

Supplementary Material

Heteroannulation of cyclic ketones: Synthesis, characterization and antitumor evaluation of some condensed azine derivatives

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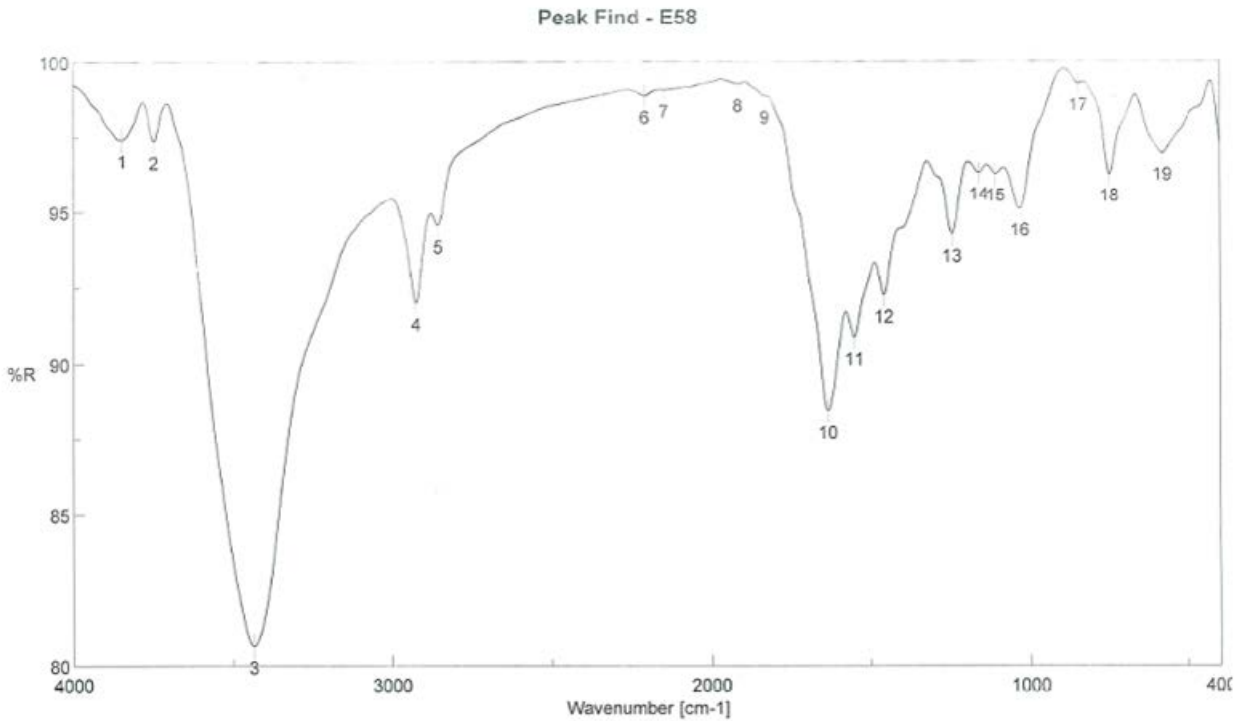
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Running Title: Heteroannulation of cyclic ketones.

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- 5- Antitumor evaluation S1



[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1	3847.29	97.4132	2	3747.01	97.36	3	3434.6	80.6656	4	2925.48	92.0129
5	2856.06	94.5459	6	2208.09	98.8739	7	2147.35	99.0681	8	1915.93	99.2567
9	1832.04	98.8647	10	1635.34	88.4186	11	1552.42	90.8622	12	1458.89	92.258
13	1245.79	94.2393	14	1160.94	96.308	15	1108.87	96.2701	16	1032.69	95.092
17	848.525	99.2763	18	751.138	96.2474	19	585.29	96.9564			

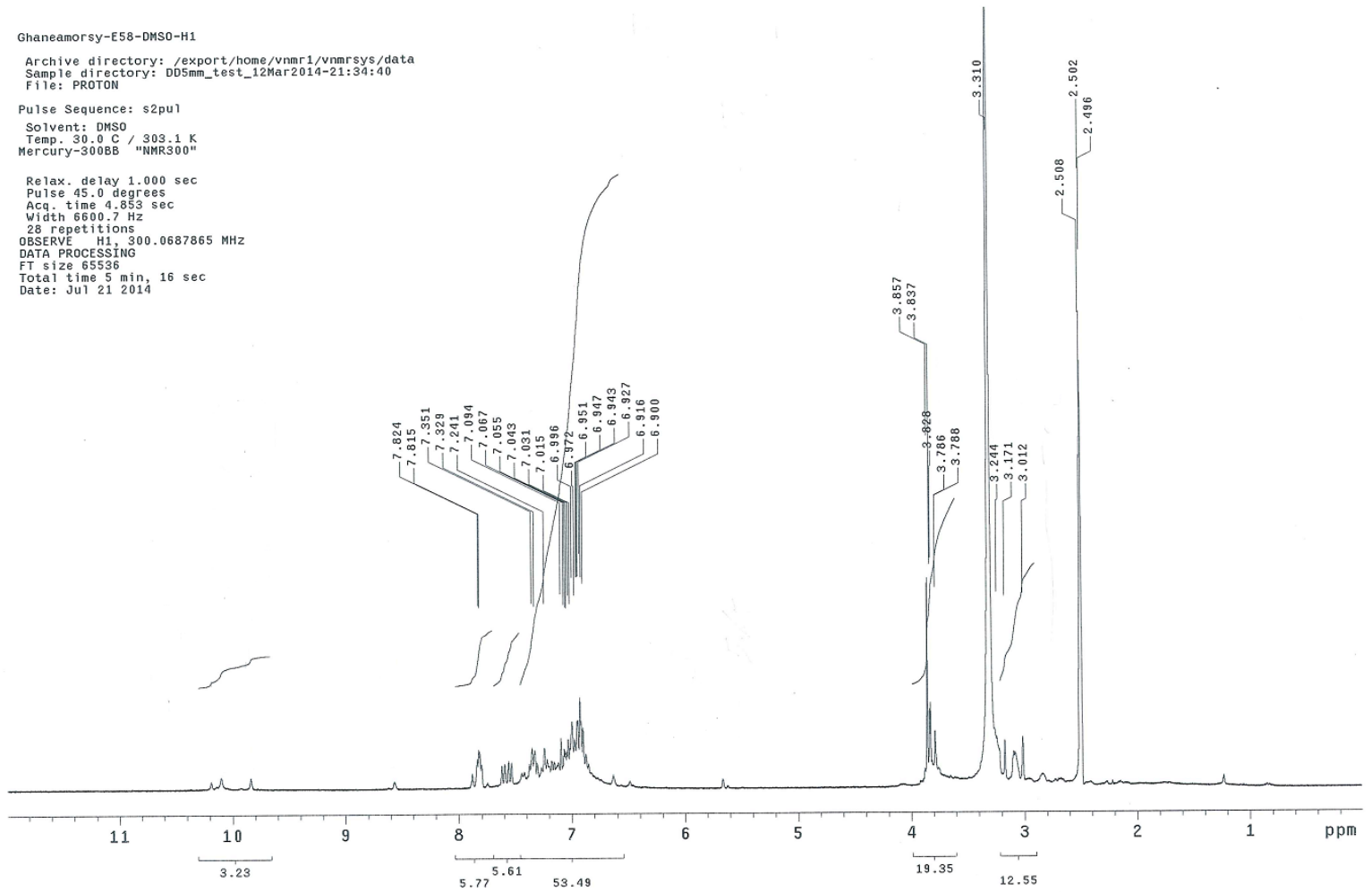
S1. IR spectrum (KBr, cm⁻¹) of compound 1

Ghaneamorsy-E58-DMSO-H1

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Sample directory: DD5mm_test_12Mar2014-21:34:40
File: PROTON

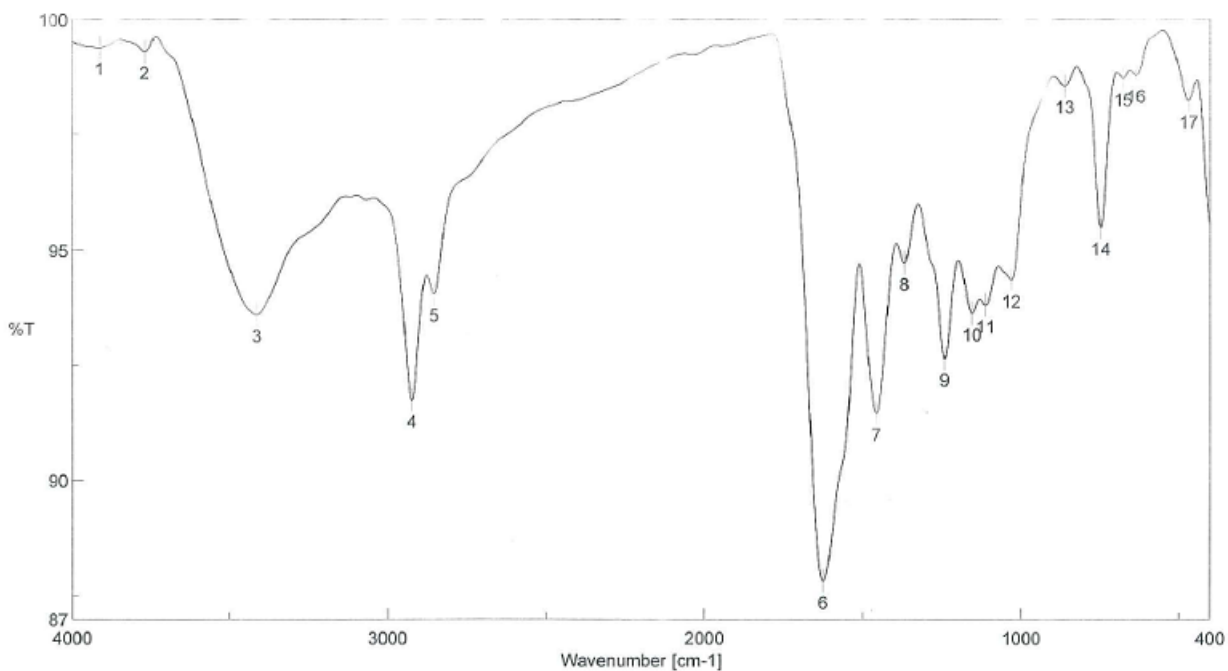
Pulse Sequence: s2pu1
Solvent: DMSO
Temp. 30.0 C / 303.1 K
Mercury-300BE "NMR300"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 4.853 sec
Width 6600.7 Hz
28 repetitions
OBSERVE H1, 300.0687865 MHz
DATA PROCESSING
F1 size 65536
Total time 5 min, 16 sec
Date: Jul 21 2014



S1. ^1H NMR spectrum (300 MHz, DMSO- d_6) of compound 1

Peak Find - E38b



[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1	3913.82	99.38125	2	3768.22	99.29530	3	3414.35	93.59963	4	2924.52	91.74218
5	2854.13	94.05332	6	1626.66	87.82288	7	1458.89	91.45398	8	1371.14	94.72494
9	1243.86	92.64562	10	1157.08	93.63259	11	1113.69	93.81184	12	1031.73	94.35777
13	863.953	98.54805	14	750.174	95.48965	15	677.856	98.70455	16	634.466	98.78675
17	468.617	98.22250									

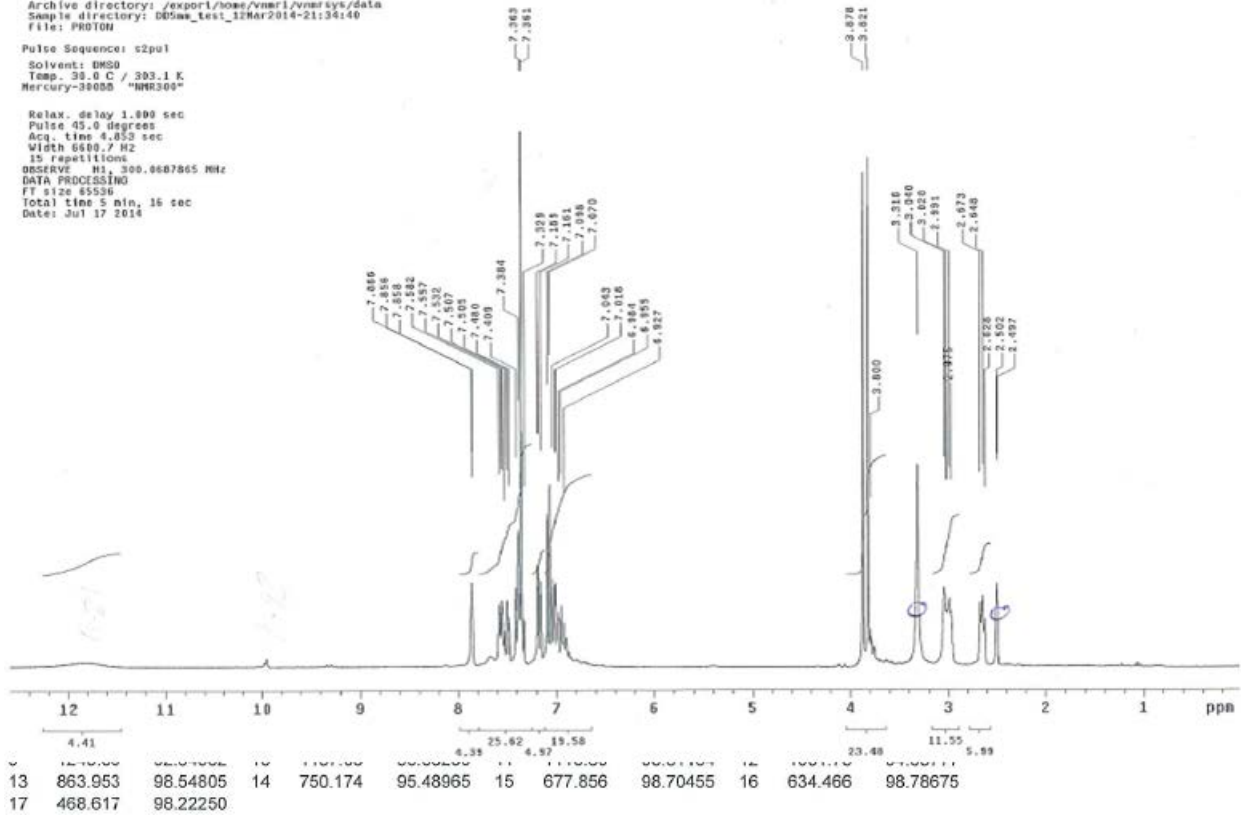
S2. IR spectrum (KBr, cm^{-1}) of compound 2

OhaneMorsy-E38b-DMSO-H1

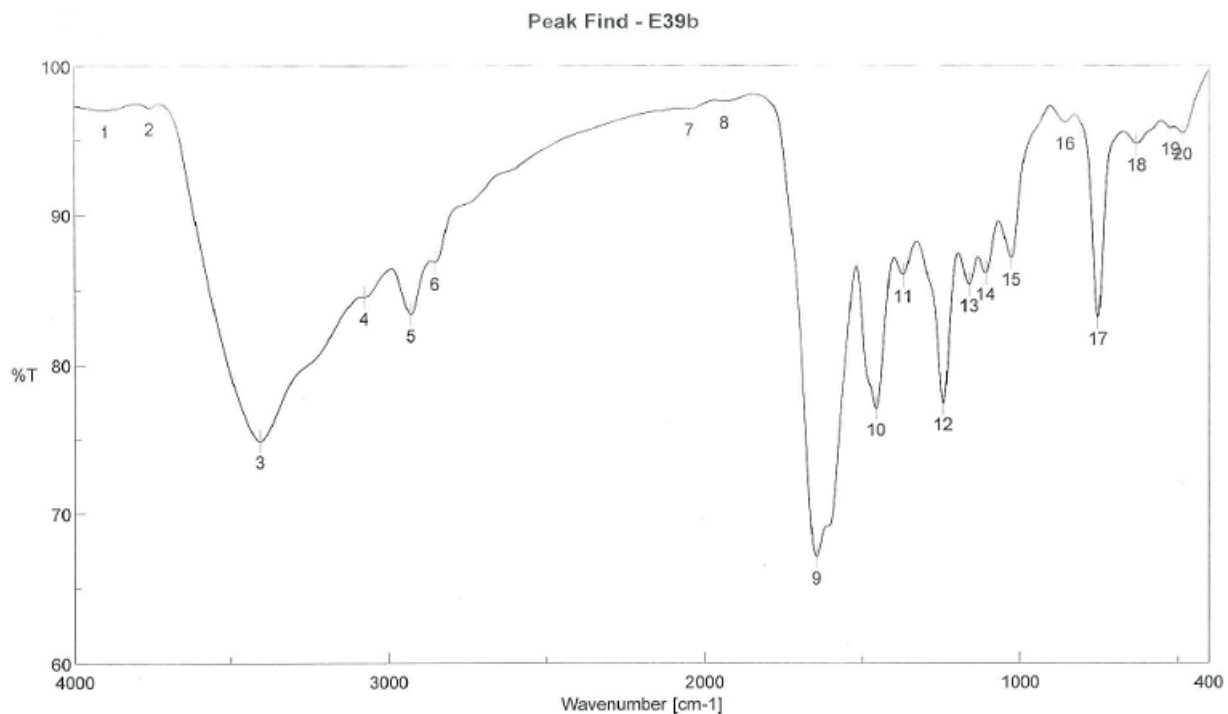
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Pulse Sequence: c2pu1
Solvent: DMSO
Temp: 30.0 C / 303.1 K
Mercury-30000 "WB300"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 4.853 sec
Width 6600.7 Hz
15 repetitions
OBSERVE N1, 300.0607865 MHz
DATA PROCESSING
FT size 85536
Total time 5 min, 16 sec
Date: Jul 17 2014



S2. ^1H NMR spectrum (300 MHz, $\text{DMSO-}d_6$) of compound 2



[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1	3902.25	97.00059	2	3756.65	97.18465	3	3408.57	74.87576	4	3076.87	84.51416
5	2930.31	83.37090	6	2854.13	86.81596	7	2048.03	97.10632	8	1938.11	97.59274
9	1646.91	67.07902	10	1457.92	77.05126	11	1372.1	85.98828	12	1244.83	77.40685
13	1162.87	85.35078	14	1110.8	86.12634	15	1028.84	87.11177	16	857.204	96.16417
17	754.995	83.16129	18	632.537	94.72434	19	521.65	95.79539	20	482.117	95.46081

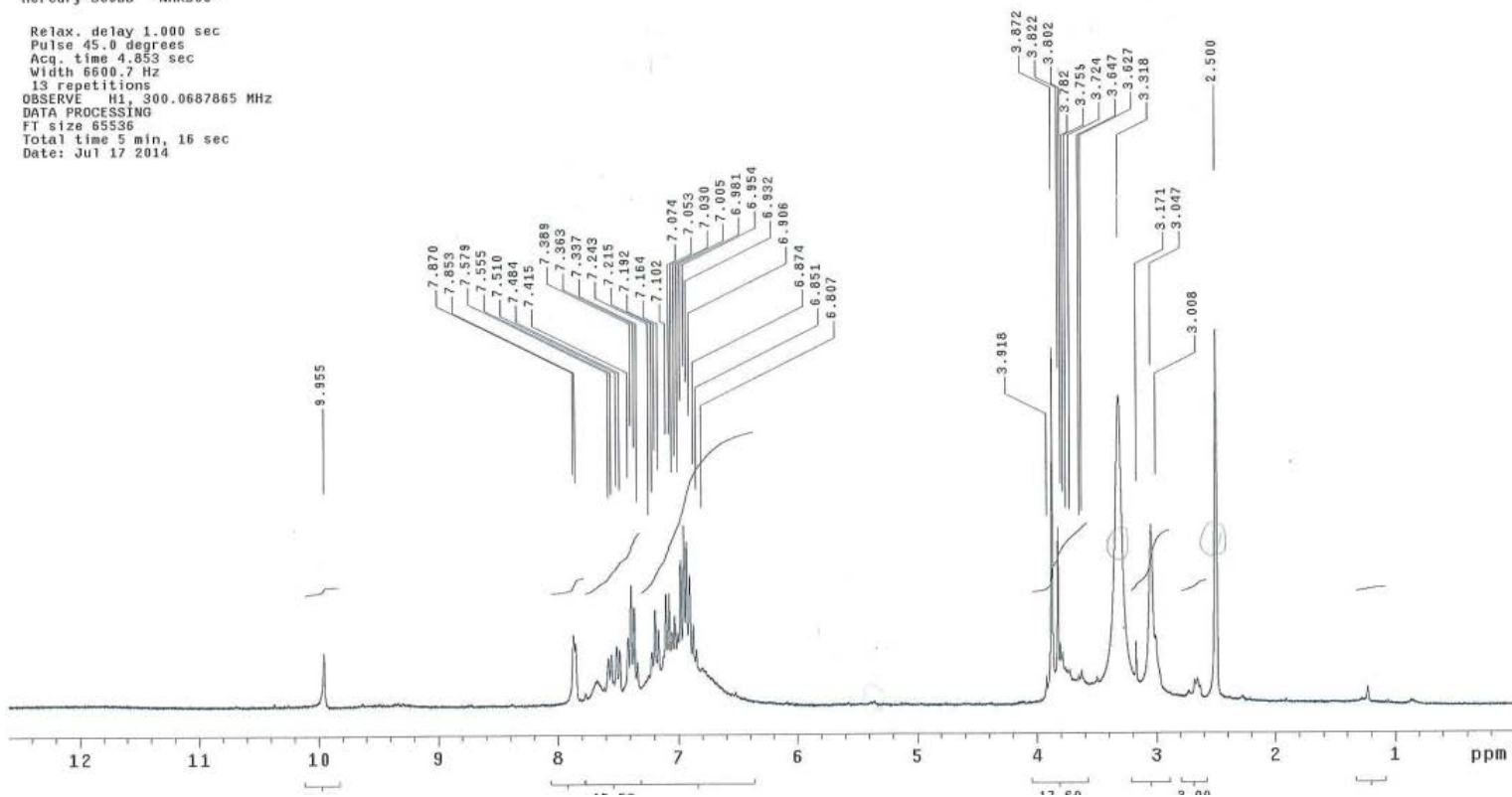
S3. IR spectrum (KBr, cm^{-1}) of compound 3

GhaneaMorsy-E39-DMSO-H1

Archive directory: /export/home/vnmr1/vnmrsys/data
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File: PROTON

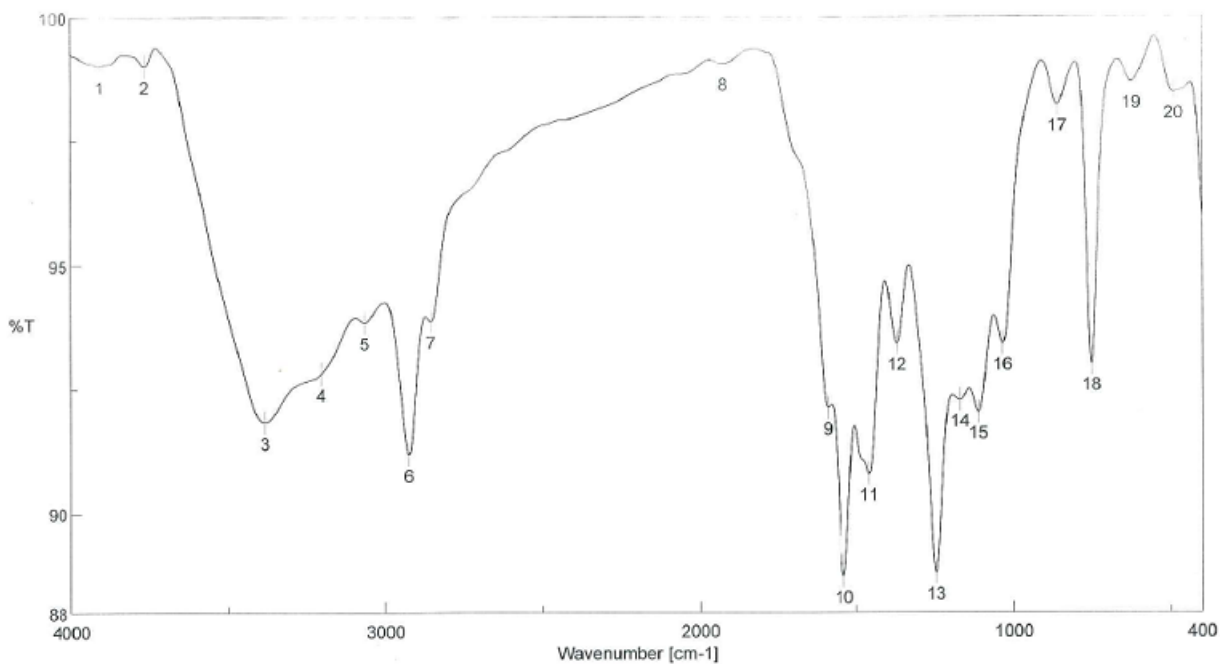
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Solvent: DMSO
Temp. 30.0 C / 303.1 K
Mercury-300BB "NMR300"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 4.853 sec
Width 6600.7 Hz
13 repetitions
OBSERVE H1, 300.0687865 MHz
DATA PROCESSING
F1 size 65536
Total time 5 min, 16 sec
Date: Jul 17 2014



S3. ^1H NMR spectrum (300 MHz, $\text{DMSO-}d_6$) of compound 3

Peak Find - E42



[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1	3907.07	99.01012	2	3764.37	99.01149	3	3383.5	91.82668	4	3205.11	92.81360
5	3086.26	93.84957	6	2925.48	91.17941	7	2857.02	93.87572	8	1928.47	99.04805
9	1592.91	92.11518	10	1541.81	88.72799	11	1459.85	90.78204	12	1371.14	93.42548
13	1244.83	88.80092	14	1170.58	92.28146	15	1112.73	92.03979	16	1035.59	93.43228
17	862.025	98.22542	18	752.102	93.02040	19	626.752	98.69072	20	491.759	98.47909

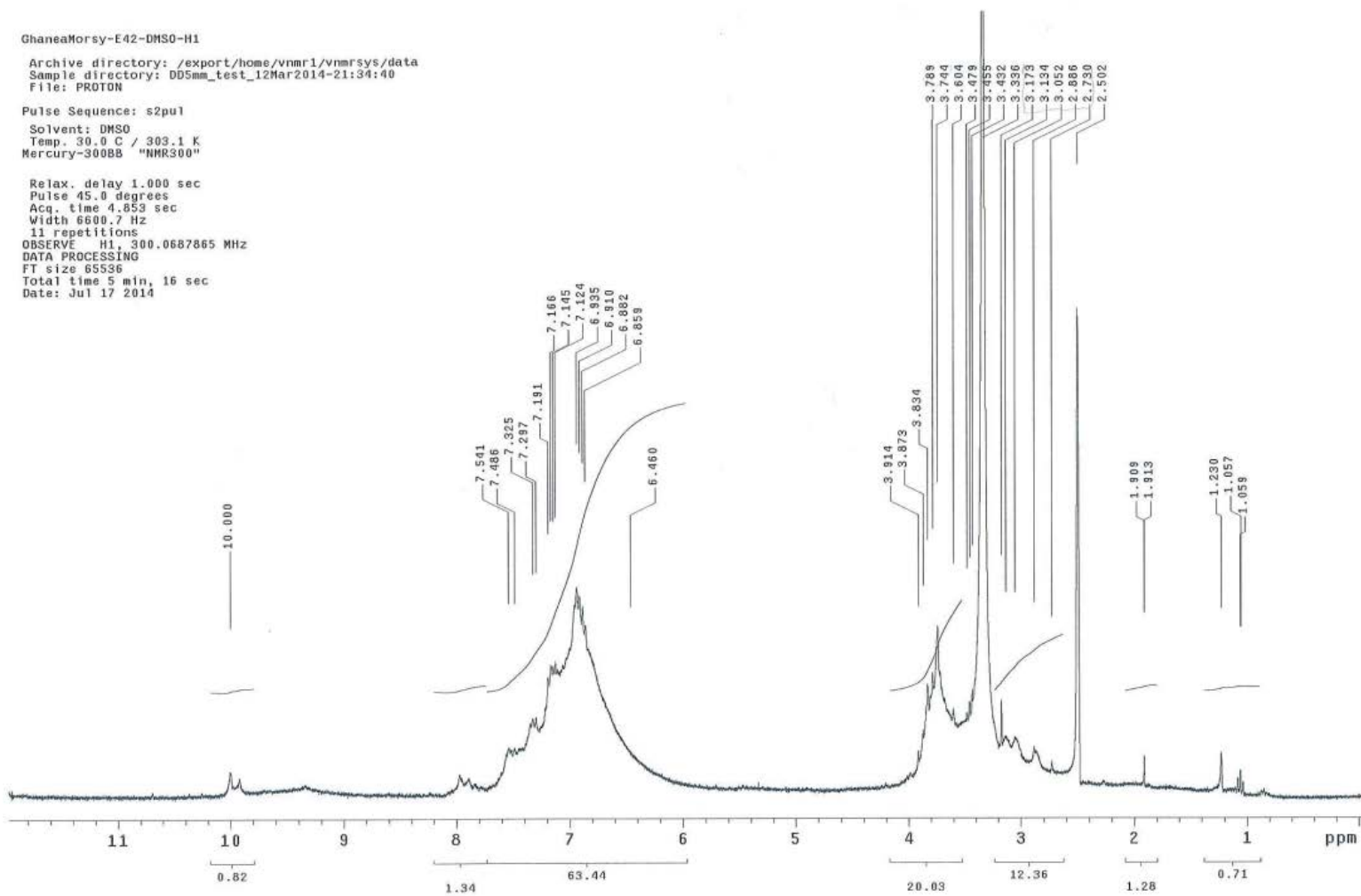
S4. IR spectrum (KBr, cm⁻¹) of compound 4

GhaneaMorsy-E42-DMSO-H1

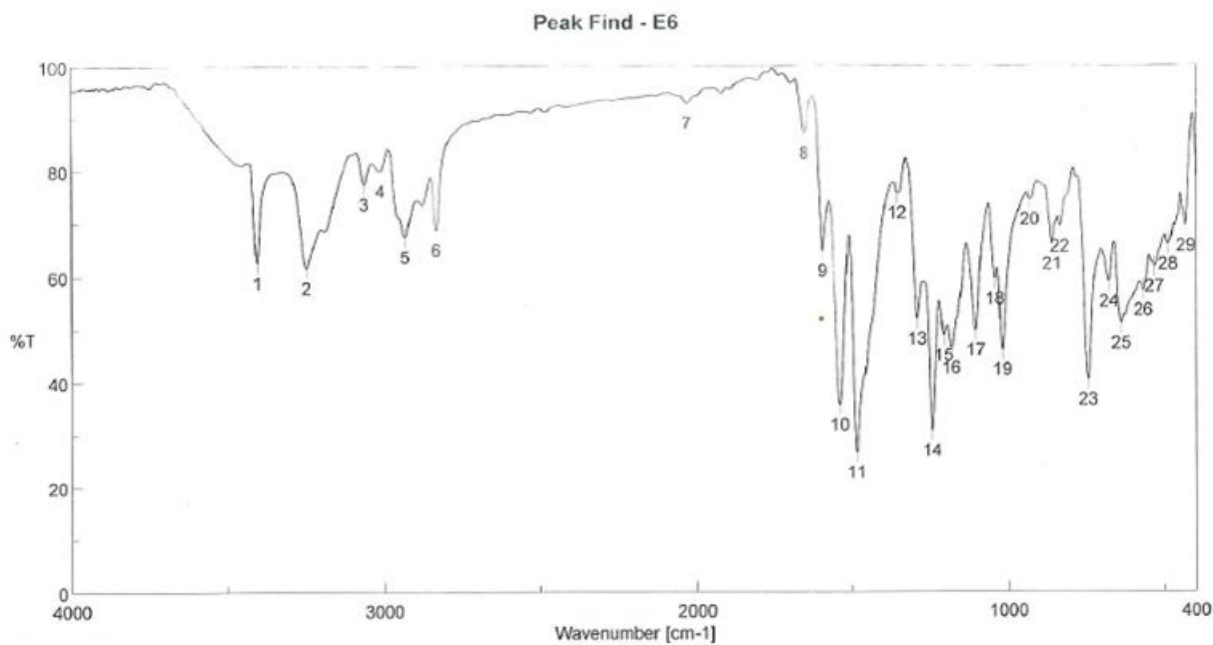
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File: PROTON

Pulse Sequence: s2pu1
Solvent: DMSO
Temp. 30.0 C / 303.1 K
Mercury-300BB "NMR300"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 4.853 sec
Width 6600.7 Hz
11 repetitions
OBSERVE H1, 300.0687865 MHz
DATA PROCESSING
FT size 65536
Total time 5 min, 16 sec
Date: Jul 17 2014



S4. ¹H NMR spectrum (300 MHz, DMSO-d₆) of compound 4



[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1	3404.71	62.67013	2	3247.54	61.69103	3	3063.37	77.45731	4	3011.3	79.95409
5	2933.2	67.45030	6	2832.92	68.73915	7	2032.6	92.86889	8	1655.59	87.04922
9	1594.84	64.79197	10	1539.88	35.57441	11	1484.92	26.51409	12	1356.68	75.76156
13	1292.07	51.98334	14	1243.86	30.68615	15	1207.22	48.85115	16	1183.11	46.48273
17	1105.01	49.83741	18	1044.26	59.55933	19	1020.16	46.14609	20	932.414	74.50311
21	862.025	66.11989	22	836.955	69.40955	23	745.352	40.40329	24	678.82	58.97649
25	640.251	51.09926	26	569.862	57.36124	27	534.185	61.79094	28	490.795	66.02766
29	433.905	69.43832									

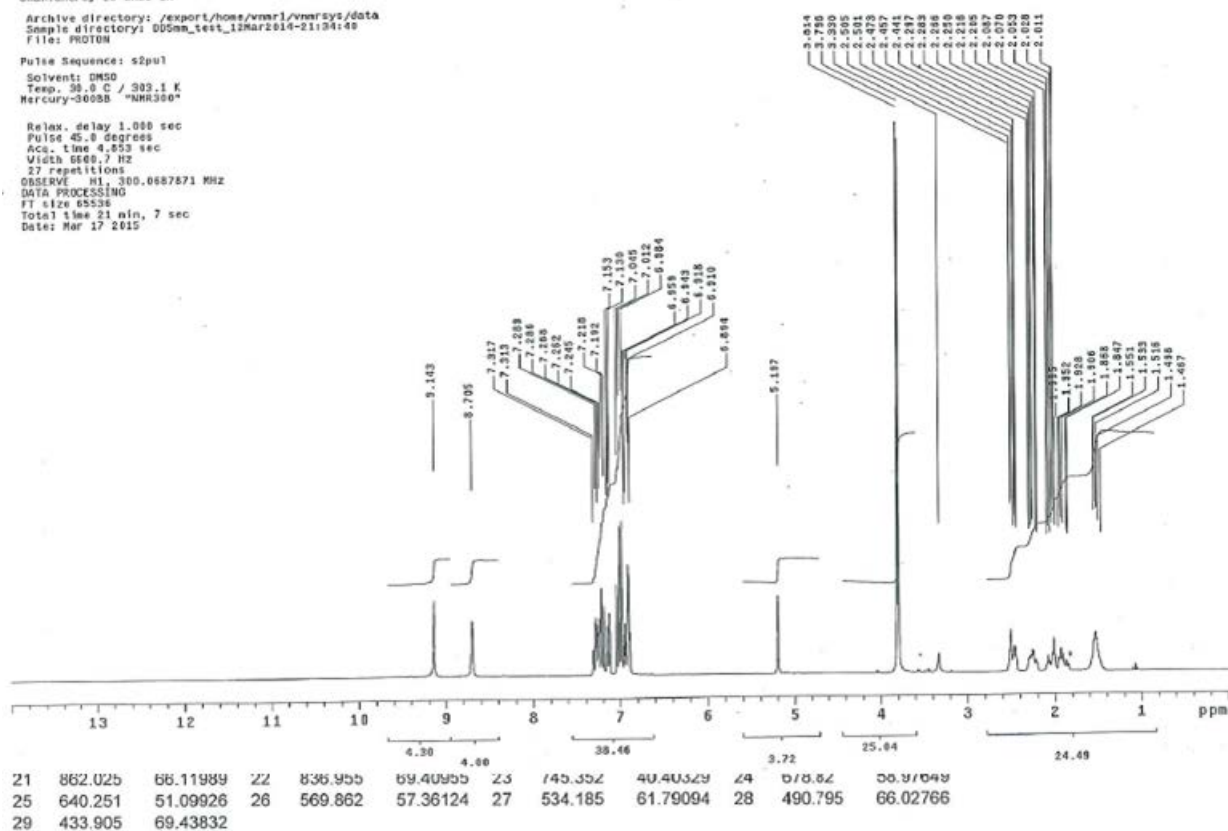
S5a. IR spectrum (KBr, cm^{-1}) of compound 7

OhanaMeray-EG-DMSO-1H

Archive directory: /export/home/vmr1/vmr/sys/data
Sample directory: 005m_test_12Mar2014-21:34:49
File: PROTDM

Pulse Sequence: s2pu1
Solvent: DMSO
Temp: 30.0 C / 303.1 K
Mercury-300SB "NMR300"

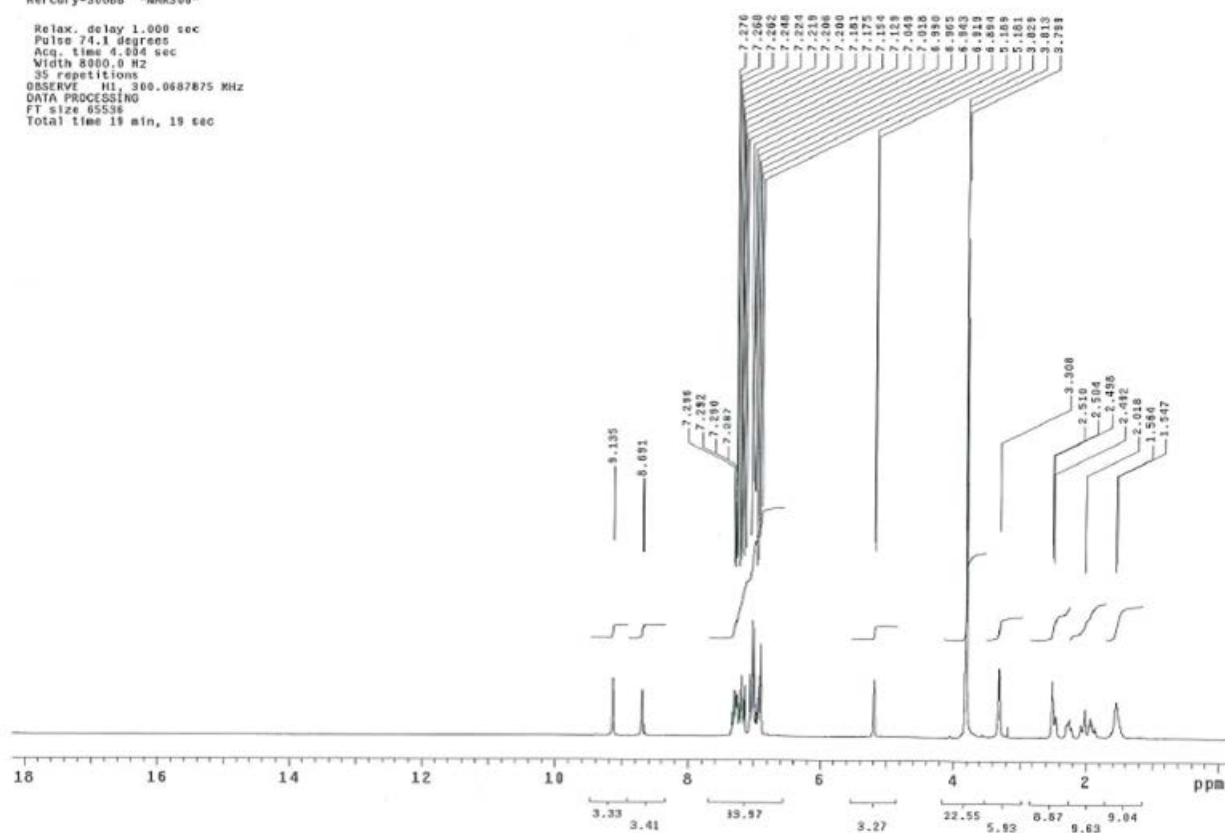
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 4.053 sec
Width 6600.7 Hz
27 repetitions
OBSERVE N1: 300.0687671 MHz
DATA PROCESSING
F1 size 85536
Total time 21 min, 7 sec
Date: Mar 17 2015



S5b. ¹H NMR spectrum (300 MHz, DMSO-*d*₆) of compound 7

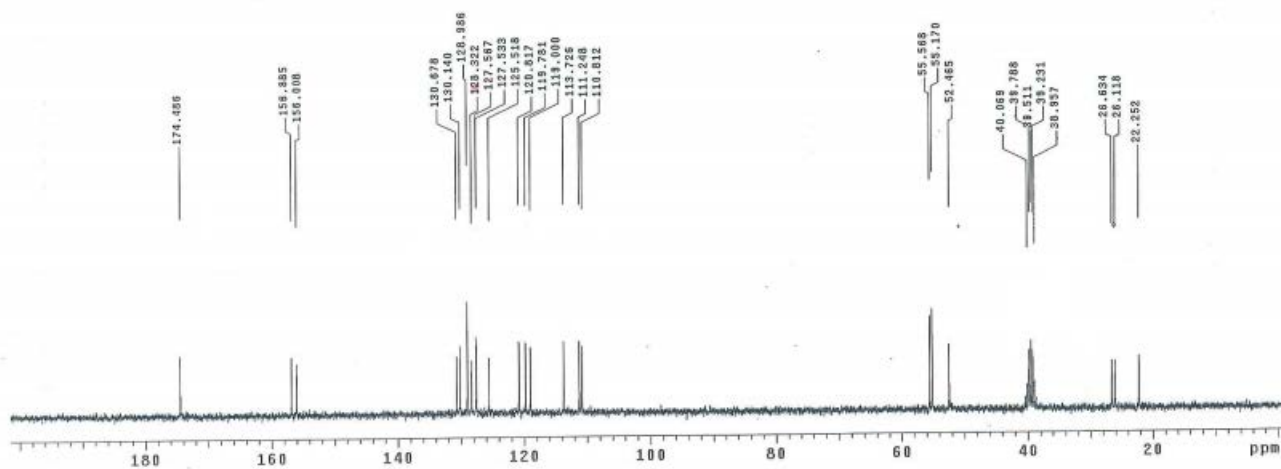
KhantMohamad-E6-DMSO-H
Pulse Sequence: s2pul
Solvent: DMSO
Temp: 30.0 C / 303.1 K
Mercury-30005 "NMR300"

Relax. delay 1.000 sec
Pulse 74.1 degrees
Acq. time 4.804 sec
Width 8000.0 HZ
35 repetitions
OBSERVE H1, 300.0607075 MHz
DATA PROCESSING
FT size 65536
Total time 19 min, 19 sec

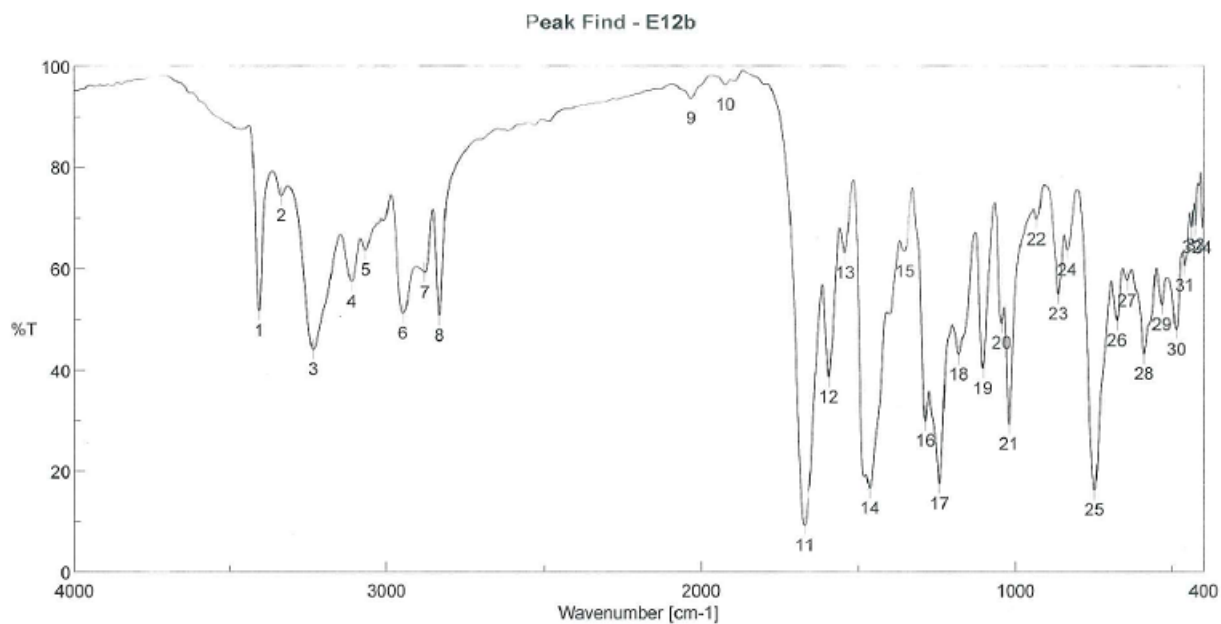


S5b. ¹H NMR spectrum (300 MHz, DMSO-*d*₆) of compound 7 (recrystallized)

KhaniaSayed-E6-DMSO-C13
Archive directory: /export/home/vnmr1/vnmrscys/data
Sample directory: D05aa_test_12Mar2014-21:34:40
File: PRDTON
Pulse Sequence: s2pul
Solvent: DMSO
Temp. 20.0 C / 303.1 K
Mercury-3000S "NMR300"
Pulse 45.0 degrees
Acq. time 1.815 sec
Width 13761.7 Hz
458 repetitions
OBSERVE C13, 75.4523854 MHz
DECOUPLE H1, 300.0782839 MHz
Power 33 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131872
Total time 3 hr, 17 min, 51 sec
Date: Mar 18 2015



S5c. ^{13}C NMR spectrum (75 MHz, DMSO- d_6) of compound 7



[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1	3407.6	51.76382	2	3336.25	74.30941	3	3235	44.13831	4	3111.58	57.42469
5	3067.23	63.67796	6	2947.66	51.23463	7	2878.24	59.23565	8	2831.95	50.76416
9	2033.57	93.54477	10	1923.65	96.25835	11	1671.02	9.11932	12	1594.84	38.61280
13	1542.77	63.09124	14	1463.71	16.50786	15	1352.82	63.37659	16	1287.25	29.93531
17	1242.9	17.45550	18	1182.15	43.08918	19	1105.01	40.31755	20	1045.23	49.34721
21	1021.12	29.28344	22	932.414	69.67442	23	862.989	55.02960	24	835.026	63.65382
25	747.281	16.18227	26	676.892	49.78593	27	645.072	57.61539	28	590.111	43.21335
29	534.185	52.92119	30	486.938	48.03564	31	460.904	60.61478	32	437.762	68.10007
33	427.155	68.51730	34	404.014	68.03063						

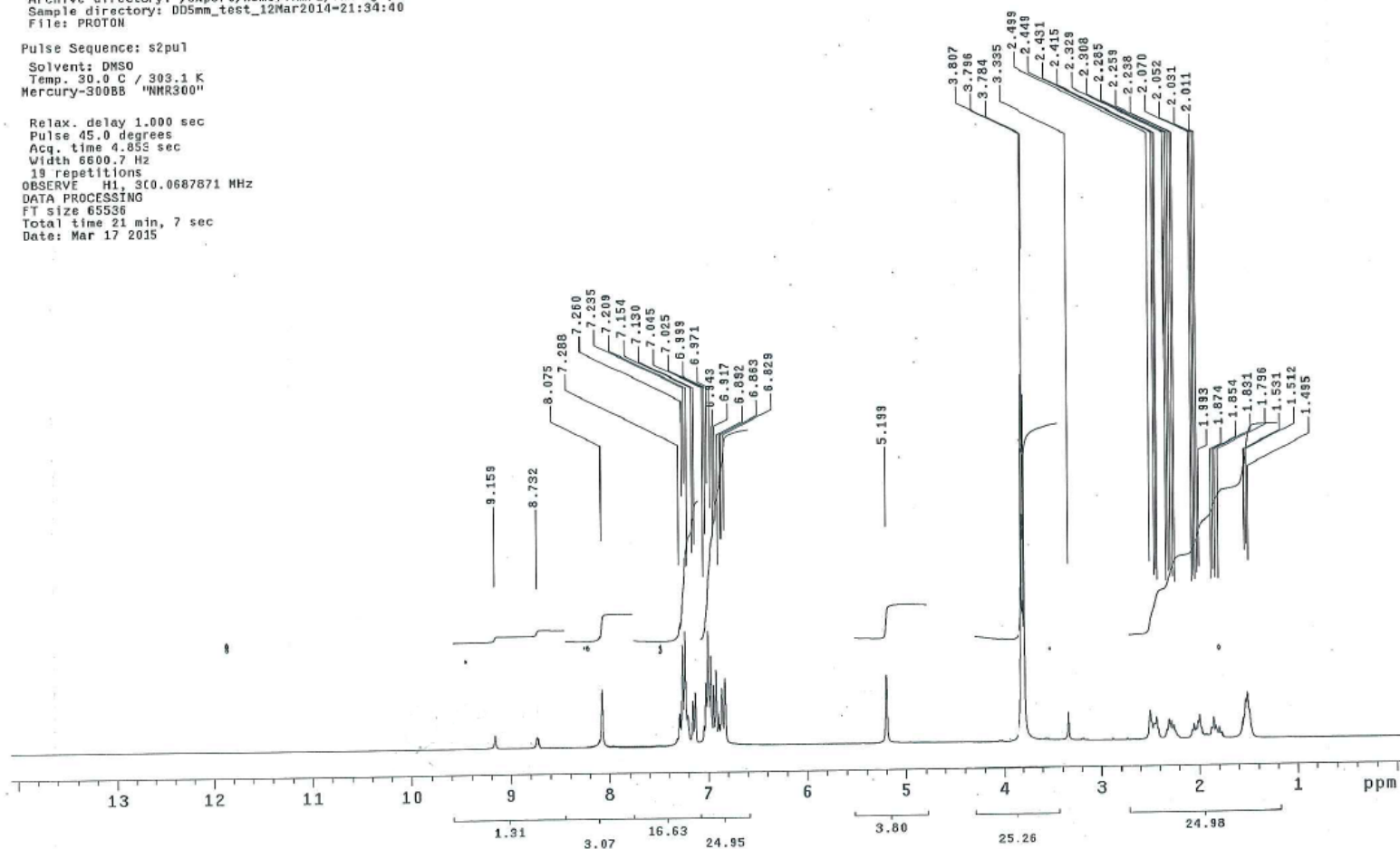
S6_a.IR spectrum (KBr, cm⁻¹) of compound 8

GhaniaMorsy-12b-DMSO-1H

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

Pulse Sequence: s2pu1
Solvent: DMSO
Temp. 30.0 C / 303.1 K
Mercury-300BB "NMR300"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 4.855 sec
Width 6600.7 Hz
18 repetitions
OBSERVE H1, 300.0687671 MHz
DATA PROCESSING
FT size 65536
Total time 21 min, 7 sec
Date: Mar 17 2015



S6b. ^1H NMR spectrum (300 MHz, $\text{DMSO-}d_6$) of compound 8

GhaniaMohamad-E12b-DMSO-H

Pulse Sequence: s2pu1

Solvent: DMSO

Temp. 30.0 C / 303.1 K

Mercury-300BB "NMR300"

