Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry
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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

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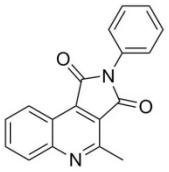
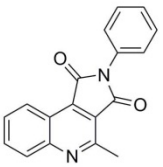
^{1}H NMR of Compound **7**



300 MHz, $CDCl_3$

^{13}C NMR of Compound **7**



75 MHz, $CDCl_3$

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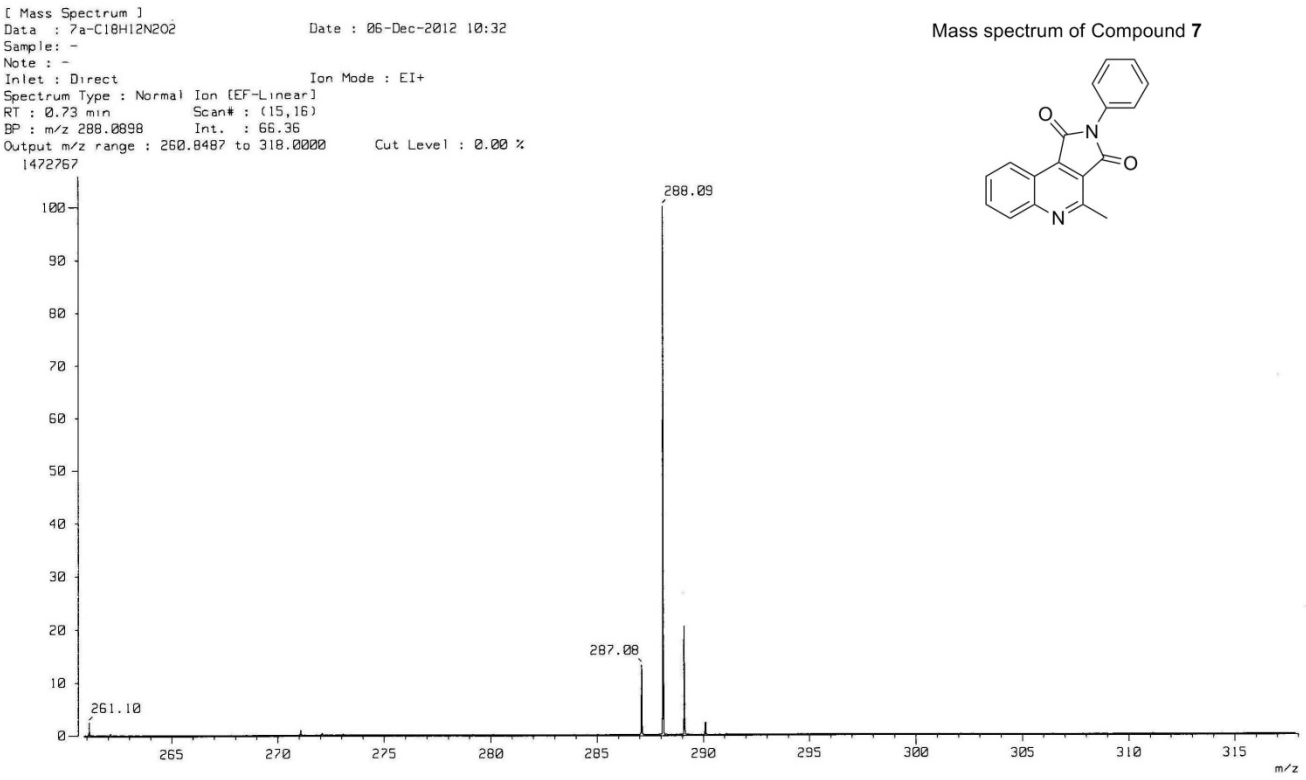

Mass spectrum of Compound **7**


```
[ Elemental Composition ]                                    Page: 1
Data  : 7a-C18H12N2O2              Date : 06-Dec-2012 10:32
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
```

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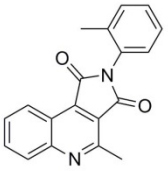
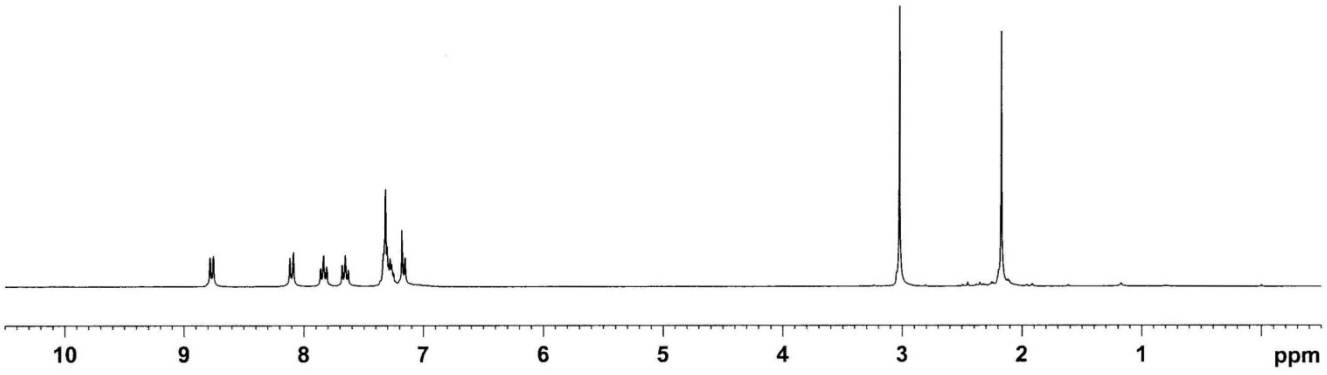
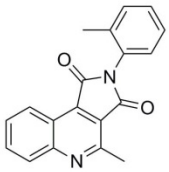
^{1}H NMR of Compound **8**



300 MHz, $CDCl_3$



^{13}C NMR of Compound **8**



75 MHz, $CDCl_3$

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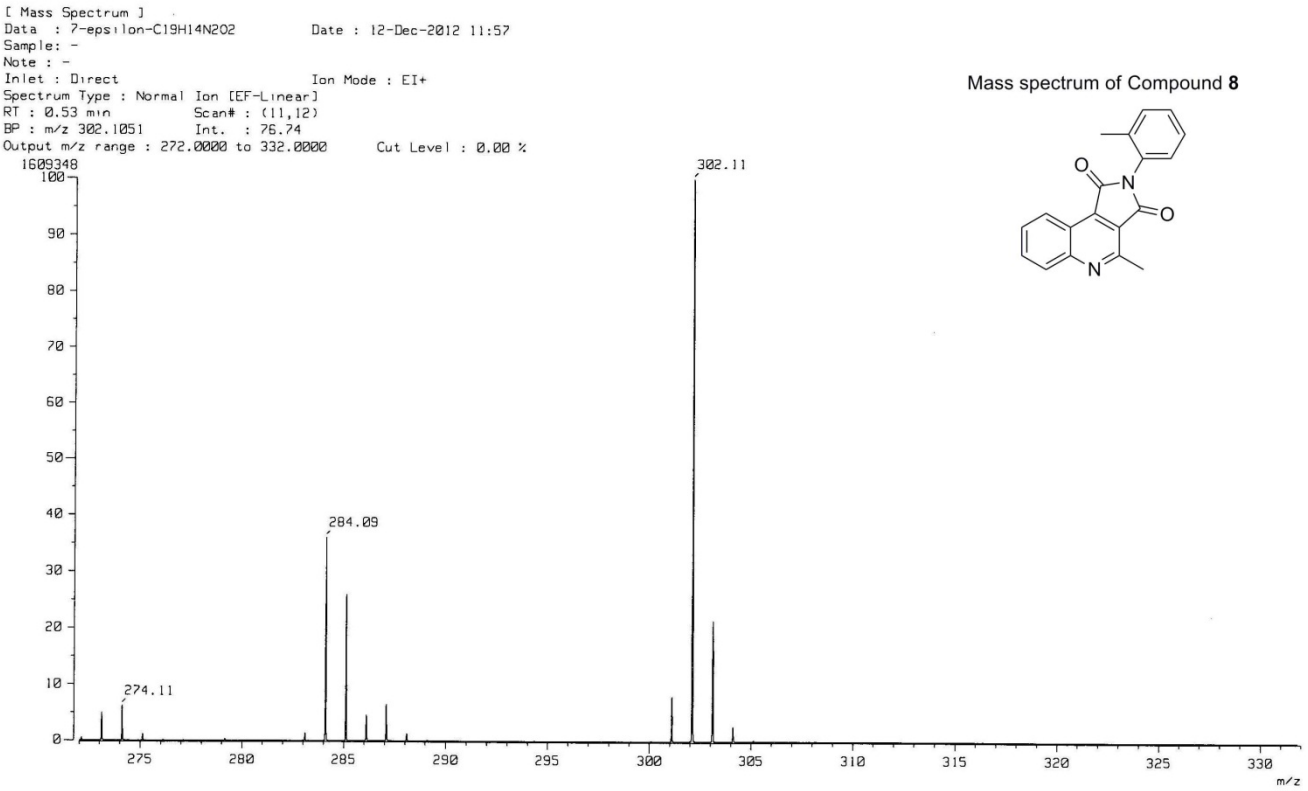

Mass spectrum of Compound **8**

[Elemental Composition] Page: 1
Data : 7-epsilon-C19H14N2O2 Date : 12-Dec-2012 11:57
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			

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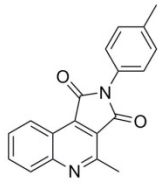
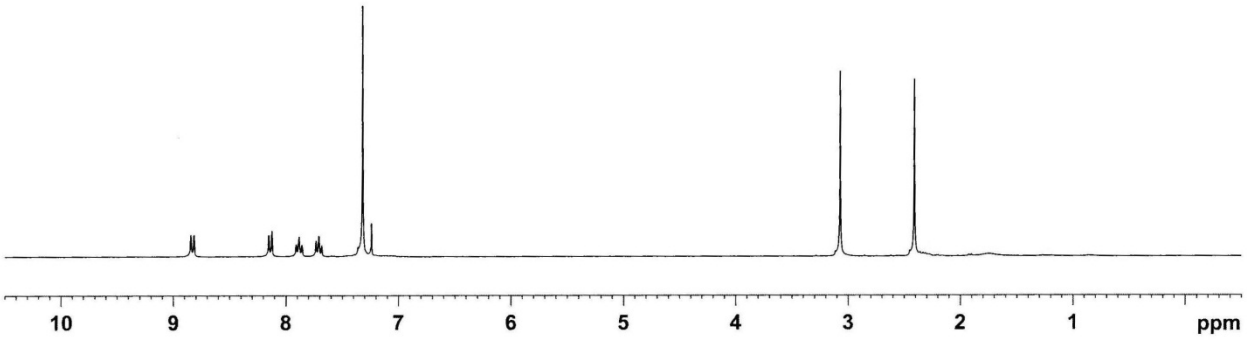
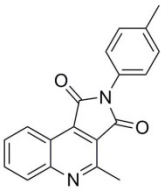
^{1}H NMR of Compound **9**



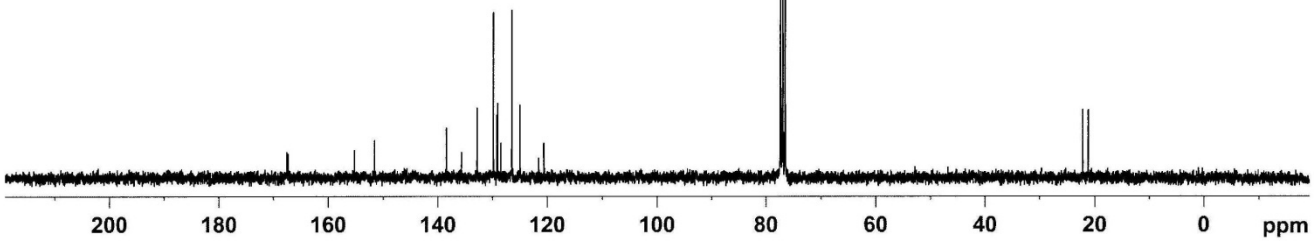
300 MHz, $CDCl_3$



^{13}C NMR of Compound **9**



75 MHz, $CDCl_3$



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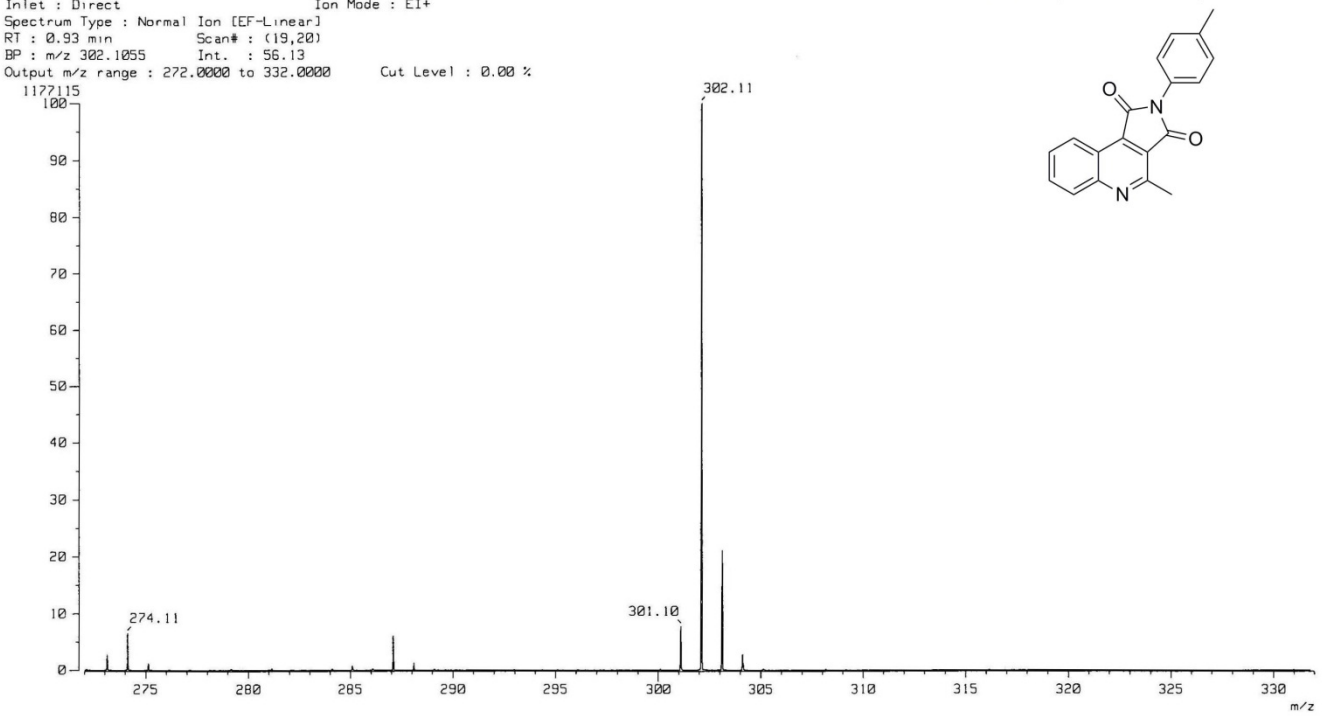
[Mass Spectrum]
Data : 7r-C19H14N2O2 Date : 12-Dec-2012 10:56
Sample: -
Note : -
Inlet : Direct Ion Mode : EI+
Spectrum Type : Normal Ion [EF-Linear]
RT : 0.93 min Scan# : (19,20)
BP : m/z 302.1055 Int. : 56.13
Output m/z range : 272.0000 to 332.0000 Cut Level : 0.00 %

Mass spectrum of Compound **9**



[Elemental Composition] Page: 1
Data : 7r-C19H14N2O2 Date : 12-Dec-2012 10:56
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			

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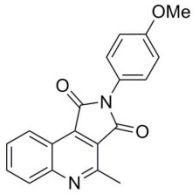
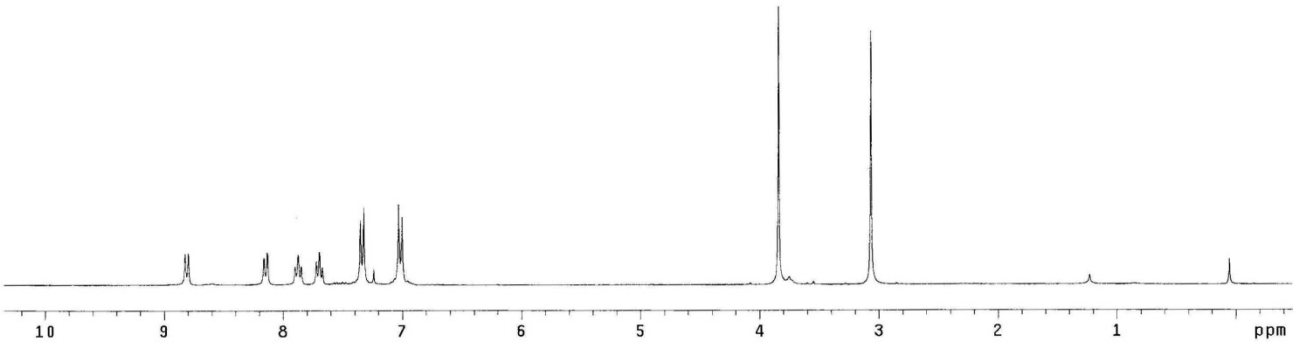
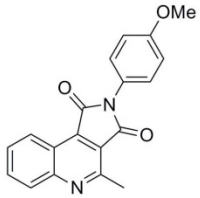
^{1}H NMR of Compound **10**



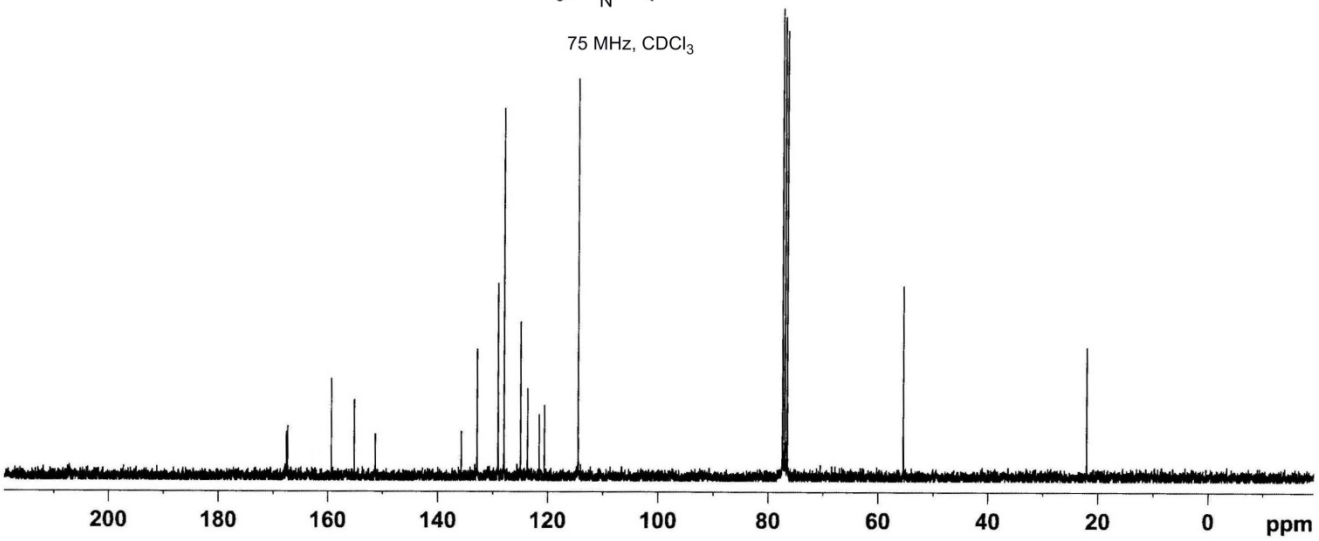
300 MHz, $CDCl_3$



^{13}C NMR of Compound **10**



75 MHz, $CDCl_3$



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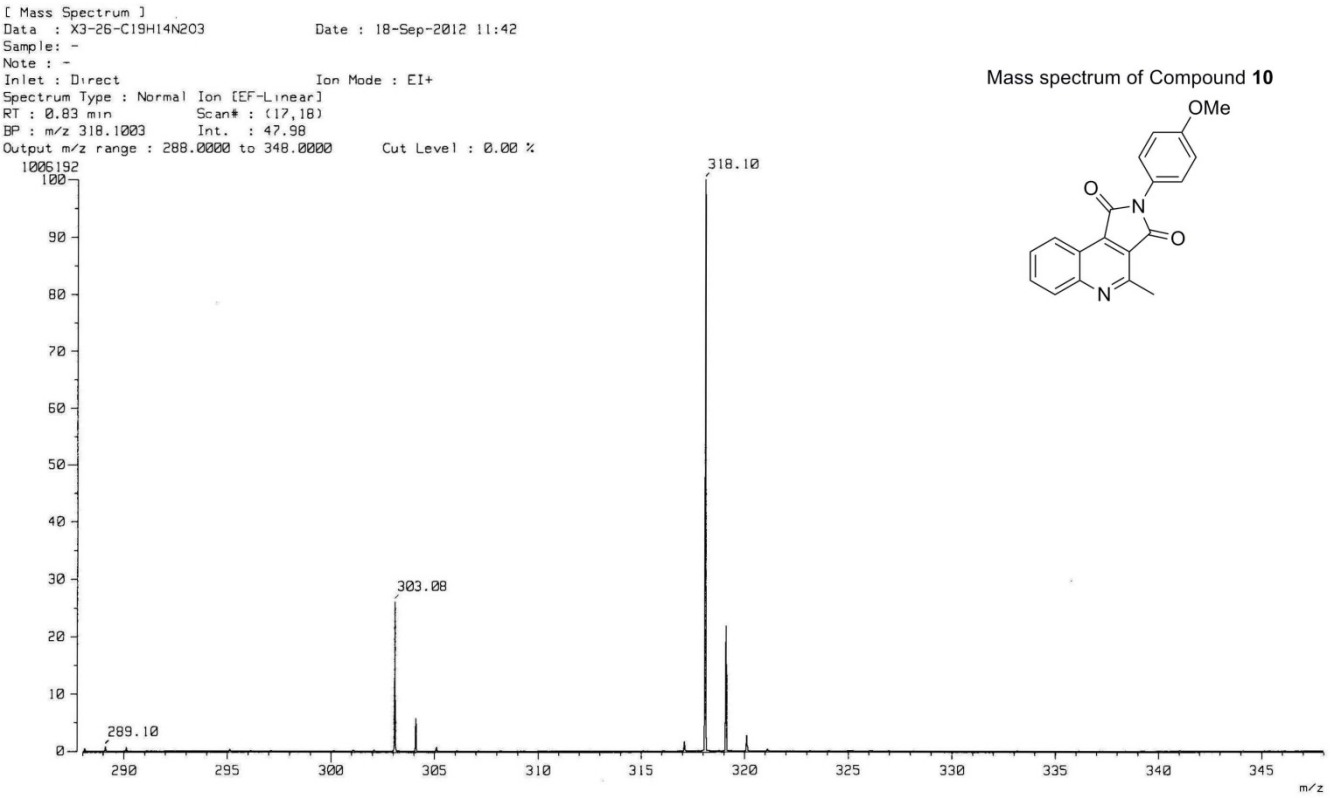

Mass spectrum of Compound **10**

[Elemental Composition] Page: 1
Data : X3-26-C19H14N2O3 Date : 18-Sep-2012 11:42
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			

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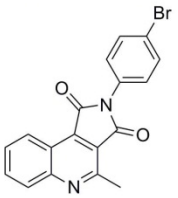
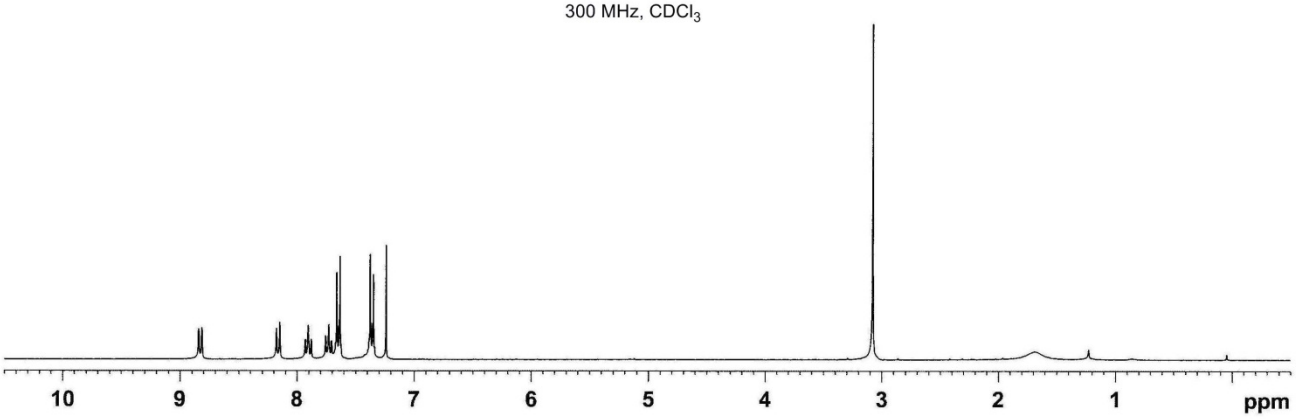
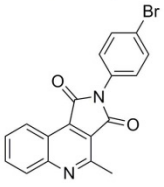
^{1}H NMR of Compound **11**



300 MHz, $CDCl_3$



^{13}C NMR of Compound **11**



150 MHz, $CDCl_3$

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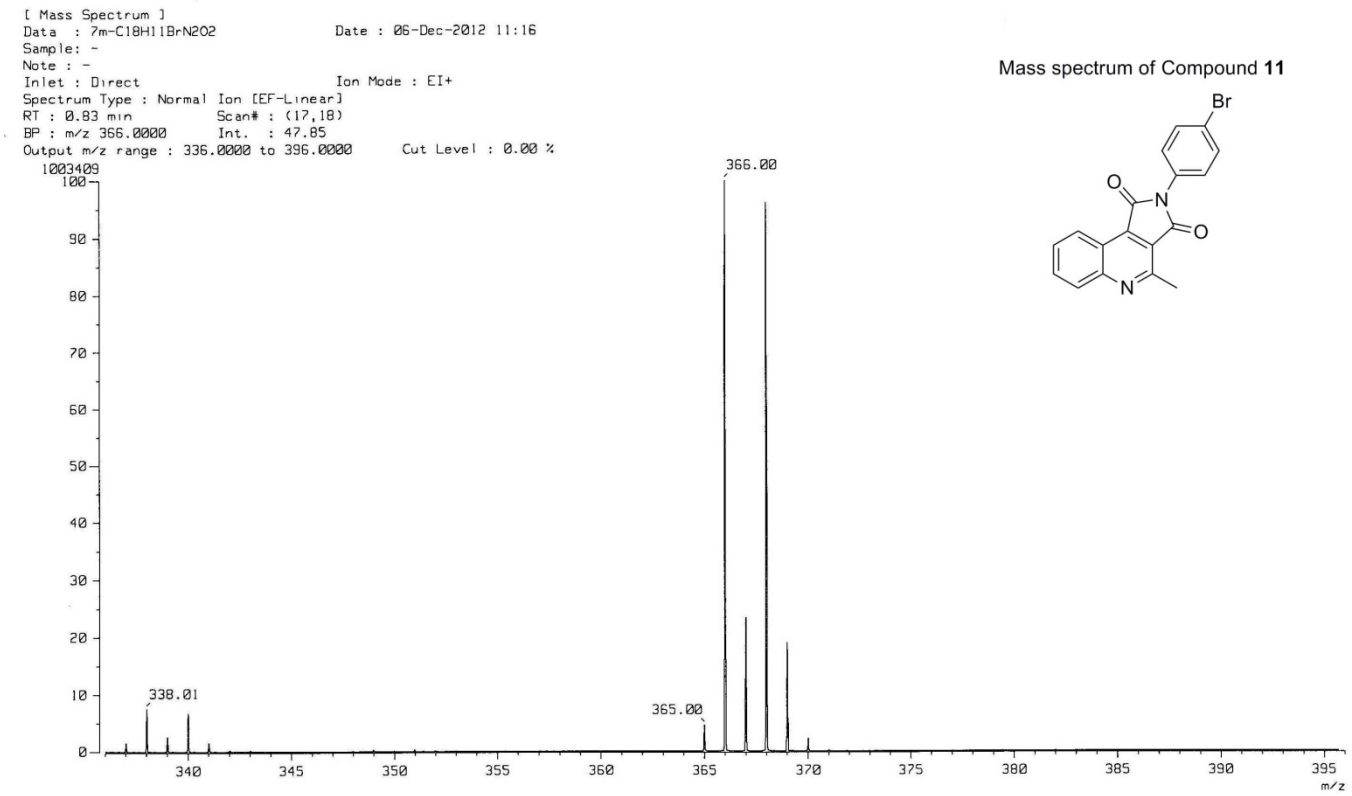

Mass spectrum of Compound **11**

[Elemental Composition] Page: 1

Data : 7m-C18H11BrN2O2 Date : 06-Dec-2012 11:16
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			

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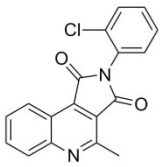
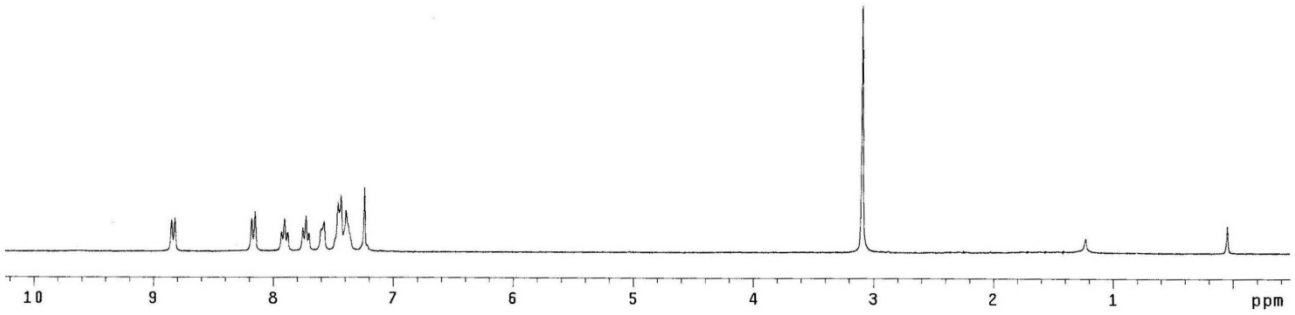
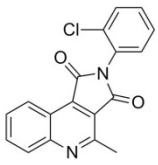
^{1}H NMR of Compound **12**



