Supporting Information

Cu-Catalyzed One-pot Synthesis of Fused oxazepinone derivatives *via* sp^2 C-H and O-H Cross-Dehydrogenative Coupling

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1. General information

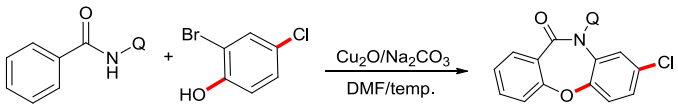
N-(quinolin-8-yl)benzamides were prepared according to literature procedures.[1-5] Other reagents were commercially available and were used without further purification. All reactions were monitored by thin-layer chromatography (TLC). ^{1}H NMR spectra were recorded on a Bruker Avance 300 spectrometer at 300 MHz, using $CDCl_3$, CD_2Cl_2 and DMSO-d_6 as solvent and tetramethylsilane (TMS) as internal standard. ^{13}C NMR spectra were run in the same instrument at 75 MHz. HRMS spectra were determined on a Q-TOF6510 spectrograph (Agilent).

2. General synthetic method of *N*-(quinolin-8-yl)benzamide[1-5]

To a solution of 8-aminoquinoline (1.00 g, 7 mmol) and Et_3N (1.1 mL, 8 mmol, 1.2 equiv) in anhydrous CH_2Cl_2 (10 mL) was cooled to 0 ℃. Benzoyl chloride (8 mmol) was added dropwise and reaction mixture was stirred at room temperature overnight. The mixture was quenched with water (15 mL) and extracted with CH_2Cl_2 (3×10 mL). Combined organic phase was dried over $MgSO_4$ and filtered, and concentrated in *vacuo*. The crude product was purified by flash chromatography on silica gel, eluting with EtOAc/hexanes to deliver the corresponding compound.

3. Optimization of Reaction Conditions

3.1 Screening of Temperature [a]

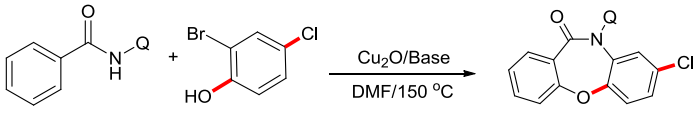


1 Q = Quinolin-8-yl **2** **3a**

Entry	temp. (^{o}C)	Yield (%)
1	110	47
2	120	78
3	130	84
4	140	90
5	160	83

[a] Reaction conditions: **1a** (0.2 mmol), **2a** (0.3 mmol), catalyst (10 mol %), Na_2CO_3 (3.5 equiv.), solvent (2 mL), in a sealed tube under air atmosphere for 6 h.

3.2 Screening of Base [a]



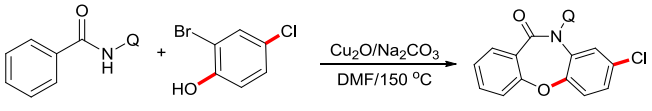
1 Q = Quinolin-8-yl **2** **3a**

Entry	**Base**	Yield (%)
1	$NaHCO_3$	N.R.
2	KOAc	N.R.
3	NaOAc	N.R.

4	DBU	N.R.
5	KOH	trace

[a] Reaction conditions: **1a** (0.2 mmol), **2a** (0.3 mmol), catalyst (10 mol %), base (3.5 equiv.), solvent (2 mL), in a sealed tube at 150 °C under air atmosphere for 6 h.

3.3 Screening of the Amount of Na_2CO_3[a]



1
Q = Quinolin-8-yl

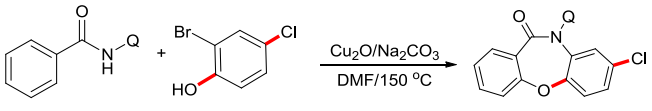
2

3a

Entry	**Na_2CO_3 (equiv.)**	Yield (%)
1	2.5	62
2	3.0	78
3	4.0	90

[a] Reaction conditions: **1a** (0.2 mmol), **2a** (0.3 mmol), catalyst (10 mol %), Na_2CO_3, solvent (2 mL), in a sealed tube at 150 °C under air atmosphere for 6 h.

3.4 Screening of the Amount of Na_2CO_3[a]



1
Q = Quinolin-8-yl

2

3a

Entry	**Compound 2 (equiv.)**	Yield (%)
1	1.0	78
2	1.2	87
3	1.5	90
4	1.7	89

[a] Reaction conditions: **1a** (0.2 mmol), **2a**, catalyst (10 mol %), Na_2CO_3 (3.5 equiv.), solvent (2 mL), in a sealed tube at 150 °C under air atmosphere for 6 h.

4. Comparison of Cu_2O and $Cu(OTf)_2$

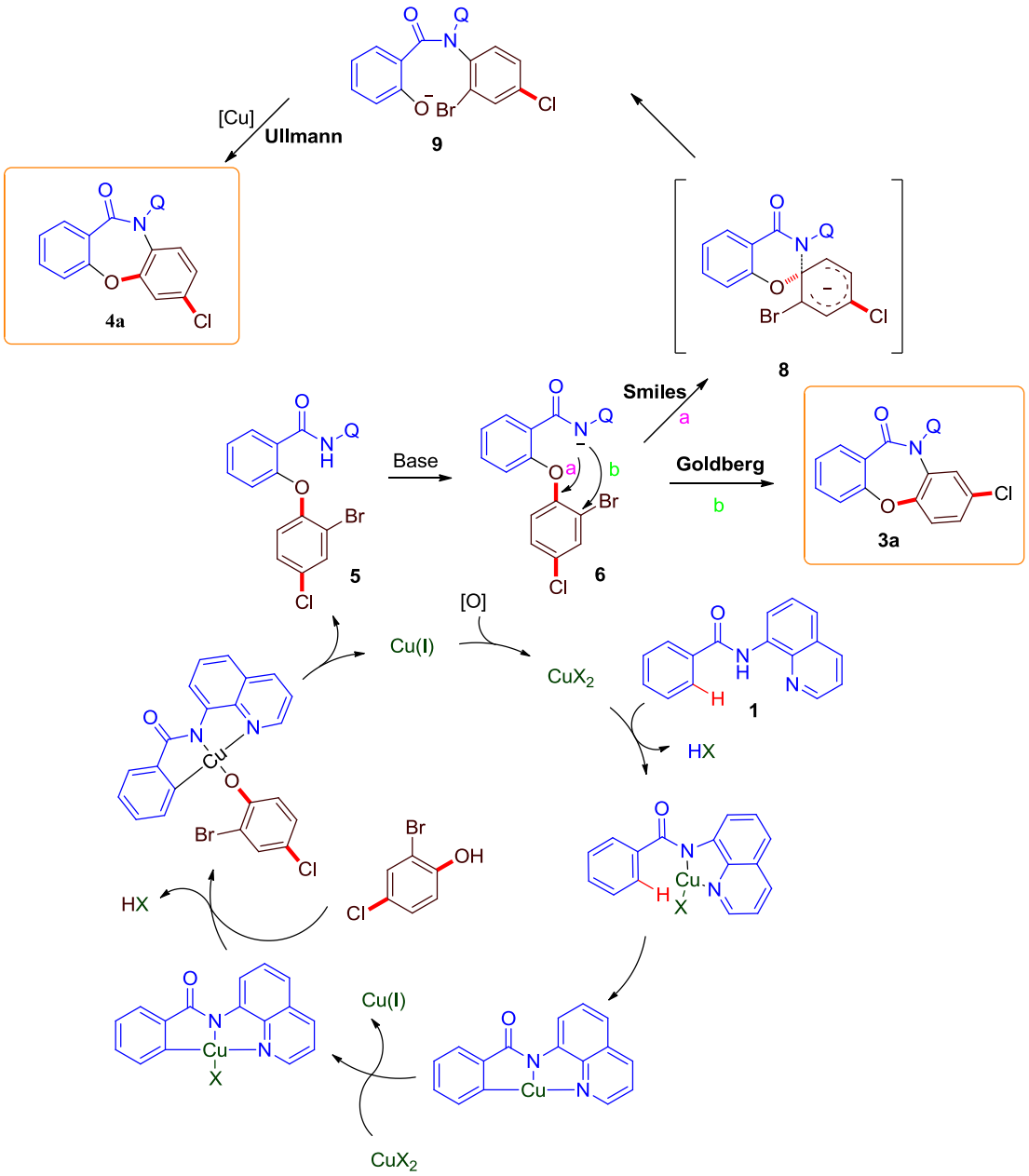
[Cu]	Brand	Purity	Quality	Price	Yield
Cu_2O	Adamas	99%	25 g	101.00 RMB	90% (10 mol% Cu_2O)
$Cu(OTf)_2$	Adamas	98%	25 g	1302.00 RMB	91% (20 mol% $Cu(OTf)_2$)

5. General experimental procedures for the synthesis of 3a

A sealable tube (10 mL) was charged with Cu_2O (3 mg, 0.050 mmol), Na_2CO_3 (75 mg, 0.70 mmol), *N*-(quinolin-8-yl)benzamide **1a** (50 mg, 0.20 mmol) and 2-bromo-4-chlorophenol **2a** (63 mg, 0.30 mmol). DMF (2 mL) was added and the tube sealed. The mixture was gradually heated to 150 ℃ for 6 h, cooled to room temperature. CH_2Cl_2 (60 mL) was added to dilute the mixture.

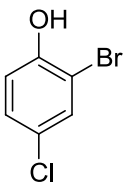
The combined organics were washed with saturated brine (25 mL), dried over $MgSO_4$, subjected to filtration, and concentrated in *vacuo*. The crude product was purified by flash chromatography on silica gel, eluting with EtOAc/hexanes to deliver the compound **3a**.

6. Plausible Mechanism of CDC-Smiles Rearrangement

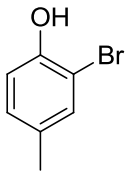


Scheme 1. Plausible Mechanism of CDC-Smiles Rearrangement

7. Substrate scope of compounds 2



2a



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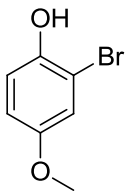

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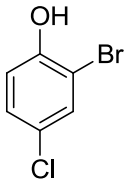
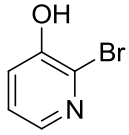


2d

2e



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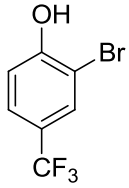

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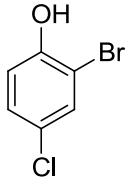
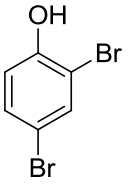
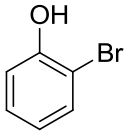


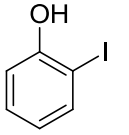
2h



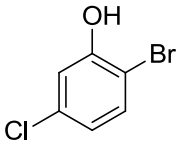
2i



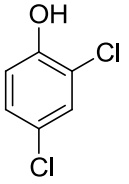
2j



2k



2l



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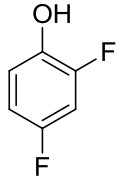


2n

8. The X-ray Crystallography Data of 4a and 3k[a]

4a (3i):

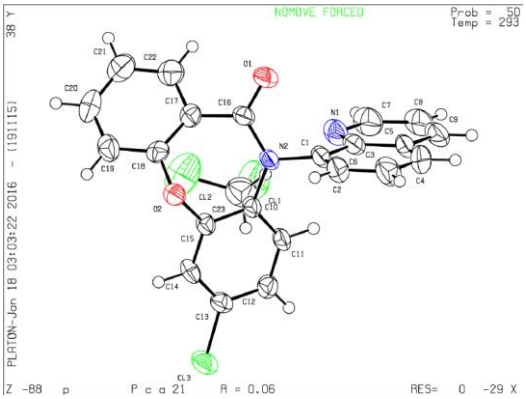


Table 1. Crystal data and structure refinement for **4a (3i)**

Bond precision:	C-C = 0.0086 A	Wavelength=0.71000	
Cell:	a=7.7032(10)	b=16.441(2)	c=14.9629(18)
	alpha=90	beta=90	gamma=90
Temperature:	293 K		
	Calculated	Reported	
Volume	1895.0(4)	1895.0(4)	
Space group	P c a 21	P c a 21	
Hall group	P 2c -2ac	P 2c -2ac	
Moiety formula	C22 H13 Cl N2 O2, C H2 Cl2	C22 H13 Cl N2 O2, C H2 Cl2	
Sum formula	C23 H15 Cl3 N2 O2	C23 H15 Cl3 N2 O2	
Mr	457.72	457.72	
Dx,g cm-3	1.604	1.604	
Z	4	4	
Mu (mm-1)	0.501	0.509	
F000	936.0	936.0	
F000'	938.09		
h,k,lmax	9,19,17	9,19,17	
Nref	3340[1745]	3058	
Tmin,Tmax			
Tmin'			
Correction method= Not given			
Data completeness= 1.75/0.92		Theta(max)= 25.000	
R(reflections)= 0.0629(2069)		wR2(reflections)= 0.1592(3058)	
S = 1.006	Npar= 271		

Table 2. Bond lengths [A] and angles [deg] for **4a**

C1	0.031(3)	0.027(2)	0.056(4)	0.004(2)	0.003(3)	0.006(2)
C2	0.048(4)	0.039(3)	0.054(4)	0.007(3)	-0.001(3)	0.007(3)
C3	0.059(5)	0.055(4)	0.063(5)	0.008(4)	-0.008(4)	0.016(3)

C4 0.065(5) 0.050(3) 0.063(5) 0.025(3) 0.006(4) 0.014(3)
C5 0.042(4) 0.028(2) 0.078(6) 0.011(3) 0.014(4) 0.009(2)
C6 0.032(3) 0.030(2) 0.065(5) 0.000(3) 0.009(3) 0.004(2)
C7 0.059(5) 0.044(3) 0.082(6) -0.015(3) 0.005(4) -0.008(3)
C8 0.061(5) 0.029(3) 0.120(8) -0.018(4) 0.027(5) -0.012(3)
C9 0.052(4) 0.028(3) 0.110(7) 0.001(3) 0.025(5) 0.005(2)
C10 0.027(3) 0.023(2) 0.047(3) 0.003(2) 0.002(2) -0.001(2)
C11 0.037(3) 0.020(2) 0.055(4) 0.004(2) 0.004(3) 0.003(2)
C12 0.034(3) 0.035(2) 0.053(4) 0.010(3) 0.003(3) -0.002(2)
C13 0.029(3) 0.037(2) 0.047(4) 0.001(3) 0.002(3) 0.006(2)
C14 0.033(3) 0.027(2) 0.046(4) 0.001(2) -0.010(3) 0.007(2)
C15 0.026(3) 0.022(2) 0.047(3) 0.001(2) -0.002(2) -0.0040(19)
C16 0.028(3) 0.028(2) 0.053(4) -0.003(2) 0.008(3) 0.001(2)
C17 0.032(3) 0.030(2) 0.044(4) 0.000(2) -0.001(3) -0.008(2)
C18 0.026(3) 0.035(3) 0.041(4) -0.001(2) 0.001(3) -0.009(2)
C19 0.045(4) 0.031(2) 0.065(5) 0.004(3) -0.003(3) -0.003(2)
C20 0.070(5) 0.052(3) 0.055(5) 0.021(3) -0.002(4) -0.014(3)
C21 0.065(5) 0.059(4) 0.053(5) 0.001(3) 0.011(4) -0.011(3)
C22 0.049(4) 0.043(3) 0.057(5) -0.006(3) 0.005(3) -0.008(2)
C23 0.074(6) 0.074(4) 0.059(5) -0.008(4) -0.001(4) 0.009(4)
Cl1 0.140(2) 0.0577(9) 0.0746(15) -0.0117(9) 0.0048(14) -0.0135(10)
Cl2 0.113(2) 0.1012(14) 0.0857(17) 0.0038(13) -0.0159(14) -0.0485(13)
Cl3 0.0337(8) 0.0461(7) 0.0897(13) 0.0057(8) 0.0083(9) 0.0105(6)
N1 0.051(3) 0.030(2) 0.066(4) -0.007(2) 0.003(3) -0.0010(19)
N2 0.028(2) 0.0218(17) 0.050(3) 0.0015(18) 0.004(2) 0.0026(15)
O1 0.033(2) 0.0427(18) 0.069(3) 0.0040(19) 0.013(2) 0.0082(18)
O2 0.028(2) 0.0262(15) 0.058(3) -0.0035(17) 0.0045(18) -0.0065(14)

3k:

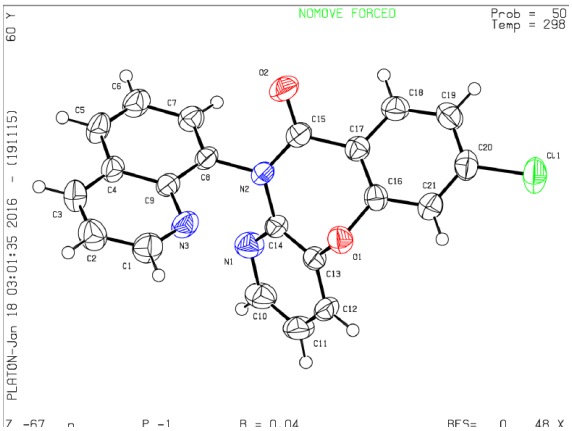


Table 1. Crystal data and structure refinement for **3k**

```
Bond precision:  C-C = 0.0030 A          Wavelength=0.71000

Cell:         a=7.1470(16)      b=7.9449(18)     c=16.405(4)
              alpha=101.767(2)  beta=96.018(2)   gamma=106.7307(18)
Temperature:  298 K

                Calculated                Reported
Volume          859.9(3)                  860.0(3)
Space group     P -1                      P -1
Hall group      -P 1                      -P 1
Moiety formula  C21 H12 Cl N3 O2          C21 H12 Cl N3 O2
Sum formula     C21 H12 Cl N3 O2          C21 H12 Cl N3 O2
Mr              373.79                    373.79
Dx,g cm-3       1.444                     1.444
Z               2                         2
Mu (mm-1)       0.240                     0.244
F000            384.0                     384.0
F000'           384.44
h,k,lmax        8,9,19                    8,9,19
Nref            3047                      3034
Tmin,Tmax       0.978,0.981
Tmin'           0.978

Correction method= Not given

Data completeness= 0.996          Theta(max)= 24.993

R(reflections)= 0.0422( 2419)     wR2(reflections)= 0.1550( 3034)

S = 1.160                 Npar= 244
```

Table 2. Bond lengths [A] and angles [deg] for **3k**

C1	0.0795(17)	0.0436(13)	0.0573(15)	0.0178(11)	0.0086(12)	0.0242(12)
C2	0.0733(16)	0.0620(15)	0.0461(13)	0.0180(11)	0.0107(11)	0.0286(13)
C3	0.0627(14)	0.0519(13)	0.0406(12)	0.0005(10)	0.0101(10)	0.0234(11)
C4	0.0414(11)	0.0356(11)	0.0424(11)	0.0025(8)	0.0105(9)	0.0139(8)
C5	0.0653(14)	0.0332(11)	0.0522(13)	-0.0023(9)	0.0088(11)	0.0213(10)
C6	0.0634(14)	0.0327(11)	0.0569(14)	0.0093(10)	0.0090(11)	0.0200(10)
C7	0.0459(12)	0.0357(11)	0.0460(12)	0.0100(9)	0.0072(9)	0.0122(9)
C8	0.0345(10)	0.0283(10)	0.0414(11)	0.0016(8)	0.0058(8)	0.0042(8)
C9	0.0335(10)	0.0306(10)	0.0418(11)	0.0052(8)	0.0081(8)	0.0082(8)
C10	0.0382(11)	0.0613(15)	0.0606(14)	0.0204(11)	0.0127(10)	0.0080(10)
C11	0.0501(13)	0.0549(15)	0.0532(14)	0.0171(11)	0.0044(11)	-0.0083(11)
C12	0.0762(15)	0.0282(10)	0.0380(11)	0.0078(9)	0.0050(11)	0.0004(10)
C13	0.0478(11)	0.0340(10)	0.0304(10)	0.0096(8)	0.0057(8)	0.0101(9)
C14	0.0371(10)	0.0336(10)	0.0330(10)	0.0064(8)	0.0031(8)	0.0046(8)
C15	0.0430(11)	0.0355(11)	0.0469(12)	0.0061(9)	0.0080(9)	0.0073(9)
C16	0.0408(10)	0.0414(11)	0.0342(10)	0.0085(8)	0.0047(8)	0.0152(9)
C17	0.0354(10)	0.0387(11)	0.0415(11)	0.0076(8)	0.0055(8)	0.0108(8)
C18	0.0406(11)	0.0437(12)	0.0522(13)	0.0133(10)	0.0127(10)	0.0097(9)
C19	0.0424(12)	0.0594(14)	0.0405(11)	0.0130(10)	0.0119(9)	0.0135(10)

C20	0.0404(11) 0.0540(13) 0.0406(12) -0.0031(10) 0.0050(9) 0.0129(10)
C21	0.0490(12) 0.0378(11) 0.0459(12) 0.0057(9) 0.0069(10) 0.0136(9)
Cl1	0.0830(5) 0.0703(5) 0.0515(4) -0.0133(3) 0.0187(3) 0.0148(4)
N1	0.0429(10) 0.0476(11) 0.0573(11) 0.0140(9) 0.0129(8) 0.0114(8)
N2	0.0392(9) 0.0284(8) 0.0406(9) 0.0018(7) 0.0079(7) 0.0044(7)
N3	0.0589(11) 0.0307(9) 0.0513(11) 0.0087(8) 0.0062(8) 0.0140(8)
O1	0.0605(9) 0.0417(8) 0.0394(8) 0.0139(6) 0.0114(7) 0.0220(7)
O2	0.0591(10) 0.0431(9) 0.0822(12) -0.0054(8) 0.0324(9) -0.0078(8)

3q:

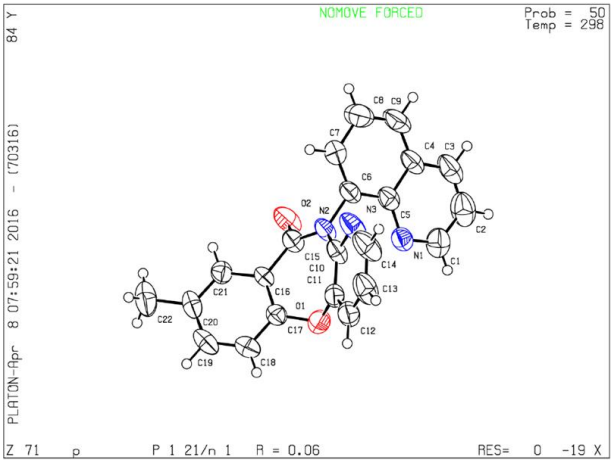


Table 1. Crystal data and structure refinement for **3q**

```
Bond precision:  C-C = 0.0059 A          Wavelength=0.71000

Cell:            a=7.928(2)     b=17.102(5)         c=25.464(7)
                 alpha=90       beta=91.235(3)      gamma=90
Temperature:     298 K

                Calculated                Reported
Volume          3451.7(16)                3451.7(16)
Space group     P 21/n                    P 1 21/n 1
Hall group      -P 2yn                    -P 2yn
Moiety formula  C22 H15 N3 O2             2(C22 H15 N3 O2)
Sum formula     C22 H15 N3 O2             C44 H30 N6 O4
Mr              353.37                    706.74
Dx,g cm-3       1.360                     1.360
Z               8                         4
Mu (mm-1)       0.088                     0.090
F000            1472.0                    1472.0
F000'           1472.58
h,k,lmax        9,20,30                   9,20,30
Nref            6106                      6090
Tmin,Tmax       0.984,0.991               0.982,0.991
Tmin'           0.982

Correction method= # Reported T Limits: Tmin=0.982 Tmax=0.991
AbsCorr = ?

Data completeness= 0.997          Theta(max)= 25.000

R(reflections)= 0.0605( 2522)     wR2(reflections)= 0.1570( 6090)

S = 0.959                 Npar= 489
```

Table 2. Bond lengths [A] and angles [deg] for **3q**

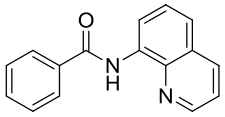
O1	0.0704(19)	0.0588(19)	0.0491(18)	0.0037(15)	0.0003(14)	-0.0071(16)
O2	0.068(2)	0.0441(18)	0.113(3)	-0.0108(16)	0.0340(19)	-0.0044(15)
N1	0.054(2)	0.044(2)	0.062(2)	0.0026(19)	0.0088(18)	-0.0011(17)
N2	0.055(2)	0.0297(19)	0.072(2)	-0.0012(17)	0.0139(18)	0.0001(17)
N3	0.062(3)	0.040(2)	0.120(3)	-0.005(2)	0.017(2)	-0.008(2)
C1	0.072(3)	0.072(4)	0.079(4)	0.016(3)	0.005(3)	0.006(3)
C2	0.074(4)	0.076(4)	0.117(5)	0.028(4)	0.019(3)	0.020(3)
C3	0.074(3)	0.042(3)	0.120(5)	0.005(3)	0.030(3)	0.010(3)
C4	0.055(3)	0.034(3)	0.085(4)	-0.004(3)	0.020(3)	0.003(2)
C5	0.043(2)	0.040(3)	0.068(3)	0.001(2)	0.014(2)	-0.008(2)
C6	0.058(3)	0.033(2)	0.065(3)	-0.003(2)	0.012(2)	-0.003(2)
C7	0.088(3)	0.049(3)	0.062(3)	0.005(2)	0.004(3)	0.005(3)
C8	0.102(4)	0.066(4)	0.082(4)	-0.021(3)	0.019(3)	-0.006(3)
C9	0.085(4)	0.042(3)	0.101(4)	-0.017(3)	0.027(3)	0.005(3)
C10	0.050(3)	0.032(2)	0.073(3)	0.004(2)	0.007(2)	0.004(2)
C11	0.058(3)	0.043(3)	0.052(3)	0.009(2)	0.006(2)	0.001(2)
C12	0.076(3)	0.049(3)	0.070(3)	0.008(2)	0.023(3)	0.006(3)
C13	0.066(3)	0.055(3)	0.122(5)	0.014(3)	0.033(3)	0.002(3)
C14	0.064(3)	0.049(3)	0.138(5)	-0.006(3)	0.024(3)	-0.011(3)
C15	0.054(3)	0.041(3)	0.061(3)	0.000(2)	0.004(2)	-0.001(2)
C16	0.044(2)	0.029(2)	0.052(3)	-0.0034(19)	-0.001(2)	-0.0006(18)
C17	0.046(2)	0.040(3)	0.050(3)	-0.001(2)	-0.003(2)	-0.0014(19)
C18	0.060(3)	0.047(3)	0.067(3)	-0.013(2)	-0.003(2)	0.001(2)
C19	0.058(3)	0.034(3)	0.094(4)	-0.008(3)	-0.021(3)	0.005(2)
C20	0.048(3)	0.039(3)	0.074(3)	0.013(2)	-0.024(2)	-0.008(2)
C21	0.054(3)	0.046(3)	0.050(3)	0.002(2)	-0.008(2)	-0.010(2)
C22	0.098(4)	0.064(3)	0.104(4)	0.032(3)	-0.027(3)	-0.023(3)
O3	0.069(2)	0.0399(17)	0.103(3)	0.0006(16)	0.0269(18)	0.0035(15)
O4	0.081(2)	0.0565(19)	0.0496(18)	-0.0029(15)	-0.0081(15)	0.0044(16)
N4	0.046(2)	0.047(2)	0.053(2)	0.0029(19)	0.0012(17)	0.0004(16)
N5	0.057(2)	0.040(2)	0.114(3)	-0.004(2)	0.013(2)	0.0092(19)
N6	0.055(2)	0.0279(19)	0.057(2)	-0.0052(16)	0.0010(17)	-0.0003(16)
C23	0.052(3)	0.034(2)	0.051(3)	-0.002(2)	0.000(2)	0.004(2)
C24	0.093(3)	0.040(3)	0.059(3)	-0.007(2)	-0.012(2)	0.004(2)
C25	0.119(4)	0.043(3)	0.050(3)	0.007(2)	0.001(3)	0.012(3)
C26	0.085(3)	0.037(3)	0.069(3)	0.003(2)	0.020(3)	0.004(2)
C27	0.046(2)	0.034(2)	0.061(3)	-0.008(2)	0.009(2)	-0.0010(19)
C28	0.038(2)	0.032(2)	0.058(3)	-0.007(2)	0.006(2)	0.0025(18)
C29	0.055(3)	0.044(3)	0.084(4)	-0.011(3)	0.011(3)	-0.017(2)
C30	0.068(3)	0.065(3)	0.074(4)	-0.015(3)	-0.012(3)	-0.017(3)
C31	0.060(3)	0.074(3)	0.054(3)	-0.004(3)	-0.007(2)	-0.002(3)
C32	0.062(3)	0.056(3)	0.146(5)	-0.009(3)	0.021(3)	0.011(3)
C33	0.083(4)	0.052(3)	0.142(5)	-0.028(3)	0.043(4)	-0.007(3)

C34	0.089(4)	0.055(3)	0.074(3)	-0.018(3)	0.022(3)	-0.011(3)
C35	0.066(3)	0.044(3)	0.053(3)	-0.012(2)	0.000(2)	-0.002(2)
C36	0.051(3)	0.029(2)	0.068(3)	-0.015(2)	0.003(2)	-0.002(2)
C37	0.050(3)	0.036(3)	0.060(3)	-0.002(2)	-0.001(2)	0.009(2)
C38	0.046(2)	0.024(2)	0.059(3)	-0.004(2)	-0.007(2)	0.0042(18)
C39	0.046(2)	0.044(3)	0.056(3)	-0.001(2)	-0.009(2)	0.003(2)
C40	0.063(3)	0.040(3)	0.074(3)	0.011(2)	-0.002(2)	-0.001(2)
C41	0.056(3)	0.031(2)	0.100(4)	0.004(3)	0.001(3)	-0.001(2)
C42	0.057(3)	0.035(3)	0.083(4)	-0.014(2)	0.004(2)	-0.003(2)
C43	0.050(3)	0.043(3)	0.071(3)	-0.005(2)	0.006(2)	0.004(2)
C44	0.128(5)	0.055(3)	0.129(5)	-0.037(3)	0.035(4)	-0.006(3)

[a] **4a**: CCDC 1449079; **3k**: CCDC 1449087; **3q**: CCDC 1473081. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www. ccdc.cam.ac.uk/data_request/cif.

9. Spectra data

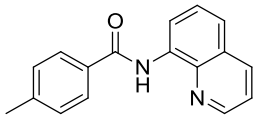
***N*-(quinolin-8-yl)benzamide** (**1a**)



This compound is known.[1, 5]

^{1}H NMR (300 MHz, $CDCl_3$): δ 10.75 (1H, s), 8.96 (1H, *J* = 7.5, 1.8 Hz, dd), 8.85 (1H, *J* = 4.2, 1.5 Hz, dd), 8.19 (1H, *J* = 8.4, 1.8 Hz, dd), 8.12-8.07 (2H, m), 7.62-7.51 (5H, m), 7.49 (1H, *J* = 8.4, 1.5 Hz, dd),; ^{13}C NMR (75 MHz, $CDCl_3$): δ 165.5, 148.3, 138.8, 136.5, 135.2, 134.6, 131.9, 128.8, 128.0, 127.5, 127.3, 121.7, 116.2; HRMS calcd for $C_{16}H_{12}N_2O$ $(M+H)^+$ 249.1022; found: 249.1021.

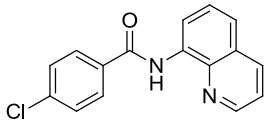
4-Methyl-*N*-(quinolin-8-yl)benzamide (**1b**)



This compound is known.[1, 5]

^{1}H NMR (400 MHz, $CDCl_3$): δ 10.72 (1H, s), 8.95 (1H, *J* = 7.6, 1.3 Hz, dd), 8.85 (1H, *J* = 4.2, 1.6 Hz, dd), 8.19 (1H, *J* = 8.2, 1.2 Hz, dd), 8.00 (1H, *J* = 8.2 Hz, d), 7.61-7.52 (2H, m), 7.49 (1H, *J* = 8.2, 4.2 Hz, dd), 7.35 (1H, *J* = 8.0 Hz, d), 2.45 (3H, s); ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.5, 148.2, 142.3, 138.8, 136.5, 134.7, 132.4, 129.5, 128.0, 127.5, 127.3, 121.7, 121.5, 116.6, 21.6; HRMS calcd for $C_{17}H_{14}N_2O$ $(M+H)^+$ 263.1179; found: 263.1176.

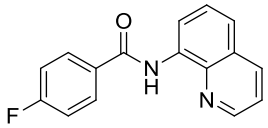
4-Chloro-*N*-(quinolin-8-yl)benzamide (**1c**)



This compound is known.[3]

^{1}H NMR (400 MHz, $CDCl_3$): δ 10.70 (1H, s), 8.91 (1H, J = 7.4, 1.4 Hz, dd), 8.85 (1H, J = 4.2, 1.6 Hz, dd), 8.19 (1H, J = 8.3, 1.4 Hz, dd), 8.03 (2H, J = 8.5 Hz, d), 7.61-7.46 (5H, m); ^{13}C NMR (100 MHz, $CDCl_3$): δ 164.3, 148.4, 138.7, 138.1, 136.5, 134.4, 133.5, 129.1, 128.7, 128.0, 127.5, 121.9, 121.8, 116.6; HRMS calcd for $C_{16}H_{11}ClN_2O$ $(M+H)^+$ 283.0633; found: 283.0650.

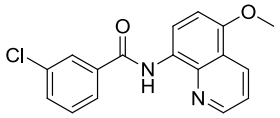
4-Fluoro-*N*-(quinolin-8-yl)benzamide (**1d**)



This compound is known.[4, 5]

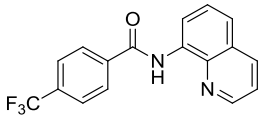
^{1}H NMR (400 MHz, $CDCl_3$): δ 10.69 (1H, s), 8.92 (1H, J = 7.4, 1.5 Hz, dd), 8.85 (1H, J = 4.2, 1.6 Hz, dd), 8.20 (1H, J = 8.2, 1.6 Hz, dd), 8.12-8.08 (2H, m), 7.62-7.53 (2H, m), 7.50 (1H, J = 8.3, 4.2 Hz, dd), 7.26-7.20 (2H, m); ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.3 ($^1J_{C,F}$ = 251, d), 164.3, 148.3, 138.8, 136.5, 134.5, 131.4, 129.7 ($^3J_{C,F}$ = 9, d), 128.0, 127.5, 121.8 ($^4J_{C,F}$ = 254.3, d), 116.6, 115.6 ($^2J_{C,F}$ = 22, d); HRMS calcd for $C_{16}H_{11}FN_2O$ $(M+H)^+$ 267.0928; found: 267.0936.

3-Chloro-*N*-(5-methoxyquinolin-8-yl)benzamide (**1e**)



^{1}H NMR (300 MHz, $CDCl_3$): δ 10.46 (1H, s), 8.89 (1H, J = 6.0, 2.4 Hz, dd), 8.84 (1H, J = 11.2 Hz, d), 8.65 (1H, J = 11.2, 2.4 Hz, dd), 8.06 (1H, J = 2.0 Hz, t), 7.96 (1H, J = 10.0 Hz, td), 7.56-7.45 (3H, m), 6.92 (1H, J = 11.2 Hz, d); ^{13}C NMR (75 MHz, $CDCl_3$): δ 163.7, 150.7, 148.7, 139.3, 137.2, 135.0, 131.6, 130.0, 127.7, 127.6, 125.2, 120.8, 120.6, 117.3, 104.4, 55.8; HRMS calcd for $C_{17}H_{13}ClN_2O_2$ $(M+H)^+$ 313.0738; found: 313.0737.

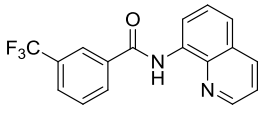
***N*-(quinolin-8-yl)-4-(trifluoromethyl)benzamide** (**1f**)



This compound is known.[1, 5]

^{1}H NMR (400 MHz, $CDCl_3$): δ 10.79 (1H, s), 8.93 (1H, J = 7.1, 1.8 Hz, dd), 8.86 (1H, J = 4.2, 1.6 Hz, dd), 8.22-8.18 (3H, m), 7.82 (2H, J = 8.2 Hz, d), 7.63-7.56 (2H, m), 7.52 (1H, J = 8.3, 4.2 Hz, m); ^{13}C NMR (100 MHz, $CDCl_3$): δ 164.1, 148.4, 138.7, 138.4, 136.6, 134.2, 133.6 ($^2J_{C,F}$ = 32, d), 128.0, 127.8, 127.5, 125.9 ($^3J_{C,F}$ = 4, d), 125.1 ($^1J_{C,F}$ = 271, d), 122.2, 121.8, 116.9; HRMS calcd for $C_{17}H_{11}F_3N_2O$ $(M+H)^+$ 317.0896; found: 317.0898.

***N*-(quinolin-8-yl)-3-(trifluoromethyl)benzamide** (**1g**)

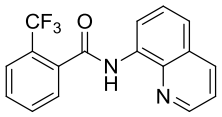


This compound is known.[4, 5]

^{1}H NMR (400 MHz, $CDCl_3$): δ 10.77 (1H, s), 8.93 (1H, J = 7.1, 1.5 Hz, dd), 8.87 (1H, J = 4.2, 1.6 Hz, dd),

8.35 (1H, s), 8.26-8.24 (1H, *J* = 7.8 Hz, d), 8.21 (1H, *J* = 8.3, 1.4 Hz, dd), 7.85 (1H, *J* = 7.8 Hz, d), 7.71 (1H, *J* = 7.8 Hz, t), 7.63 (2H, m) 7.51 (1H, *J* = 8.2, 4.2 Hz, dd); ^{13}C NMR (100 MHz, $CDCl_3$): δ 148.5, 138.7, 136.5, 136.0, 134.2, 131.2 ($^2J_{C,F}$ = 33, t), 130.3, 129.4, 128.4 ($^3J_{C,F}$ = 4, d), 128.0, 127.4, 125.1 ($^1J_{C,F}$ = 271, d), 124.6 ($^3J_{C,F}$ = 4, d), 122.2, 121.8; HRMS calcd for $C_{17}H_{11}F_3N_2O$ $(M+H)^+$ 317.0896; found: 317.0898.

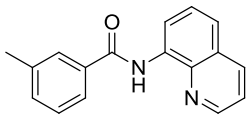
_N_-(quinolin-8-yl)-2-(trifluoromethyl)benzamide (1h)



This compound is known.[5]

^{1}H NMR (400 MHz, $CDCl_3$): δ 10.17 (1H, s), 8.94 (1H, *J* = 7.0, 1.9 Hz, dd), 8.76 (1H, *J* = 4.2, 1.1 Hz, dd), 8.19 (1H, *J* = 4.2, 1.1 Hz, dd), 7.80-7.75 (2H, m), 7.70 (1H, J = 7.3 Hz, t), 7.63-7.56 (3H, m), 7.46 (1H, *J* = 8.3, 4.2 Hz, dd),; ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.9, 148.3, 138.4, 136.4, 136.2, 134.3, 132.2, 130.2, 128.5, 128.0, 127.9 ($^2J_{C,F}$ = 32, d), 127.5 ($^1J_{C,F}$ = 252, d), 127.4, 126.76 ($^3J_{C,F}$ = 5, t), 122.3, 121.8, 117.0; HRMS calcd for $C_{17}H_{11}F_3N_2O$ $(M+H)^+$ 317.0896; found: 317.0902.

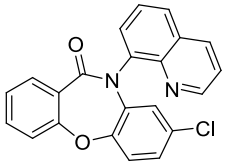
3-Methyl-_N_-(quinolin-8-yl)benzamide (1i)



This compound is known.[2]

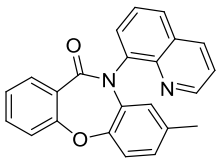
^{1}H NMR (400 MHz, $CDCl_3$): δ 10.67 (1H, s), 8.94 (1H, *J* = 7.6, 1.2 Hz, dd), 8.81 (1H, *J* = 4.2, 1.6 Hz, dd), 8.12 (1H, *J* = 8.3, 1.6 Hz, dd), 7.87-7.84 (2H, m), 7.62-7.51 (5H, m), 7.57 (1H, *J* = 8.1 Hz, t), 7.49 (1H, J = 8.2, 1.2 Hz, dd), 7.42-7.34 (3H, m), 2.45 (3H, t); ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.7, 148.3, 138.8, 138.7, 136.4, 135.2, 134.7, 132.6, 128.7, 128.1, 128.0, 127.4, 124.2, 121.67, 121.65, 116.5, 21.5; HRMS calcd for $C_{17}H_{14}N_2O$ $(M+H)^+$ 263.1179; found: 263.1180.

8-chloro-10-(quinolin-8-yl)dibenzo[b,f][1,4]oxazepin-11(10H)-one 3a



The title compound **3a** was prepared according to general procedure. A purification by flash chromatography in petroleum ether : ethyl acetate = 5 : 1 gave the title compound as a colourless oil (67 mg, 90%).^{1}H NMR (400 MHz, CD_2Cl_2): δ 8.96 (1H, *J* = 4.2, 2.5 Hz, dd), 8.34 (1H, *J* =8.3, 1.6 Hz, dd), 8.03 (1H, *J* = 8.2, 1.3 Hz, dd), 7.93 (1H, *J* = 7.7, 1.6 Hz, dd), 7.85 (1H, *J* = 7.3, 1.2 Hz, dd), 7.73 (1H, *J* = 7.8 Hz, t) 7.60-7.51 (2H, m), 7.36-7.31 (3H, m), 7.08 (1H, *J* = 8.6, 2.4 Hz, dd), 6.67 (1H, *J* = 2.4 Hz, d); ^{13}C NMR (75 MHz, CD_2Cl_2): δ 190.81, 164.21, 150.76, 134.89, 133.45, 131.01, 129.17, 128.70, 127.97, 125.44, 124.51, 114.79, 114.69, 113.87, 113.76, 108.87, 55.55; HRMS calcd for $C_{22}H_{13}ClN_2O_2$ $(M+H)^+$ 373.0738; found: 373.0732.

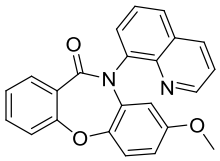
8-methyl-10-(quinolin-8-yl)dibenzo[b,f][1,4]oxazepin-11(10H)-one 3b



The title compound **3b** was prepared according to general procedure. A purification by flash chromatography in petroleum ether : ethyl acetate = 4 : 1 gave the title compound as a colourless oil (49 mg, 68%). ^{1}H NMR (300 MHz, $CDCl_3$): δ 9.02 (1H, *J* = 7.5, 1.2 Hz, dd), 8.57 (1H, *J* =4.2, 1.8 Hz, dd), 8.39 (1H, *J* = 7.8, 1.8 Hz,

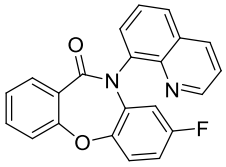
dd), 8.12 (1H, *J* = 8.1, 1.5 Hz, dd), 7.60-7.48 (3H, m), 7.43-7.33 (2H, m), 7.24 (1H, *J* = 7.5, 0.6 Hz, dd), 7.18 (1H, *J* = 8.1, 1.5 Hz, dd), 7.12 (1H, *J* = 8.1 Hz, d), 6.76 (1H, *J* = 8.4, 0.9 Hz, dd), 2.38 (3H, s); ^{13}C NMR (75 MHz, $CDCl_3$): δ 163.16, 155.74, 149.88, 148.11, 139.13, 136.49, 135.96, 135.54, 134.27, 132.89, 132.37, 129.64, 127.93, 127.42, 124.13, 123.26, 122.25, 121.56, 121.43, 119.18, 116.36, 115.65, 20.60; HRMS calcd for $C_{23}H_{16}N_2O_2$ $(M+H)^+$ 353.1285; found: 353.1285.

8-methoxy-10-(quinolin-8-yl)dibenzo[b,f][1,4]oxazepin-11(10H)-one 3c



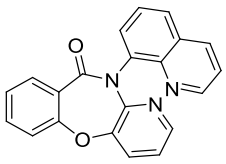
The title compound **3c** was prepared according to general procedure. A purification by flash chromatography in petroleum ether : ethyl acetate = 3 : 1 gave the title compound as a colourless oil (45 mg, 62%). ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.97 (1H, *J* = 4.2, 1.5 Hz, dd), 8.26 (1H, *J* = 8.4, 1.5 Hz, dd), 7.96-7.90 (2H, m), 7.81 (1H, *J* = 7.5, 1.5 Hz, dd), 7.66 (1H, *J* = 7.8 Hz, t), 7.51-7.44 (2H, m), 7.27 (1H, s), 7.25 (2H, *J* = 6.0 Hz, d), 6.59 (1H, *J* = 8.7, 3.0 Hz, dd), 6.18 (1H, *J* = 3.0 Hz, d); ^{13}C NMR (75 MHz, $CDCl_3$): δ 166.86, 160.69, 156.71, 151.36, 147.30, 144.92, 139.91, 136.46, 136.39, 133.50, 132.46, 130.11, 129.39, 128.89, 127.15, 126.88, 125.24, 121.82, 121.67, 119.66, 110.58, 109.95, 55.46; HRMS calcd for $C_{23}H_{16}N_2O_3$ $(M+H)^+$ 369.1234; found: 369.1235.

8-fluoro-10-(quinolin-8-yl)dibenzo[b,f][1,4]oxazepin-11(10H)-one 3d



The title compound **3d** was prepared according to general procedure. A purification by flash chromatography in petroleum ether : ethyl acetate = 5 : 1 gave the title compound as a colourless oil (58 mg, 82%). ^{1}H NMR (400 MHz, DMSO-d_6): δ 8.95 (1H, *J* = 4.4, 1.6 Hz, dd), 8.50 (1H, *J* =8.4, 1.6 Hz, dd), 8.14 (1H, *J* = 8.4, 1.2 Hz, dd), 7.95 (1H, *J* = 7.2, 0.8 Hz, dd), 7.82 (1H, *J* = 8.0, 1.6 Hz, dd), 7.77 (1H, *J* = 7.6 Hz, t), 7.65 (1H, *J* = 7.6, 1.2 Hz, dd), 7.61 (1H, *J* = 4.0 Hz, q), 7.54 (1H, *J* = 9.2, 5.6 Hz, dd), 7.48 (1H, *J* = 7.6 Hz, d),7.38-7.34 (1H, m), 6.99-6.98 (1H, m), 6.36 (1H, *J* = 10.0, 3.2 Hz, dd); ^{13}C NMR (100 MHz, DMSO-d_6): δ 166.14, 160.34 ($^1J_{C,F}$ = 241.0, d), 160.14, 151.98, 149.37 ($^4J_{C,F}$ = 2.0, d), 144.31, 139.01, 137.14, 137.01 ($^3J_{C,F}$ = 10.0, d), 134.81, 132.35, 131.02, 129.87, 129.62, 127.30, 126.85, 126.25, 123.48 ($^3J_{C,F}$ = 10.0, d), 122.67, 120.55, 113.07 ($^2J_{C,F}$ = 23.0, d), 110.96 ($^2J_{C,F}$ = 23.0, d); HRMS calcd for $C_{22}H_{13}FN_2O_2$ $(M+H)^+$ 357.1034; found: 357.1011.

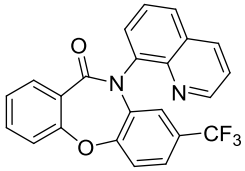
11-(quinolin-8-yl)benzo[f]pyrido[3,2-b][1,4]oxazepin-10(11H)-one 3e



The title compound **3e** was prepared according to general procedure. A purification by flash chromatography in petroleum ether : ethyl acetate = 4 : 1 gave the title compound as a colourless oil (57 mg, 85%). ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.87 (1H, *J* = 2.7 Hz, d), 8.22 (1H, *J* = 8.1 Hz, d), 8.00-7.86 (4H, m), 7.69-7.62 (2H, m), 7.55-7.49 (1H, m), 7.41 (1H, *J* = 4.2 Hz, q), 7.32-7.22 (2H, m), 7.02 (1H, *J* = 7.8, 4.8 Hz, dd); ^{13}C NMR (75 MHz, $CDCl_3$): δ 166.25, 159.58, 150.71, 149.17, 148.40, 144.79, 138.73, 136.30, 133.76, 132.82, 130.34, 129.59, 129.31, 128.53, 126.84, 126.34, 125.71, 121.43, 120.86, 119.65; HRMS calcd for $C_{21}H_{13}N_3O_2$

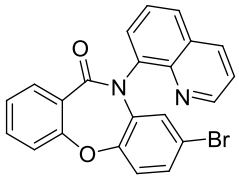
$(M+H)^+$ 340.1081; found: 340.1063.

10-(quinolin-8-yl)-8-(trifluoromethyl)dibenzo[b,f][1,4]oxazepin-11(10H)-one 3f



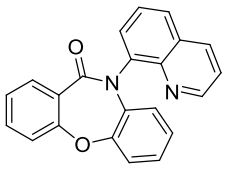
The title compound **3f** was prepared according to general procedure. A purification by flash chromatography in petroleum ether : ethyl acetate = 5 : 1 gave the title compound as a colourless oil (70 mg, 86%). ^{1}H NMR (400 MHz, DMSO-d_6): δ 8.94 (1H, J = 4.0, 1.6 Hz, dd), 8.53 (1H, J =8.0, 1.2 Hz, dd), 8.18 (1H, J = 8.4, 0.8 Hz, dd), 7.98-7.95 (2H, m),7.85 (1H, J = 7.6, 1.2 Hz, dd), 7.79 (1H, J = 8.0 Hz, t), 7.71 (1H, J = 8.4, 2.0 Hz, td), 7.63-7.58 (2H, m),7.42 (1H, J = 7.6, 0.8 Hz, td),7.35 (1H, J = 8.4, 1.6 Hz, dd), 6.80 (1H, J = 8.8 Hz, d); ^{13}C NMR (100 MHz, DMSO-d_6): δ 166.11, 159.70, 152.62, 151.94, 144.31, 139.52, 138.94, 137.13, 134.96, 132.35, 131.07, 129.91, 129.64, 127.28, 126.76 ($^2J_{C,F}$ = 33.0, d), 126.69, 126.53, 125.22 ($^1J_{C,F}$ = 271.0, d), 125.09, 123.29 ($^3J_{C,F}$ = 4.0, d), 122.67, 120.75, 119.57 ($^3J_{C,F}$ = 4.0, d); HRMS calcd for $C_{23}H_{13}F_3N_2O_2$ $(M+H)^+$ 407.1002; found: 407.0971.

8-bromo-10-(quinolin-8-yl)dibenzo[b,f][1,4]oxazepin-11(10H)-one 3g



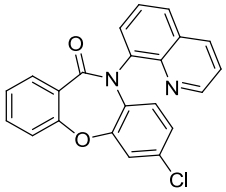
The title compound **3g** was prepared according to general procedure. A purification by flash chromatography in petroleum ether : ethyl acetate = 5 : 1 gave the title compound as a colourless oil (69 mg, 83%). ^{1}H NMR (400 MHz, DMSO-d_6): δ 8.98 (1H, J = 4.4, 1.6 Hz, dd), 8.52 (1H, J =8.0, 1.2 Hz, dd), 8.17 (1H, J = 8.4, 1.2 Hz, dd), 8.01 (1H, J = 7.2, 1.2 Hz, dd), 7.86 (1H, J = 7.6, 1.6 Hz, dd), 7.80 (1H, J = 7.6 Hz, t), 7.70 (1H, J = 8.0, 1.6 Hz, td), 7.64 (1H, J = 4.4 Hz, q), 7.51 (2H, J = 7.2 Hz, t), 7.42 (1H, J = 7.6, 0.8 Hz, td), 7.35 (1H, J = 8.4, 4.4Hz, dd), 6.76 (1H, J = 2.4 Hz, d); ^{13}C NMR (100 MHz, DMSO-d_6): δ 166.06, 159.93, 152.41, 152.02, 144.28, 138.92, 137.38, 137.17, 134.83, 132.37, 131.15, 129.92, 129.60, 129.27, 127.30, 126.77, 126.55, 126.37, 124.14, 122.70, 120.61, 117.67; HRMS calcd for $C_{22}H_{13}BrN_2O_2$ $(M+H)^+$ 417.0233; found: 417.0243.

10-(quinolin-8-yl)dibenzo[b,f][1,4]oxazepin-11(10H)-one 3h



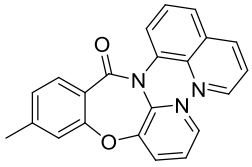
The title compound **3h** was prepared according to general procedure. A purification by flash chromatography in petroleum ether : ethyl acetate = 5 : 1 gave the title compound as a colourless oil (X = Br, 54 mg, 80%; X = I, 51 mg, 75%). ^{1}H NMR (400 MHz, DMSO-d_6): δ 8.93 (1H, J = 4.4, 2.0 Hz, dd), 8.53 (1H, J =8.4, 1.6 Hz, dd), 8.15 (1H, J = 8.4, 1.6 Hz, dd), 7.89 (1H, J = 8.4, 1.2 Hz, dd), 7.78-7.72 (2H, m), 7.66-7.60 (2H, m), 7.48-7.45 (2H, m), 7.38 (1H, J = 7.6, 0.8 Hz, td), 7.15 (1H, J = 7.6, 1.2 Hz, td), 6.98 (1H, J = 8.4, 1.6 Hz, td), 6.60 (1H, J = 7.6,1.6 Hz, dd); ^{13}C NMR (100 MHz, DMSO-d_6): δ 166.18, 160.29, 153.07, 151.85, 144.57, 139.63, 137.08, 135.75, 134.60, 132.24, 130.86, 129.57, 129.54, 127.29, 127.14, 126.53, 126.20, 126.11, 124.35, 122.58, 121.99, 120.61; HRMS calcd for $C_{22}H_{14}N_2O_2$ $(M+H)^+$ 339.1128; found: 339.1137.

7-chloro-10-(quinolin-8-yl)dibenzo[b,f][1,4]oxazepin-11(10H)-one 3i (4a)



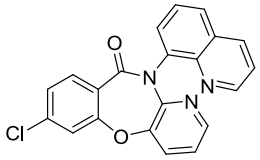
The title compound **3i** was prepared according to general procedure. A purification by flash chromatography in petroleum ether : ethyl acetate = 5 : 1 gave the title compound as a colourless oil (65 mg, 87%). ^{1}H NMR (400 MHz, CD_2Cl_2): δ 8.99 (1H, *J* = 4.0, 1.2 Hz, dd), 8.40 (1H, *J* = 8.0, 1.2 Hz, dd), 8.05 (1H, *J* = 8.4, 1.2 Hz, dd), 7.94 (1H, *J* = 8.4, 2.0 Hz, dd), 7.86 (1H, *J* = 8.4, 1.2 Hz, dd), 7.76 (1H, *J* = 8.0 Hz, t), 7.62-7.56 (2H, m), 7.42 (1H, *J* = 2.4 Hz, d), 7.37-7.33 (2H, m), 6.91 (1H, *J* = 8.8, 2.4 Hz, dd), 6.63 (1H, *J* = 8.4 Hz, d); ^{13}C NMR (100 MHz, CD_2Cl_2): δ 166.16, 159.99, 153.53, 150.90, 139.19, 137.08, 134.77, 133.77, 132.28, 130.63, 130.38, 129.49, 129.03, 126.89, 126.76, 125.62, 125.45, 125.14, 121.93, 121.77, 119.90; HRMS calcd for $C_{22}H_{13}ClN_2O_2$ $(M+H)^+$ 373.0738; found: 373.0740.

7-methyl-11-(quinolin-8-yl)benzo[f]pyrido[3,2-b][1,4]oxazepin-10(11H)-one 3j



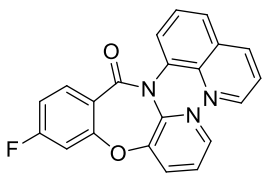
The title compound **3j** was prepared according to general procedure. A purification by flash chromatography in petroleum ether : ethyl acetate = 5 : 1 gave the title compound as a colourless oil (46 mg, 65%). ^{1}H NMR (300 MHz, CD_2Cl_2): δ 8.73 (1H, *J* = 4.2, 1.8 Hz, dd), 8.17 (1H, *J* =8.4, 1.8 Hz, dd), 7.86 (1H, *J* =8.4, 1.5 Hz, dd), 7.81 (1H, *J* =4.8, 1.5 Hz, dd), 7.77 (1H, *J* =7.5, 1.5 Hz, dd), 7.71 (1H, *J* = 7.8 Hz, d), 7.61-7.54 (2H, m), 7.34 (1H, *J* = 4.2 Hz, q), 7.06-7.02 (2H, m), 6.94 (1H, *J* =8.1, 4.8 Hz, dd), 2.33 (3H, s); ^{13}C NMR (75 MHz, CD_2Cl_2): δ 166.48, 159.75, 151.07, 149.48, 148.47, 145.80, 144.96, 144.79, 139.27, 136.70, 132.60, 131.05, 130.11, 129.59, 128.76, 126.91, 126.60, 124.13, 121.93, 121.30, 120.56, 21.56; HRMS calcd for $C_{22}H_{15}N_3O_2$ $(M+H)^+$ 354.1237; found: 354.1225.

7-chloro-11-(quinolin-8-yl)benzo[f]pyrido[3,2-b][1,4]oxazepin-10(11H)-one 3k



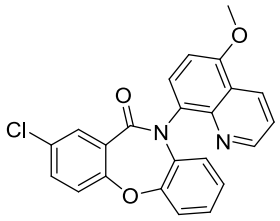
The title compound **3k** was prepared according to general procedure. A purification by flash chromatography in petroleum ether : ethyl acetate = 5 : 1 gave the title compound as a colourless oil (63 mg, 85%). ^{1}H NMR (300 MHz, CD_2Cl_2): δ 8.83 (1H, *J* = 4.2, 1.8 Hz, dd), 8.29 (1H, *J* =8.1 Hz, d), 7.98-7.94 (2H, m), 7.93-7.84 (2H, m), 7.72-7.67 (2H, m), 7.46 (1H, *J* = 4.2 Hz, q), 7.40 (1H, *J* = 2.1 Hz, d), 7.34 (1H, *J* = 8.4, 2.1 Hz, dd), 7.08 (1H, *J* = 8.1, 4.8 Hz, dd); ^{13}C NMR (75 MHz, CD_2Cl_2): δ 165.55, 160.04, 151.08, 149.05, 148.11, 145.22, 139.50, 138.89, 136.75, 133.98, 130.96, 130.23, 129.59, 128.92, 126.61, 126.51, 125.78, 122.00, 121.54, 120.75; HRMS calcd for $C_{21}H_{12}ClN_3O_2$ $(M+H)^+$ 374.0691; found: 374.0695.

7-fluoro-11-(quinolin-8-yl)benzo[f]pyrido[3,2-b][1,4]oxazepin-10(11H)-one 3l



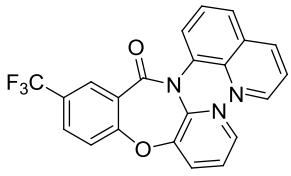
The title compound **3l** was prepared according to general procedure. A purification by flash chromatography in petroleum ether : ethyl acetate = 5 : 1 gave the title compound as a colourless oil (56 mg, 78%). ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.85 (1H, J = 5.2, 1.5 Hz, dd), 8.19 (1H, J = 8.1, 1.5 Hz, dd), 8.02-7.97 (1H, m), 7.96 (1H, J = 7.8, 1.5 Hz, dd), 7.90 (2H, J = 7.8, 1.2 Hz, td), 7.67-7.58 (2H, m), 7.38 (1H, J = 4.2 Hz, q), 7.04-6.96 (3H, m); ^{13}C NMR (75 MHz, $CDCl_3$): δ 167.25 ($^{1}J_{C,F}$ = 254.3, d), 165.20, 160.66 ($^{3}J_{C,F}$ = 11.3, d), 150.73, 148.83, 147.85, 145.07, 144.62, 138.53, 136.24, 134.77 ($^{3}J_{C,F}$ = 9.8, d), 130.30, 129.60, 129.27, 128.59, 126.25, 123.14 ($^{4}J_{C,F}$ = 3.0, d), 121.44, 120.93, 113.39 ($^{2}J_{C,F}$ = 21.0, d), 107.50 ($^{2}J_{C,F}$ = 23.3, d); HRMS calcd for $C_{21}H_{12}FN_3O_2$ $(M+H)^+$ 358.0986; found: 358.0966.

2-chloro-10-(5-methoxyquinolin-8-yl)dibenzo[b,f][1,4]oxazepin-11(10H)-one 3m



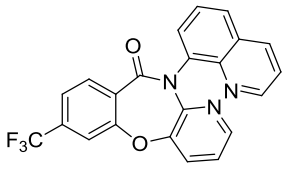
The title compound **3m** was prepared according to general procedure. A purification by flash chromatography in petroleum ether : ethyl acetate = 4 : 1 gave the title compound as a colourless oil (64 mg, 80%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.95 (1H, J = 4.0, 1.2 Hz, dd), 8.67 (1H, J = 8.4, 1.2 Hz, dd), 7.92 (1H, J = 2.4 Hz, d), 7.68 (1H, J = 8.4 Hz, d), 7.47-7.41 (2H, m), 7.30 (1H, J = 8.0, 1.2 Hz, dd), 7.23 (1H, J = 8.8 Hz, d), 7.07 (1H, J = 8.0, 1.2 Hz, td), 6.92-6.86 (2H, m), 6.68 (1H, J = 8.4, 1.2 Hz, dd); ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.76, 158.97, 155.58, 152.88, 151.54, 145.12, 135.91, 133.22, 132.34, 132.15, 131.42, 130.75, 129.96, 128.63, 125.90, 125.71, 124.40, 121.63, 121.31, 121.26, 120.96, 104.22, 56.00; HRMS calcd for $C_{23}H_{15}ClN_2O_3$ $(M+H)^+$403.0844; found: 403.0844.

11-(quinolin-8-yl)-8-(trifluoromethyl)benzo[f]pyrido[3,2-b][1,4]oxazepin-10(11H)-one 3n



The title compound **3n** was prepared according to general procedure. A purification by flash chromatography in petroleum ether : ethyl acetate = 5 : 1 gave the title compound as a colourless oil (67 mg, 82%). ^{1}H NMR (300 MHz, CD_2Cl_2): δ 8.76 (1H, J = 3.9 Hz, d), 8.23 (1H, J = 8.1 Hz, d), 8.16 (1H, J = 2.1 Hz, d), 7.91-7.85 (2H, m), 7.79-7.72 (2H, m), 7.65-7.60 (2H, m), 7.51-7.44 (2H, m), 7.01 (1H, J = 8.1, 4.8 Hz, dd); ^{13}C NMR (100 MHz, CD_2Cl_2): δ 164.83, 161.65, 150.29, 148.38, 147.49, 145.02, 140.57, 138.03, 136.05, 130.81 ($^{3}J_{C,F}$ = 6.0, d), 130.70 ($^{3}J_{C,F}$ = 5.0, d), 130.67, 130.43, 129.92, 129.25, 128.66, 128.10 ($^{2}J_{C,F}$ = 33.0, d), 127.37, 126.54, 121.65, 121.30, 120.88; HRMS calcd for $C_{22}H_{12}F_3N_3O_2$ $(M+H)^+$ 408.0954; found: 408.0948.

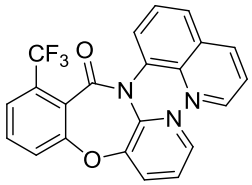
11-(quinolin-8-yl)-7-(trifluoromethyl)benzo[f]pyrido[3,2-b][1,4]oxazepin-10(11H)-one 3o



The title compound **3o** was prepared according to general procedure. A purification by flash chromatography in petroleum ether : ethyl acetate = 5 : 1 gave the title compound as a colourless oil (68 mg, 84%). ^{1}H NMR (400 MHz, CD_2Cl_2): δ 8.85 (1H, J = 4.2, 1.6 Hz, dd), 8.31 (1H, J = 8.2, 1.1 Hz, dd), 8.11 (1H, J = 8.1 Hz, d),

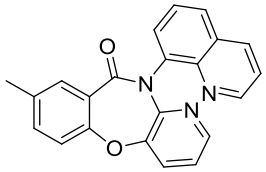
8.00-7.96 (2H, m), 7.89 (1H, *J* = 7.3, 1.2 Hz, dd), 7.75-7.70 (2H, m), 7.65 (1H, s), 7.62 (1H, *J* = 8.1 Hz, d), 7.48 (1H, *J* = 8.3, 4.2 Hz, dd), 7.10 (1H, *J* = 8.0, 4.7 Hz, dd); ^{13}C NMR (100 MHz, CD_2Cl_2): δ 164.96, 159.36, 150.72, 148.46, 147.80, 144.94, 144.25, 138.35, 136.39, 135.32 ($^2J_{C,F}$ = 33.0, d), 133.55, 130.48, 130.22, 129.89, 129.22, 128.62, 126.23, 124.52 ($^1J_{C,F}$ = 271.0, d), 122.37 ($^3J_{C,F}$ = 3.0, d), 121.65, 121.27, 117.45 ($^3J_{C,F}$ = 3.0, d); HRMS calcd for $C_{22}H_{12}F_3N_3O_2$ $(M+H)^+$ 408.0954; found: 408.0945.

11-(quinolin-8-yl)-9-(trifluoromethyl)benzo[f]pyrido[3,2-b][1,4]oxazepin-10(11H)-one 3p



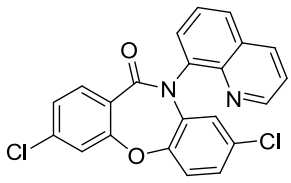
The title compound **3p** was prepared according to general procedure. A purification by flash chromatography in petroleum ether : ethyl acetate = 5 : 1 gave the title compound as a colourless oil (65 mg, 80%). ^{1}H NMR (300 MHz, CD_2Cl_2): δ 8.77 (1H, br, s), 8.29 (1H, *J* = 8.1 Hz, d), 8.01-7.97 (3H, m), 7.78-7.59 (5H, m), 8.44 (1H, br, s), 7.10 (1H, *J* = 7.8, 4.5 Hz, dd); ^{13}C NMR (100 MHz, CD_2Cl_2): δ 164.59, 160.90, 150.52, 149.23, 144.95, 143.81, 137.80, 136.35, 132.52, 131.99 ($^2J_{C,F}$ = 32.0, d), 131.02, 129.44, 129.39, 128.63, 126.28, 124.74 ($^3J_{C,F}$ = 5.0, d), 124.52 ($^1J_{C,F}$ = 272.0, d), 123.79, 121.56, 121.15; HRMS calcd for $C_{22}H_{12}F_3N_3O_2$ $(M+H)^+$ 408.0954; found: 408.0948.

8-methyl-11-(quinolin-8-yl)benzo[f]pyrido[3,2-b][1,4]oxazepin-10(11H)-one 3q



The title compound **3q** was prepared according to general procedure. A purification by flash chromatography in petroleum ether : ethyl acetate = 5 : 1 gave the title compound as a colourless oil (45 mg, 63%). ^{1}H NMR (300 MHz, CD_2Cl_2): δ 8.74 (1H, *J* = 4.2, 1.8 Hz, dd), 8.17 (1H, *J* = 8.1, 1.5 Hz, dd), 7.86 (1H, *J* = 8.1, 1.5 Hz, dd), 7.80 (1H, *J* = 4.5, 1.5 Hz, dd), 7.75 (1H, *J* = 7.5, 1.5 Hz dd), 7.62-7.53 (3H, m), 7.35 (1H, *J* = 4.2 Hz, q), 7.27 (1H, *J* = 8.1, 1.8 Hz, dd), 7.14 (1H, *J* = 8.1 Hz, d),6.93 (1H, *J* = 8.1, 4.8 Hz, dd), 2.27 (3H, s); ^{13}C NMR (75 MHz, CD_2Cl_2): δ 166.674, 157.83, 151.06, 149.47, 148.70, 144.77, 139.35, 136.76, 136.06, 134.94, 132.81, 130.92, 130.01, 129.61, 128.80, 126.66, 121.97, 121.34, 119.91, 20.81; HRMS calcd for $C_{22}H_{15}N_3O_2$ $(M+H)^+$ 354.1237; found: 354.1247.

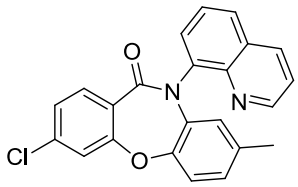
3,8-dichloro-10-(quinolin-8-yl)dibenzo[b,f][1,4]oxazepin-11(10H)-one 3r



The title compound **3r** was prepared according to general procedure. A purification by flash chromatography in petroleum ether : ethyl acetate = 5 : 1 gave the title compound as a colourless oil (70 mg, 86%). ^{1}H NMR (300 MHz, CD_2Cl_2): δ 8.85 (1H, *J* = 3.9, 1.5 Hz, dd), 8.25 (1H, *J* = 8.1, 1.5 Hz, dd), 7.94 (1H, *J* = 8.1, 1.2 Hz, dd), 7.76-7.70 (2H, m), 7.64 (1H, *J* = 8.1 Hz, t), 7.45 (1H, *J* = 3.9 Hz, q), 7.28 (1H, *J* = 2.1 Hz, d), 7.23 (2H, *J* = 8.1, 1.5 Hz, dd), 6.99 (1H, *J* = 8.7, 2.4 Hz, dd), 6.55 (1H, *J* = 2.4 Hz, d); ^{13}C NMR (75 MHz, CD_2Cl_2): δ 165.70, 160.70, 151.77, 144.81, 139.37, 139.29, 137.10, 136.94, 133.65, 131.07, 130.69, 129.94,

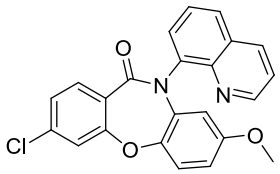
129.73, 127.07, 126.41, 126.23, 125.82, 124.46, 123.02, 122.46, 120.83; HRMS calcd for $C_{22}H_{12}Cl_2N_2O_2$ $(M+H)^+$ 407.0349; found: 407.0371.

3-chloro-8-methyl-10-(quinolin-8-yl)dibenzo[b,f][1,4]oxazepin-11(10H)-one 3s



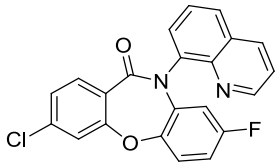
The title compound **3s** was prepared according to general procedure. A purification by flash chromatography in petroleum ether : ethyl acetate = 4 : 1 gave the title compound as a colourless oil (55 mg, 71%). ^{1}H NMR (300 MHz, CD_2Cl_2): δ 9.01 (1H, J = 2.7 Hz, d), 8.43 (1H, J = 7.8 Hz, d), 8.04 (1H, J = 7.8, 0.9 Hz, dd), 7.86-7.79 (2H, m), 7.75 (1H, J = 7.8 Hz, t), 7.61 (1H, J = 3.9 Hz, q), 7.34 (1H, J = 0.9 Hz, d), 7.28-7.22 (2H, m), 6.93 (1H, J = 8.1, 1.5 Hz, dd), 6.46 (1H, J = 1.8 Hz, d), 2.01 (3H, s); ^{13}C NMR (75 MHz, CD_2Cl_2): δ 166.020, 161.230, 151.563, 151.157, 139.901, 138.997, 136.918, 136.158, 135.418, 133.531, 130.707, 129.846, 129.310, 127.047, 126.254, 126.020, 124.966, 122.289, 121.417, 120.775, 20.840; HRMS calcd for $C_{23}H_{15}ClN_2O_2$ $(M+H)^+$ 387.0895; found: 387.0894.

3-chloro-8-methoxy-10-(quinolin-8-yl)dibenzo[b,f][1,4]oxazepin-11(10H)-one 3t



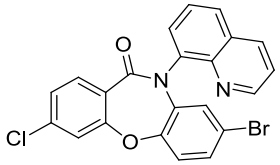
The title compound **3t** was prepared according to general procedure. A purification by flash chromatography in petroleum ether : ethyl acetate = 3 : 1 gave the title compound as a colourless oil (63 mg, 78%). ^{1}H NMR (300 MHz, CD_2Cl_2): δ 8.97 (1H, J = 4.2, 1.8 Hz, dd), 8.35 (1H, J = 8.4, 1.8Hz, dd), 8.03 (1H, J = 8.1, 1.5 Hz, dd), 7.87-7.82 (2H, m), 7.74 (1H, J = 7.8 Hz, t), 7.55 (1H, J = 4.2 Hz, q), 7.38 (1H, J = 1.8 Hz, d), 7.32 (2H, J = 8.7, 2.4 Hz, dd), 6.66 (1H, J = 8.7, 2.7 Hz, dd), 6.21 (1H, J = 2.7Hz, d), 3.50 (3H, s); ^{13}C NMR (75 MHz, CD_2Cl_2): δ 166.01, 161.26, 157.40, 151.65, 147.10, 145.00, 139.79, 139.08, 136.87, 136.52, 130.62, 129.87, 129.43, 127.05, 126.17, 126.00, 122.32, 122.10, 120.72, 110.90, 110.38, 55.81; HRMS calcd for $C_{23}H_{15}ClN_2O_3$ $(M+H)^+$ 403.0844; found: 403.0839.

3-chloro-8-fluoro-10-(quinolin-8-yl)dibenzo[b,f][1,4]oxazepin-11(10H)-one 3u



The title compound **3u** was prepared according to general procedure. A purification by flash chromatography in petroleum ether : ethyl acetate = 5 : 1 gave the title compound as a colourless oil (64 mg, 82%). ^{1}H NMR (300 MHz, CD_2Cl_2): δ 8.97 (1H, J = 4.2, 1.5 Hz, dd), 8.36 (1H, J = 8.1, 1.5Hz, dd), 8.05 (1H, J = 8.1, 1.5 Hz, dd), 7.89-7.83 (2H, m), 7.75 (1H, J = 8.1 Hz, t), 7.56 (1H, J = 4.2 Hz, q), 7.41-7.31 (3H, m), 6.86-6.79 (1H, m), 6.41 (1H, J = 9.9, 3.0 Hz, dd); ^{13}C NMR (75 MHz, CD_2Cl_2): δ 165.76, 161.59 ($^1J_{C,F}$ = 242.3, d), 160.87, 151.78, 149.18 ($^4J_{C,F}$ = 3.0, d), 144.86, 139.44, 139.37, 137.17 ($^3J_{C,F}$ = 9.8, d), 136.92, 133.65, 130.61, 129.93, 129.93, 129.70, 127.10, 126.32, 125.88, 122.87 ($^3J_{C,F}$ = 9.8, d), 122.45, 120.81, 112.86 ($^2J_{C,F}$ = 23.3, d), 111.71 ($^2J_{C,F}$ = 27.0, d); HRMS calcd for$C_{22}H_{12}ClFN_2O_2$ $(M+H)^+$ 391.0644; found: 391.0640.

8-bromo-3-chloro-10-(quinolin-8-yl)dibenzo[b,f][1,4]oxazepin-11(10H)-one 3v



The title compound **3v** was prepared according to general procedure. A purification by flash chromatography in petroleum ether : ethyl acetate = 5 : 1 gave the title compound as a colourless oil (80 mg, 89%). ^{1}H NMR (400 MHz, CD_2Cl_2): δ 8.99 (1H, J = 4.4, 1.6 Hz, dd), 8.40 (1H, J = 8.0, 0.8 Hz, dd), 8.07 (1H, J = 8.0, 0.8 Hz, dd), 7.89-7.83 (2H, m), 7.77 (1H, J = 8.0 Hz, t), 7.59 (1H, J = 4.4 Hz, q), 7.39 (1H, J = 2.0 Hz, d), 7.35 (1H, J = 8.4, 2.0 Hz, dd), 7.29-7.26 (2H, m), 6.82 (1H, J = 2.0 Hz, d); ^{13}C NMR (100 MHz, CD_2Cl_2): δ 165.28, 160.25, 151.97, 151.03, 138.97, 138.68, 136.96, 133.37, 130.57, 129.55, 129.31, 128.92, 127.03, 126.84, 125.99, 125.39, 122.99, 122.03, 120.38, 118.12; HRMS calcd for $C_{22}H_{12}BrClN_2O_2$ $(M+H)^+$ 450.9843; found: 450.9843.

10. References

1. L. Grigorjeva; O. Daugulis. *Org. Lett.*, **2014**, *16*, 4684–4687.

2. F. R. Gou; X. C. Wang; P. F. Huo; H. P. Bi; Z. H. Guan; Y. M. Liang. *Org. Lett.*, **2009**, *11*, 5726–5729.

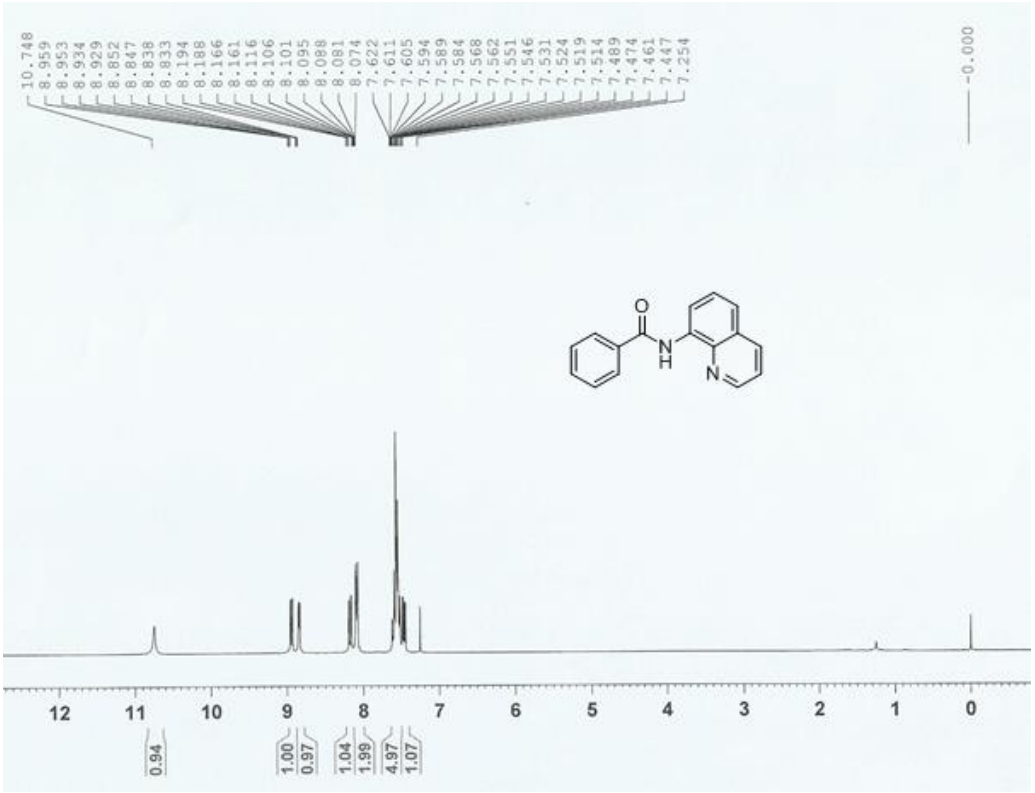
3. A. M. Suess; M. Z. Ertem; C. J. Cramer; S. S. Stahl. *J. Am. Chem. Soc.*, **2013**, *135*, 9797–9804.

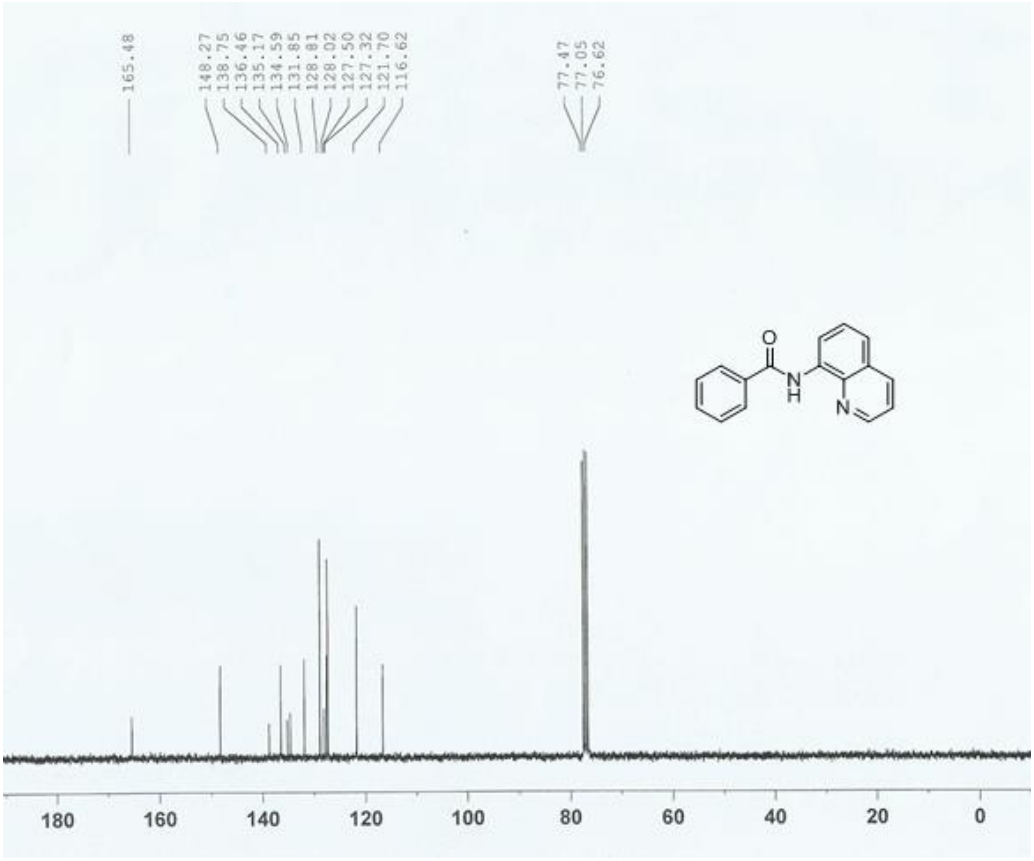
4. L. D. Tran, J. Roane and O. Daugulis, *Angew. Chem. Int. Ed.*, **2013**, *52*, 6043–6046.

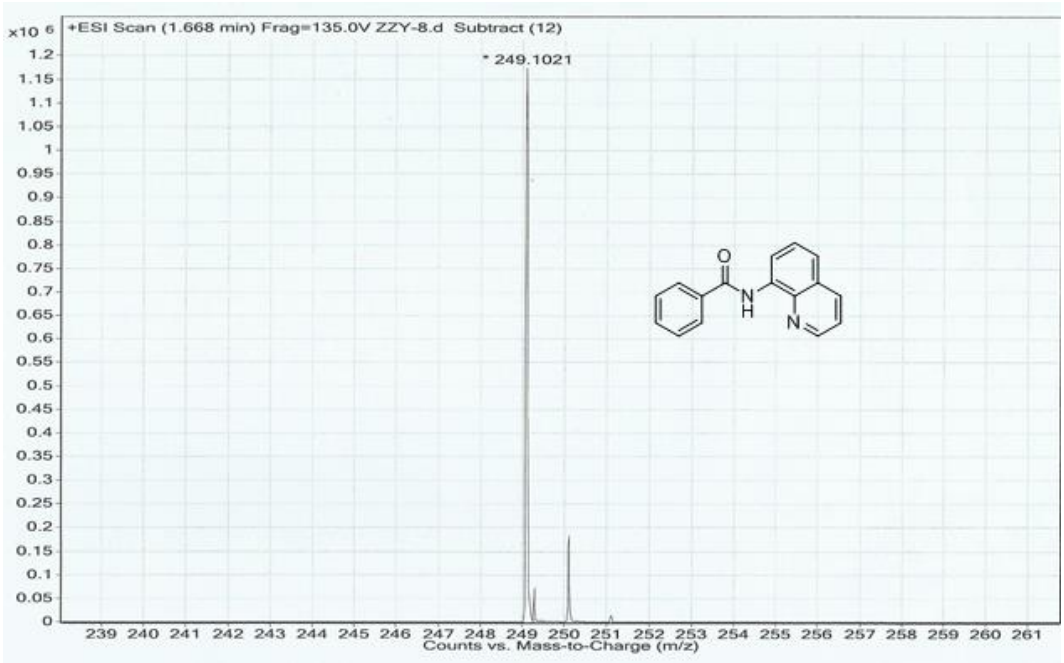
5. D. Katayev; K. F. Pfister; T. Wendling; L. J. Goo ßen. *Chem. Eur. J.*, **2014**, *20*, 9902–9905.

11. ^{1}H NMR and ^{13}C NMR spectra

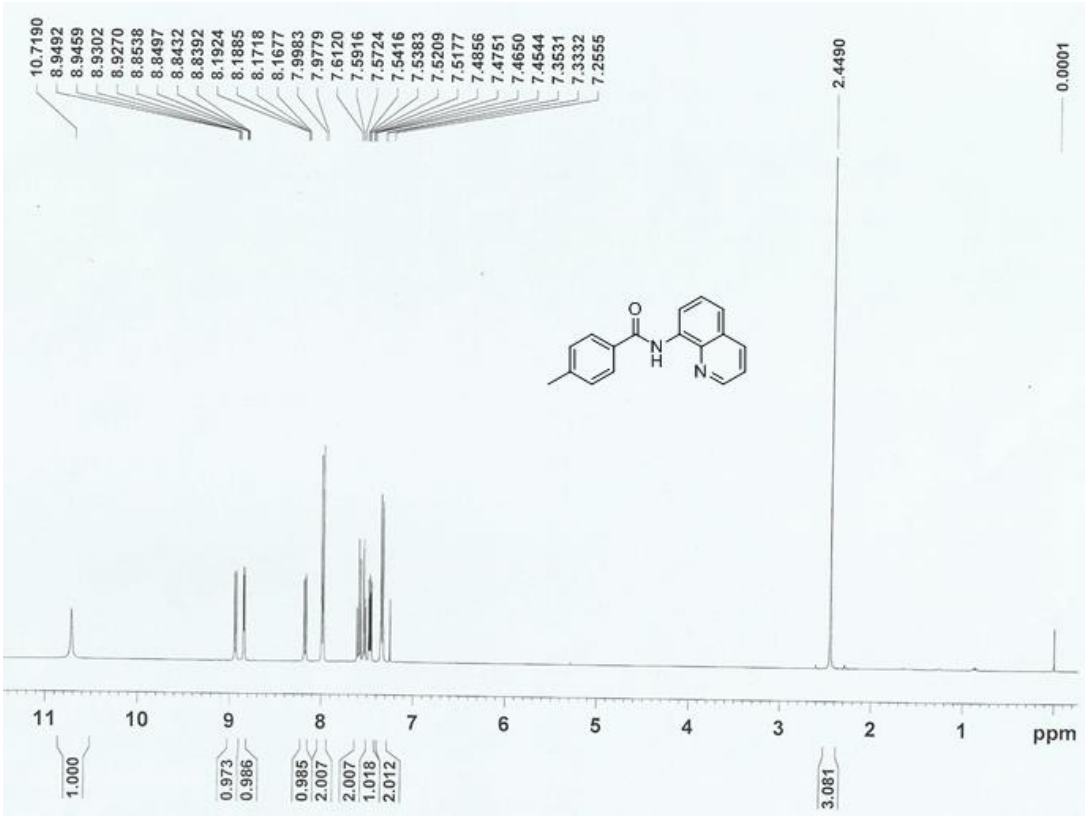
***N*-(quinolin-8-yl)benzamide (1a)**







4-methyl-*N*-(quinolin-8-yl)benzamide (**1b**)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8.9459
8.9302
8.9270
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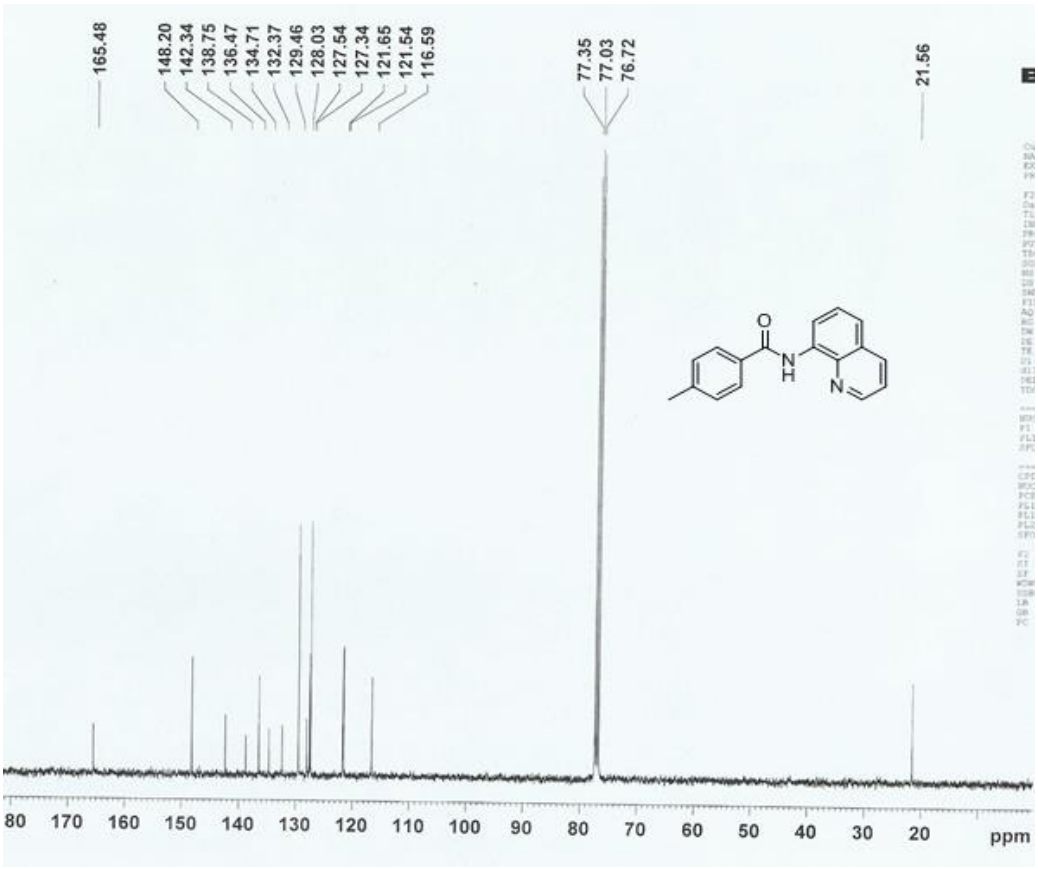
8.8497
8.8432
8.8392
8.1924
8.1885
8.1718
8.1677
7.9983
7.9779
7.6120
7.5916
7.5724
7.5416
7.5383
7.5209
7.5177
7.4856
7.4751
7.4650
7.4544
7.3531
7.3332
7.2555
2.4490
0.0001
O
N
H
N
11
10
9
8
7
6
5
4
3
2
1
ppm
1.000
0.973
0.986
0.985
2.007
2.007
1.018
2.012
3.081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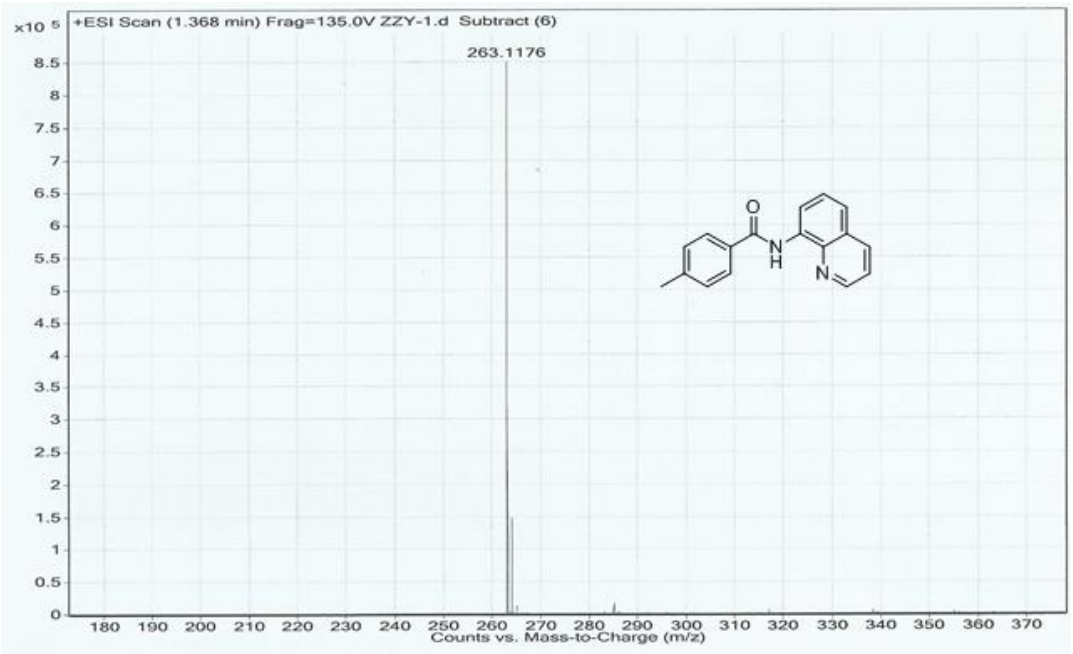
138.75
136.47
134.71
132.37
129.46
128.03
127.54
127.34
121.65
121.54
116.59
77.35
77.03
76.72
21.56
O
N
H
N
80 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm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O
N
H
N
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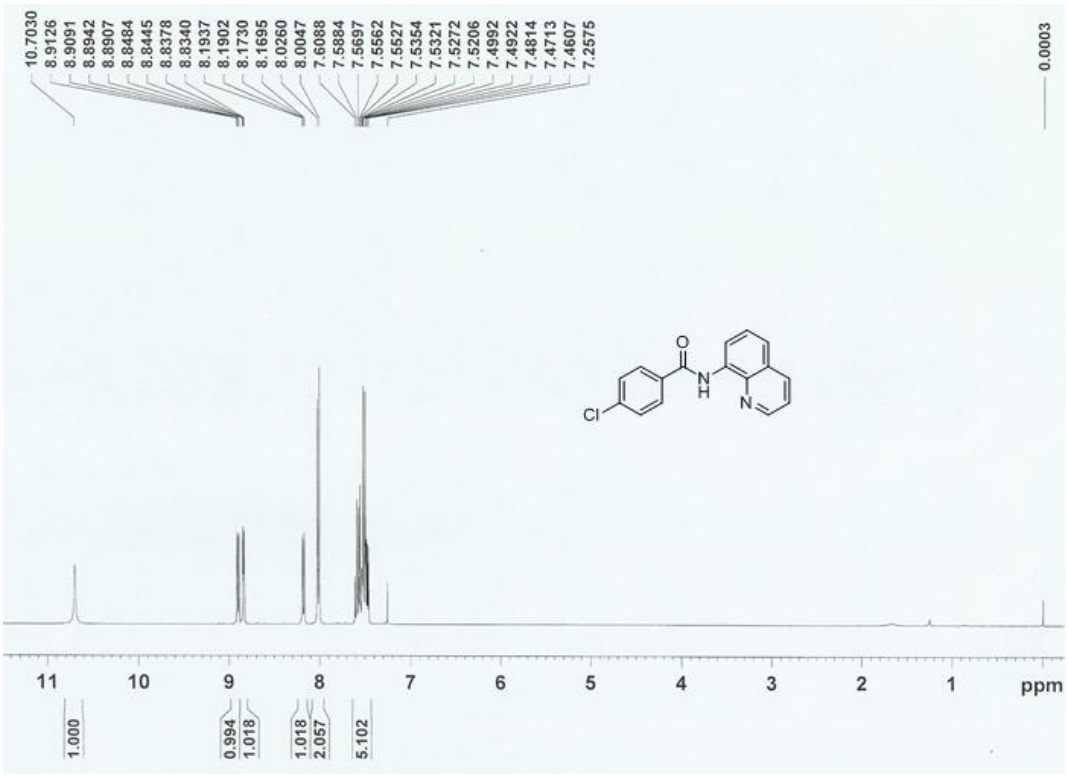
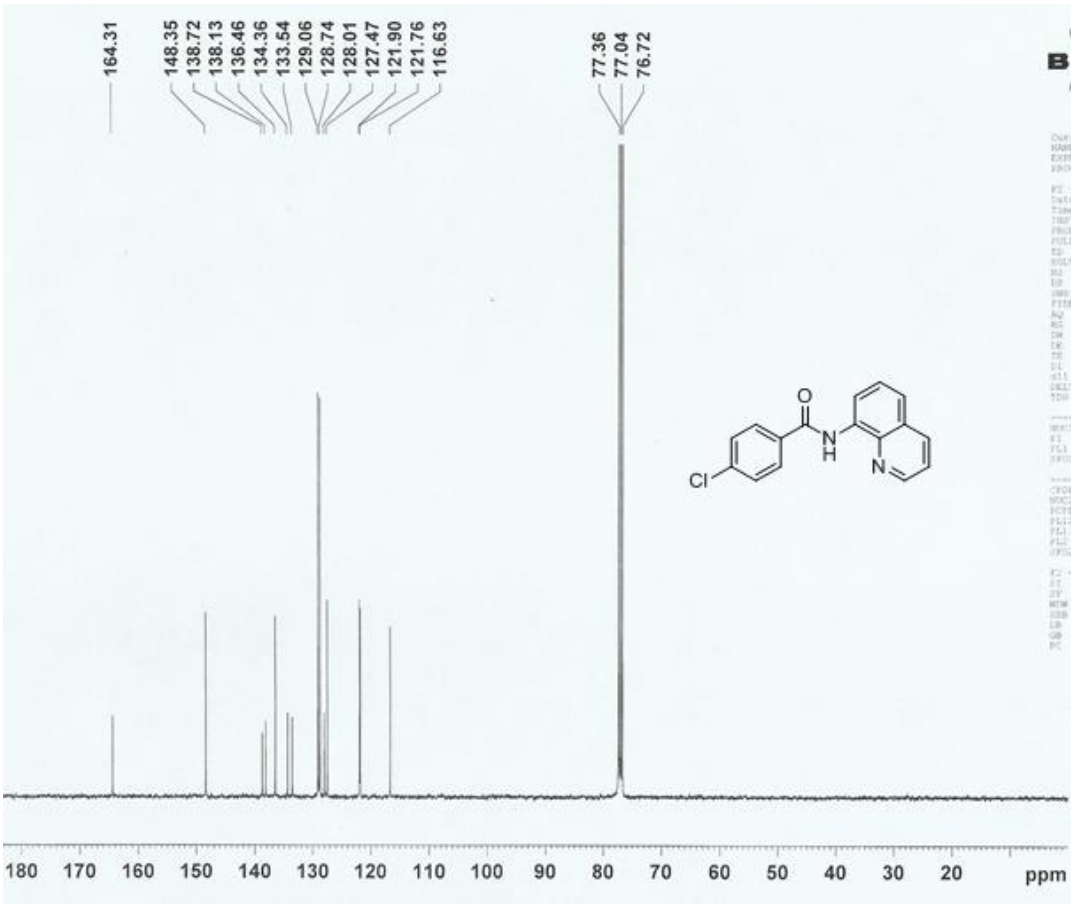
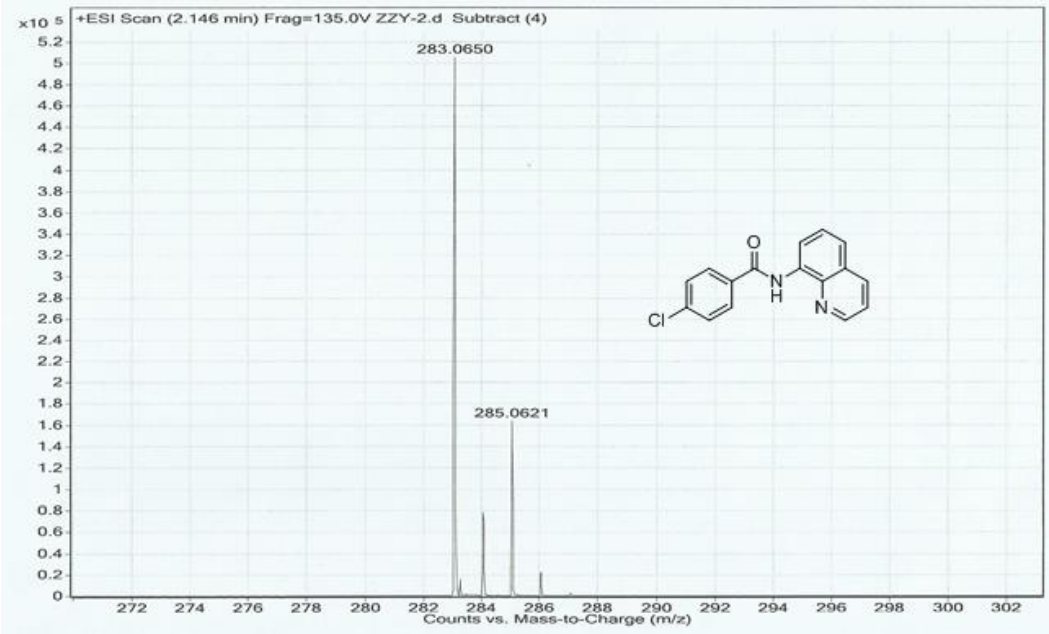
Counts vs. Mass-to-Charge (m/z)

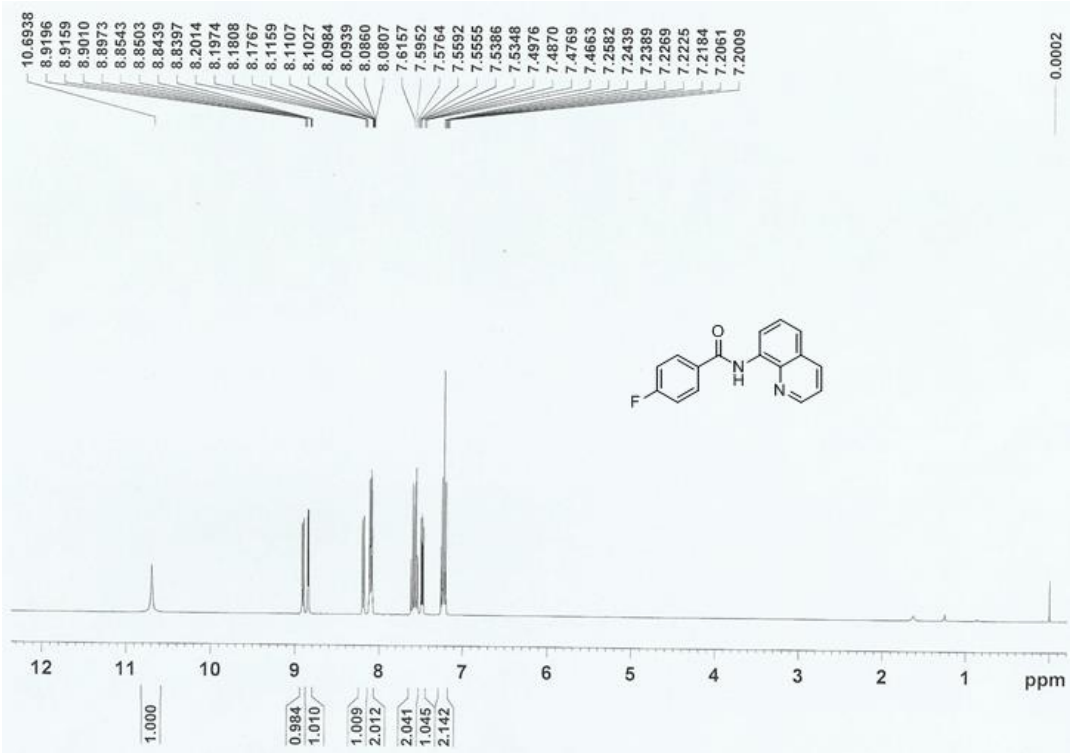
4-chloro-*N*-(quinolin-8-yl)benzamide (1c)

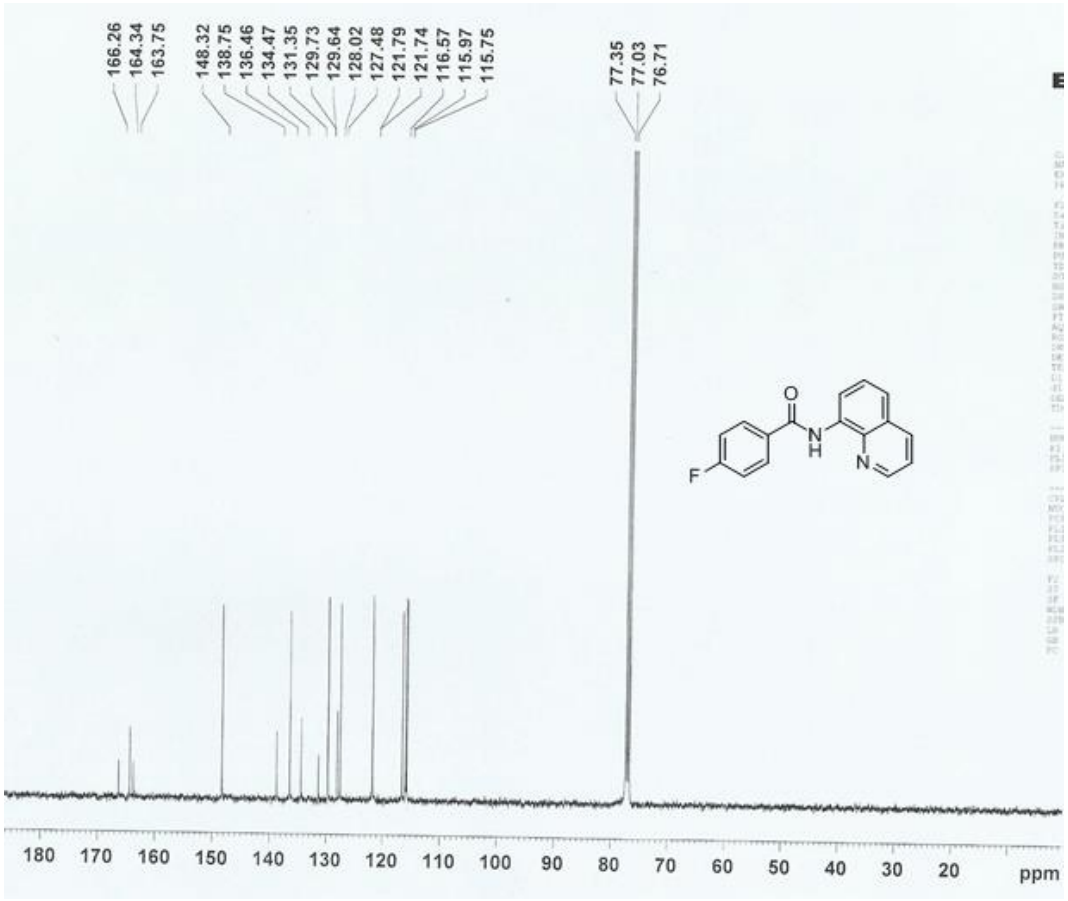






4-fluoro-*N*-(quinolin-8-yl)benzamide (**1d**)

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134.47
131.35
129.73
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128.02
127.48
121.79
121.74
116.57
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77.35
77.03
76.71
O
N
H
F
N
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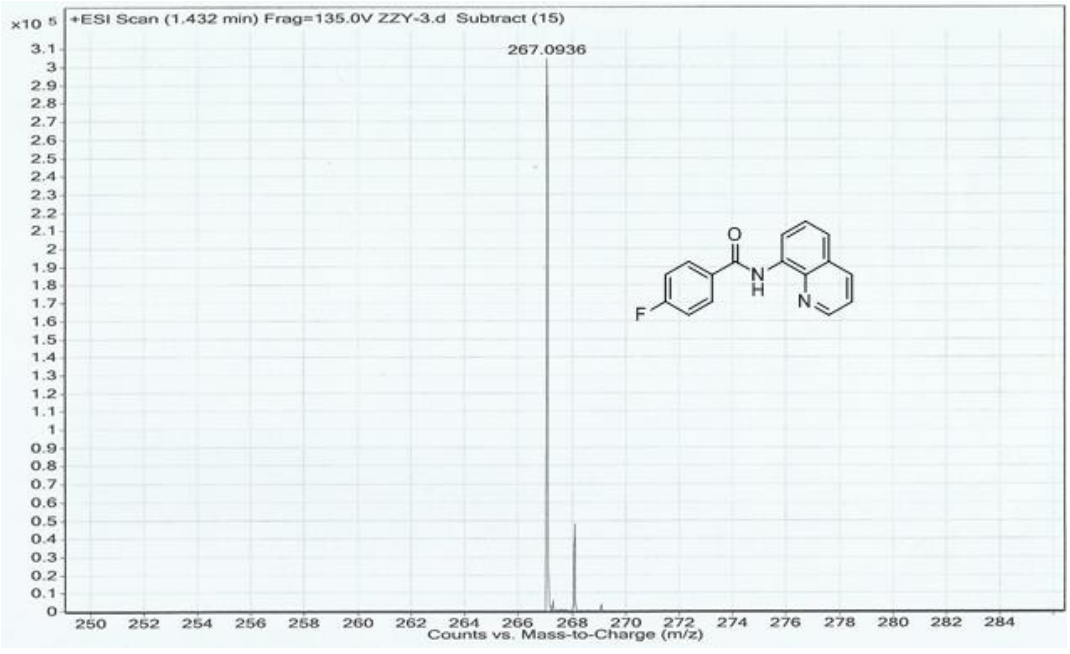
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2.9
2.8
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2.6
2.5
2.4
2.3
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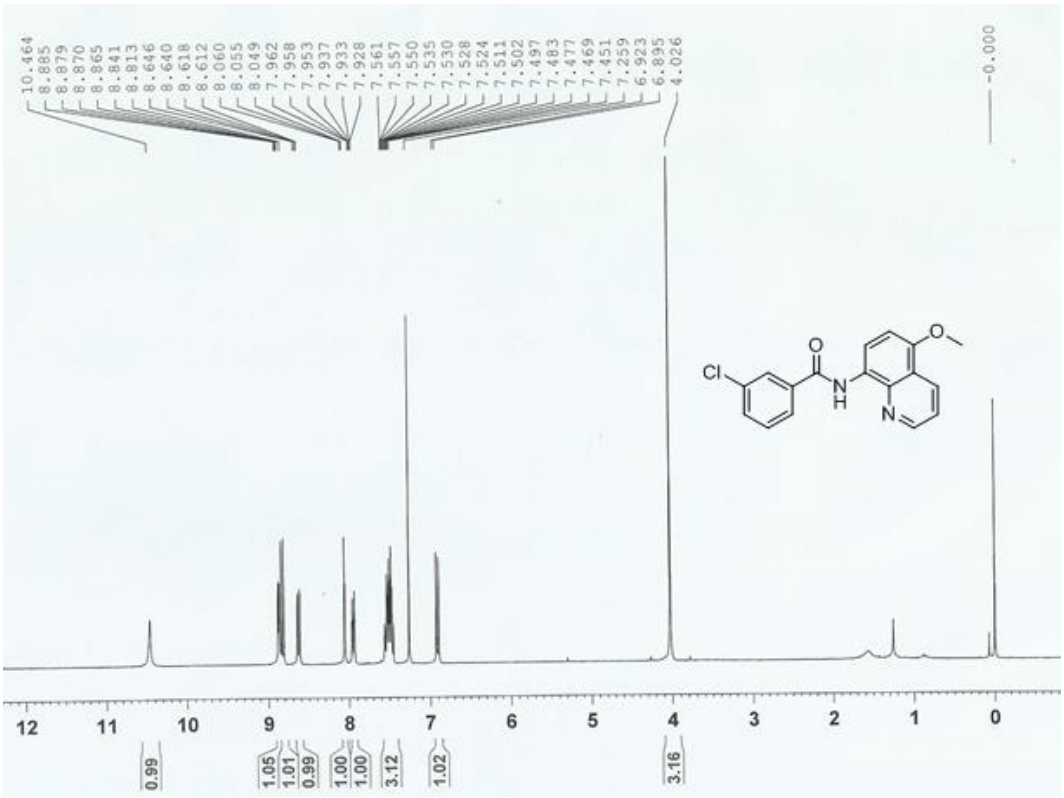
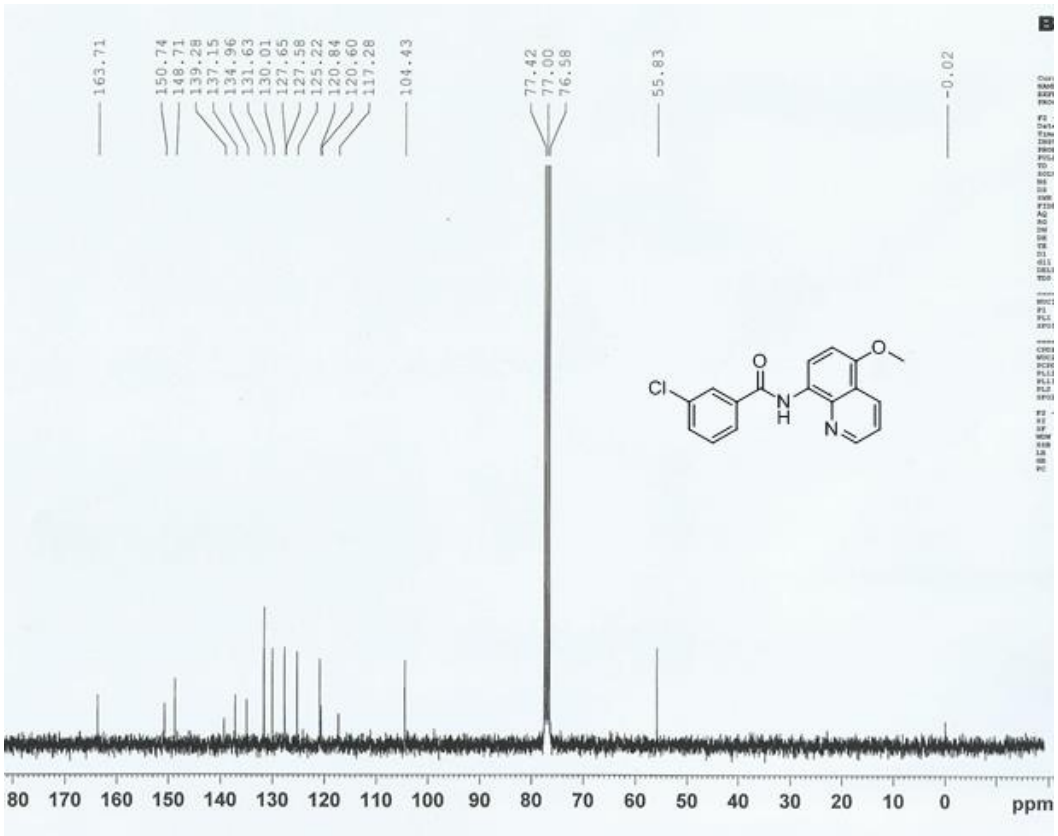
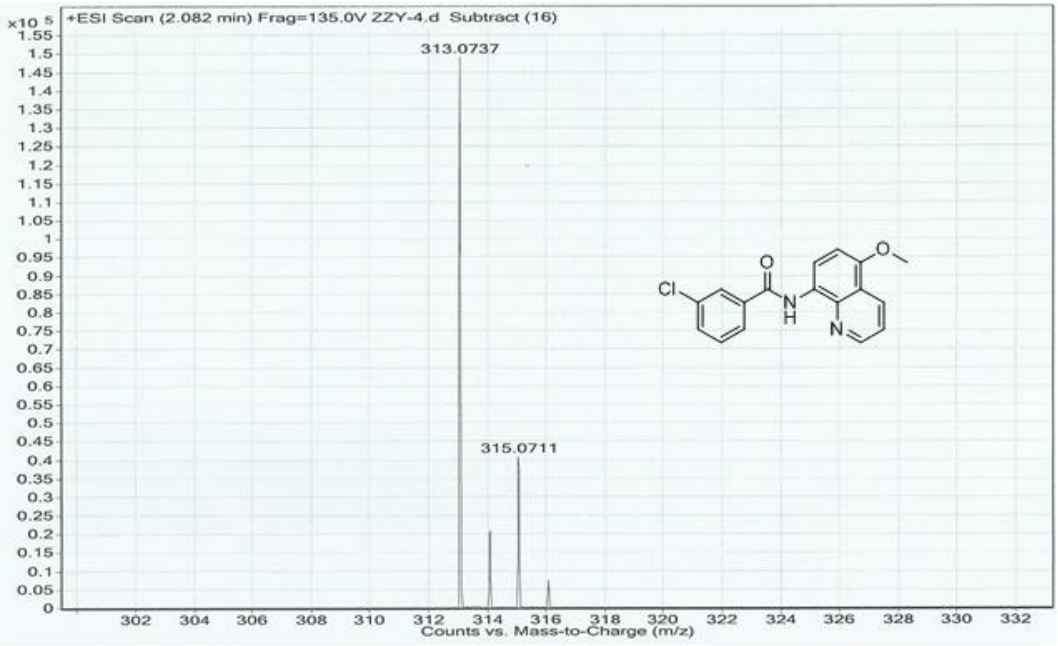
2.1
2
1.9
1.8
1.7
1.6
1.5
1.4
1.3
1.2
1.1
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
250 252 254 256 258 260 262 264 266 268 270 272 274 276 278 280 282 284
Counts vs. Mass-to-Charge (m/z)
O
N
H
F
N

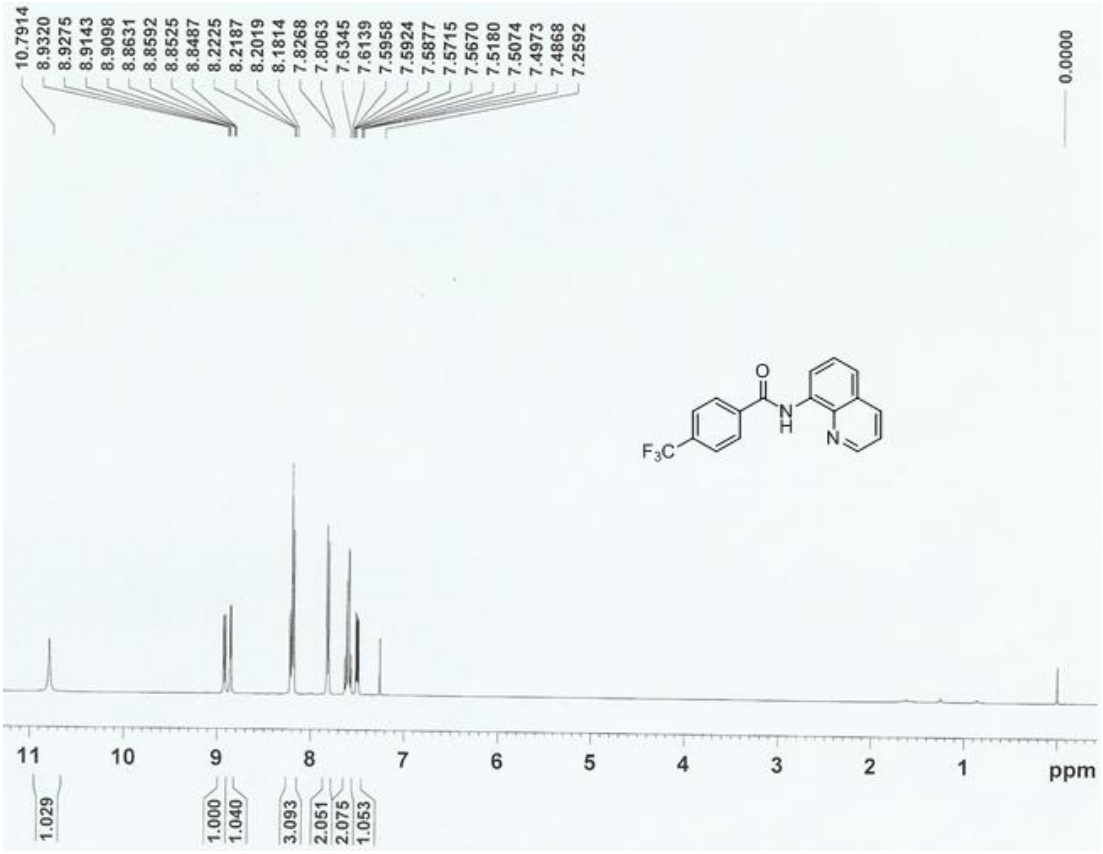
3-chloro-*N*-(5-methoxyquinolin-8-yl)benzamide (**1e**)

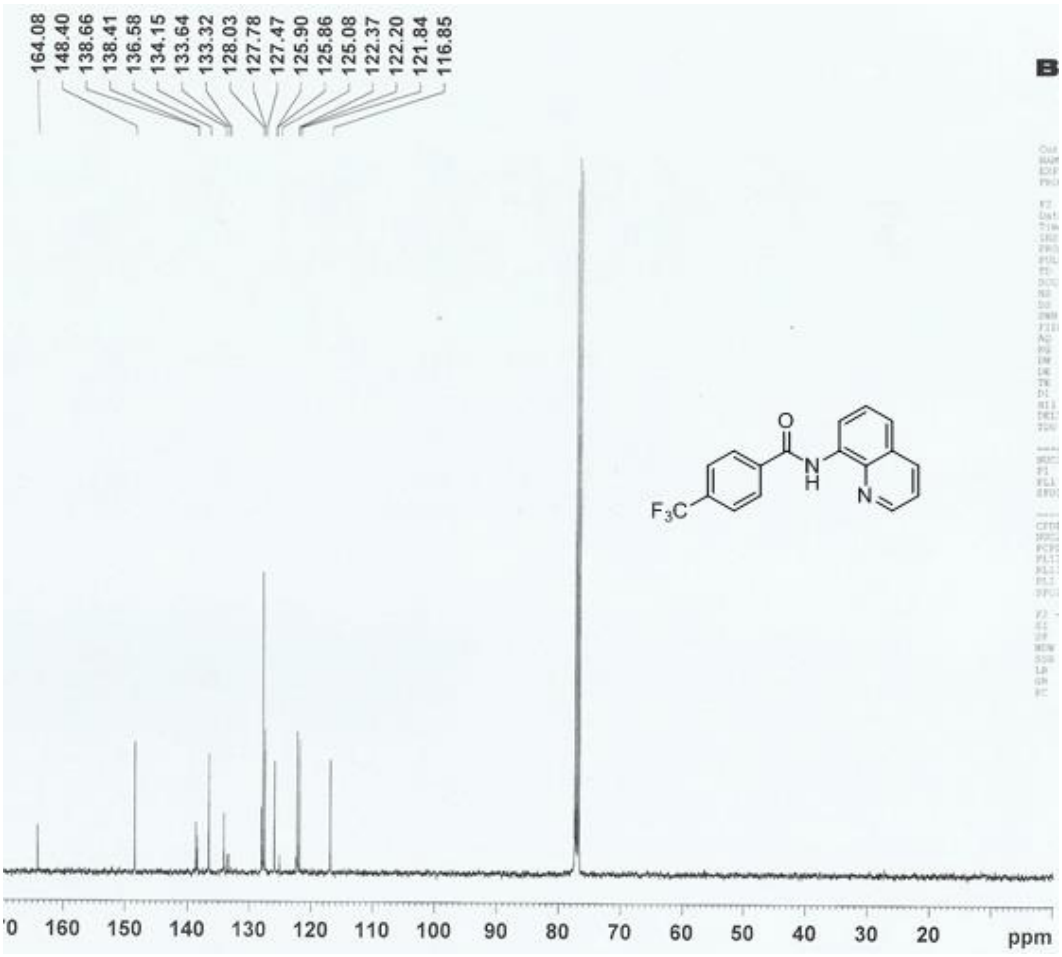






***N*-(quinolin-8-yl)-4-(trifluoromethyl)benzamide (1f)**

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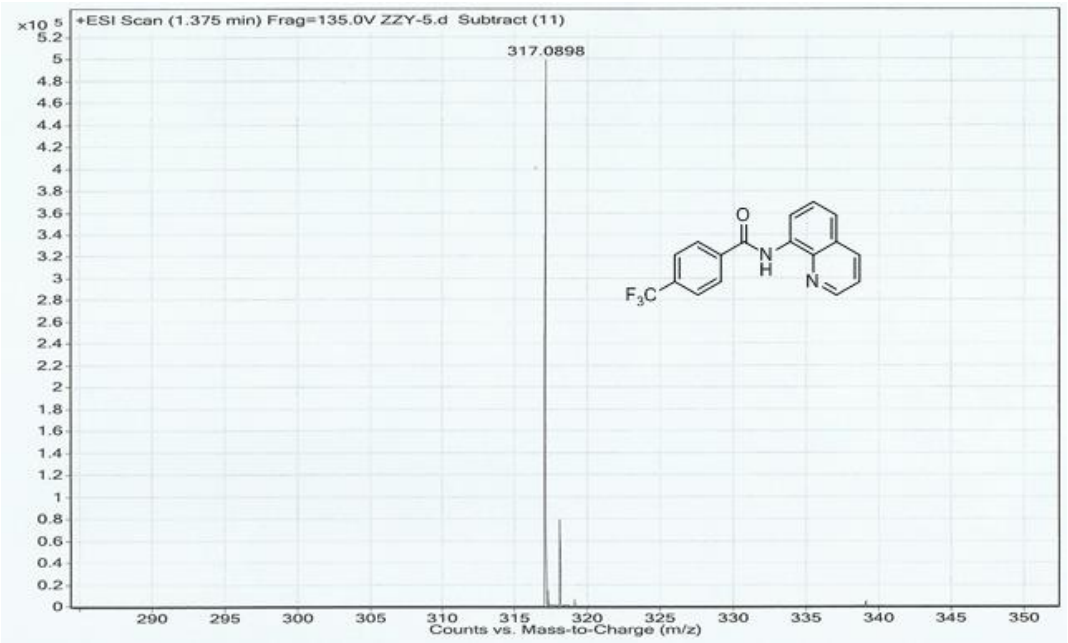
138.66
138.41
136.58
134.15
133.64
133.32
128.03
127.78
127.47
125.90
125.86
125.08
122.37
122.20
121.84
116.85
B
O
N
H
N
F3C
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm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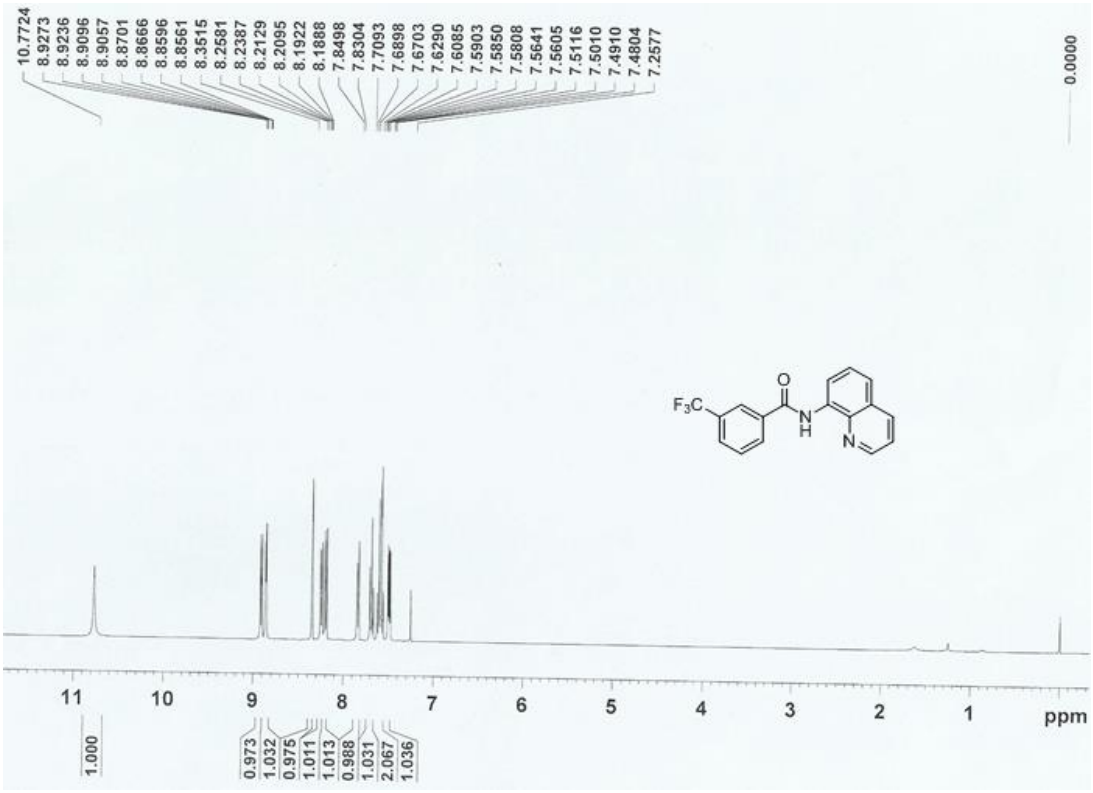
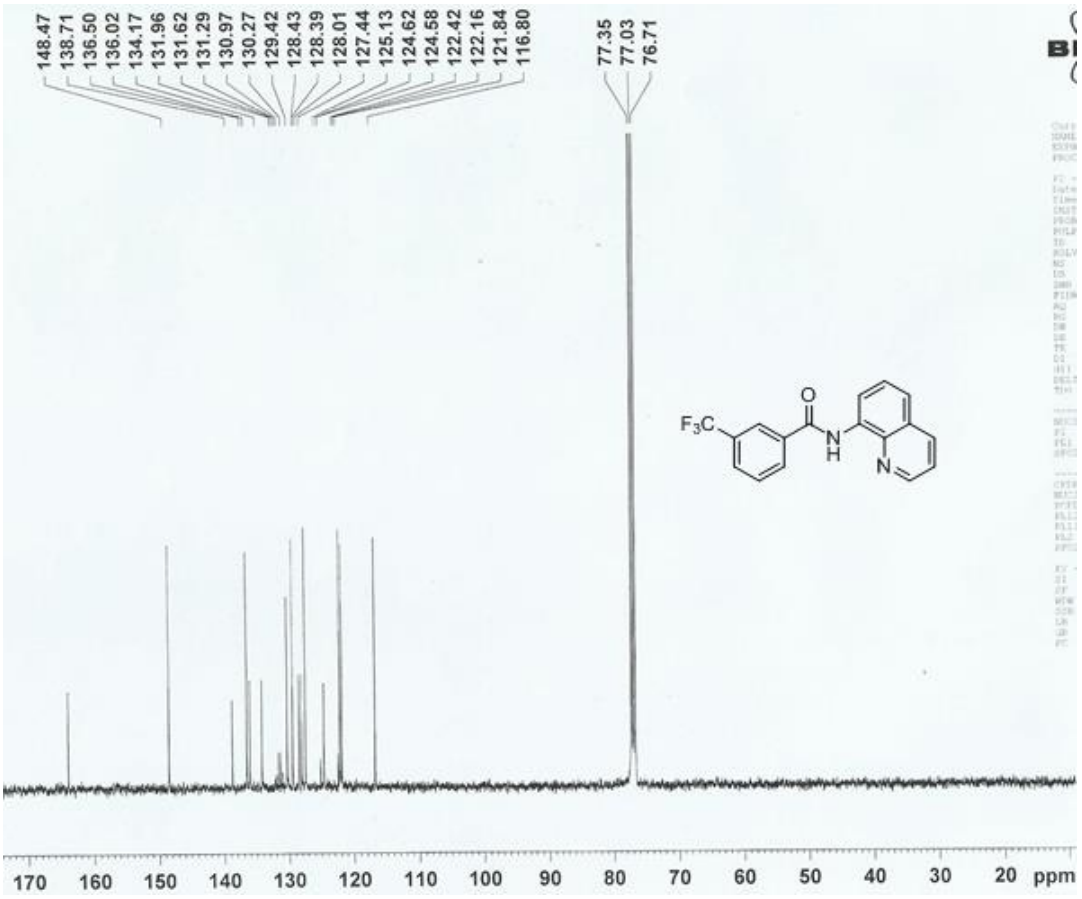
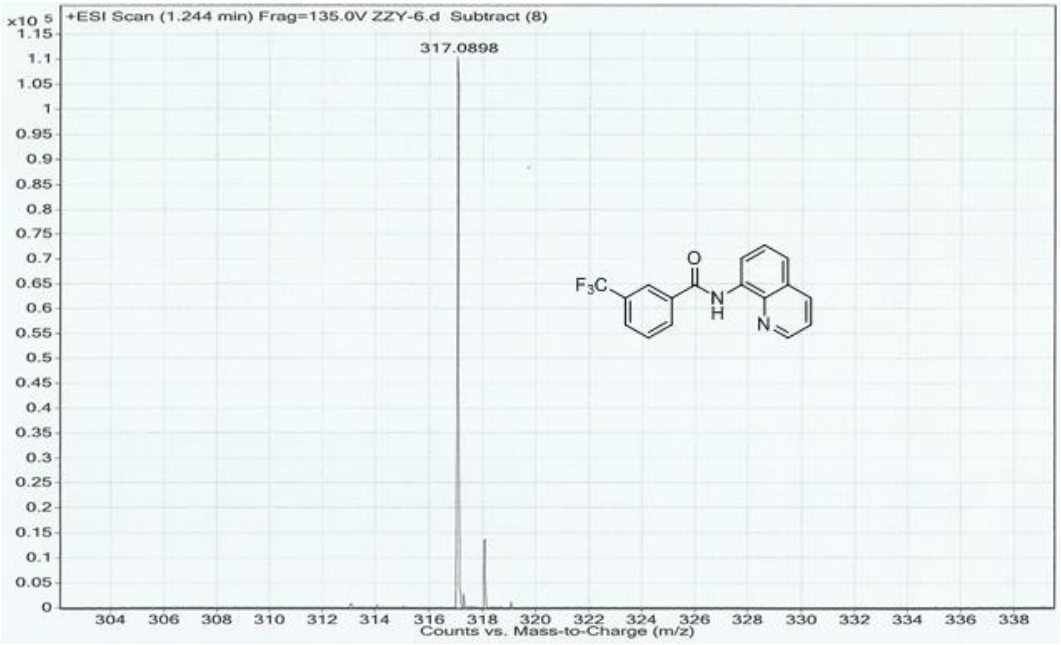
+ESI Scan (1.375 min) Frag=135.0V ZZY-5.d Subtract (11)
317.0898
O
N
H
N
F3C
Counts vs. Mass-to-Charge (m/z)

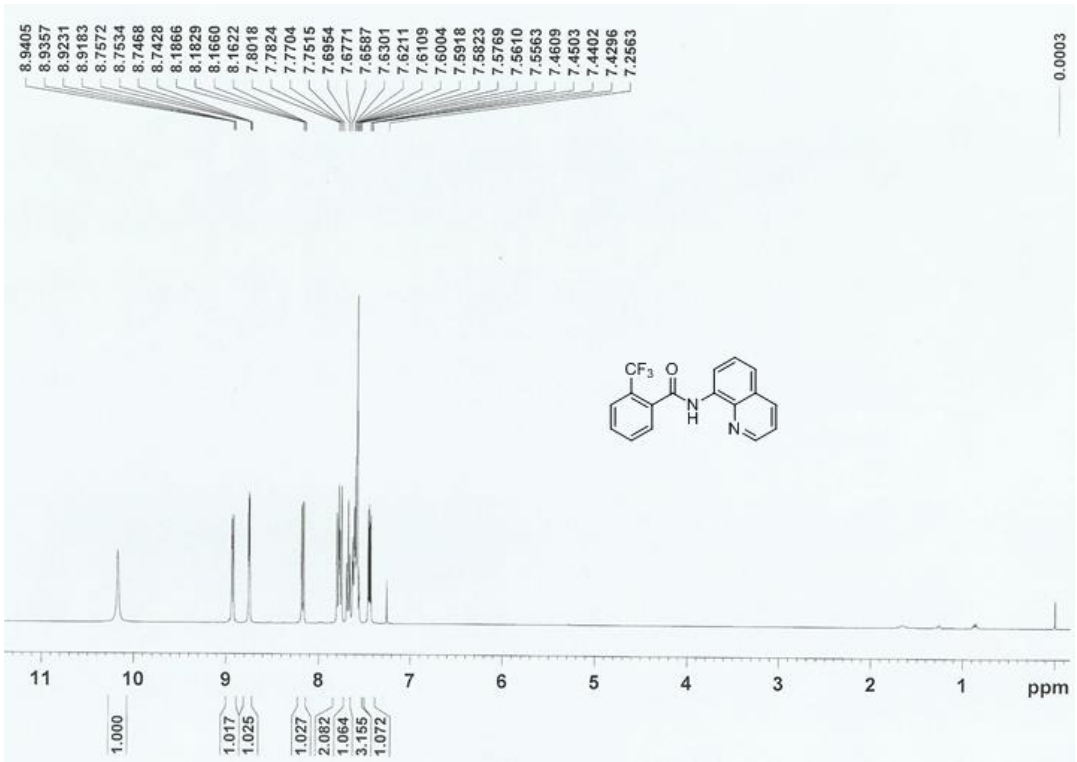
***N*-(quinolin-8-yl)-3-(trifluoromethyl)benzamide (1g)**

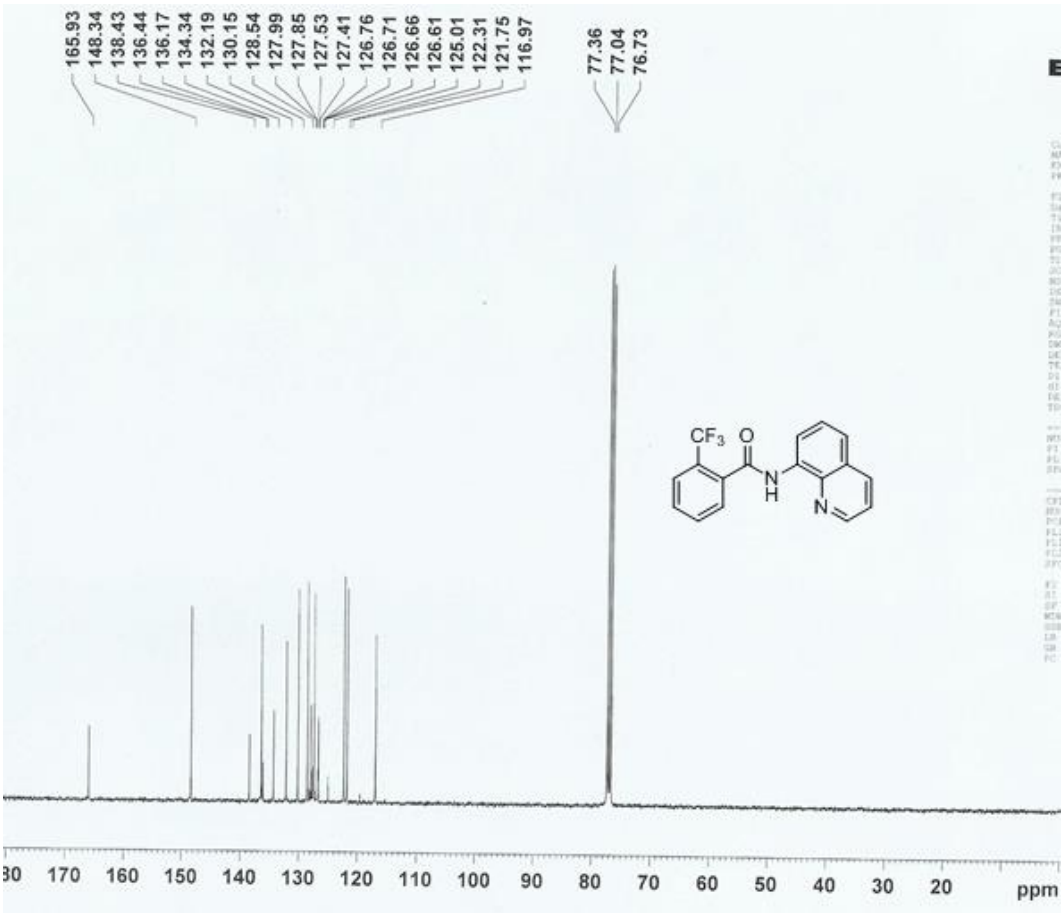


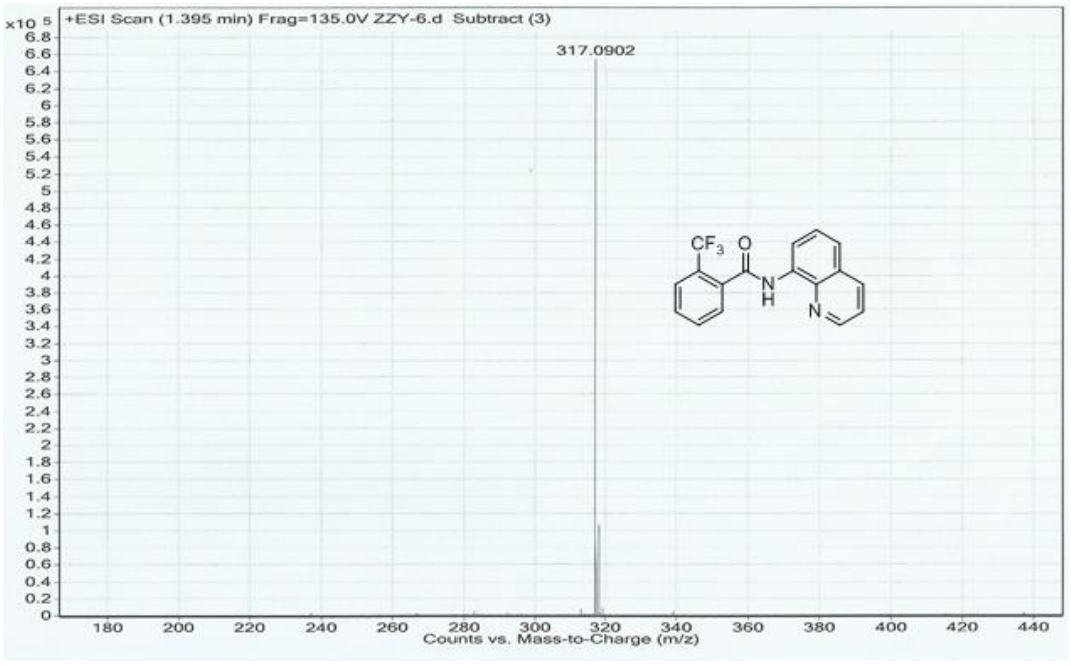




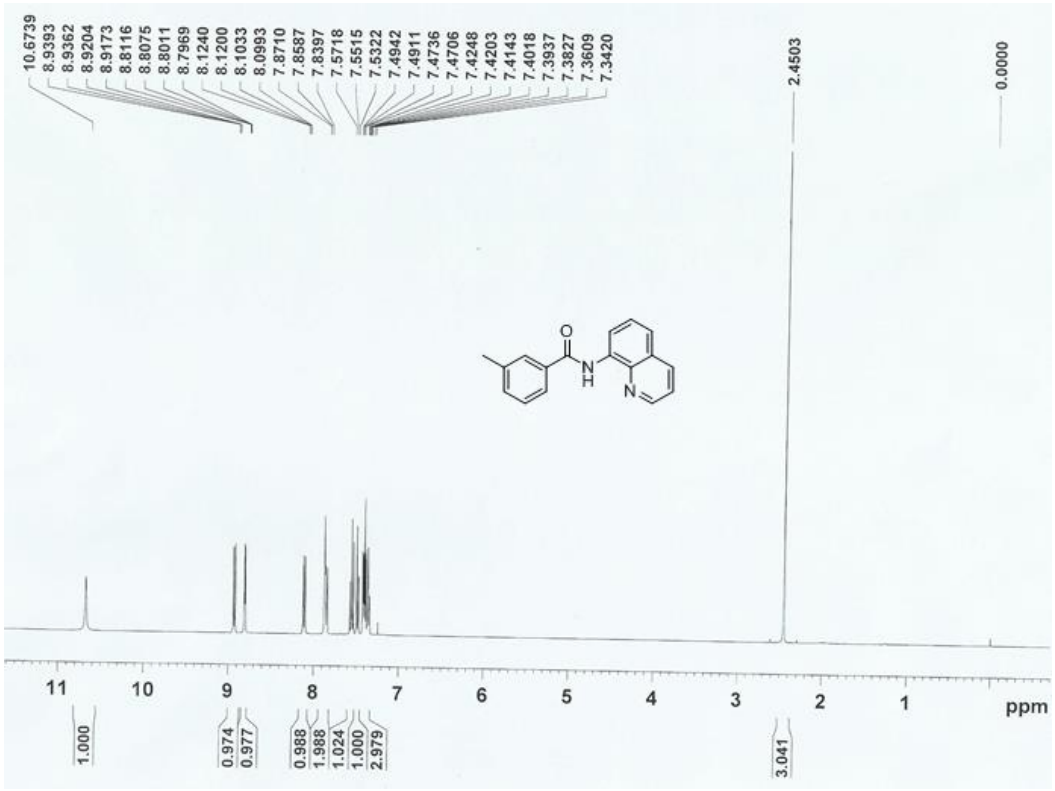
***N*-(quinolin-8-yl)-2-(trifluoromethyl)benzamide (1h)**

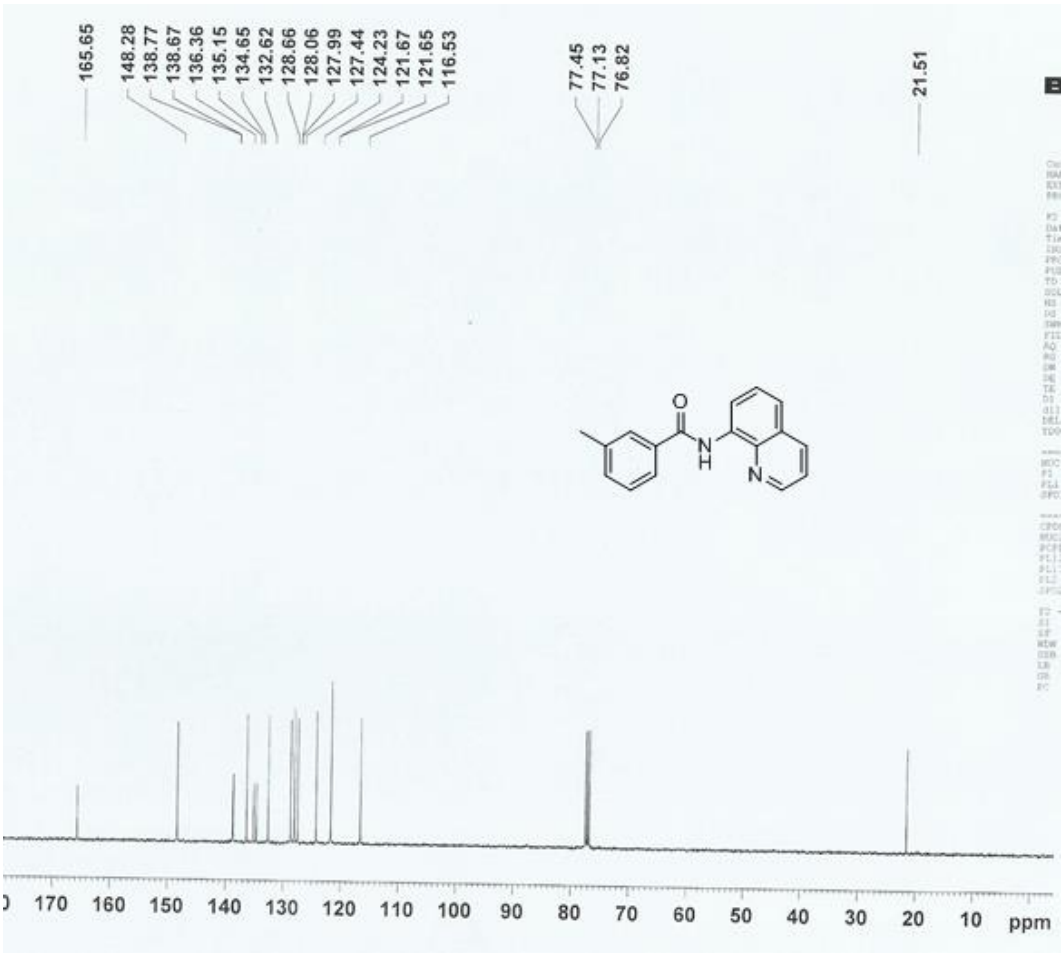


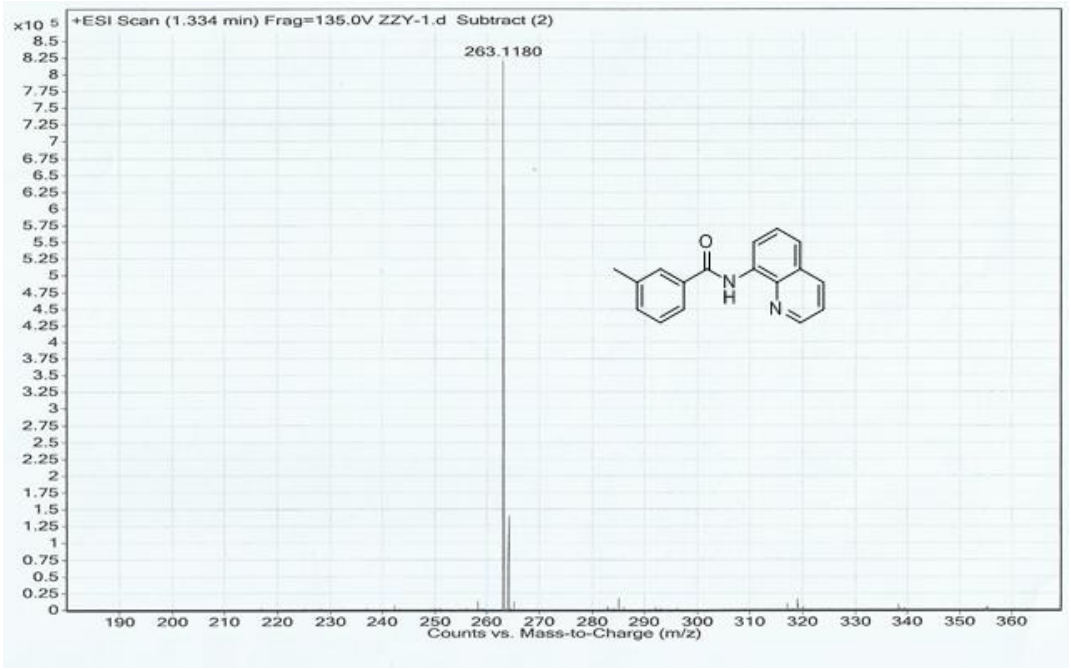

165.93
148.34
138.43
136.44
136.17
134.34
132.19
130.15
128.54
127.99
127.85
127.53
127.41
126.76
126.71
126.66
126.61
125.01
122.31
121.75
116.97
77.36
77.04
76.73
CF3
O
N
H
N
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


x10 5
+ESI Scan (1.395 min) Frag=135.0V ZZY-6.d Subtract (3)
317.0902
CF3
O
N
H
N
180
200
220
240
260
280
300
320
340
360
380
400
420
440
Counts vs. Mass-to-Charge (m/z)

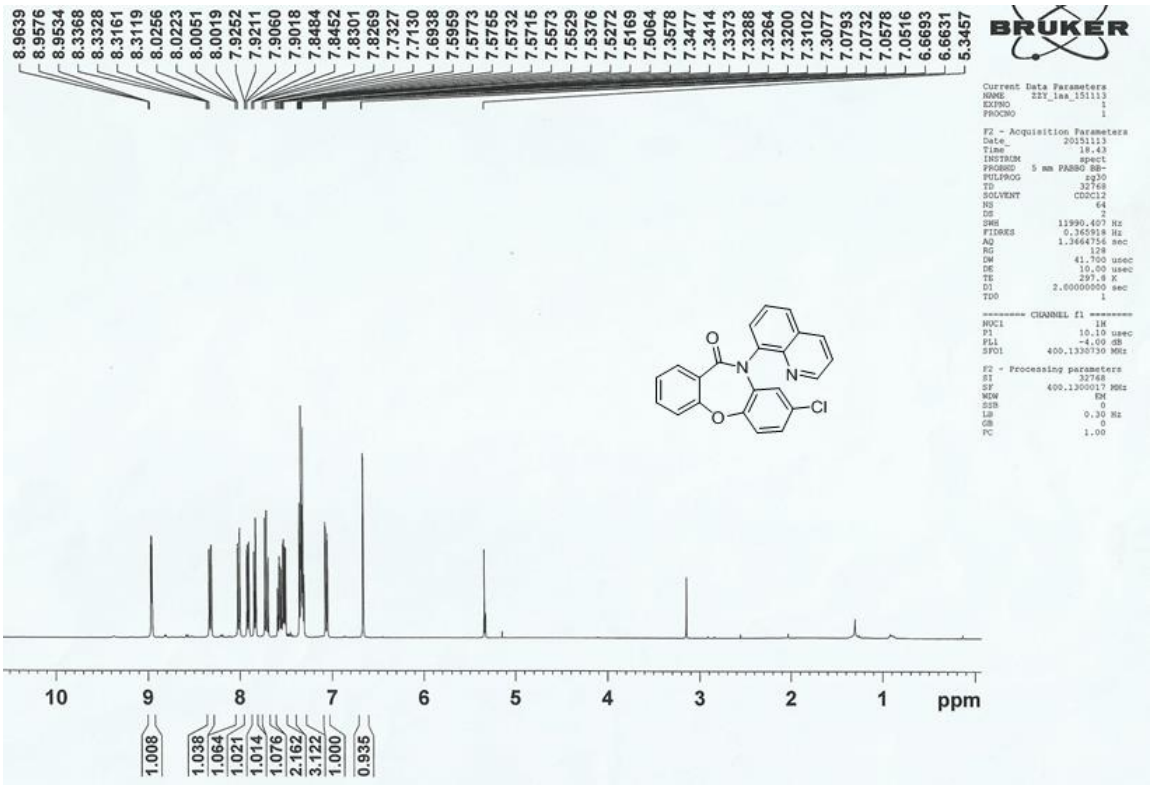
3-methyl-*N*-(quinolin-8-yl)benzamide (**1i**)

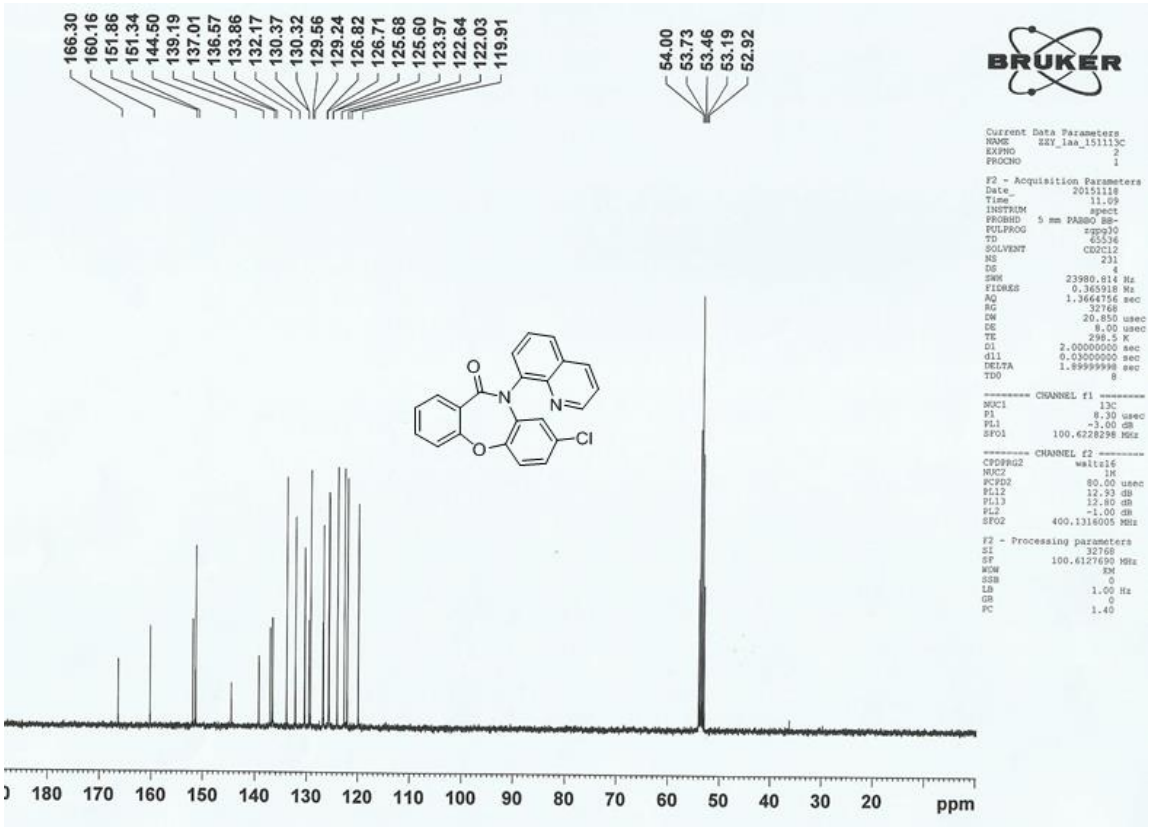


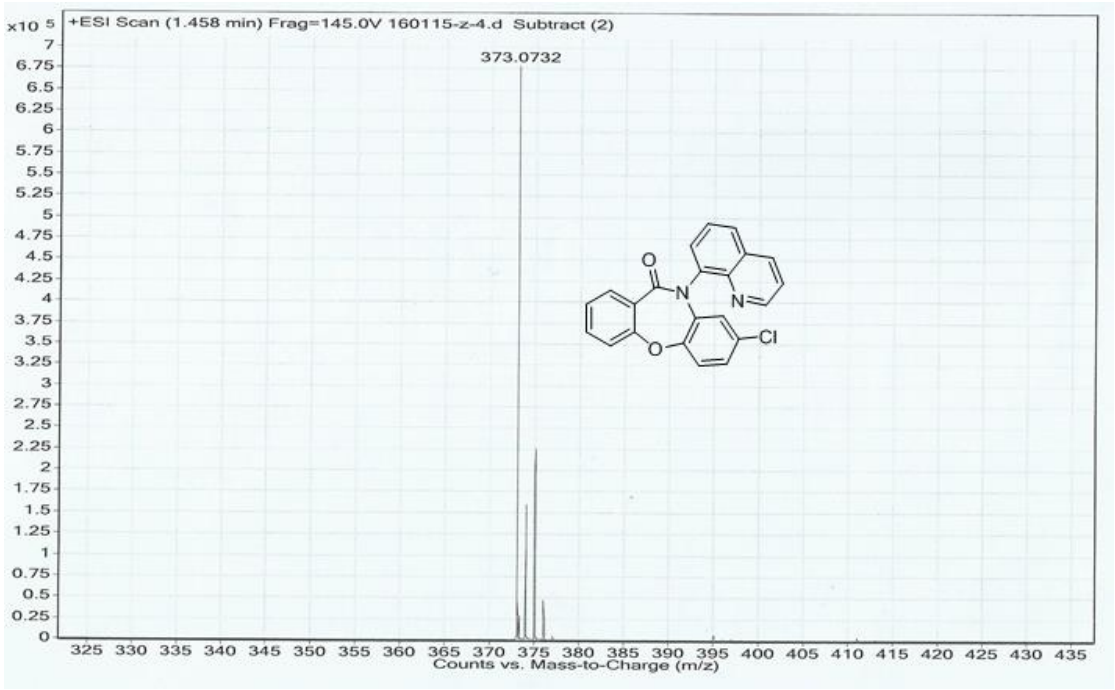




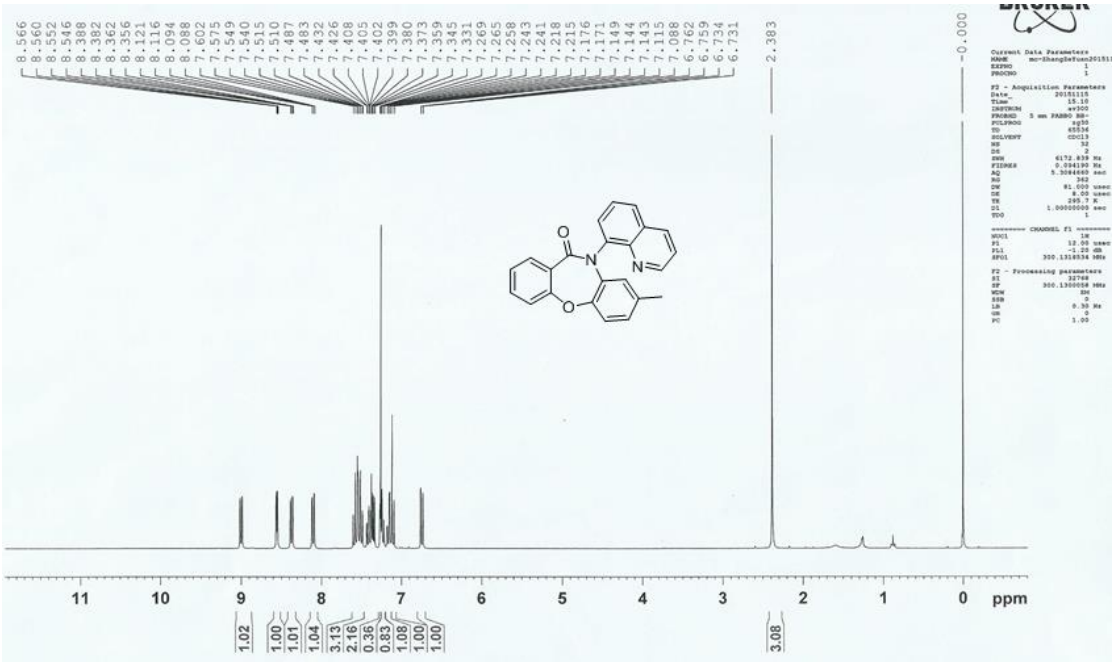
8-chloro-10-(quinolin-8-yl)dibenzo[b,f][1,4]oxazepin-11(10H)-one 3a

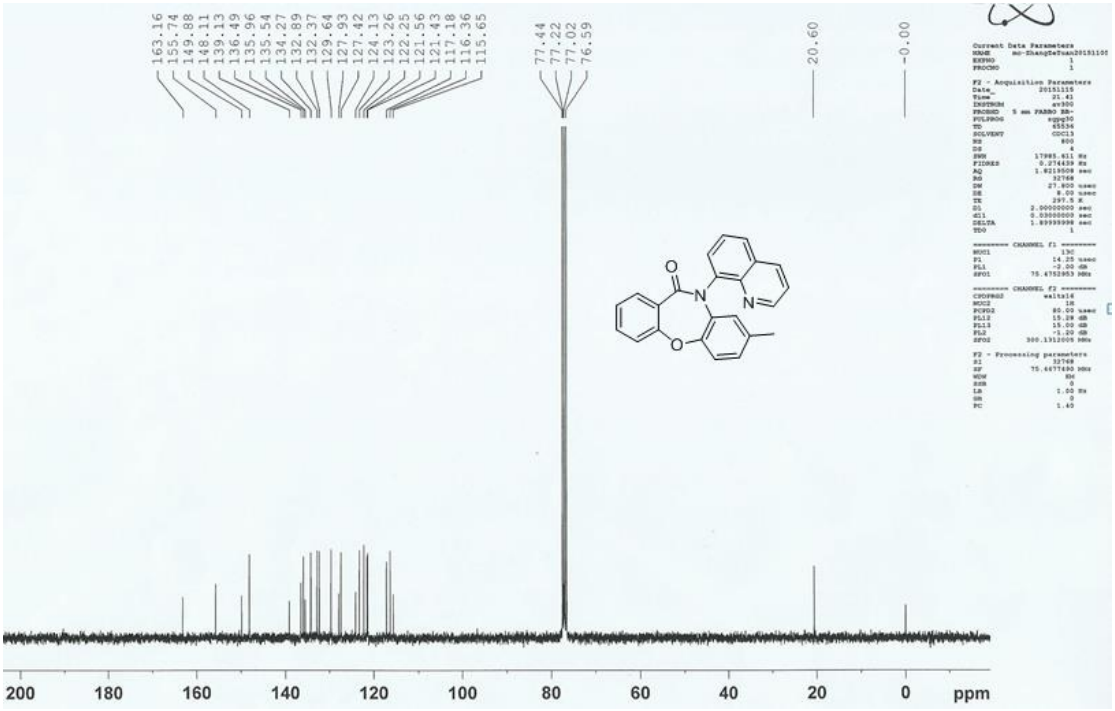


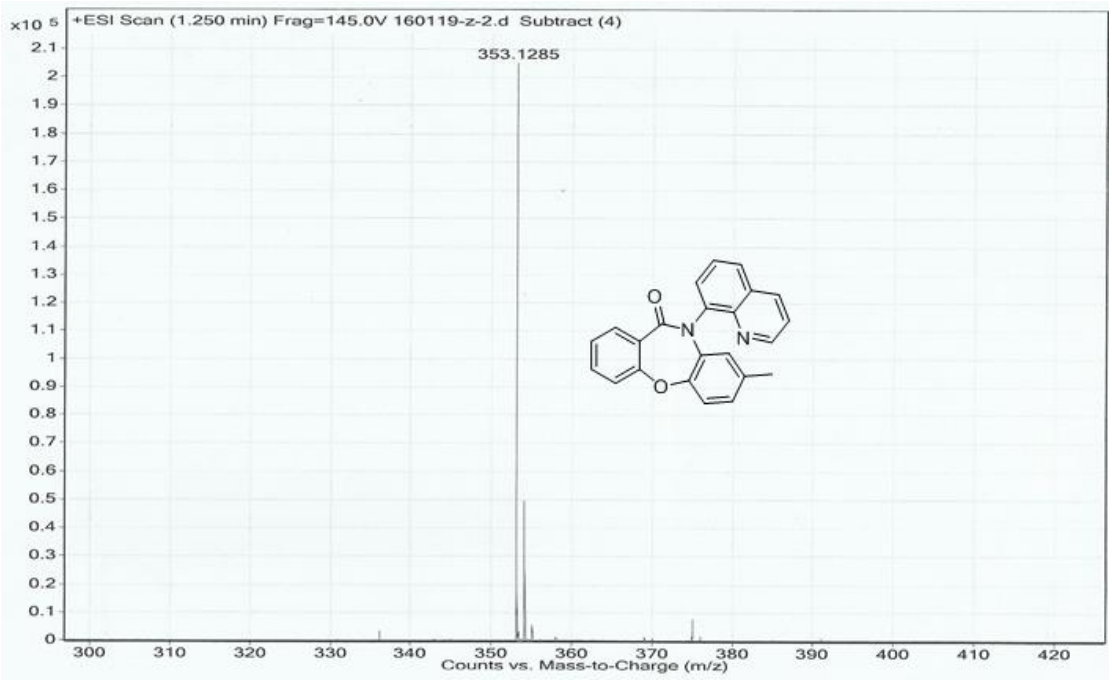

166.30
160.16
151.86
151.34
144.50
139.19
137.01
136.57
133.86
132.17
130.37
130.32
129.56
129.24
126.82
126.71
125.68
125.60
123.97
122.64
122.03
119.91
54.00
53.73
53.46
53.19
52.92
BRUKER
Current Data Parameters
NAME ZZY_laa_151113C
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20151118
Time 11.09
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CD2Cl2
NS 231
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 32768
DW 20.850 usec
DE 8.00 usec
TE 298.5 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 8
======== CHANNEL f1 ========
NUC1 13C
P1 8.30 usec
PL1 -3.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 12.93 dB
PL13 12.80 dB
PL2 -1.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
O
N
N
Cl
O
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20
ppm


x10 5
+ESI Scan (1.458 min) Frag=145.0V 160115-z-4.d Subtract (2)
373.0732
O
N
N
Cl
O
325 330 335 340 345 350 355 360 365 370 375 380 385 390 395 400 405 410 415 420 425 430 435
Counts vs. Mass-to-Charge (m/z)

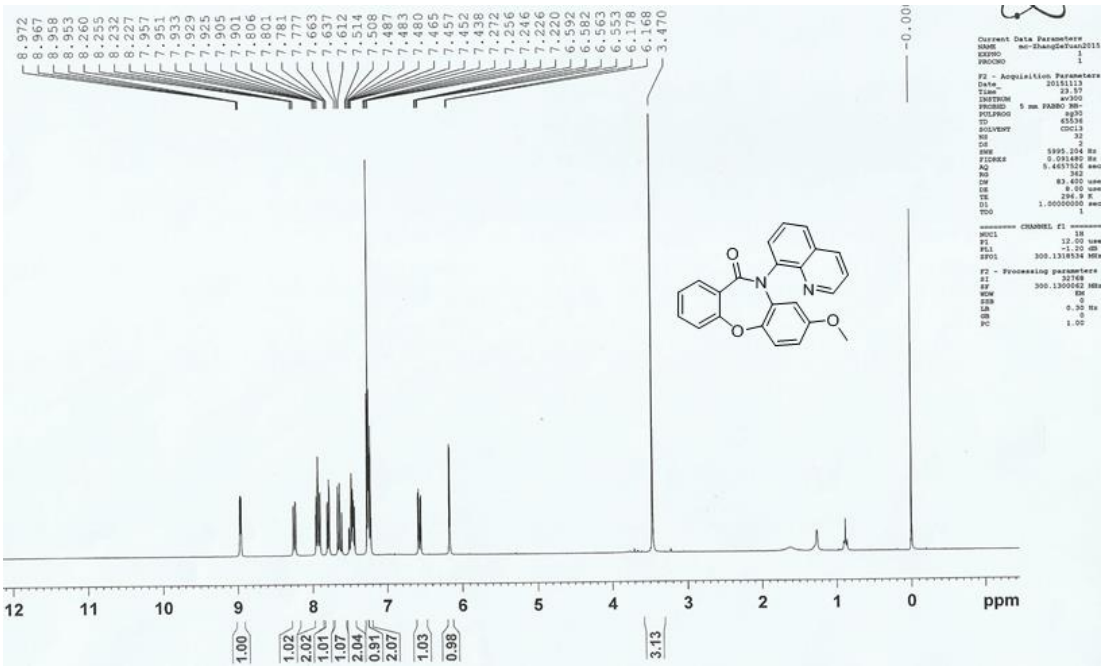
8-methyl-10-(quinolin-8-yl)dibenzo[b,f][1,4]oxazepin-11(10H)-one 3b

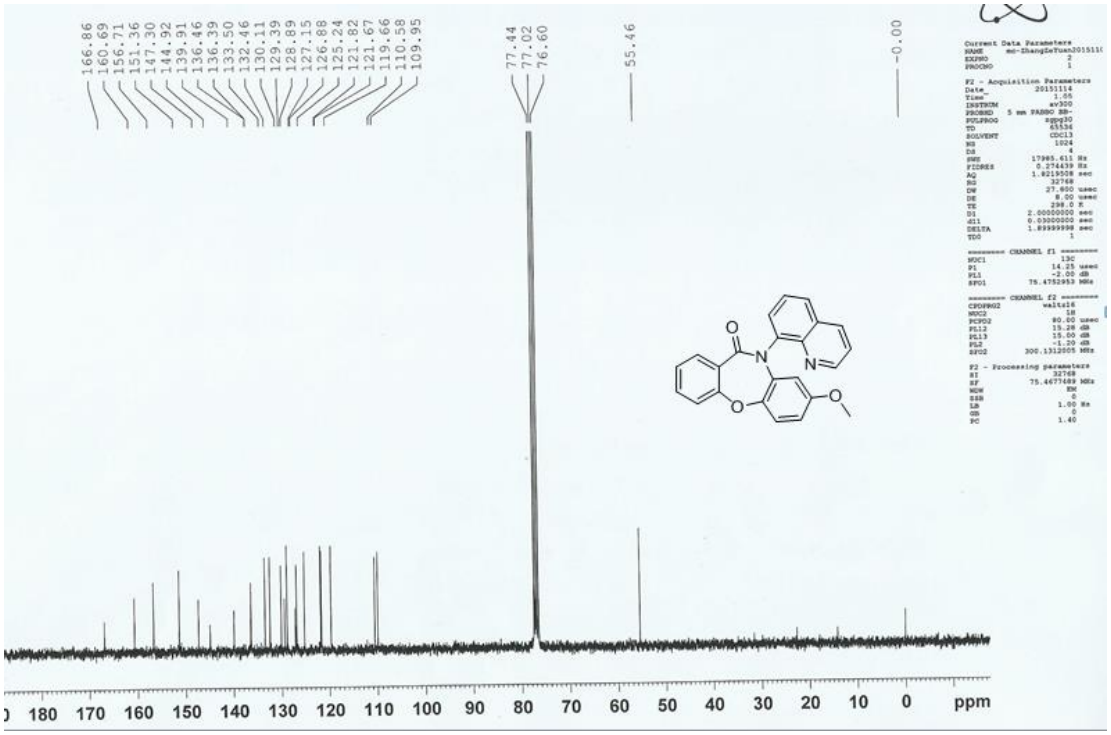


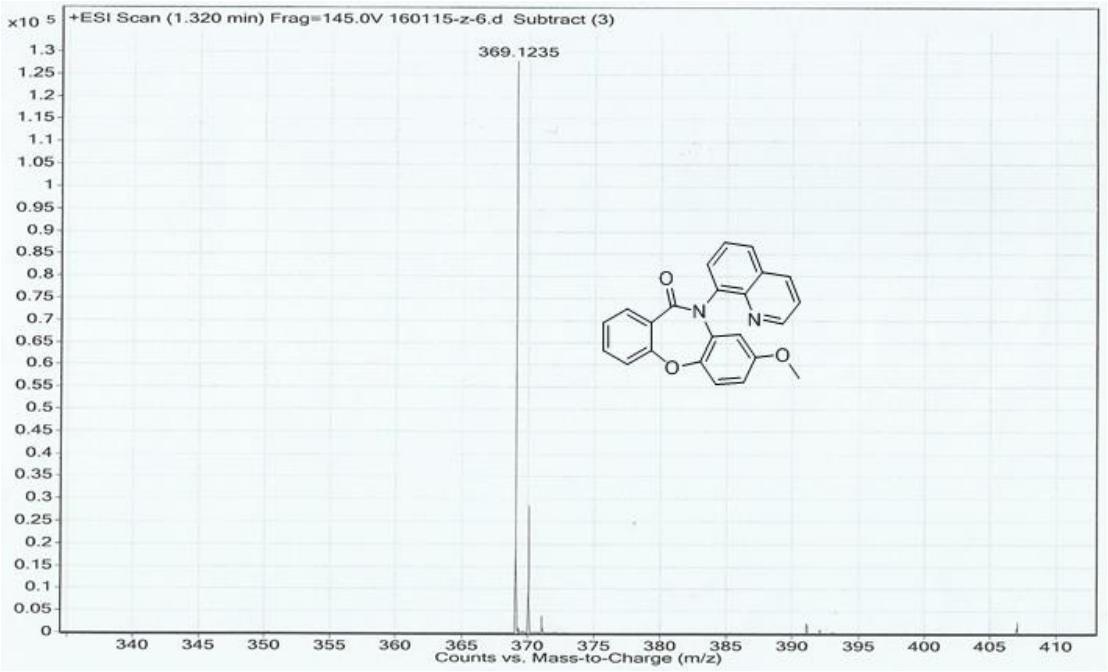




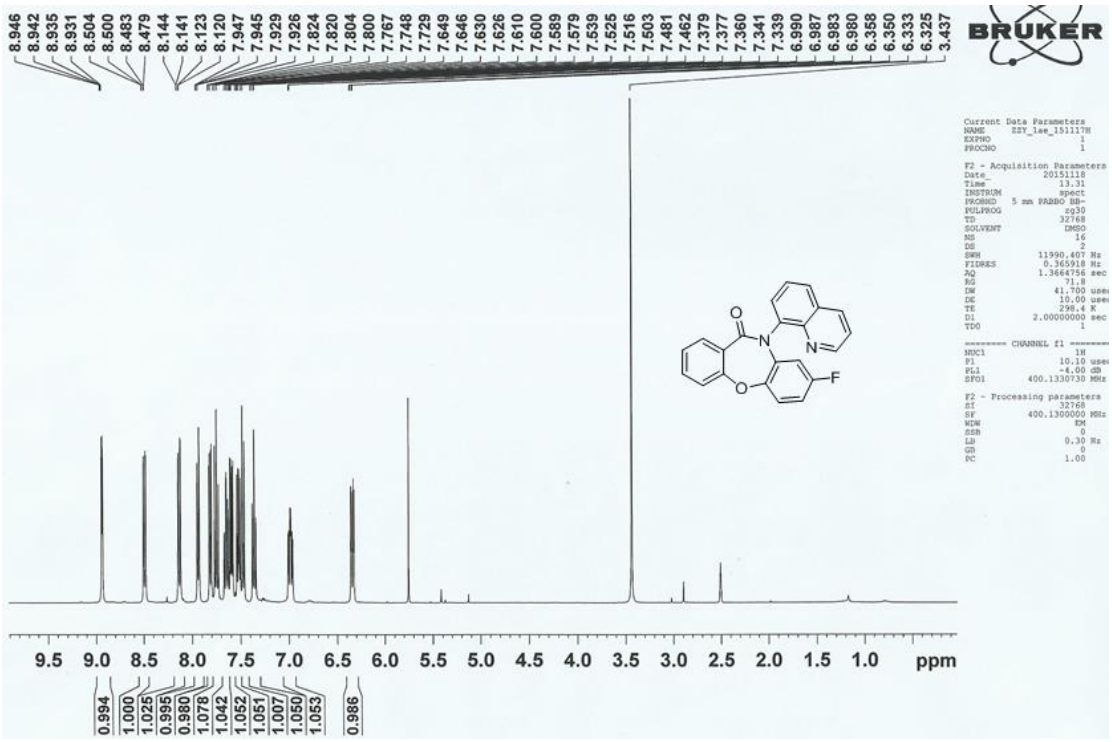
8-methoxy-10-(quinolin-8-yl)dibenzo[b,f][1,4]oxazepin-11(10H)-one 3c

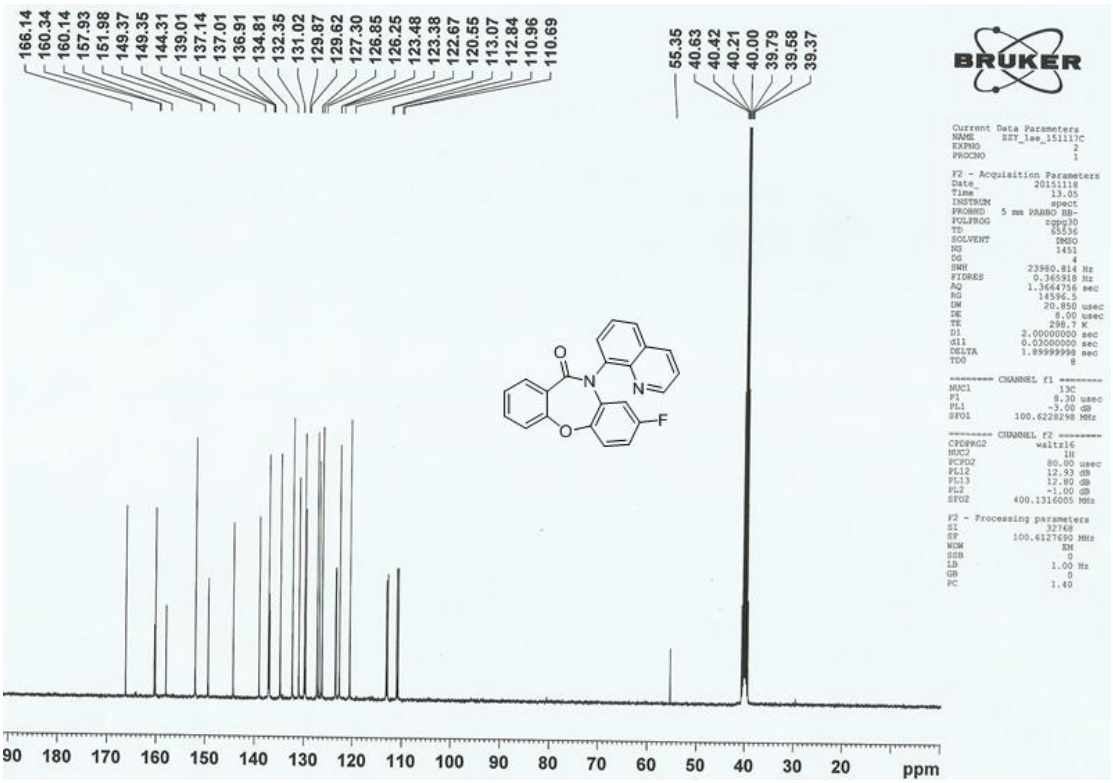


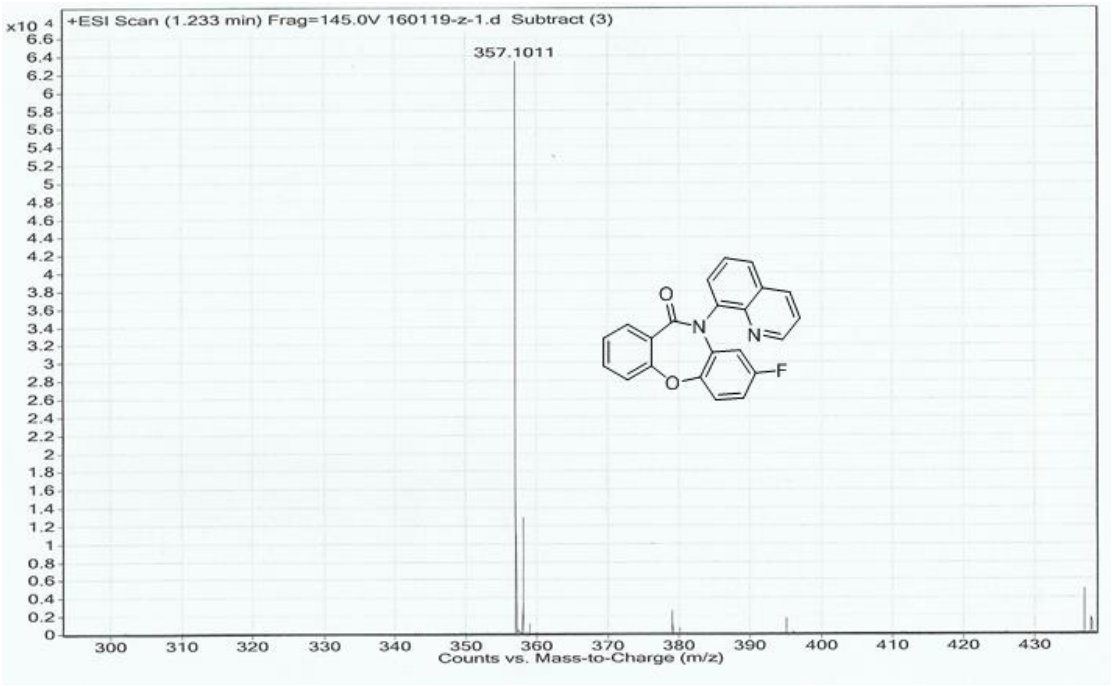

166.86
160.69
156.71
151.36
147.30
144.92
139.91
136.46
136.39
133.50
132.46
130.11
129.39
128.89
127.15
126.88
125.24
121.82
121.67
119.66
110.58
109.95
77.44
77.02
76.60
55.46
0.00
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


x10 5
+ESI Scan (1.320 min) Frag=145.0V 160115-z-6.d Subtract (3)
369.1235
1.3
1.25
1.2
1.15
1.1
1.05
1
0.95
0.9
0.85
0.8
0.75
0.7
0.65
0.6
0.55
0.5
0.45
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
340 345 350 355 360 365 370 375 380 385 390 395 400 405 410
Counts vs. Mass-to-Charge (m/z)

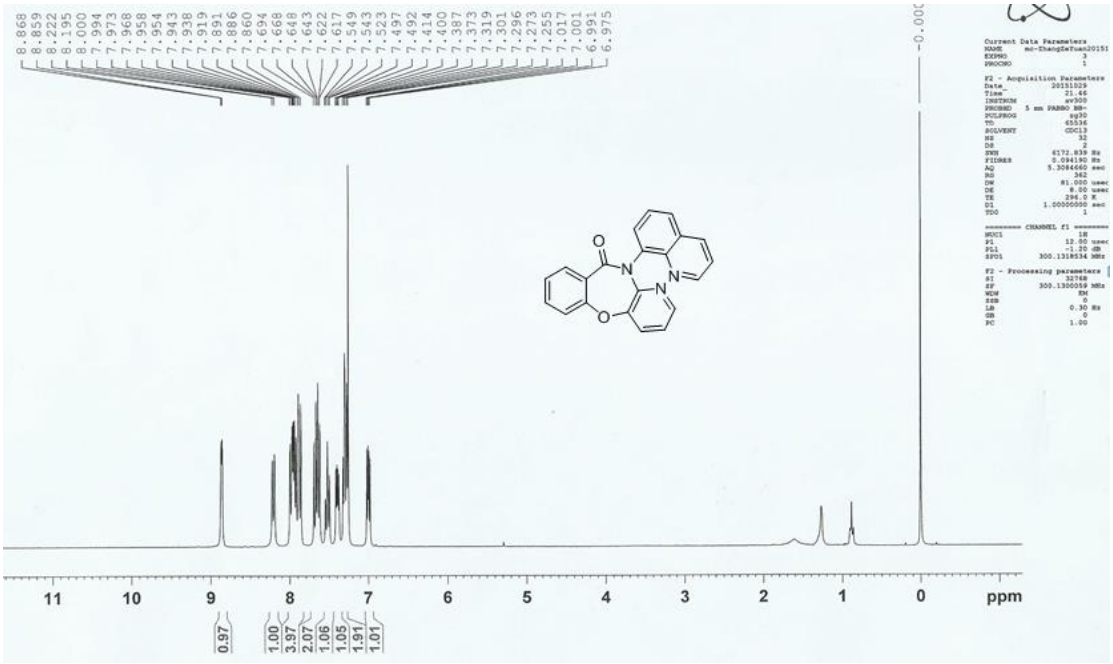
8-fluoro-10-(quinolin-8-yl)dibenzo[b,f][1,4]oxazepin-11(10H)-one 3d

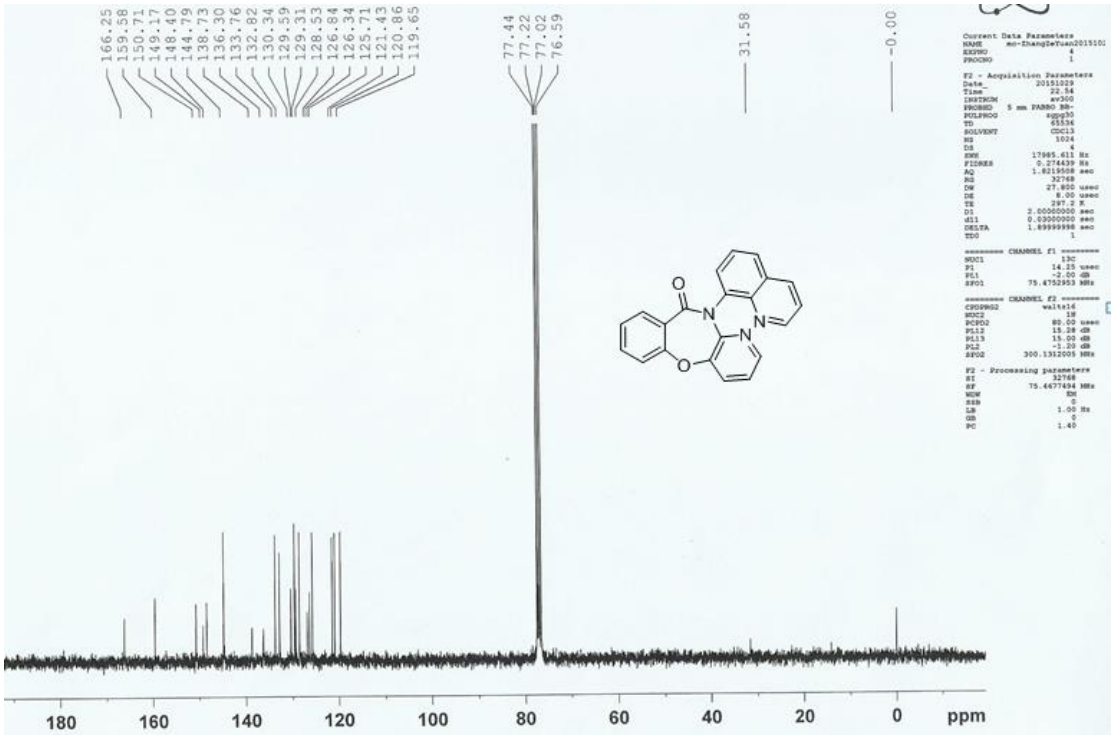


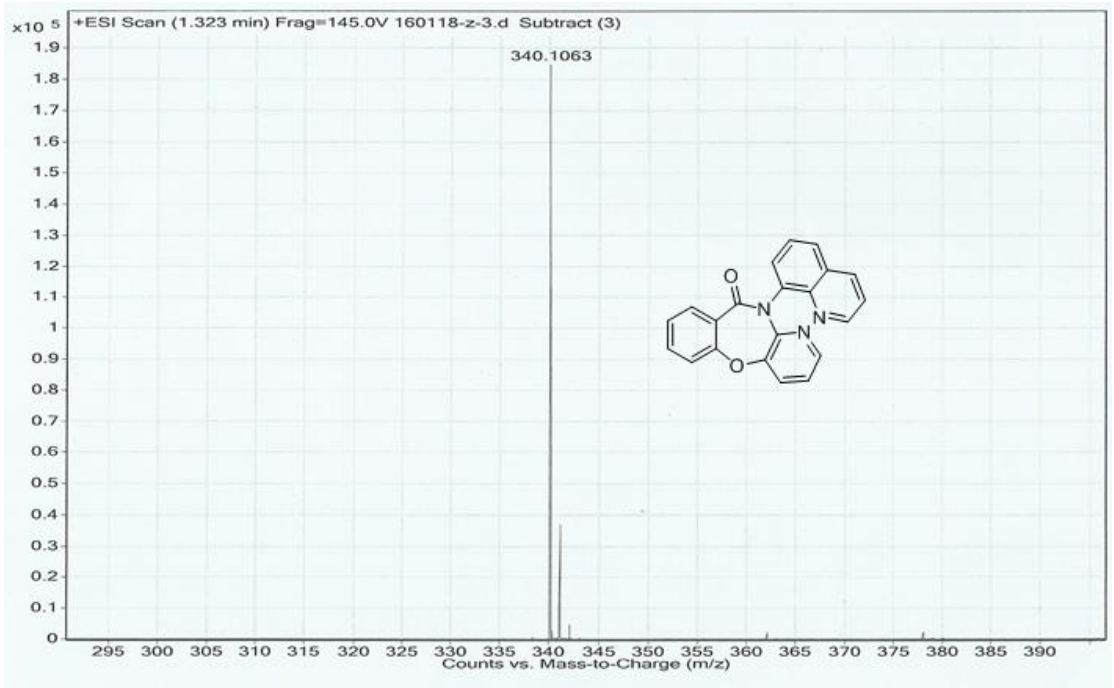




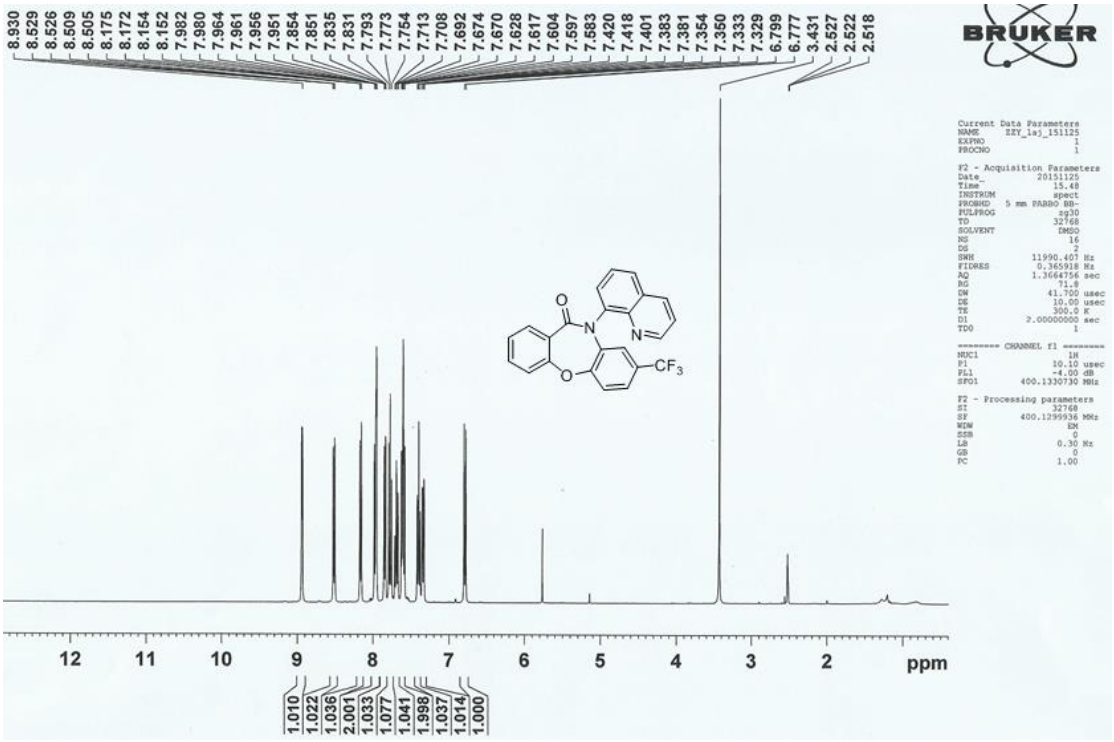
11-(quinolin-8-yl)benzo[f]pyrido[3,2-b][1,4]oxazepin-10(11H)-one 3e

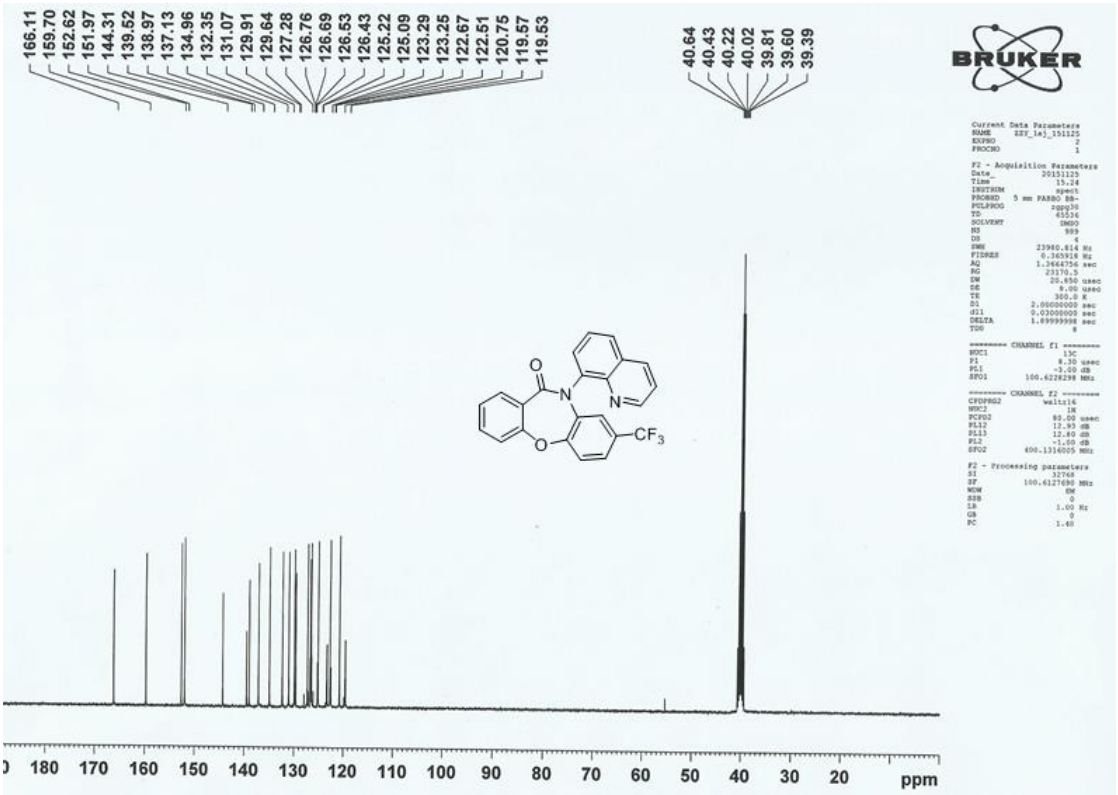


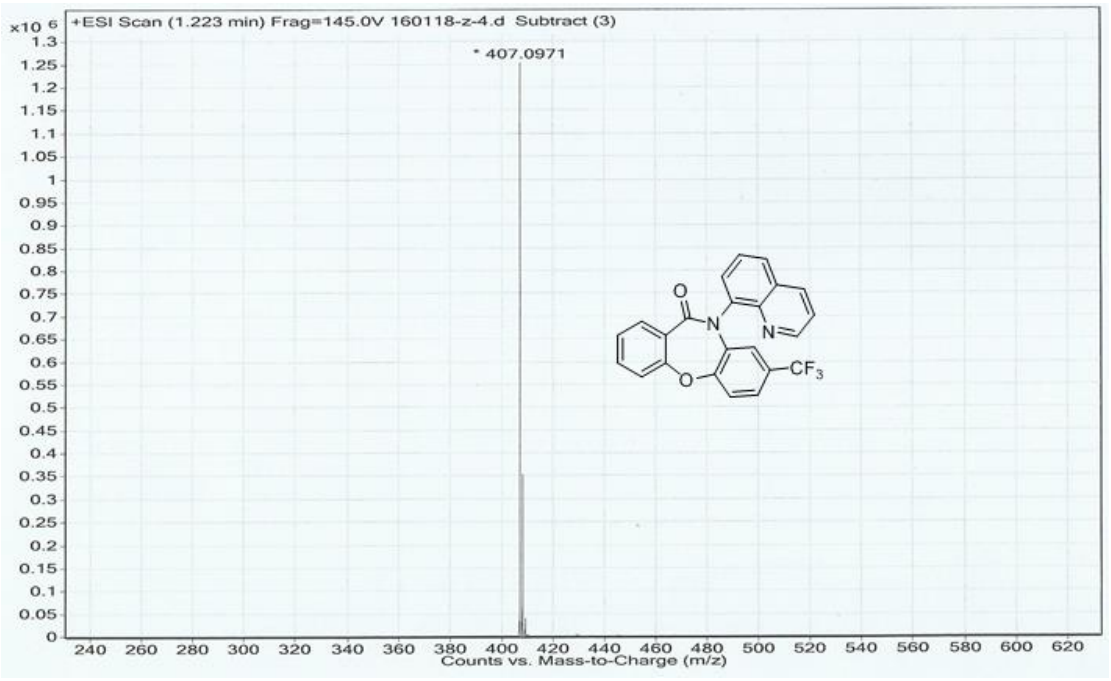

166.25
159.58
150.71
149.17
148.40
144.79
138.73
136.30
133.76
132.82
130.34
129.59
129.31
128.53
126.84
126.34
125.71
121.43
120.86
119.65
77.44
77.22
77.02
76.59
31.58
0.00
180
160
140
120
100
80
60
40
20
0
ppm


x10 5
+ESI Scan (1.323 min) Frag=145.0V 160118-z-3.d Subtract (3)
340.1063
Counts vs. Mass-to-Charge (m/z)

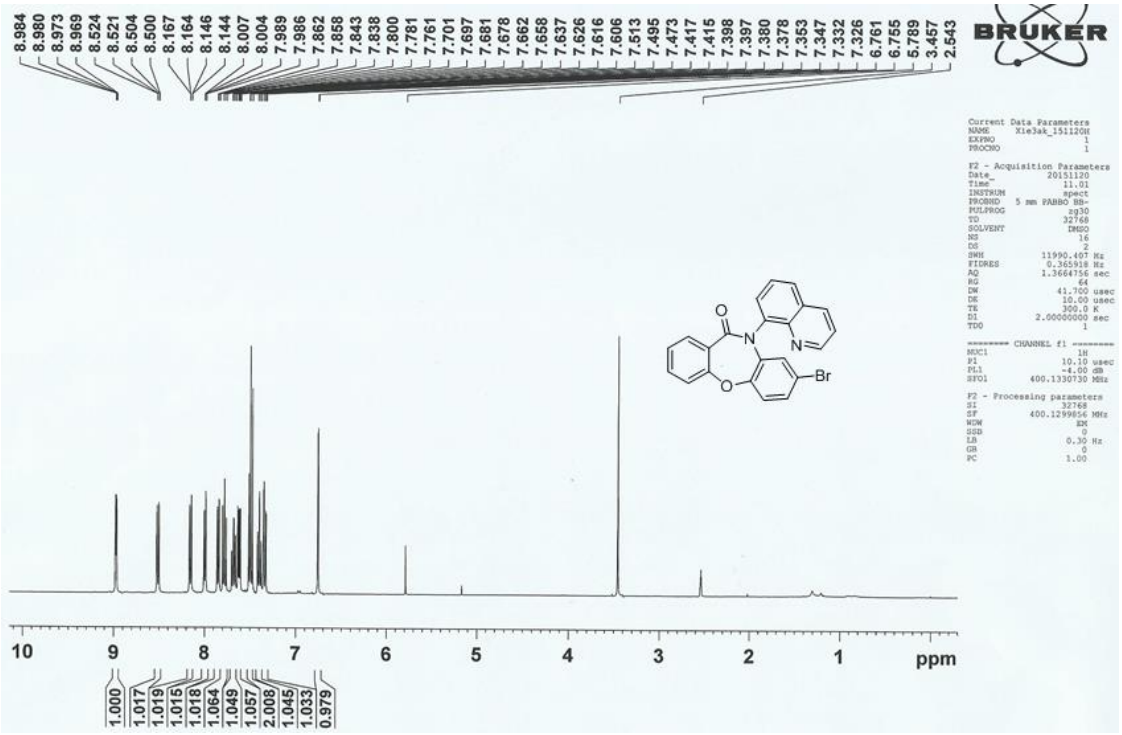
10-(quinolin-8-yl)-8-(trifluoromethyl)dibenzo[b,f][1,4]oxazepin-11(10H)-one 3f

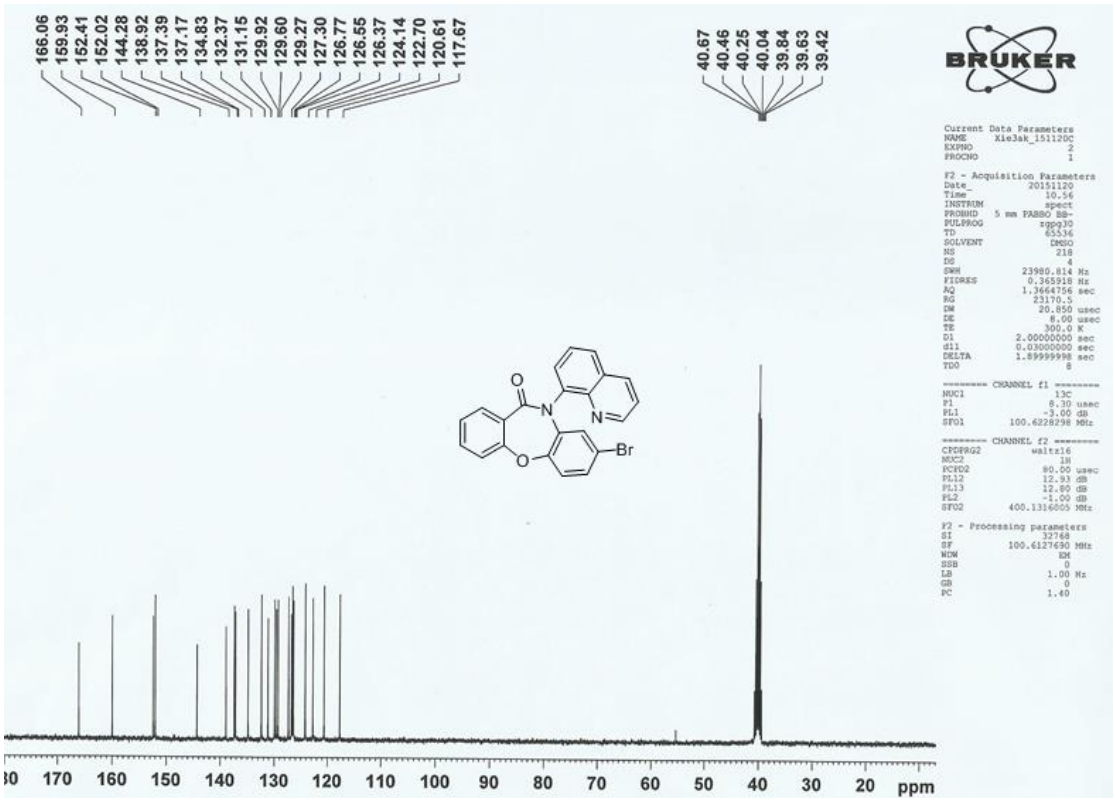


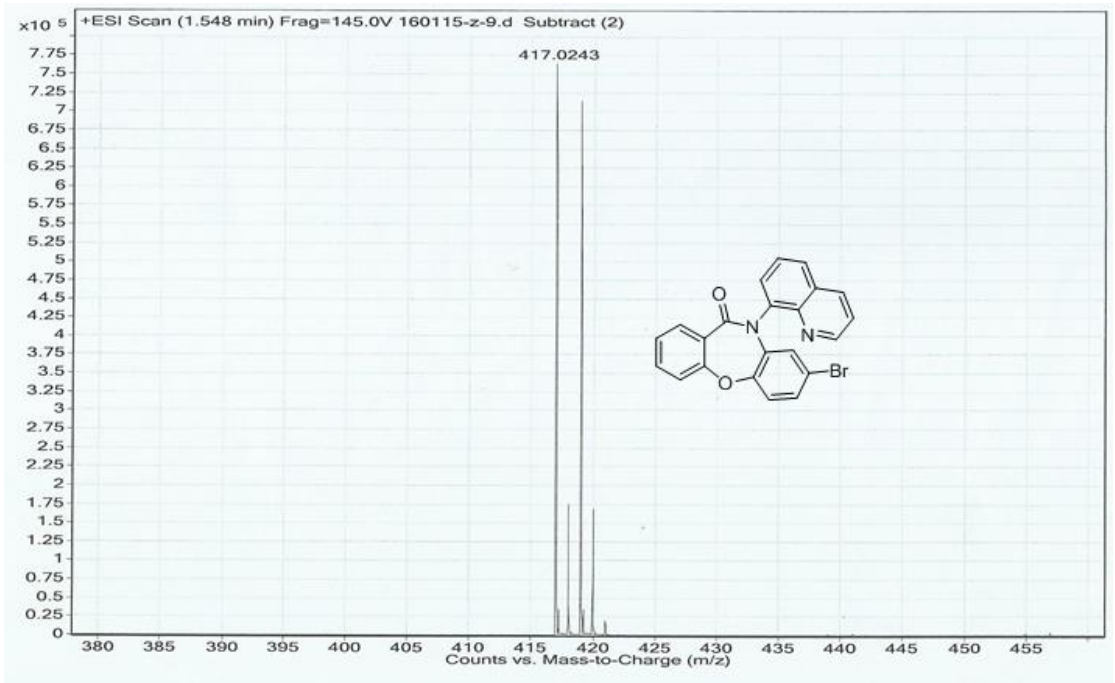




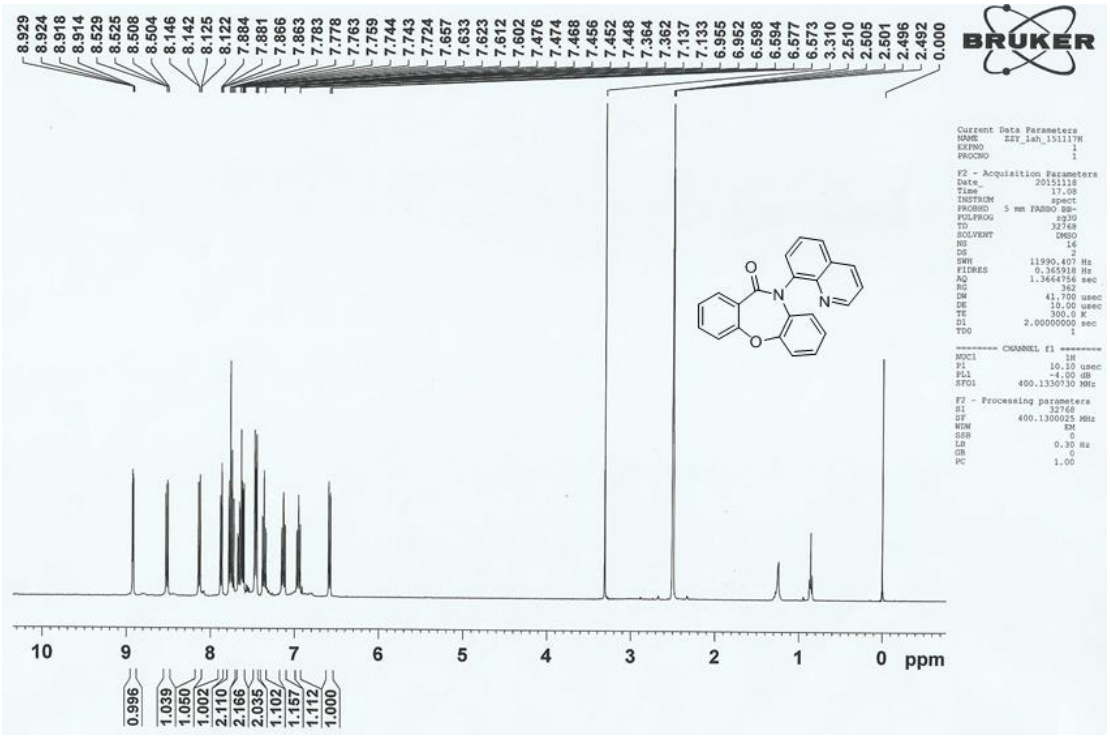
8-bromo-10-(quinolin-8-yl)dibenzo[b,f][1,4]oxazepin-11(10H)-one 3g

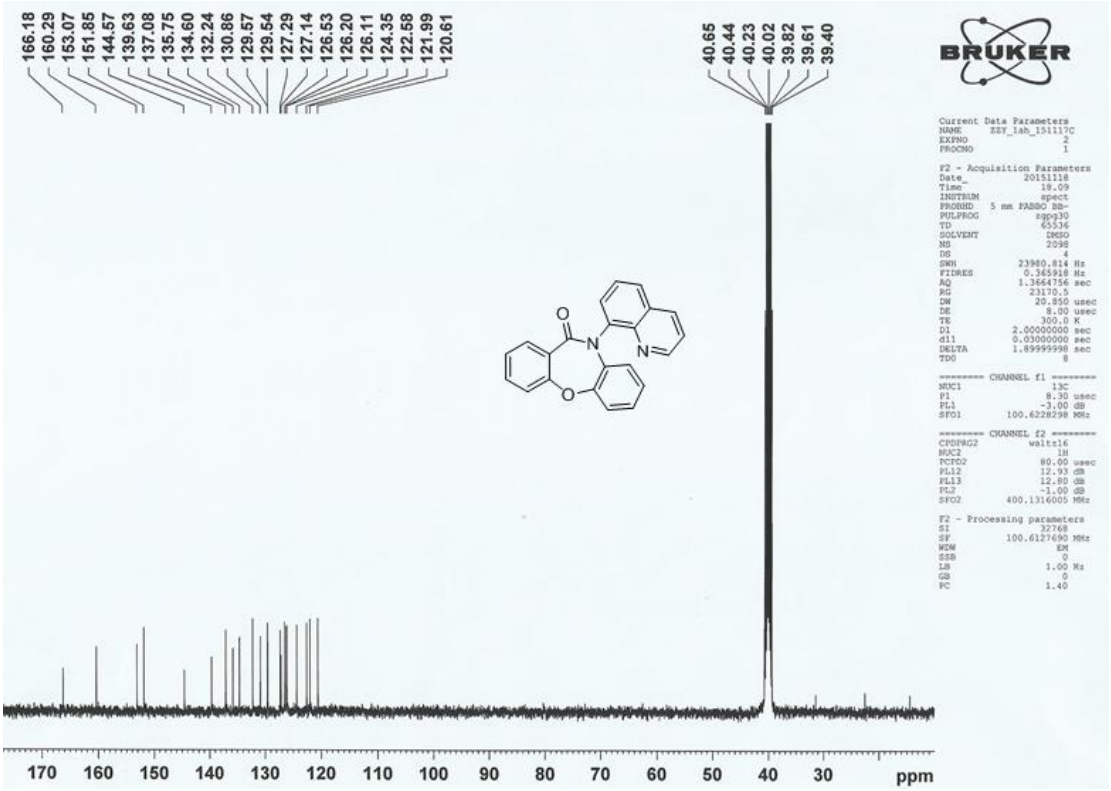


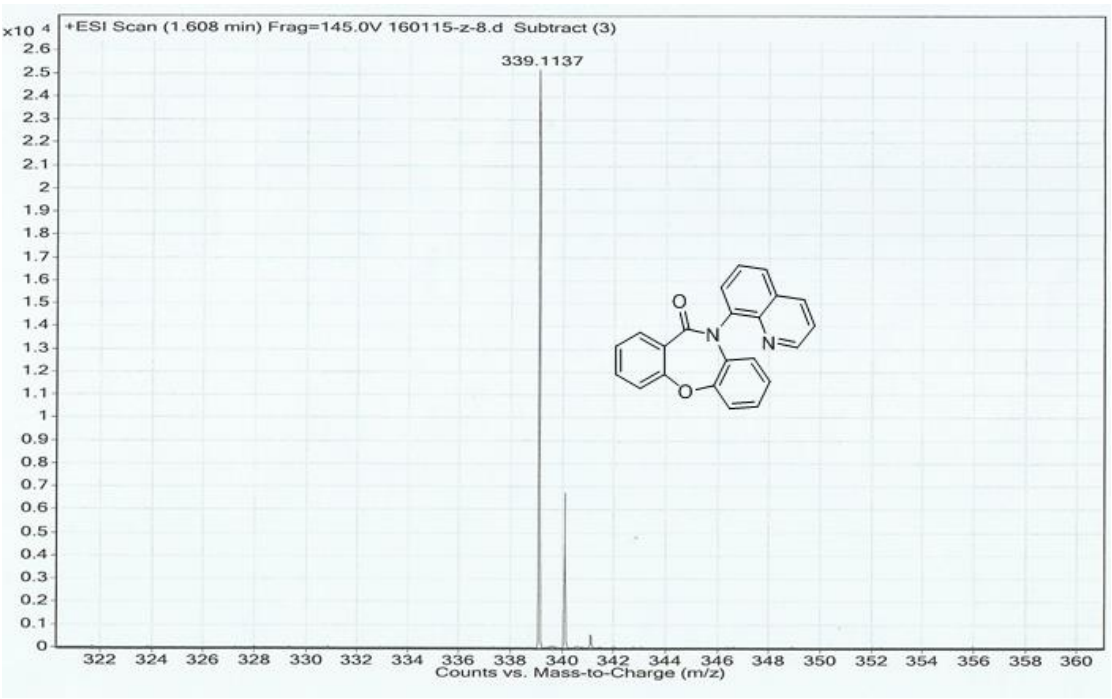

166.06
159.93
152.41
152.02
144.28
138.92
137.39
137.17
134.83
132.37
131.15
129.92
129.60
129.27
127.30
126.77
126.55
126.37
124.14
122.70
120.61
117.67
40.67
40.46
40.25
40.04
39.84
39.63
39.42
BRUKER
Current Data Parameters
NAME Xie3ak_151120C
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20151120
Time 10.56
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 218
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 23170.5
DW 20.850 usec
DE 8.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 8
======== CHANNEL f1 ========
NUC1 13C
P1 8.30 usec
PL1 -3.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 12.93 dB
PL13 12.80 dB
PL2 -1.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
O
N
N
Br
O
30 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


x10 5
+ESI Scan (1.548 min) Frag=145.0V 160115-z-9.d Subtract (2)
417.0243
7.75
7.5
7.25
7
6.75
6.5
6.25
6
5.75
5.5
5.25
5
4.75
4.5
4.25
4
3.75
3.5
3.25
3
2.75
2.5
2.25
2
1.75
1.5
1.25
1
0.75
0.5
0.25
0
380 385 390 395 400 405 410 415 420 425 430 435 440 445 450 455
Counts vs. Mass-to-Charge (m/z)
O
N
N
Br
O

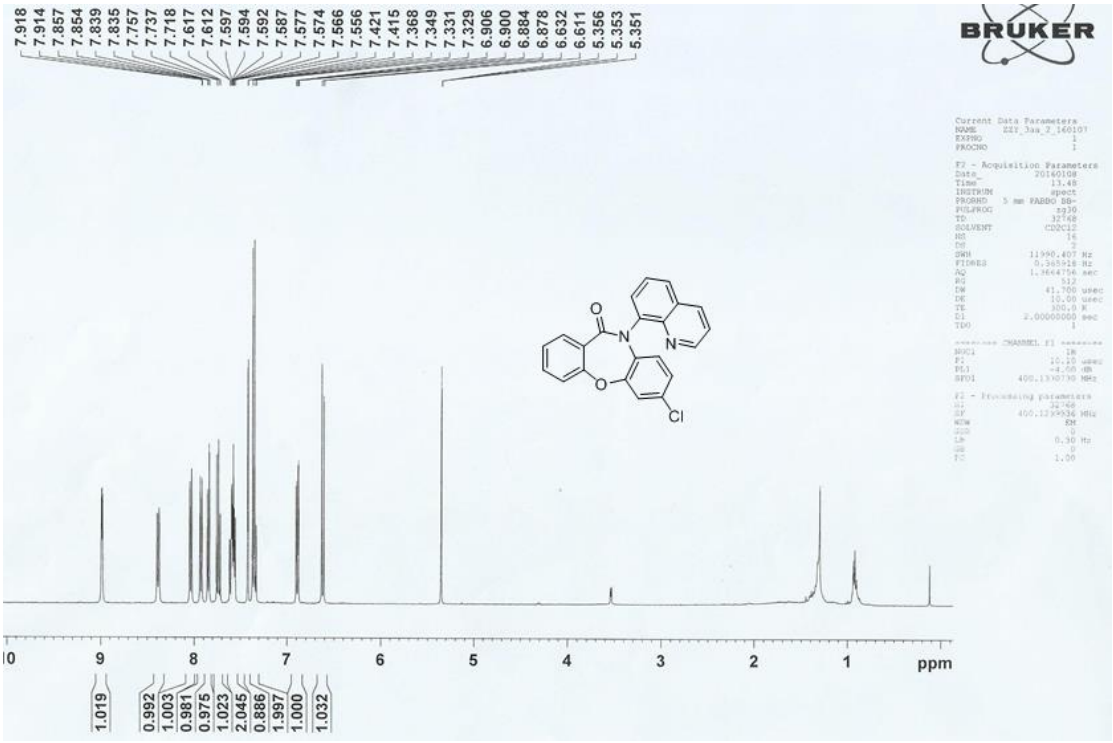
10-(quinolin-8-yl)dibenzo[b,f][1,4]oxazepin-11(10H)-one 3h

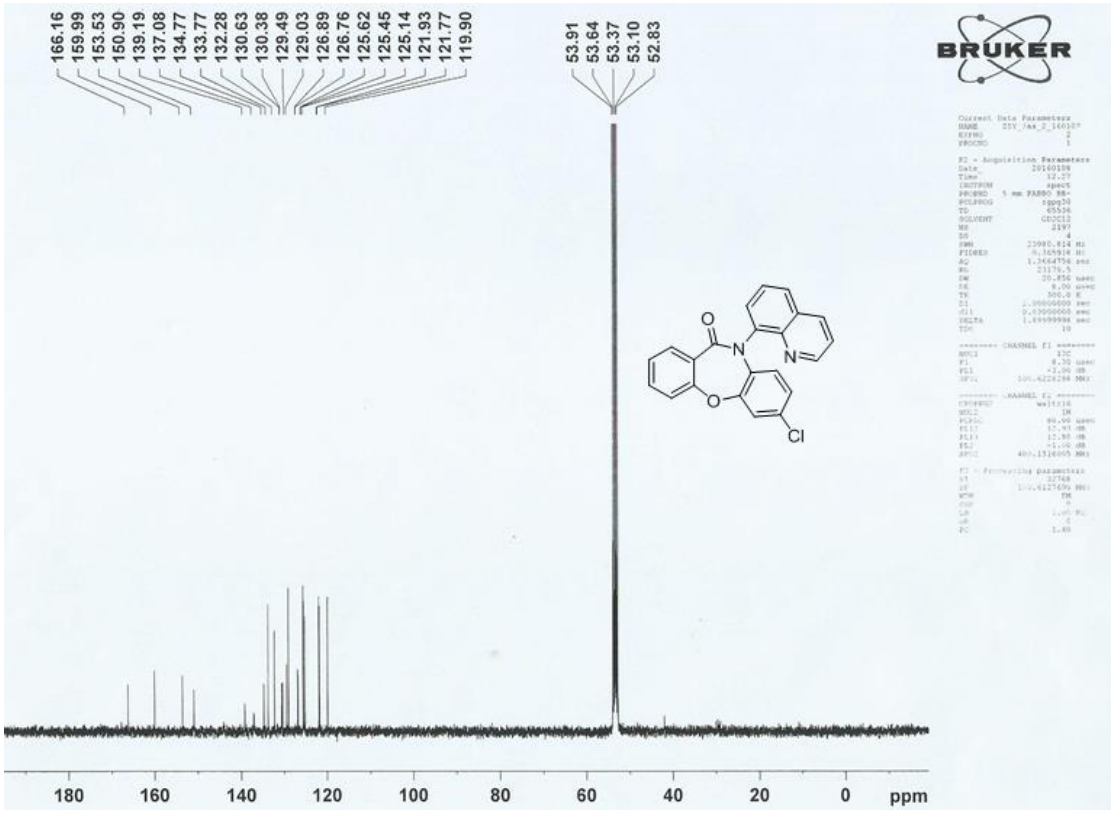


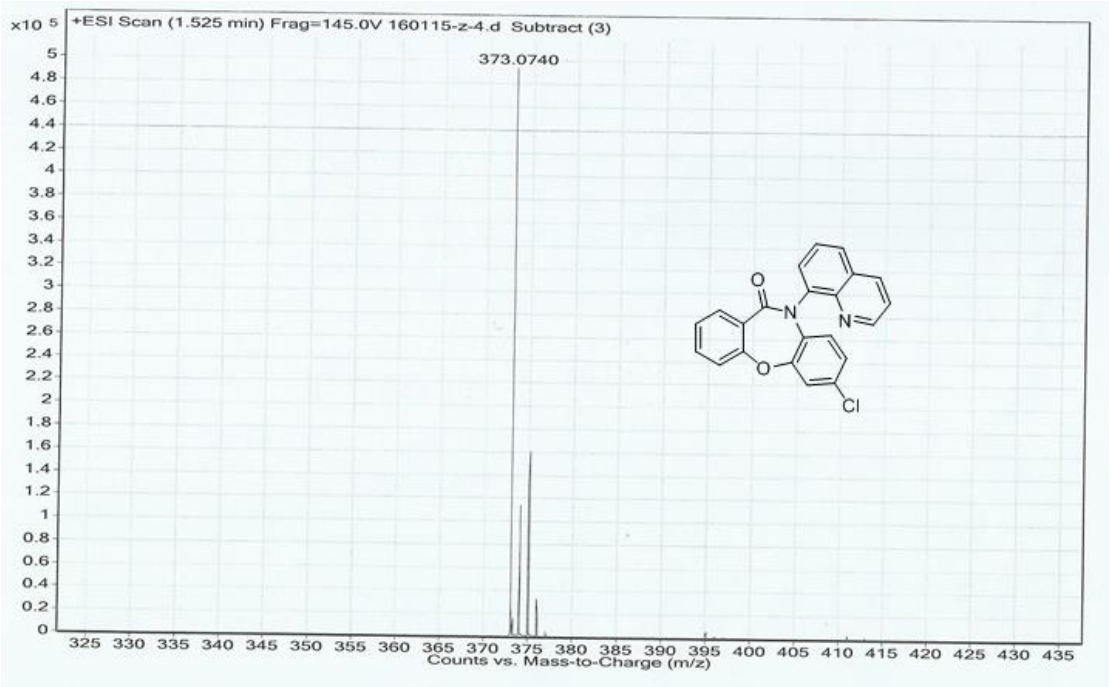




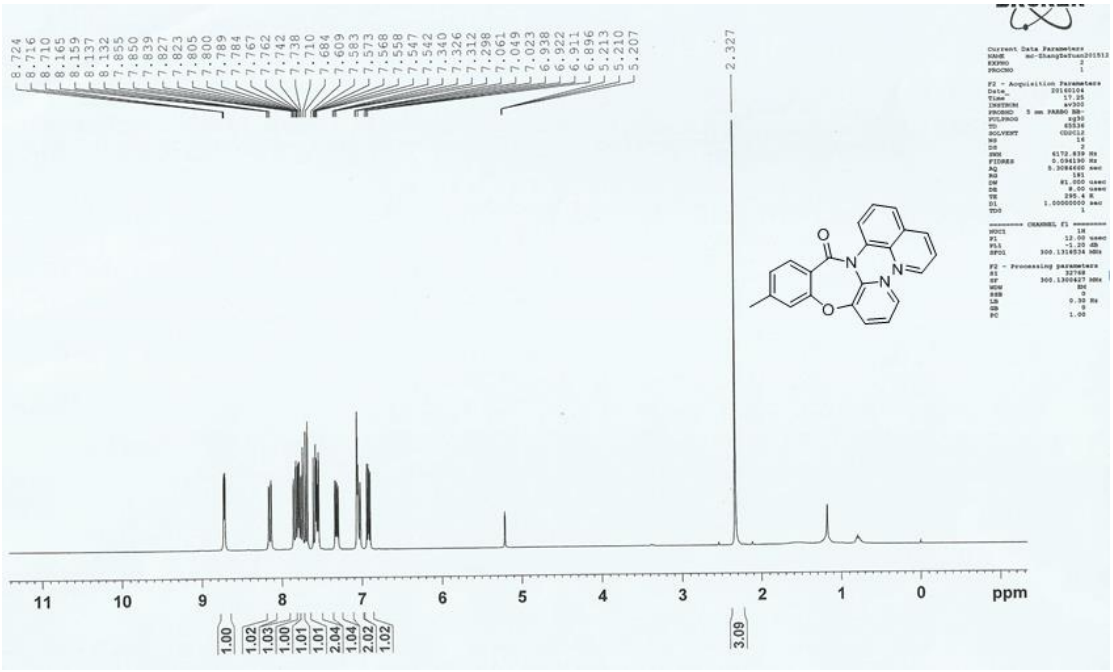
7-chloro-10-(quinolin-8-yl)dibenzo[b,f][1,4]oxazepin-11(10H)-one 3i

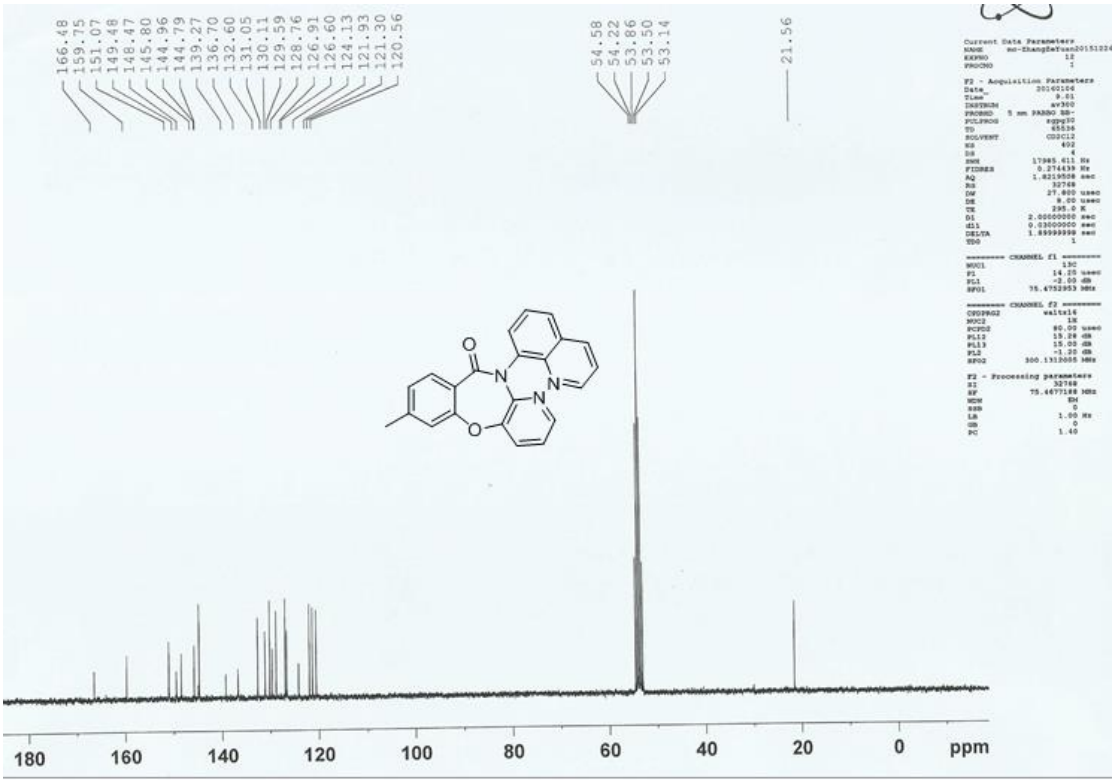


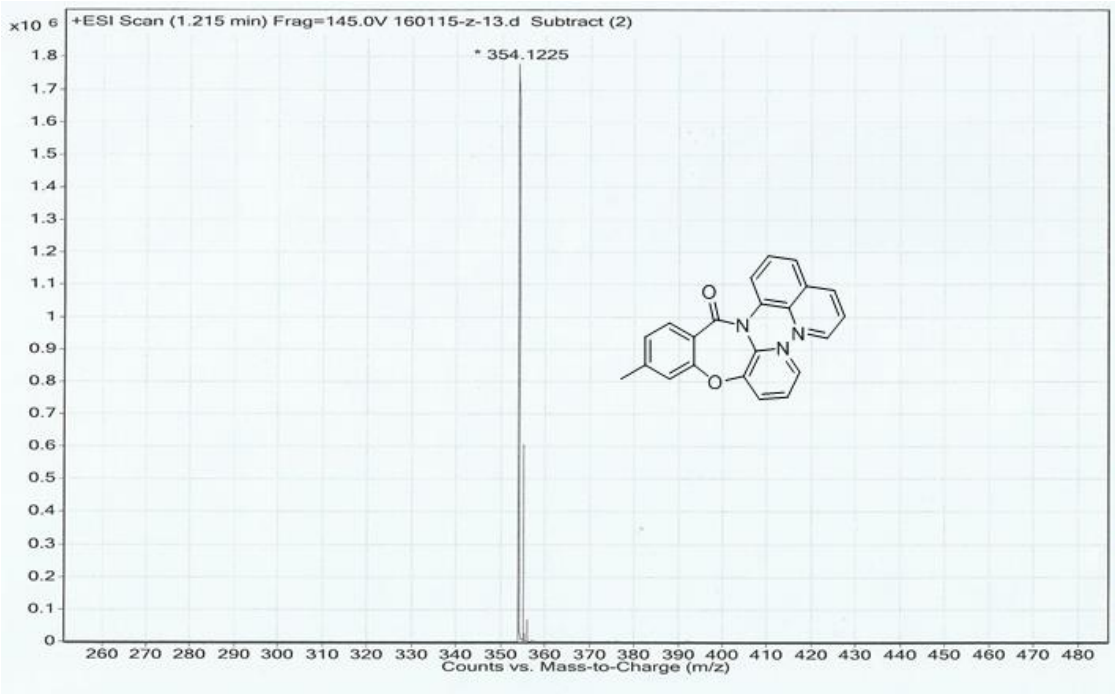

166.16
159.99
153.53
150.90
139.19
137.08
134.77
133.77
132.28
130.63
130.38
129.49
129.03
126.89
126.76
125.62
125.45
125.14
121.93
121.77
119.90
53.91
53.64
53.37
53.10
52.83
BRUKER
O
N
N
O
Cl
180
160
140
120
100
80
60
40
20
0
ppm


x10 5
+ESI Scan (1.525 min) Frag=145.0V 160115-z-4.d Subtract (3)
373.0740
O
N
N
O
Cl
Counts vs. Mass-to-Charge (m/z)

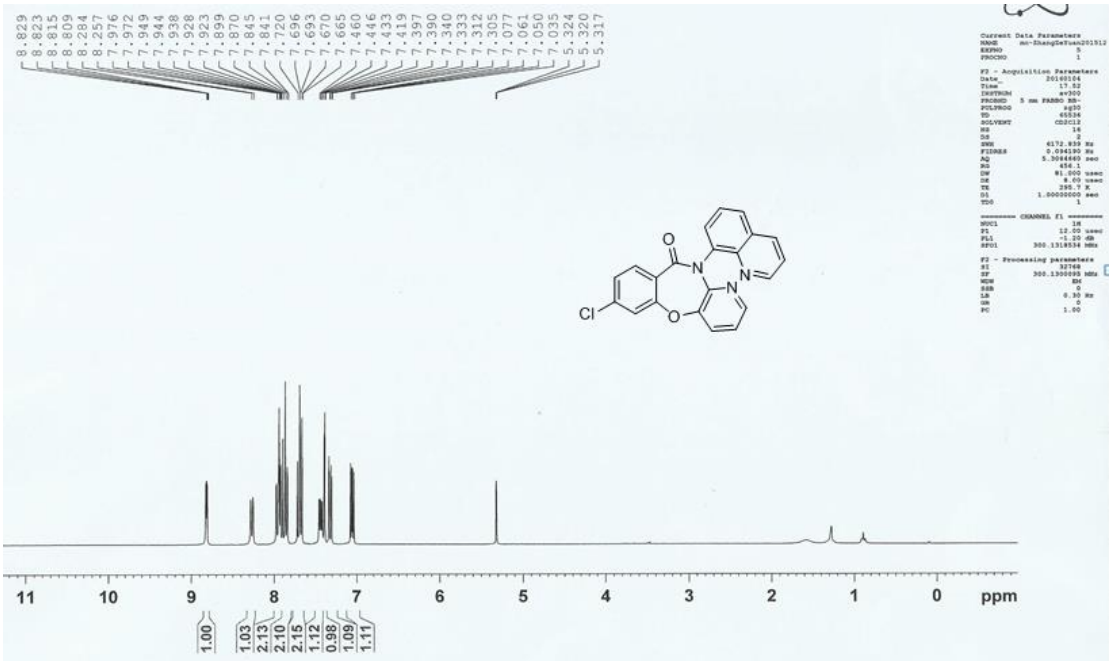
7-methyl-11-(quinolin-8-yl)benzo[f]pyrido[3,2-b][1,4]oxazepin-10(11H)-one 3j

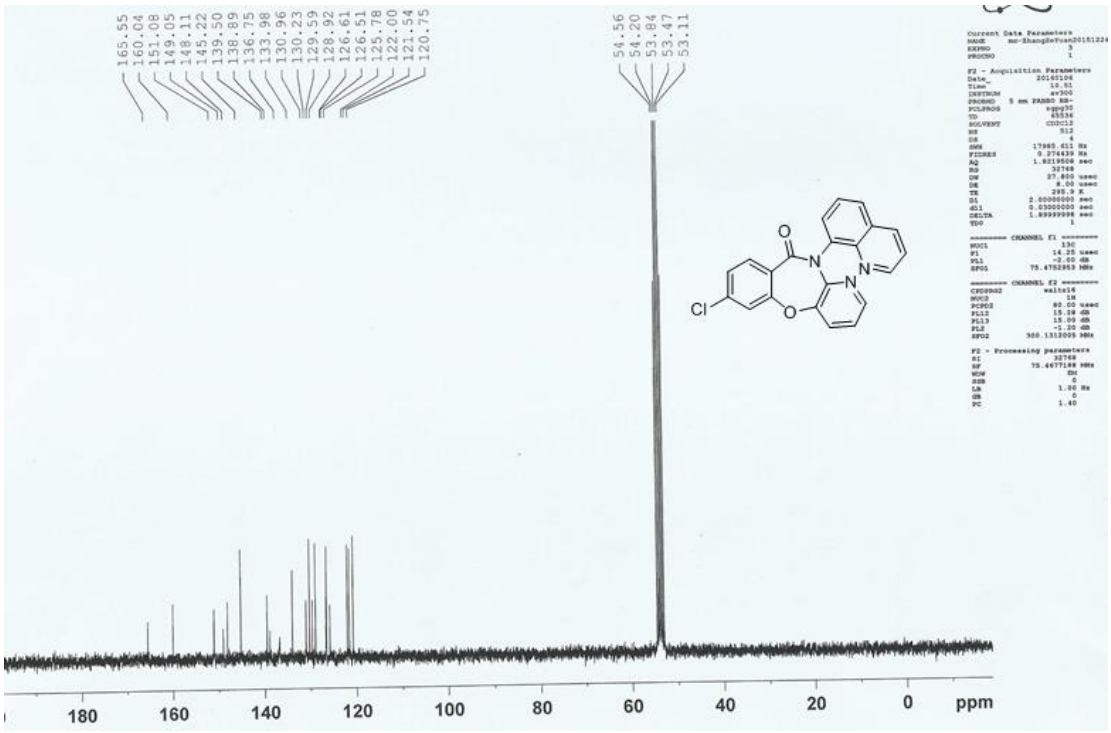


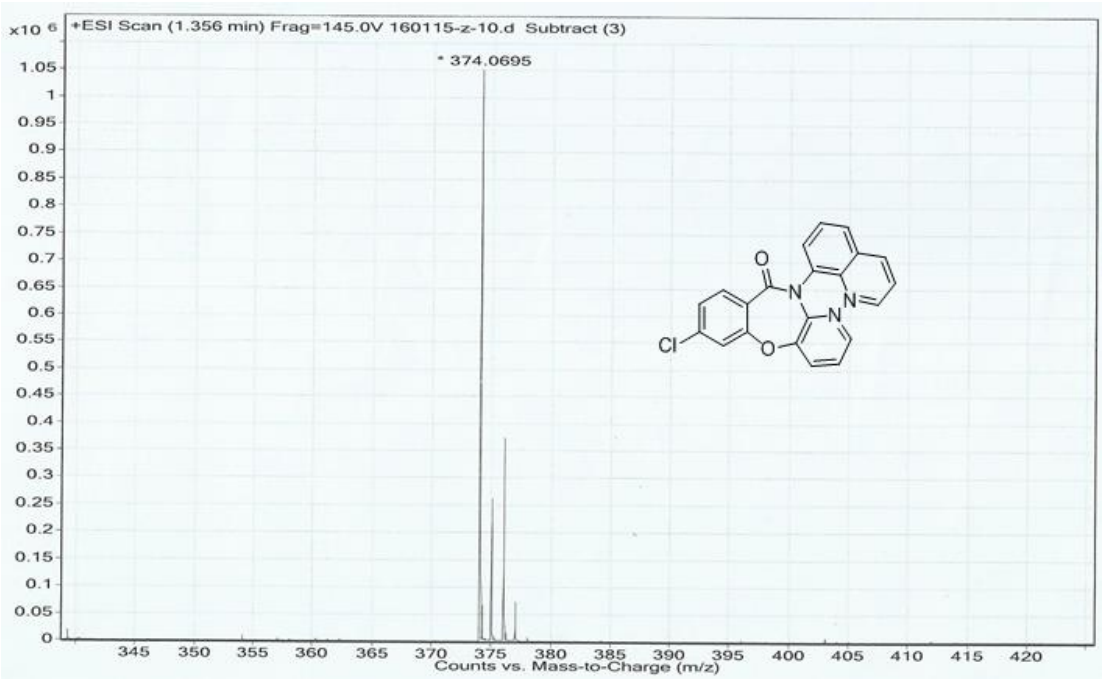




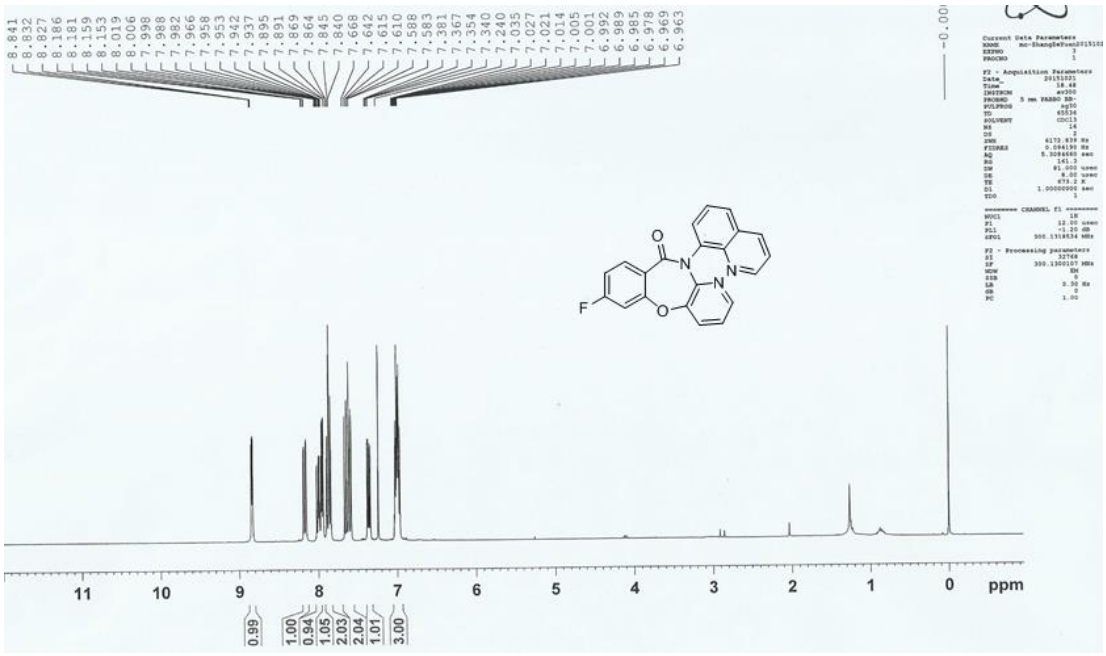
7-chloro-11-(quinolin-8-yl)benzo[f]pyrido[3,2-b][1,4]oxazepin-10(11H)-one 3k

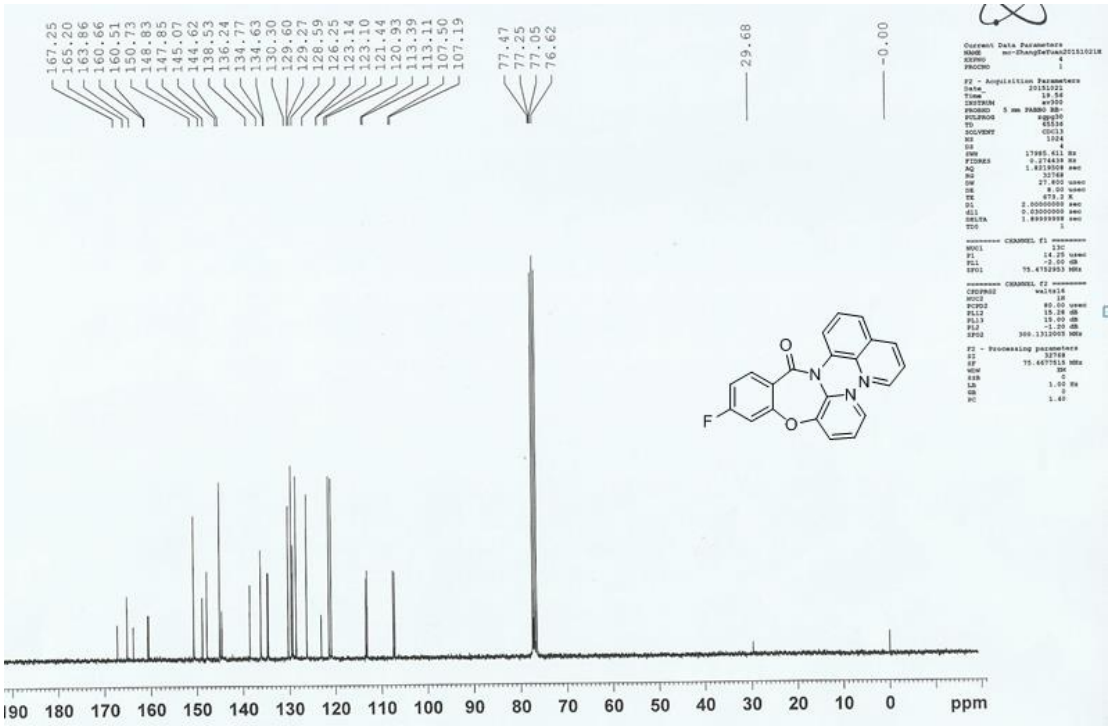


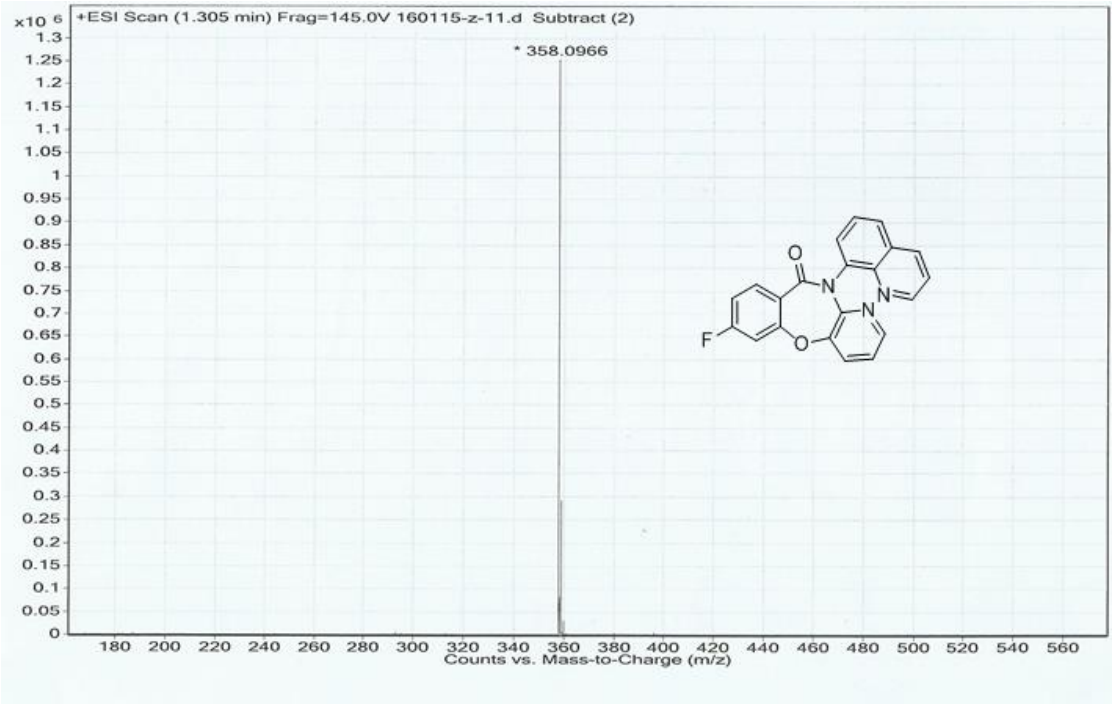

165.55
160.04
151.08
149.05
148.11
145.22
139.50
138.89
136.75
133.98
130.96
130.23
129.59
128.92
126.61
126.51
125.78
122.00
121.54
120.75
54.56
54.20
53.84
53.47
53.11
Cl
O
N
N
O
180
160
140
120
100
80
60
40
20
0
ppm


x10 6
+ESI Scan (1.356 min) Frag=145.0V 160115-z-10.d Subtract (3)
* 374.0695
1.05
1
0.95
0.9
0.85
0.8
0.75
0.7
0.65
0.6
0.55
0.5
0.45
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
345
350
355
360
365
370
375
380
385
390
395
400
405
410
415
420
Counts vs. Mass-to-Charge (m/z)
Cl
O
N
N
O

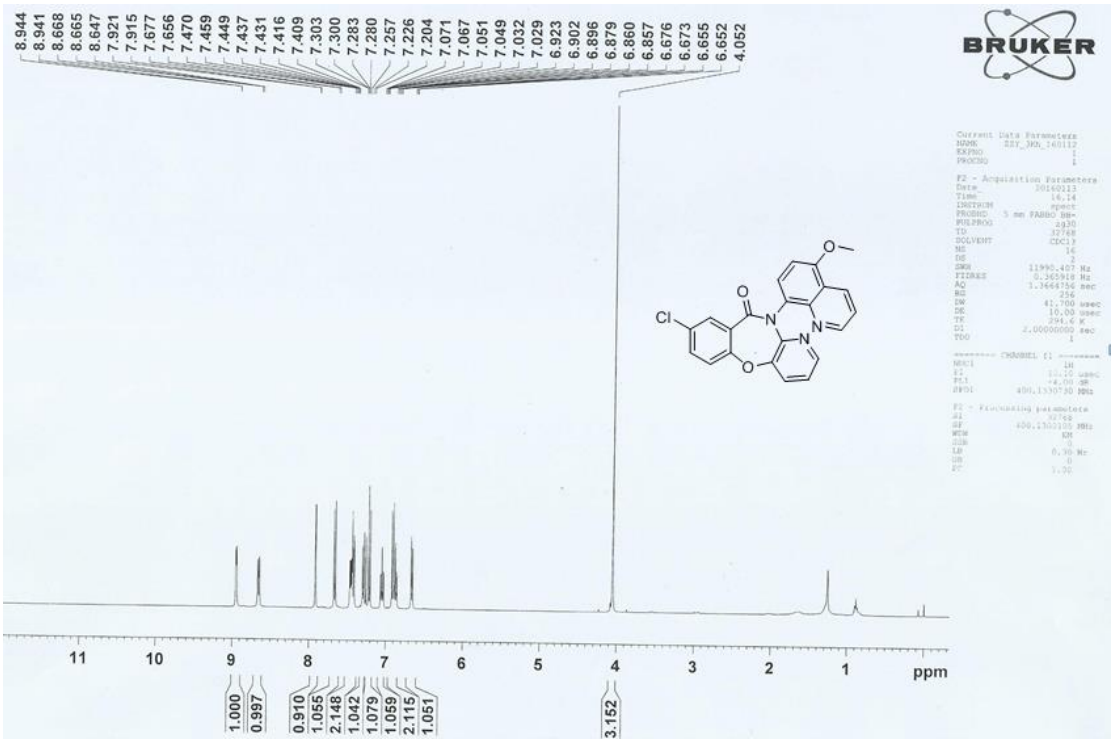
7-fluoro-11-(quinolin-8-yl)benzo[f]pyrido[3,2-b][1,4]oxazepin-10(11H)-one 3l

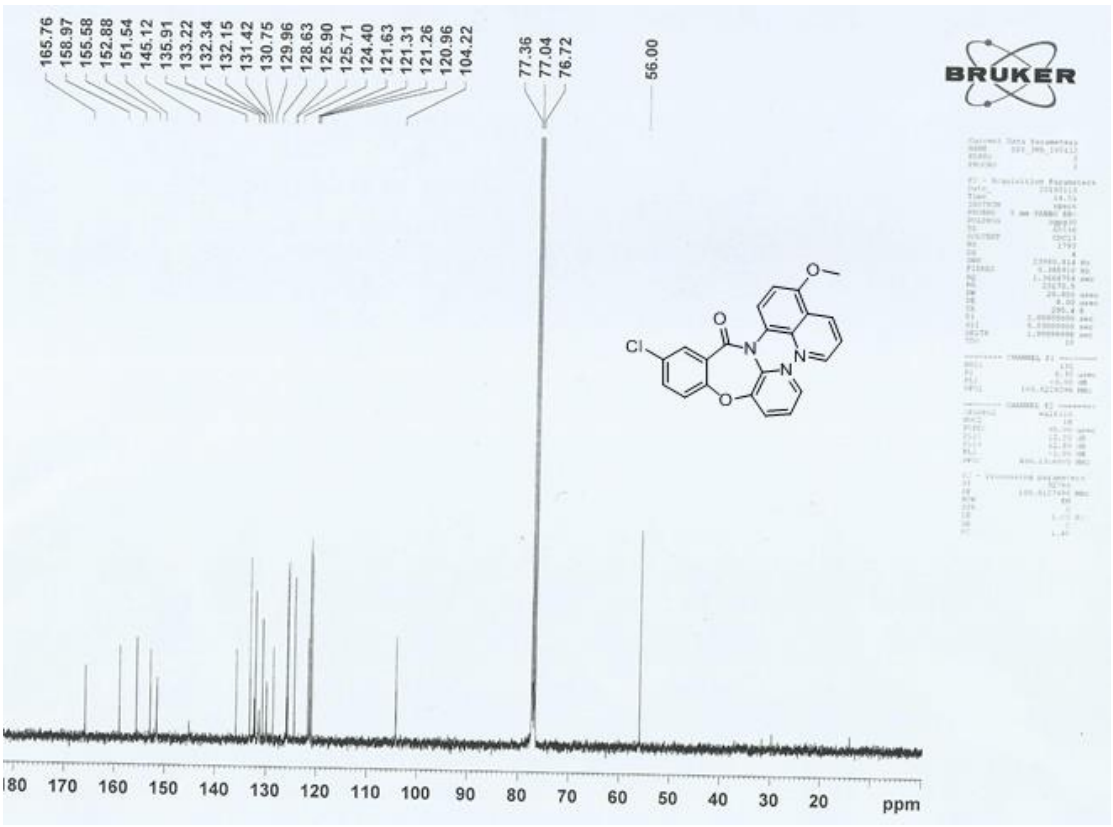


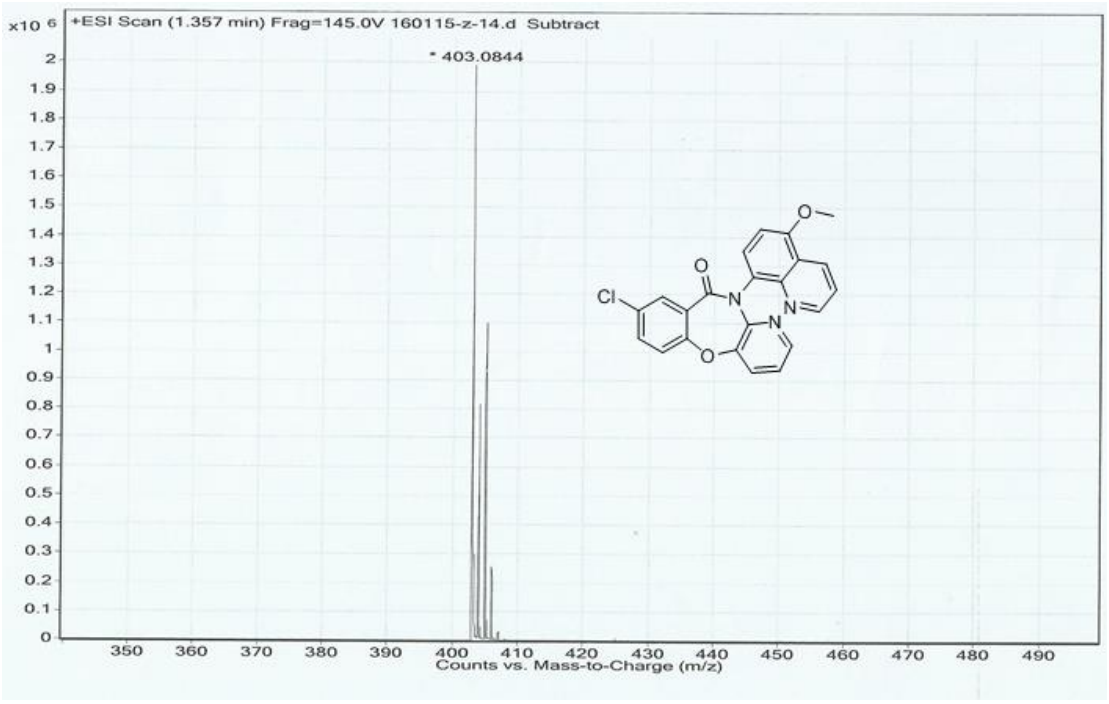




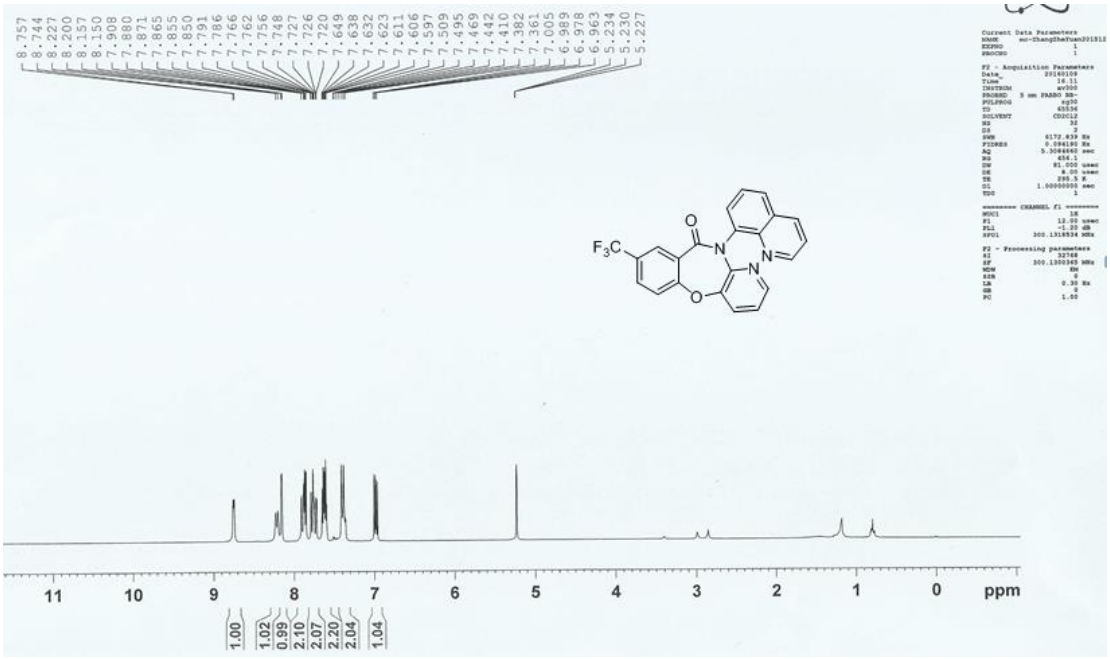
2-chloro-10-(5-methoxyquinolin-8-yl)dibenzo[b,f][1,4]oxazepin-11(10H)-one 3m

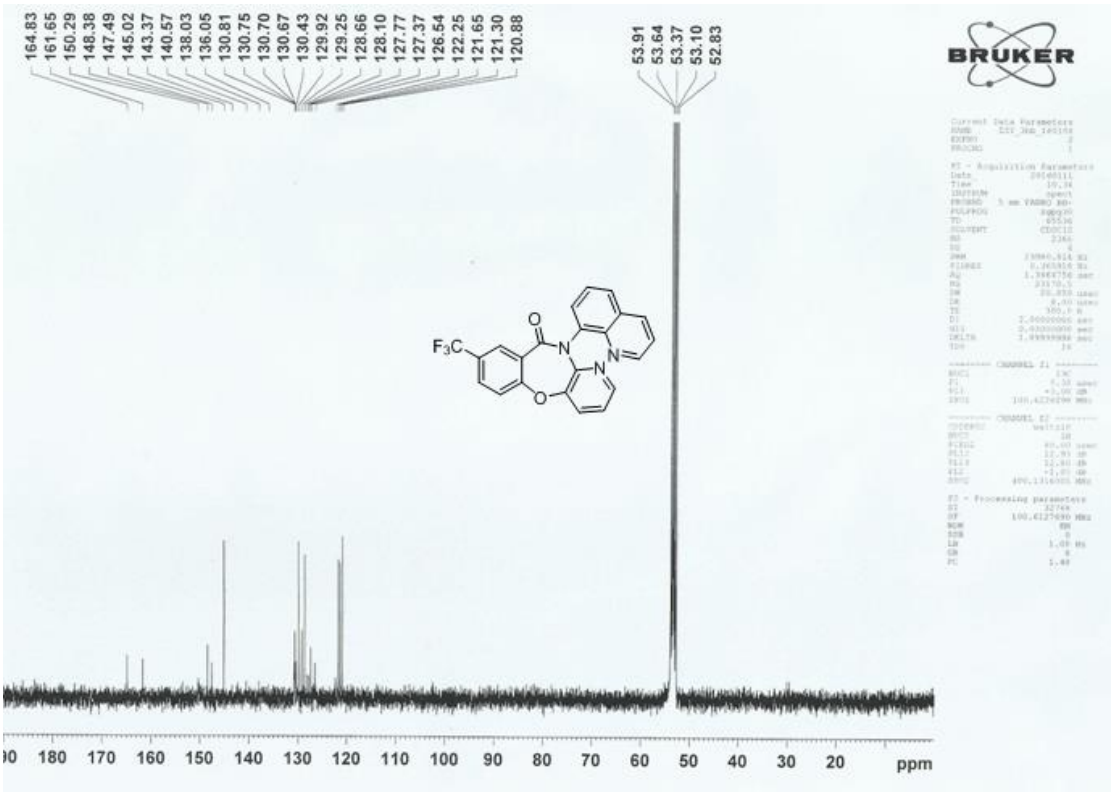


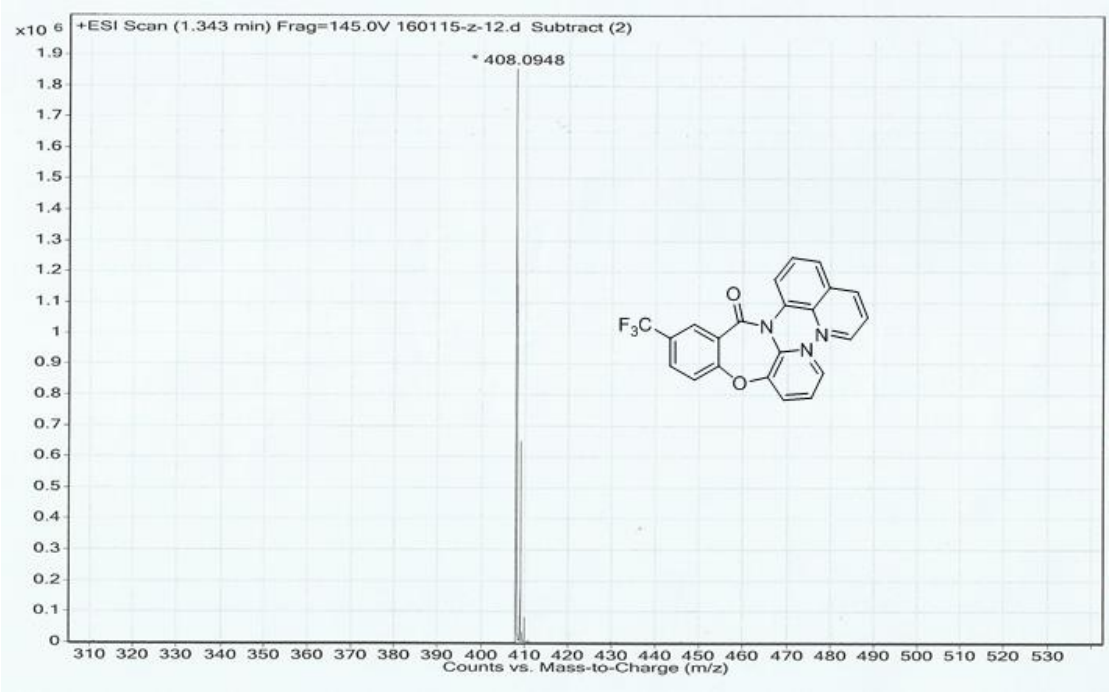

165.76
158.97
155.58
152.88
151.54
145.12
135.91
133.22
132.34
132.15
131.42
130.75
129.96
128.63
125.90
125.71
124.40
121.63
121.31
121.26
120.96
104.22
77.36
77.04
76.72
56.00
BRUKER
Cl
O
N
N
O
O
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


x10 6
+ESI Scan (1.357 min) Frag=145.0V 160115-z-14.d Subtract
403.0844
2
1.9
1.8
1.7
1.6
1.5
1.4
1.3
1.2
1.1
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
Cl
O
N
N
O
O
350 360 370 380 390 400 410 420 430 440 450 460 470 480 490
Counts vs. Mass-to-Charge (m/z)

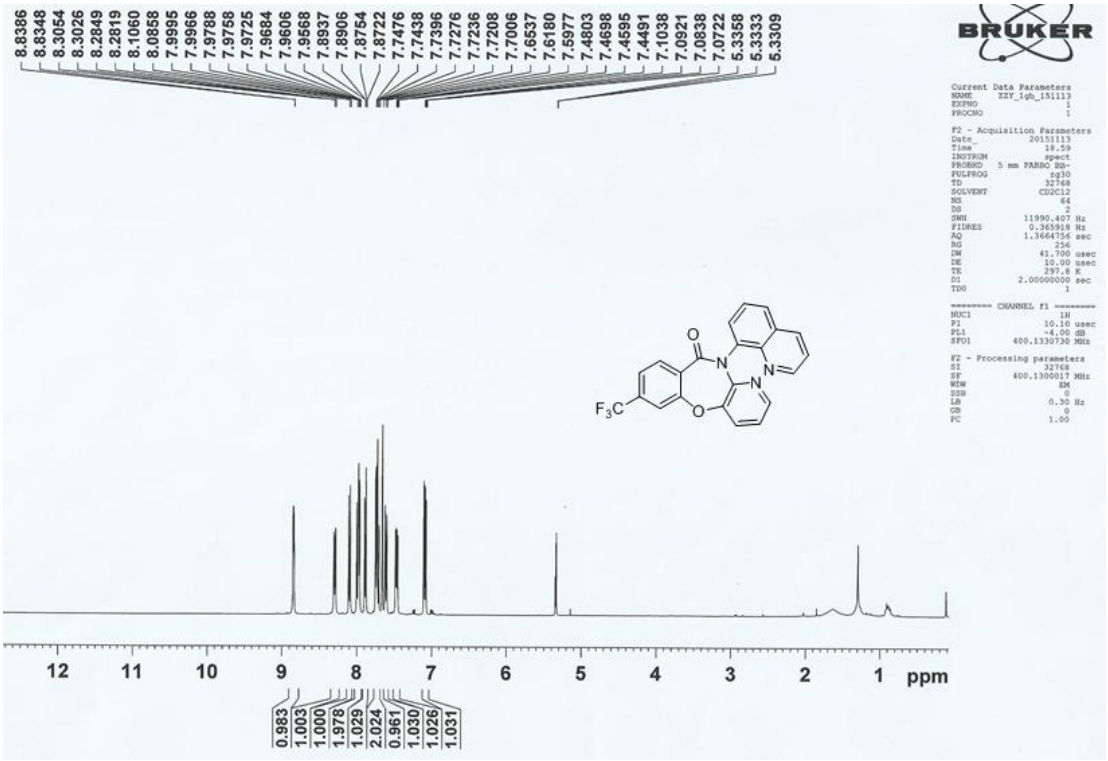
11-(quinolin-8-yl)-8-(trifluoromethyl)benzo[f]pyrido[3,2-b][1,4]oxazepin-10(11H)-one 3n

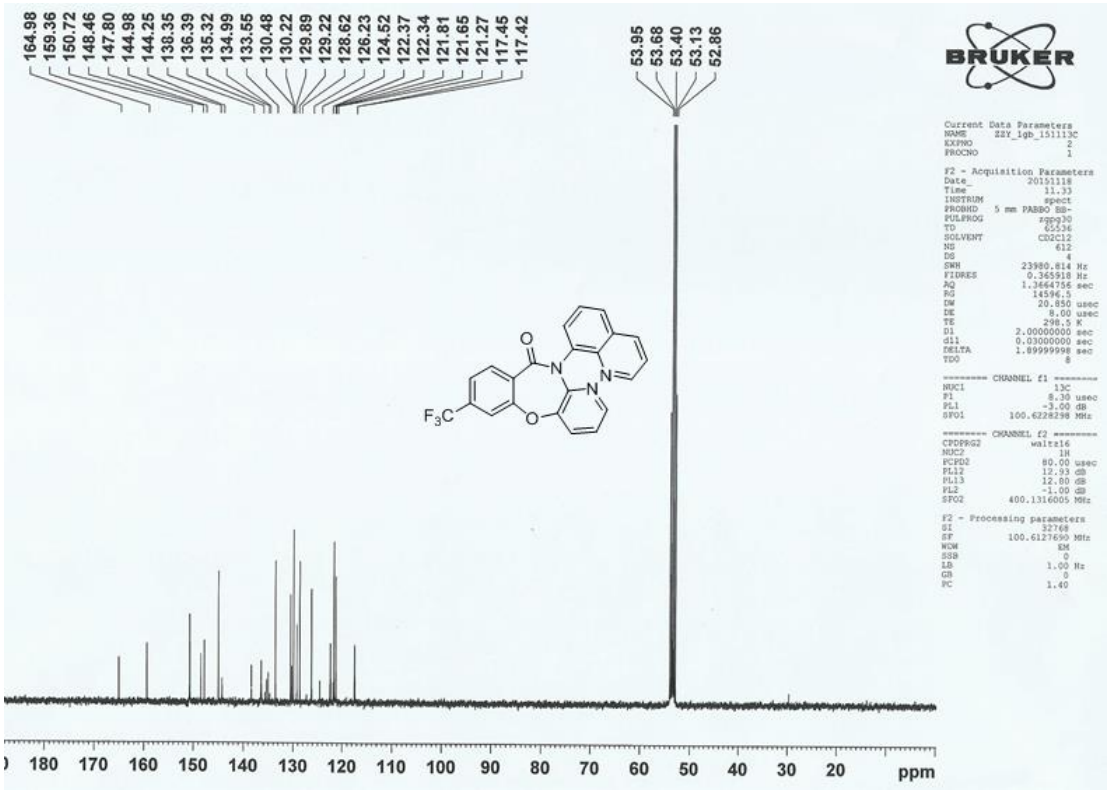


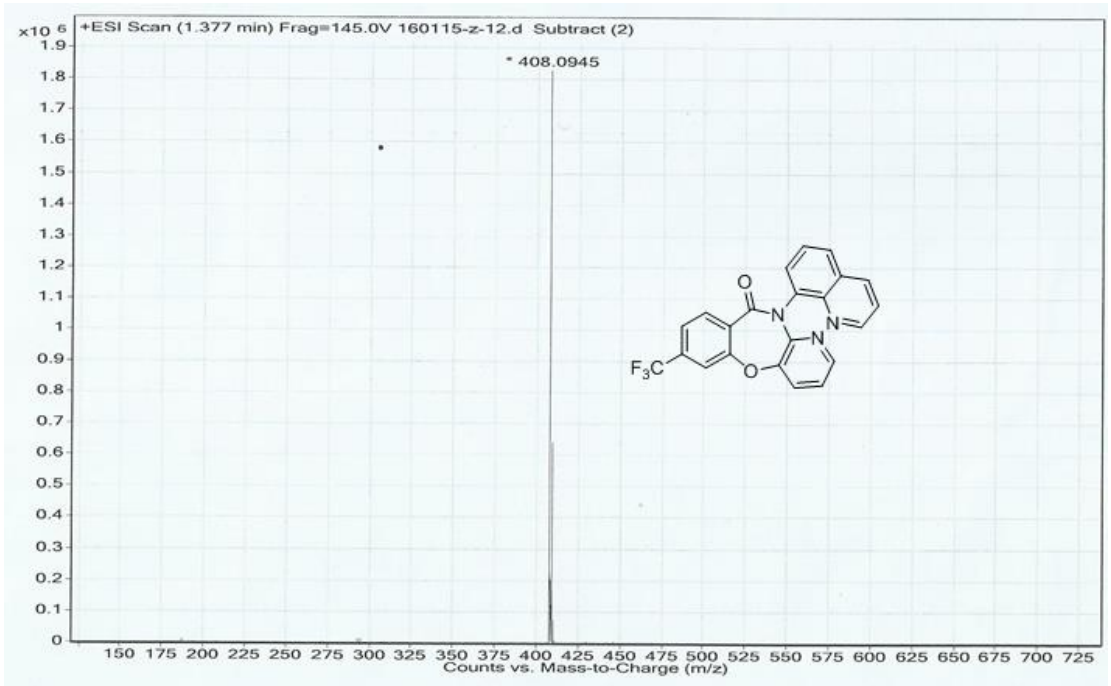




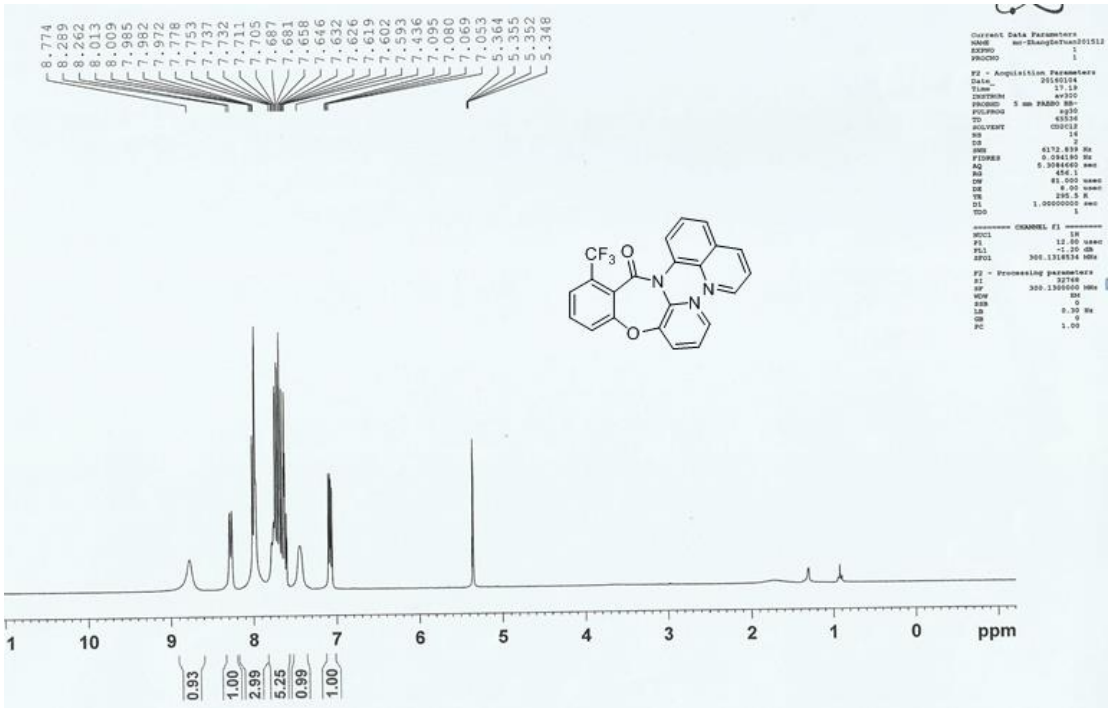
11-(quinolin-8-yl)-7-(trifluoromethyl)benzo[f]pyrido[3,2-b][1,4]oxazepin-10(11H)-one 3o

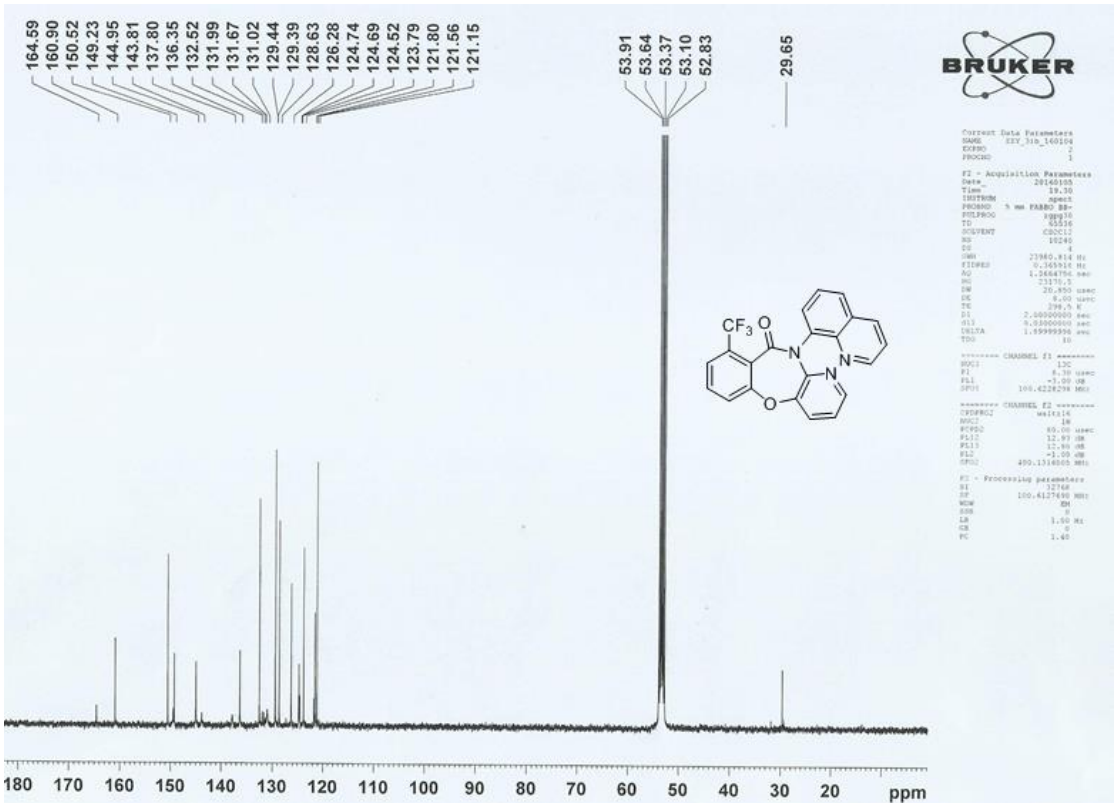


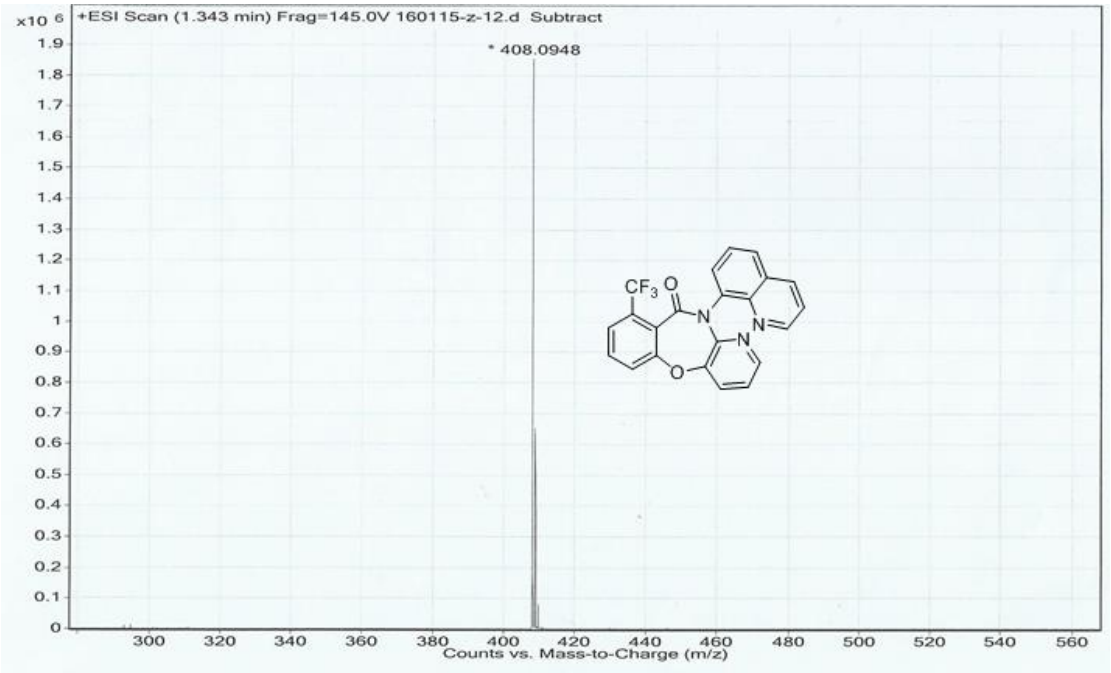

164.98
159.36
150.72
148.46
147.80
144.98
144.25
138.35
136.39
135.32
134.99
133.55
130.48
130.22
129.89
129.22
128.62
126.23
124.52
122.37
122.34
121.81
121.65
121.27
117.45
117.42
53.95
53.68
53.40
53.13
52.86
BRUKER
Current Data Parameters
NAME ZZY_1gb_151113c
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20151118
Time 11.33
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CD2Cl2
NS 612
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 14596.5
DW 20.850 usec
DE 8.00 usec
TE 298.5 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 8
======== CHANNEL f1 ========
NUC1 13C
P1 8.30 usec
PL1 -3.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 12.93 dB
PL13 12.80 dB
PL2 -1.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
O
N
N
N
O
F3C
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


x10 6
+ESI Scan (1.377 min) Frag=145.0V 160115-z-12.d Subtract (2)
* 408.0945
1.9
1.8
1.7
1.6
1.5
1.4
1.3
1.2
1.1
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
O
N
N
N
O
F3C
150 175 200 225 250 275 300 325 350 375 400 425 450 475 500 525 550 575 600 625 650 675 700 725
Counts vs. Mass-to-Charge (m/z)

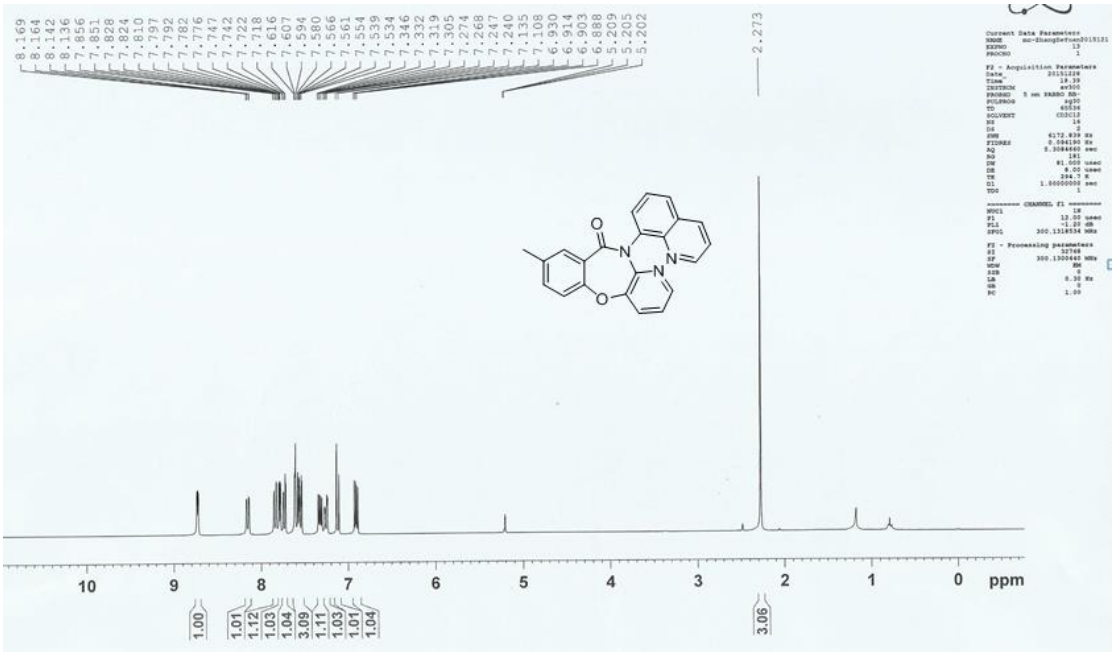
11-(quinolin-8-yl)-9-(trifluoromethyl)benzo[f]pyrido[3,2-b][1,4]oxazepin-10(11H)-one 3p

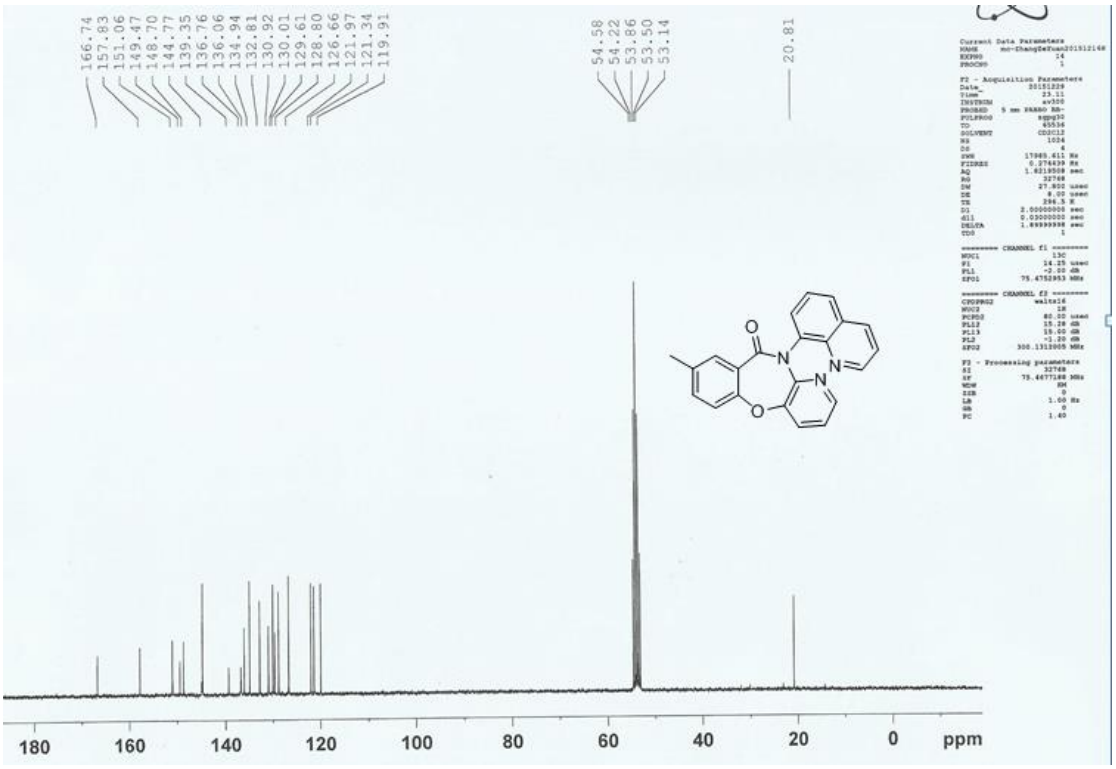


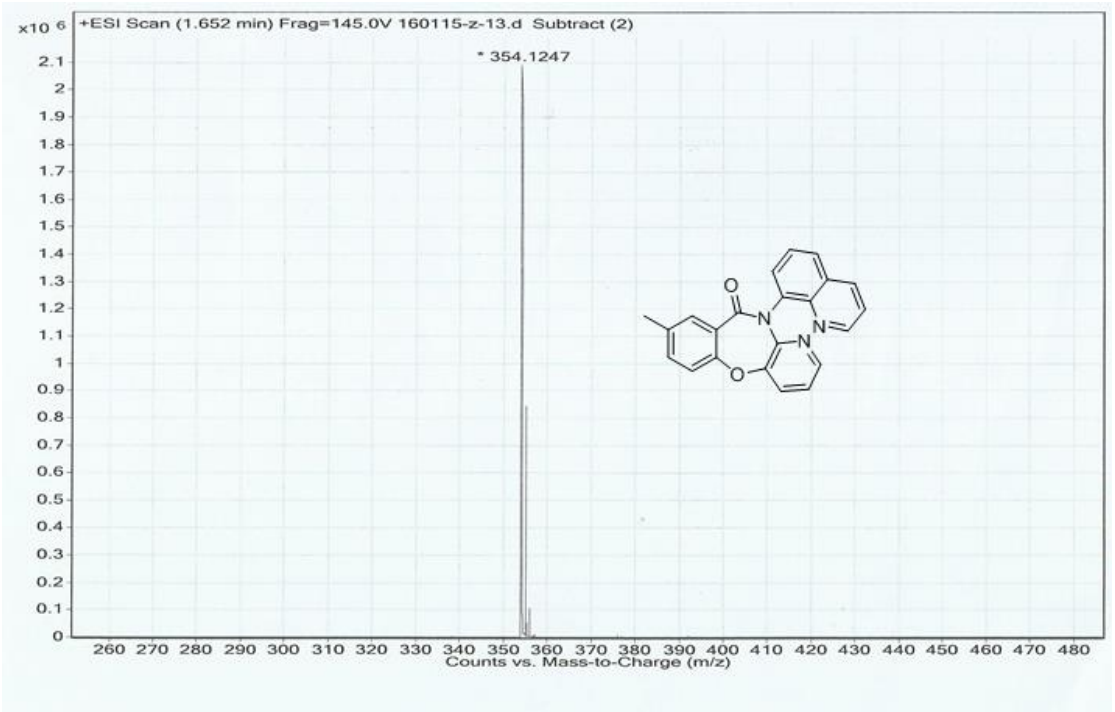




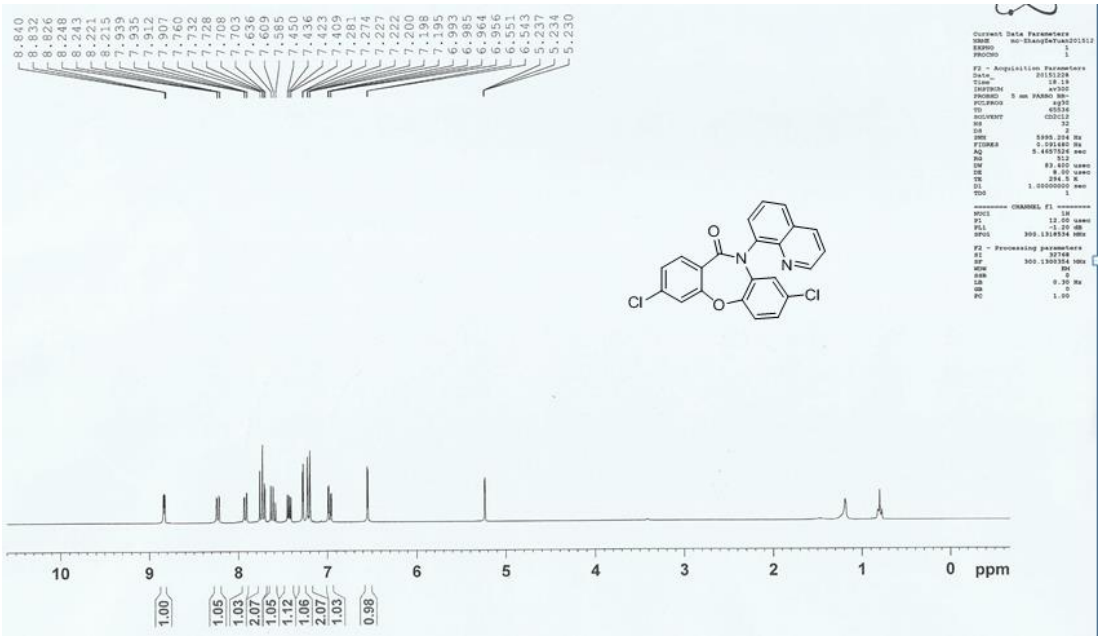
8-methyl-11-(quinolin-8-yl)benzo[f]pyrido[3,2-b][1,4]oxazepin-10(11H)-one 3q

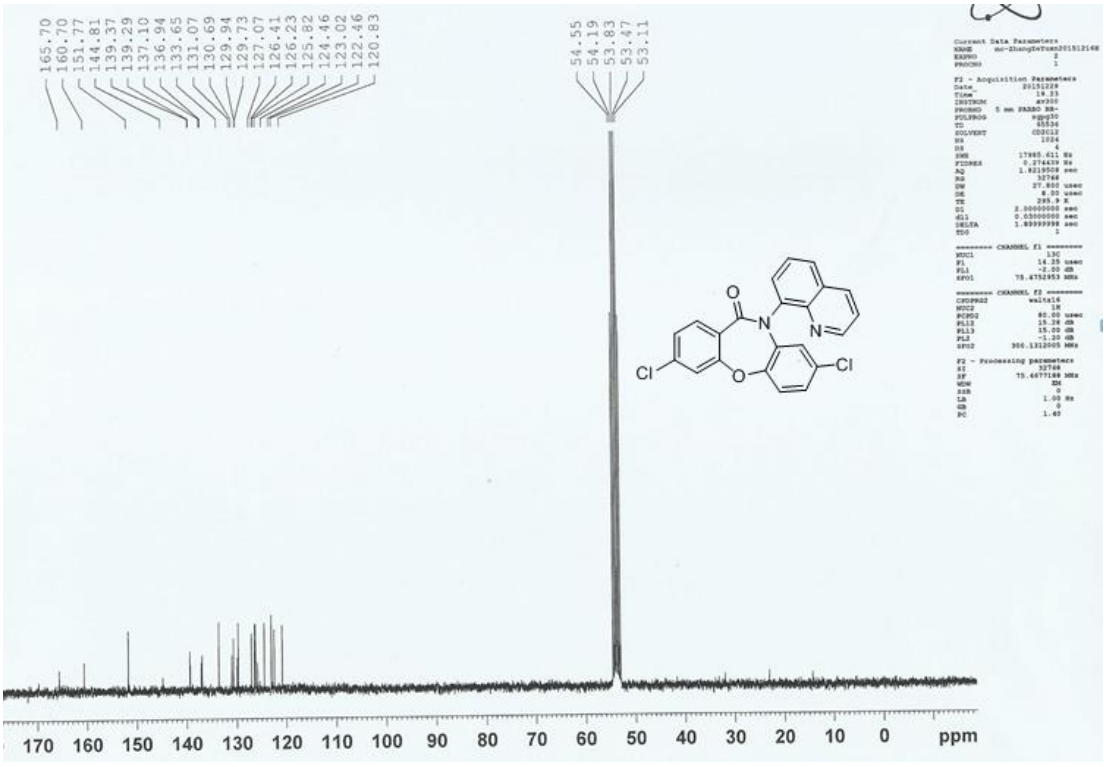


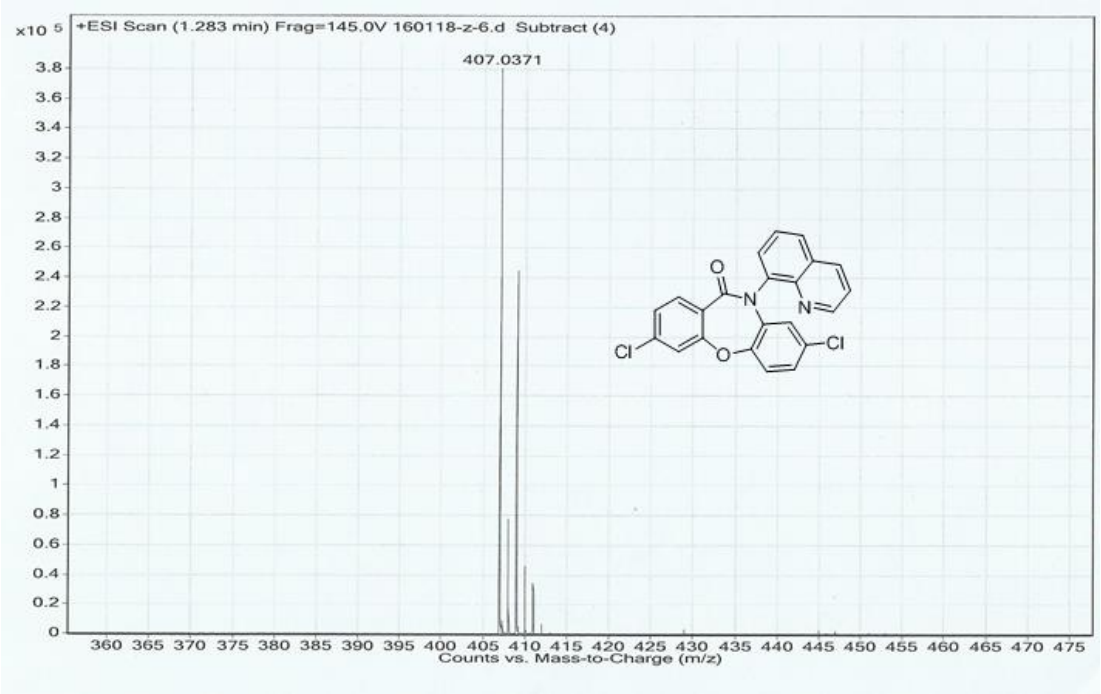

166.74
157.83
151.06
149.47
148.70
144.77
139.35
136.76
136.06
134.94
132.81
130.92
130.01
129.61
128.80
126.66
121.97
121.34
119.91
54.58
54.22
53.86
53.50
53.14
20.81
180
160
140
120
100
80
60
40
20
0
ppm


x10 6
+ESI Scan (1.652 min) Frag=145.0V 160115-z-13.d Subtract (2)
* 354.1247
2.1
2
1.9
1.8
1.7
1.6
1.5
1.4
1.3
1.2
1.1
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
260 270 280 290 300 310 320 330 340 350 360 370 380 390 400 410 420 430 440 450 460 470 480
Counts vs. Mass-to-Charge (m/z)

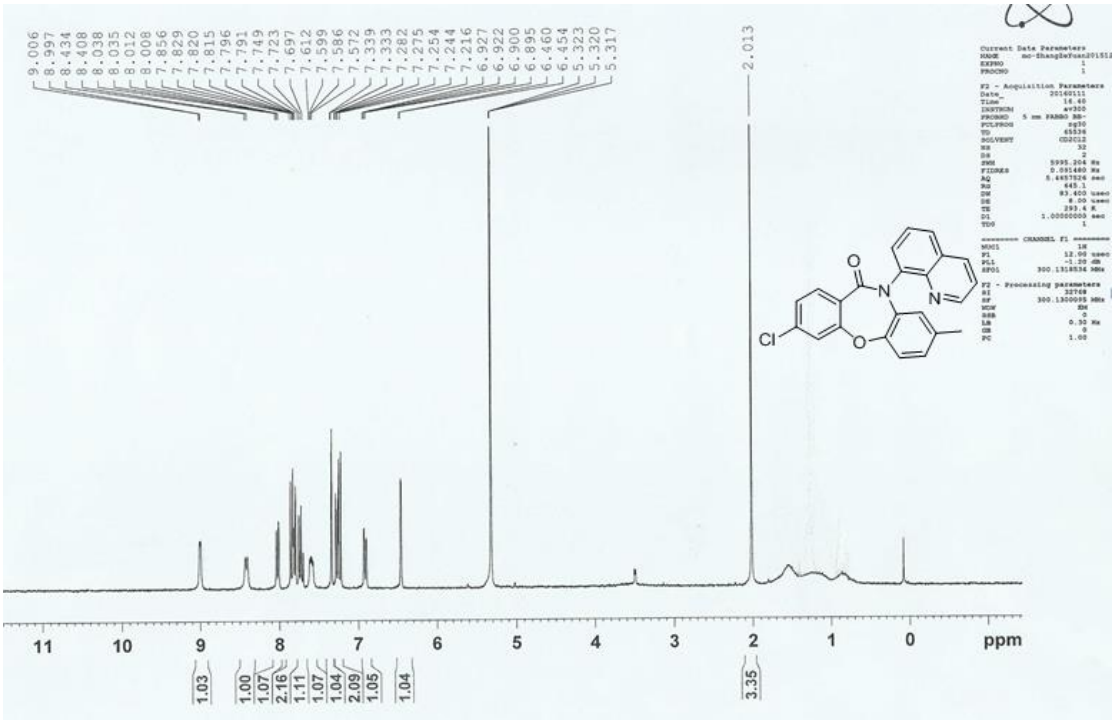
3,8-dichloro-10-(quinolin-8-yl)dibenzo[b,f][1,4]oxazepin-11(10H)-one 3r

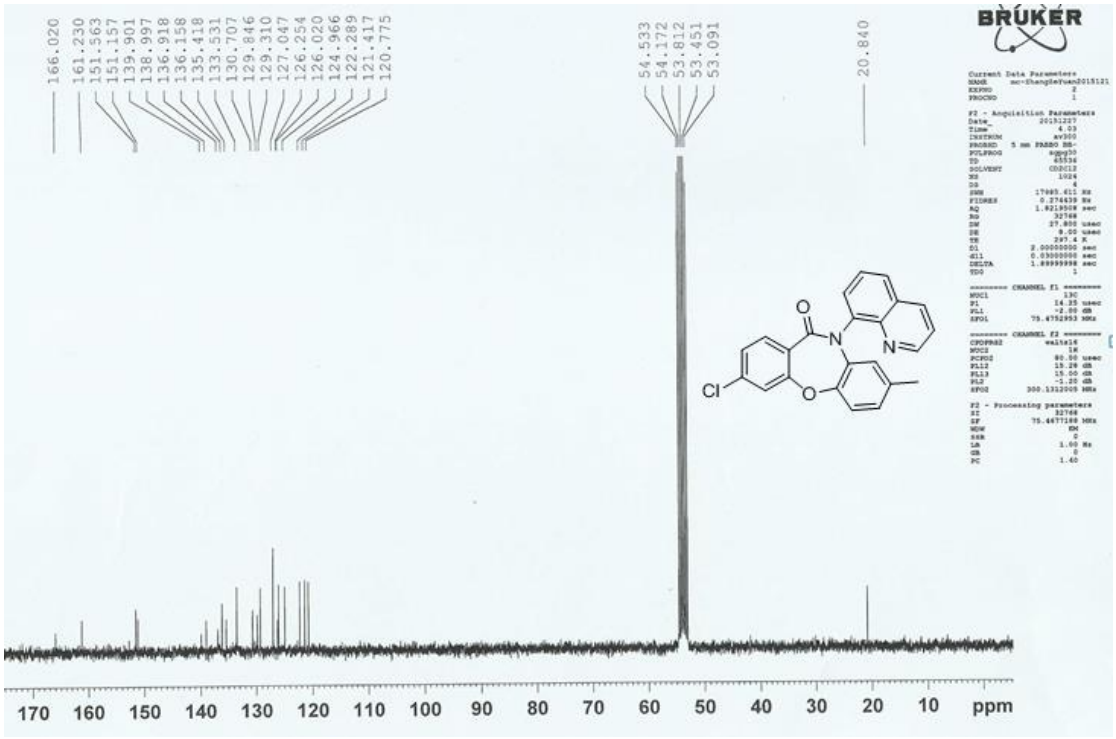


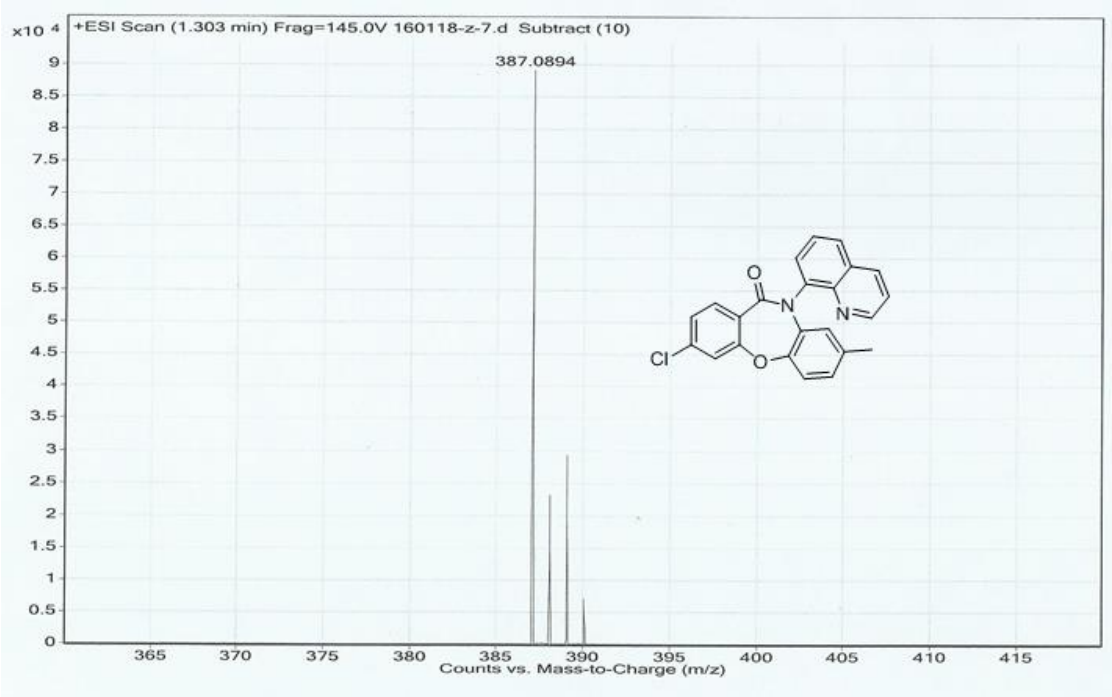




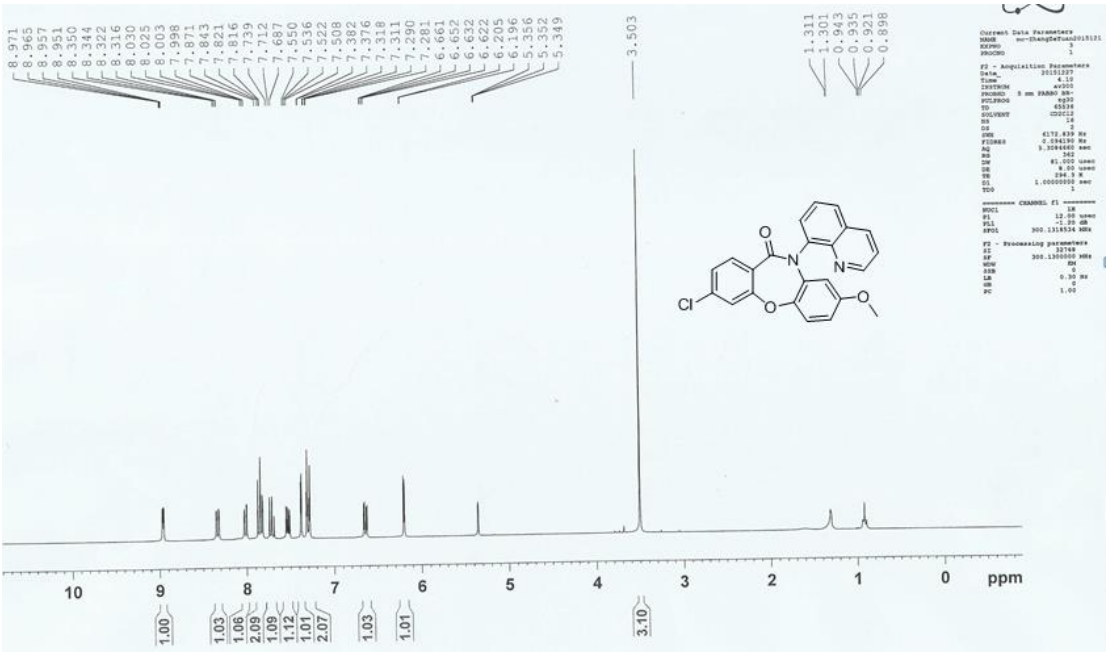
3-chloro-8-methyl-10-(quinolin-8-yl)dibenzo[b,f][1,4]oxazepin-11(10H)-one 3s

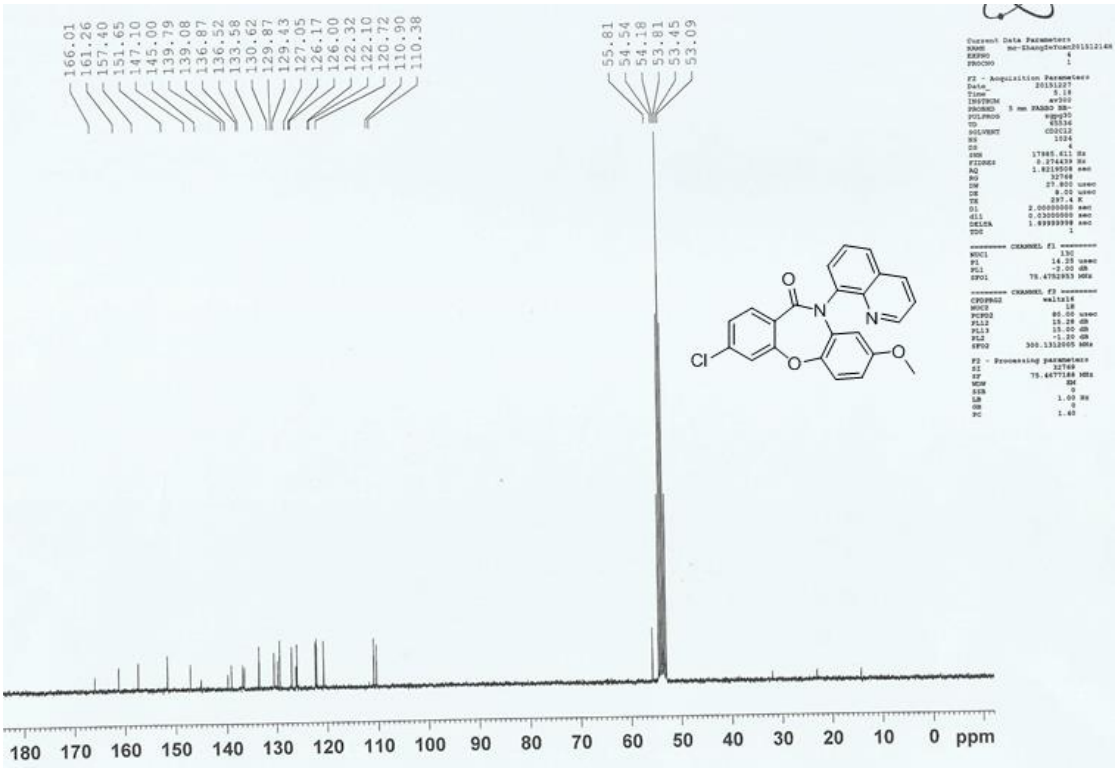


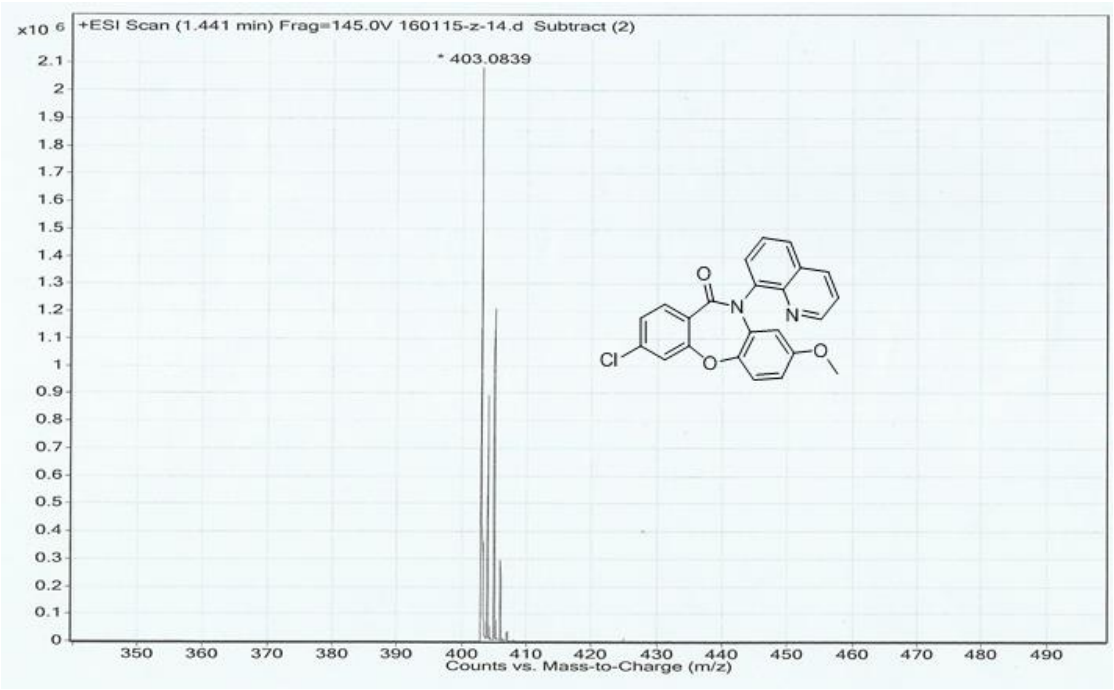

166.020
161.230
151.563
151.157
139.901
138.997
136.918
136.158
135.418
133.531
130.707
129.846
129.310
127.047
126.254
126.020
124.966
122.289
121.417
120.775
54.533
54.172
53.812
53.451
53.091
20.840
BRUKER
Cl
O
N
N
O
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


x10 4
+ESI Scan (1.303 min) Frag=145.0V 160118-z-7.d Subtract (10)
387.0894
Cl
O
N
N
O
9
8.5
8
7.5
7
6.5
6
5.5
5
4.5
4
3.5
3
2.5
2
1.5
1
0.5
0
365 370 375 380 385 390 395 400 405 410 415
Counts vs. Mass-to-Charge (m/z)

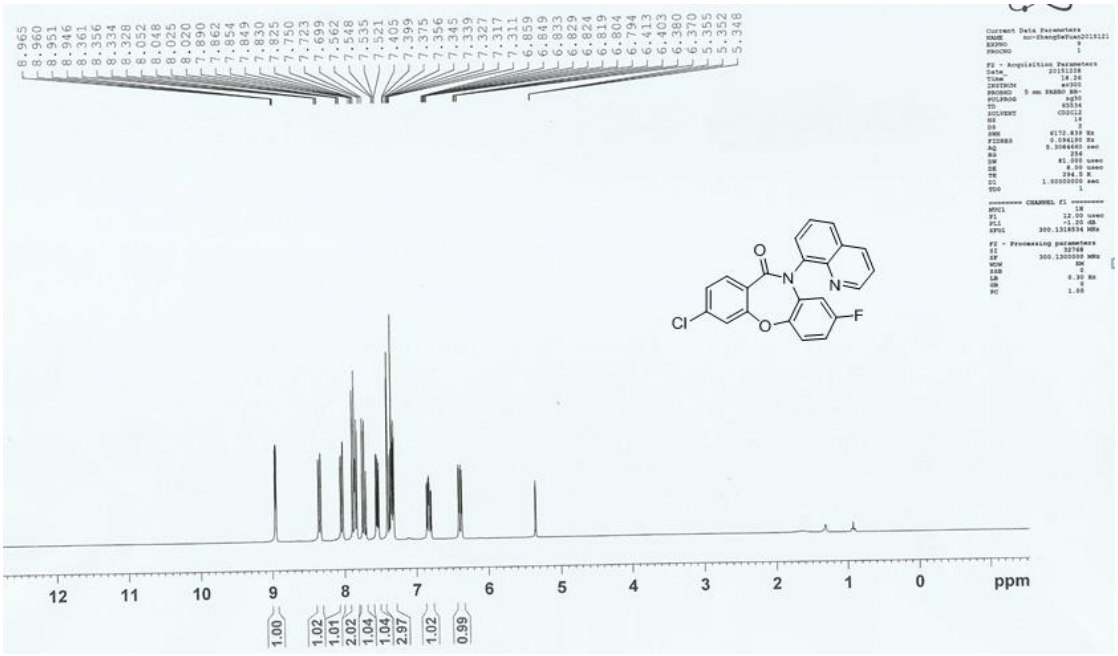
3-chloro-8-methoxy-10-(quinolin-8-yl)dibenzo[b,f][1,4]oxazepin-11(10H)-one 3t

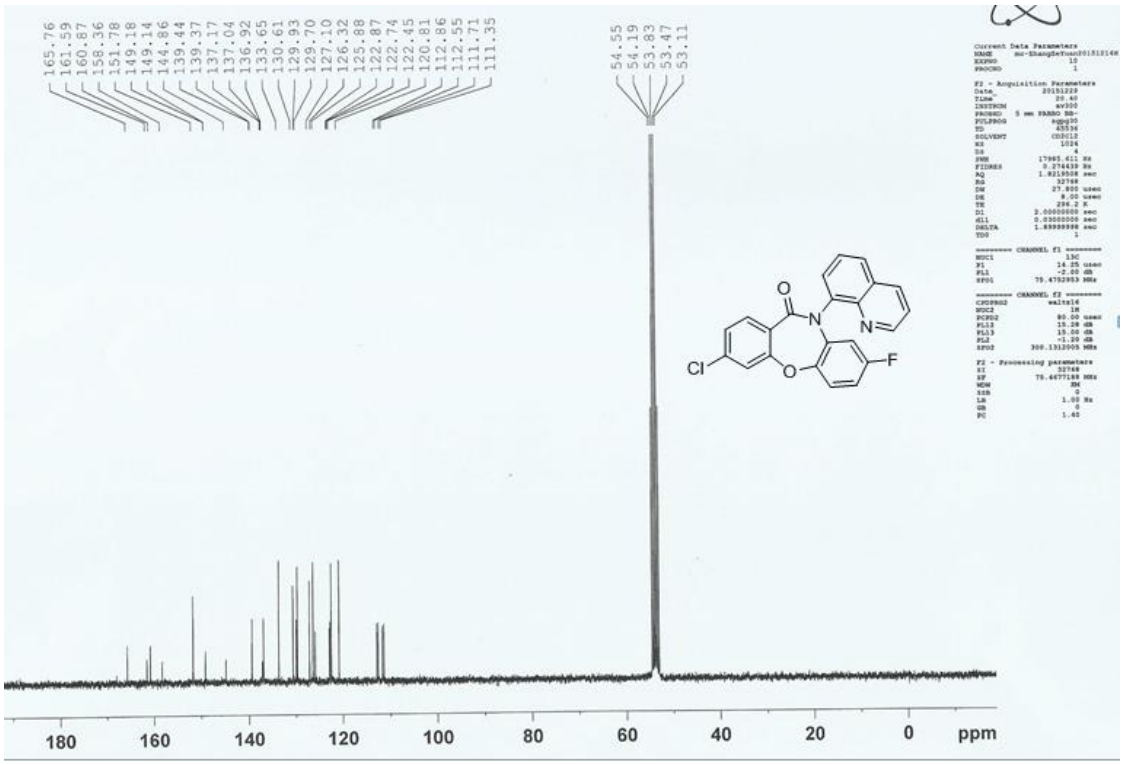


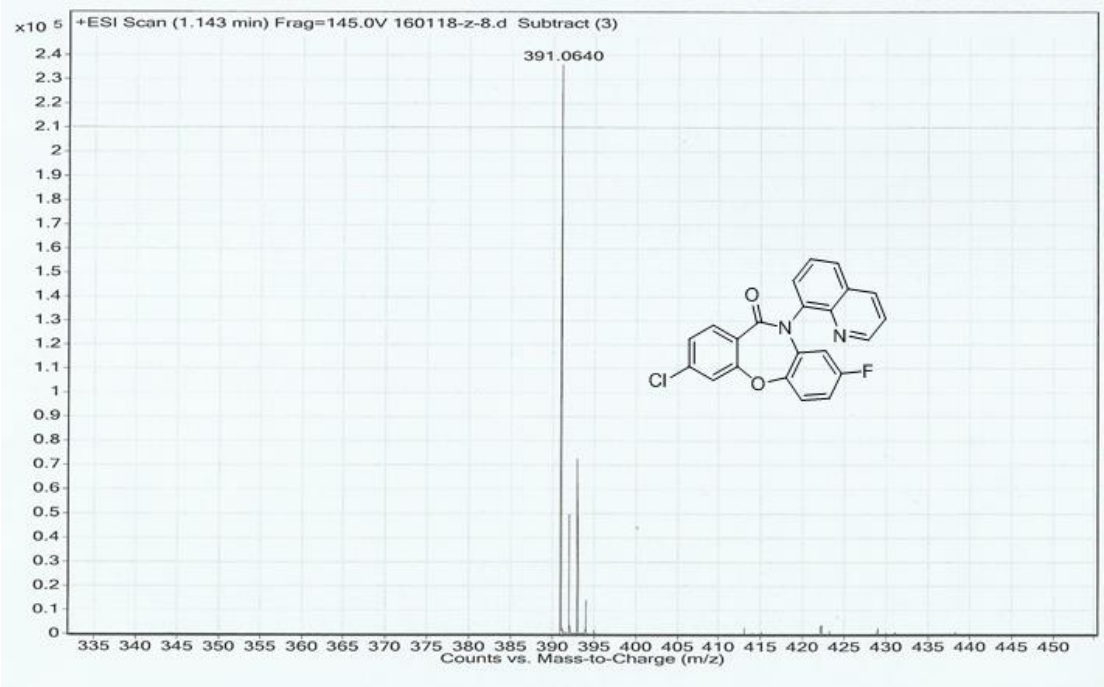




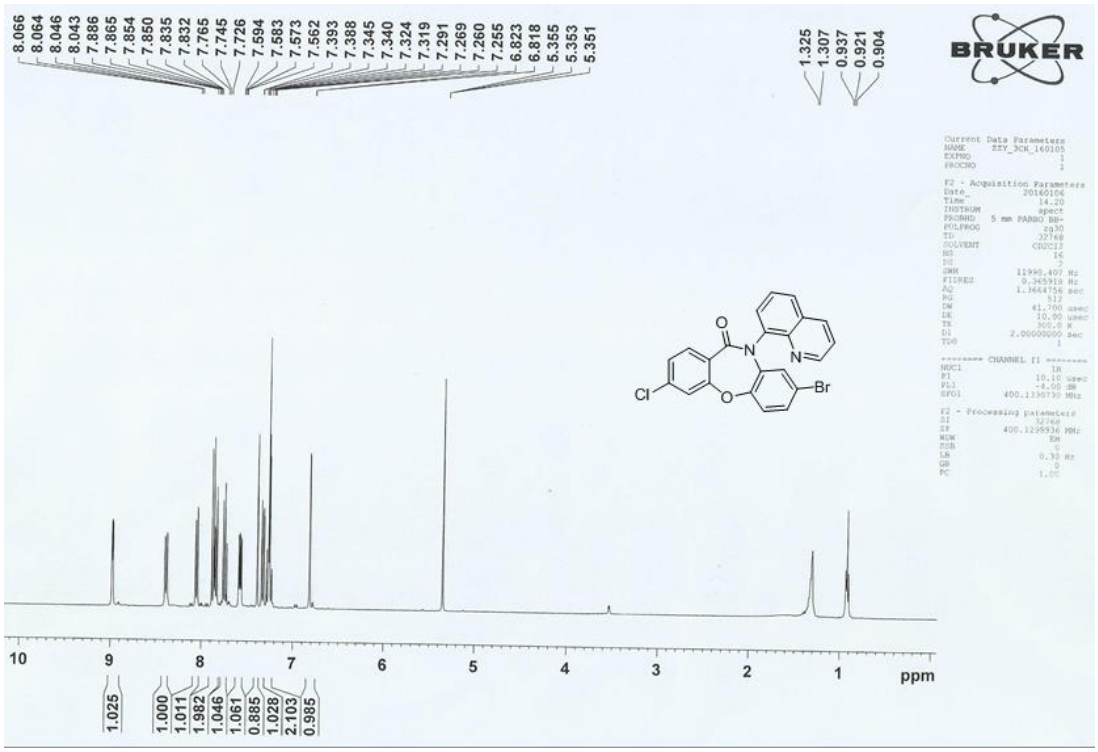
3-chloro-8-fluoro-10-(quinolin-8-yl)dibenzo[b,f][1,4]oxazepin-11(10H)-one 3u

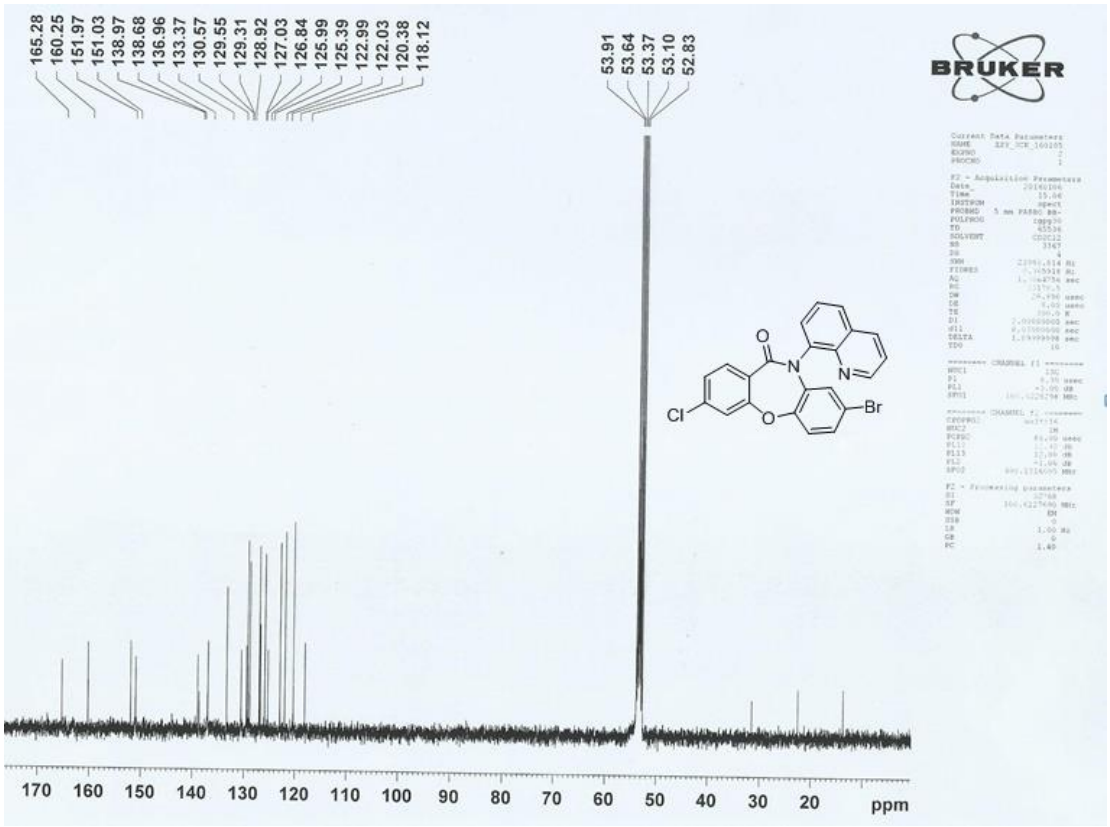


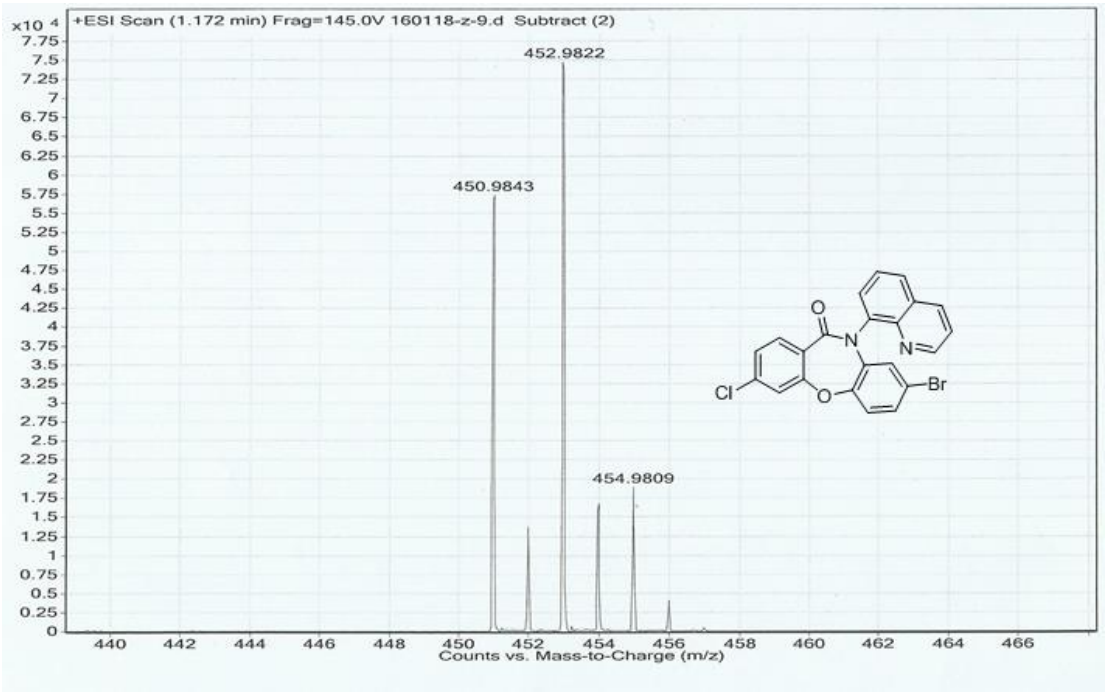

165.76
161.59
160.87
158.36
151.78
149.18
149.14
144.86
139.44
139.37
137.17
137.04
136.92
133.65
130.61
129.93
129.70
127.10
126.32
125.88
122.87
122.74
122.45
120.81
112.86
112.55
111.71
111.35
54.55
54.19
53.83
53.47
53.11
O
N
N
Cl
O
F
180
160
140
120
100
80
60
40
20
0
ppm


x10 5
+ESI Scan (1.143 min) Frag=145.0V 160118-z-8.d Subtract (3)
391.0640
2.4
2.3
2.2
2.1
2
1.9
1.8
1.7
1.6
1.5
1.4
1.3
1.2
1.1
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
335 340 345 350 355 360 365 370 375 380 385 390 395 400 405 410 415 420 425 430 435 440 445 450
Counts vs. Mass-to-Charge (m/z)
O
N
N
Cl
O
F

8-bromo-3-chloro-10-(quinolin-8-yl)dibenzo[b,f][1,4]oxazepin-11(10H)-one 3v






+ESI Scan (1.172 min) Frag=145.0V 160118-z-9.d Subtract (2)
x10 4
452.9822
450.9843
454.9809
O
N
N
Cl
O
Br
Counts vs. Mass-to-Charge (m/z)