Relax. delay 1.000 sec

Pulse 74.1 degrees

Acq. time 4.004 sec

Width 8000.0 Hz

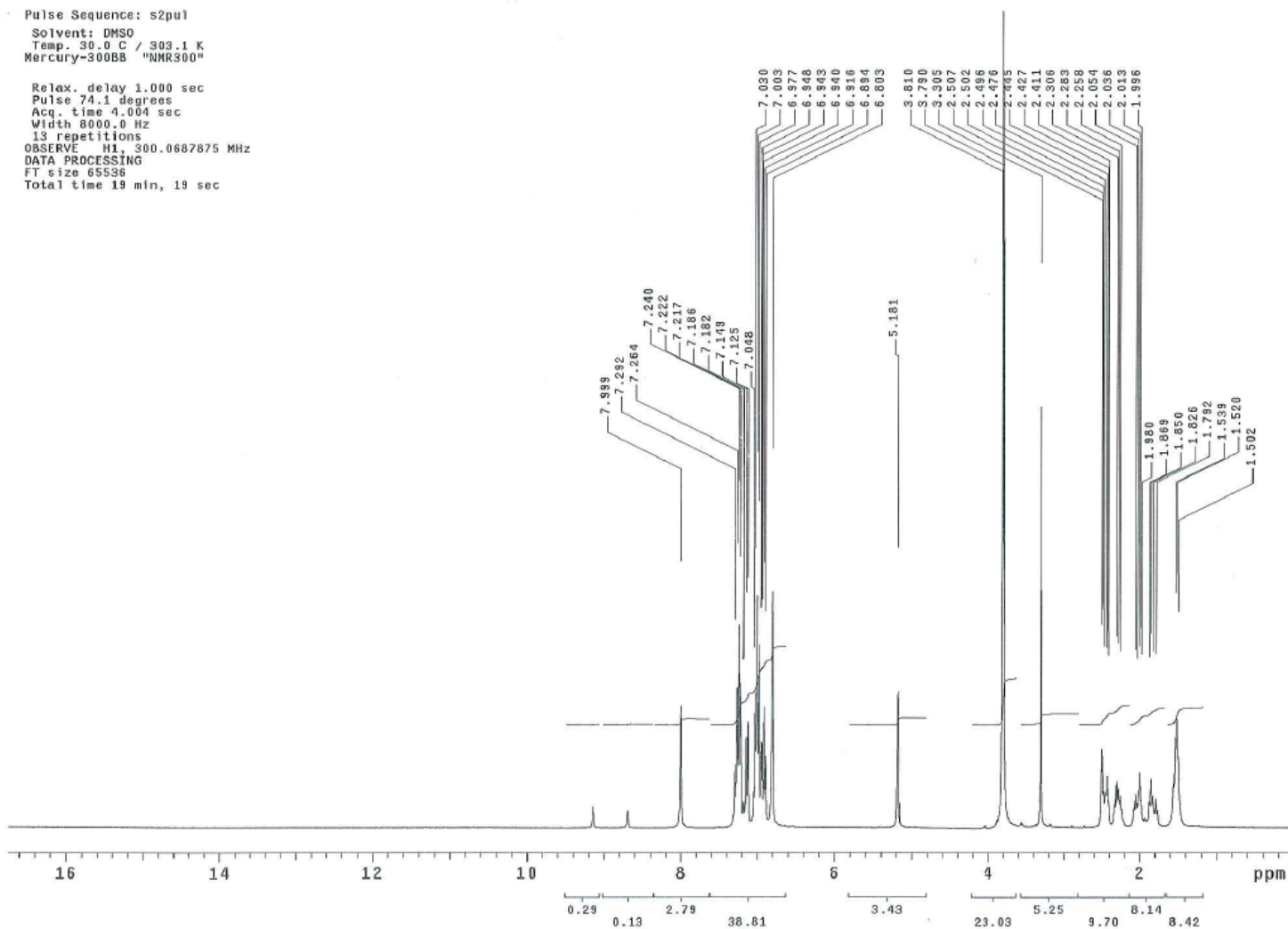
13 repetitions

OBSERVE H1, 300.0687875 MHz

DATA PROCESSING

FT size 65536

Total time 19 min, 19 sec



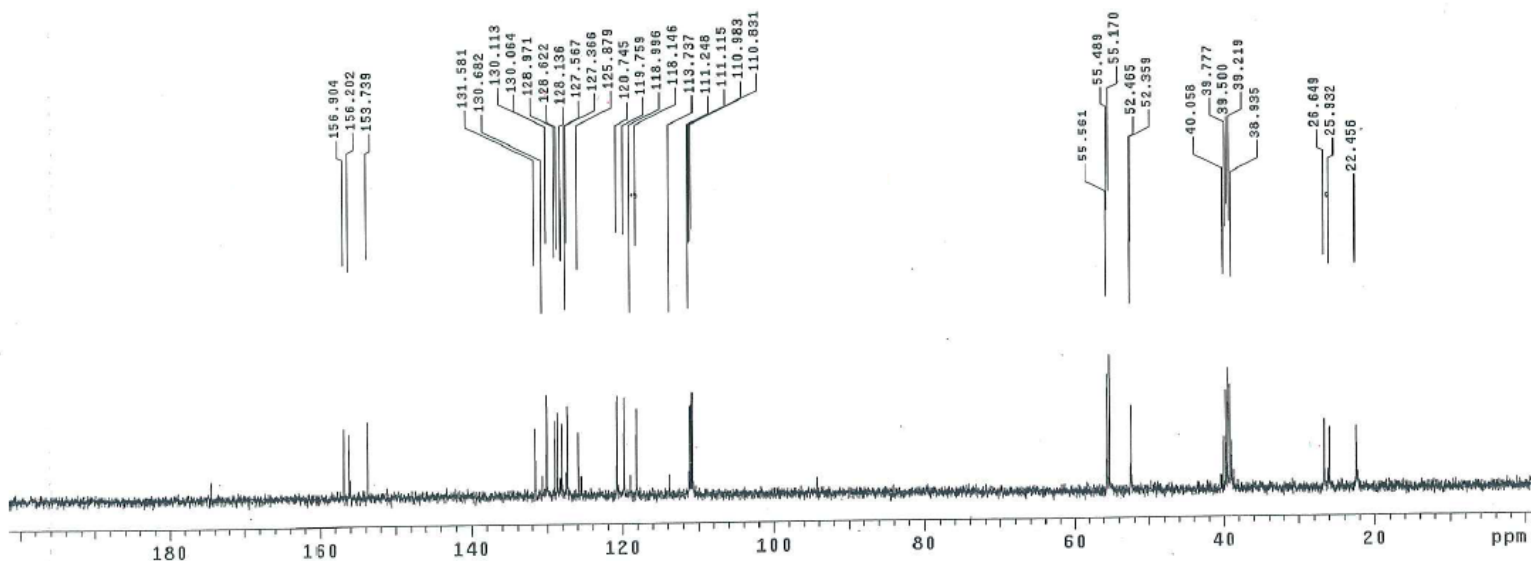
S6b. ^1H NMR spectrum (300 MHz, $\text{DMSO-}d_6$) of compound 8 (recrystallized)

KhaniaSayed-12b-DMSO-C13

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

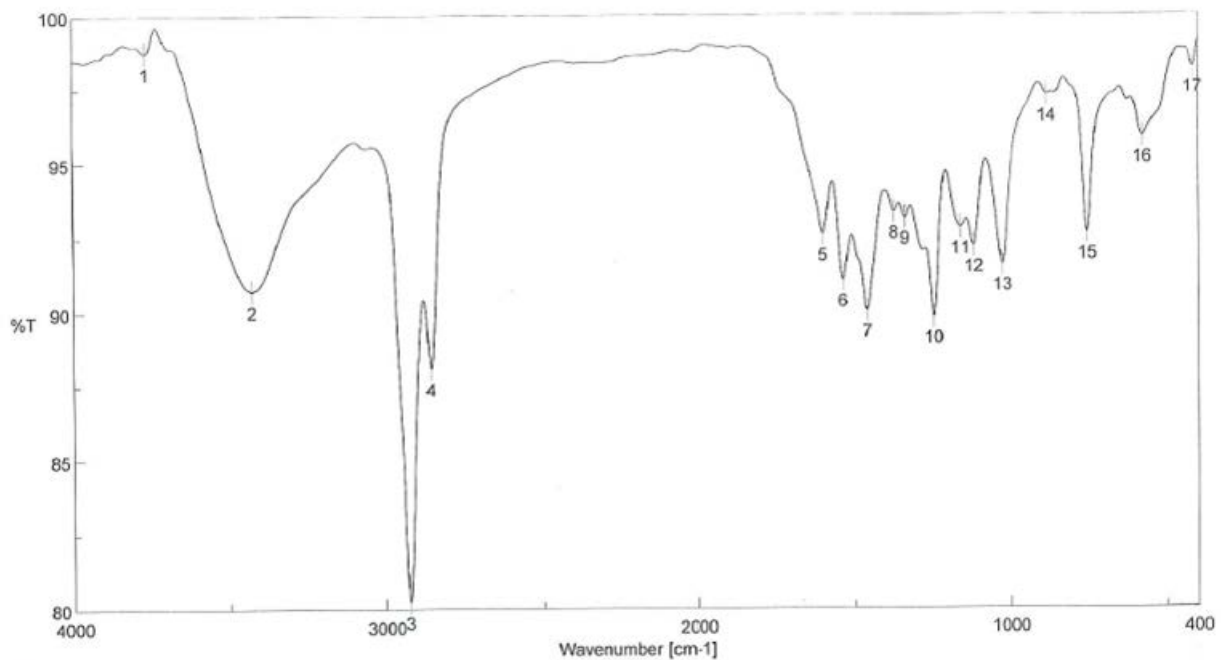
Pulse Sequence: s2pul
Solvent: DMSO
Temp. 30.0 C / 303.1 K
Mercury-300BB "NMR300"

Pulse 45.0 degrees
Acq. time 1.815 sec
Width 18761.7 Hz
536 repetitions
OBSERVE C13, 75.4523954 MHz
DECOUPLE H1, 300.0702830 MHz
Power 53 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 3 hr, 17 min, 51 sec
Date: Mar 18 2015



S6c. ^{13}C NMR spectrum (75 MHz, DMSO- d_6) of compound 8

Peak Find - E28



[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1	3770.15	98.76314	2	3427.85	90.73800	3	2924.52	80.24010	4	2856.06	88.10795
5	1600.63	92.61578	6	1536.02	91.08023	7	1458.89	90.04934	8	1374.03	93.35133
9	1338.36	93.15968	10	1245.79	89.82976	11	1159.97	92.83221	12	1117.55	92.21955
13	1024.98	91.59732	14	882.274	97.26966	15	753.066	92.64864	16	577.576	95.86507
17	417.513	98.21755									

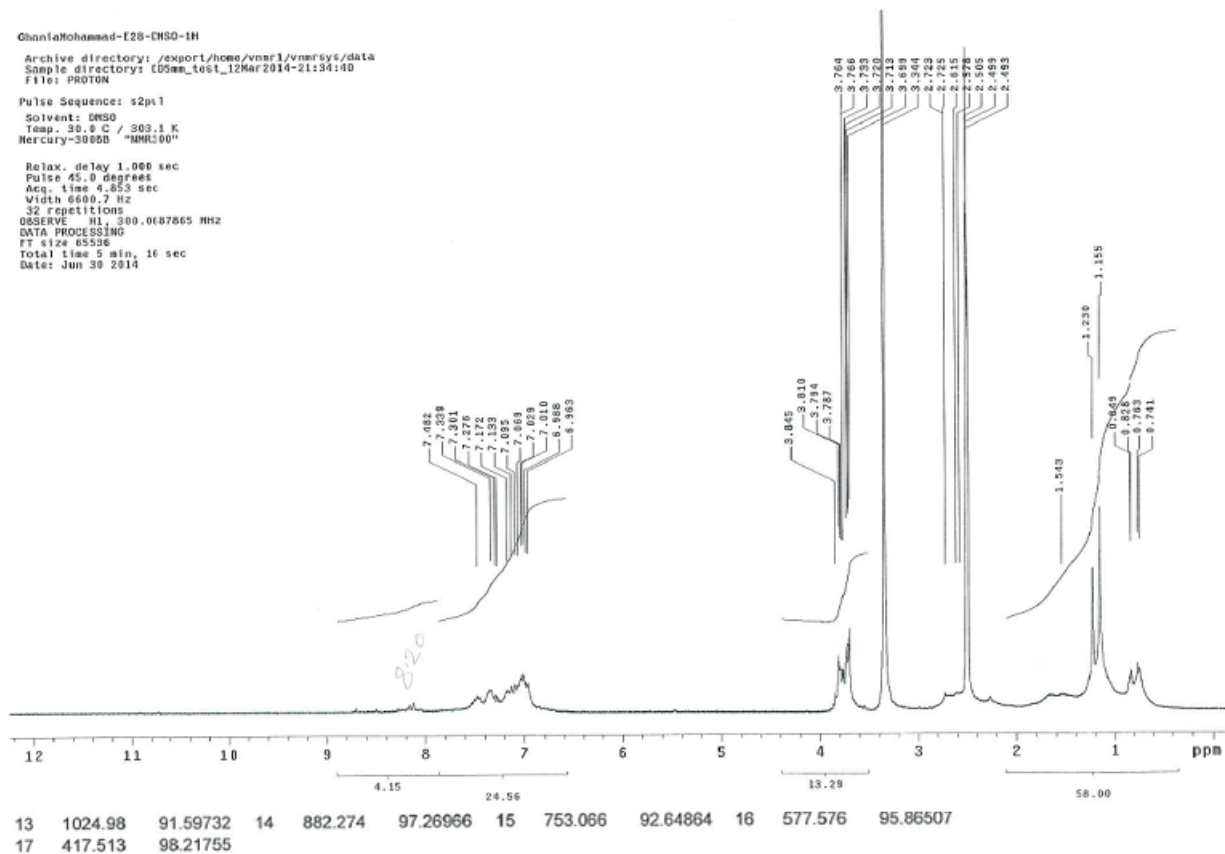
S7a. IR spectrum (KBr, cm^{-1}) of compound 9

ChaoMohaamed-128-CHSO-1H

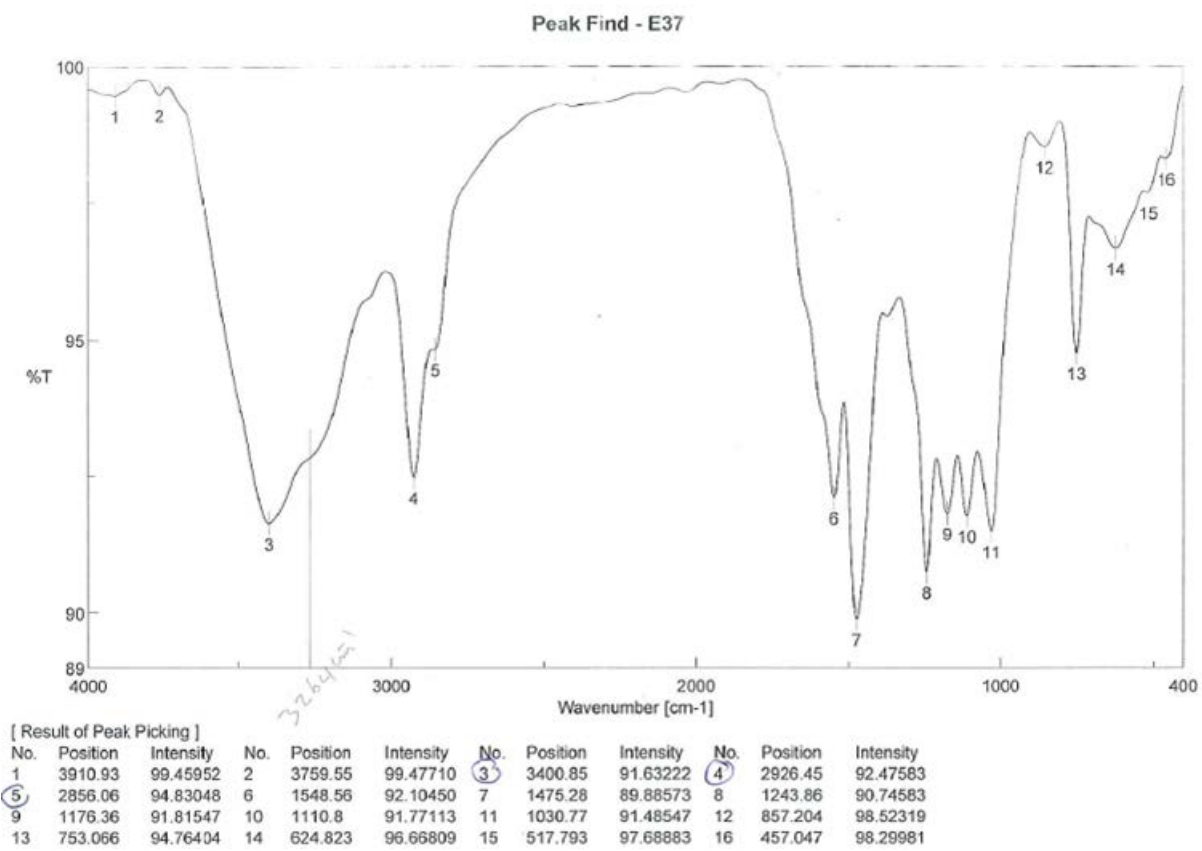
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File: PROTON

Pulse Sequence: s2pt1
Solvent: DMSO
Temp. 30.0 C / 303.1 K
Mercury-3000B "NMR300"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 4.853 sec
Width 6600.7 Hz
32 repetitions
OBSERVE H1, 300.0087865 MHz
DATA PROCESSING
FT size 65536
Total time 5 min, 16 sec
Date: Jun 30 2014



S7_b. ¹H NMR spectrum (300 MHz, DMSO-*d*₆) of compound 9



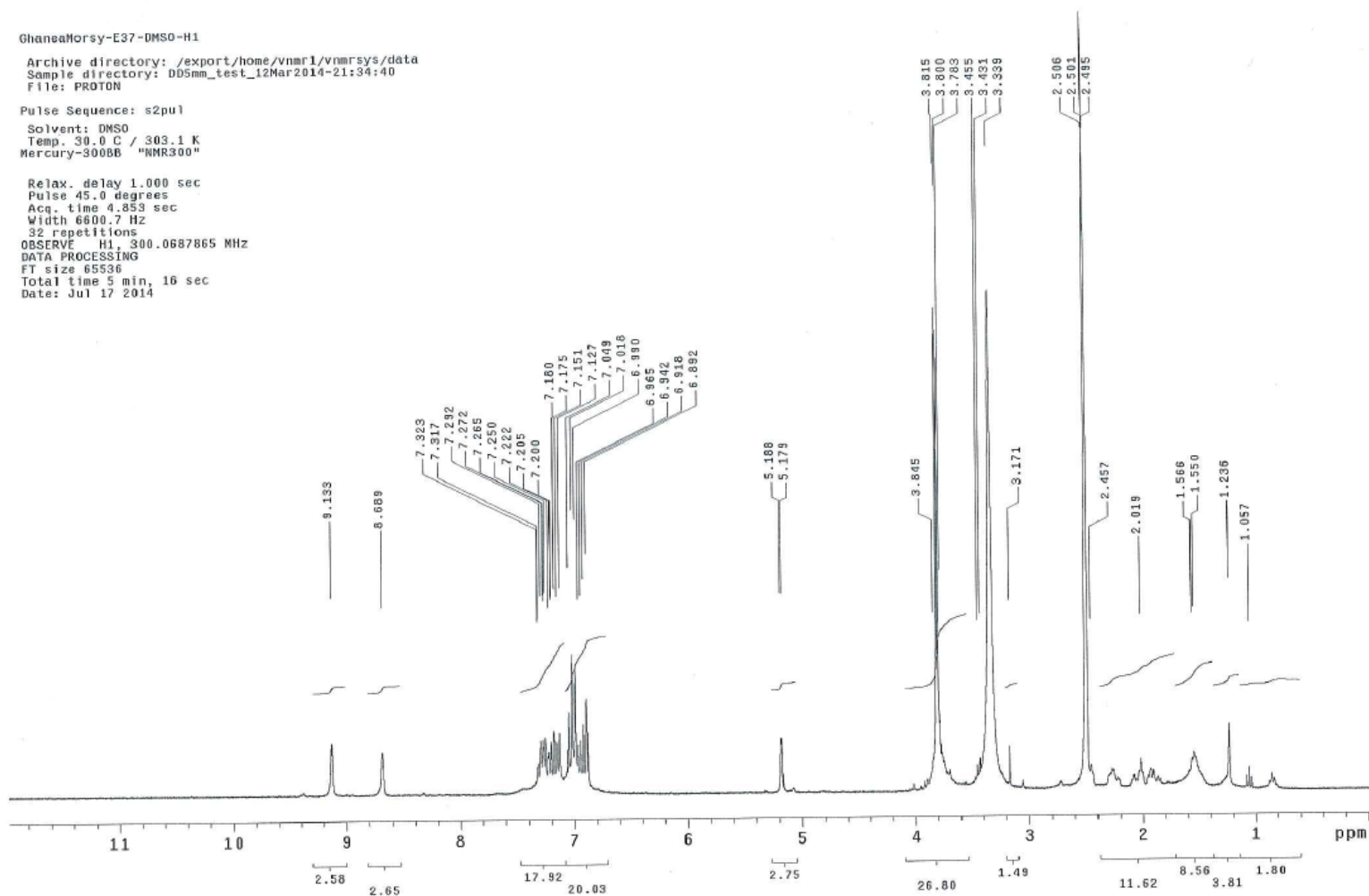
S8a. IR spectrum (KBr, cm^{-1}) of compound 10

GhaneaMorsy-E37-DMSO-H1

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

Pulse Sequence: s2pu1
Solvent: DMSO
Temp. 30.0 C / 303.1 K
Mercury-300BB "NMR300"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 4.853 sec
Width 6600.7 Hz
32 repetitions
OBSERVE H1, 300.0687865 MHz
DATA PROCESSING
FT size 65536
Total time 5 min, 16 sec
Date: Jul 17 2014



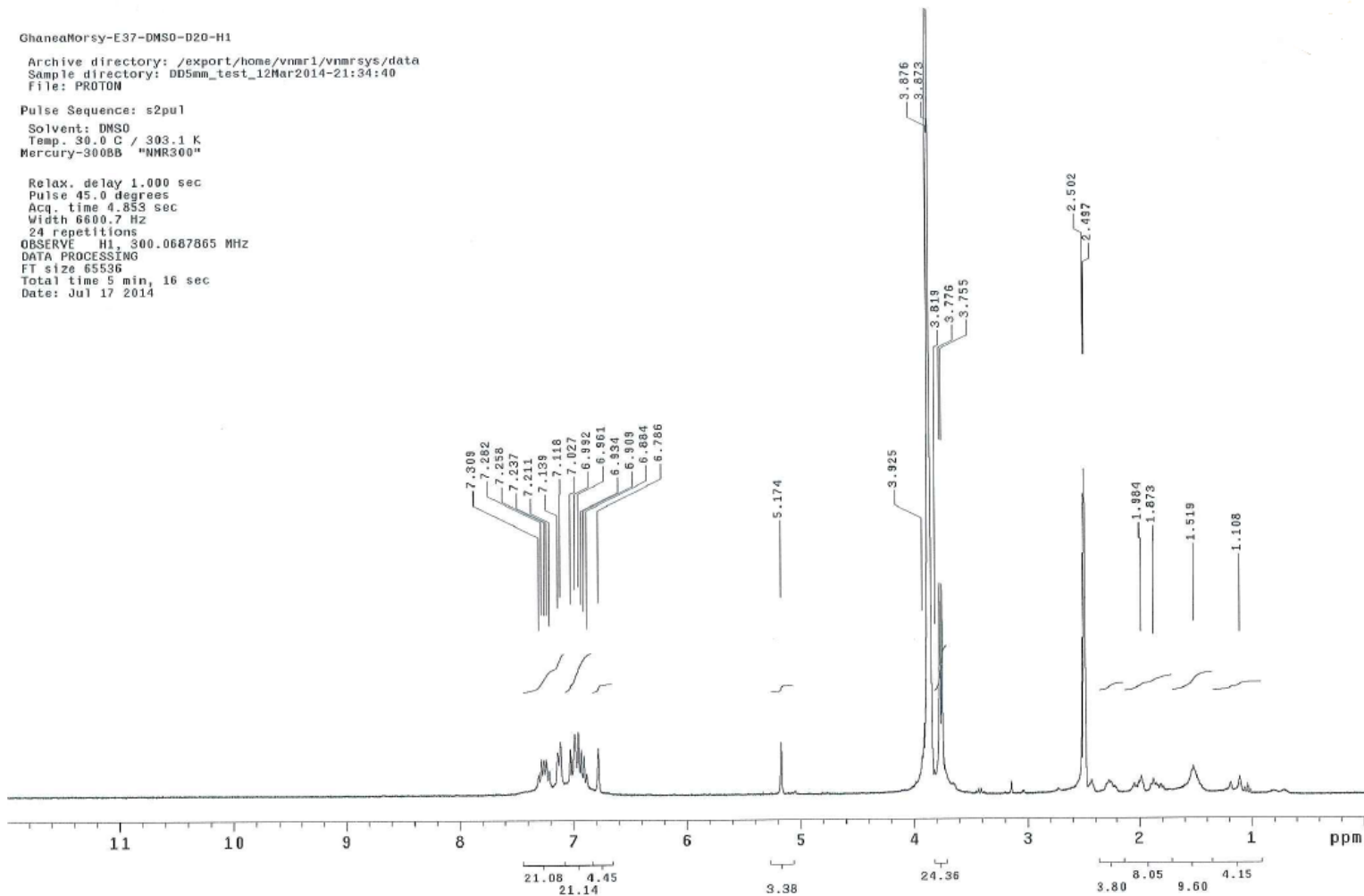
S8b. ^1H NMR spectrum (300 MHz, $\text{DMSO-}d_6$) of compound 10

GhaneaMorsy-E37-DMSO-D2O-H1

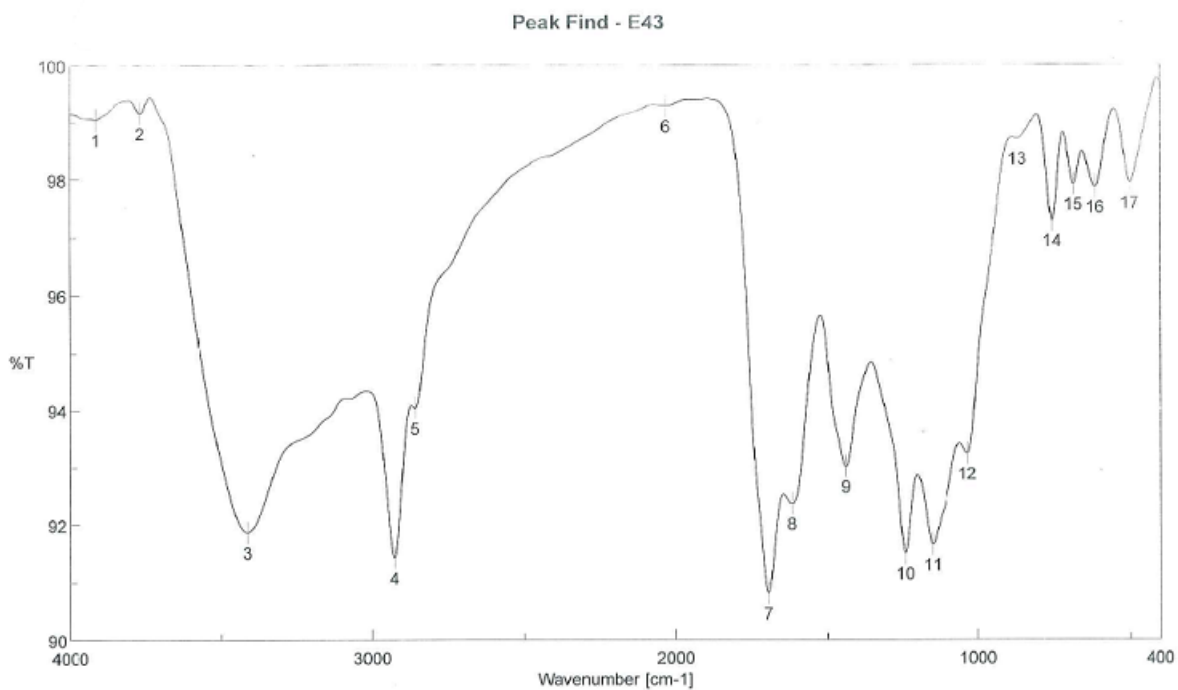
Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: DD5mm_test_12Mar2014-21:34:40
File: PROTON

Pulse Sequence: s2pu1
Solvent: DMSO
Temp. 30.0 C / 303.1 K
Mercury-300BB "NMR300"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 4.853 sec
Width 6600.7 Hz
24 repetitions
OBSERVE H1, 300.0687865 MHz
DATA PROCESSING
FT size 65536
Total time 5 min, 16 sec
Date: Jul 17 2014



S8b. ¹H NMR spectrum (300 MHz, DMSO-D₂O) of compound 10



[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1	3911.9	99.04807	2	3763.4	99.15662	3	3411.46	91.86352	4	2927.41	91.42448
5	2859.92	94.03410	6	2034.53	99.27702	7	1696.09	90.80791	8	1618.95	92.35915
9	1440.56	93.00827	10	1243.86	91.49924	11	1152.26	91.65218	12	1036.55	93.23637
13	871.667	98.71235	14	757.888	97.29163	15	688.463	97.91861	16	617.109	97.86836
17	503.33	97.94212									

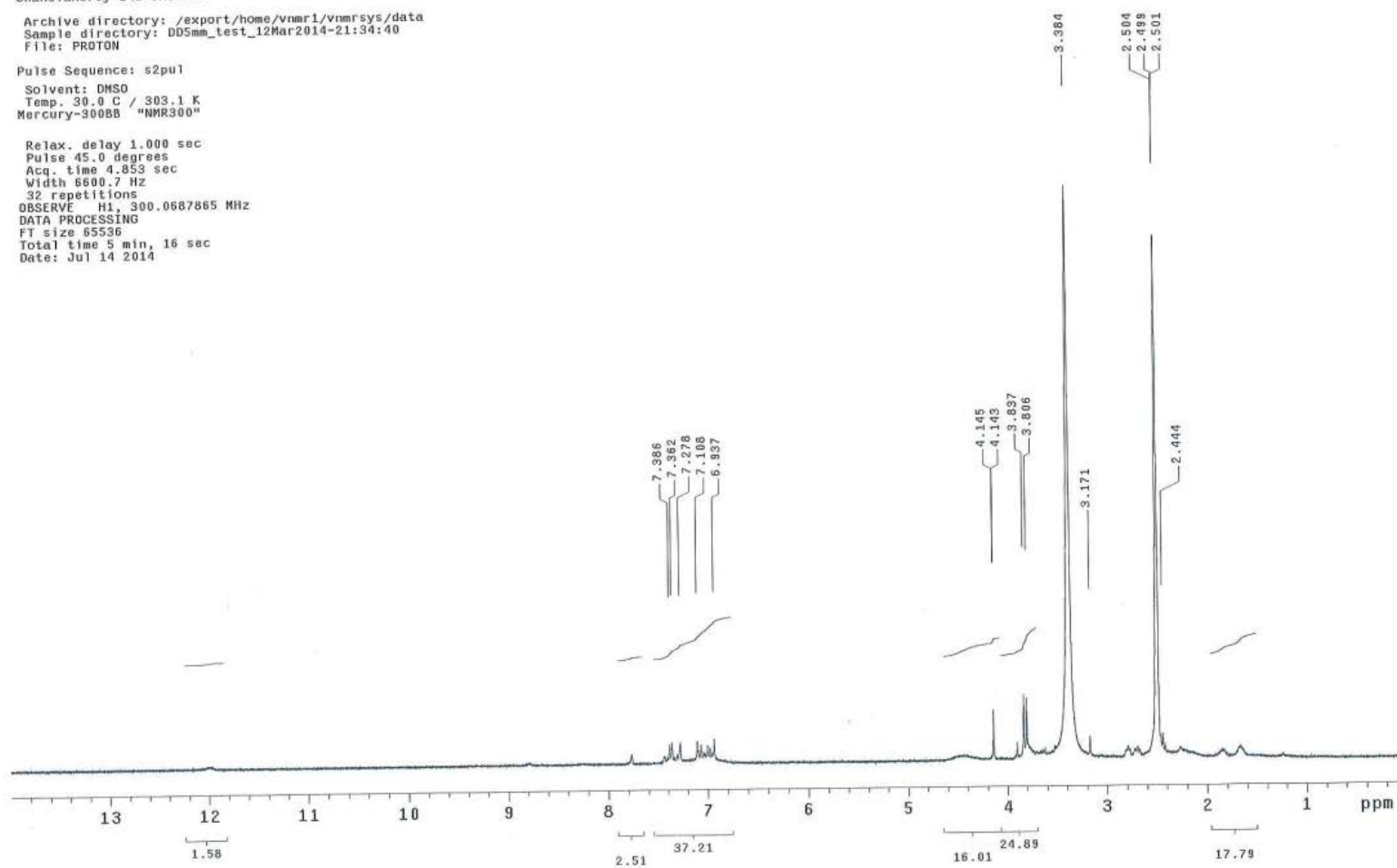
S9_a. IR spectrum (KBr, cm⁻¹) of compound 11

GhaneliMorsy-E43-DMSO-1H

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Sample directory: DD5mm_test_12Mar2014-21:34:40
File: PROTON

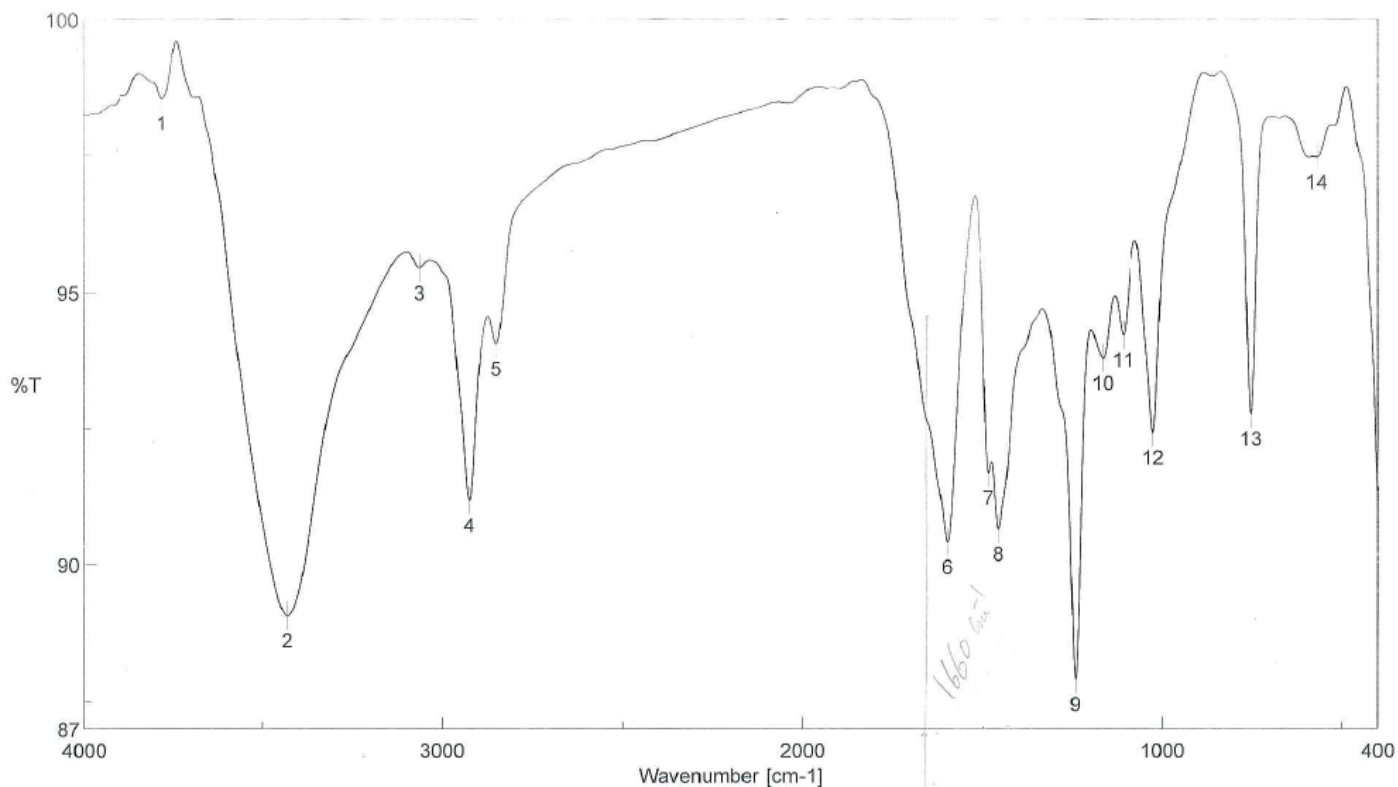
Pulse Sequence: s2pu1
Solvent: DMSO
Temp. 30.0 C / 303.1 K
Mercury-300BB "NMR300"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 4.853 sec
Width 6600.7 Hz
32 repetitions
OBSERVE H1, 300.0687865 MHz
DATA PROCESSING
F1 size 65536
Total time 5 min, 16 sec
Date: Jul 14 2014



