

Electronic Supplementary Information

Efficient One-Step Synthesis of Pyrrolo[3,4-c]quinoline-1,3-dione Derivatives by Organocatalytic Cascade Reactions of Isatins and β -Ketoamides

Likai Xia and Yong Rok Lee*

School of Chemical Engineering, Yeungnam University, Gyeongsan 712-749, Republic of Korea

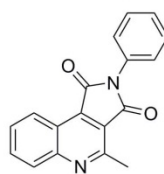
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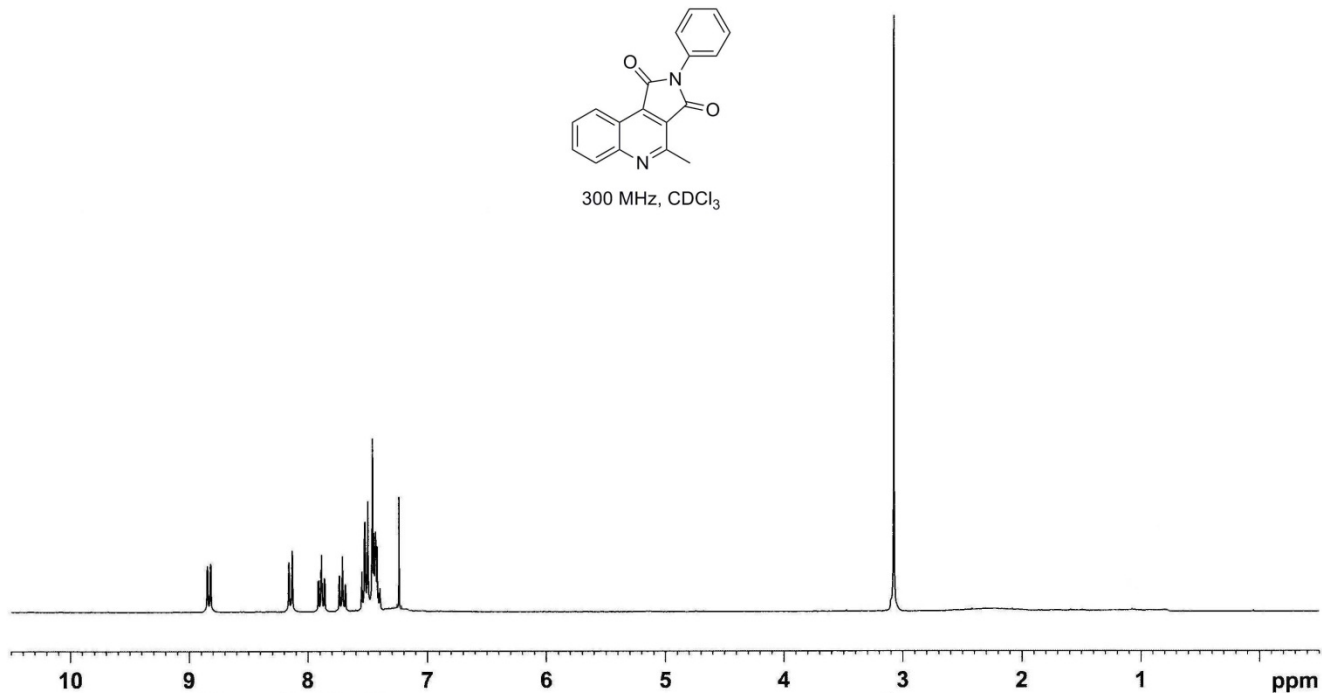
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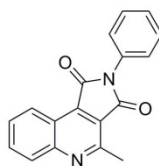
¹H NMR of Compound 7



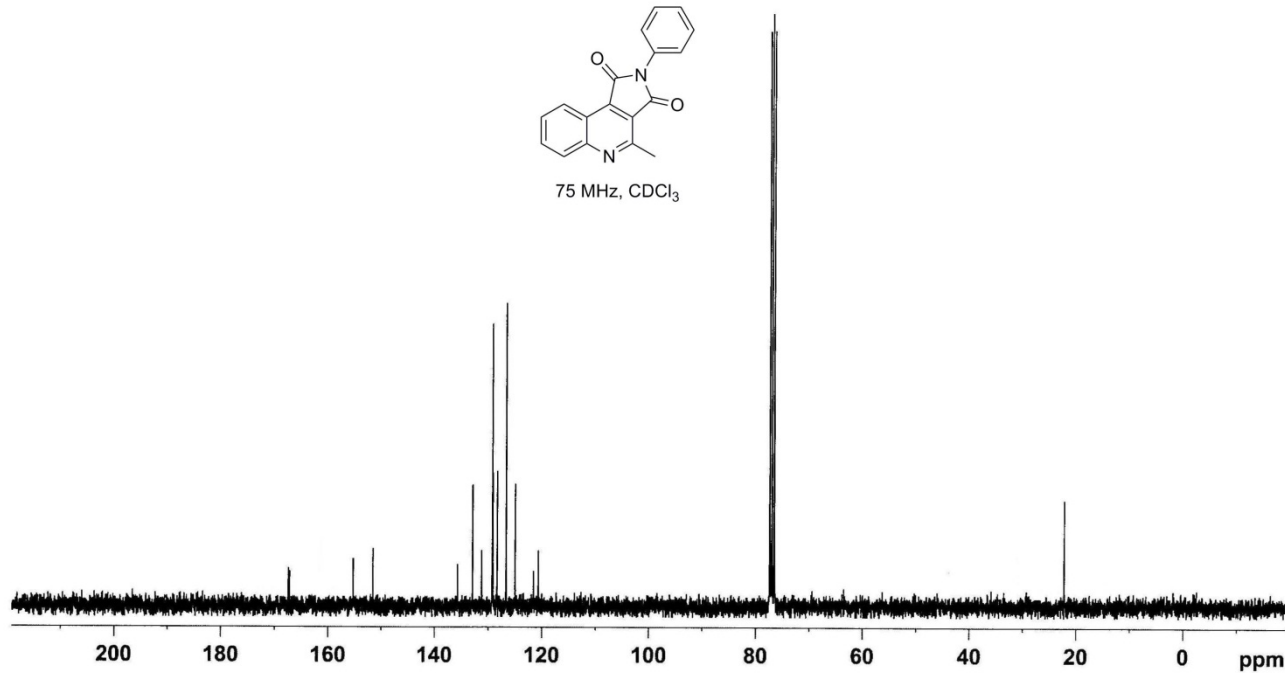
300 MHz, CDCl₃



¹³C NMR of Compound 7

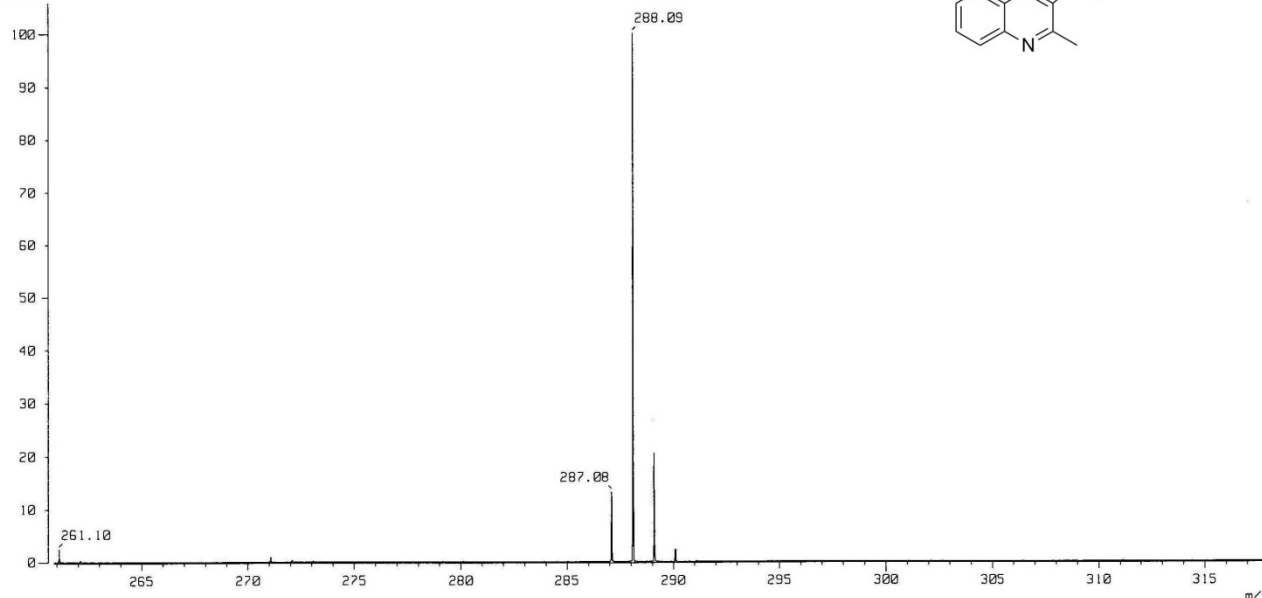
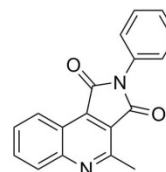


75 MHz, CDCl₃



[Mass Spectrum]
Data : 7a-C18H12N2O2 Date : 06-Dec-2012 10:32
Sample: -
Note: -
Inlet : Direct Ion Mode : EI+
Spectrum Type : Normal Ion [EF-Linear]
RT : 0.73 min Scan# : (15,16)
BP : m/z 288.0898 Int. : 66.36
Output m/z range : 260.0487 to 318.0000 Cut Level : 0.00 %
1472767

Mass spectrum of Compound 7



[Elemental Composition]

Data : 7a-C18H12N2O2

Date : 06-Dec-2012 10:32

Page: 1

Sample: -

Note: -

Inlet : Direct

Ion Mode : EI+

RT : 0.73 min

Scan#: (15,16)

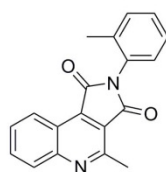
Elements : C 18/0, H 12/0, N 2/0, O 2/0

Mass Tolerance : 1000ppm, 2mmu if m/z < 2, 3mmu if m/z > 3

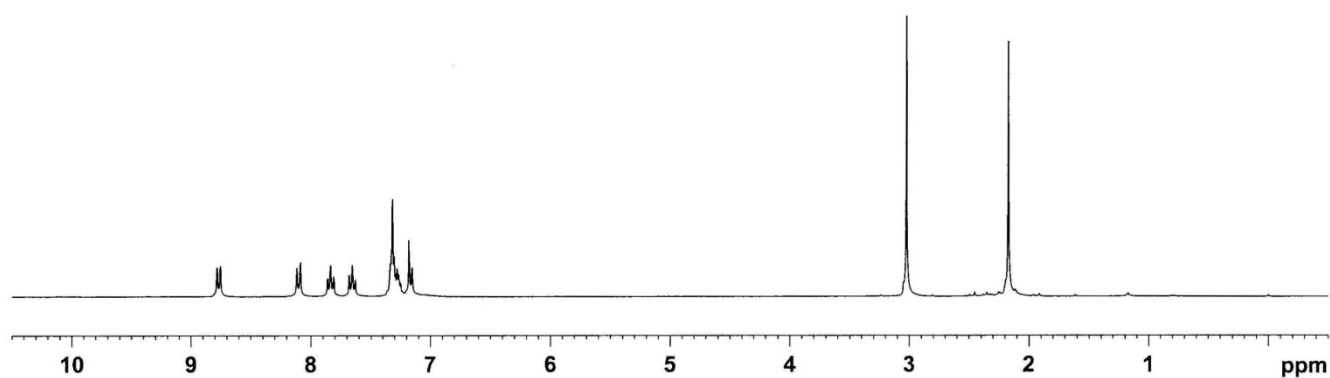
Unsaturation (U.S.) : -0.5 - 100.0

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
287.0822	13.2	+0.5 / +0.1	14.5	C 18 H 11 N 2 O 2
288.0898	100.0	-0.4 / -0.1	14.0	C 18 H 12 N 2 O 2
289.0924	20.5			

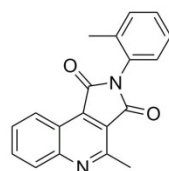
¹H NMR of Compound **8**



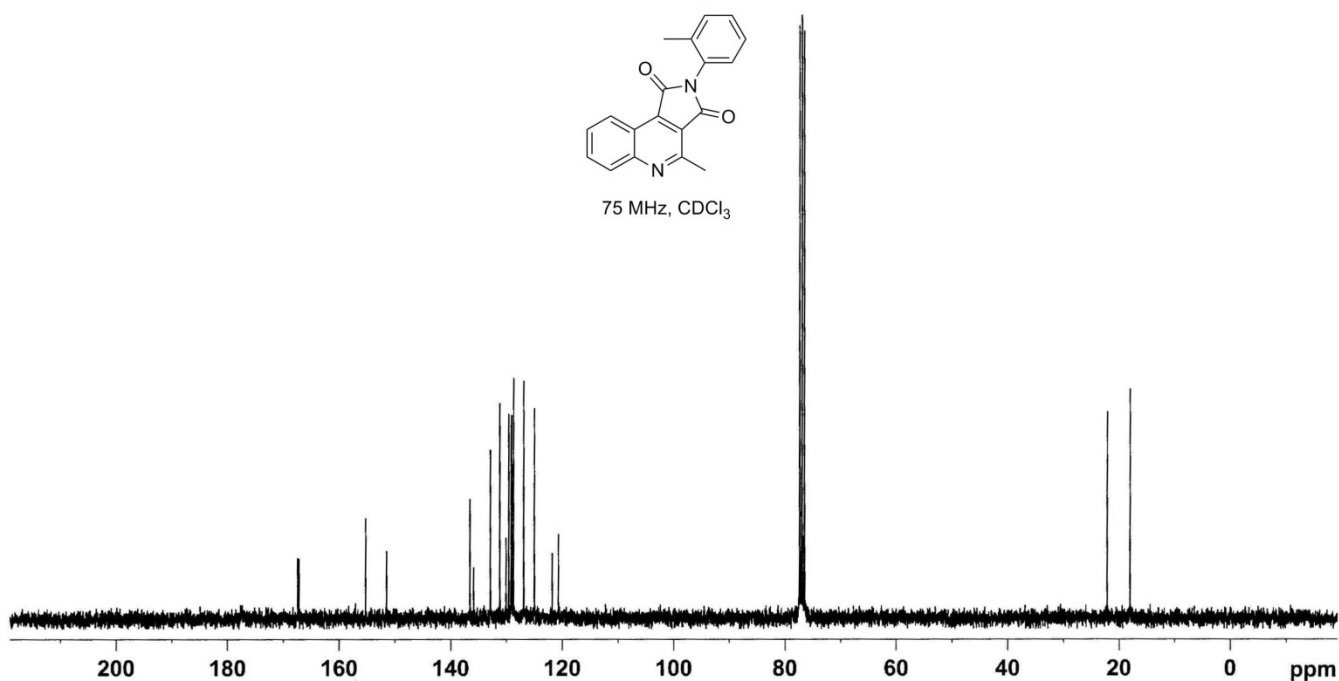
300 MHz, CDCl₃



¹³C NMR of Compound **8**

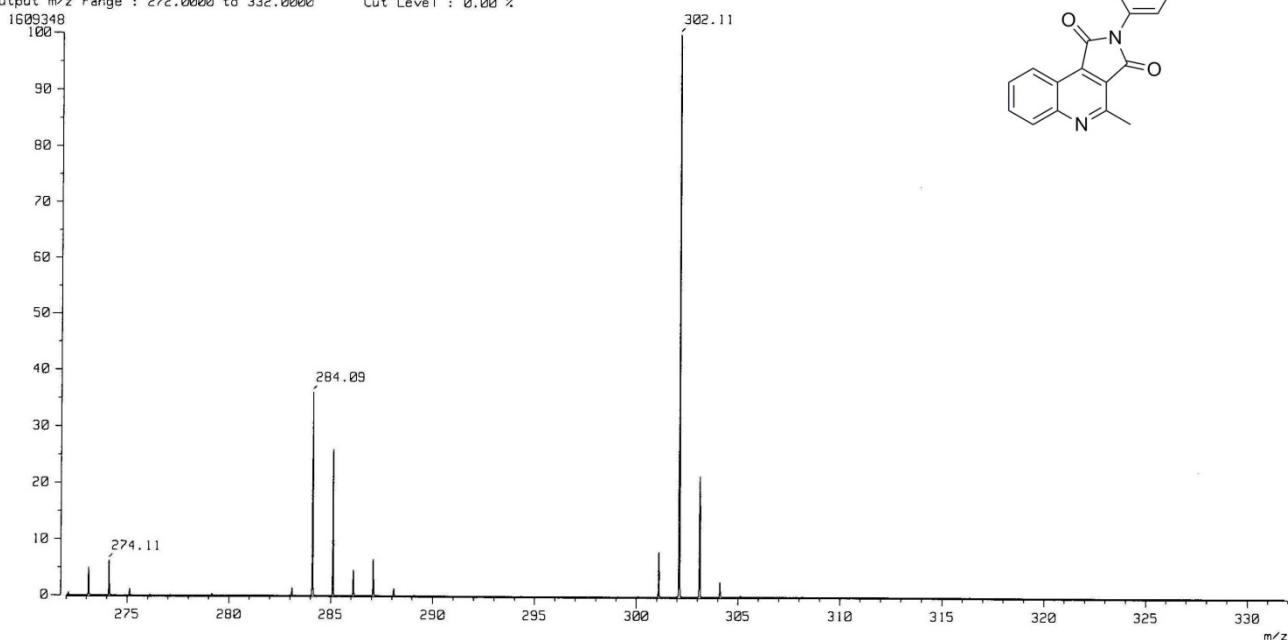
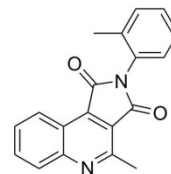


75 MHz, CDCl₃



[Mass Spectrum]
Data : 7-epsilon-C19H14N2O2 Date : 12-Dec-2012 11:57
Sample: -
Note: -
Inlet : Direct Ion Mode : EI+
Spectrum Type : Normal Ion [EF-Linear]
RT : 0.53 min Scan# : (11,12)
BP : m/z 302.1051 Int. : 76.74
Output m/z range : 272.0000 to 332.0000 Cut Level : 0.00 %

Mass spectrum of Compound 8



[Elemental Composition]

Data : 7-epsilon-C19H14N2O2

Date : 12-Dec-2012 11:57

Page: 1

Sample: -

Note: -

Inlet : Direct

Ion Mode : EI+

RT : 0.53 min

Scan#: (11,12)

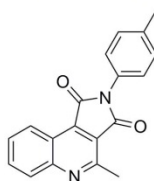
Elements : C 19/0, H 14/0, N 2/0, O 2/0

Mass Tolerance : 1000ppm, 2mmu if m/z < 2, 3mmu if m/z > 3

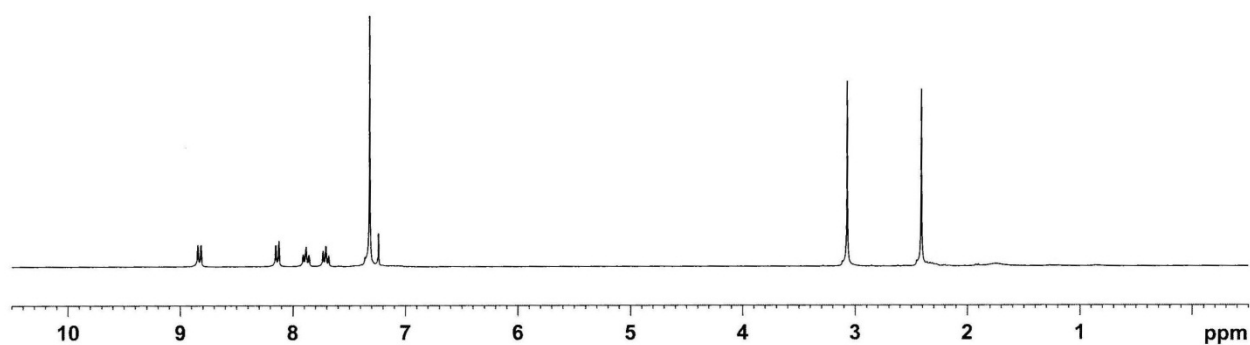
Unsaturation (U.S.) : -0.5 - 100.0

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
284.0949	36.0	-0.1 / +0.0	15.0	C 19 H 12 N 2 O
285.1018	26.0	-3.5 / -1.0	14.5	C 19 H 13 N 2 O
302.1051	100.0	-1.4 / -0.4	14.0	C 19 H 14 N 2 O 2
303.1080	21.5			

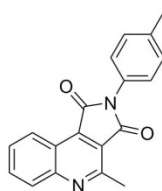
^1H NMR of Compound 9



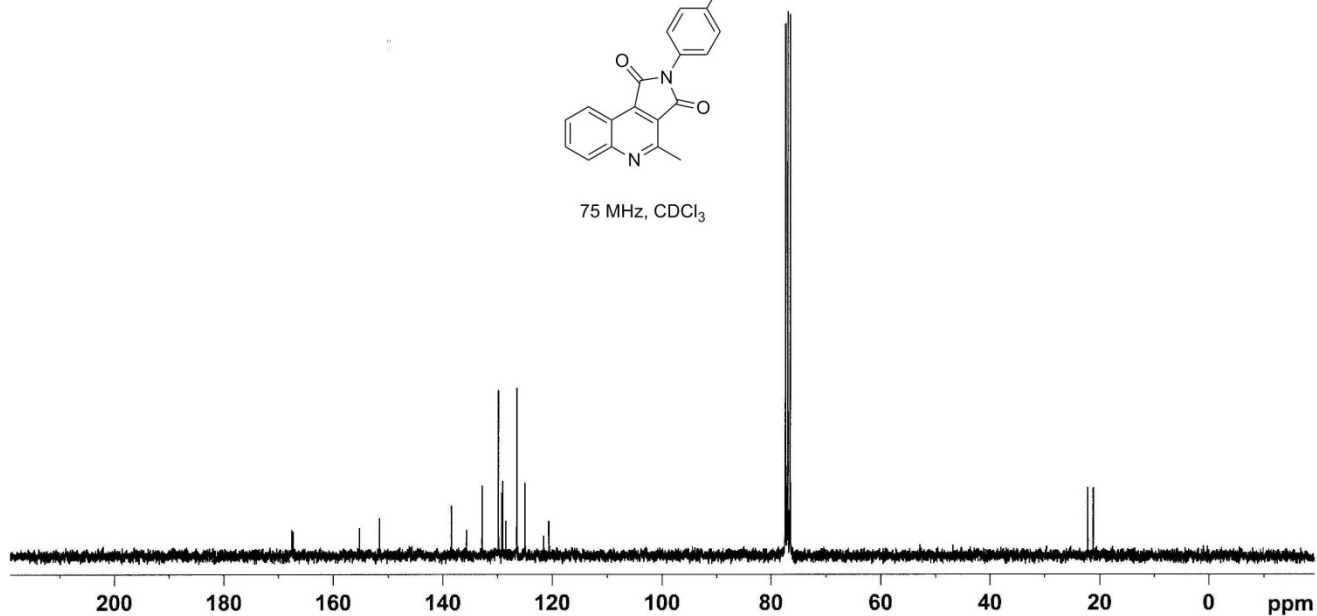
300 MHz, CDCl_3



^{13}C NMR of Compound 9

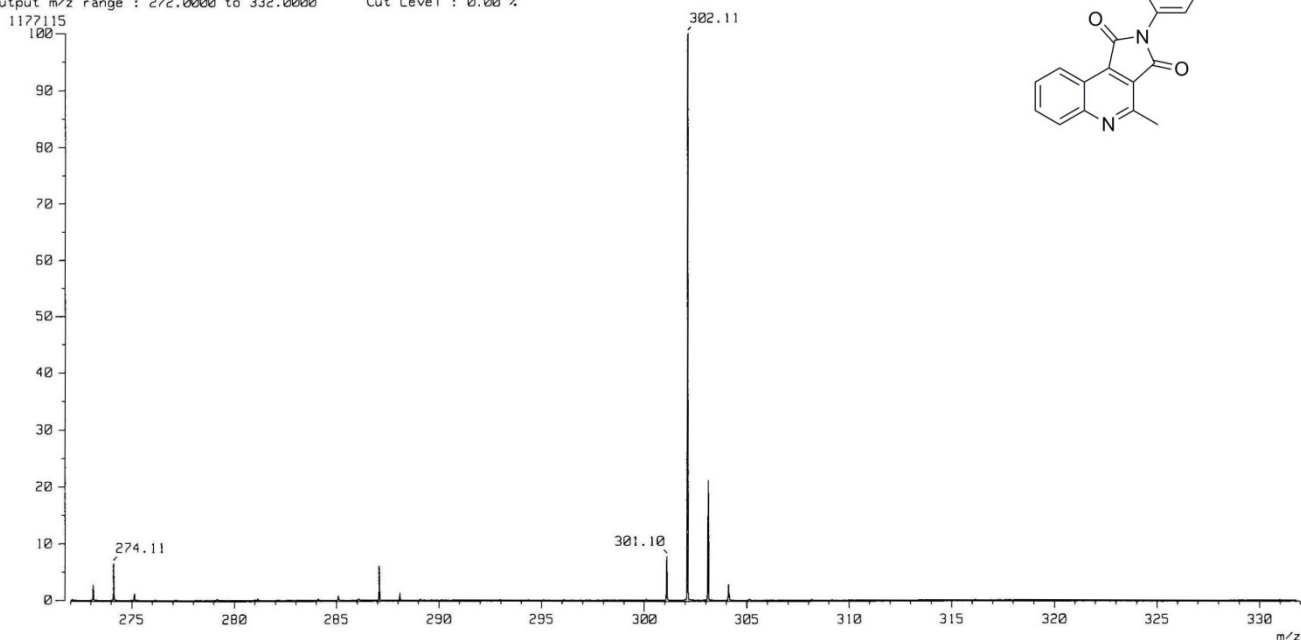
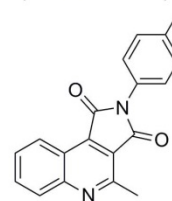


75 MHz, CDCl_3



[Mass Spectrum]
Data : 7r-C19H14N2O2 Date : 12-Dec-2012 10:56
Sample: -
Note: -
Inlet: Direct Ion Mode: EI+
Spectrum Type: Normal Ion [EF-Linear]
RT: 0.93 min Scan#: (19,20)
BP: m/z 302.1055 Int.: 56.13
Output m/z range: 272.0000 to 332.0000 Cut Level: 0.00 %

Mass spectrum of Compound 9



[Elemental Composition]

Data : 7r-C19H14N2O2

Date : 12-Dec-2012 10:56

Page: 1

Sample: -

Note: -

Inlet: Direct

Ion Mode: EI+

RT: 0.93 min

Scan#: (19,20)

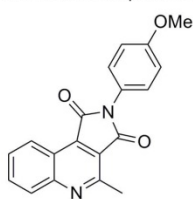
Elements: C 19/0, H 14/0, N 2/0, O 2/0

Mass Tolerance: 1000ppm, 2mmu if m/z < 2, 3mmu if m/z > 3

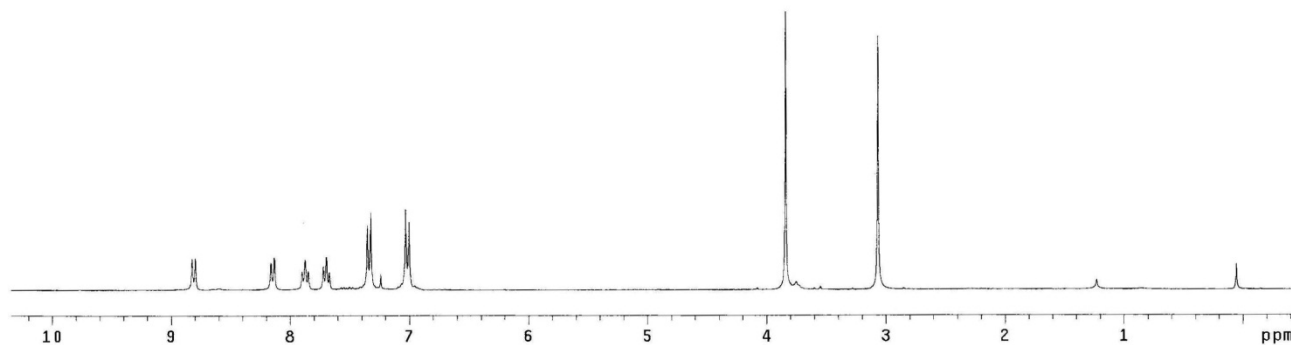
Unsaturation (U.S.): -0.5 - 100.0

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
302.1055	100.0	-0.2 / -0.1	14.0	C 19 H 14 N 2 O 2
303.1085	21.1			

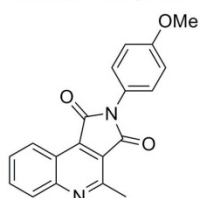
¹H NMR of Compound **10**



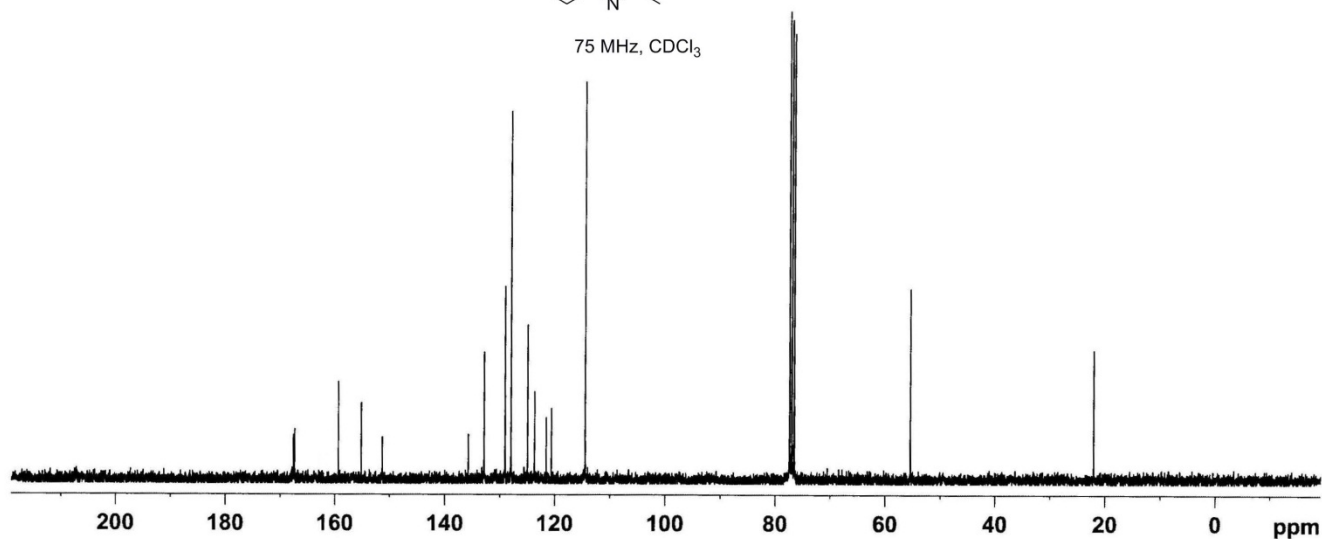
300 MHz, CDCl₃



¹³C NMR of Compound **10**

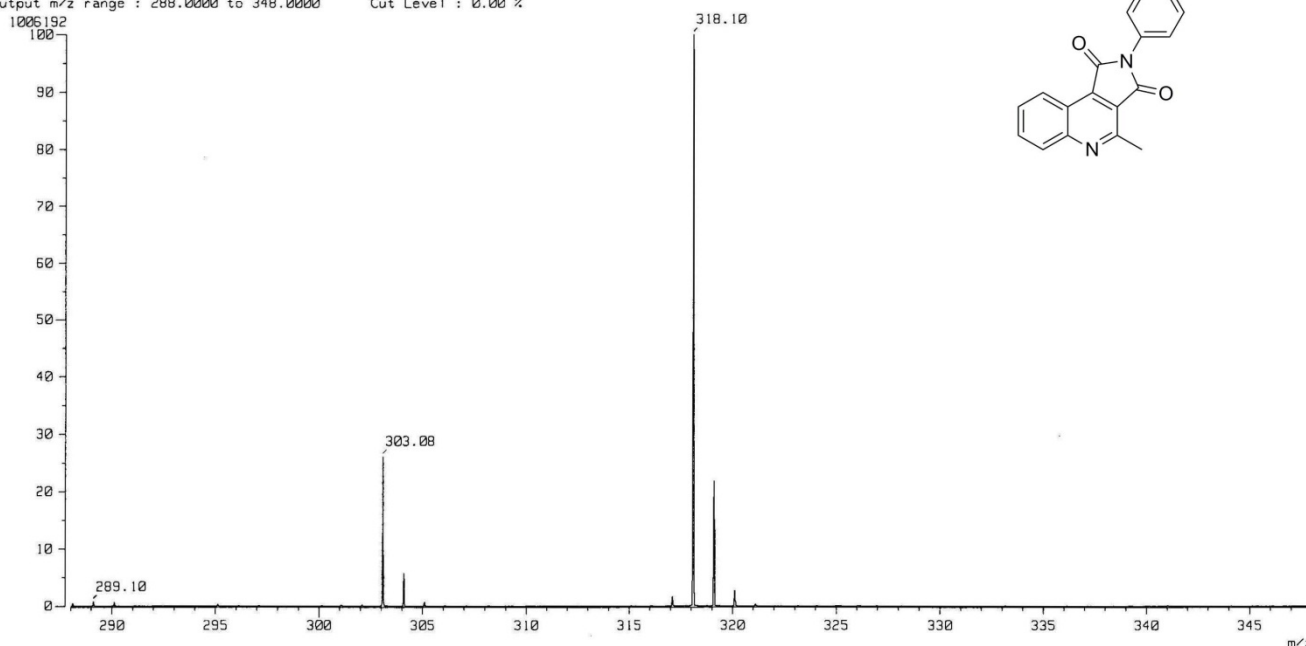
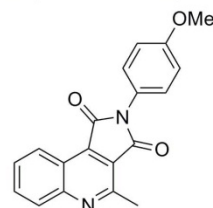


75 MHz, CDCl₃



[Mass Spectrum]
Data : X3-26-C19H14N2O3 Date : 18-Sep-2012 11:42
Sample: -
Note: -
Inlet: Direct Ion Mode: EI+
Spectrum Type: Normal Ion [EF-Linear]
RT: 0.83 min Scan#: (17,18)
BP: m/z 318.1003 Int.: 47.98
Output m/z range: 288.0000 to 348.0000 Cut Level: 0.00 %

Mass spectrum of Compound 10



[Elemental Composition]

Data : X3-26-C19H14N2O3

Date : 18-Sep-2012 11:42

Page: 1

Sample: -

Note: -

Inlet: Direct

Ion Mode: EI+

RT: 0.83 min

Scan#: (17,18)

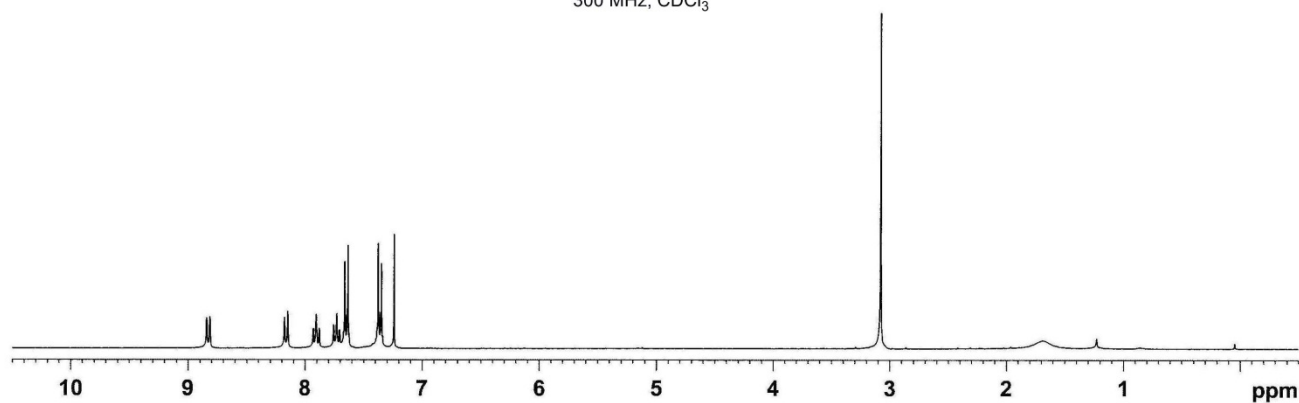
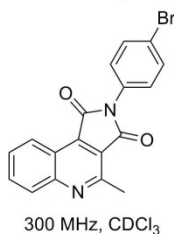
Elements: C 19/0, H 14/0, N 2/0, O 3/0

Mass Tolerance: 1000ppm, 2mmu if m/z < 2, 3mmu if m/z > 3

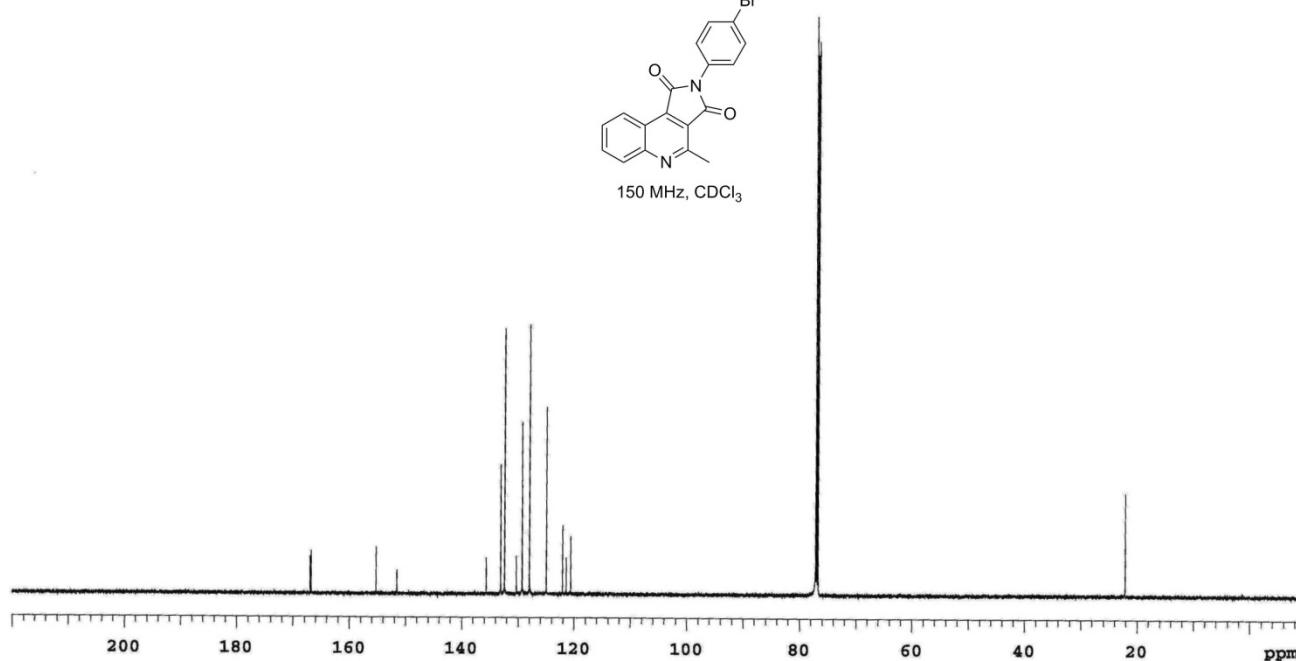
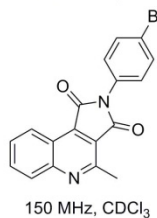
Unsaturation (U.S.): -0.5 - 100.0

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
303.0771	26.2	+0.3 / +0.1	14.5	C 18 H 11 N 2 O 3
318.1003	100.0	-0.6 / -0.2	14.0	C 19 H 14 N 2 O 3
319.1028	21.9			

¹H NMR of Compound 11

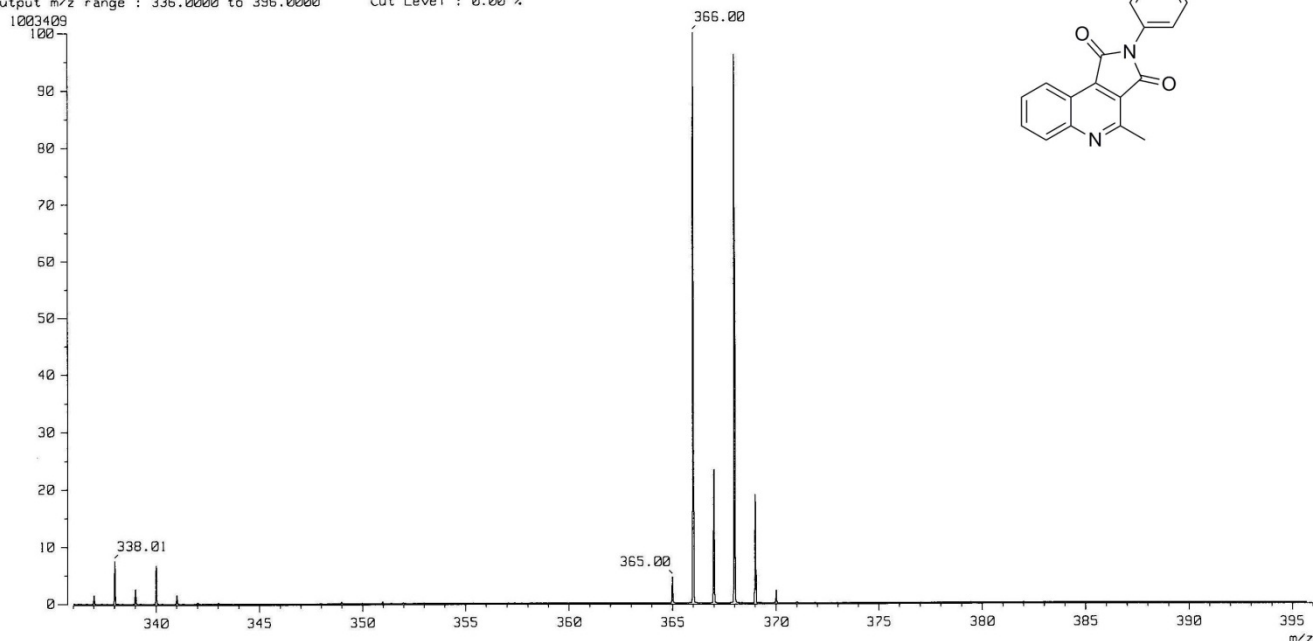
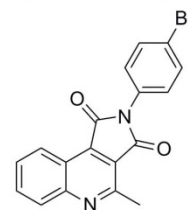


¹³C NMR of Compound 11



[Mass Spectrum]
Data : 7m-C18H11BrN2O2 Date : 06-Dec-2012 11:16
Sample: -
Note: -
Inlet : Direct Ion Mode : EI+
Spectrum Type : Normal Ion [EF-Linear]
RT : 0.83 min Scan#: (17,18)
BP : m/z 366.0000 Int. : 47.85
Output m/z range : 335.0000 to 396.0000 Cut Level : 0.00 %

Mass spectrum of Compound 11



[Elemental Composition]

Data : 7m-C18H11BrN2O2

Date : 06-Dec-2012 11:16

Page: 1

Sample: -

Note: -

Inlet : Direct

Ion Mode : EI+

RT : 0.83 min

Scan#: (17,18)

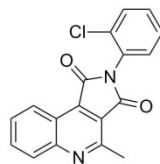
Elements : C 18/0, H 11/0, Br 1/0, N 2/0, O 2/0

Mass Tolerance : 1000ppm, 2mmu if m/z < 2, 3mmu if m/z > 3

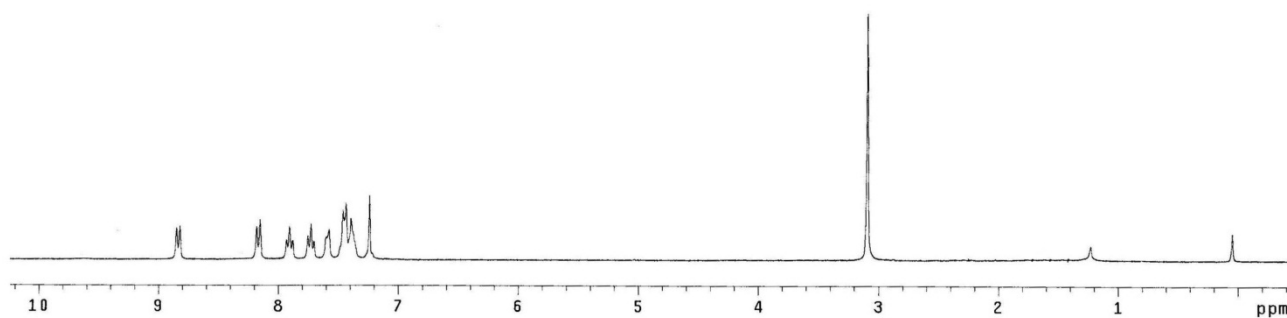
Unsaturation (U.S.) : -0.5 - 100.0

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
366.0000	100.0	-1.0 / -0.4	14.0	C 18 H 11 Br N 2 O 2
367.0012	23.4			
367.9976	96.2			
369.0013	19.0			

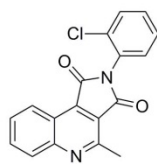
¹H NMR of Compound 12



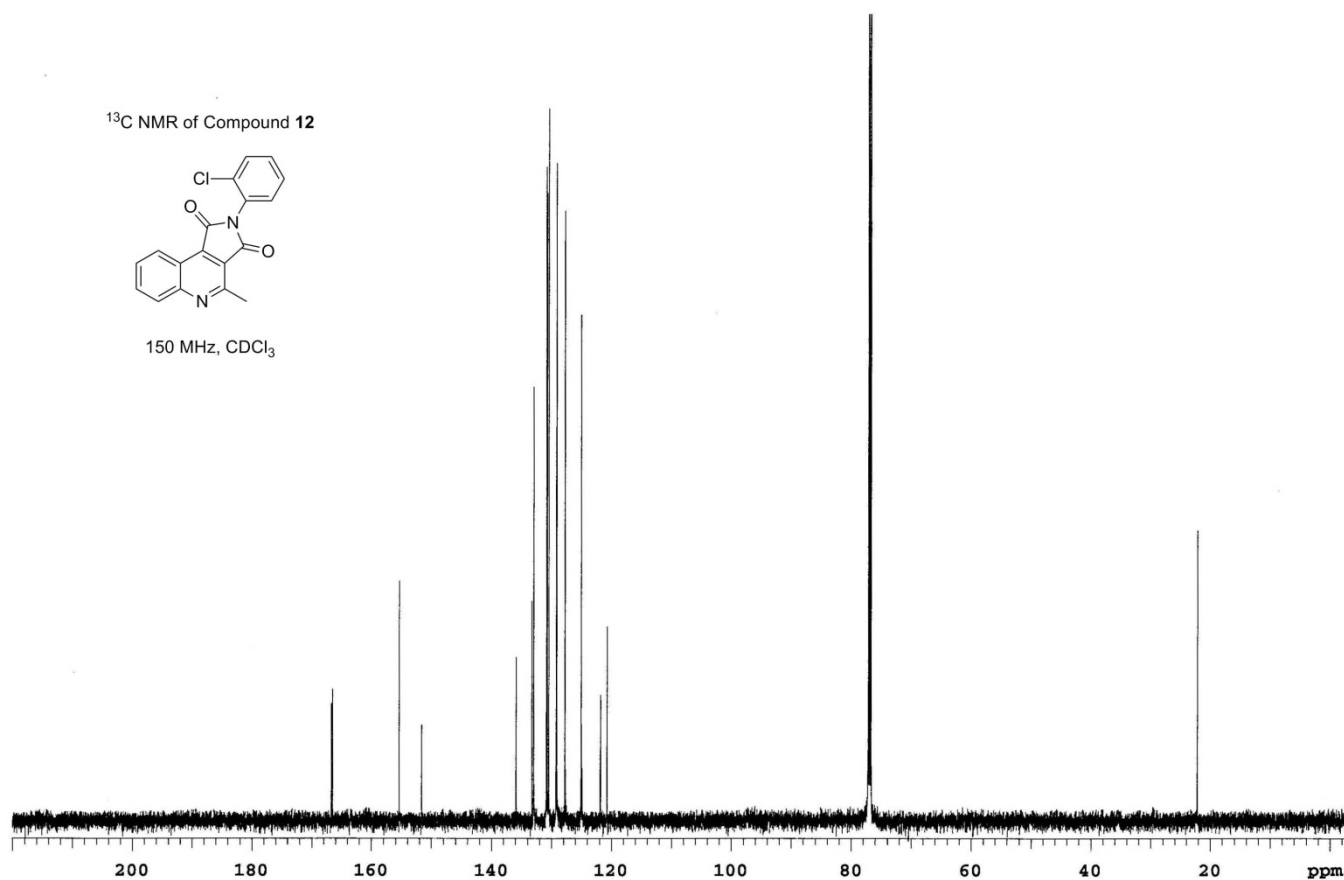
300 MHz, CDCl₃



¹³C NMR of Compound 12

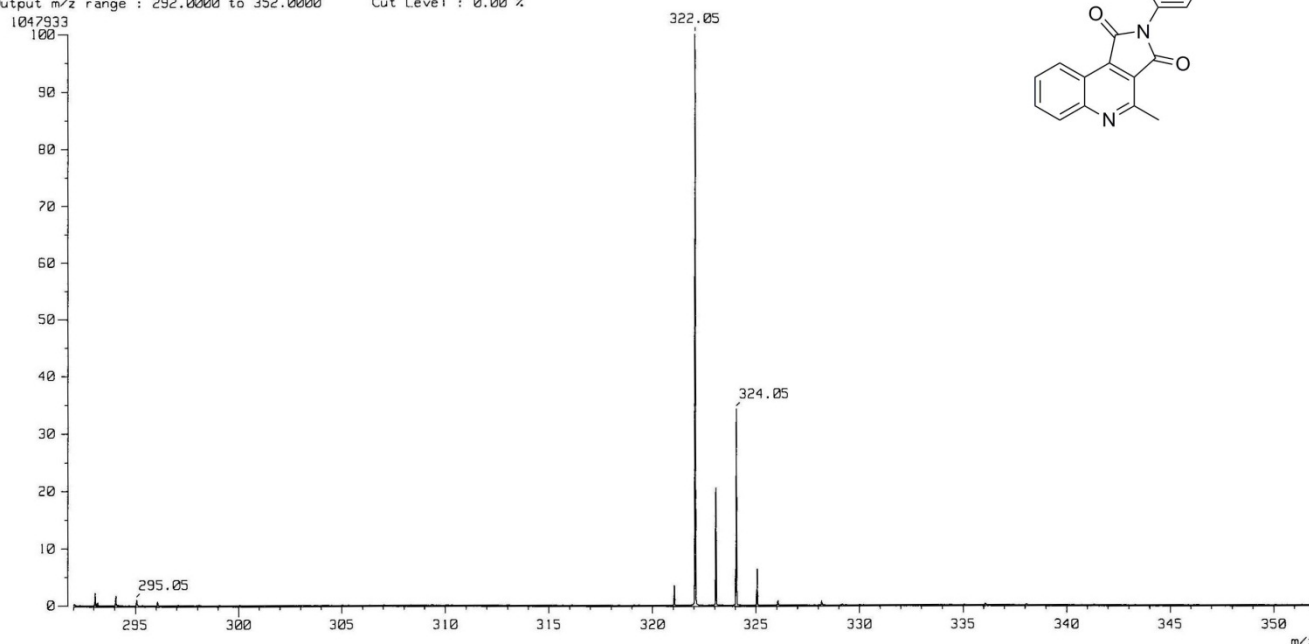
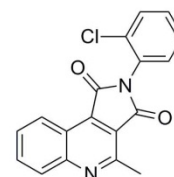


150 MHz, CDCl₃



[Mass Spectrum]
Data : 7z-C18H11ClN2O2 Date : 12-Dec-2012 11:36
Sample: -
Note: -
Inlet : Direct Ion Mode : EI+
Spectrum Type : Normal Ion [EF-Linear]
RT : 0.78 min Scan# : (16,17)
BP : m/z 322.0511 Int. : 49.97
Output m/z range : 292.0000 to 352.0000 Cut Level : 0.00 %

Mass spectrum of Compound 12



[Elemental Composition]

Data : 7z-C18H11ClN2O2

Date : 12-Dec-2012 11:36

Page: 1

Sample: -

Note: -

Inlet : Direct

Ion Mode : EI+

RT : 0.78 min

Scan#: (16,17)

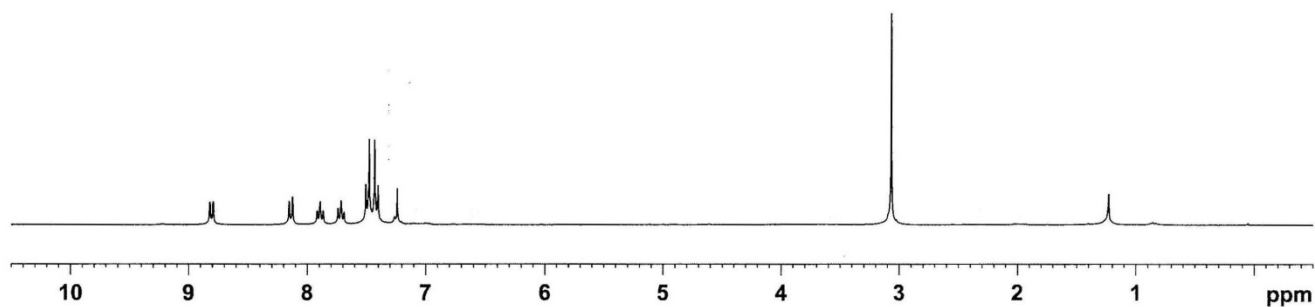
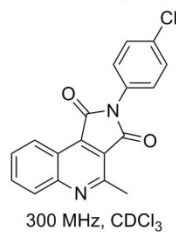
Elements : C 18/0, H 11/0, Cl 1/0, N 2/0, O 2/0

Mass Tolerance : 1000ppm, 2mmu if m/z < 2, 3mmu if m/z > 3

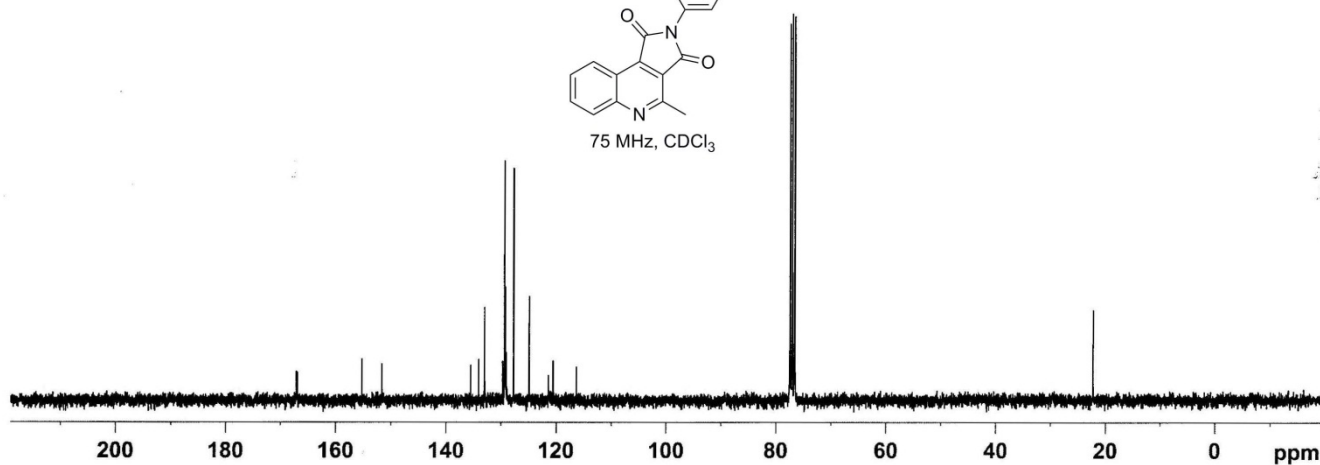
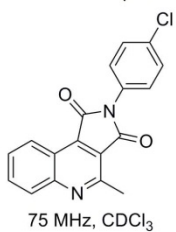
Unsaturation (U.S.) : -0.5 - 100.0

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
322.0511	100.0	+0.6 / +0.2	14.0	C 18 H 11 Cl N 2 O 2
323.0539	20.6			
324.0479	34.2			

¹H NMR of Compound 13

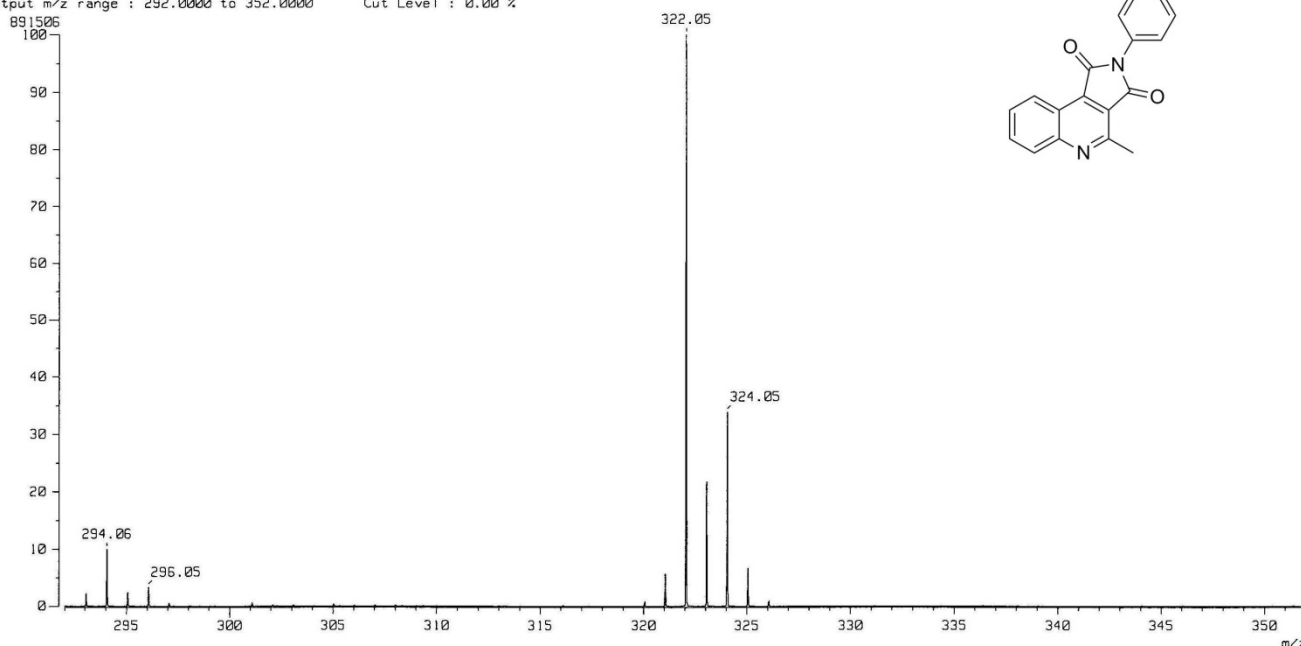
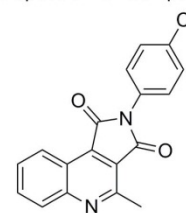


¹³C NMR of Compound 13



[Mass Spectrum]
Data : 7v-C18H11ClN2O2 Date : 12-Dec-2012 11:16
Sample: -
Note: -
Inlet : Direct Ion Mode : EI+
Spectrum Type : Normal Ion [EF-Linear]
RT : 0.68 min Scan# : (14,15)
BP : m/z 322.0507 Int. : 42.51
Output m/z range : 292.0000 to 352.0000 Cut Level : 0.00 %

Mass spectrum of Compound 13



[Elemental Composition]

Data : 7v-C18H11ClN2O2

Date : 12-Dec-2012 11:16

Page: 1

Sample: -

Note: -

Inlet : Direct

Ion Mode : EI+

RT : 0.68 min

Scan#: (14,15)

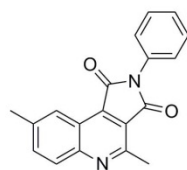
Elements : C 18/0, H 11/0, Cl 1/0, N 2/0, O 2/0

Mass Tolerance : 1000ppm, 2mmu if m/z < 2, 3mmu if m/z > 3

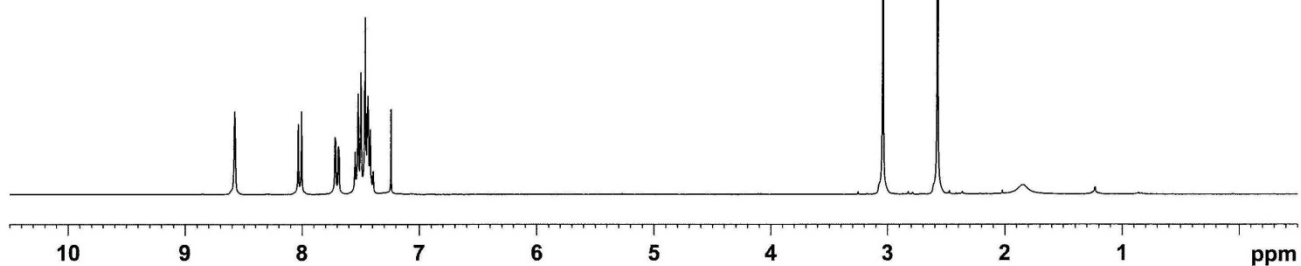
Unsaturation (U.S.) : -0.5 - 100.0

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
294.0557	10.0	-0.9 / -0.3	13.0	C 17 H 11 Cl N 2 O
322.0507	100.0	-0.7 / -0.2	14.0	C 18 H 11 Cl N 2 O 2
323.0527	21.8			
324.0494	33.9			

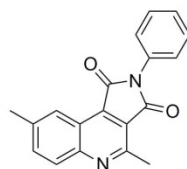
¹H NMR of Compound **14**



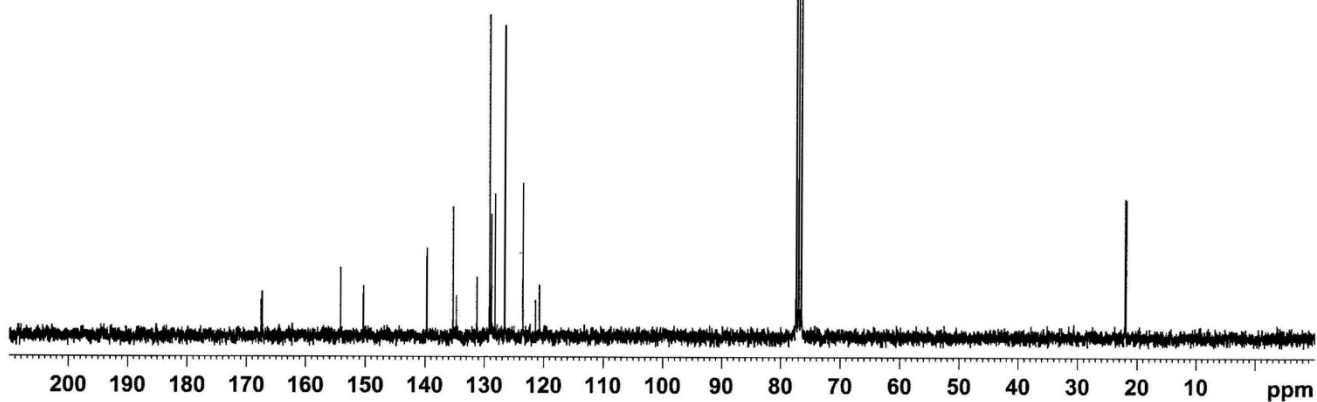
300 MHz, CDCl₃



¹³C NMR of Compound **14**

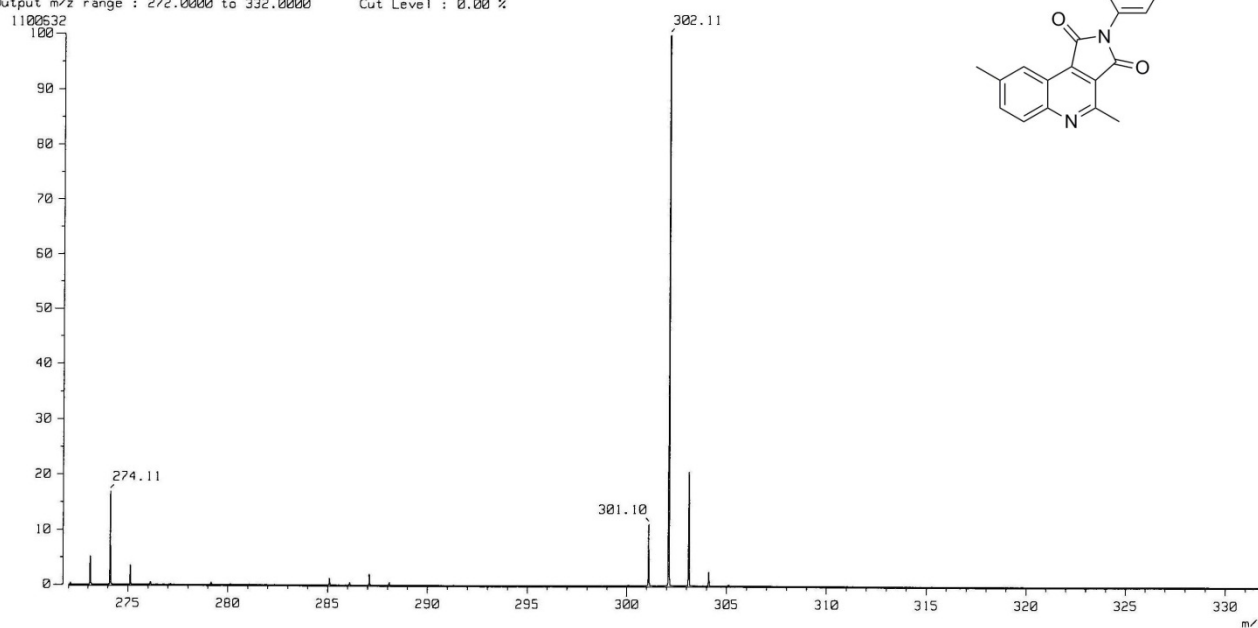
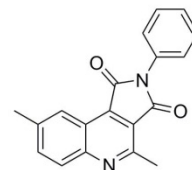


75 MHz, CDCl₃



[Mass Spectrum]
Data : 7e-C19H14N2O2 Date : 06-Dec-2012 10:51
Sample: -
Note: -
Inlet : Direct Ion Mode : EI+
Spectrum Type : Normal Ion [EF-Linear]
RT : 0.98 min Scan# : (20,21)
BP : m/z 302.1057 Int. : 52.48
Output m/z range : 272.0000 to 332.0000 Cut Level : 0.00 %

Mass spectrum of Compound 14



[Elemental Composition]

Data : 7e-C19H14N2O2

Date : 06-Dec-2012 10:51

Page: 1

Sample: -

Note: -

Inlet : Direct

Ion Mode : EI+

RT : 0.98 min

Scan#: (20,21)

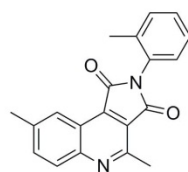
Elements : C 19/0, H 14/0, N 2/0, O 2/0

Mass Tolerance : 1000ppm, 2mmu if m/z < 2, 3mmu if m/z > 3

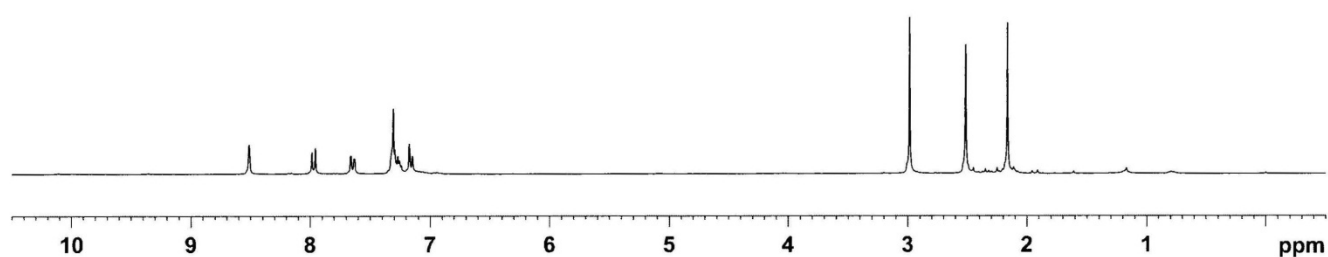
Unsaturation (U.S.) : -0.5 - 100.0

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
274.1104	17.0	-0.8 / -0.2	13.0	C 18 H 14 N 2 O
301.0973	11.2	-1.4 / -0.4	14.5	C 19 H 13 N 2 O 2
302.1057	100.0	+0.4 / +0.1	14.0	C 19 H 14 N 2 O 2
303.1080	20.7			

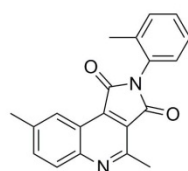
^1H NMR of Compound 15



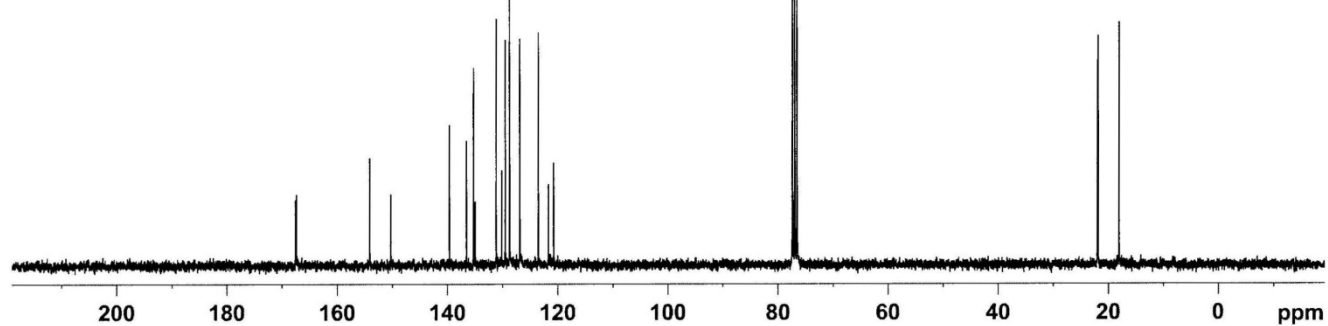
300 MHz, CDCl_3



^{13}C NMR of Compound 15

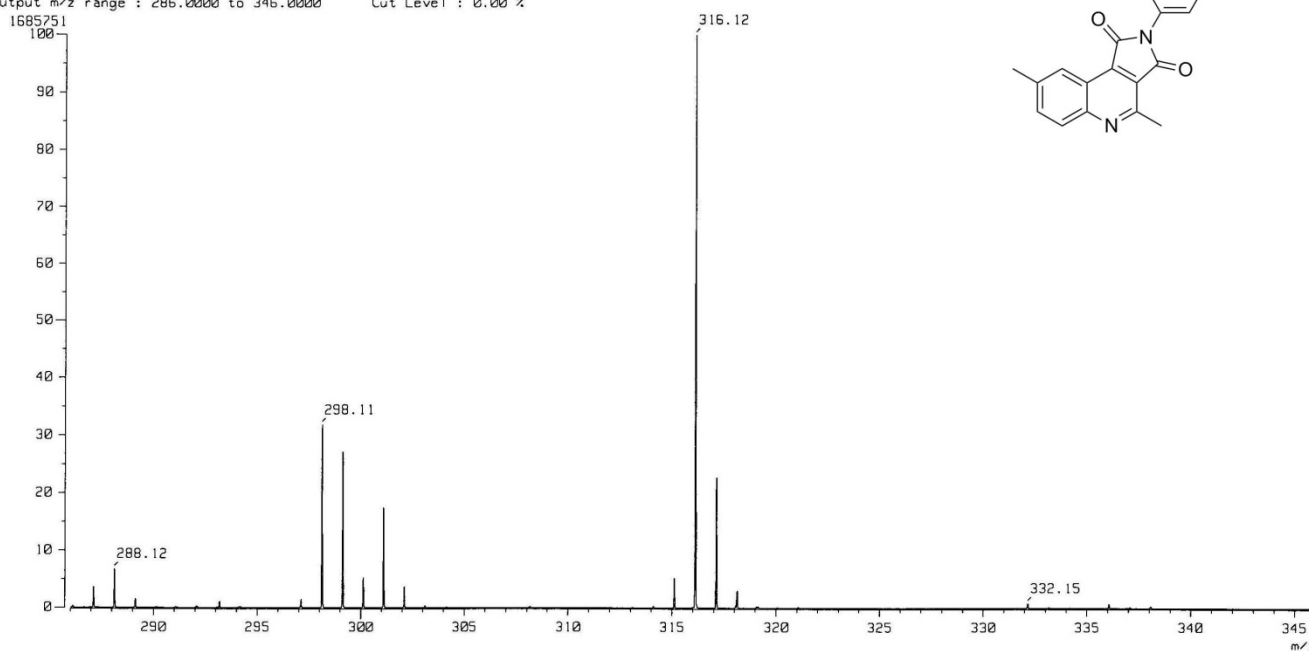
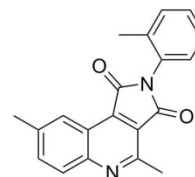


75 MHz, CDCl_3



[Mass Spectrum]
Data : 7-theta-C20H16N2O2 Date : 12-Dec-2012 14:45
Sample: -
Note: -
Inlet : Direct Ion Mode : EI+
Spectrum Type : Normal Ion [EF-Linear]
RT : 0.68 min Scan#: (14,15)
BP : m/z 316.1209 Int. : 80.38
Output m/z range : 286.0000 to 346.0000 Cut Level : 0.00 %

Mass spectrum of Compound 15



[Elemental Composition]

Data : 7-theta-C20H16N2O2

Date : 12-Dec-2012 14:45

Page: 1

Sample: -

Note: -

Inlet : Direct

Ion Mode : EI+

RT : 0.68 min

Scan#: (14,15)

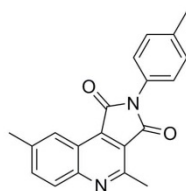
Elements : C 20/0, H 16/0, N 2/0, O 2/0

Mass Tolerance : 1000ppm, 2mmu if m/z < 2, 3mmu if m/z > 3

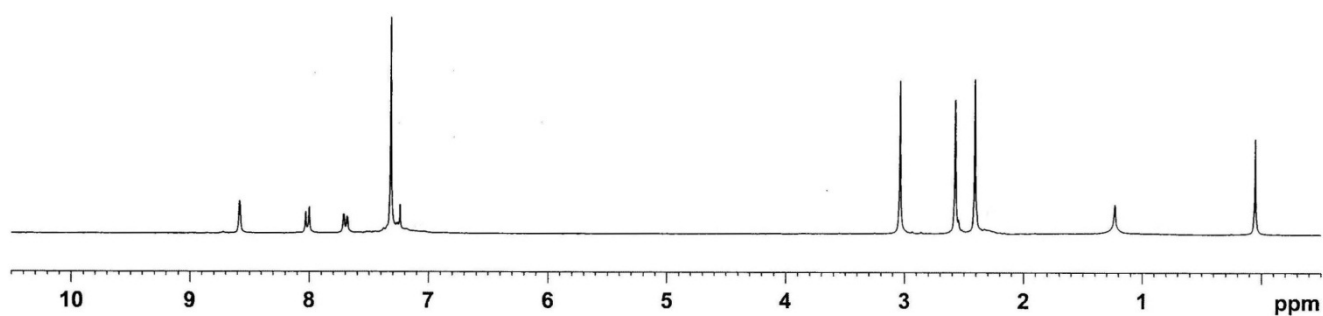
Unsaturation (U.S.) : -0.5 - 100.0

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
298.1106	31.9	-0.2 / +0.0	15.0	C 20 H 14 N 2 O
299.1158	27.1	-8.8 / -2.6	14.5	C 20 H 15 N 2 O
301.0979	17.5	+0.6 / +0.2	14.5	C 19 H 13 N 2 O 2
316.1209	100.0	-0.7 / -0.2	14.0	C 20 H 16 N 2 O 2
317.1249	22.8			

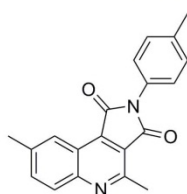
¹H NMR of Compound **16**



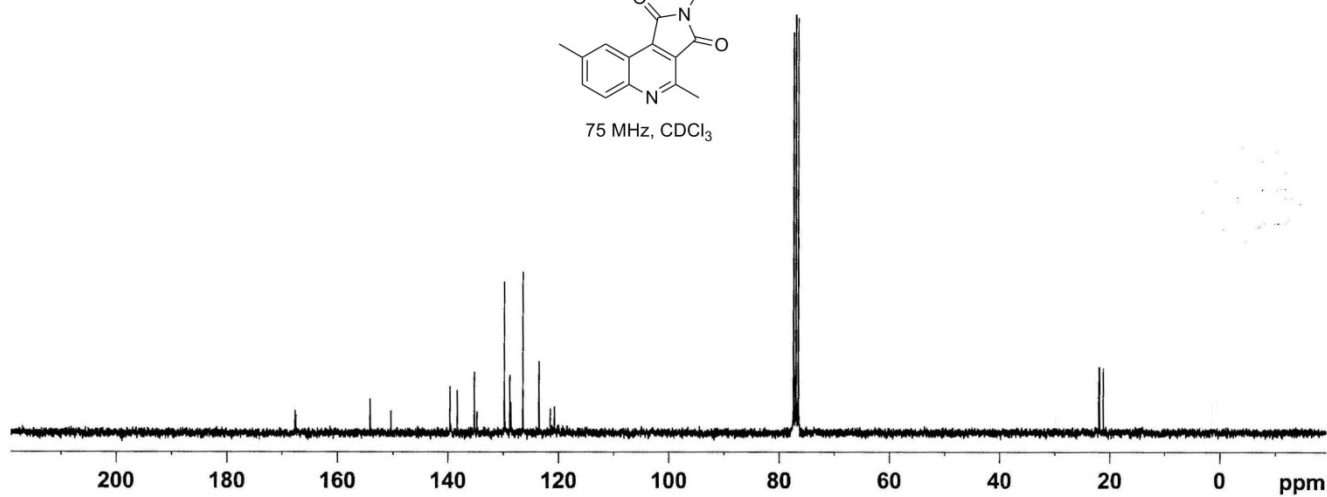
300 MHz, CDCl₃



¹³C NMR of Compound **16**

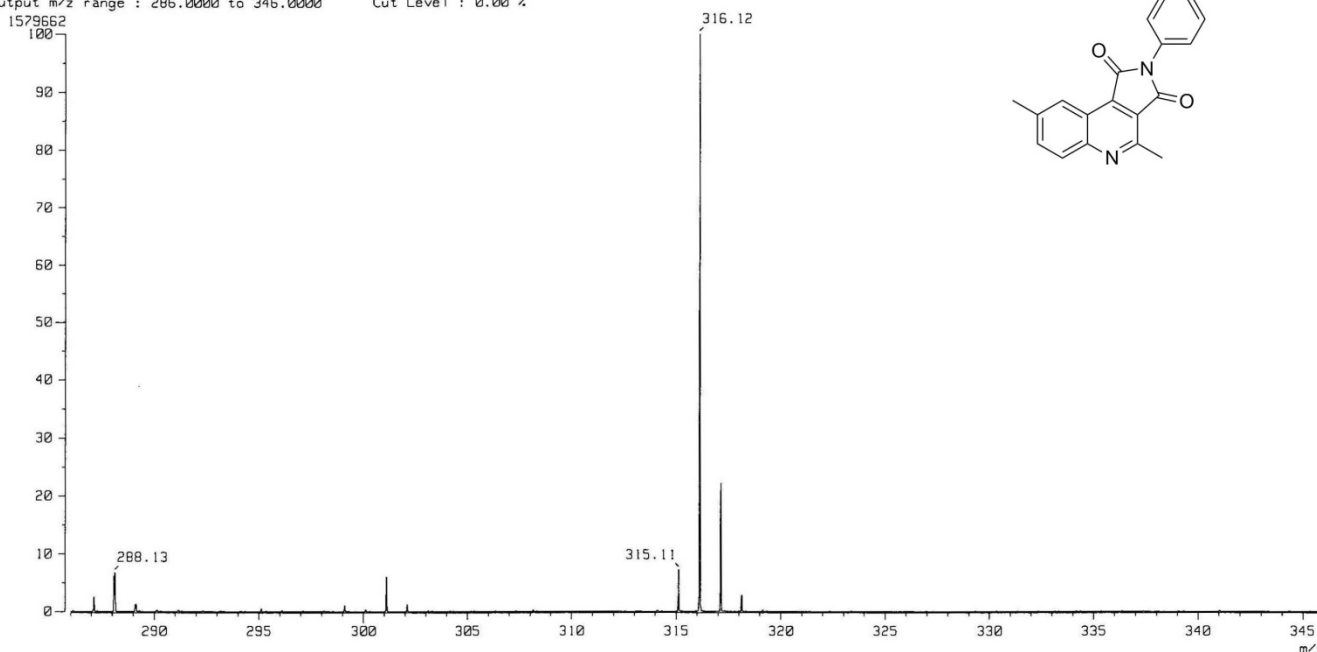
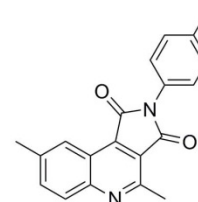


75 MHz, CDCl₃



[Mass Spectrum]
Data : 7u-C20H16N2O2 Date : 12-Dec-2012 11:12
Sample: -
Note: -
Inlet : Direct Ion Mode : EI+
Spectrum Type : Normal Ion [EF-Linear]
RT : 0.73 min Scan#: (15,16)
BP : m/z 316.1212 Int. : 75.32
Output m/z range : 286.0000 to 346.0000 Cut Level : 0.00 %

Mass spectrum of Compound 16



[Elemental Composition]

Data : 7u-C20H16N2O2

Date : 12-Dec-2012 11:12

Page: 1

Sample: -

Note: -

Inlet : Direct

Ion Mode : EI+

RT : 0.73 min

Scan#: (15,16)

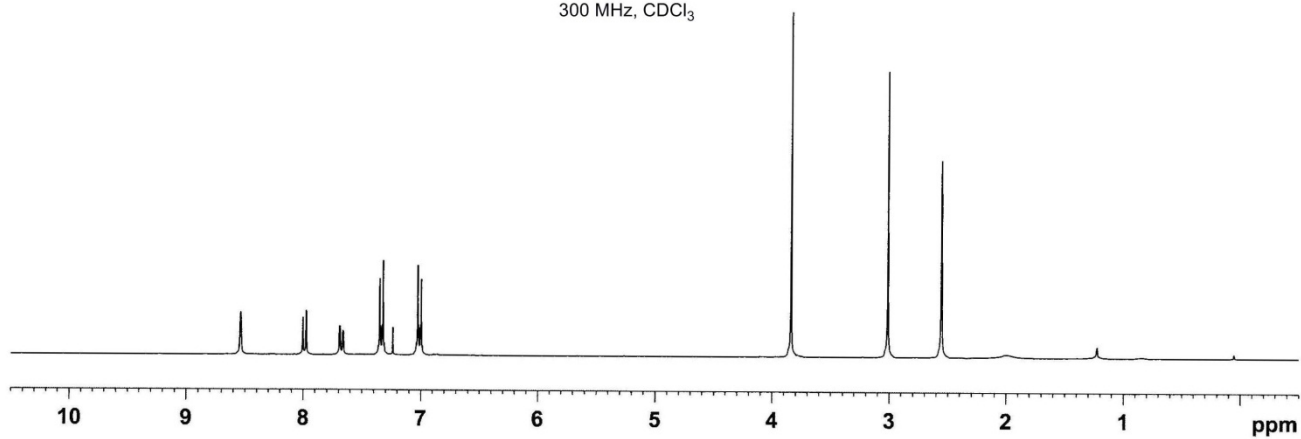
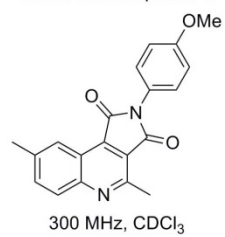
Elements : C 20/0, H 16/0, N 2/0, O 2/0

Mass Tolerance : 1000ppm, 2mmu if m/z < 2, 3mmu if m/z > 3

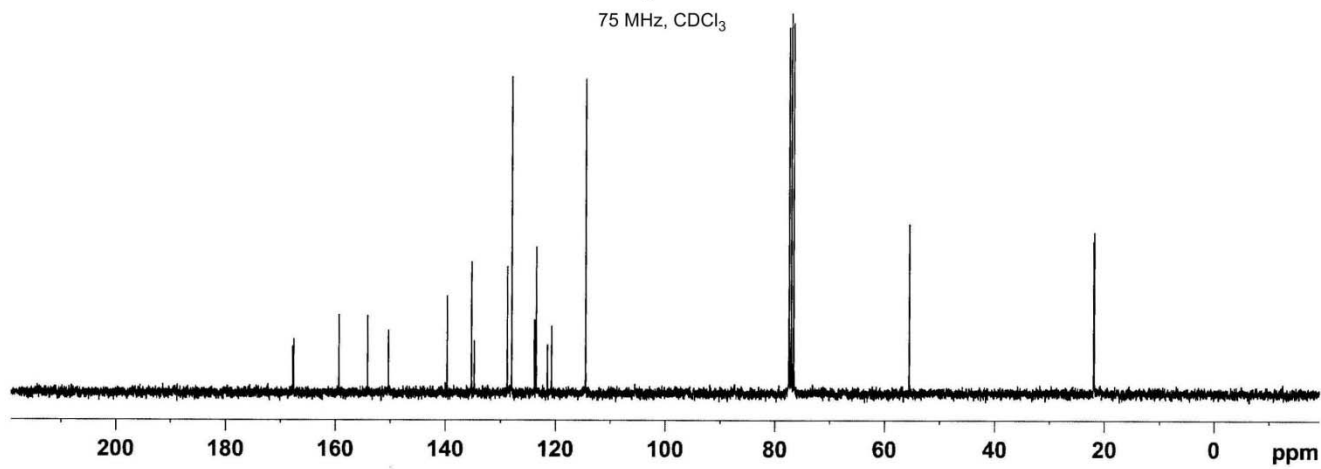
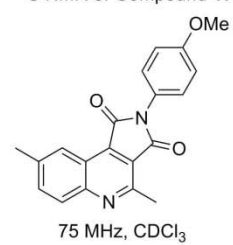
Unsaturation (U.S.) : -0.5 - 100.0

Observed m/z	Int%	Err[ppm / mmu]	U.S. Composition
316.1212	100.0	+0.0 / +0.0	14.0 C 20 H 16 N 2 O 2
317.1255	22.2		

¹H NMR of Compound 17

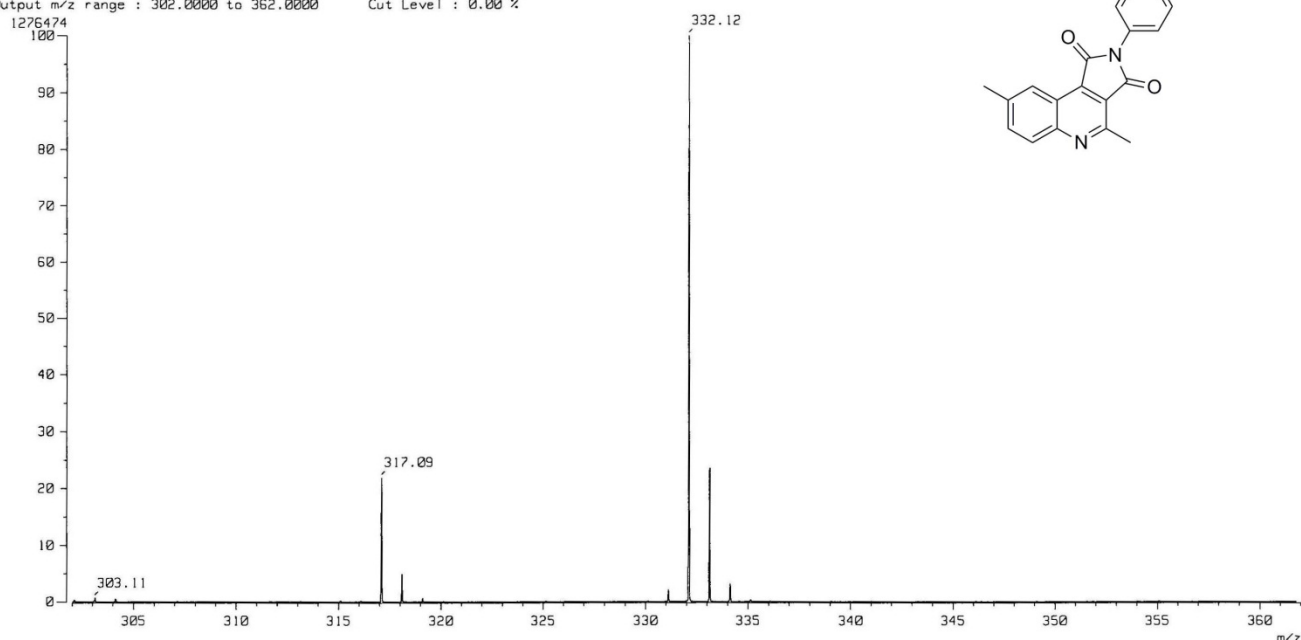
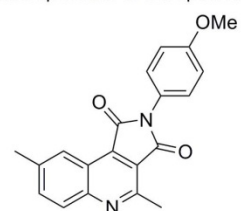


¹³C NMR of Compound 17



[Mass Spectrum]
Data : 7k-C20H16N2O3 Date : 06-Dec-2012 11:06
Sample: -
Note: -
Inlet: Direct Ion Mode: EI+
Spectrum Type: Normal Ion [EF-Linear]
RT: 0.73 min Scan#: (15,16)
BP: m/z 332.1162 Int.: 60.87
Output m/z range: 302.0000 to 362.0000 Cut Level: 0.00 %

Mass spectrum of Compound 17



[Elemental Composition]

Data : 7k-C20H16N2O3

Date : 06-Dec-2012 11:06

Page: 1

Sample: -

Note: -

Inlet: Direct

Ion Mode: EI+

RT: 0.73 min

Scan#: (15,16)

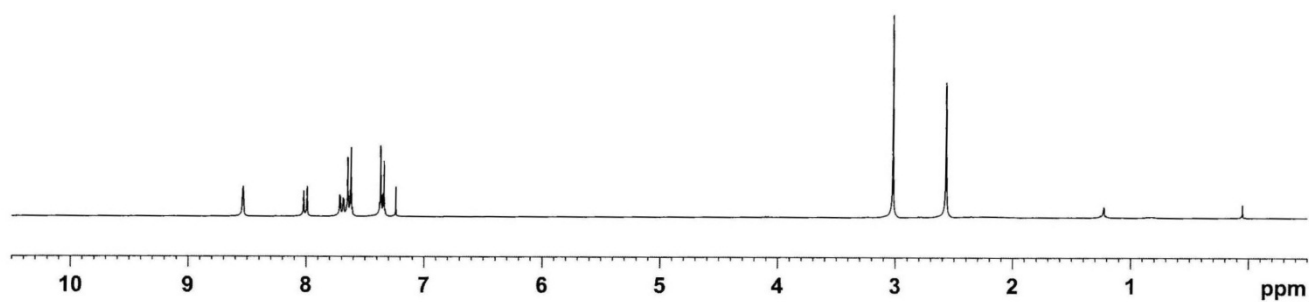
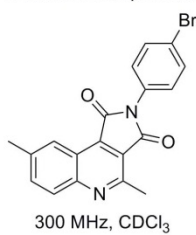
Elements: C 20/0, H 16/0, N 2/0, O 3/0

Mass Tolerance: 1000ppm, 2mmu if m/z < 2, 3mmu if m/z > 3

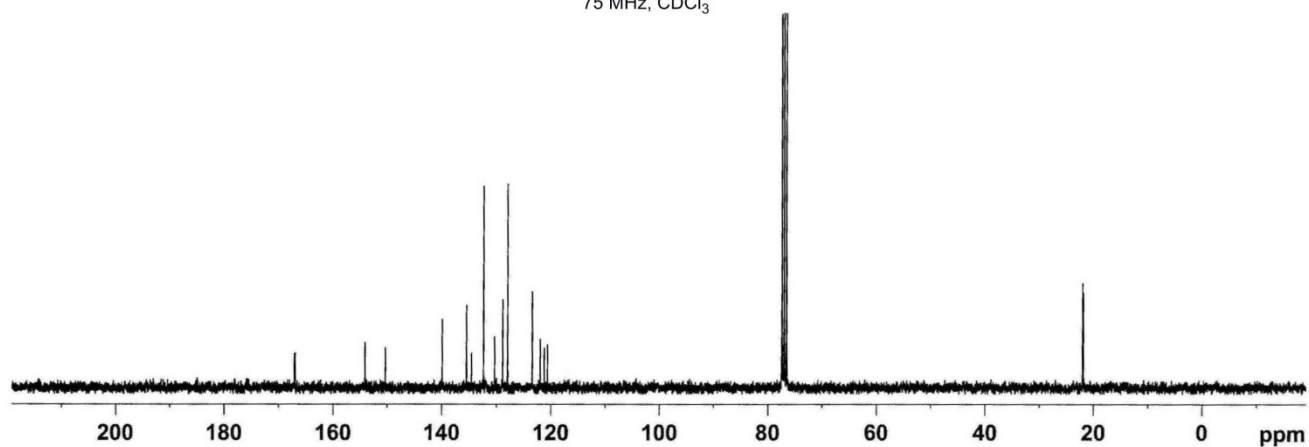
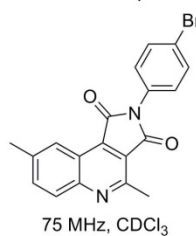
Unsaturation (U.S.): -0.5 - 100.0

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
317.0925	22.0	-0.4 / -0.1	14.5	C 19 H 13 N 2 O 3
332.1162	100.0	+0.3 / +0.1	14.0	C 20 H 16 N 2 O 3
333.1185	23.6			

¹H NMR of Compound **18**

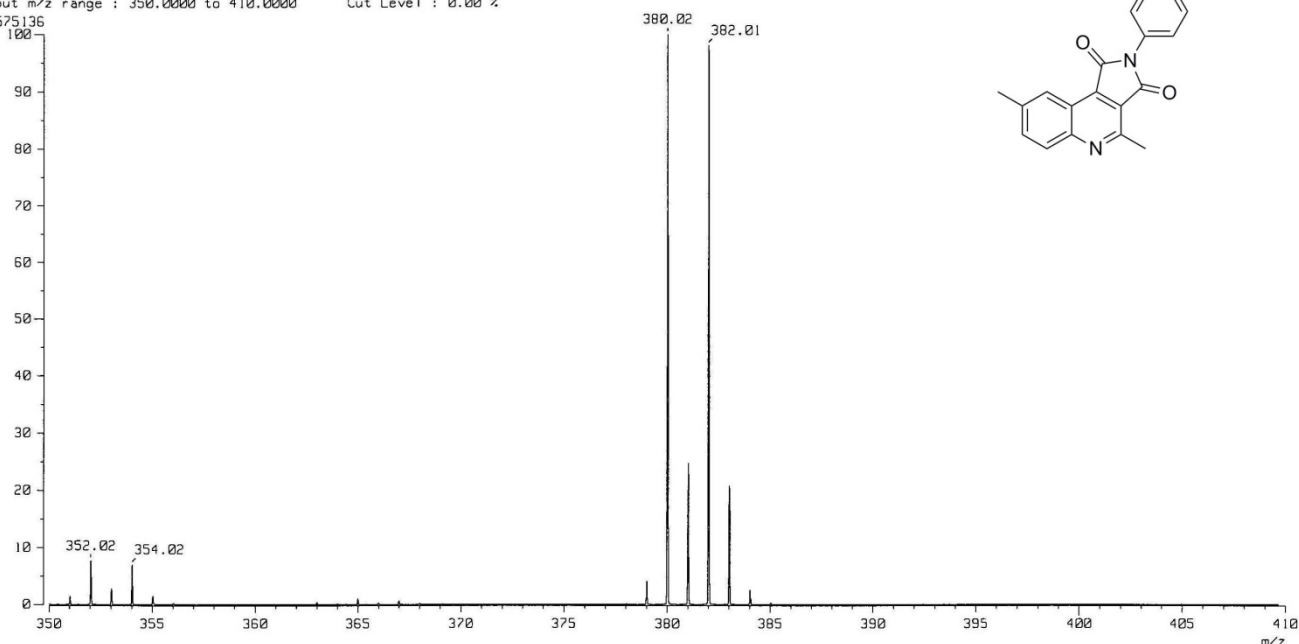
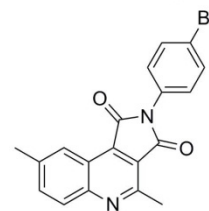


¹³C NMR of Compound **18**



[Mass Spectrum]
Data : 7p-C19H13BrN2O2 Date : 06-Dec-2012 11:31
Sample : -
Note : -
Inlet : Direct Ion Mode : EI+
Spectrum Type : Normal Ion [EF-Linear]
RT : 0.58 min Scan# : (12,13)
BP : m/z 380.0160 Int. : 75.11
Output m/z range : 350.0000 to 410.0000 Cut Level : 0.00 %

Mass spectrum of Compound 18



[Elemental Composition]

Data : 7p-C19H13BrN2O2

Date : 06-Dec-2012 11:31

Page: 1

Sample: -

Note : -

Inlet : Direct

Ion Mode : EI+

RT : 0.58 min

Scan#: (12,13)

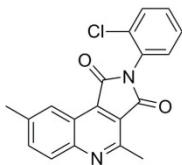
Elements : C 19/0, H 13/0, Br 1/0, N 2/0, O 2/0

Mass Tolerance : 1000ppm, 2mmu if m/z < 2, 3mmu if m/z > 3

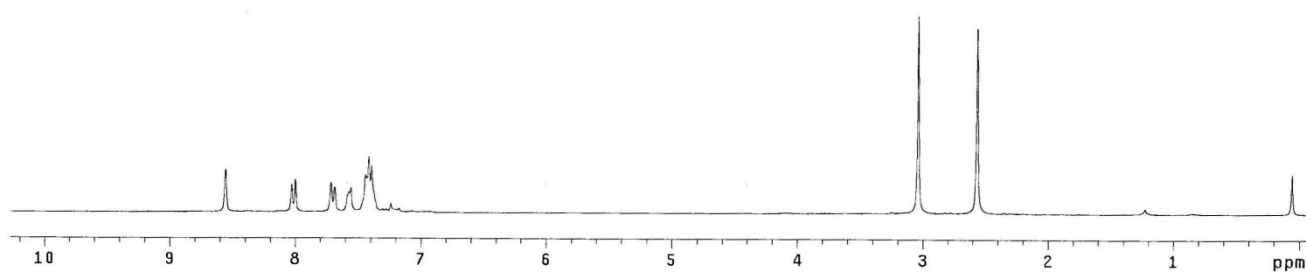
Unsaturation (U.S.) : -0.5 - 100.0

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
380.0160	100.0	-0.1 / +0.0	14.0	C 19 H 13 Br N 2 O 2
381.0167	24.8			
382.0141	98.1			
383.0172	20.9			

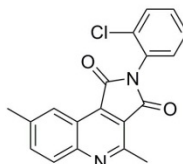
¹H NMR of Compound **19**



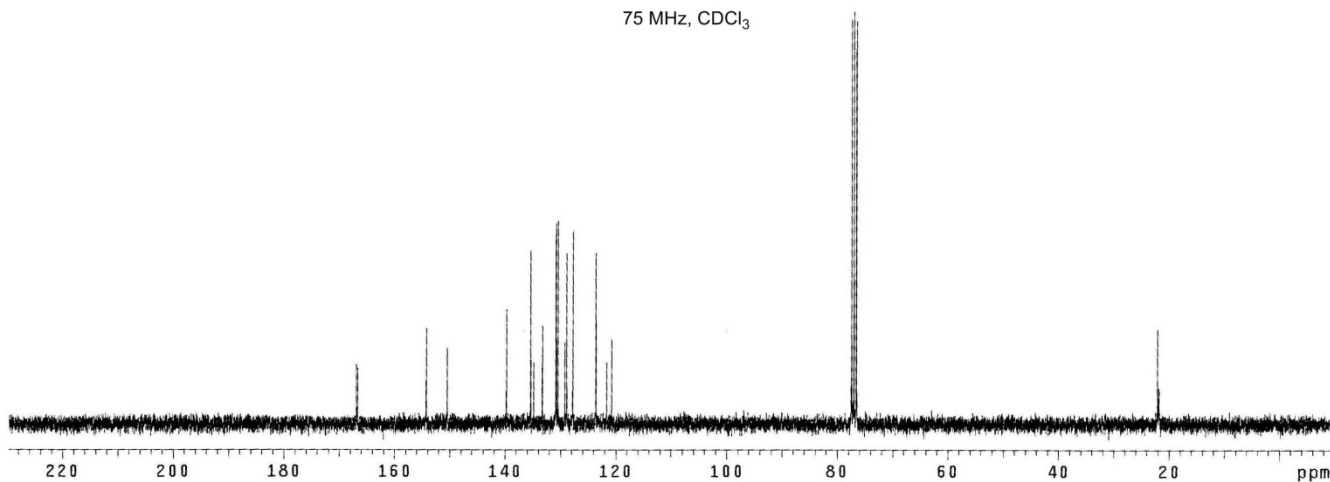
300 MHz, CDCl₃



¹³C NMR of Compound **19**

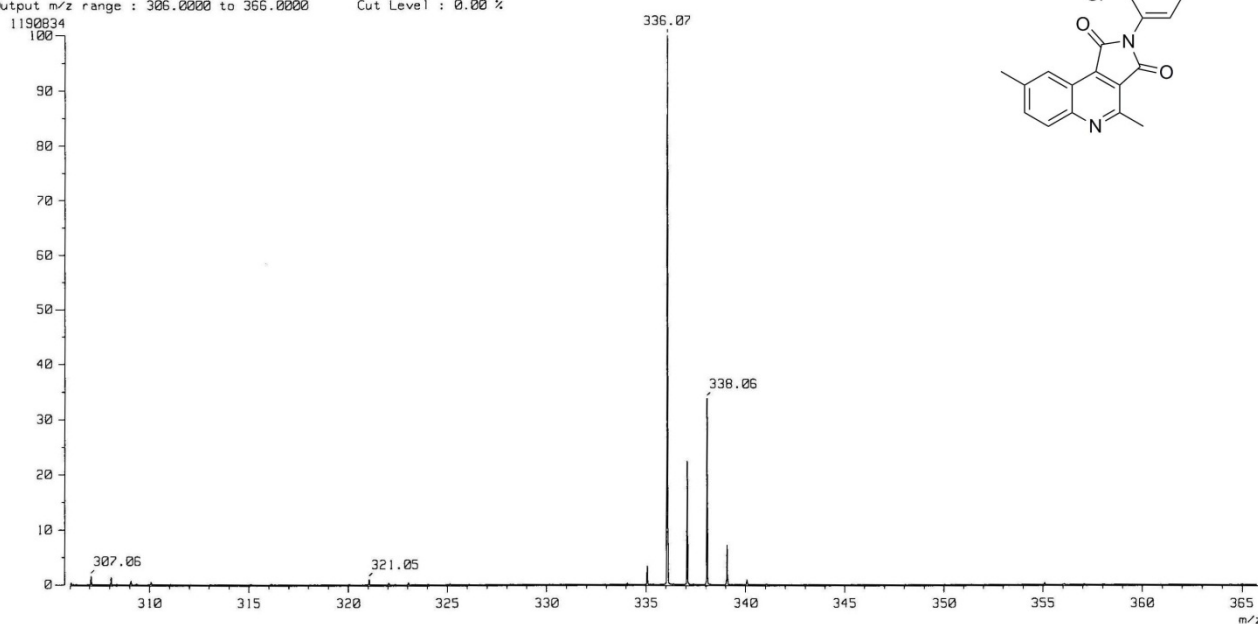
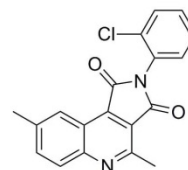


75 MHz, CDCl₃



[Mass Spectrum]
Data : 7-gamma-C19H13ClN2O2 Date : 12-Dec-2012 11:52
Sample: -
Note: -
Inlet: Direct Ion Mode: EI+
Spectrum Type: Normal Ion [EF-Linear]
RT: 0.58 min Scan#: (12,13)
BP: m/z 336.0665 Int.: 56.78
Output m/z range: 306.0000 to 366.0000 Cut Level: 0.00 %

Mass spectrum of Compound 19



[Elemental Composition]

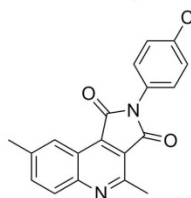
Data : 7-gamma-C19H13ClN2O2
Sample: -
Note: -
Inlet: Direct
RT: 0.58 min
Elements: C 19/0, H 13/0, Cl 1/0, N 2/0, O 2/0
Mass Tolerance: 1000ppm, 2mmu if m/z < 2, 3mmu if m/z > 3
Unsaturation (U.S.): -0.5 - 100.0

Date : 12-Dec-2012 11:52

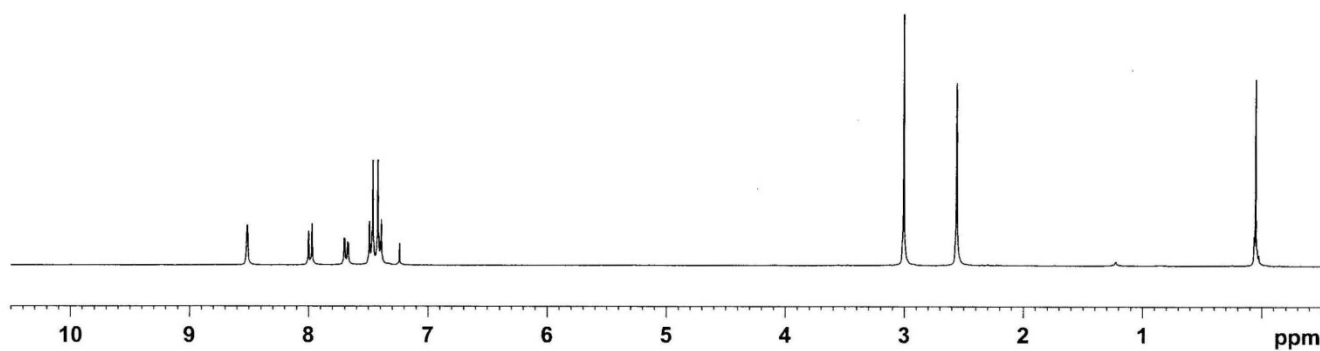
Page: 1

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
336.0665	100.0	-0.1 / +0.0	14.0	C 19 H 13 Cl N 2 O 2
337.0697	22.5			
338.0629	33.8			

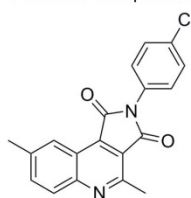
¹H NMR of Compound **20**



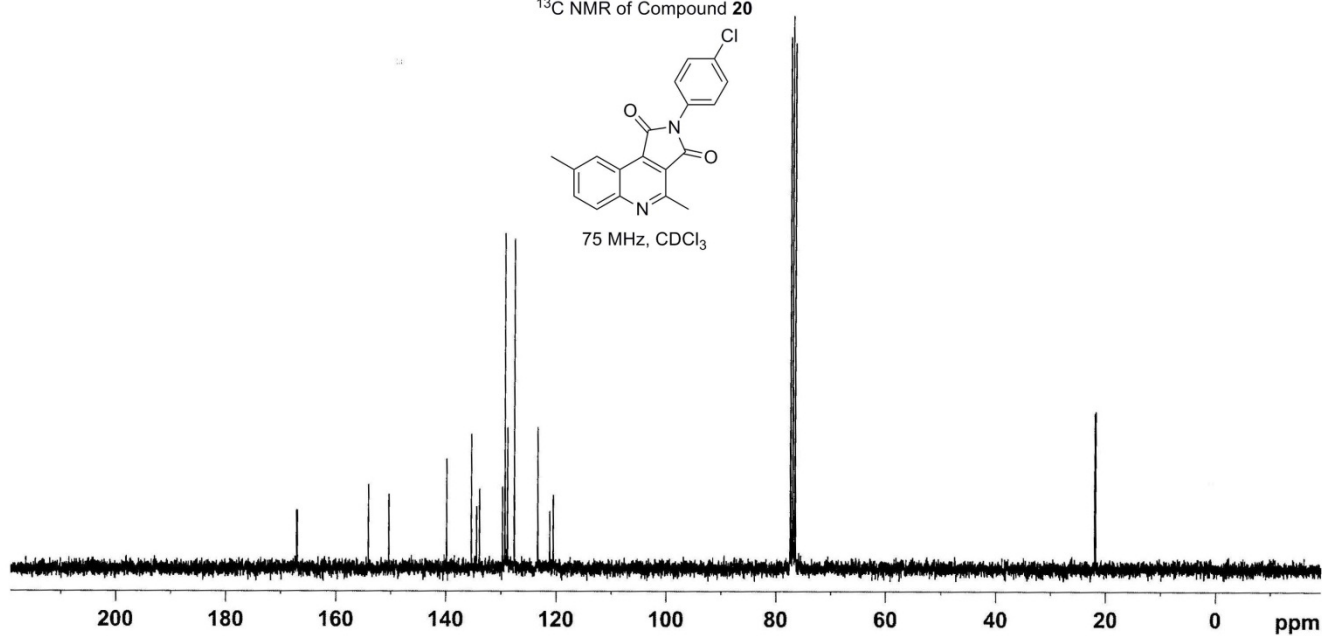
300 MHz, CDCl₃



¹³C NMR of Compound **20**

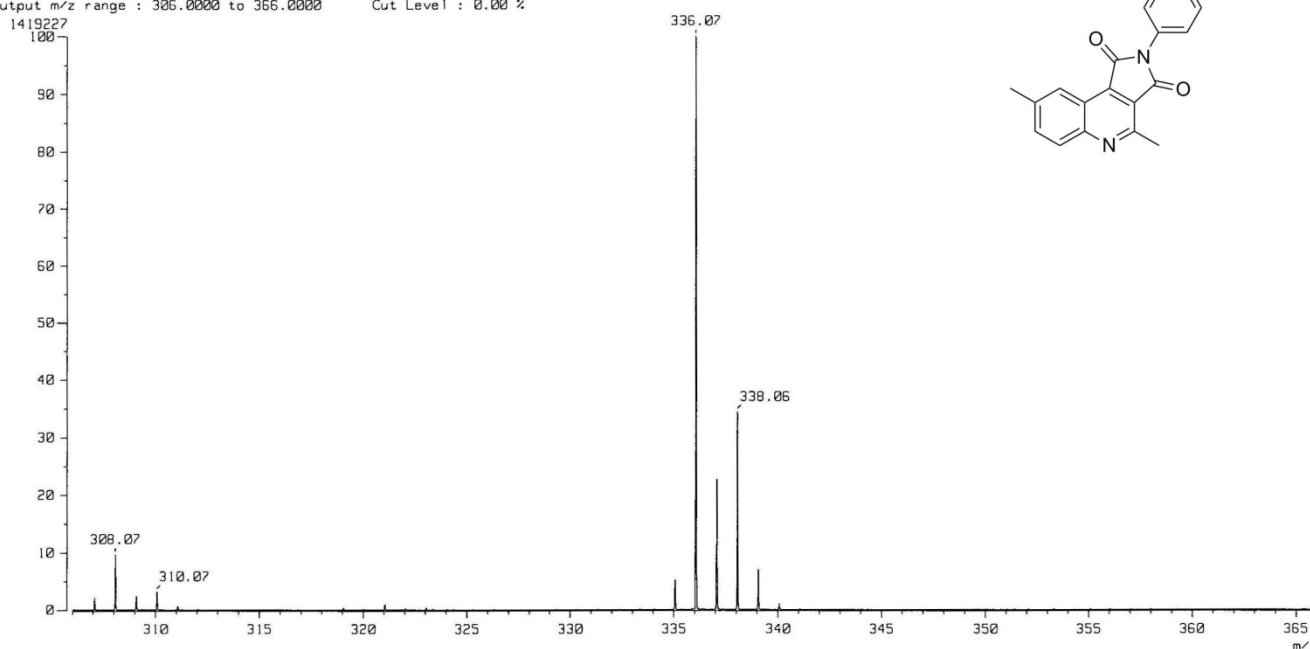
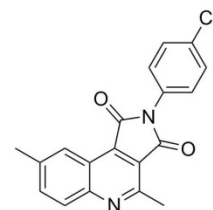


75 MHz, CDCl₃



[Mass Spectrum]
Data : 7y-C19H13ClN2O2 Date : 12-Dec-2012 11:31
Sample: -
Note: -
Inlet : Direct Ion Mode : EI+
Spectrum Type : Normal Ion [EF-Linear]
RT : 0.58 min Scan# : (12,13)
BP : m/z 336.0664 Int. : 67.67
Output m/z range : 305.0000 to 366.0000 Cut Level : 0.00 %

Mass spectrum of Compound 20



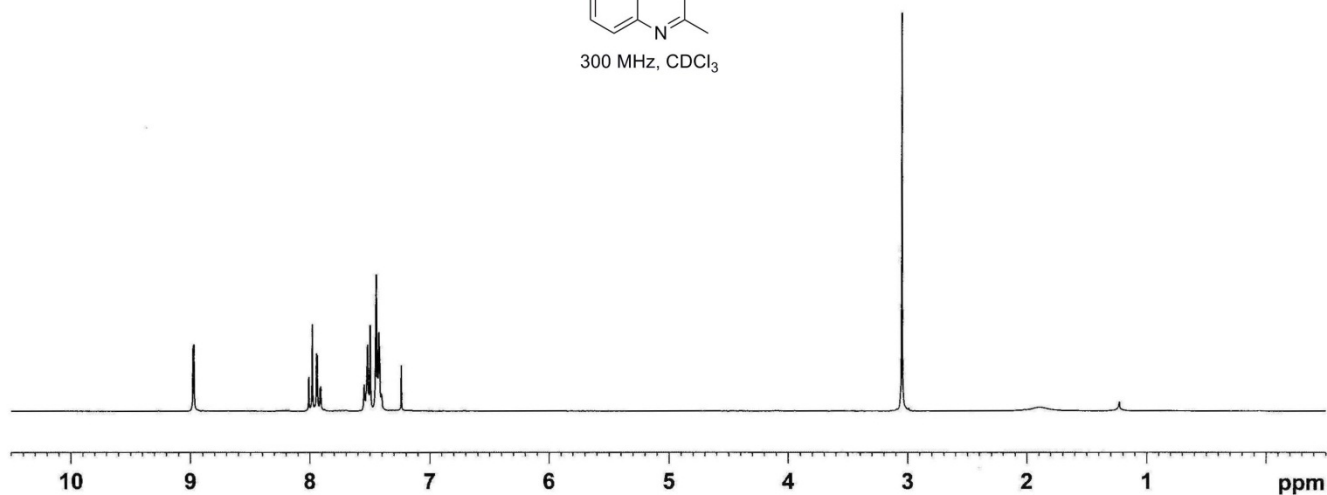
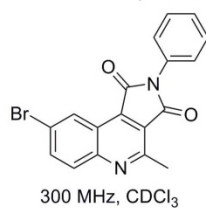
[Elemental Composition]

Page: 1

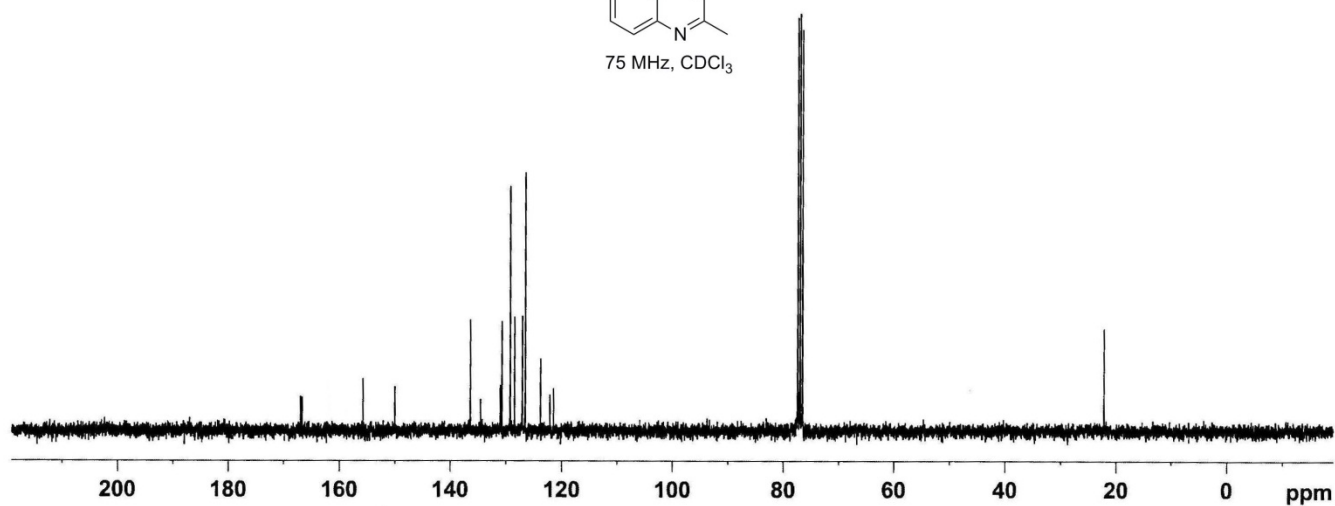
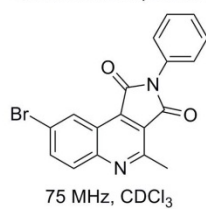
Data : 7y-C19H13ClN2O2 Date : 12-Dec-2012 11:31
Sample: -
Note: -
Inlet : Direct Ion Mode : EI+
RT : 0.58 min Scan#: (12,13)
Elements : C 19/0, H 13/0, Cl 1/0, N 2/0, O 2/0
Mass Tolerance : 1000ppm, 2mmu if m/z < 2, 3mmu if m/z > 3
Unsaturation (U.S.) : -0.5 - 100.0

Observed m/z	Int%	Err[ppm / mmu]	U.S. Composition
336.0664	100.0	-0.4 / -0.1	14.0 C 19 H 13 Cl N 2 O 2
337.0697	22.7		
338.0642	34.4		

¹H NMR of Compound **21**

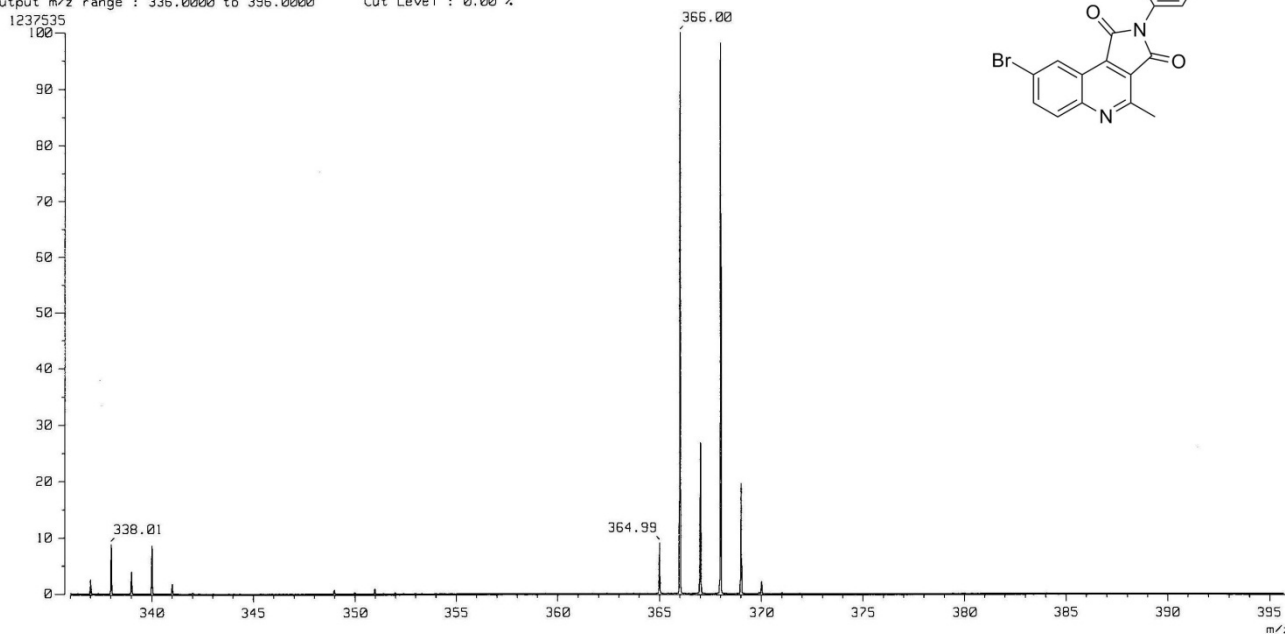
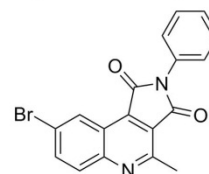


¹³C NMR of Compound **21**



[Mass Spectrum]
Data : 7b-C18H11BrN2O2 Date : 06-Dec-2012 10:37
Sample: -
Note: -
Inlet: Direct Ion Mode: EI+
Spectrum Type: Normal Ion [EF-Linear]
RT: 0.88 min Scan#: (18,19)
BP: m/z 366.0001 Int.: 59.01
Output m/z range: 335.0000 to 396.0000 Cut Level: 0.00 %

Mass spectrum of Compound **21**



[Elemental Composition]

Data : 7b-C18H11BrN2O2

Date : 06-Dec-2012 10:37

Page: 1

Sample: -

Note: -

Inlet: Direct

Ion Mode: EI+

RT: 0.88 min

Scan#: (18,19)

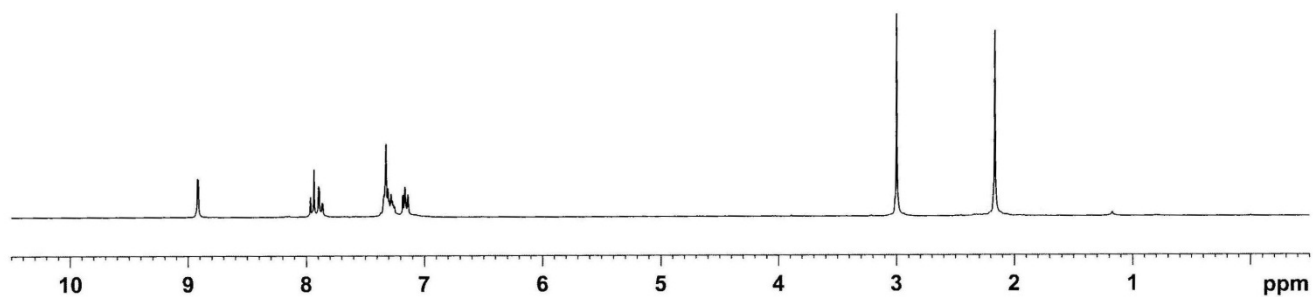
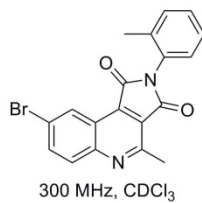
Elements : C 18/0, H 11/0, Br 1/0, N 2/0, O 2/0

Mass Tolerance : 1000ppm, 2mmu if m/z < 2, 3mmu if m/z > 3

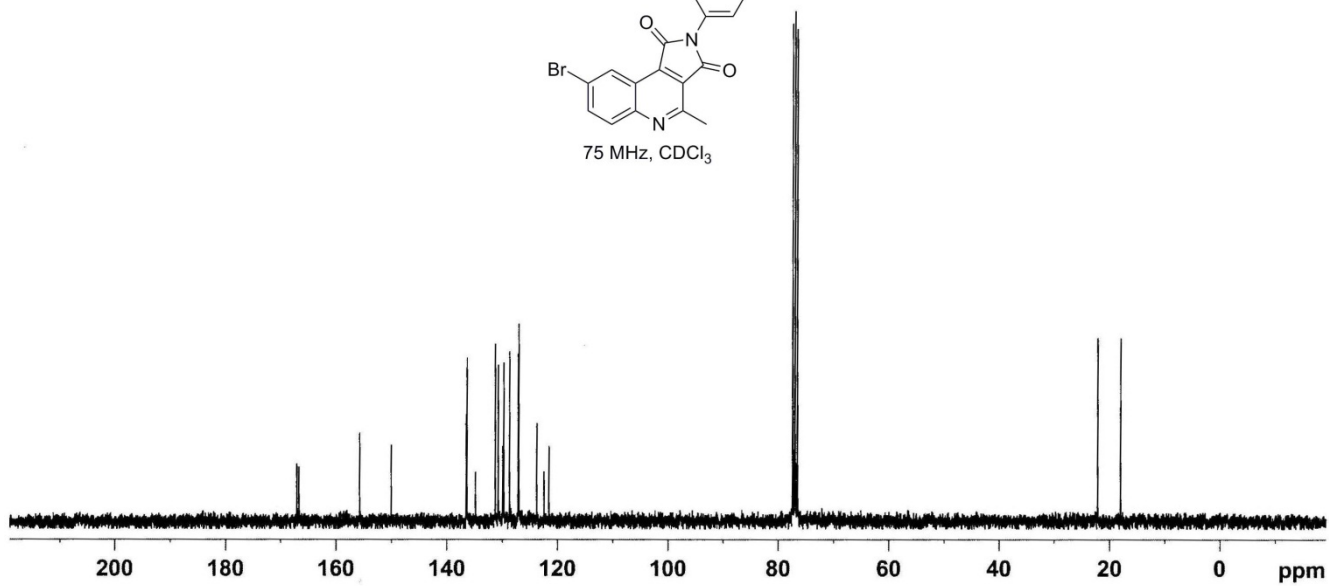
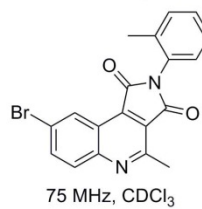
Unsaturation (U.S.) : -0.5 - 100.0

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
366.0001	100.0	-0.7 / -0.3	14.0	C 18 H 11 Br N 2 O 2
366.9999	26.9			
367.9973	98.2			
369.0015	19.7			

¹H NMR of Compound **22**

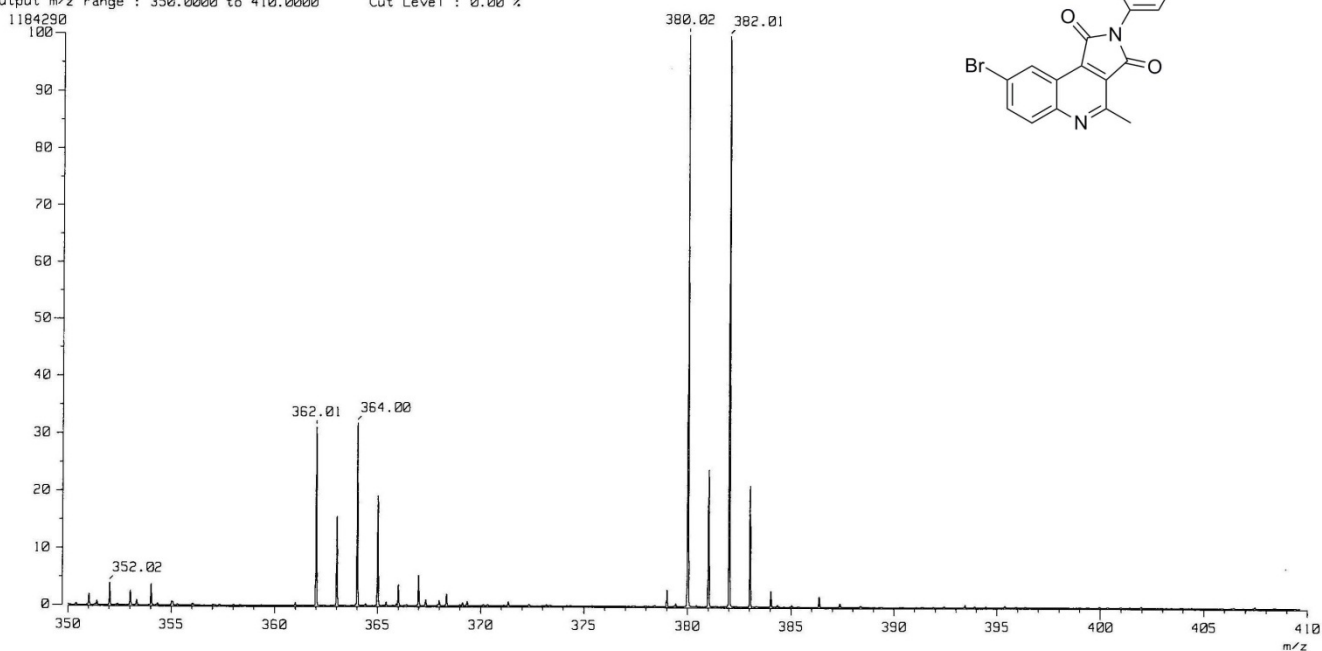
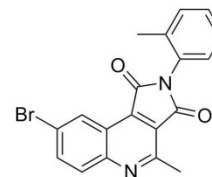


¹³C NMR of Compound **22**



[Mass Spectrum]
Data : 7-zeta-C19H13BrN2O2 Date : 12-Dec-2012 12:02
Sample: -
Note: -
Inlet : Direct Ion Mode : EI+
Spectrum Type : Normal Ion [EF-Linear]
RT : 0.78 min Scan# : (16,17)
BP : m/z 380.0159 Int. : 56.47
Output m/z range : 350.0000 to 410.0000 Cut Level : 0.00 %

Mass spectrum of Compound 22



[Elemental Composition]

Page: 1

Data : 7-zeta-C19H13BrN2O2

Date : 12-Dec-2012 12:02

Sample: -

Note: -

Inlet : Direct

Ion Mode : EI+

RT : 0.78 min

Scan#: (16,17)

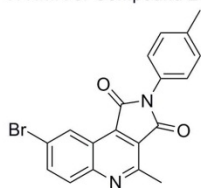
Elements : C 19/0, H 13/0, Br 1/0, N 2/0, O 2/0

Mass Tolerance : 1000ppm, 2mmu if m/z < 2, 3mmu if m/z > 3

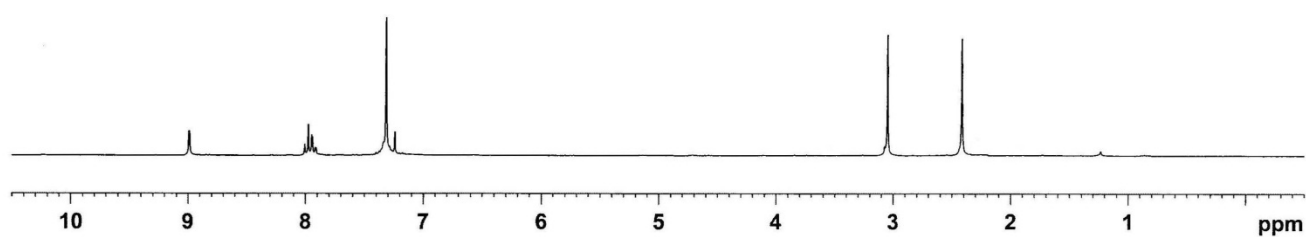
Unsaturation (U.S.) : -0.5 - 100.0

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
362.0051	31.1	-1.1 / -0.4	15.0	C 19 H 11 Br N 2 O
363.0097	15.6			
364.0019	31.9			
365.0041	19.3	-2.8 / -1.0	14.0	C 19 H 12 Br N O 2
380.0159	100.0	-0.3 / -0.1	14.0	C 19 H 13 Br N 2 O 2
381.0167	23.9			
382.0138	99.8			
383.0160	21.1			

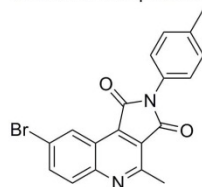
^1H NMR of Compound **23**



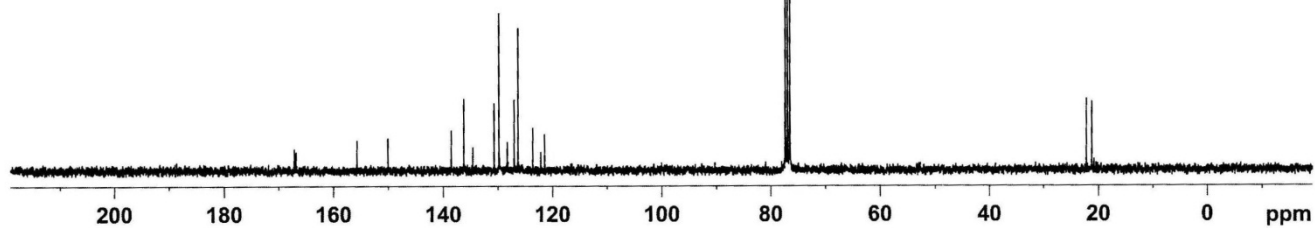
300 MHz, CDCl_3



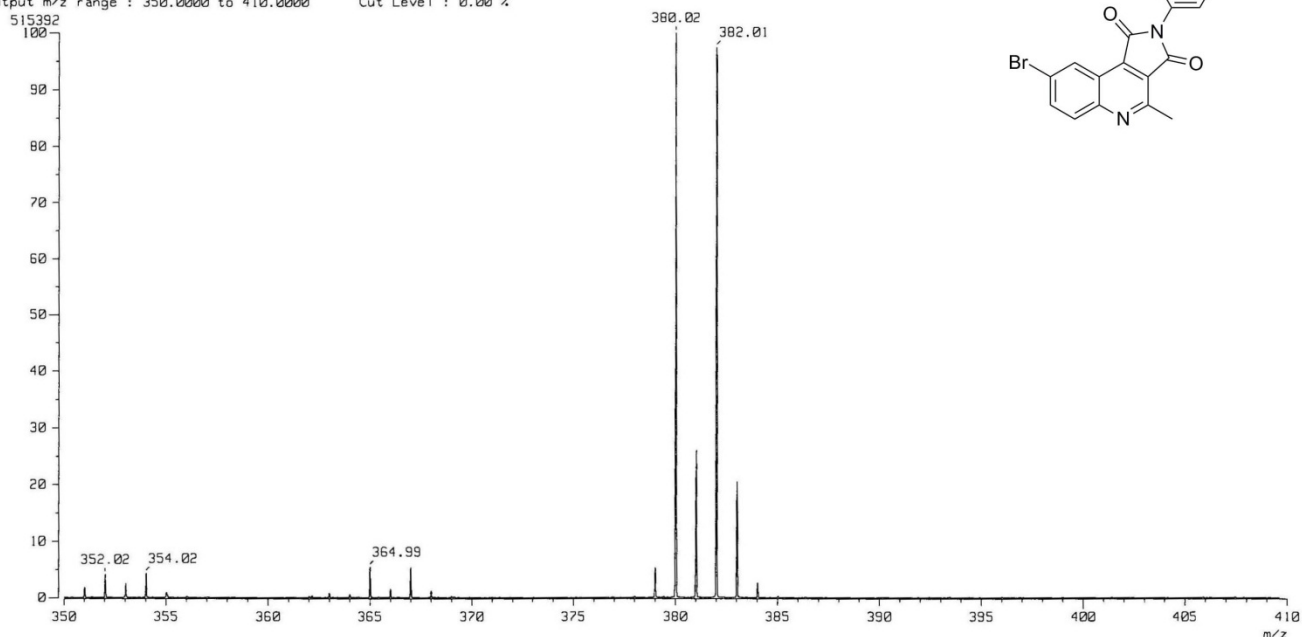
^{13}C NMR of Compound **23**



75 MHz, CDCl_3



[Mass Spectrum]
Data : 7s-C19H13BrN2O2 Date : 12-Dec-2012 11:00
Sample: -
Note : -
Inlet : Direct Ion Mode : EI+
Spectrum Type : Normal Ion [EF-Linear]
RT : 0.83 min Scan# : (17,18)
BP : m/z 380.0158 Int. : 24.58
Output m/z range : 350.0000 to 410.0000 Cut Level : 0.00 %



[Elemental Composition]

Data : 7s-C19H13BrN2O2

Date : 12-Dec-2012 11:00

Page: 1

Sample: -

Note : -

Inlet : Direct

Ion Mode : EI+

RT : 0.83 min

Scan#: (17,18)

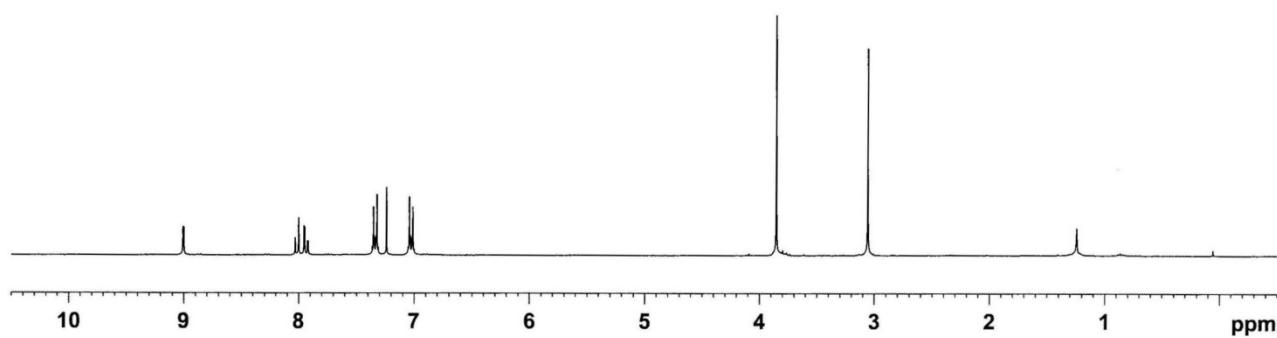
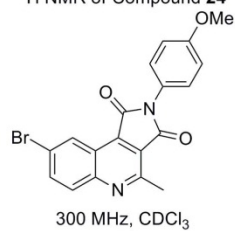
Elements : C 19/0, H 13/0, Br 1/0, N 2/0, O 2/0

Mass Tolerance : 1000ppm, 2mmu if m/z < 2, 3mmu if m/z > 3

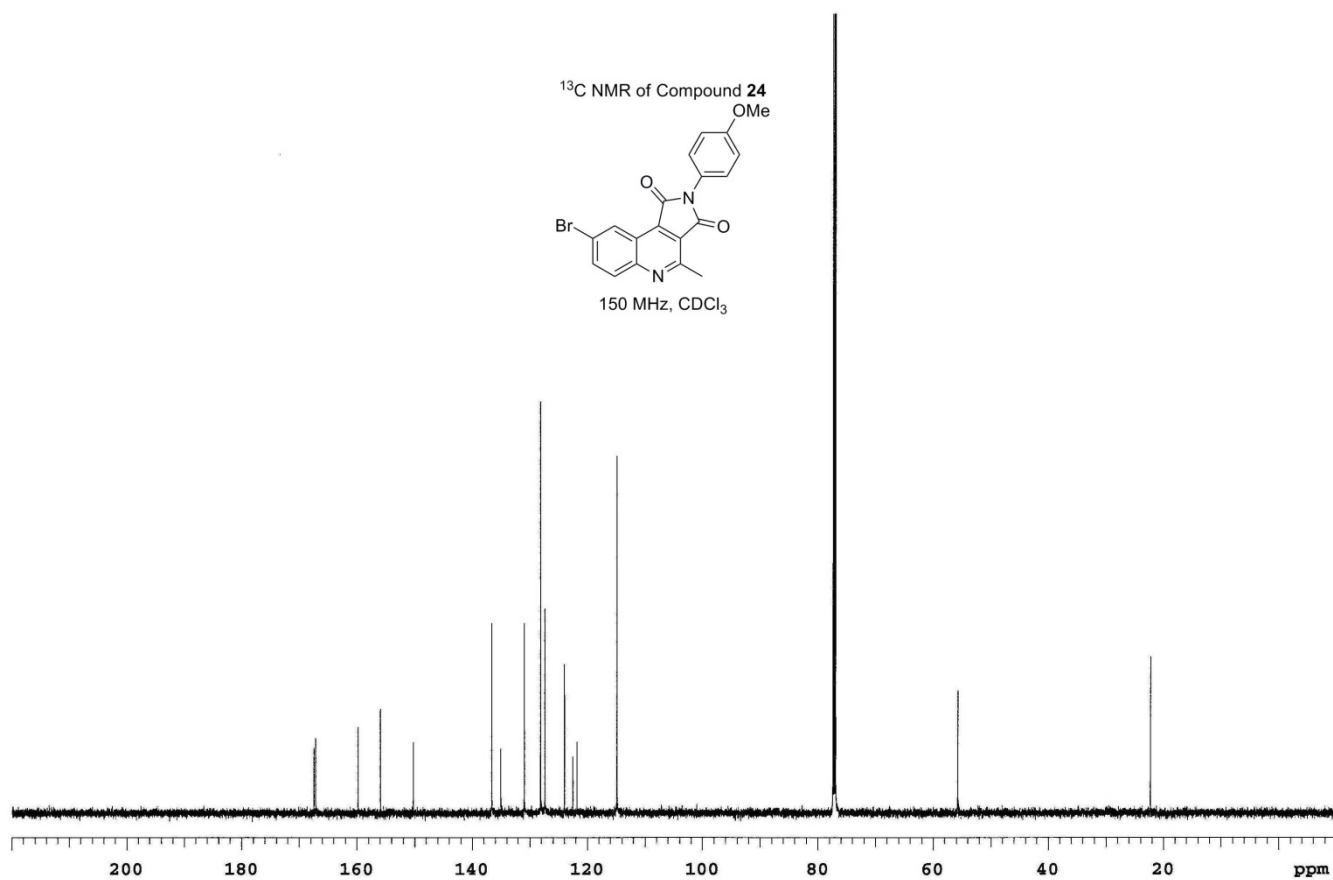
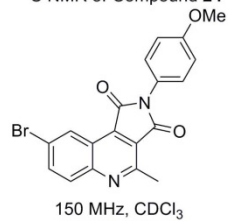
Unsaturation (U.S.) : -0.5 - 100.0

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
380.0158	100.0	-0.7 / -0.3	14.0	C 19 H 13 Br N 2 O 2
381.0158	26.1			
382.0135	97.5			
383.0173	20.6			

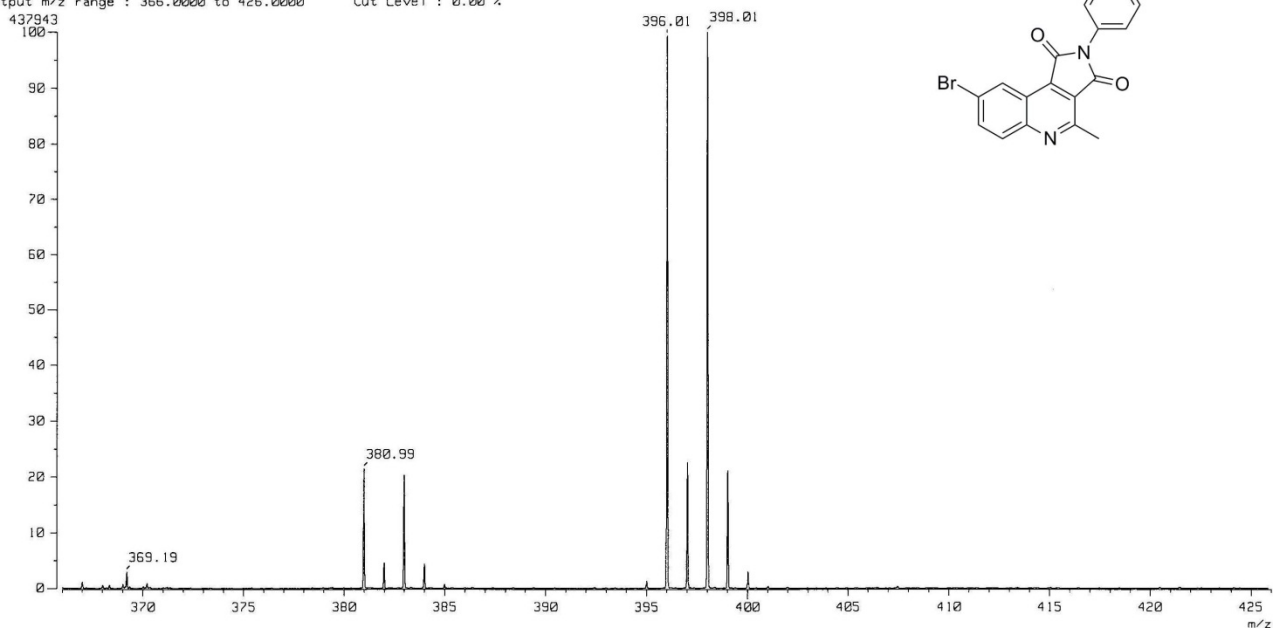
¹H NMR of Compound **24**



¹³C NMR of Compound **24**



[Mass Spectrum]
Data : X3-27-C19H13BrN2O3 Date : 18-Sep-2012 11:47
Sample: -
Note: -
Inlet : Direct Ion Mode : EI+
Spectrum Type : Normal Ion [EF-Linear]
RT : 0.88 min Scan#: (18,19)
BP : m/z 398.0094 Int. : 20.88
Output m/z range : 366.0000 to 426.0000 Cut Level : 0.00 %



[Elemental Composition]

Data : X3-27-C19H13BrN2O3

Date : 18-Sep-2012 11:47

Page: 1

Sample: -

Note: -

Inlet : Direct

Ion Mode : EI+

RT : 0.88 min

Scan#: (18,19)

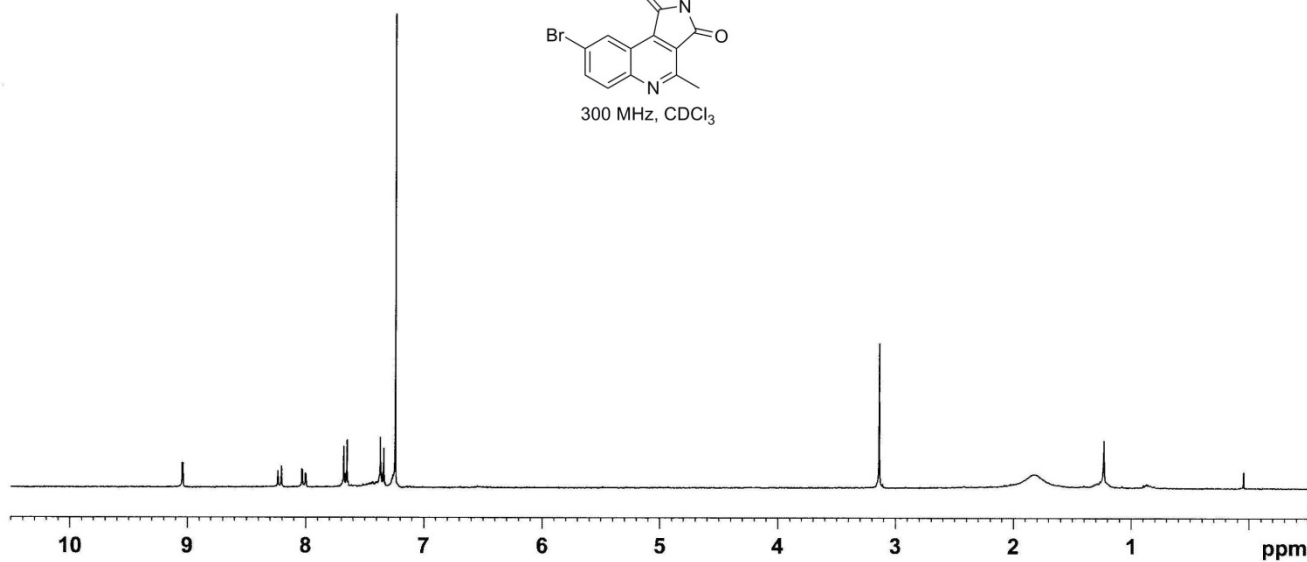
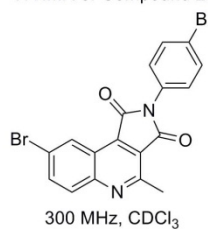
Elements : C 19/0, H 13/0, Br 1/0, N 2/0, O 3/0

Mass Tolerance : 1000ppm, 2mmu if m/z < 2, 3mmu if m/z > 3

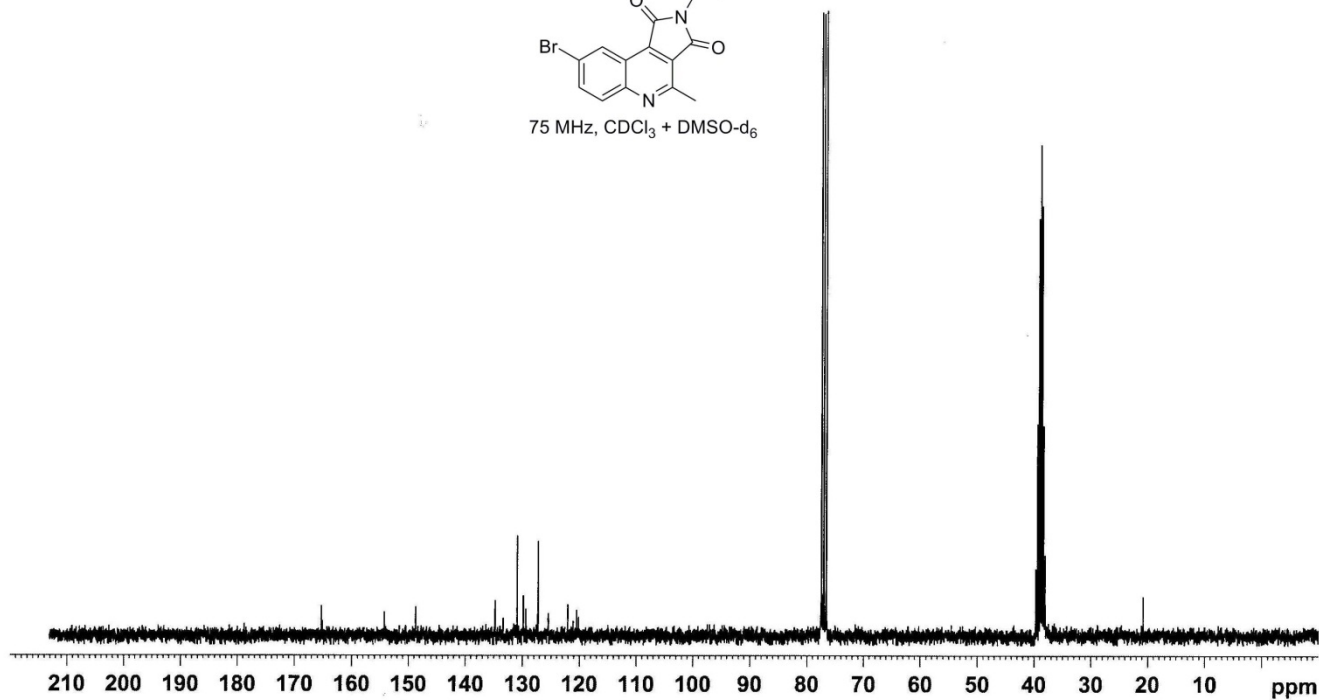
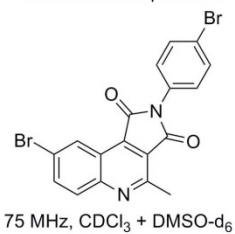
Unsaturation (U.S.) : -0.5 - 100.0

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
380.9876	21.4	+0.4 / +0.2	14.5	C 18 H 10 Br N 2 O 3
382.9846	20.4			
396.0110	99.3	+0.1 / +0.0	14.0	C 19 H 13 Br N 2 O 3
397.0132	22.6			
398.0094	100.0			
399.0126	21.1			

¹H NMR of Compound **25**

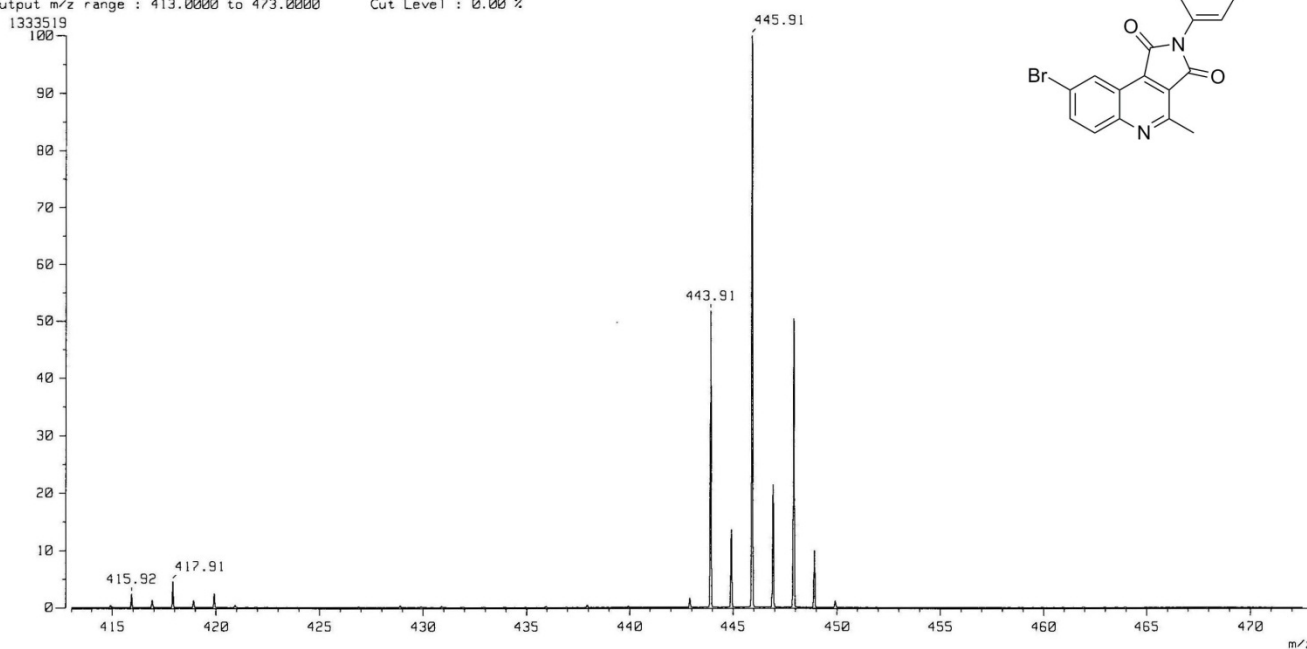
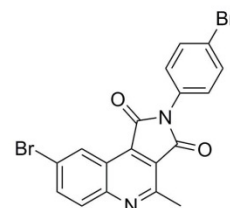


¹³C NMR of Compound **25**



[Mass Spectrum]
Data : 7n-C18H10Br2N2O2 Date : 06-Dec-2012 11:20
Sample: -
Note: -
Inlet: Direct Ion Mode: EI+
Spectrum Type: Normal Ion [EF-Linear]
RT: 0.98 min Scan#: (20,21)
BP: m/z 445.9103 Int.: 63.59
Output m/z range: 413.0000 to 473.0000 Cut Level: 0.00 %

Mass spectrum of Compound 25



[Elemental Composition]

Data : 7n-C18H10Br2N2O2

Date : 06-Dec-2012 11:20

Page: 1

Sample: -

Note: -

Inlet: Direct

Ion Mode: EI+

RT: 0.98 min

Scan#: (20,21)

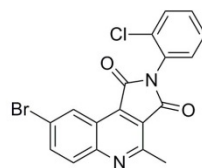
Elements: C 18/0, H 10/0, Br 2/0, N 2/0, O 2/0

Mass Tolerance: 1000ppm, 2mmu if m/z < 2, 3mmu if m/z > 3

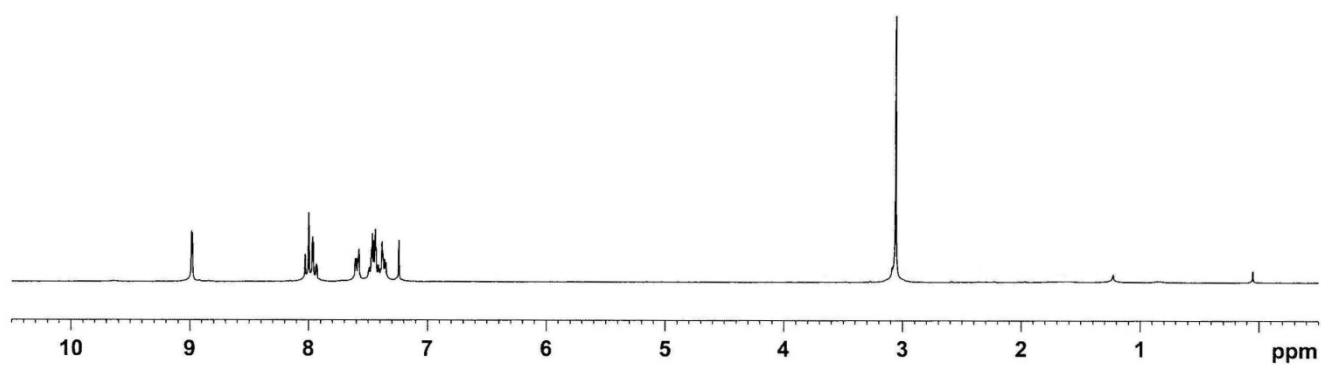
Unsaturation (U.S.): -0.5 - 100.0

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
443.9111	51.8	+0.5 / +0.2	14.0	C 18 H 10 Br 2 N 2 O 2
444.9117	13.6			
445.9103	100.0			
446.9123	21.4			
447.9095	50.4			

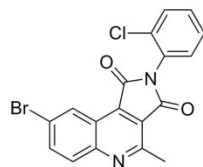
^1H NMR of Compound **26**



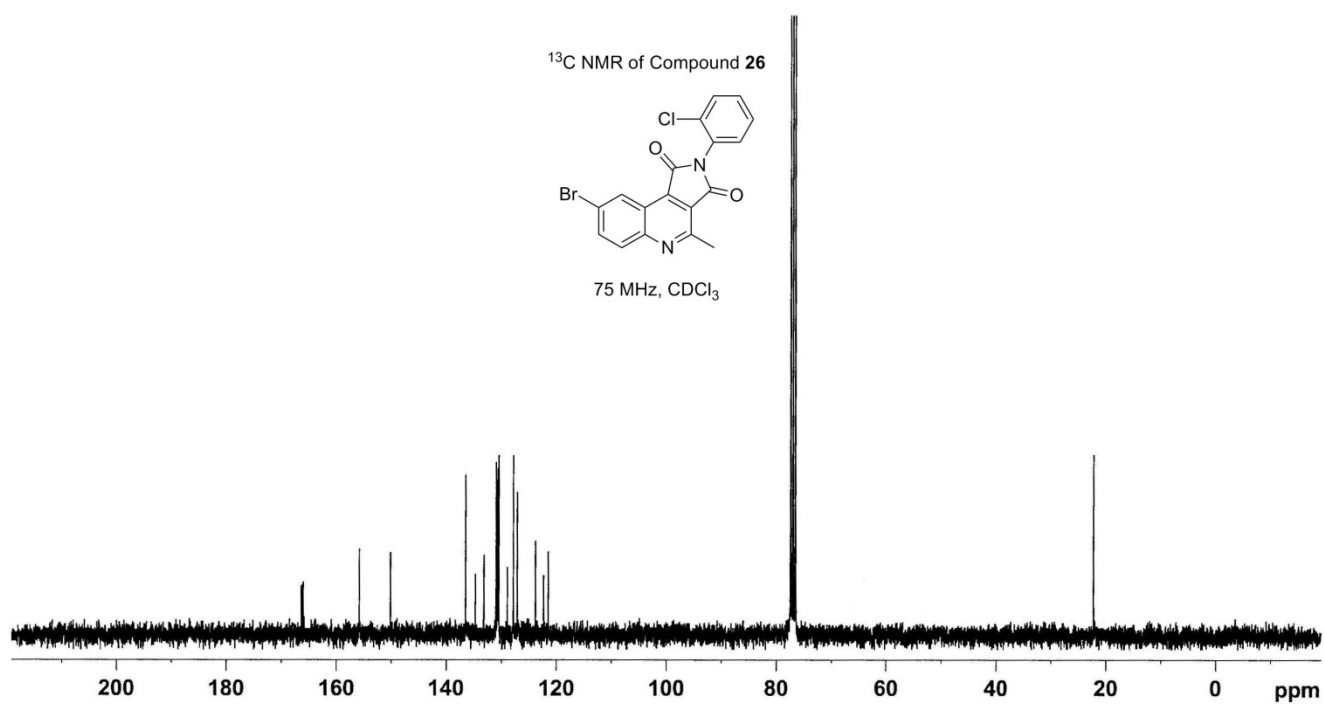
300 MHz, CDCl_3



^{13}C NMR of Compound **26**

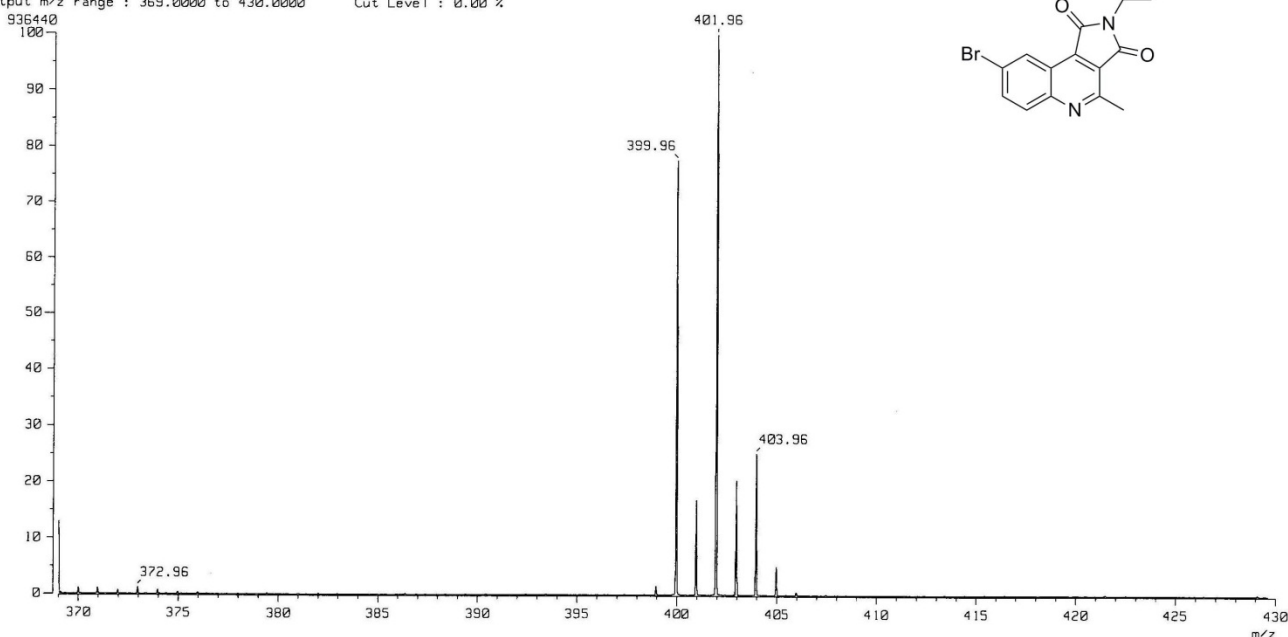
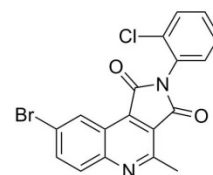


75 MHz, CDCl_3



[Mass Spectrum]
Data : 7-alpha-Cl₁₈H₁₀BrClN₂O₂ Date : 12-Dec-2012 11:40
Sample: -
Note: -
Inlet : Direct Ion Mode : EI+
Spectrum Type : Normal Ion [EF-Linear]
RT : 0.53 min Scan# : (11,12)
BP : m/z 401.9570 Int. : 44.65
Output m/z range : 369.0000 to 430.0000 Cut Level : 0.00 %

Mass spectrum of Compound 26



[Elemental Composition]

Data : 7-alpha-Cl₁₈H₁₀BrClN₂O₂

Date : 12-Dec-2012 11:40

Page: 1

Sample: -

Note: -

Inlet : Direct

Ion Mode : EI+

RT : 0.53 min

Scan#: (11,12)

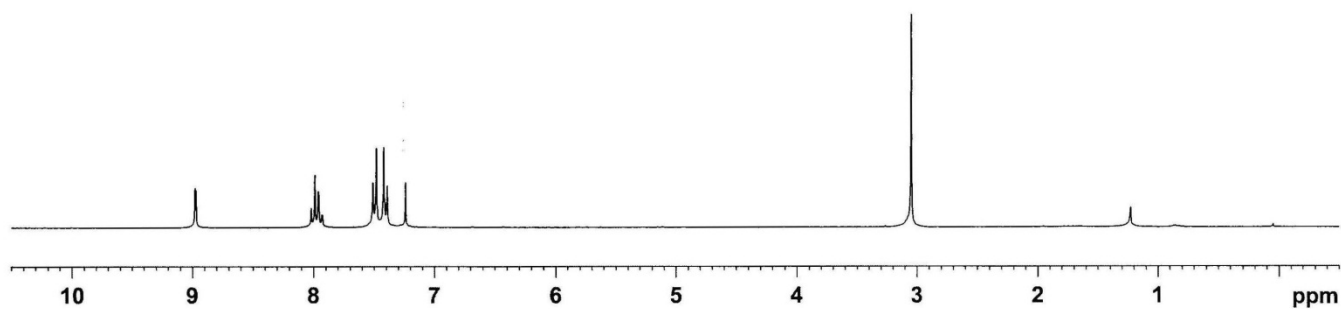
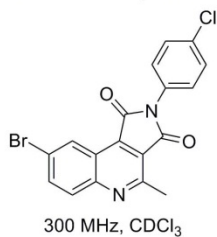
Elements : C 18/0, H 10/0, Br 1/0, Cl 1/0, N 2/0, O 2/0

Mass Tolerance : 1000ppm, 2mmu if m/z < 2, 3mmu if m/z > 3

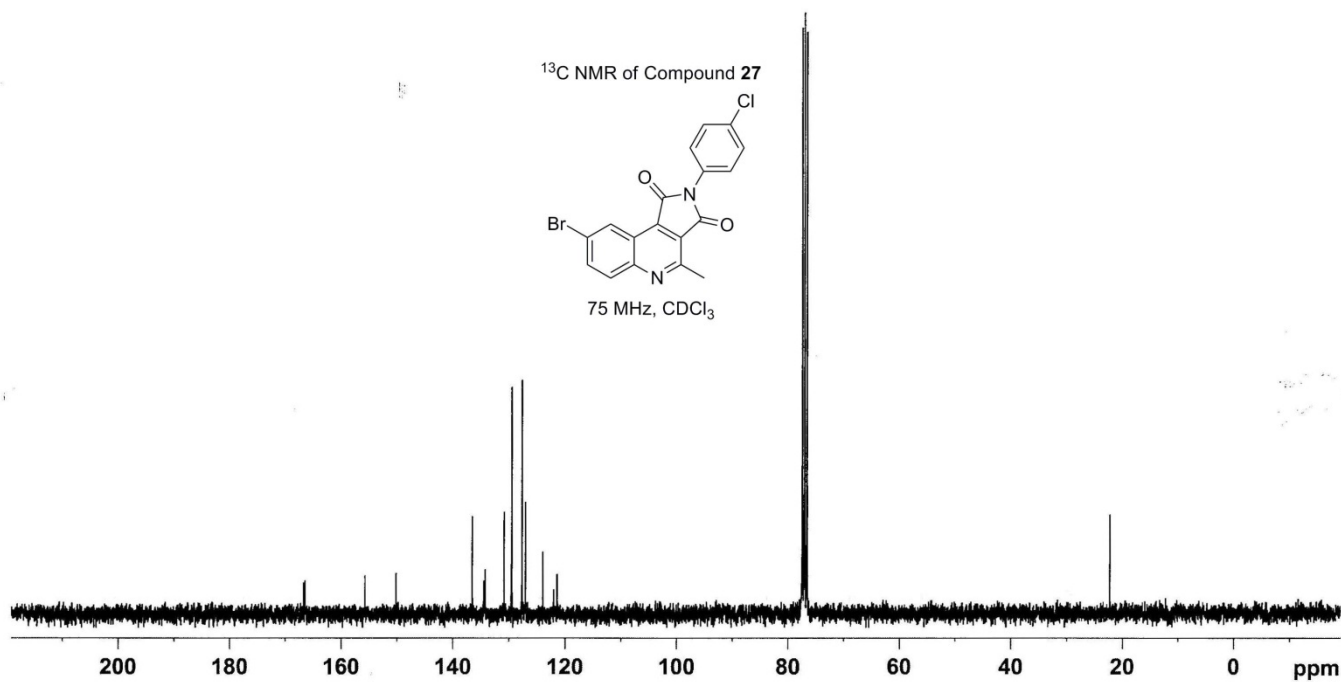
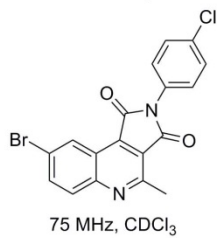
Unsaturation (U.S.) : -0.5 - 100.0

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
399.9613	77.7	-0.4 / -0.1	14.0	C 18 H 10 Br Cl N 2 O 2
400.9624	17.0			
401.9570	100.0			
402.9604	20.5			
403.9572	25.2			

¹H NMR of Compound 27

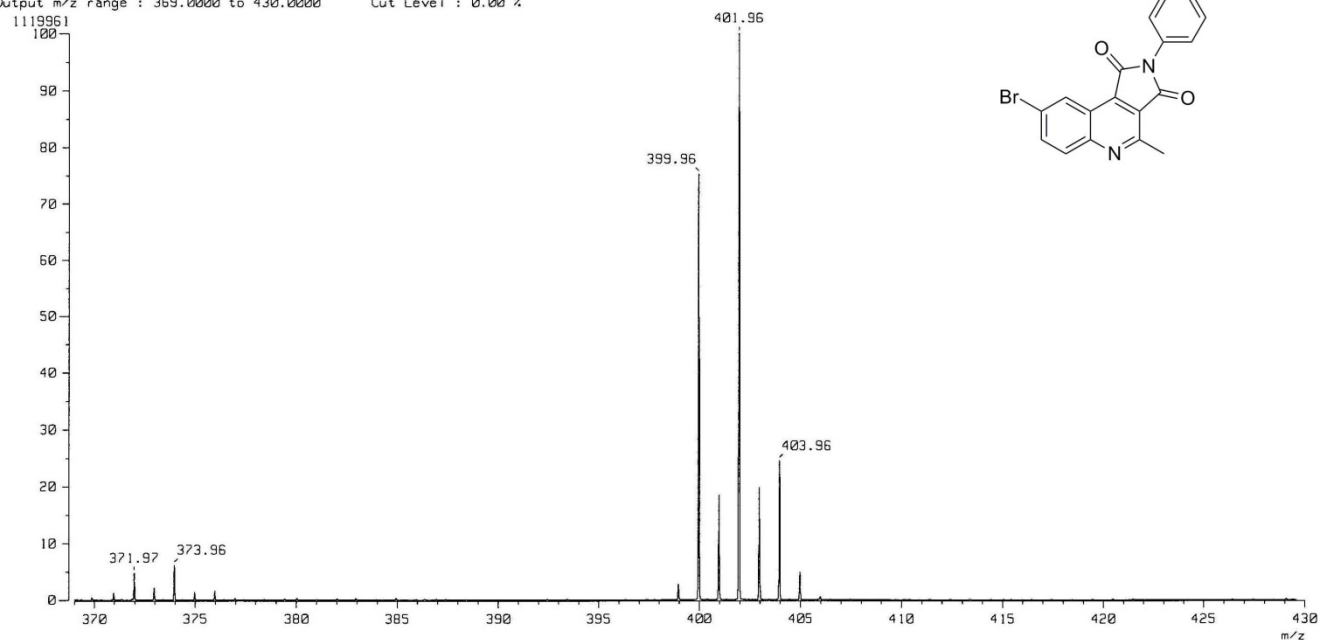
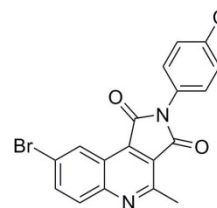


¹³C NMR of Compound 27



[Mass Spectrum]
Data : 7w-C18H10BrClN2O2 Date : 12-Dec-2012 11:21
Sample: -
Note: -
Inlet : Direct Ion Mode : EI+
Spectrum Type : Normal Ion (EF-Linear)
RT : 1.28 min Scan#: (26,27)
BP : m/z 401.9587 Int. : 53.40
Output m/z range : 369.0000 to 430.0000 Cut Level : 0.00 %

Mass spectrum of Compound 27



[Elemental Composition]

Data : 7w-C18H10BrClN2O2

Date : 12-Dec-2012 11:21

Page: 1

Sample: -

Note: -

Inlet : Direct

Ion Mode : EI+

RT : 1.28 min

Scan#: (26,27)

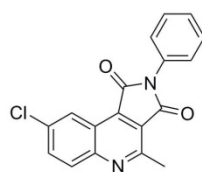
Elements : C 18/0, H 10/0, Br 1/0, Cl 1/0, N 2/0, O 2/0

Mass Tolerance : 1000ppm, 2mmu if m/z < 2, 3mmu if m/z > 3

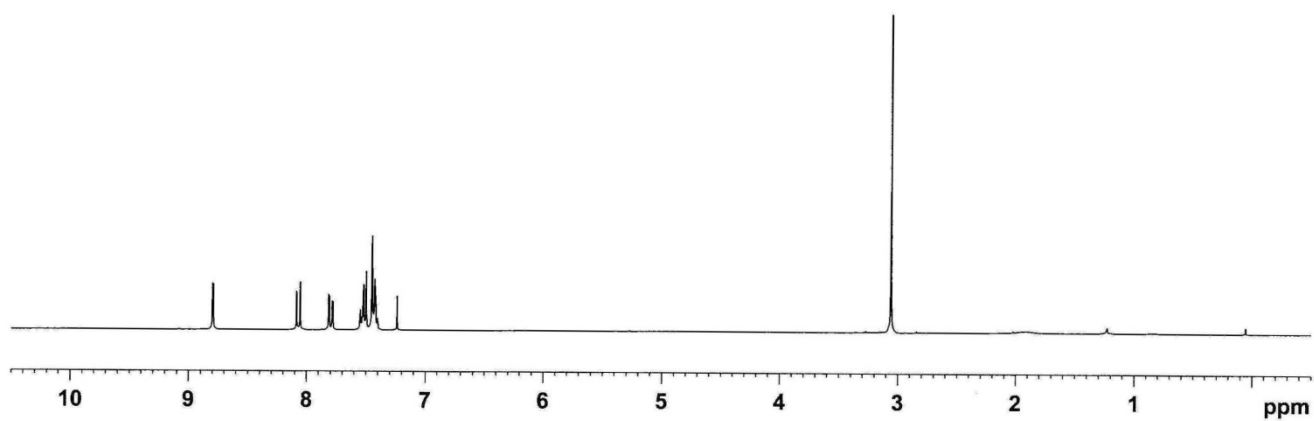
Unsaturation (U.S.) : -0.5 - 100.0

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
399.9612	75.2	-0.6 / -0.2	14.0	C 18 H 10 Br Cl N 2 O 2
400.9617	18.5			
401.9587	100.0			
402.9601	19.8			
403.9554	24.5			

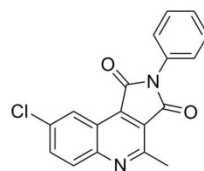
¹H NMR of Compound **28**



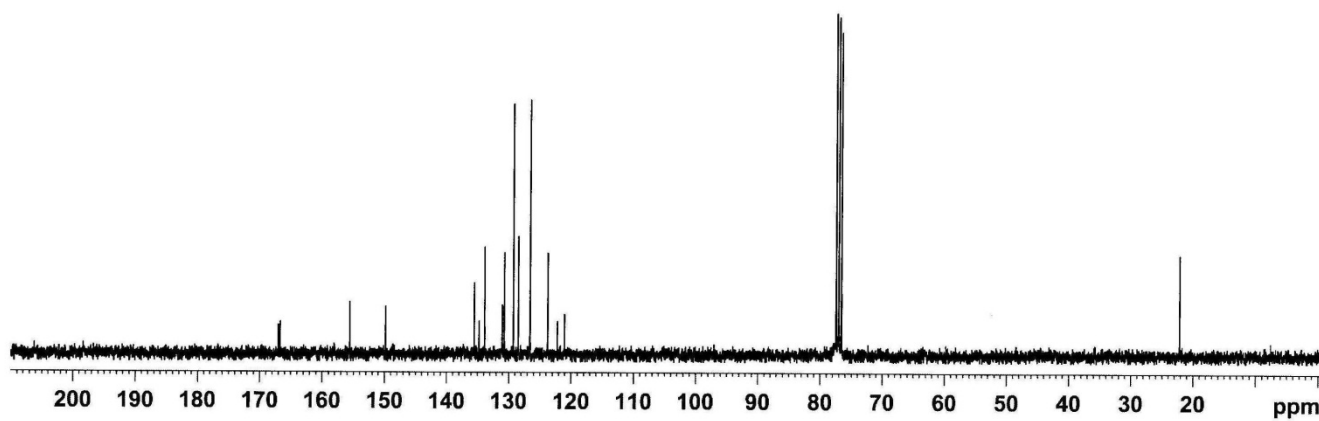
300 MHz, CDCl₃



¹³C NMR of Compound **28**

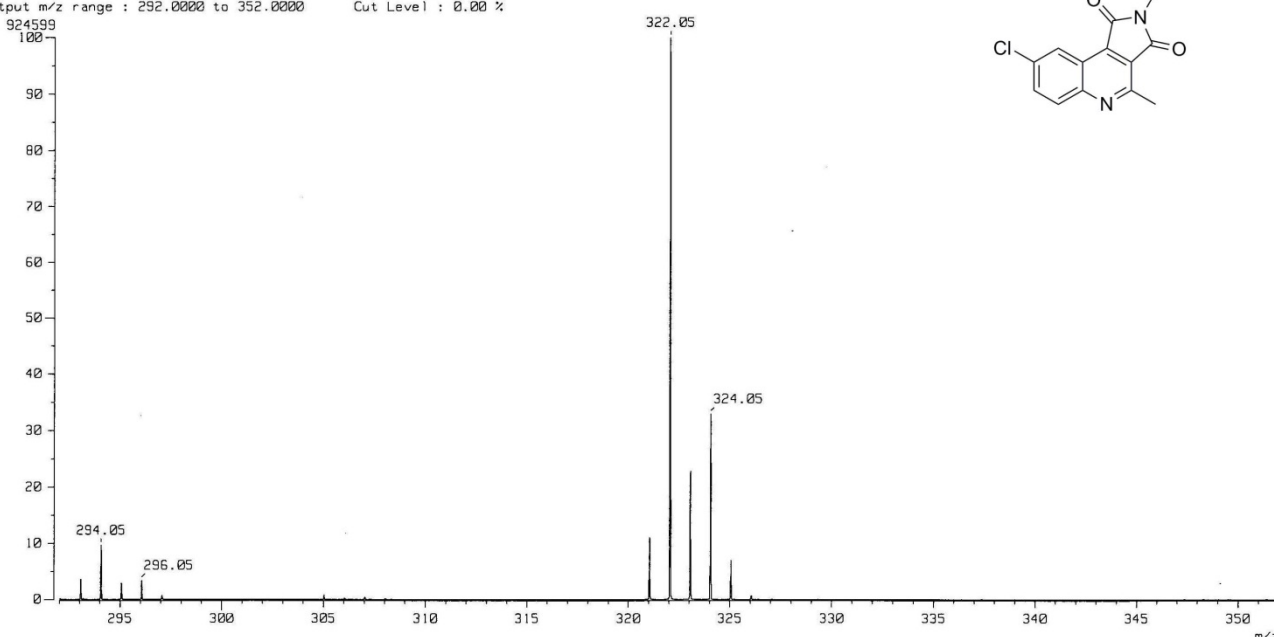
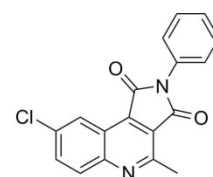


75 MHz, CDCl₃



[Mass Spectrum]
Data : 7c-Cl₁₈H₁₁ClN₂O₂ Date : 06-Dec-2012 10:42
Sample: -
Note: -
Inlet: Direct Ion Mode: EI+
Spectrum Type: Normal Ion [EF-Linear]
RT: 0.58 min Scan#: (12,13)
BP: m/z 322.0508 Int.: 44.09
Output m/z range: 292.0000 to 352.0000 Cut Level: 0.00 %

Mass spectrum of Compound 28



[Elemental Composition]

Data : 7c-Cl₁₈H₁₁ClN₂O₂

Date : 06-Dec-2012 10:42

Page: 1

Sample: -

Note: -

Inlet: Direct

Ion Mode: EI+

RT: 0.58 min

Scan#: (12,13)

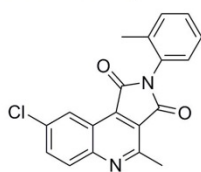
Elements: C 18/0, H 11/0, Cl 1/0, N 2/0, O 2/0

Mass Tolerance: 1000ppm, 2mmu if m/z < 2, 3mmu if m/z > 3

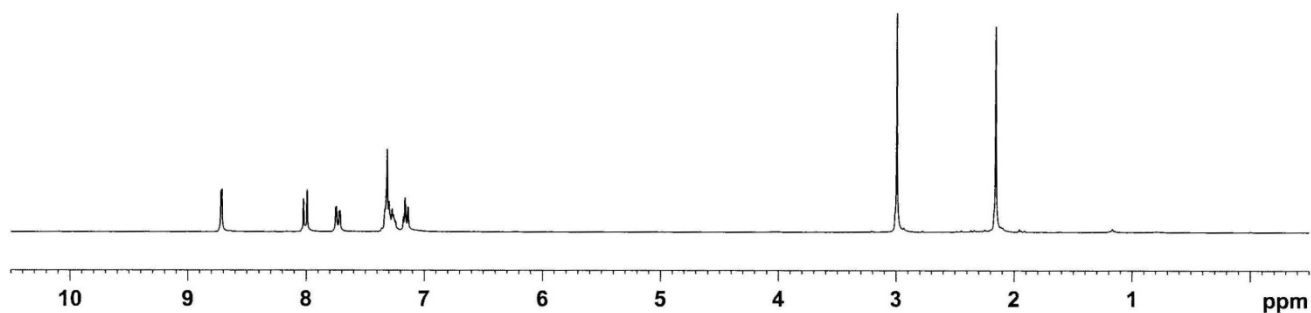
Unsaturation (U.S.): -0.5 - 100.0

Observed m/z	Int%	Err [ppm / mmu]	U.S.	Composition
321.0429	11.1	-0.6 / -0.2	14.5	C 18 H 10 Cl N 2 O 2
322.0508	100.0	-0.5 / -0.2	14.0	C 18 H 11 Cl N 2 O 2
323.0515	22.8			
324.0486	33.0			

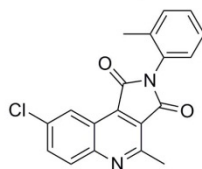
¹H NMR of Compound **29**



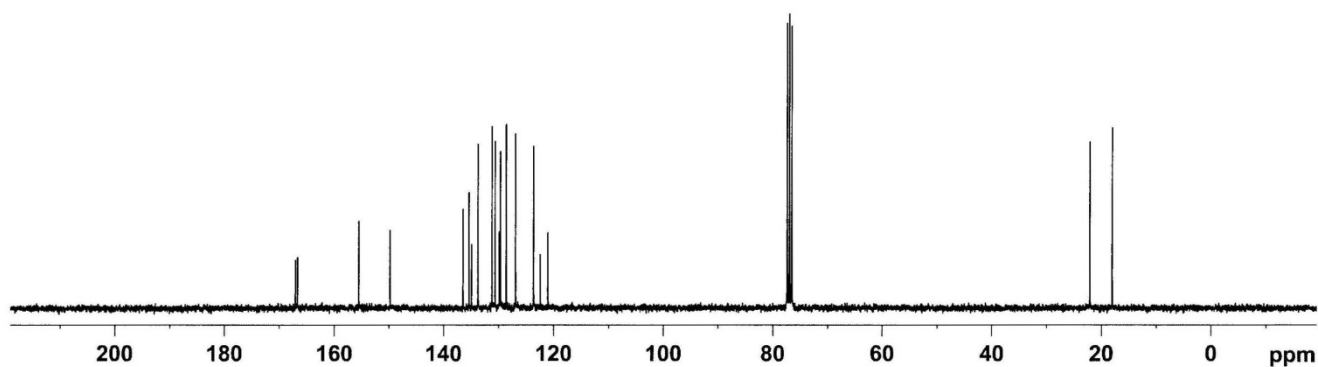
300 MHz, CDCl₃



¹³C NMR of Compound **29**

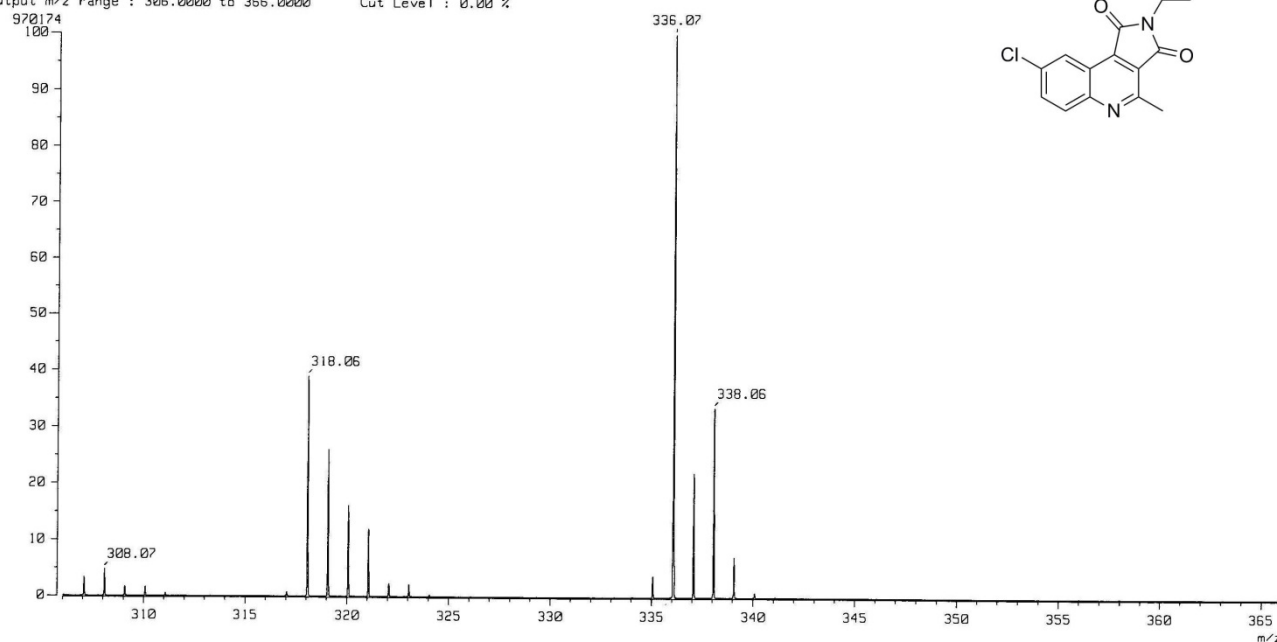
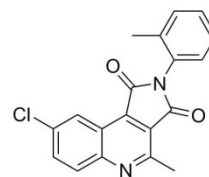


75 MHz, CDCl₃



[Mass Spectrum]
Data : 7-eta-C19H13ClN2O2 Date : 12-Dec-2012 14:40
Sample: -
Note: -
Inlet : Direct Ion Mode : EI+
Spectrum Type : Normal Ion (EF-Linear)
RT : 0.68 min Scan#: (14,15)
BP : m/z 336.0664 Int. : 46.26
Output m/z range : 305.0000 to 365.0000 Cut Level : 0.00 %

Mass spectrum of Compound 29



[Elemental Composition]

Data : 7-eta-C19H13ClN2O2

Date : 12-Dec-2012 14:40

Page: 1

Sample: -

Note: -

Inlet : Direct

Ion Mode : EI+

RT : 0.68 min

Scan#: (14,15)

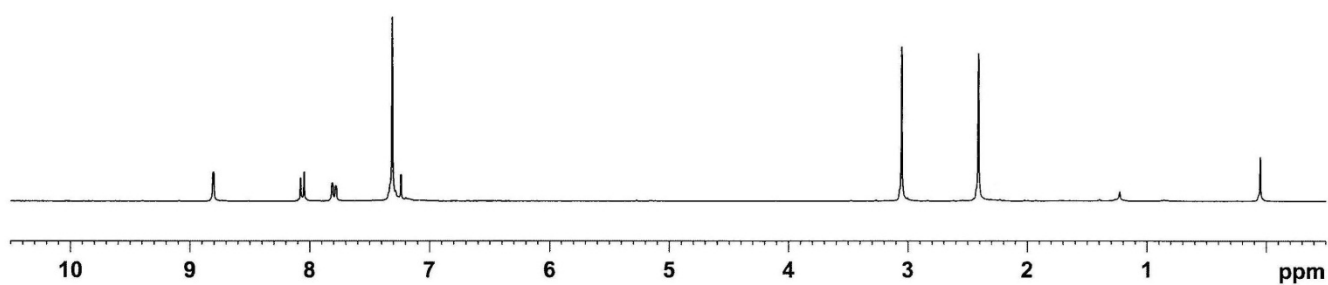
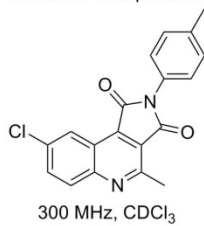
Elements : C 19/0, H 13/0, Cl 1/0, N 2/0, O 2/0

Mass Tolerance : 1000ppm, 2mmu if m/z < 2, 3mmu if m/z > 3

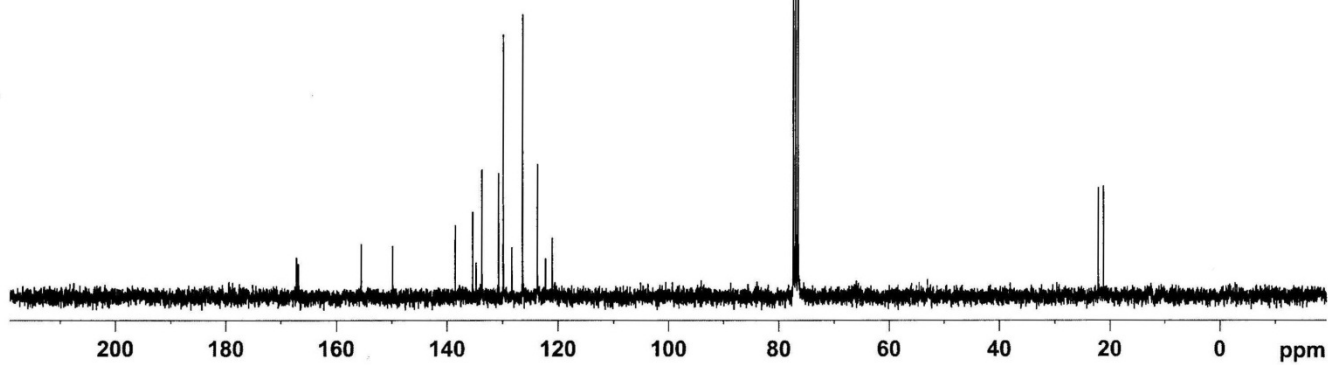
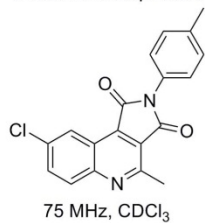
Unsaturation (U.S.) : -0.5 - 100.0

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
318.0554	39.0	-1.8 / -0.6	15.0	C 19 H 11 Cl N 2 O
319.0605	26.1			
320.0544	16.2			
321.0527	12.0	-9.1 / -2.9	14.0	C 19 H 12 Cl N O 2
336.0664	100.0	-0.5 / -0.2	14.0	C 19 H 13 Cl N 2 O 2
337.0683	22.1			
338.0638	33.6			

¹H NMR of Compound **30**

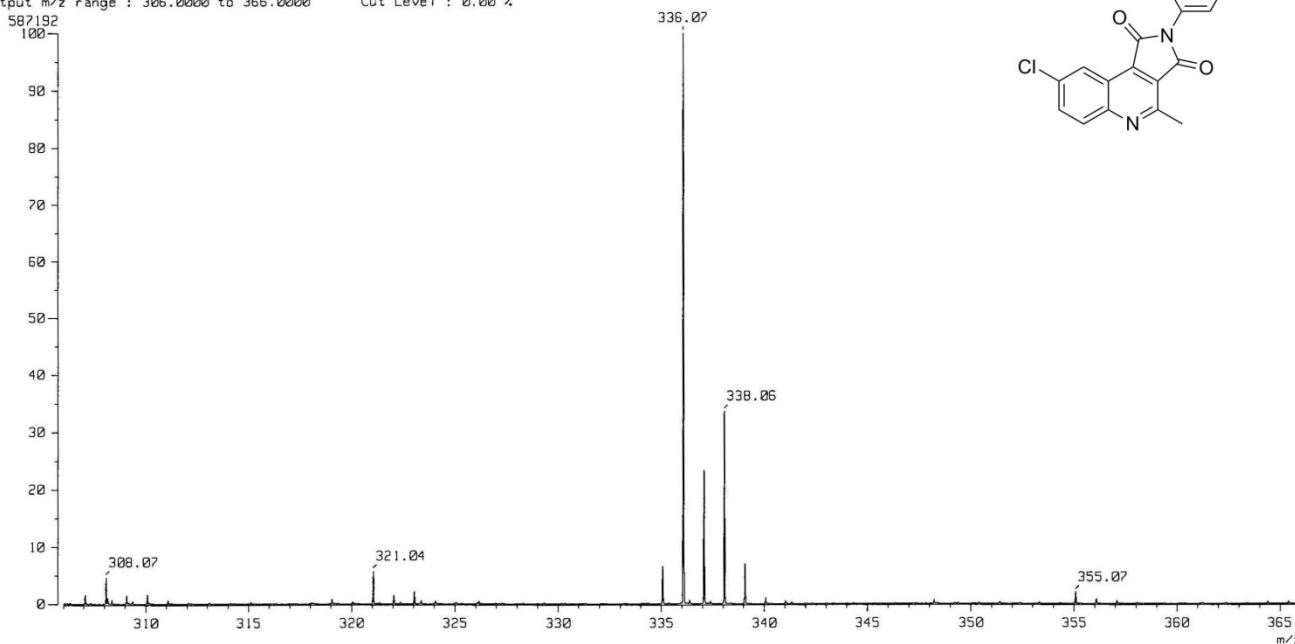
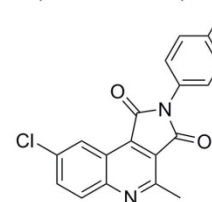


¹³C NMR of Compound **30**



[Mass Spectrum]
Data : 7t-C19H13ClN2O2 Date : 12-Dec-2012 11:05
Sample: -
Note: -
Inlet: Direct Ion Mode: EI+
Spectrum Type: Normal Ion [EF-Linear]
RT: 0.48 min Scan#: (10,11)
BP: m/z 336.0664 Int.: 28.00
Output m/z range: 306.0000 to 366.0000 Cut Level: 0.00 %

Mass spectrum of Compound 30



[Elemental Composition]

Data : 7t-C19H13ClN2O2

Date : 12-Dec-2012 11:05

Page: 1

Sample: -

Note: -

Inlet: Direct

Ion Mode: EI+

RT: 0.48 min

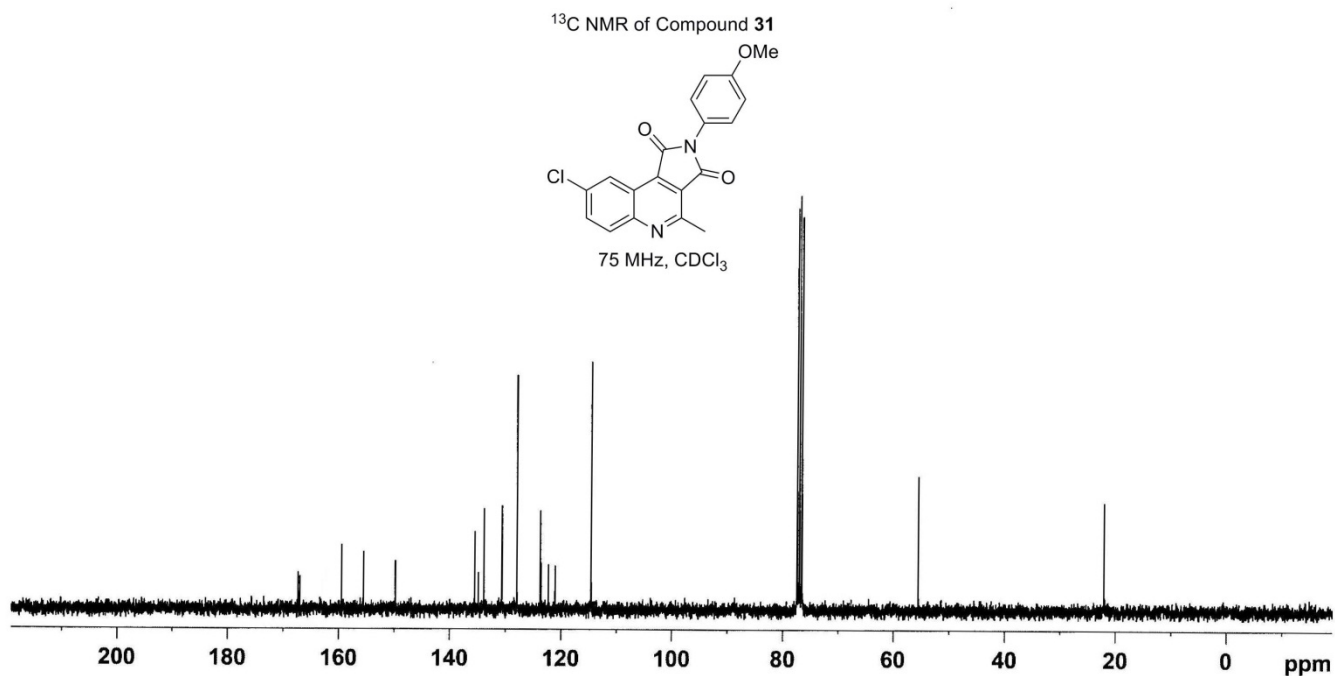
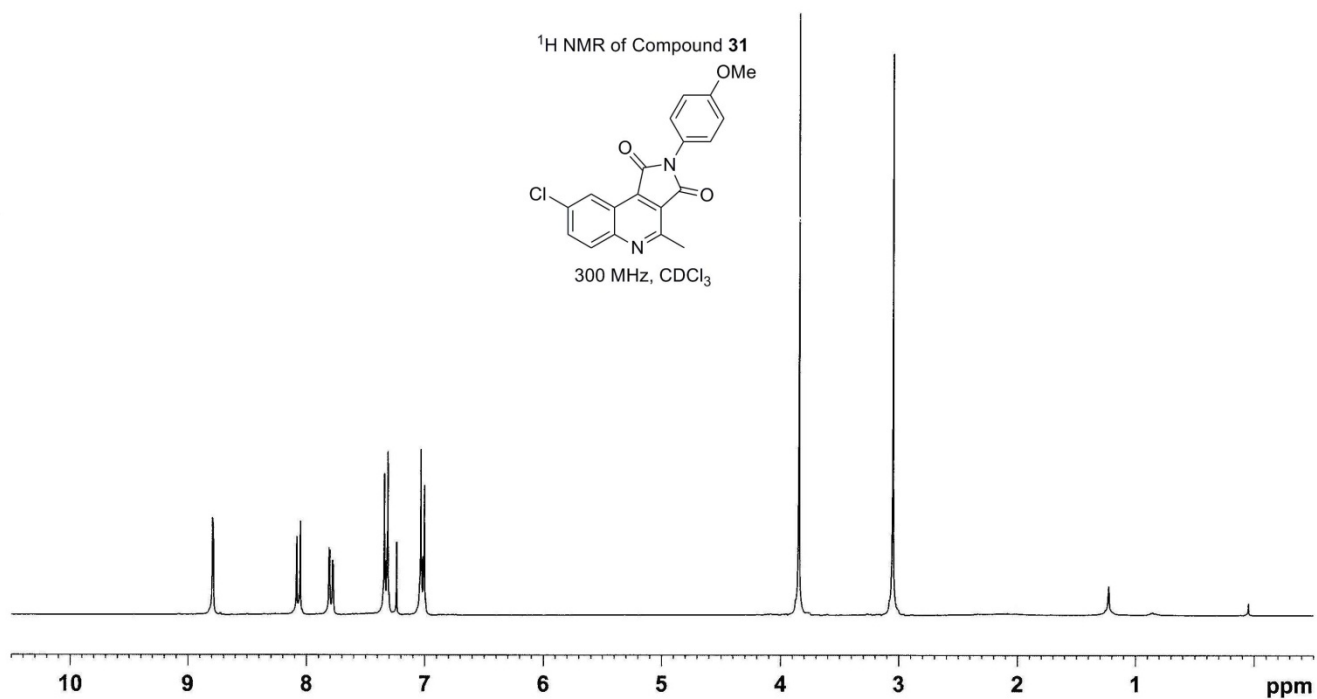
Scan#: (10,11)

Elements: C 19/0, H 13/0, Cl 1/0, N 2/0, O 2/0

Mass Tolerance: 1000ppm, 2mmu if m/z < 2, 3mmu if m/z > 3

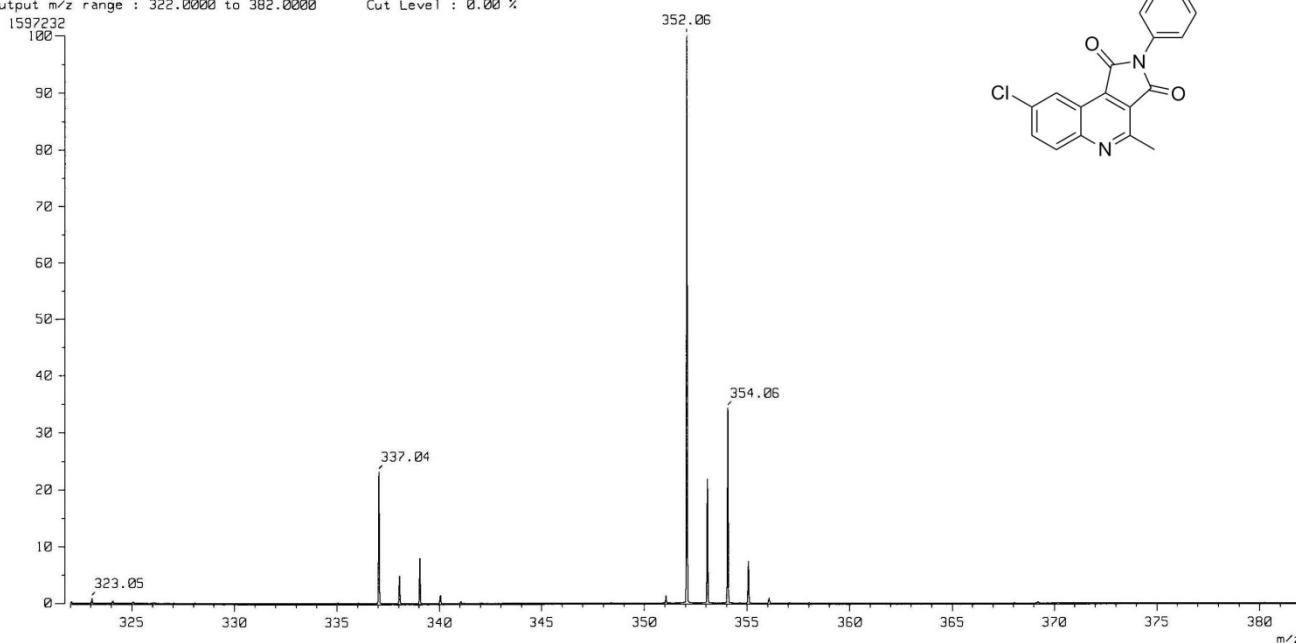
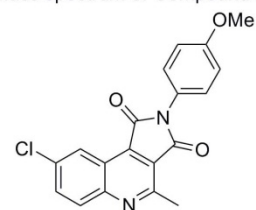
Unsaturation (U.S.): -0.5 - 100.0

Observed m/z	Int%	Err[ppm / mmu]	U.S. Composition
336.0664	100.0	-0.4 / -0.1	14.0 C 19 H 13 Cl N 2 O 2
337.0692	23.4		
338.0638	33.6		



[Mass Spectrum]
Data : X3-28-C19H13ClN2O3 Date : 18-Sep-2012 11:53
Sample: -
Note: -
Inlet : Direct Ion Mode : EI+
Spectrum Type : Normal Ion [EF-Linear]
RT : 1.23 min Scan#: (25,26)
BP : m/z 352.0612 Int. : 76.16
Output m/z range : 322.0000 to 382.0000 Cut Level : 0.00 %

Mass spectrum of Compound 31



[Elemental Composition]

Data : X3-28-C19H13ClN2O3

Date : 18-Sep-2012 11:53

Page: 1

Sample: -

Note: -

Inlet : Direct

Ion Mode : EI+

RT : 1.23 min

Scan#: (25,26)

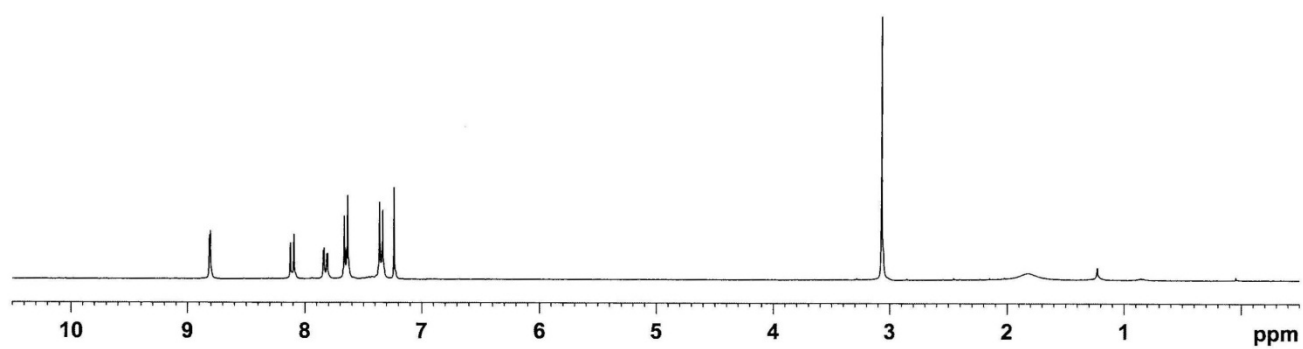
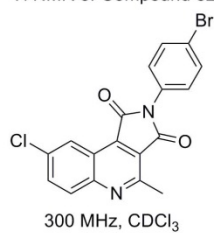
Elements : C 19/0, H 13/0, Cl 1/0, N 2/0, O 3/0

Mass Tolerance : 1000ppm, 2mmu if m/z < 2, 3mmu if m/z > 3

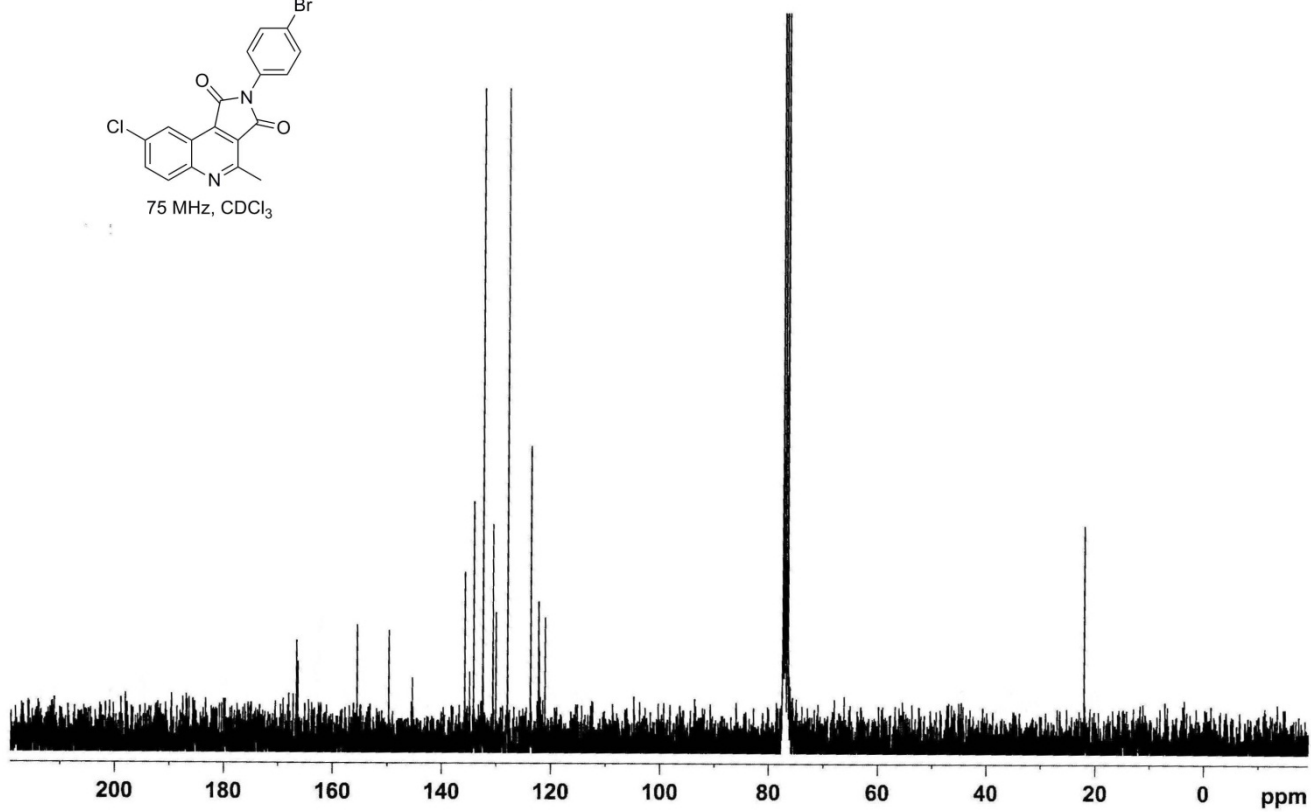
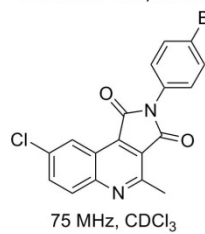
Unsaturation (U.S.) : -0.5 - 100.0

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
337.0383	23.2	+0.8 / +0.3	14.5	C 18 H 10 Cl N 2 O 3
352.0612	100.0	-0.6 / -0.2	14.0	C 19 H 13 Cl N 2 O 3
353.0633	21.9			
354.0592	34.3			

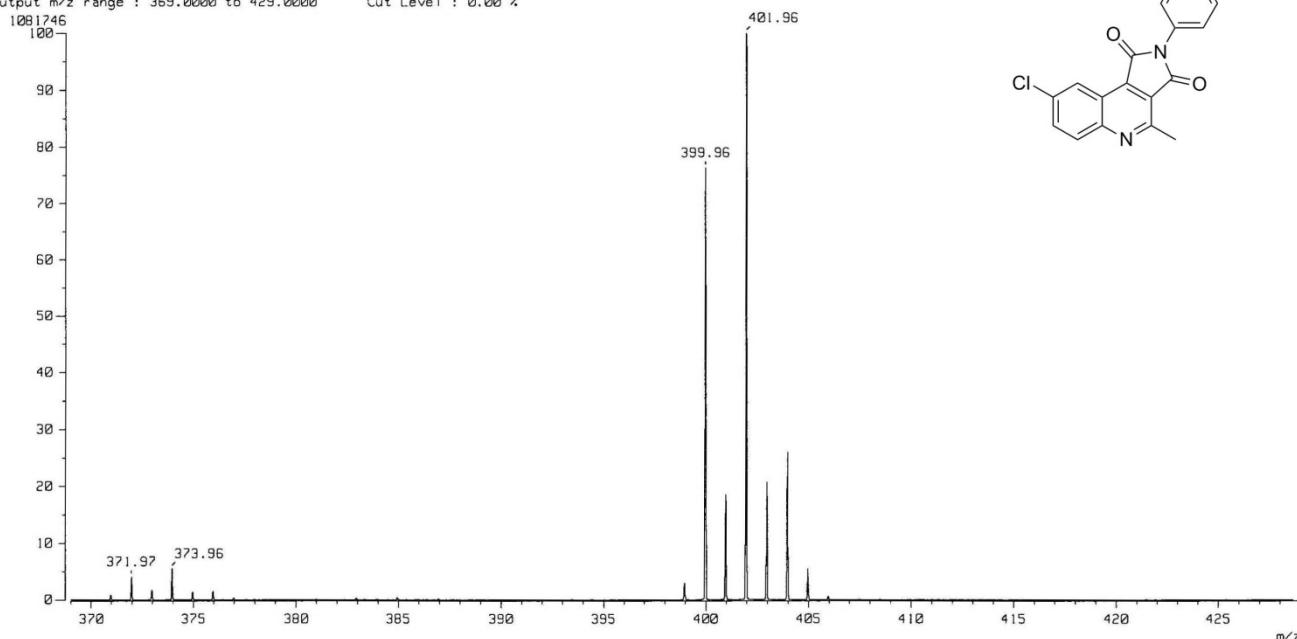
^1H NMR of Compound **32**



^{13}C NMR of Compound **32**



[Mass Spectrum]
Data : 7o-C18H10BrClN2O2 Date : 06-Dec-2012 11:26
Sample: -
Note: -
Inlet: Direct Ion Mode: EI+
Spectrum Type: Normal Ion [EF-Linear]
RT: 0.93 min Scan#: (19,20)
BP: m/z 401.9586 Int.: 51.58
Output m/z range: 369.0000 to 429.0000 Cut Level: 0.00 %



[Elemental Composition]

Data : 7o-C18H10BrClN2O2

Date : 06-Dec-2012 11:26

Page: 1

Sample: -

Note: -

Inlet: Direct

Ion Mode: EI+

RT: 0.93 min

Scan#: (19,20)

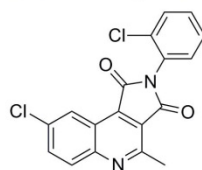
Elements: C 18/0, H 10/0, Br 1/0, Cl 1/0, N 2/0, O 2/0

Mass Tolerance: 1000ppm, 2mmu if m/z < 2, 3mmu if m/z > 3

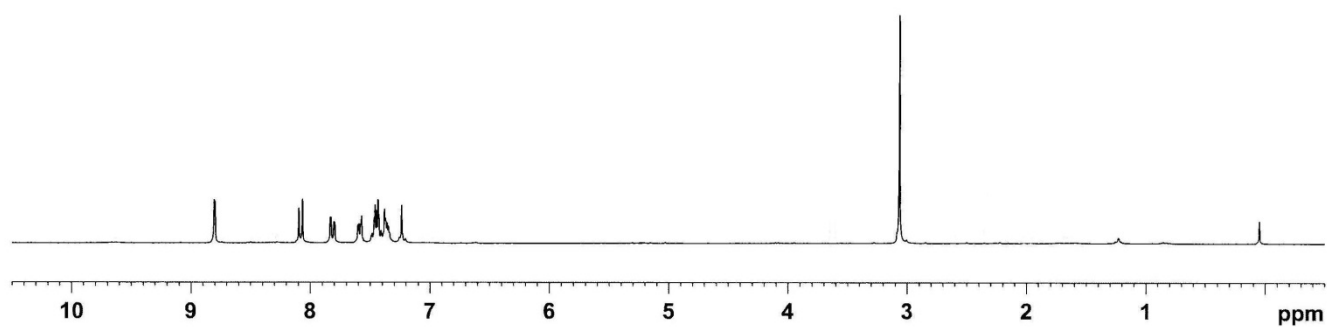
Unsaturation (U.S.): -0.5 - 100.0

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
399.9618	76.3	+0.9 / +0.4	14.0	C 18 H 10 Br Cl N 2 O 2
400.9625	18.6			
401.9586	100.0			
402.9617	20.7			
403.9567	26.0			

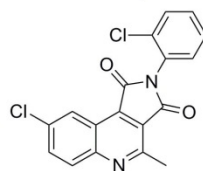
¹H NMR of Compound **33**



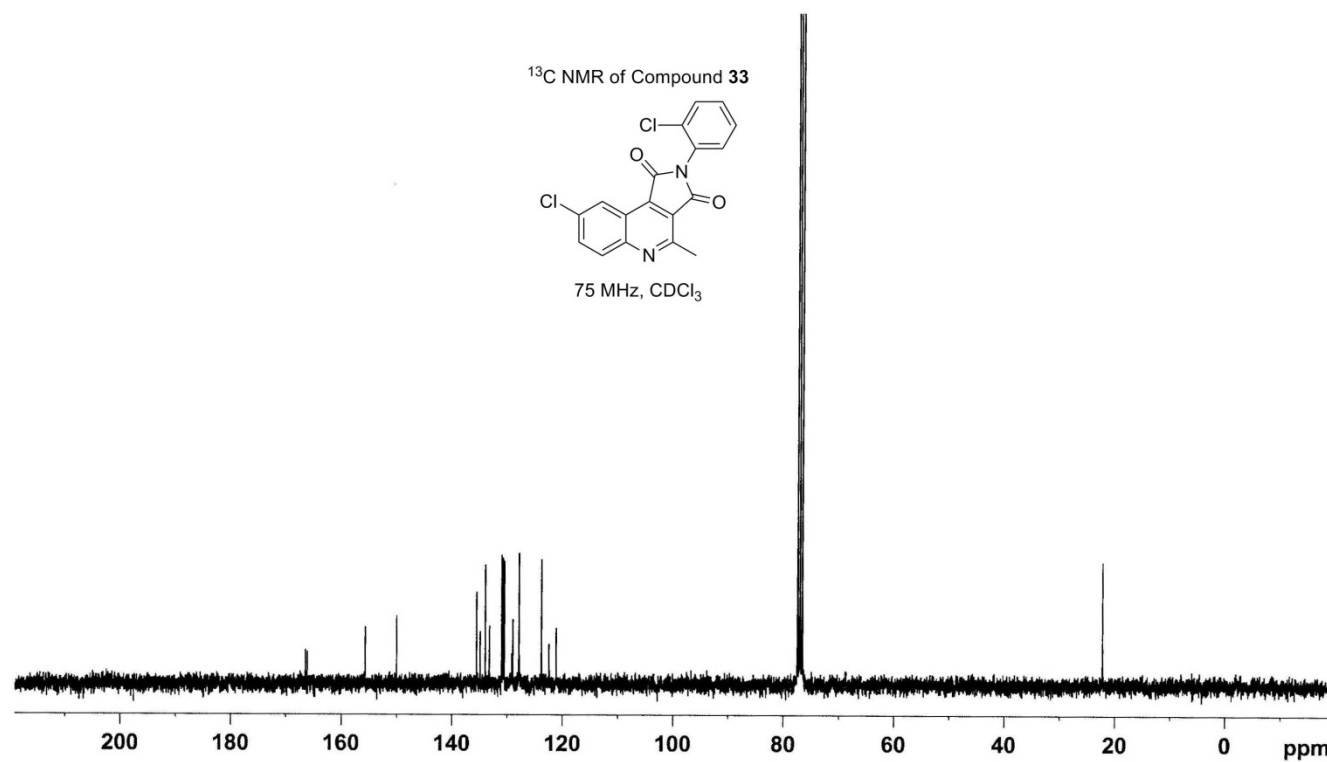
300 MHz, CDCl₃



¹³C NMR of Compound **33**

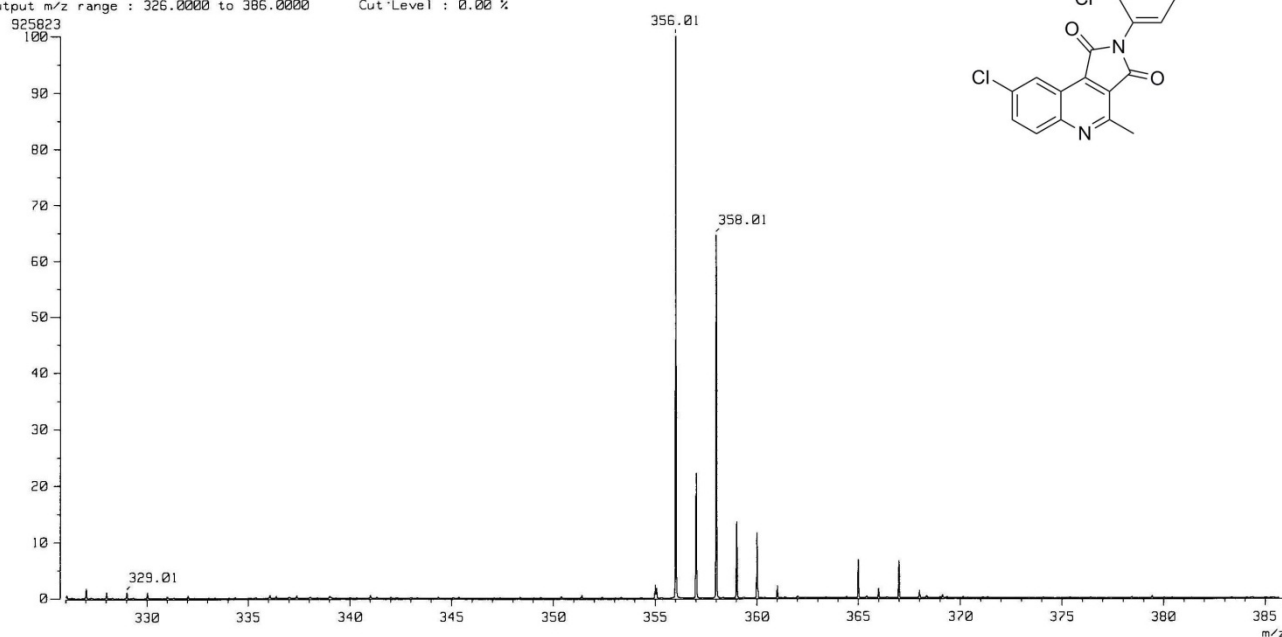
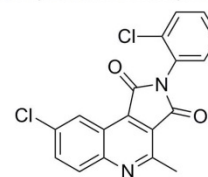


75 MHz, CDCl₃



[Mass Spectrum]
Data : 7-beta-Cl₁₈H₁₀Cl₂N₂O₂ Date : 12-Dec-2012 11:48
Sample: -
Note: -
Inlet : Direct Ion Mode : EI+
Spectrum Type : Normal Ion [EF-Linear]
RT : 0.63 min Scan# : (13,14)
BP : m/z 356.0119 Int. : 44.15
Output m/z range : 326.0000 to 386.0000 Cut-Level : 0.00 %

Mass spectrum of Compound 33



[Elemental Composition]

Data : 7-beta-Cl₁₈H₁₀Cl₂N₂O₂

Date : 12-Dec-2012 11:48

Page: 1

Sample: -

Note: -

Inlet : Direct

Ion Mode : EI+

RT : 0.63 min

Scan#: (13,14)

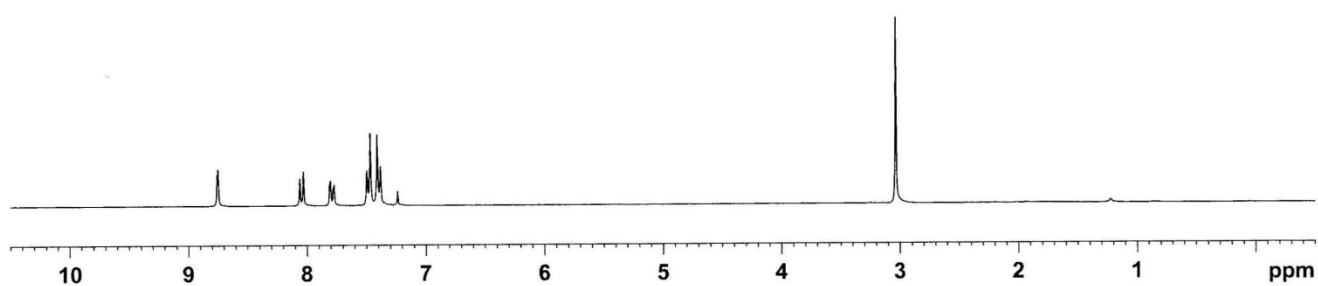
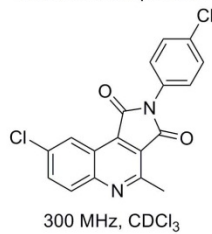
Elements : C 18/0, H 10/0, Cl 2/0, N 2/0, O 2/0

Mass Tolerance : 1000ppm, 2mmu if m/z < 2, 3mmu if m/z > 3

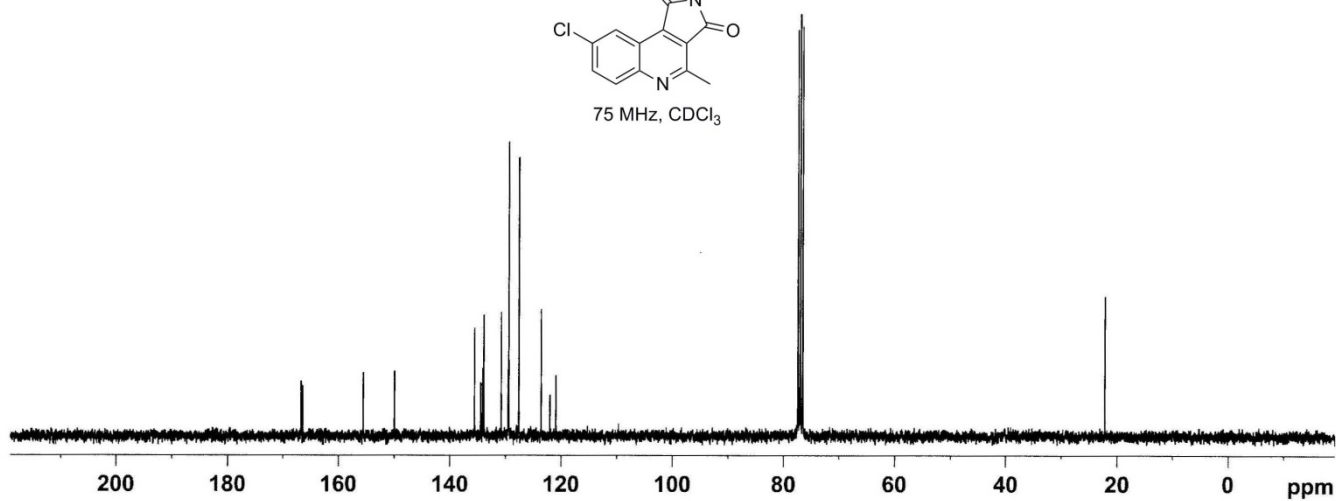
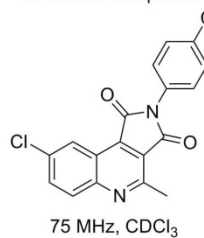
Unsaturation (U.S.) : -0.5 - 100.0

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
356.0119	100.0	-0.2 / -0.1	14.0	C 18 H 10 Cl 2 N 2 O 2
357.0155	22.2			
358.0085	64.6			
359.0122	13.6			
360.0068	11.7			

¹H NMR of Compound **34**

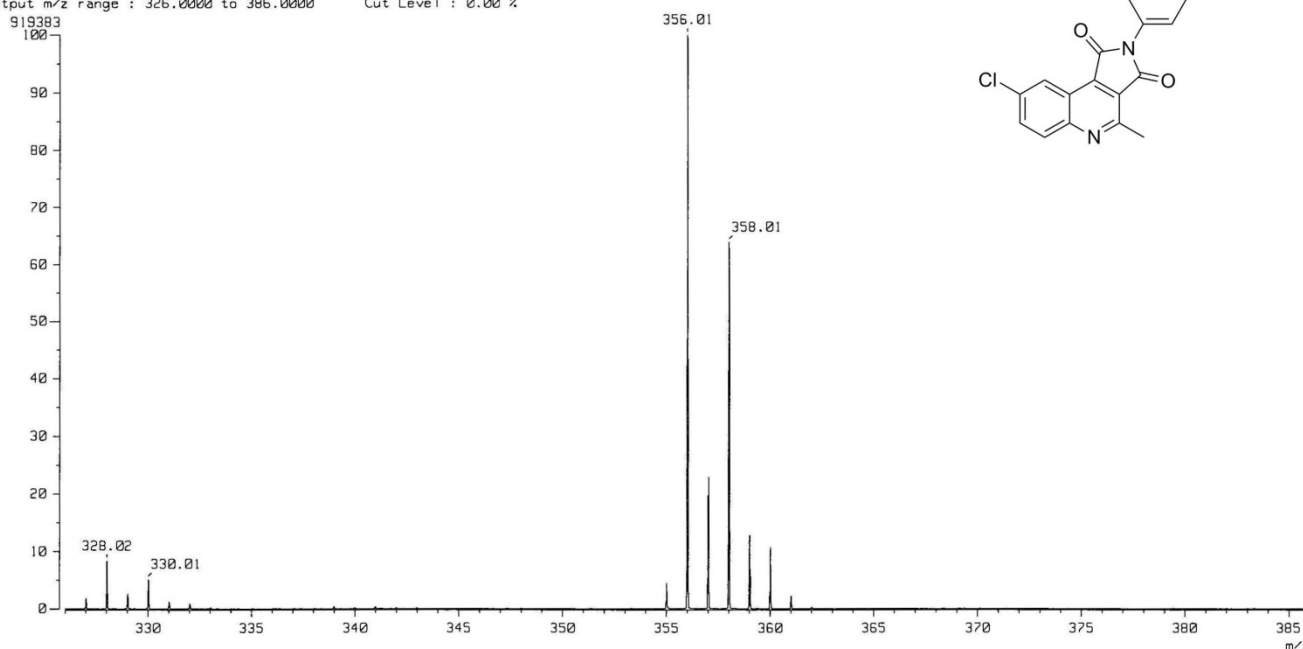
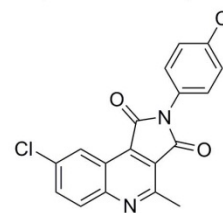


¹³C NMR of Compound **34**



[Mass Spectrum]
Data : 7x-C18H10Cl2N2O2 Date : 12-Dec-2012 11:27
Sample: -
Note: -
Inlet : Direct Ion Mode : EI+
Spectrum Type : Normal Ion [EF-Linear]
RT : 0.68 min Scan#: (14,15)
BP : m/z 356.0118 Int. : 43.84
Output m/z range : 326.0000 to 386.0000 Cut Level : 0.00 %

Mass spectrum of Compound **34**



[Elemental Composition]

Data : 7x-C18H10Cl2N2O2

Date : 12-Dec-2012 11:27

Page: 1

Sample: -

Note: -

Inlet : Direct

Ion Mode : EI+

RT : 0.68 min

Scan#: (14,15)

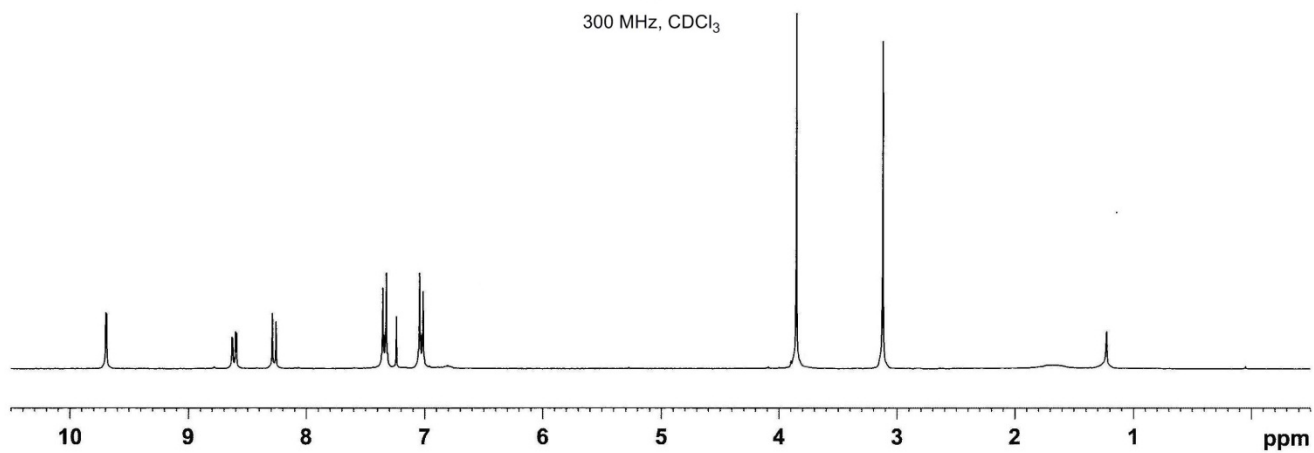
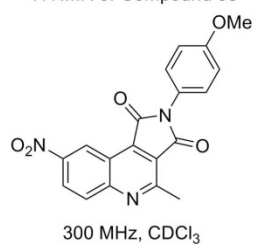
Elements : C 18/0, H 10/0, Cl 2/0, N 2/0, O 2/0

Mass Tolerance : 1000ppm, 2mmu if m/z < 2, 3mmu if m/z > 3

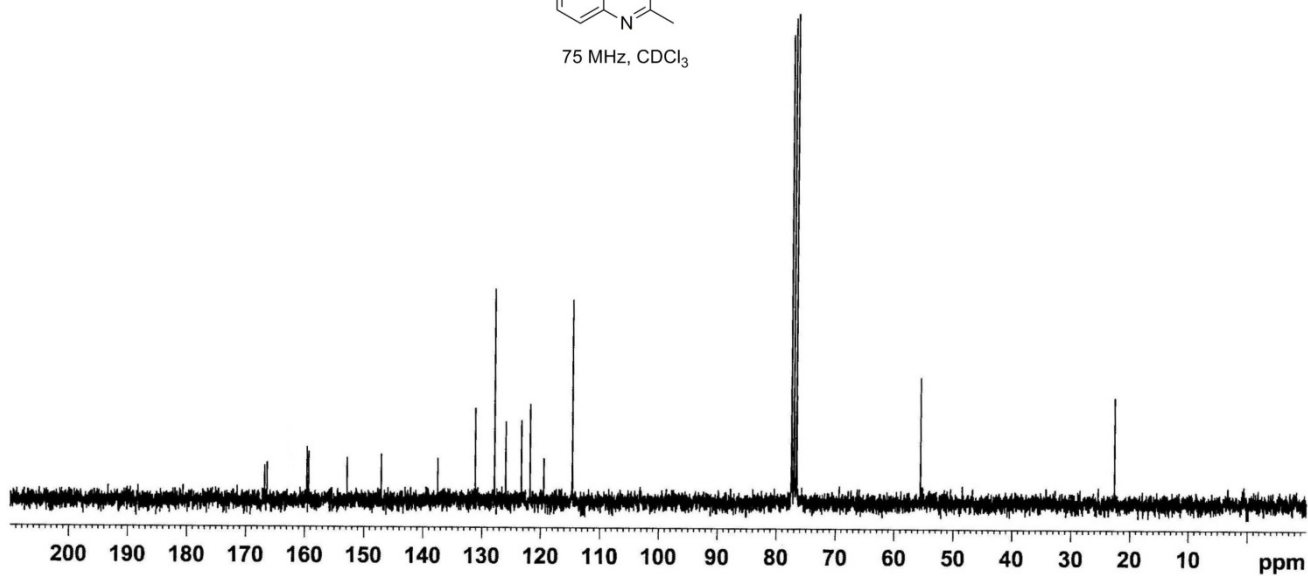
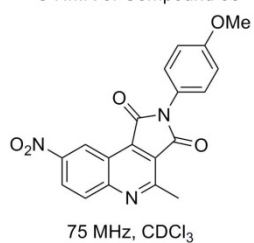
Unsaturation (U.S.) : -0.5 - 100.0

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
356.0118	100.0	-0.4 / -0.2	14.0	C 18 H 10 Cl 2 N 2 O 2
357.0120	23.0			
358.0086	63.9			
359.0101	12.9			
360.0058	10.8			

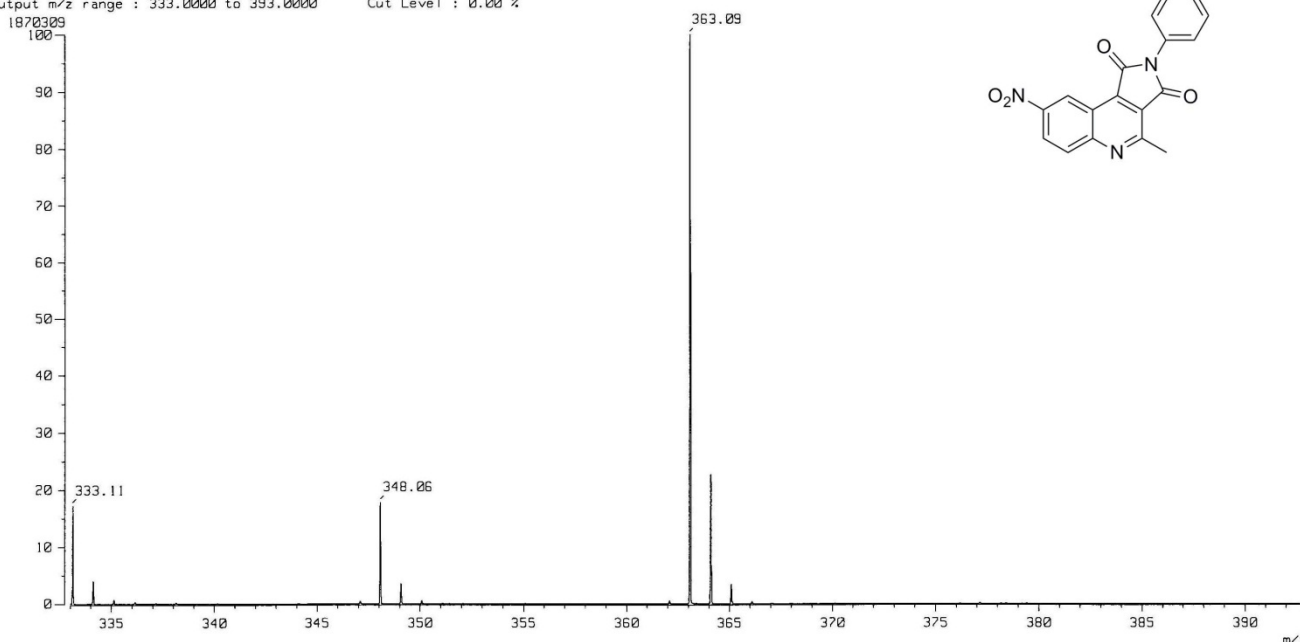
¹H NMR of Compound **35**



¹³C NMR of Compound **35**



[Mass Spectrum]
Data : 71-C19H13N3O5 Date : 06-Dec-2012 11:11
Sample: -
Note: -
Inlet: Direct Ion Mode: EI+
Spectrum Type: Normal Ion [EF-Linear]
RT: 0.83 min Scan#: (17,18)
BP: m/z 363.0855 Int.: 89.18
Output m/z range: 333.0000 to 393.0000 Cut Level: 0.00 %



[Elemental Composition]

Data : 71-C19H13N3O5

Date : 06-Dec-2012 11:11

Page: 1

Sample: -

Note: -

Inlet: Direct

Ion Mode: EI+

RT: 0.83 min

Scan#: (17,18)

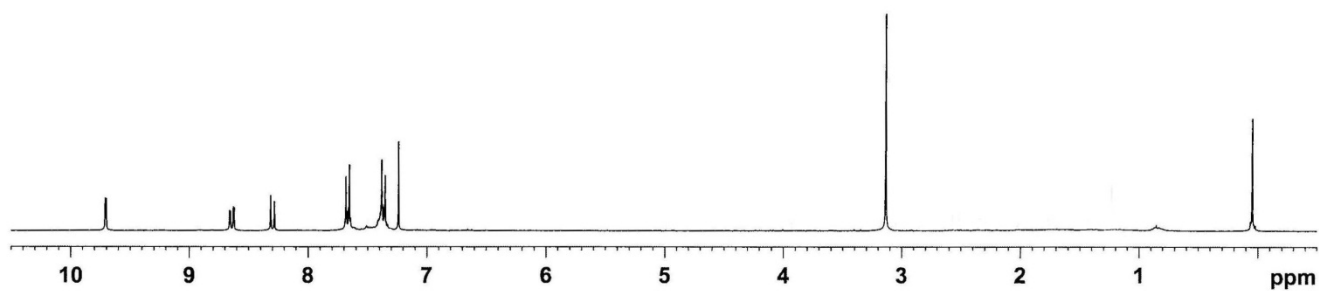
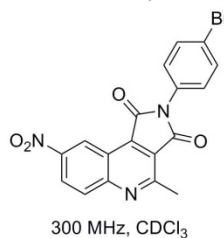
Elements: C 19/0, H 13/0, N 3/0, O 5/0

Mass Tolerance: 1000ppm, 2mmu if m/z < 2, 3mmu if m/z > 3

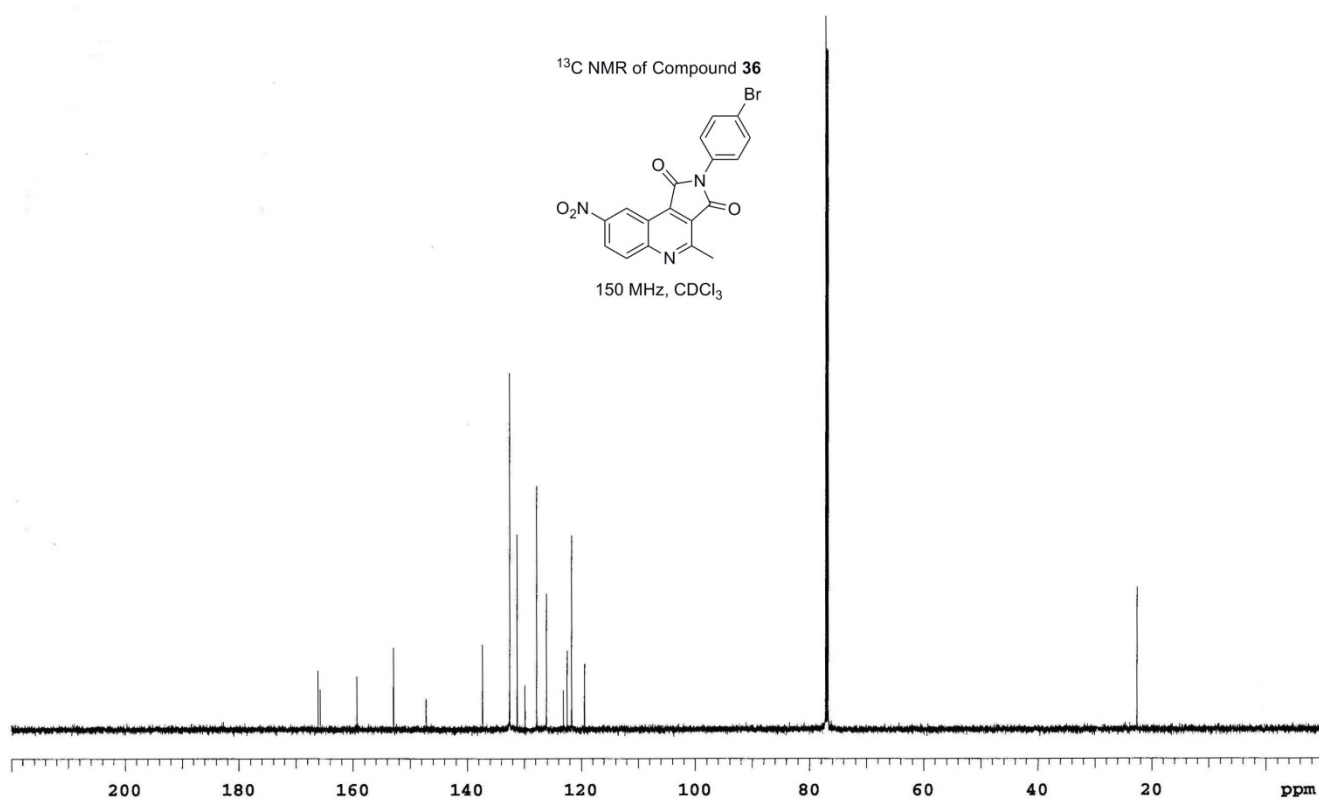
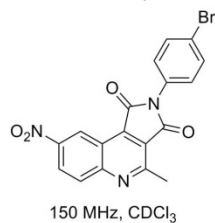
Unsaturation (U.S.): -0.5 - 100.0

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
333.1103	17.3			
348.0623	17.9	+0.9 / +0.3	15.5	C 18 H 10 N 3 O 5
363.0855	100.0	+0.1 / +0.0	15.0	C 19 H 13 N 3 O 5
364.0887	22.7			

¹H NMR of Compound **36**

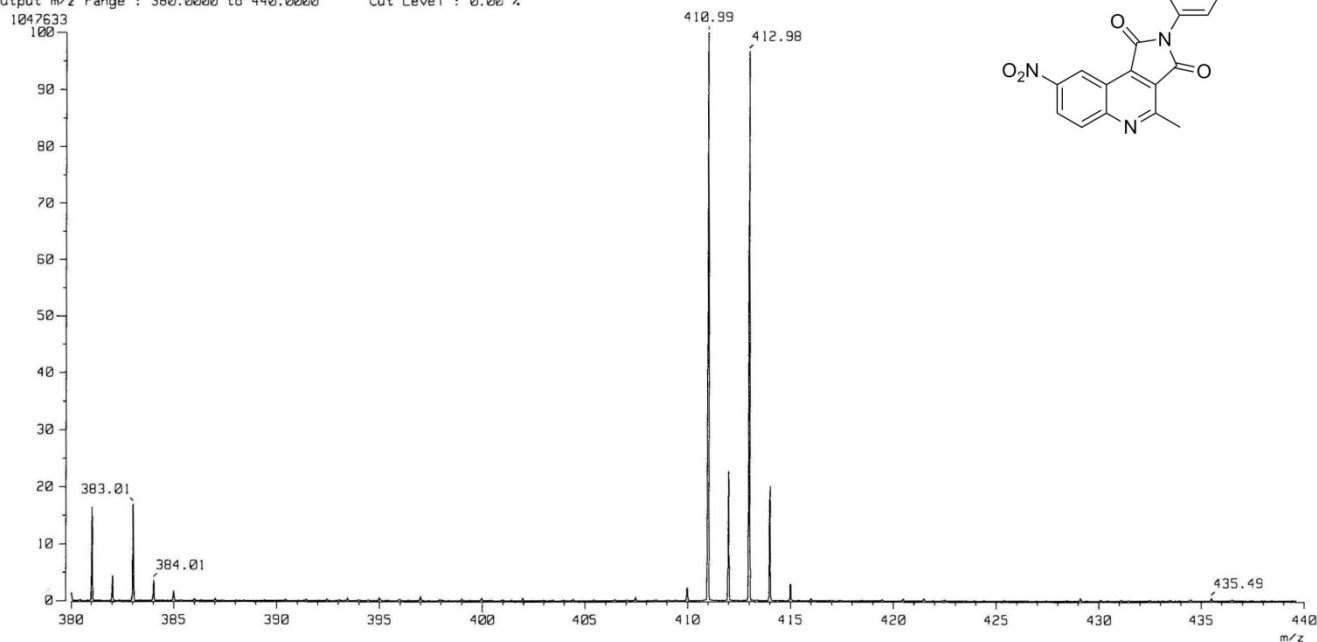
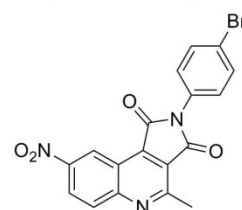


¹³C NMR of Compound **36**



[Mass Spectrum]
Data : 7q-C18H10BrN3O4 Date : 06-Dec-2012 11:35
Sample: -
Note: -
Inlet : Direct Ion Mode : EI+
Spectrum Type : Normal Ion [EF-Linear]
RT : 1.18 min Scan#: (24,25)
BP : m/z 410.9855 Int. : 49.96
Output m/z range : 380.0000 to 440.0000 Cut Level : 0.00 %

Mass spectrum of Compound 36



[Elemental Composition]

Data : 7q-C18H10BrN3O4

Date : 06-Dec-2012 11:35

Page: 1

Sample: -

Note: -

Inlet : Direct

Ion Mode : EI+

RT : 1.18 min

Scan#: (24,25)

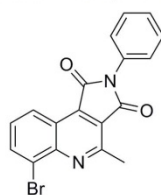
Elements : C 18/0, H 10/0, Br 1/0, N 3/0, O 4/0

Mass Tolerance : 1000ppm, 2mmu if m/z < 2, 3mmu if m/z > 3

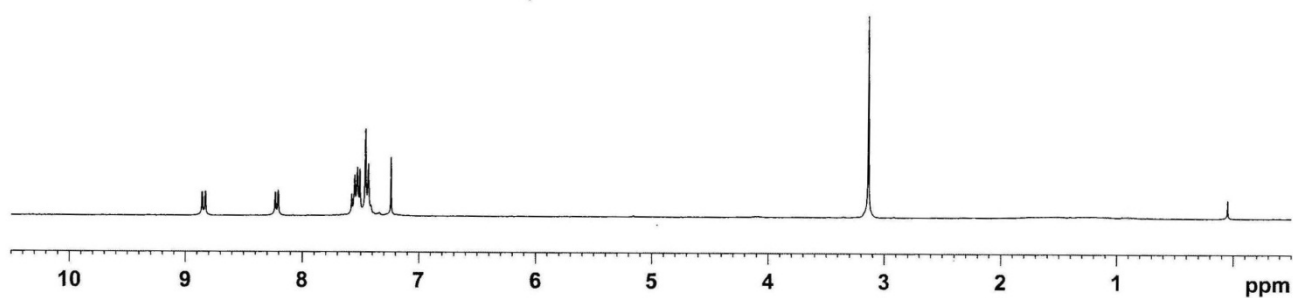
Unsaturation (U.S.) : -0.5 - 100.0

Observed m/z	Int%	Err[ppm / mmu]	U.S. Composition
381.0082	16.5		
383.0063	17.0		
410.9855	100.0	+0.1 / +0.0	15.0 C 18 H 10 Br N 3 O 4
411.9844	22.8		
412.9803	96.7		
413.9850	20.1		

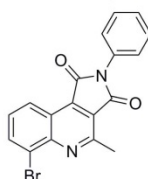
^1H NMR of Compound 37



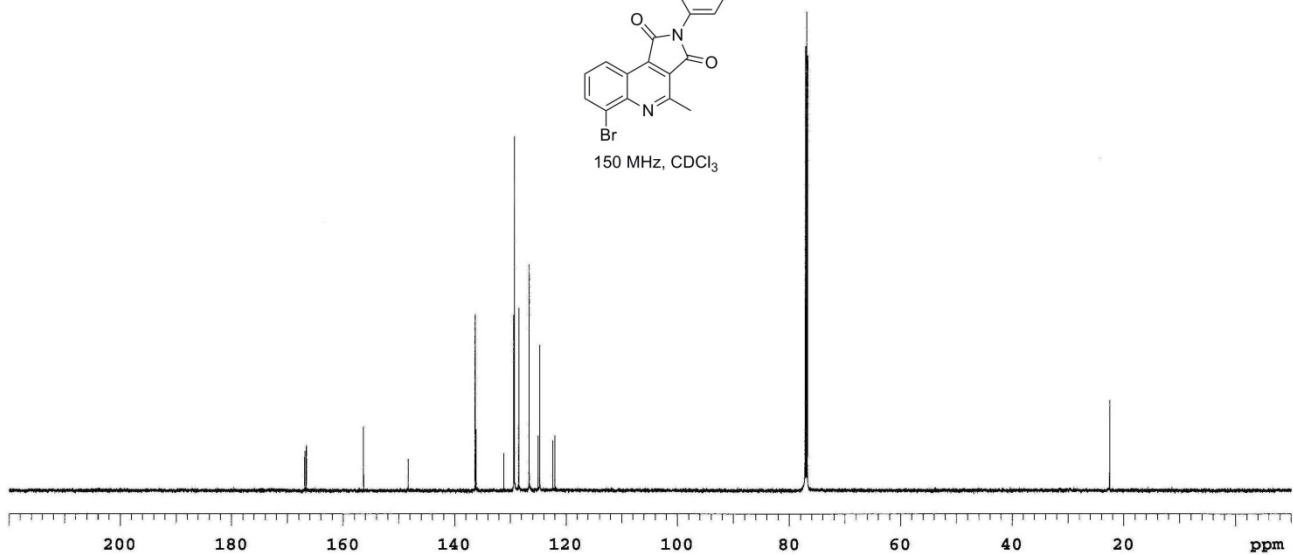
300 MHz, CDCl_3



^{13}C NMR of Compound 37

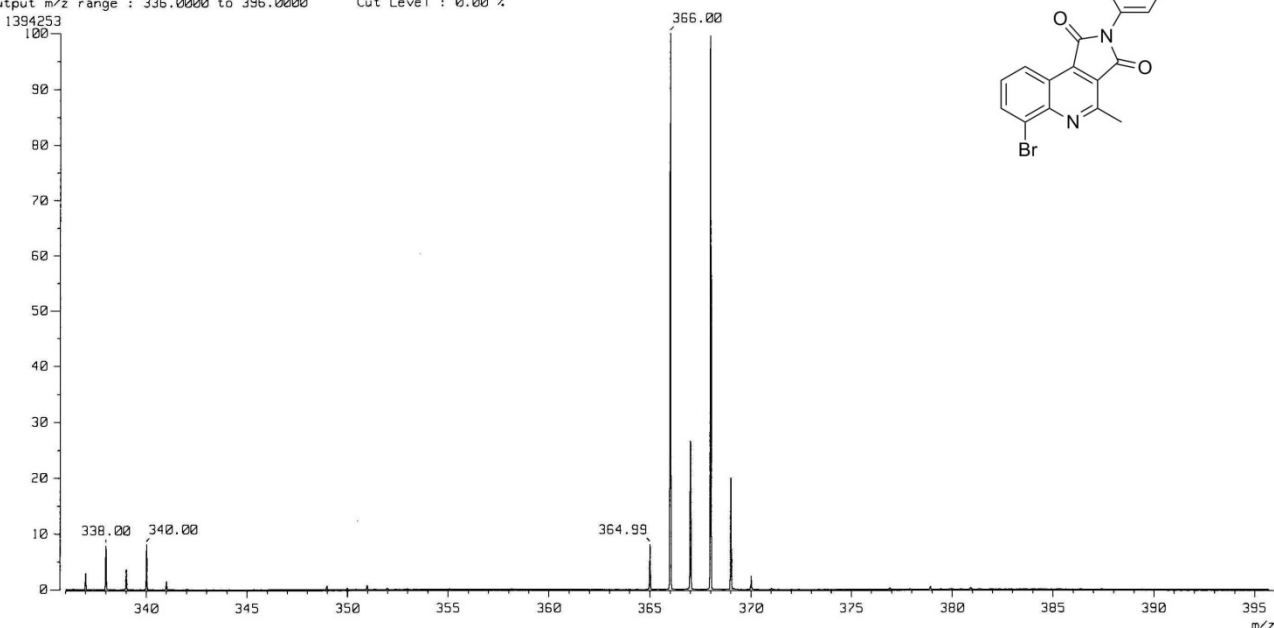
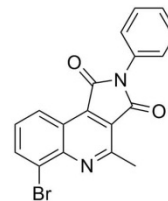


150 MHz, CDCl_3



[Mass Spectrum]
Data : 7d-C18H11BrN2O2 Date : 06-Dec-2012 10:47
Sample: -
Note: -
Inlet : Direct Ion Mode : EI+
Spectrum Type : Normal Ion [EF-Linear]
RT : 0.63 min Scan#: (13,14)
BP : m/z 365.0002 Int. : 65.48
Output m/z range : 336.0000 to 396.0000 Cut Level : 0.00 %

Mass spectrum of Compound 37



[Elemental Composition]

Data : 7d-C18H11BrN2O2

Date : 06-Dec-2012 10:47

Page: 1

Sample: -

Note: -

Inlet : Direct

Ion Mode : EI+

RT : 0.63 min

Scan#: (13,14)

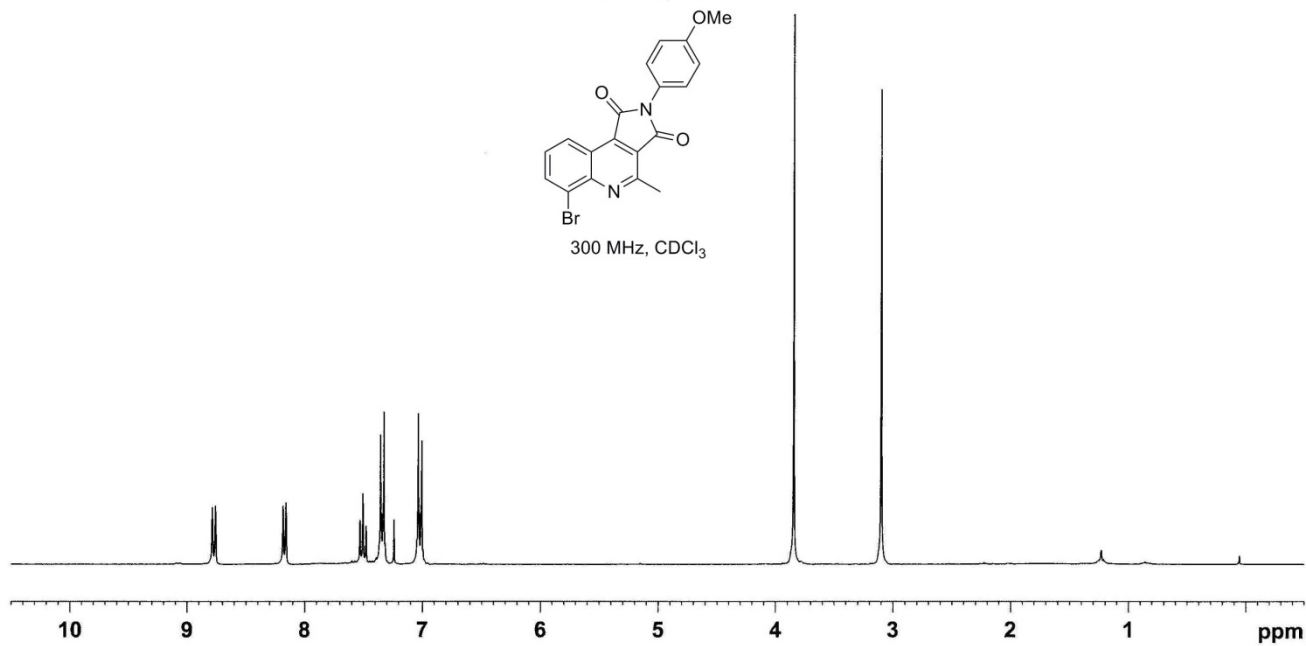
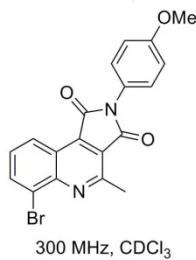
Elements : C 18/0, H 11/0, Br 1/0, N 2/0, O 2/0

Mass Tolerance : 1000ppm, 2mmu if m/z < 2, 3mmu if m/z > 3

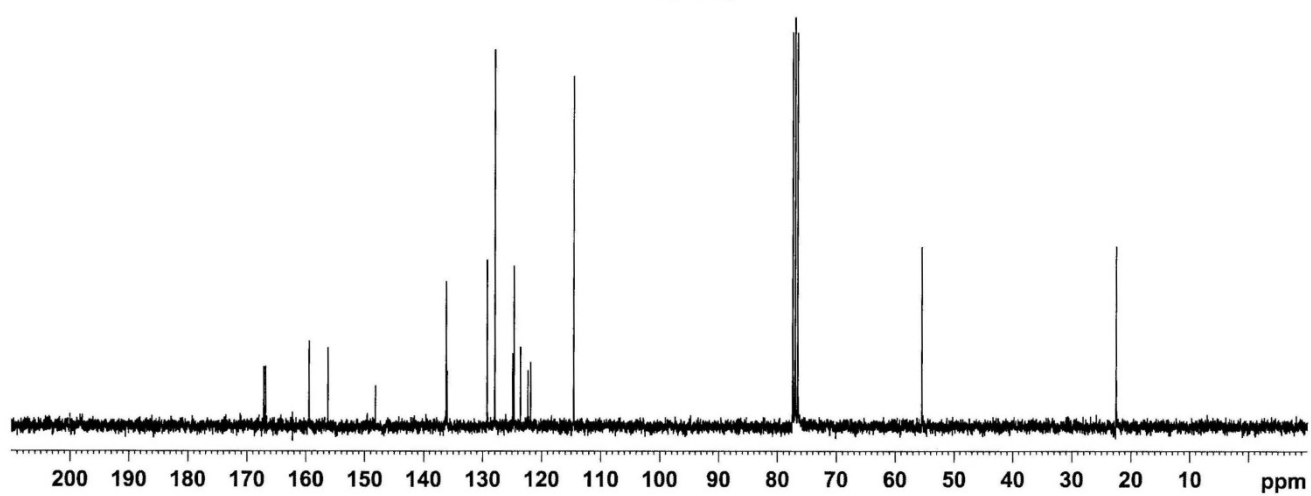
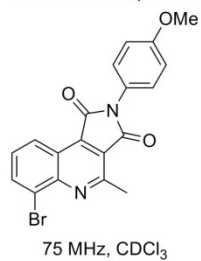
Unsaturation (U.S.) : -0.5 - 100.0

Observed m/z	Int%	Err[ppm / mmu]	U.S. Composition
366.0002	100.0	-0.6 / -0.2	14.0 C 18 H 11 Br N 2 O 2
366.9993	26.7		
367.9980	99.6		
369.0007	20.1		

¹H NMR of Compound 38

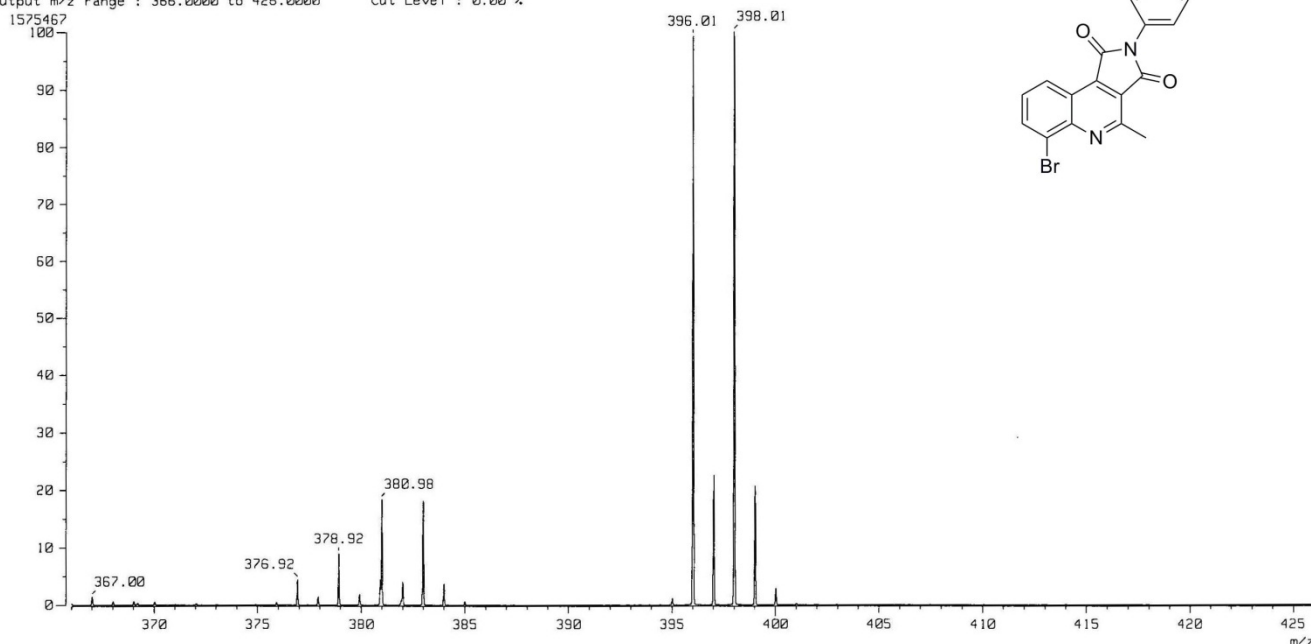
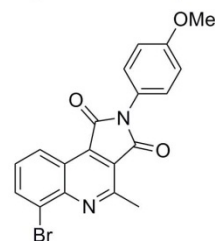


¹³C NMR of Compound 38



[Mass Spectrum]
Data : X3-29-C19H13BrN2O3 Date : 18-Sep-2012 11:58
Sample: -
Note: -
Inlet: Direct Ion Mode: EI+
Spectrum Type: Normal Ion [EF-Linear]
RT: 1.03 min Scan#: (21,22)
BP: m/z 398.0110 Int.: 75.12
Output m/z range: 366.0000 to 426.0000 Cut Level: 0.00 %

Mass spectrum of Compound 38



[Elemental Composition]

Data : X3-29-C19H13BrN2O3

Date : 18-Sep-2012 11:58

Page: 1

Sample: -

Note: -

Inlet: Direct

Ion Mode: EI+

RT: 1.03 min

Scan#: (21,22)

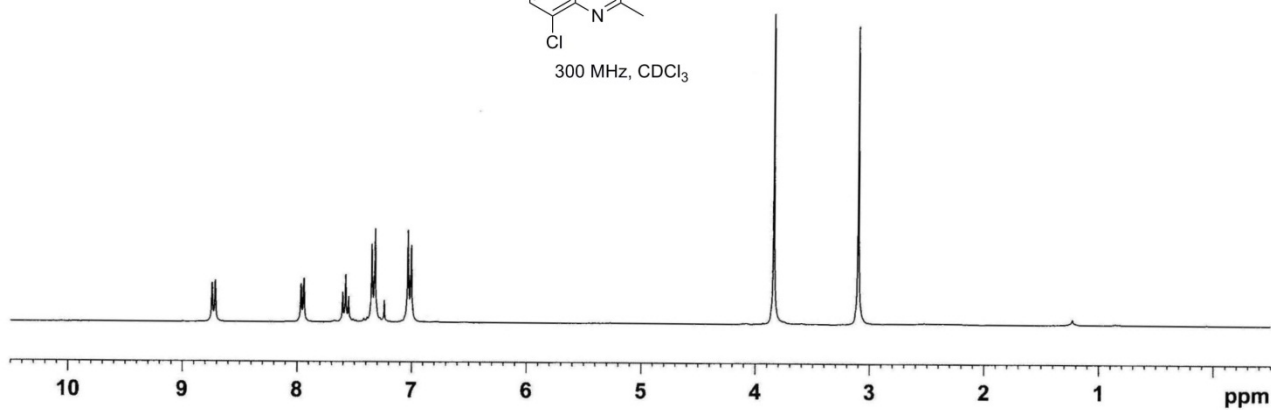
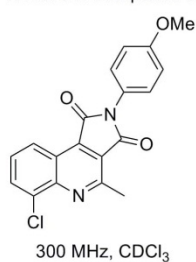
Elements: C 19/0, H 13/0, Br 1/0, N 2/0, O 3/0

Mass Tolerance: 1000ppm, 2mmu if m/z < 2, 3mmu if m/z > 3

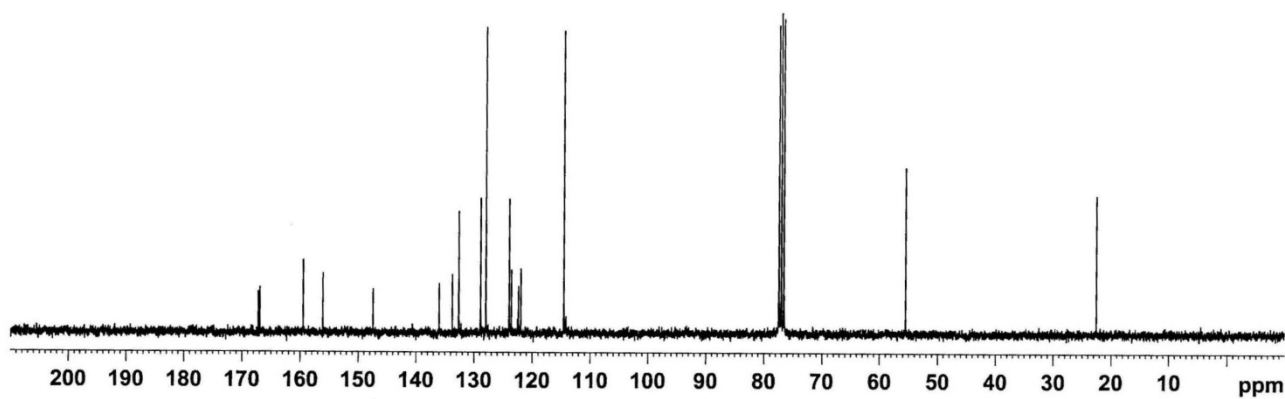
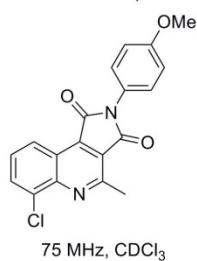
Unsaturation (U.S.): -0.5 - 100.0

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
380.9759	18.4			
382.9871	18.2			
396.0113	99.2	+0.8 / +0.3	14.0	C 19 H 13 Br N 2 O 3
397.0146	22.6			
398.0110	100.0			
399.0143	20.8			

¹H NMR of Compound **39**

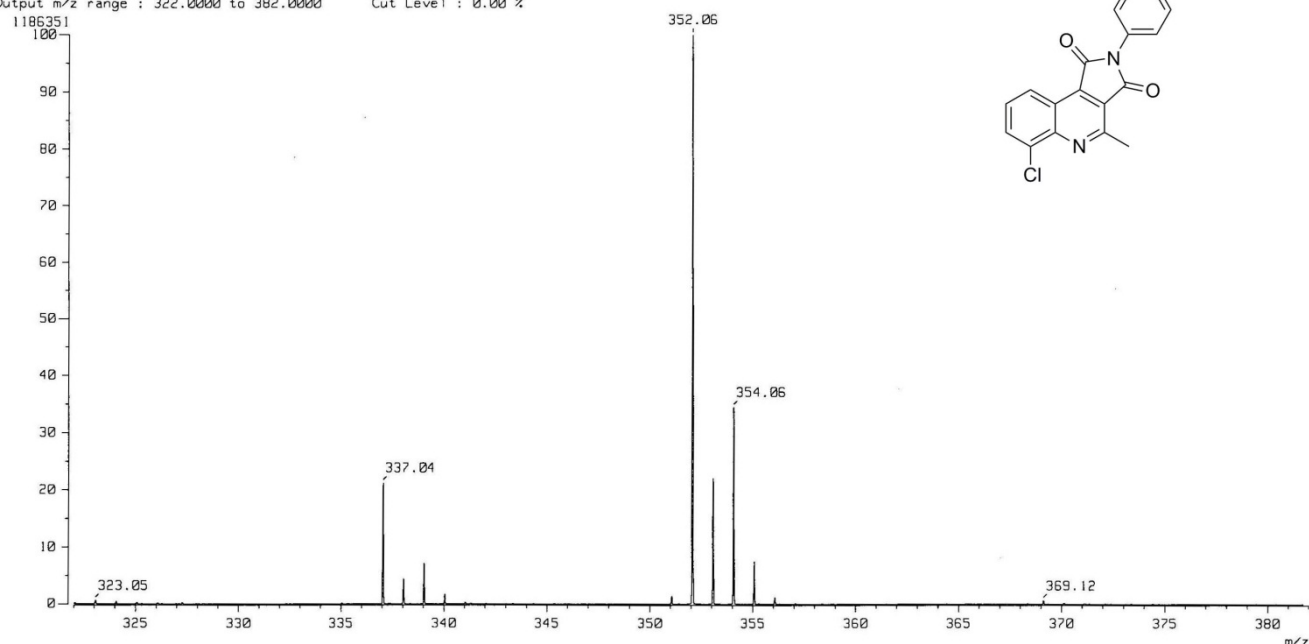
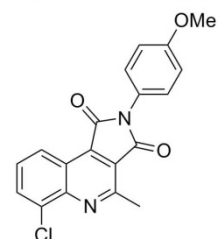


¹³C NMR of Compound **39**



[Mass Spectrum]
Data : 7j-C19H13ClN2O3 Date : 06-Dec-2012 11:00
Sample: -
Note: -
Inlet : Direct Ion Mode : EI+
Spectrum Type : Normal Ion [EF-Linear]
RT : 0.98 min Scan#: (20,21)
BP : m/z 352.0612 Int. : 56.57
Output m/z range : 322.0000 to 382.0000 Cut Level : 0.00 %

Mass spectrum of Compound 39



[Elemental Composition]

Data : 7j-C19H13ClN2O3

Date : 06-Dec-2012 11:00

Page: 1

Sample: -

Note: -

Inlet : Direct

Ion Mode : EI+

RT : 0.98 min

Scan#: (20,21)

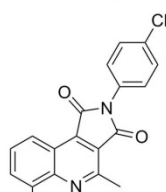
Elements : C 19/0, H 13/0, Cl 1/0, N 2/0, O 3/0

Mass Tolerance : 1000ppm, 2mmu if m/z < 2, 3mmu if m/z > 3

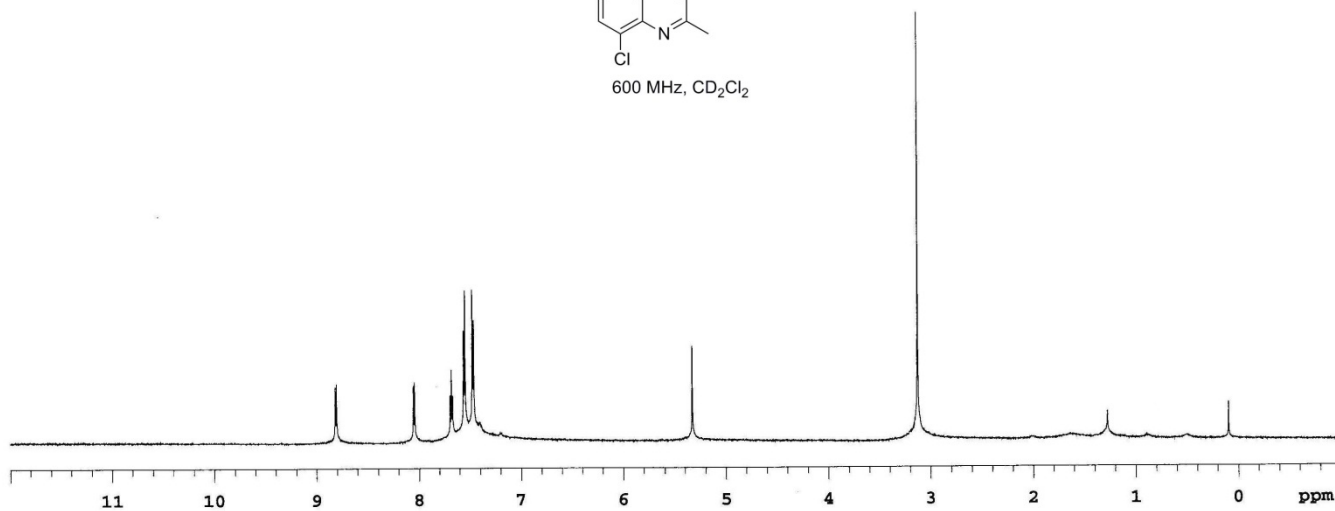
Unsaturation (U.S.) : -0.5 - 100.0

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
337.0384	21.2	+1.1 / +0.4	14.5	C 18 H 10 Cl N 2 O 3
352.0612	100.0	-0.9 / -0.3	14.0	C 19 H 13 Cl N 2 O 3
353.0634	22.1			
354.0590	34.5			

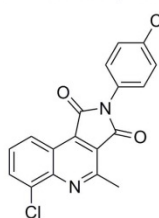
¹H NMR of Compound **40**



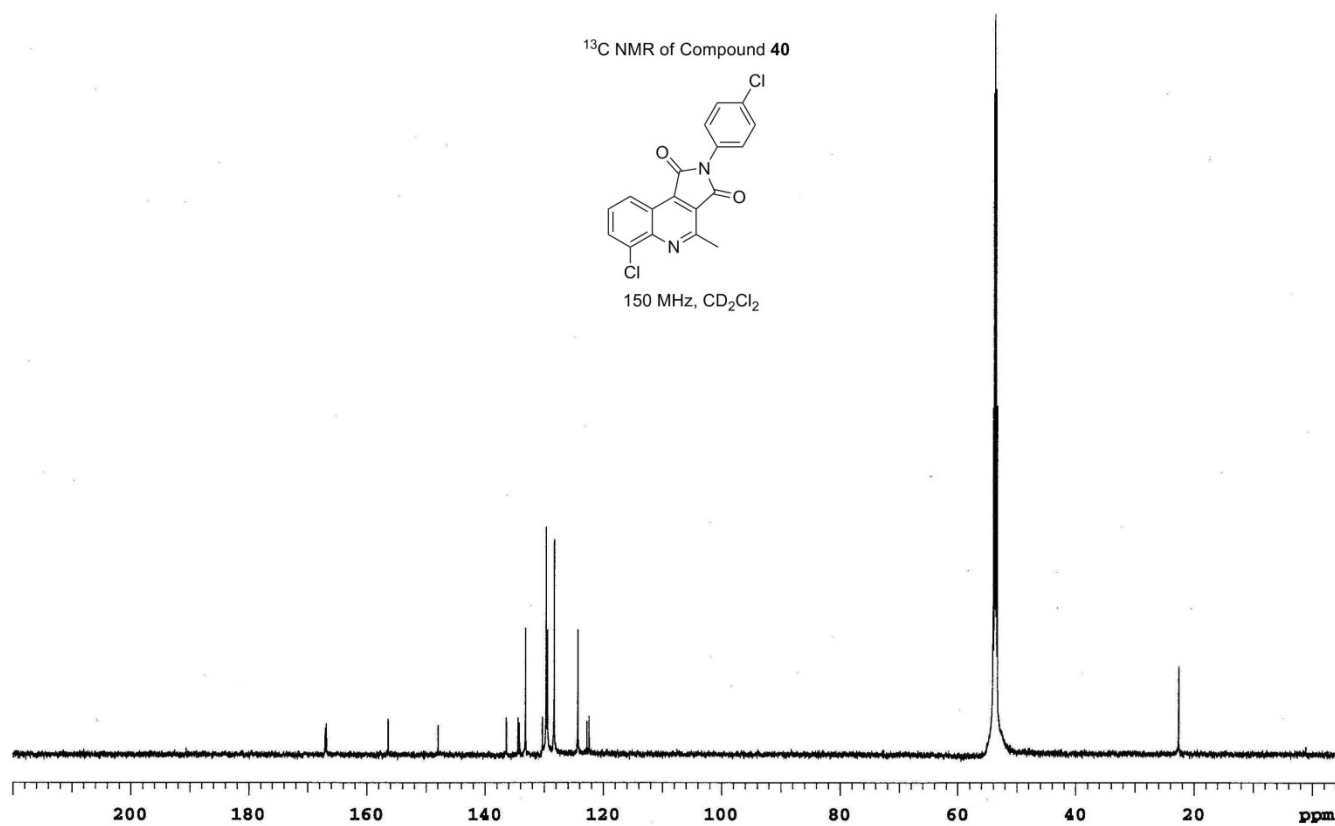
600 MHz, CD₂Cl₂



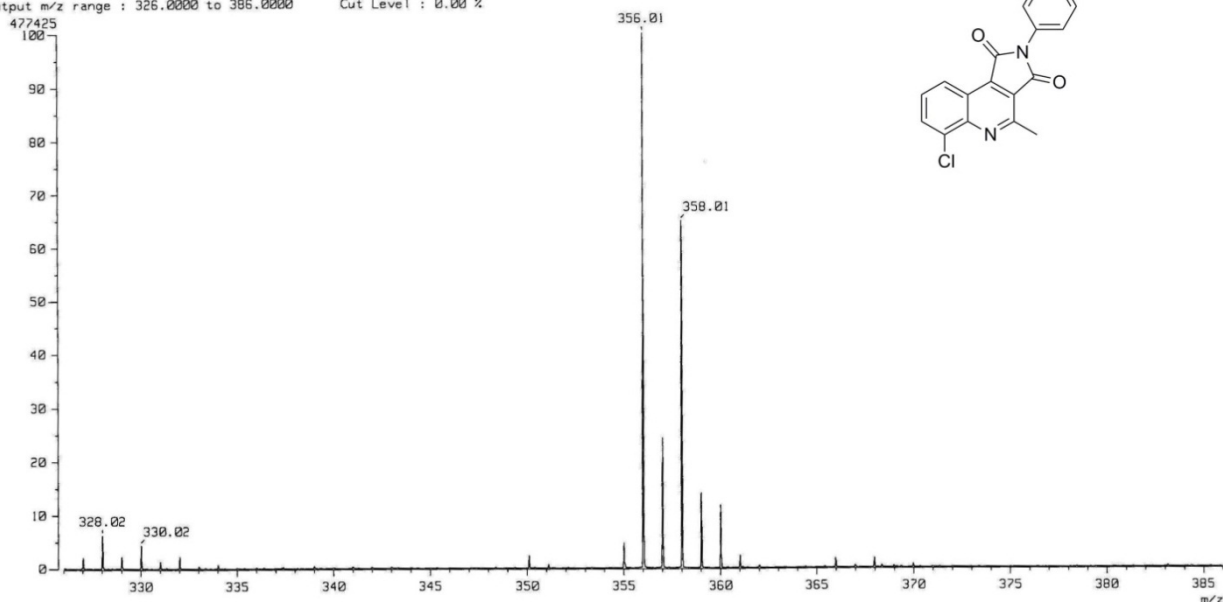
¹³C NMR of Compound **40**



150 MHz, CD₂Cl₂



[Mass Spectrum]
Data : X6-10-C18H10Cl2N2O2 Date : 20-Feb-2013 17:19
Sample: -
Note: -
Inlet: Direct Ion Mode: EI+
Spectrum Type: Normal Ion [EF-Linear]
RT: 0.83 min Scan#: (17,18)
BP: m/z 356.0122 Int.: 22.77
Output m/z range: 325.0000 to 385.0000 Cut Level: 0.00 %



[Elemental Composition]

Data : X6-10-C18H10Cl2N2O2

Date : 20-Feb-2013 17:19

Page: 1

Sample: -

Note: -

Inlet: Direct

Ion Mode: EI+

RT: 0.83 min

Scan#: (17,18)

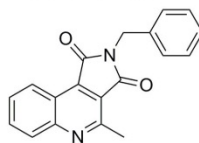
Elements: C 18/0, H 10/0, Cl 2/0, N 2/0, O 2/0

Mass Tolerance: 1000ppm, 2mmu if m/z < 2, 3mmu if m/z > 3

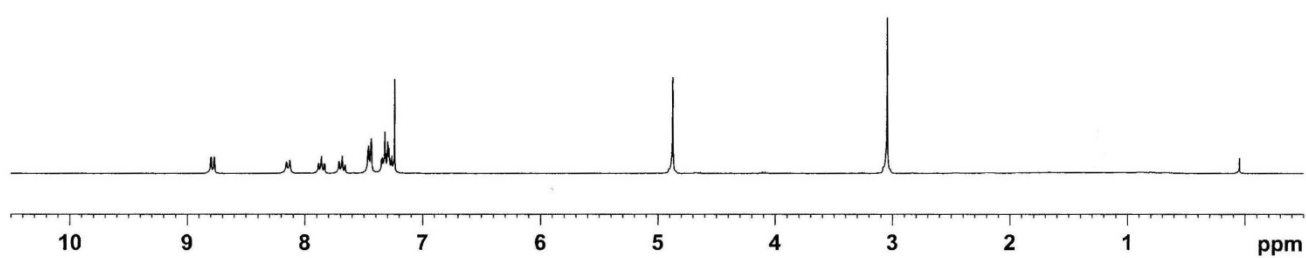
Unsaturation (U.S.): -0.5 - 100.0

Observed m/z	Int%	Err[ppm / mmu]	U.S. Composition
356.0122	100.0	+0.9 / +0.3	14.0 C 18 H 10 Cl 2 N 2 O 2
357.0154	24.3		
358.0108	64.9		
359.0119	14.1		
360.0085	11.8		

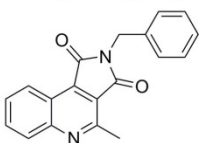
¹H NMR of Compound **41**



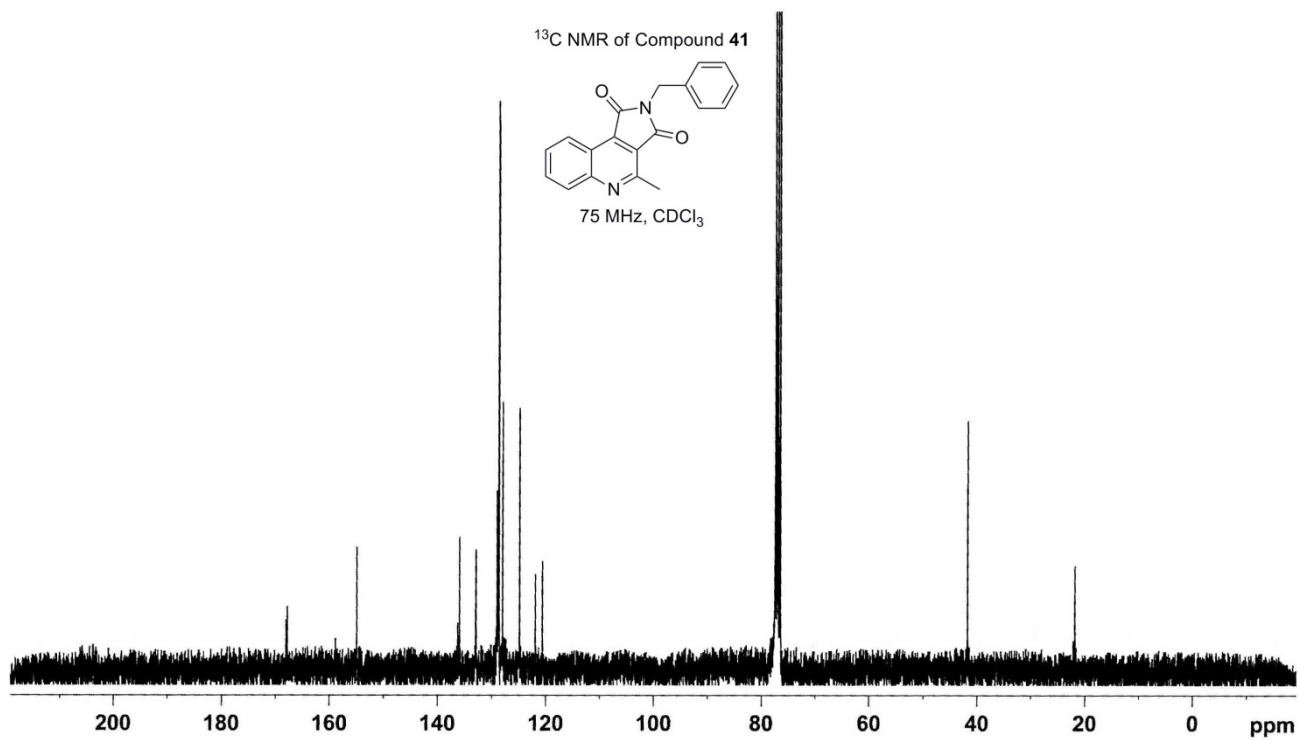
300 MHz, CDCl₃



¹³C NMR of Compound **41**

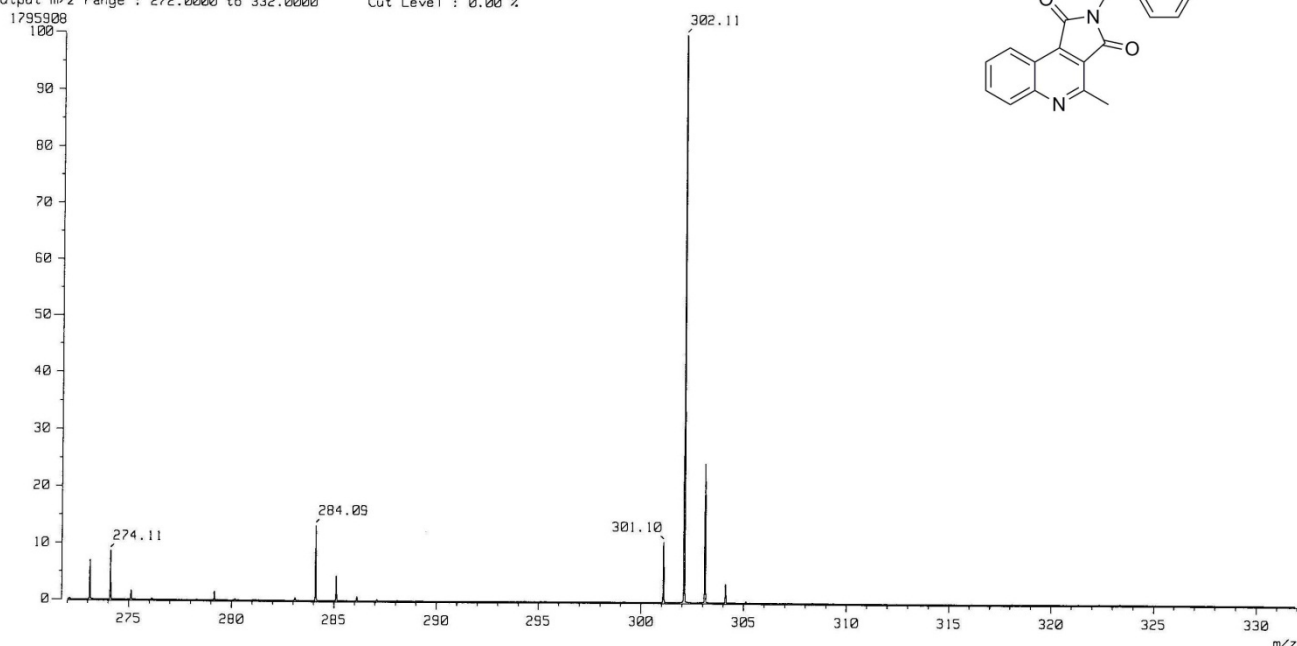
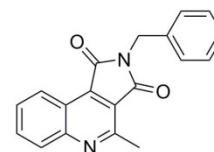


75 MHz, CDCl₃



[Mass Spectrum]
Data : 7-mu-C19H14N2O2 Date : 12-Dec-2012 15:10
Sample: -
Note: -
Inlet : Direct Ion Mode : EI+
Spectrum Type : Normal Ion [EF-Linear]
RT : 0.53 min Scan# : (11,12)
BP : m/z 302.1054 Int. : 85.64
Output m/z range : 272.0000 to 332.0000 Cut Level : 0.00 %

Mass spectrum of Compound 41



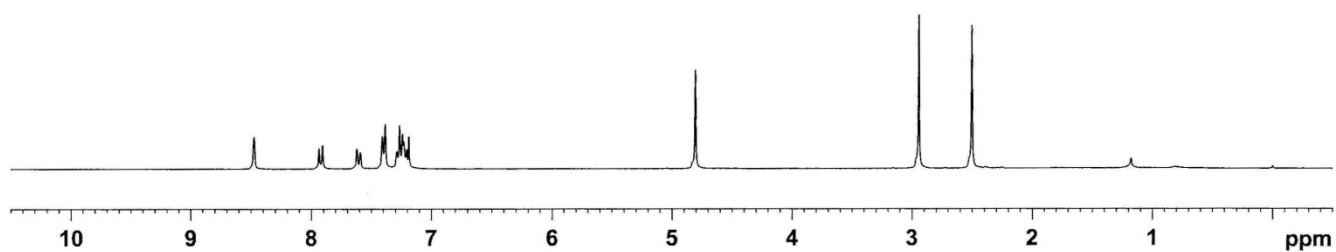
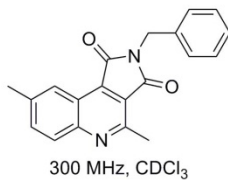
[Elemental Composition]

Page: 1

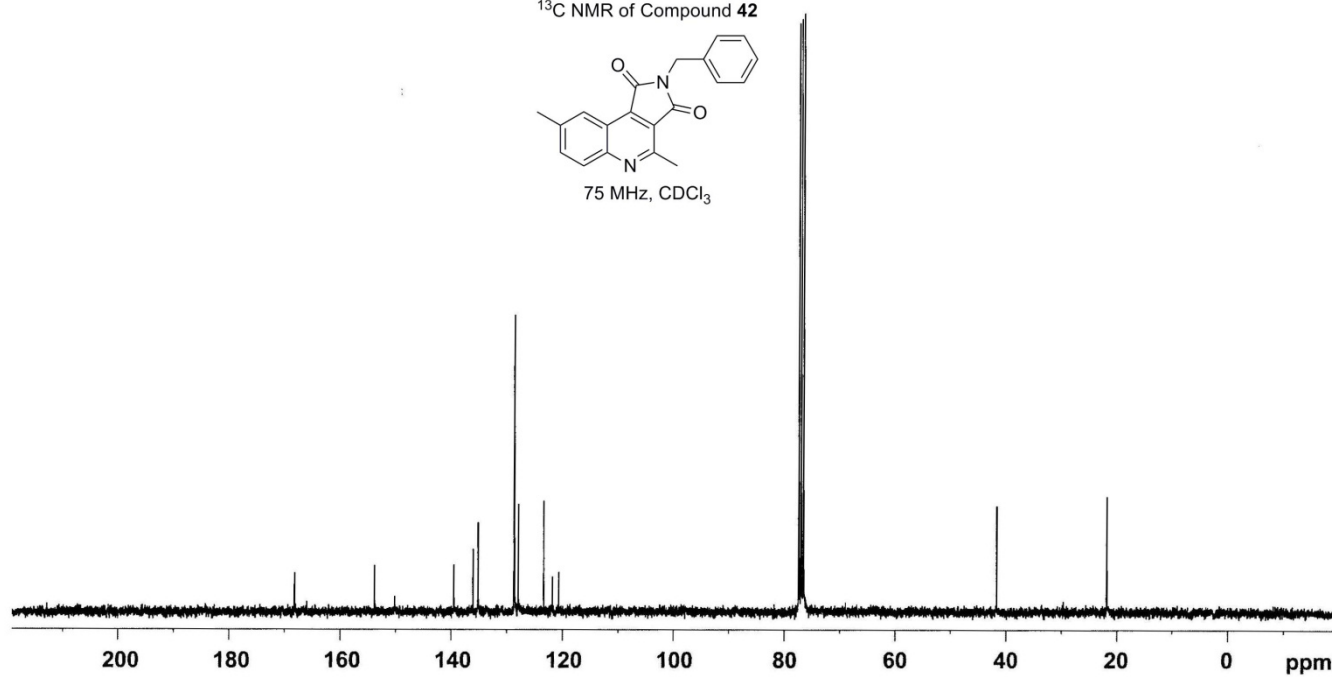
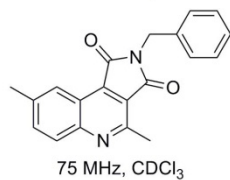
Data : 7-mu-C19H14N2O2 Date : 12-Dec-2012 15:10
Sample: -
Note: -
Inlet : Direct Ion Mode : EI+
RT : 0.53 min Scan#: (11,12)
Elements : C 19/0, H 14/0, N 2/0, O 2/0
Mass Tolerance : 1000ppm, 2mmu if m/z < 2, 3mmu if m/z > 3
Unsaturation (U.S.) : -0.5 - 100.0

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
284.0945	13.3	-1.6 / -0.5	15.0	C 19 H 12 N 2 O
301.0973	10.7	-1.4 / -0.4	14.5	C 19 H 13 N 2 O 2
302.1054	100.0	-0.3 / -0.1	14.0	C 19 H 14 N 2 O 2
303.1086	24.4			

¹H NMR of Compound **42**

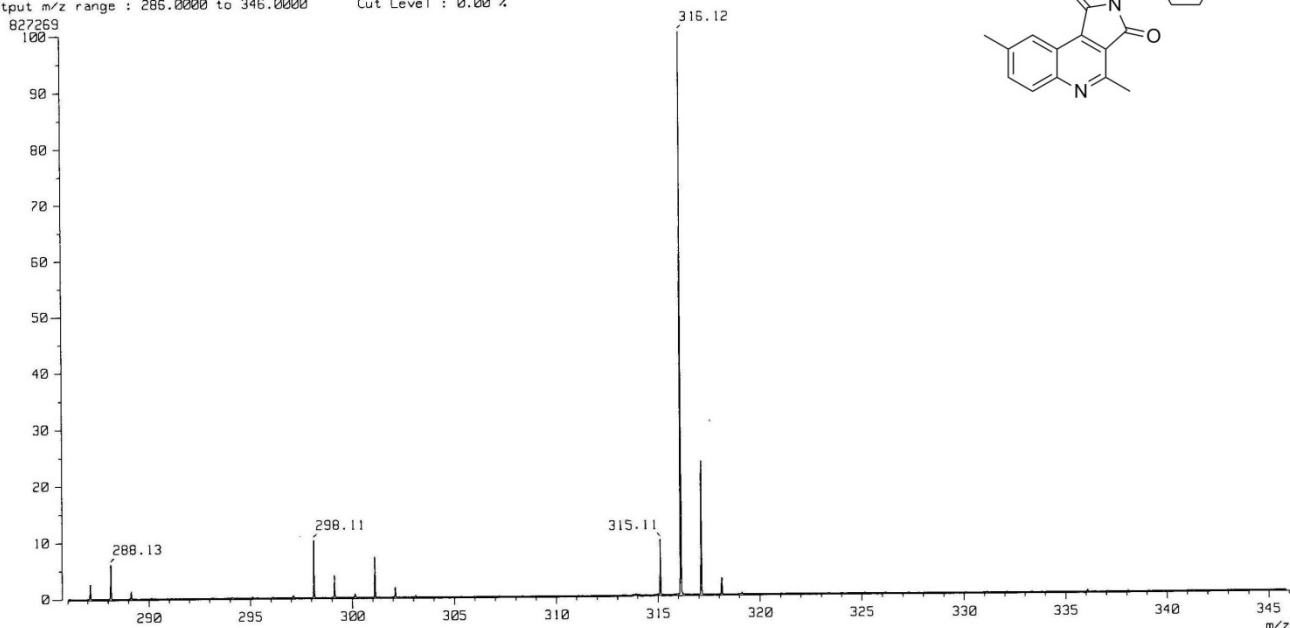
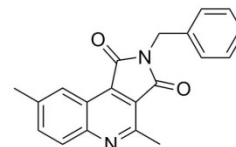


¹³C NMR of Compound **42**



[Mass Spectrum]
Data : 7Final-C20H16N2O2 Date : 12-Dec-2012 15:25
Sample: -
Note: -
Inlet: Direct Ion Mode: EI+
Spectrum Type: Normal Ion [EF-Linear]
RT: 0.43 min Scan#: (9,10)
BP: m/z 316.1209 Int.: 39.45
Output m/z range: 285.0000 to 346.0000 Cut Level: 0.00 %

Mass spectrum of Compound 42



[Elemental Composition]

Data : 7Final-C20H16N2O2

Date : 12-Dec-2012 15:25

Page: 1

Sample: -

Note: -

Inlet: Direct

Ion Mode: EI+

RT: 0.43 min

Scan#: (9,10)

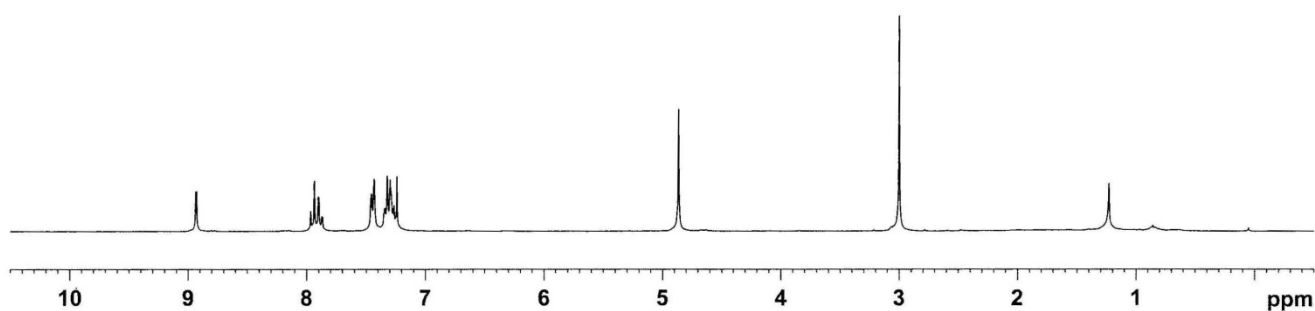
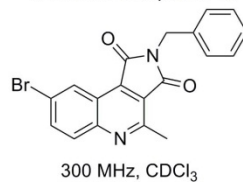
Elements: C 20/0, H 16/0, N 2/0, O 2/0

Mass Tolerance: 1000ppm, 2mmu if m/z < 2, 3mmu if m/z > 3

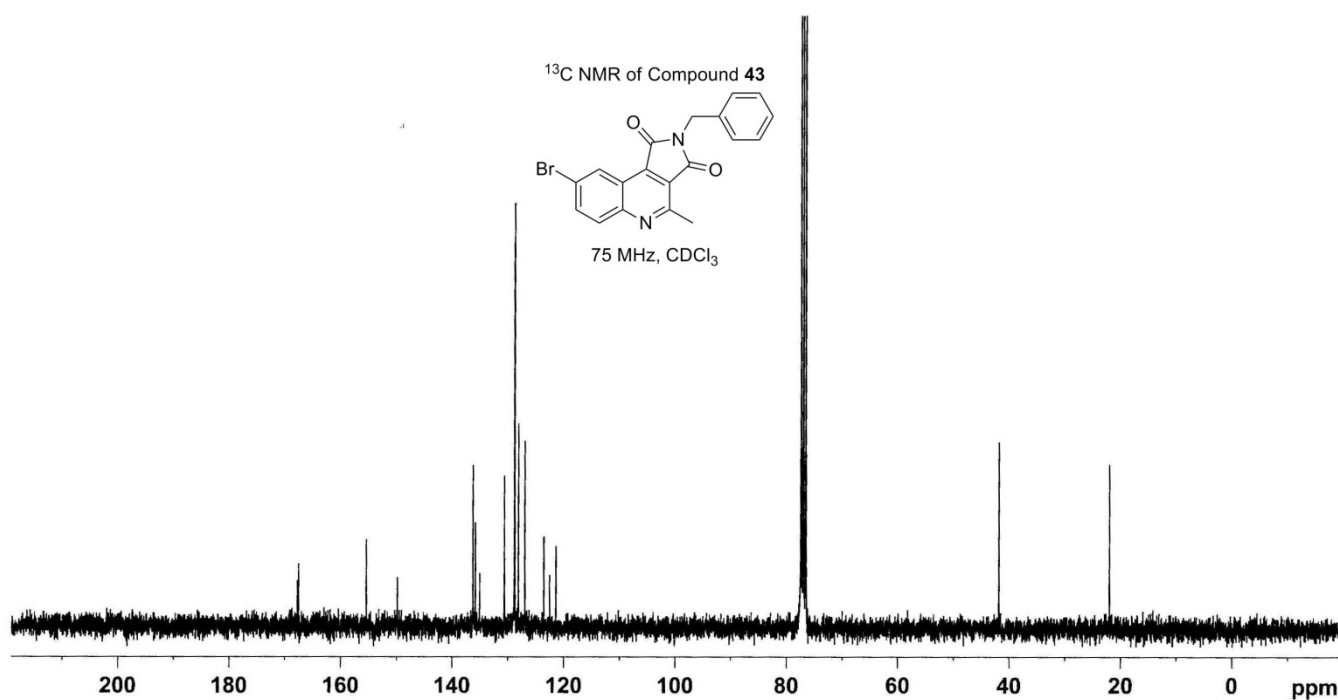
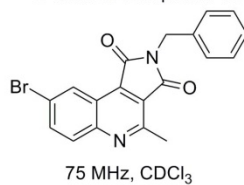
Unsaturation (U.S.): -0.5 - 100.0

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
298.1104	10.2	-0.8 / -0.2	15.0	C 20 H 14 N 2 O
316.1209	100.0	-0.8 / -0.3	14.0	C 20 H 16 N 2 O 2
317.1241	23.7			

¹H NMR of Compound **43**

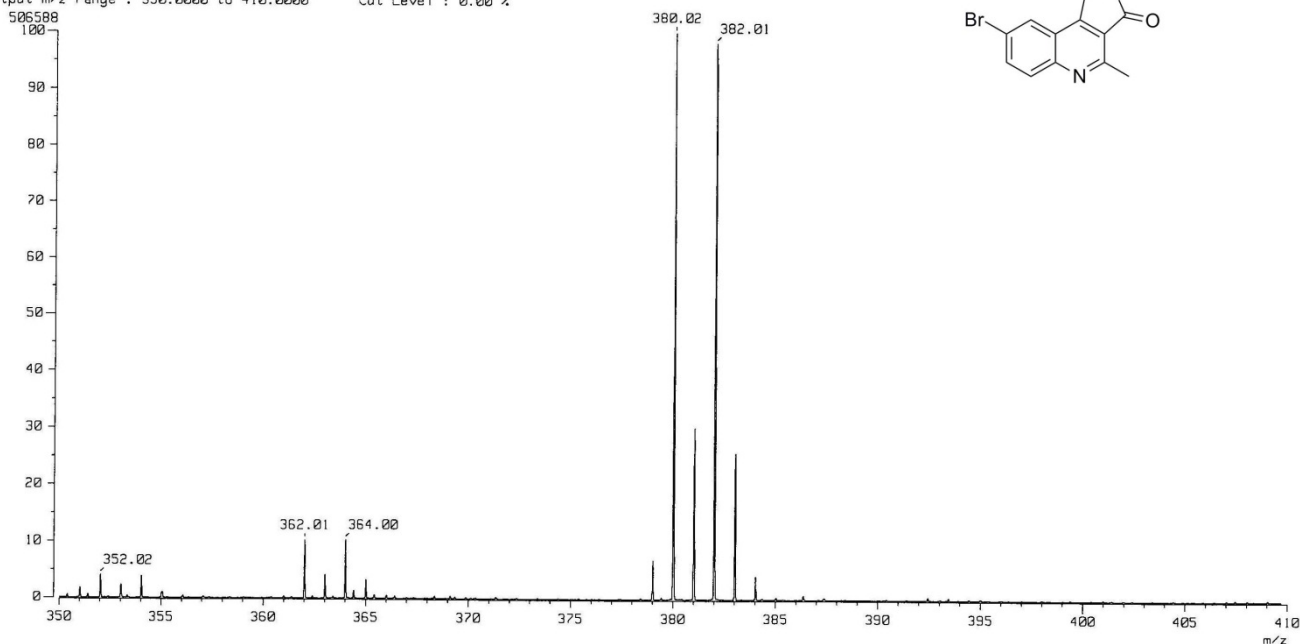
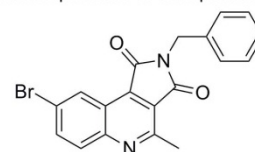


¹³C NMR of Compound **43**



[Mass Spectrum]
Data : 7-nu-C19H13BrN2O2 Date : 12-Dec-2012 15:15
Sample: -
Note: -
Inlet : Direct Ion Mode : EI+
Spectrum Type : Normal Ion [EF-Linear]
RT : 0.33 min Scan# : (7,8)
BP : m/z 380.0158 Int. : 24.15
Output m/z range : 350.0000 to 410.0000 Cut Level : 0.00 %

Mass spectrum of Compound 43



[Elemental Composition]

Data : 7-nu-C19H13BrN2O2

Date : 12-Dec-2012 15:15

Page: 1

Sample: -

Note: -

Inlet : Direct

Ion Mode : EI+

RT : 0.33 min

Scan#: (7,8)

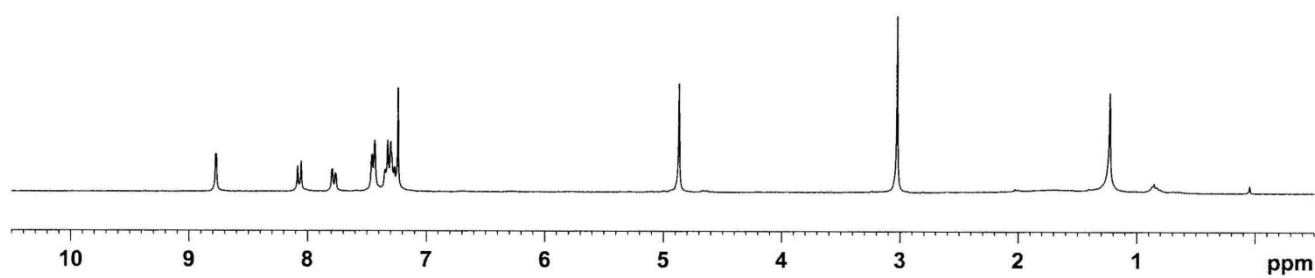
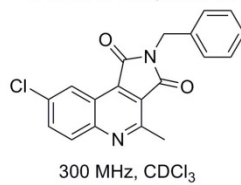
Elements : C 19/0, H 13/0, Br 1/0, N 2/0, O 2/0

Mass Tolerance : 1000ppm, 2mmu if m/z < 2, 3mmu if m/z > 3

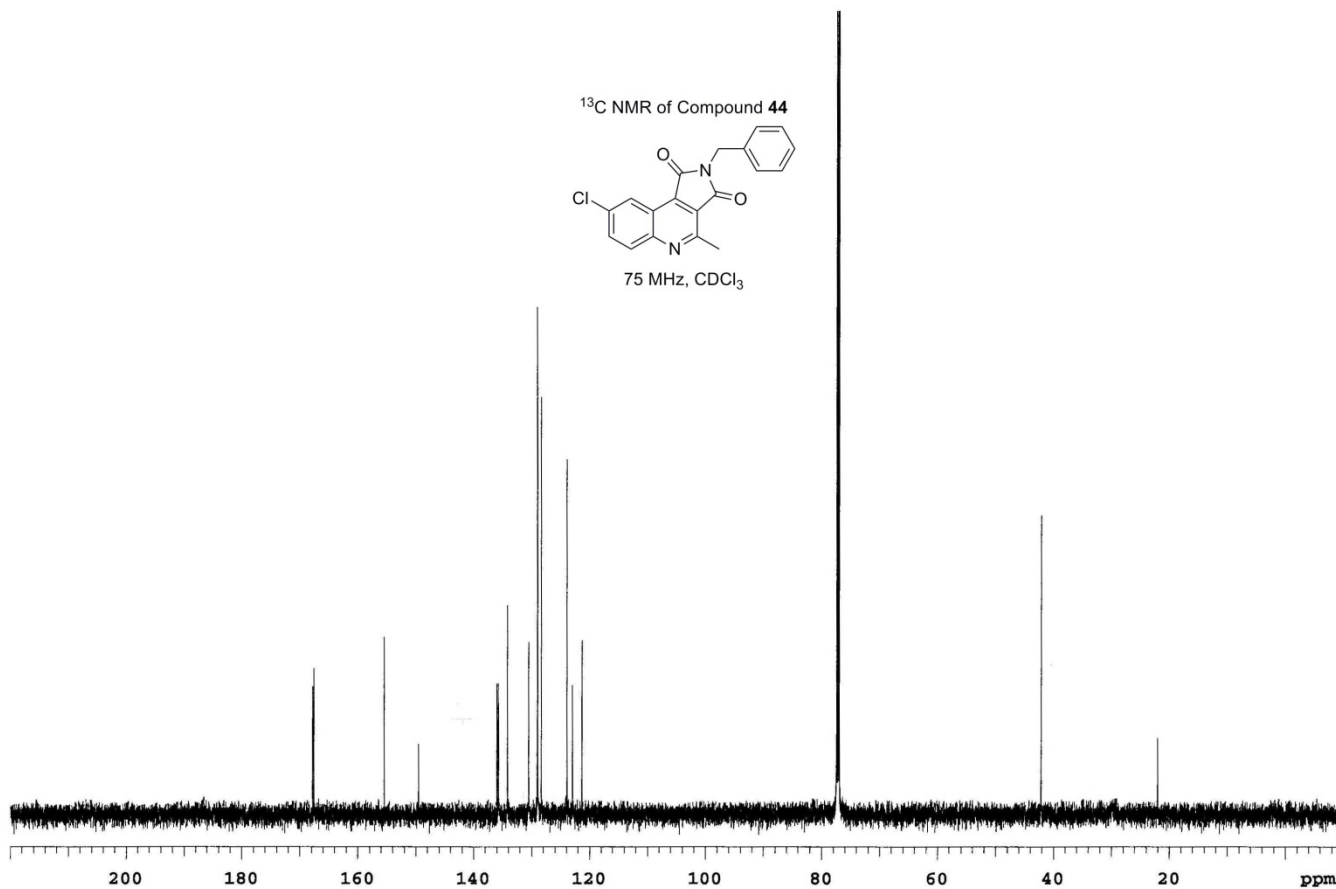
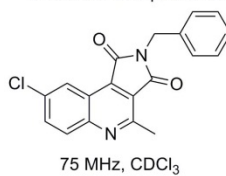
Unsaturation (U.S.) : -0.5 - 100.0

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
362.0058	10.3	+1.0 / +0.4	15.0	C 19 H 11 Br N 2 O
364.0025	10.4			
380.0158	100.0	-0.6 / -0.2	14.0	C 19 H 13 Br N 2 O 2
381.0160	30.2			
382.0145	98.2			
383.0163	25.8			

¹H NMR of Compound **44**

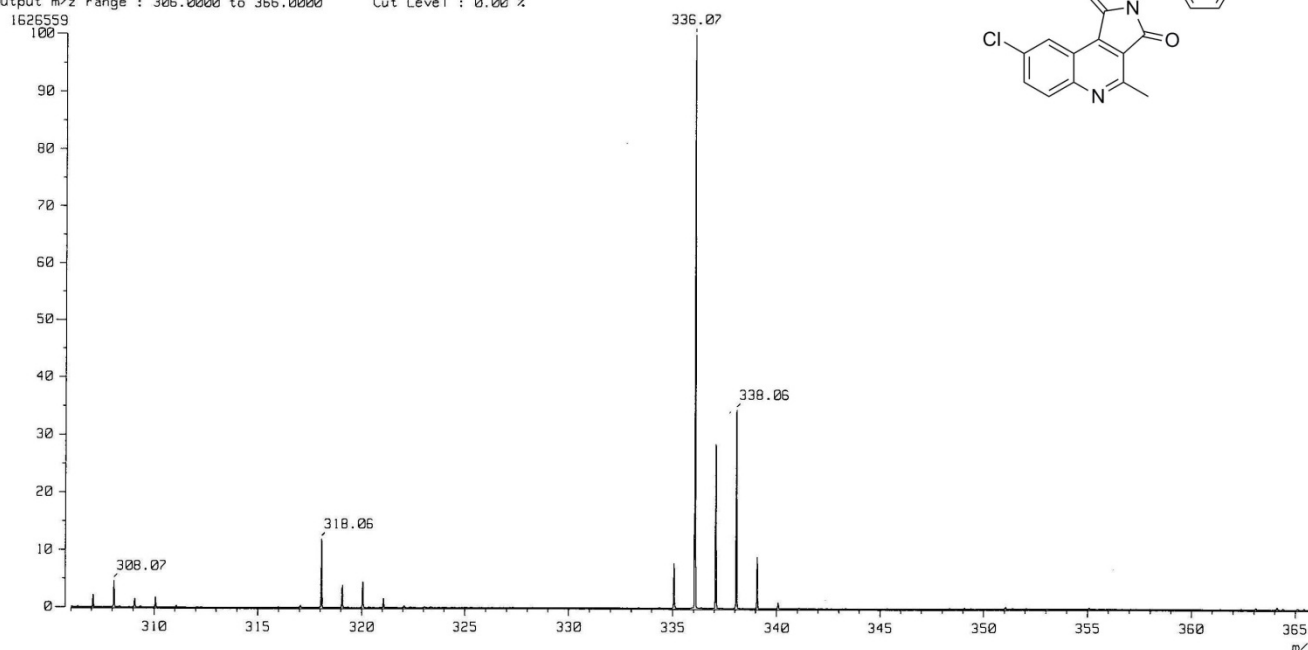
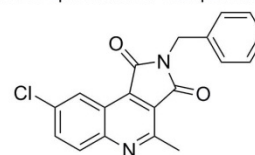


¹³C NMR of Compound **44**



[Mass Spectrum]
Data : 7-xi-C19H13ClN2O2 Date : 12-Dec-2012 15:20
Sample: -
Note: -
Inlet : Direct Ion Mode : EI+
Spectrum Type : Normal Ion [EF-Linear]
RT : 0.53 min Scan#: (11,12)
BP : m/z 336.0653 Int. : 77.56
Output m/z range : 306.0000 to 366.0000 Cut Level : 0.00 %

Mass spectrum of Compound 44



[Elemental Composition]

Data : 7-xi-C19H13ClN2O2

Date : 12-Dec-2012 15:20

Page: 1

Sample: -

Note: -

Inlet : Direct

Ion Mode : EI+

RT : 0.53 min

Scan#: (11,12)

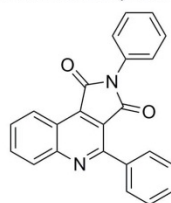
Elements : C 19/0, H 13/0, Cl 1/0, N 2/0, O 2/0

Mass Tolerance : 1000ppm, 2mmu if m/z < 2, 3mmu if m/z > 3

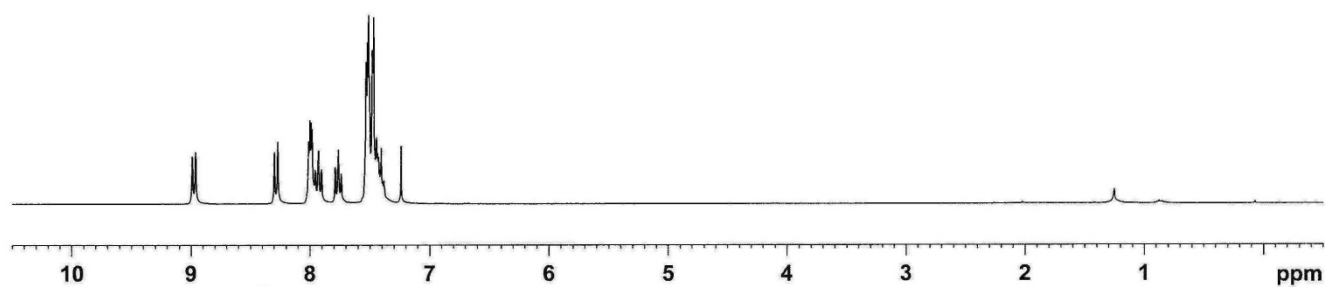
Unsaturation (U.S.) : -0.5 - 100.0

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
318.0558	12.0	-0.5 / -0.2	15.0	C 19 H 11 Cl N 2 O
336.0663	100.0	-0.7 / -0.2	14.0	C 19 H 13 Cl N 2 O 2
337.0683	28.6			
338.0646	34.5			

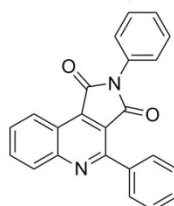
^1H NMR of Compound **45**



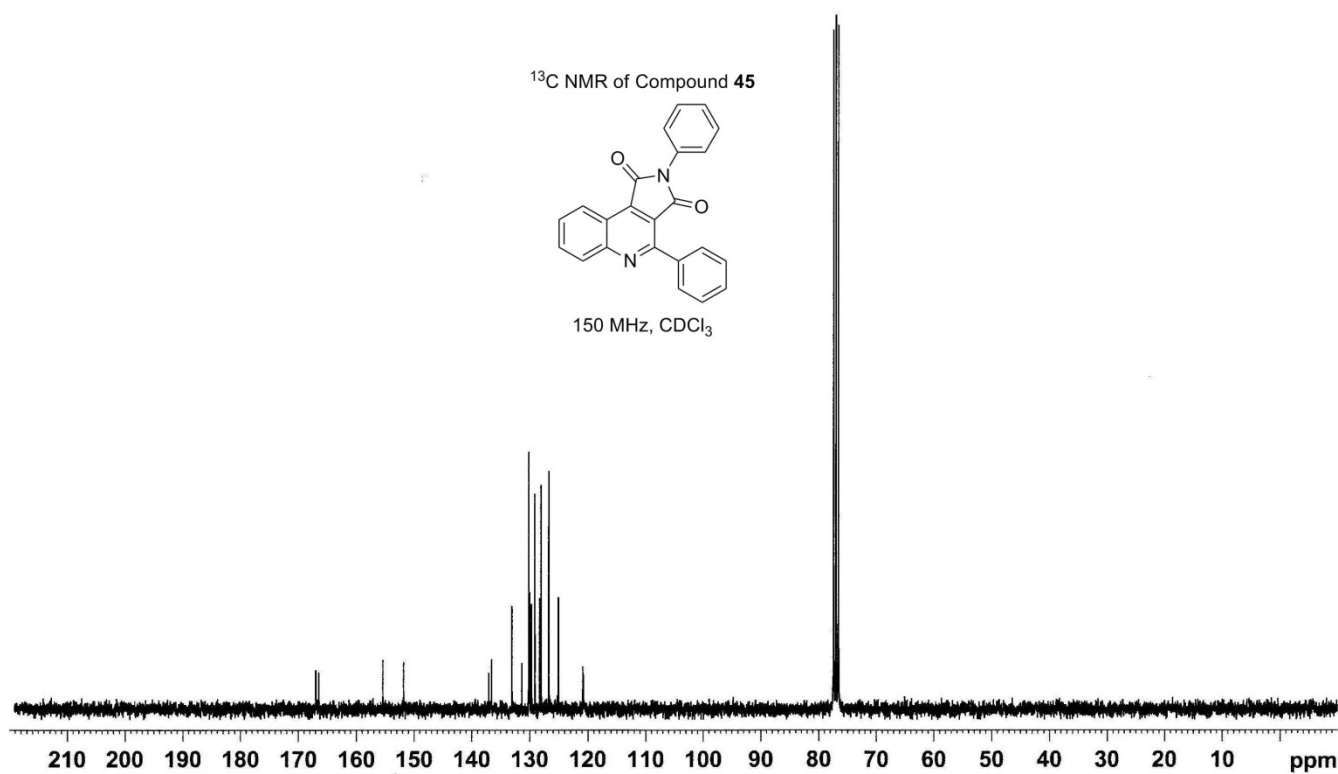
300 MHz, CDCl_3



^{13}C NMR of Compound **45**

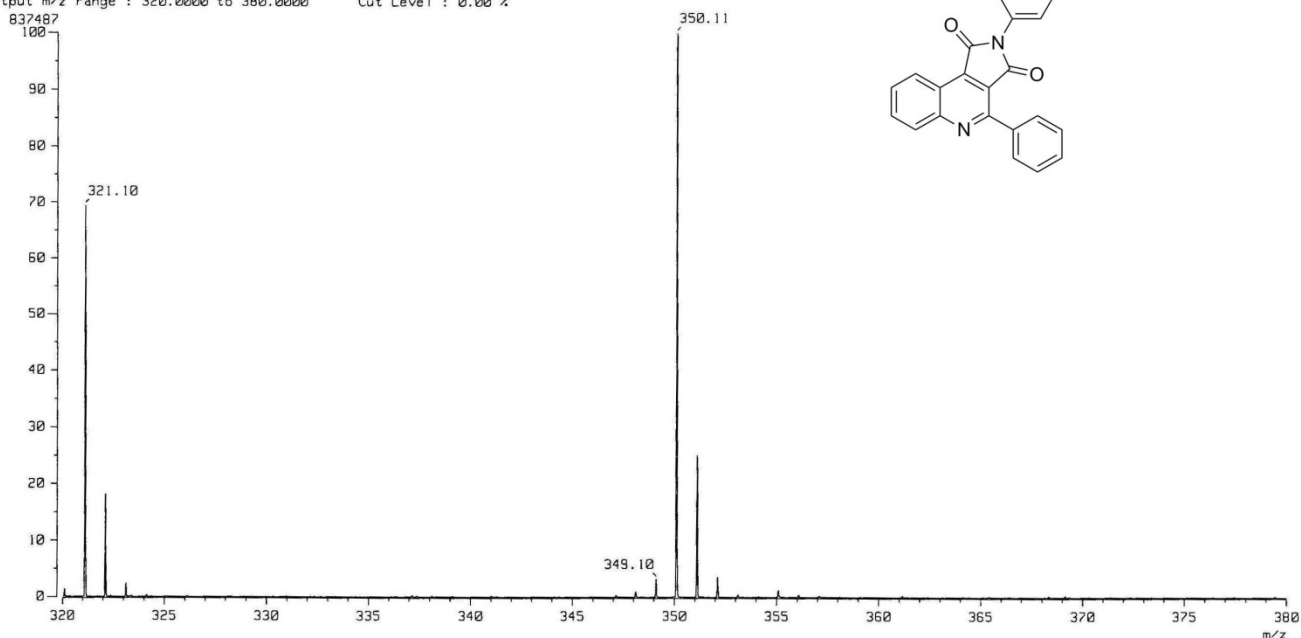


150 MHz, CDCl_3



[Mass Spectrum]
Data : X6-9-C23H14N2O2 Date : 20-Feb-2013 17:14
Sample: -
Note: -
Inlet : Direct Ion Mode : EI+
Spectrum Type : Normal Ion [EF-Linear]
RT : 0.78 min Scan# : (16,17)
BP : m/z 350.1057 Int. : 39.93
Output m/z range : 320.0000 to 380.0000 Cut Level : 0.00 %

Mass spectrum of Compound 45



[Elemental Composition]

Data : X6-9-C23H14N2O2

Date : 20-Feb-2013 17:14

Page: 1

Sample: -

Note: -

Inlet : Direct

Ion Mode : EI+

RT : 0.78 min

Scan#: (16,17)

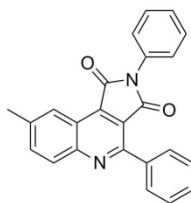
Elements : C 23/0, H 14/0, N 2/0, O 2/0

Mass Tolerance : 1000ppm, 2mmu if m/z < 2, 3mmu if m/z > 3

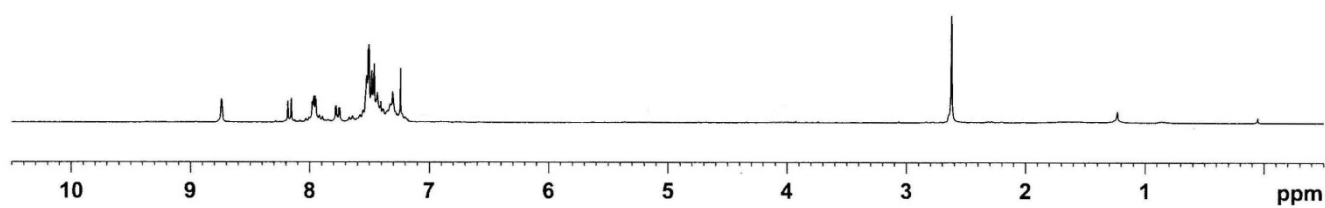
Unsaturation (U.S.) : -0.5 - 100.0

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
321.1034	69.4	+2.0 / +0.6	17.5	C 22 H 13 N 2 O
322.1068	18.2			
350.1057	100.0	+0.5 / +0.2	18.0	C 23 H 14 N 2 O 2
351.1100	25.1			

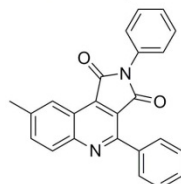
¹H NMR of Compound **46**



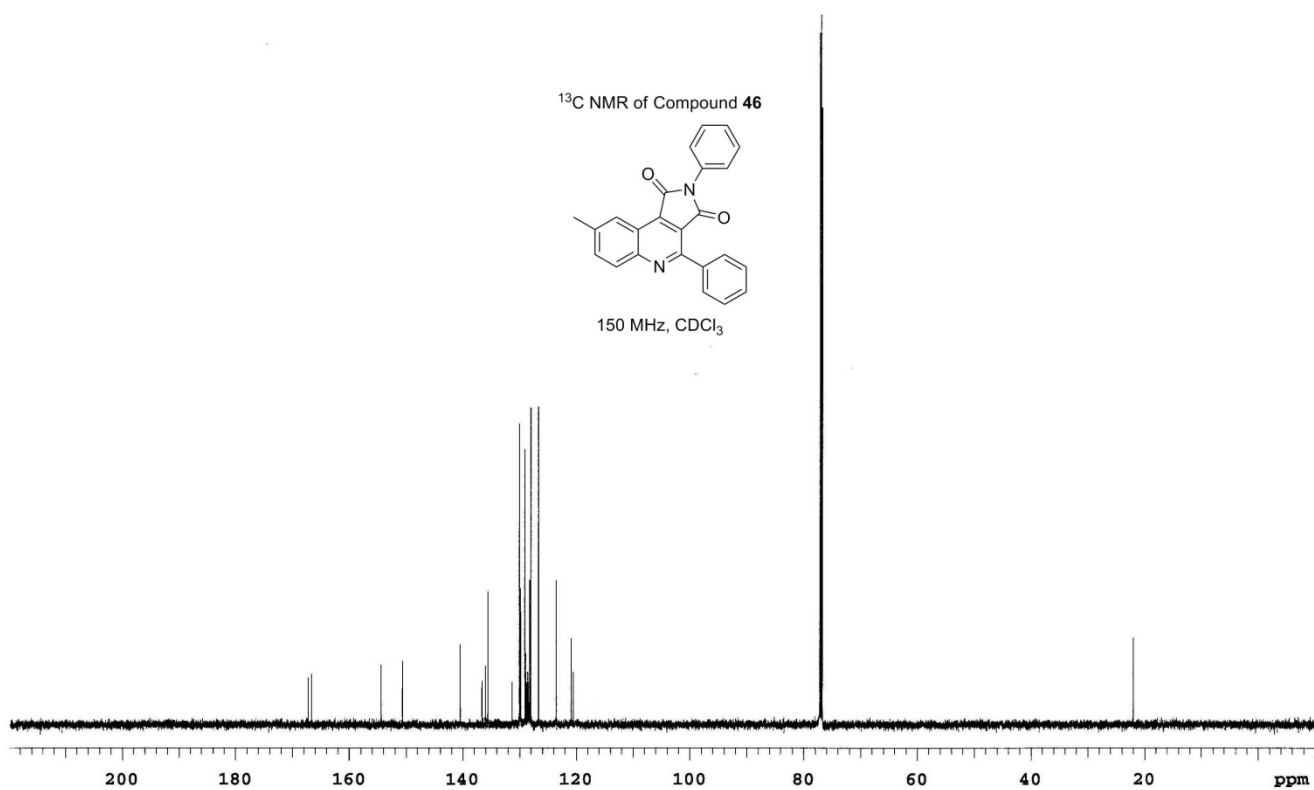
300 MHz, CDCl₃



¹³C NMR of Compound **46**

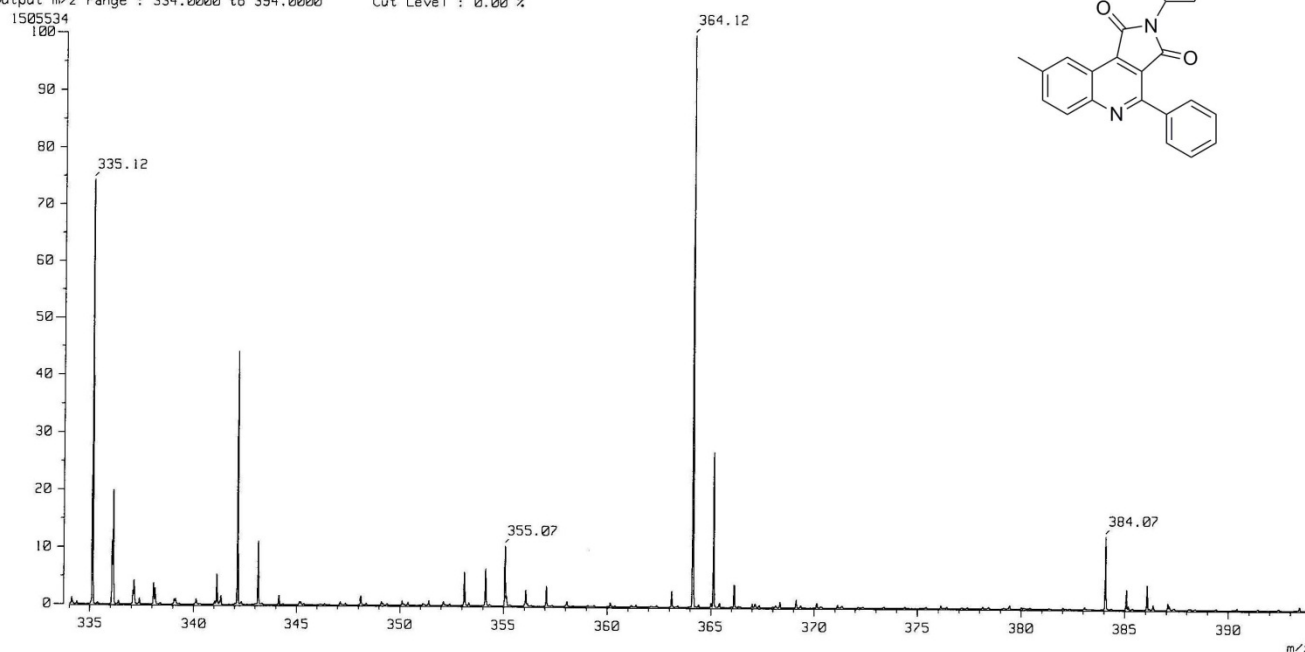
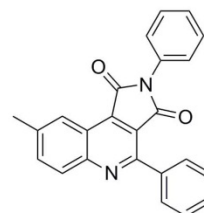


150 MHz, CDCl₃



[Mass Spectrum]
Data : 7-lambda-C24H16N2O2 Date : 12-Dec-2012 15:06
Sample: -
Note: -
Inlet: Direct Ion Mode: EI+
Spectrum Type: Normal Ion [EF-Linear]
RT: 1.33 min Scan#: (27,28)
BP: m/z 364.1215 Int.: 71.79
Output m/z range: 334.0000 to 394.0000 Cut Level: 0.00 %

Mass spectrum of Compound 46



[Elemental Composition]

Data : 7-lambda-C24H16N2O2

Date : 12-Dec-2012 15:06

Page: 1

Sample: -

Note: -

Inlet: Direct

Ion Mode: EI+

RT: 1.33 min

Scan#: (27,28)

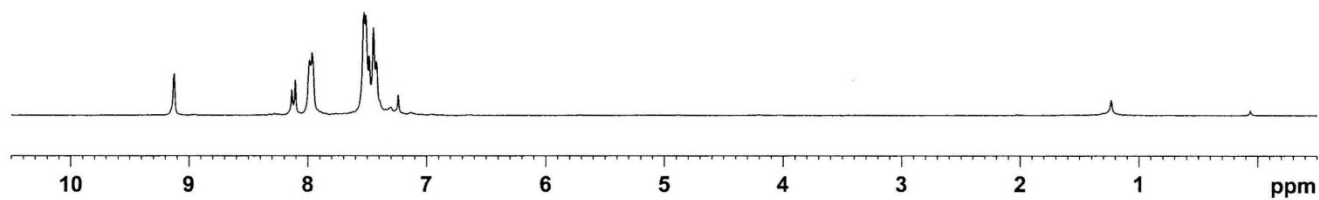
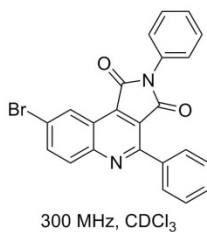
Elements: C 24/0, H 16/0, N 2/0, O 2/0

Mass Tolerance: 1000ppm, 2mmu if m/z < 2, 3mmu if m/z > 3

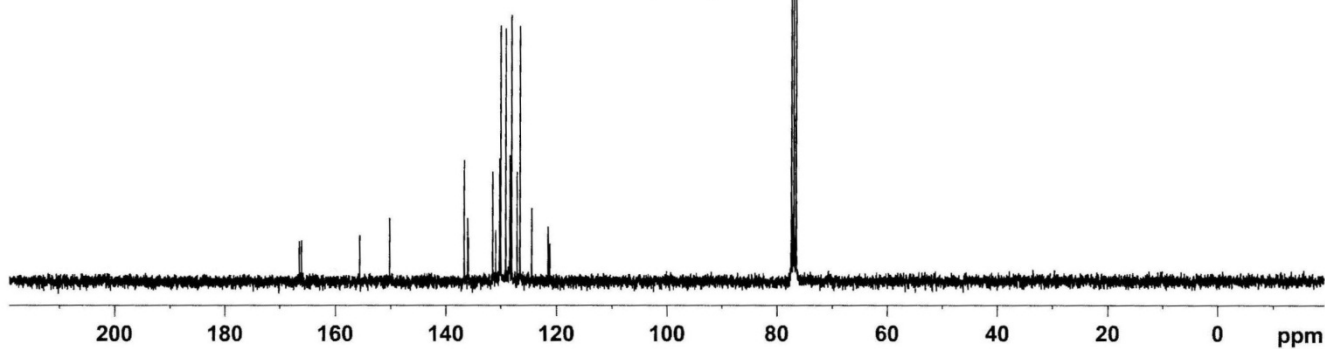
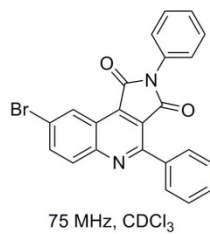
Unsaturation (U.S.): -0.5 - 100.0

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
335.1190	74.4	+1.7 / +0.6	17.5	C 23 H 15 N 2 O
336.1028	20.0	+1.1 / +0.4	17.5	C 23 H 14 N O 2
342.1367	44.2			
343.1390	11.2			
355.0659	10.6			
364.1215	100.0	+0.9 / +0.3	18.0	C 24 H 16 N 2 O 2
365.1245	27.0			
384.0671	12.8			

¹H NMR of Compound **47**

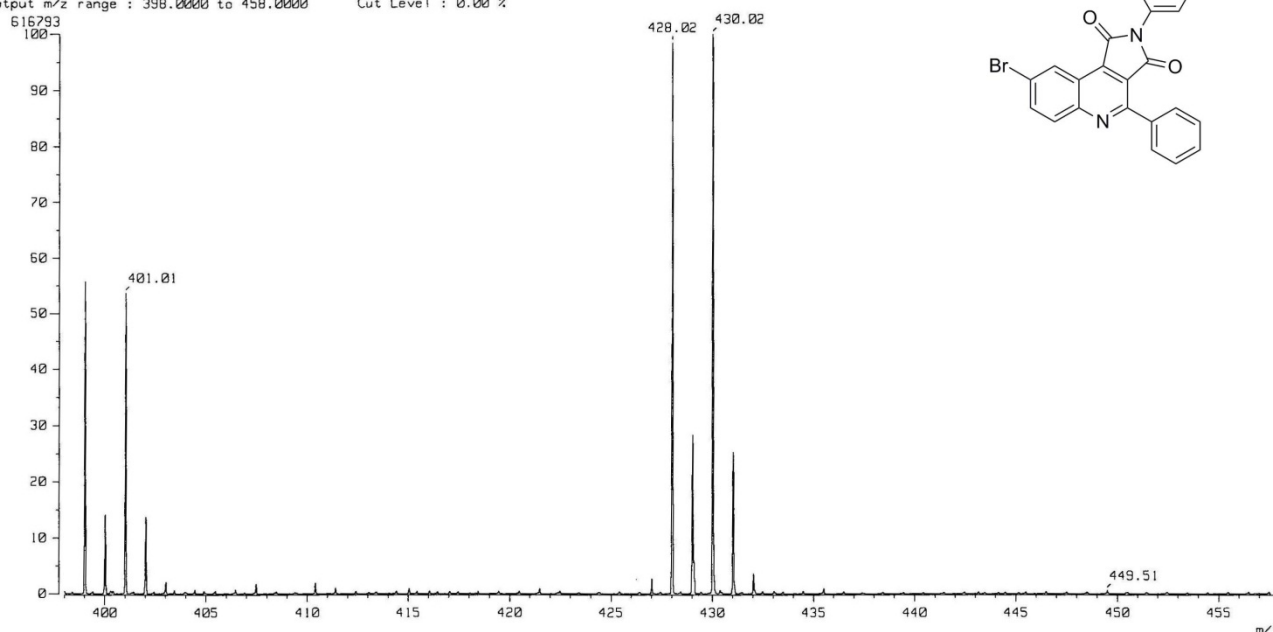
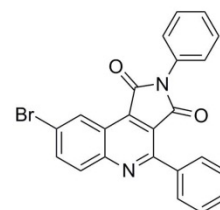


¹³C NMR of Compound **47**



[Mass Spectrum]
Data : 7-iota-C23H13BrN2O2 Date : 12-Dec-2012 14:50
Sample: -
Note: -
Inlet : Direct Ion Mode : EI+
Spectrum Type : Normal Ion [EF-Linear]
RT : 0.78 min Scan# : (16,17)
BP : m/z 430.0162 Int. : 29.41
Output m/z range : 398.0000 to 458.0000 Cut Level : 0.00 %

Mass spectrum of Compound 47



[Elemental Composition]

Data : 7-iota-C23H13BrN2O2

Date : 12-Dec-2012 14:50

Page: 1

Sample: -

Note: -

Inlet : Direct

Ion Mode : EI+

RT : 0.78 min

Scan#: (16,17)

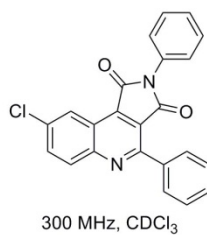
Elements : C 23/0, H 13/0, Br 1/0, N 2/0, O 2/0

Mass Tolerance : 1000ppm, 2mmu if m/z < 2, 3mmu if m/z > 3

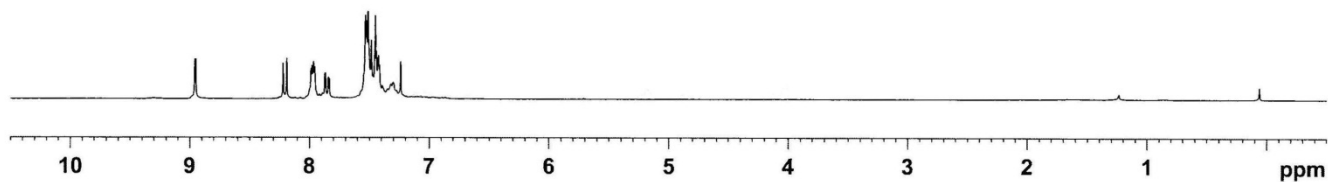
Unsaturation (U.S.) : -0.5 - 100.0

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
399.0136	55.8	+0.7 / +0.3	17.5	C 22 H 12 Br N 2 O
400.0146	14.2			
401.0122	53.7			
402.0103	13.8	-6.5 / -2.6	16.5	C 22 H 13 Br N O 2
428.0163	98.5	+0.6 / +0.3	18.0	C 23 H 13 Br N 2 O 2
429.0192	28.4			
430.0162	100.0			
431.0219	25.3			

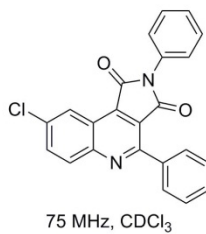
^1H NMR of Compound **48**



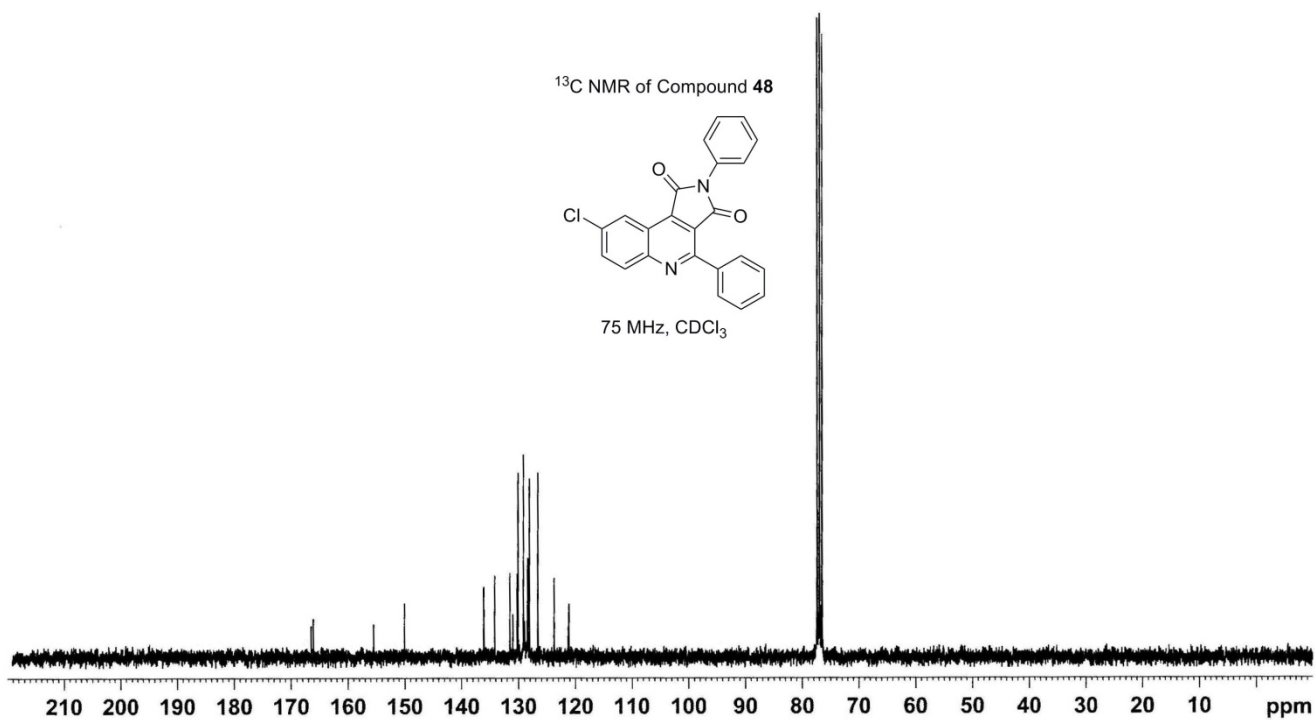
300 MHz, CDCl_3



^{13}C NMR of Compound **48**

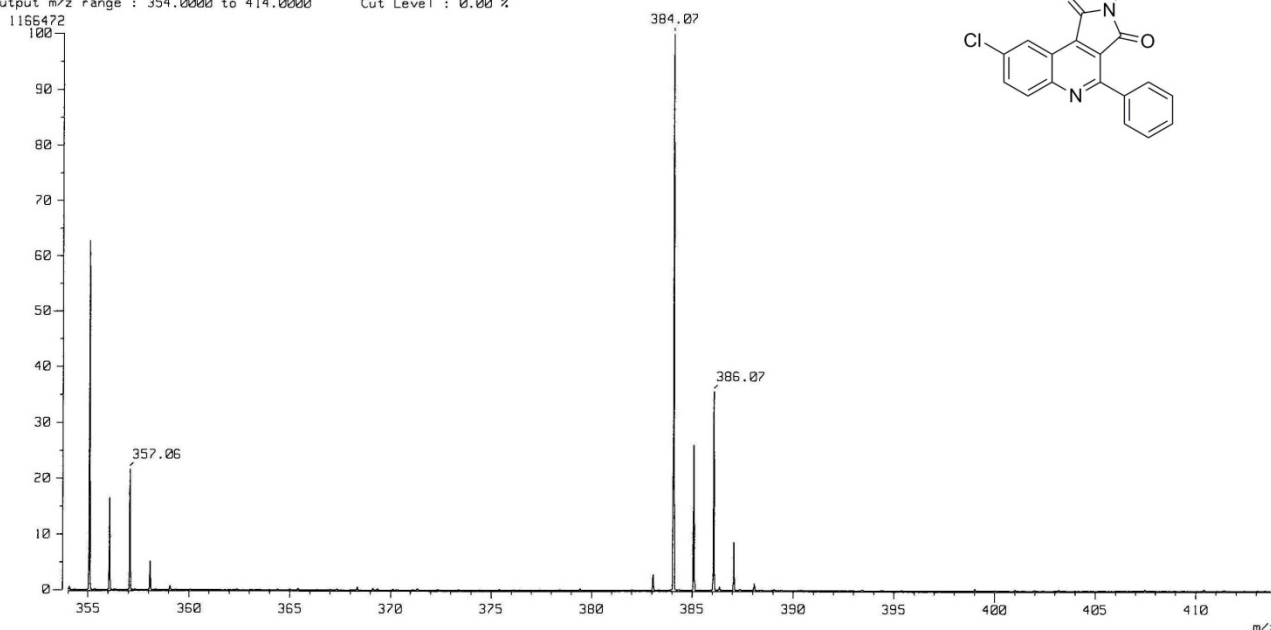
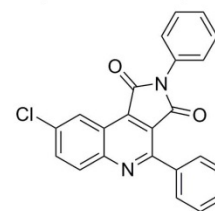


75 MHz, CDCl_3



[Mass Spectrum]
Data : 7-kappa-C23H13ClN2O2 Date : 12-Dec-2012 14:56
Sample: -
Note: -
Inlet : Direct Ion Mode : EI+
Spectrum Type : Normal Ion [EF-Linear]
RT : 0.73 min Scan# : (15,16)
BP : m/z 384.0664 Int. : 55.62
Output m/z range : 354.0000 to 414.0000 Cut Level : 0.00 %

Mass spectrum of Compound 48



[Elemental Composition]

Page: 1

Data : 7-kappa-C23H13ClN2O2

Date : 12-Dec-2012 14:56

Sample: -

Note: -

Inlet : Direct

Ion Mode : EI+

RT : 0.73 min

Scan#: (15,16)

Elements : C 23/0, H 13/0, Cl 1/0, N 2/0, O 2/0

Mass Tolerance : 1000ppm, 2mmu if m/z < 2, 3mmu if m/z > 3

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

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
355.0641	62.7	+0.7 / +0.2	17.5	C 22 H 12 Cl N 2 O
356.0670	16.6			
357.0620	21.7			
384.0664	100.0	-0.4 / -0.1	18.0	C 23 H 13 Cl N 2 O 2
385.0701	26.1			
386.0662	35.7			

X-ray crystal data for compound **39**

Table 1. Crystal data and structure refinement for No10.

Identification code	No10	
Empirical formula	C ₁₉ H ₁₃ Cl N ₂ O ₃	
Formula weight	352.76	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 12.3101(17) Å	α = 90°.
	b = 8.8146(13) Å	β = 97.891(3)°.
	c = 14.675(2) Å	γ = 90°.
Volume	1577.3(4) Å ³	
Z	4	
Density (calculated)	1.486 Mg/m ³	
Absorption coefficient	0.264 mm ⁻¹	
F(000)	728	
Crystal size	0.28 x 0.20 x 0.17 mm ³	
Theta range for data collection	1.67 to 28.33°.	
Index ranges	-16<=h<=16, -7<=k<=11, -19<=l<=18	
Reflections collected	11357	
Independent reflections	3924 [R(int) = 0.0464]	
Completeness to theta = 28.33°	99.8 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	3924 / 0 / 228	
Goodness-of-fit on F ²	1.079	
Final R indices [I>2sigma(I)]	R1 = 0.0498, wR2 = 0.1131	
R indices (all data)	R1 = 0.1194, wR2 = 0.1728	
Largest diff. peak and hole	0.414 and -0.531 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for No10. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	3082(2)	4670(3)	6793(2)	33(1)
C(1)	2245(2)	3673(4)	6952(2)	34(1)
O(1)	2137(2)	3121(3)	7688(1)	43(1)
C(2)	2965(3)	5123(4)	5863(2)	37(1)
O(2)	3578(2)	5975(3)	5544(2)	49(1)
C(3)	1958(2)	4340(3)	5411(2)	32(1)
C(4)	1546(2)	3477(3)	6050(2)	32(1)
C(5)	589(2)	2588(3)	5815(2)	32(1)
C(6)	134(2)	1624(4)	6426(2)	37(1)
C(7)	-780(2)	788(4)	6101(2)	42(1)
C(8)	-1279(2)	930(4)	5183(2)	42(1)
C(9)	-857(3)	1874(4)	4593(2)	39(1)
Cl(1)	-1482(1)	2022(1)	3465(1)	51(1)
C(10)	122(2)	2730(3)	4878(2)	34(1)
N(2)	533(2)	3607(3)	4236(2)	38(1)
C(11)	1448(2)	4394(4)	4484(2)	36(1)
C(12)	1892(3)	5300(4)	3763(2)	45(1)
C(13)	3901(2)	5237(4)	7500(2)	35(1)
C(14)	3593(2)	6059(4)	8221(2)	37(1)
C(15)	4360(2)	6560(4)	8935(2)	36(1)
C(16)	5462(2)	6231(4)	8919(2)	37(1)
O(3)	6283(2)	6651(3)	9594(2)	48(1)
C(17)	5967(3)	7350(4)	10398(2)	49(1)
C(18)	5777(3)	5448(4)	8180(2)	46(1)
C(19)	5000(3)	4931(4)	7478(2)	45(1)

Table 3. Bond lengths [Å] and angles [°] for No10.

N(1)-C(1)	1.398(4)
N(1)-C(2)	1.411(4)
N(1)-C(13)	1.433(4)
C(1)-O(1)	1.208(3)
C(1)-C(4)	1.487(4)
C(2)-O(2)	1.204(4)
C(2)-C(3)	1.493(4)
C(3)-C(4)	1.359(4)
C(3)-C(11)	1.419(4)
C(4)-C(5)	1.417(4)
C(5)-C(6)	1.406(4)
C(5)-C(10)	1.420(4)
C(6)-C(7)	1.374(4)
C(6)-H(6)	0.9500
C(7)-C(8)	1.408(4)
C(7)-H(7)	0.9500
C(8)-C(9)	1.354(5)
C(8)-H(8)	0.9500
C(9)-C(10)	1.435(4)
C(9)-Cl(1)	1.733(3)
C(10)-N(2)	1.369(4)
N(2)-C(11)	1.330(4)
C(11)-C(12)	1.488(4)
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-C(14)	1.378(4)
C(13)-C(19)	1.384(4)
C(14)-C(15)	1.383(4)
C(14)-H(14)	0.9500
C(15)-C(16)	1.391(4)
C(15)-H(15)	0.9500
C(16)-O(3)	1.365(3)
C(16)-C(18)	1.385(4)
O(3)-C(17)	1.433(4)
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800

C(17)-H(17C)	0.9800
C(18)-C(19)	1.384(4)
C(18)-H(18)	0.9500
C(19)-H(19)	0.9500

C(1)-N(1)-C(2)	111.1(2)
C(1)-N(1)-C(13)	124.0(2)
C(2)-N(1)-C(13)	124.7(3)
O(1)-C(1)-N(1)	125.2(3)
O(1)-C(1)-C(4)	128.9(3)
N(1)-C(1)-C(4)	105.9(2)
O(2)-C(2)-N(1)	124.5(3)
O(2)-C(2)-C(3)	130.0(3)
N(1)-C(2)-C(3)	105.5(3)
C(4)-C(3)-C(11)	121.5(3)
C(4)-C(3)-C(2)	108.6(3)
C(11)-C(3)-C(2)	129.9(3)
C(3)-C(4)-C(5)	121.2(3)
C(3)-C(4)-C(1)	108.9(3)
C(5)-C(4)-C(1)	129.9(3)
C(6)-C(5)-C(4)	124.7(3)
C(6)-C(5)-C(10)	121.8(3)
C(4)-C(5)-C(10)	113.5(3)
C(7)-C(6)-C(5)	118.8(3)
C(7)-C(6)-H(6)	120.6
C(5)-C(6)-H(6)	120.6
C(6)-C(7)-C(8)	120.9(3)
C(6)-C(7)-H(7)	119.6
C(8)-C(7)-H(7)	119.6
C(9)-C(8)-C(7)	120.7(3)
C(9)-C(8)-H(8)	119.6
C(7)-C(8)-H(8)	119.6
C(8)-C(9)-C(10)	121.1(3)
C(8)-C(9)-Cl(1)	119.9(3)
C(10)-C(9)-Cl(1)	119.0(3)
N(2)-C(10)-C(5)	125.3(3)
N(2)-C(10)-C(9)	118.1(3)
C(5)-C(10)-C(9)	116.6(3)
C(11)-N(2)-C(10)	119.1(3)

N(2)-C(11)-C(3)	119.4(3)
N(2)-C(11)-C(12)	117.8(3)
C(3)-C(11)-C(12)	122.8(3)
C(11)-C(12)-H(12A)	109.5
C(11)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(11)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(14)-C(13)-C(19)	119.6(3)
C(14)-C(13)-N(1)	119.9(3)
C(19)-C(13)-N(1)	120.5(3)
C(13)-C(14)-C(15)	121.2(3)
C(13)-C(14)-H(14)	119.4
C(15)-C(14)-H(14)	119.4
C(14)-C(15)-C(16)	119.2(3)
C(14)-C(15)-H(15)	120.4
C(16)-C(15)-H(15)	120.4
O(3)-C(16)-C(18)	116.3(3)
O(3)-C(16)-C(15)	124.0(3)
C(18)-C(16)-C(15)	119.7(3)
C(16)-O(3)-C(17)	117.1(2)
O(3)-C(17)-H(17A)	109.5
O(3)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
O(3)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(19)-C(18)-C(16)	120.6(3)
C(19)-C(18)-H(18)	119.7
C(16)-C(18)-H(18)	119.7
C(18)-C(19)-C(13)	119.8(3)
C(18)-C(19)-H(19)	120.1
C(13)-C(19)-H(19)	120.1

Symmetry transformations used to generate equivalent atoms: