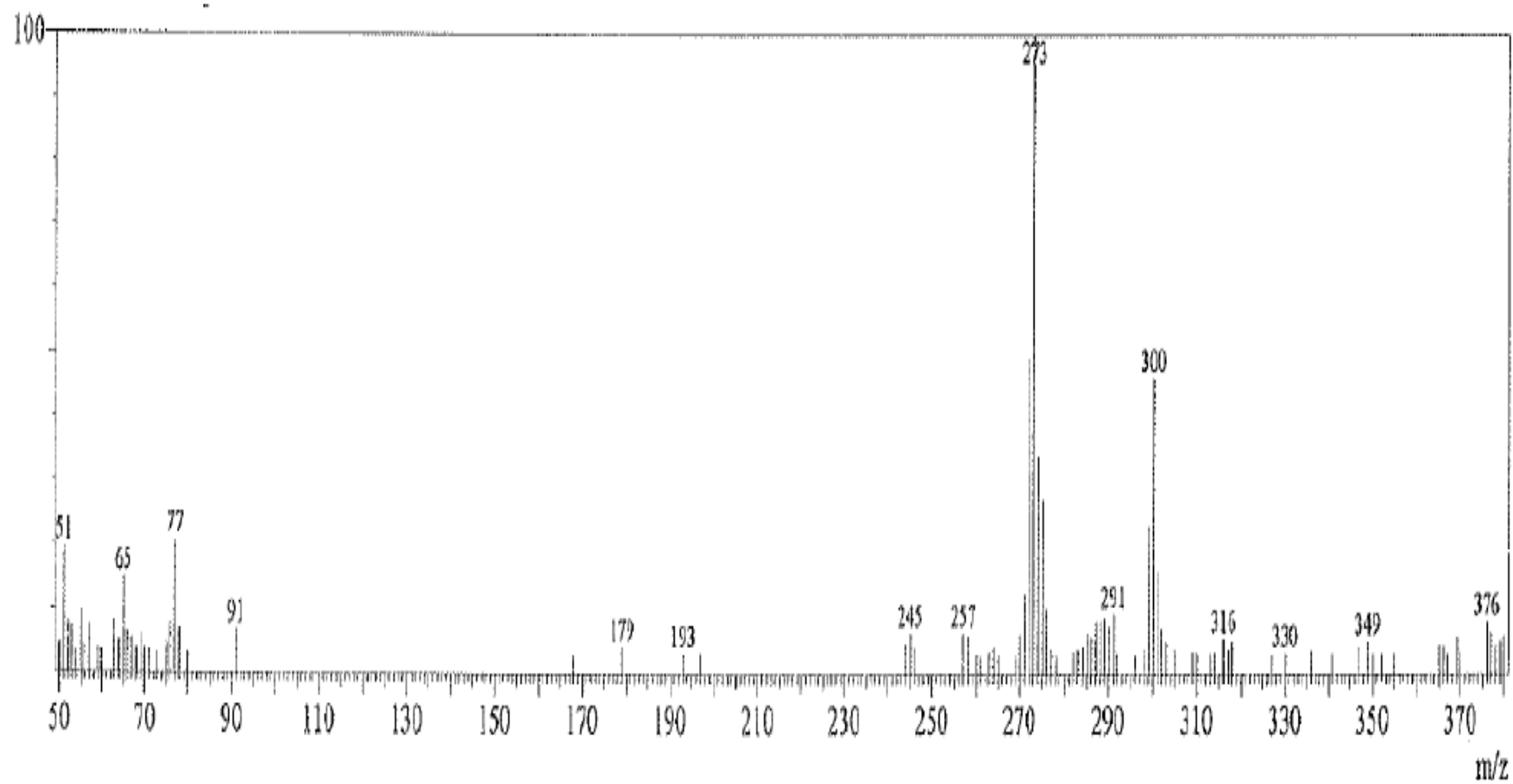


Figure S11: Mass spectrum of compound **3b**.

nmr1.ac 100000-HS23-DMSO-C13

Archive directory: /export/home/vnmr1/vnmr/sys/data
Sample directory: D05mm_test_12Mar2014-21:34:40
File: PROTON

Pulse Sequence: s2pul

Solvent: DMSO
Ambient temperature
Mercury-300BB "NMR300"

Pulse 45.0 degrees
Acq. time 1.707 sec
Width 18761.7 Hz
2216 repetitions
OBSERVE C13, 75.4523437 MHz
DECOUPLE H1, 300.0702830 MHz
Power 34 dB
Continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 21 hr, 47 min, 2 sec
Date: Jan 30 2020

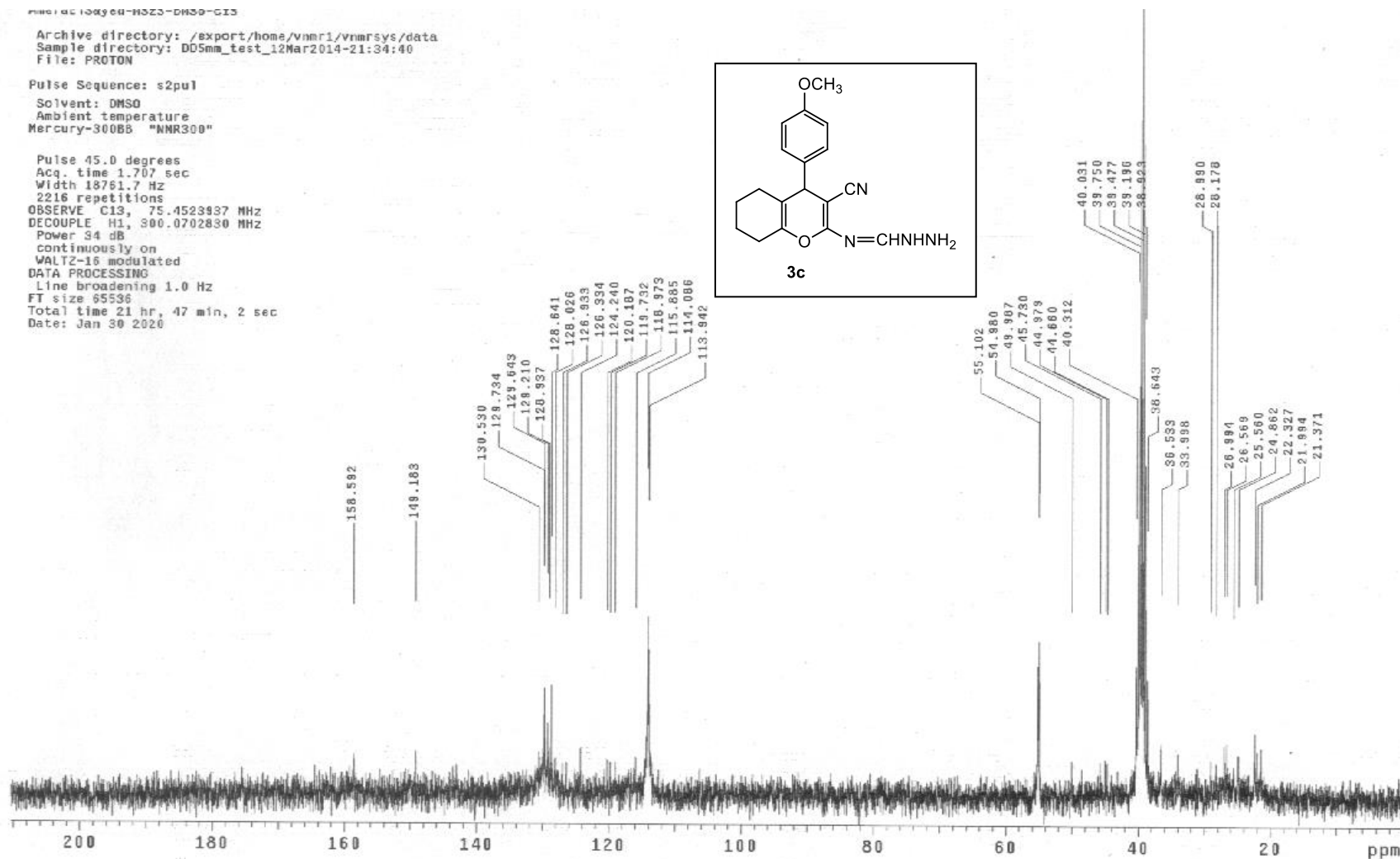
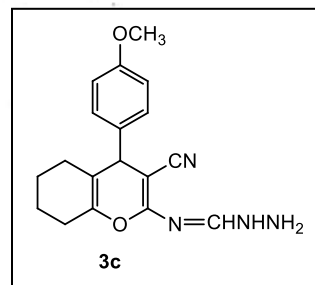


Figure S12: ¹³C NMR spectrum of compound 3c.

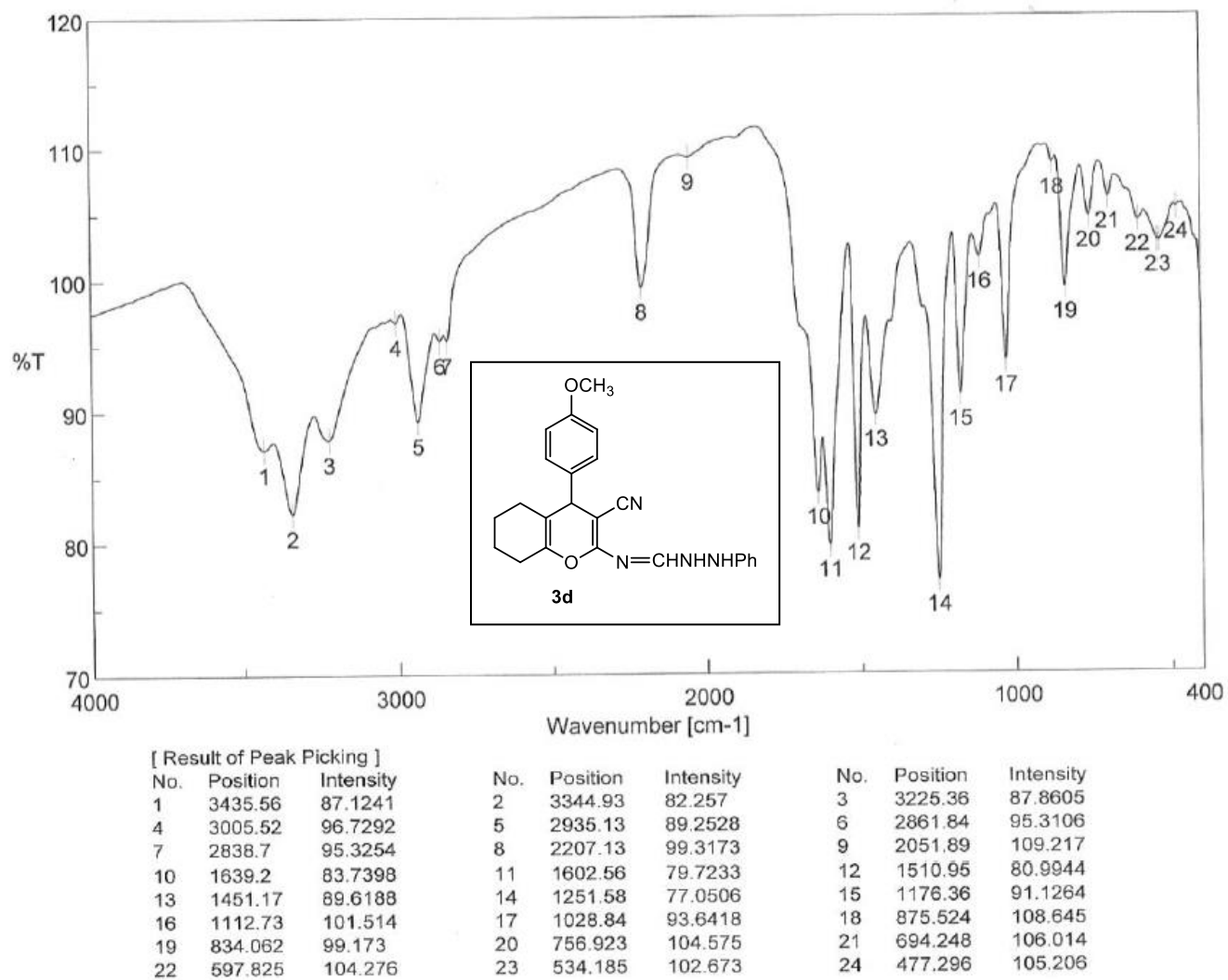


Figure S13: IR spectrum of compound **3d**.

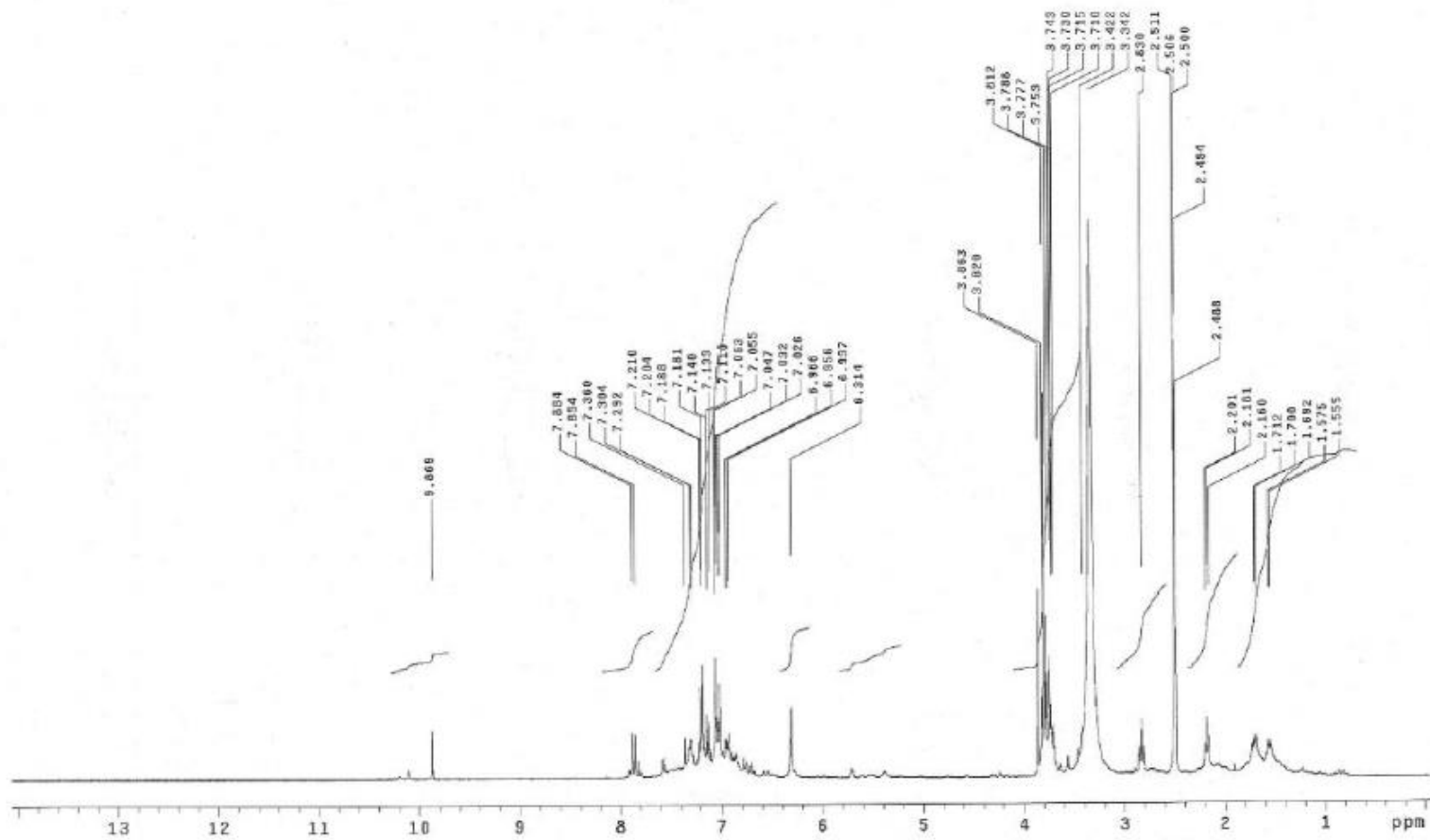
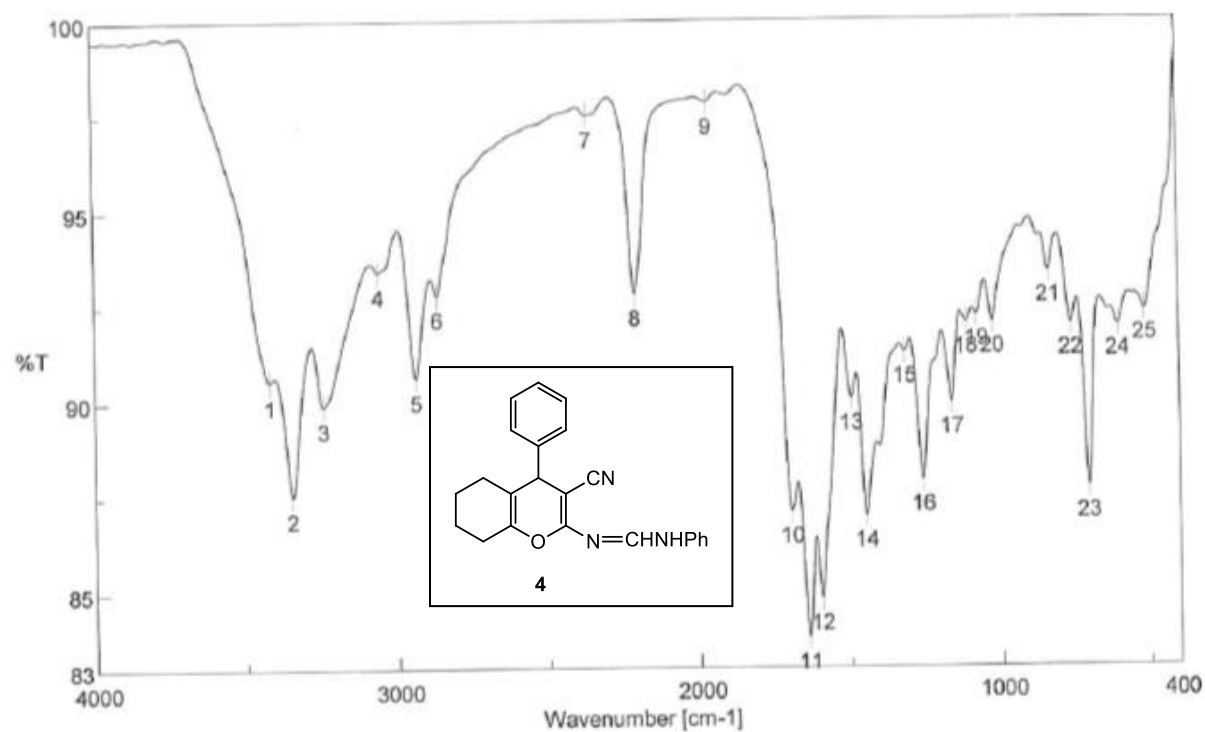


Figure S14: ¹H NMR spectrum of compound 3d.



[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1	3417.24	90.5229	2	3346.85	87.5254	3	3242.72	89.8877
4	3058.55	93.3954	5	2935.13	90.6139	6	2862.81	92.7824
7	2362.37	97.5011	8	2210.02	92.8075	9	1962.22	97.8367
10	1694.16	87.078	11	1640.16	83.7828	12	1596.77	84.7966
13	1495.53	90.0316	14	1447.31	86.9553	15	1317.14	91.2472
16	1259.29	87.8875	17	1161.9	89.9195	18	1112.73	92.0113
19	1078.01	92.2166	20	1025.94	92.0134	21	835.026	93.3505
22	761.744	91.9623	23	704.855	87.6892	24	604.574	91.9318
25	513.936	92.331						

Figure S15: IR spectrum of compound 4.

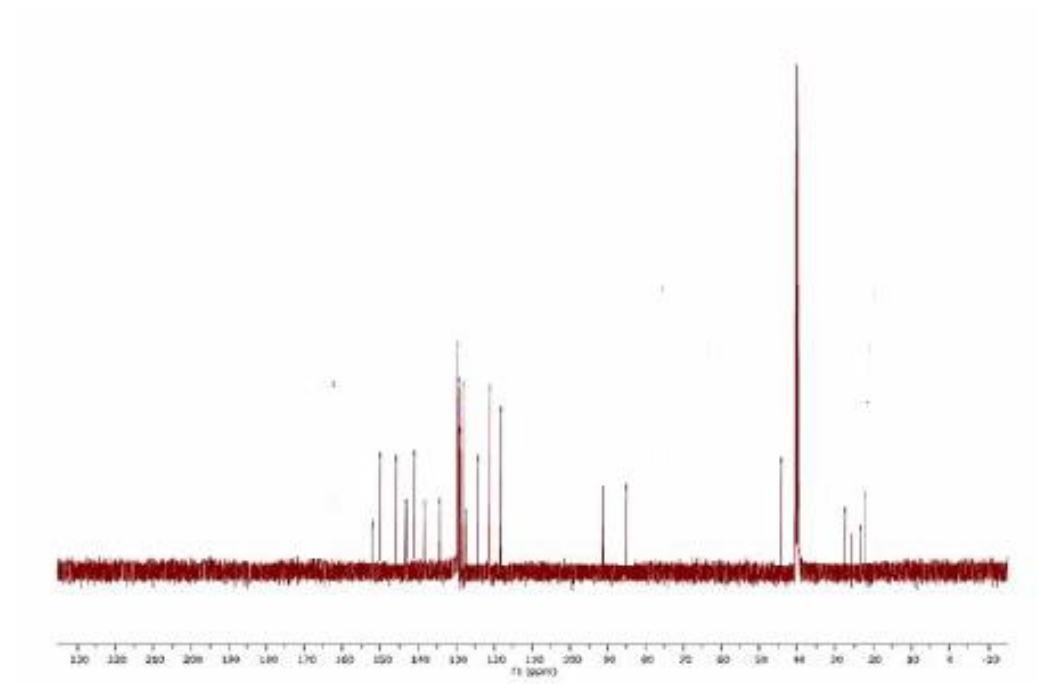


Figure S16: ^{13}C NMR spectrum of compound **4**.

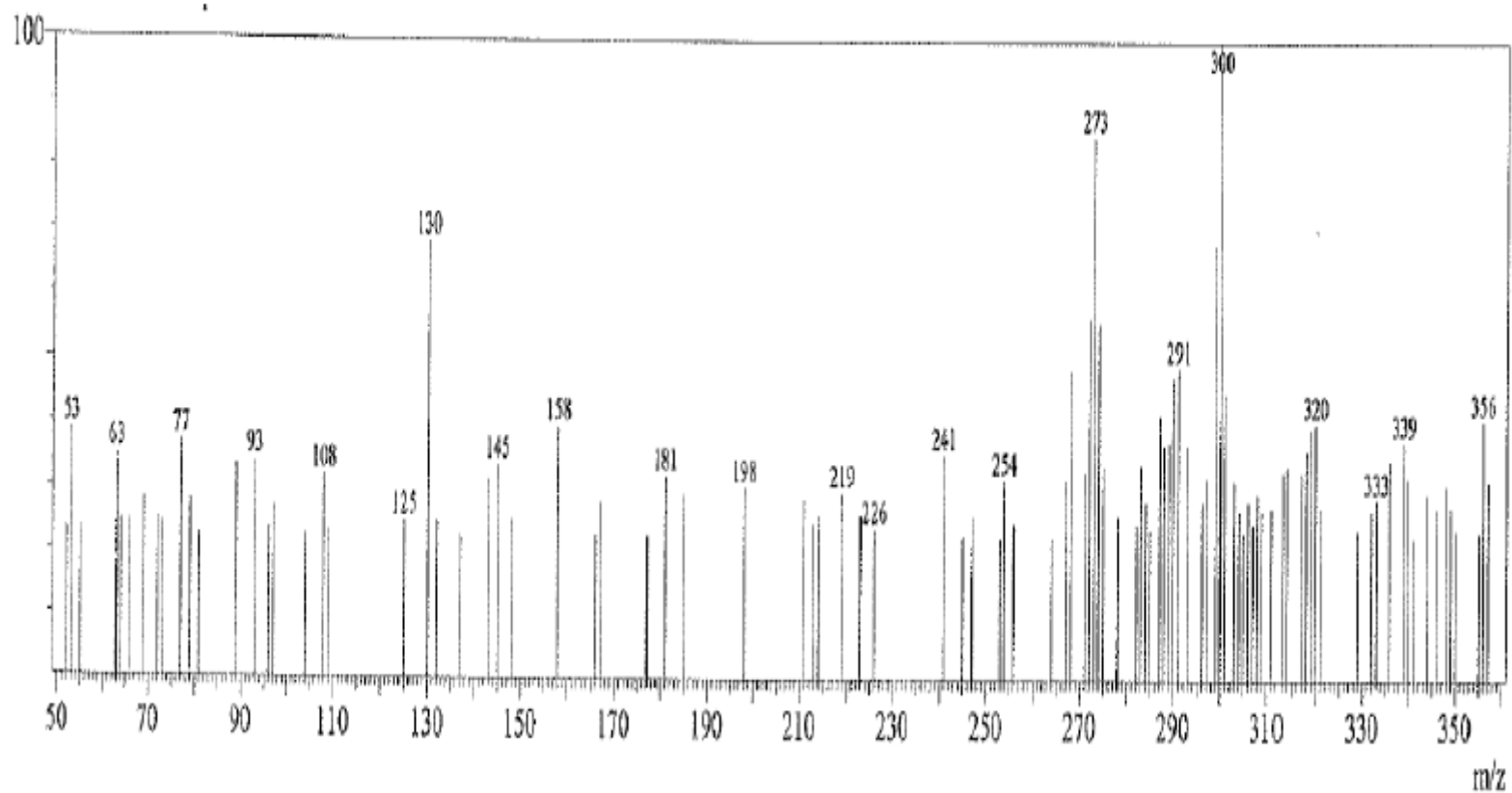


Figure S17: Mass spectrum of compound 4.

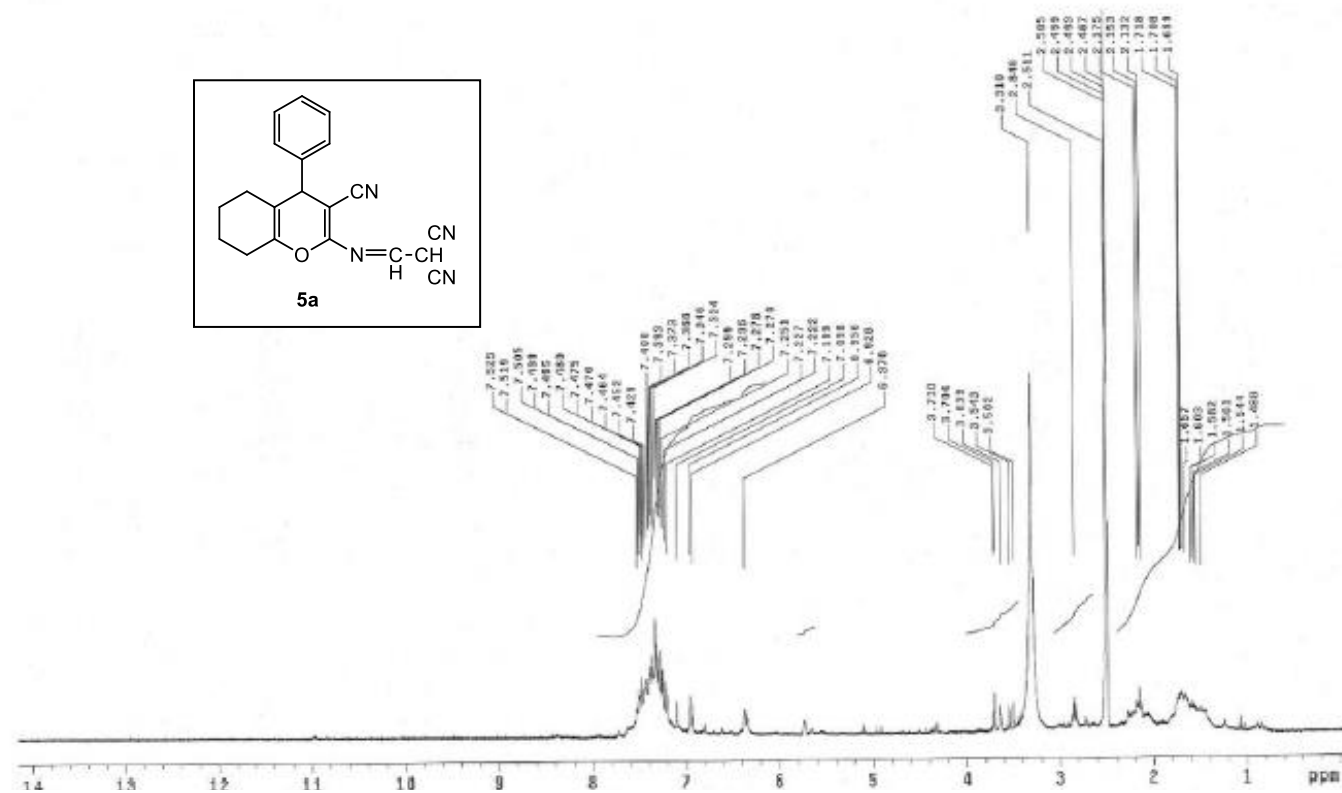


Figure S18: ¹H NMR spectrum of compound 5a.

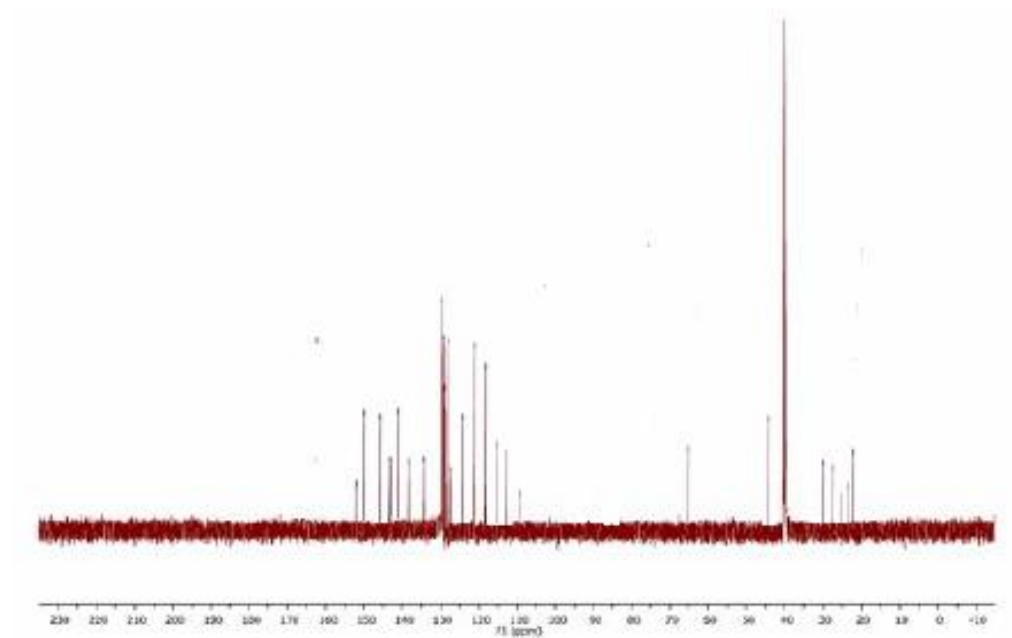


Figure S19: ^{13}C NMR spectrum of compound **5a**.

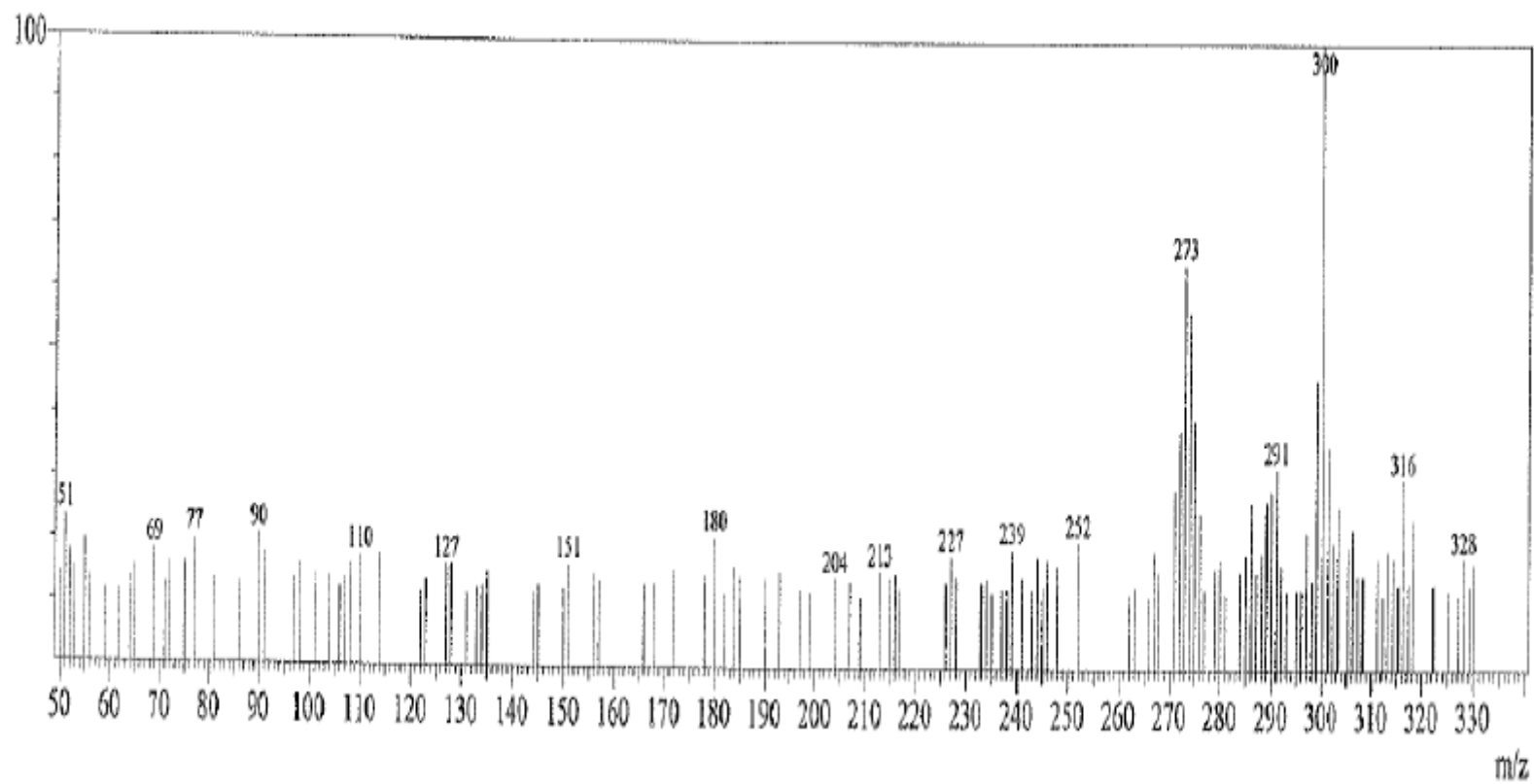


Figure S20: Mass spectrum of compound 5a.

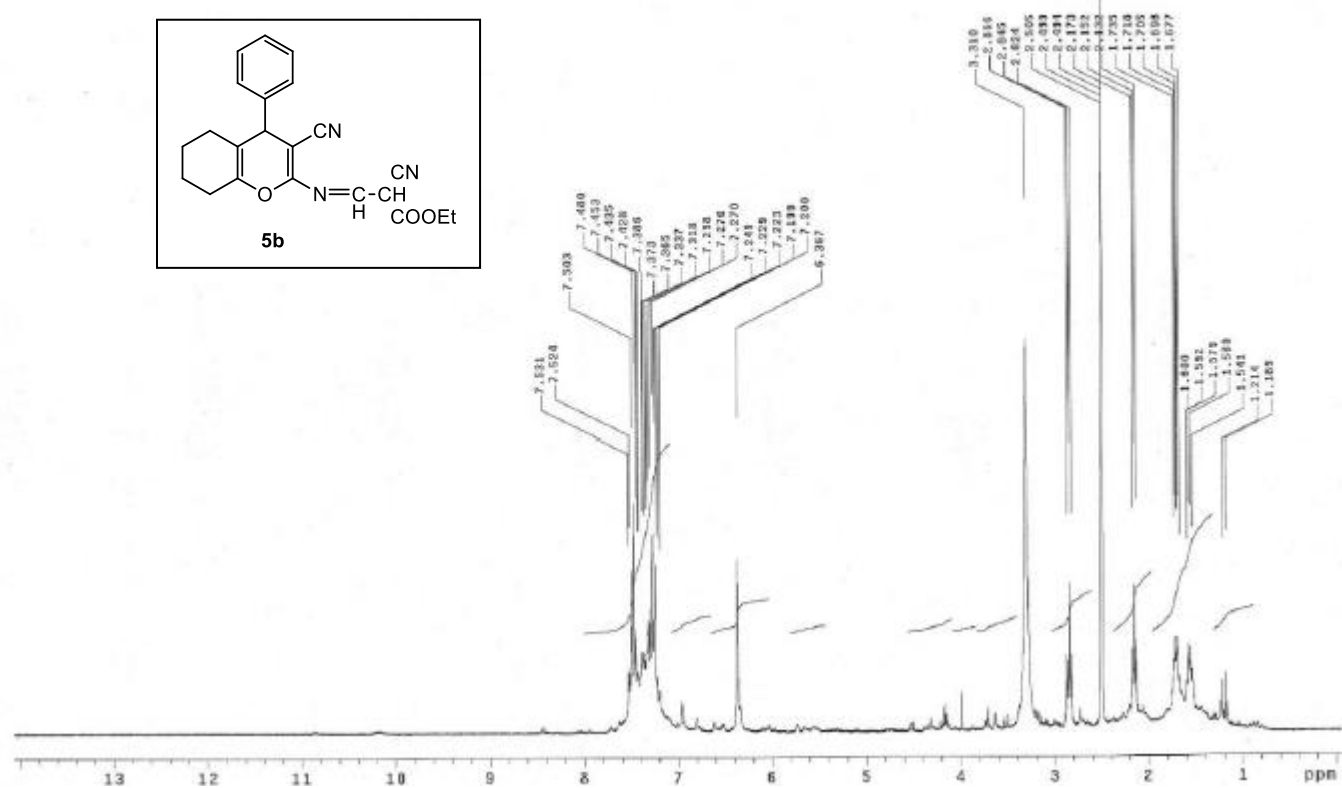


Figure S21: ¹H NMR spectrum of compound **5b**.