300 MHz, $CDCl_3$



^{13}C NMR of Compound **12**



150 MHz, $CDCl_3$

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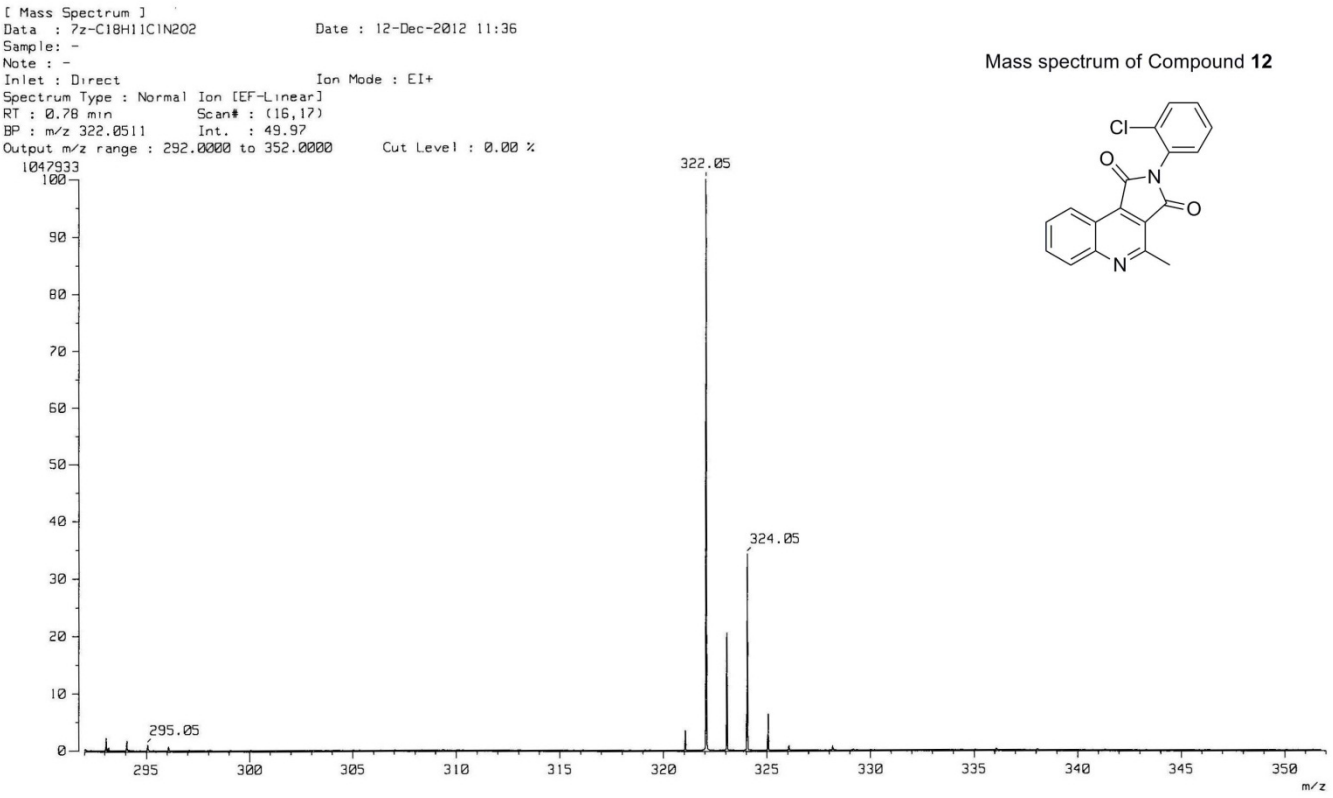

Mass spectrum of Compound **12**


```
[ Elemental Composition ]                                    Page: 1
Data  : 7z-C18H11ClN2O2              Date : 12-Dec-2012 11:36
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
```

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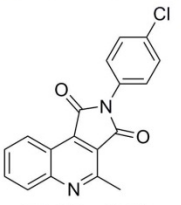
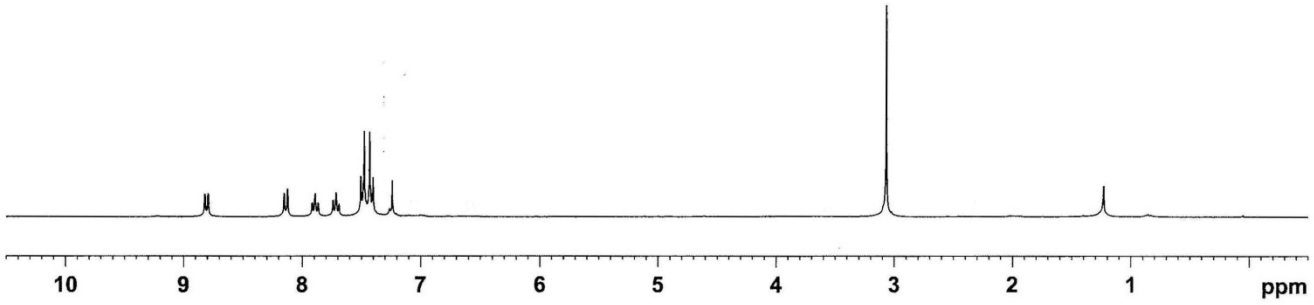
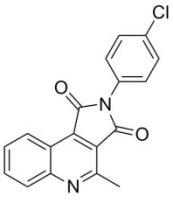
^{1}H NMR of Compound **13**



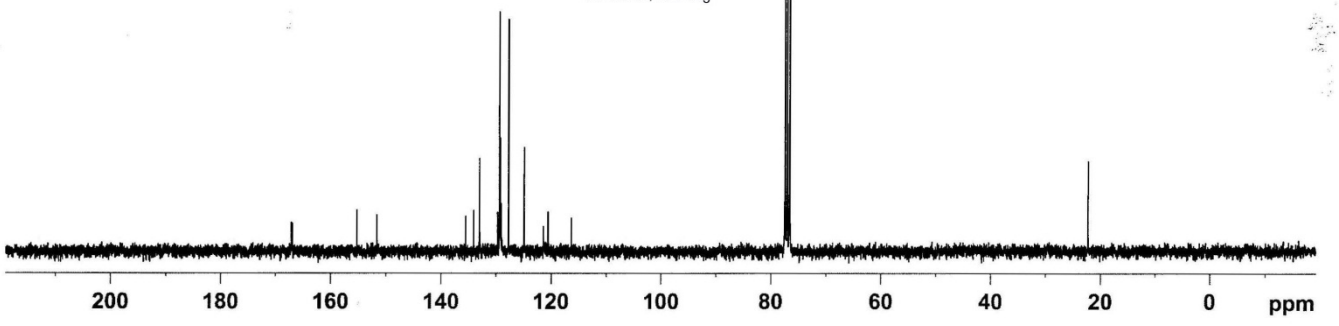
300 MHz, $CDCl_3$



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



75 MHz, $CDCl_3$



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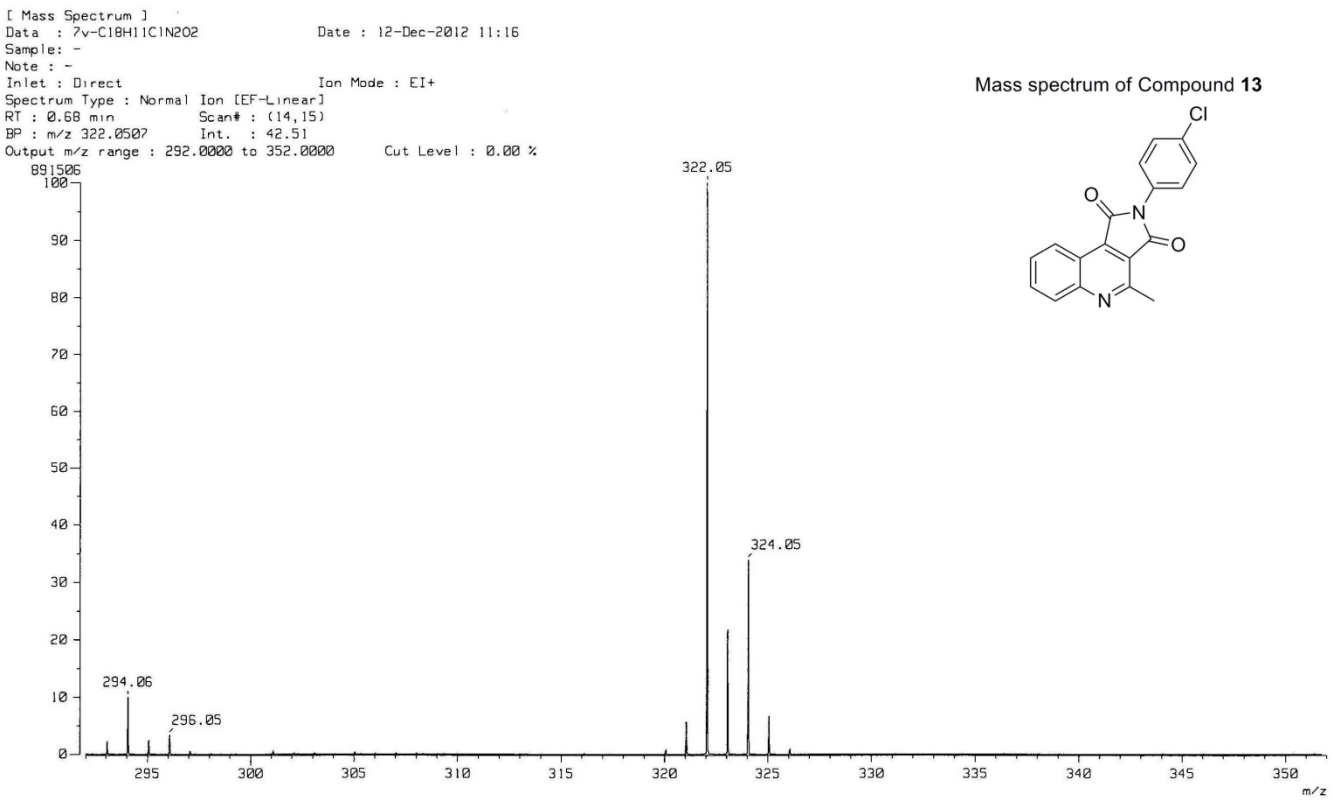

Mass spectrum of Compound **13**

[Elemental Composition] Page: 1
Data : 7v-C18H11ClN2O2 Date : 12-Dec-2012 11:16
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			

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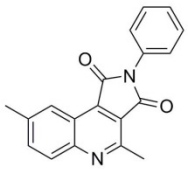
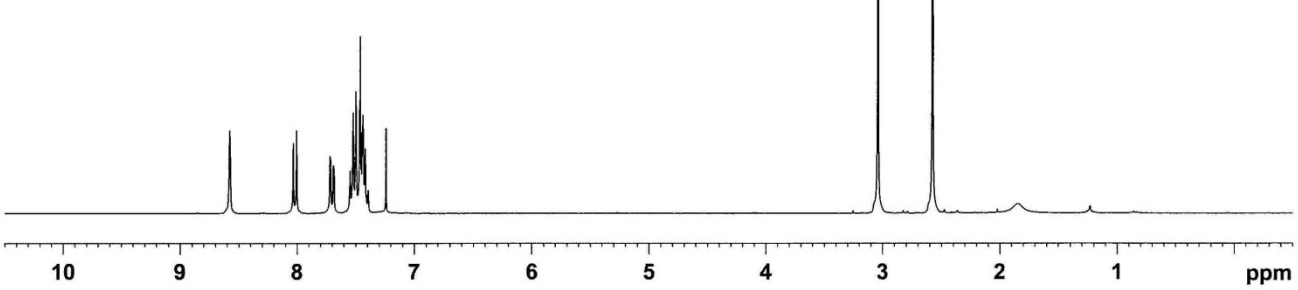
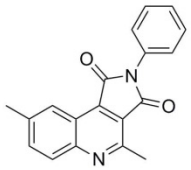
^{1}H NMR of Compound **14**



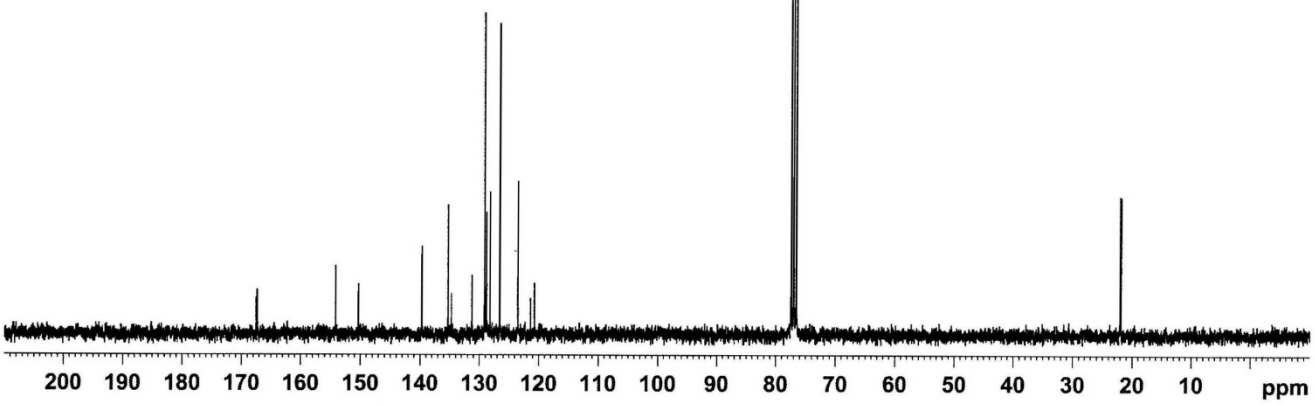
300 MHz, $CDCl_3$



^{13}C NMR of Compound **14**



75 MHz, $CDCl_3$



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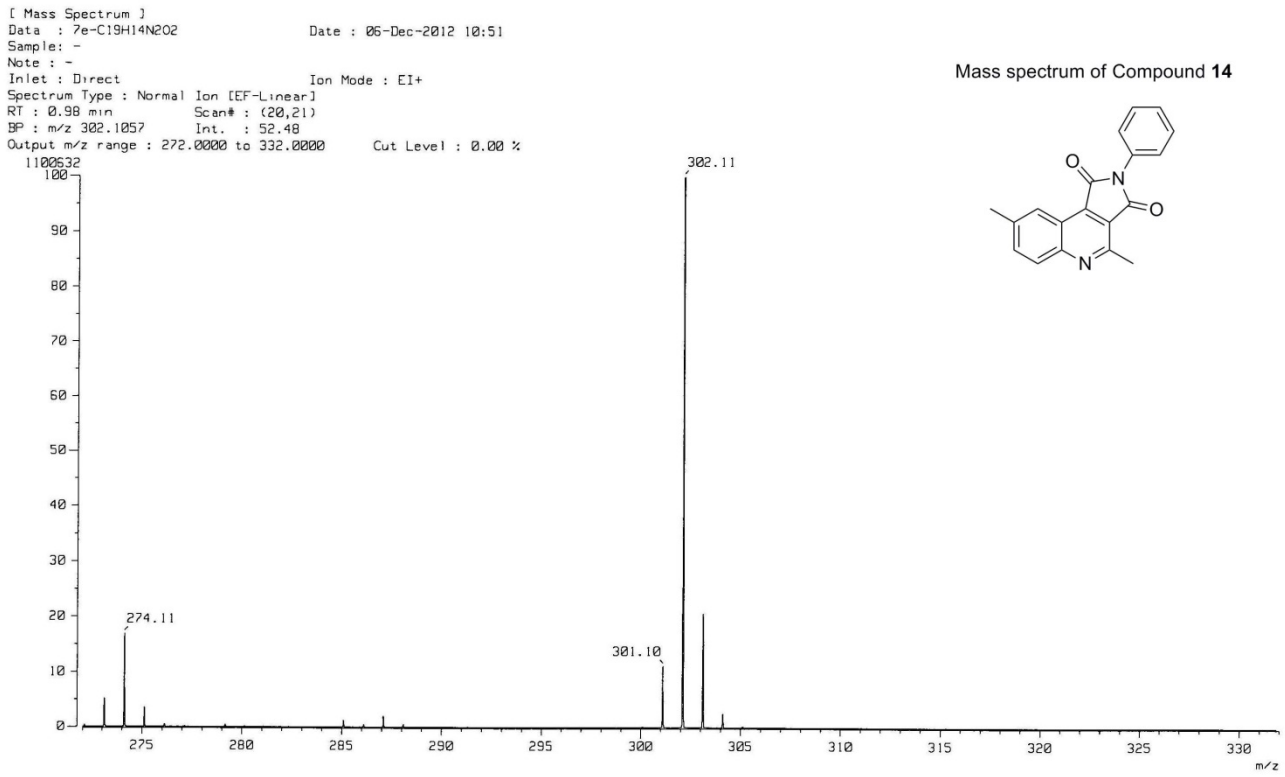

Mass spectrum of Compound **14**

[Elemental Composition] Page: 1

Data : 7e-C19H14N2O2 Date : 06-Dec-2012 10:51
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			

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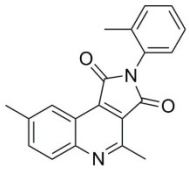
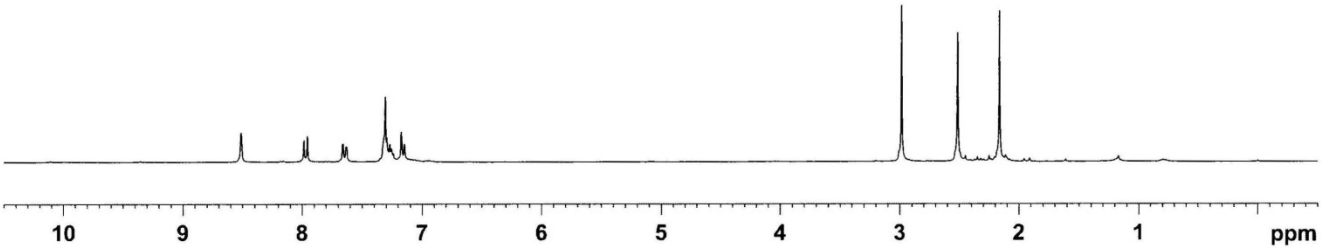
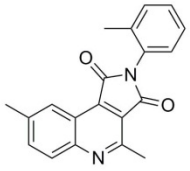
^{1}H NMR of Compound **15**



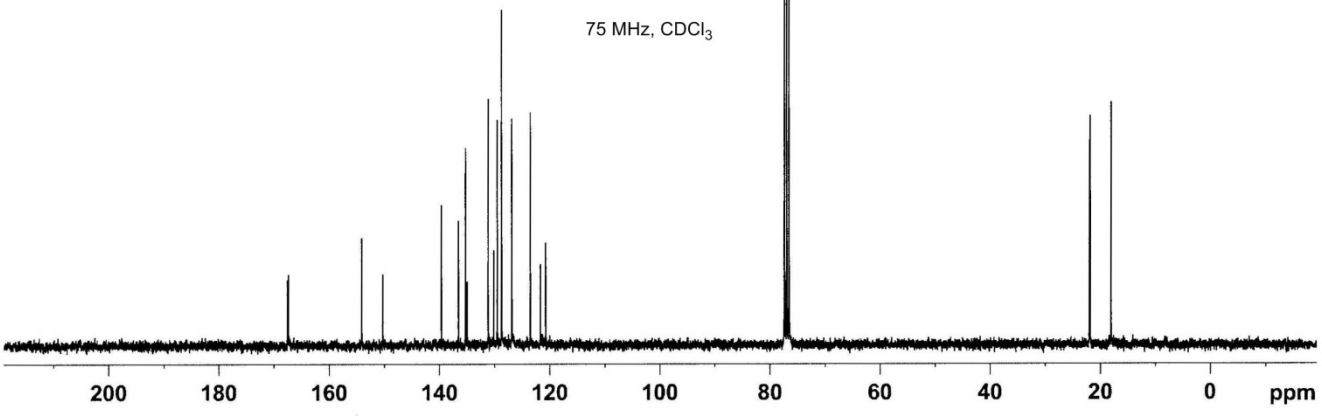
300 MHz, $CDCl_3$



^{13}C NMR of Compound **15**



75 MHz, $CDCl_3$



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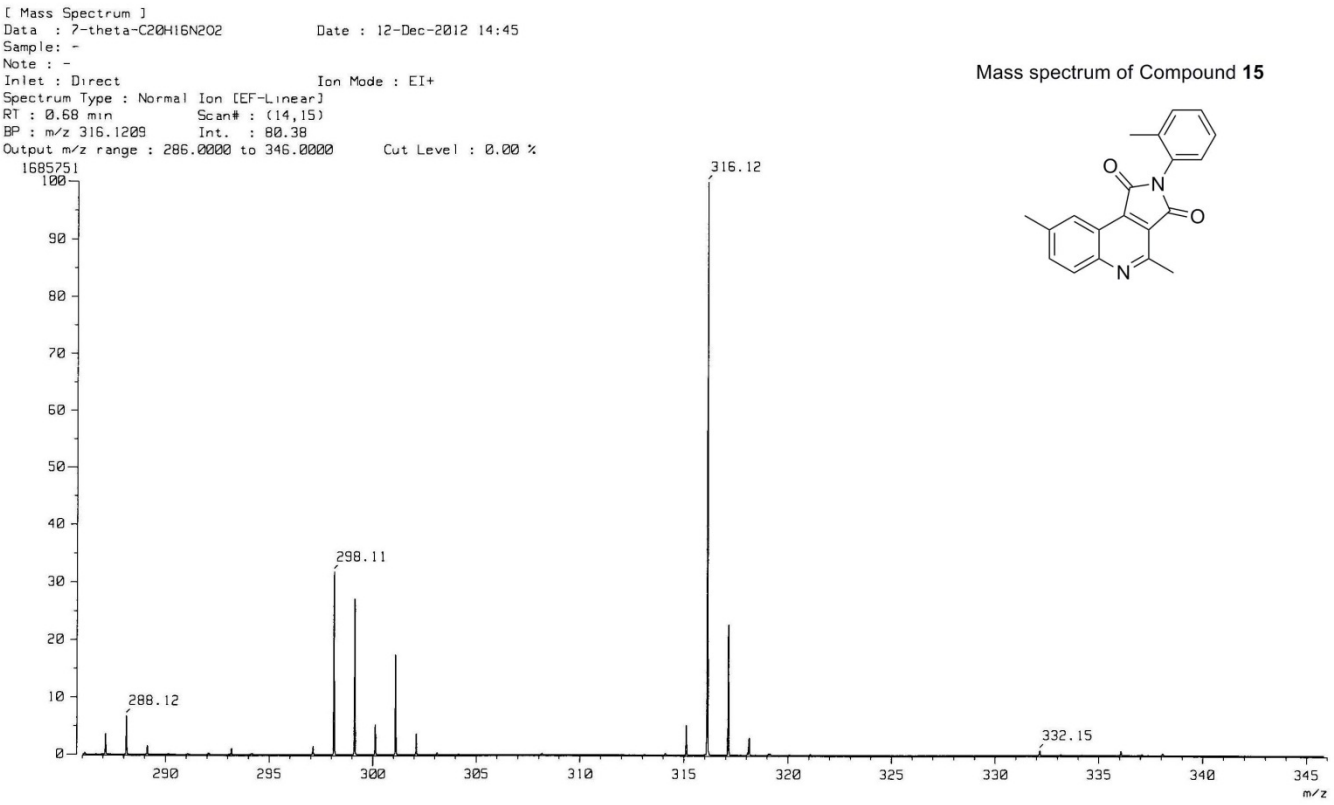

Mass spectrum of Compound **15**

[Elemental Composition] Page: 1

Data : 7-theta-C20H16N2O2 Date : 12-Dec-2012 14:45
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			

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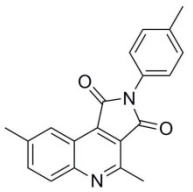
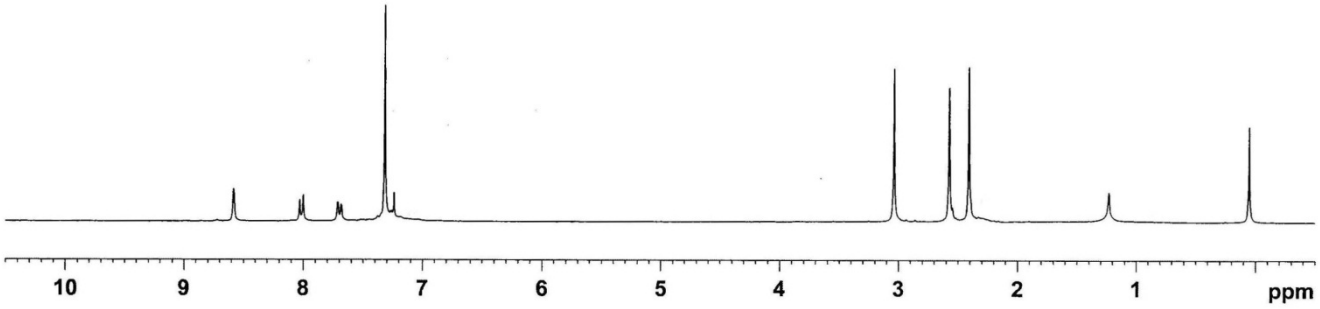
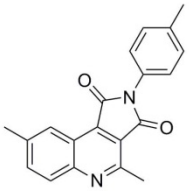
^{1}H NMR of Compound **16**



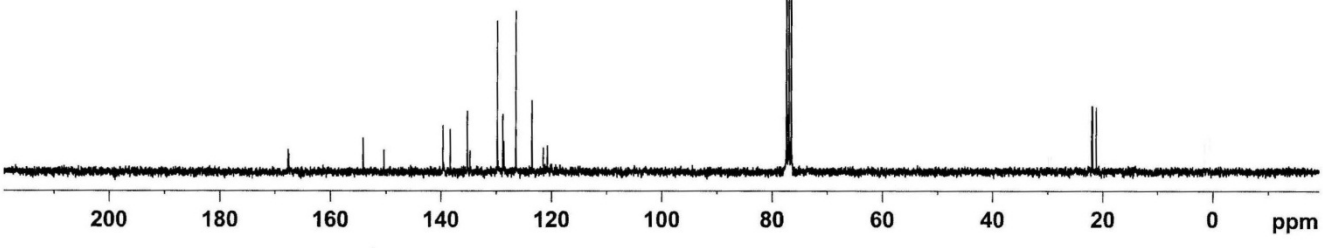
300 MHz, $CDCl_3$



^{13}C NMR of Compound **16**



75 MHz, $CDCl_3$



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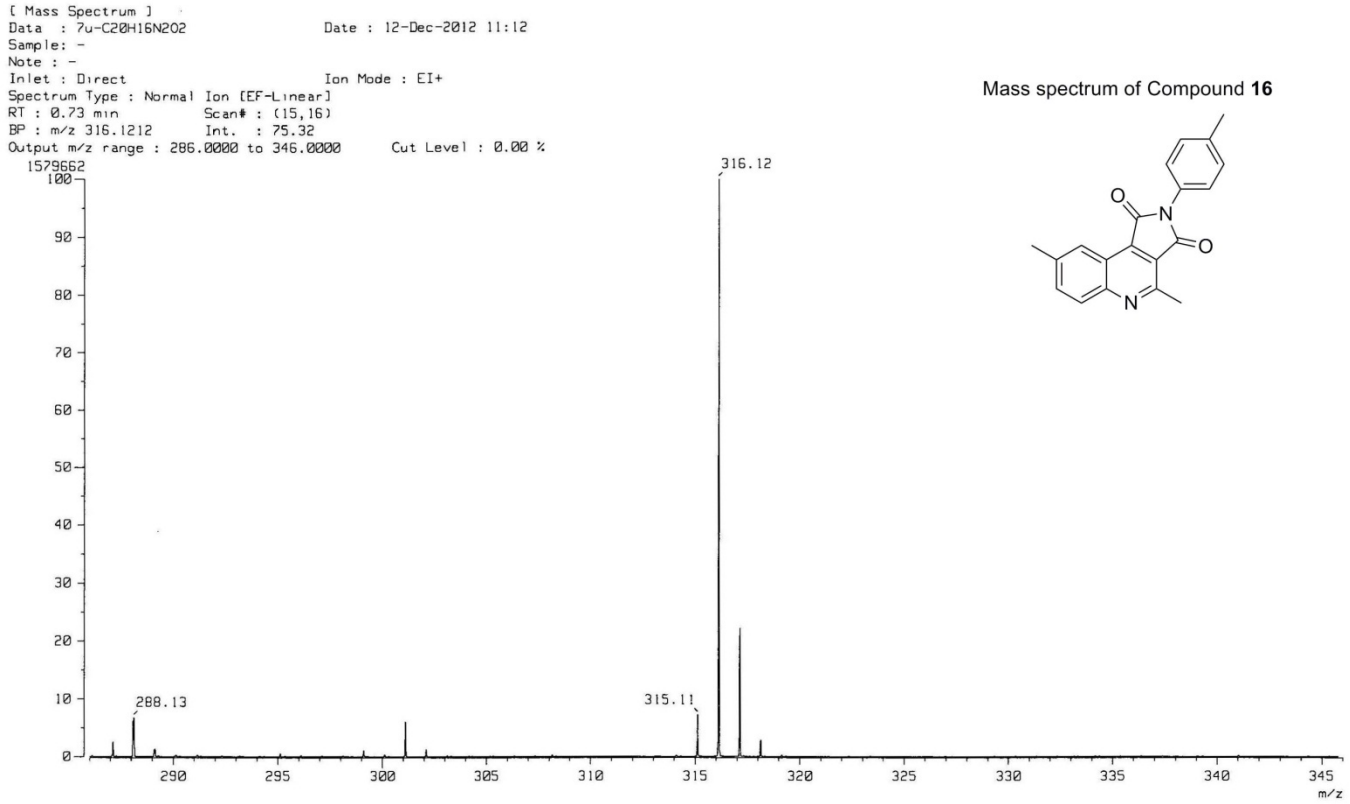

Mass spectrum of Compound **16**


```
[ Elemental Composition ]                                    Page: 1
Data  : 7u-C20H16N2O2                Date : 12-Dec-2012 11:12
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
```

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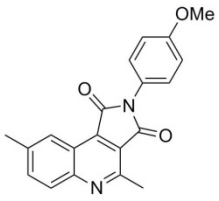
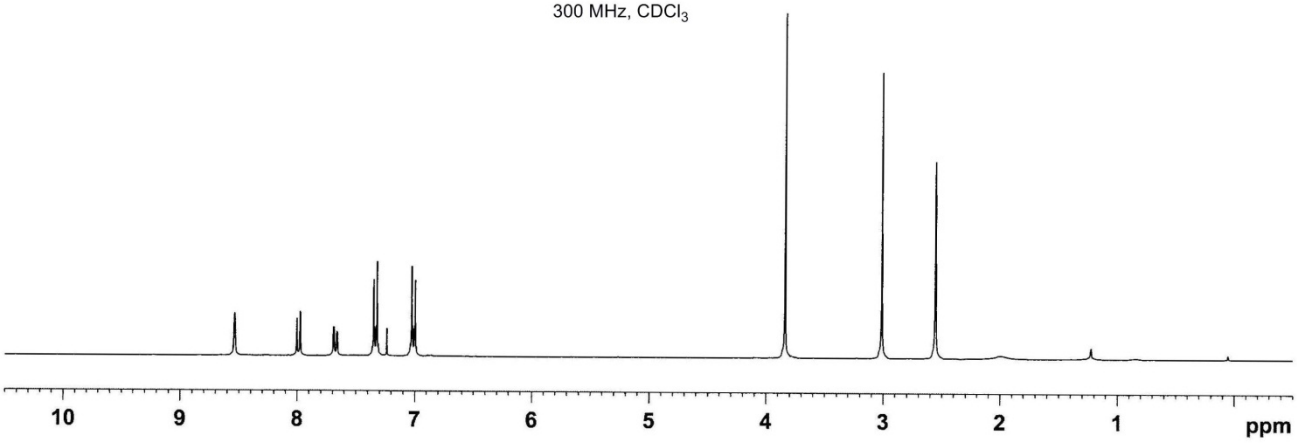
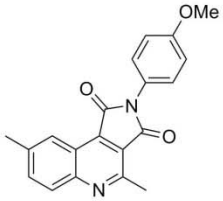
^{1}H NMR of Compound **17**



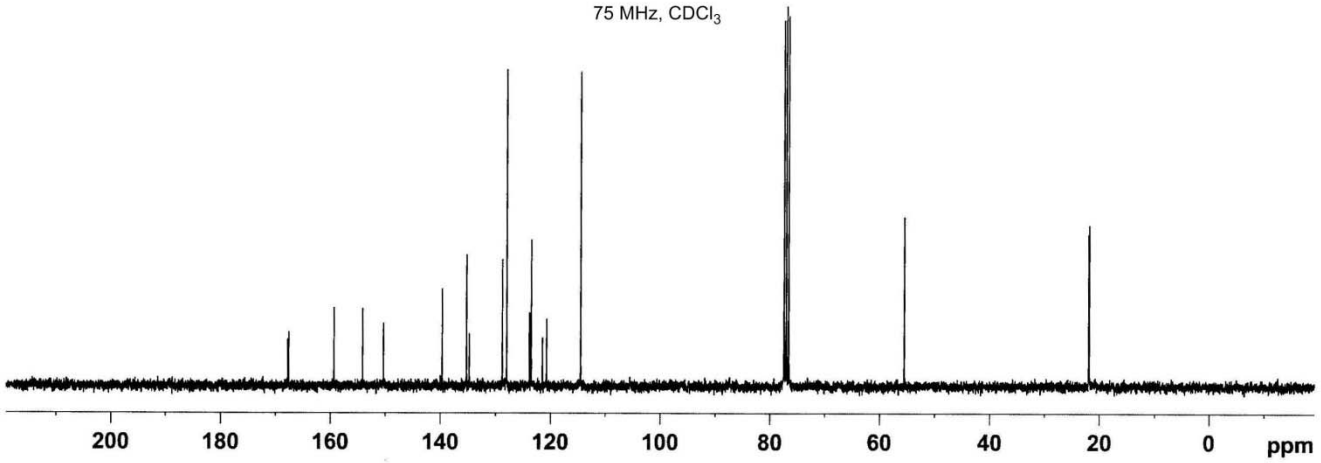
300 MHz, $CDCl_3$



^{13}C NMR of Compound **17**



75 MHz, $CDCl_3$



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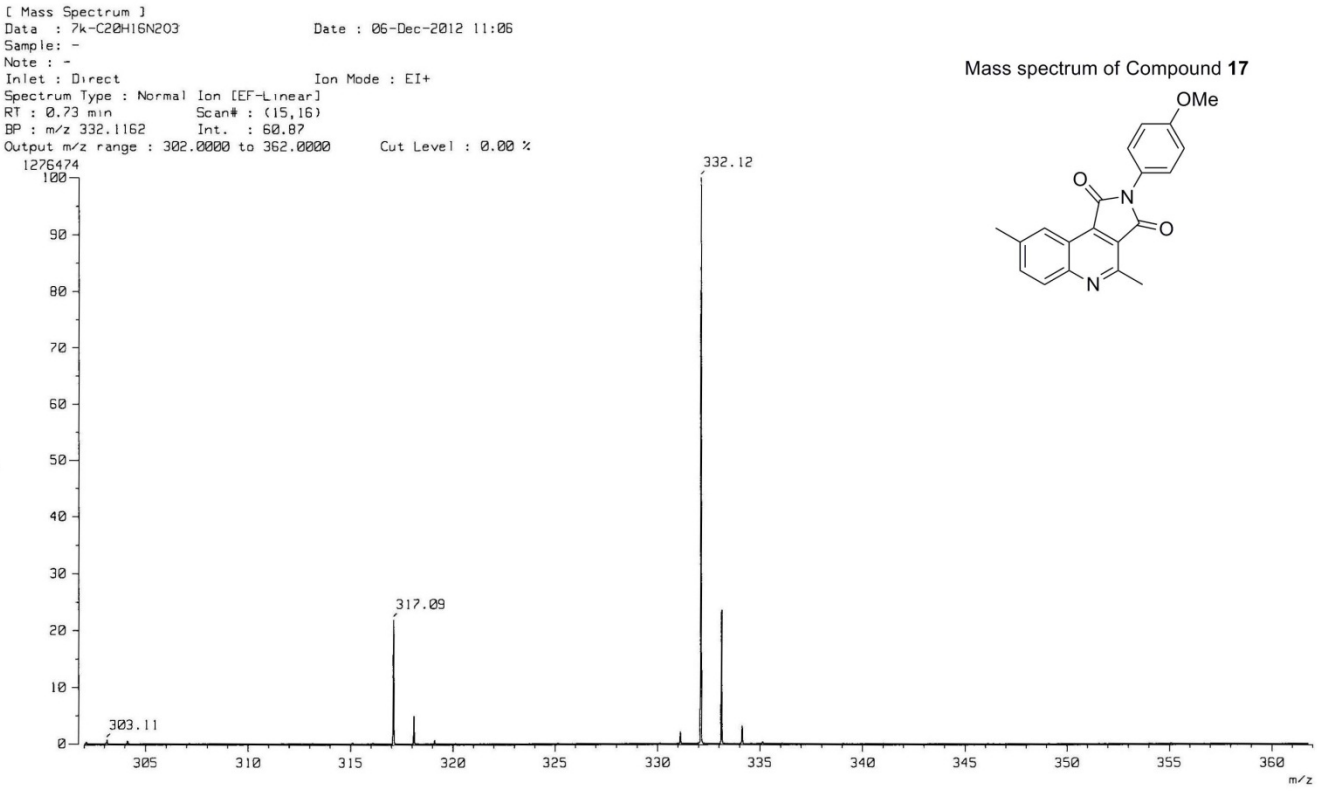

Mass spectrum of Compound **17**

[Elemental Composition] Page: 1
Data : 7k-C20H16N2O3 Date : 06-Dec-2012 11:06
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			

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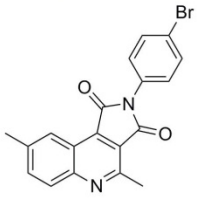
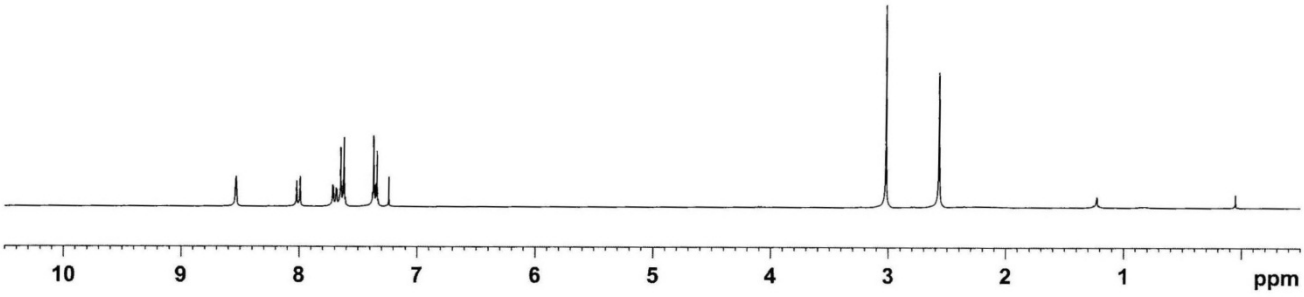
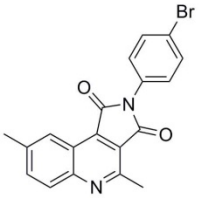
^{1}H NMR of Compound **18**



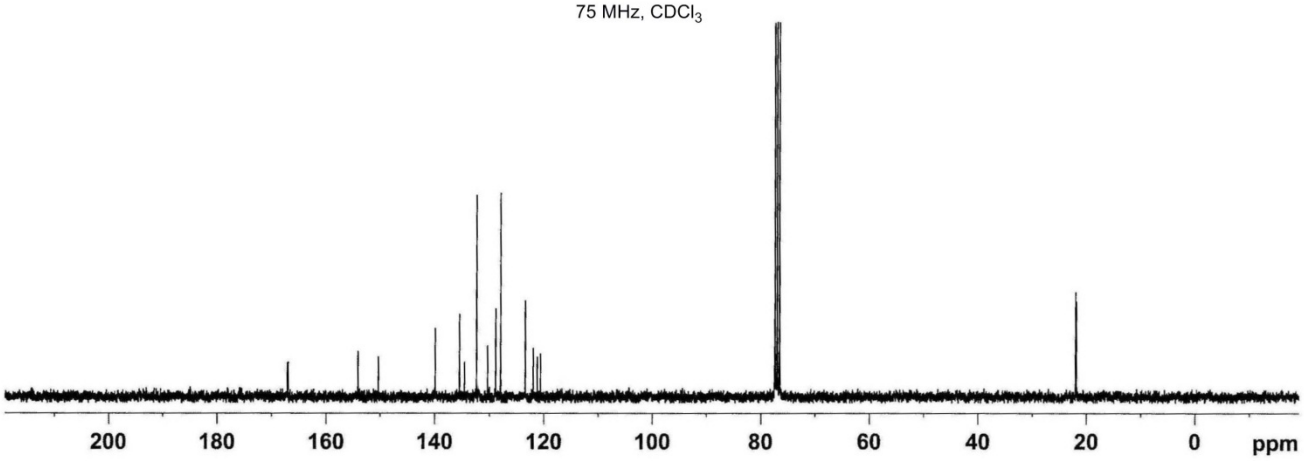
300 MHz, $CDCl_3$



^{13}C NMR of Compound **18**



75 MHz, $CDCl_3$



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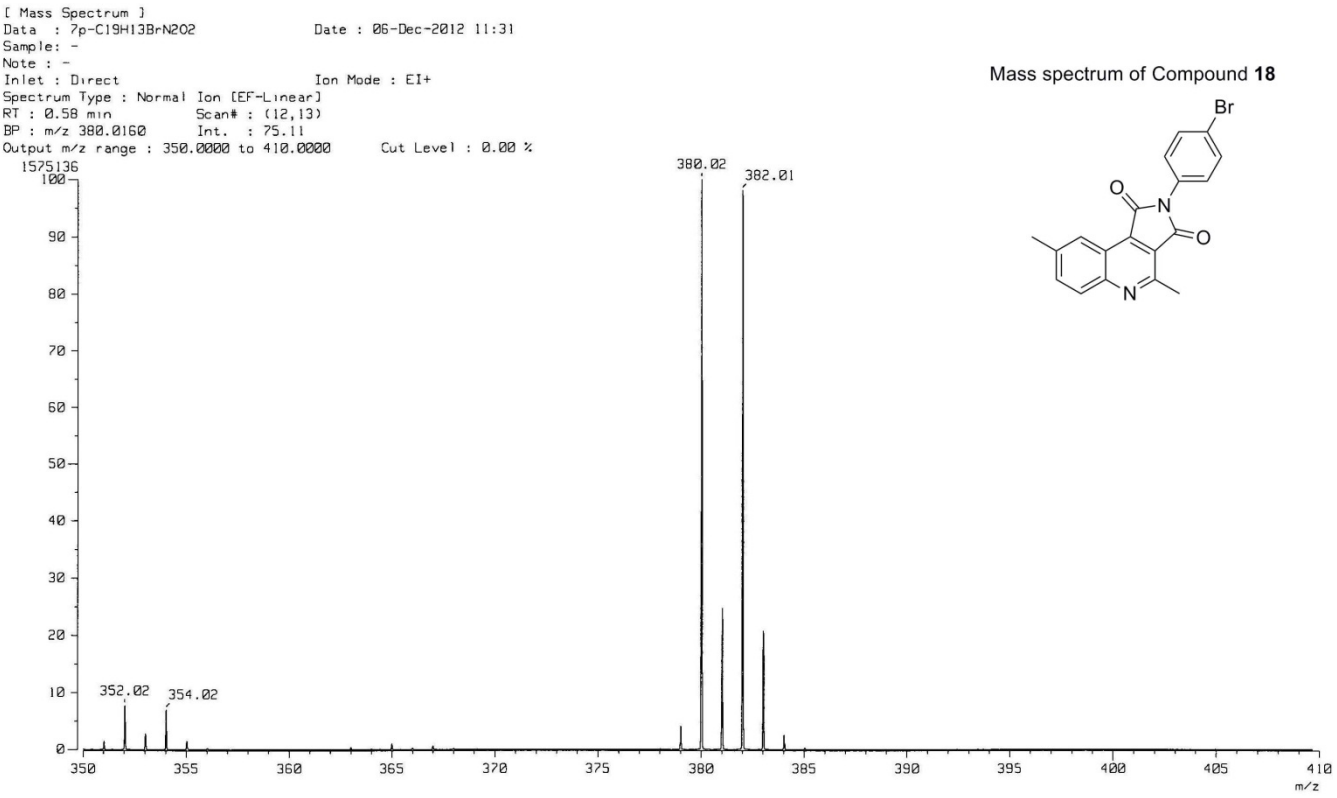

Mass spectrum of Compound **18**

[Elemental Composition] Page: 1
Data : 7p-C19H13BrN2O2 Date : 06-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, 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			

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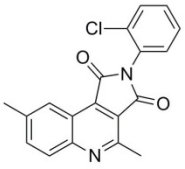
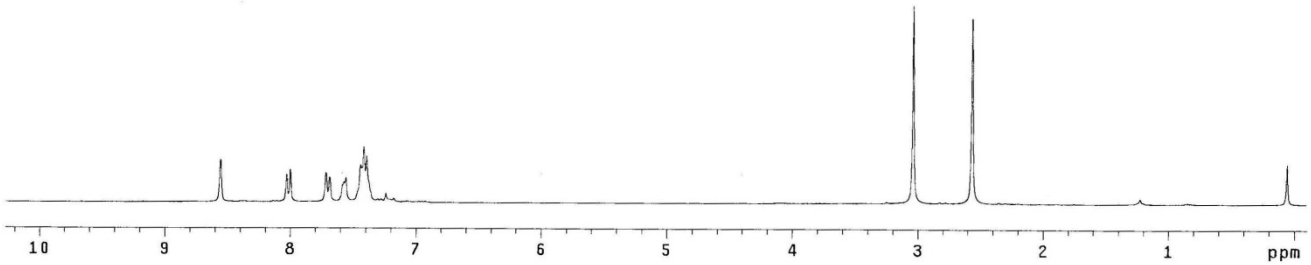
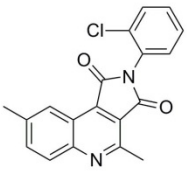
^{1}H NMR of Compound **19**



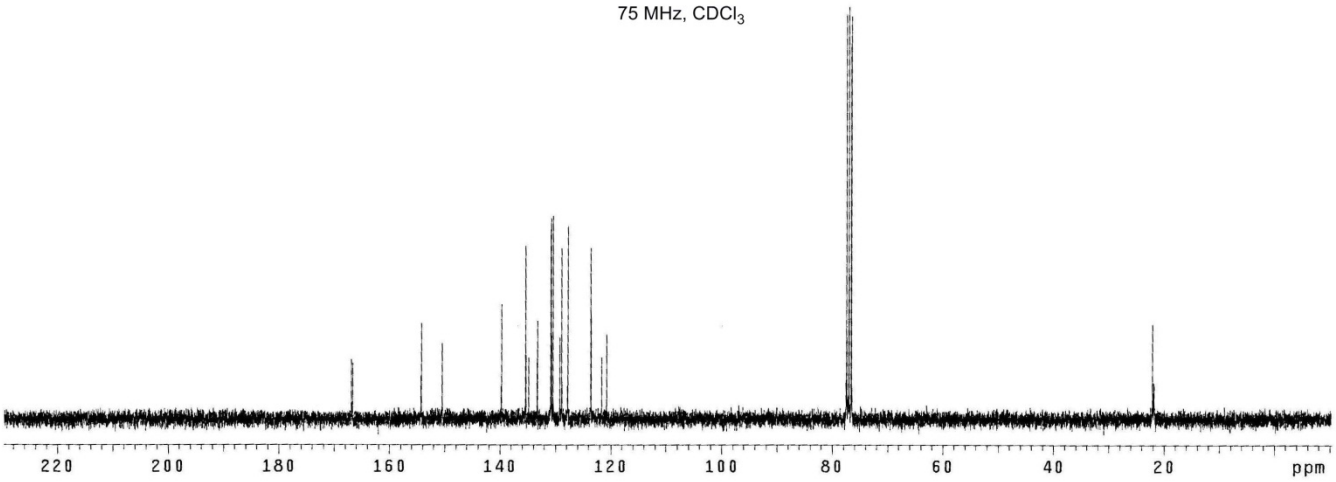
300 MHz, $CDCl_3$



^{13}C NMR of Compound **19**



75 MHz, $CDCl_3$



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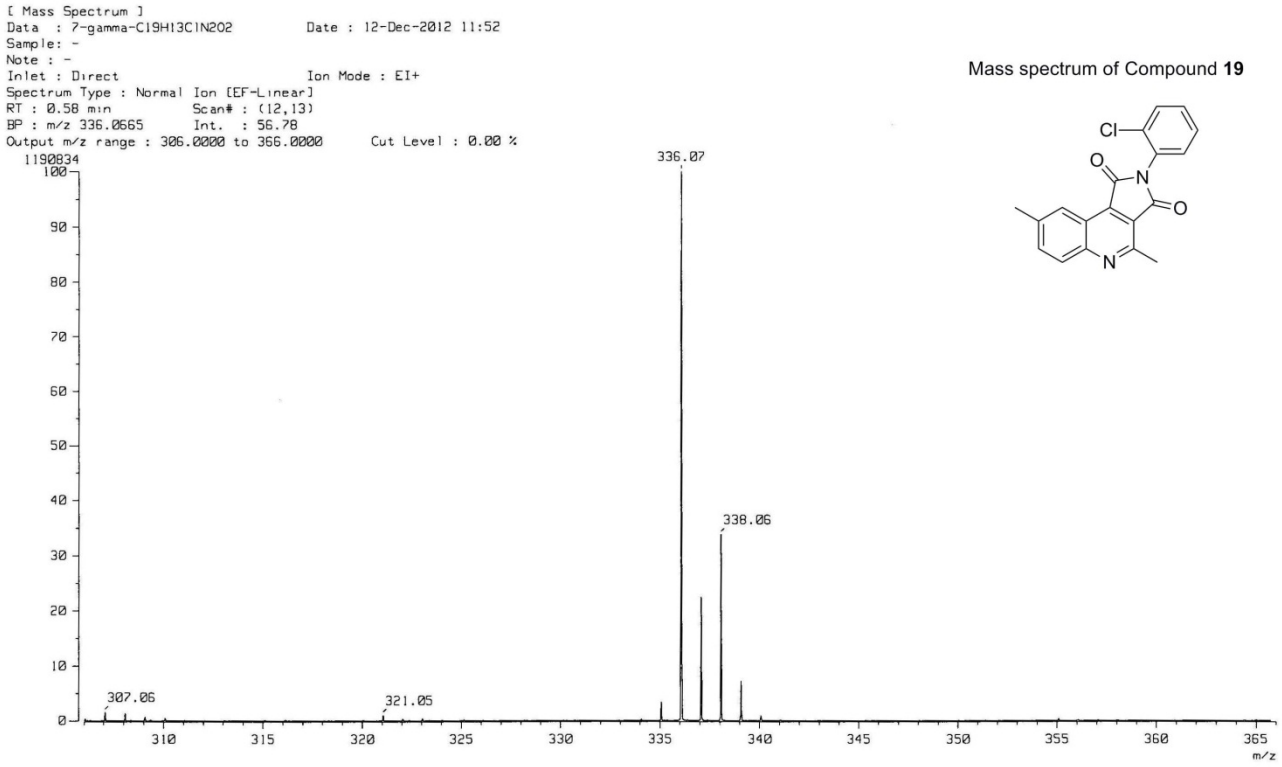

Mass spectrum of Compound **19**

[Elemental Composition] Page: 1
Data : 7-gamma-C19H13ClN2O2 Date : 12-Dec-2012 11:52
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
336.0665	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			

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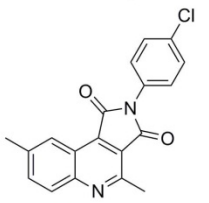
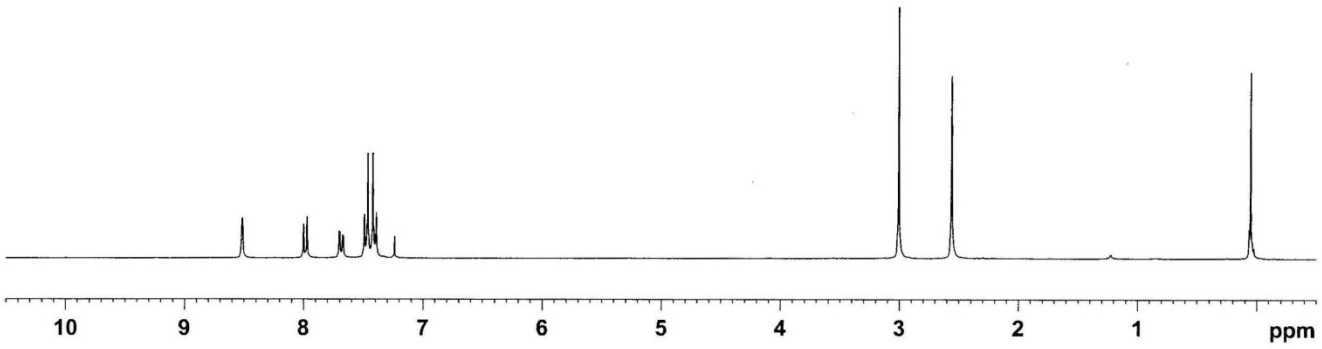
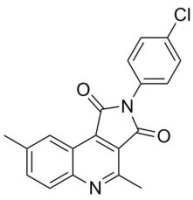
^{1}H NMR of Compound **20**



300 MHz, $CDCl_3$



^{13}C NMR of Compound **20**



75 MHz, $CDCl_3$

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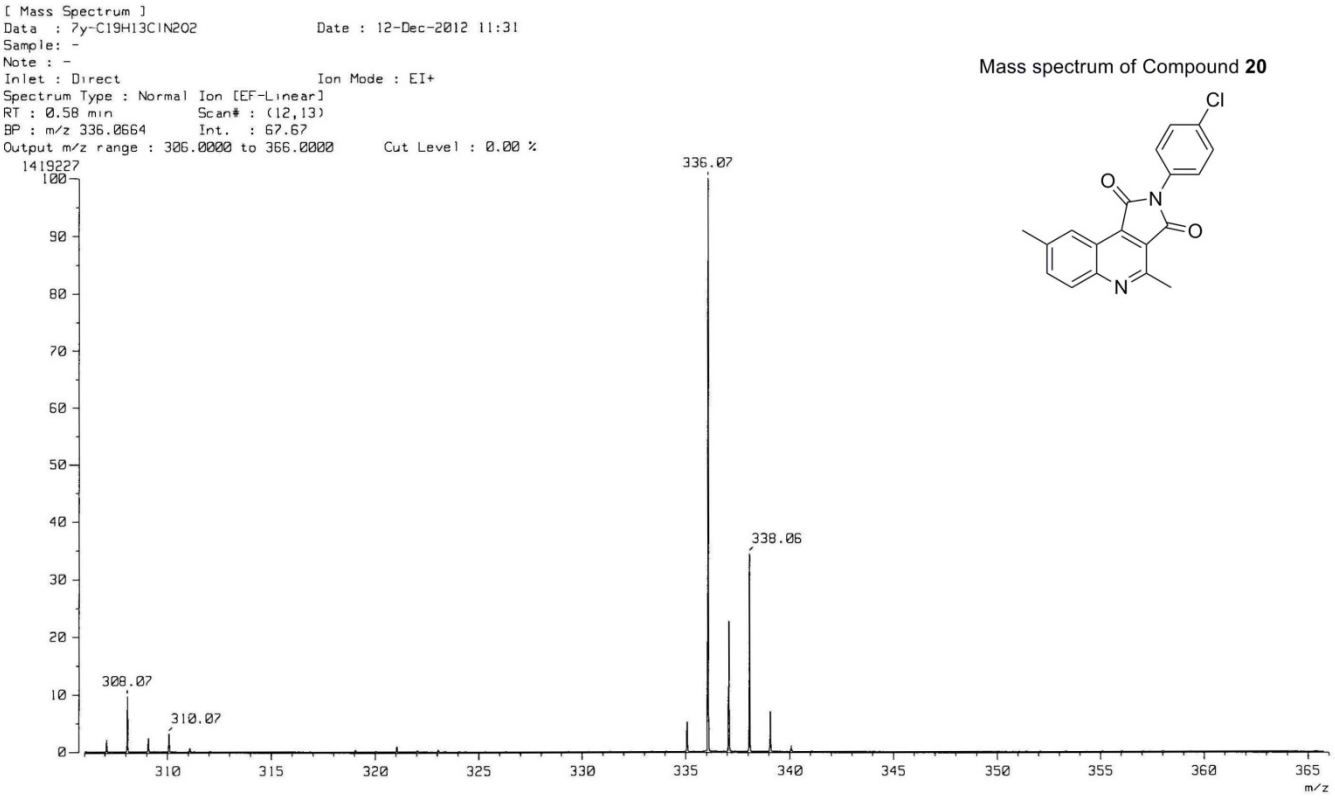

Mass spectrum of Compound **20**

[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			

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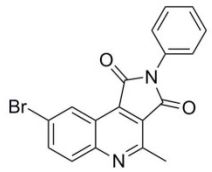
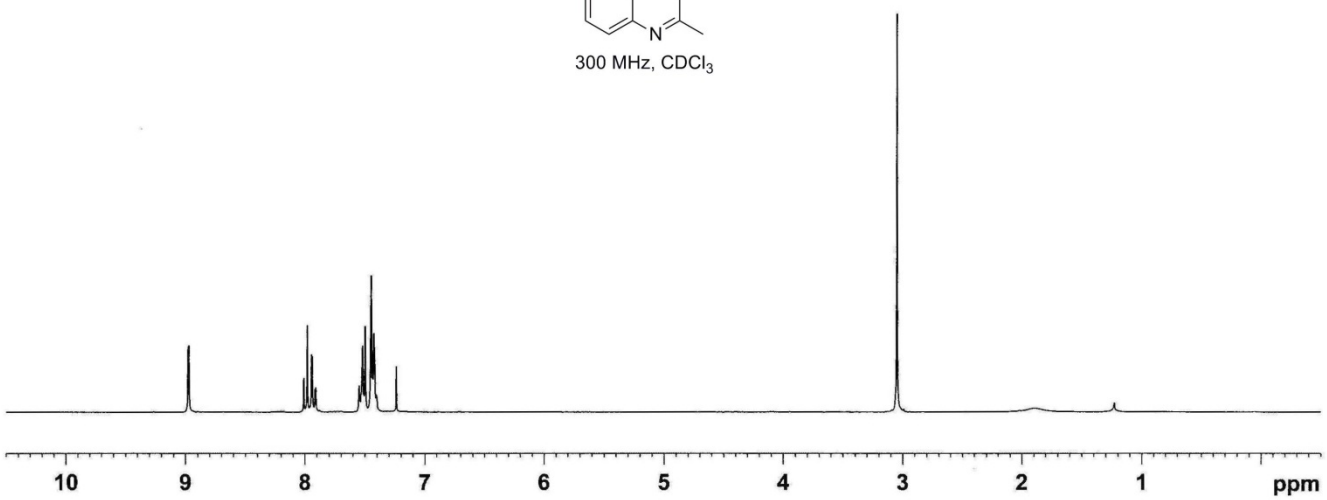
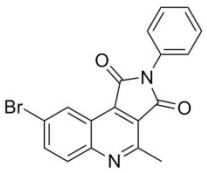
^{1}H NMR of Compound **21**



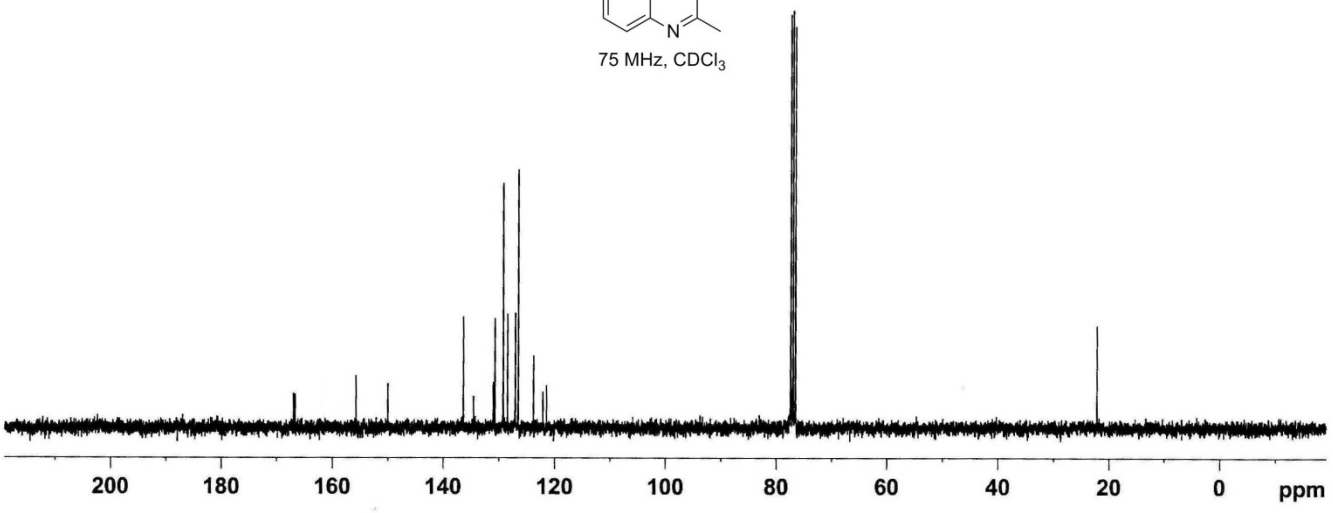
300 MHz, $CDCl_3$



^{13}C NMR of Compound **21**



75 MHz, $CDCl_3$



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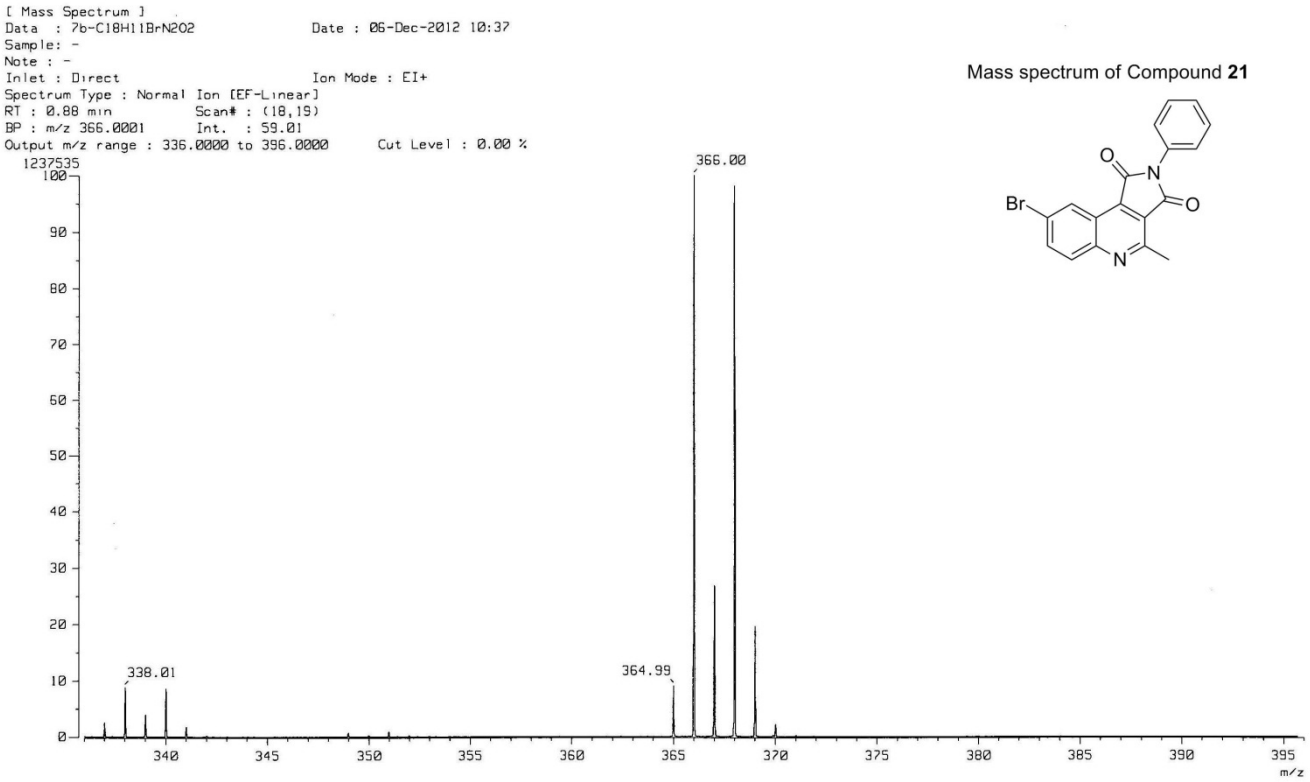

Mass spectrum of Compound **21**

[Elemental Composition] Page: 1

Data : 7b-C18H11BrN2O2 Date : 06-Dec-2012 10:37
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			