S9b. ¹H NMR spectrum (300 MHz, DMSO-*d*₆) of compound 11

Peak Find - E65b

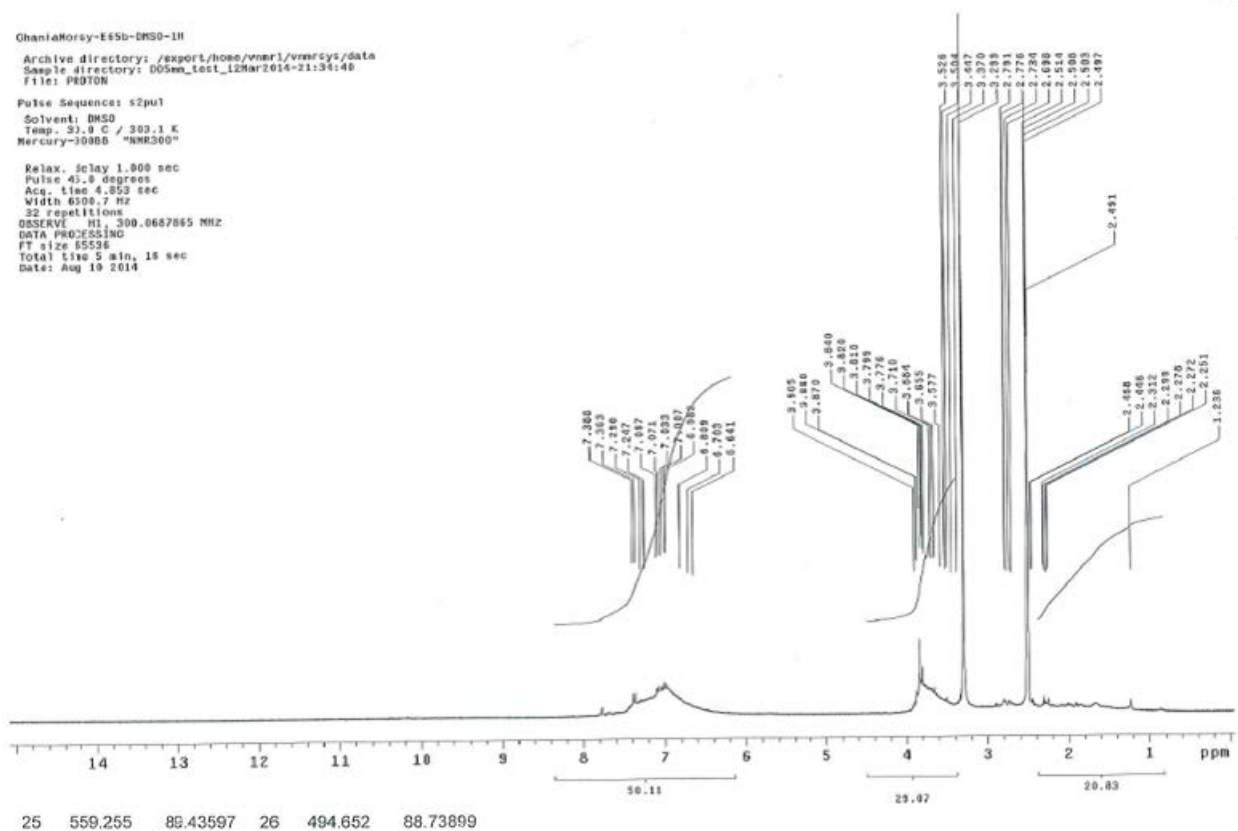


[Result of Peak Picking]

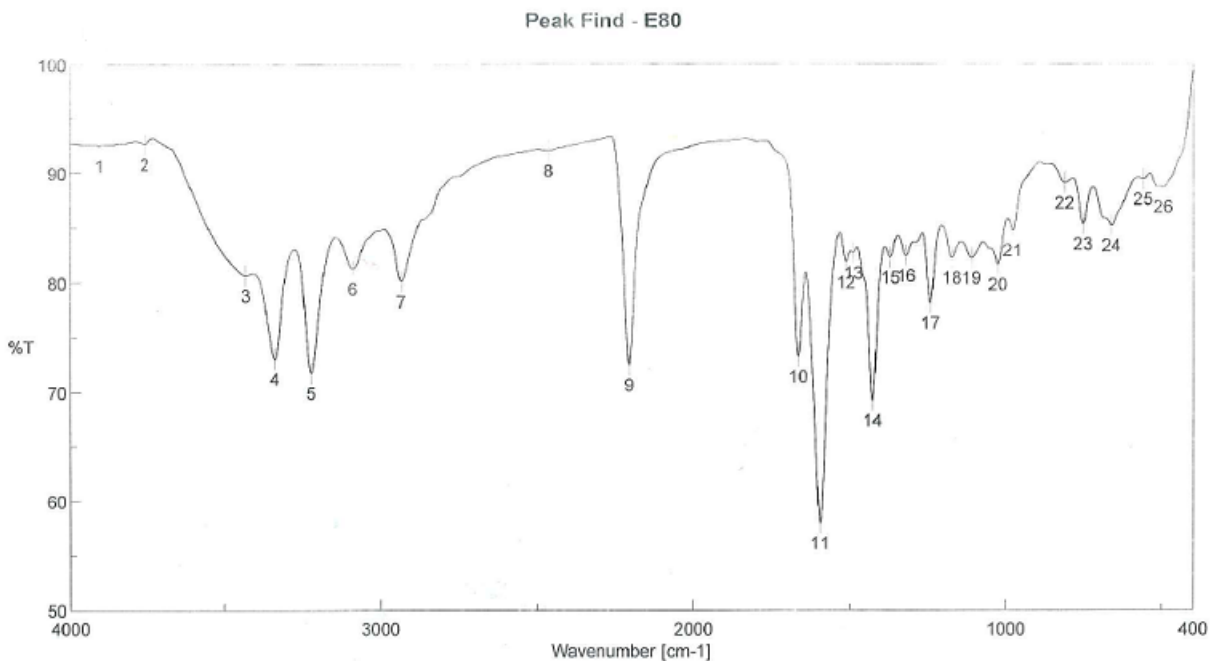
No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1	3778.83	98.54137	2	3429.78	89.06640	3	3064.33	95.44338	4	2925.48	91.17744
5	2851.24	94.06120	6	1600.63	90.41415	7	1486.85	91.68355	8	1458.89	90.64905
9	1244.83	87.90830	10	1168.65	93.79612	11	1111.76	94.21937	12	1026.91	92.42641
13	753.066	92.76951	14	570.826	97.46294						

S10a. IR spectrum (KBr, cm⁻¹) of compound 13

OhaniaKorsy-E55b-DMSO-1H
 Archive directory: /export/home/vmr1/vmr/sys/data
 Sample directory: D05ma_test_12Mar2014-21:34:48
 File: PROTON
 Pulse Sequence: s2pu1
 Solvent: DMSO
 Temp: 31.9 C / 303.1 K
 Mercury-300SD "NMR300"
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 4.553 sec
 Width 6508.7 Hz
 32 repetitions
 OBSERVE HI, 300.0687865 MHz
 DATA PROCESSING
 FT size 65536
 Total time 5 min, 15 sec
 Date: Aug 10 2014



S10b. ^1H NMR spectrum (300 MHz, $\text{DMSO-}d_6$) of compound 13



[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1	3907.07	92.46972	2	3758.58	92.61684	3	3433.64	80.64453	4	3340.1	73.03141
5	3223.43	71.73652	6	3089.4	81.26193	7	2935.13	80.11257	8	2464.58	92.02169
9	2205.2	72.52130	10	1664.27	73.26752	11	1593.88	57.95969	12	1511.92	81.89087
13	1488.78	82.72935	14	1427.07	69.23699	15	1370.18	82.33361	16	1320.04	82.45583
17	1241.93	78.17953	18	1172.51	82.28985	19	1109.83	82.27370	20	1024.98	81.66831
21	977.733	84.76556	22	811.885	89.08572	23	753.066	85.34871	24	661.464	85.21179
25	559.255	88.43597	26	494.652	88.73899						

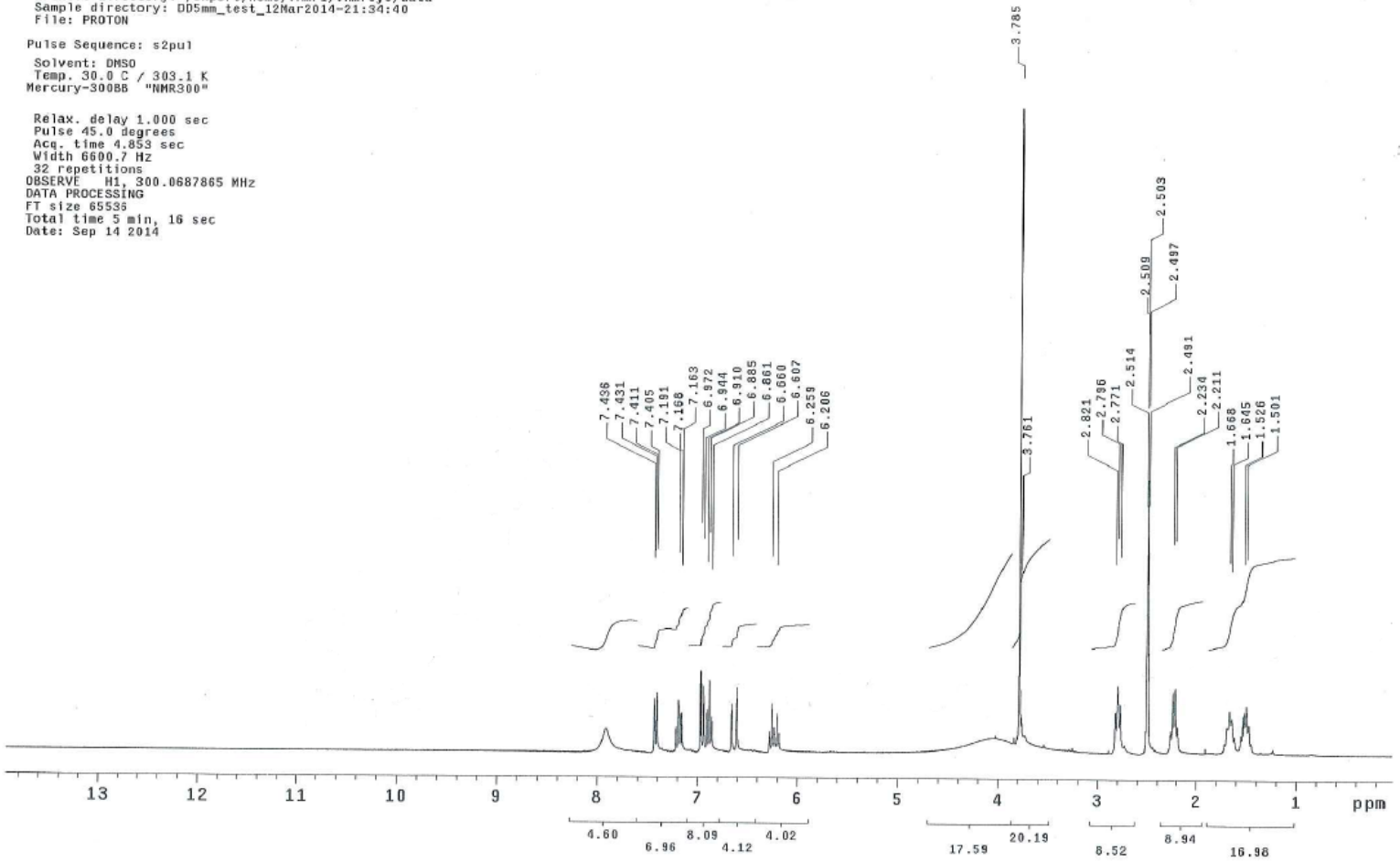
S11a. IR spectrum (KBr, cm^{-1}) of compound 16

GhaneyaMorsy-E80-DMSO-1H

Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: DD5mm_test_12Mar2014-21:54:40
File: PROTON

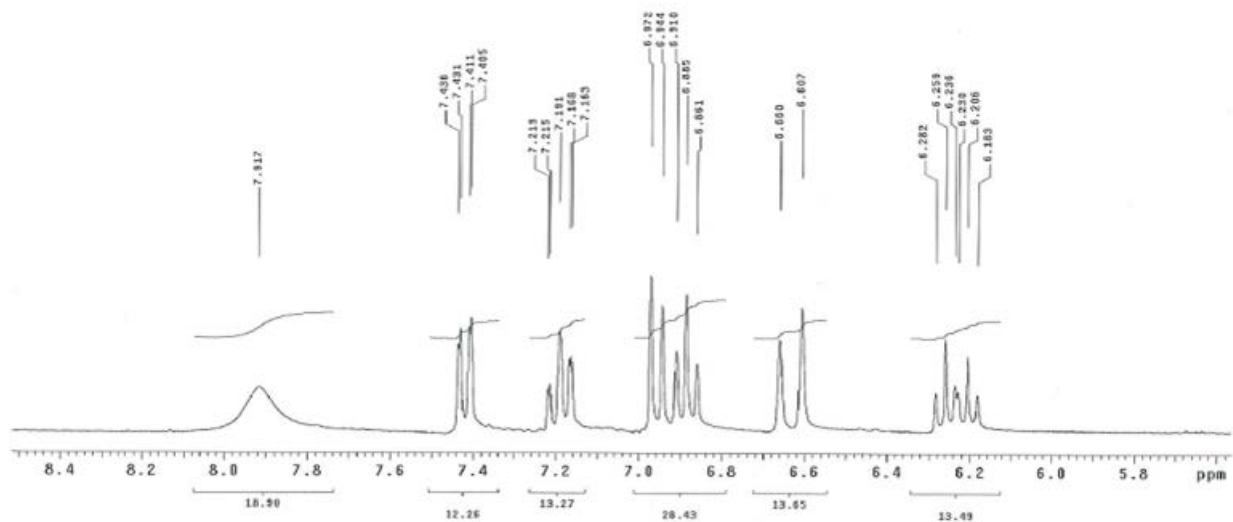
Pulse Sequence: s2pu1
Solvent: DMSO
Temp. 30.0 C / 303.1 K
Mercury-300BB "NMR300"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 4.853 sec
Width 6600.7 Hz
32 repetitions
OBSERVE H1, 300.0687865 MHz
DATA PROCESSING
FT size 65535
Total time 5 min, 16 sec
Date: Sep 14 2014



S11b. ^1H NMR spectrum (300 MHz, $\text{DMSO-}d_6$) of compound 16

Ghaneyamorsy-189-DR50-1H
Archive directory: /export/home/vnar1/vnarsys/data
Sample directory: D05mm_test_12Mar2014-21:24:40
File: PROTON
Pulse Sequence: s2pu1
Solvent: DMSO
Temp: 30.0 C / 303.1 K
Mercury-30000 "NMR300"
Relax. delay 1.000 sec
Pulse 45.0 degree
Acq. time 4.153 sec
Width 6600.7 Hz
32 repetitions
OBSERVE W1, 300.0507865 MHz
DATA PROCESSING
F1 size 65536
Total time 5 min, 16 sec
Date: Sep 14 1014



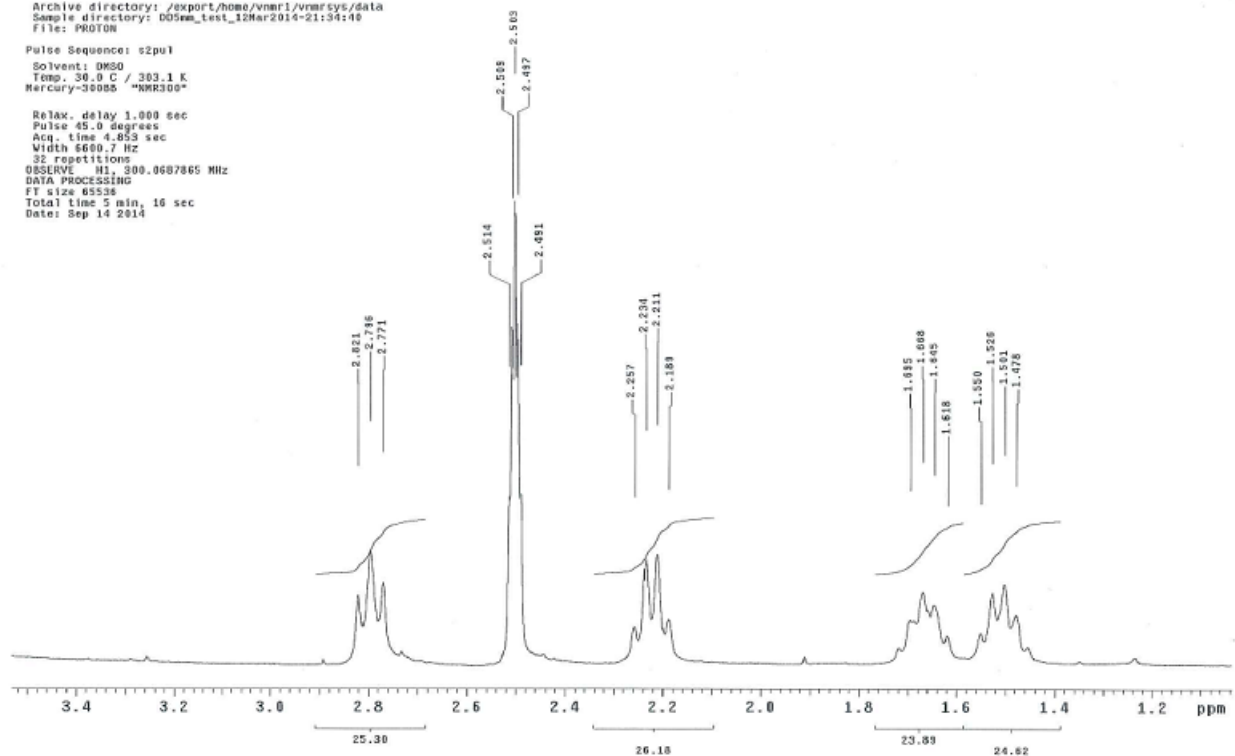
S11b. ^1H NMR spectrum (300 MHz, $\text{DMSO-}d_6$) of compound 16 (*Magnified area*)

GhansyaMorsy-E80-DMSO-1H

Archive directory: /export/home/vmr1/vmrSYS/data
Sample directory: D05em_test_12Mar2014-21:34:40
File: PROTON

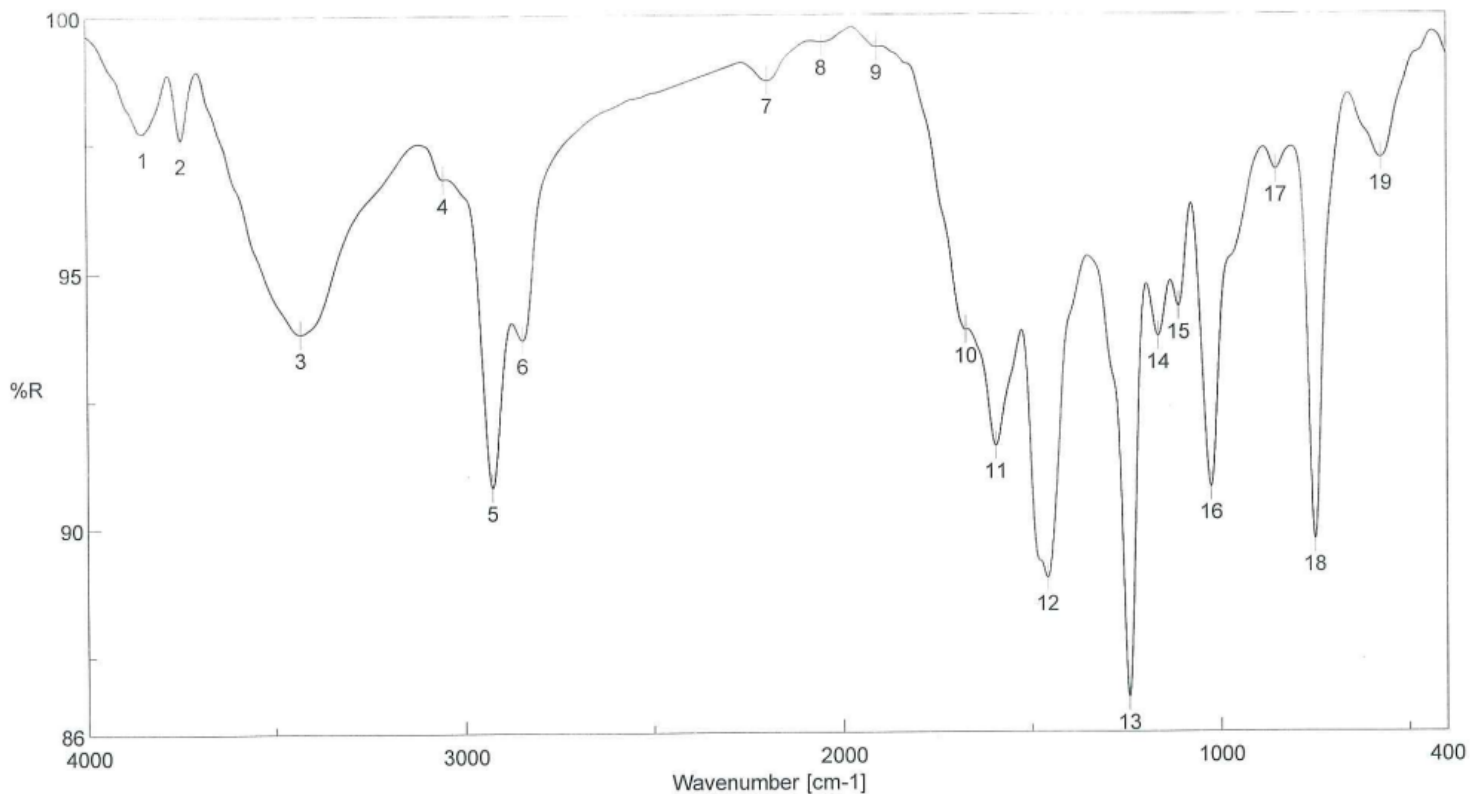
Pulse Sequence: s2pu1
Solvent: DMSO
Temp. 30.0 C / 303.1 K
Mercury-30006 "MRK300"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 4.853 sec
Width 6600.7 Hz
32 repetitions
OBSERVE H1, 300.0687865 MHz
DATA PROCESSING
FT size 65536
Total time 5 min, 16 sec
Date: Sep 14 2014



S11_b. ¹H NMR spectrum (300 MHz, DMSO-*d*₆) of compound 16 (*Magnified area*)

Peak Find - E63



[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1	3848.26	97.7177	2	3747.01	97.5879	3	3432.67	93.8097	4	3055.66	96.7941
5	2927.41	90.7926	6	2846.42	93.6721	7	2197.49	98.7054	8	2053.82	99.4617
9	1908.22	99.3585	10	1674.87	93.8485	11	1594.84	91.5844	12	1458.89	88.994
13	1242.9	86.6773	14	1164.79	93.7204	15	1111.76	94.2983	16	1025.94	90.7722
17	853.347	96.9477	18	751.138	89.7399	19	575.647	97.1617			

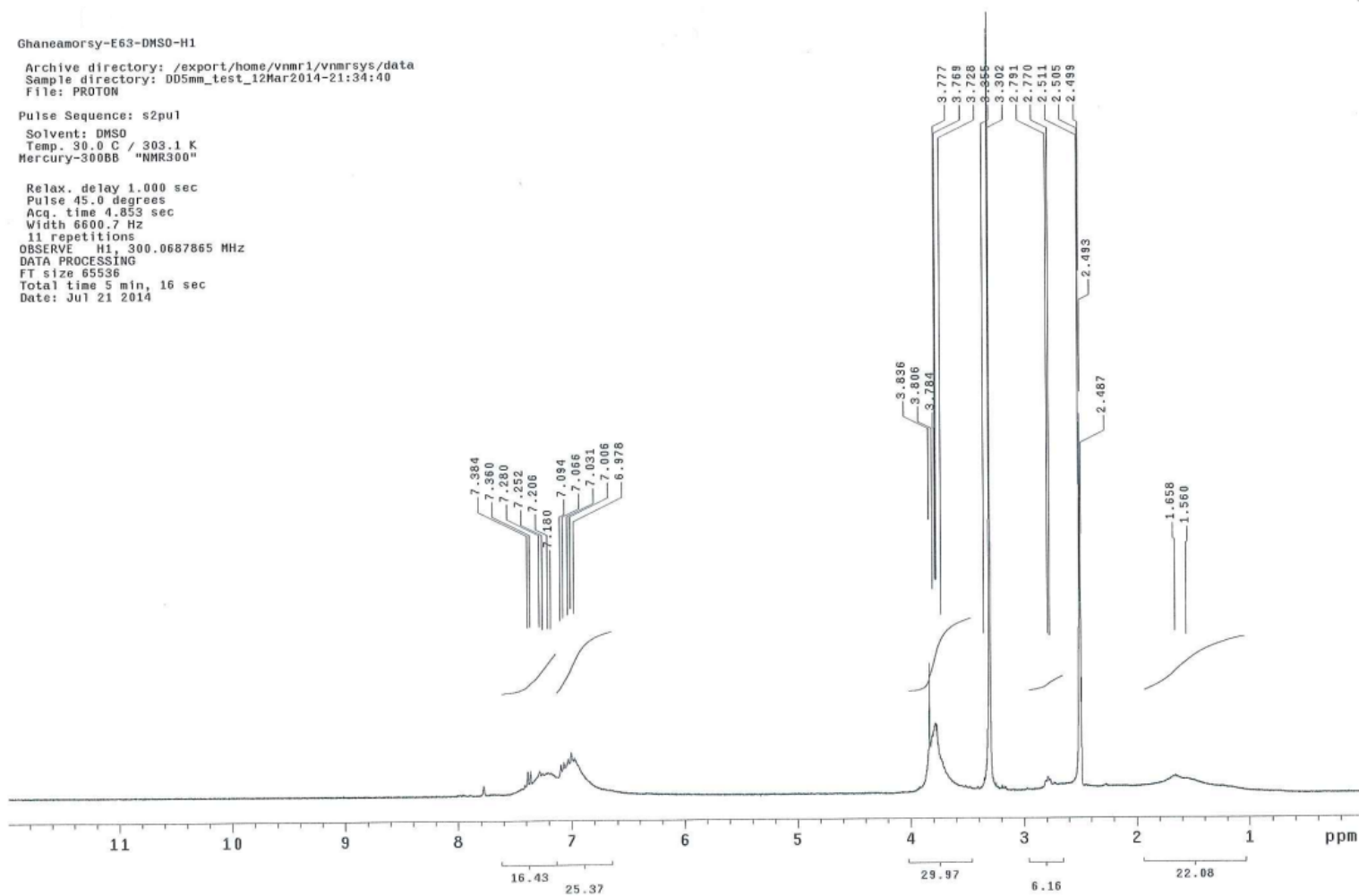
S12a. IR spectrum (KBr, cm⁻¹) of compound 17

Ghaneamorsy-E63-DMSO-H1

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

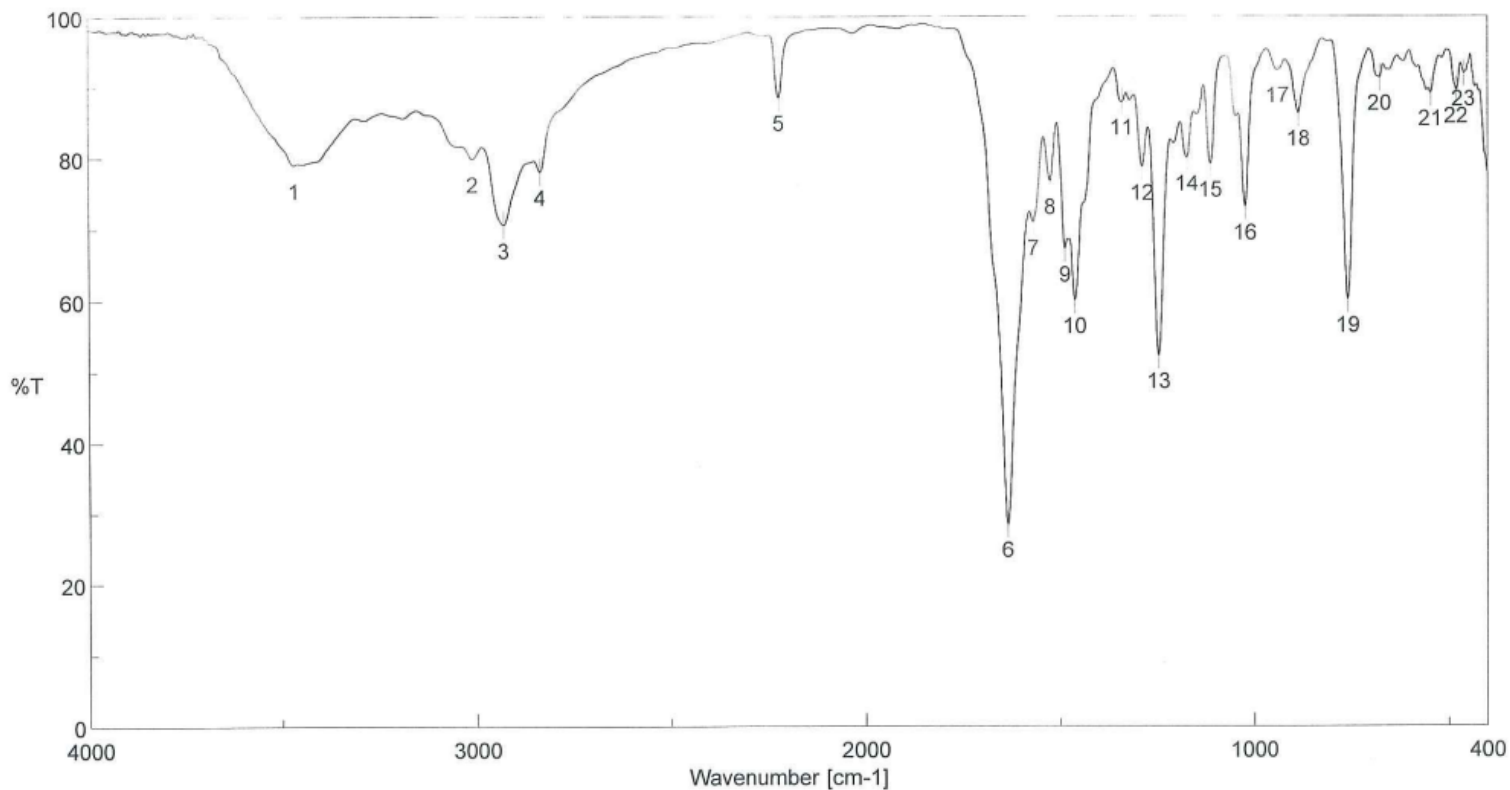
Pulse Sequence: s2pu1
Solvent: DMSO
Temp. 30.0 C / 303.1 K
Mercury-300BB "NMR300"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 4.853 sec
Width 6600.7 Hz
11 repetitions
OBSERVE H1, 300.0687865 MHz
DATA PROCESSING
FT size 65536
Total time 5 min, 16 sec
Date: Jul 21 2014



S12b. ¹H NMR spectrum (300 MHz, DMSO-d₆) of compound 17

Peak Find - E4



[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
①	3468.35	78.96292	②	3011.3	79.83396	③	2932.23	70.56142	4	2837.74	78.02757
⑤	2223.52	88.42147	⑥	1635.34	28.43761	7	1569.77	70.95975	8	1526.38	76.68094
9	1487.81	67.21743	10	1462.74	60.03839	11	1341.25	87.82886	12	1288.22	78.63858
13	1246.75	52.29260	14	1173.47	79.96577	15	1112.73	79.08384	16	1023.05	73.09677
17	939.163	92.36802	18	886.131	86.25280	19	759.816	60.17382	20	676.892	91.25376
21	546.72	89.05956	22	481.153	89.44514	23	461.868	91.85877			

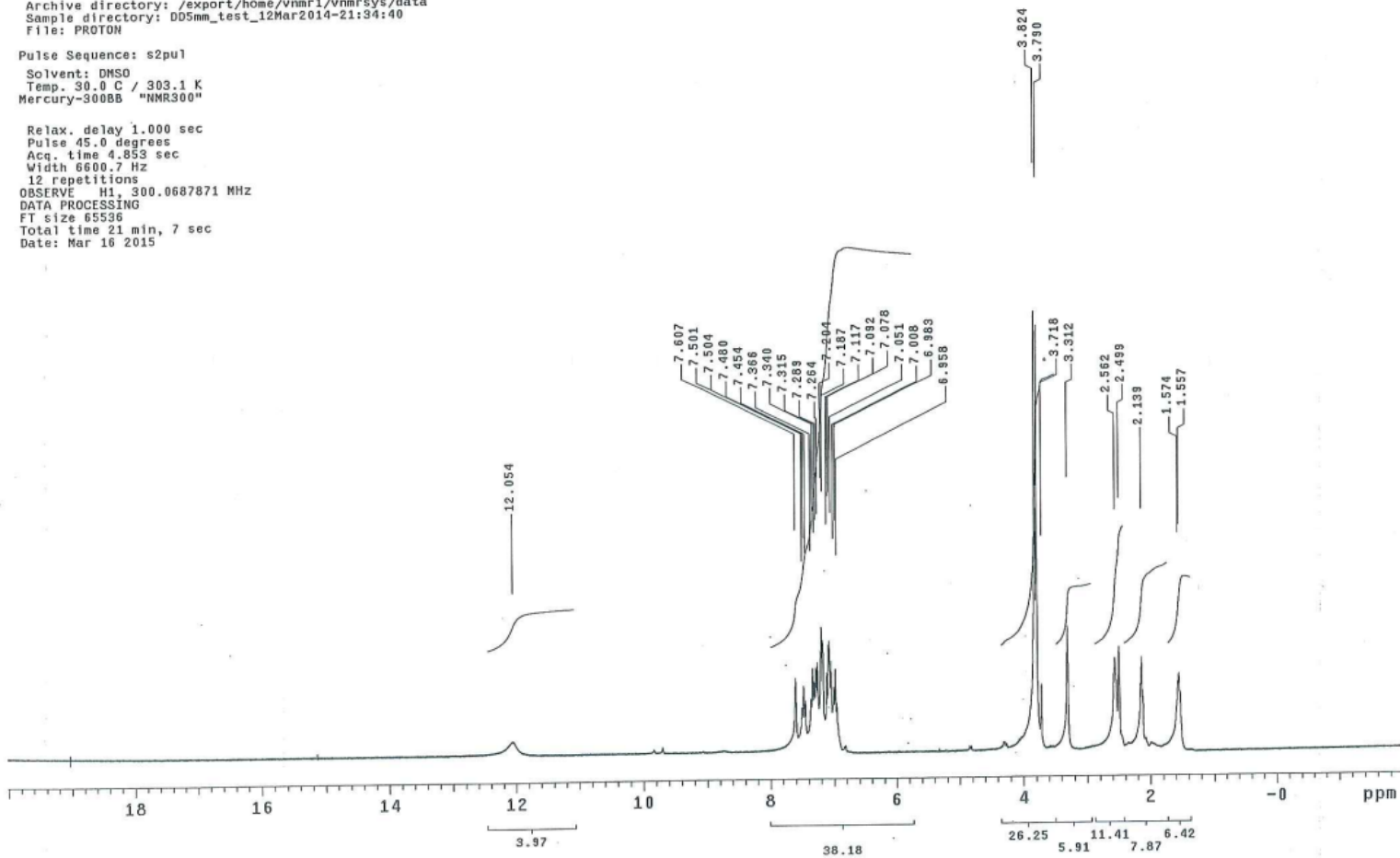
S13a. IR spectrum (KBr, cm⁻¹) of compound 21

KhaniaSayed-E4-DMSO-H

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

Pulse Sequence: s2pu1
Solvent: DMSO
Temp. 30.0 C / 303.1 K
Mercury-300BB "NMR300"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 4.853 sec
Width 6600.7 Hz
12 repetitions
OBSERVE H1, 300.0687871 MHz
DATA PROCESSING
FT size 65536
Total time 21 min, 7 sec
Date: Mar 16 2015



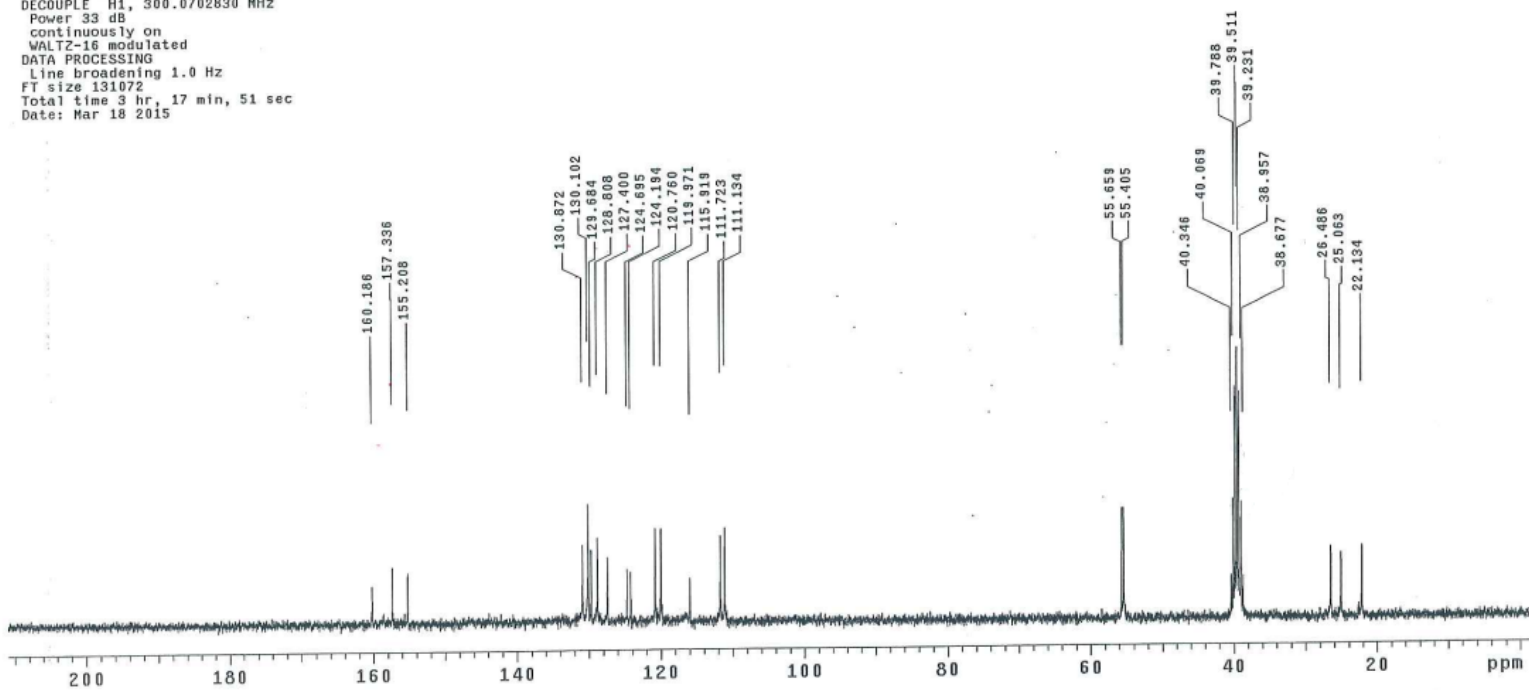
S13b. ^1H NMR spectrum (300 MHz, $\text{DMSO-}d_6$) of compound 21

GhaniaMorsy-E4-DMSO-C13

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

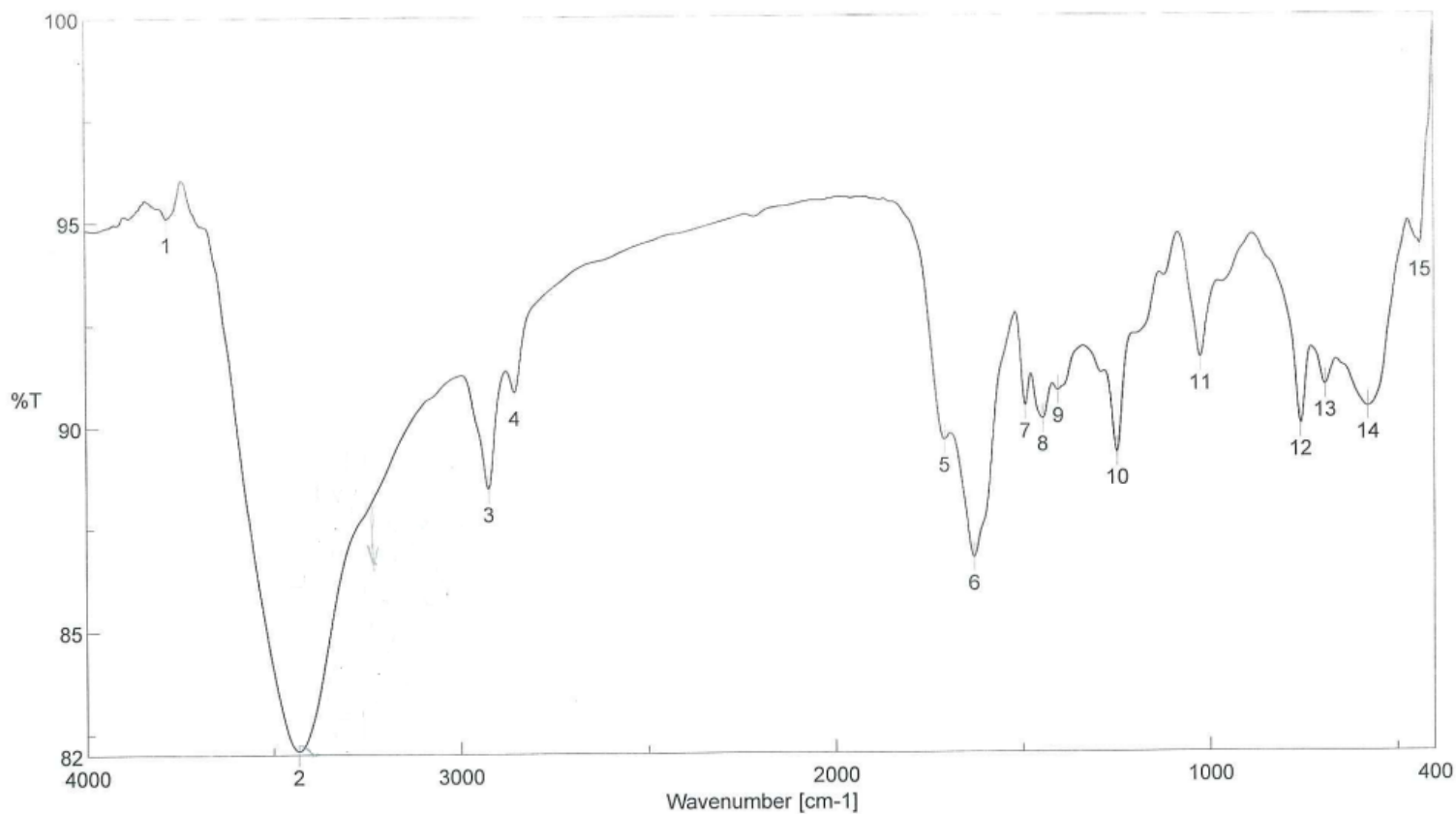
Pulse Sequence: s2pu1
Solvent: DMSO
Temp. 30.0 C / 303.1 K
Mercury-300BB "NMR300"

Pulse 45.0 degrees
Acq. time 1.815 sec
Width 18761.7 Hz
2248 repetitions
OBSERVE C13, 75.4523954 MHz
DECOUPLE H1, 300.0702830 MHz
Power 33 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 3 hr, 17 min, 51 sec
Date: Mar 18 2015



S13c. ^{13}C NMR spectrum (75 MHz, $\text{DMSO-}d_6$) of compound 21

Peak Find - E67



[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1	3781.72	95.09843	2	3432.67	82.08977	3	2924.52	88.46484	4	2854.13	90.83206
5	1707.66	89.62933	6	1628.59	86.73815	7	1491.67	90.45927	8	1445.39	90.14161
9	1403.92	90.83438	10	1246.75	89.31385	11	1024.02	91.62869	12	755.959	89.99448
13	690.391	90.94867	14	576.612	90.41011	15	437.762	94.35038			

S14_a. IR spectrum (KBr, cm⁻¹) of compound 23

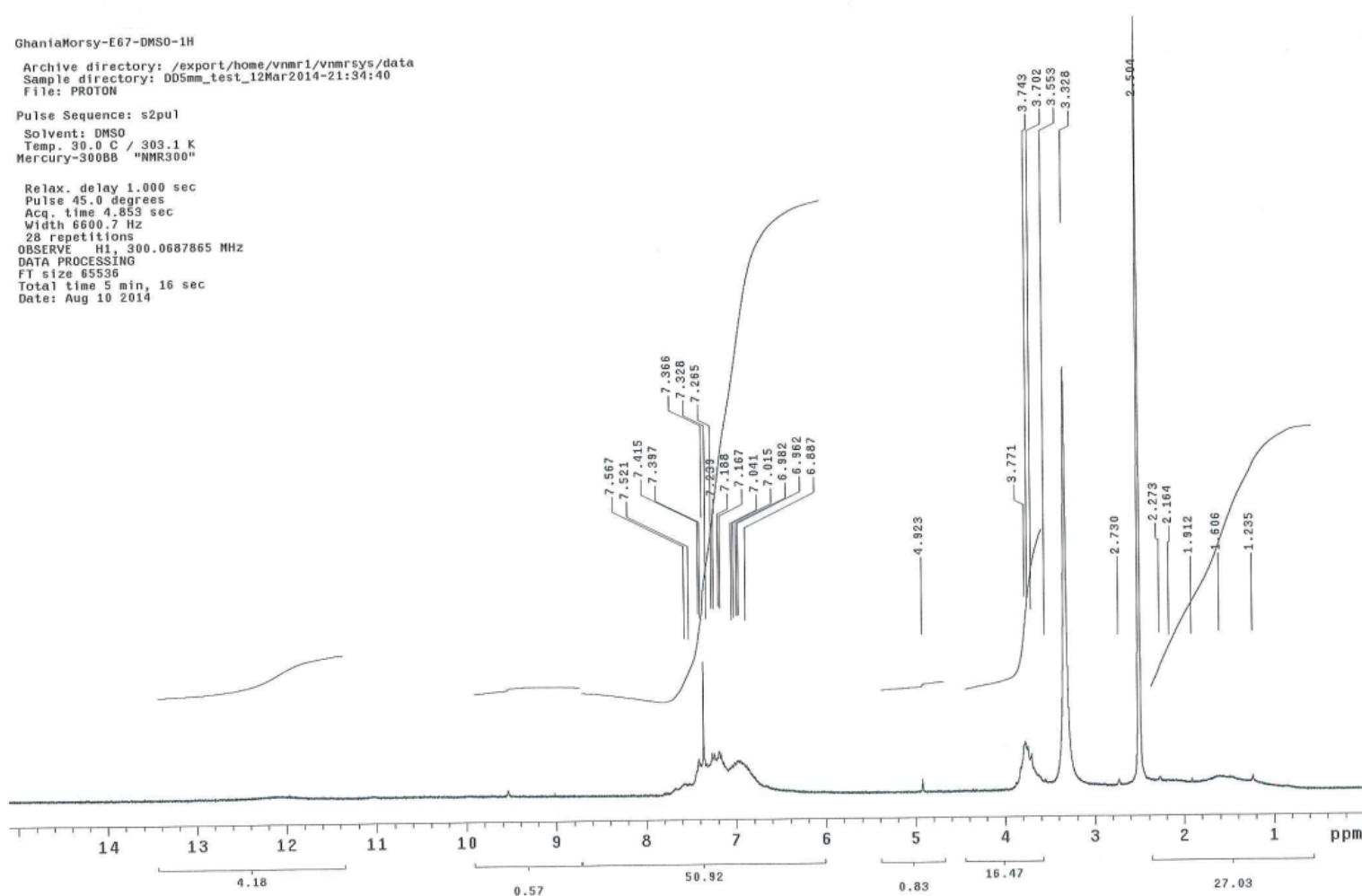
GhaniaMorsy-E67-DMSO-1H

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

Pulse Sequence: s2pu1

Solvent: DMSO
Temp. 30.0 C / 303.1 K
Mercury-300BB "NMR300"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 4.853 sec
Width 6600.7 Hz
28 repetitions
OBSERVE H1, 300.0687865 MHz
DATA PROCESSING
F1 size 65536
Total time 5 min, 16 sec
Date: Aug 10 2014



S14b. ¹H NMR spectrum (300 MHz, DMSO-*d*₆) of compound 23

Antitumor evaluation S1

Table S1 *Effect of compounds 1, 13, 16, 17 and 21 on the growth of three human tumor cell lines*

Sample ID	Compound	GI ₅₀ (μg L ⁻¹)(% Growth)		
		MCF-7	NCI-H460	SF-268
E53	1	20.23 ± 4.50	18.28 ± 4.21	42.62 ± 4.80
E65b	13	14.27 ± 6.07	18.15 ± 4.05	20.27 ± 2.40
E80	16	4.16 ± 1.09	7.25 ± 1.30	12.80 ± 3.90
E63	17	13.48 ± 4.22	6.09 ± 1.88	4.62 ± 1.12
E4	21	22.31 ± 3.40	18.29 ± 2.40	28.11 ± 10.30
	Doxorubicin	0.04 ± 0.008	0.09 ± 0.008	0.09 ± 0.007



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Table 1 Effect of compounds ----- on the growth of three human tumor cell lines

Compound	GI ₅₀ (μg L ⁻¹)(% Growth)		
	MCF-7	NCI-H460	SF-268
E53	20.23 ± 4.50	18.28 ± 4.21	42.62 ± 4.80
E80	4.16 ± 1.09	7.25 ± 1.30	12.80 ± 3.90
E4	22.31 ± 3.40	18.29 ± 2.40	28.11 ± 10.30
E65b	14.27 ± 6.07	18.15 ± 4.05	20.27 ± 2.40
E63	13.48 ± 4.22	6.09 ± 1.88	4.62 ± 1.12
E60	60.34 ± 12.36	58.20 ± 6.58	18.60 ± 2.09
Doxorubicin	0.04 ± 0.008	0.09 ± 0.008	0.09 ± 0.007

Results are given in concentrations that were able to cause 50 % of cell growth inhibition (GI₅₀) after a continuous exposure of 48 h and show means ± SEM of three-independent experiments performed in duplicate.

Against MCF-7

Compound	Viability rate (%)	IC ₅₀ (mg/ml)		
		0.1 μg/ml	1 μg/ml	10 μg/ml
E53	55.81 ± 9.12	50.39 ± 6.88	44.21 ± 8.92	20.22 ± 2.02
E80	90.22 ± 6.47	88.87 ± 5.41	80.42 ± 6.80	6.80 ± 2.93
E4	70.41 ± 12.46	68.20 ± 9.34	66.13 ± 10.68	20.50 ± 5.50
E65b	64.55 ± 2.53	62.40 ± 2.59	58.40 ± 6.31	11.01 ± 3.24

Handwritten signature and stamp in Arabic, including the word 'center'.

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E36	80.41 ± 4.49	76.21 ± 6.39	70.18 ± 5.63	8.44 ± 1.29
E60	78.54 ± 2.19	68.38 ± 8.39	62.31 ± 5.32	12.12 ± 3.37

Against NCI-H460

Compound	Viability rate (%)			IC ₅₀ (µg/ml)
	0.1 µg/ml	1 µg/ml	10 µg/ml	
E53	68.21 ± 6.80	58.63 ± 2.90	52.08 ± 6.72	18.29 ± 1.89
E80	87.28 ± 6.52	76.64 ± 5.83	70.93 ± 4.09	6.78 ± 2.61
E4	72.57 ± 3.60	65.28 ± 6.84	58.74 ± 6.03	18.22 ± 2.64
E65b	48.26 ± 4.53	40.56 ± 3.28	36.41 ± 4.68	30.42 ± 4.84
E36	92.58 ± 5.82	86.09 ± 5.93	80.51 ± 6.83	5.59 ± 1.25
E60	68.28 ± 3.05	59.41 ± 3.29	55.93 ± 6.82	19.26 ± 5.62

Results are given in concentrations that were able to cause 50 % of cell growth inhibition (GI₅₀) after a continuous exposure of 48 h and show means ± SEM of three-independent experiments performed in duplicate.

Handwritten signature and date: 1/1/14

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Against SF-268

Compound	Viability rate (%)			IC ₅₀ (µg/ml)
	0.1 µg/ml	1 µg/ml	10 µg/ml	
E53	78.23 ± 4.46	72.30 ± 4.27	68.21 ± 4.53	42.30 ± 3.40
E80	80.42 ± 8.73	72.20 ± 4.80	63.44 ± 3.26	8.32 ± 1.90
E4	68.22 ± 5.31	60.19 ± 3.59	55.52 ± 2.49	12.33 ± 1.30
E65b	73.46 ± 8.20	66.39 ± 2.09	58.73 ± 5.90	27.52 ± 1.63
E36	84.77 ± 2.40	75.21 ± 3.49	66.42 ± 5.70	6.73 ± 1.69
E60	52.40 ± 4.63	46.27 ± 2.89	42.72 ± 3.62	58.48 ± 3.09

1. Campaigne, E., *Comprehen. Heter. Chem.*, **1984**, 4, 863.
2. Skehan, P., Storeng, R., Scudiero, D., Monks, A., McMahon, J., Vistica, D., Warren, J. T., Bokesch, H., Kenny, S., Boyd, M. R., *J. Natl. Cancer Inst.*, **1990**, 82, 1107.
3. Monks, A., Scudiero, D., Skehan, P., Shoemaker, R., Paul, K., Vistica, D., Hose, C., Langley, J., Cronise, P., Vaigro-Wolff, A., Gray-Goodr M., Campbell, H., Mayo, J., Boyd, J. M., *J. Natl. Cancer Inst.*, **1991**, 83, 757.



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