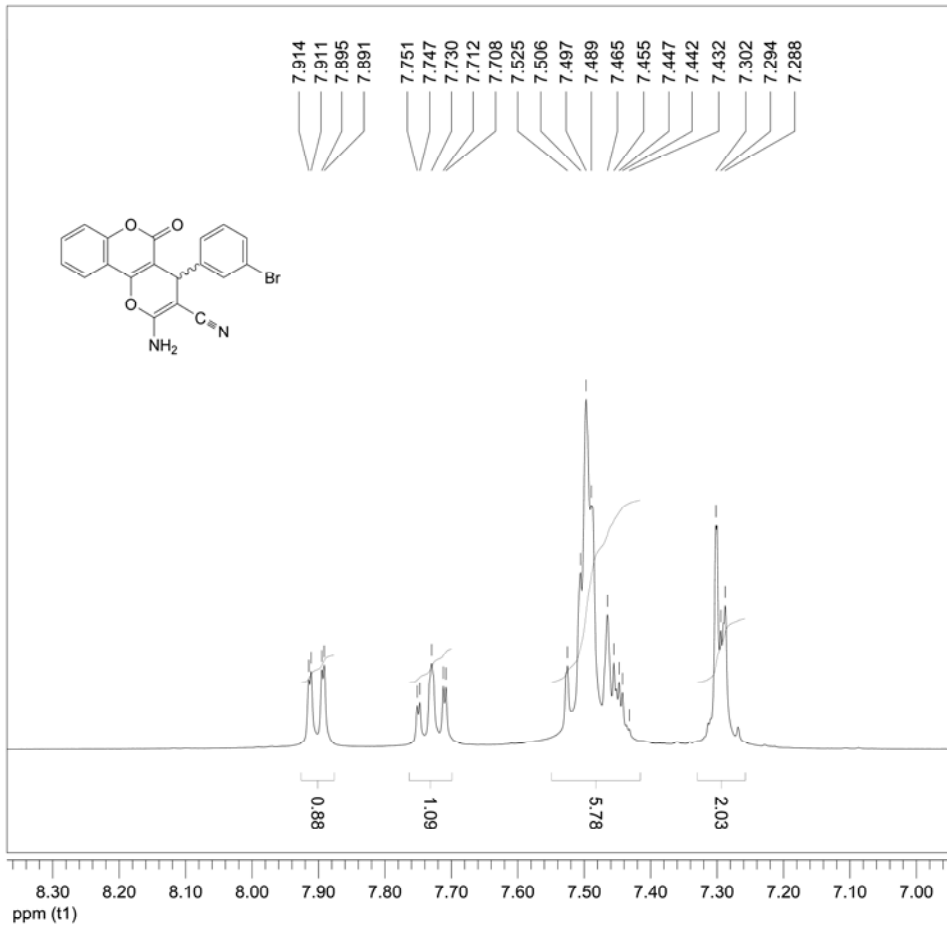


Instrument Specifications:
 NMR Spectrometer 400 MHz, Avance III 400
 Bruker, Germany

Date:
 29 Jul 2012
Spectrum Title:
 Khodabakhshi (KH1)
 DMSO-1H NMR
Frequency (MHz):
 (f1) 400.130
Original Points Count:
 (f1) 32768
Actual Points Count:
 (f1) 32768
Acquisition Time (sec):
 (f1) 3.8928
Spectral Width (ppm):
 (f1) 21.037
Pulse Program:
 Unknown



Instrument Specifications:
NMR Spectrometer 400 MHz, Avance II 400
Bruker, Germany

Date:
29 Jul 2012

Spectrum Title:
Khodabakhshi (KH1)
DMSO-1H NMR

Frequency (MHz):
(f1) 400.130

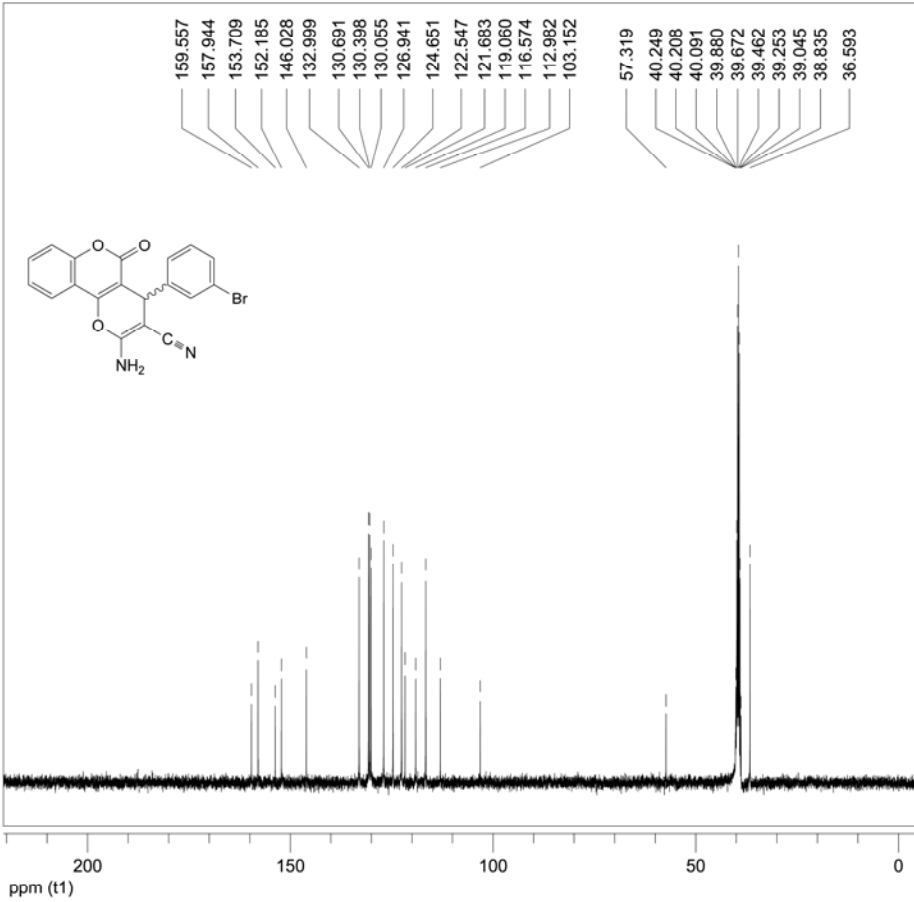
Original Points Count:
(f1) 32768

Actual Points Count:
(f1) 32768

Acquisition Time (sec):
(f1) 3.8928

Spectral Width (ppm):
(f1) 21.037

Pulse Program:
Unknown



Instrument Specifications:
NMR Spectrometer 400 MHz, Avance II 400
Bruker, Germany

Date:

29 Jul 2012

Spectrum Title:

Khodabakhshi (KH1)

DMSO-13C NMR

Frequency (MHz):

(f1) 100.613

Original Points Count:

(f1) 32768

Actual Points Count:

(f1) 32768

Acquisition Time (sec):

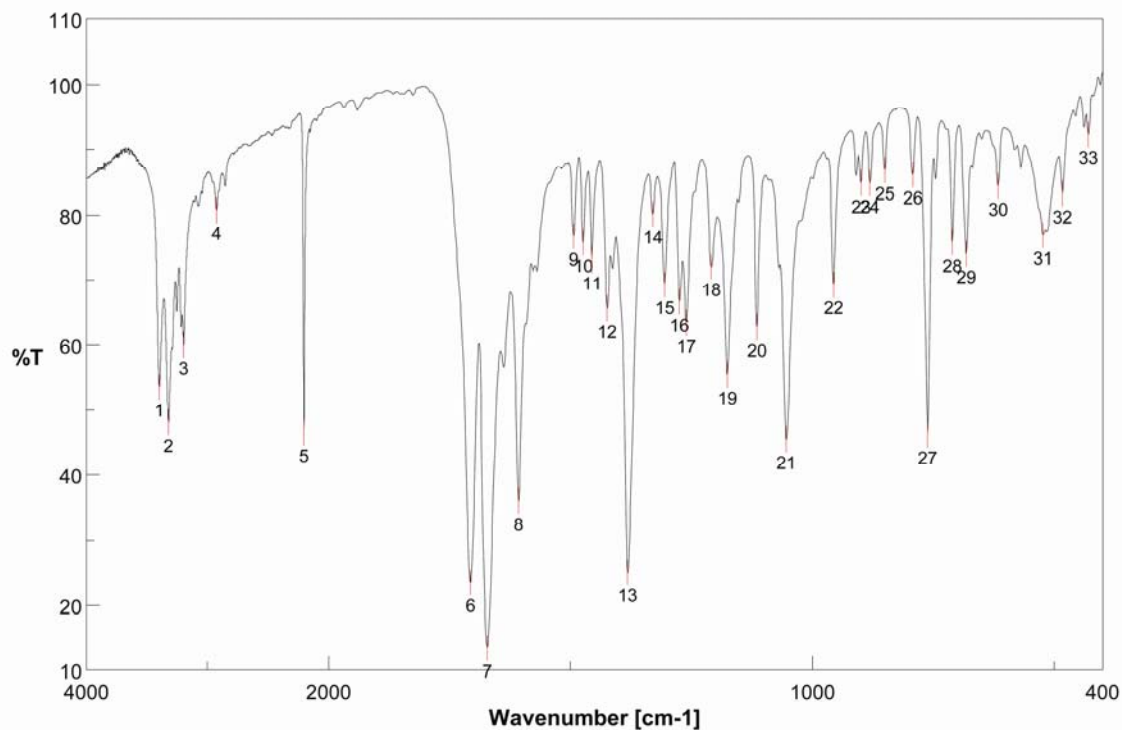
(f1) 1.2583

Spectral Width (ppm):

(f1) 258.830

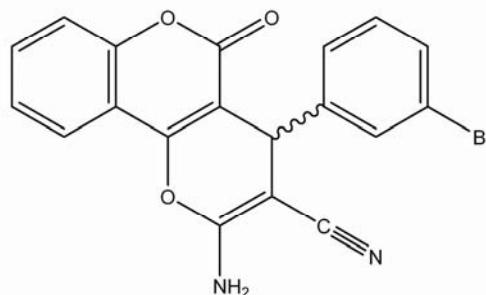
Pulse Program:

Unknown

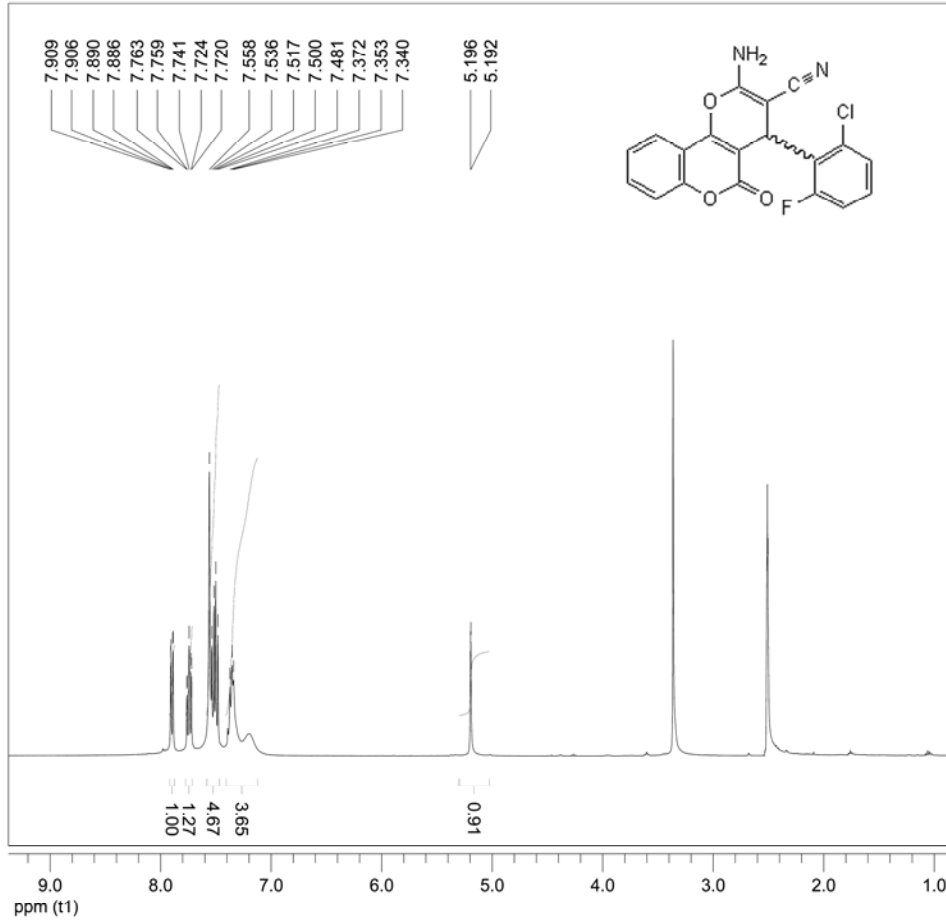


Accumulation Auto (24)
 Resolution 4 cm-1
 Zero Filling ON
 Apodization Cosine
 Gain Auto (2)
 Scanning Speed Auto (2 mm/sec)
 Date/Time 2012/06/30 ط.ب.ظ:6:16
 Update 2012/06/30 ط.ب.ظ:6:18
 Operator
 File Name
 Sample Name
 Comment

Memory#2



No.	cm-1	%T	No.	cm-1	%T	No.	cm-1	%T
1	3396.99	5.35E+001	2	3321.78	4.81E+001	3	3195.47	6.00E+001
4	2924.52	8.07E+001	5	2202.31	4.66E+001	6	1706.69	2.35E+001
7	1671.98	1.35E+001	8	1607.38	3.61E+001	9	1493.6	7.67E+001
10	1473.35	7.58E+001	11	1455.99	7.31E+001	12	1424.17	6.56E+001
13	1381.75	2.51E+001	14	1329.68	8.02E+001	15	1305.57	6.92E+001
16	1274.72	6.66E+001	17	1260.25	6.34E+001	18	1209.15	7.20E+001
19	1175.4	5.55E+001	20	1114.65	6.27E+001	21	1053.91	4.55E+001
22	956.52	6.92E+001	23	899.63	8.48E+001	24	881.309	8.49E+001
25	850.454	8.68E+001	26	792.6	8.61E+001	27	761.744	4.62E+001
28	710.64	7.58E+001	29	681.713	7.40E+001	30	616.145	8.44E+001
31	523.579	7.69E+001	32	483.081	8.33E+001	33	430.048	9.23E+001



Instrument Specifications:
NMR Spectrometer 400 MHz, Avance III 400
Bruker, Germany

Date:
29 Jul 2012

Spectrum Title:
Khoda bakhshi (KH2)
DMSO-1H NMR

Frequency (MHz):
(f1) 400.130

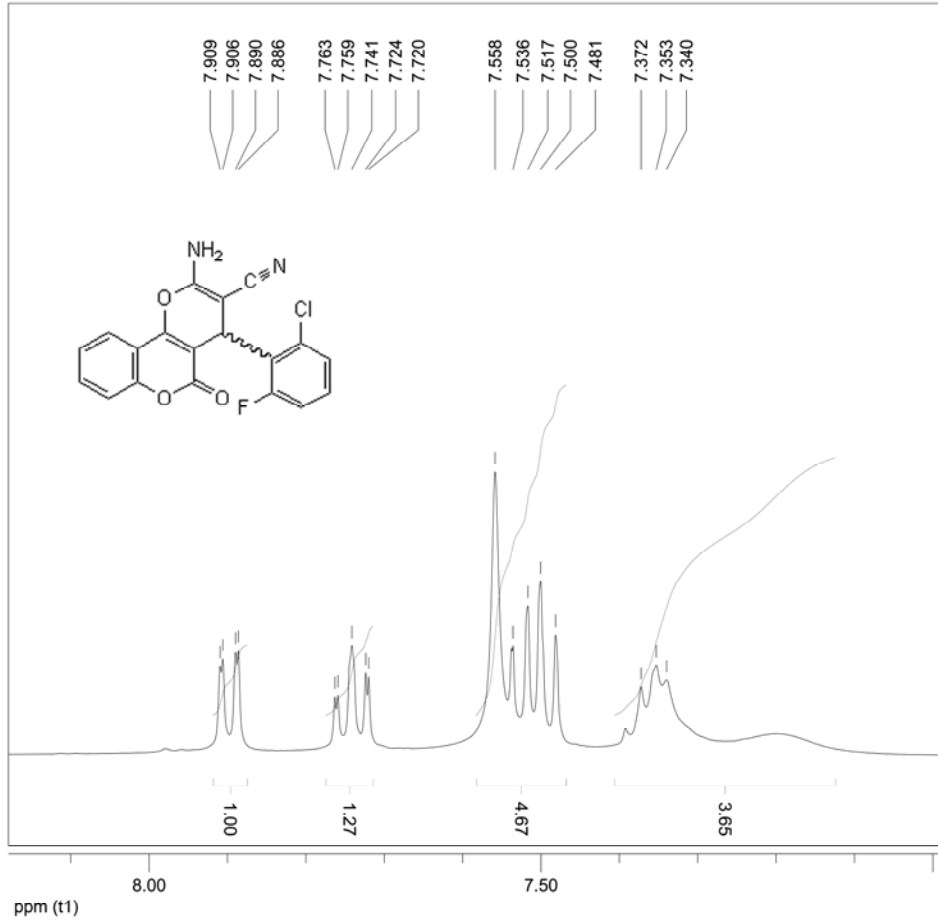
Original Points Count:
(f1) 32768

Actual Points Count:
(f1) 32768

Acquisition Time (sec):
(f1) 3.8928

Spectral Width (ppm):
(f1) 21.037

Pulse Program:
Unknown



Instrument Specifications:
NMR Spectrometer 400 MHz, Avance II 400
Bruker, Germany

Date:
29 Jul 2012

Spectrum Title:
Khoda bakhshi (KH2)
DMSO-1H NMR

Frequency (MHz):
(f1) 400.130

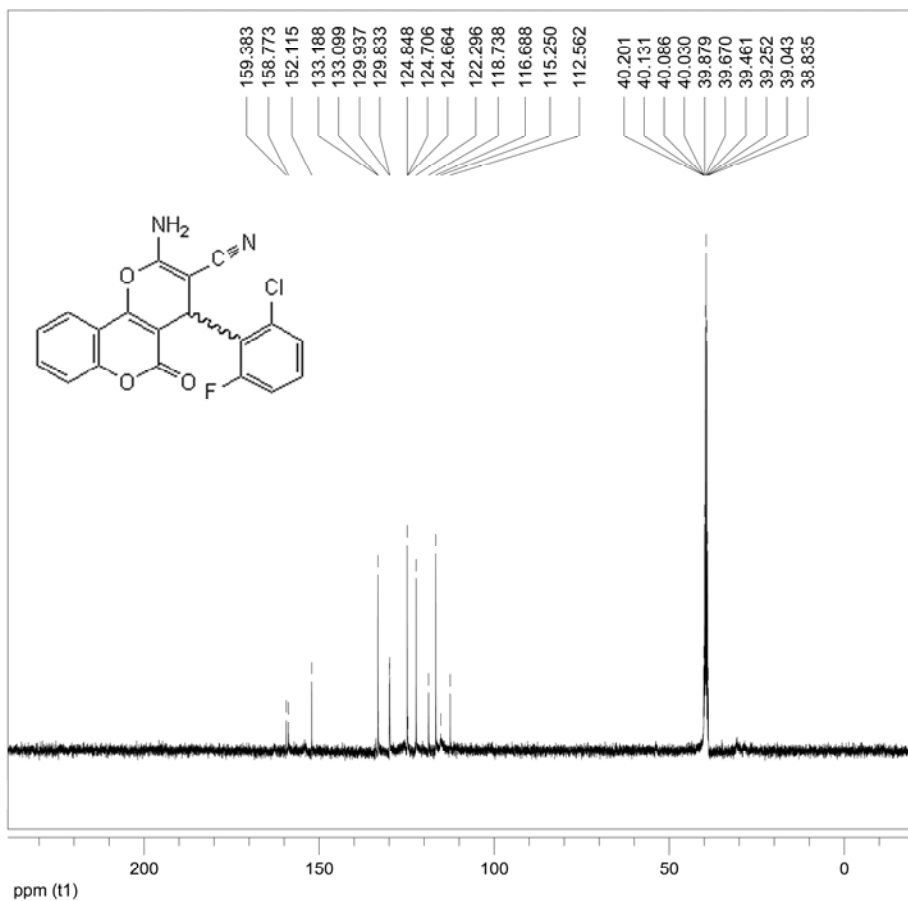
Original Points Count:
(f1) 32768

Actual Points Count:
(f1) 32768

Acquisition Time (sec):
(f1) 3.8928

Spectral Width (ppm):
(f1) 21.037

Pulse Program:
Unknown

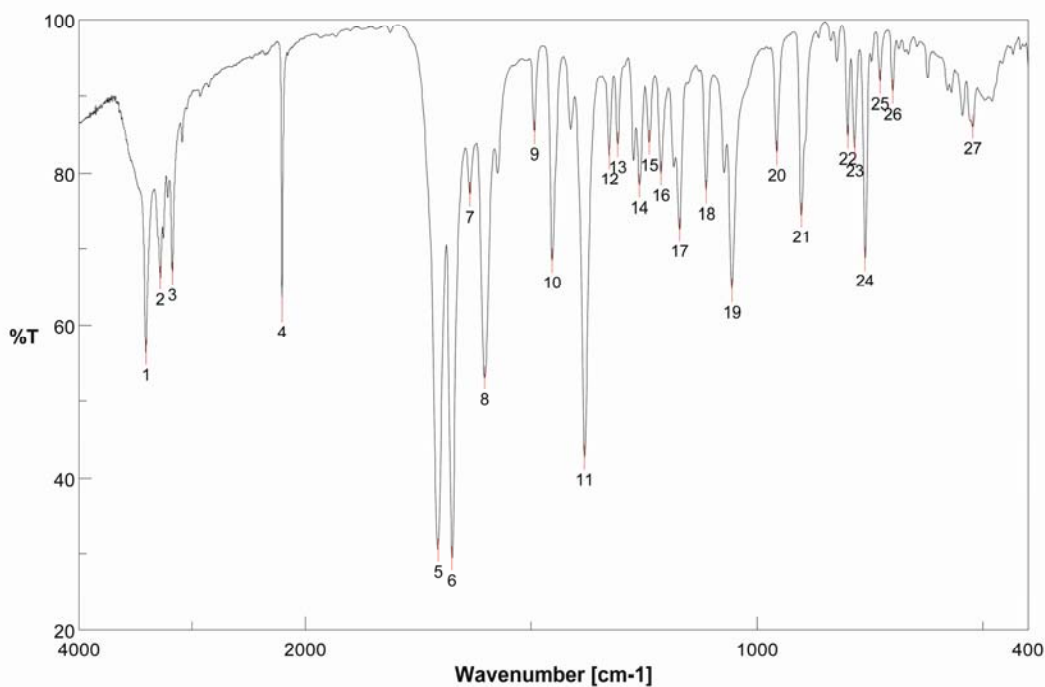


Instrument Specifications:
NMR Spectrometer 400 MHz, Avance III 400
Bruker, Germany

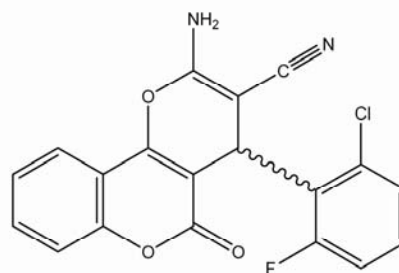
Date:
29 Jul 2012
Document's Title:
CNMR.mrc

Spectrum Title:

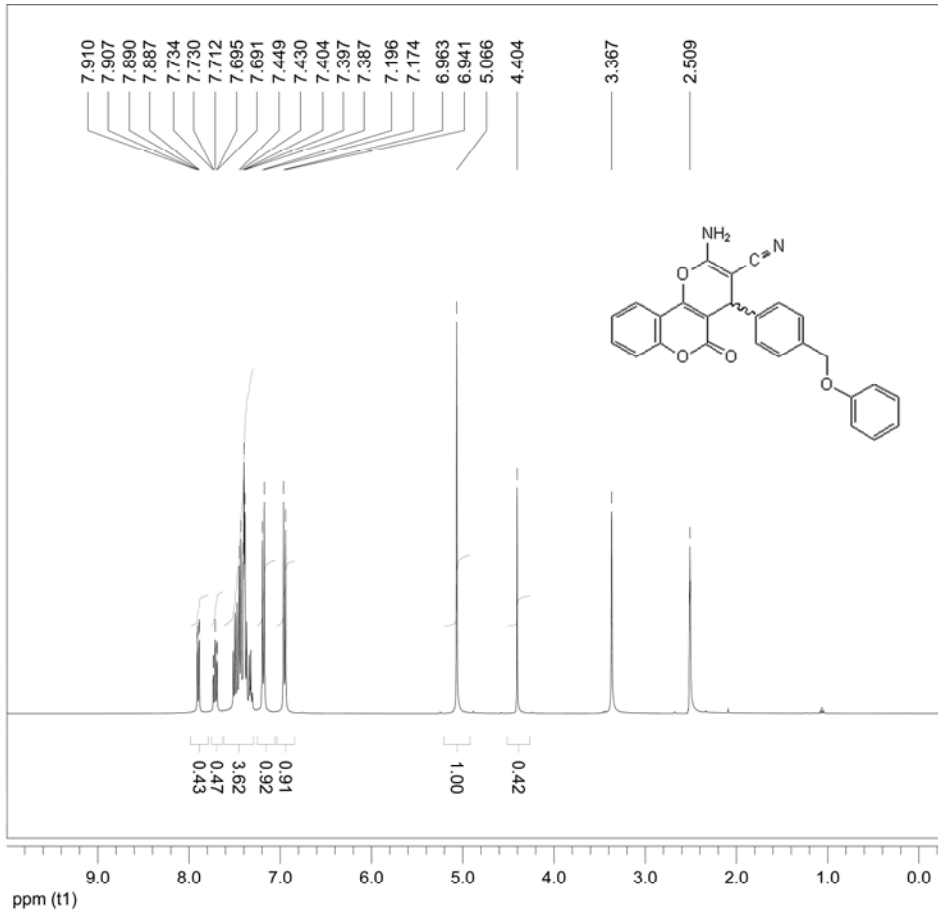
Frequency (MHz):
(f1) 100.613
Original Points Count:
(f1) 32768
Actual Points Count:
(f1) 32768
Acquisition Time (sec):
(f1) 1.2583
Spectral Width (ppm):
(f1) 258.830
Pulse Program:
Unknown



Accumulation Auto (21)
 Resolution 4 cm-1
 Zero Filling ON
 Apodization Cosine
 Gain Auto (2)
 Scanning Speed Auto (2 mm/sec)
 Date/Time 2012/06/30 ب.ظ 7:16
 Update 2012/06/30 ب.ظ 7:16
 Operator
 File Name
 Sample Name
 Comment



No.	cm-1	%T	No.	cm-1	%T	No.	cm-1	%T
1	3408.57	5.64E+001	2	3280.32	6.62E+001	3	3175.22	6.68E+001
4	2203.27	6.20E+001	5	1705.73	3.06E+001	6	1674.87	2.94E+001
7	1635.34	7.72E+001	8	1602.56	5.31E+001	9	1492.63	8.54E+001
10	1453.1	6.85E+001	11	1381.75	4.27E+001	12	1326.79	8.21E+001
13	1308.46	8.37E+001	14	1260.25	7.84E+001	15	1238.08	8.40E+001
16	1213.01	7.99E+001	17	1171.54	7.26E+001	18	1112.73	7.75E+001
19	1055.84	6.46E+001	20	956.52	8.27E+001	21	901.558	7.45E+001
22	799.35	8.47E+001	23	783.922	8.33E+001	24	760.78	6.87E+001
25	727.996	9.20E+001	26	700.033	9.07E+001	27	522.615	8.61E+001



Instrument Specifications:
NMR Spectrometer 400 MHz, Avance II 400
Bruker, Germany

Date:

29 Jul 2012

Spectrum Title:

Khodabakhshi (KH4)
DMSO-1H NMR

Frequency (MHz):

(f1) 400.130

Original Points Count:

(f1) 32768

Actual Points Count:

(f1) 32768

Acquisition Time (sec):

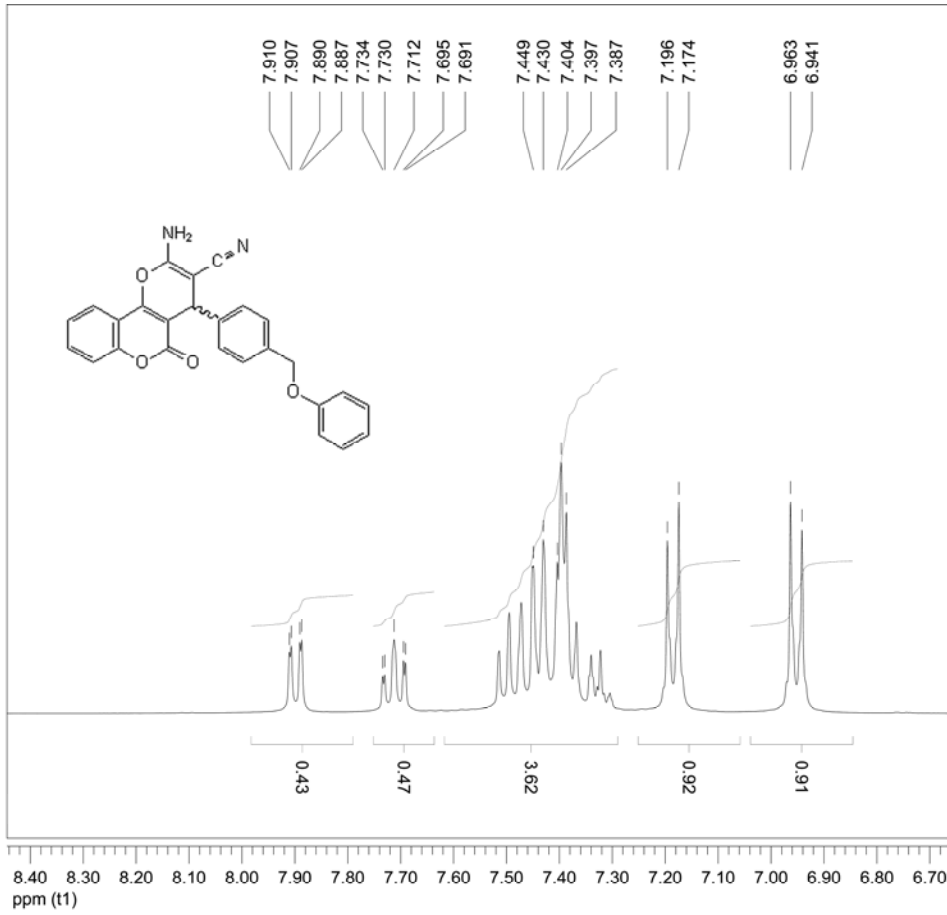
(f1) 3.8928

Spectral Width (ppm):

(f1) 21.037

Pulse Program:

Unknown



Instrument Specifications:
NMR Spectrometer 400 MHz, Avance II 400
Bruker, Germany

Date:
29 Jul 2012

Spectrum Title:
Khodabakhshi (KH4)
DMSO-1H NMR

Frequency (MHz):
(f1) 400.130

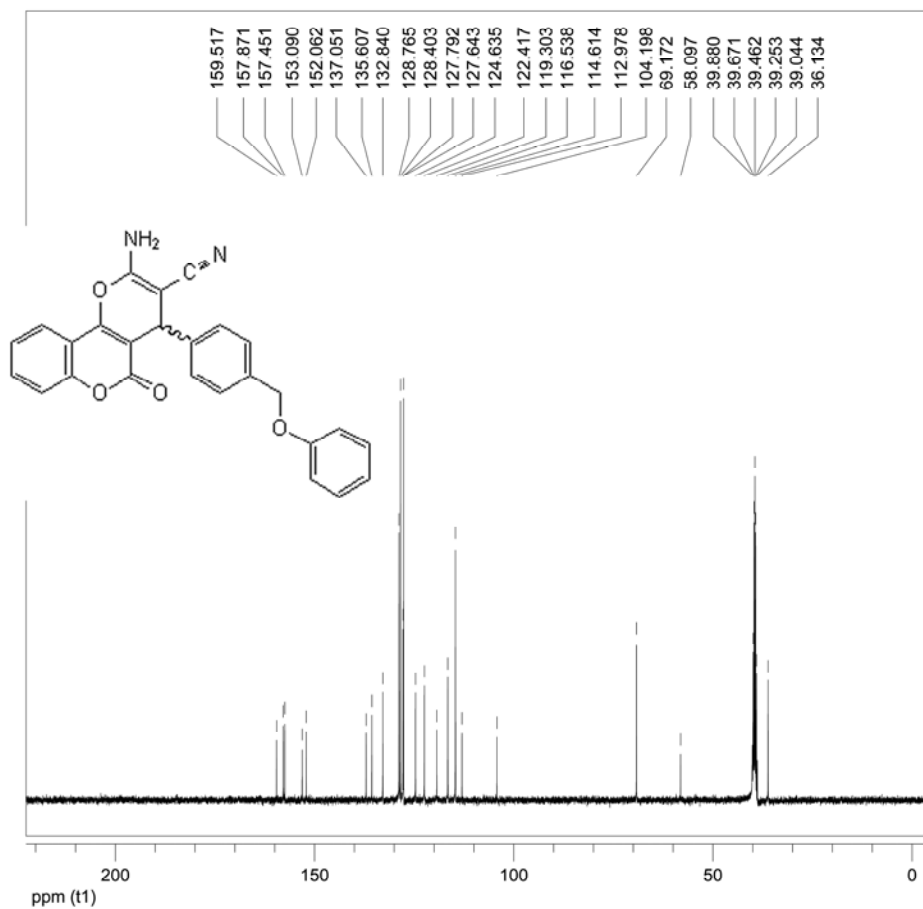
Original Points Count:
(f1) 32768

Actual Points Count:
(f1) 32768

Acquisition Time (sec):
(f1) 3.8928

Spectral Width (ppm):
(f1) 21.037

Pulse Program:
Unknown



Instrument Specifications:
NMR Spectrometer 400 MHz, Avance III 400
Bruker, Germany

Date:
29 Jul 2012

Spectrum Title:
Khodabakhshi (KH4)
DMSO-13C NMR

Frequency (MHz):
(f1) 100.613

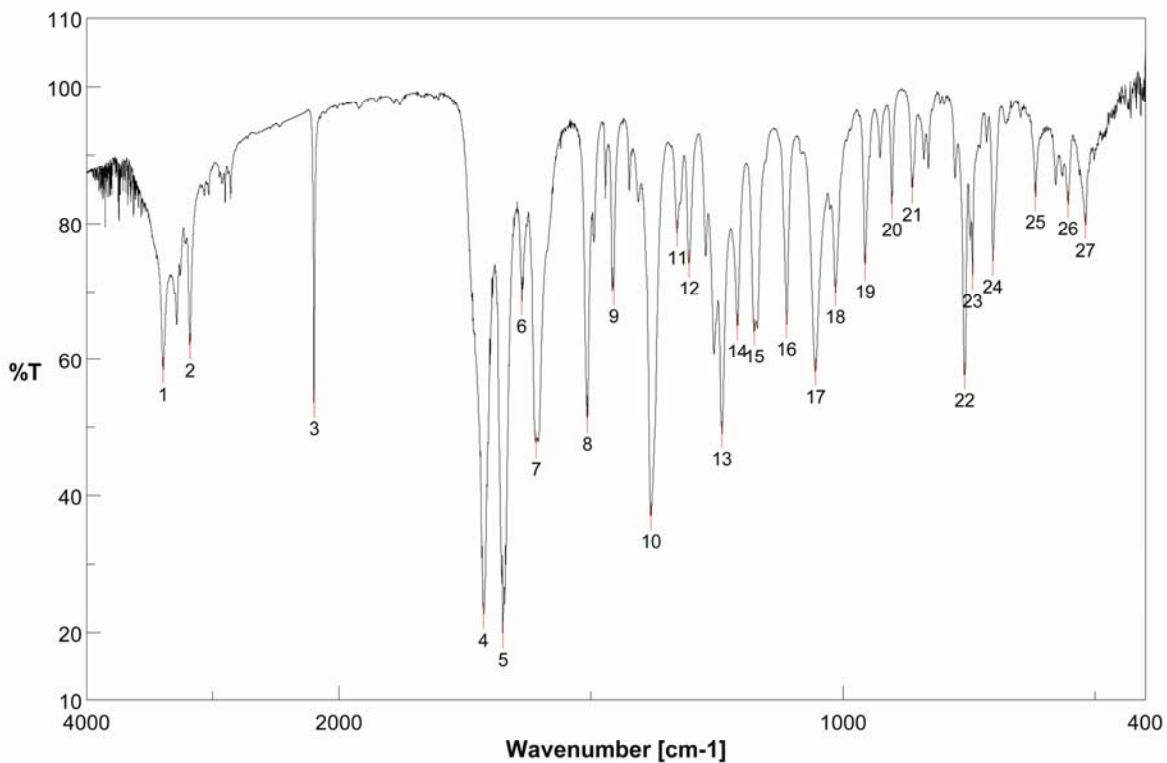
Original Points Count:
(f1) 32768

Actual Points Count:
(f1) 32768

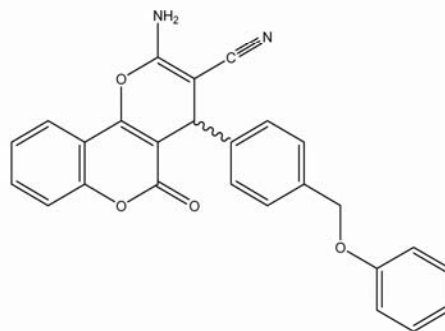
Acquisition Time (sec):
(f1) 1.2583

Spectral Width (ppm):
(f1) 258.830

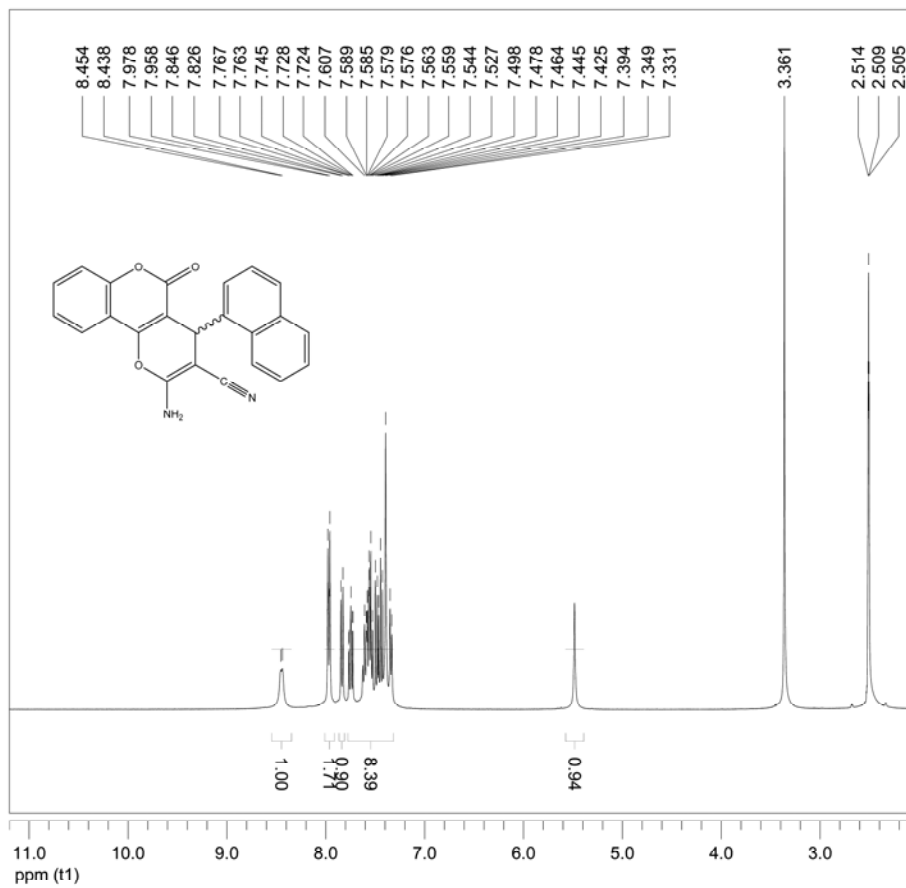
Pulse Program:
Unknown



Accumulation Auto (23)
 Resolution 1 cm-1
 Zero Filling ON
 Apodization Cosine
 Gain Auto (2)
 Scanning Speed Auto (2 mm/sec)
 Date/Time 2012/06/30 ب.ظ:5:21
 Update 2012/06/30 ب.ظ:5:41
 Operator
 File Name 4-coum+bezyloxybenaldehyde+Malon
 Sample Name
 Comment



No.	cm-1	%T	No.	cm-1	%T	No.	cm-1	%T
1	3391.45	5.84E+001	2	3180.04	6.19E+001	3	2196.04	5.34E+001
4	1712.96	2.24E+001	5	1674.39	1.97E+001	6	1636.79	6.85E+001
7	1608.58	4.75E+001	8	1506.37	5.12E+001	9	1454.55	7.00E+001
10	1381.02	3.70E+001	11	1328.95	7.86E+001	12	1305.33	7.41E+001
13	1240	4.90E+001	14	1209.39	6.48E+001	15	1175.88	6.40E+001
16	1111.76	6.51E+001	17	1054.63	5.81E+001	18	1014.86	6.99E+001
19	956.279	7.37E+001	20	903.005	8.27E+001	21	862.507	8.49E+001
22	759.334	5.76E+001	23	742.942	7.22E+001	24	702.926	7.44E+001
25	618.074	8.39E+001	26	553.47	8.28E+001	27	518.999	7.97E+001



Instrument Specifications:
NMR Spectrometer 400 MHz, Avance II 400
Bruker, Germany

Date:
29 Jul 2012

Spectrum Title:
Khodabakhshi (KH3)
DMSO-1H NMR

Frequency (MHz):
(f1) 400.130

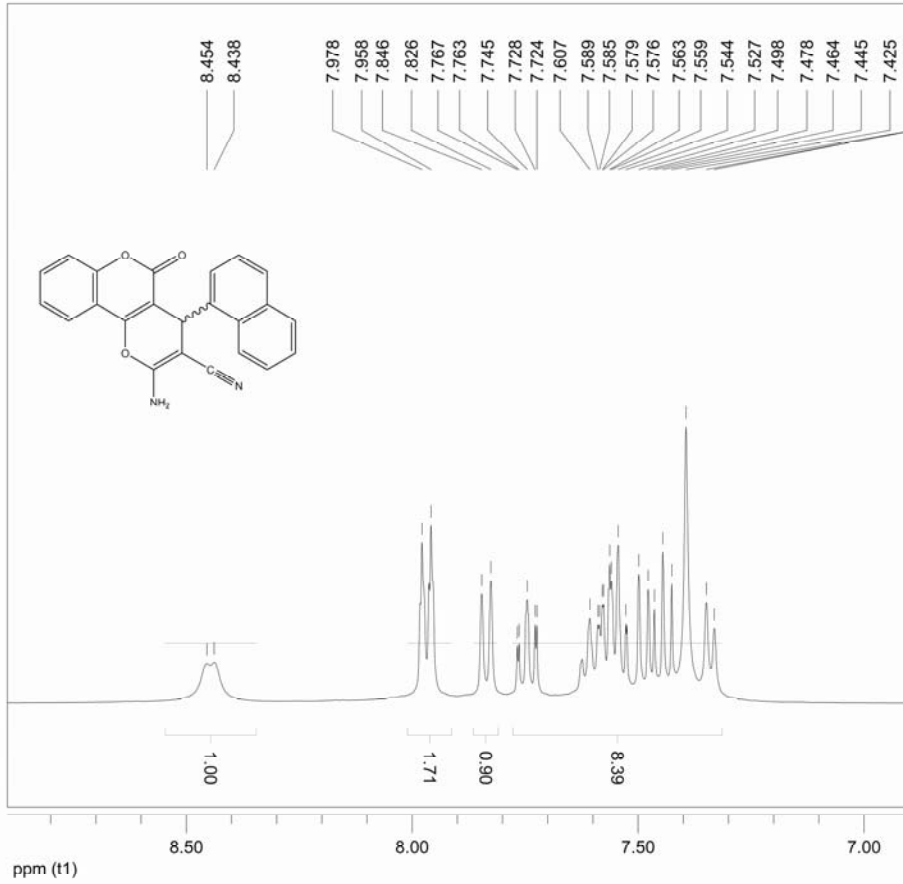
Original Points Count:
(f1) 32768

Actual Points Count:
(f1) 32768

Acquisition Time (sec):
(f1) 3.8928

Spectral Width (ppm):
(f1) 21.037

Pulse Program:
Unknown



Instrument Specifications:
NMR Spectrometer 400 MHz, Avance III 400
Bruker, Germany

Date:

29 Jul 2012

Spectrum Title:

Khodabakhshi (Expand-KH3)
DMSO-1H NMR

Frequency (MHz):

(f1) 400.130

Original Points Count:

(f1) 32768

Actual Points Count:

(f1) 32768

Acquisition Time (sec):

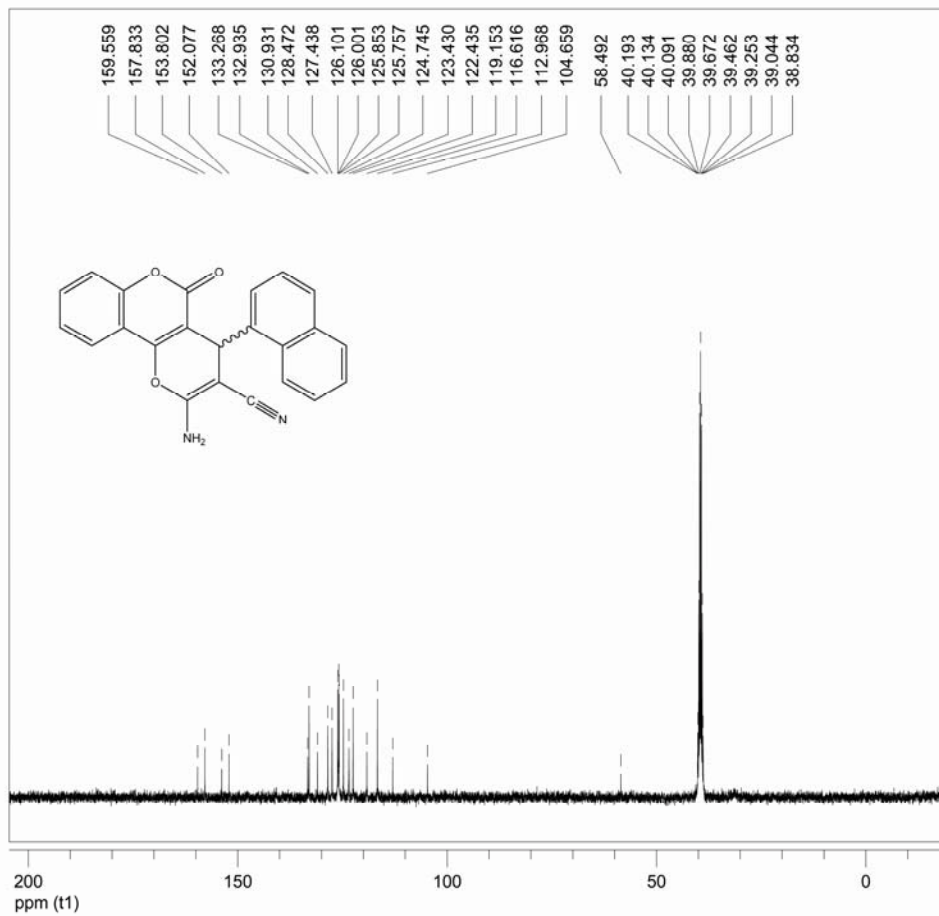
(f1) 3.8928

Spectral Width (ppm):

(f1) 21.037

Pulse Program:

Unknown



Instrument Specifications:
NMR Spectrometer 400 MHz, Avance II 400
Bruker, Germany

Date:

30 Jul 2012

Spectrum Title:

Khodabakhshi (KH3)
DMSO-13C NMR

Frequency (MHz):

(f1) 100.613

Original Points Count:

(f1) 32768

Actual Points Count:

(f1) 32768

Acquisition Time (sec):

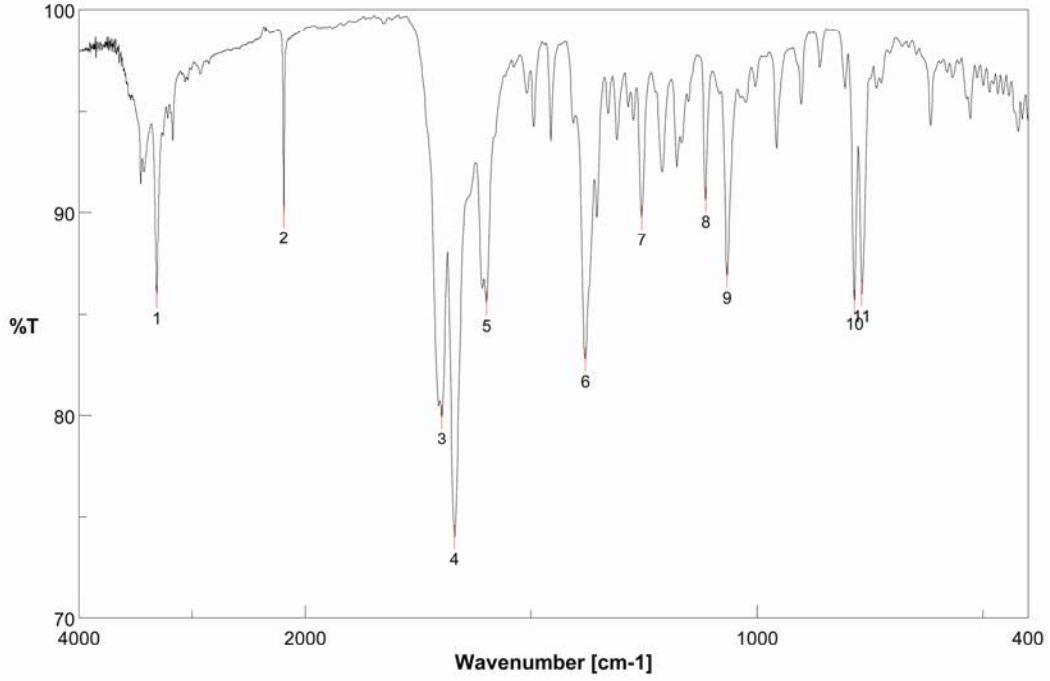
(f1) 1.2583

Spectral Width (ppm):

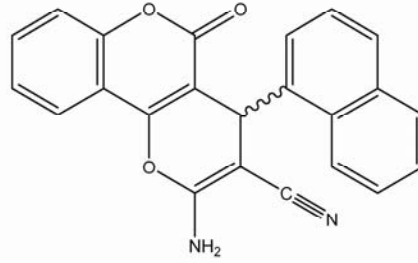
(f1) 258.830

Pulse Program:

Unknown



Accumulation Auto (17)
 Resolution 4 cm-1
 Zero Filling ON
 Apodization Cosine
 Gain Auto (1)
 Scanning Speed Auto (2 mm/sec)
 Date/Time 2012/06/30 7:01
 Update 2012/06/30 7:03
 Operator
 File Name
 Sample Name
 Comment Memory#3



No.	cm-1	%T	No.	cm-1	%T	No.	cm-1	%T
1	3312.14	8.59E+001	2	2188.81	8.98E+001	3	1697.05	7.99E+001
4	1669.09	7.40E+001	5	1598.7	8.55E+001	6	1379.82	8.28E+001
7	1255.43	8.97E+001	8	1113.69	9.06E+001	9	1066.44	8.69E+001
10	784.886	8.56E+001	11	768.494	8.60E+001			

Characterization data of new compounds

Compound (4i). IR (KBr): 3396, 3321, 3195, 2202, 1706, 1671, 1607, 1381, 1053 cm^{-1} . ^1H NMR (DMSO, 400 MHz): δ 7.90 (dd, 1H, $J=7.8, 1.2$ Hz), 7.75-7.70 (m, 1H), 7.52-7.43 (m, 6H), 7.30-7.28 (m, 2H), 4.50 (s, 1H) ppm. ^{13}C NMR (DMSO, 100 MHz): δ 159.55, 157.94, 153.70, 152.18, 146.02, 132.99, 130.69, 130.39, 130.05, 126.94, 124.65, 122.54, 121.68, 119.05, 116.57, 112.98, 103.15, 57.31, 36.59. Anal. Calcd. for $\text{C}_{19}\text{H}_{11}\text{BrN}_2\text{O}_3$: C, 57.74; H, 2.81; N, 7.09 %. Found: C, 58.05; H, 2.68; N, 7.16 %.

Compound (4j). IR (KBr): 3408, 3280, 3175, 2203, 1705, 1674, 1602, 1381, 1055 cm^{-1} . ^1H NMR (DMSO, 400 MHz): δ 7.90 (dd, 1H, $J=7.8, 1.2$ Hz), 7.76-7.72 (m, 1H), 7.55-7.48 (m, 4H), 7.55-7.19 (m, 3H), 5.19 (d, 1H, $J=1.6$ Hz). ^{13}C NMR (DMSO, 100 MHz): δ 159.38, 158.77, 152.11, 133.18, 133.09, 129.93, 129.83, 124.84, 124.70, 124.66, 122.29, 118.73, 116.68, 115.25, 112.56, 38.83 ppm. Anal. Calcd. for $\text{C}_{19}\text{H}_{10}\text{ClFN}_2\text{O}_3$: C, 61.89; H, 2.73; N, 7.60 %. Found: C, 61.90; H, 2.55; N, 7.72 %.

Compound (4k). IR (KBr): 3391, 3180, 2196, 1712, 1674, 1608, 1381, 1240, 1054 cm^{-1} . ^1H NMR (DMSO, 400 MHz): δ 7.90 (dd, 1H, $J=8.0$ Hz), 7.73-7.69 (m, 1H), 7.44-7.38 (m, 7H), 7.18 (d, 2H, $J=8.8$ Hz), 6.95 (d, 2H, $J=8.8$ Hz), 5.06 (s, 2H), 4.40 (s, 1H). ^{13}C NMR (DMSO, 100 MHz): δ 159.51, 157.87, 157.45, 153.09, 152.06, 137.05, 135.60, 132.83, 128.76, 128.40, 127.79, 127.64, 124.63, 122.41, 119.30, 116.53, 114.61, 112.97, 104.19, 69.17, 58.09, 36.13. Anal. Calcd. for $\text{C}_{26}\text{H}_{18}\text{N}_2\text{O}_4$: C, 73.92; H, 4.29; N, 6.63 %. Found: C, 74.15; H, 4.15; N, 6.79 %.

Compound (4l). IR (KBr): 3340, 3312, 2188, 1697, 1669, 1598, 1379, 1066 cm^{-1} . ^1H NMR (DMSO, 400 MHz): δ 8.44 (d, 1H, $J=6.4$ Hz), 7.96 (d, 2H, $J=8.0$ Hz), 7.83 (d, 1H, $J=8.0$ Hz), 7.76-7.33 (m, 8H), 5.48 (s, 1H). ^{13}C NMR (DMSO, 100 MHz): δ 159.55, 157.83, 153.80, 152.07, 133.26, 132.93, 130.93, 128.47, 127.43, 126.10, 126.00, 125.85, 125.75, 124.74, 123.43, 122.43, 119.15, 116.61, 112.96, 104.65, 58.49 ppm. Anal. Calcd. for $\text{C}_{23}\text{H}_{14}\text{N}_2\text{O}_3$: C, 75.40; H, 3.85; N, 7.65 %. Found: C, 75.65; H, 3.70; N, 7.53 %.