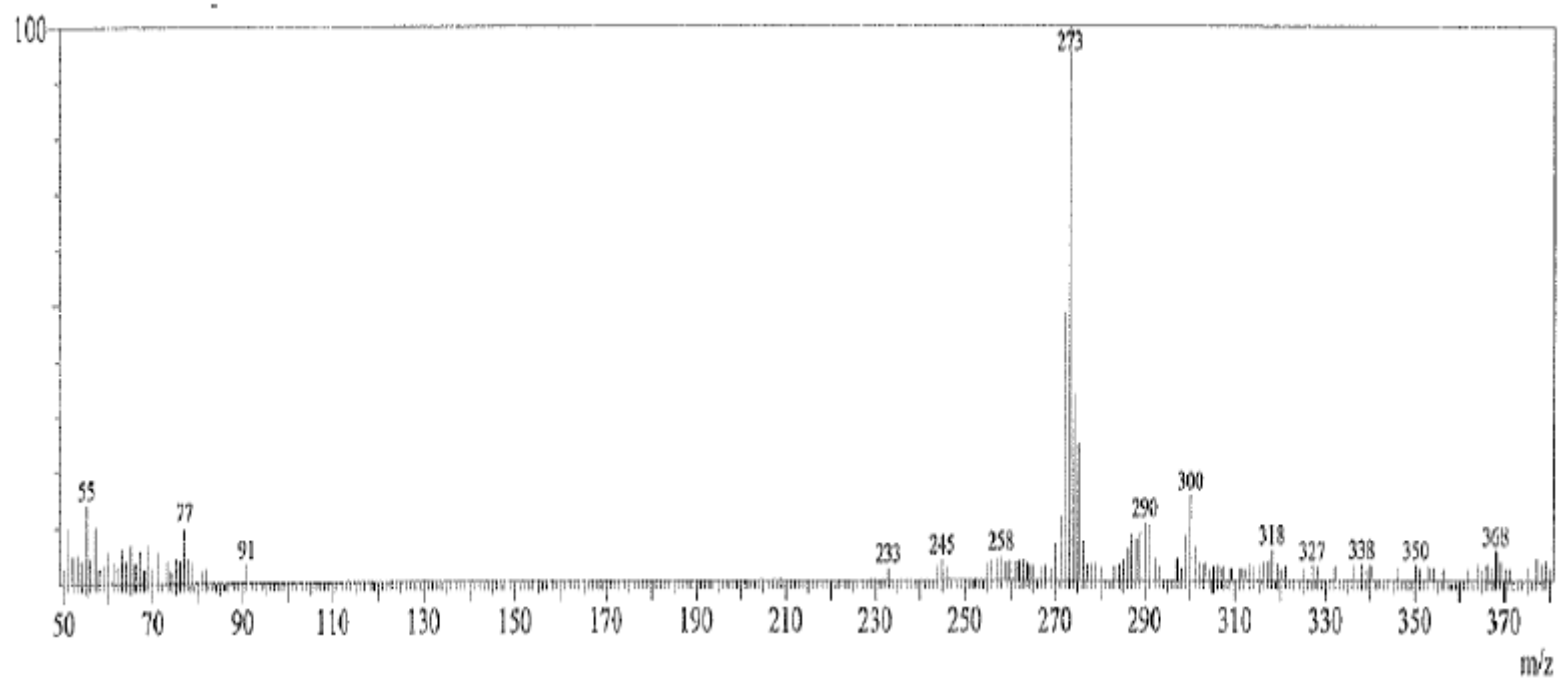


Figure S22: Mass spectrum of compound **5b**.

AmeralSayed-MS1-DMSO-C13

Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: DD5mm_test_12Mar2014-21:34:40
File: PROTON

Pulse Sequence: s2pu1
Solvent: DMSO
Ambient temperature
Mercury-300BB "NMR300"

Pulse 45.0 degrees
Acq. time 1.707 sec
Width 18761.7 Hz
2760 repetitions
OBSERVE C13, 75.4523920 MHz
DECOUPLE H1, 300.0702830 MHz
Power 34 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 21 hr, 47 min, 2 sec
Date: Jan 13 2020

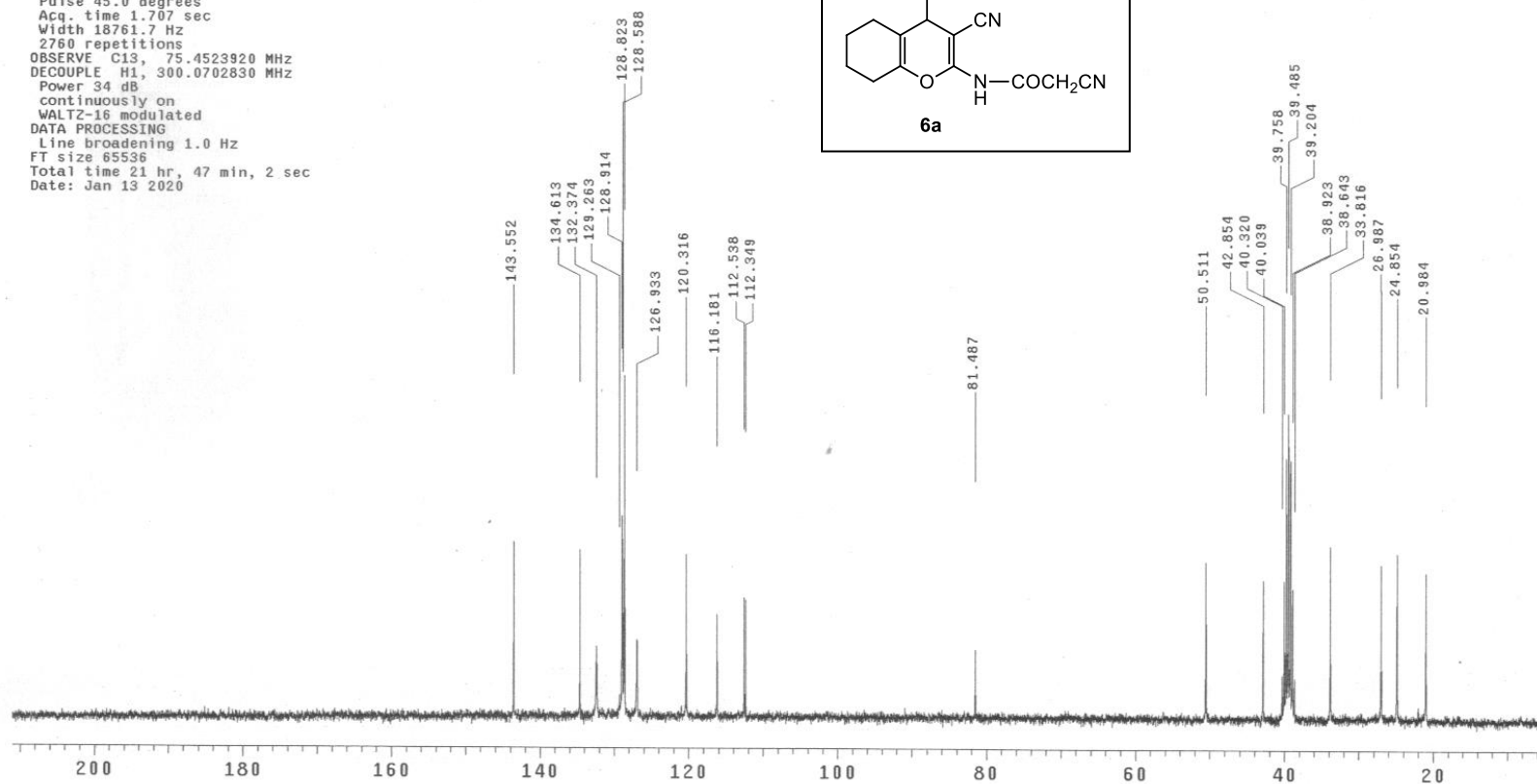
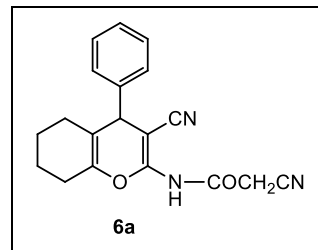


Figure S23: ^{13}C NMR spectrum of compound 6a.

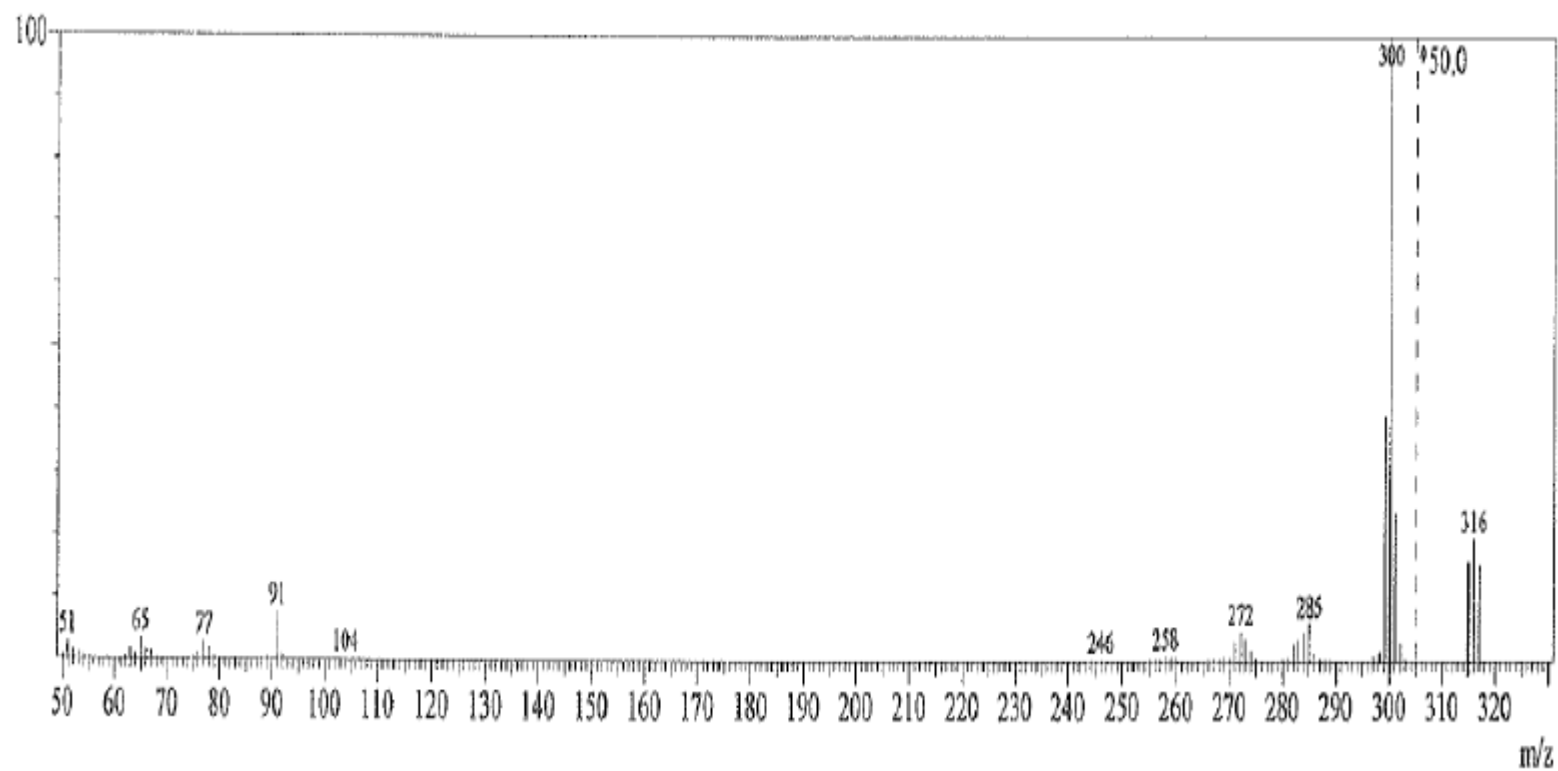


Figure S24: Mass spectrum of compound **6a**.

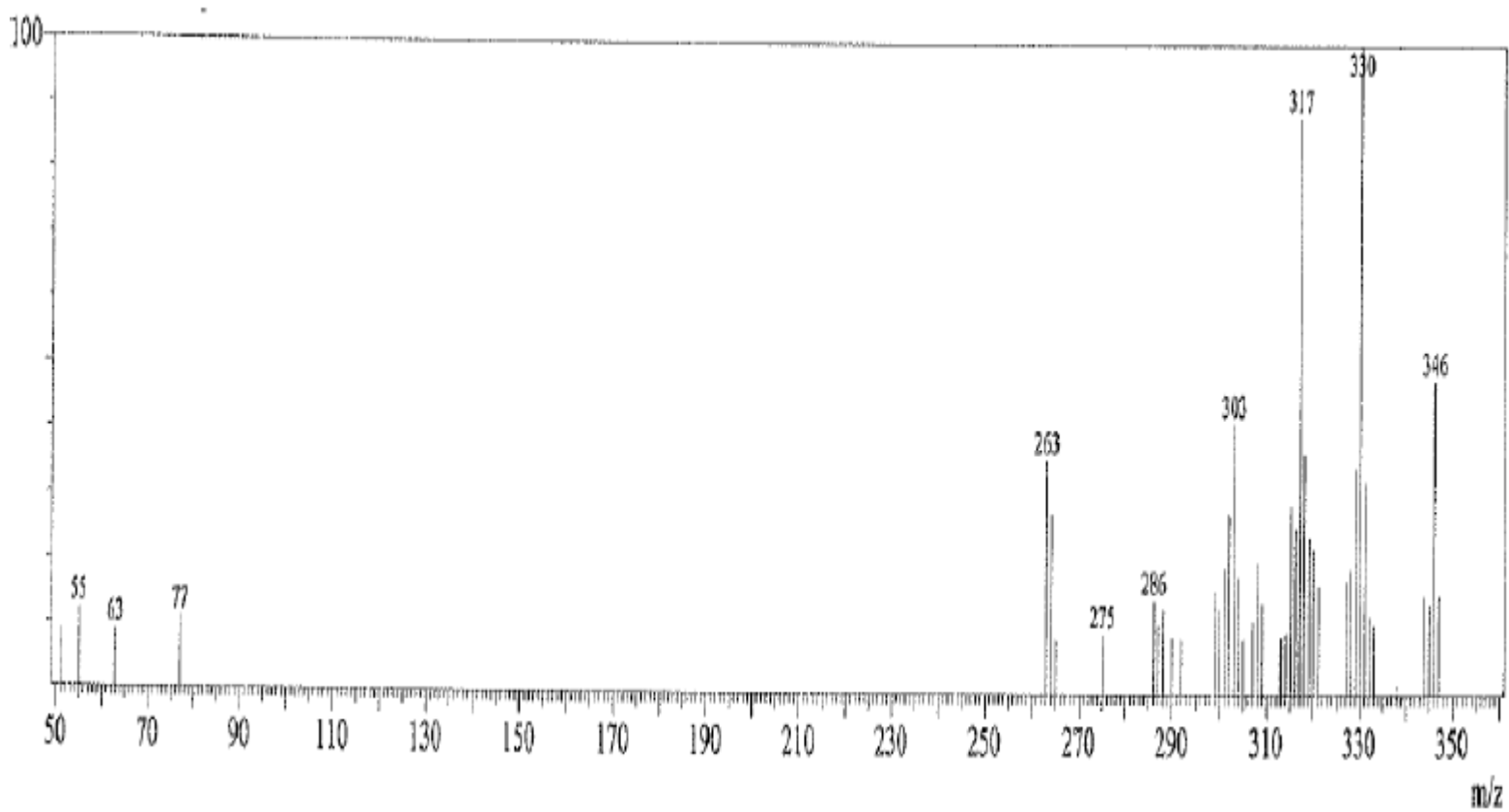


Figure S25: Mass spectrum of compound **6b**.

AmeeraAlSayed-MS10-DMSO-C13

Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: D05mm_test_12Mar2014-21:34:40
File: PROTON

Pulse Sequence: s2pu1

Solvent: DMSO
Ambient temperature
Mercury-300BB "NMR300"

Pulse 45.0 degrees
Acq. time 1.707 sec
Width 18761.7 Hz
2320 repetitions
OBSERVE C13, 75.4523937 MHz
DECOUPLE H1, 300.0702830 MHz
Power 34 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 21 hr, 47 min, 2 sec
Date: Feb 3 2020

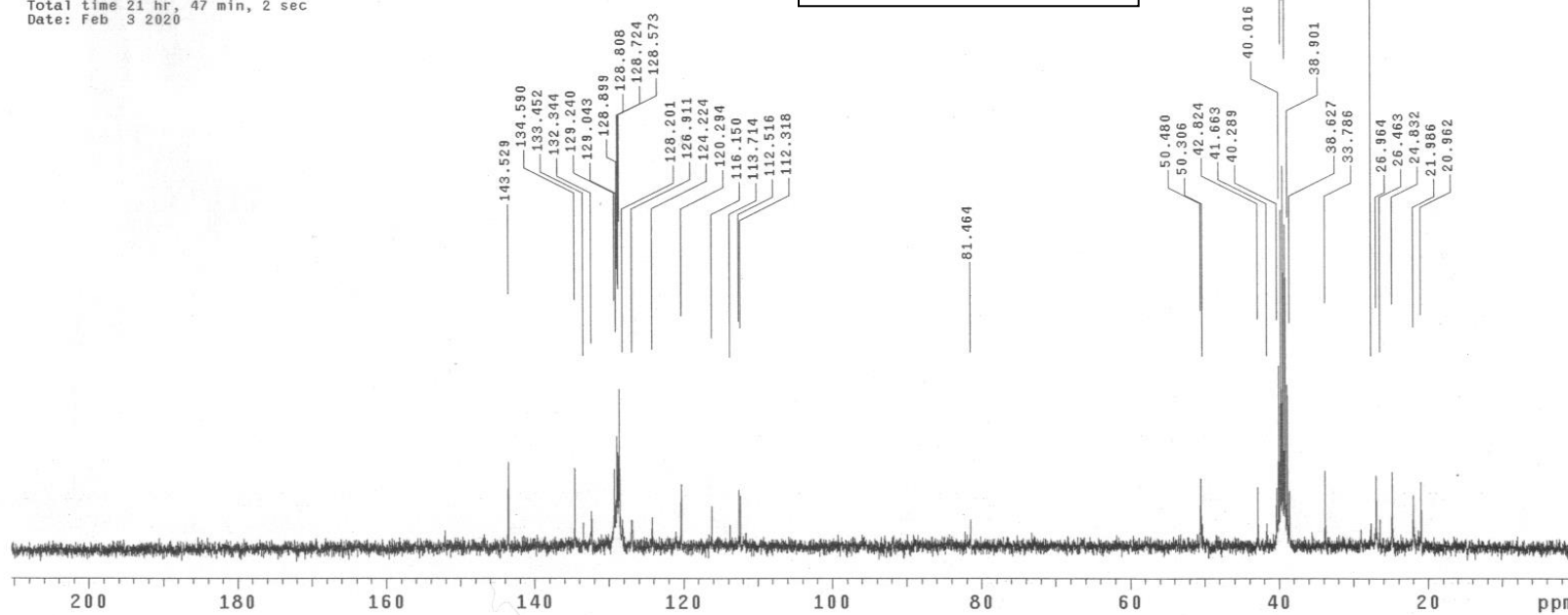
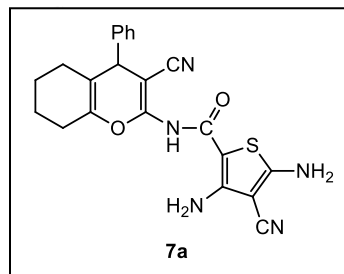


Figure S26: ¹³C NMR spectrum of compound 7a.

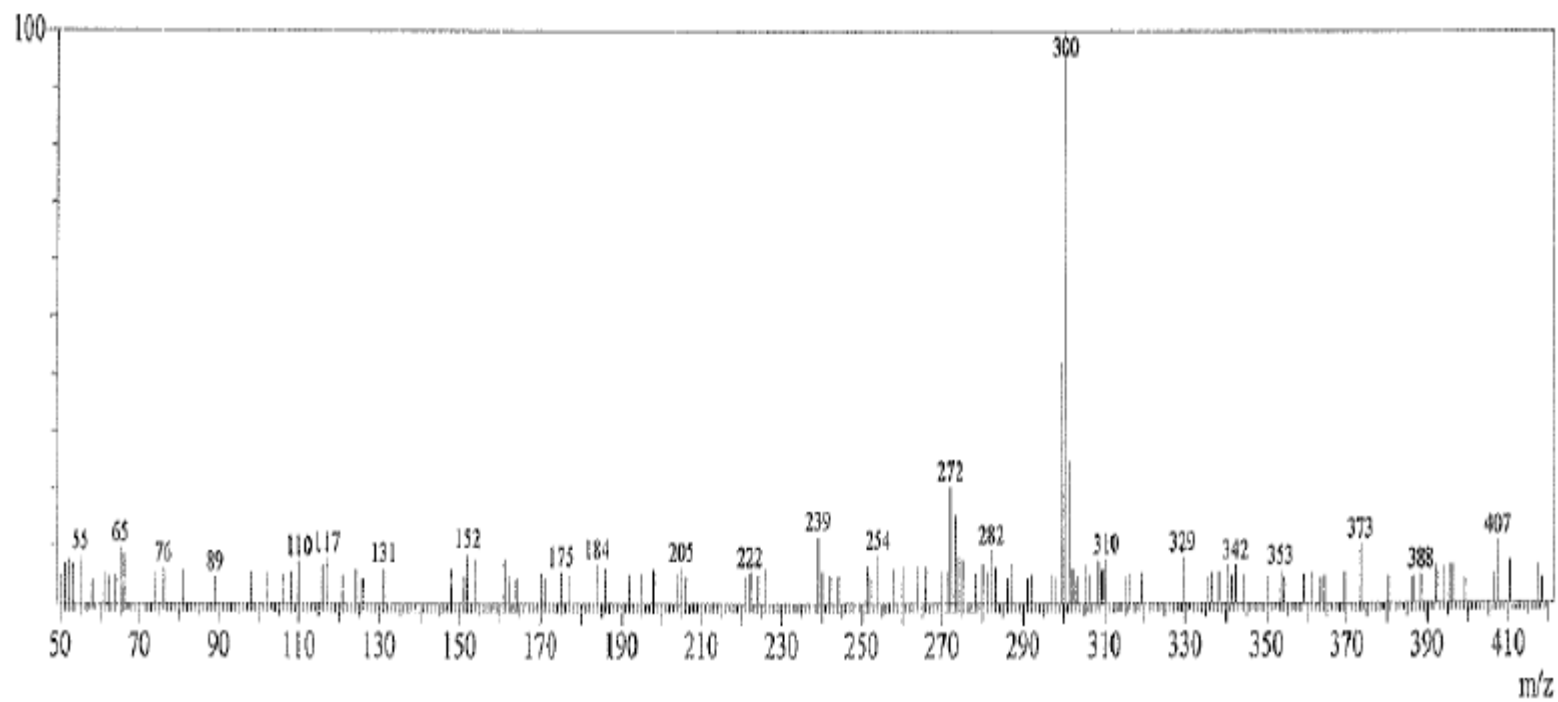
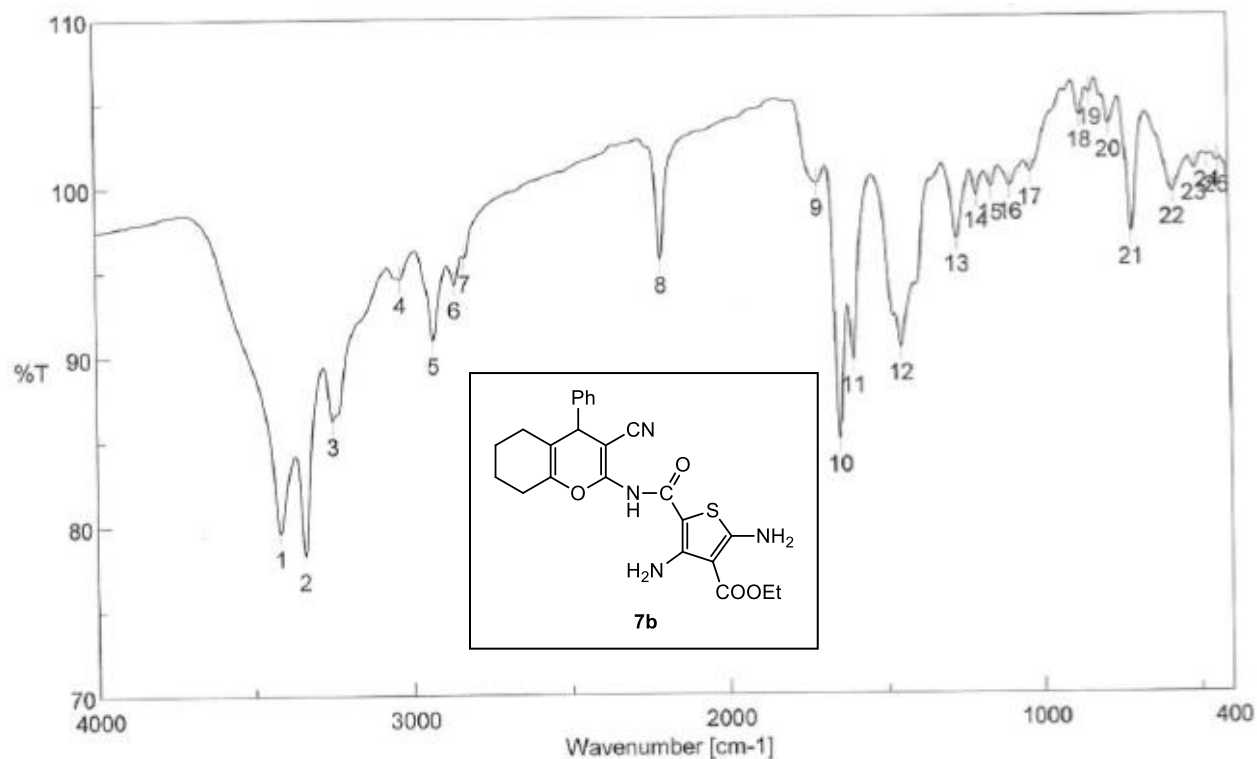


Figure S27: Mass spectrum of compound **7a**.



[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1	3418.21	79.6287	2	3340.1	78.2855	3	3251.4	86.2487
4	3035.41	94.5687	5	2933.2	90.9642	6	2864.74	94.2377
7	2831.95	95.8217	8	2209.06	95.6575	9	1709.59	100.143
10	1645.95	85.0313	11	1601.59	89.6972	12	1450.21	90.4214
13	1271.82	96.7864	14	1207.22	99.3675	15	1160.94	99.8256
16	1100.19	99.8804	17	1033.66	100.718	18	874.56	104.076
19	840.812	105.406	20	781.029	103.499	21	710.64	97.1546
22	579.504	99.4986	23	508.151	100.899	24	466.689	101.616
25	435.834	101.334						

Figure S28: IR spectrum of compound **7b**.

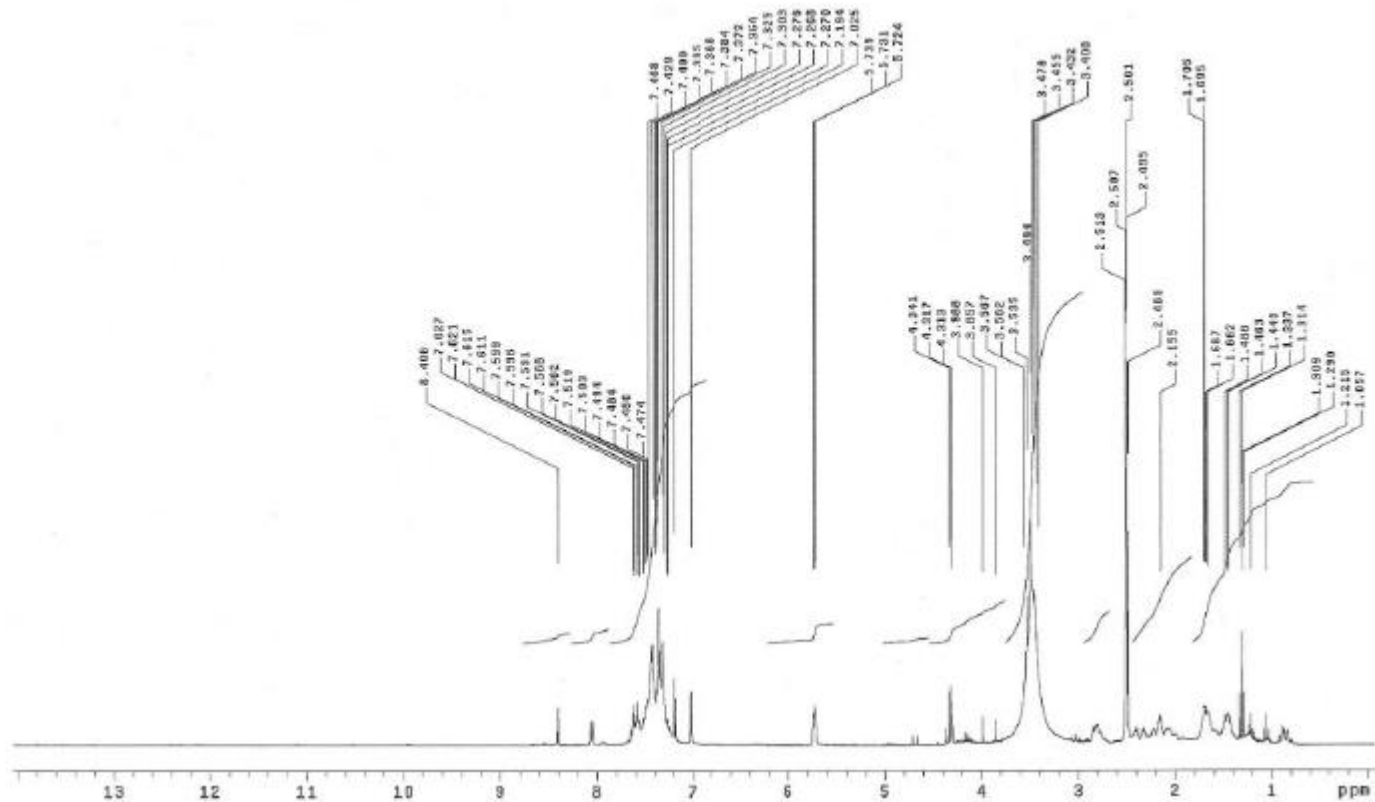


Figure S29: ¹H NMR spectrum of compound **7b**.

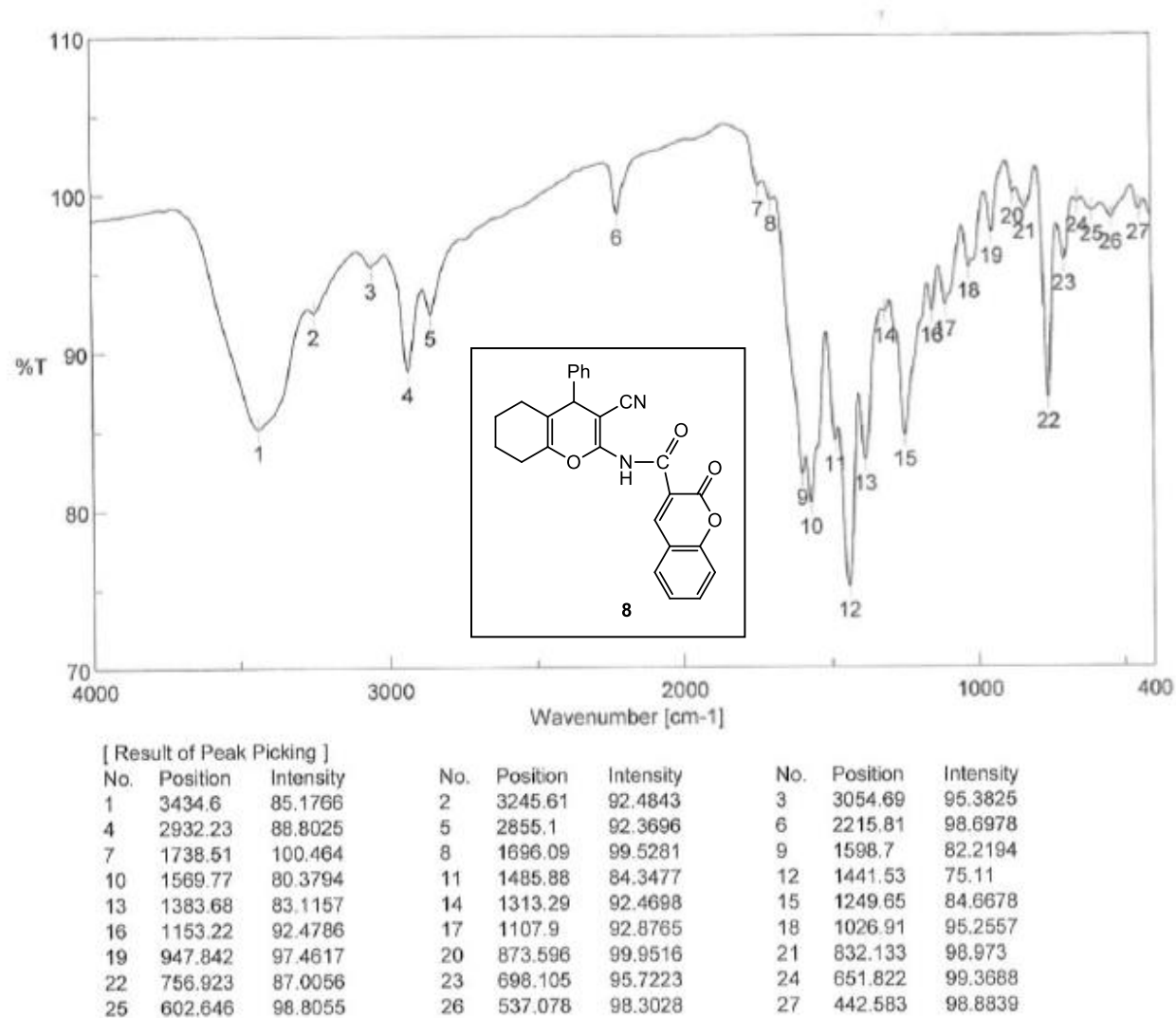


Figure S30: IR spectrum of compound **8**.

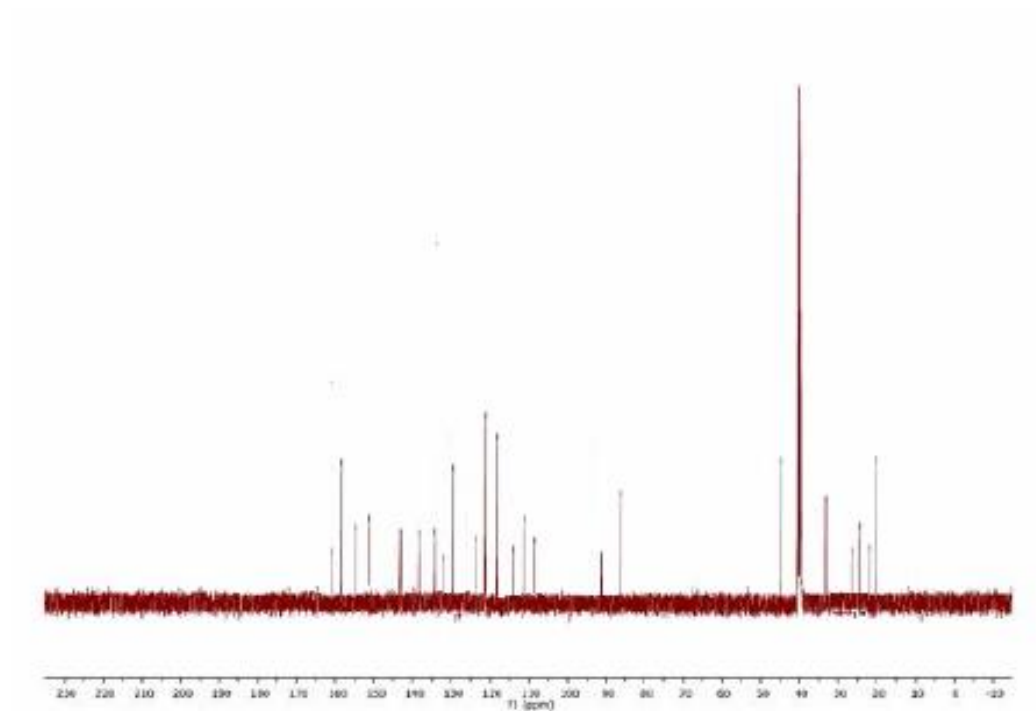


Figure S31: ^{13}C NMR spectrum of compound **8**.

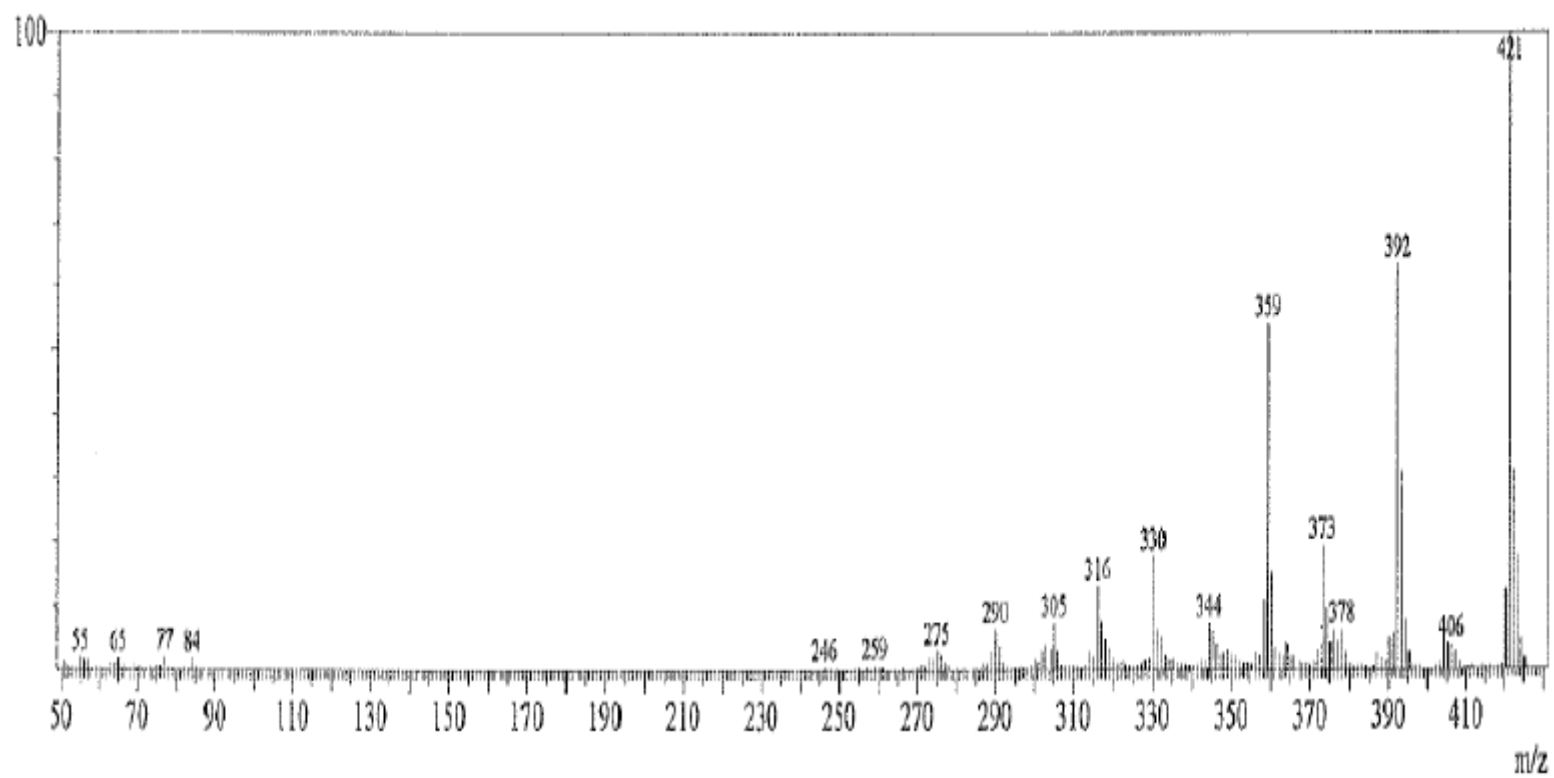


Figure S32: Mass spectrum of compound **8**.

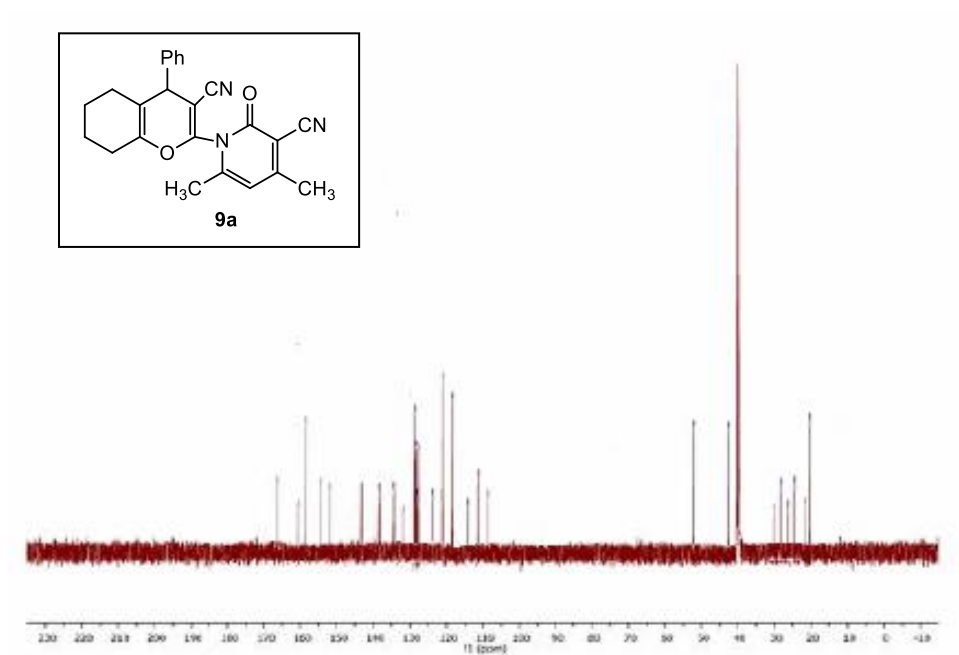


Figure S33: ^{13}C NMR spectrum of compound **9a**.

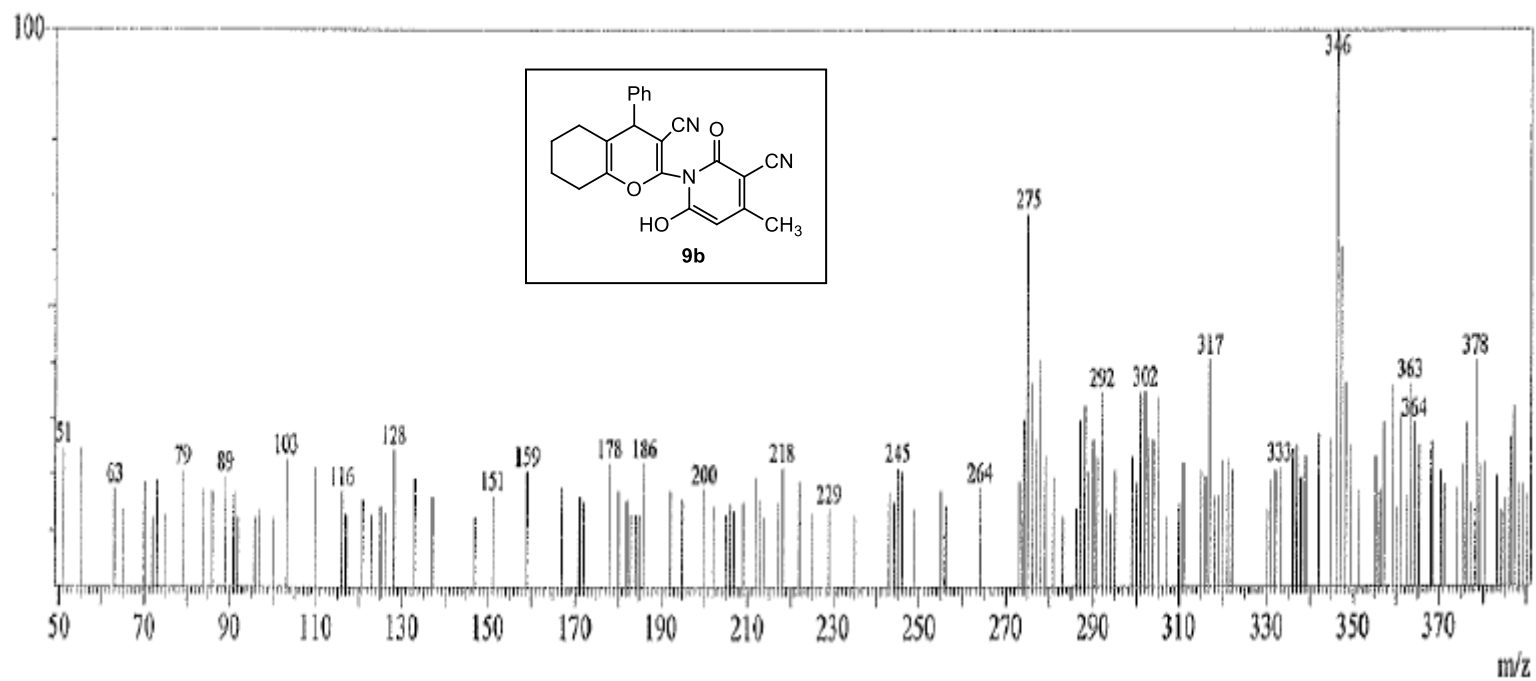


Figure S34: Mass spectrum of compound **9b**.

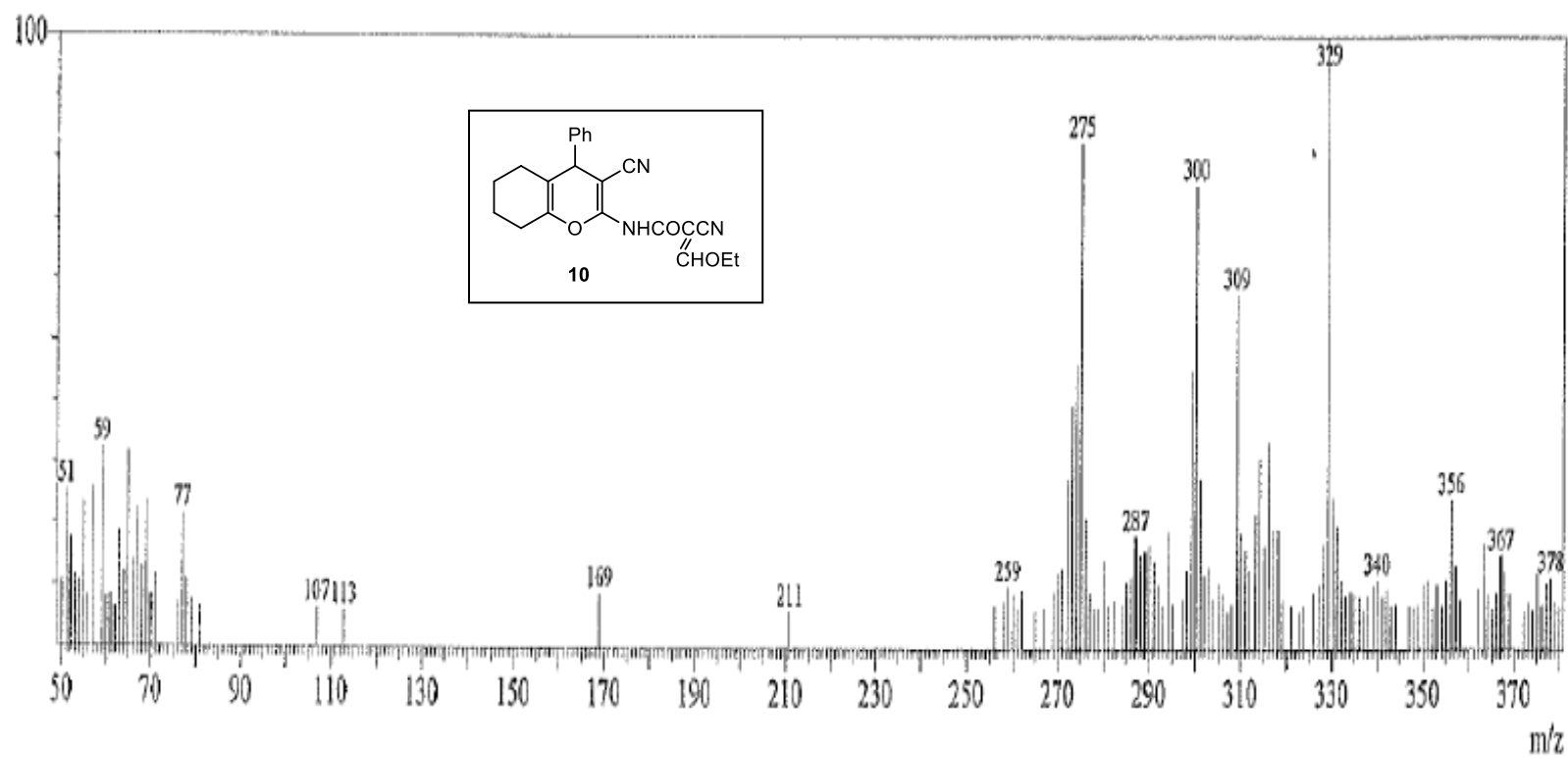


Figure S35: Mass spectrum of compound **10**.

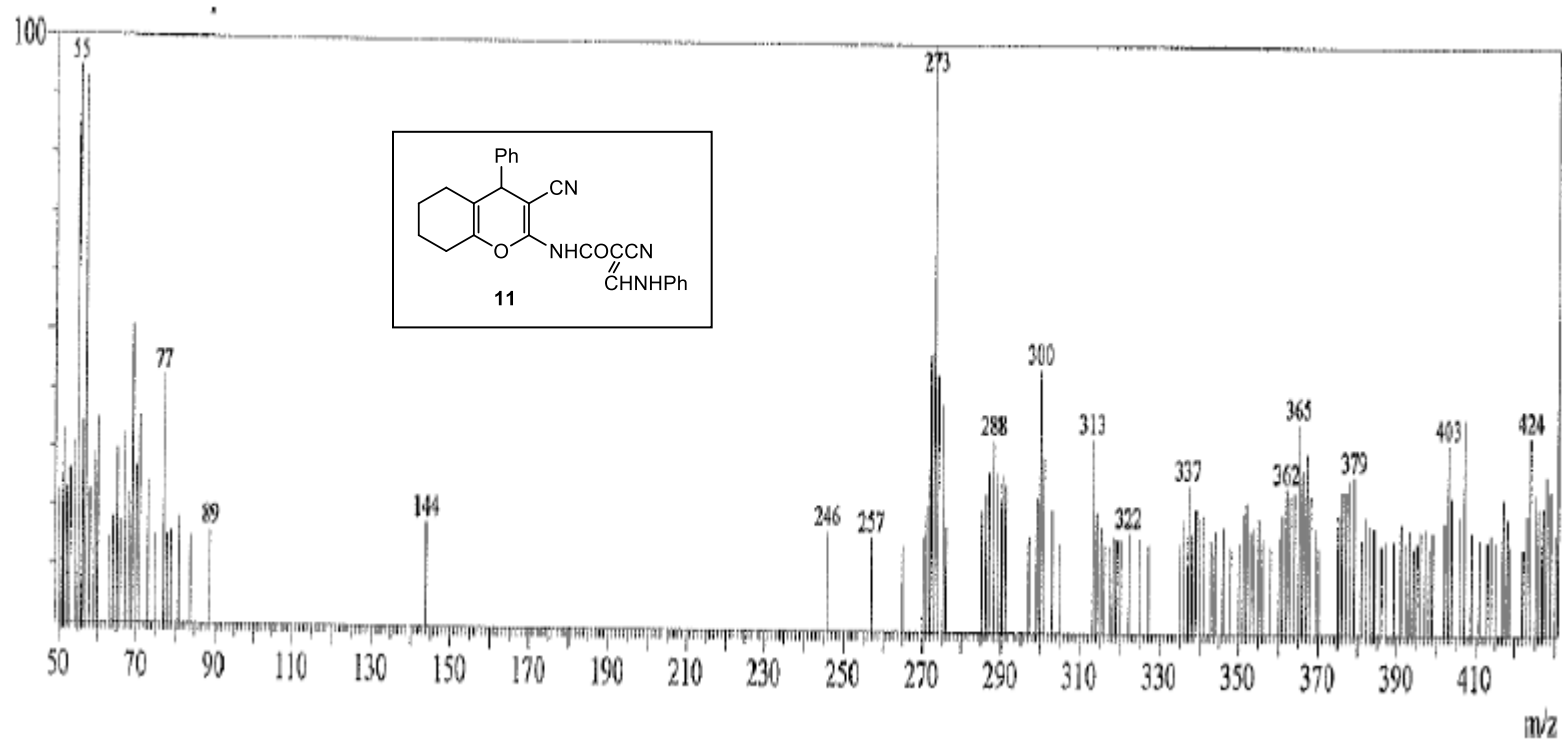


Figure S36: Mass spectrum of compound **11**.

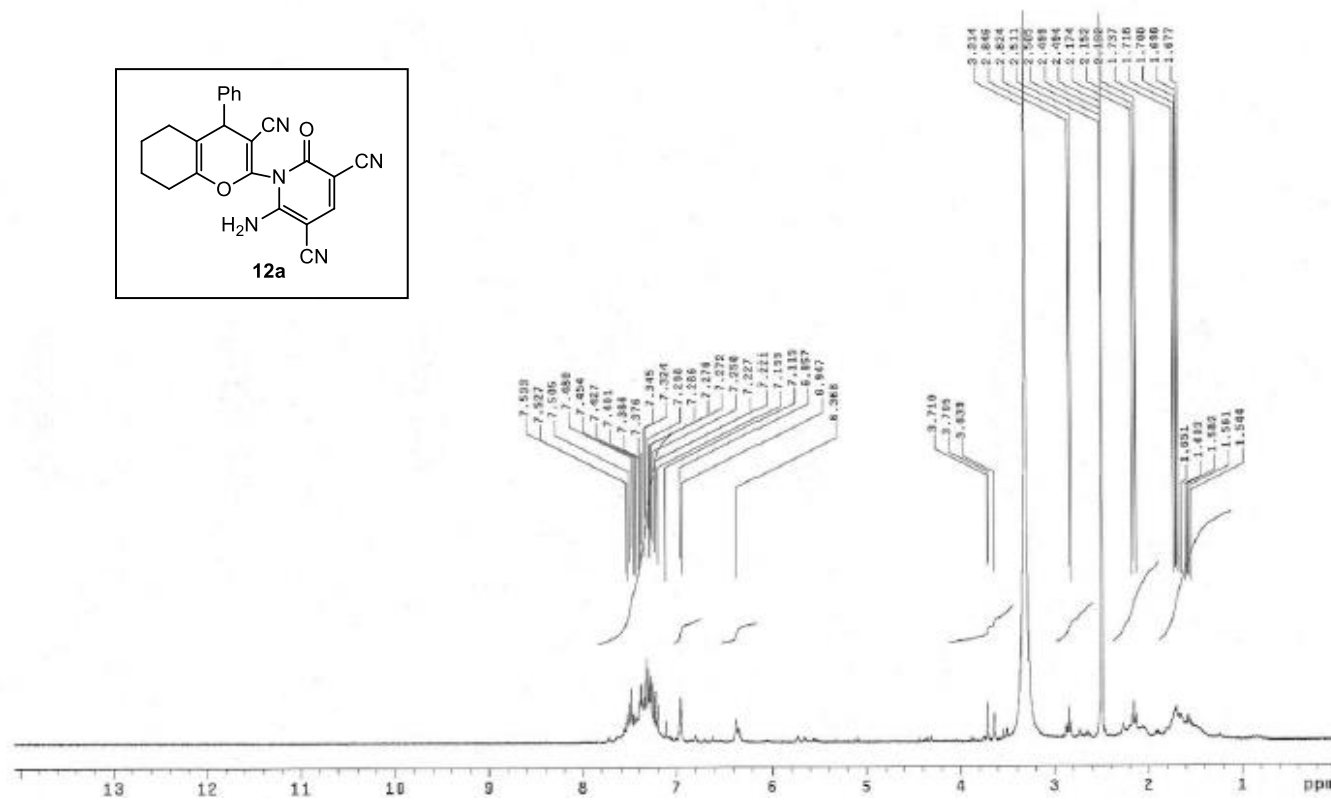


Figure S37: ¹H NMR spectrum of compound **12a**.

AmeraE1Sayed-MS18C-DMSO-C13

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Sample directory: D05mm_test_12Mar2014-21:34:40
File: PROTON

Pulse Sequence: s2pu1

Solvent: DMSO
Ambient temperature
Mercury-300BB "NMR300"

Pulse 45.0 degrees
Acq. time 1.707 sec
Width 18761.7 Hz
3640 repetitions
OBSERVE C13, 75.4523885 MHz
DECOUPLE H1, 300.0702830 MHz
Power 34 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 21 hr, 47 min, 2 sec
Date: Feb 20 2020

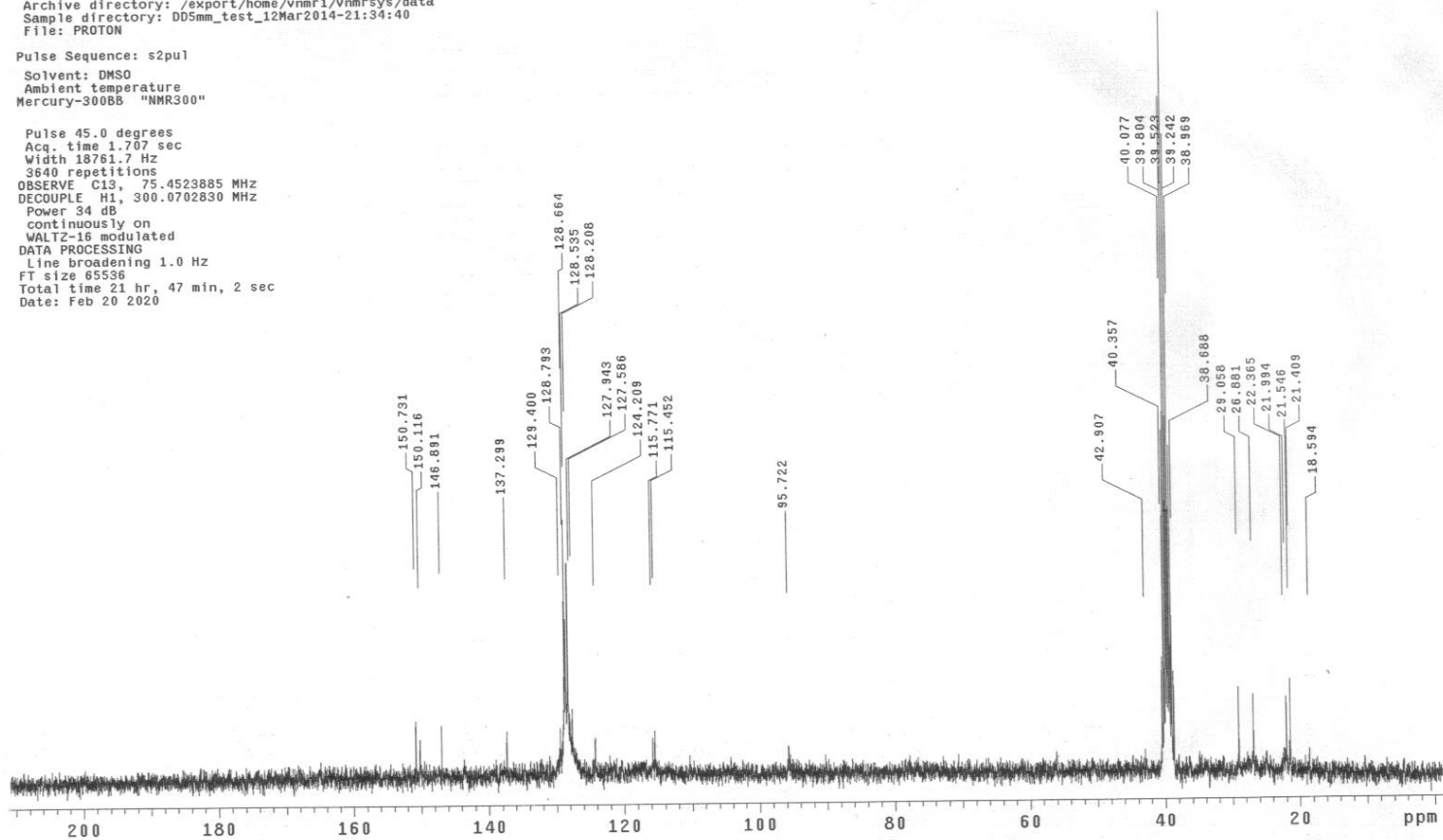


Figure S38: ^{13}C NMR spectrum of compound 12a.

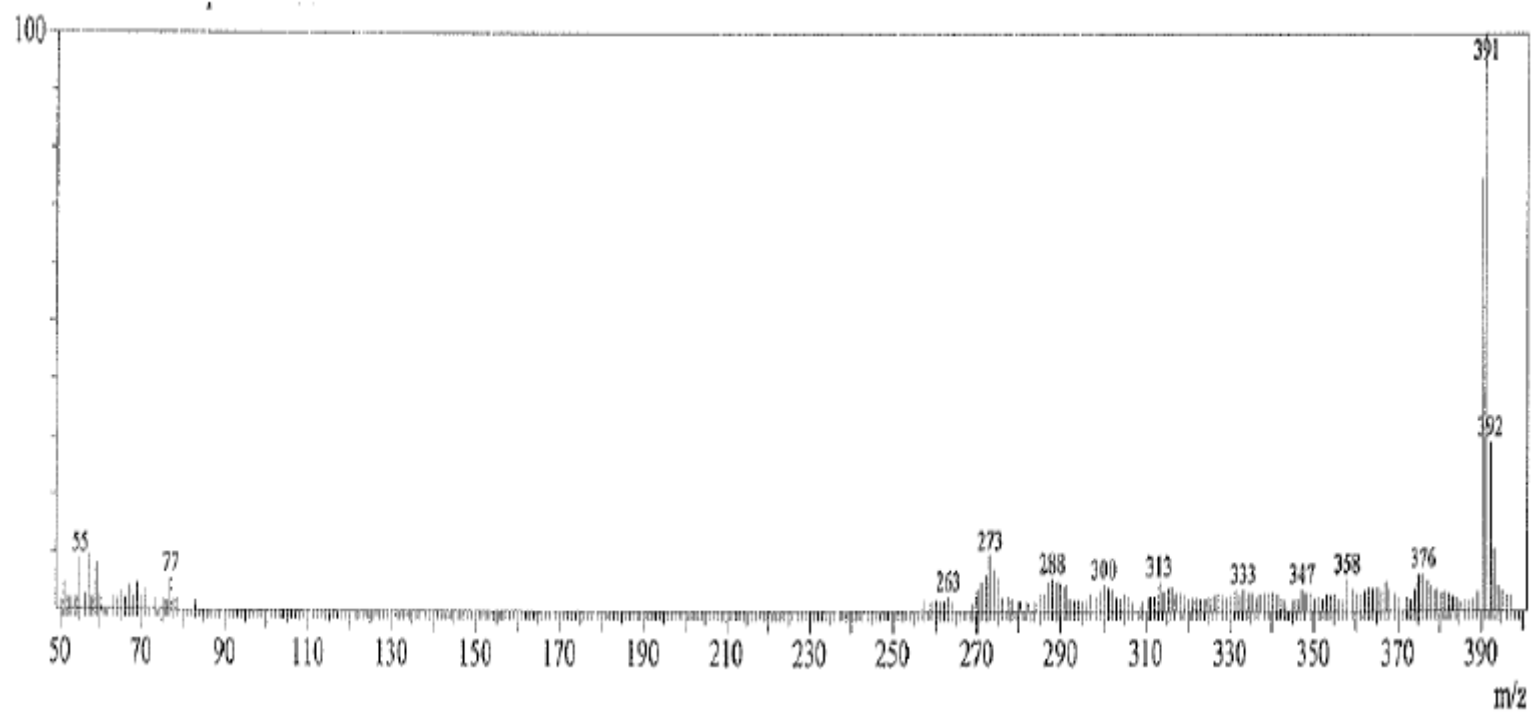


Figure S39: Mass spectrum of compound **12a**.

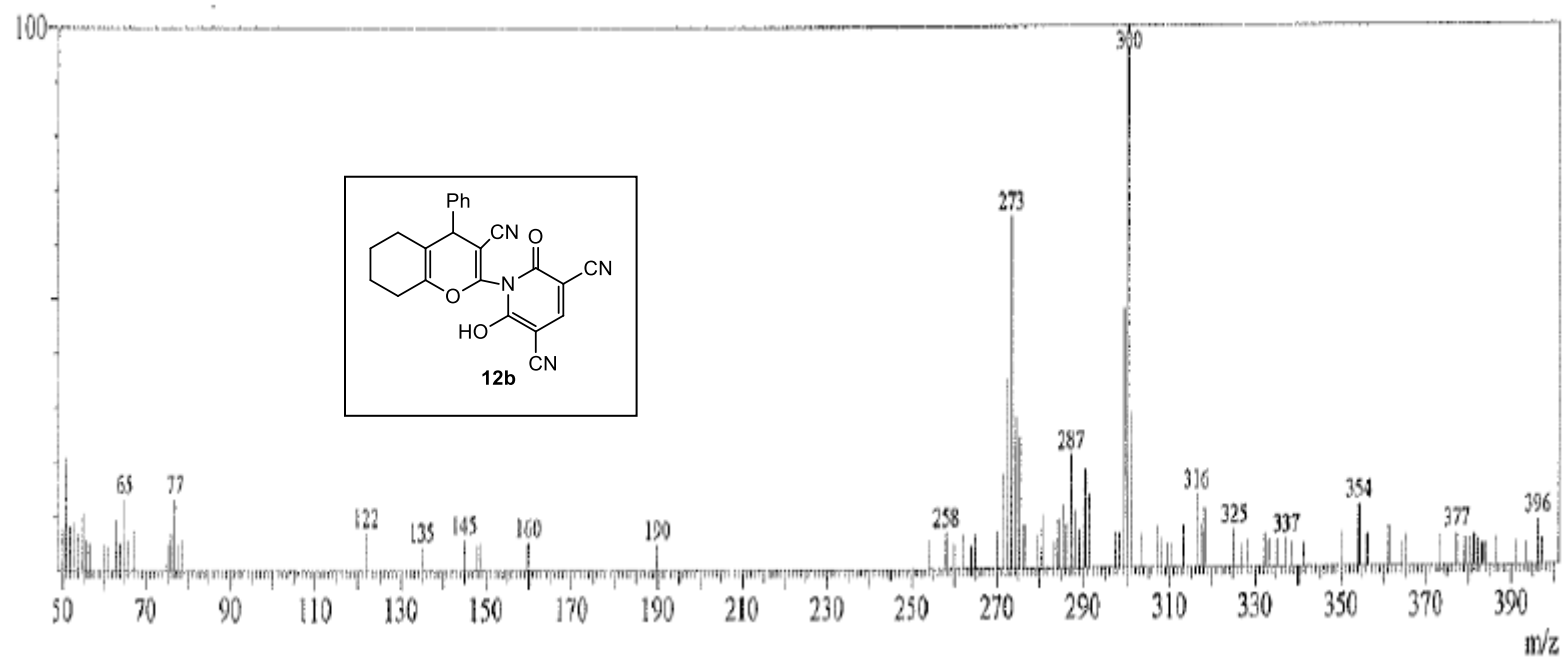


Figure S40: Mass spectrum of compound **12b**.