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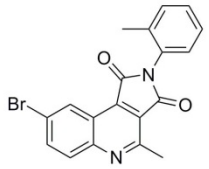
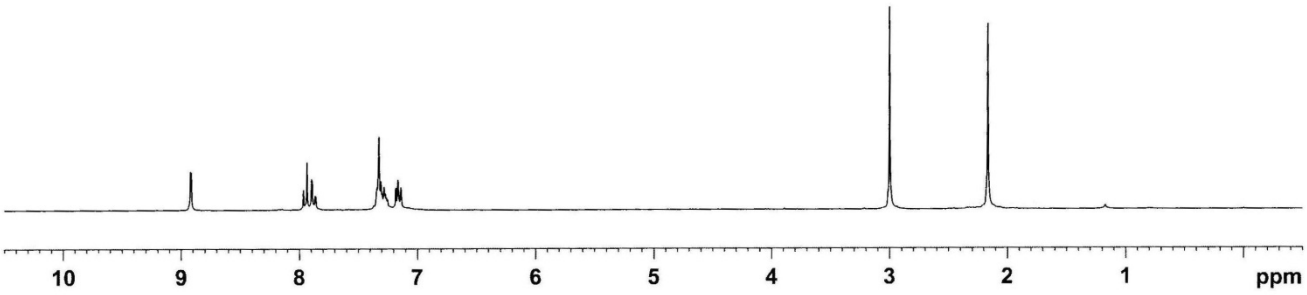
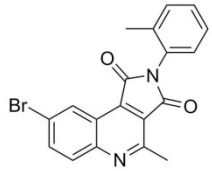
^{1}H NMR of Compound **22**



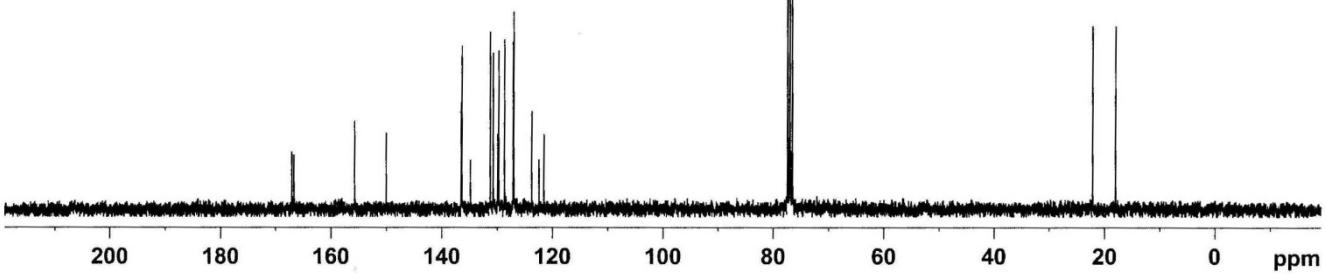
300 MHz, $CDCl_3$



^{13}C NMR of Compound **22**



75 MHz, $CDCl_3$



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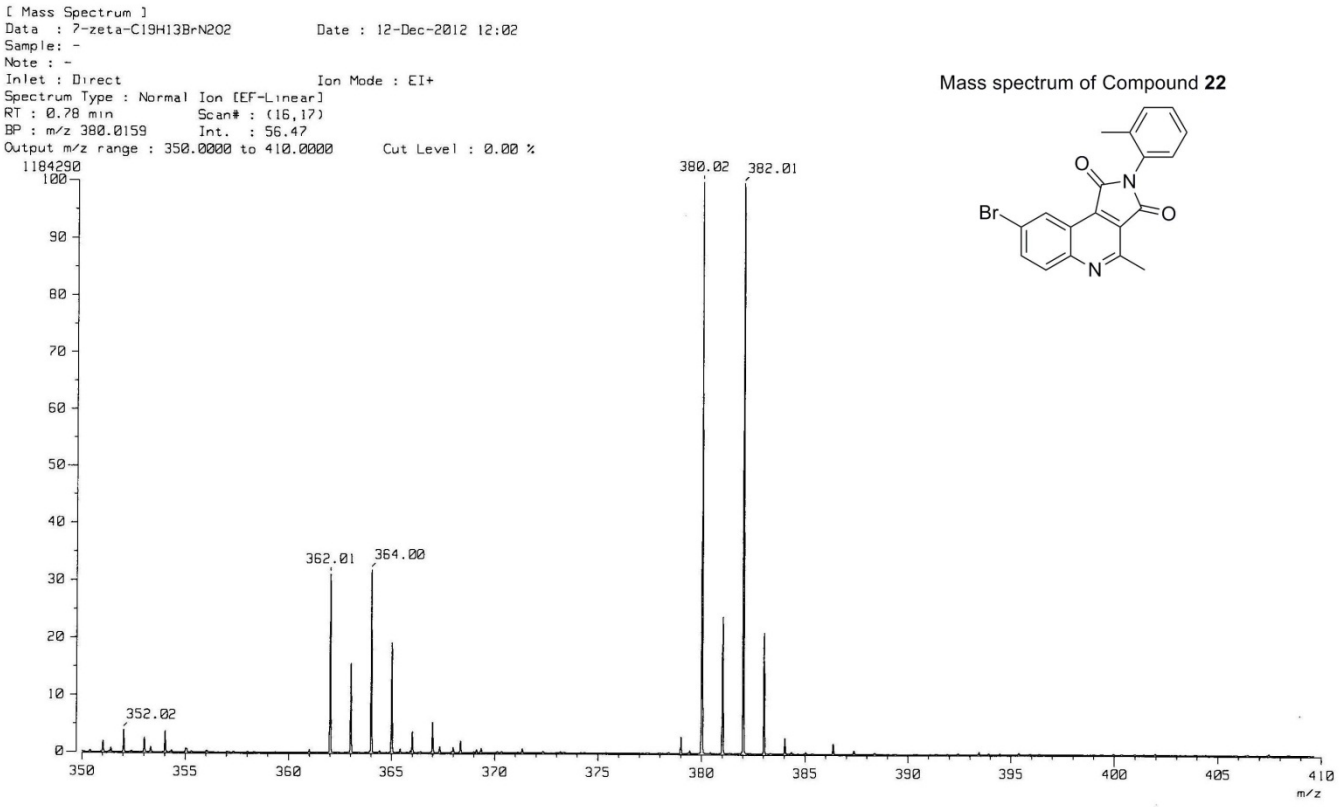

Mass spectrum of Compound **22**

[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			

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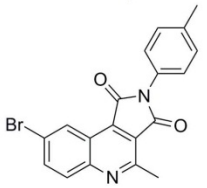
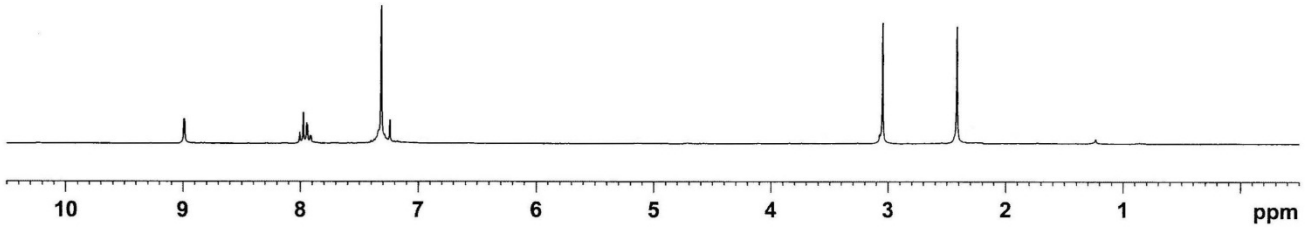
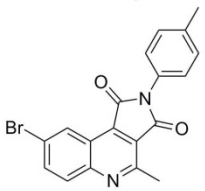
^{1}H NMR of Compound **23**



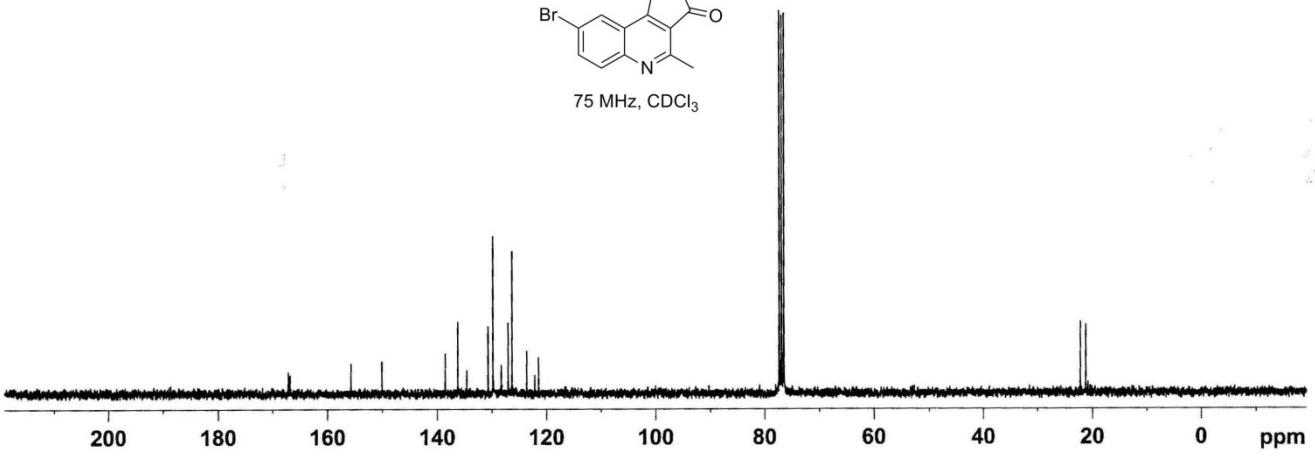
300 MHz, $CDCl_3$



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



75 MHz, $CDCl_3$



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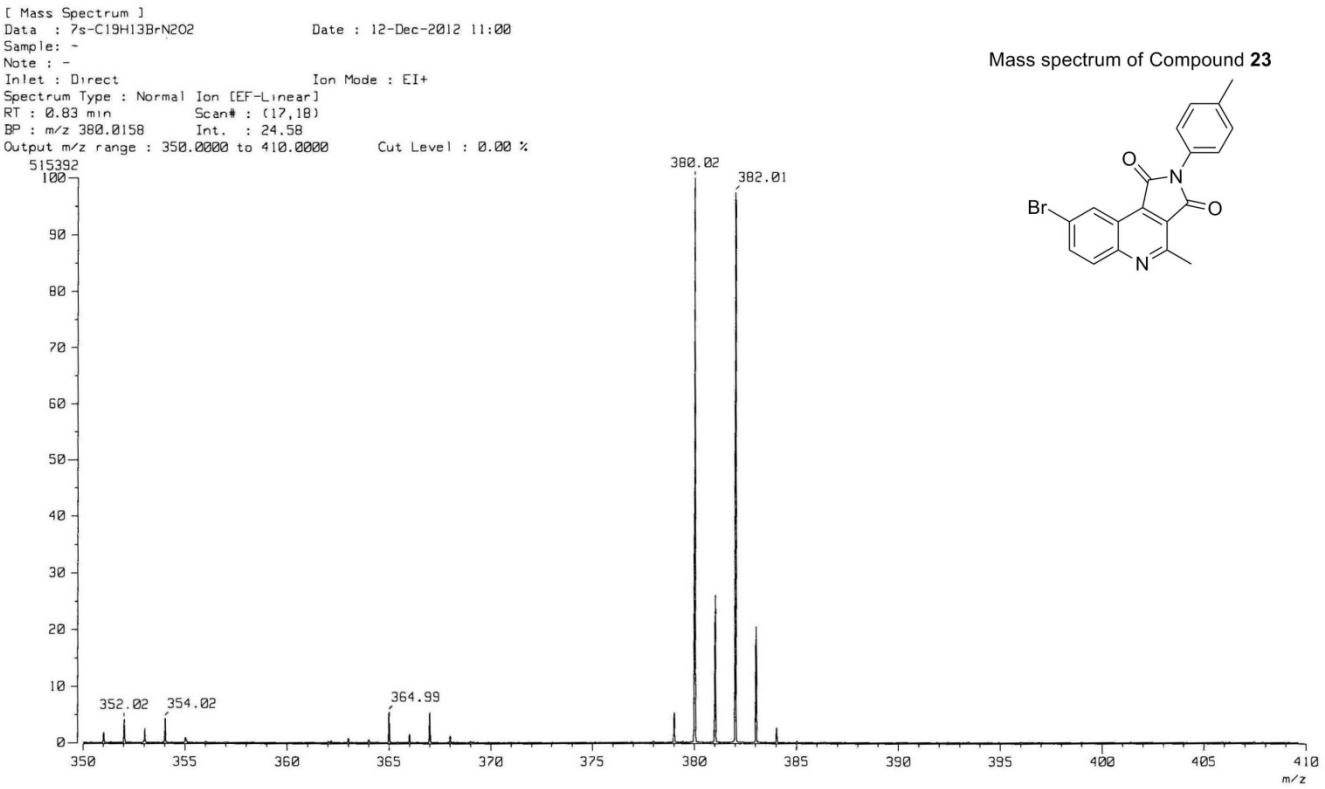

Mass spectrum of Compound **23**

[Elemental Composition] Page: 1
Data : 7s-C19H13BrN2O2 Date : 12-Dec-2012 11:00
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			

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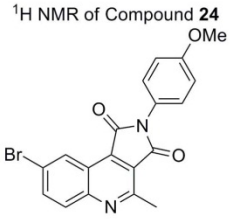
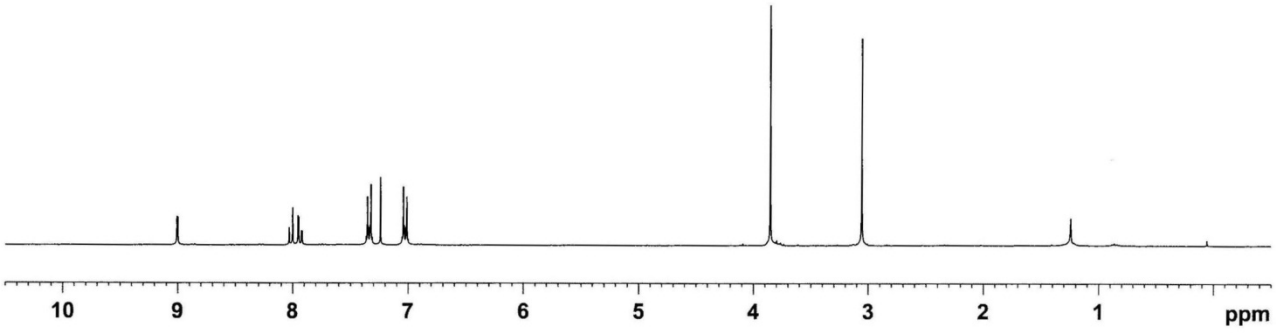
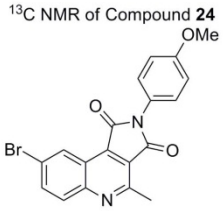
^{1}H NMR of Compound **24**



300 MHz, $CDCl_3$



^{13}C NMR of Compound **24**



150 MHz, $CDCl_3$

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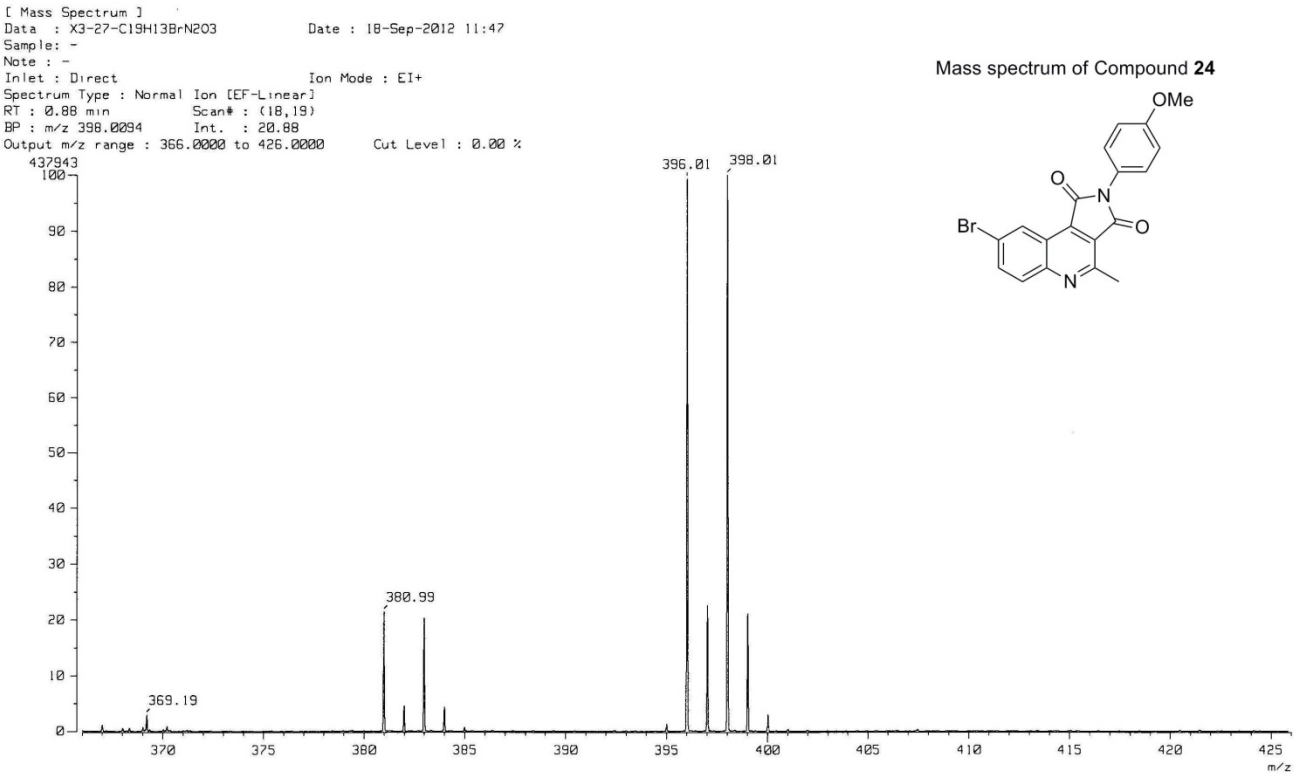
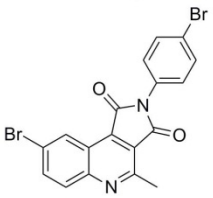


Mass spectrum of Compound **24**

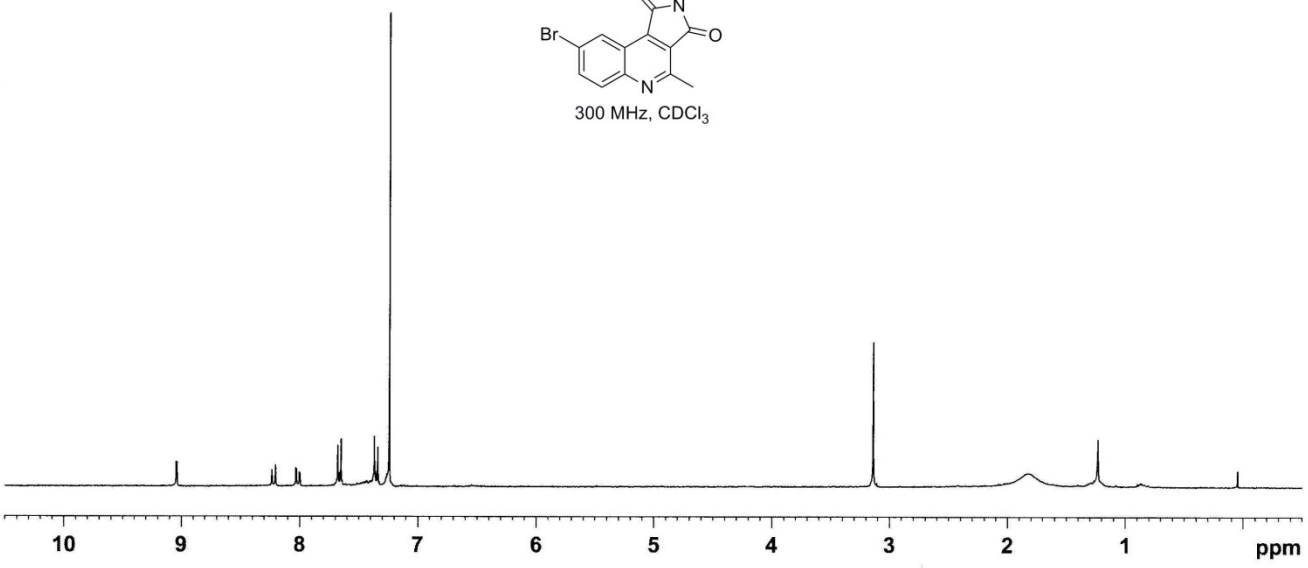
[Elemental Composition] Page: 1
Data : X3-27-C19H13BrN2O3 Date : 18-Sep-2012 11:47
Sample: -
Note : -
Inlet : Direct Ion Mode : EI+
RT : 0.88 min Scan#: (18,19)
Elements : C 19/0, H 13/0, Br 1/0, N 2/0, O 3/0
Mass Tolerance : 1000ppm, 2mmu if m/z < 2, 3mmu if m/z > 3
Unsaturation (U.S.) : -0.5 - 100.0

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			

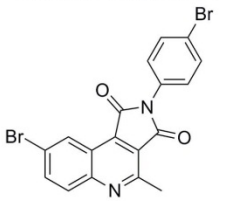
^{1}H NMR of Compound **25**



300 MHz, $CDCl_3$



^{13}C NMR of Compound **25**



75 MHz, $CDCl_3$ + DMSO-d_6

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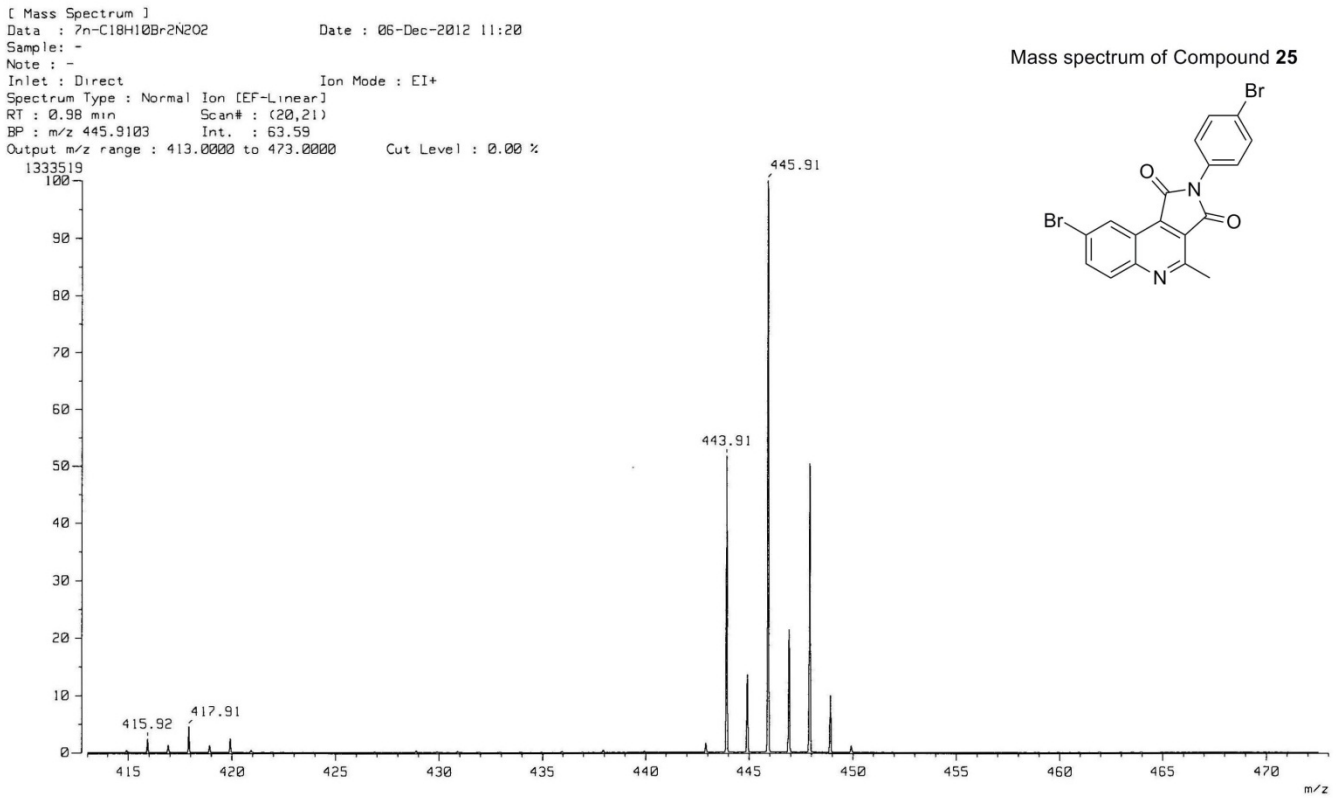

Mass spectrum of Compound **25**

[Elemental Composition] Page: 1
Data : 7n-C18H10Br2N2O2 Date : 06-Dec-2012 11:20
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			

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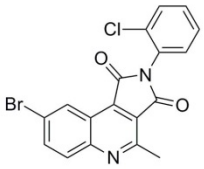
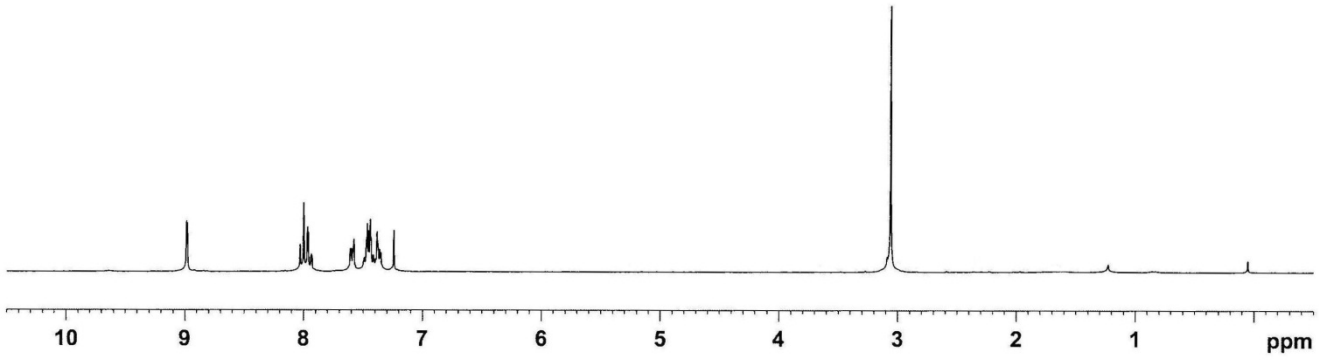
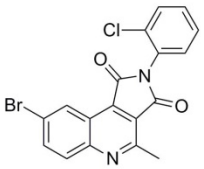
^{1}H NMR of Compound **26**



300 MHz, $CDCl_3$



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



75 MHz, $CDCl_3$

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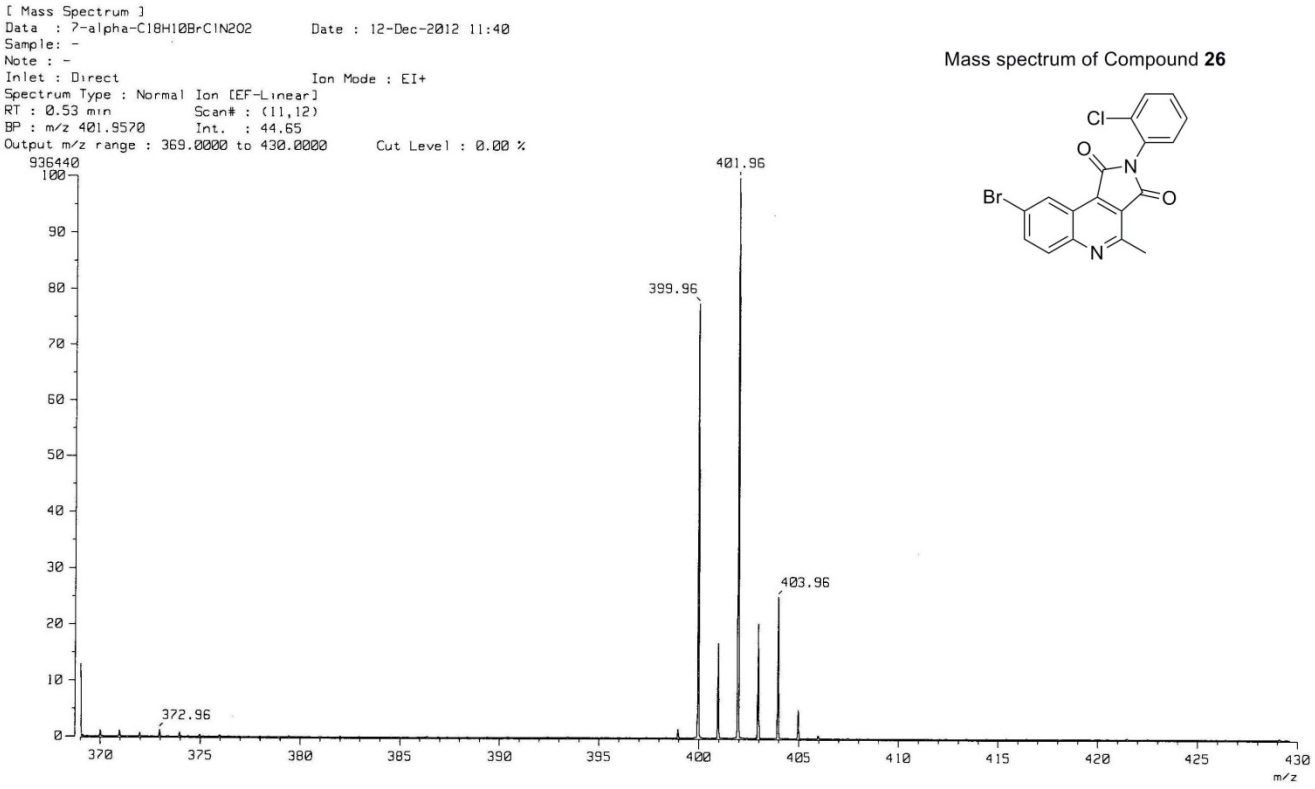

Mass spectrum of Compound **26**

[Elemental Composition] Page: 1
Data : 7-alpha-C18H10BrClN2O2 Date : 12-Dec-2012 11:40
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			

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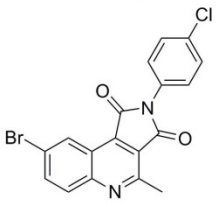
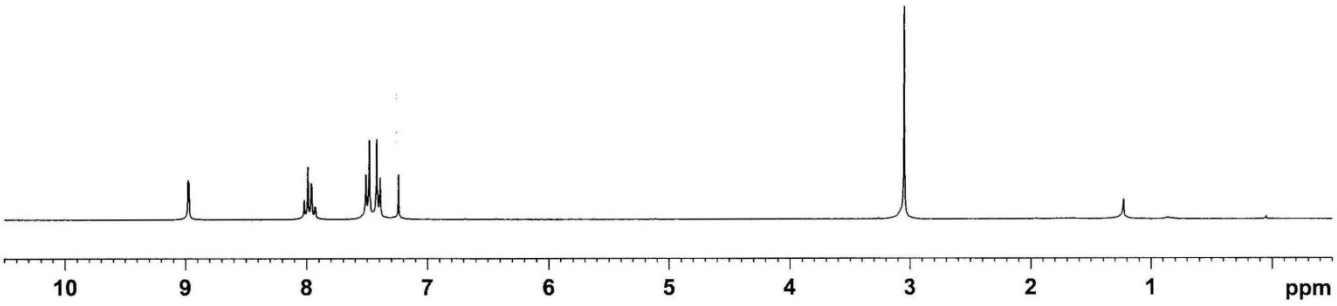
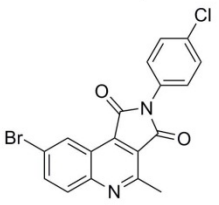
^{1}H NMR of Compound **27**



300 MHz, $CDCl_3$



^{13}C NMR of Compound **27**



75 MHz, $CDCl_3$

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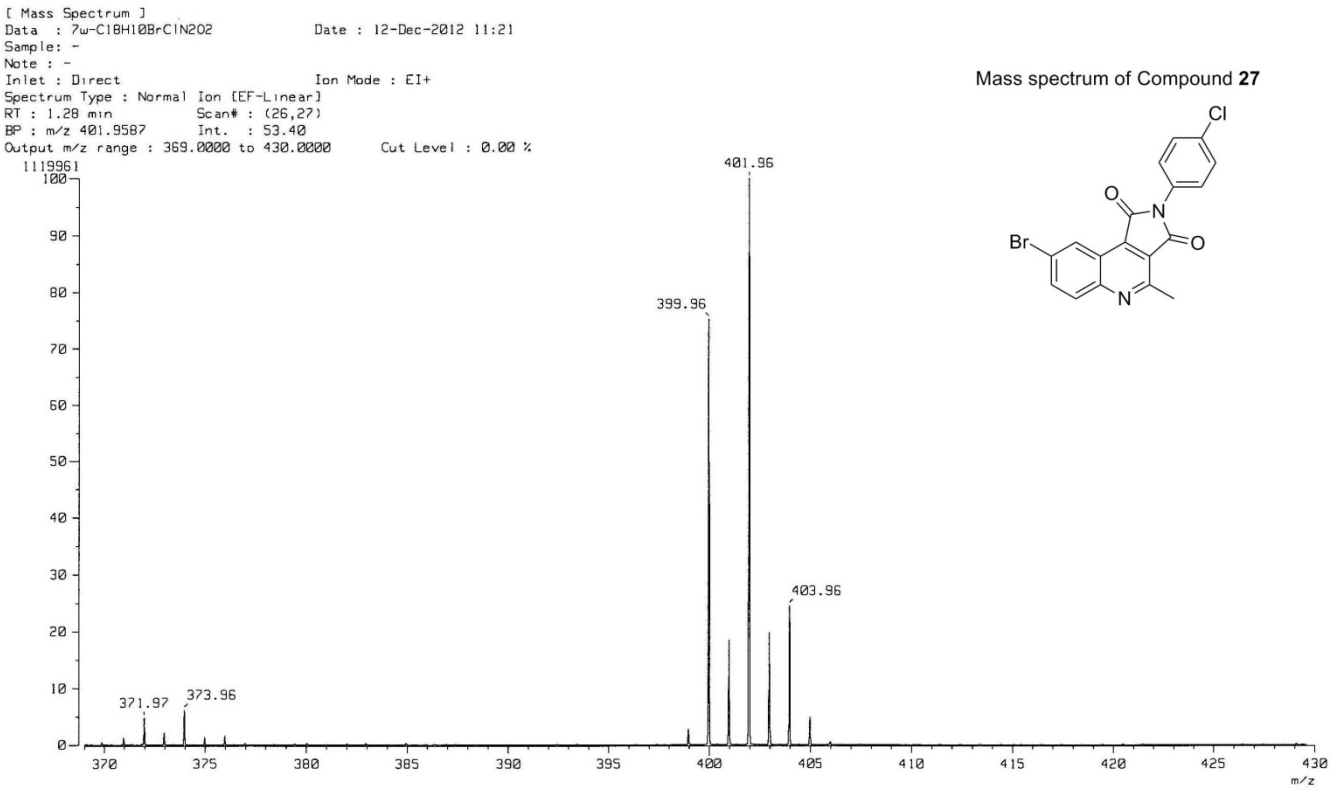

Mass spectrum of Compound **27**

[Elemental Composition] Page: 1
Data : 7w-C18H10BrClN2O2 Date : 12-Dec-2012 11:21
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			

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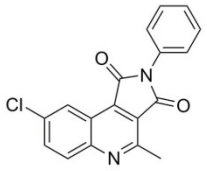
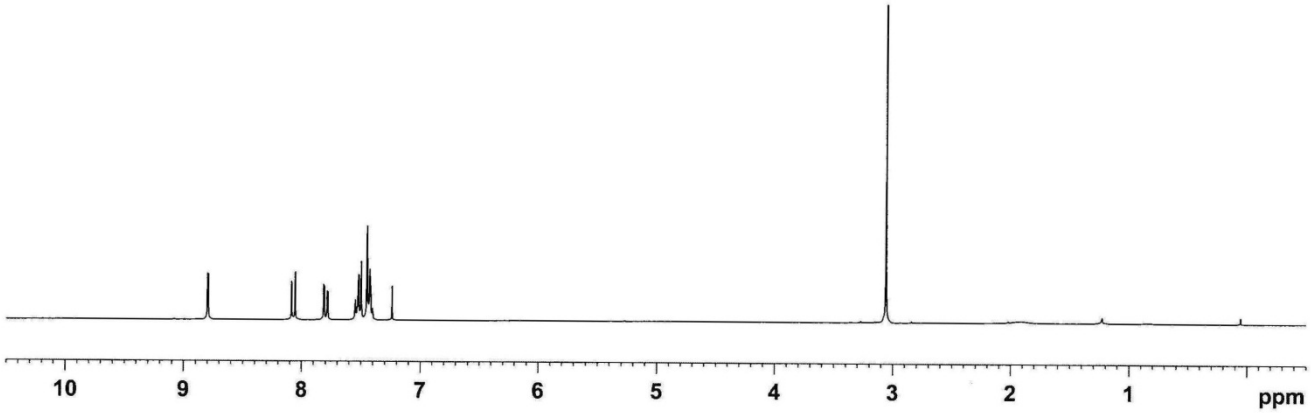
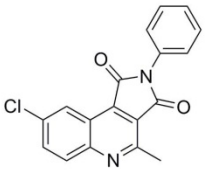
^{1}H NMR of Compound **28**



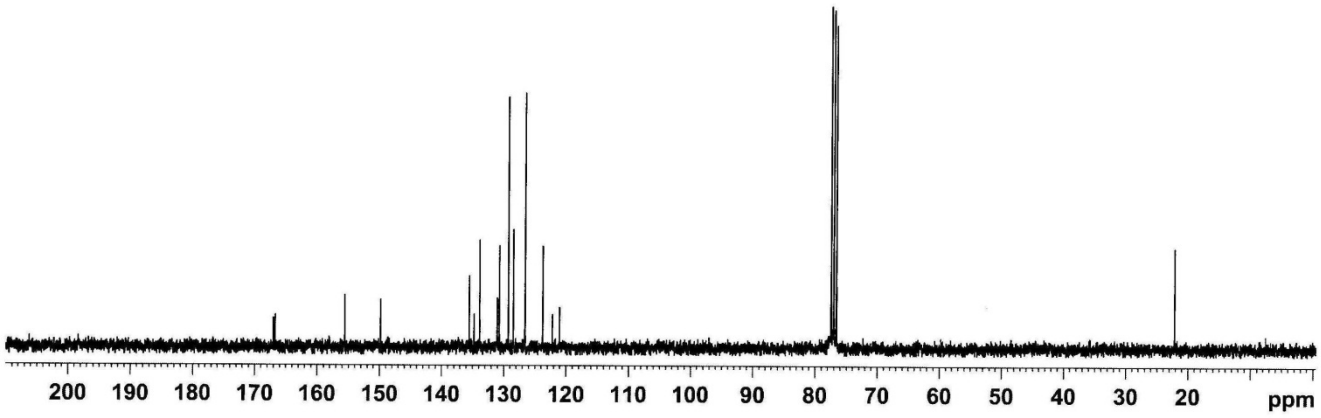
300 MHz, $CDCl_3$



^{13}C NMR of Compound **28**



75 MHz, $CDCl_3$



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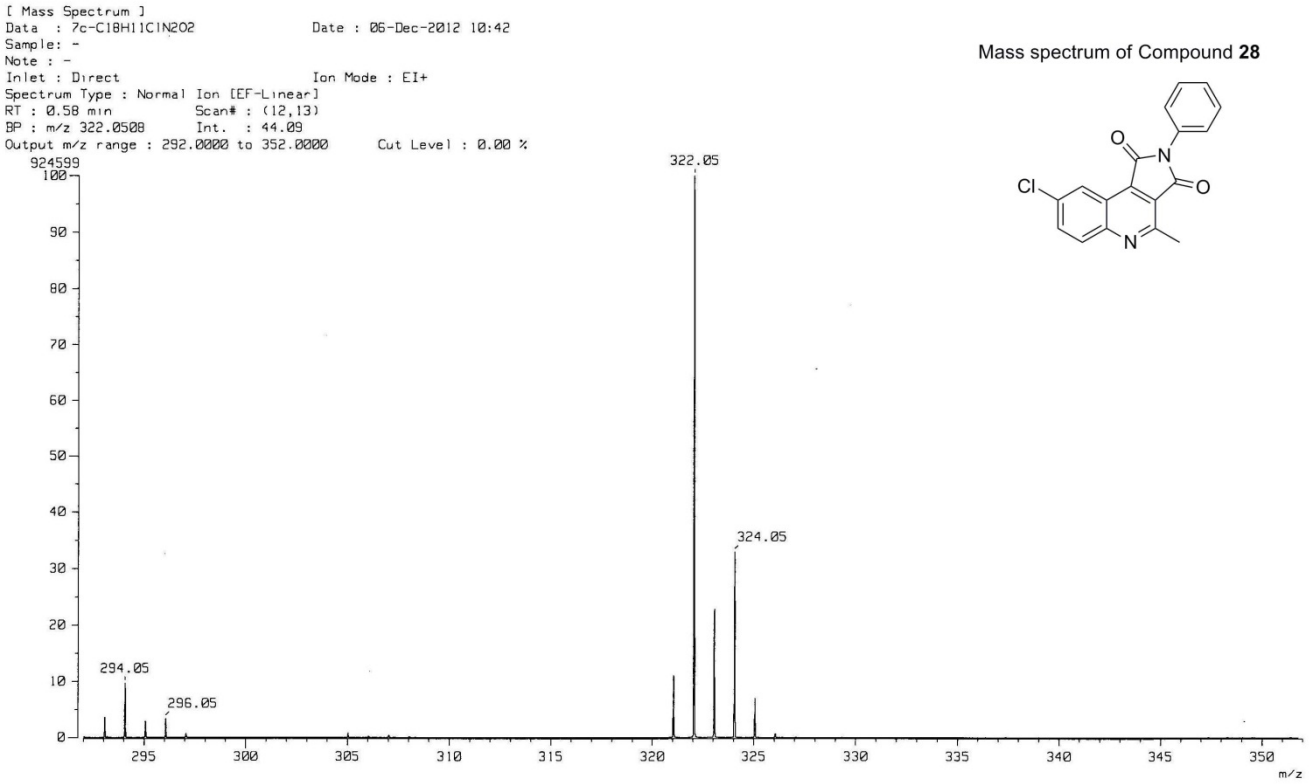
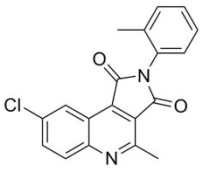
Mass spectrum of Compound **28**



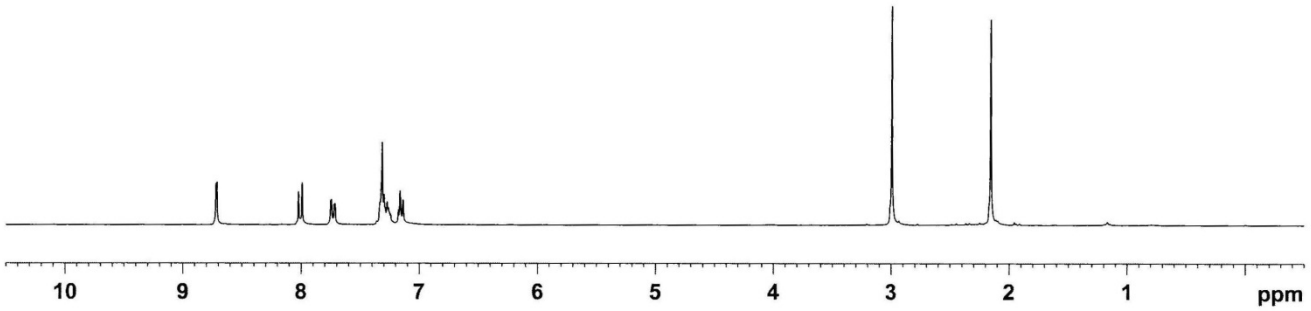
[Elemental Composition] Page: 1
Data : 7c-C18H11ClN2O2 Date : 06-Dec-2012 10:42
Sample: -
Note : -
Inlet : Direct Ion Mode : EI+
RT : 0.58 min Scan#: (12,13)
Elements : C 18/0, H 11/0, Cl 1/0, N 2/0, O 2/0
Mass Tolerance : 1000ppm, 2mmu if m/z < 2, 3mmu if m/z > 3
Unsaturation (U.S.) : -0.5 - 100.0

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			

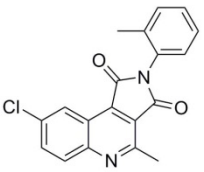
^{1}H NMR of Compound **29**



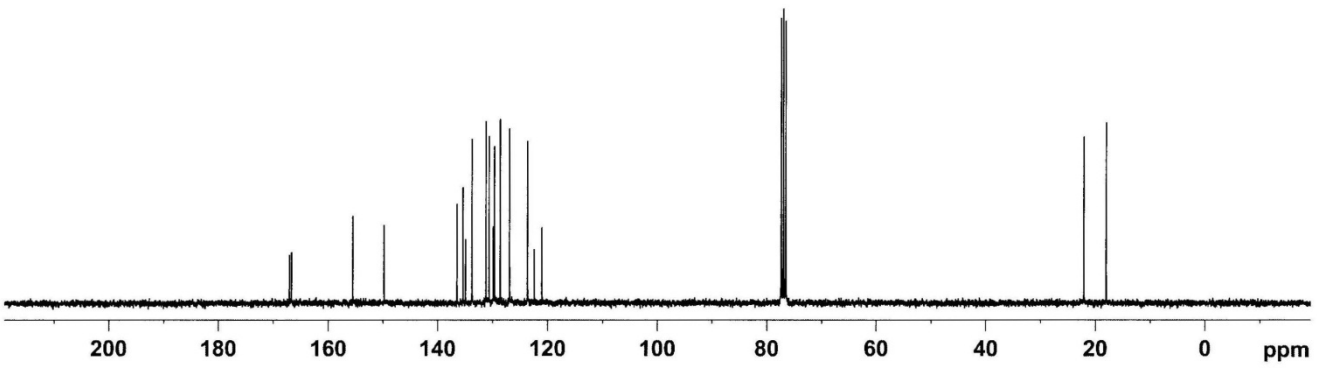
300 MHz, $CDCl_3$



^{13}C NMR of Compound **29**



75 MHz, $CDCl_3$



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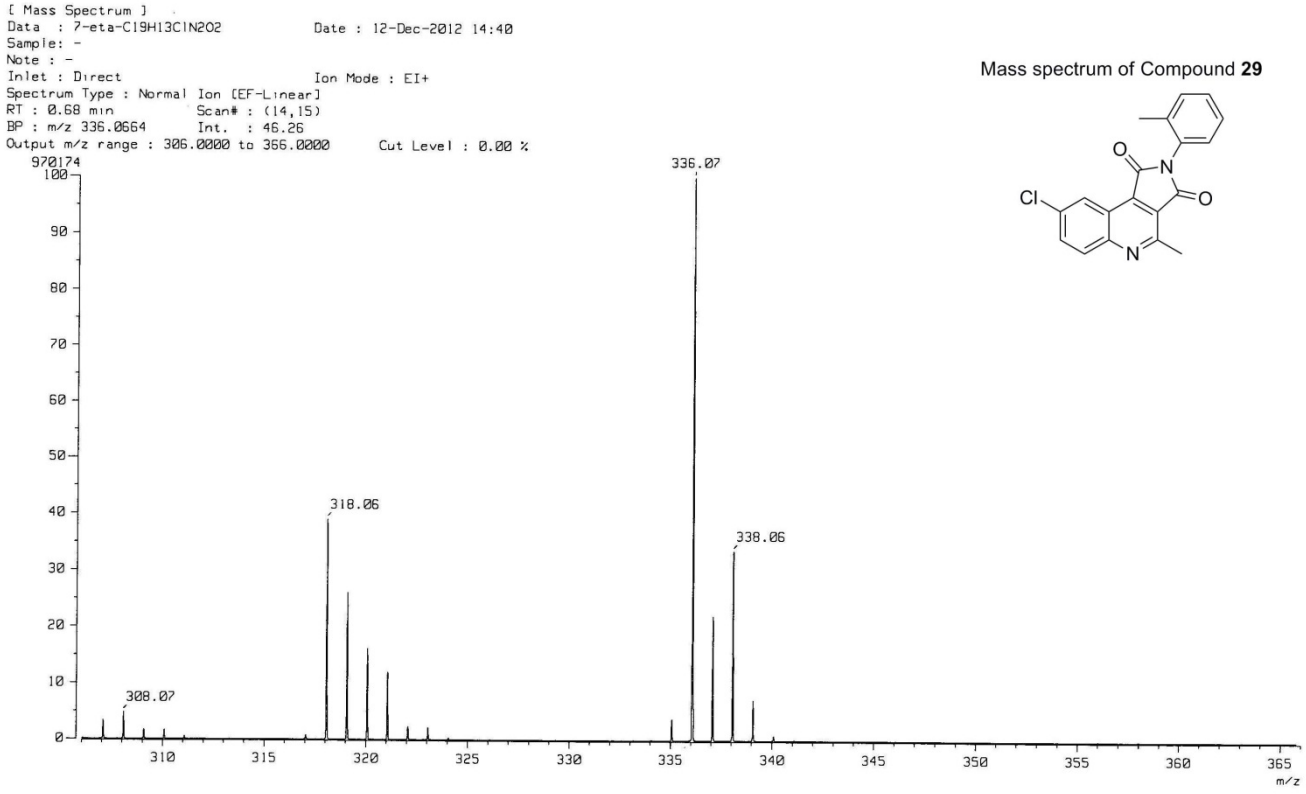

Mass spectrum of Compound **29**

[Elemental Composition] Page: 1
Data : 7-eta-C19H13ClN2O2 Date : 12-Dec-2012 14:40
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			

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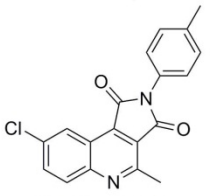
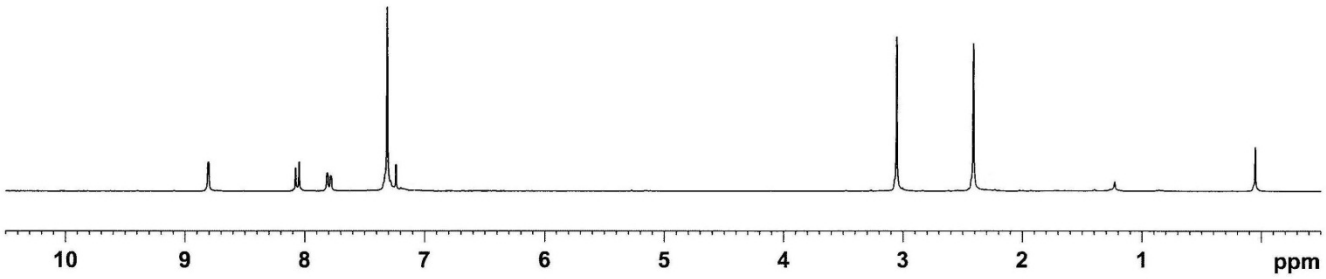
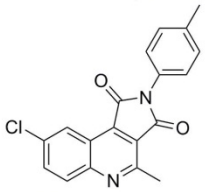
^{1}H NMR of Compound **30**



300 MHz, $CDCl_3$



^{13}C NMR of Compound **30**



75 MHz, $CDCl_3$

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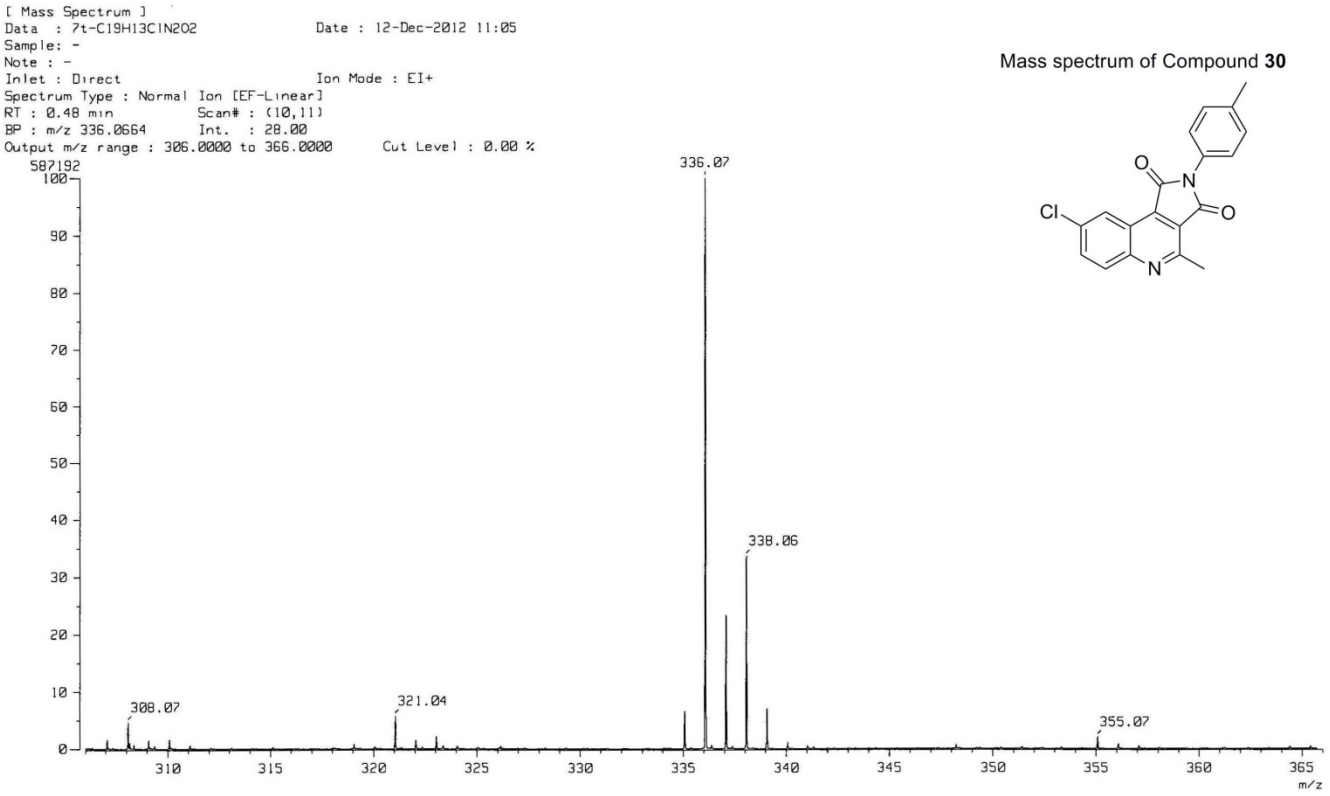

Mass spectrum of Compound **30**

[Elemental Composition] Page: 1
Data : 7t-C19H13ClN2O2 Date : 12-Dec-2012 11:05
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			

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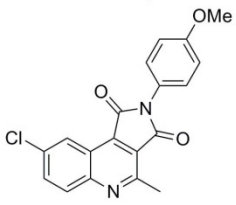
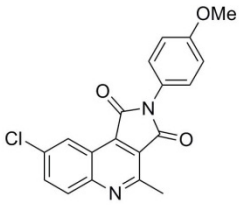
^{1}H NMR of Compound **31**

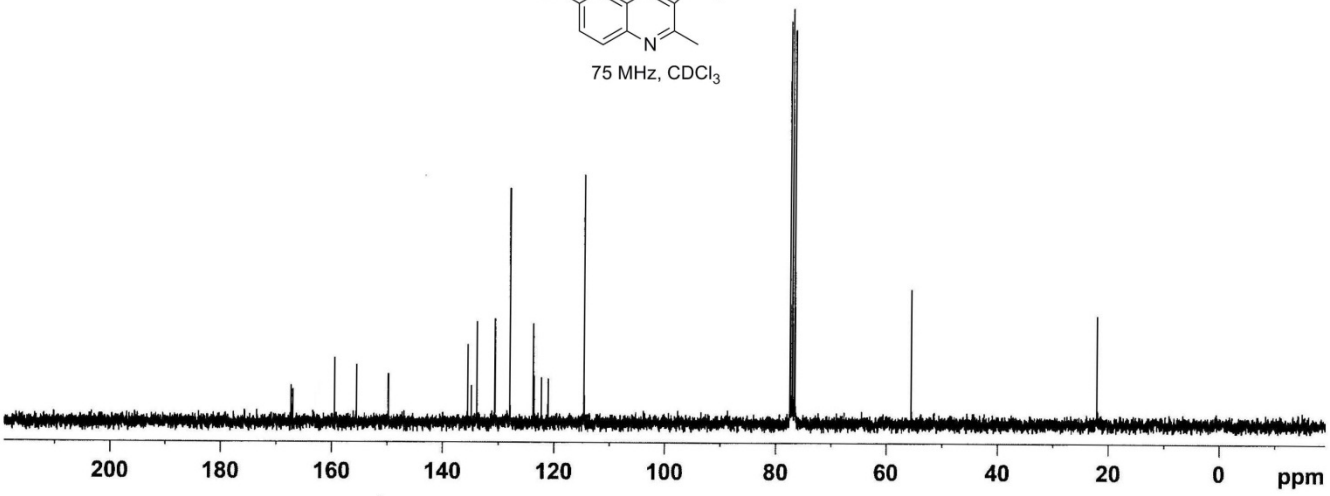


300 MHz, $CDCl_3$

^{13}C NMR of Compound **31**



75 MHz, $CDCl_3$



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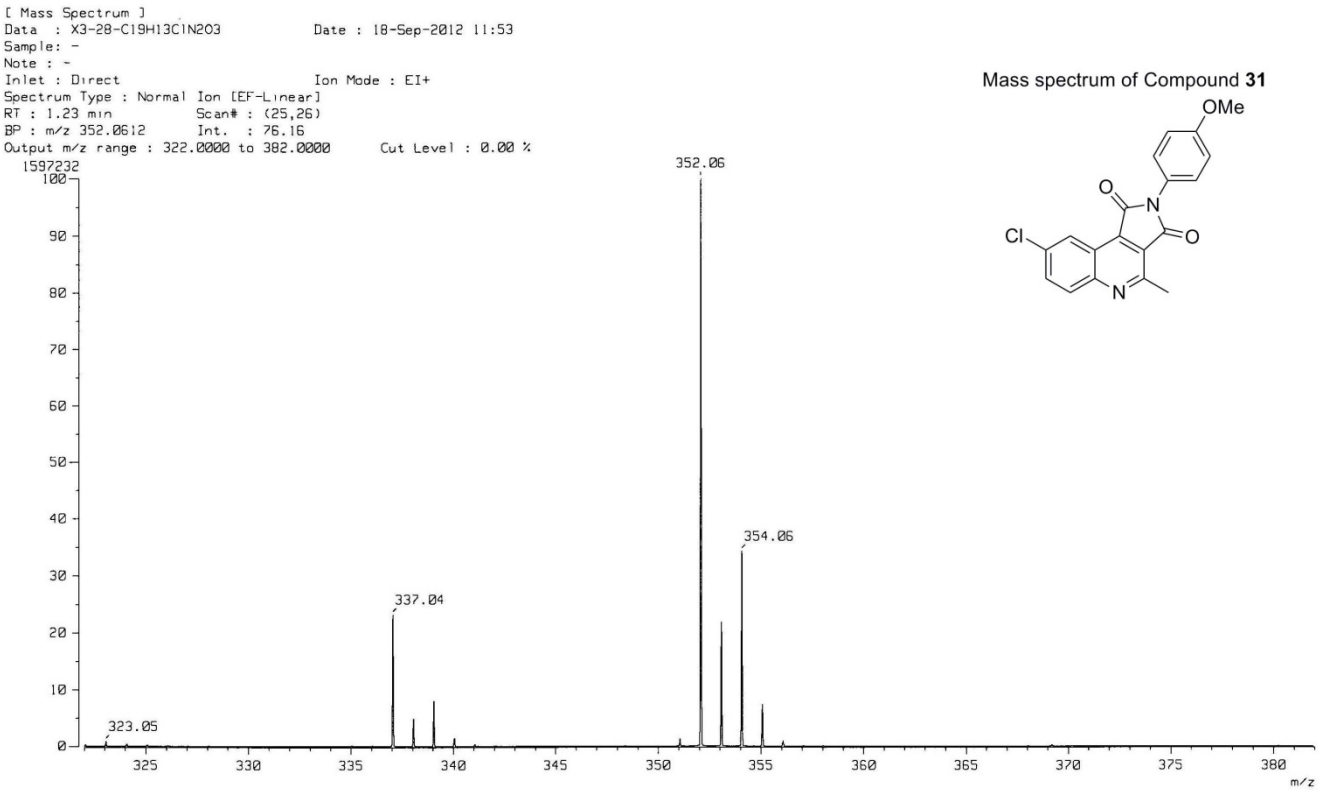

Mass spectrum of Compound **31**

[Elemental Composition] Page: 1
Data : X3-28-C19H13ClN2O3 Date : 18-Sep-2012 11:53
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			

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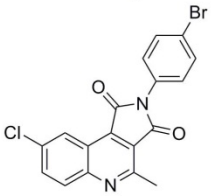
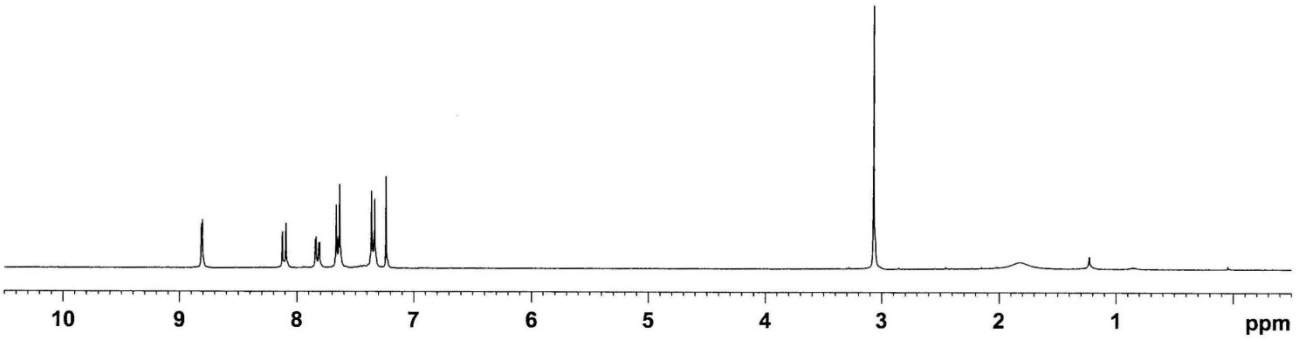
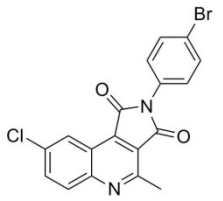
^{1}H NMR of Compound **32**



300 MHz, $CDCl_3$



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



75 MHz, $CDCl_3$

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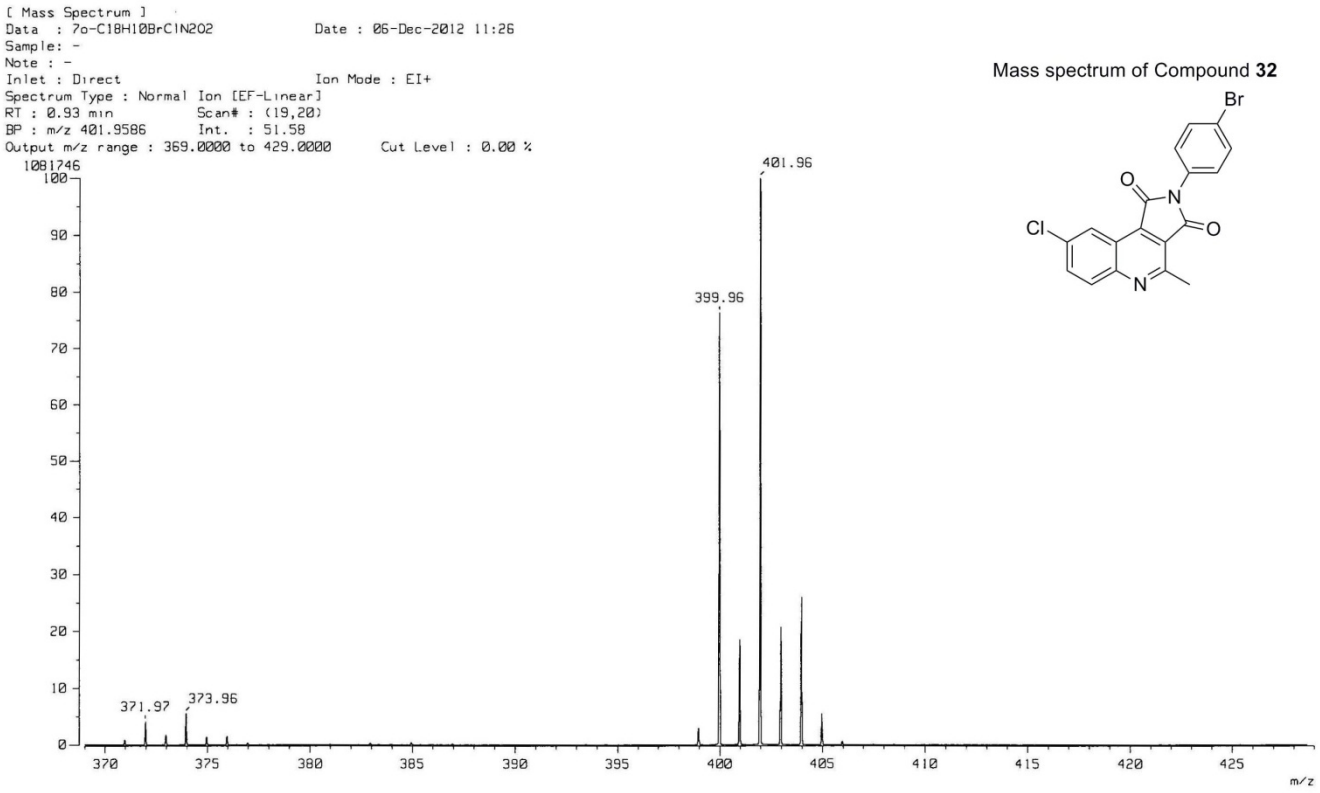
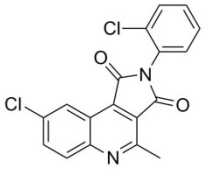


Mass spectrum of Compound **32**

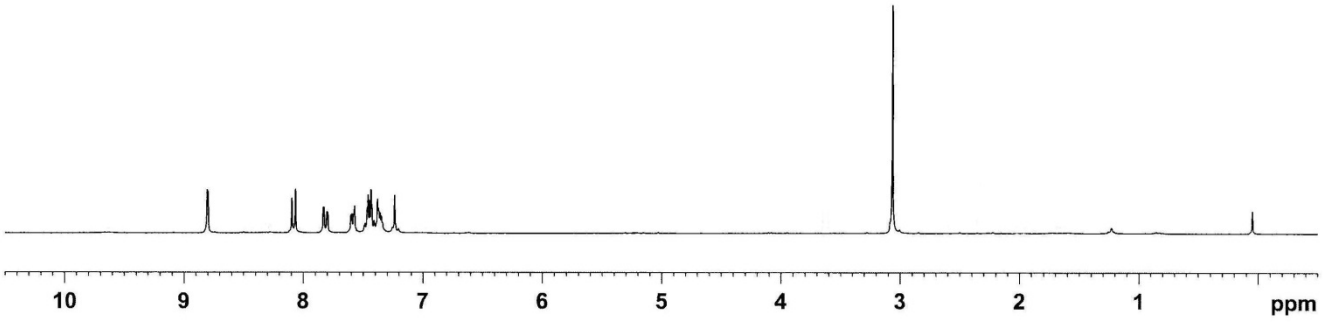
[Elemental Composition] Page: 1
Data : 7o-C18H10BrClN2O2 Date : 06-Dec-2012 11:26
Sample: -
Note : -
Inlet : Direct Ion Mode : EI+
RT : 0.93 min Scan#: (19,20)
Elements : C 18/0, H 10/0, Br 1/0, Cl 1/0, N 2/0, O 2/0
Mass Tolerance : 1000ppm, 2mmu if m/z < 2, 3mmu if m/z > 3
Unsaturation (U.S.) : -0.5 - 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			

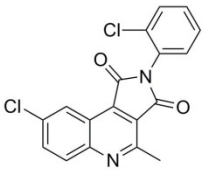
^{1}H NMR of Compound **33**



300 MHz, $CDCl_3$



^{13}C NMR of Compound **33**



75 MHz, $CDCl_3$

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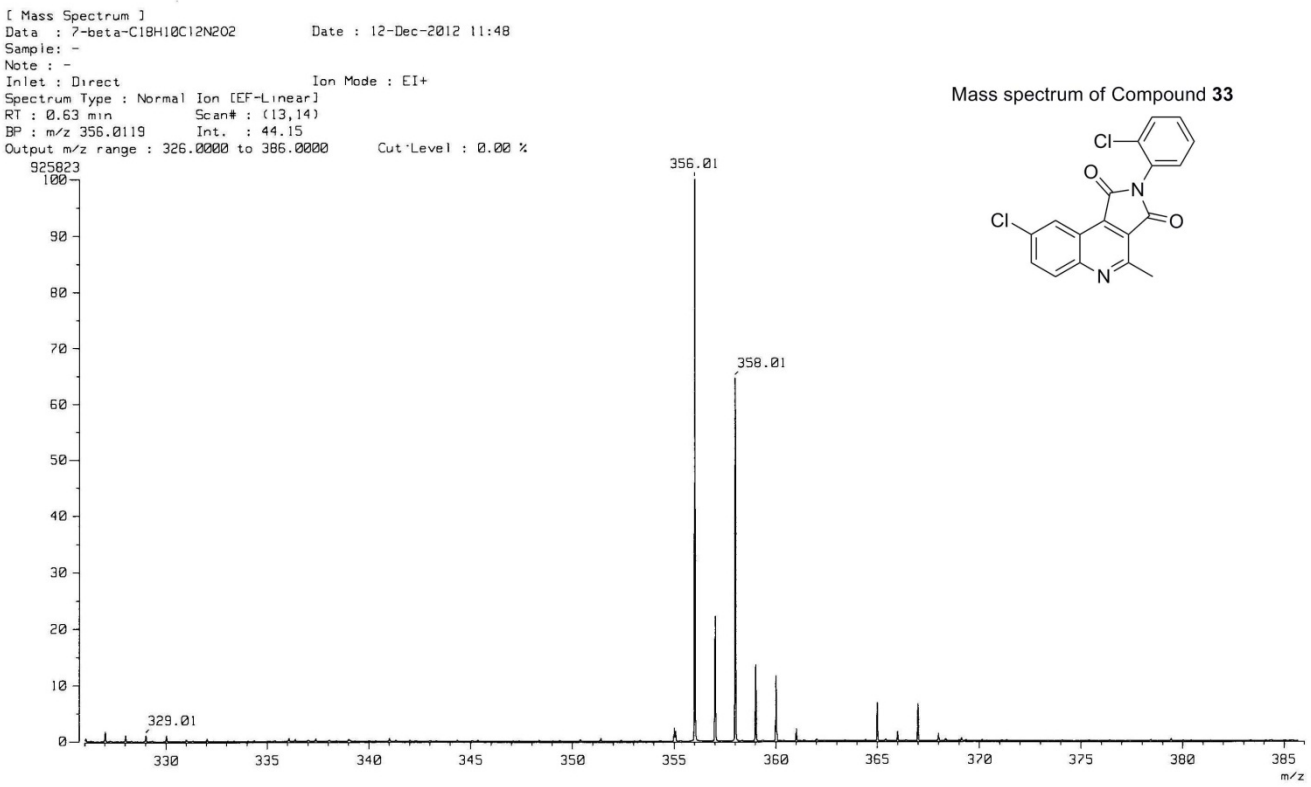

Mass spectrum of Compound **33**

[Elemental Composition] Page: 1
Data : 7-beta-C18H10Cl2N2O2 Date : 12-Dec-2012 11:48
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			

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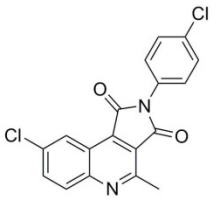
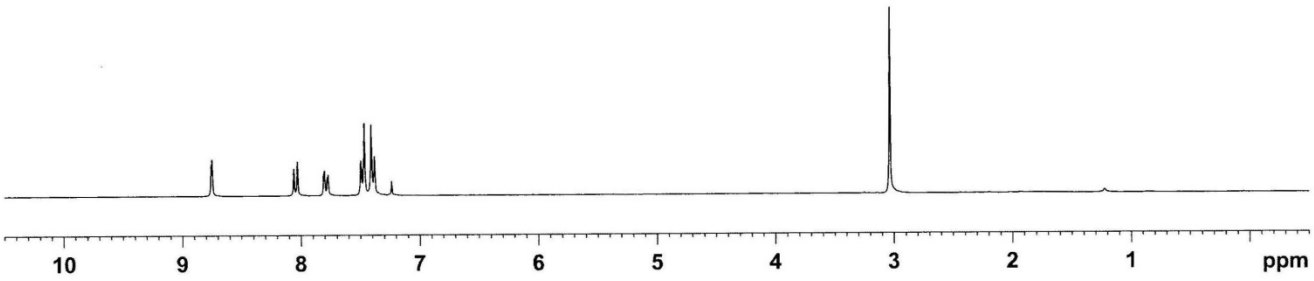
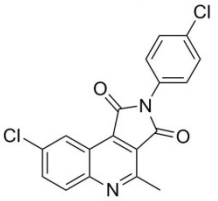
^{1}H NMR of Compound **34**



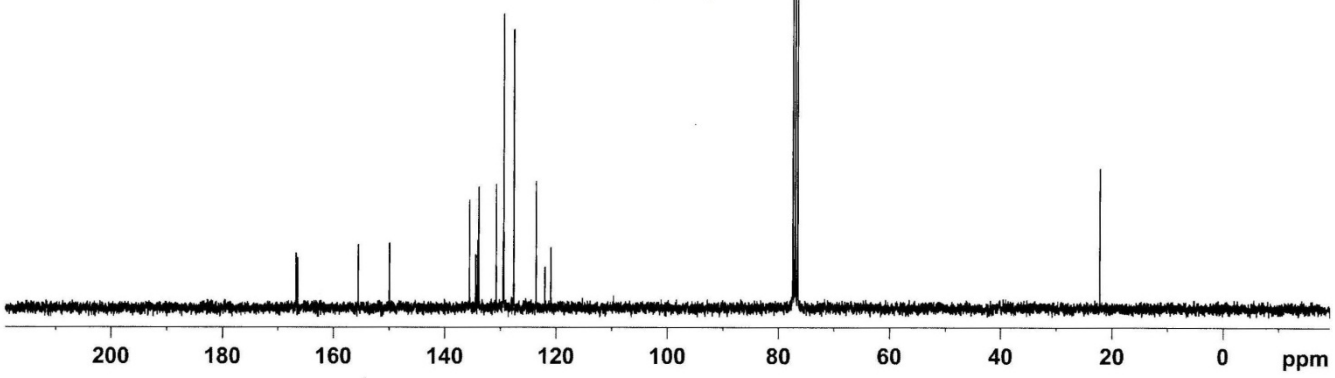
300 MHz, $CDCl_3$

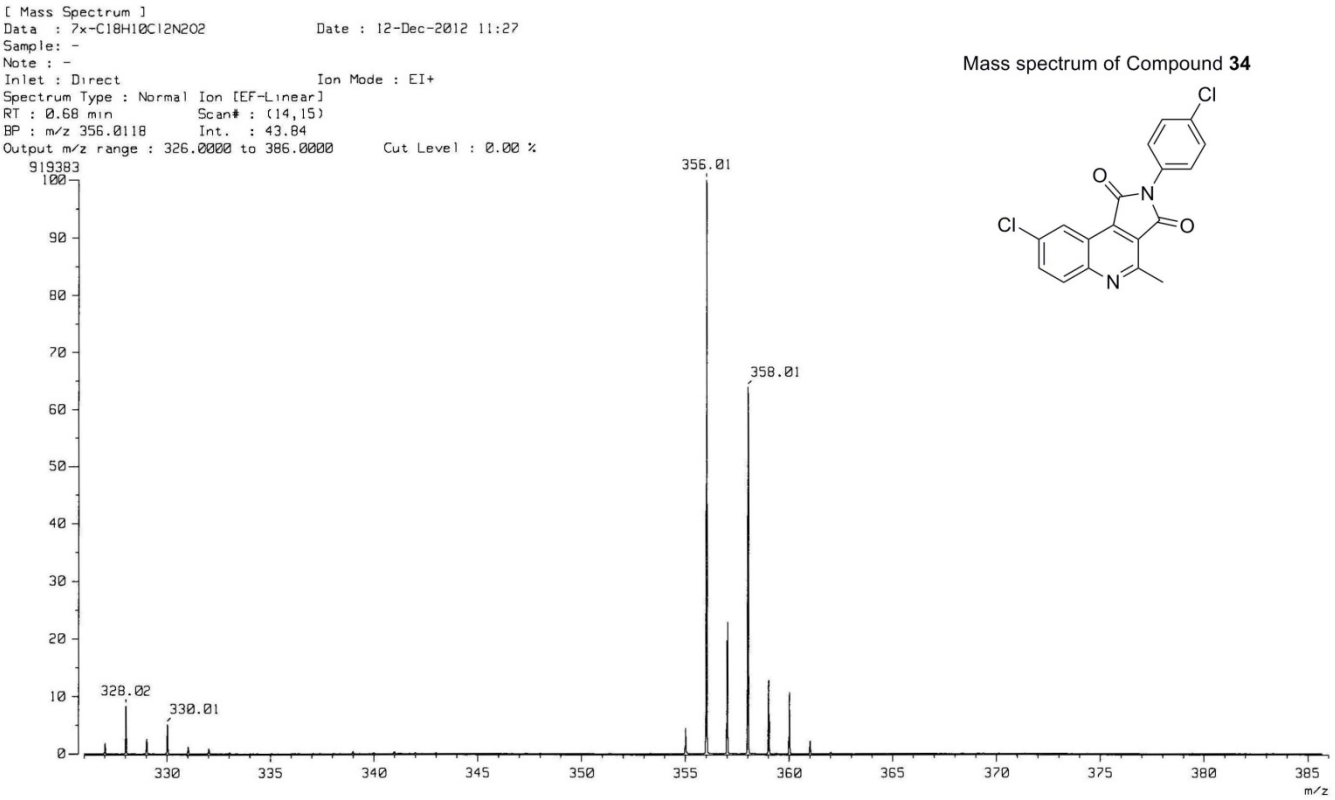


^{13}C NMR of Compound **34**



75 MHz, $CDCl_3$





Mass spectrum of Compound **34**

[Elemental Composition] Page: 1
Data : 7x-C18H10Cl2N2O2 Date : 12-Dec-2012 11:27
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			

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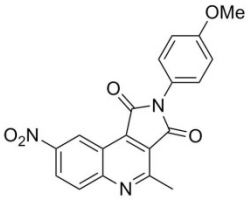
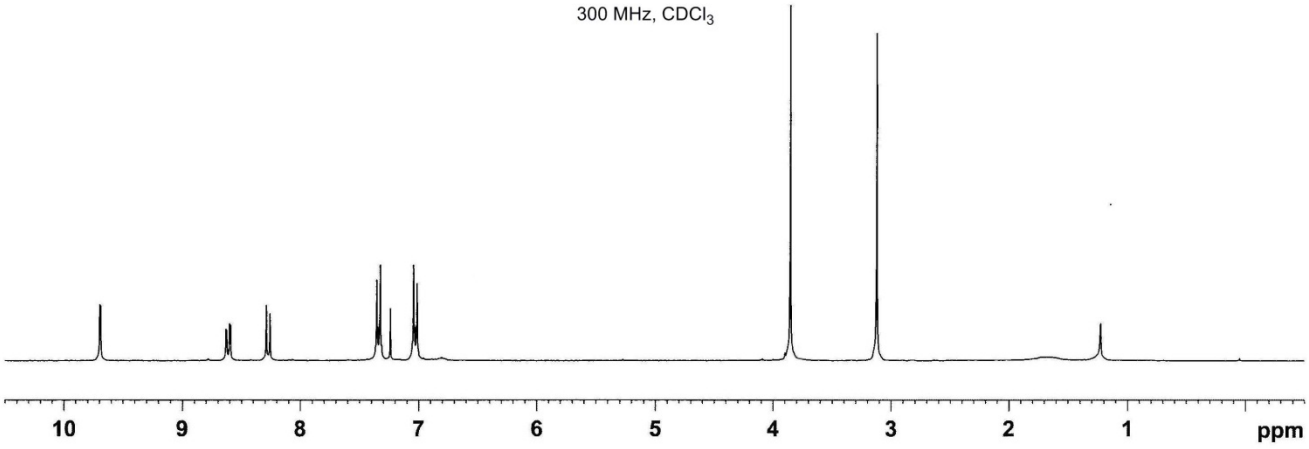
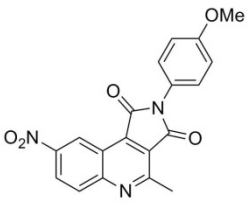
^{1}H NMR of Compound **35**



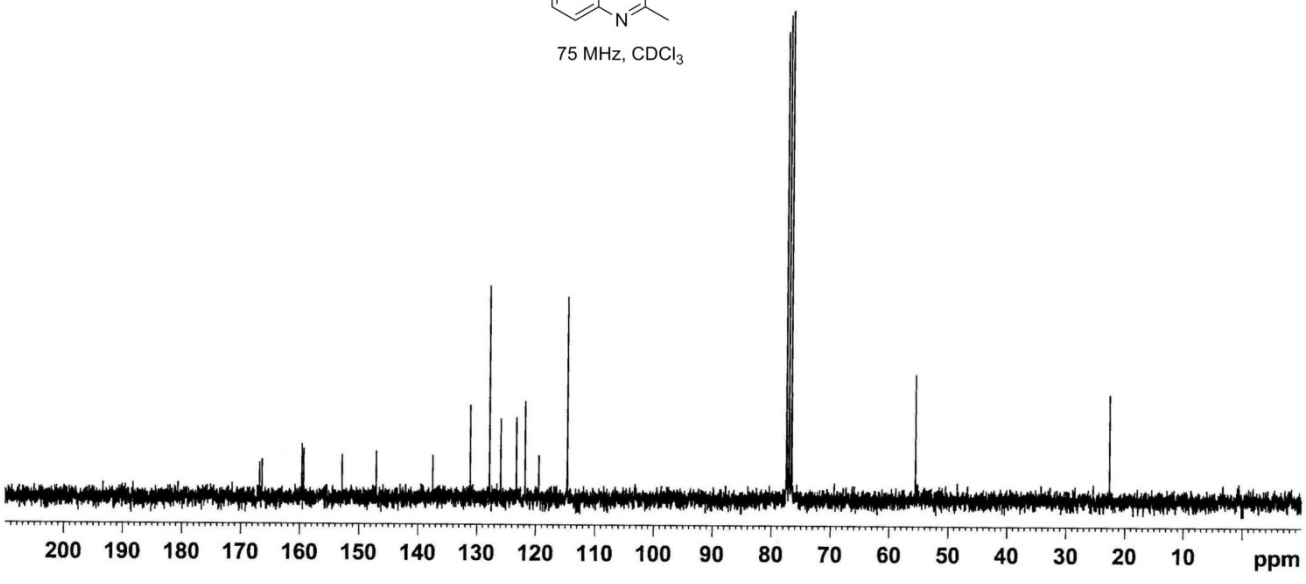
300 MHz, $CDCl_3$



^{13}C NMR of Compound **35**



75 MHz, $CDCl_3$



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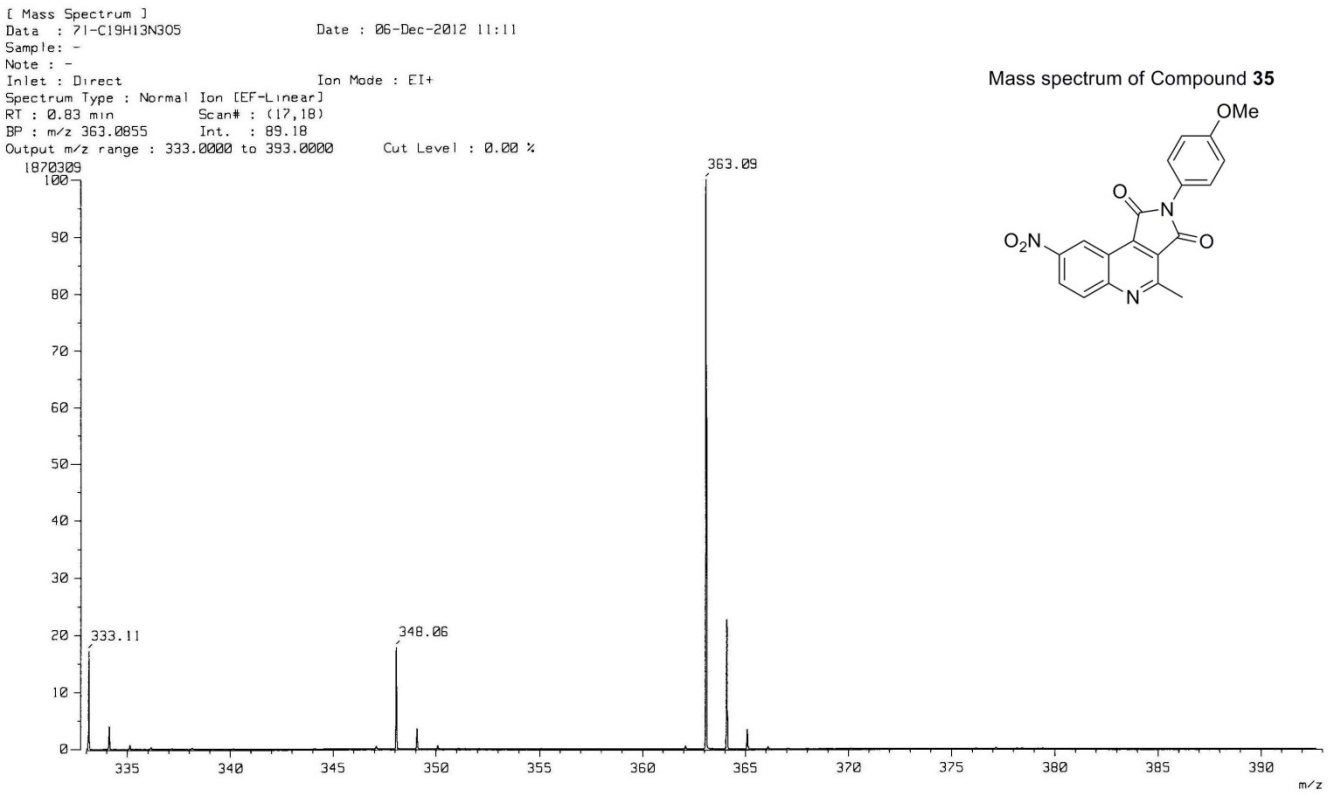

Mass spectrum of Compound **35**

[Elemental Composition] Page: 1
Data : 7l-C19H13N3O5 Date : 06-Dec-2012 11:11
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			

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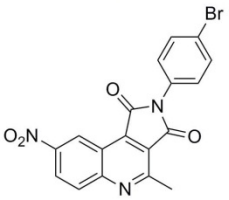
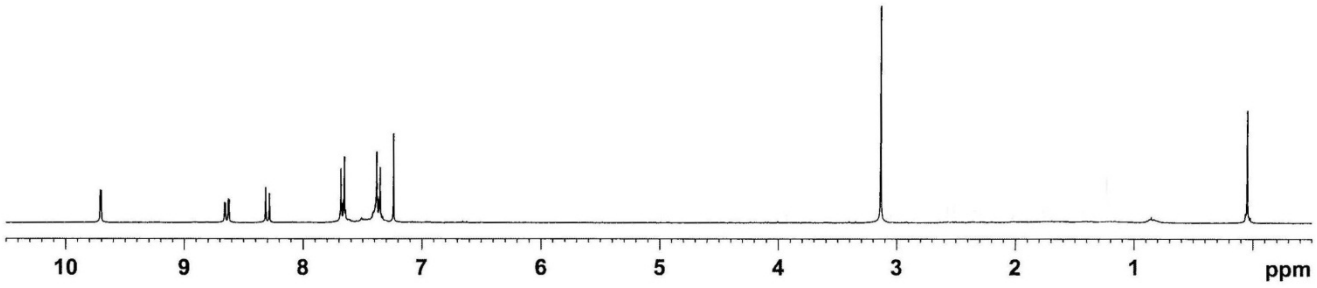
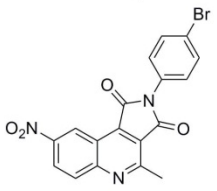
^{1}H NMR of Compound **36**



300 MHz, $CDCl_3$



^{13}C NMR of Compound **36**



150 MHz, $CDCl_3$

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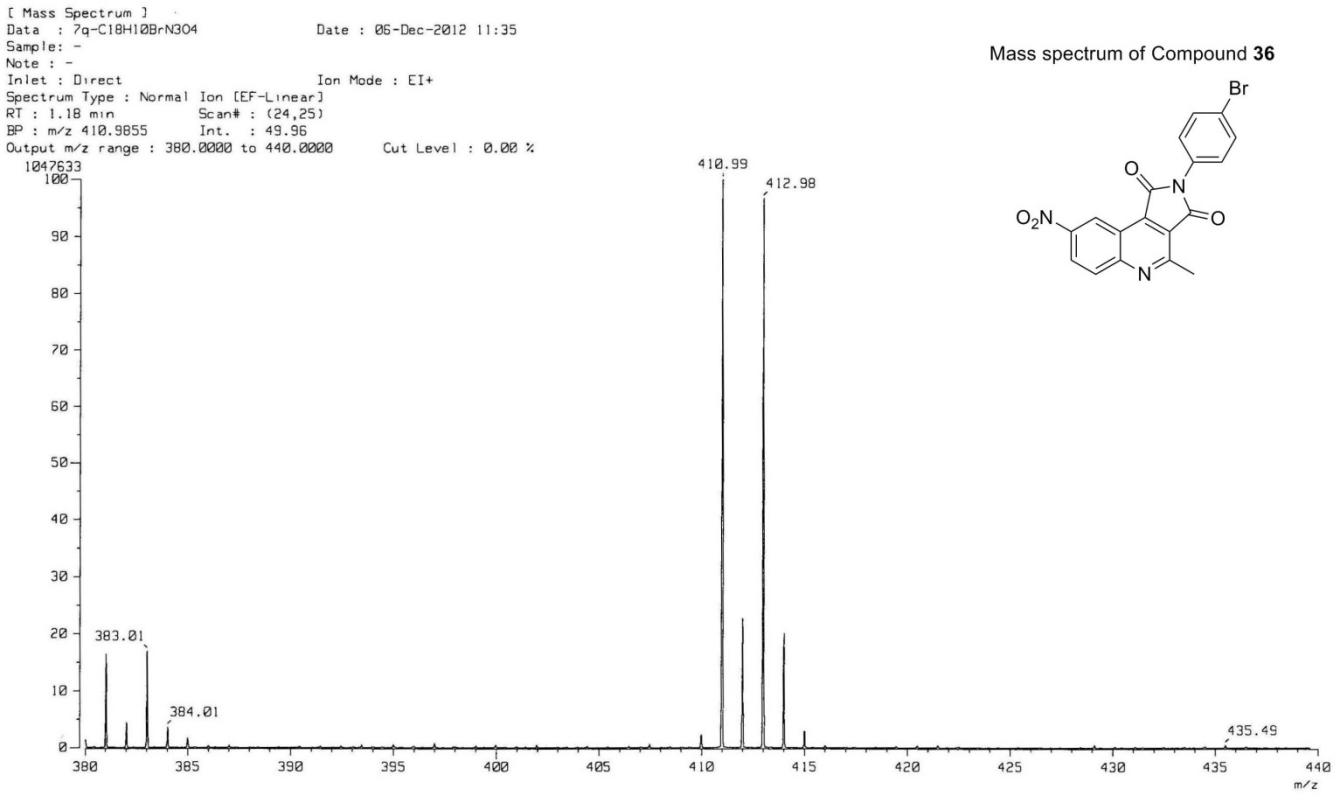

Mass spectrum of Compound **36**

[Elemental Composition] Page: 1
Data : 7q-C18H10BrN3O4 Date : 06-Dec-2012 11:35
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			

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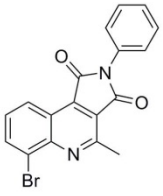
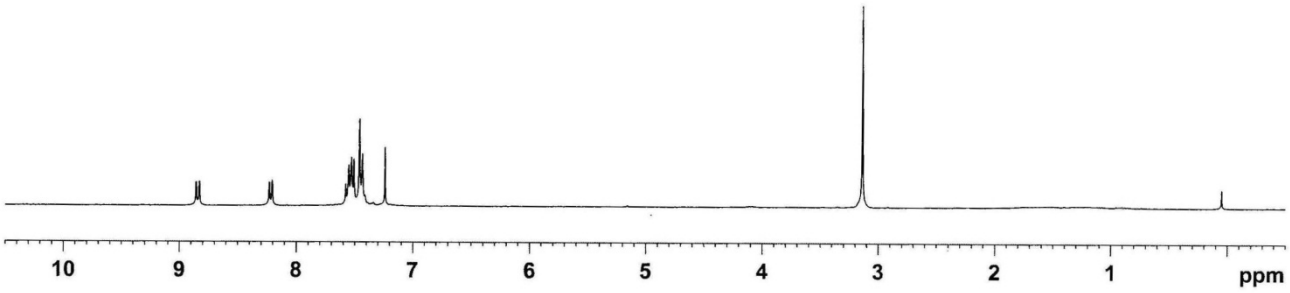
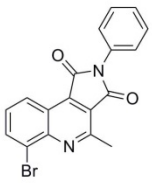
^{1}H NMR of Compound **37**



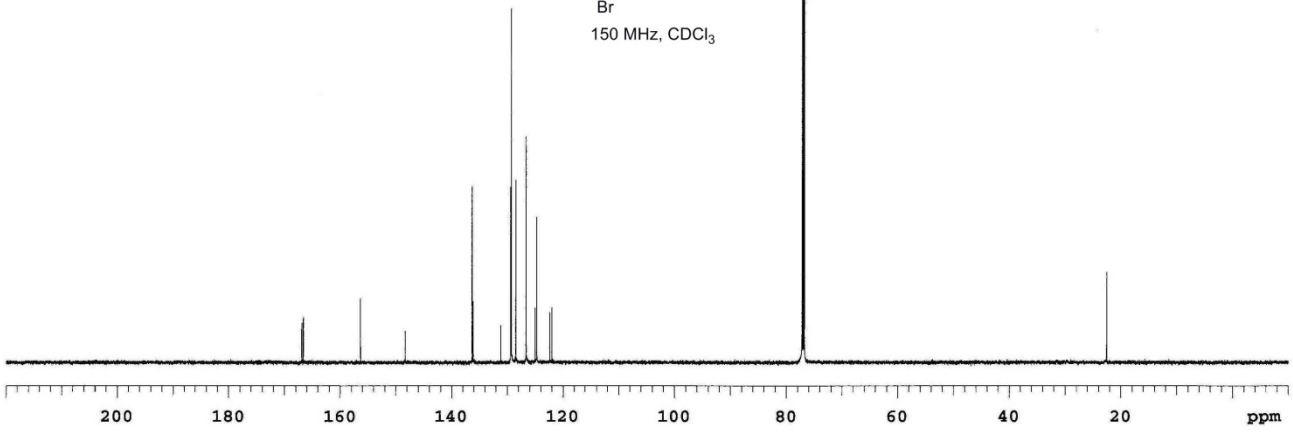
300 MHz, $CDCl_3$



^{13}C NMR of Compound **37**



150 MHz, $CDCl_3$



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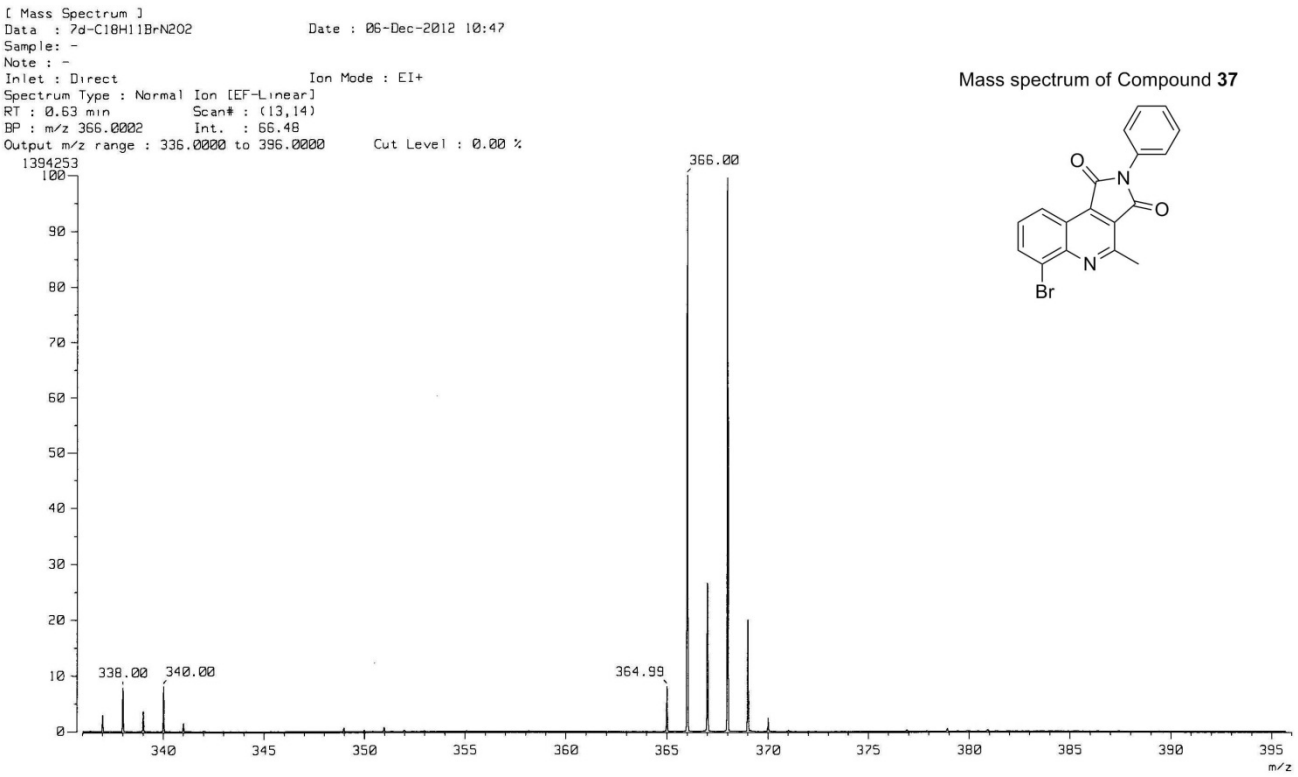

Mass spectrum of Compound **37**

[Elemental Composition] Page: 1

Data : 7d-C18H11BrN2O2 Date : 06-Dec-2012 10:47

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			

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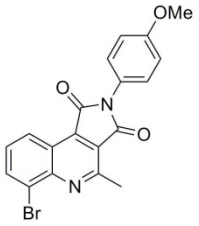
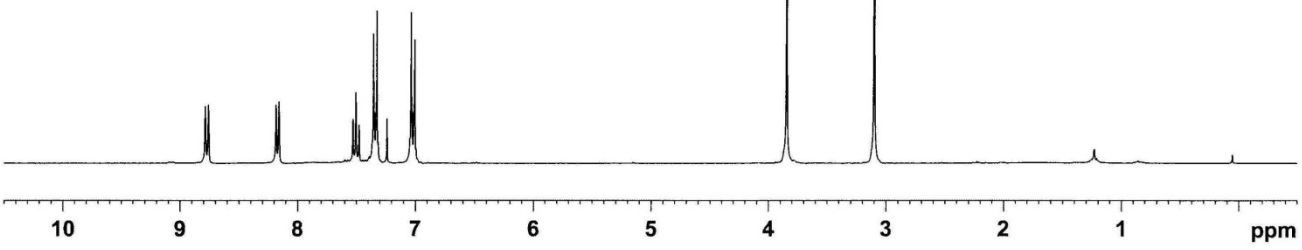
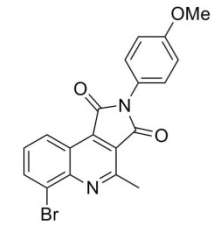
^{1}H NMR of Compound **38**



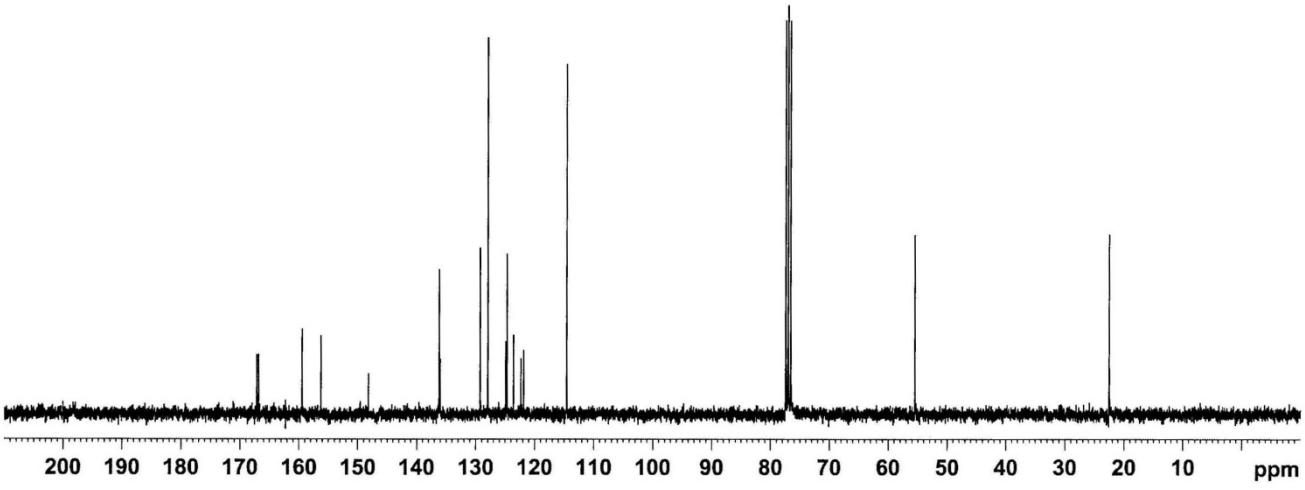
300 MHz, $CDCl_3$



^{13}C NMR of Compound **38**



75 MHz, $CDCl_3$



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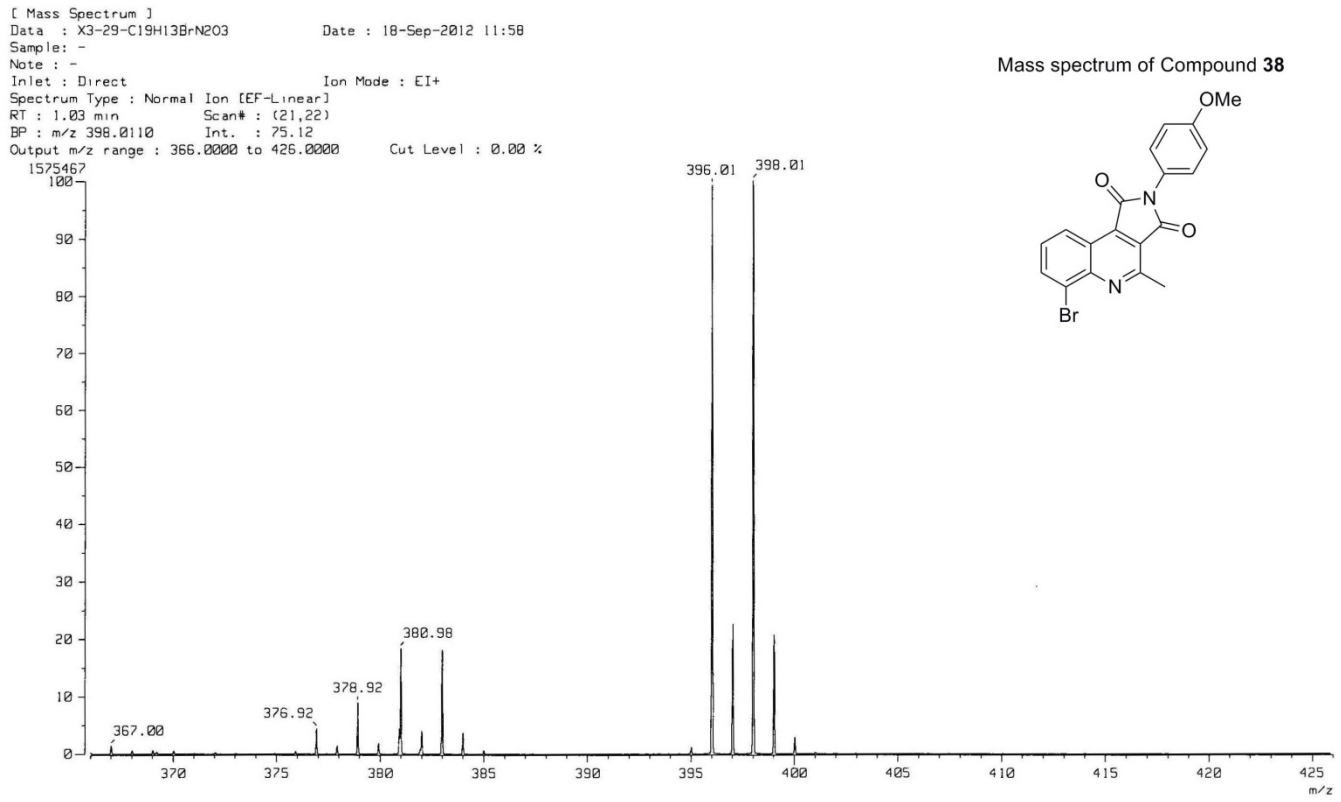

Mass spectrum of Compound **38**

[Elemental Composition] Page: 1
Data : X3-29-C19H13BrN2O3 Date : 18-Sep-2012 11:58
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			

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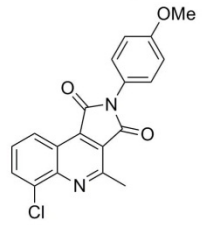
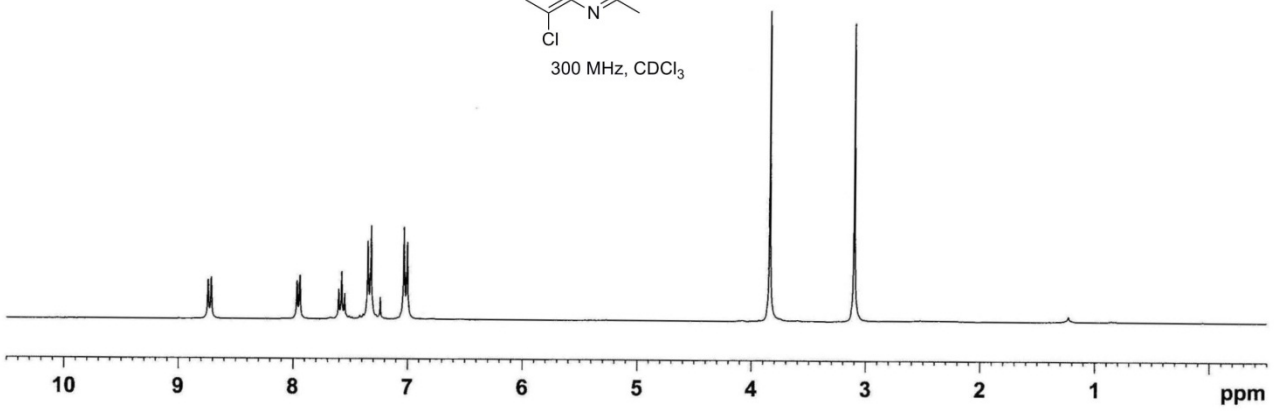
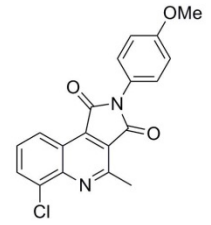
^{1}H NMR of Compound **39**



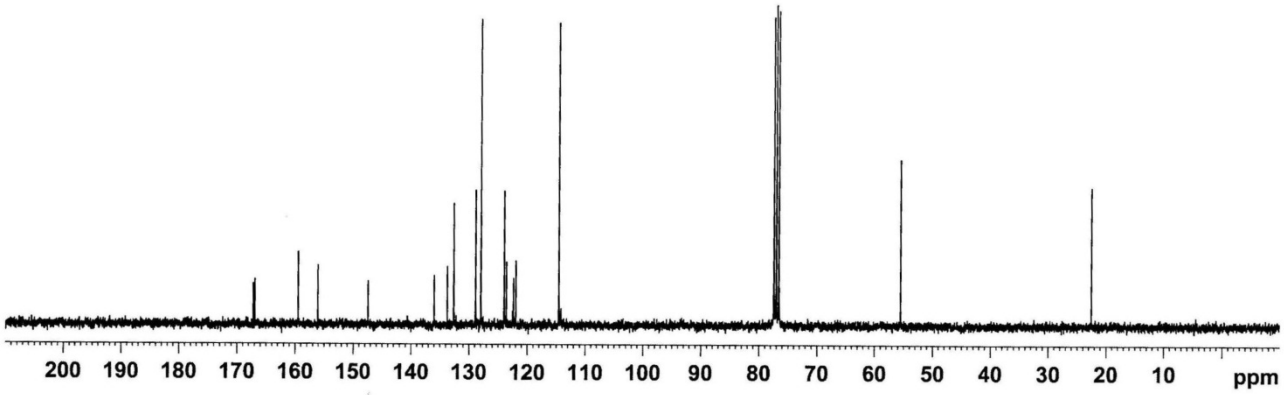
300 MHz, $CDCl_3$



^{13}C NMR of Compound **39**



75 MHz, $CDCl_3$



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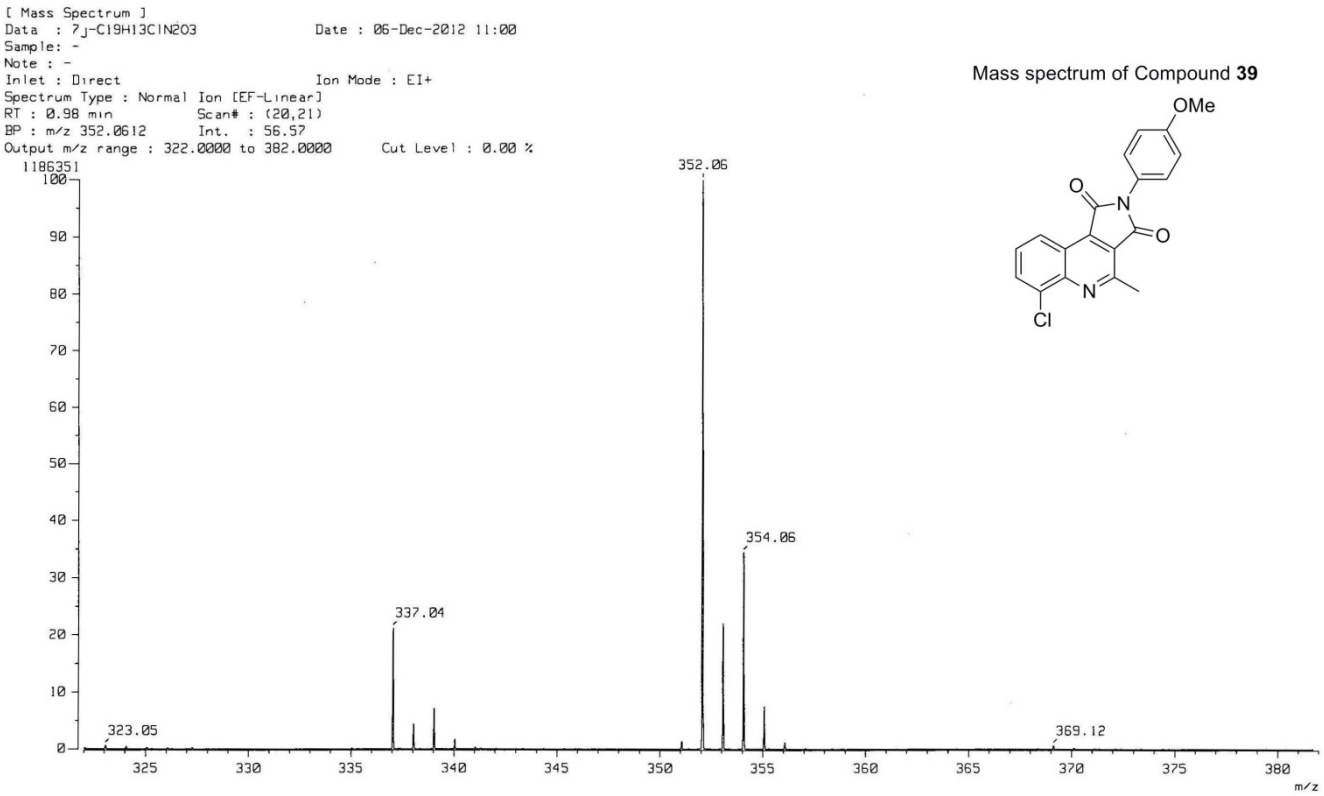

Mass spectrum of Compound **39**

[Elemental Composition] Page: 1
Data : 7j-C19H13ClN2O3 Date : 06-Dec-2012 11:00
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			

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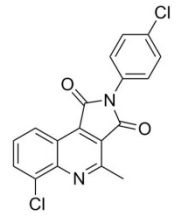
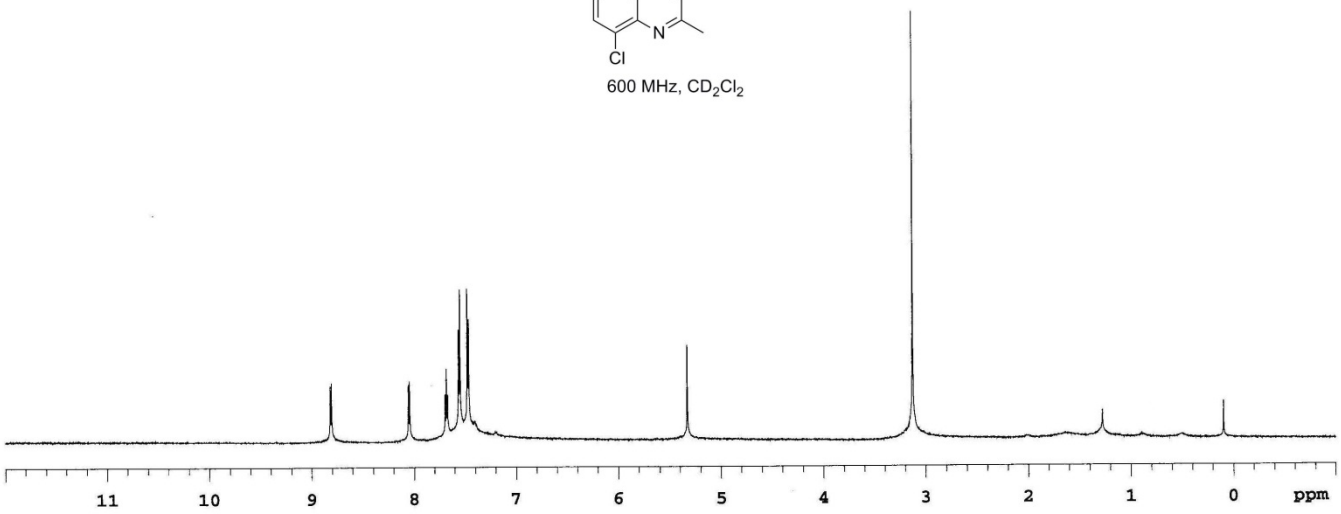
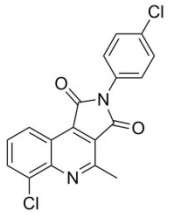
^{1}H NMR of Compound **40**



600 MHz, CD_2Cl_2



^{13}C NMR of Compound **40**



150 MHz, CD_2Cl_2

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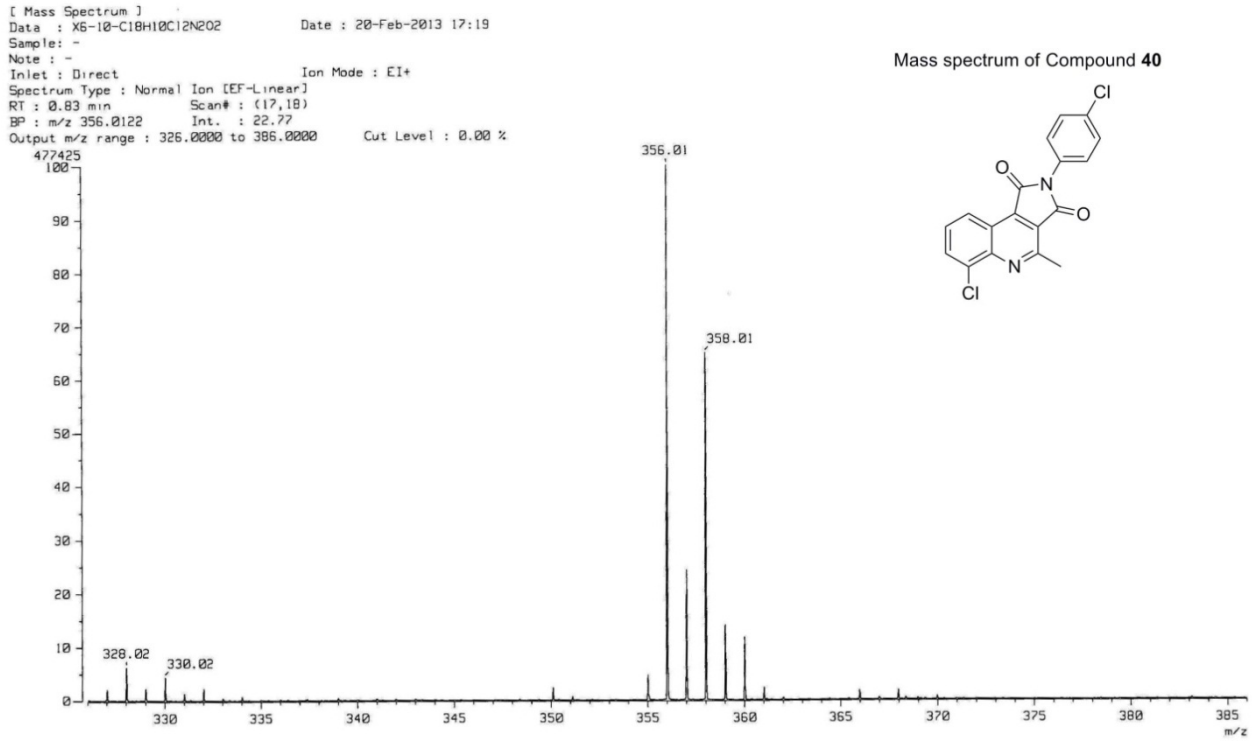

Mass spectrum of Compound **40**

Page: 1

[Elemental Composition]
Data : X6-10-C18H10Cl2N2O2 Date : 20-Feb-2013 17:19
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			

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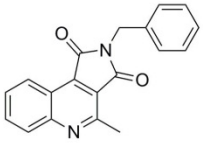
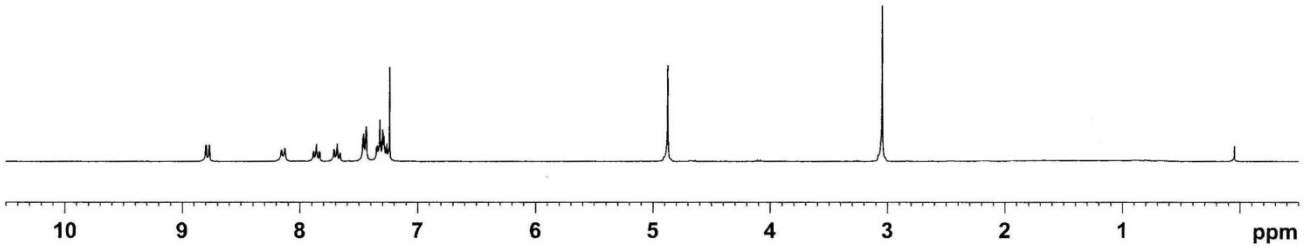
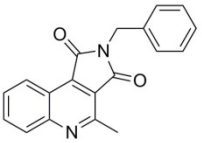
^{1}H NMR of Compound **41**



300 MHz, $CDCl_3$



^{13}C NMR of Compound **41**



75 MHz, $CDCl_3$

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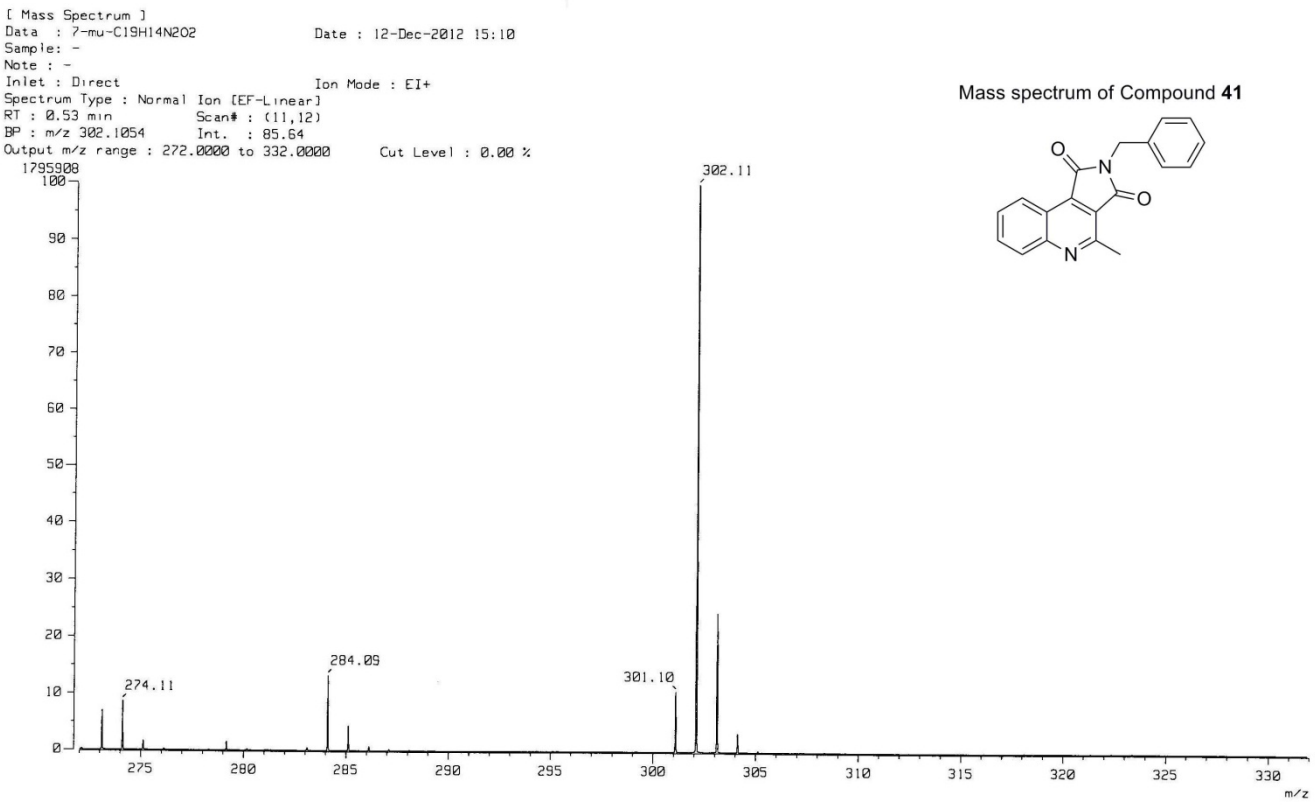

Mass spectrum of Compound **41**

[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			

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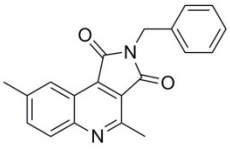
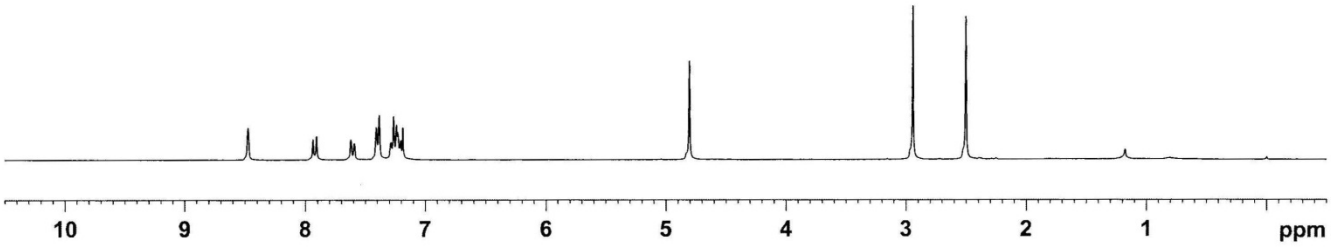
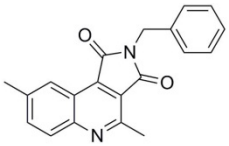
^{1}H NMR of Compound **42**



300 MHz, $CDCl_3$



^{13}C NMR of Compound **42**



75 MHz, $CDCl_3$

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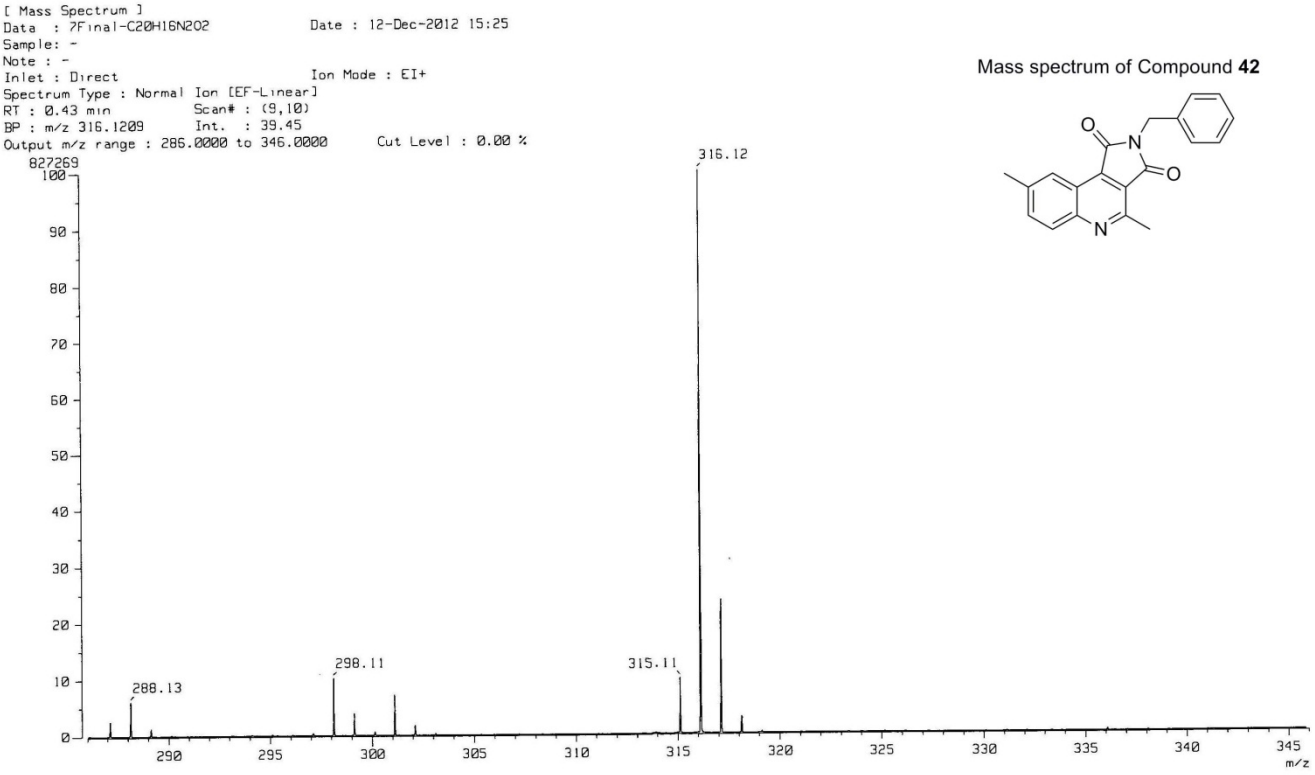

Mass spectrum of Compound **42**

[Elemental Composition] Page: 1

Data : 7Final-C20H16N2O2 Date : 12-Dec-2012 15:25
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			

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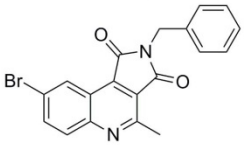
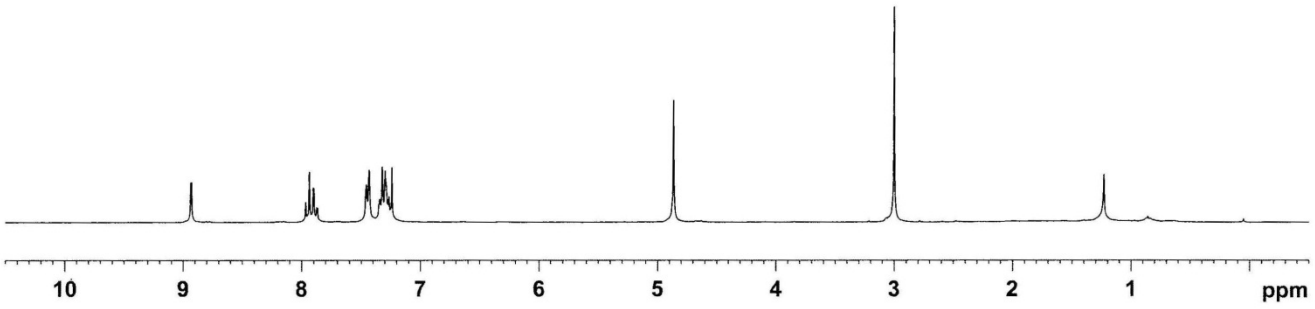
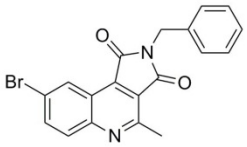
^{1}H NMR of Compound **43**



300 MHz, $CDCl_3$



^{13}C NMR of Compound **43**



75 MHz, $CDCl_3$

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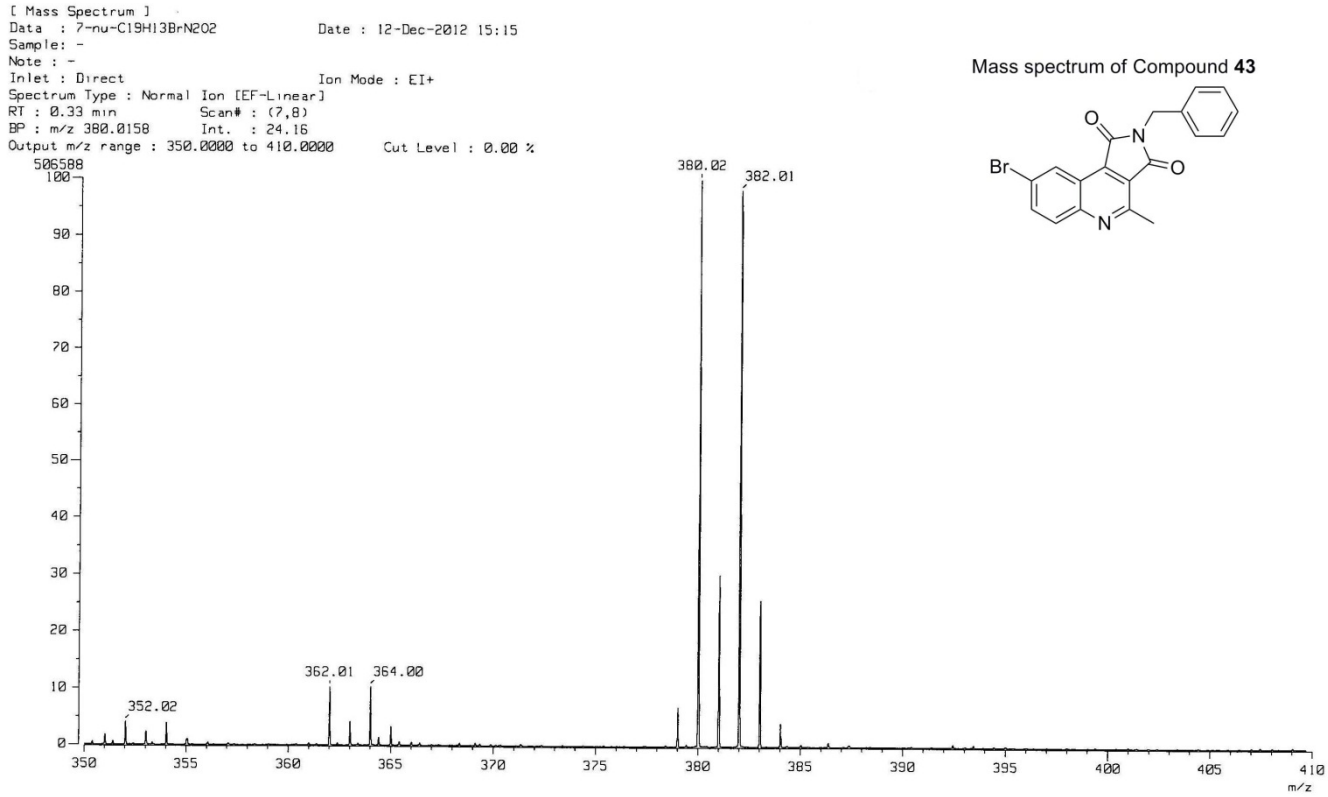

Mass spectrum of Compound **43**

[Elemental Composition] Page: 1
Data : 7-nu-C19H13BrN2O2 Date : 12-Dec-2012 15:15
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			

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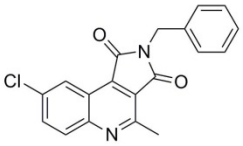
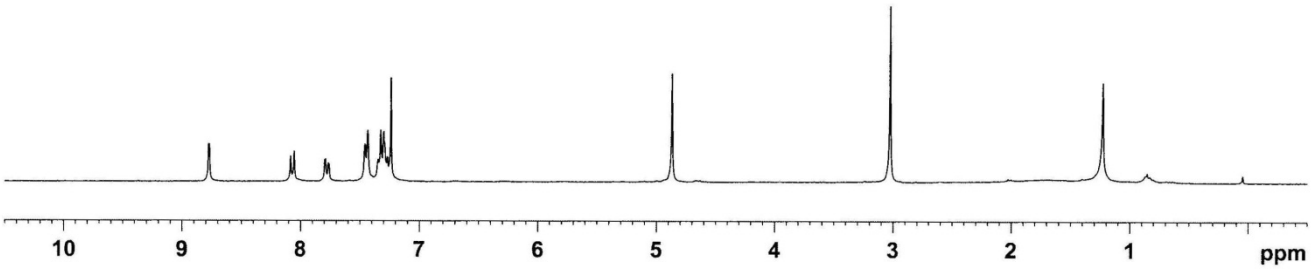
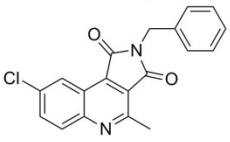
^{1}H NMR of Compound **44**



300 MHz, $CDCl_3$



^{13}C NMR of Compound **44**



75 MHz, $CDCl_3$

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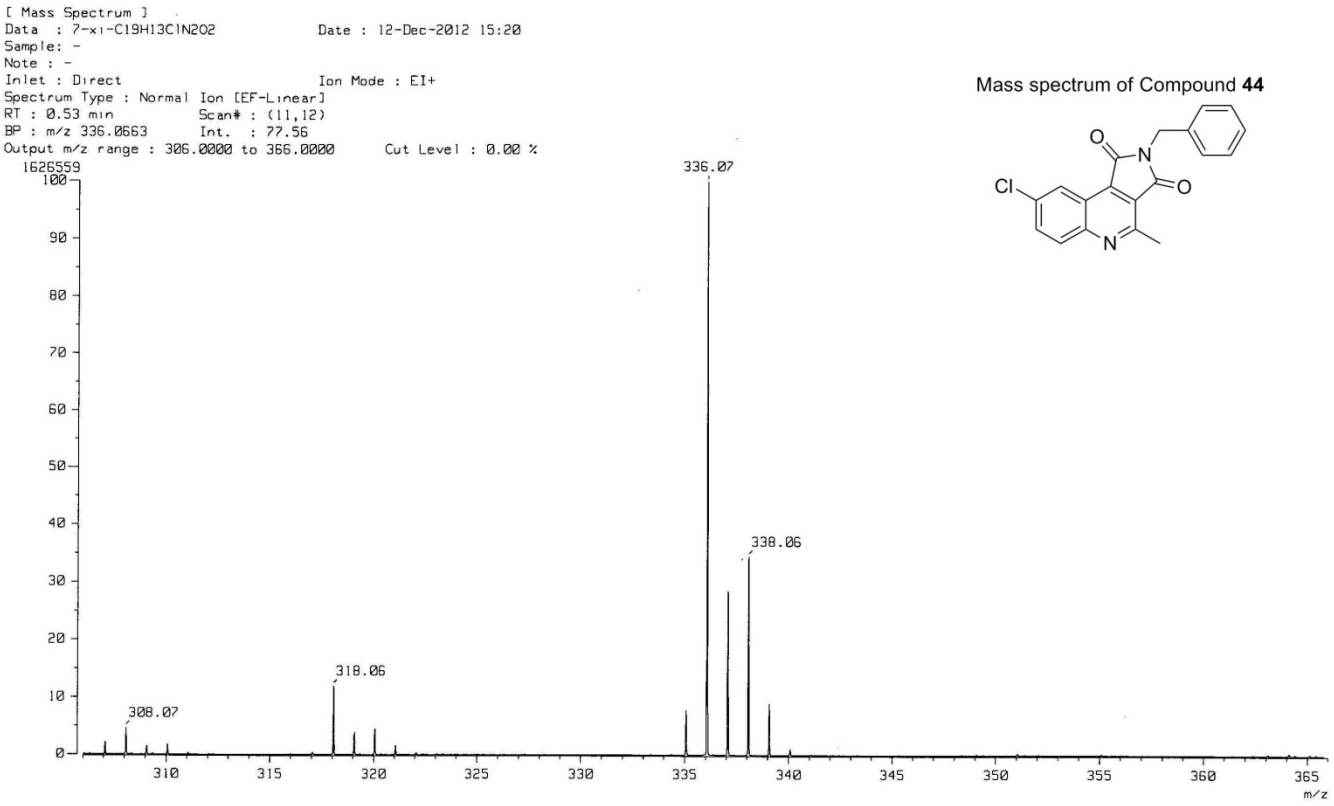
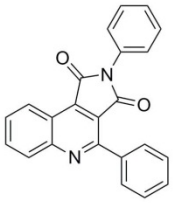


Mass spectrum of Compound **44**

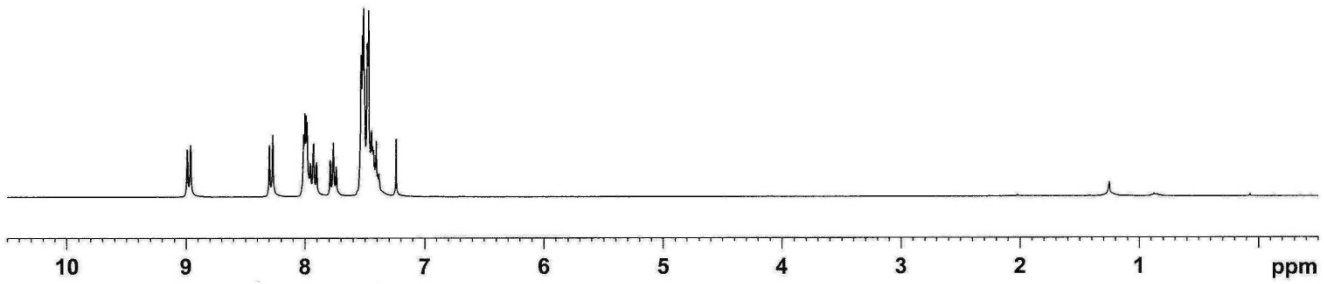
[Elemental Composition] Page: 1
Data : 7-xi-C19H13ClN2O2 Date : 12-Dec-2012 15:20
Sample: -
Note : -
Inlet : Direct Ion Mode : EI+
RT : 0.53 min Scan#: (11,12)
Elements : C 19/0, H 13/0, Cl 1/0, N 2/0, O 2/0
Mass Tolerance : 1000ppm, 2mmu if m/z < 2, 3mmu if m/z > 3
Unsaturation (U.S.) : -0.5 - 100.0

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			

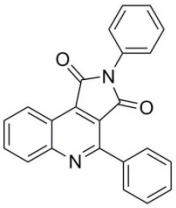
^{1}H NMR of Compound **45**



300 MHz, $CDCl_3$



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



150 MHz, $CDCl_3$

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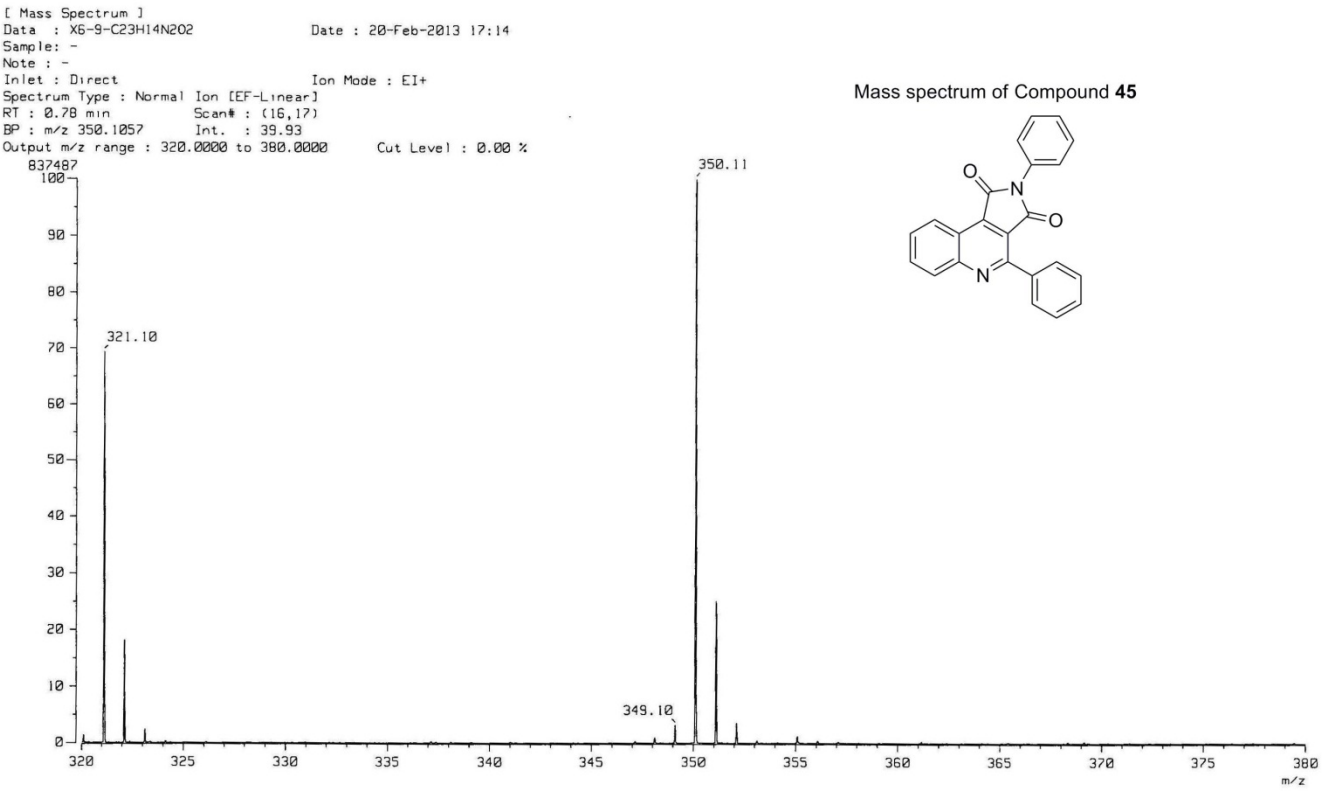

Mass spectrum of Compound **45**


```
[ Elemental Composition ]                                        Page: 1
Data  : X6-9-C23H14N2O2              Date : 20-Feb-2013 17:14
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
```

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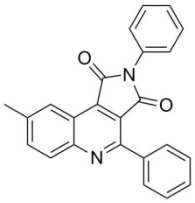
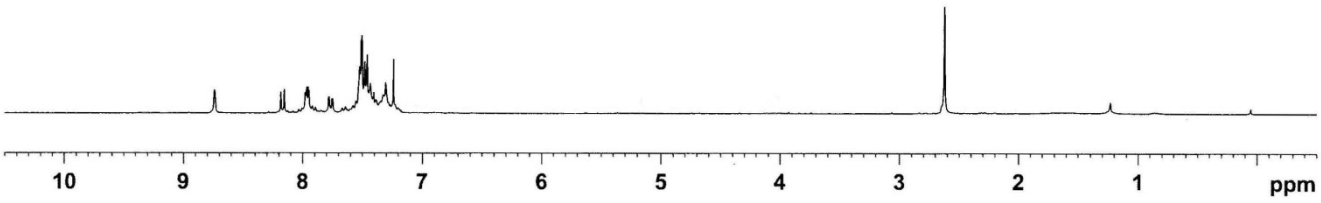
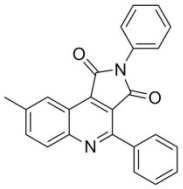
^{1}H NMR of Compound **46**



300 MHz, $CDCl_3$



^{13}C NMR of Compound **46**



150 MHz, $CDCl_3$

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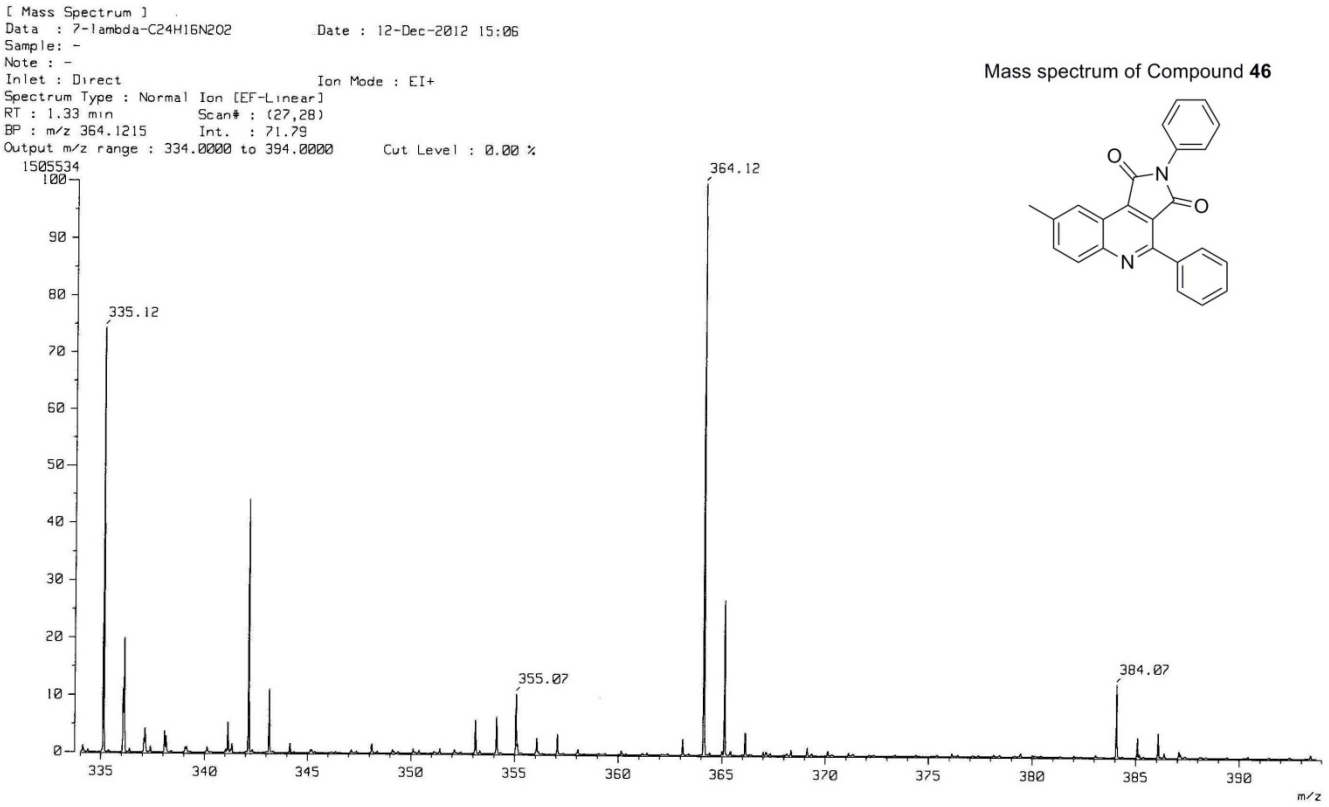

Mass spectrum of Compound **46**

[Elemental Composition] Page: 1

Data : 7-lambda-C24H16N2O2 Date : 12-Dec-2012 15:06
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			

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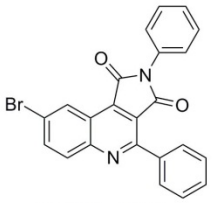
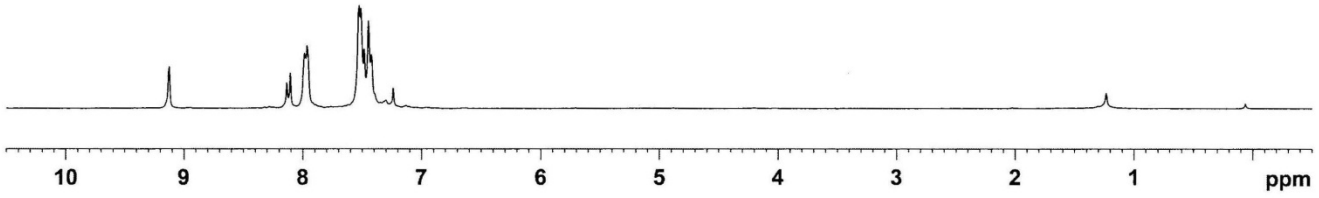
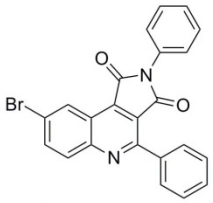
^{1}H NMR of Compound **47**



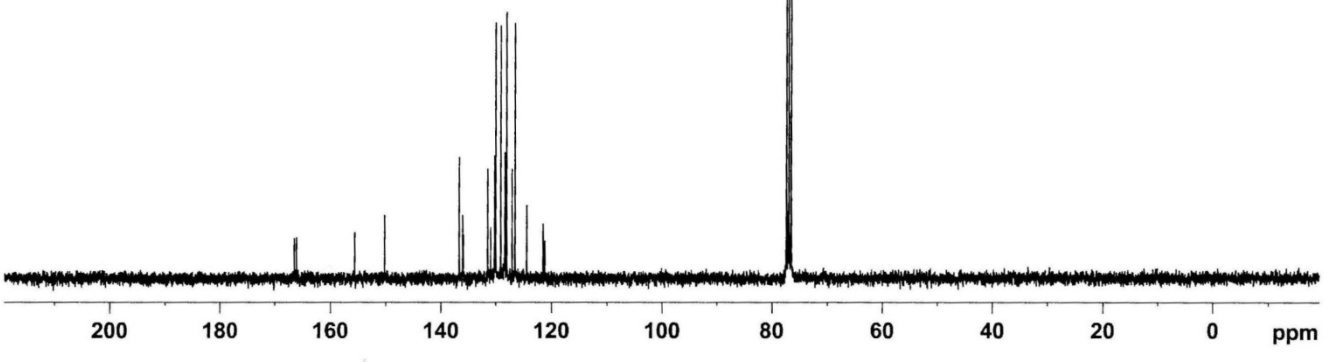
300 MHz, $CDCl_3$



^{13}C NMR of Compound **47**



75 MHz, $CDCl_3$



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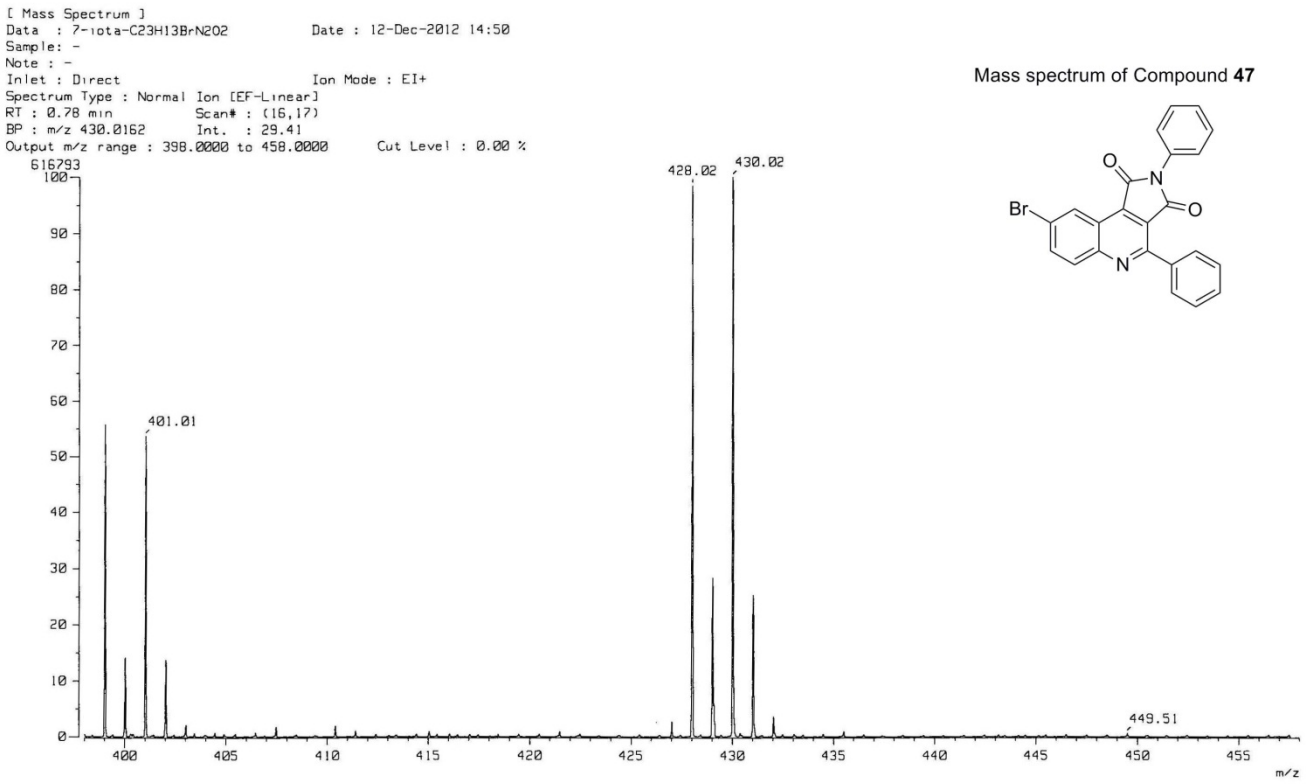

Mass spectrum of Compound **47**

[Elemental Composition] Page: 1
Data : 7-iota-C23H13BrN2O2 Date : 12-Dec-2012 14:50
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			

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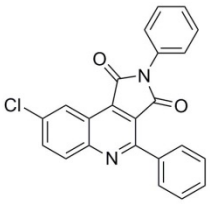
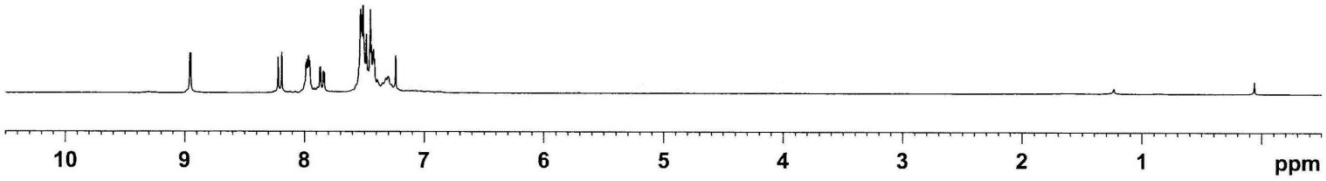
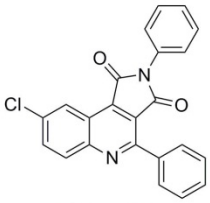
^{1}H NMR of Compound **48**



300 MHz, $CDCl_3$



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



75 MHz, $CDCl_3$

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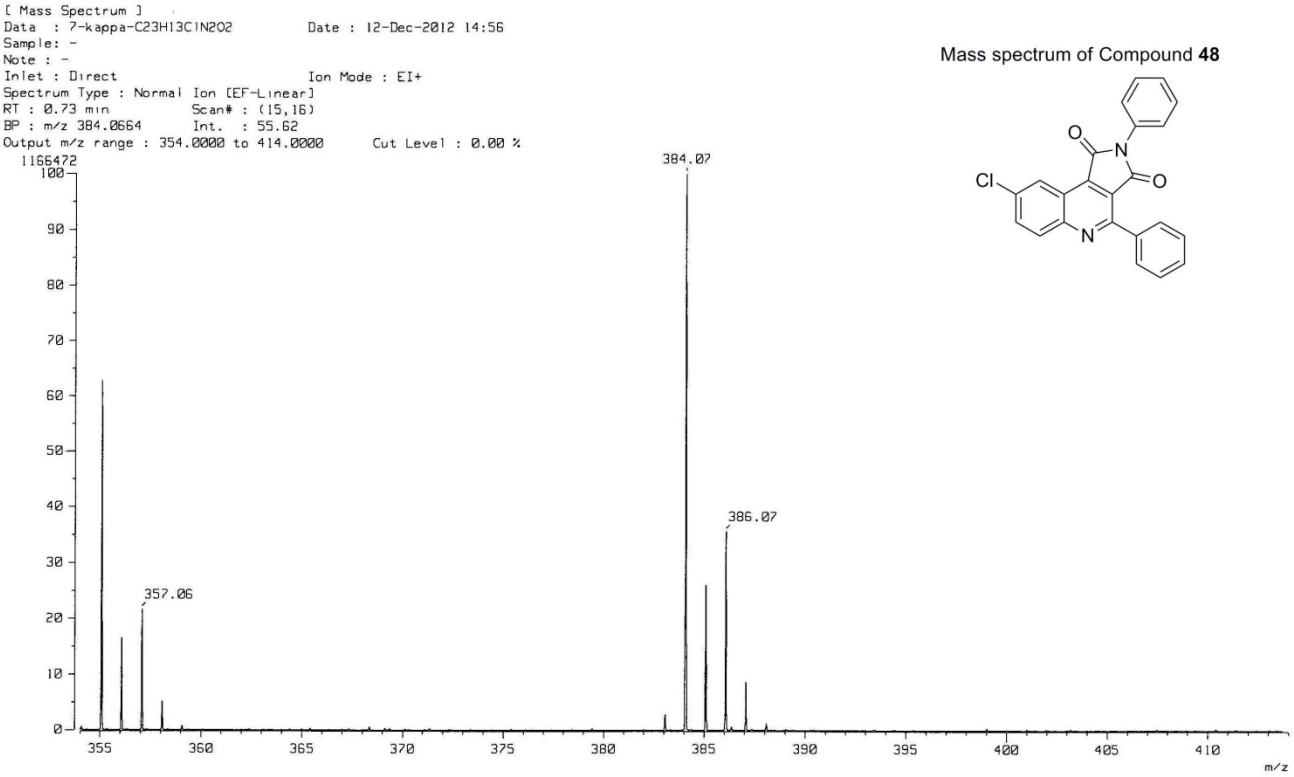

Mass spectrum of Compound **48**

[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			

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

Table 1. Crystal data and structure refinement for No10.

Identification code	No10	
Empirical formula	$C_{19}H_{13}ClN_2O_3$	
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 $e.Å^{-3}$	

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Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 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)

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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

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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)

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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: