

Supporting Information

Regioselective Synthesis of Novel and Diverse Naphtho[1,2-*b*]furan-3-carboxamides and Benzofuran-3-carboxamides by Cascade Formal [3 + 2] Cycloaddition

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Naphtho[1,2-*b*]furans

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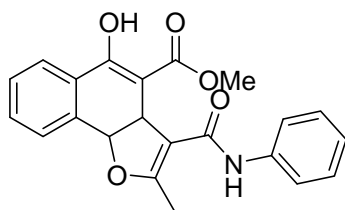
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Benzofurans

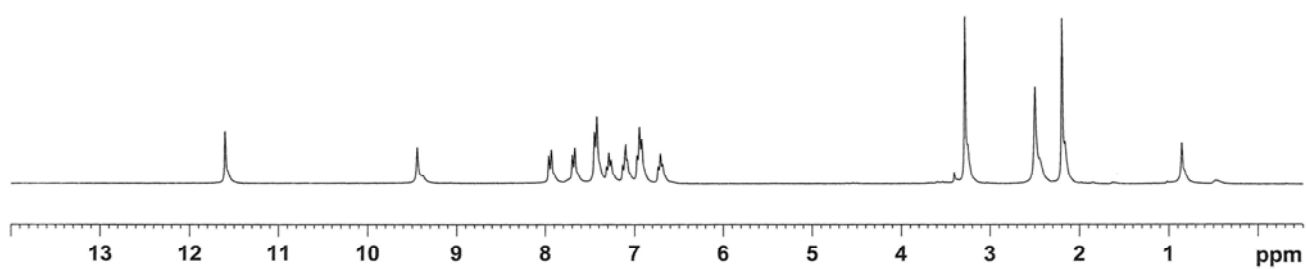
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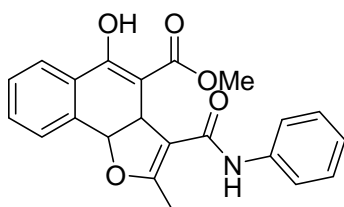
¹H NMR of Compound 7



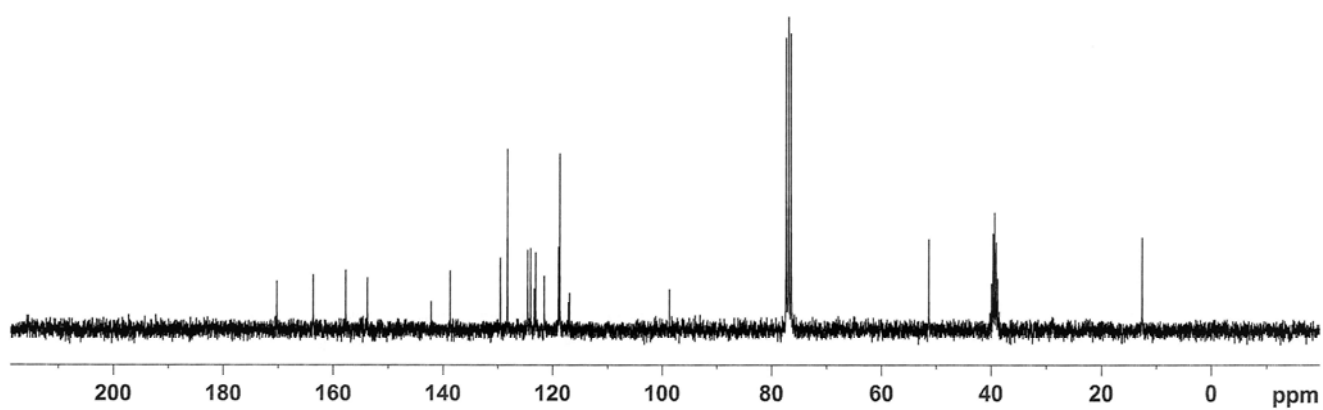
300 MHz, CDCl₃ + DMSO-d₆



¹³C NMR of Compound 7

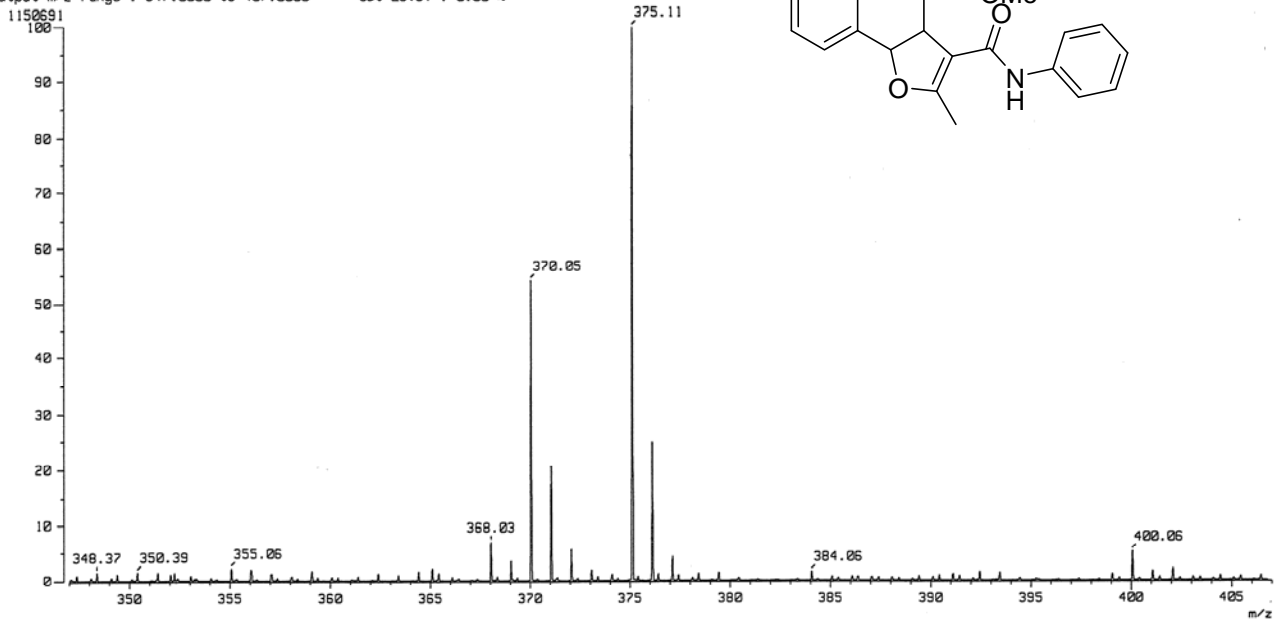
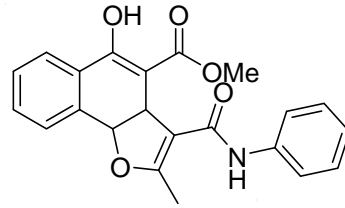


75 MHz, CDCl₃ + DMSO-d₆



[Mass Spectrum]
 Date : 02-Dec-2013 11:37
 Sample : -
 Note : -
 Inlet : Direct Ion Mode : EI+
 Spectrum Type : Normal Ion (EF-Linear)
 RT : 1.08 min Scan# : (22,23)
 BP : m/z 375.1104 Int. : 54.87
 Output m/z range : 347.0000 to 407.0000 Cut Level : 0.00 %

Mass Spectrum of Compound 7

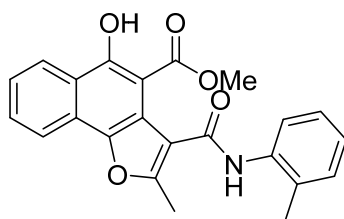


[Elemental Composition]

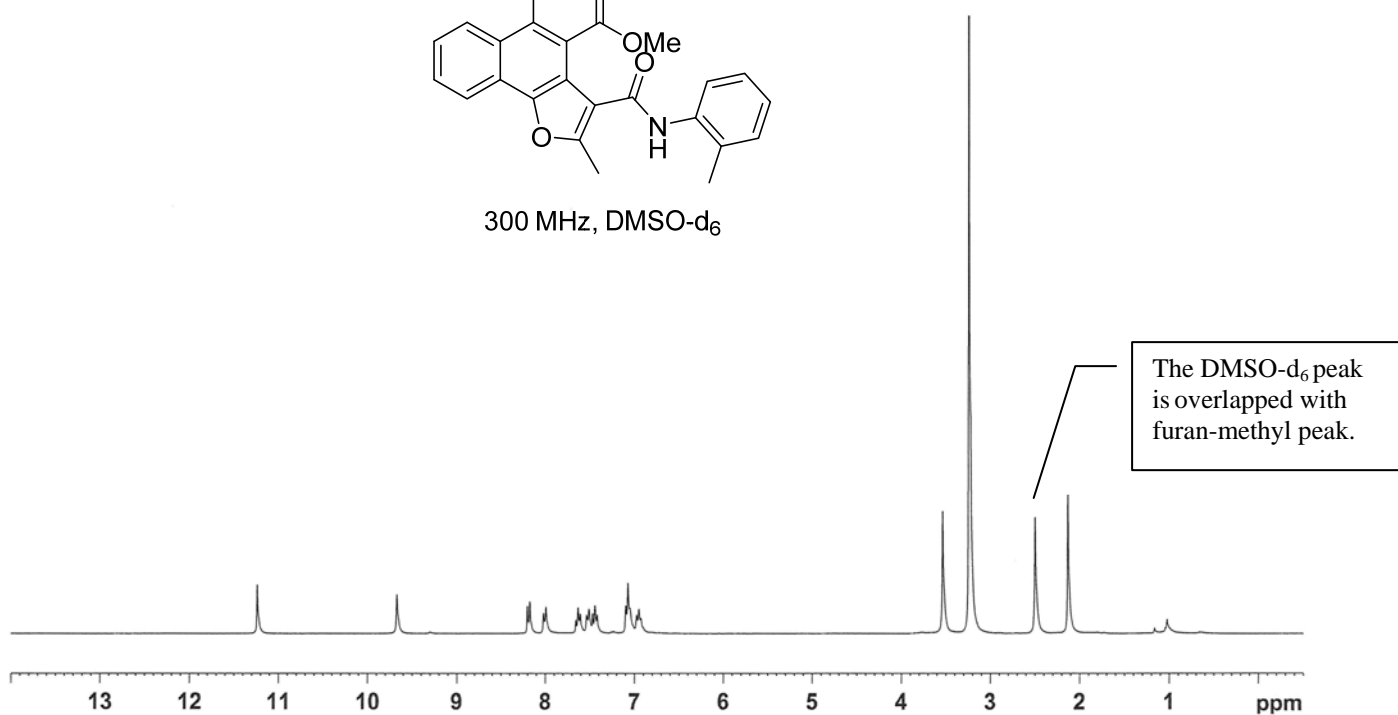
Data : x9-1-C22H19NO5 Date : 02-Dec-2013 11:37
 Sample : -
 Note : -
 Inlet : Direct Ion Mode : EI+
 RT : 1.08 min Scan# : (22,23)
 Elements : C 22/0, H 19/0, N 1/0, O 5/0
 Mass Tolerance : 1000ppm, 1mmu if m/z < 1, 3mmu if m/z > 3
 Unsaturation (U.S.) : -0.5 - 100.0

Observed m/z	Int%	Err [ppm / mmu]	U.S. Composition
370.0477	54.2		
371.0526	20.7		
375.1104	100.0	-0.7 / -0.3	15.0 C 22 H 17 N O 5
376.1136	25.0		

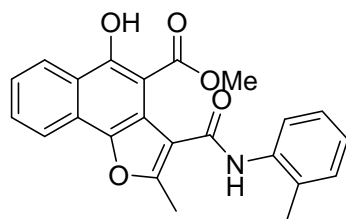
¹H NMR of Compound **8**



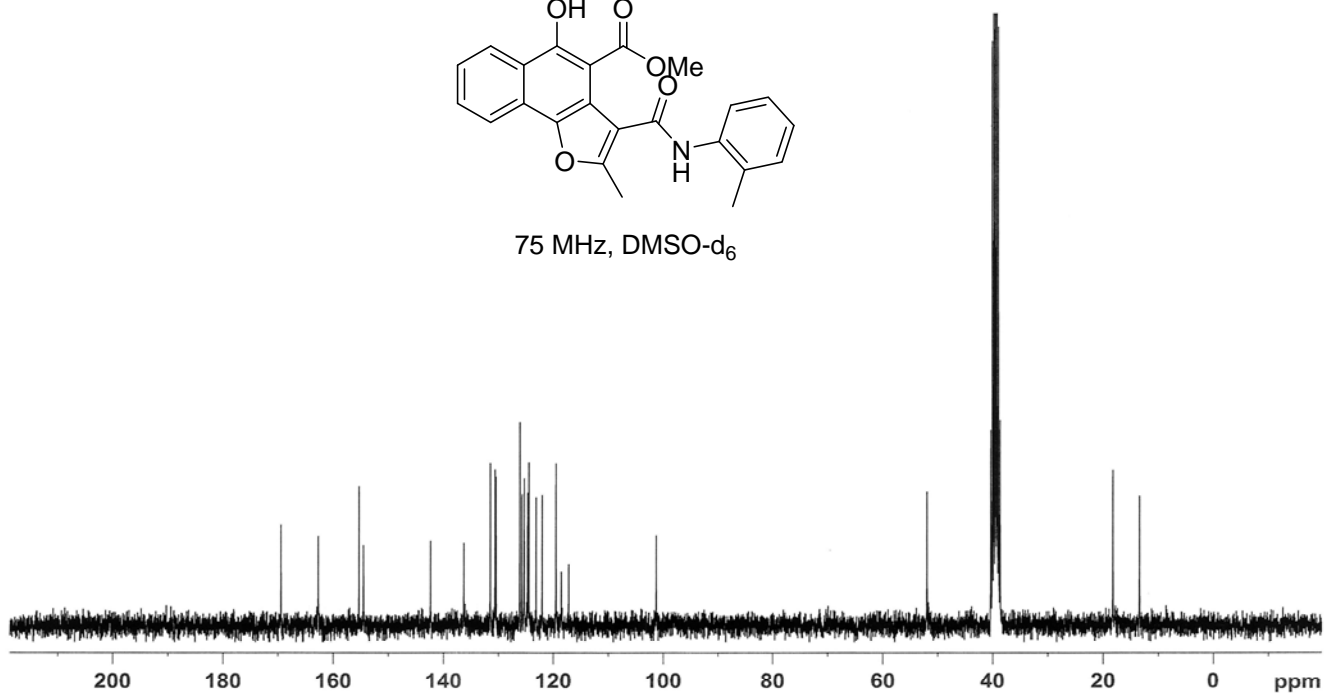
300 MHz, DMSO-d₆



¹³C NMR of Compound **8**

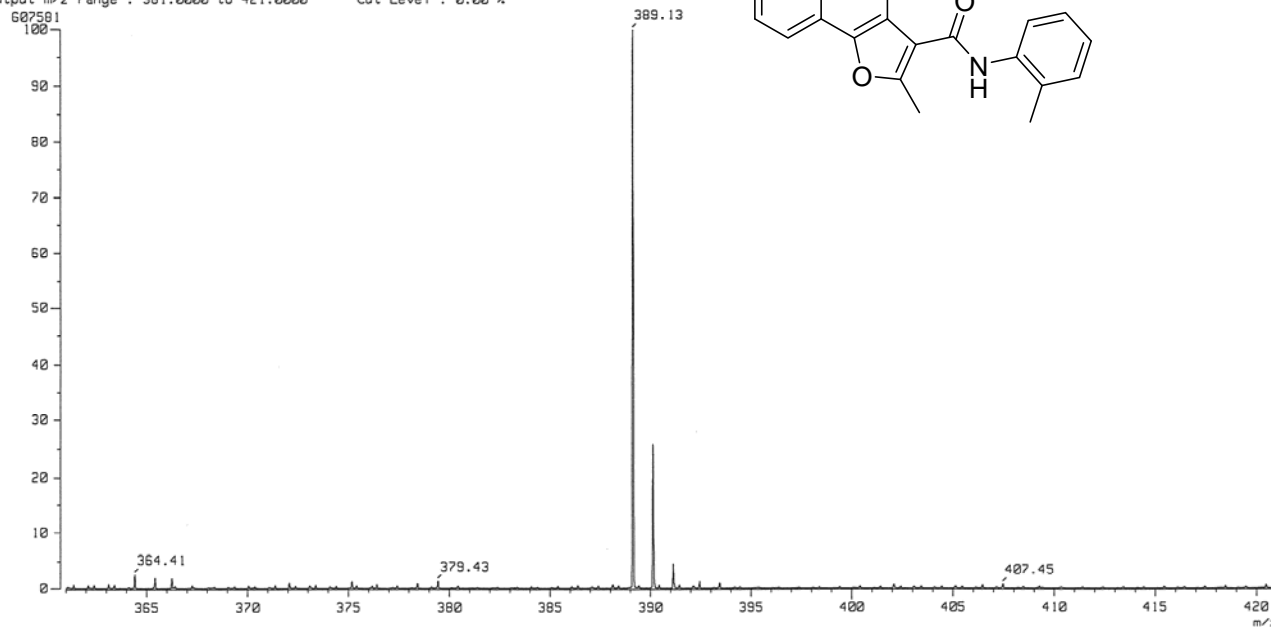
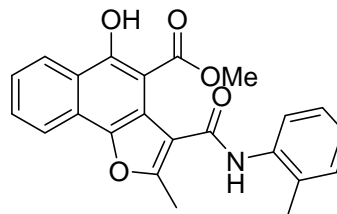


75 MHz, DMSO-d₆



[Mass Spectrum]
 Date : 04-Nov-2013 13:41
 Sample : -
 Note : -
 Inlet : Direct Ion Mode : EI+
 Spectrum Type : Normal Ion [EF-Linear]
 RT : 0.88 min Scan# : (18,19)
 BP : m/z 389.1261 Int. : 28.97
 Output m/z range : 351.0000 to 421.0000 Cut Level : 0.00 %

Mass Spectrum of Compound 8

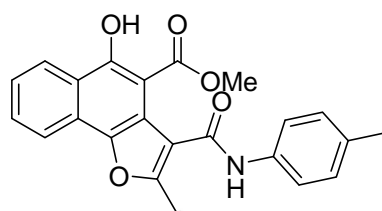


[Elemental Composition]

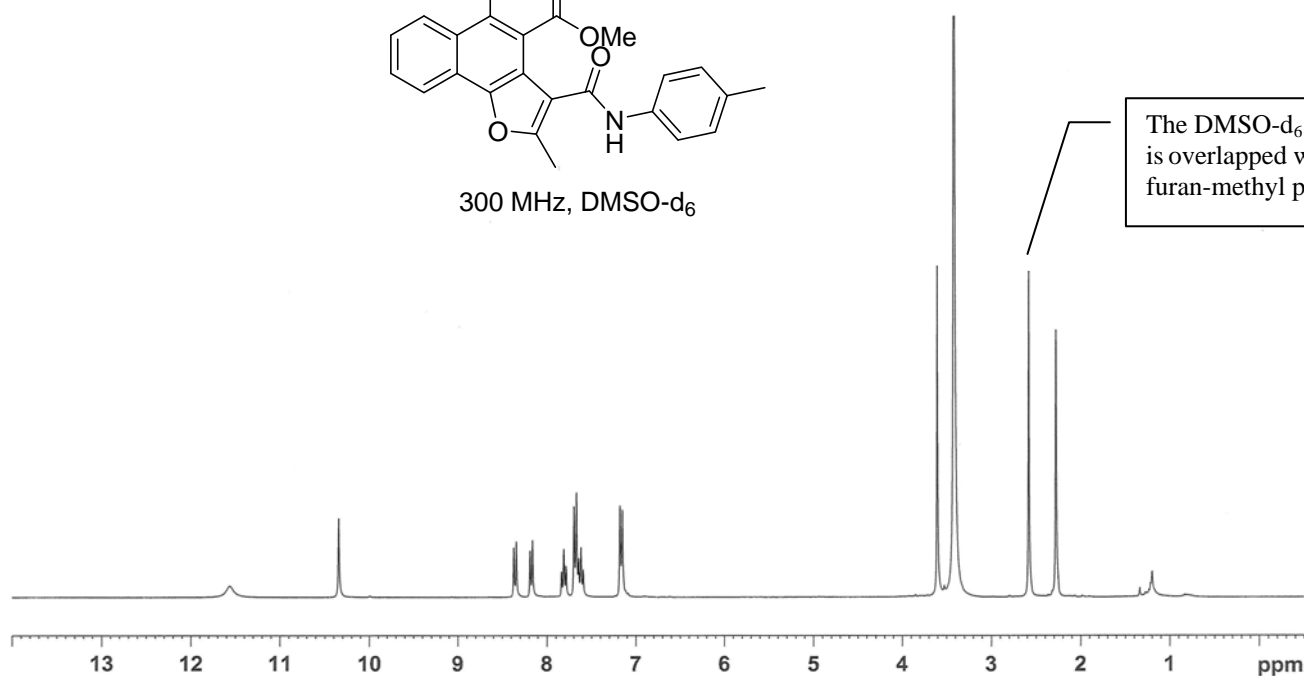
Data : x9-2-C23H21NO5 Date : 04-Nov-2013 13:41
 Sample : -
 Note : -
 Inlet : Direct Ion Mode : EI+
 RT : 0.88 min Scan# : (18,19)
 Elements : C 23/0, H 21/0, N 1/0, O 5/0
 Mass Tolerance : 1000ppm, 1mmu if m/z < 1, 3mmu if m/z > 3
 Unsaturation (U.S.) : -0.5 - 100.0

Observed m/z	Int%	Err [ppm / mmu]	U.S. Composition
389.1261	100.0	-0.6 / -0.2	15.0 C 23 H 19 N O 5
390.1309	25.8		

¹H NMR of Compound 9

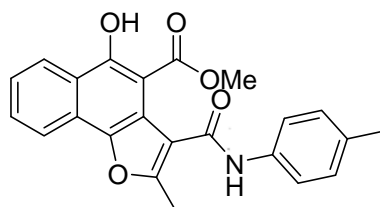


300 MHz, DMSO-d₆

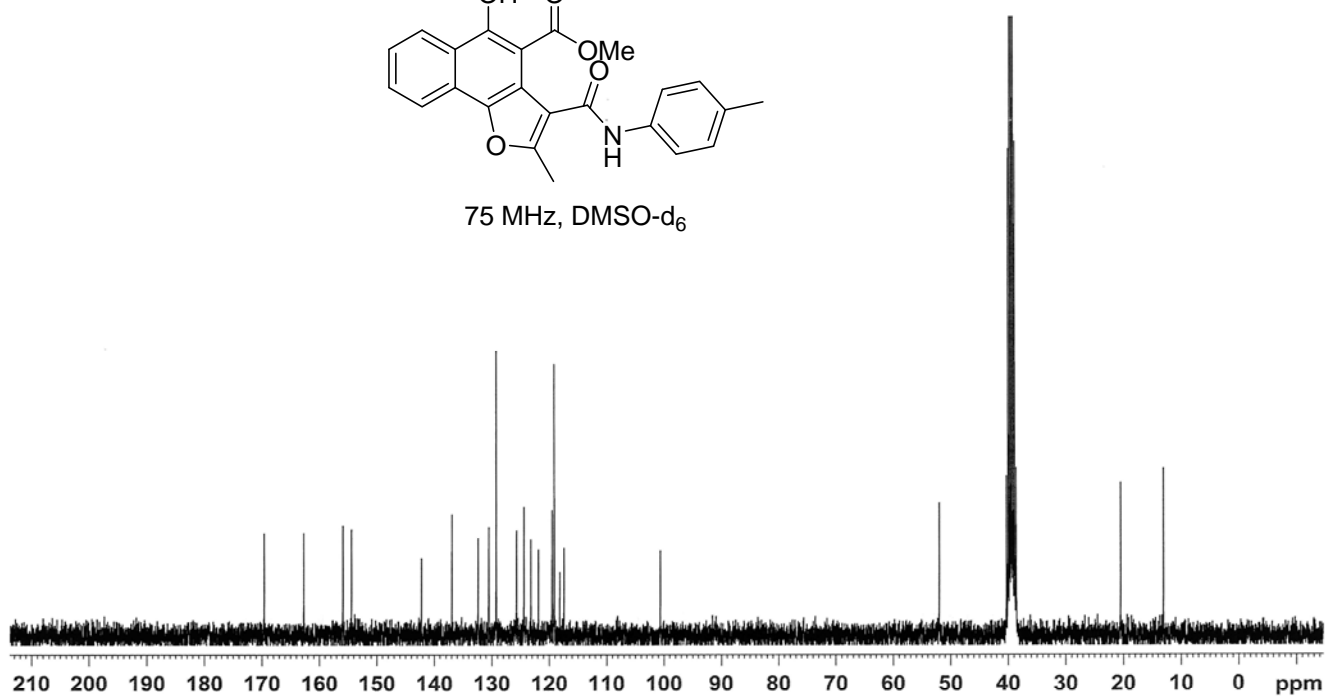


The DMSO-d₆ peak is overlapped with furan-methyl peak.

¹³C NMR of Compound 9

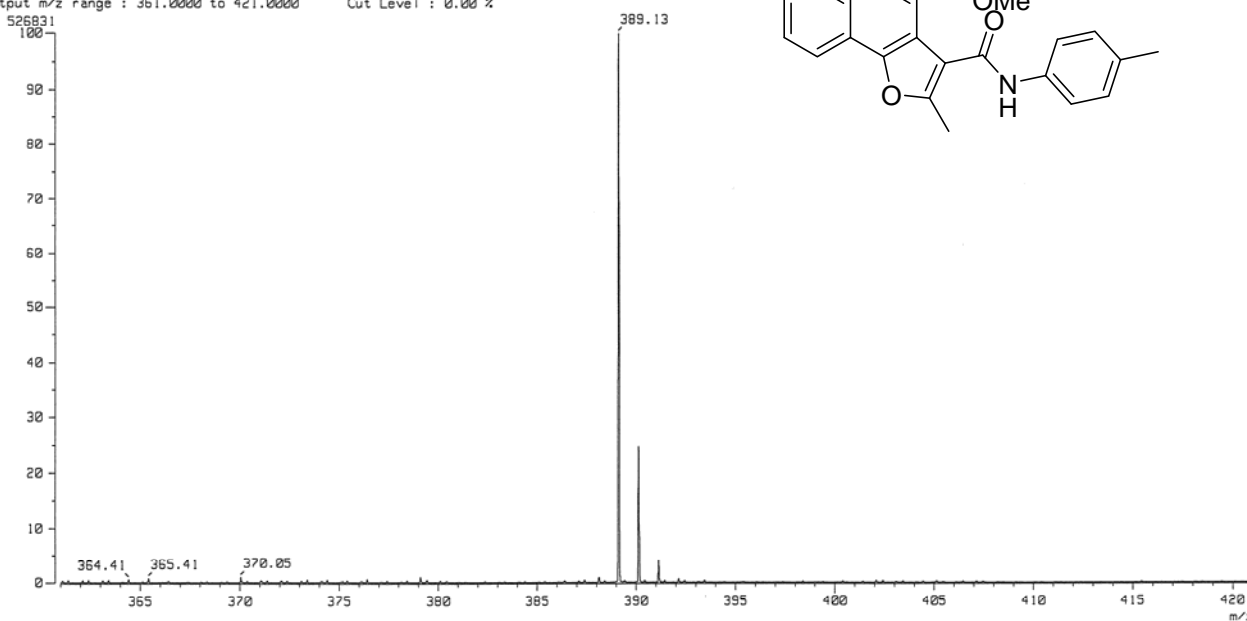
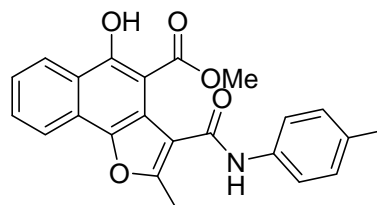


75 MHz, DMSO-d₆



[Mass Spectrum]
 Date : 04-Nov-2013 14:01
 Sample : -
 Note : -
 Inlet : Direct Ion Mode : EI+
 Spectrum Type : Normal Ion [EF-Linear]
 RT : 1.08 min Scan# : (22,23)
 BP : m/z 389.1265 Int. : 25.12
 Output m/z range : 351.0000 to 421.0000 Cut Level : 0.00 %

Mass Spectrum of Compound 9

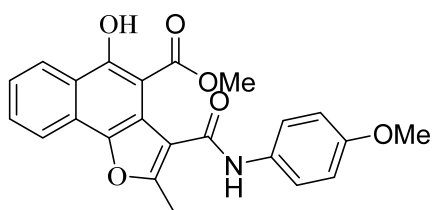


[Elemental Composition]

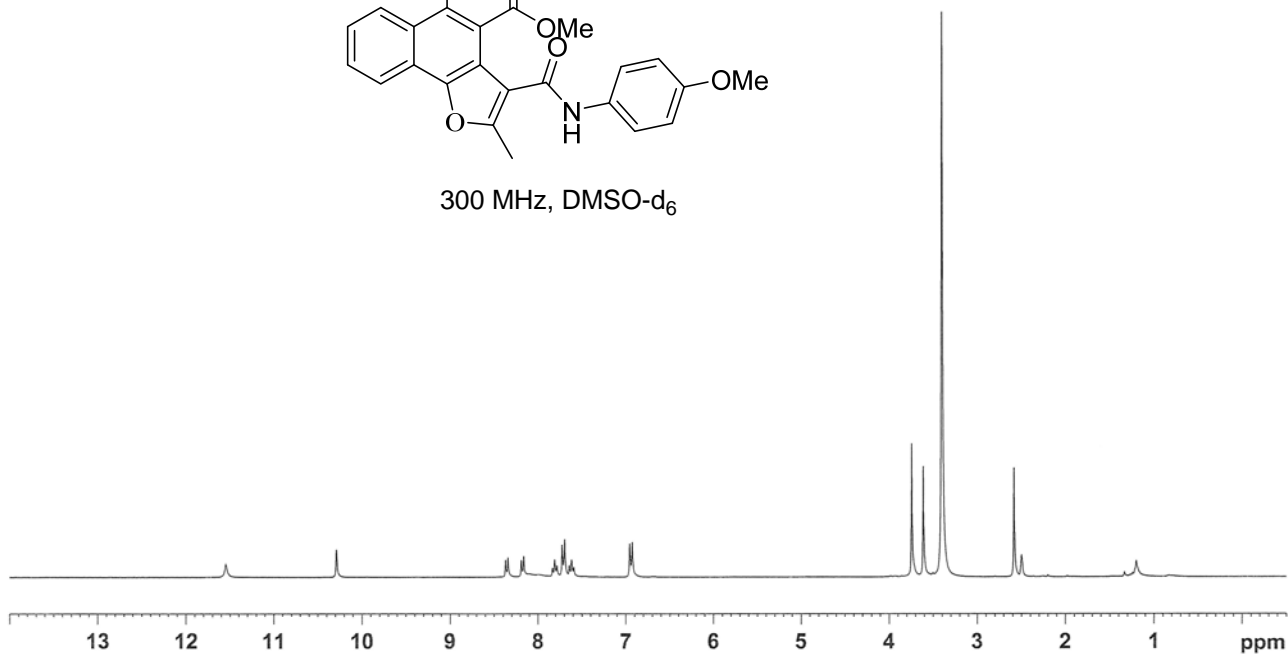
Date : 04-Nov-2013 14:01
 Data : x9-3-C23H21NO5
 Sample : -
 Note : -
 Inlet : Direct Ion Mode : EI+
 RT : 1.08 min Scan# : (22,23)
 Elements : C 23/0, H 21/0, N 1/0, O 5/0
 Mass Tolerance : 1000ppm, 1mmu if m/z < 1, 2mmu if m/z > 2
 Unsaturation (U.S.) : -0.5 - 100.0

Observed m/z	Int%	Err [ppm / mmu]	U.S. Composition
389.1265	100.0	+0.4 / +0.2	15.0 C 23 H 19 N O 5
390.1313	24.8		

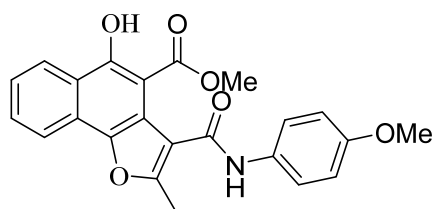
¹H NMR of Compound 10



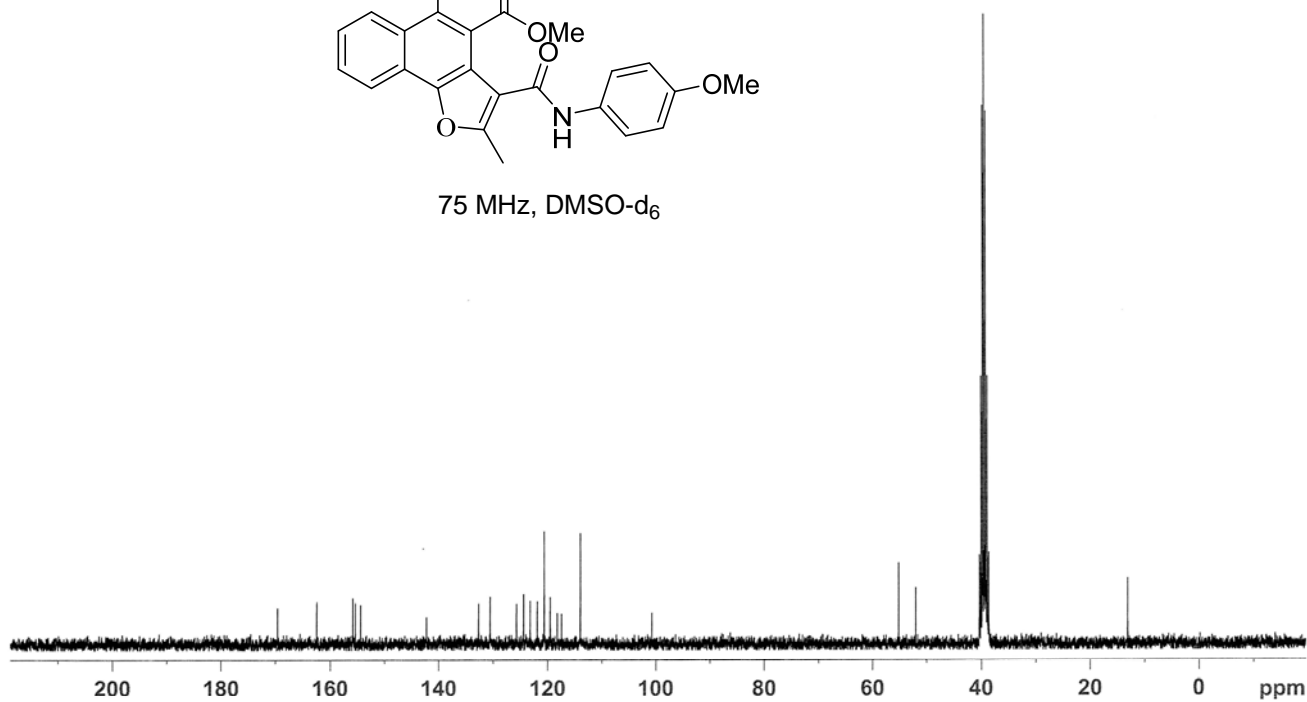
300 MHz, DMSO-d₆



¹³C NMR of Compound 10

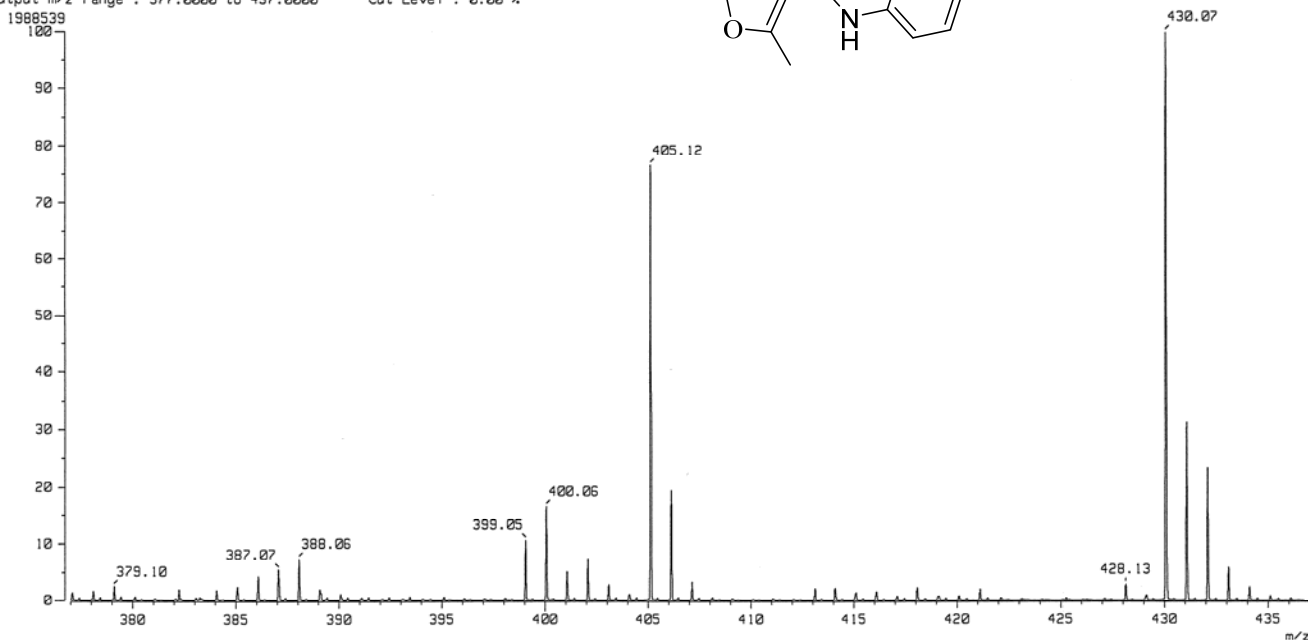
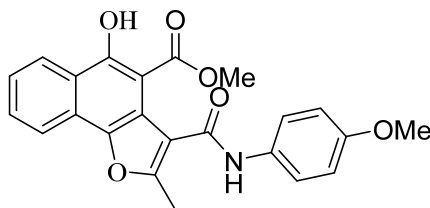


75 MHz, DMSO-d₆



Mass Spectrum of Compound 10

[Mass Spectrum]
 Data : x9-4-C23H21NO6 Date : 04-Nov-2013 14:06
 Sample : -
 Note : -
 Inlet : Direct Ion Mode : EI+
 Spectrum Type : Normal Ion [EF-Linear]
 RT : 1.58 min Scan# : (32,33)
 BP : m/z 430.0706 Int. : 94.82
 Output m/z range : 377.0000 to 437.0000 Cut Level : 0.00 %



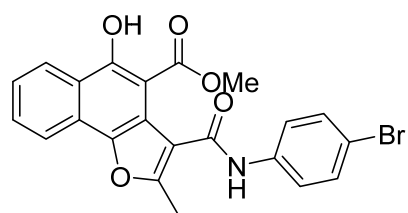
[Elemental Composition]

Data : x9-4-C23H21NO6 Date : 04-Nov-2013 14:06
 Sample : -
 Note : -
 Inlet : Direct Ion Mode : EI+
 RT : 1.58 min Scan# : (32,33)
 Elements : C 23/0, H 21/0, N 1/0, O 6/0
 Mass Tolerance : 1000ppm, 1mmu if m/z < 1, 3mmu if m/z > 3
 Unsaturation (U.S.) : -0.5 - 100.0

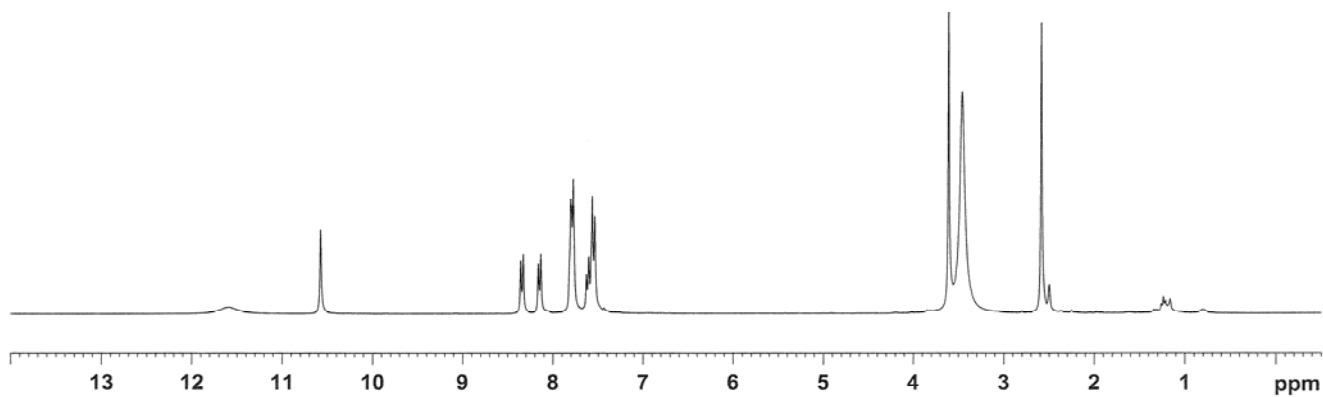
Page: 1

Observed m/z	Int%	Err [ppm / mmu]	U.S. Composition
399.0516	10.7		
400.0596	16.6		
405.1215	76.6	+0.5 / +0.2	15.0 C 23 H 19 N O 6
406.1235	19.5		
430.0706	100.0		
431.0744	31.4		
432.0840	23.4		

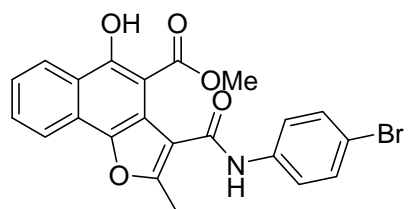
¹H NMR of Compound 11



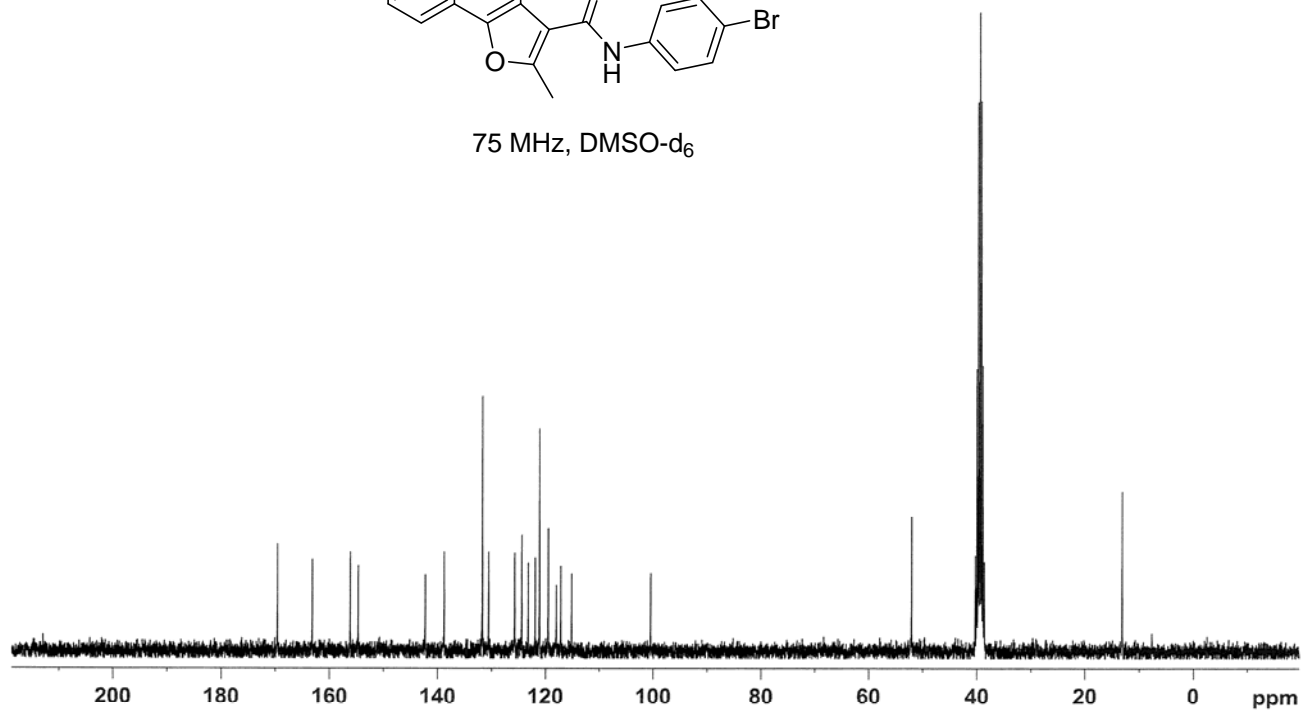
300 MHz, DMSO-d₆



¹³C NMR of Compound 11

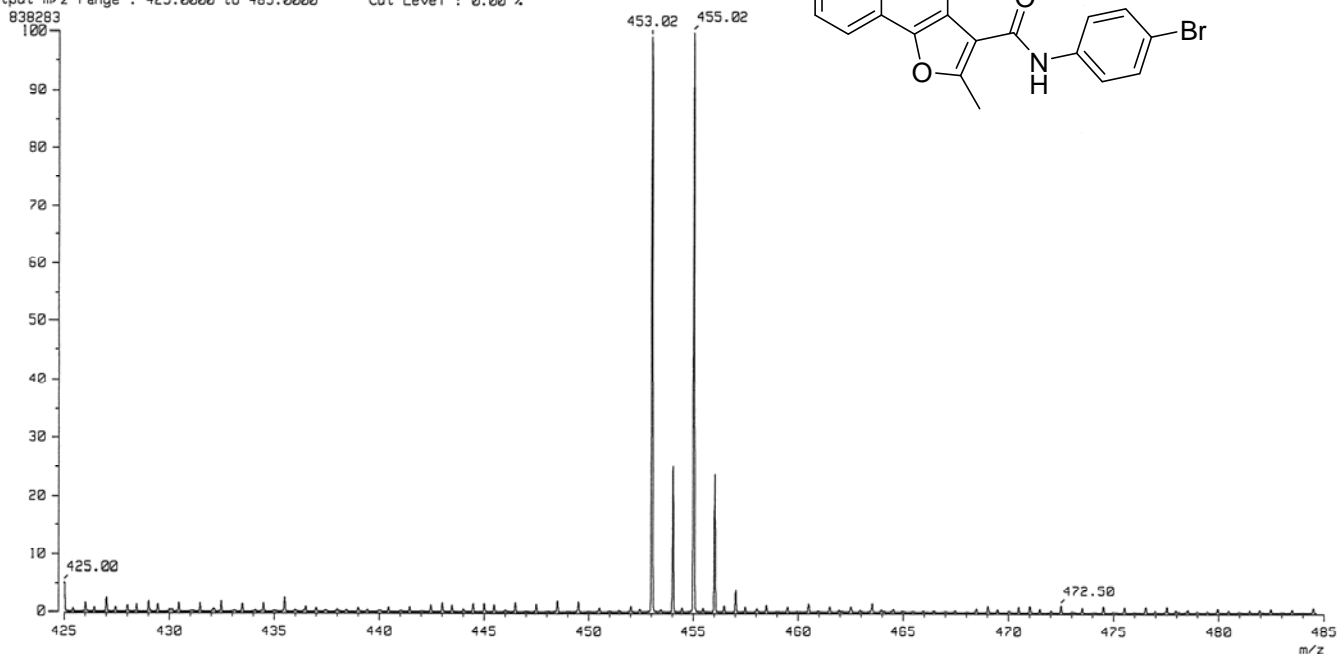
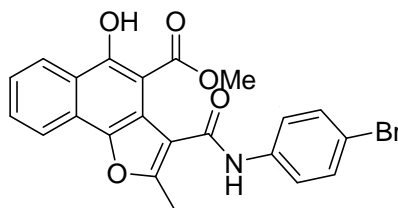


75 MHz, DMSO-d₆



[Mass Spectrum]
 Data : x9-5-C22H18BrNO5 Date : 04-Nov-2013 14:13
 Sample : -
 Note : -
 Inlet : Direct Ion Mode : EI+
 Spectrum Type : Normal Ion [EF-Linear]
 RT : 1.53 min Scan# : (31,32)
 BP : m/z 455.0211 Int. : 39.97
 Output m/z range : 425.0000 to 485.0000 Cut Level : 0.00 %

Mass Spectrum of Compound 11

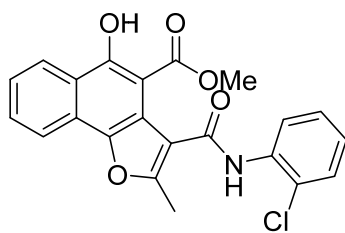


[Elemental Composition]

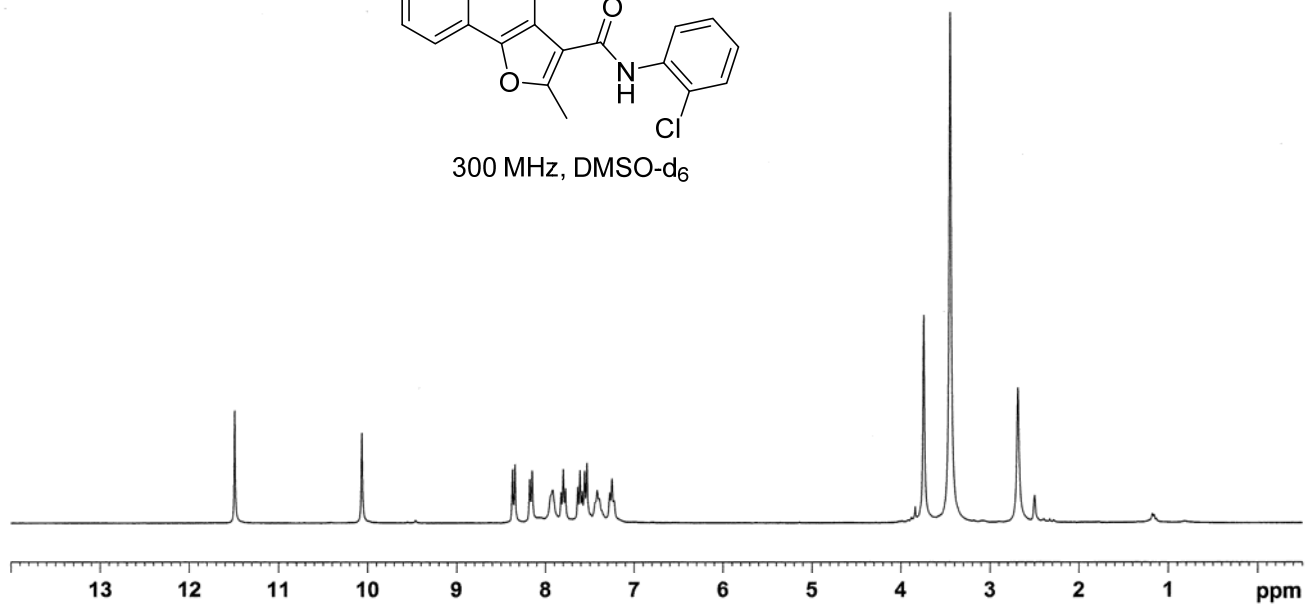
Data : x9-5-C22H18BrNO5 Date : 04-Nov-2013 14:13
 Sample : -
 Note : -
 Inlet : Direct Ion Mode : EI+
 RT : 1.53 min Scan#: (31,32)
 Elements : C 22/0, H 18/0, Br 1/0, N 1/0, O 5/0
 Mass Tolerance : 1mmu
 Unsaturation (U.S.) : -0.5 - 100.0

Observed m/z	Int%	Err [ppm / mmu]	U.S. Composition
453.0214	99.3	+0.4 / +0.2	15.0 C 22 H 16 Br N O 5
454.0277	25.2		
455.0211	100.0		
456.0230	23.9		

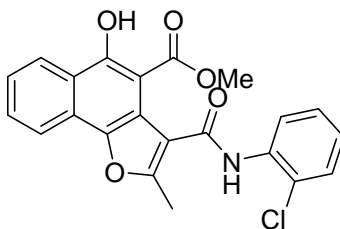
¹H NMR of Compound 12



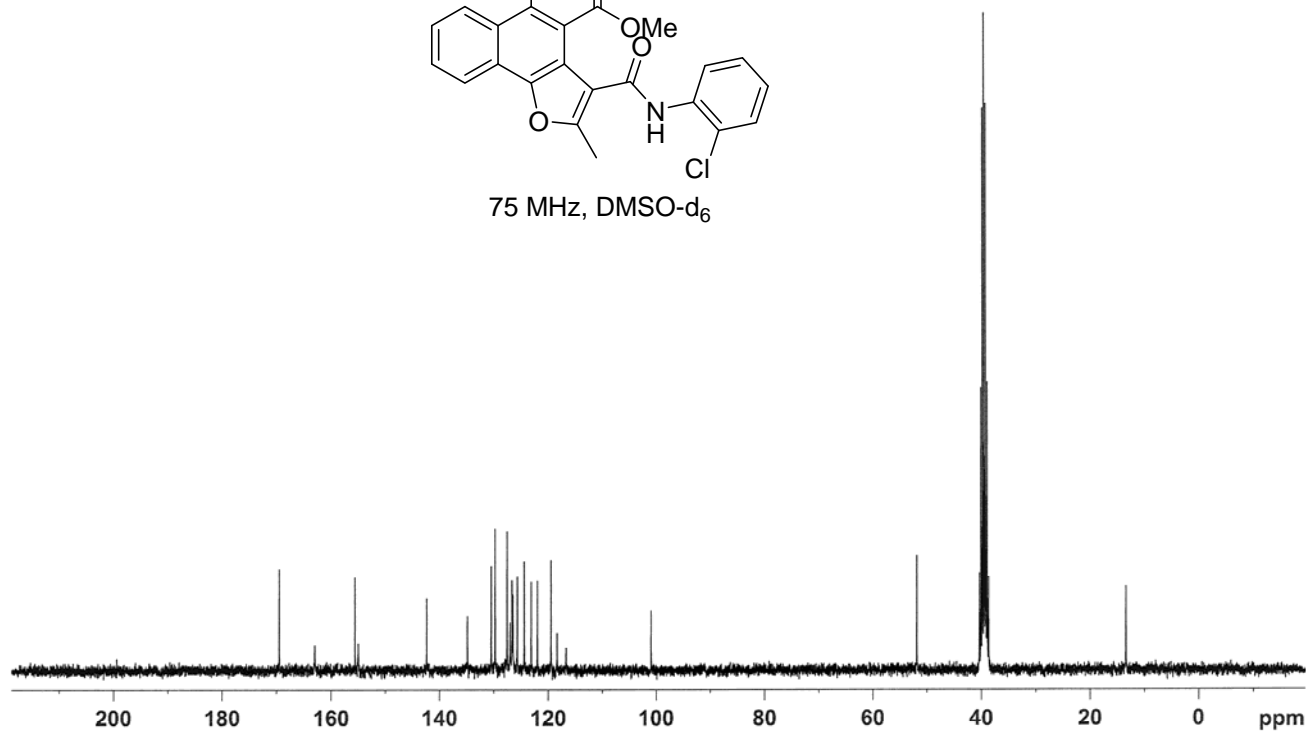
300 MHz, DMSO-d₆



¹³C NMR of Compound 12

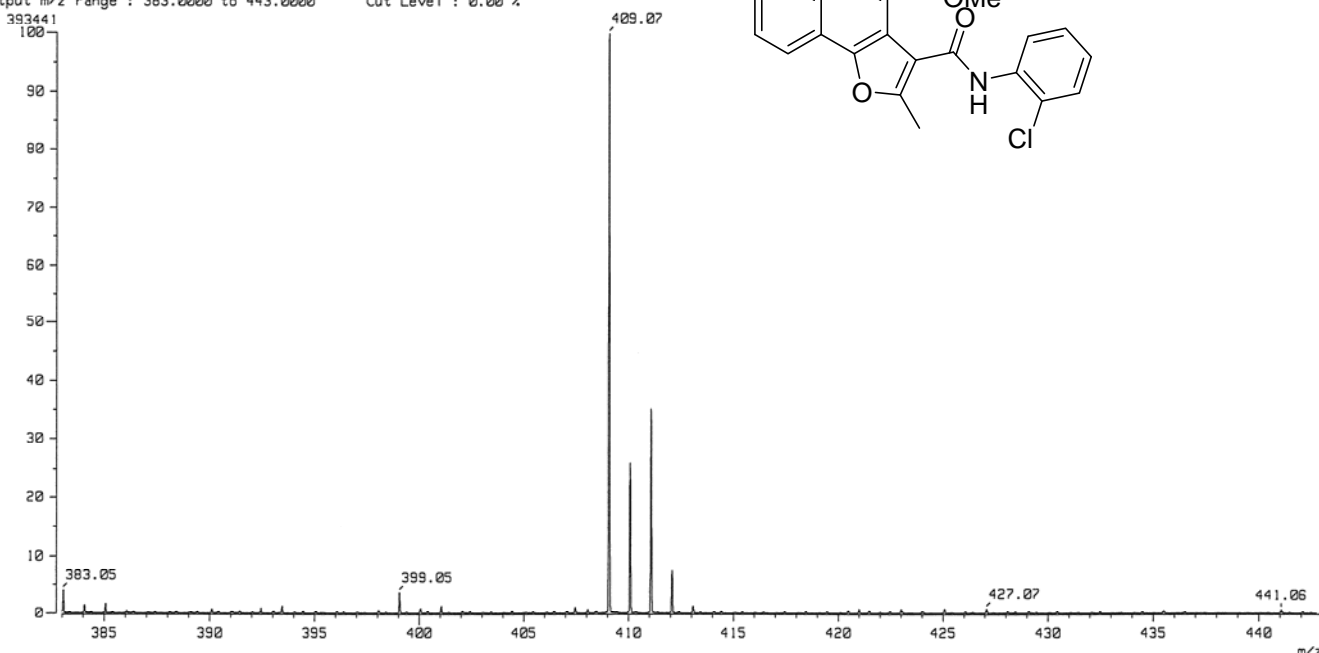
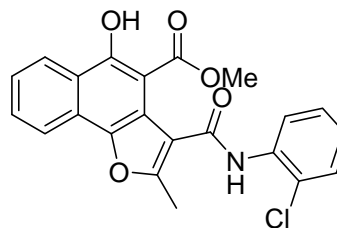


75 MHz, DMSO-d₆



[Mass Spectrum]
 Data : x9-6-C22H20ClNO5 Date : 04-Nov-2013 14:18
 Sample : -
 Note : -
 Inlet : Direct Ion Mode : EI+
 Spectrum Type : Normal Ion [EF-Linear]
 RT : 1.08 min Scan# : (22,23)
 BP : m/z 409.0716 Int. : 18.76
 Output m/z range : 383.0000 to 443.0000 Cut Level : 0.00 %

Mass Spectrum of Compound 12

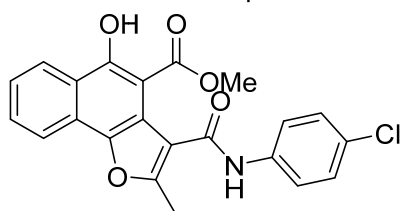


[Elemental Composition]

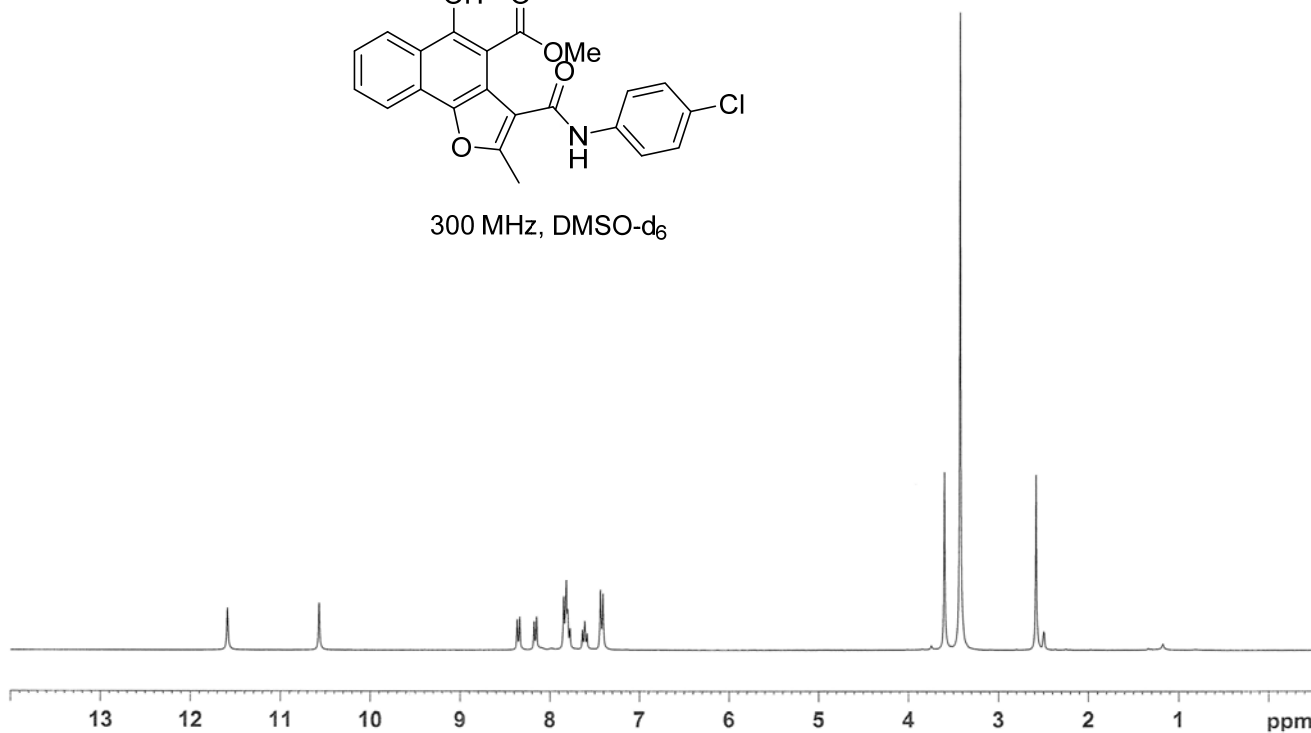
Data : x9-6-C22H20ClNO5 Date : 04-Nov-2013 14:18
 Sample : -
 Note : -
 Inlet : Direct Ion Mode : EI+
 RT : 1.08 min Scan# : (22,23)
 Elements : C 22/0, H 20/0, Cl 1/0, N 1/0, O 5/0
 Mass Tolerance : 1000ppm, 1mmu if m/z < 1, 3mmu if m/z > 3
 Unsaturation (U.S.) : -0.5 - 100.0

Observed m/z	Int%	Err [ppm / mmu]	U.S. Composition
409.0716	100.0	-0.3 / -0.1	15.0 C 22 H 16 Cl N O 5
410.745	26.0		
411.0692	35.3		

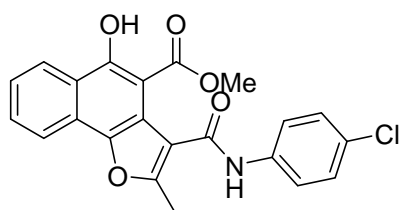
¹H NMR of Compound 13



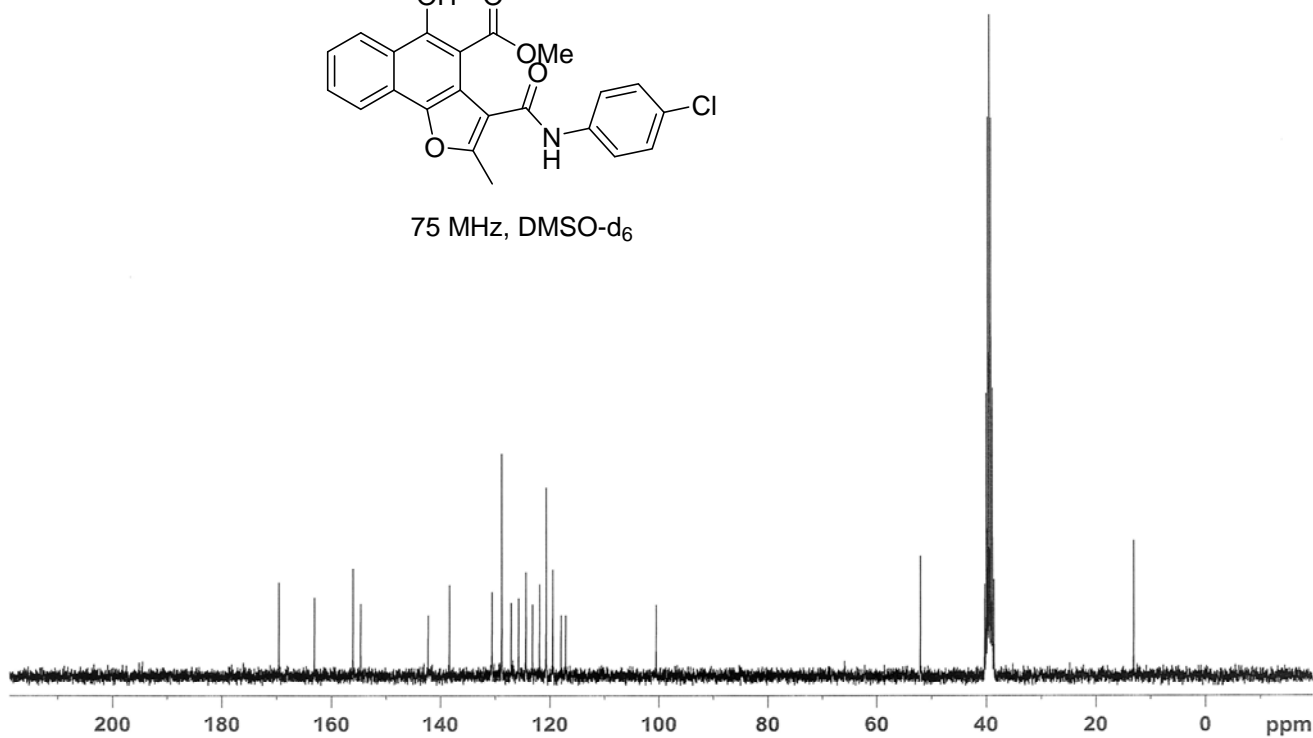
300 MHz, DMSO-d₆



¹³C NMR of Compound 13

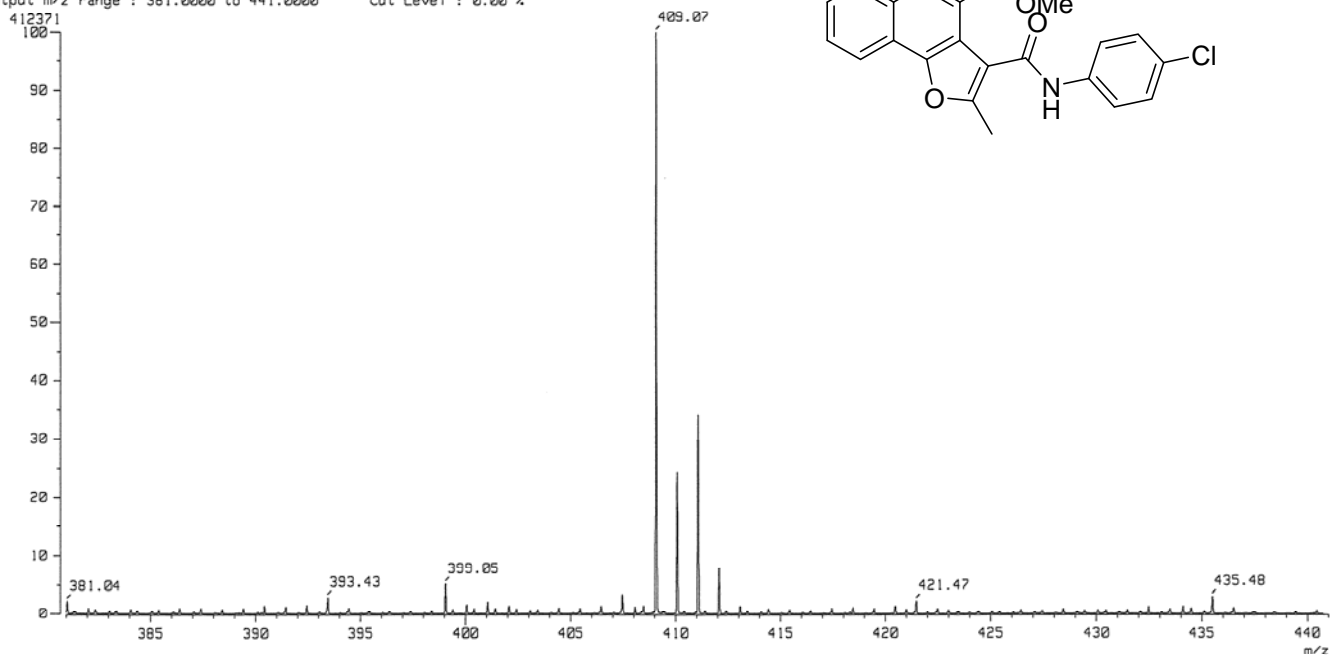
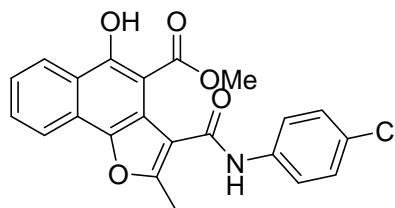


75 MHz, DMSO-d₆



[Mass Spectrum]
 Date : 04-Nov-2013 14:22
 Sample : -
 Note : -
 Inlet : Direct Ion Mode : EI+
 Spectrum Type : Normal Ion [EF-Linear]
 RT : 0.93 min Scan# : (19,20)
 BP : m/z 409.0717 Int. : 19.66
 Output m/z range : 381.0000 to 441.0000 Cut Level : 0.00 %

Mass Spectrum of Compound 13

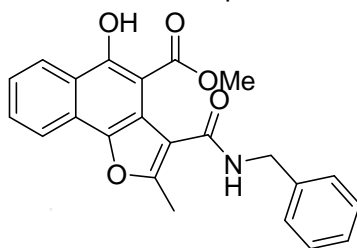


[Elemental Composition]

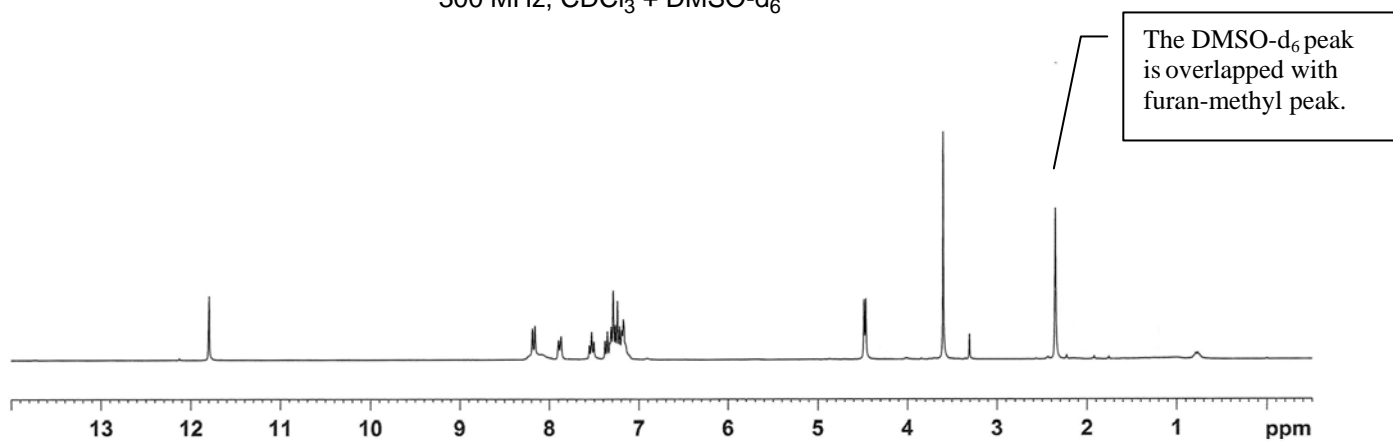
Data : x9-7-C22H18ClNO5 Date : 04-Nov-2013 14:22
 Sample : -
 Note : -
 Inlet : Direct Ion Mode : EI+
 RT : 0.93 min Scan# : (19,20)
 Elements : C 22/0, H 18/0, Cl 1/0, N 1/0, O 5/0
 Mass Tolerance : 1000ppm, 1mmu if m/z < 1, 3mmu if m/z > 3
 Unsaturation (U.S.) : -0.5 - 100.0

Observed m/z	Int%	Err [ppm / mmu]	U.S.	Composition
409.0717	100.0	+0.0 / +0.0	15.0	C 22 H 16 Cl N O 5
410.0747	24.4			
411.0691	34.2			

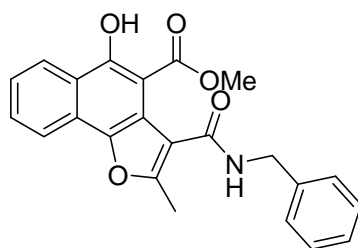
¹H NMR of Compound 14



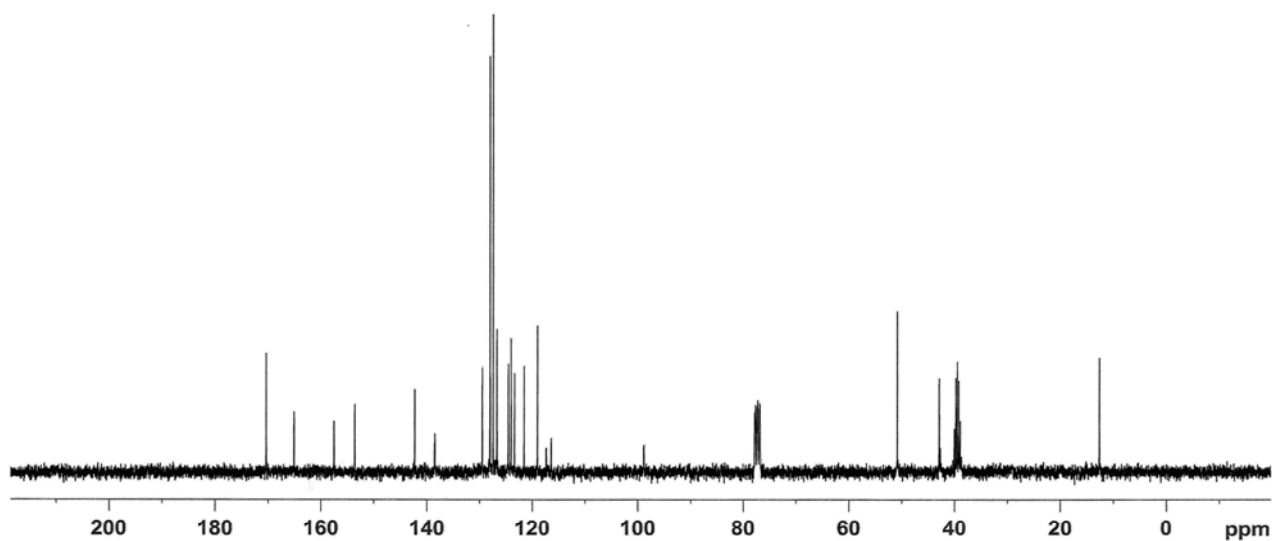
300 MHz, CDCl₃ + DMSO-d₆



¹³C NMR of Compound 14

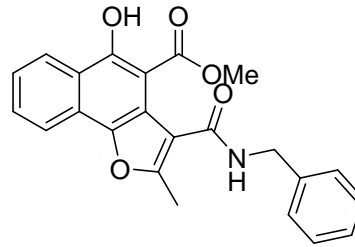


75 MHz, CDCl₃ + DMSO-d₆



[Mass Spectrum]
 Date : 04-Nov-2013 14:26
 Sample : -
 Note : -
 Inlet : Direct Ion Mode : EI+
 Spectrum Type : Normal Ion [EF-Linear]
 RT : 1.33 min Scan# : (27,28)
 BP : m/z 389.1262 Int. : 46.12
 Output m/z range : 361.0000 to 421.0000 Cut Level : 0.00 %

Mass Spectrum of Compound 14

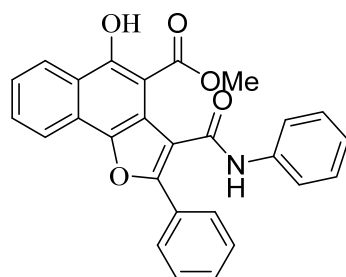


[Elemental Composition]

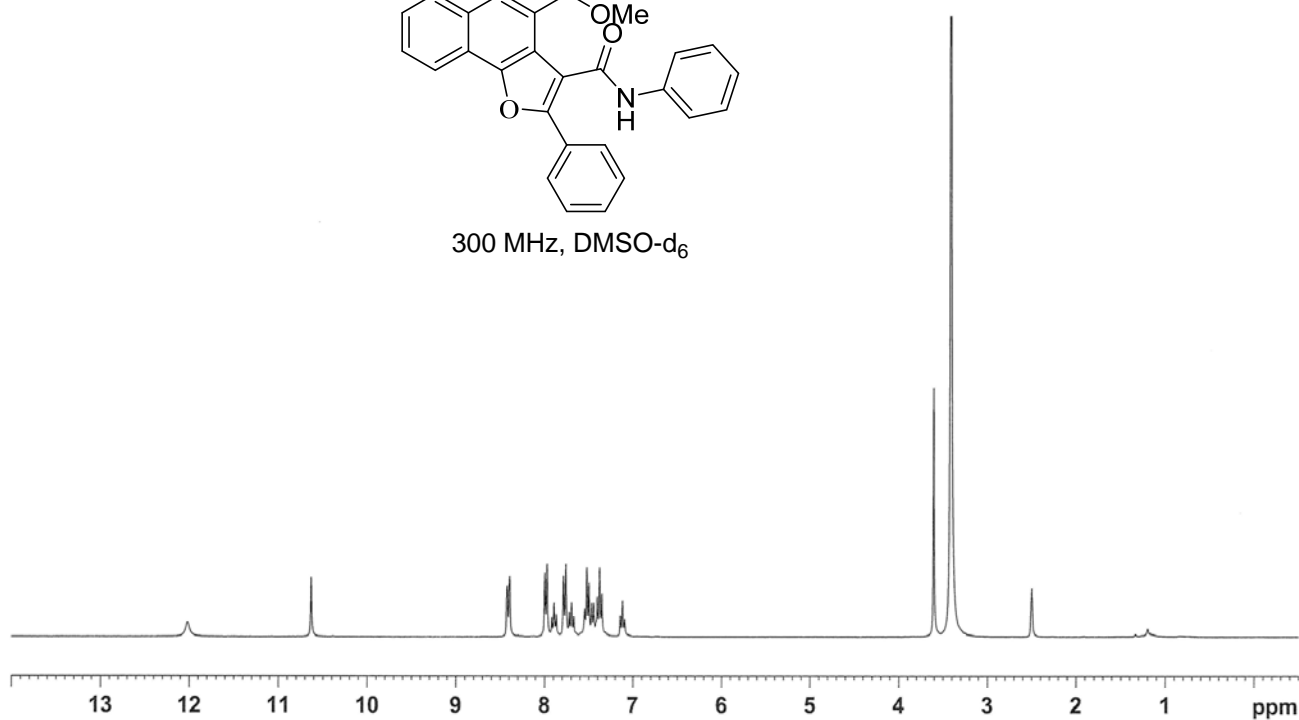
Data : x9-8-C23H21NO5 Date : 04-Nov-2013 14:26
 Sample : -
 Note : -
 Inlet : Direct Ion Mode : EI+
 RT : 1.33 min Scan# : (27,28)
 Elements : C 23/0, H 21/0, N 1/0, O 5/0
 Mass Tolerance : 1000ppm, 1mmu if m/z < 1, 3mmu if m/z > 3
 Unsaturation (U.S.) : -0.5 - 100.0

Observed m/z	Int%	Err [ppm / mmu]	U.S.	Composition
389.1262	100.0	-0.4 / -0.2	15.0	C 23 H 19 N O 5
390.1306	26.3			

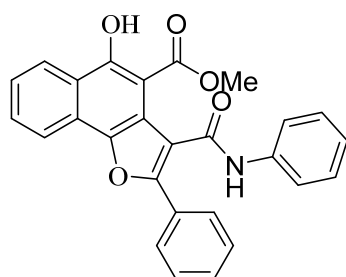
¹H NMR of Compound 15



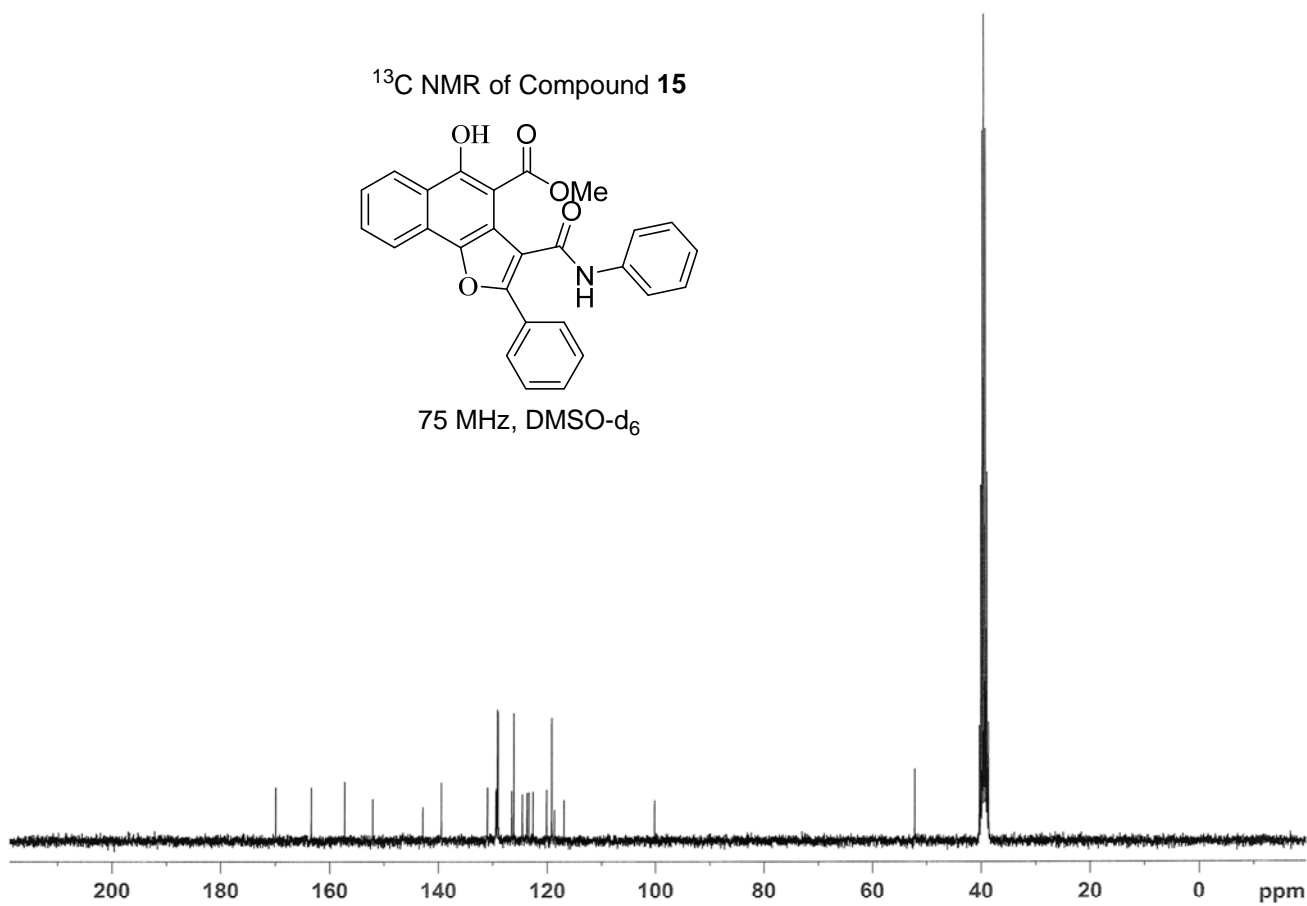
300 MHz, DMSO-d₆



¹³C NMR of Compound 15

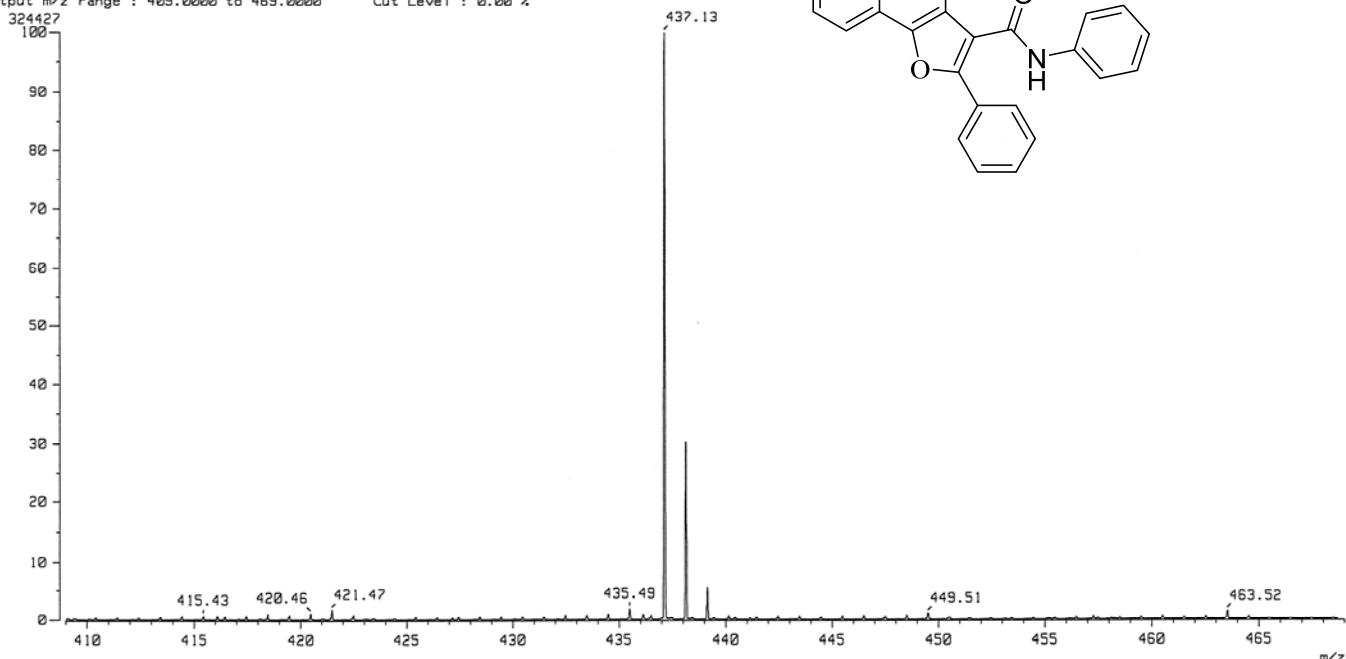
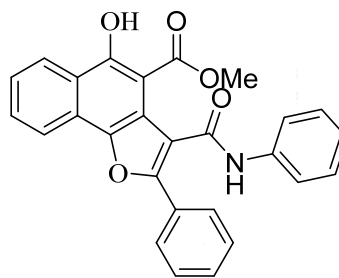


75 MHz, DMSO-d₆



[Mass Spectrum]
 Data : x9-9-C27H21NO5 Date : 04-Nov-2013 14:31
 Sample : -
 Note : -
 Inlet : Direct Ion Mode : EI+
 Spectrum Type : Normal Ion [EF-Linear]
 RT : 1.08 min Scan# : (22,23)
 BP : m/z 437.1266 Int. : 15.47
 Output m/z range : 409.0000 to 469.0000 Cut Level : 0.00 %

Mass Spectrum of Compound 15

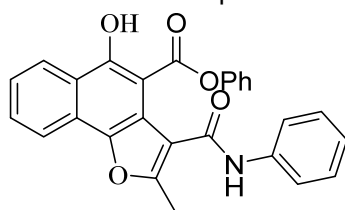


[Elemental Composition]

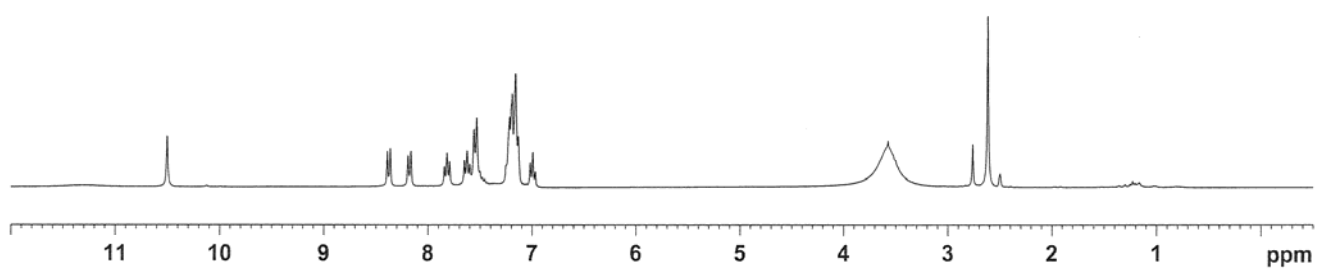
Data : x9-9-C27H21NO5 Date : 04-Nov-2013 14:31
 Sample : -
 Note : -
 Inlet : Direct Ion Mode : EI+
 RT : 1.08 min Scan#: (22,23)
 Elements : C 27/0, H 21/0, N 1/0, O 5/0
 Mass Tolerance : 1000ppm, 1mmu if m/z < 1, 2mmu if m/z > 2
 Unsaturation (U.S.) : -0.5 - 100.0

Observed m/z	Int%	Err [ppm / mmu]	U.S. Composition
437.1266	100.0	+0.7 / +0.3	19.0 C 27 H 19 N O 5
438.1314	30.4		

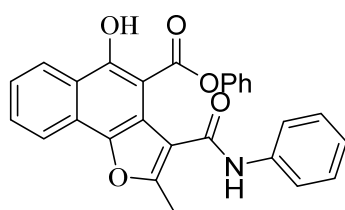
¹H NMR of Compound 16



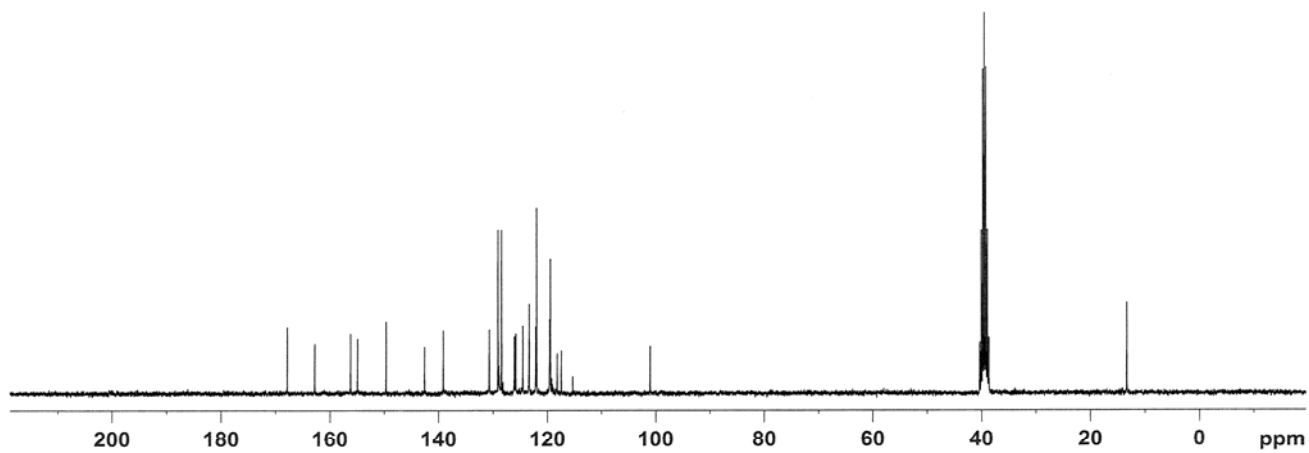
300 MHz, DMSO-d₆



¹³C NMR of Compound 16

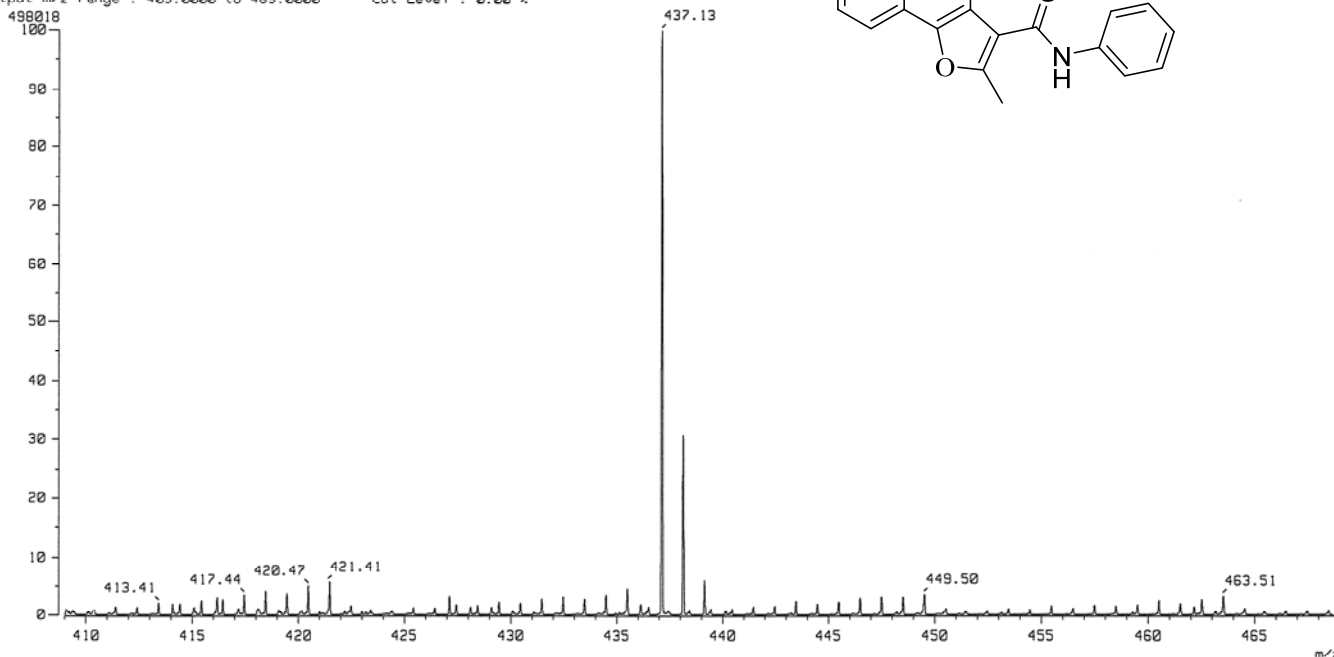
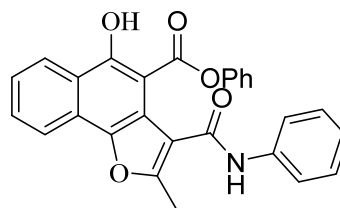


75 MHz, DMSO-d₆



[Mass Spectrum]
 Data : x9-10-C27H21NO5 Date : 04-Nov-2013 14:36
 Sample : -
 Note : -
 Inlet : Direct Ion Mode : EI+
 Spectrum Type : Normal Ion [EF-Linear]
 RT : 1.28 min Scan# : (26,27)
 BP : m/z 437.1261 Int. : 23.75
 Output m/z range : 409.0000 to 469.0000 Cut Level : 0.00 %

Mass Spectrum of Compound 16

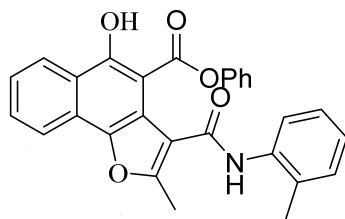


[Elemental Composition]

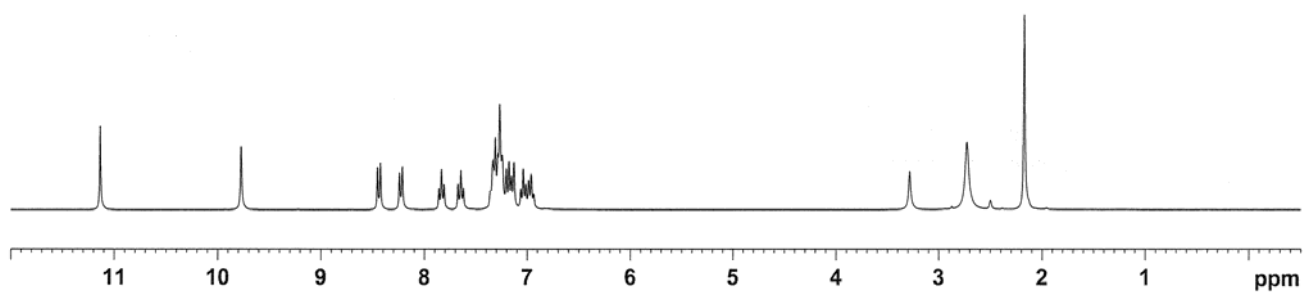
Data : x9-10-C27H21NO5 Date : 04-Nov-2013 14:36
 Sample : -
 Note : -
 Inlet : Direct Ion Mode : EI+
 RT : 1.28 min Scan#: (26,27)
 Elements : C 27/0, H 21/0, N 1/0, O 5/0
 Mass Tolerance : 1000ppm, 1mmu if m/z < 1, 3mmu if m/z > 3
 Unsaturation (U.S.) : -0.5 - 100.0

Observed m/z	Int%	Err [ppm / mmu]	U.S. Composition
437.1261	100.0	-0.4 / -0.2	19.0 C 27 H 19 N O 5
438.1299	30.9		

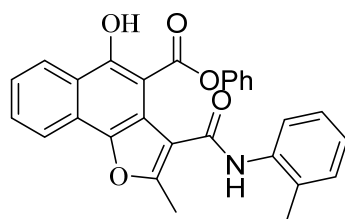
¹H NMR of Compound 17



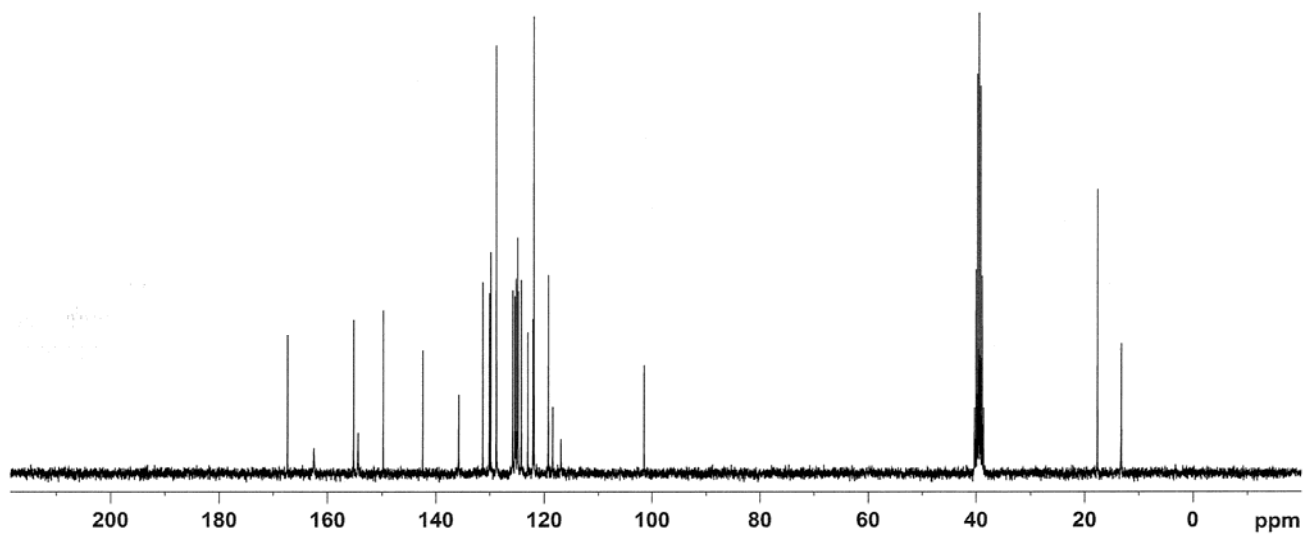
300 MHz, DMSO-d₆



¹³C NMR of Compound 17

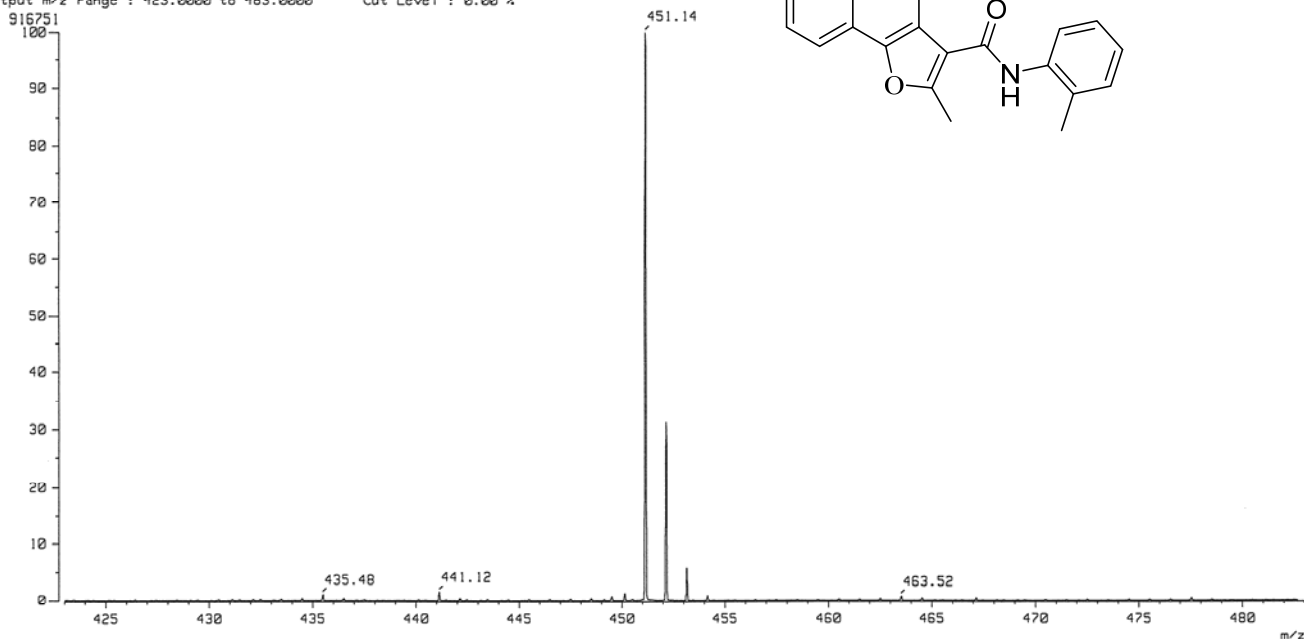
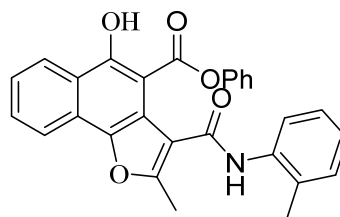


75 MHz, DMSO-d₆



[Mass Spectrum]
 Date : 04-Nov-2013 14:43
 Sample : -
 Note : -
 Inlet : Direct Ion Mode : EI+
 Spectrum Type : Normal Ion [EF-Linear]
 RT : 1.13 min Scan# : (23,24)
 BP : m/z 451.1417 Int. : 43.71
 Output m/z range : 423.0000 to 483.0000 Cut Level : 0.00 %

Mass Spectrum of Compound 17

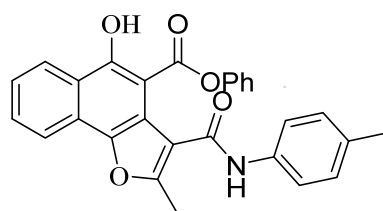


[Elemental Composition]

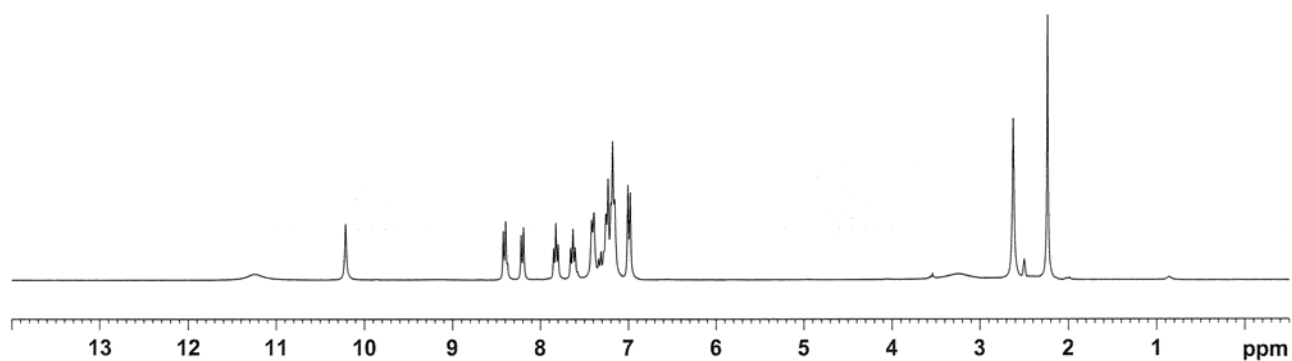
Data : x9-11-C28H23NO5 Date : 04-Nov-2013 14:43
 Sample : -
 Note : -
 Inlet : Direct Ion Mode : EI+
 RT : 1.13 min Scan# : (23,24)
 Elements : C 28/0, H 23/0, N 1/0, O 5/0
 Mass Tolerance : 1000ppm, 1mmu if m/z < 1, 3mmu if m/z > 3
 Unsaturation (U.S.) : -0.5 - 100.0

Observed m/z	Int%	Err [ppm / mmu]	U.S. Composition
451.1417	100.0	-0.6 / -0.2	19.0 C 28 H 21 N O 5
452.1462	31.3		

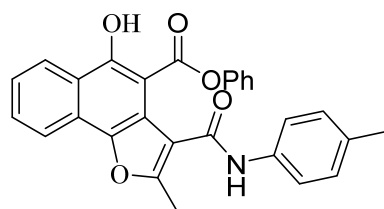
¹H NMR of Compound **18**



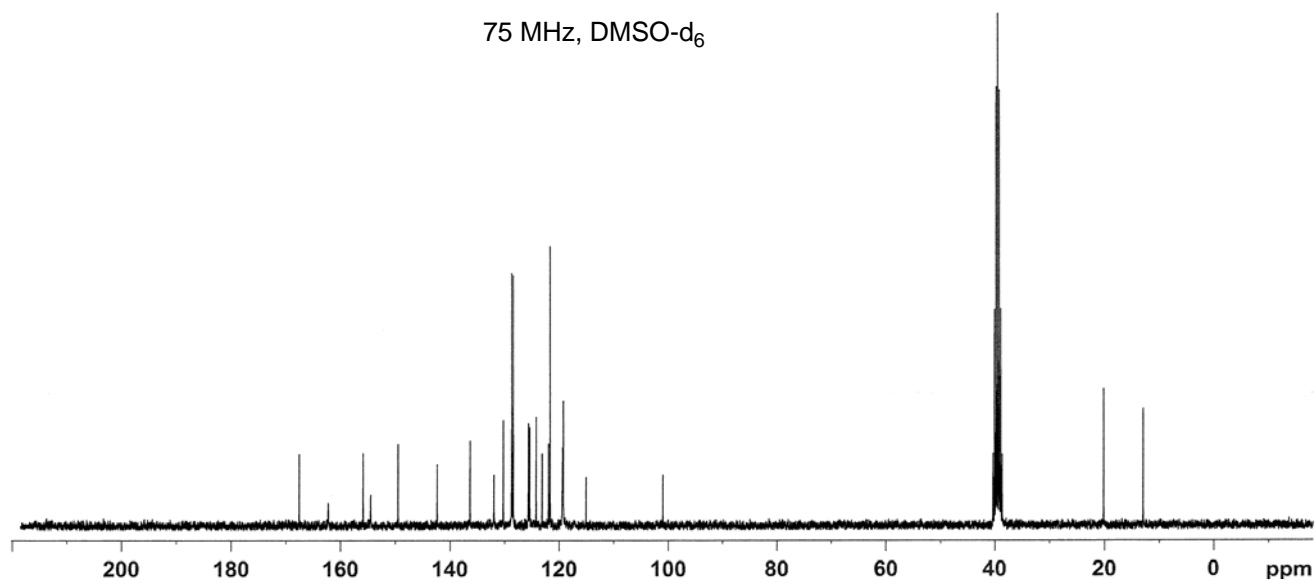
300 MHz, DMSO-d₆



¹³C NMR of Compound **18**

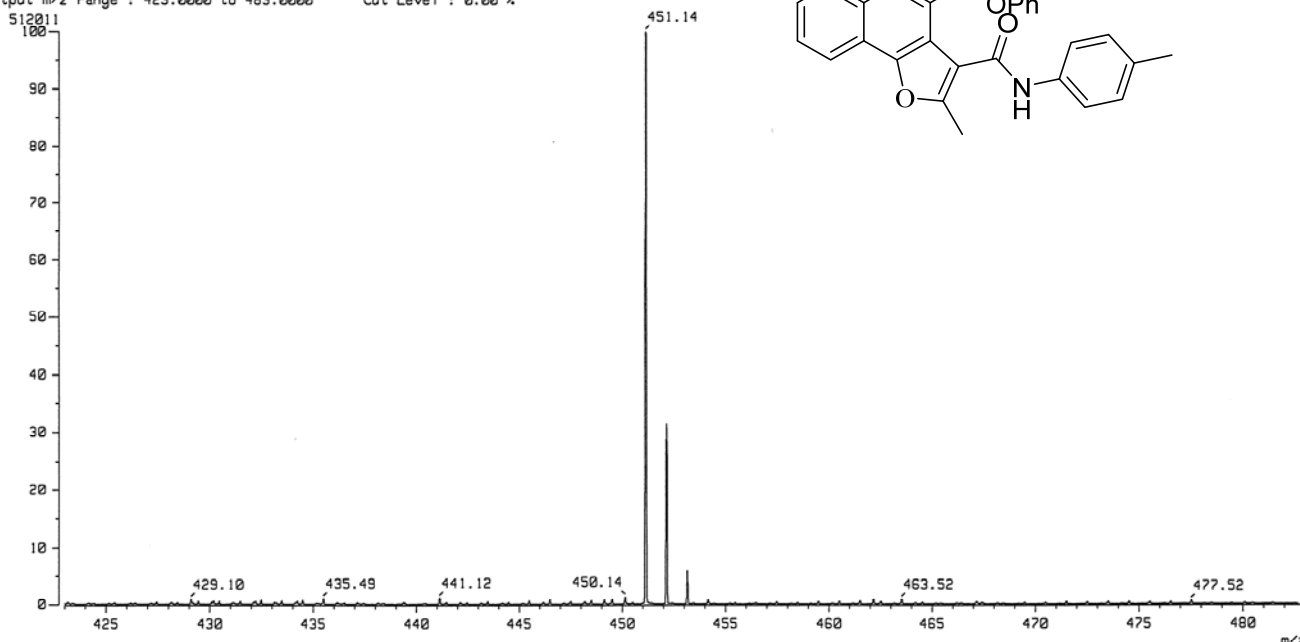
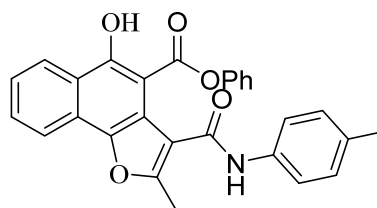


75 MHz, DMSO-d₆



[Mass Spectrum]
 Date : 04-Nov-2013 14:46
 Sample : -
 Note : -
 Inlet : Direct Ion Mode : EI+
 Spectrum Type : Normal Ion [EF-Linear]
 RT : 1.63 min Scan# : (33,34)
 BP : m/z 451.1422 Int. : 24.41
 Output m/z range : 423.0000 to 483.0000 Cut Level : 0.00 %

Mass Spectrum of Compound 18

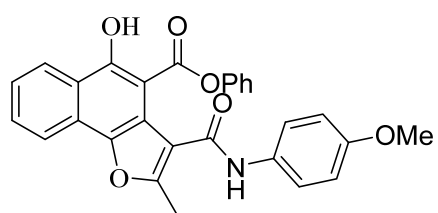


[Elemental Composition]

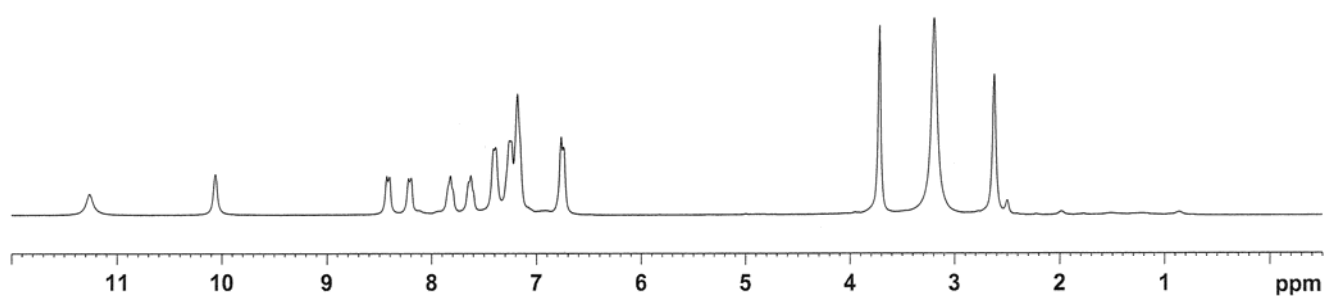
Data : x9-12-C28H23NO5 Date : 04-Nov-2013 14:46
 Sample : -
 Note : -
 Inlet : Direct Ion Mode : EI+
 RT : 1.63 min Scan# : (33,34)
 Elements : C 28/0, H 23/0, N 1/0, O 5/0
 Mass Tolerance : 1000ppm, 1mmu if m/z < 1, 3mmu if m/z > 3
 Unsaturation (U.S.) : -0.5 - 100.0

Observed m/z	Int%	Err [ppm / mmu]	U.S. Composition
451.1422	100.0	+0.5 / +0.2	19.0 C 28 H 21 N O 5
452.1457	31.5		

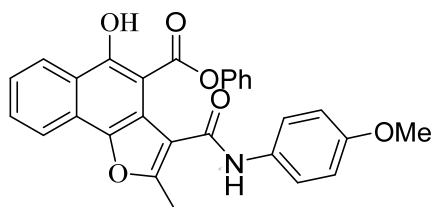
¹H NMR of Compound 19



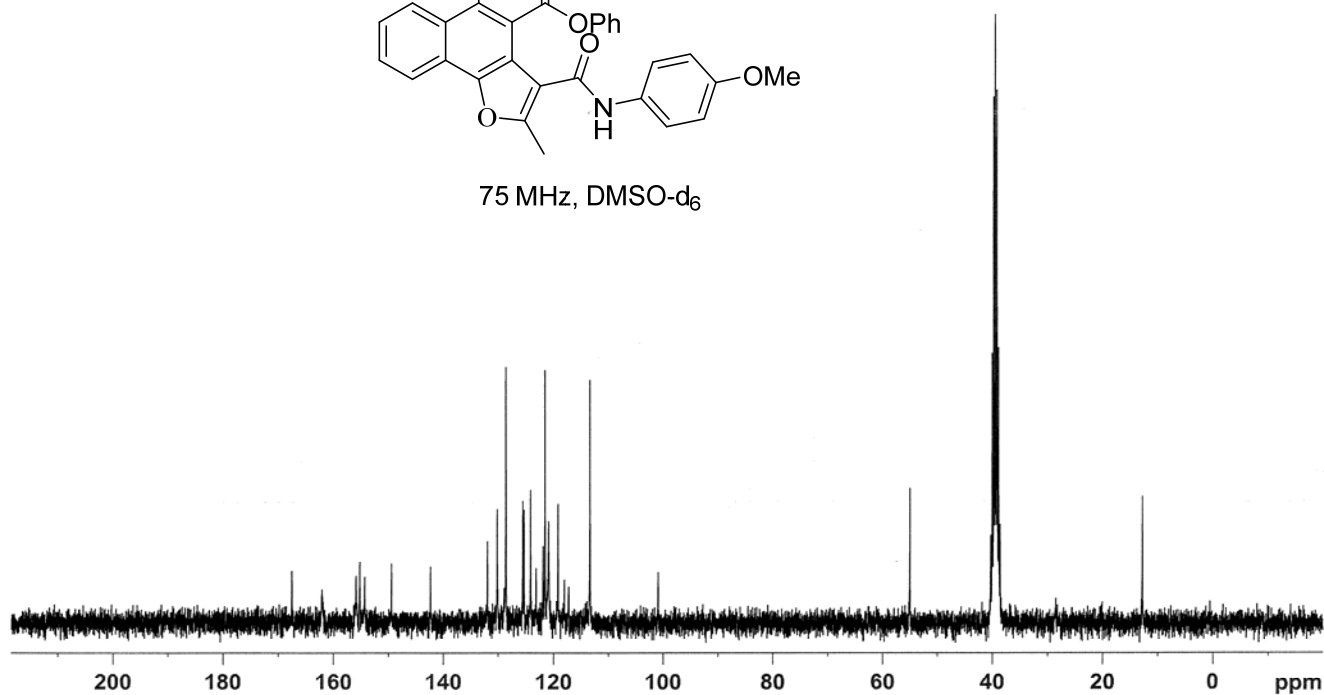
300 MHz, DMSO-d₆



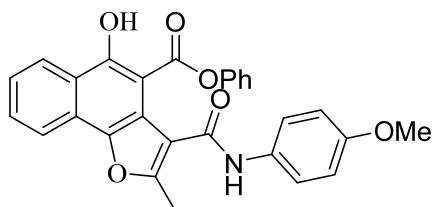
¹³C NMR of Compound 19



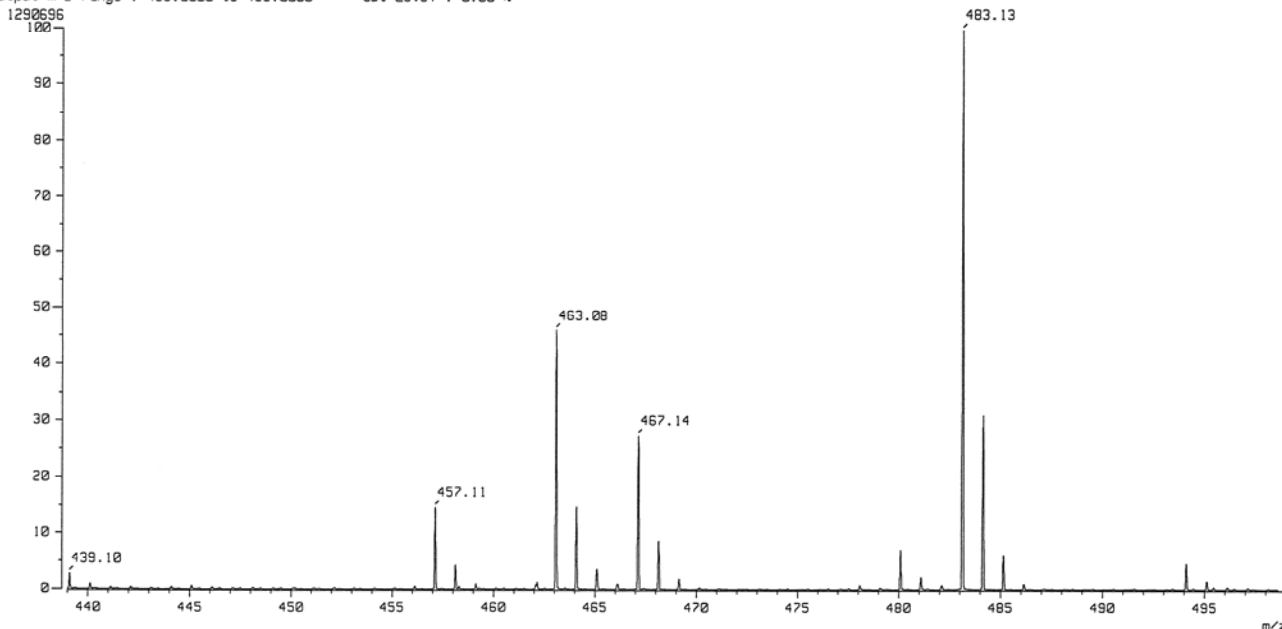
75 MHz, DMSO-d₆



Mass Spectrum of Compound 19



[Mass Spectrum]
 Data : x9-13-C28H23NO6 Date : 04-Nov-2013 14:51
 Sample : -
 Note : -
 Inlet : Direct Ion Mode : EI+
 Spectrum Type : Normal Ion [EF-Linear]
 RT : 1.38 min Scan# : (28,29)
 BP : m/z 483.1311 Int. : 61.55
 Output m/z range : 439.0000 to 499.0000 Cut Level : 0.00 %

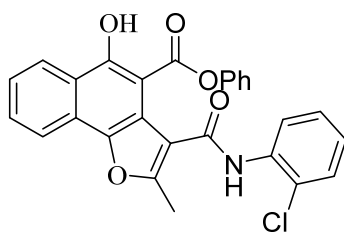


[Elemental Composition]

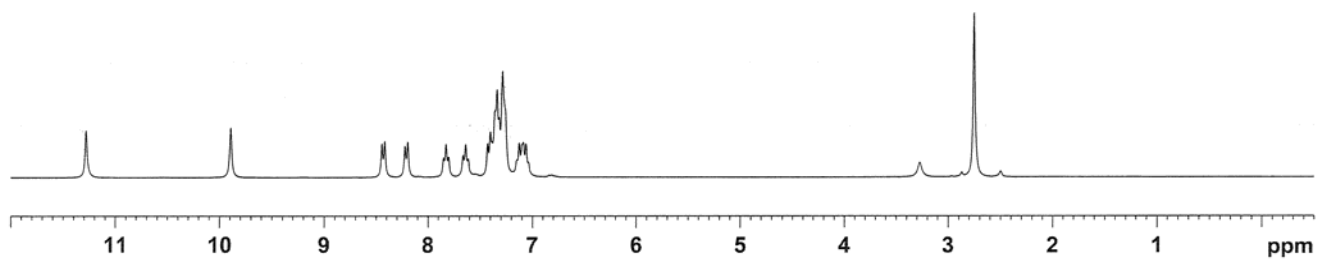
Data : x9-13-C28H23NO6 Date : 04-Nov-2013 14:51
 Sample : -
 Note : -
 Inlet : Direct Ion Mode : EI+
 RT : 1.38 min Scan#: (28,29)
 Elements : C 28/0, H 23/0, N 1/0, O 6/0
 Mass Tolerance : 1000ppm, 1mmu if m/z < 1, 3mmu if m/z > 3
 Unsaturation (U.S.) : -0.5 - 100.0

Observed m/z	Int%	Err [ppm / mmu]	U.S. Composition
457.1142	14.7		
463.0780	46.1		
464.0827	14.8		
467.1366	27.4	-0.6 / -0.3	19.0 C 28 H 21 N O 6
483.1311	100.0		
484.1335	31.0		

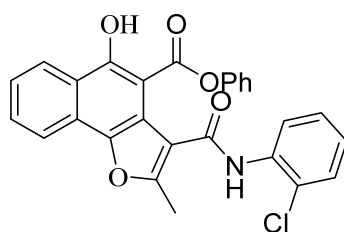
¹H NMR of Compound **20**



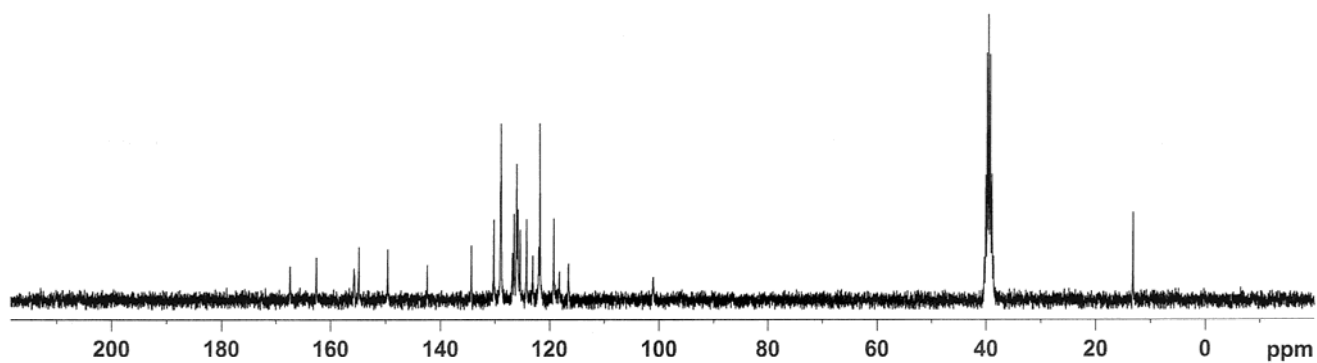
300 MHz, DMSO-d₆



¹³C NMR of Compound **20**

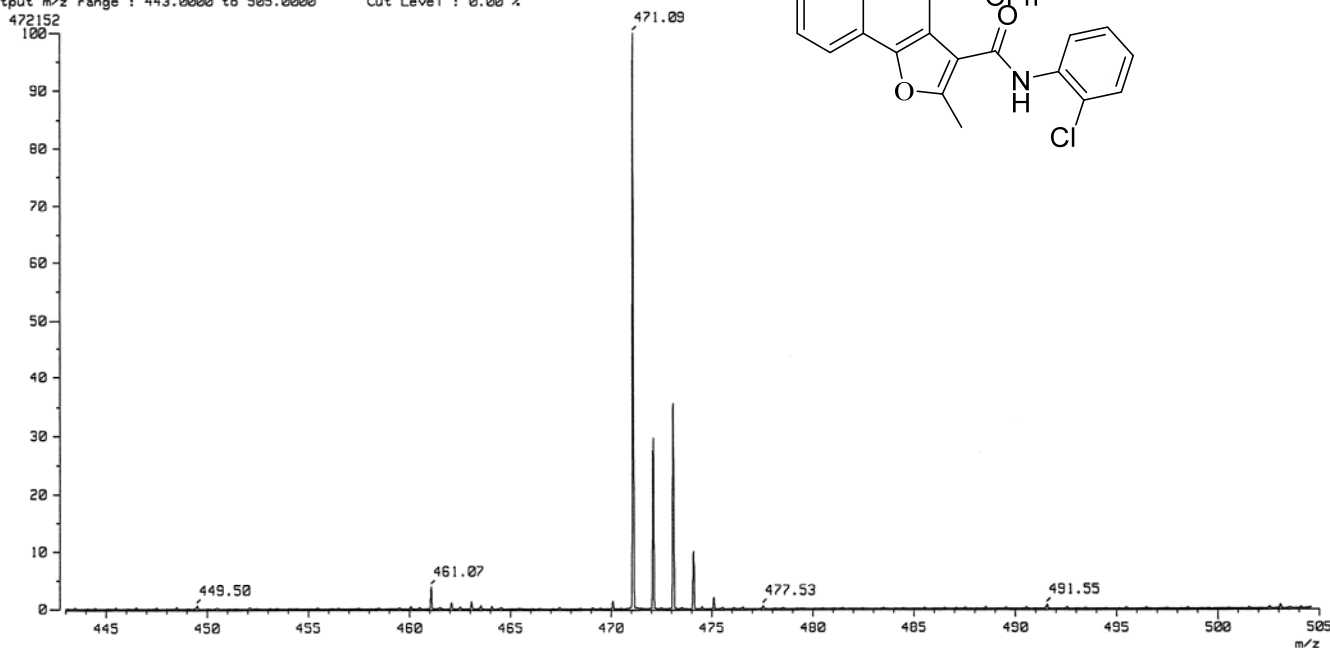
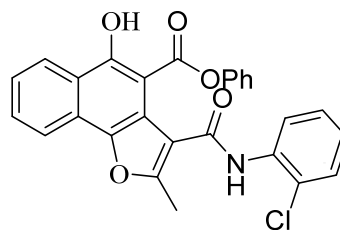


75 MHz, DMSO-d₆



[Mass Spectrum]
 Data : x9-14-C27H22ClNO5 Date : 04-Nov-2013 14:56
 Sample : -
 Note : -
 Inlet : Direct Ion Mode : EI+
 Spectrum Type : Normal Ion [EF-Linear]
 RT : 1.18 min Scan# : (24,25)
 BP : m/z 471.0873 Int. : 22.51
 Output m/z range : 443.0000 to 505.0000 Cut Level : 0.00 %

Mass Spectrum of Compound 20



[Elemental Composition]

Data : x9-14-C27H22ClNO5
 Sample : -
 Note : -

Date : 04-Nov-2013 14:56

Page: 1

Inlet : Direct

Ion Mode : EI+

RT : 1.18 min

Scan#: (24,25)

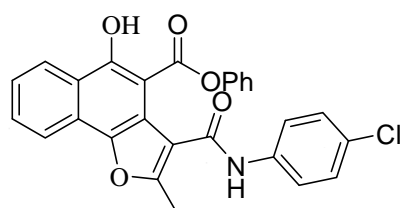
Elements : C 27/0, H 22/0, Cl 1/0, N 1/0, O 5/0

Mass Tolerance : 1000ppm, 1mmu if m/z < 1, 2mmu if m/z > 2

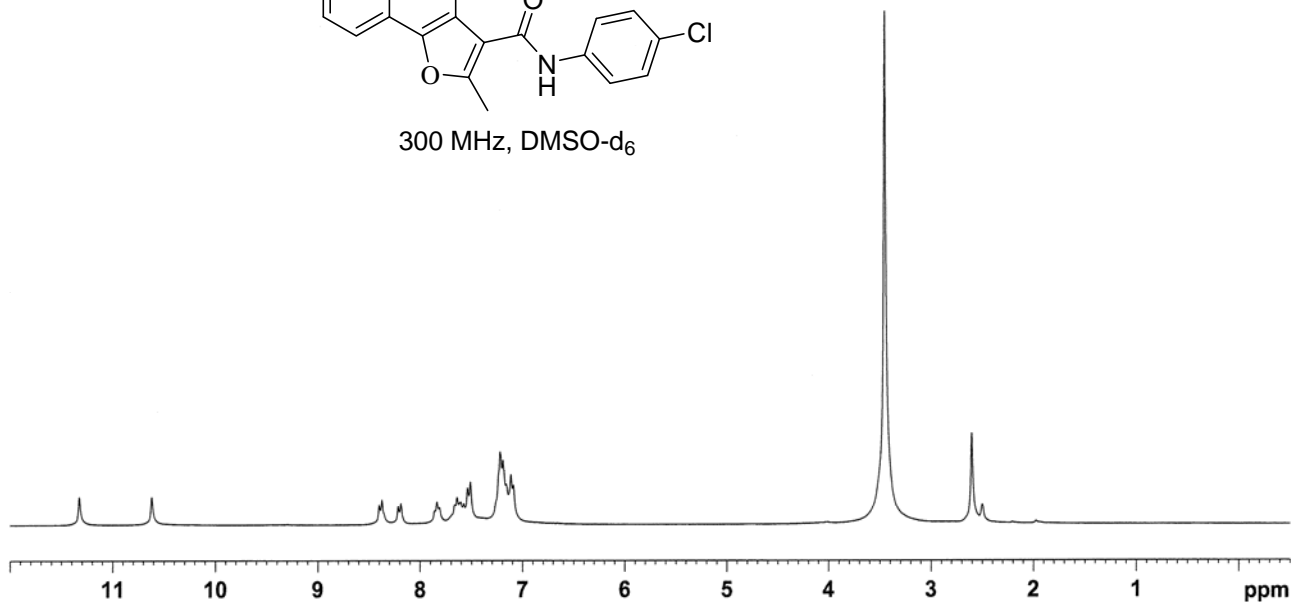
Unsaturation (U.S.) : -0.5 - 100.0

Observed m/z	Int%	Err [ppm / mmu]	U.S. Composition
471.0873	100.0	-0.1 / -0.1	19.0 C 27 H 18 Cl N O 5
472.0923	29.7		
473.0851	35.6		
474.0884	10.0		

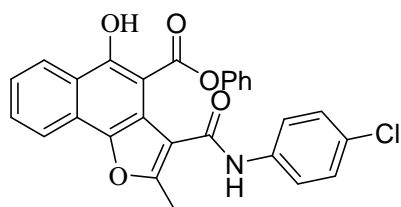
¹H NMR of Compound 21



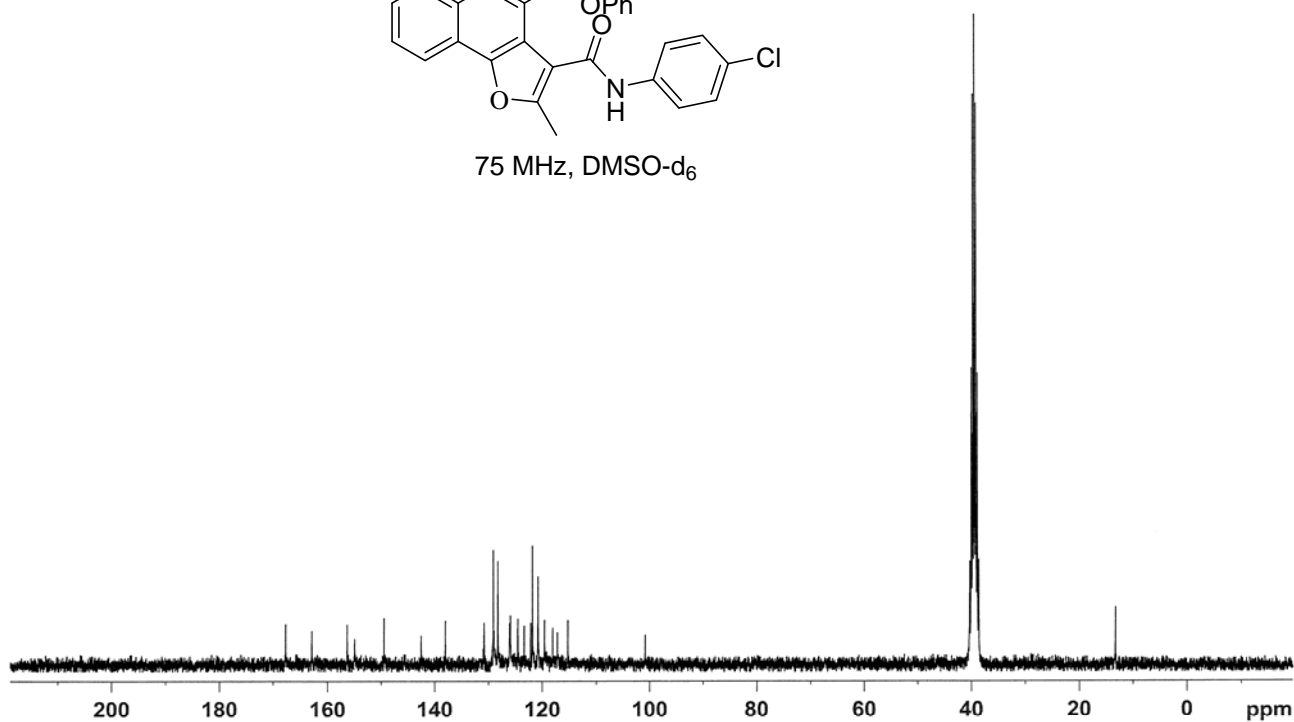
300 MHz, DMSO-d₆



¹³C NMR of Compound 21

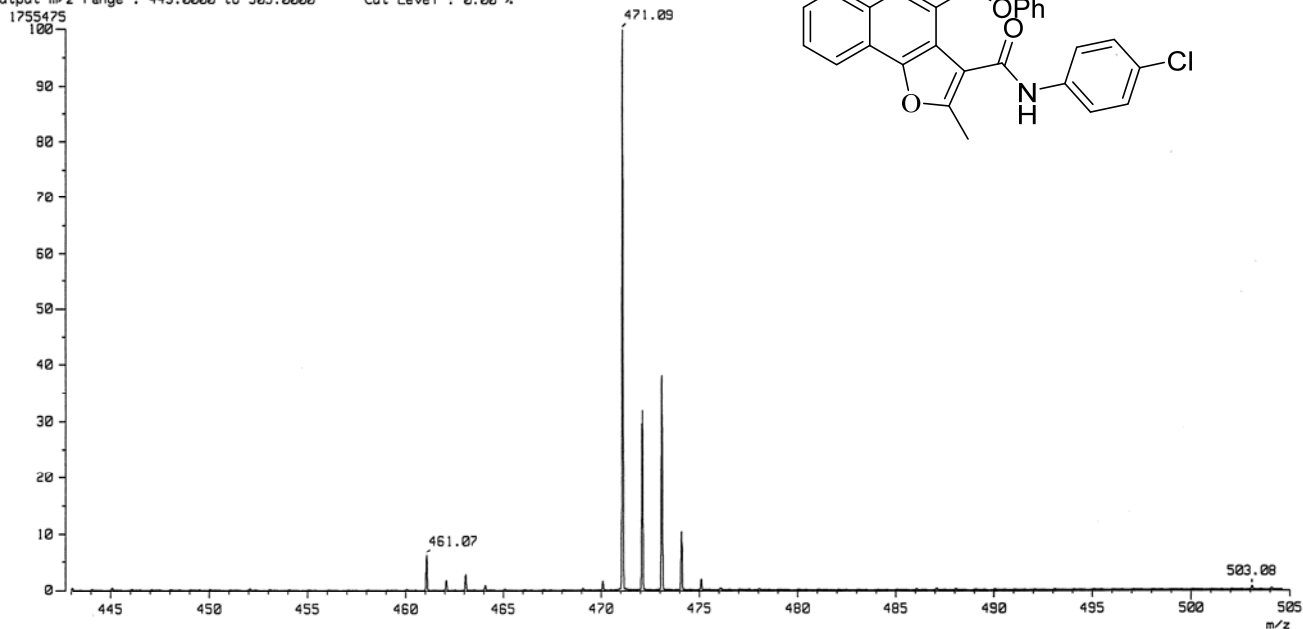
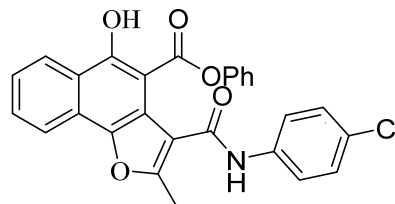


75 MHz, DMSO-d₆



[Mass Spectrum]
 Date : 04-Nov-2013 15:01
 Sample : -
 Note : -
 Inlet : Direct Ion Mode : EI+
 Spectrum Type : Normal Ion [EF-Linear]
 RT : 1.83 min Scan# : (37,38)
 BP : m/z 471.0872 Int. : 83.71
 Output m/z range : 443.0000 to 505.0000 Cut Level : 0.00 %

Mass Spectrum of Compound 21



[Elemental Composition]

Data : x9-15-C27H20ClNO5

Date : 04-Nov-2013 15:01

Page: 1

Sample : -

Note : -

Inlet : Direct

Ion Mode : EI+

RT : 1.83 min

Scan#: (37,38)

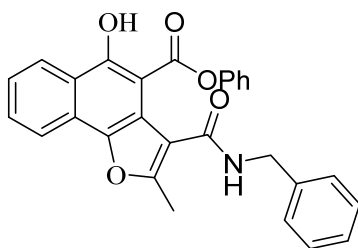
Elements : C 27/0, H 20/0, Cl 1/0, N 1/0, O 5/0

Mass Tolerance : 1000ppm, 1mmu if m/z < 1, 3mmu if m/z > 3

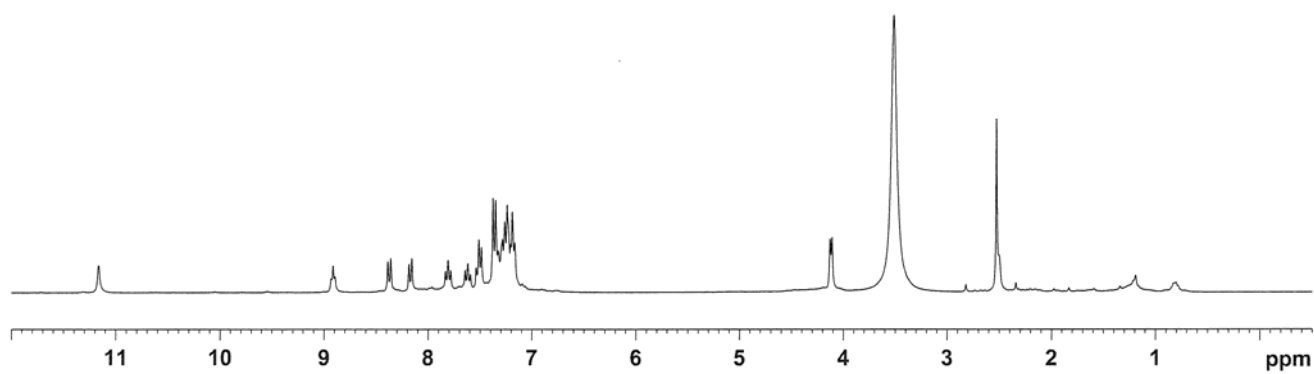
Unsaturation (U.S.) : -0.5 - 100.0

Observed m/z	Int%	Err [ppm / mmu]	U.S. Composition
471.0872	100.0	-0.3 / -0.1	19.0 C 27 H 18 Cl N O 5
472.0909	31.9		
473.0858	38.2		
474.0878	10.4		

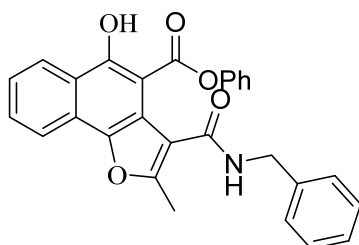
¹H NMR of Compound 22



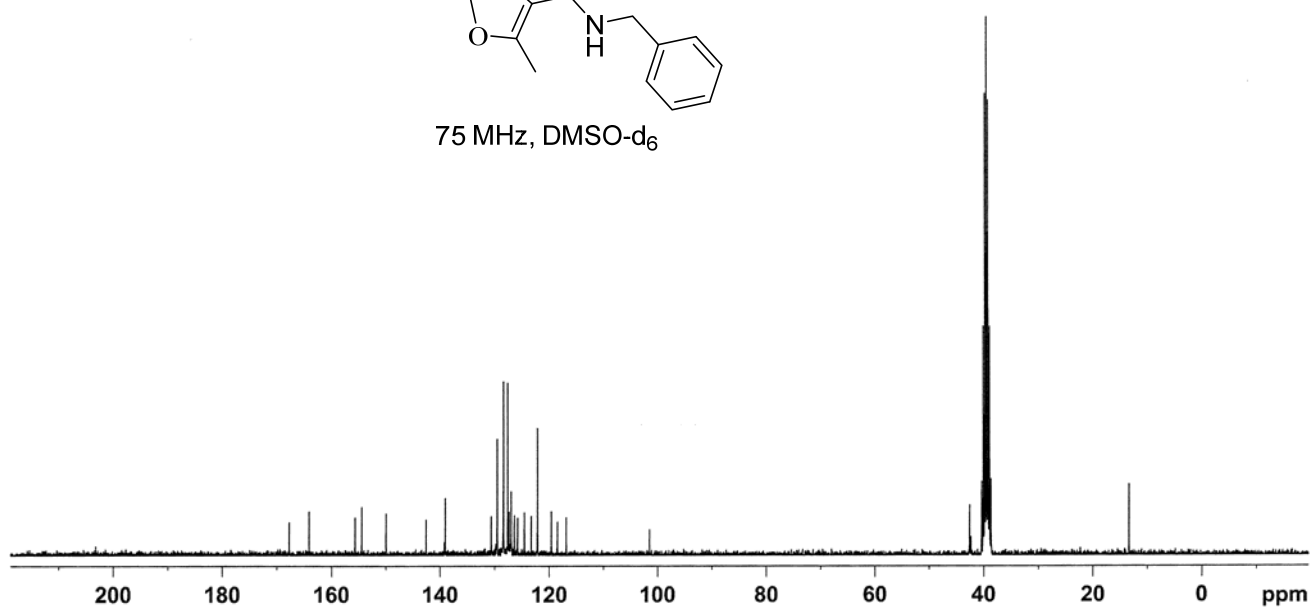
300 MHz, DMSO-d₆



¹³C NMR of Compound 22



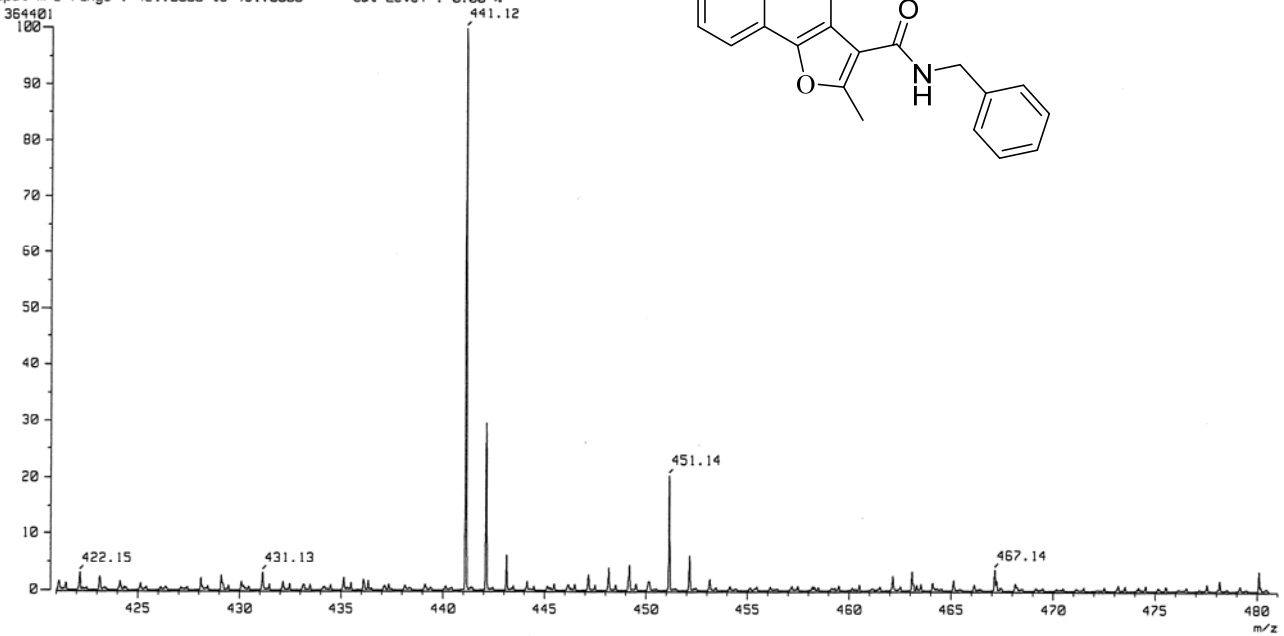
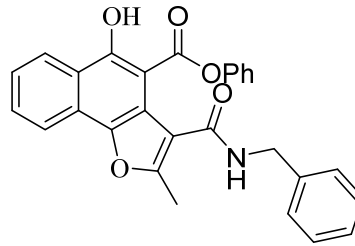
75 MHz, DMSO-d₆



[Mass Spectrum]
 Data : X9-16-C28H21NO5
 Sample: -
 Note: -
 Inlet : Direct
 Spectrum Type : Normal Ion [EF-Linear]
 RT : 1.68 min Scan# : (34,35)
 BP : m/z 441.1217 Int. : 17.38
 Output m/z range : 421.0000 to 481.0000

Date : 29-Nov-2013 13:56

Mass Spectrum of Compound 22



[Elemental Composition]

Data : X9-16-C28H21NO5

Date : 29-Nov-2013 13:56

Page: 1

Sample: -
 Note: -

Inlet : Direct
 RT : 1.68 min

Ion Mode : EI+
 Scan#: (34,35)

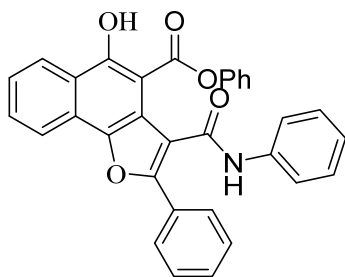
Elements : C 28/0, H 21/0, N 1/0, O 5/0

Mass Tolerance : 1000ppm, 1mmu if m/z < 1, 3mmu if m/z > 3

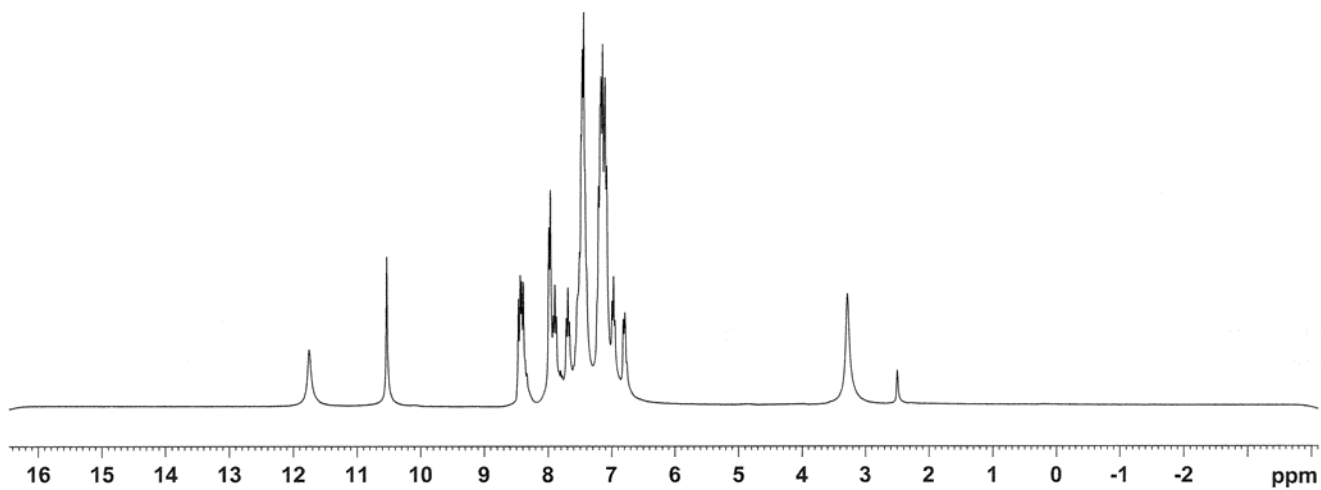
Unsaturation (U.S.) : -0.5 - 100.0

Observed m/z	Int%	Err[ppm / mmu]	U.S. Composition
441.1217	100.0		
442.1251	29.7		
451.1419	20.5	-0.1 / -0.1	19.0 C 28 H 21 N O 5

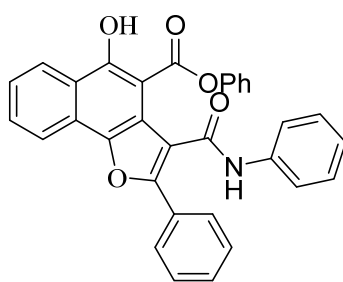
¹H NMR of Compound 23



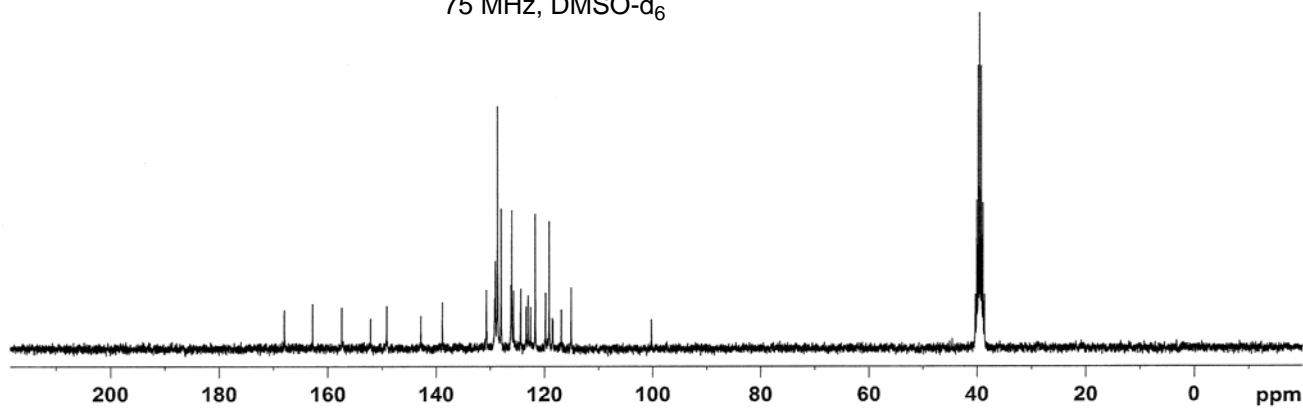
300 MHz, DMSO-d₆



¹³C NMR of Compound 23

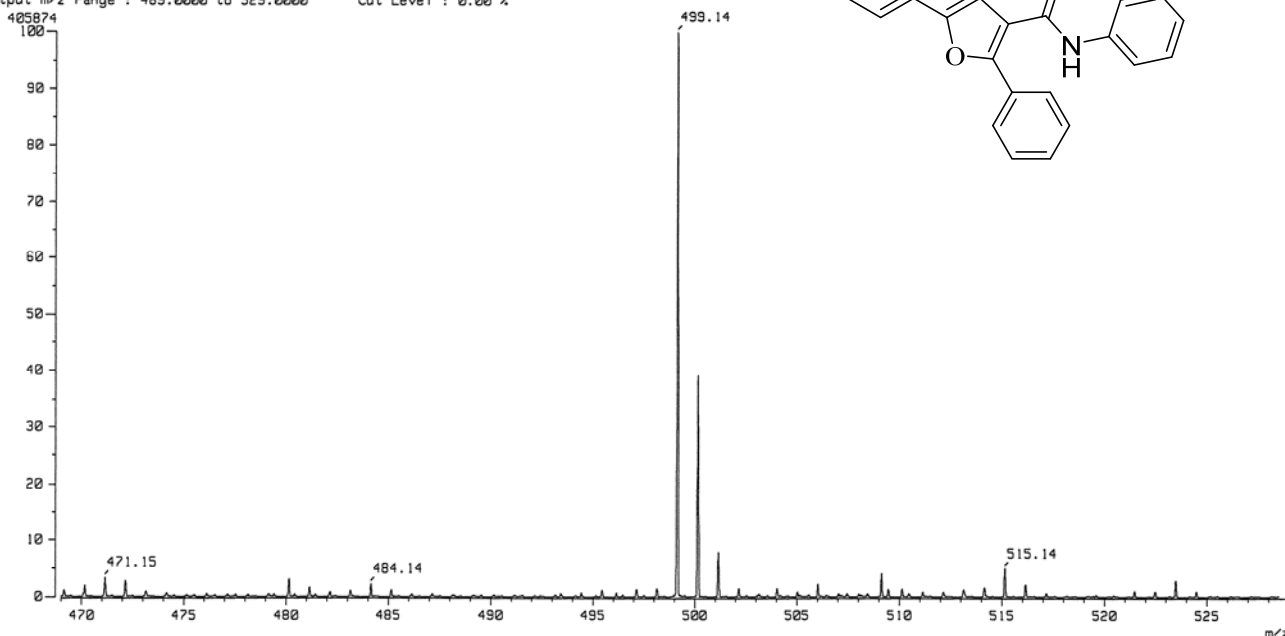
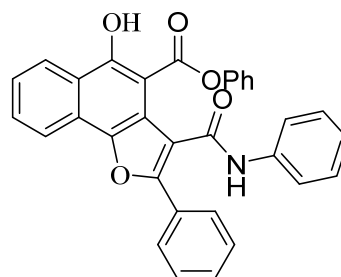


75 MHz, DMSO-d₆



[Mass Spectrum]
 Date : 29-Nov-2013 15:02
 Sample : -
 Note : -
 Inlet : Direct Ion Mode : EI+
 Spectrum Type : Normal Ion [EF-Linear]
 RT : 1.53 min Scan# : (31,32)
 BP : m/z 499.1422 Int. : 19.35
 Output m/z range : 469.0000 to 529.0000 Cut Level : 0.00 %

Mass Spectrum of Compound 23



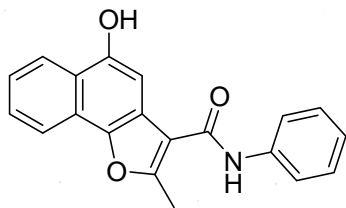
[Elemental Composition]

Page: 1

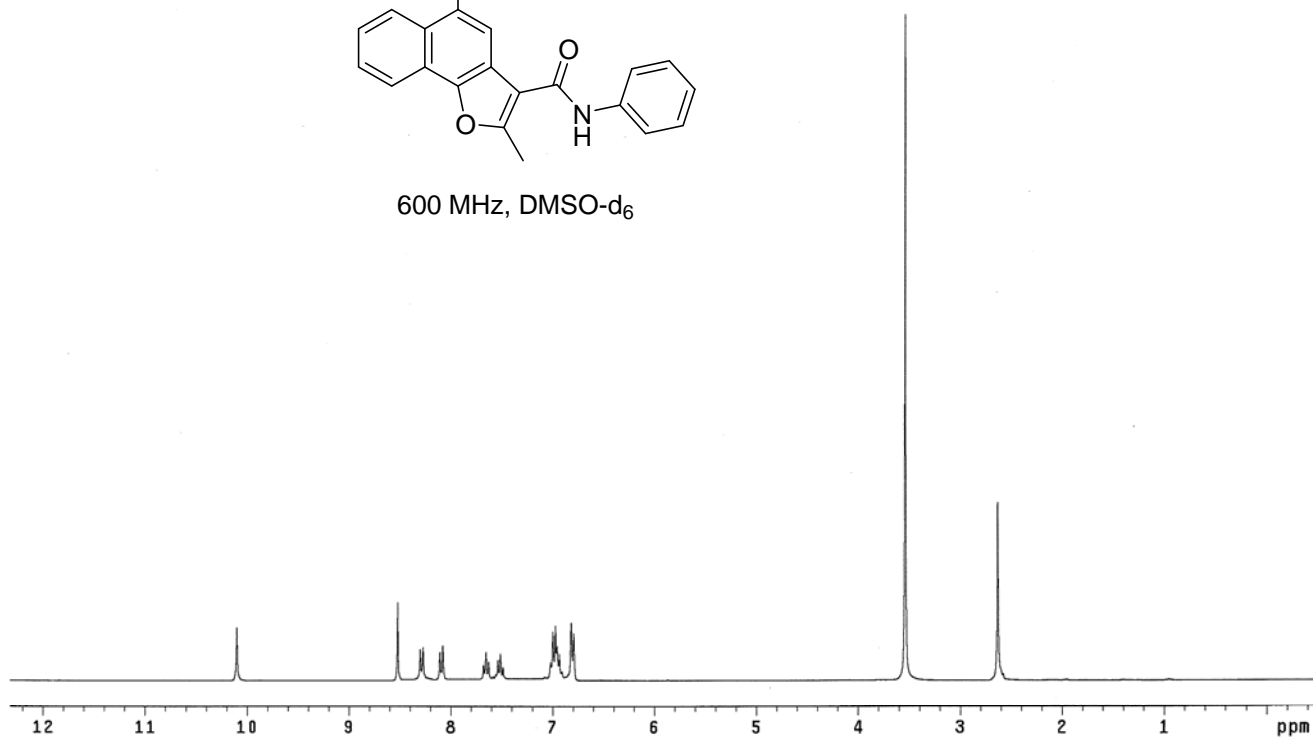
Data : x9-17-C32H21NO5 Date : 29-Nov-2013 15:02
 Sample : -
 Note : -
 Inlet : Direct Ion Mode : EI+
 RT : 1.53 min Scan# : (31,32)
 Elements : C 32/0, H 21/0, N 1/0, O 5/0
 Mass Tolerance : 1000ppm, 1mmu if m/z < 1, 3mmu if m/z > 3
 Unsaturation (U.S.) : -0.5 - 100.0

Observed m/z	Int%	Err [ppm / mmu]	U.S.	Composition
499.1422	100.0	+0.5 / +0.3	23.0	C 32 H 21 N O 5
500.1451	39.2			

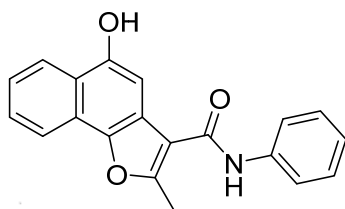
¹H NMR of Compound **26**



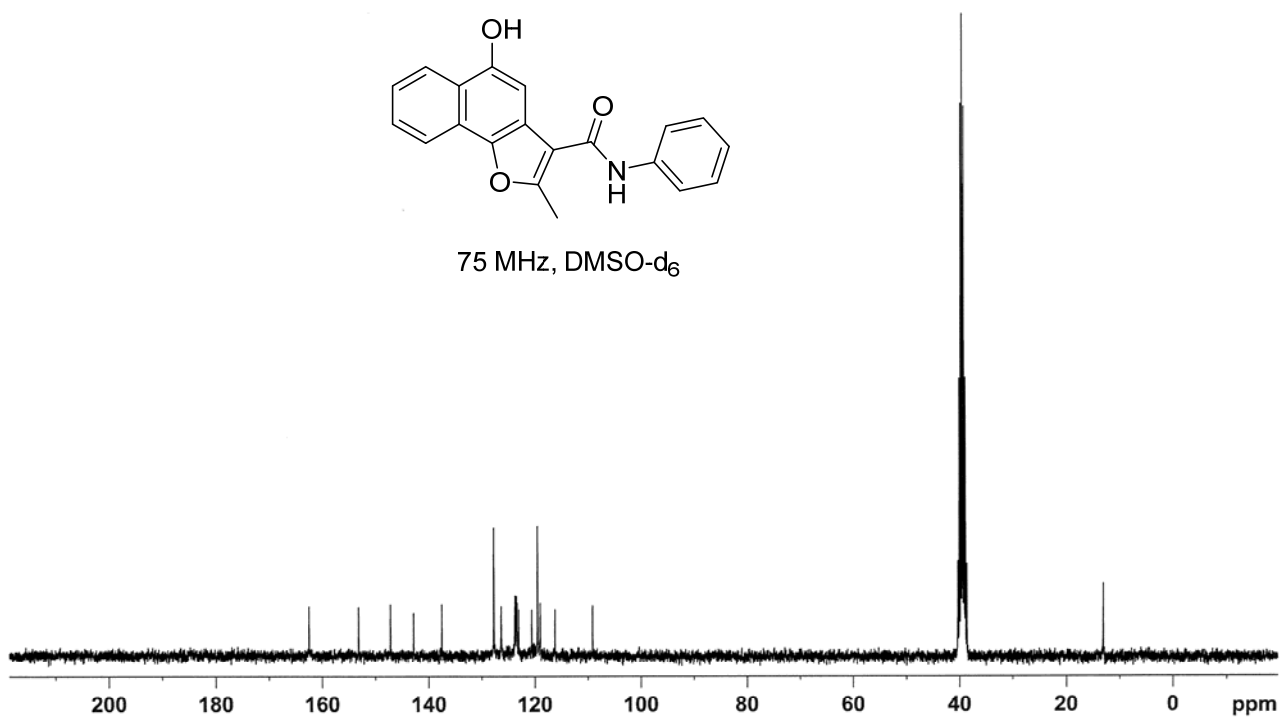
600 MHz, DMSO-d₆



¹³C NMR of Compound **26**

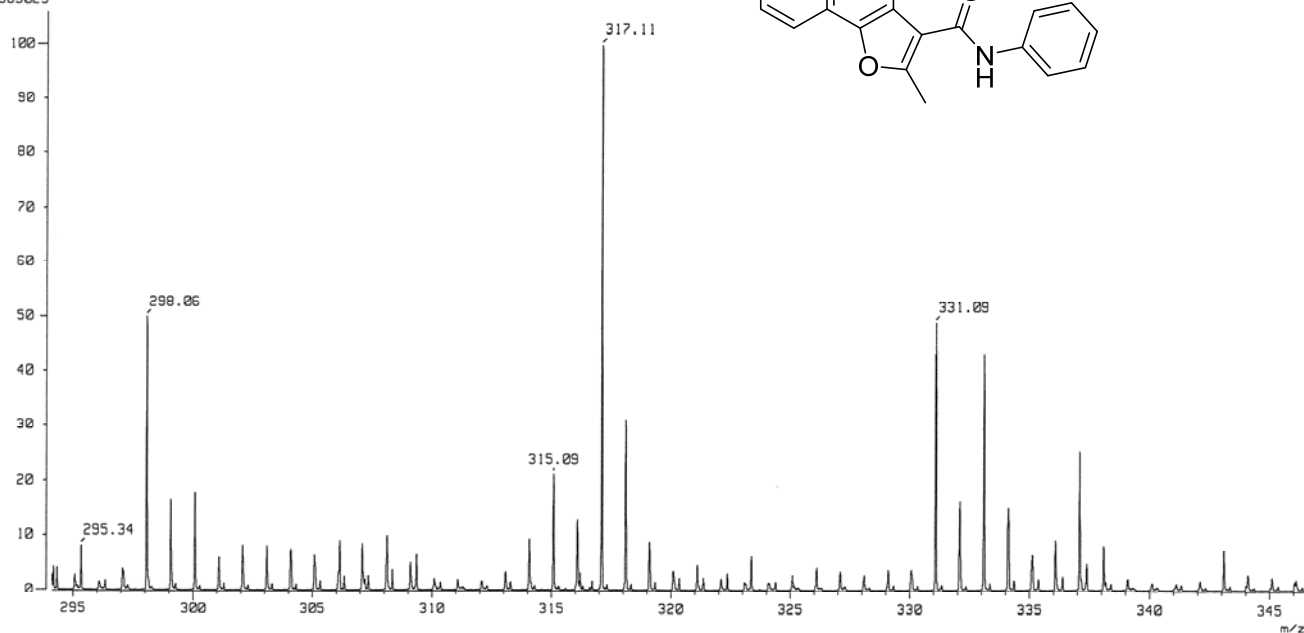
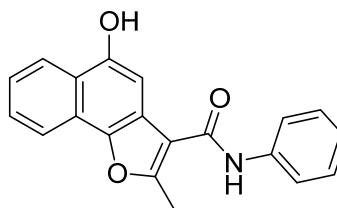


75 MHz, DMSO-d₆



[Mass Spectrum]
 Data : x9-18-C20H15NO3 Date : 29-Nov-2013 15:07
 Sample: -
 Note: -
 Inlet : Direct Ion Mode : EI+
 Spectrum Type : Normal Ion [EF-Linear]
 RT : 1.78 min Scan# : (36,37)
 BP : m/z 317.1051 Int. : 25.46
 Output m/z range : 294.1217 to 346.4659 Cut Level : 0.00 %
 565025

Mass Spectrum of Compound 26



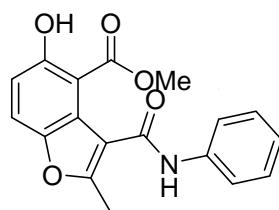
[Elemental Composition]

Data : x9-18-C20H15NO3 Date : 29-Nov-2013 15:07
 Sample: -
 Note: -
 Inlet : Direct Ion Mode : EI+
 RT : 1.78 min Scan#: (36,37)
 Elements : C 20/0, H 15/0, N 1/0, O 3/0
 Mass Tolerance : 1000ppm, 1mmu if m/z < 1, 3mmu if m/z > 3
 Unsaturation (U.S.) : -0.5 - 100.0

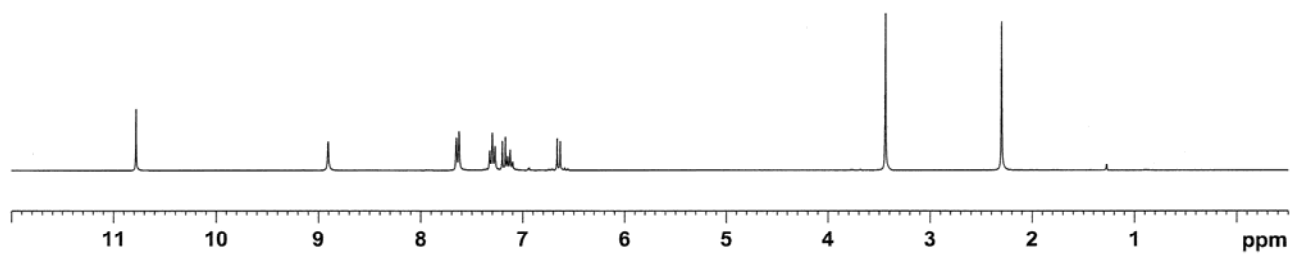
Page: 1

Observed m/z	Int%	Err [ppm / mmu]	U.S.	Composition
298.0647	50.0	+5.6 / +1.7	16.0	C 20 H 10 O 3
299.0710	16.7	+0.7 / +0.2	15.5	C 20 H 11 O 3
300.0789	18.0	+0.9 / +0.3	15.0	C 20 H 12 O 3
315.0909	21.2	+4.1 / +1.3	15.0	C 20 H 13 N O 3
316.0889	12.8			
317.1051	100.0	-0.3 / -0.1	14.0	C 20 H 15 N O 3
318.1070	31.2			
331.0870	49.1			
332.0888	16.5			
333.1033	43.3			
334.1174	15.3			
337.0868	25.5			

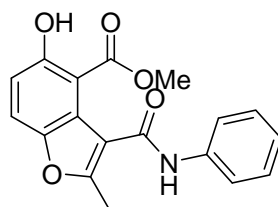
¹H NMR of Compound 27



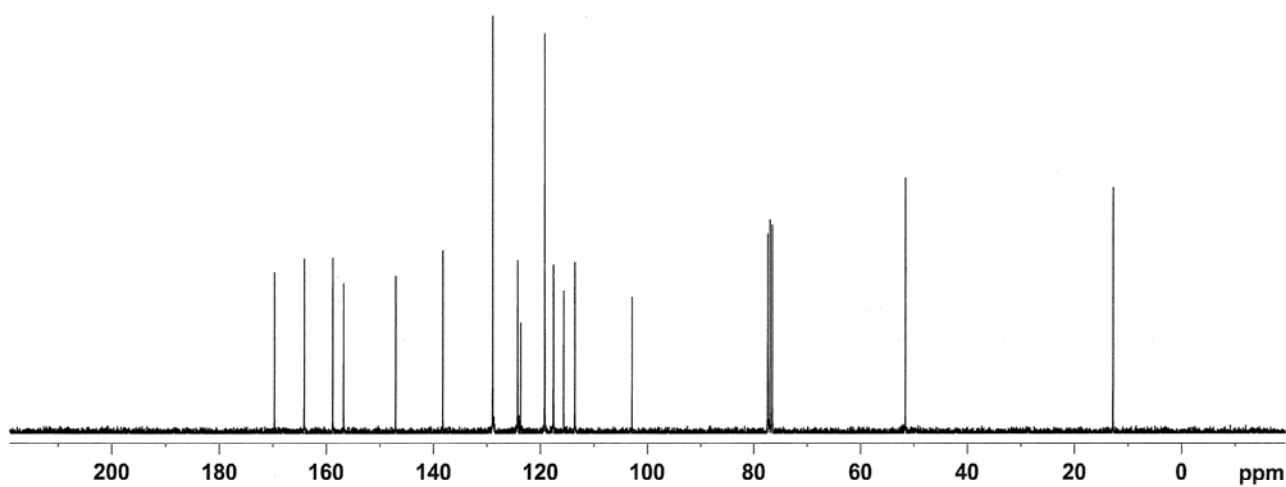
300 MHz, CDCl₃



¹³C NMR of Compound 27

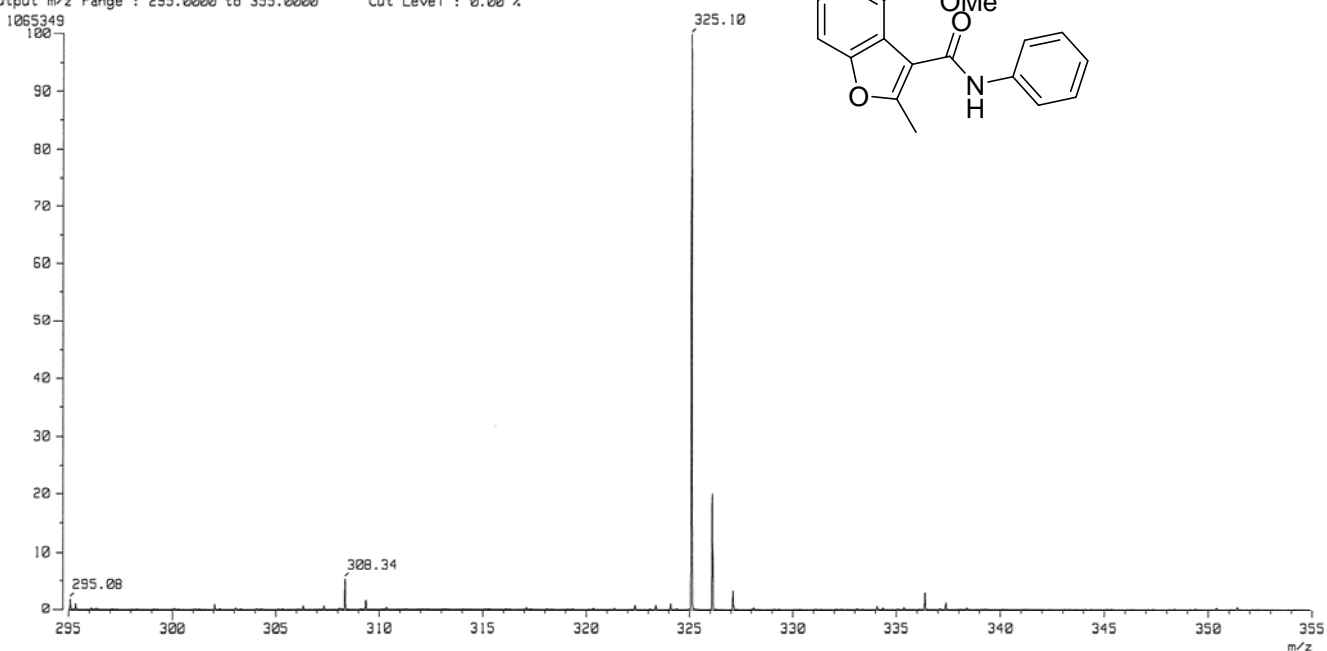
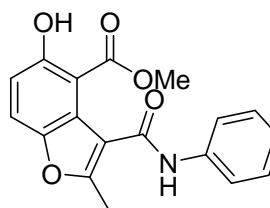


75 MHz, CDCl₃



[Mass Spectrum]
 Date : 29-Nov-2013 15:14
 Sample : -
 Note : -
 Inlet : Direct Ion Mode : EI+
 Spectrum Type : Normal Ion [EF-Linear]
 RT : 0.58 min Scan# : (12,13)
 BP : m/z 325.0952 Int. : 50.00
 Output m/z range : 295.0000 to 355.0000 Cut Level : 0.00 %

Mass Spectrum of Compound 27



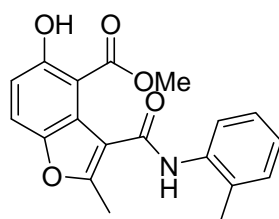
[Elemental Composition]

Data : X9-19-C18H15NO5 Date : 29-Nov-2013 15:14
 Sample : -
 Note : -
 Inlet : Direct Ion Mode : EI+
 RT : 0.58 min Scan# : (12,13)
 Elements : C 18/0, H 15/0, N 1/0, O 5/0
 Mass Tolerance : 1000ppm, 1mmu if m/z < 1, 3mmu if m/z > 3
 Unsaturation (U.S.) : -0.5 - 100.0

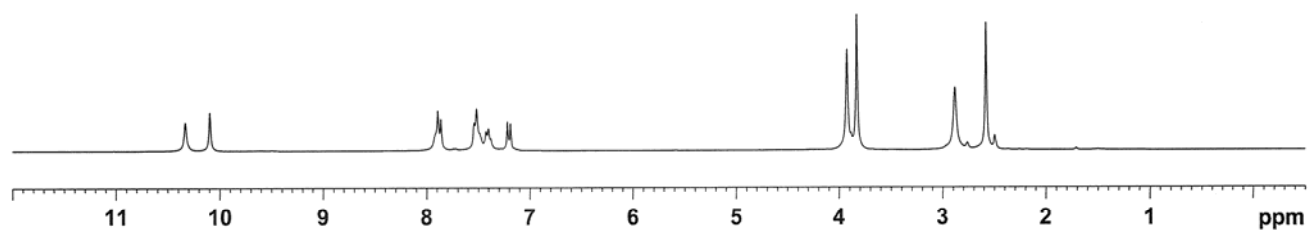
Page: 1

Observed m/z	Int%	Err [ppm / mmu]	U.S.	Composition
325.0952	100.0	+0.4 / +0.1	12.0	C 18 H 15 N O 5
326.0996	20.2			

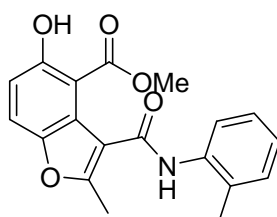
¹H NMR of Compound 28



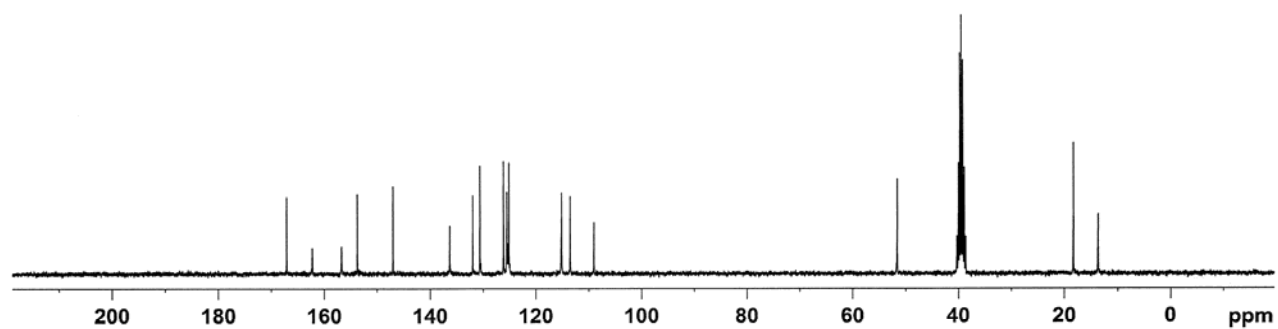
300 MHz, DMSO-d₆



¹³C NMR of Compound 28

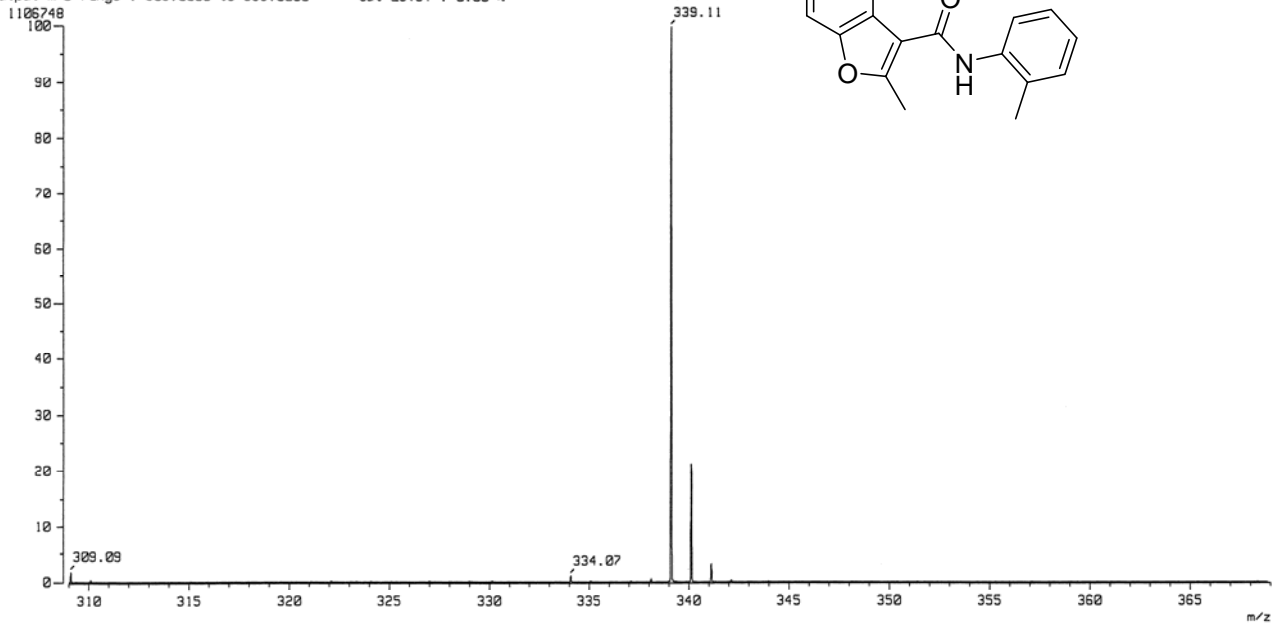
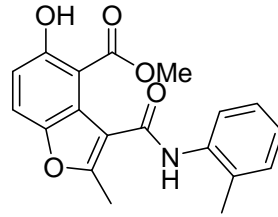


75 MHz, DMSO-d₆



[Mass Spectrum]
 Date : x9-43-C19H17NO5 Date : 29-Nov-2013 16:37
 Sample: -
 Note : -
 Inlet : Direct Ion Mode : EI+
 Spectrum Type : Normal Ion [EF-Linear]
 RT : 0.58 min Scan# : (12,13)
 BP : m/z 339.1106 Int. : 52.77
 Output m/z range : 309.0000 to 369.0000 Cut Level : 0.00 %

Mass Spectrum of Compound 28



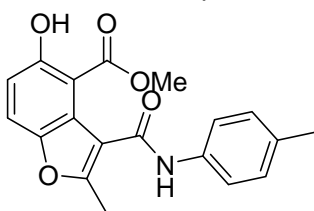
[Elemental Composition]

Data : x9-43-C19H17NO5 Date : 29-Nov-2013 16:37
 Sample: -
 Note : -
 Inlet : Direct Ion Mode : EI+
 RT : 0.58 min Scan#: (12,13)
 Elements : C 19/0, H 17/0, N 1/0, O 5/0
 Mass Tolerance : 1000ppm, 1mmu if m/z < 1, 3mmu if m/z > 3
 Unsaturation (U.S.) : -0.5 - 100.0

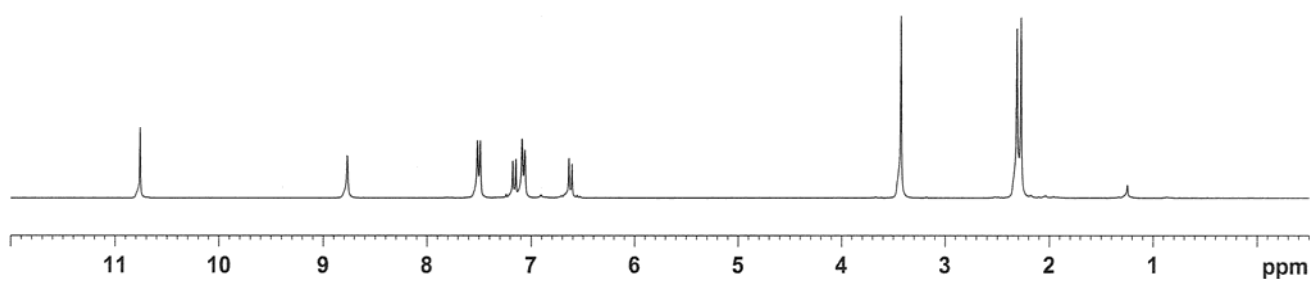
Page: 1

Observed m/z	Int%	Err [ppm / mmu]	U.S. Composition
339.1106	100.0	-0.3 / -0.1	12.0 C 19 H 17 N O 5
340.1144	21.4		

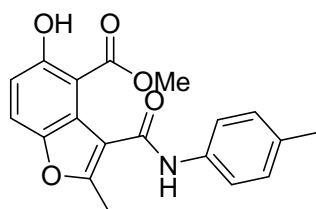
¹H NMR of Compound **29**



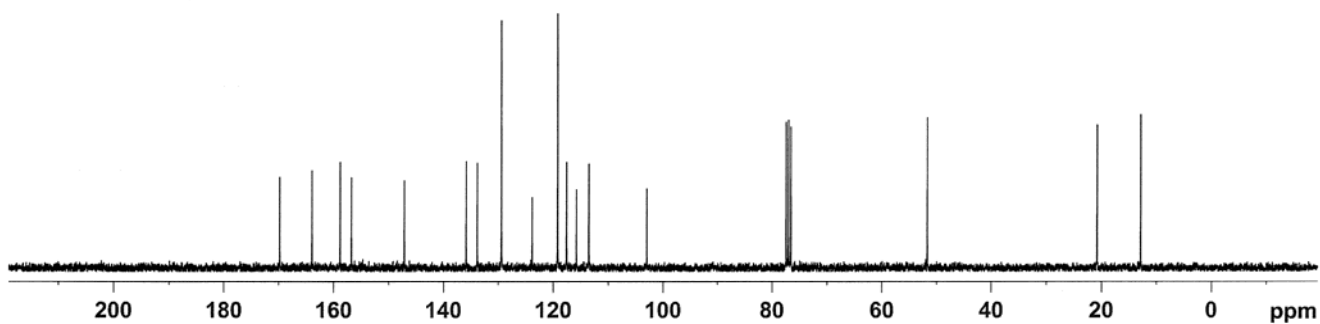
300 MHz, CDCl₃



¹³C NMR of Compound **29**

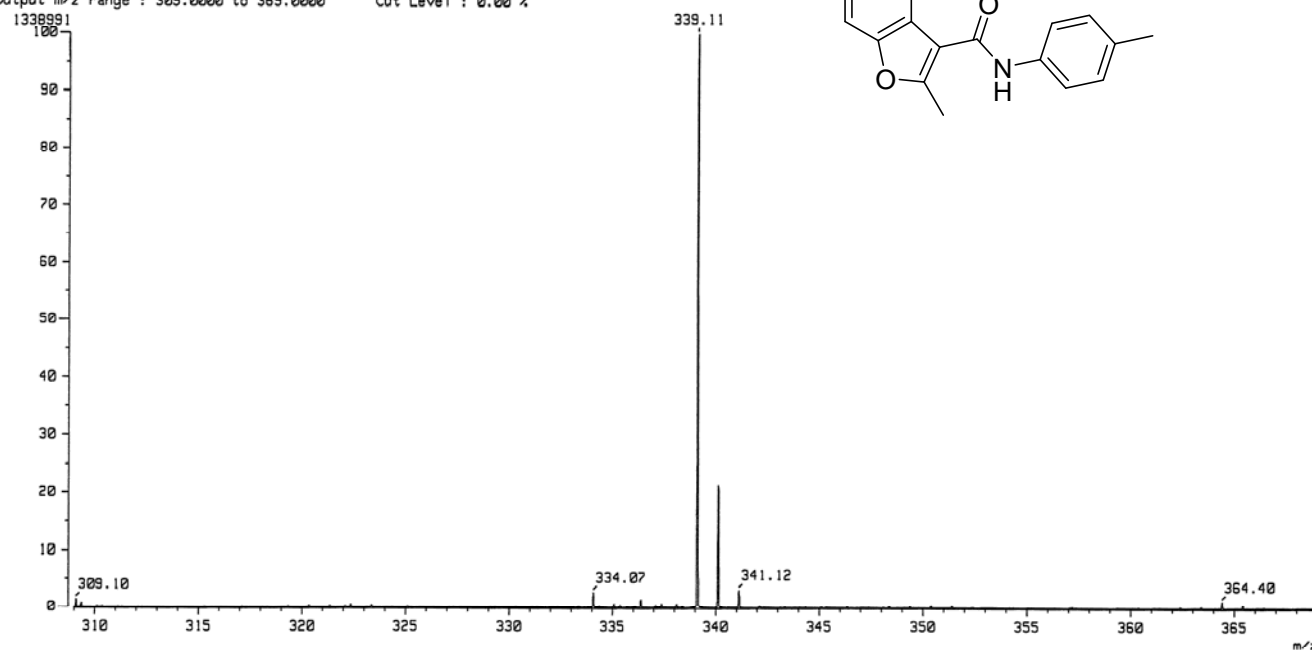
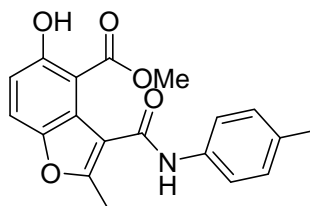


75 MHz, CDCl₃



[Mass Spectrum]
 Date : 29-Nov-2013 15:17
 Sample : -
 Note : -
 Inlet : Direct Ion Mode : EI+
 Spectrum Type : Normal Ion [EF-Linear]
 RT : 0.53 min Scan# : (11,12)
 BP : m/z 339.1104 Int. : 63.85
 Output m/z range : 309.0000 to 369.0000 Cut Level : 0.00 %

Mass Spectrum of Compound 29

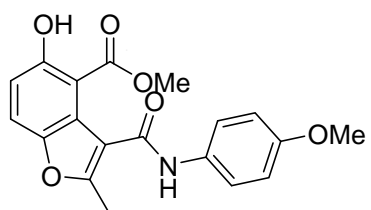


[Elemental Composition]

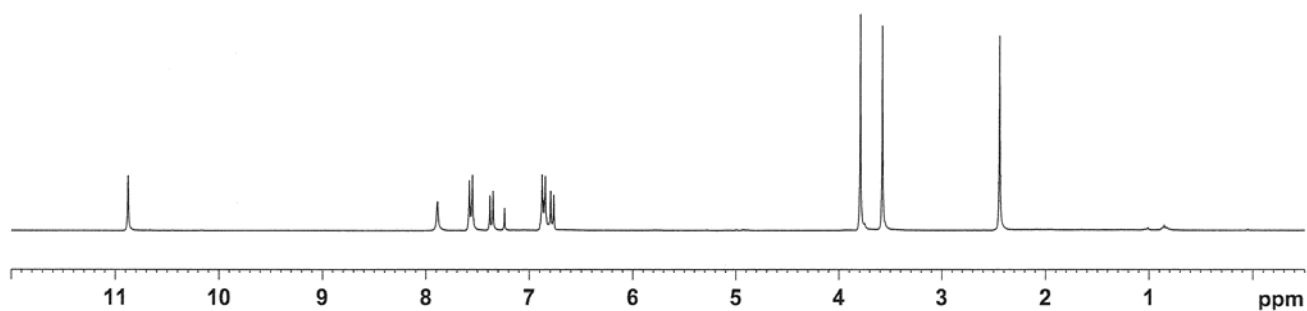
Data : x9-20-C19H17NO5 Date : 29-Nov-2013 15:17
 Sample : -
 Note : -
 Inlet : Direct Ion Mode : EI+
 RT : 0.53 min Scan# : (11,12)
 Elements : C 19/0, H 17/0, N 1/0, O 5/0
 Mass Tolerance : 1000ppm, 1mmu if m/z < 1, 3mmu if m/z > 3
 Unsaturation (U.S.) : -0.5 - 100.0

Observed m/z	Int%	Err [ppm / mmu]	U.S. Composition
339.1104	100.0	-0.9 / -0.3	12.0 C 19 H 17 N O 5
340.1144	21.4		

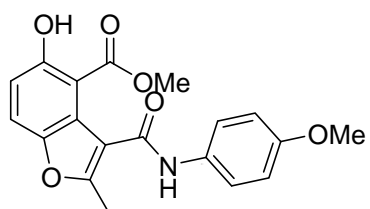
¹H NMR of Compound 30



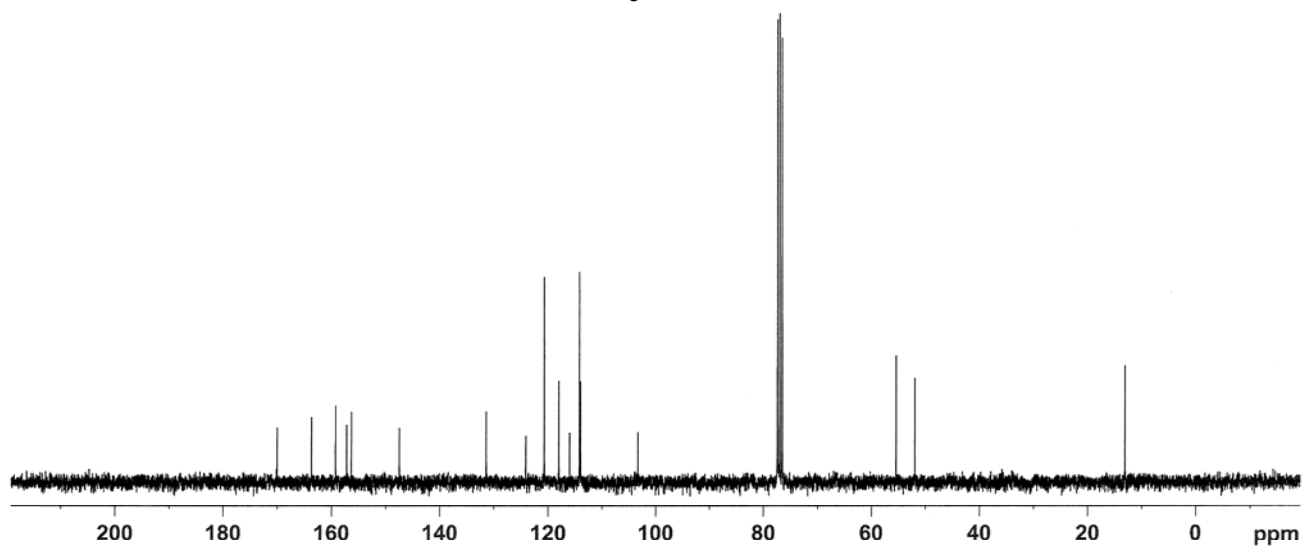
300 MHz, CDCl₃



¹³C NMR of Compound 30

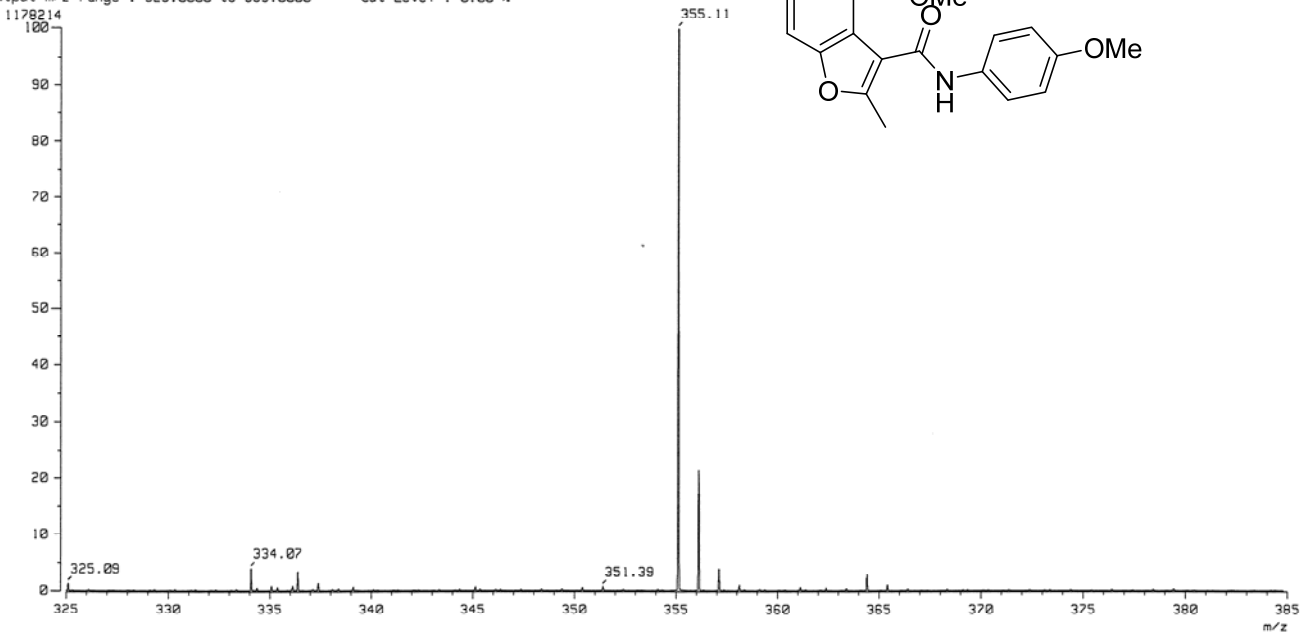
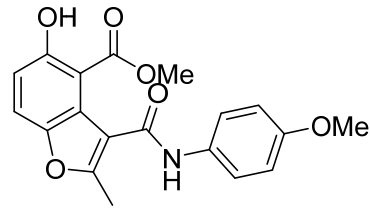


75 MHz, CDCl₃



[Mass Spectrum]
 Data : x9-21-C19H17NO6 Date : 29-Nov-2013 15:20
 Sample : -
 Note : -
 Inlet : Direct Ion Mode : EI+
 Spectrum Type : Normal Ion [EF-Linear]
 RT : 0.73 min Scan# : (15,16)
 BP : m/z 355.1056 Int. : 56.18
 Output m/z range : 325.0000 to 385.0000 Cut Level : 0.00 %

Mass Spectrum of Compound 30

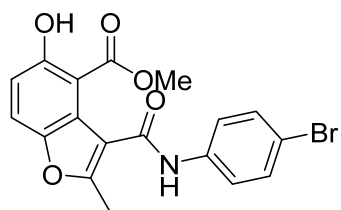


[Elemental Composition]

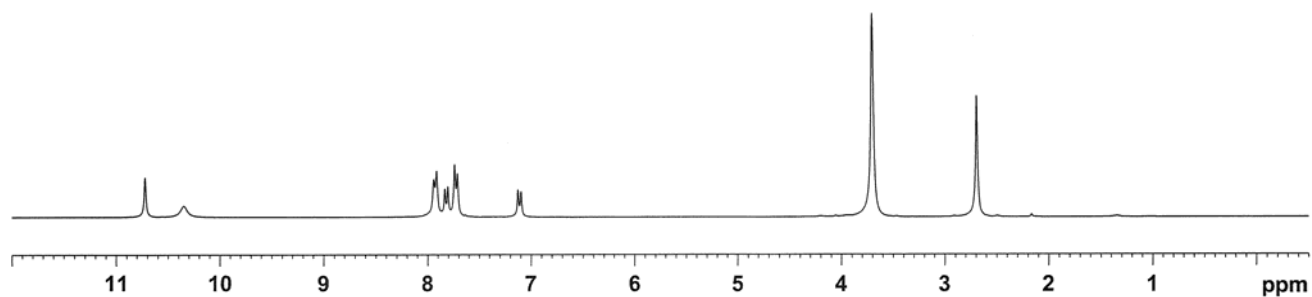
Data : x9-21-C19H17NO6 Date : 29-Nov-2013 15:20
 Sample : -
 Note : -
 Inlet : Direct Ion Mode : EI+
 RT : 0.73 min Scan# : (15,16)
 Elements : C 19/0, H 17/0, N 1/0, O 6/0
 Mass Tolerance : 1000ppm, 1mmu if m/z < 1, 3mmu if m/z > 3
 Unsaturation (U.S.) : -0.5 - 100.0

Observed m/z	Int%	Err [ppm / mmu]	U.S. Composition
355.1056	100.0	+0.1 / +0.0	12.0 C 19 H 17 N O 6
356.1096	21.5		

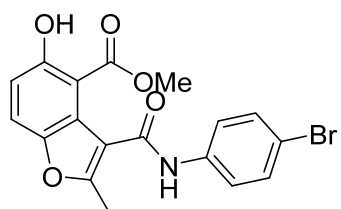
¹H NMR of Compound 31



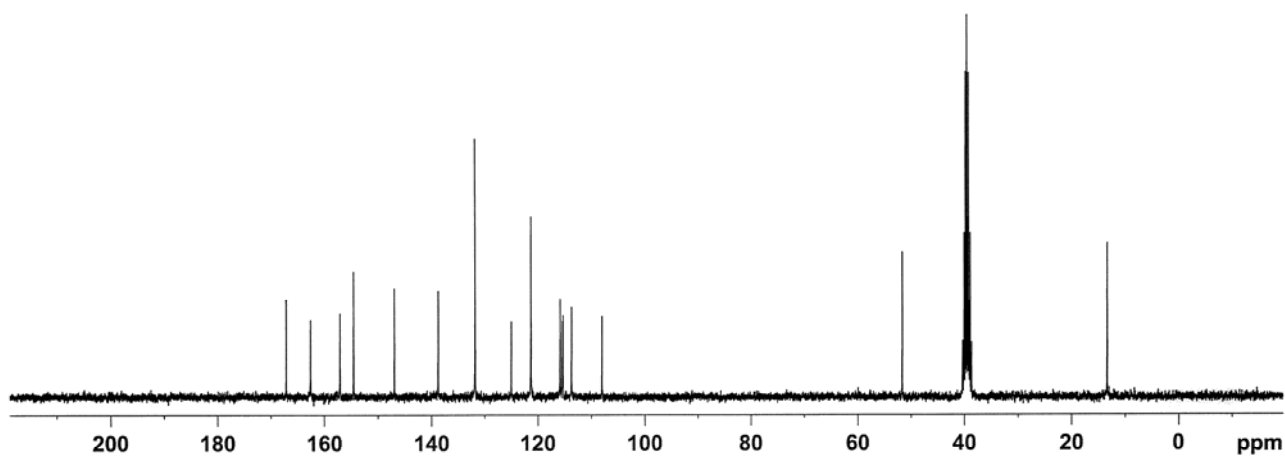
300 MHz, DMSO-d₆



¹³C NMR of Compound 31

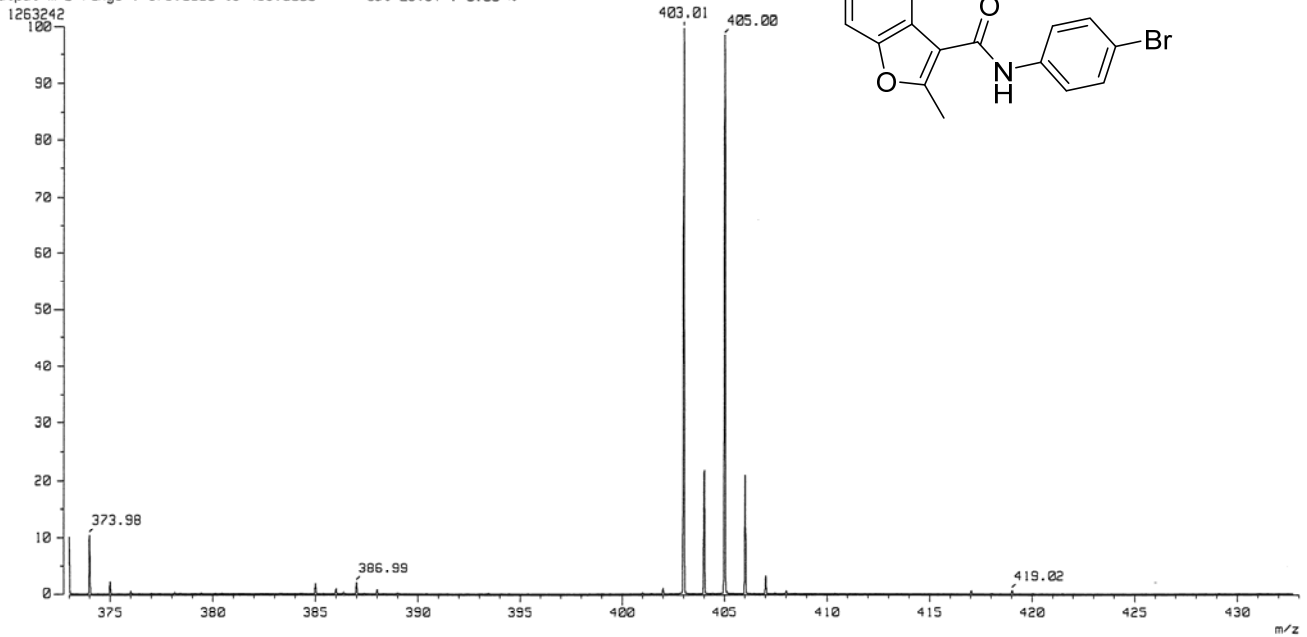
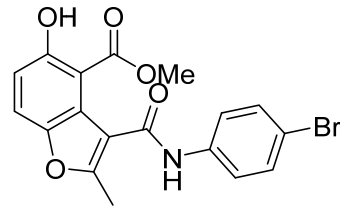


75 MHz, DMSO-d₆



[Mass Spectrum]
 Data : x9-42-C18H14BrNO5 Date : 29-Nov-2013 16:33
 Sample : -
 Note : -
 Inlet : Direct Ion Mode : EI+
 Spectrum Type : Normal Ion [EF-Linear]
 RT : 0.58 min Scan# : (12,13)
 BP : m/z 403.0056 Int. : 60.24
 Output m/z range : 373.0000 to 433.0000 Cut Level : 0.00 %

Mass Spectrum of Compound 31



[Elemental Composition]

Data : x9-42-C18H14BrNO5

Date : 29-Nov-2013 16:33

Page: 1

Sample: -

Note : -

Inlet : Direct

Ion Mode : EI+

RT : 0.58 min

Scan#: (12,13)

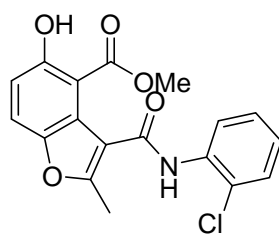
Elements : C 18/0, H 14/0, Br 1/0, N 1/0, O 5/0

Mass Tolerance : 1000ppm, 1mmu if m/z < 1, 3mmu if m/z > 3

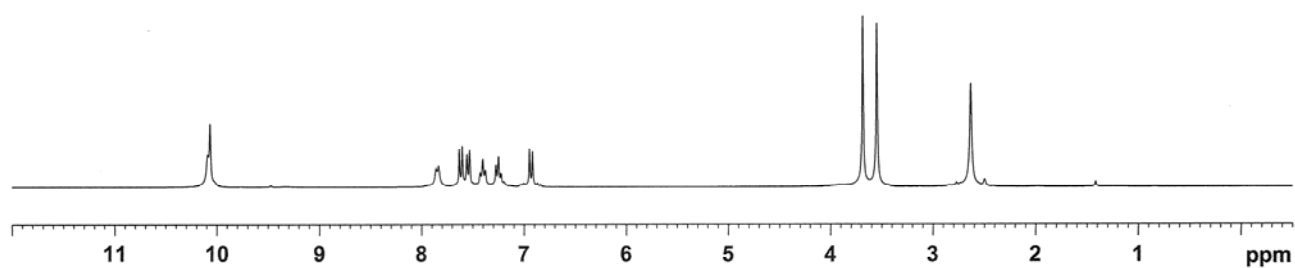
Unsaturation (U.S.) : -0.5 - 100.0

Observed m/z	Int%	Err [ppm / mmu]	U.S. Composition
373.9843	10.5		
403.0056	100.0	+0.1 / +0.1	12.0 C 18 H 14 Br N O 5
404.0078	22.0		
405.0044	98.7		
406.0074	21.1		

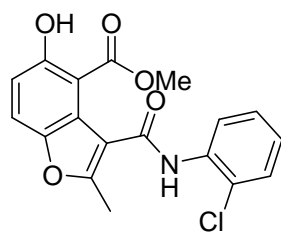
¹H NMR of Compound **32**



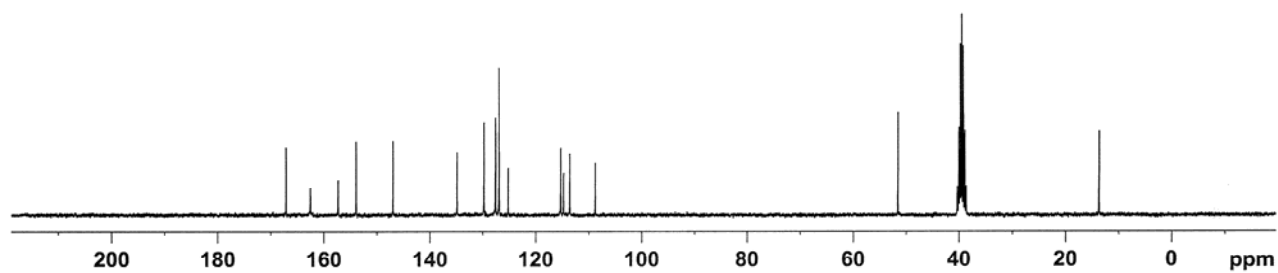
300 MHz, DMSO-d₆



¹³C NMR of Compound **32**

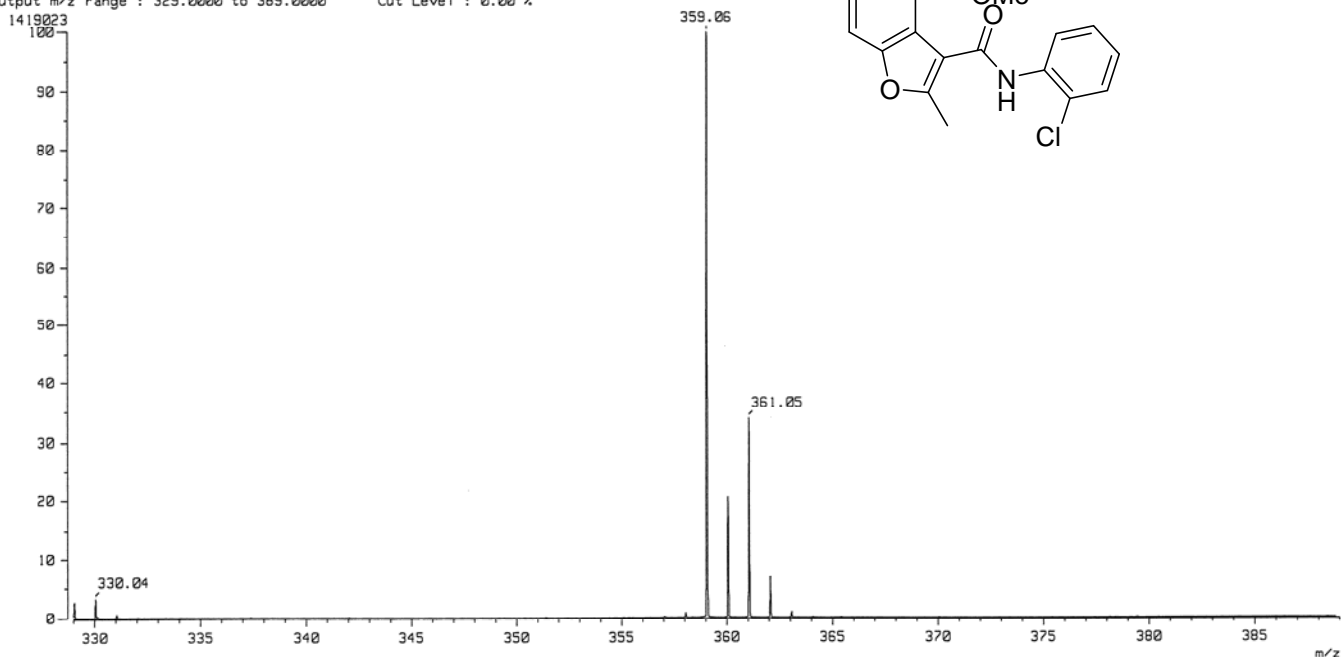
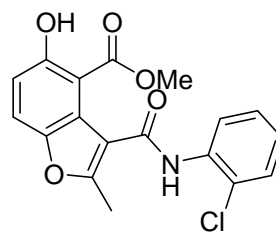


75 MHz, DMSO-d₆



[Mass Spectrum]
 Date : x9-41-C18H14ClNO5 Date : 29-Nov-2013 16:30
 Sample : -
 Note : -
 Inlet : Direct Ion Mode : EI+
 Spectrum type : Normal Ion [EF-Linear]
 RT : 0.53 min Scan# : (11,12)
 BP : m/z 359.0559 Int. : 67.66
 Output m/z range : 329.0000 to 389.0000 Cut Level : 0.00 %

Mass Spectrum of Compound 32

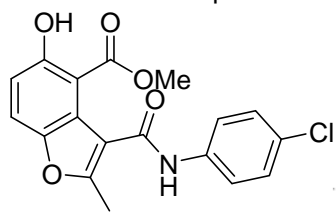


[Elemental Composition]

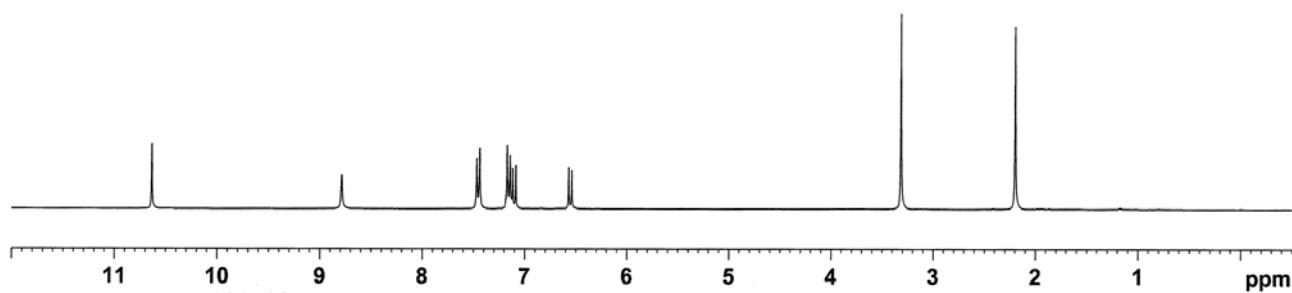
Data : x9-41-C18H14ClNO5 Date : 29-Nov-2013 16:30
 Sample : -
 Note : -
 Inlet : Direct Ion Mode : EI+
 RT : 0.53 min Scan# : (11,12)
 Elements : C 18/0, H 14/0, Cl 1/0, N 1/0, O 5/0
 Mass Tolerance : 1000ppm, 1mmu if m/z < 1, 3mmu if m/z > 3
 Unsaturation (U.S.) : -0.5 - 100.0

Observed m/z	Int%	Err [ppm / mmu]	U.S. Composition
359.0559	100.0	-0.3 / -0.1	12.0 C 18 H 14 Cl N O 5
360.0593	20.6		
361.0546	34.0		

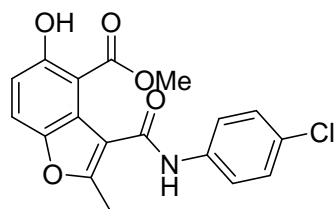
¹H NMR of Compound 33



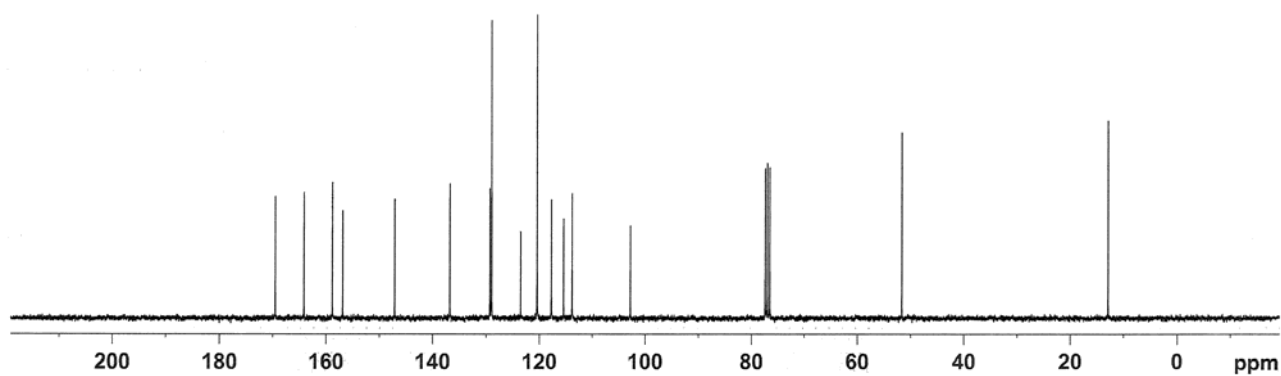
300 MHz, CDCl₃



¹³C NMR of Compound 33

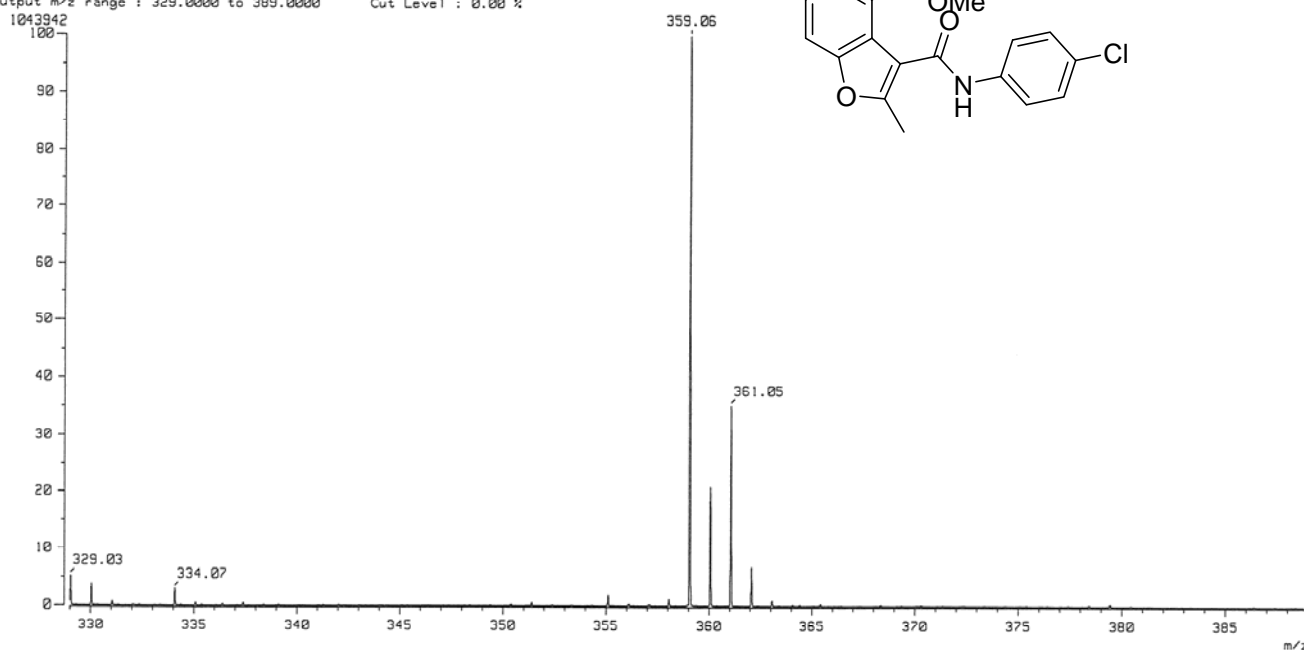
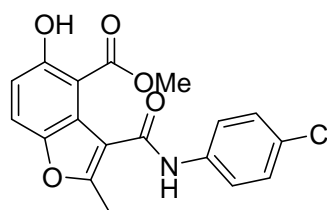


75 MHz, CDCl₃



[Mass Spectrum]
 Data : x9-22-C18H14ClNO5 Date : 29-Nov-2013 15:24
 Sample : -
 Note : -
 Inlet : Direct Ion Mode : EI+
 Spectrum Type : Normal Ion [EF-Linear]
 RT : 0.58 min Scan# : (12,13)
 BP : m/z 359.0562 Int. : 49.78
 Output m/z range : 329.0000 to 389.0000 Cut Level : 0.00 %

Mass Spectrum of Compound 33



[Elemental Composition]

Data : x9-22-C18H14ClNO5

Date : 29-Nov-2013 15:24

Page: 1

Sample: -

Note : -

Inlet : Direct

Ion Mode : EI+

RT : 0.58 min

Scan#: (12,13)

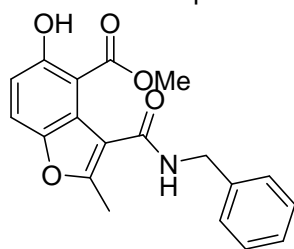
Elements : C 18/0, H 14/0, Cl 1/0, N 1/0, O 5/0

Mass Tolerance : 1000ppm, 1mmu if m/z < 1, 3mmu if m/z > 3

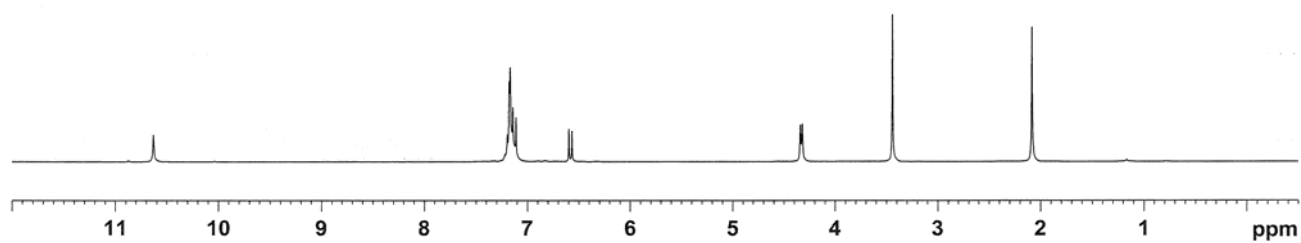
Unsaturation (U.S.) : -0.5 - 100.0

Observed m/z	Int%	Err [ppm / mmu]	U.S.	Composition
359.0562	100.0	+0.5 / +0.2	12.0	C 18 H 14 Cl N O 5
360.0583	21.1			
361.0533	35.2			

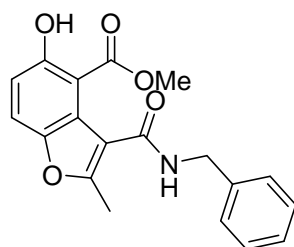
¹H NMR of Compound 34



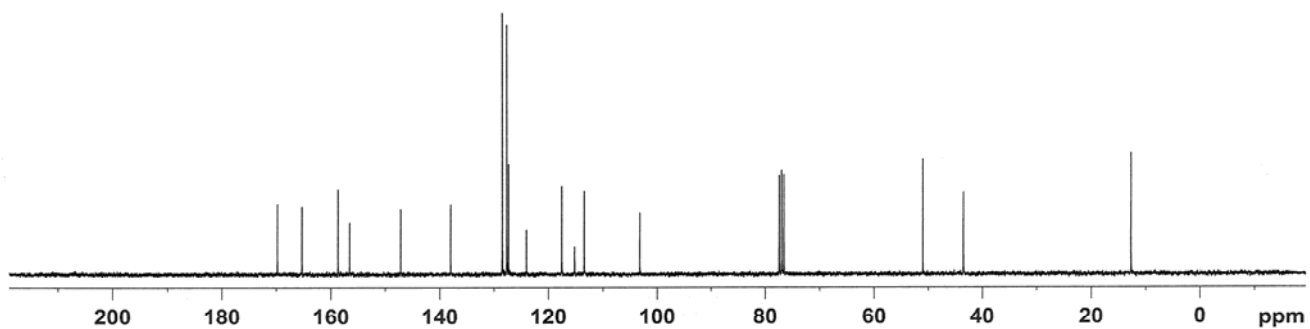
300 MHz, CDCl₃



¹³C NMR of Compound 34

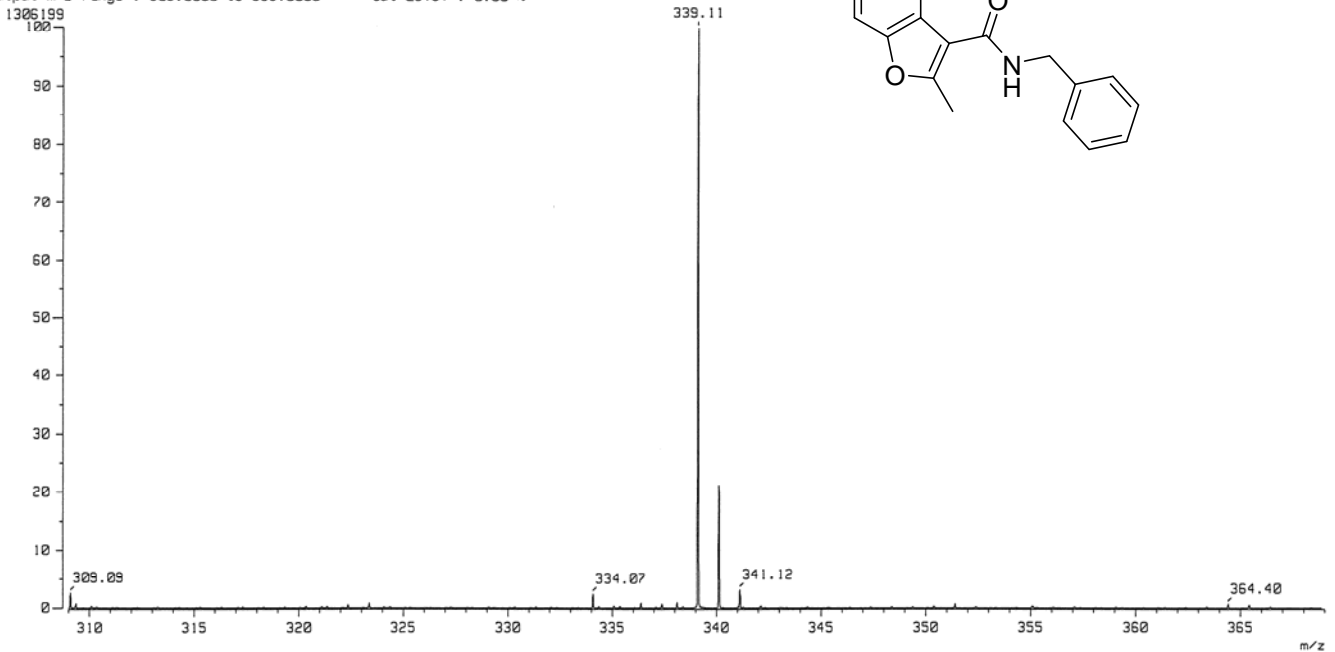
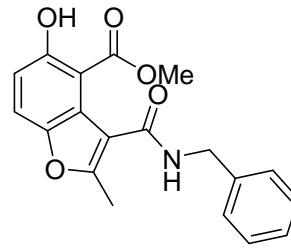


75 MHz, CDCl₃



[Mass Spectrum]
 Date : 29-Nov-2013 15:28
 Data : x9-23-C19H17NO5
 Sample : -
 Note : -
 Inlet : Direct Ion Mode : EI+
 Spectrum Type : Normal Ion [EF-Linear]
 RT : 0.63 min Scan# : (13,14)
 BP : m/z 339.1108 Int. : 62.28
 Output m/z range : 309.0000 to 369.0000 Cut Level : 0.00 %

Mass Spectrum of Compound 34

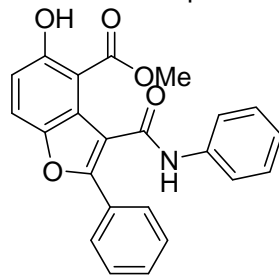


[Elemental Composition]

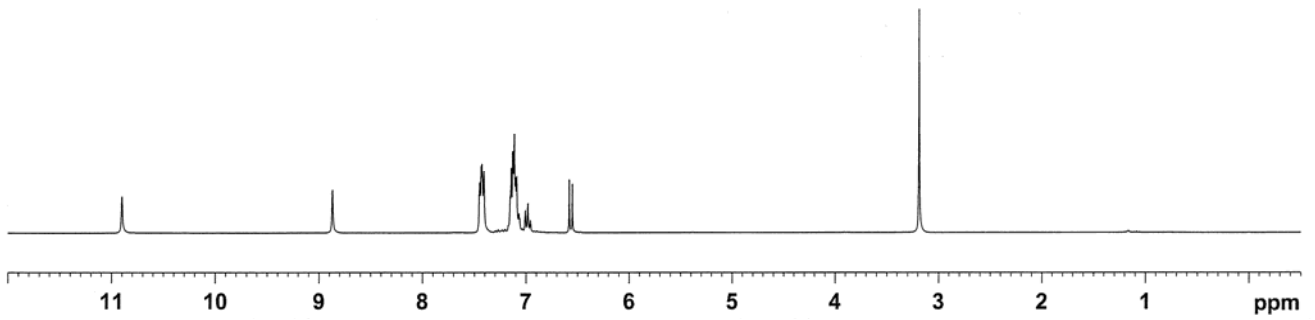
Date : 29-Nov-2013 15:28
 Data : x9-23-C19H17NO5
 Sample : -
 Note : -
 Inlet : Direct Ion Mode : EI+
 RT : 0.63 min Scan# : (13,14)
 Elements : C 19/0, H 17/0, N 1/0, O 5/0
 Mass Tolerance : 1000ppm, 1mmu if m/z < 1, 3mmu if m/z > 3
 Unsaturation (U.S.) : -0.5 - 100.0

Observed m/z	Int%	Err [ppm / mmu]	U.S. Composition
339.1108	100.0	+0.4 / +0.1	12.0 C 19 H 17 N O 5
340.1134	21.2		

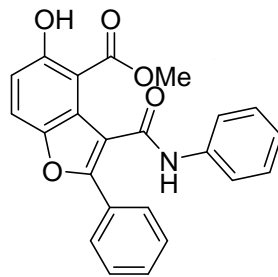
¹H NMR of Compound 35



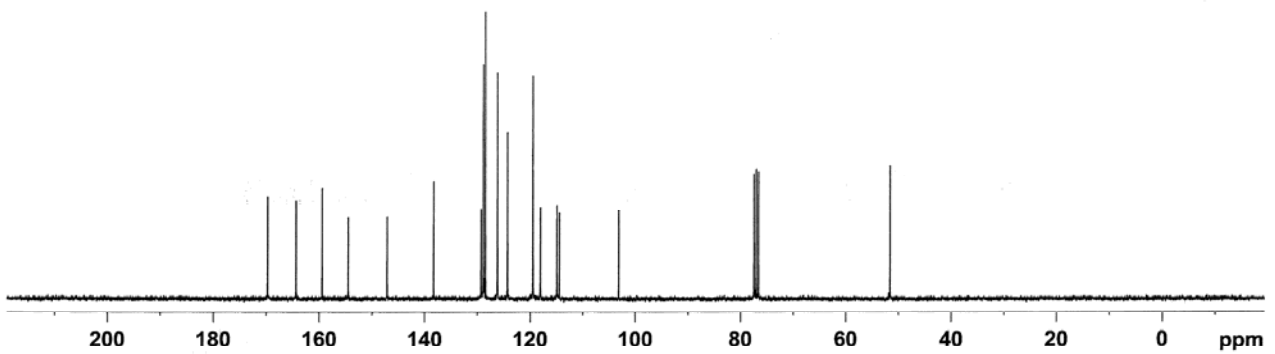
300 MHz, CDCl₃



¹³C NMR of Compound 35

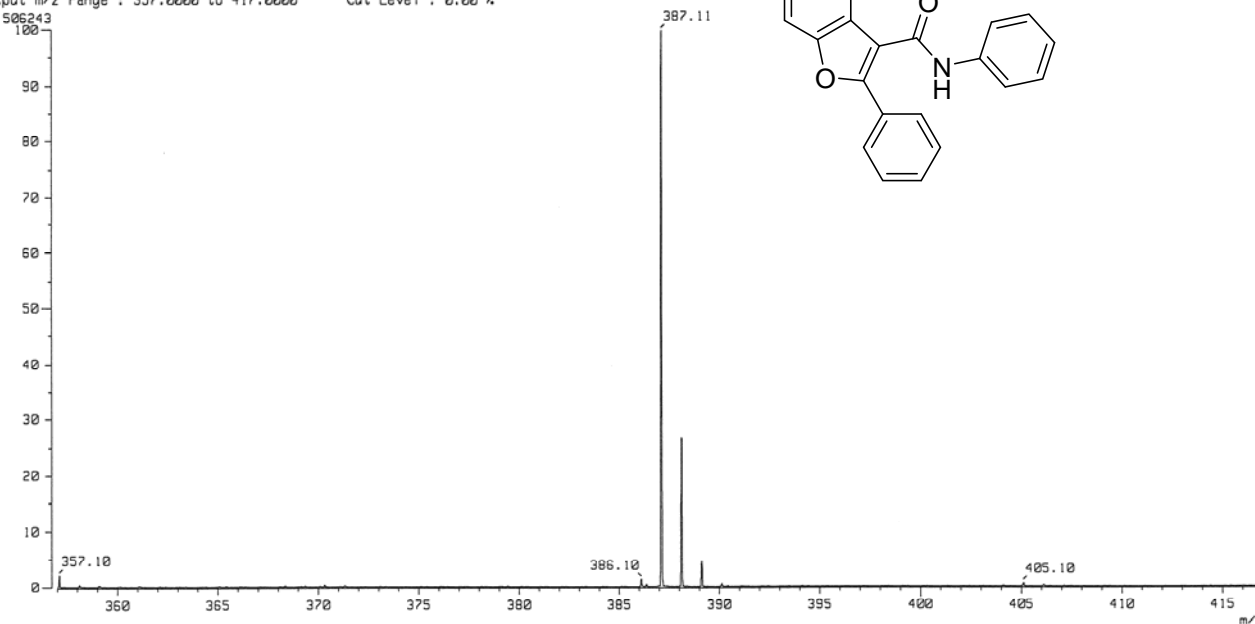
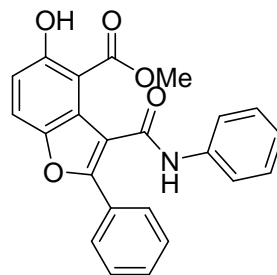


75 MHz, CDCl₃



[Mass Spectrum]
 Data : x9-24-C23H17NO5 Date : 29-Nov-2013 15:31
 Sample : -
 Note : -
 Inlet : Direct Ion Mode : EI+
 Spectrum Type : Normal Ion [EF-Linear]
 RT : 0.98 min Scan# : (20,21)
 BP : m/z 387.1107 Int. : 24.14
 Output m/z range : 357.0000 to 417.0000 Cut Level : 0.00 %

Mass Spectrum of Compound 35



[Elemental Composition]

Data : x9-24-C23H17NO5

Date : 29-Nov-2013 15:31

Page: 1

Sample: -

Note : -

Inlet : Direct

Ion Mode : EI+

RT : 0.98 min

Scan#: (20,21)

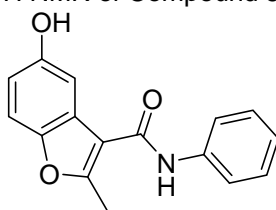
Elements : C 23/0, H 17/0, N 1/0, O 5/0

Mass Tolerance : 1000ppm, 1mmu if m/z < 1, 3mmu if m/z > 3

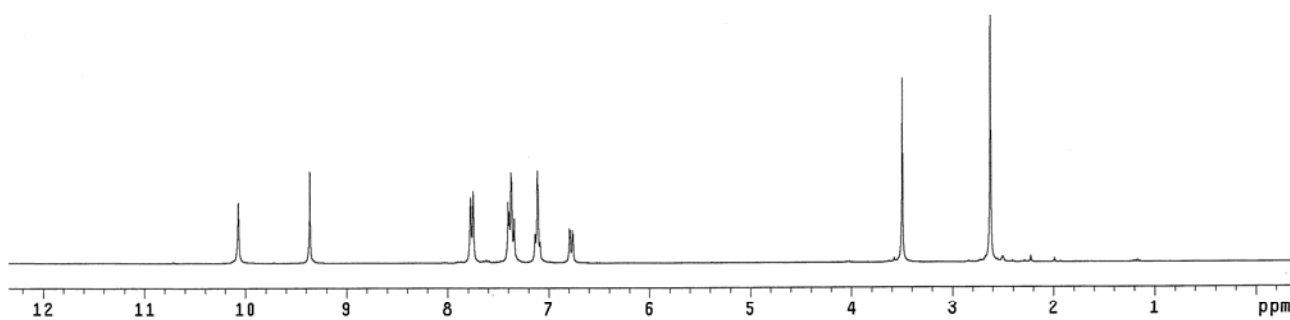
Unsaturation (U.S.) : -0.5 - 100.0

Observed m/z	Int%	Err [ppm / mmu]	U.S. Composition
387.1107	100.0	+0.2 / +0.1	16.0 C 23 H 17 N O 5
388.1141	26.8		

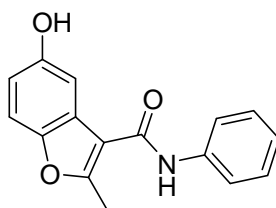
¹H NMR of Compound 36



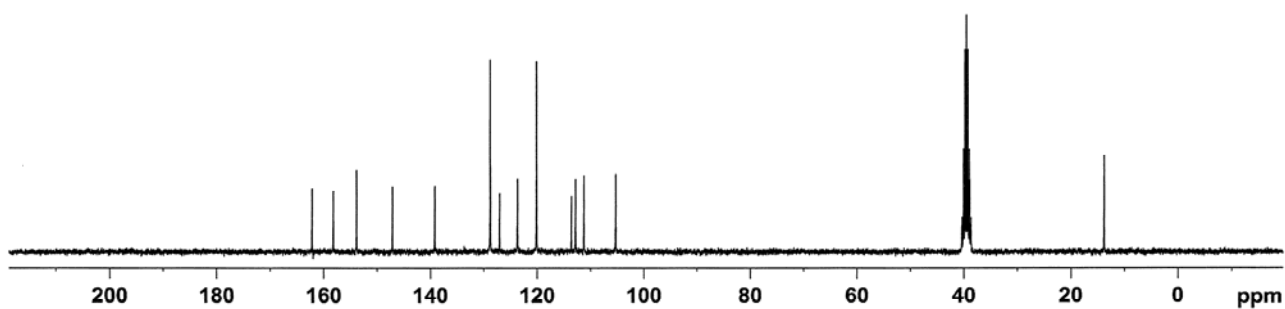
300 MHz, DMSO-d₆



¹³C NMR of Compound 36

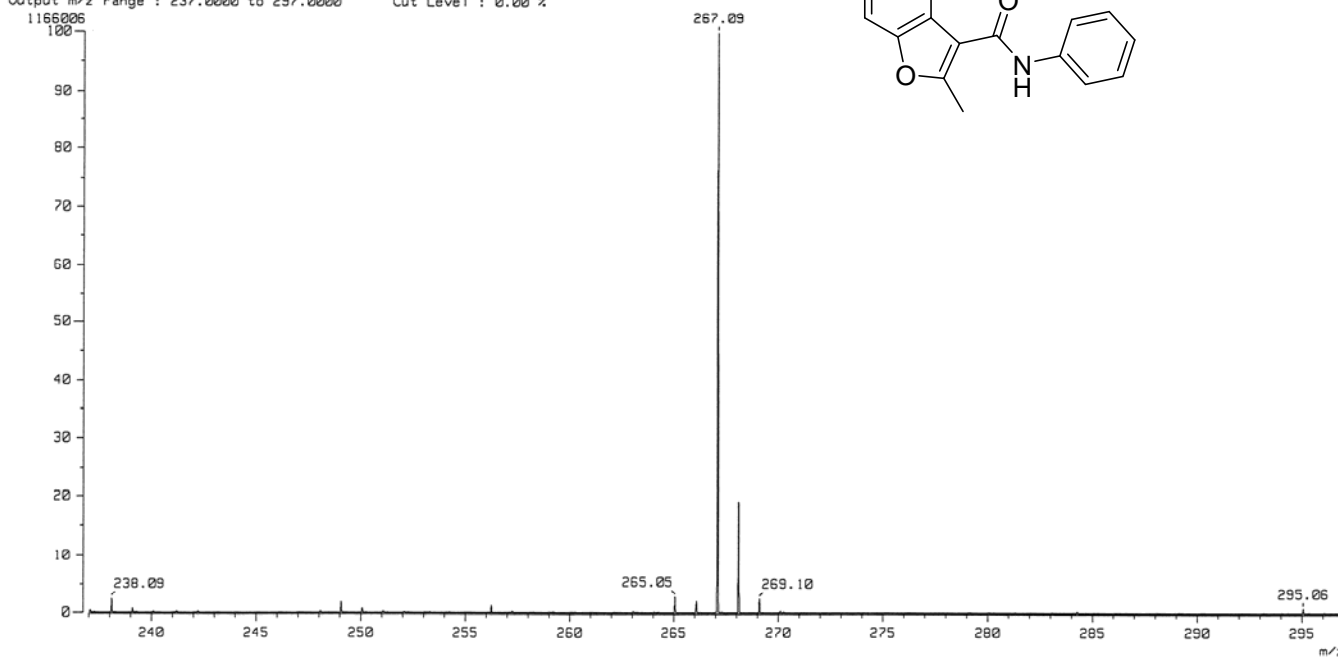
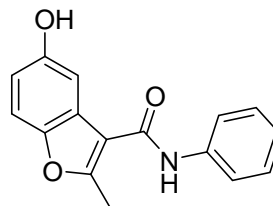


75 MHz, DMSO-d₆



[Mass Spectrum]
 Date : 29-Nov-2013 15:35
 Sample : -
 Note : -
 Inlet : Direct Ion Mode : EI+
 Spectrum Type : Normal Ion [EF-Linear]
 RT : 0.78 min Scan# : (16,17)
 BP : m/z 267.0898 Int. : 55.60
 Output m/z range : 237.0000 to 297.0000 Cut Level : 0.00 %

Mass Spectrum of Compound 36

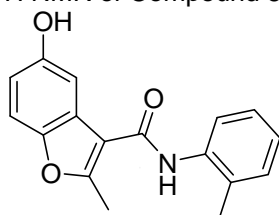


[Elemental Composition]

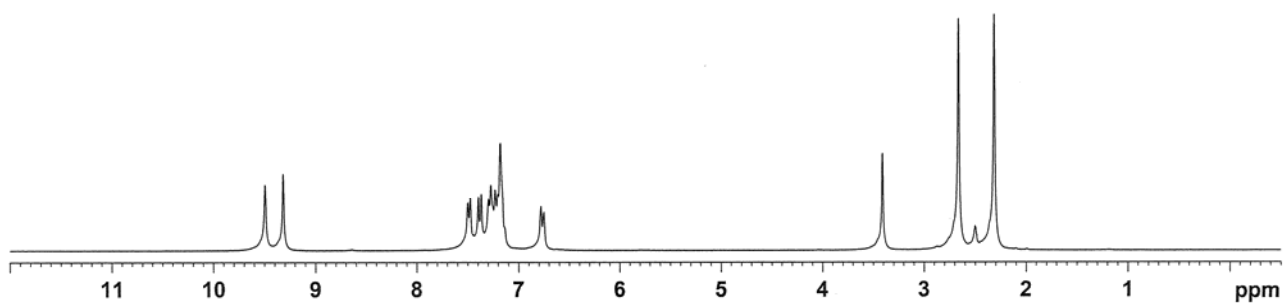
Data : x9-25-C16H13NO3 Date : 29-Nov-2013 15:35
 Sample : -
 Note : -
 Inlet : Direct Ion Mode : EI+
 RT : 0.78 min Scan# : (16,17)
 Elements : C 16/0, H 13/0, N 1/0, O 3/0
 Mass Tolerance : 1000ppm, 1mmu if m/z < 1, 3mmu if m/z > 3
 Unsaturation (U.S.) : -0.5 - 100.0

Observed m/z	Int%	Err [ppm / mmu]	U.S.	Composition
267.0898	100.0	+1.0 / +0.3	11.0	C 16 H 13 N O 3
268.0929	19.2			

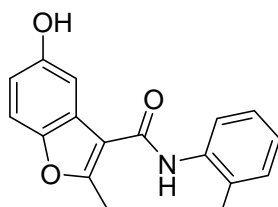
¹H NMR of Compound 37



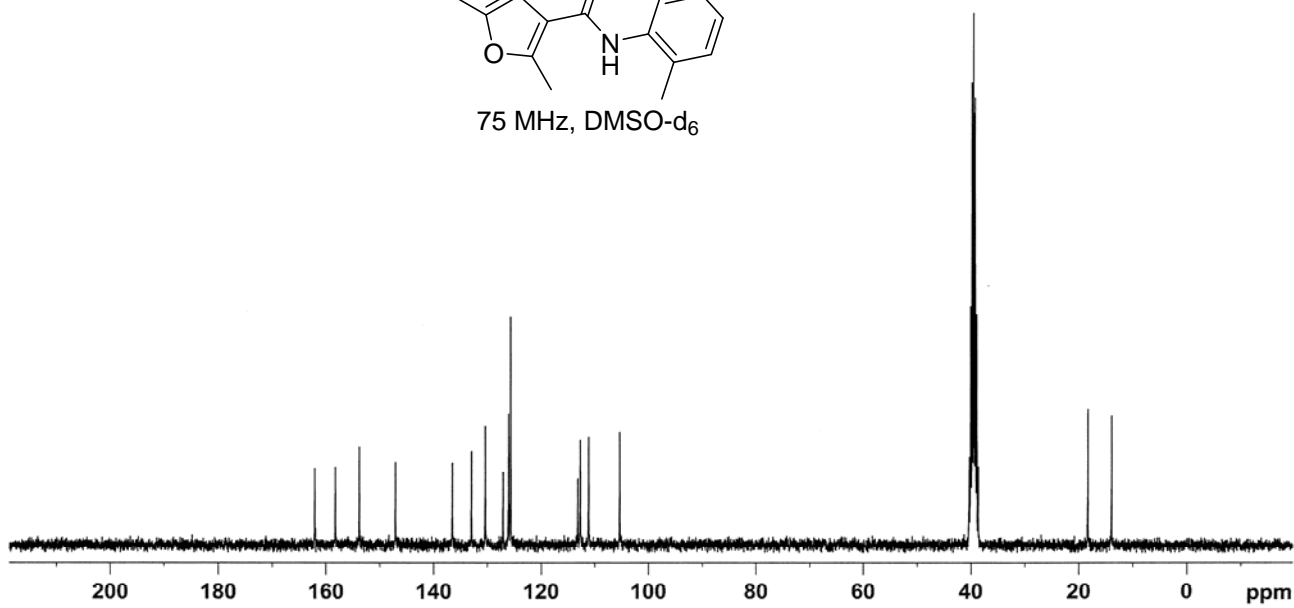
300 MHz, DMSO-d₆



¹³C NMR of Compound 37

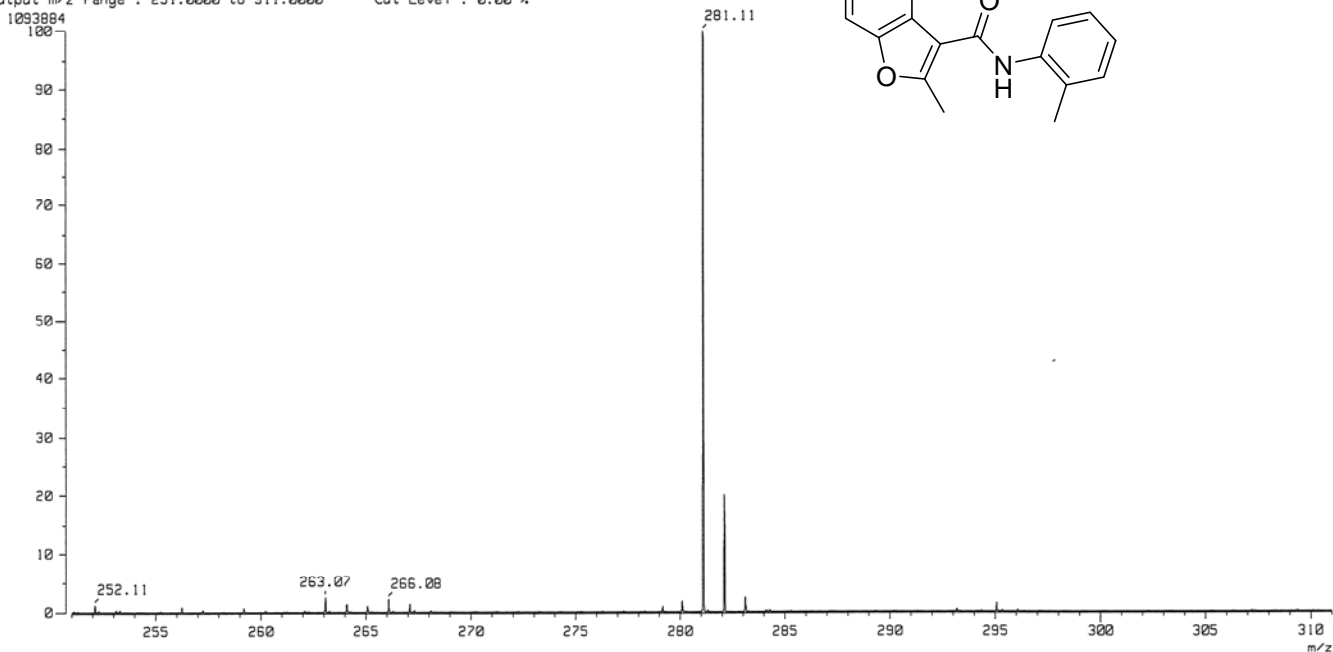
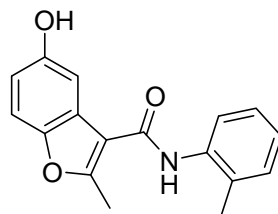


75 MHz, DMSO-d₆



[Mass Spectrum]
 Date : 29-Nov-2013 15:39
 Sample : -
 Note : -
 Inlet : Direct Ion Mode : EI+
 Spectrum Type : Normal Ion [EF-Linear]
 RT : 0.63 min Scan# : (13,14)
 BP : m/z 281.1053 Int. : 52.16
 Output m/z range : 251.0000 to 311.0000 Cut Level : 0.00 %

Mass Spectrum of Compound 37

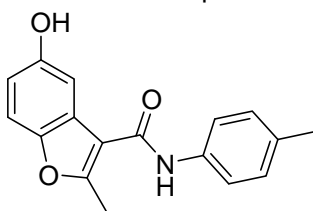


[Elemental Composition]

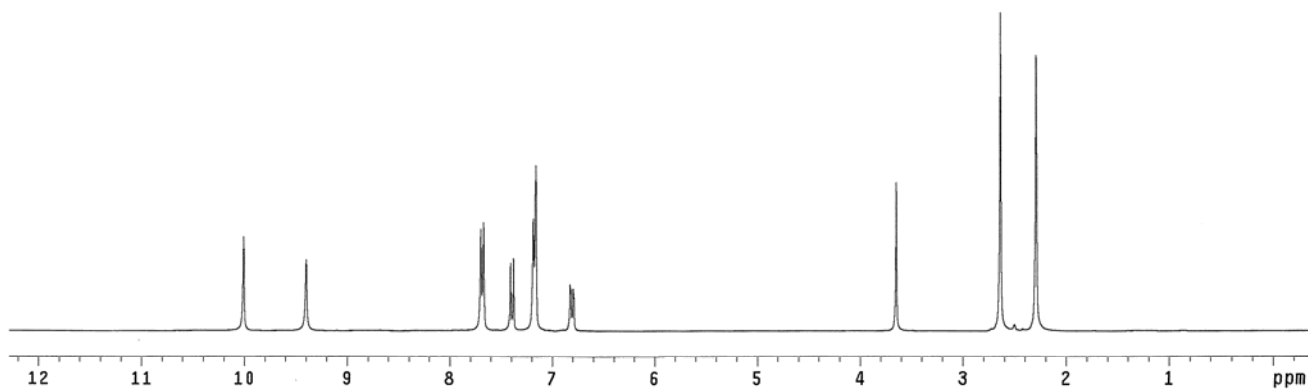
Data : x9-26-C17H15NO3 Date : 29-Nov-2013 15:39
 Sample : -
 Note : -
 Inlet : Direct Ion Mode : EI+
 RT : 0.63 min Scan# : (13,14)
 Elements : C 17/0, H 15/0, N 1/0, O 3/0
 Mass Tolerance : 1000ppm, 1mmu if m/z < 1, 3mmu if m/z > 3
 Unsaturation (U.S.) : -0.5 - 100.0

Observed m/z	Int%	Err [ppm / mmu]	U.S.	Composition
281.1053	100.0	+0.5 / +0.2	11.0	C 17 H 15 N O 3
282.1097	20.1			

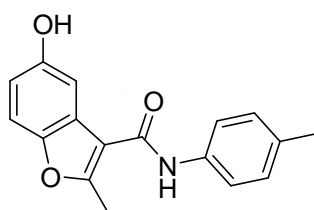
¹H NMR of Compound 38



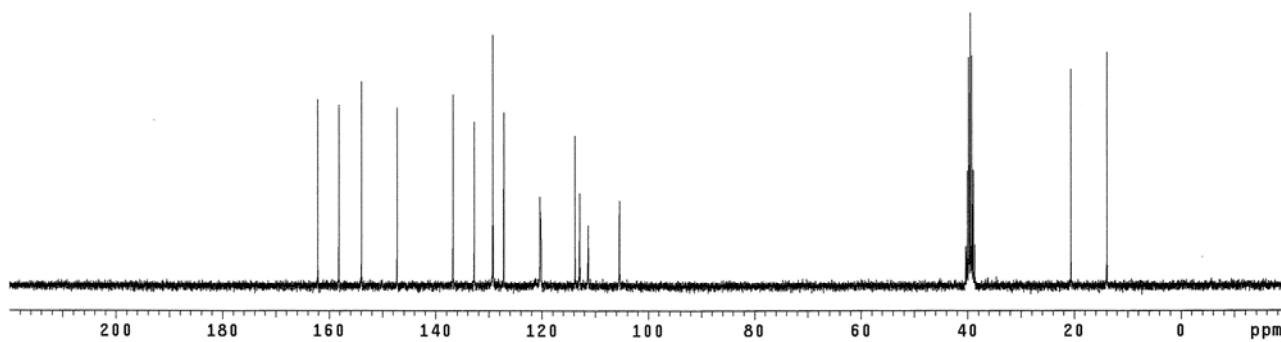
300 MHz, CDCl₃



¹³C NMR of Compound 38

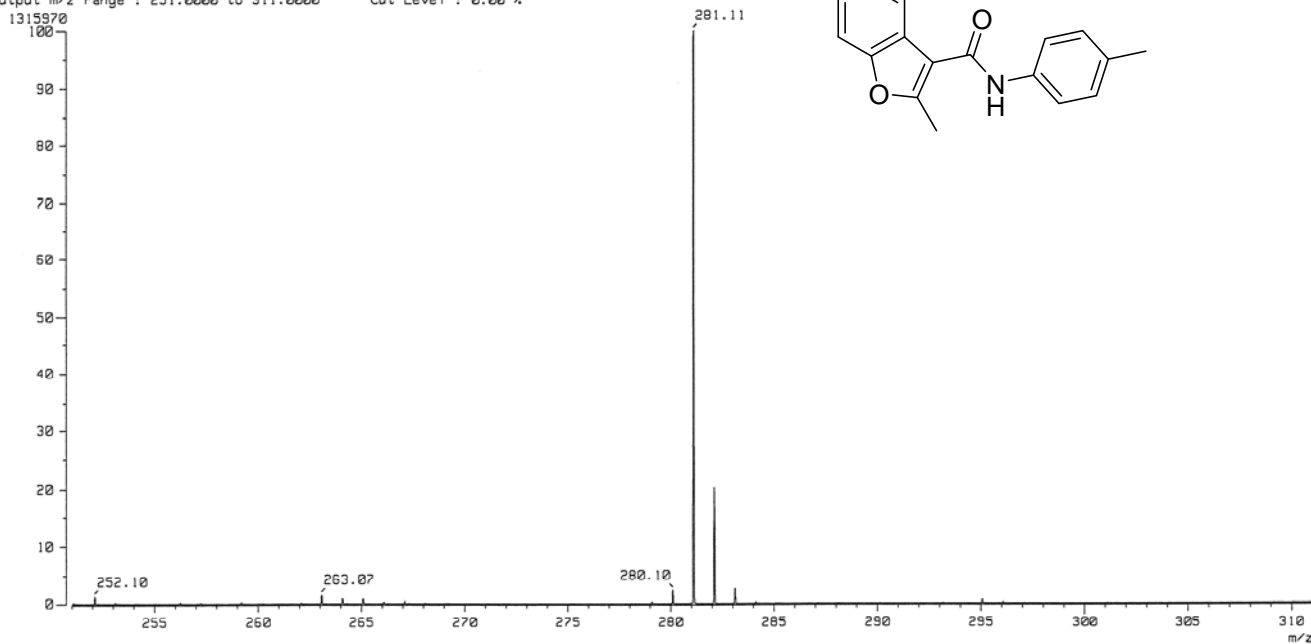
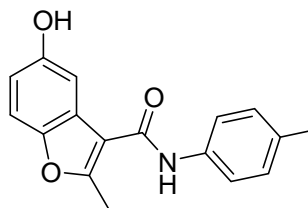


75 MHz, CDCl₃



[Mass Spectrum]
 Data : x9-27-C17H15NO3 Date : 29-Nov-2013 15:42
 Sample : -
 Note : -
 Inlet : Direct Ion Mode : EI+
 Spectrum Type : Normal Ion [EF-Linear]
 RT : 0.53 min Scan# : (11,12)
 BP : m/z 281.1055 Int. : 62.75
 Output m/z range : 251.0000 to 311.0000 Cut Level : 0.00 %

Mass Spectrum of Compound 38

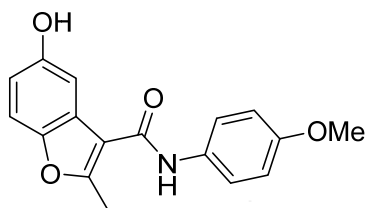


[Elemental Composition]

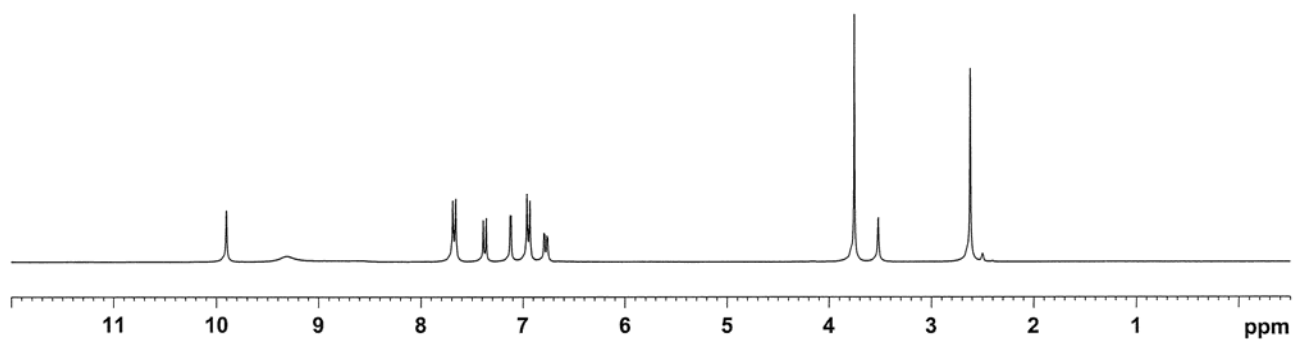
Data : x9-27-C17H15NO3 Date : 29-Nov-2013 15:42
 Sample : -
 Note : -
 Inlet : Direct Ion Mode : EI+
 RT : 0.53 min Scan# : (11,12)
 Elements : C 17/0, H 15/0, N 1/0, O 3/0
 Mass Tolerance : 1000ppm, 1mmu if m/z < 1, 3mmu if m/z > 3
 Unsaturation (U.S.) : -0.5 - 100.0

Observed m/z	Int%	Err [ppm / mmu]	U.S. Composition
281.1055	100.0	+1.1 / +0.3	11.0 C 17 H 15 N O 3
282.1086	20.2		

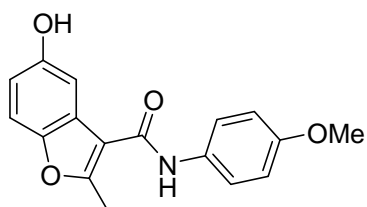
¹H NMR of Compound **39**



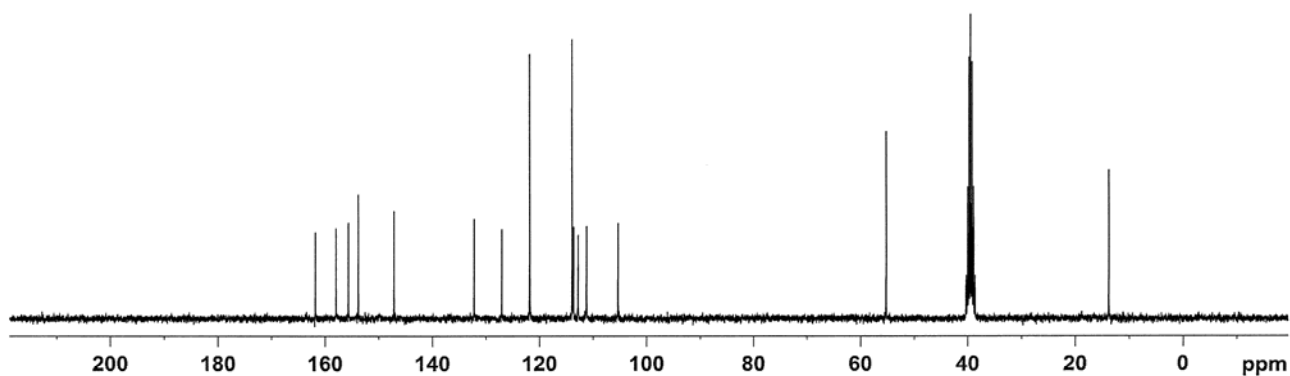
300 MHz, DMSO-d₆



¹³C NMR of Compound **39**

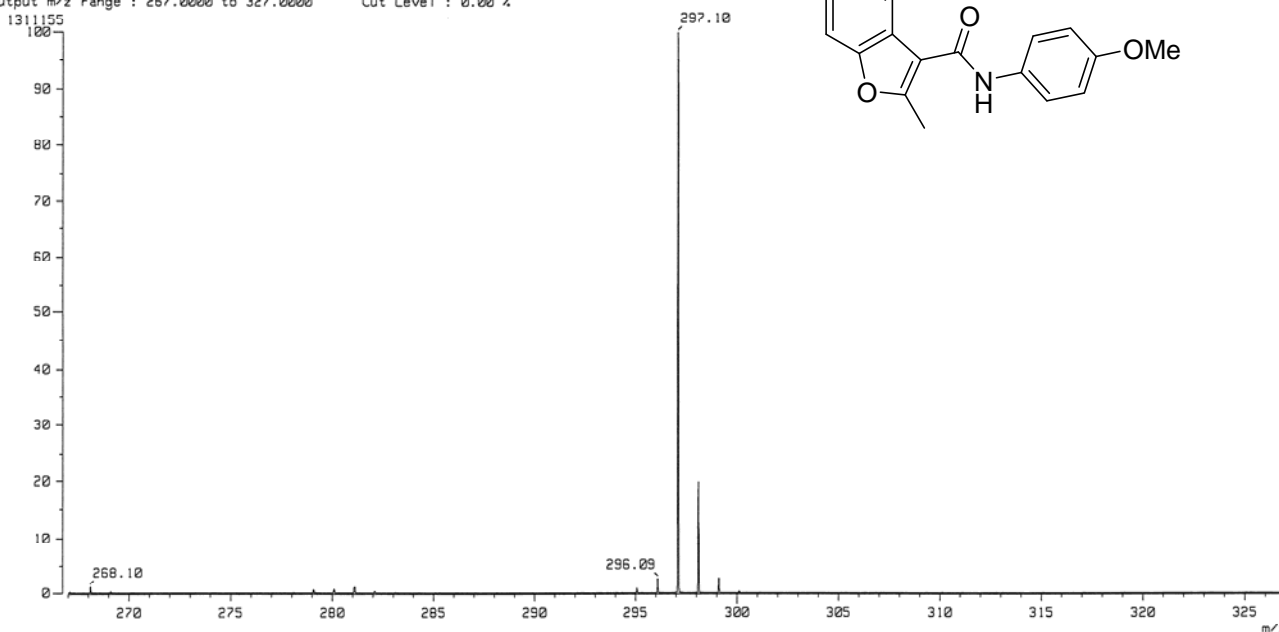
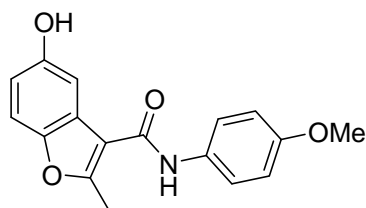


75 MHz, DMSO-d₆



[Mass Spectrum]
 Data : x9-28-C17H15NO4 Date : 29-Nov-2013 15:45
 Sample : -
 Note : -
 Inlet : Direct Ion Mode : EI+
 Spectrum Type : Normal Ion [EF-Linear]
 RT : 0.73 min Scan# : (15,16)
 BP : m/z 297.1003 Int. : 62.52
 Output m/z range : 267.0000 to 327.0000 Cut Level : 0.00 %

Mass Spectrum of Compound 39

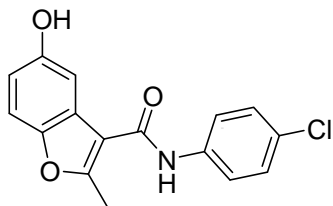


[Elemental Composition]

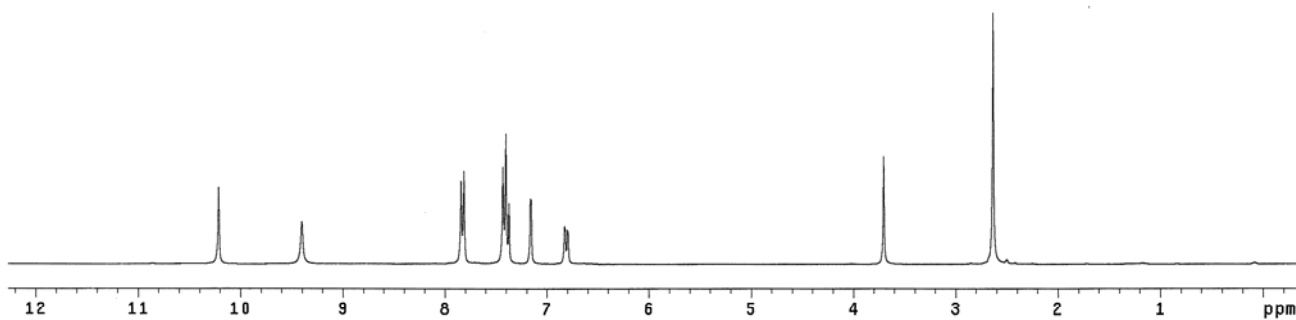
Data : x9-28-C17H15NO4 Date : 29-Nov-2013 15:45
 Sample : -
 Note : -
 Inlet : Direct Ion Mode : EI+
 RT : 0.73 min Scan# : (15,16)
 Elements : C 17/0, H 15/0, N 1/0, O 4/0
 Mass Tolerance : 1000ppm, 1mmu if m/z < 1, 3mmu if m/z > 3
 Unsaturation (U.S.) : -0.5 - 100.0

Observed m/z	Int%	Err [ppm / mmu]	U.S. Composition
297.1003	100.0	+0.5 / +0.1	11.0 C 17 H 15 N O 4
298.1026	19.8		

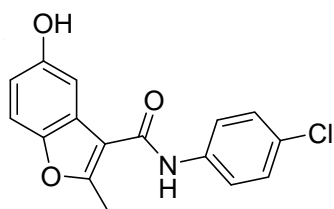
¹H NMR of Compound **40**



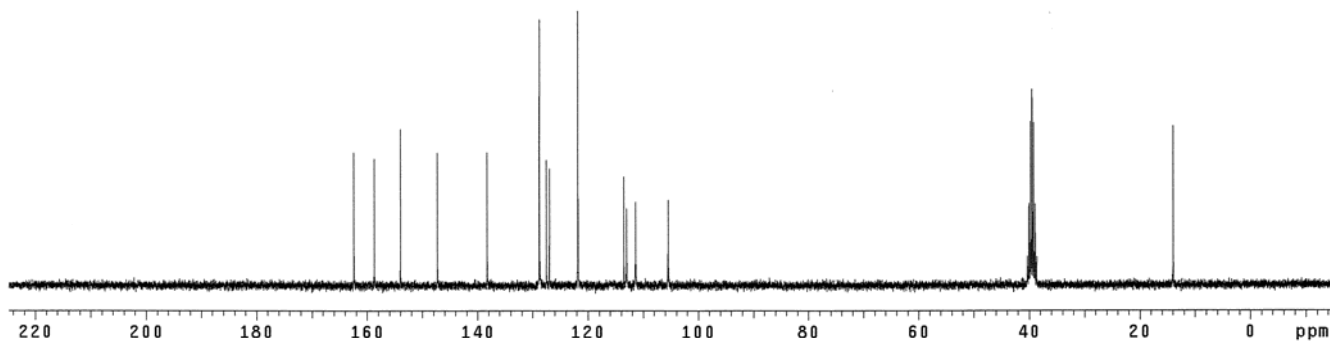
600 MHz, DMSO-d₆



¹³C NMR of Compound **40**

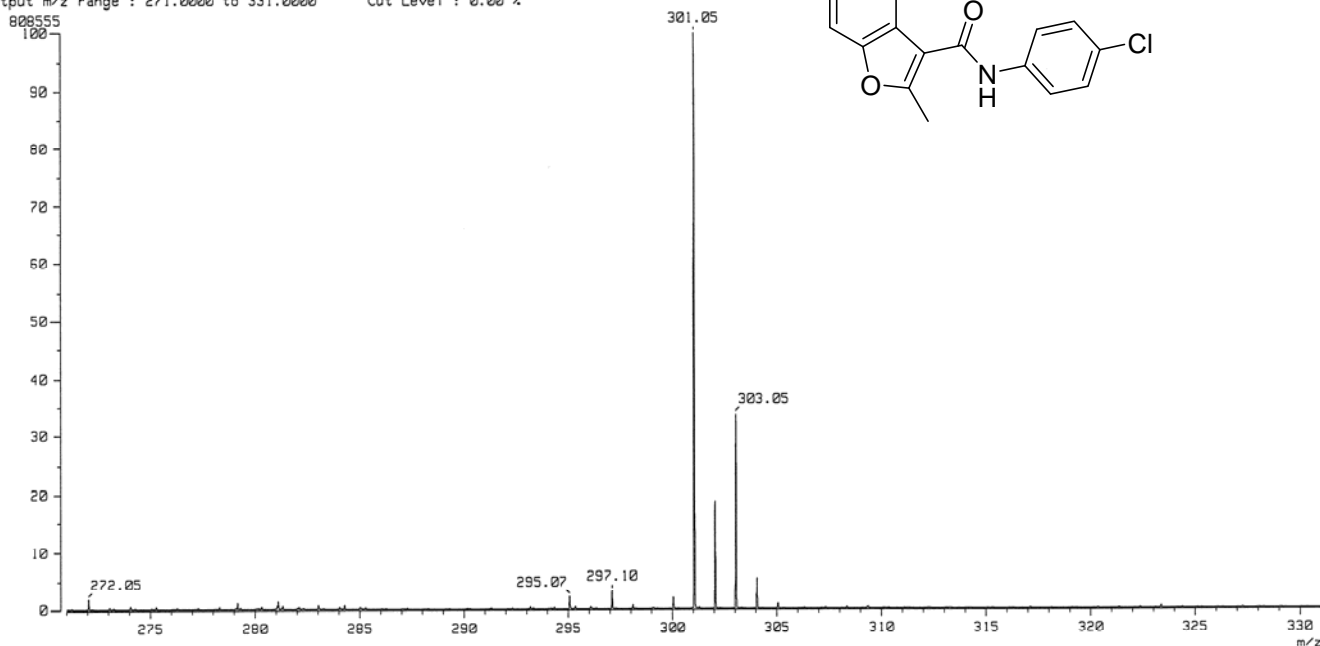
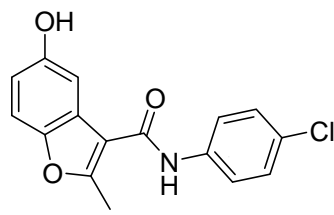


150 MHz, DMSO-d₆



[Mass Spectrum]
 Data : x9-29-C16H12ClNO3 Date : 29-Nov-2013 15:48
 Sample : -
 Note : -
 Inlet : Direct Ion Mode : EI+
 Spectrum Type : Normal Ion [EF-Linear]
 RT : 0.73 min Scan# : (15,16)
 BP : m/z 301.0508 Int. : 38.55
 Output m/z range : 271.0000 to 331.0000 Cut Level : 0.00 %

Mass Spectrum of Compound 40



[Elemental Composition]

Data : x9-29-C16H12ClNO3
 Sample : -
 Note : -

Date : 29-Nov-2013 15:48

Page: 1

Inlet : Direct
 RT : 0.73 min

Ion Mode : EI+
 Scan#: (15,16)

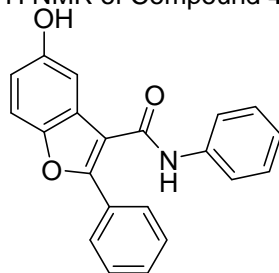
Elements : C 16/0, H 12/0, Cl 1/0, N 1/0, O 3/0

Mass Tolerance : 1000ppm, 1mmu if m/z < 1, 3mmu if m/z > 3

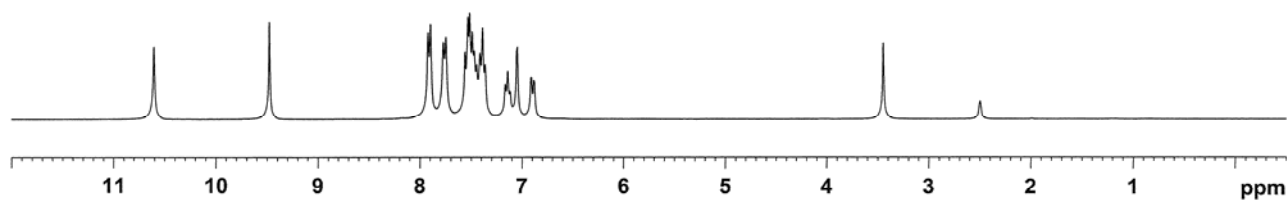
Unsaturation (U.S.) : -0.5 - 100.0

Observed m/z	Int%	Err [ppm / mmu]	U.S. Composition
301.0508	100.0	+0.7 / +0.2	11.0 C 16 H 12 Cl N O 3
302.0544	18.9		
303.0491	33.9		

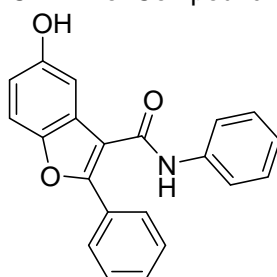
¹H NMR of Compound 41



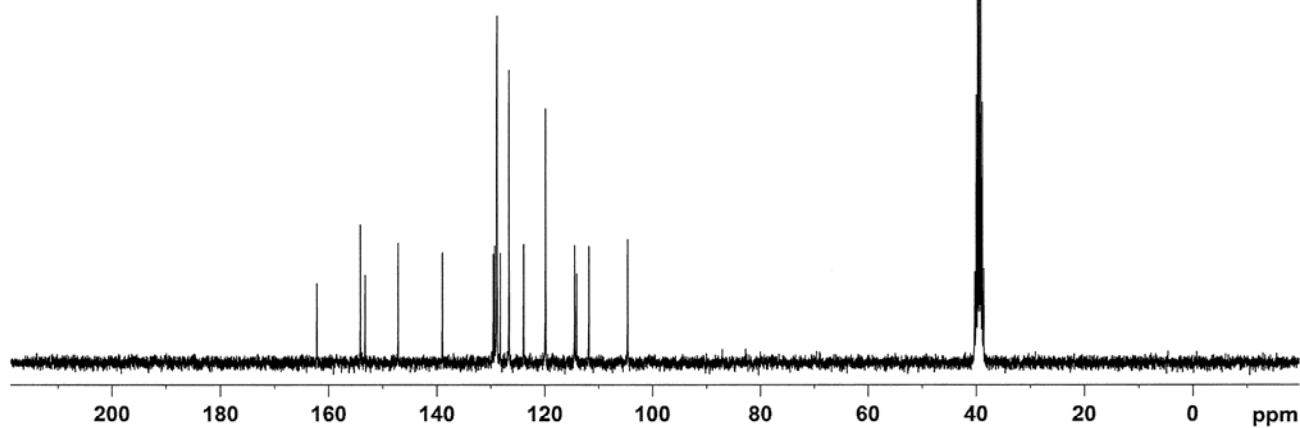
300 MHz, DMSO-d₆



¹³C NMR of Compound 41

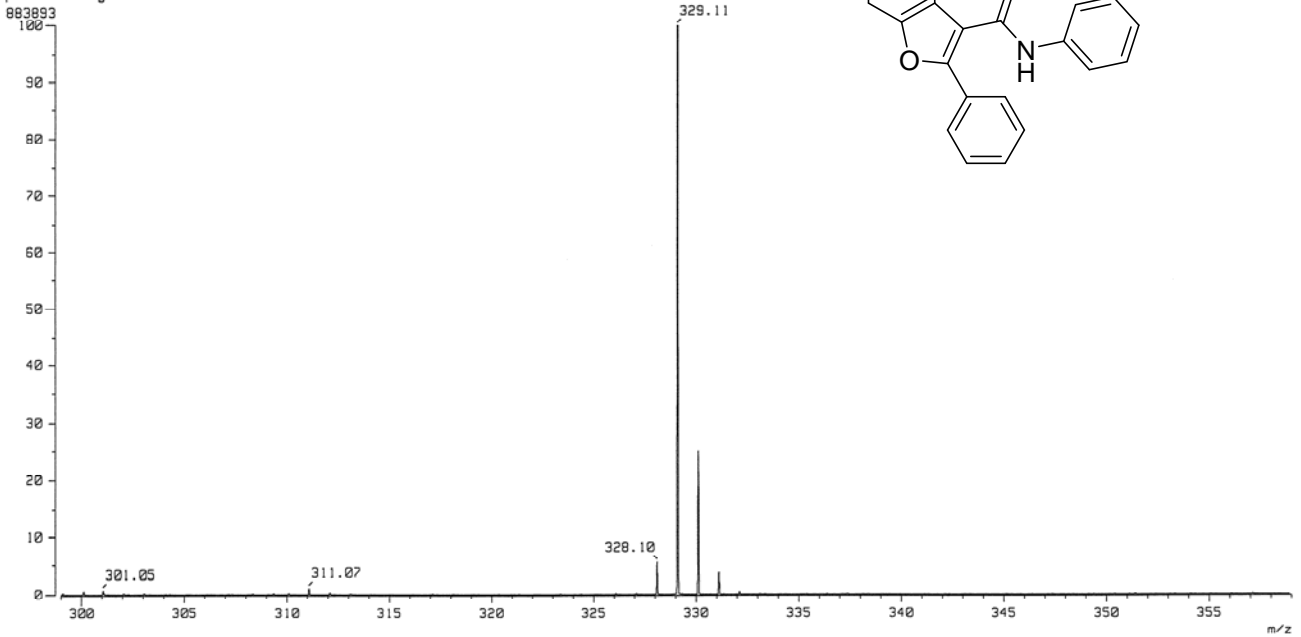
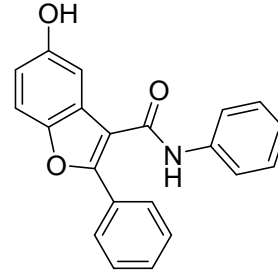


75 MHz, DMSO-d₆



[Mass Spectrum]
 Data : x9-30-C21H15NO3 Date : 29-Nov-2013 15:52
 Sample: -
 Note: -
 Inlet : Direct Ion Mode : EI+
 Spectrum Type : Normal Ion [EF-Linear]
 RT : 0.78 min Scan# : (16,17)
 BP : m/z 329.1050 Int. : 42.15
 Output m/z range : 299.0000 to 359.0000 Cut Level : 0.00 %

Mass Spectrum of Compound 41



[Elemental Composition]

Data : x9-30-C21H15NO3 Date : 29-Nov-2013 15:52
 Sample: -
 Note: -
 Inlet : Direct Ion Mode : EI+
 RT : 0.78 min Scan#: (16,17)
 Elements : C 21/0, H 15/0, N 1/0, O 3/0
 Mass Tolerance : 1000ppm, 1mmu if m/z < 1, 3mmu if m/z > 3
 Unsaturation (U.S.) : -0.5 - 100.0

Observed m/z	Int%	Err [ppm / mmu]	U.S. Composition
329.1050	100.0	-0.6 / -0.2	15.0 C 21 H 15 N O 3
330.1084	25.0		