Electronic Supplementary Material (ESI) for Green Chemistry.

Highly-Efficient Palladium-Catalyzed Aminocarbonylation/S_NAr Approach to Dibenzoxazepinones

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1. General considerations

Nuclear Magnetic Resonance spectra were recorded on Bruker Avance 300 and Bruker ARX 400 spectrometers. All ^{1}H NMR experiments were reported in δ units, parts per million (ppm), and were measured relative to residual chloroform (7.26 ppm) or DMSO (2.5 ppm) in the deuterated solvent. All ^{13}C NMR spectra were reported in ppm relative to deuterochloroform (77.0 ppm) or [D_6]DMSO (39.5 ppm) and all were obtained with 1H decoupling. All coupling constants J were reported in Hz. The following abbreviations were used to describe peak splitting patterns when appropriate: s = singlet, d = doublet, t = triplet, dd = doublet of doublet, m = multiplet and br s = broad singlet. All measurements were carried out at room temperature unless otherwise stated. Electron impact (EI) mass spectra were recorded on AMD 402 mass spectrometer (70 eV). High resolution mass spectra (HRMS) were recorded on Agilent 6210. The data were given as mass units per charge (m/z). Gas chromatography analysis was performed on an Agilent HP-5890 instrument with a FID detector and HP-5 capillary column (polydimethylsiloxane with 5 % phenyl groups, 30 m, 0.32 mm i.d., 0.25 μm film thickness) using argon as carrier gas. The products were isolated from the reaction mixture by column chromatography on silica gel 60, 0.063-0.2 mm, 70-230 mesh (Merck).

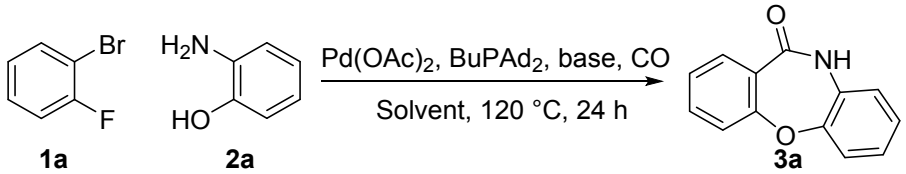
2. Materials

DMSO (99.8 %), DMA (anhydrous, 99.8 %) was purchased from Sigma-Aldrich and used without further purification. All Chemicals were commercial available and were used without further purification unless otherwised noted.

3. **Representative procedure for the synthesis of dibenzoxazepinones**

A vial (6 mL) was charged with $Pd(OAc)_2$ (2 mol%), $BuPAd_2$ (6 mol%), 2-aminophenol (0,5 mmol) and a magnetic stirring bar. Then, 1-bromo-2-fluorobenzene (0.5 mmol), DBU (3.0 equiv), and DMSO (2.0 mL) were injected under argon by using a syringe. The vial (or several vials) was placed in an alloy plate, which was transferred into a 300 mL autoclave of the 4560 series from Parr Instruments under argon atmosphere. After flushing the autoclave three times with CO, a pressure of 10 bar of CO was adjusted at ambient temperature. Then, the reaction was performed for 24 h at 120^0C. After the reaction was complete, the autoclave was cooled down with ice-water mixture to room temperature and the pressure was released carefully. The solution was diluted with ethyl acetate and then silica gel was added into the solution. After evaporation of the organic solvent, the crude product was purified by column chromatography using ethyl acetate/*n*-pentane.

Table S1. Optimization of Reaction Conditions.[a]



1a **2a** **3a**

Entry	CO (bar)	Base	Solvent	Yield (%)[b]
1	10	DBU	DMA	78 (75)[c]
2	10	DBU	DMF	34
3	10	DBU	NMP	58
4	10	DBU	DMSO	86 (82)
5	10	DBU	MeCN	25
6	10	DBU	1,4-dioxane	19
7	10	DBU	Toluene	0

8	10	DABCO	DMSO	51
9	10	DIPEA	DMSO	70
10	10	K_2CO_3	DMSO	43
11	10	K_2CO_3	MeCN	8[d]
12	10	K_2CO_3	MeCN	19
13	10	DBU	DMSO	47[e]
14	5	DBU	DMSO	67 (64)
15	10	DBU	DMSO	53[f]

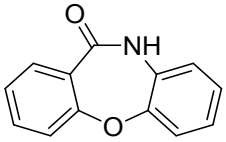
[a] Unless otherwise stated, the reaction was conducted on 0.50 mmol scale (2mol% $Pd(OAc)_2$, 6 mol% $BuPAd_2$, 0.50 mmol of **1a**, 0.50 mmol of **2a**, 1.5 mmol base) with 2.0 mL solvent. Reaction temperature was 120 ^{0}C. Reaction time was 24 h. [b] Yields were determined by GC with hexadecane as an internal standard; yields in parentheses are for the isolated product. [c] Reaction time was 32 h. [d] 2 mol% $Pd(OAc)_2$, 2 mol% DPPP. [e] 1 mol% $Pd(OAc)_2$, 3 mol% $BuPAd_2$. [f] Reaction temperature was 100 ^{0}C. Ad = adamantyl, Bu = *n*-butyl, DABCO =1,4-diazabicyclo[2.2.2]octane, DBU = 1,8-Diazabicyclo[5.4.0]undec-7-ene, DIPEA = *N,N'*-diisopropylethylamine, DMA = *N,N*-dimethylacetamide, DMF = *N,N*-dimethylformamide, DMSO = dimethyl sulfoxide, DPPP = 1,3-bis(diphenylphosphino) propane. NMP = *N*-methyl-2-pyrrolidone.

4. The preparation of intermediate 2-fluoro-N-(2-hydroxyphenyl)benzamide

2-fluoro-*N*-(2-hydroxyphenyl)benzamide was synthesized according to the previous report.[1] The 2-fluorobenzoyl chloride was added dropwise to a solution of 2-aminophenol (1.95 g, 18 mmol) and Et_3N (5 mL, 36 mmol) in dry THF (30 mL) at 0 °C. After the addition of the acid chloride, the mixture was allowed to warm up to room temperature overnight while stirring under a nitrogen atmosphere. After stirring overnight, the mixture was diluted with water (100 mL) and neutralized with 4% HCl to pH 7. The precipitated amide was then filtered off over a glass filter and washed with 4% HCl and copious amounts of water. The washed product was dried in vacuo without further purification.

5. Analytic data

Dibenzo[b,f][1,4]oxazepin-11(10*H*)-one[2] (3a)



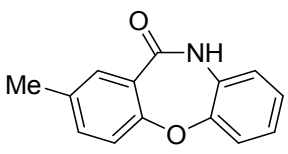
^{1}H NMR (300 MHz, [D$_6$]DMSO): δ = 10.53 (s, 1H), 7.77 (d, *J* = 8.0 Hz, 1H), 7.52-7.50 (t, *J* = 7.6 Hz, 1H), 7.36-7.29 (m, 3H), 7.19-7.12 (m, 3H)

^{13}C NMR (75 MHz, [D$_6$]DMSO): δ = 167.55, 159.86, 150.96, 134.50, 132.00, 130.64, 125.93, 125.83, 125.23, 125.13, 121.70, 121.33, 120.85.

GC-MS (EI, 70 eV): m/z (%) = 211 (M^+, 100), 183 (48), 154 (83), 127 (28), 76 (33), 63 (31), 50 (37), 38 (15).

HRMS (EI): calcd. for $[C_{13}H_9O_2N]^+$: 211.06278; found: 211.06295.

2-methyldibenzo[b,f][1,4]oxazepin-11(10H)-one (3b)



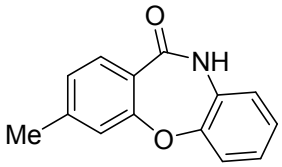
^{1}H NMR (300 MHz, [D$_6$]DMSO): δ = 10.49 (br s, 1H), 7.56 (d, *J* = 2.2 Hz, 1H), 7.40 (dd, *J* = 3.0, 7.8 Hz, 1H), 7.30 (td, *J* = 1.2, 7.2 Hz, 1H), 7.22 (d, *J* = 8.4 Hz, 1H), 7.18-7.10 (m, 3H), 2.30 (s, 3H).

^{13}C NMR (75 MHz, [D$_6$]DMSO): δ = 165.8, 156.8, 150.5, 134.8, 134.6, 131.2, 131.1, 125.8, 125.2, 121.1, 120.3, 20.0.

GC-MS (EI, 70 eV): m/z (%) = 225 (M^+, 100), 197 (38), 168 (28), 154 (20), 143 (8), 115 (10), 89 (16), 77 (14), 63(29), 52 (21), 39 (21).

HRMS (EI): calcd. for $[C_{14}H_{11}O_2N]^+$: 225.07843; found: 225.07825.

3-methyldibenzo[b,f][1,4]oxazepin-11(10H)-one (3c)

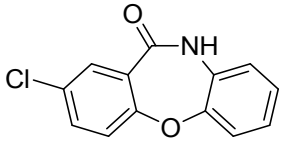


^{1}H NMR (400 MHz, [D$_6$]DMSO): δ = 10.43 (br s, 1H), 7.66 (dd, *J* = 1.2 Hz, 8.0 Hz, 1H), 7.30 (d, *J* = 7.2 Hz, 1H), 7.18-7.15 (m, 3H), 7.14-7.11 (m, 2H), 2.36 (s, 3H).

^{13}C NMR (100 MHz, [D$_6$]DMSO): δ = 165.70, 158.71, 150.23, 145.13, 131.21, 131.16, 126.06, 125.83, 125.07, 122.71, 121.49, 121.25, 120.78, 20.77.

GC-MS (EI, 70 eV): m/z (%) = 225 (M^+, 100), 197 (30), 168 (23), 154 (14).

2-chlorodibenzo[b,f][1,4]oxazepin-11(10H)-one[3] (3d)



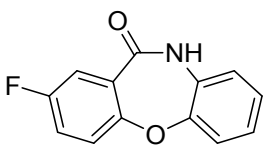
^{1}H NMR (300 MHz, [D$_6$]DMSO): δ = 10.7 (br s, 1H), 7.72 (d, *J* = 2.7 Hz, 1H), 7.68 (dd, *J* = 3.0, 8.6 Hz, 1H), 7.21-7.12 (m, 3H).

^{13}C NMR (75 MHz, [D$_6$]DMSO): δ = 164.4, 157.6, 150.1, 134.0, 130.7, 130.5, 129.4, 127.3, 126.2, 125.5, 122.8, 121.8, 121.3.

GC-MS (EI, 70 eV): m/z (%) = 245 (M^+, 100), 210 (28), 188 (29), 154 (27), 126 (20), 110 (12), 92 (11), 63 (34), 52 (26).

HRMS (EI): calcd. for $[C_{13}H_8O_2NCl]^+$ 245.02381; found 245.02417.

2-fluorodibenzo[b,f][1,4]oxazepin-11(10H)-one (3e)



^{1}H NMR (300 MHz, [D$_6$]DMSO): δ = 10.68 (br s, 1H), 7.50 (dd, *J* = 2.1, 8.7 Hz, 2H), 7.46-7.41 (m, 1H), (dd, *J* = 1.5, 6.9 Hz, 1H), 7.20-7.14 (m, 3H).

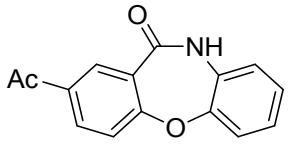
^{13}C NMR (75 MHz, [D$_6$]DMSO): δ = 164.5 (d, *J* = 1.7 Hz), 158.8 (d, *J* = 240.5 Hz), 155.1 (d, *J* = 2.3 Hz), 150.4, 130.8, 127.2 (d, *J* = 7.8 Hz), 126.07, 125.43, 122.72 (d, *J* = 8.5 Hz), 121.72, 121.22, 121.1 (d, *J* = 23.6 Hz), 117.0 (d, *J* = 24.9 Hz).

^{19}F NMR (282 MHz, [D$_6$]DMSO): δ = -116.7 (q, *J* = 5.6 Hz).

GC-MS (EI, 70 eV): m/z (%) = 229 (M^+, 100), 201 (40), 172 (73), 146 (14), 94 (32), 63 (25), 52 (28), 38 (8).

HRMS (EI): calcd. for $[C_{13}H_8O_2NF]^+$ 229.05336; found: 229.05331.

2-acetyldibenzo[b,f][1,4]oxazepin-11(10H)-one (3f)



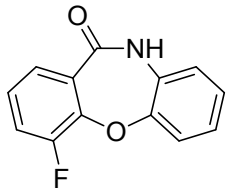
^{1}H NMR (300 MHz, [D$_6$]DMSO): δ = 10.72 (br s, 1H), 8.32 (d, *J* = 2.4 Hz, 1H), 8.17 (dd, *J* = 2.1, 8.4 Hz, 1H), 7.48 (d, *J* = 8.4 Hz, 1H), 7.37 (d, *J* = 7.8 Hz, 1H), 7.22-7.16 (m, 3H), 2.59 (s, 3H).

^{13}C NMR (75 MHz, [D$_6$]DMSO): δ = 196.2, 165.0, 162.0, 149.7, 134.1, 134.0, 132.0, 130.7, 126.3, 125.4, 121.7, 121.4, 121.2, 26.7.

GC-MS (EI, 70 eV): m/z (%) = 253 (M^+, 100), 238 (91), 210 (73), 182 (35), 153 (18), 127 (23), 75 (10), 63 (14), 43 (26).

HRMS (EI): calcd. for $[C_{15}H_{11}O_3N]^+$ 253.07334; found: 253.07364.

4-fluorodibenzo[b,f][1,4]oxazepin-11(10H)-one (3g)



^{1}H NMR (300 MHz, [D$_6$]DMSO): δ = 10.68 (br s, 1H), 7.64-7.56 (m, 2H), 7.33-7.27 (m, 2H), 7.26-7.12 (m, 3H).

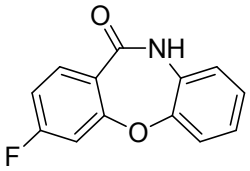
^{13}C NMR (75 MHz, [D$_6$]DMSO): δ = 164.6 (d, *J* = 2.3 Hz), 152.5 (d, *J* = 245.2 Hz), 150.1, 146.2 (d, *J* = 13.5Hz), 130.9, 128.0, 126.5 (d, *J* = 4.5 Hz), 126.4, 125.9 (d, *J* = 7.5 Hz), 125.4, 121.9, 121.2, 120.7 (d, *J* = 18.8 Hz)

^{19}F NMR (282 MHz, [D$_6$]DMSO): δ = -133.2 (q, *J* = 5.6 Hz).

GC-MS (EI, 70 eV): m/z (%) = 229 (M^+, 100), 201 (35), 172 (49), 100 (20).

HRMS (EI): calcd. for $[C_{13}H_8O_2NF]^+$ 229.05336, found 229.05325.

3-fluorodibenzo[b,f][1,4]oxazepin-11(10H)-one (3h)



^{1}H NMR (300 MHz, [D$_6$]DMSO): δ = 10.57 (br s, 1H), 7.84 (dd, *J* = 6.9, 8.9 Hz,1H), 7.36-7.30 (m ,2H), 7.24-7.12 (m, 4H).

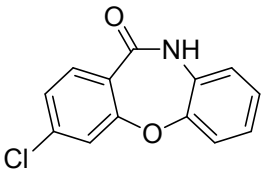
^{13}C NMR (75 MHz, [D$_6$]DMSO): δ = 165.0 (d, *J* = 251.3 Hz), 164.8, 160.0 (d, *J* = 12.0 Hz), 149.8, 133.5 (d, *J* = 10.5 Hz), 130.9, 126.2, 125.3, 122.3 (d, *J* = 3.8 Hz), 121.6, 121.3, 112.9 (d, *J* = 21.0 Hz), 108.2 (d, *J* =24.0 Hz).

^{19}F NMR (282 MHz, [D$_6$]DMSO): δ = -104.5 (q, *J* = 8.5 Hz).

GC-MS (EI, 70 eV): m/z (%) = 229 (M^+, 100), 201 (33), 172 (49), 94 (15).

HRMS (EI): calcd. for $[C_{13}H_8O_2NF]^+$ 229.05336; found 229. 05321.

3-chlorodibenzo[b,f][1,4]oxazepin-11(10H)-one (3i)



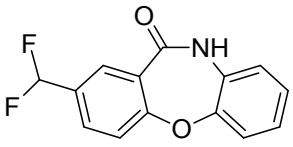
^{1}H NMR (300 MHz, [D$_6$]DMSO): δ = 10.62 (br s, 1H), 7.78 (d, *J* = 8.4 Hz, 1H), 7.56 (d, *J* = 1.8 Hz, 1H), 7.42-7.35 (m, 2H), 7.24-7.12 (m, 3H).

^{13}C NMR (75 MHz, [D$_6$]DMSO): δ = 164.8, 159.1, 149.9, 138.1, 132.9, 130.9, 126.2, 125.7, 125.4, 124.6, 121.7, 121.4, 120.9.

GC-MS (EI, 70 eV): m/z (%) = 245 (M^+, 100), 217 (29), 154 (34), 63 (17).

HRMS (EI): calcd. for $[C_{13}H_8O_2NCl]^+$ 245.02381; found 245.02360; calcd. for $[C_{13}H_8O_2N^{37}Cl]^+$ 247.02086; found 247.02094.

2-(difluoromethyl)dibenzo[b,f][1,4]oxazepin-11(10H)-one (3j)



^{1}H NMR (300 MHz, [D$_6$]DMSO): δ = 10.69 (br s, 1H), 7.98 (q, *J* = 1.2 Hz, 1H), (dt, *J* = 1.2, 8.4 Hz, 1H), (d, *J* = 8.1 Hz, 1H), 7.36 (d, *J* = 7.5 Hz, 1H), 7.22-7.13 (m, 3H), 7.10 (t, *J* = 55.5 Hz, 1H).

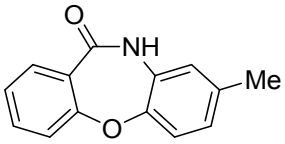
^{13}C NMR (75 MHz, [D$_6$]DMSO): δ = 164.9, 160.4, 149.9, 131.6 (t, *J* = 6.0 Hz), 131.2 (t, *J* = 23.0 Hz), 130.8, 129.3 (t, *J* = 6.8 Hz), 126.2, 126.0, 125.4, 121.7, 121.6, 121.4, 114.0 (t, *J* = 234.0 Hz)

^{19}F NMR (282 MHz, [D$_6$]DMSO) : δ = -109.1 (d, *J* = 56.4 Hz).

GC-MS (EI, 70 eV): m/z (%) = 261 (M^+, 100), 233 (33), 204 (17), 154 (27), 63 (15).

HRMS (EI): calcd. for $[C_{14}H_9O_2NF]^+$ 261.05959; found 261.05940.

8-methyldibenzo[b,f][1,4]oxazepin-11(10H)-one (3l)



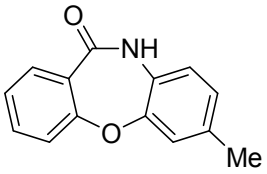
^{1}H NMR (300 MHz, [D$_6$]DMSO): δ = 10.47, 7.76 (dd, *J* = 1.8, 7.8 Hz, 1H), 7.63-7.57 (m ,1H), 7.33-7.28 (m, 2H), (d, *J* = 2.4, 8.1 Hz), 6.95-6.91 (m, 2H), 2.23 (s, 3H).

^{13}C NMR (75 MHz, [D$_6$]DMSO): δ = 195.9, 159.0, 148.3, 135.2, 134.3, 131.3, 130.7, 125.7, 125.6, 125.3, 121.7, 120.9, 120.5.

GC-MS (EI, 70 eV): m/z (%) = 225 (M^+, 100), 210 (15), 196 (69), 168 (23), 154 (19), 76 (27), 50 (30), 39 (24).

HRMS (EI): calcd. for $[C_{14}H_{11}O_2N]^+$ 225.07843; found 225.07837.

7-methyldibenzo[b,f][1,4]oxazepin-11(10H)-one[5] (3m)



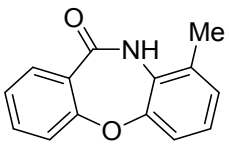
^{1}H NMR (300 MHz, [D$_6$]DMSO): δ = 10.44 (br s, 1H), 7.76 (dd, *J* = 1.8, 7.5 Hz, 1H), 7.63-7.57 (m, 1H), 7.33-7.28 (m, 2H), 7.15 (s, 1H), 7.06-6.69 (m, 2H), 2.26 (s, 3H).

^{13}C NMR (75 MHz, [D$_6$]DMSO): δ = 165.7, 158.9, 150.3, 134.9, 134.2, 131.3, 128.4, 126.3, 128.4, 125.8, 125.3, 121.5, 121.3, 120.6, 20.1.

GC-MS (EI, 70 eV): m/z (%) = 225 (M^+, 100), 196 (37), 168 (19).

HRMS (EI): calcd. for $[C_{14}H_{11}O_2N]^+$ 225.07843; found 225.07842.

9-methyldibenzo[b,f][1,4]oxazepin-11(10H)-one (3n)



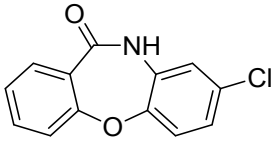
^{1}H NMR (400 MHz, [D$_6$]DMSO) : δ = 9.94 (br s, 1H), 7.73 (dd, J = 7.8, 2.0 Hz, 1H), 7.61-7.57 (m ,1H), 7.35-7.29 (m, 2H), 7.19 (1H, dd, *J* = 5.4, 4.0 Hz), 7.07-7.05 (m, 2H), 2.33 (s, 3H).

^{13}C NMR (75 MHz, [D$_6$]DMSO) : δ = 166.0, 159.5, 152.5, 134.0, 131.5, 131.1, 129.5, 127.5, 126.2, 125.5, 125.4, 120.4, 118.7, 17.8.

GC-MS (EI, 70 eV): m/z (%) = 225 (M^+, 100), 210 (36), 196 (58), 168 (35), 76 (30), 39 (22).

HRMS (EI): calcd. for $[C_{14}H_{11}O_2N]^+$ 225.07843; found 225.07835.

8-chlorodibenzo[b,f][1,4]oxazepin-11(10H)-one[6] (3o)



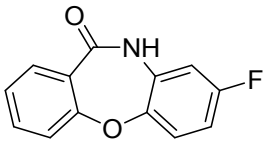
^{1}H NMR (300 MHz, [D$_6$]DMSO): δ = 10.62 (br s, 1H), 7.78 (dd, *J* = 1.8, 7.7 Hz, 1H), 7.67-7.61 (m, 1H), 7.39-7.31 (m, 3H), 7.20-7.17(m, 2H).

^{13}C NMR (75 MHz, [D$_6$]DMSO): δ = 165.5, 158.4, 149.0, 134.7, 132.6, 131.4, 129.4, 125.7, 125.3, 124.7, 123.0, 120.9, 120.6.

GC-MS (EI, 70 eV): m/z (%) = 245 (M^+, 83), 210 (100), 182 (42), 154 (62), 127 (25), 76 (51), 63 (38), 50 (42).

HRMS (EI): calcd. for $[C_{13}H_8O_2NCl]^+$: 245.02381; found 245.02397; calcd. for $[C_{13}H_8O_2N^{37}Cl]^+$: 247.02086; found 247.02160

8-fluorodibenzo[b,f][1,4]oxazepin-11(10H)-one (3p)



^{1}H NMR (300 MHz, [D$_6$]DMSO): δ = 10.62 (br s, 1H), 7.78 (dd, *J* = 1.8, 7.5 Hz, 1H), 7.69-7.60 (m ,1H), 7.40-7.30 (m, 3H), 7.00-6.95 (m, 2H).

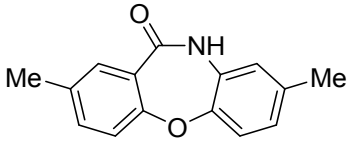
^{13}C NMR (75 MHz, [D$_6$]DMSO): δ = 165.6, 159.0 (d, *J* = 239.3 Hz), 158.6, 146.5 (d, *J* = 2.3Hz), 134.6, 132.5 (d, *J* = 11.3 Hz), 131.4, 125.5, 125.4, 122.6 (d, *J* = 10.5 Hz), 120.5, 111.3 (d, *J* = 23.3 Hz), 108.0 (d, J = 26.3 Hz).

^{19}F NMR (282 MHz, [D$_6$]DMSO): δ = -116.0 (q, *J* = 8.5 Hz).

GC-MS (EI, 70 eV): m/z (%) = 229 (M^+, 100), 201 (32), 172 (78), 145 (20), 76 (36).

HRMS (EI): calcd. for $[C_{13}H_8O_2NF]^+$: 229.05336; found 229.05352.

2,8-dimethyldibenzo[b,f][1,4]oxazepin-11(10H)-one (3r)



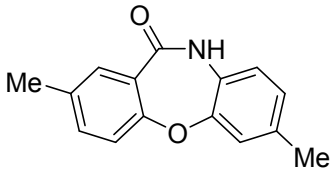
^{1}H NMR (300 MHz, [D$_6$]DMSO): δ = 10.41 (br s, 1H), 7.55 (d, *J* = 1.8 Hz), 7.40-7.37 (m, 1H), 7.20-7.15 (m, 2H), 6.94-6.89 (m, 2H), 2.30 (s, 3H), 2.23 (s, 3H).

^{13}C NMR (75 MHz, [D$_6$]DMSO): δ = 165.9, 156.9, 148.4, 135.0, 134.7, 134.5, 121.2, 130.8, 125.5, 125.3, 121.6, 120.8, 120.2, 20.3, 20.1.

GC-MS (EI, 70 eV): m/z (%) = 239 (M^+, 100), 224 (17), 210 (59), 167 (13).

HRMS (EI): calcd. for $[C_{15}H_{13}O_2N]^+$: 239.09408; found 239.09461.

2,7-dimethyldibenzo[b,f][1,4]oxazepin-11(10H)-one (3s)



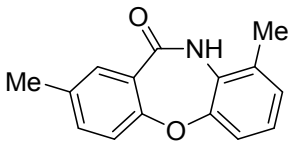
^{1}H NMR (300 MHz, [D$_6$]DMSO): δ = 10.38 (br s,1H), 7.55(d, *J* = 2.1 Hz, 1H), 7.41-7.37 (m, 1H), 7.19(d, *J* = 8.1Hz), 7.12 (s, 1H), 7.04-6.96 (m, 2H), 2.30 (s, 3H), 2.25 (s, 3H).

^{13}C NMR (75 MHz, [D$_6$]DMSO): δ = 165.9, 156.9, 148.4, 135.0, 134.7, 134.5, 131.2, 130.8, 125.5, 125.3, 121.7, 120.8, 120.3, 20.3, 20.1.

GC-MS (EI, 70 eV): m/z (%) = 239 (M^+, 100), 224 (13), 210 (38)

HRMS (EI): calcd. for $[C_{15}H_{13}O_2N]^+$: 239.09408; found 239.09427.

2,9-dimethyldibenzo[b,f][1,4]oxazepin-11(10H)-one (3t)



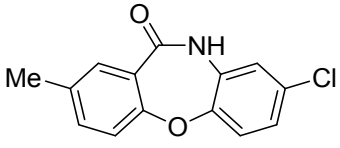
^{1}H NMR (300 MHz, [D$_6$]DMSO): δ = 9.90 (br s, 1H), (dd, J = 0.9 Hz, 2.1 Hz, 1H), 7.39-7.36 (m, 1H), 7.22-7.15 (m, 2H), 7.06-7.04 (m, 2H), 2.31 (s, 3H), 2.29 (s, 3H).

^{13}C NMR (75 MHz, [D$_6$]DMSO): δ = 166.1, 157.4, 152.6, 134.7, 134.4, 131.4, 131.0, 129.5, 127.3, 125.7, 125.3, 120.1, 118.6, 20.1, 17.8..

GC-MS (EI, 70 eV): m/z (%) = 239 (M^+, 100), 224 (34), 210 (51), 194 (13), 167(14), 77 (15).

HRMS (EI): calcd. for $[C_{15}H_{13}O_2N]^+$ 239.09408; found 239. 09467.

8-chloro-2-methyldibenzo[b,f][1,4]oxazepin-11(10H)-one (3u)



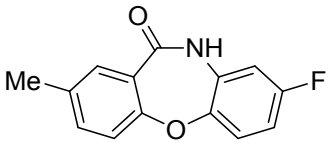
^{1}H NMR (300 MHz, [D$_6$]DMSO): δ = 10.57 (br s, 1H), 7.57 (dd, *J* = 0.9, 2.1 Hz, 1H), 7.42 (d, *J* = 8.1 Hz, 1H), 7.36-7.32 (m, 1H), 7.24 (d, *J* = 8.1 Hz, 1H), 7.19-7.16 (m, 2H), 2.30 (s, 3H).

^{13}C NMR (75 MHz, [D$_6$]DMSO): δ = 165.1, 155.9, 148.6, 134.5, 134.4, 132.1, 130.8, 128.8, 124.2, 124.0, 122.3, 120.3, 119.9.

GC-MS (EI, 70 eV): m/z (%) = 259 (M^+, 78), 224 (100), 196 (30), 168 (34).

HRMS (ESI): calcd. for $[C_{14}H_{10}{}^{35}ClNO_2 + Na]^+$ 282.02923, found 282.02864; calcd. for $[C_{14}H_{10}{}^{37}ClNO_2 + Na]^+$ 284.02669, found 284.02599.

8-fluoro-2-methyldibenzo[b,f][1,4]oxazepin-11(10H)-one (3v)



^{1}H NMR (300 MHz, [D$_6$]DMSO): δ = 10.56 (br s, 1H), 7.56 (d, J = 2.1 Hz, 1H), 7.43-7.40 (m, 1H), (7.37-7.32 (m, 1H), (d, *J* = 8.1 Hz, 1H), 6.99-6.93 (m, 2H), 2.30 (s, 3H).

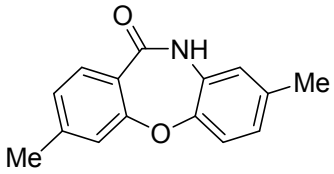
^{13}C NMR (75 MHz, [D$_6$]DMSO): δ = 165.7, 158.9 (d, *J* = 240.0 Hz), 156.6, 146.7 (d, *J* = 2.3 Hz), 135.0, 134.8, 132.5 (d, *J* = 11.3 Hz), 131.3, 124.9, 122.5 (d, *J* = 9.8 Hz), 120.3, 111.3 (d, *J* = 22.5 Hz), 107.9 (d, *J* = 26.3 Hz), 20.1.

^{19}F NMR (282 Hz, [D$_6$]DMSO) : δ = -116.2 (q, *J* = 19.7 Hz).

GC-MS (EI, 70 eV): m/z (%) = 243 (M^+, 100), 215 (23), 186 (26), 172 (23), 89 (13).

HRMS (EI): calcd. for $[C_{14}H_{10}O_2NF]^+$ 243.06901; found 243.06964.

3,8-dimethyldibenzo[b,f][1,4]oxazepin-11(10H)-one (3w)



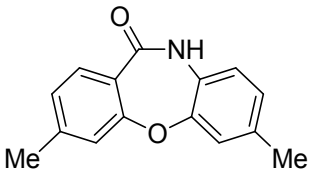
^{1}H NMR (300 MHz, [D$_6$]DMSO): δ = 10.37 (br s, 1H), 7.64 (d, *J* = 8.4 Hz, 1H), 7.18-7.10 (m, 3H), 6. 93 (s, 1H), 6.93-6.90 (m, 1H), 2.35 (s, 3H), 2.23 (s, 3H).

^{13}C NMR (75 MHz, [D$_6$]DMSO): δ = 165.8, 158.8, 148.2, 145.0, 135.1, 131.1, 130.8, 125.9, 125.5, 122.8, 121.6, 120.9, 120.7, 20.8, 20.3.

GC-MS (EI, 70 eV): m/z (%) = 239 (M^+, 100), 224 (15), 210 (64).0

HRMS (EI): calcd. for $[C_{15}H_{13}O_2N]^+$ 239.09408; found 239.09460.

3,7-dimethyldibenzo[b,f][1,4]oxazepin-11(10H)-one (3x)



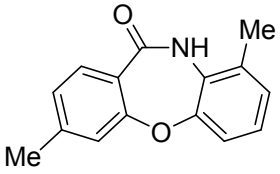
^{1}H NMR (300 MHz, [D$_6$]DMSO): δ = 10.34 (br s, 1H), 7.64 (d, *J* = 7.8 Hz, 1H), 7.14-7.09 (m, 3H), 7.04-6.95 (m, 2H), 2.34 (s, 3H), 2.25 (s, 3H).

^{13}C NMR (75 MHz, [D$_6$]DMSO): δ = 165.7, 158.7, 150.1, 145.0, 134.8, 131.1, 128.5, 126.2, 126.0, 122.8, 121.5, 121.2, 120.8, 20.8, 20.1.

GC-MS (EI, 70 eV): m/z (%) = 239 (M^+, 100), 210 (41), 182 (14)

HRMS (EI): calcd. for $[C_{15}H_{13}O_2N]^+$ 239.09408; found 239.09462.

3,9-dimethyldibenzo[b,f][1,4]oxazepin-11(10H)-one (3y)



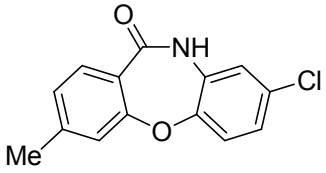
^{1}H NMR (300 MHz, [D$_6$]DMSO): δ = 9.84 (br s, 1H), 7.61 (d, *J* = 7.8 Hz,1H), 7.18-7.10 (m, 3H), 7.05-7.04 (m, 2H), 2.34 (s, 3H), 2.31 (s, 3H).

^{13}C NMR (75 MHz, [D$_6$]DMSO): δ = 165.94, 159.33, 152.35, 144.77, 131.35, 130.86, 129.55, 127.39, 126.11, 125.24, 123.23, 120.56, 118.76, 20.81, 17.76.

GC-MS (EI, 70 eV): m/z (%) = 239 (M^+, 100), 224 (31), 210 (53), 195 (13), 182 (11).

HRMS (EI): calcd. for $[C_{15}H_{13}O_2N]^+$ 239.09408; found 239.09456.

8-chloro-3-methyldibenzo[b,f][1,4]oxazepin-11(10H)-one (3z)



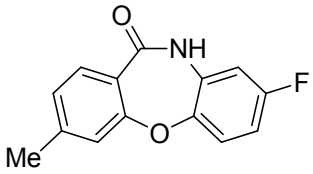
^{1}H NMR (300 MHz, [D$_6$]DMSO): δ = 10.52 (br s, 1H), 7.66 (d, *J* = 1.8 Hz, 1H), 7.34 (d, J = 8.4 Hz, 1H), 7.19-7,13 (m, 4H), 2.36 (s, 3H).

^{13}C NMR (75 MHz, [D$_6$]DMSO): δ = 165.48, 158.26, 148.87, 145.49, 132.69, 131.25, 129.35, 126.33, 124.60, 122.93, 122.34, 120.78, 20.79.

GC-MS (EI, 70 eV): m/z (%) = 259 (M^+, 77), 224 (100), 196 (28), 168 (36), 89 (19), 63 (17).

HRMS (EI): calcd. for $[C_{14}H_{10}O_2NCl]^+$ 259.03946, found 259.04015.

8-fluoro-3-methyldibenzo[b,f][1,4]oxazepin-11(10H)-one (3aa)



^{1}H NMR (300 MHz, [D$_6$]DMSO): δ = 10.52 (br s, 1H), (d, *J* = 7.8 Hz, 1H), 7.37-7.32 (m, 2H), 7.18 (s ,1H), 7.14 (dt, *J* = 8.1, 0.9 Hz, 1H), 6.99-6.94 (m, 2H), 2.36 (s, 3H).

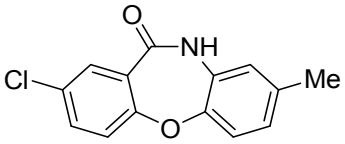
^{13}C NMR (75 MHz, [D$_6$]DMSO): δ = 165.56, 158.94 (d, *J* = 240.0 Hz), 158.49, 146.39 (d, *J* = 2.6 Hz), 145.41, 132.59 (d, *J* = 11.3 Hz), 131.21, 126.20, 122.58 (d, *J* = 10.0 Hz), 122.43, 120.72, 111.19 (d, *J* = 23.0 Hz), 107.90 (d, *J* = 26.2 Hz), 20.77.

^{19}F NMR (282 MHz, [D$_6$]DMSO): δ = -116.1 (q, *J* = 19.8 Hz)

GC-MS (EI, 70 eV): m/z (%) = 243 (M^+, 100), 215 (26), 186 (28), 172 (21), 89 (16).

HRMS (EI): calcd. for $[C_{14}H_{10}O_2NF]^+$ 243.06901; found 243.06871.

2-chloro-8-methyldibenzo[b,f][1,4]oxazepin-11(10H)-one (3ab)



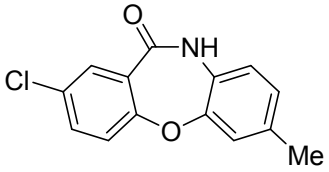
^{1}H NMR (300 MHz, [D$_6$]DMSO): δ = 10.59 (br s, 1H), 7.70 (d, *J* = 2.7 Hz, 1H), 7.65 (dd, *J* = 3.0, 8.6 Hz, 1H), 7.36 (d, *J* = 8.7 Hz, 1H), 7.15 (s, 1H), 7.06-6.98 (m, 2H), 2.25 (s, 3H).

^{13}C NMR (75 MHz, [D$_6$]DMSO): δ = 164.3, 157.8, 150.0, 135.2, 133.9, 130.5, 129.3, 128.0, 127.4, 126.6, 122.8, 122.5, 20.1.

GC-MS (EI, 70 eV): m/z (%) = 259 (M^+, 100), 244(14), 230 (54), 167 (18), 83 (15).

HRMS (ESI, m/z): calcd. for $[C_{14}H_{10}{}^{35}ClNO_2 + Na]^+$ 282.02923, found 282.02916; calcd. for $[C_{14}H_{10}{}^{37}ClNO_2 + Na]^+$ 284.02669, found 284.02654.

2-chloro-7-methyldibenzo[b,f][1,4]oxazepin-11(10H)-one (3ac)



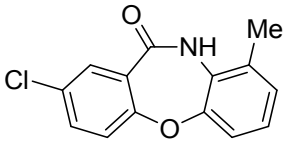
^{1}H NMR (300 MHz, [D$_6$]DMSO): δ = 10.59 (br s, 1H), 7.71-7.64 (m, 2H), 7.38 (d, *J* = 8.4 Hz, 1H), 7.16 (s, 1H), 7.06-6.99 (m, 2H), 2.26 (s, 3H).

^{13}C NMR (75 MHz, [D$_6$]DMSO): δ = 164.34, 157.58, 150.01, 135.22, 133.89, 130.52, 129.33, 127.99, 127.40, 126.60, 122.78, 121.50, 20.11.

GC-MS (EI, 70 eV): m/z (%) = 259 (M^+, 100), 230 (32), 224 (17), 167 (18).

HRMS (ESI): calcd. for $[C_{14}H_{10}{}^{35}ClNO_2 + Na]^+$ 282.02923, found 282.02899; calcd. for $[C_{14}H_{10}{}^{37}ClNO_2 + Na]^+$ 284.02669, found 284.02616.

2-chloro-9-methyldibenzo[b,f][1,4]oxazepin-11(10H)-one (3ad)



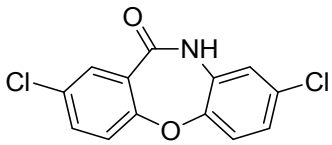
^{1}H NMR (300 MHz, [D$_6$]DMSO): δ = 10.11(br s, 1H), 7.69-7.63 (m, 2H), 7.39 (dt, *J* = 8.4 Hz, 1.5Hz, 1H), 7.21 (t, *J* = 4.8 Hz, 1H), 7.09-7.06 (m, 2H), 2.49 (s, 3H).

^{13}C NMR (75 MHz, [D$_6$]DMSO): δ = 164.68, 158.16, 152.30, 133.69, 131.77, 130.33, 129.47, 129.11, 127.87, 127.72, 125.61, 122.55, 118.75, 17.74.

GC-MS (EI, 70 eV): m/z (%) = 259(M^+, 100), 244 (29), 230 (45), 167 (20).

HRMS (ESI): calcd. for $[C_{14}H_{10}{}^{35}ClNO_2 + Na]^+$ 282.02923, found 282.02940; calcd. for $[C_{14}H_{10}{}^{37}ClNO_2 + Na]^+$ 284.02669, found 284.02675.

2,8-dichlorodibenzo[b,f][1,4]oxazepin-11(10H)-one (3ae)



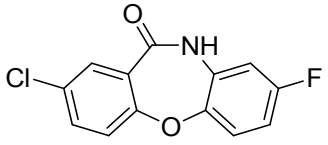
^{1}H NMR (300 MHz, [D$_6$]DMSO): δ = 10.76 (s, 1H), 7.69-7.63 (m, 2H), 7.40-7.34 (m, 2H), 7.20-7.16 (m, 2H).

^{13}C NMR (75 MHz, [D$_6$]DMSO): δ = 164.32, 157.09, 148.77, 134.28, 132.07, 130.54, 129.76, 129.70, 126.85, 125.09, 122.98, 122.80, 121.07.

GC-MS (EI, 70 eV): m/z (%) = 279 (M^+, 81), 244 (100), 216 (34), 188 (42), 75 (23), 63 (24).

HRMS (ESI): calcd. for $[C_{13}H_7{}^{35}Cl_2NO_2 + Na]^+$ 301.97460, found 301.97514; calcd. for $[C_{13}H_7{}^{37}Cl_2NO_2 + Na]^+$ 203.97184, found 303.97218.

2-chloro-8-fluorodibenzo[b,f][1,4]oxazepin-11(10H)-one (3af)



^{1}H NMR (300 MHz, [D$_6$]DMSO): δ = 10.77 (br s, 1H), 7.73-7.68 (m, 2H), 7.43-7.38 (m, 2H), 7.03-6.95 (m, 2H).

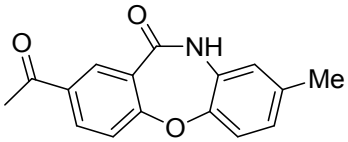
^{13}C NMR (75 MHz, [D$_6$]DMSO): δ = 164.2, 159.1 (d, *J* = 240.0 Hz), 138.3, 134.2, 132.9, 132.1 (d, *J* = 11.3 Hz), 127.0, 125.9, 124.4 (d, *J* = 9.8 Hz), 122.8, 120.9, 111.6 (d, *J* = 23.3 Hz), 108.2 (d, *J* = 26.3 Hz)

^{19}F NMR (282 MHz, [D$_6$]DMSO): δ = -115.6 (q, *J* = 8.5 Hz).

GC-MS (EI, 70 eV): m/z (%) = 263 (M^+, 100), 235 (23), 200 (16), 172 (57), 75 (19).

HRMS (EI): calcd. for $[C_{13}H_7{}^{35}ClFNO_2 + Na]^+$ 286.00416, found 286.00498; calcd. for $[C_{13}H_7{}^{37}ClFNO_2 + Na]^+$ 288.00157, found 288.00216

2-acetyl-8-methyldibenzo[b,f][1,4]oxazepin-11(10H)-one (3ag)



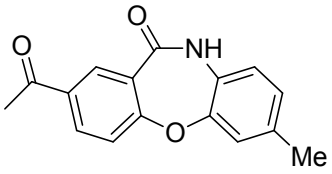
^{1}H NMR (300 MHz, [D$_6$]DMSO): δ = 10.65 (br s, 1H), 8.31 (d, *J* = 2.4 Hz, 1H), 8.16 (dd, *J* = 2.1, 8.4 Hz, 1H), 7.45 (d, *J* = 8.4 Hz, 1H), 7. 24 (d, *J* = 7.8 Hz), 6.97-6.93 (m, 2H), 2.59 (s, 3H), 2.24 (s, 3H).

^{13}C NMR (75 MHz, [D$_6$]DMSO): δ = 196.22, 165.09, 162.16, 147.61, 135.65, 134.03, 133.85, 131.98, 130.28, 125.83, 125.68, 121.83, 121.15, 121.06, 26.70, 20.29.

GC-MS (EI, 70 eV): m/z (%) = 267 (M^+, 100), 252 (41), 238 (28), 224 (26), 196 (17), 167 (12), 126 (10).

HRMS (ESI): calcd. for $[C_{16}H_{13}NO_3 + Na]^+$ 290.07876, found 290.07871.

2-acetyl-7-methyldibenzo[b,f][1,4]oxazepin-11(10H)-one (3ah)



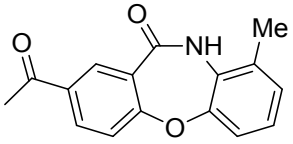
^{1}H NMR (300 MHz, [D$_6$]DMSO): δ = 10.61 (br s, 1H), 8.32 (d, *J* = 2.4 Hz, 1H), 8.16 (dd, *J* = 2.4, 8.4 Hz, 1H), (d, *J* = 7.45 Hz, 8.4 Hz), 7.19 (s, 1H), 7.08-7.00 (m, 2H), 2.59 (s, 3H), 2.26 (s, 3H).

^{13}C NMR (75 MHz, [D$_6$]DMSO): δ = 196.2, 164.9, 162.0, 149.6, 135.2, 134.0, 133.9, 132.0, 128.0, 126.7, 125.7, 121.6, 121.5, 121.2, 26.7, 20.1.

GC-MS (EI, 70 eV): m/z (%) = 267 (M^+, 100), 252 (38), 224 (35), 196 (16).

HRMS (ESI): calcd. for $[C_{16}H_{13}NO_3 + Na]^+$ 290.07876, found 290.07895.

2-acetyl-9-methyldibenzo[b,f][1,4]oxazepin-11(10H)-one) (3ai)



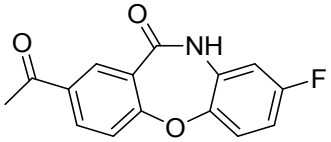
^{1}H NMR (300 MHz, [D$_6$]DMSO): δ = 10.13 (br s, 1H), 8.28 (d, *J* = 2.1 Hz, 1H), 8.16-8.13 (m ,1H), 7.48 (d, *J* = 8.4 Hz, 1H), 7.25-7.22 (m, 1H), 7.10-7.08 (m, 2H), 2.59 (s, 3H), 2.33 (s, 3H).

^{13}C NMR (75 MHz, [D$_6$]DMSO): δ = 196.23, 165.31, 162.62, 151.87, 134.06, 133.73, 131.75, 129.12, 127.84, 126.25, 125.61, 121.01, 118.87, 26.70, 17.75.

GC-MS (EI, 70 eV): m/z (%) = 267 (M+, 100), 252 (54), 238 (19), 224 (23), 208 (13), 196 (16).

HRMS (ESI): calcd. for $[C_{16}H_{13}NO_3 + Na]^+$ 290.07876, found 290.07893.

2-acetyl-8-fluorodibenzo[b,f][1,4]oxazepin-11(10H)-one (3ak)



^{1}H NMR (300 MHz, [D$_6$]DMSO): δ = 10.79 (br s, 1H), 8.32 (d, *J* = 2.1 Hz), 8.20-8.16 (m, 1H), 7.49 (d, *J* = 8.4 Hz, 1H), 7.44-7.40 (m ,1H), 7.04-6.97 (m, 2H), 2.59 (s, 3H).

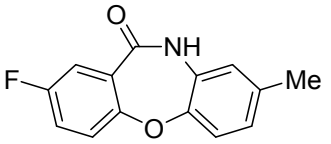
^{13}C NMR (75 MHz, [D$_6$]DMSO): δ = 196.2, 164.9, 161.8, 159.2 (d, *J* = 240.8 Hz), 145.8 (d, *J* = 2.3 Hz), 134.3, 134.1, 132.1 (d, *J* = 11.3 Hz), 132.0, 125.4, 122.8 (d, *J* = 9.8 Hz), 121.2, 111.6 (d, *J* = 23.3Hz), 108.2 (d, *J* = 26.3Hz), 26.7.

^{19}F NMR (282 MHz, [D$_6$]DMSO): δ = -115.5 (q, *J* = 8.5 Hz).

GC-MS (EI, 70 eV): m/z (%) = 271 (M^+, 100), 256 (91), 228 (25), 200 (21), 172 (17), 75 (15), 43 (14).

HRMS (ESI): calcd. for $[C_{15}H_{10}FNO_3 + Na]^+$ 294.05369, found 294.05361.

2-fluoro-8-methyldibenzo[b,f][1,4]oxazepin-11(10H)-one (3al)



^{1}H NMR (300 MHz, [D$_6$]DMSO): δ = 10.62 (br s, 1H), 7.50-7.44 (m, 2H), 7.40-7.38 (m, 1H), 7.21 (dd, *J* = 7.1 Hz, 2.1 Hz, 1H), 6.95 (s, 1H), 6.95-6.92 (m, 1H), 2.24 (s, 3H).

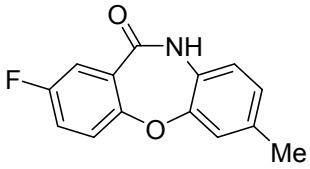
^{13}C NMR (75 MHz, [D$_6$]DMSO): δ = 164.6 (d, *J* = 2.3 Hz), 158.7 (d, *J* = 240 Hz), 155.2 (d, *J* = 2.3 Hz), 148.3, 135.4, 130.4, 127.3 (d, *J* = 8.3 Hz), 125.8, 122.6 (d, *J* = 8.3 Hz), 121.8, 121.2, 120.9, 117.0 (d, *J* = 25.5 Hz), 20.3.

^{19}F NMR (282 MHz, [D$_6$]DMSO): δ = -116.8 (q, *J* = 7.9 Hz).

GC-MS (EI, 70 eV): m/z (%) = 243 (M^+, 100), 228 (13), 214 (61), 186 (18), 172 (13), 94 (12).

HRMS (ESI): calcd. for $[C_{14}H_{10}FNO_2 + Na]^+$ 266.05878, found 266.05908.

2-fluoro-7-methyldibenzo[b,f][1,4]oxazepin-11(10H)-one (3am)



^{1}H NMR (300 MHz, [D$_6$]DMSO): δ = 10.58 (br s, 1H), 7.50-7.36 (m, 3H), 7.16 (s, 1H), 7.06-6.98 (m, 2H), 2.26 (s, 3H).

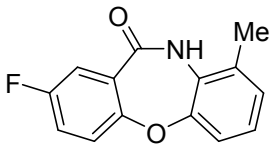
^{13}C NMR (75 MHz, [D$_6$]DMSO): δ = 164.5, 158.8 (d, *J* = 240.0 Hz), 155.1, 155.0, 150.3, 135.2, 128.1, 127.3 (d, *J* = 7.5 Hz), 126.5, 122.7 (d, *J* = 8.3 Hz), 121.4 (d, *J* =2.3 Hz), 121.0 (d, *J* = 23.3 Hz), 117.0 (d, *J* = 24.8 Hz), 20.1.

^{19}F NMR (282 MHz, [D$_6$]DMSO): δ = -166.7 (q, *J* = 8.4 Hz)

GC-MS (EI, 70 eV): m/z (%) = 243 (M^+, 100), 215 (72).

HRMS (EI): calcd. for $[C_{14}H_{10}O_2NF]^+$ 243.06901; found 243.06939.

2-fluoro-9-methyldibenzo[b,f][1,4]oxazepin-11(10H)-one (3an)



^{1}H NMR (300 MHz, [D$_6$]DMSO): δ = 10.01, 7.48-7.41 (m, 3H), 7.22-7.18 (m, 1H), 7.22-7.18 (m, 1H), 7.08-7.07 (m, 2H), 2.32 (s, 3H).

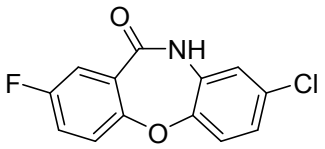
^{13}C NMR (75 MHz, [D$_6$]DMSO): δ = 164.8, 158.8 (d, *J* = 240.8 Hz), 155.7, 152.5, 131.7, 129.2, 127.7 (d, *J* = 8.3 Hz), 127.6, 125.6, 122.5 (d, *J* = 8.3 Hz), 120.8 (d, *J* = 23.3 Hz), 118.7, 116.8 (d, *J* = 24.8 Hz), 17.7.

^{19}F NMR (282 MHz, [D$_6$]DMSO): δ = -116.5 (m, *J* = 6.8 Hz).

GC-MS (EI, 70 eV): m/z (%) = 243 (M^+, 100), 228 (26), 214 (52), 186 (22), 94 (10).

HRMS (ESI): calcd. for $[C_{14}H_{10}FNO_2 + Na]^+$ 266.05878, found 266.05903.

8-chloro-2-fluorodibenzo[b,f][1,4]oxazepin-11(10H)-one (3ao)



^{1}H NMR (300 MHz, [D$_6$]DMSO): δ = 10.76 (br s, 1H), 7.53-7.48 (m, 2H), 7.44-7.37 (m, 2H), 7.22-7.19 (m, 2H).

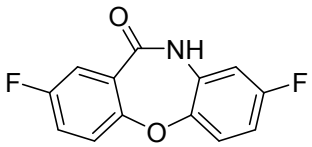
^{13}C NMR (75 MHz, [D$_6$]DMSO): δ = 164.3, 158.9 (d, *J* = 240.5 Hz), 154.6, 149.0, 132.3, 129.6, 126.9 (d, *J* = 7.5 Hz), 125.0, 122.9, 122.8 (d, *J* = 8.0 Hz), 121.4 (d, *J* = 23.2 Hz), 121.0, 117.1 (d, *J* = 25.1 Hz).

^{19}F NMR (282 MHz, [D$_6$]DMSO): δ = -116.2 (q, *J* = 7.9 Hz).

GC-MS (EI, 70 eV): m/z (%) = 263 (M^+, 100), 235 (65).

HRMS (EI): calcd. for $[C_{13}H_7O_2N^{35}ClF]^+$ 263.01439, found 263.01466; calcd. for $[C_{13}H_7O_2N^{37}ClF]^+$ 265.01144, found 265.01195.

2,8-difluorodibenzo[b,f][1,4]oxazepin-11(10H)-one (3ap)



^{1}H NMR (300 MHz, [D$_6$]DMSO): δ = 10.76 (br s, 1H), 7.52-7.47 (m, 2H), 7.45-7.37 (m, 2H), 7.03-6.95 (m, 2H).

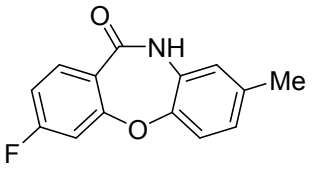
^{13}C NMR (75 MHz, [D$_6$]DMSO): δ = 164.4, 159.0 (d, *J* = 240.0 Hz), 158.8 (d, *J* = 240.8 Hz), 154.9, 154.8 (d, *J* = 5.6 Hz), 146.6 (d, *J* = 2.3 Hz), 132.2 (d, *J* = 11.3 Hz), 127.0 (d, *J* = 7.7 Hz), 122.7, 122.7 (d, *J* = 15.9 Hz), 121.4 (d, *J* = 23.3 Hz), 117.1 (d, *J* = 25.0 Hz), 111.6 (d, *J* = 23.5 Hz), 108.2 (d, *J* = 26.5 Hz).

^{19}F NMR (282 MHz, [D$_6$]DMSO): δ = -115.8 (q, *J* = 6.8 Hz), -116.4 (q, *J* = 6.5 Hz)

GC-MS (EI, 70 eV): m/z (%) = 247 (M^+, 100), 219 (35).

HRMS (EI): calcd. for $[C_{13}H_7O_2NF_2]^+$ 247.04394; found 247.04438.

3-fluoro-8-methyldibenzo[b,f][1,4]oxazepin-11(10H)-one (3aq)



^{1}H NMR (300 MHz, [D$_6$]DMSO): δ = 10.50 (br s, 1H), 7.83 (dd, *J* = 6.6 Hz, 8.9 Hz, 1H), (dd, *J* = 2.4 Hz, 9.5 Hz, 1H), 7.21-7.15 (m, 1H), 6.95 (s, 1H), 6.95-6.92 (m, 1H), 2.24 (s, 3H).

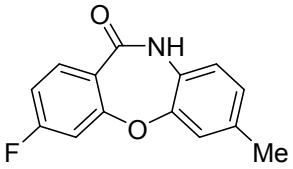
^{13}C NMR (75 MHz, [D$_6$]DMSO): δ = 164.95 (d, *J* = 250.9 Hz), 164.88, 160.11 (d, *J* = 11.8 Hz), 147.77, 135.54, 133.51 (d, *J* = 10.6 Hz), 130.47, 125.66, 122.41 (d, *J* = 3.2Hz), 121.74, 120.96, 112.78 (d, *J* = 21.5 Hz), 108.06 (d, *J* = 23.6 Hz), 20.30.

^{19}F NMR (282 MHz, [D$_6$]DMSO): δ = -104.6 (q, *J* = 8.2 Hz).

GC-MS (EI, 70 eV): m/z (%) = 243 (M^+, 100), 228 (13), 214 (82), 186 (23), 172 (15), 94 (40).

HRMS (ESI): calcd. for $[C_{14}H_{10}FNO_2 + Na]^+$ 266.05878, found 266.05864.

3-fluoro-7-methyldibenzo[b,f][1,4]oxazepin-11(10H)-one (3ar)



^{1}H NMR (300 MHz, [D$_6$]DMSO): δ = 10.47 (br s, 1H), 7.83 (dd, *J* = 6.9 Hz, 8.7 Hz 1H), 7.28 (dd, *J* = 2.4 Hz, 9.5 Hz, 1H), 7.21-7.15 (m, 2H), 7.06-6.98 (m, 2H), 2.26 (s, 3H).

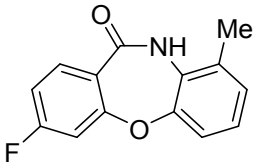
^{13}C NMR (75 MHz, [D$_6$]DMSO): δ =

^{19}F NMR (282 MHz, [D$_6$]DMSO): δ = -104.6 (d, *J* = 8.2 Hz).

GC-MS (EI, 70 eV): m/z (%) = 243 (M^+, 100), 214 (50), 186 (21), 172 (11), 94 (12).

HRMS (ESI): calcd. for $[C_{14}H_{10}FNO_2 + Na]^+$ 266.05878, found 266.05848.

3-fluoro-9-methyldibenzo[b,f][1,4]oxazepin-11(10H)-one (3as)



^{1}H NMR (300 MHz, [D$_6$]DMSO): δ = 9.99 (br s, 1H), 7.63 (dd, *J* = 8.7 Hz, 6.6 Hz, 1H), (dd, *J* = 2.4 Hz, 9.5 Hz, 1H), 7.21-7.15 (m, 2H), 7.08-7.06 (m, 2H), 3.32 (s, 3H).

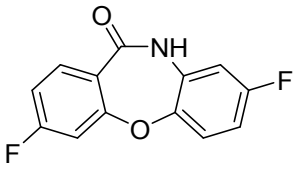
^{13}C NMR (75 MHz, [D$_6$]DMSO): δ = 165.05, 164.8 (d, *J* = 250.5 Hz), 160.5 (d, *J* = 11.3 Hz), 151.98, 133.27 (d, *J* = 10.5 Hz), 131.58, 129.28, 127.74, 125.42, 122.9 (d, *J* = 3.0 Hz), 118.79, 113.0 (d, *J* = 21.8 Hz), 108.0, 17.73.

^{19}F NMR (282 MHz, [D$_6$]DMSO): δ = -104.6 (d, *J* = 8.5 Hz).

GC-MS (EI, 70 eV): m/z (%) = 243 (M^+, 100), 228 (26), 214 (52), 186 (22).

HRMS (ESI): calcd. for $[C_{14}H_{10}FNO_2 + Na]^+$ 266.05878, found 266.05881.

3,8-difluorodibenzo[b,f][1,4]oxazepin-11(10H)-one (3au)



^{1}H NMR (300 MHz, [D$_6$]DMSO): δ =

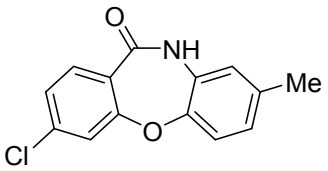
^{13}C NMR (75 MHz, [D$_6$]DMSO): δ = 165.10 (d, *J* = 251.2 Hz), 164.63, 159.13 (d, *J* = 240.8 Hz), 159.83 (d, J = Hz), 146.00 (d, *J* = 2.3 Hz), 133.62 (d, *J* = 10.5 Hz), 132.32 (d, *J* = 11.3 Hz), 124.49, 122.74 (d, *J* = 9.8 Hz), 122.48 (d, *J* = 3.8 Hz), 122.10 (d, *J* = 3.8 Hz), 113.10 (d, *J* = 21.8 Hz) , 111.48 (d, J = Hz), 108.30 (d, J = 9.0 Hz), 107.97 (d, *J* = 11.3 Hz).

^{19}F NMR (282 MHz, [D$_6$]DMSO): δ = -104.0 (q, *J* = 8.5 Hz), -115.6 (q, *J* = 8.5 Hz).

GC-MS (EI, 70 eV): m/z (%) = 247 (M^+, 100), 230 (11), 219 (24), 190 (54), 171 (14), 94 (26).

HRMS (ESI): calcd. for $[C_{13}H_7F_2NO_2 + Na]^+$ 270.03371, found 270.03304.

3-chloro-8-methyldibenzo[b,f][1,4]oxazepin-11(10H)-one (3av)



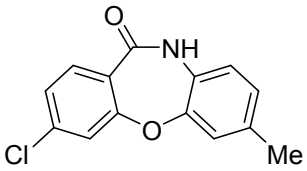
^{1}H NMR (300 MHz, [D$_6$]DMSO): δ = 10.55 (br s, 1H), 7.77 (d, *J* = 8.4 Hz, 1H), 7.52-7.51 (m, 1H), 7.40 (dd, *J* = 2.1, 8.4 Hz, 1H), 7.23 (d, *J* = 9.0 Hz, 1H), 6.96-6.94 (m, 2H), 2.24 (s, 3H).

^{13}C NMR (75 MHz, [D$_6$]DMSO): δ = 164.9, 159.3, 147.9, 138.0, 135.6, 132.8, 130.4, 125.7, 125.6, 124.7, 121.8, 121.0, 120.8, 20.3.

GC-MS (EI, 70 eV): m/z (%) = 259 (M^+ ,100), 244(13), 230 (60), 167 (17).

HRMS (ESI): calcd. for $[C_{14}H_{10}O_2NCl]^+$ 259.03946, found 259.03966; calcd. for $[C_{14}H_{10}O_2N^{37}Cl]^+$ 261.03651, found 261.03721.

3-chloro-7-methyldibenzo[b,f][1,4]oxazepin-11(10H)-one (3aw)



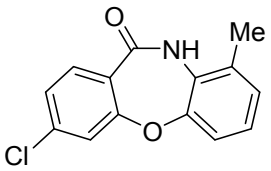
^{1}H NMR (300 MHz, [D$_6$]DMSO): δ = 10. 53 (br s, 1H), 7.77 (d, J = 8.4 Hz, 1H), 7.52 (d, *J* = 2.1 Hz,1H), 7.40 (dd, J = 2.1, 8.4 Hz, 1H), 7.19 (s, 1H), 7.06-6.99 (m ,2H).

^{13}C NMR (75 MHz, [D$_6$]DMSO): δ = 164.8, 159.2, 149.8, 138.0, 135.1, 132.8, 128.1, 126.7, 125.6, 124.7, 121.6, 121.4, 120.9, 20.1.

GC-MS (EI, 70 eV): m/z (%) = 259 (M^+, 100), 230 (39), 167 (17).

HRMS (EI): calcd. for $[C_{14}H_{10}O_2NCl]^+$ 259.03946, found 259.03997; calcd. for $[C_{14}H_{10}O_2N^{37}Cl]^+$ 261.03651, found 261.03730.

3-chloro-9-methyldibenzo[b,f][1,4]oxazepin-11(10H)-one (3ax)



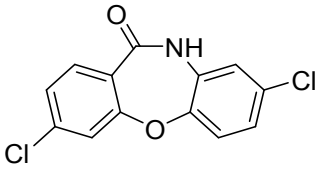
^{1}H NMR (300 MHz, [D$_6$]DMSO): δ =

^{13}C NMR (75 MHz, [D$_6$]DMSO): δ =

GC-MS (EI, 70 eV): m/z (%) = 259 (M^+, 100), 244 (26), 230 (53), 167 (20).

HRMS (EI): calcd. for $[C_{14}H_{10}O_2NCl]^+$ 259.03946, found 259.02988; calcd. for $[C_{14}H_{10}O_2N^{37}Cl]^+$ 261.03651, found 261.03727.

3,8-dichlorodibenzo[b,f][1,4]oxazepin-11(10H)-one (3ay)



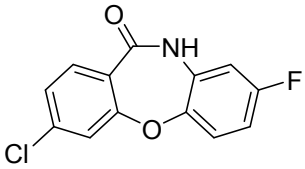
^{1}H NMR (300 MHz, [D$_6$]DMSO): δ = 10.70 (br s, 1H), (dd, *J* = 1.2, 8.2 Hz, 1H), 7.59-7.57 (m, 1H), 7.45-7.40 (m, 2H), 7.24-7.21 (m ,2H).

^{13}C NMR (75 MHz, [D$_6$]DMSO): δ = 164.6, 158.7, 148.5, 128.3, 132.9, 132.3, 129.8, 126.0, 124.9, 124.3, 123.1, 121.0, 120.9.

GC-MS (EI, 70 eV): m/z (%) = 279 (M^+, 72), 244 (100), 216 (33), 188 (40), 75 (23).

HRMS (EI): calcd. for $[C_{13}H_7O_2NCl_2]^+$ 278.98484, found 278.98486; calcd. for $[C_{13}H_7O_2NCl^{37}Cl]^+$ 280.98189, found 280.98191.

3-chloro-8-fluorodibenzo[b,f][1,4]oxazepin-11(10H)-one (3az)



^{1}H NMR (300 MHz, [D$_6$]DMSO): δ = 10.70 (br s, 1H), 7.79 (d, *J* = 8.4 Hz, 1H), 7.57 (d, *J* = 2.1 Hz, 1H), 7.44-7.40 (m, 2H), 7.04-6.95 (m ,2H).

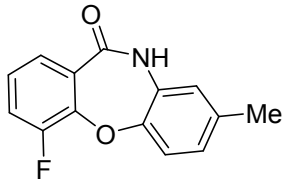
^{13}C NMR (75 MHz, [D$_6$]DMSO): δ = 164.6, 159.1 (d, *J* = 240.0 Hz), 158.9, 146.0 (d, *J* = 2.3 Hz), 138.3 , 132.9, 132.2 (d, *J* = 11.3 Hz), 125.9, 124.5, 124.4, 122.8 (d, *J* = 10.5 Hz), 120.9, 111.6 (d, *J* = 23.3Hz).

^{19}F NMR (282 MHz, [D$_6$]DMSO): δ = -115.56 (q, *J* = 8.2 Hz).

GC-MS (EI, 70 eV): m/z (%) = 263 (M^+, 100), 253 (28), 172 (55), 75 (20).

HRMS (EI): calcd. for $[C_{13}H_7O_2NClF]^+$ 263.01439, found 263.01415; calcd. for $[C_{13}H_7O_2N^{37}ClF]^+$ 265.01144, found 265.01186.

4-fluoro-8-methyldibenzo[b,f][1,4]oxazepin-11(10H)-one (3ba)



^{1}H NMR (300 MHz, [D$_6$]DMSO) : δ = 10.62 (br s, 1H), 7.61-7.55 (m, 2H), 7.33-7.26 (m, 1H), 7.19-7.16 (m, 1H), 6.98-6.94 (m, 2H), 2.24 (s, 3H).

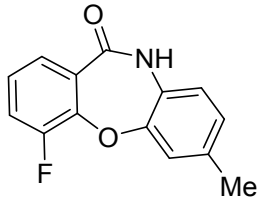
^{13}C NMR (75 MHz, [D$_6$]DMSO): δ = 164.8 (d, *J* = 2.3 Hz), 152.4 (d, *J* = 245.2 Hz), 148.1, 146.4, 146.2, 135.8, 130.4, 128.1, 126.4 (d, *J* = 3.8 Hz), 125.8 (d, *J* = 7.5 Hz), 122.0, 120.9, 120.6 (d, *J* = 18.0 Hz), 20.3.

^{19}F NMR (282 MHz, [D$_6$]DMSO): δ = -133.2 (q, *J* = 4.6 Hz)

GC-MS (EI, 70 eV): m/z (%) = 243 (M^+, 100), 228 (14), 214 (70), 186 (17), 172 (13), 94 (12).

HRMS (EI): cacld. for $[C_{14}H_{10}O_2NF]^+$ 243.06901, found 243.06909.

4-fluoro-7-methyldibenzo[b,f][1,4]oxazepin-11(10H)-one (3bb)



^{1}H NMR (300 MHz, [D$_6$]DMSO): δ = 10.59 (br s, 1H), 7.62-7.55 (m, 2H), 7.34-7.27 (m, 1H), 7.13 (s, 1H), 7.09-7.00 (m, 2H), 2.27 (s, 3H).

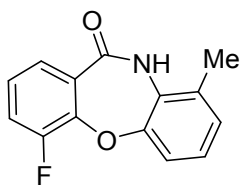
^{13}C NMR (75 MHz, [D$_6$]DMSO): δ = 164.6 (d, *J* = 3.8 Hz), 152.5 (d, *J* = 246.0 Hz), 150.0, 146.2 (d , *J* = 13.5 Hz), 135.3, 128.1, 128.0, 126.8, 126.4 (d, *J* = 3.8 Hz), 125.8 (d, *J* = 6.8 Hz), 121.5 (d, *J* = 17.3 Hz), 120.6 (d, *J* = 18.8 Hz), 20.1.

^{19}F NMR (282 MHz, [D$_6$]DMSO): δ = -133.1 (q, *J* = 4.8 Hz).

GC-MS (EI, 70 eV): m/z (%) = 243 (M^+, 100), 228 (9), 214 (48), 186 (22), 172 (12).

HRMS (EI): cacld. for $[C_{14}H_{10}FNO_2]^+$ 243.06901, found 243.06916.

4-fluoro-9-methyldibenzo[b,f][1,4]oxazepin-11(10H)-one (3bc)



^{1}H NMR (300 MHz, [D$_6$]DMSO): δ = 10.10 (br s, 1H), 7.61-7.52 (m, 2H), 7.34-7.27 (m, 1H), 7.18-7.13 (m, 1H), 7.12-7.06 (m, 2H), 2.33 (s, 3H).

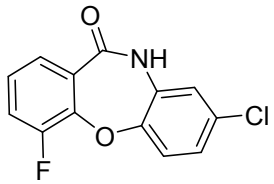
^{13}C NMR (75 MHz, [D$_6$]DMSO): δ = 164.9 (d, *J* = 3.0 Hz), 152.4 (d, *J* = 246.0 Hz), 146.7 (d, *J* = 13.5 Hz), 152.3, 132.0, 129.2, 128.5, 128.0, 126.2 (d, *J* = 3.8 Hz), 126.0 (d, *J* = 7.5 Hz), 125.6, 120.4 (d, *J* = 18.0 Hz), 118.7, 17.8.

^{19}F NMR (282 MHz, [D$_6$]DMSO): δ = -133.5 (q, *J* = 5.1 Hz).

GC-MS (EI, 70 eV): m/z (%) = 243 (M^+, 100), 228 (27), 214 (57), 186 (22).

HRMS (EI): cacld. for $[C_{14}H_{10}FNO_2]^+$ 243.06901, found243.06933

8-chloro-4-fluorodibenzo[b,f][1,4]oxazepin-11(10H)-one (3bd)



^{1}H NMR (300 MHz, [D$_6$]DMSO): δ = 10.77 (br s, 1H), 7.66-7.57 (m, 2H), 7.37-7.30 (m, 2H), 7.24-7.19 (m, 2H).

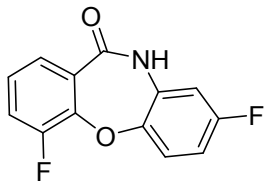
^{13}C NMR (75 MHz, [D$_6$]DMSO): δ = -132.98 (q, *J* = 5.1 Hz)

^{19}F NMR (282 MHz, [D$_6$]DMSO): δ = 164.45 (d, *J* = 3.2 Hz), 152.39 (d, *J* = 246.0 Hz), 148.72, 132.35, 129.94, 127.60, 126.55 (d, *J* = 3.7 Hz), 126.20 (d, *J* = 6.9 Hz), 124.97, 122.89, 121.23, 121.02 (d, *J* = 18.5 Hz)

GC-MS (EI, 70 eV): m/z (%) = 263 (M^+, 100), 228 (100), 200 (41), 172 (57), 94 (23).

HRMS (EI): cacld. for $[C_{13}H_7F_1{}^{35}ClNO_2]^+$ 263.01439, found 263.01380; cacld. for $[C_{13}H_7F_1{}^{37}ClNO_2]^+$ 265.01144, found 265.01087.

4,8-difluorodibenzo[b,f][1,4]oxazepin-11(10H)-one (3be)



^{1}H NMR (300 MHz, [D$_6$]DMSO): δ = 10.77 (br s, 1H), 7.63-7.59 (m, 2H), 7.37-7.32 (m, 2H), 7.03-6.96 (m, 2H).

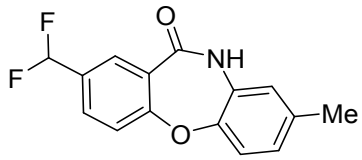
^{13}C NMR (75 MHz, [D$_6$]DMSO): δ = 164.5 (d, *J* = 3.0 Hz), 159.2 (d, *J* = 240.8 Hz), 152.4 (d, *J* = 246.0 Hz), 146.25 (d, *J* = 2.3 Hz), 150.0 (d, *J* = 13.5 Hz), 132.3 (d, *J* = 11.3 Hz), 127.7, 126.5 (d, *J* = 3.8 Hz), 126.1 (d, *J* = 7.5 Hz), 122.6 (d, *J* = 9.8 Hz), 121.0 (d, *J* = 18.8 Hz), 111.6 (d, *J* = 23.3 Hz), 108.4 (d, *J* = 26.3 Hz).

^{19}F NMR (282 MHz, [D$_6$]DMSO): δ = -115.27 (q, *J* = 8.5 Hz), --133.11 (q, *J* = 5.6 Hz).

GC-MS (EI, 70 eV): m/z (%) = 247 (M^+, 100), 219 (24), 190 (58), 172 (16), 94 (18).

HRMS (EI): cacld. for $[C_{13}H_7F_2NO_2]^+$ 247.04394, found 247.04428.

2-(difluoromethyl)-8-methyldibenzo[b,f][1,4]oxazepin-11(10H)-one (3bf)



^{1}H NMR (300 MHz, [D$_6$]DMSO): δ = 10.63 (br s, 1H), 7.97 (m ,1H), (dt, *J* = 1.2, 8.4 Hz, 1H), 7.47 (1H, J = 8.4 Hz, 2d), 7.47 (d, *J* = 8.4 Hz, 1H), 7.23 (d, *J* = 7.8 Hz, 1H), 7.1 (t, *J* = 55.5 Hz, 1H), 6.97-6.93 (m ,2H), 2.24 (s, 3H).

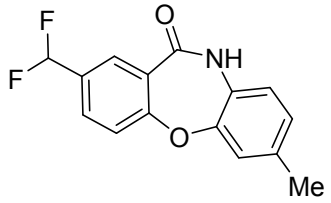
^{13}C NMR (75 MHz, [D$_6$]DMSO): δ = 165.0, 160.5, 147.9, 135.6, 131.5 (t, *J* = 5.0 Hz), 131.4 (t, *J* = 23.0 Hz), 130.3, 129.3 (t, *J* = 6.0 Hz), 126.0, 125.8, 121.8, 121.5, 121.0, 114.0 (t, *J* = 234.8 Hz), 20.3.

^{19}F NMR (282 MHz, [D$_6$]DMSO): δ = -109.11 (d, *J* = 62.0 Hz).

GC-MS (EI, 70 eV): m/z (%) = 275 (M^+, 100), 246 (72), 51 (20).

HRMS (EI): calcd. for $[C_{15}H_{11}O_2NF_2]^+$ 275.07524, found 275.07505.

2-(difluoromethyl)-7-methyldibenzo[b,f][1,4]oxazepin-11(10H)-one (3bg)



^{1}H NMR (300 MHz, [D$_6$]DMSO): δ = 10.60 (br s, 1H), 7.97 (s, 1H), 7.80-7.80 (m, 1H), 7.49-7.44 (m, 1H), 7.28-6.91 (m, 4H), 2.26 (s, 3H).

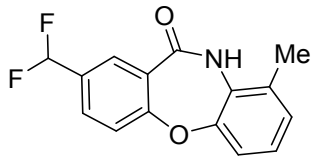
^{13}C NMR (75 MHz, [D$_6$]DMSO): δ = 164.87, 160.42, 149.80, 135.17, 131.45, 131.15 (t, *J* = 28.5Hz), 129.26 (t, *J* = 6.8 Hz) , 128.04, 126.63, 126.06, 121.55, 121.48, 114.02 (t, *J* = 234.8 Hz), 20.08.

^{19}F NMR (282 MHz, [D$_6$]DMSO): δ = -109.12 (d, *J* = 55.6 Hz)

GC-MS (EI, 70 eV): m/z (%) = 275 (M^+, 100), 246 (48), 218 (15), 196 (13), 167 (19).

HRMS (EI): calcd. for $[C_{15}H_{11}O_2NF_2]^+$ 275.07524, found 275.07527.

2-(difluoromethyl)-9-methyldibenzo[b,f][1,4]oxazepin-11(10H)-one (3bh)



^{1}H NMR (300 MHz, [D$_6$]DMSO): δ = .11 (br s, 1H), 7.93 (s, 1H), .86-7.79 (m, 1H), 7.51-7.48 (m, 1H), (m, 4H), 2.33 (s, 3H).

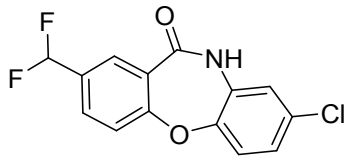
^{13}C NMR (75 MHz, [D$_6$]DMSO): δ = 165.21, 160.99, 152.10, 131.75, 131.60, 131.30 (t, *J* = 23.3 Hz), 131.22, 129.16, 128.98 (t, *J* = 6.0 Hz), 127.76, 126.57, 125.57, 124.77, 121.35, 118.82, 114.01(t, *J* = 234.0 Hz), 110.87, 17.75.

^{19}F NMR (282 MHz, [D$_6$]DMSO): δ = -109.11 (d, *J* = 55.6 Hz).

GC-MS (EI, 70 eV): m/z (%) = 275 (M^+, 100), 260 (27), 246 (63), 218 (16), 167 (20), 125 (17), 51 (30).

HRMS (EI): calcd. for $[C_{15}H_{11}O_2NF_2]^+$ 275.07524, found 275.07523.

8-chloro-2-(difluoromethyl)dibenzo[b,f][1,4]oxazepin-11(10H)-one (3bi)



^{1}H NMR (300 MHz, [D$_6$]DMSO) : δ = 10.78 (br s, 1H), 7.98 (s, 1H), 7.86 (d, *J* = 8.4 Hz, 1H), 7.53 (d, *J* = 8.4 Hz, 1H), 7.43-7.40 (m,1H), 7.24-7.21 (m, 2H), 7.11 (t, *J* = 55.5 Hz, 1H)

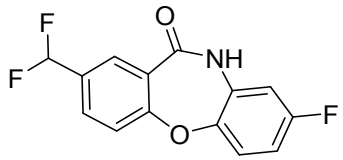
^{13}C NMR (75 MHz, [D$_6$]DMSO) : δ = 164.7, 159.9, 148.6, 132.3, 131.9 (t, *J* = 5.3 Hz), 131.4 (t, *J* = 22.5 Hz), 129.8, 129.4 (t, *J* = 6.8 Hz), 125.6, 125.0, 123.1, 121.7, 121.1, 113.9 (t, *J* = 234.8 Hz).

^{19}F NMR (282 MHz, [D$_6$]DMSO): δ = -109.3 (d, *J* = 56.4 Hz).

GC-MS (EI, 70 eV): m/z (%) = 295 (M^+, 78), 260 (100), 232 (35), 204 (36).

HRMS (EI): calcd. for $[C_{14}H_8O_2NClF_2]^+$ 295.02061, found 295.02089; calcd. for $[C_{14}H_8O_2N^{37}ClF_2]^+$ 297.01766, found 297.01842.

2-(difluoromethyl)-8-fluorodibenzo[b,f][1,4]oxazepin-11(10H)-one (3bj)



^{1}H NMR (300 MHz, [D$_6$]DMSO): δ = 10.77 (br s, 1H), 8.05-7.83 (m, 2H), 7.61-7.39 (m, 2H), 7.28-6.97 (m, 2H).

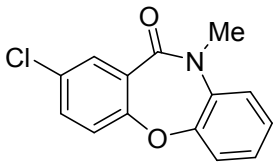
^{13}C NMR (75 MHz, [D$_6$]DMSO): δ = 164.79, 160.18, 159.1 (d, *J* = 240.7 Hz), 146.11, 132.20 (d, *J* = 11.3 Hz), 131.82 (t, *J* = 6.0 Hz), 131.37 (t, *J* = 23.3 Hz), 129.34 (t, *J* = 6.8 Hz), 125.72, 122.80 (d, *J* = 9.8 Hz), 121.59, 113.96 (*t*, *J* = 234.8 Hz), 111.60 (d, *J* = 22.5 Hz), 108.20 (d, *J* = 26.3 Hz).

^{19}F NMR (282 MHz, [D$_6$]DMSO): δ = -109.2 (d, *J* = 56.4 Hz), -115.6 (q, *J* = 8.5 Hz).

GC-MS (EI, 70 eV): m/z (%) = 279 (M^+, 100), 251 (26), 172 (37), 125 (14).

HRMS (EI): calcd. for $[C_{14}H_8O_2NF_3]^+$ 279.05016, found 279.05047.

2-chloro-10-methyldibenzo[b,f][1,4]oxazepin-11(10H)-one (5a)



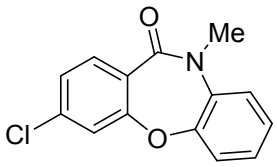
^{1}H NMR (300 MHz, [D$_6$]DMSO): δ = 7.71-7.63 (m, 2H), 7.50-7.47 (m, 1H), 7.43-7.38 (m ,2H), 7.33-7.22 (m, 2H), 3.50 (s, 3H).

^{13}C NMR (75 MHz, [D$_6$]DMSO): δ = 163.83, 158.60, 152.64, 134.99, 133.61, 130.97, 129.45, 127.51, 126.65, 126.43, 123.38, 122.11, 121.14, 36.34.

GC-MS (EI, 70 eV): m/z (%) = 259 (M^+, 100), 231 (19), 215 (42), 202 (14), 168 (23).

HRMS (EI): calcd. for $[C_{14}H_{10}O_2NCl]^+$ 259.03946, found 259.03935; calcd. for $[C_{14}H_{10}O_2N^{37}Cl]^+$ 261.03651, found 261.03677.

3-chloro-10-methyldibenzo[b,f][1,4]oxazepin-11(10H)-one (5b)



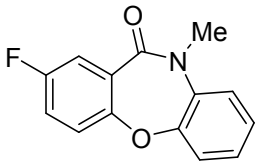
^{1}H NMR (300 MHz, [D$_6$]DMSO): δ = (d, *J* = 8.4 Hz, 1H), 7.57-7.56 (m, 1H), 7.50-7.37 (m, 3H), 7.34-7.22 (m, 2H), 3.49 (s, 3m).

^{13}C NMR (75 MHz, [D$_6$]DMSO): δ = 164.23, 160.17, 152.40, 137.63, 135.08, 133.26, 126.56, 126.48, 125.80, 124.84, 123.27, 121.25, 120.25, 36.24.

GC-MS (EI, 70 eV): m/z (%) = 259 (M^+, 100), 231 (22), 216 (37), 168 (22), 75 (12), 63 (13).

HRMS (EI): calcd. for $[C_{14}H_{10}O_2NCl]^+$ 259.03946, found 259.03060; calcd. for $[C_{14}H_{10}O_2N^{37}Cl]^+$ 261.03651, found 261.03723.

2-fluoro-10-methyldibenzo[b,f][1,4]oxazepin-11(10H)-one (5c)



^{1}H NMR (300 MHz, [D$_6$]DMSO): δ = 7.50-7.38 (m, 5H), 7.32-7.21 (m, 2H), 3.5 (s, 3H).

^{13}C NMR (100 MHz, [D$_6$]DMSO): δ = 163.9 (d, *J* = 3.0 Hz), 158.8 (d, *J* = 240.0 Hz), 156.1 (d, *J* = 3.0 Hz), 152.9, 135.1, 127.4 (d, *J* = 7.1 Hz), 126.6, 126.3, 123.3, 122.0 (d, *J* = 8.0 Hz), 121.1, 120.7 (d, *J* = 23.1 Hz), 117.5 (d, *J* = 25.1 Hz), 36.3.

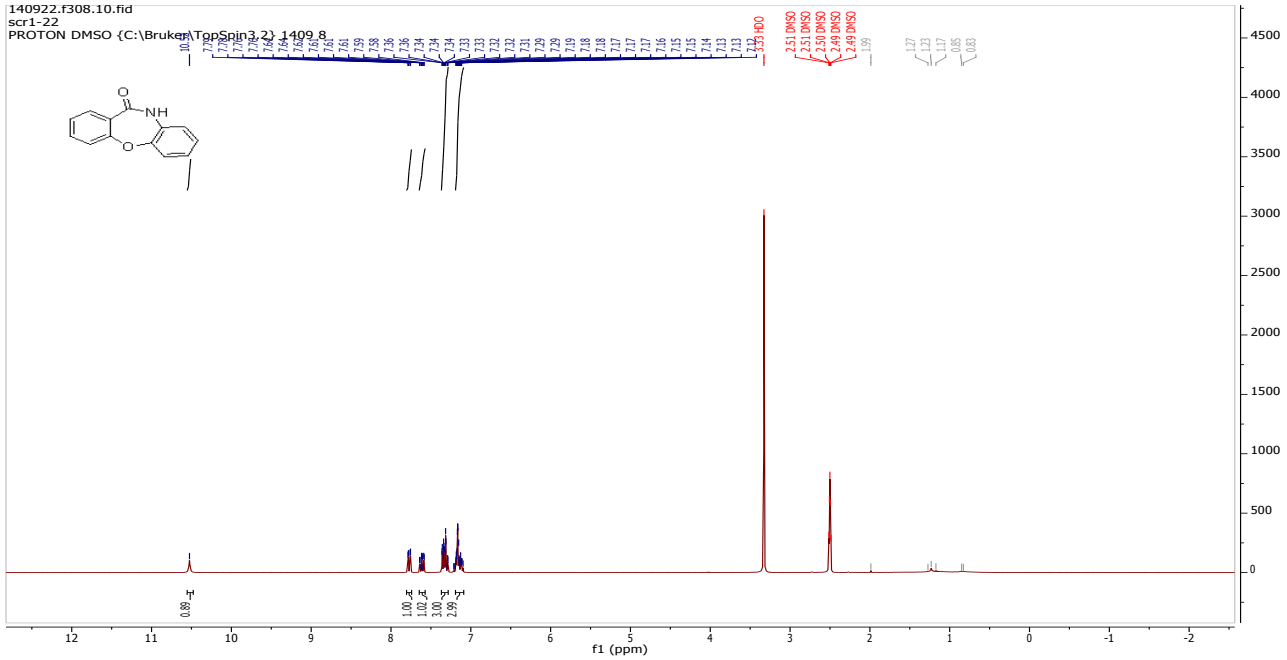
^{19}F NMR (282 MHz, [D$_6$]DMSO): δ = -116.6 (q, *J* = 19.7 Hz)

GC-MS (EI, 70 eV): m/z (%) = 243 (M^+, 100), 226 (15), 214 (22), 200 (35), 186 (36).

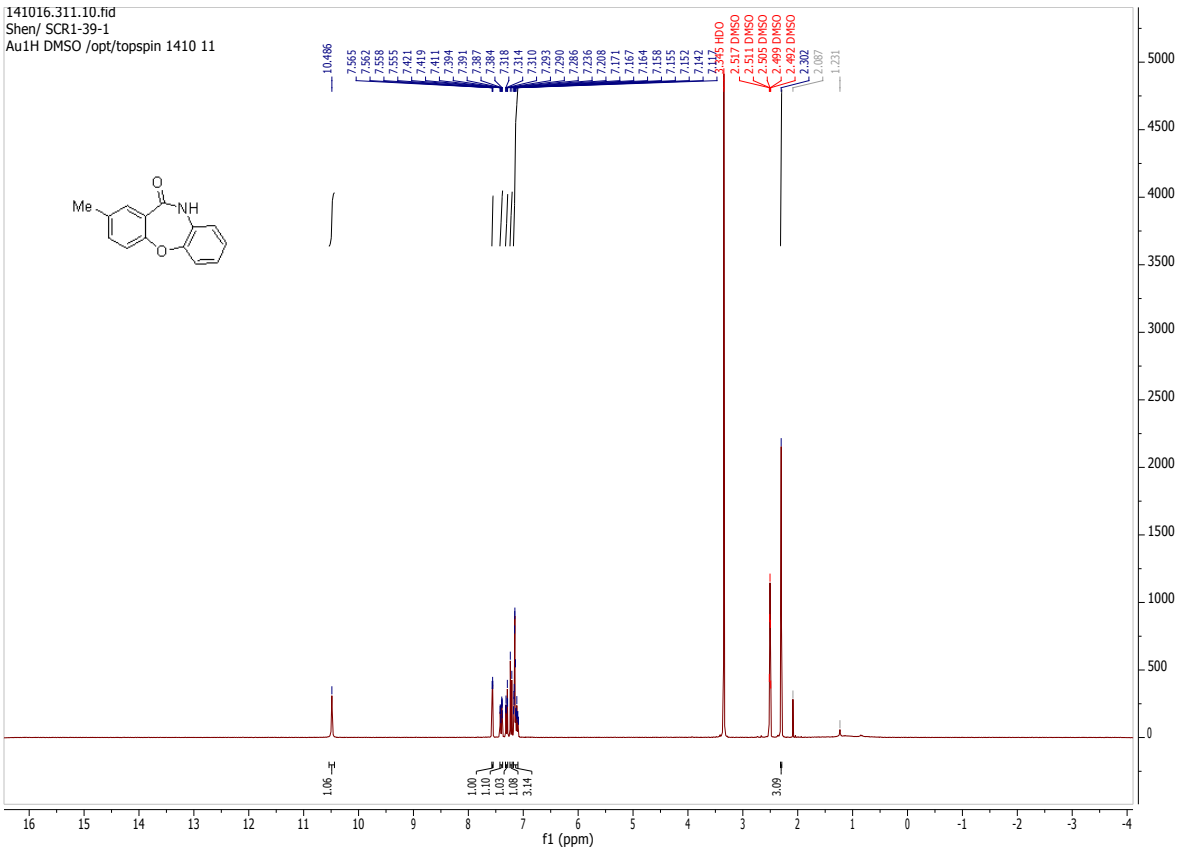
HRMS (EI): calcd. for $[C_{14}H_{10}O_2NF]^+$ 243.06901, found 243.06835.

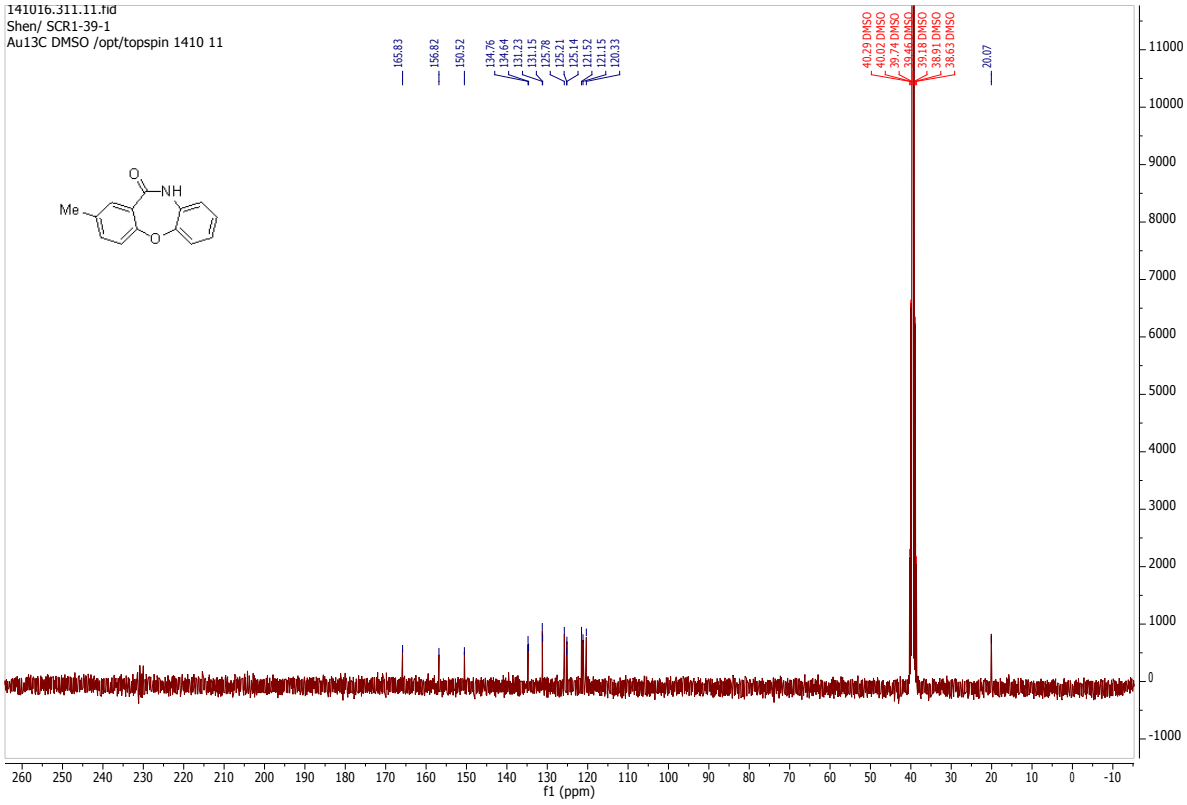
5. Spectrum Copies

Dibenzo[b,f][1,4]oxazepin-11(10*H*)-one[1] (3a)

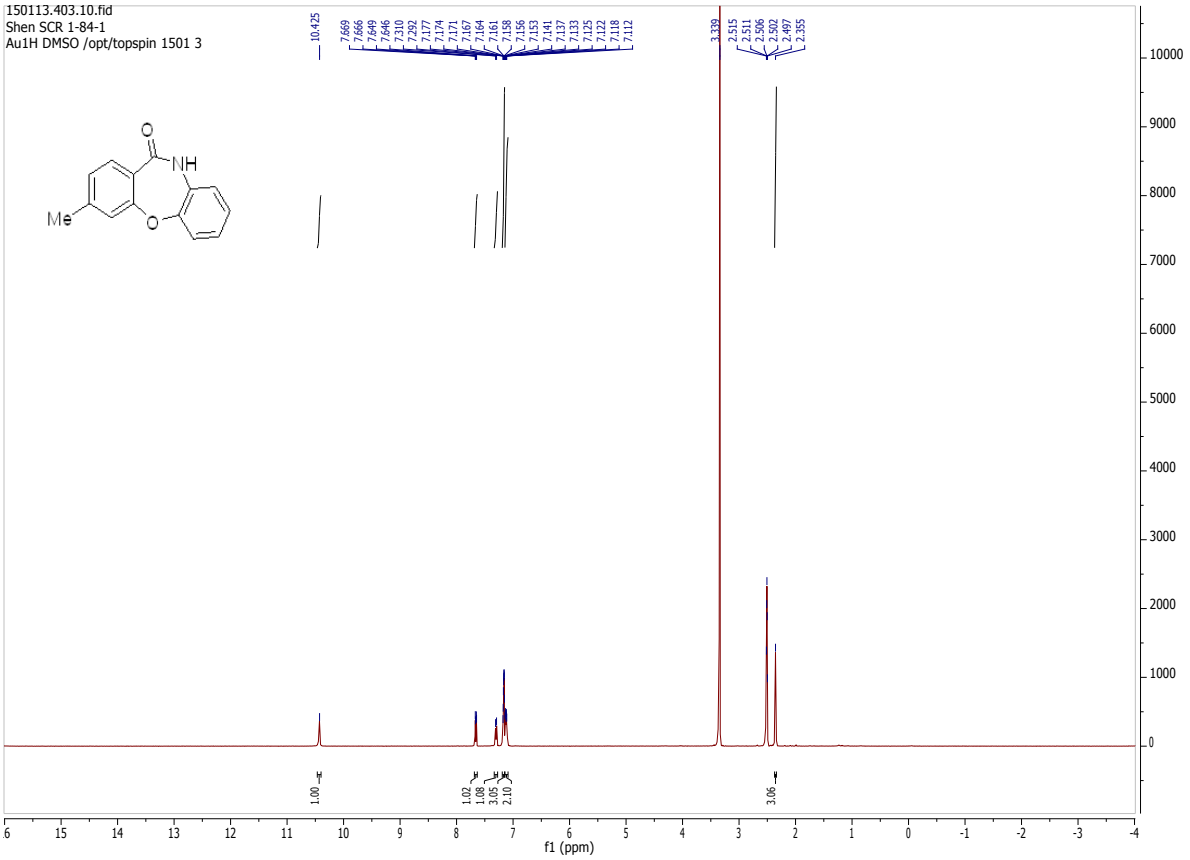


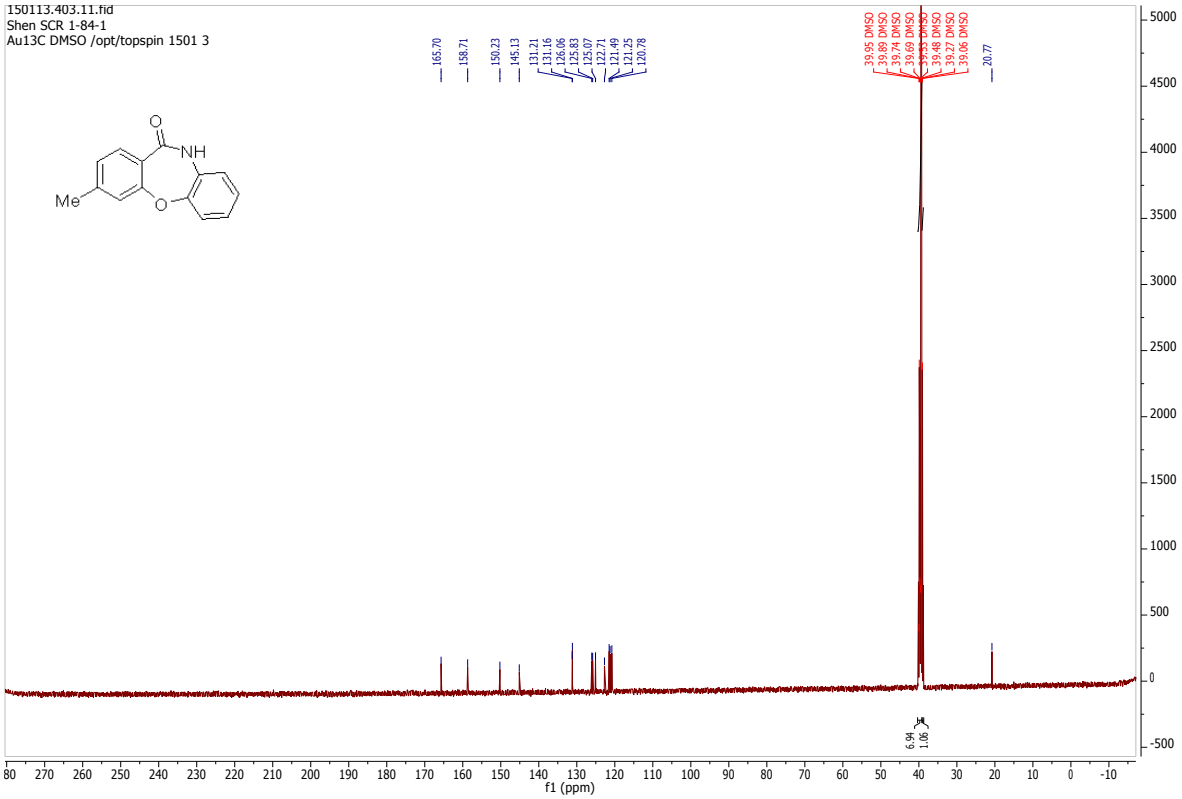
2-methyldibenzo[b,f][1,4]oxazepin-11(10H)-one (3b)



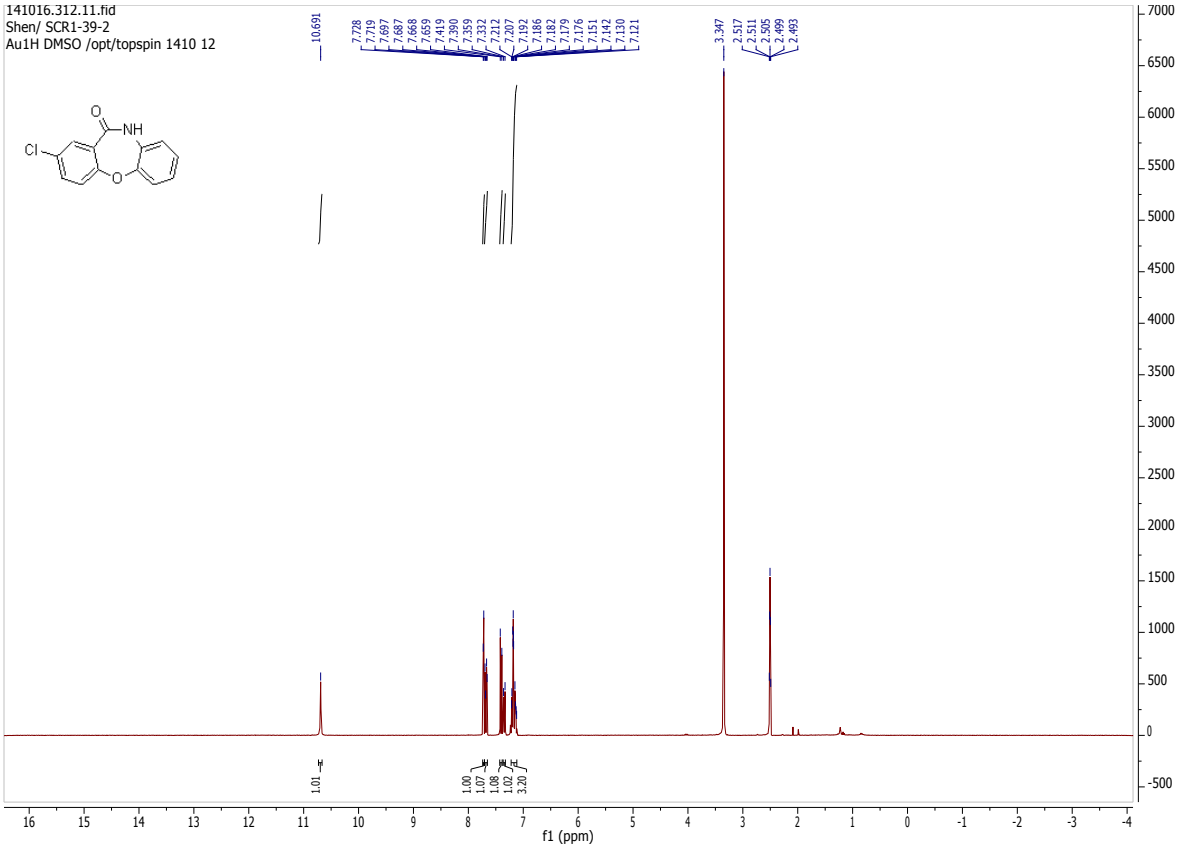


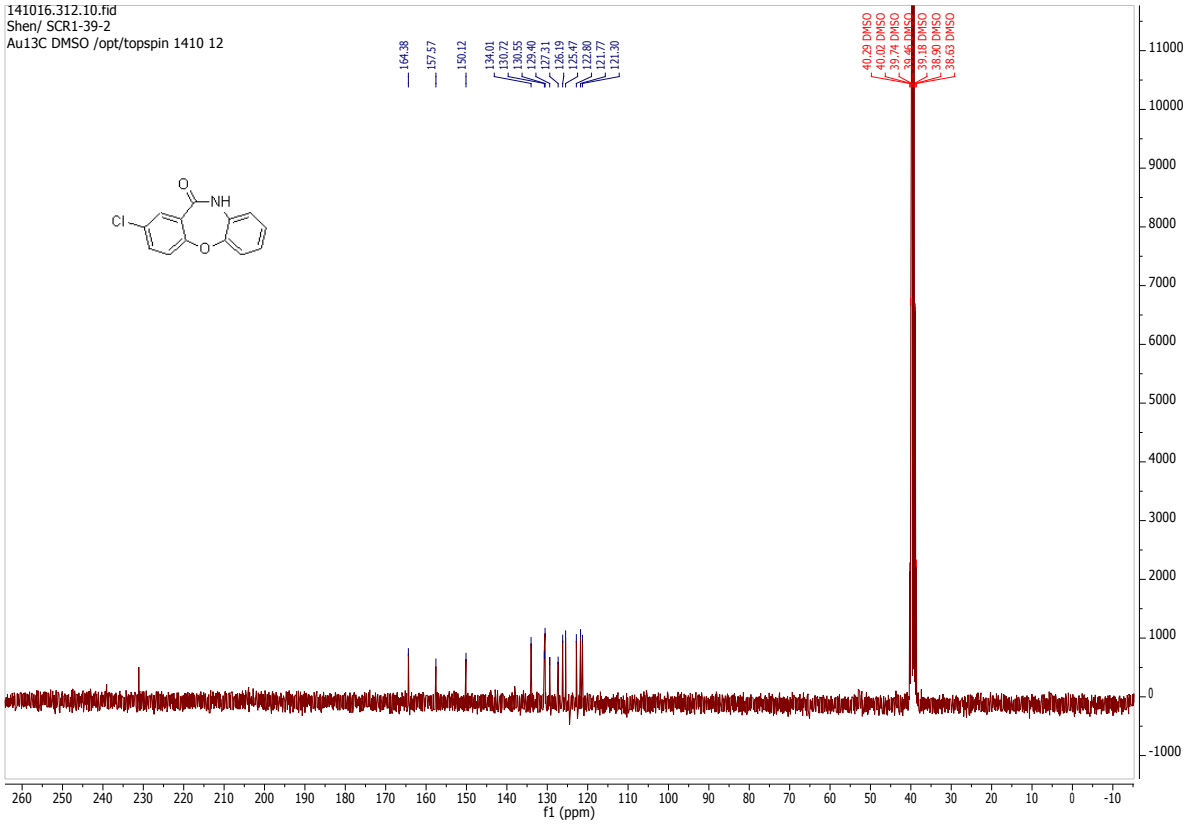
3-methyldibenzo[b,f][1,4]oxazepin-11(10H)-one (3c)



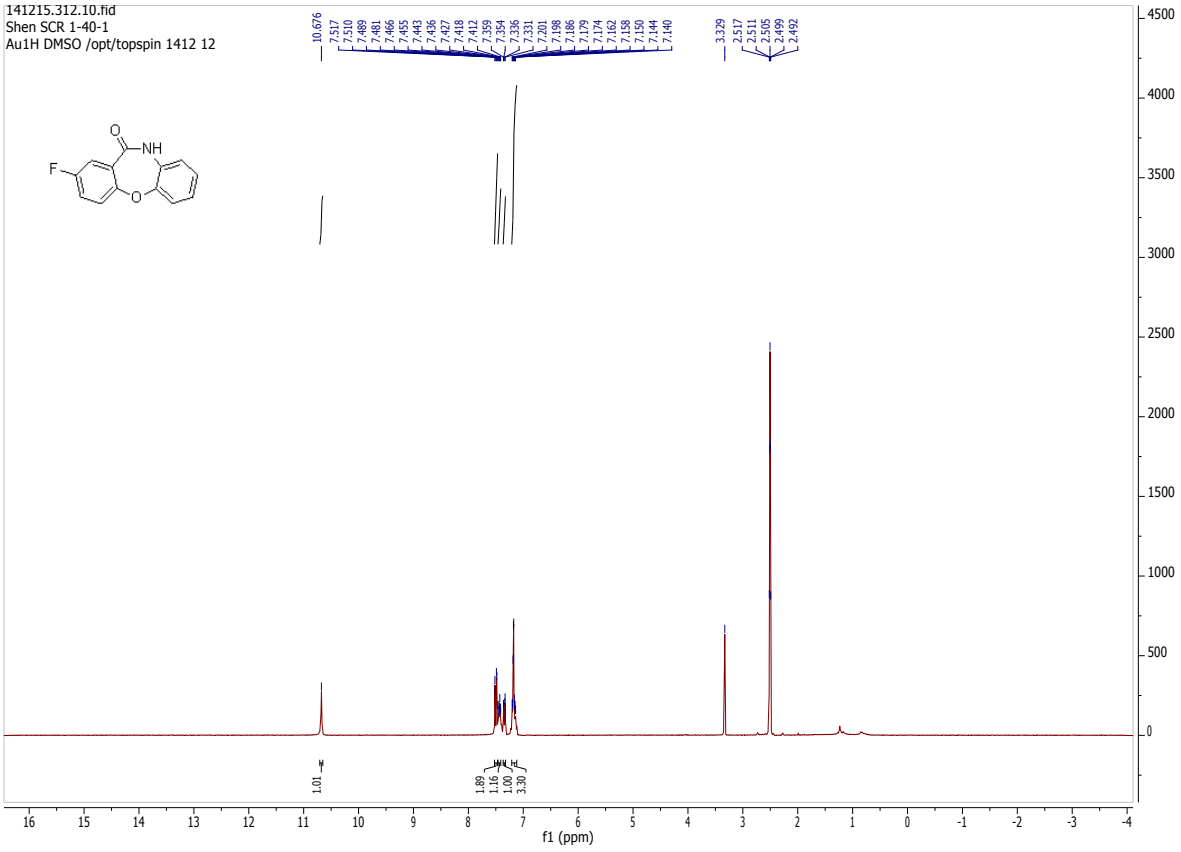


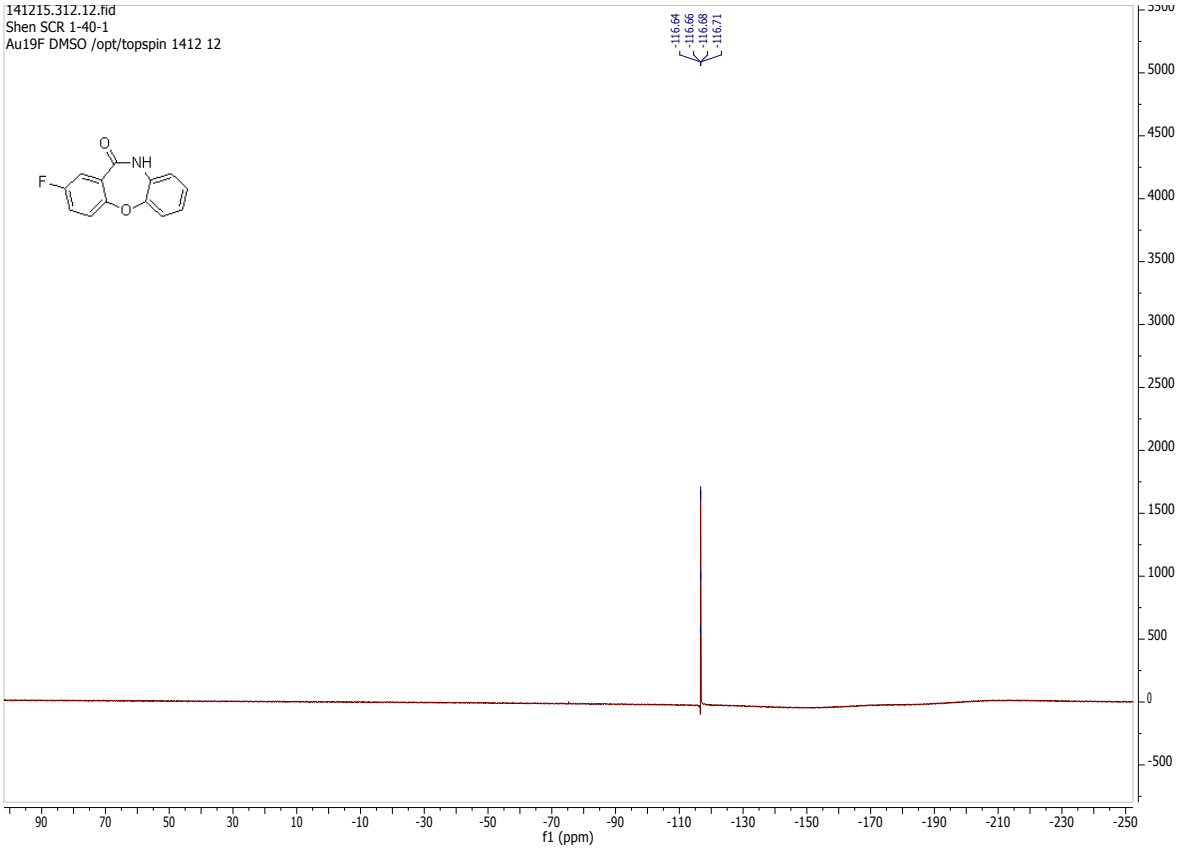
2-chlorodibenzo[b,f][1,4]oxazepin-11(10H)-one[2] (3d)





2-fluorodibenzo[b,f][1,4]oxazepin-11(10H)-one (3e)

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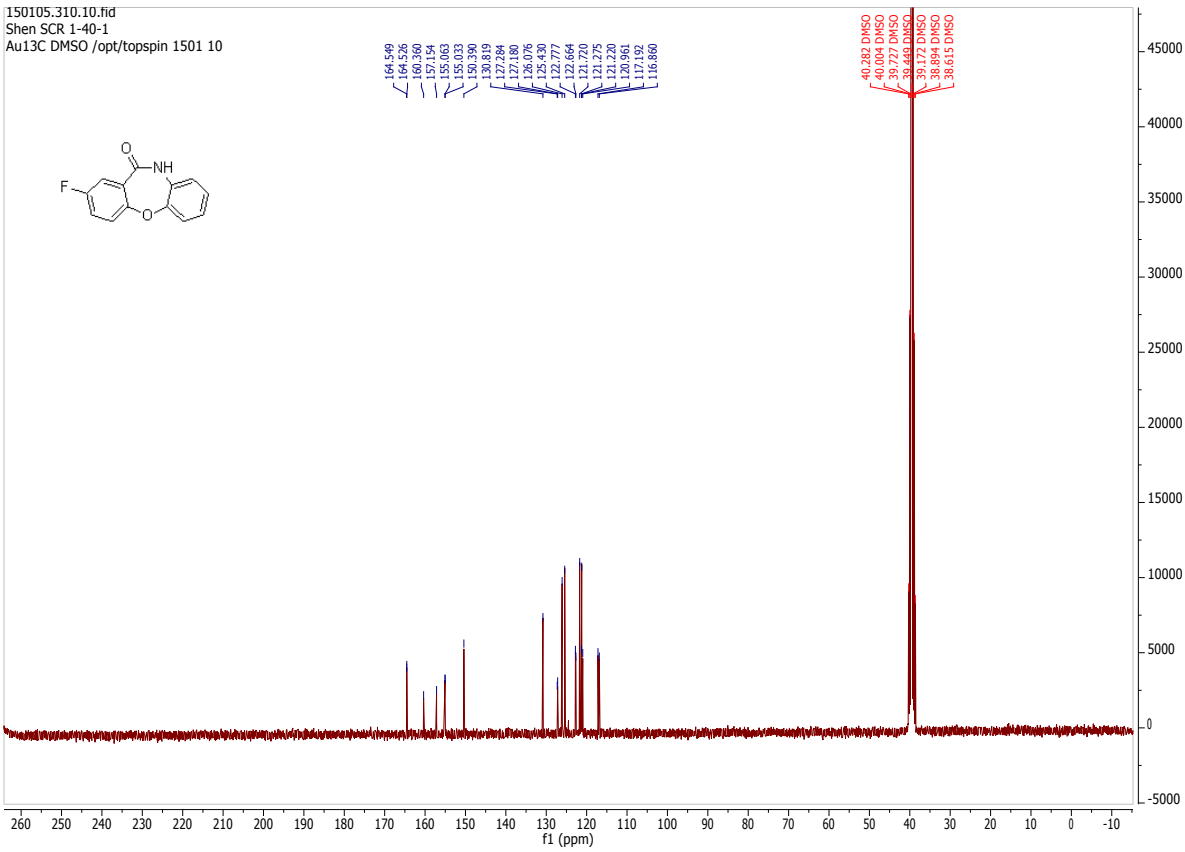
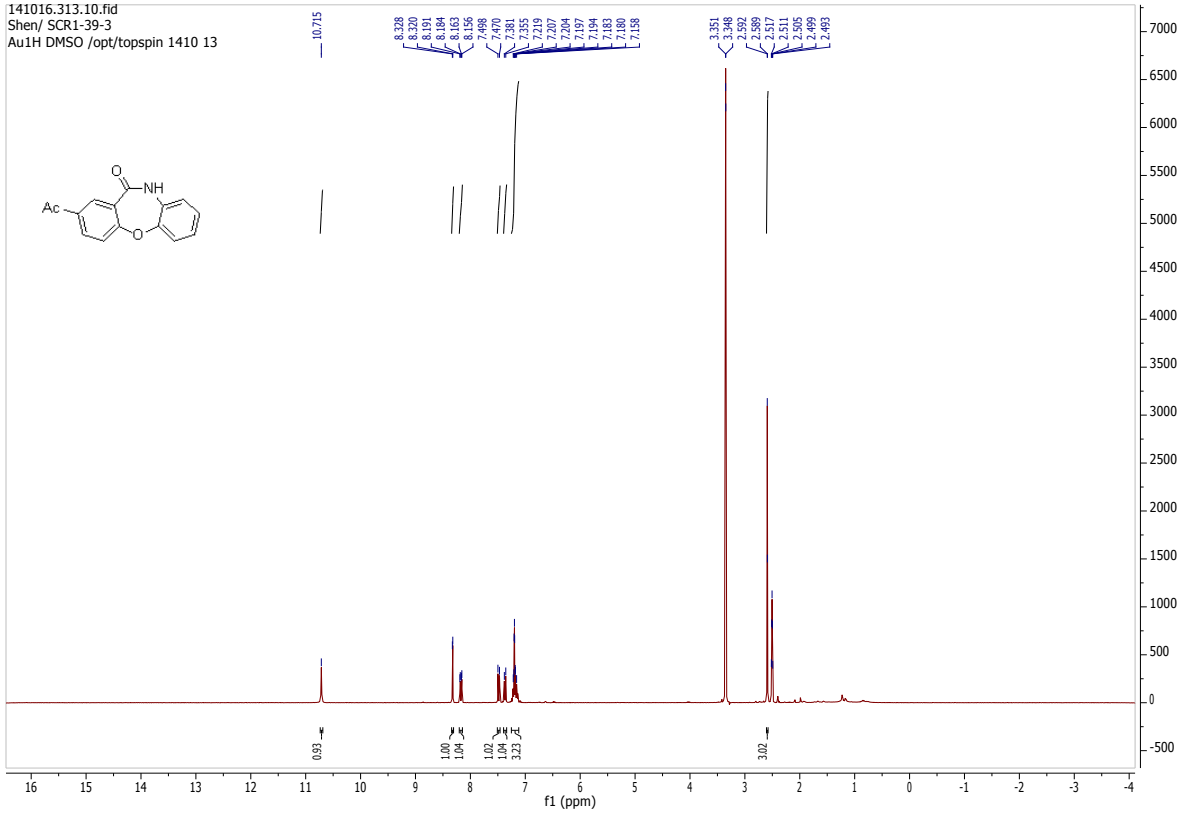
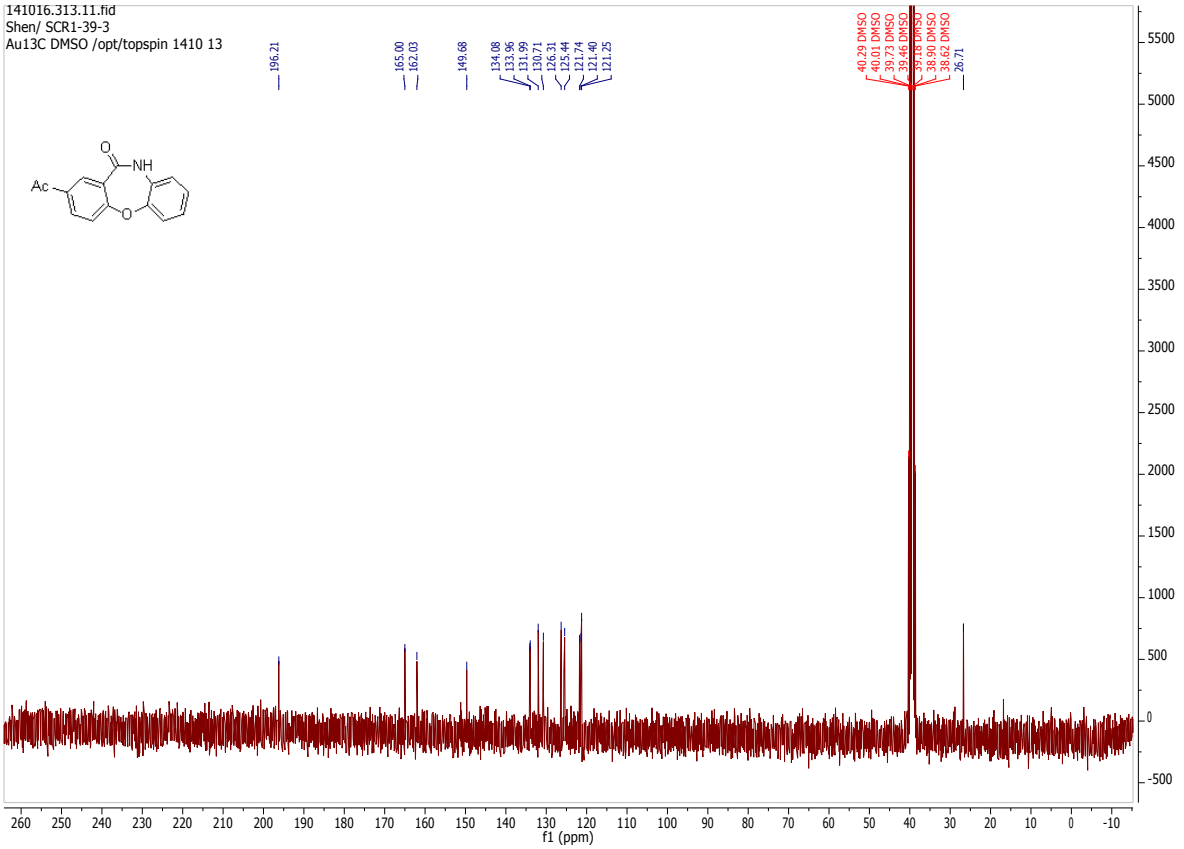
F
O
f1 (ppm)

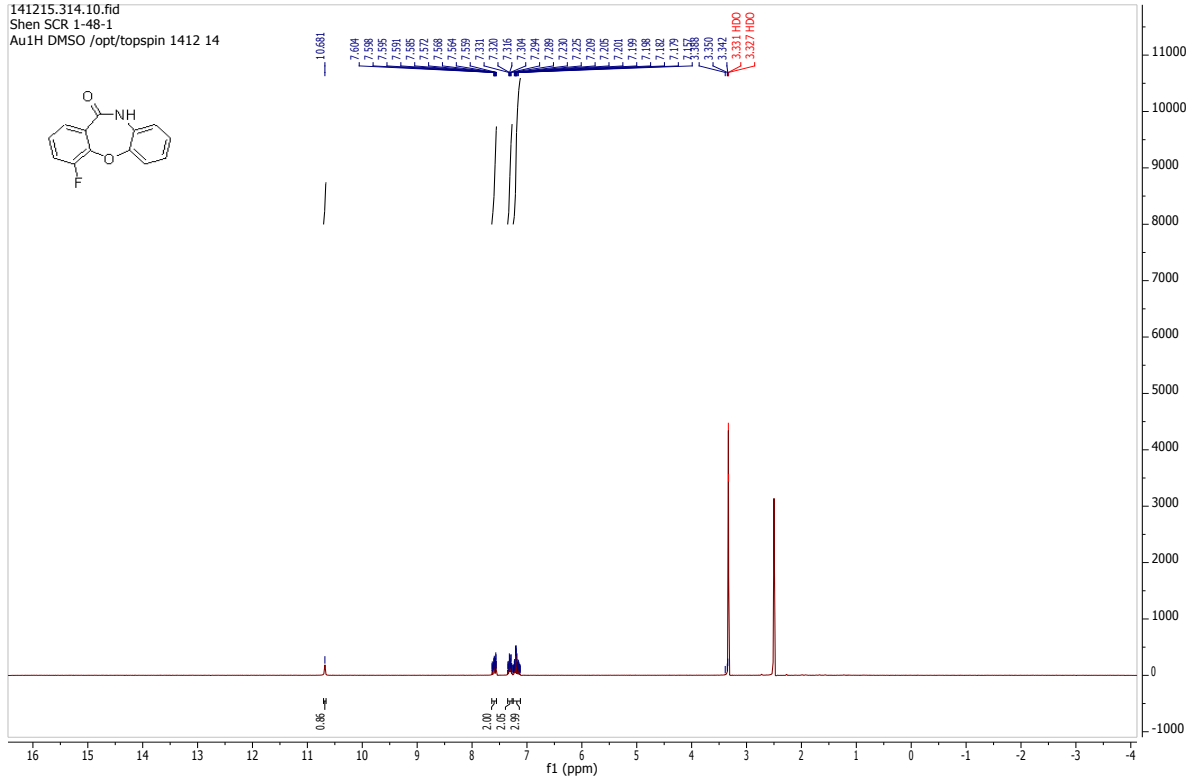

150105.310.10.fid
Shen SCR 1-40-1
Au13C DMSO /opt/topspin 1501 10
164.549
164.326
160.190
157.194
155.063
155.033
150.390
130.819
127.284
127.180
126.076
125.439
122.777
122.664
121.720
121.275
121.228
120.961
117.192
116.860
40.282 DMSO
40.064 DMSO
39.727 DMSO
39.490 DMSO
39.172 DMSO
38.894 DMSO
38.615 DMSO
O
NH
F
O
f1 (ppm)

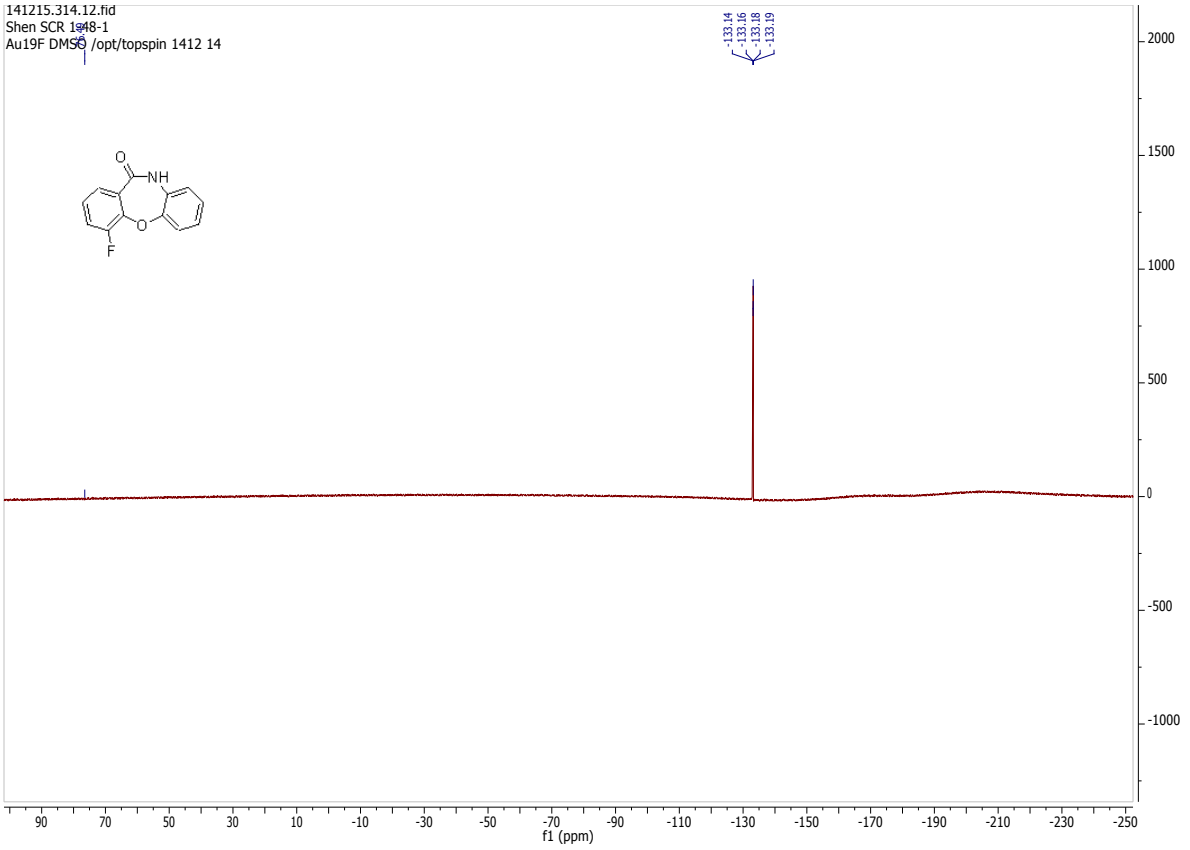
2-acetyldibenzo[b,f][1,4]oxazepin-11(10H)-one (3f)

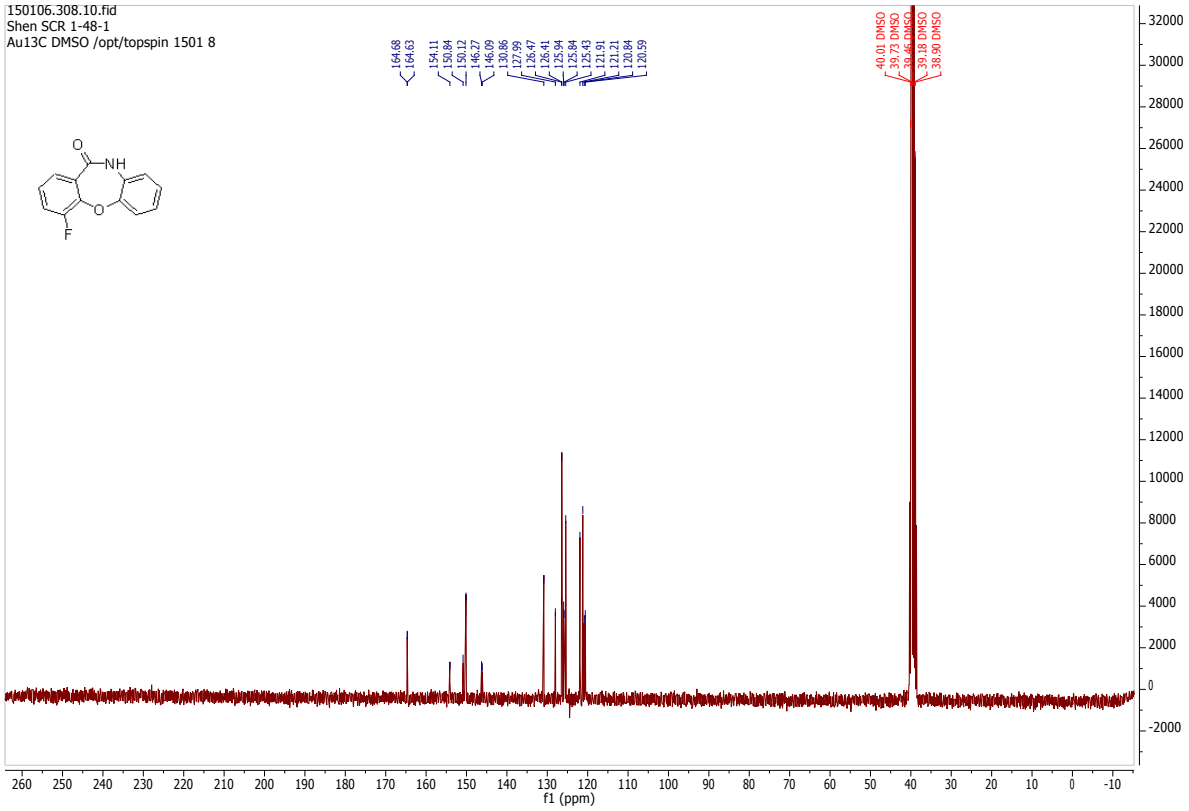




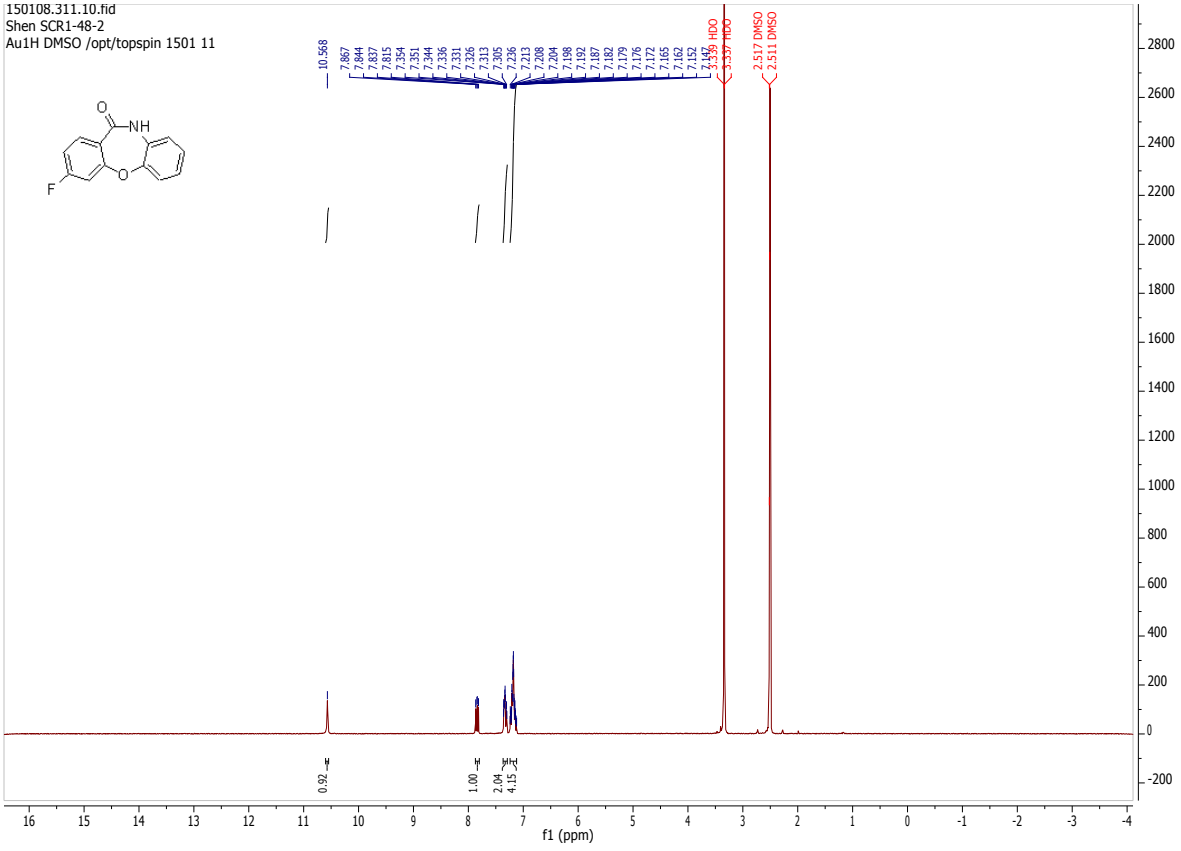
4-fluorodibenzo[b,f][1,4]oxazepin-11(10H)-one (3g)

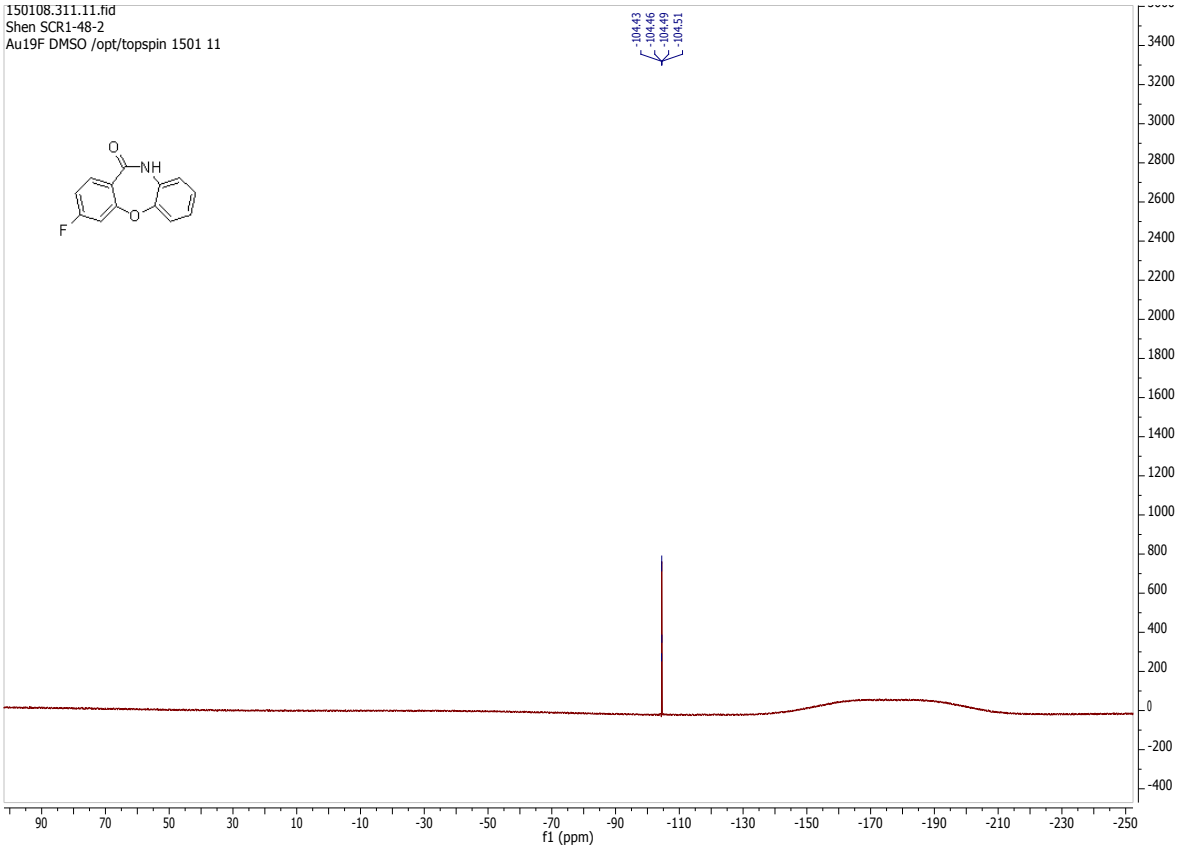


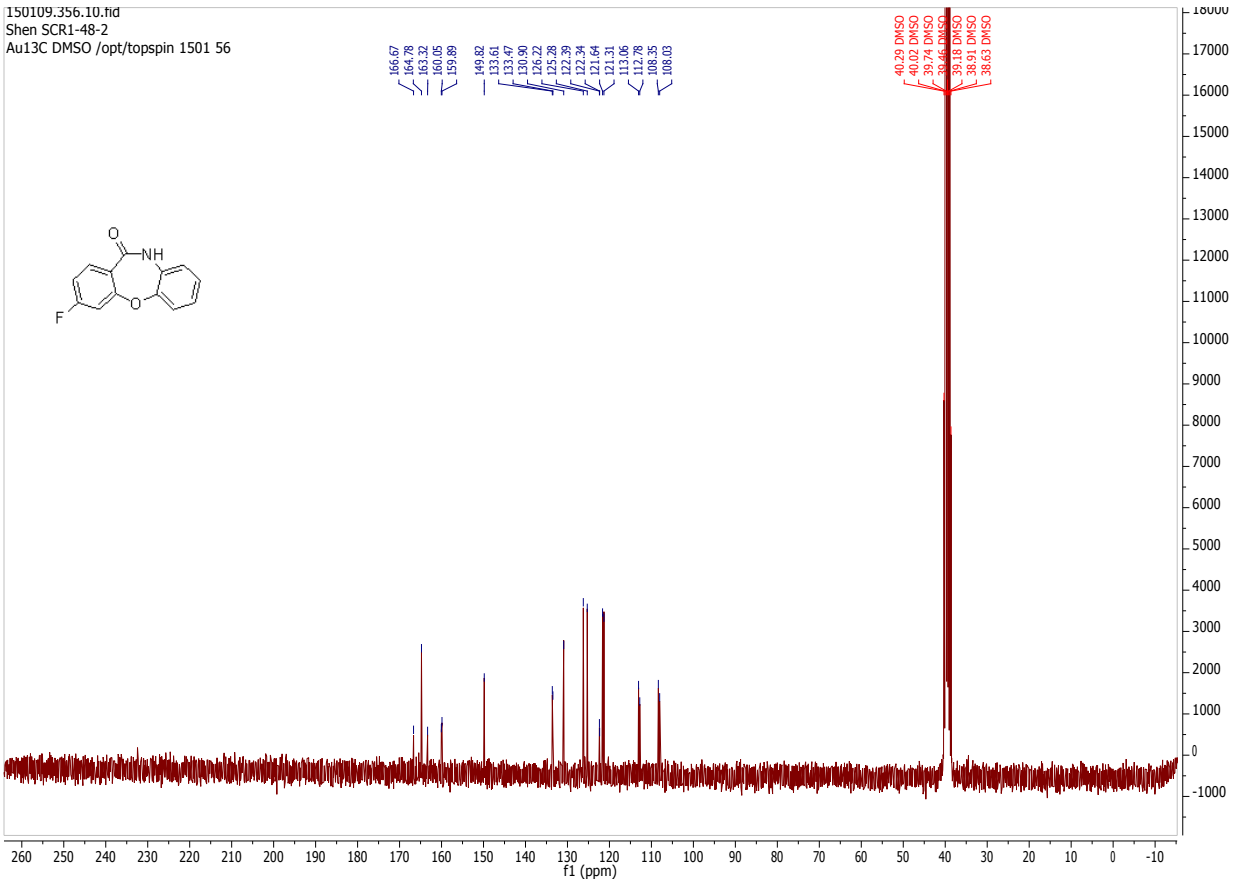




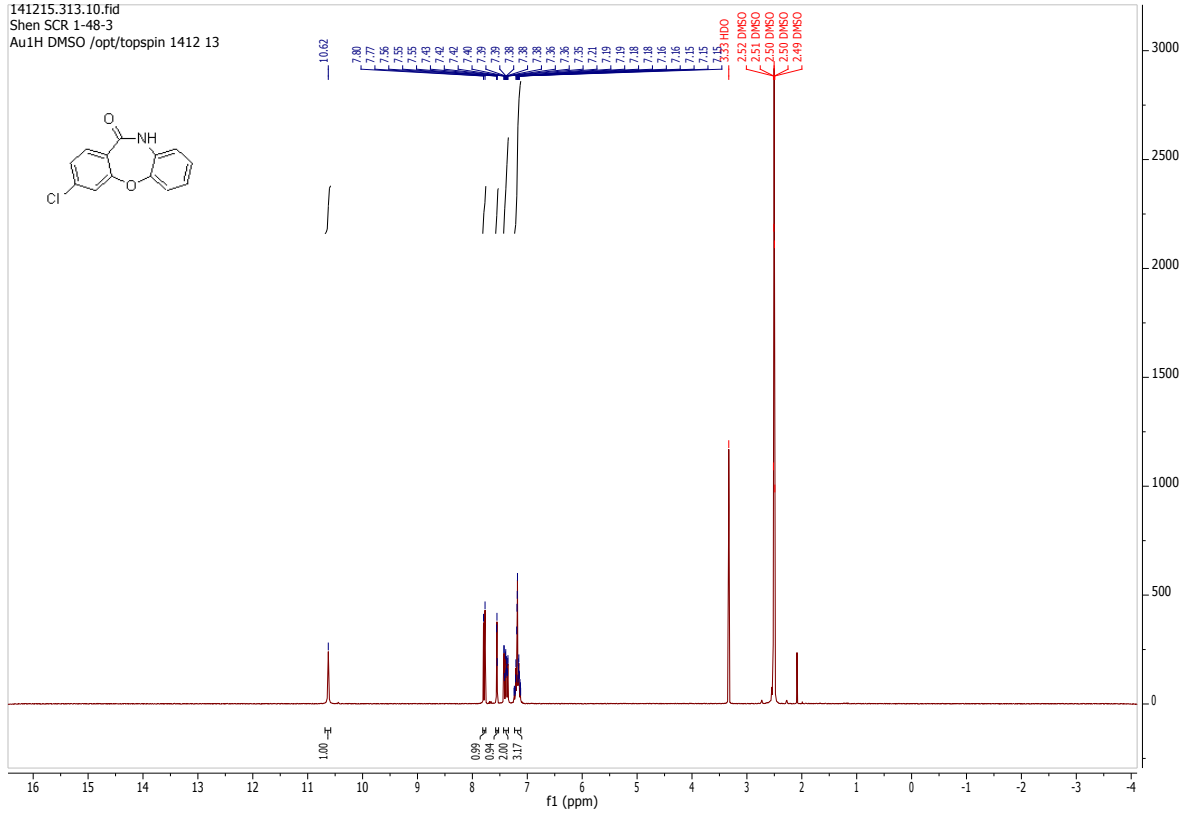
3-fluorodibenzo[b,f][1,4]oxazepin-11(10H)-one[3] (3h)

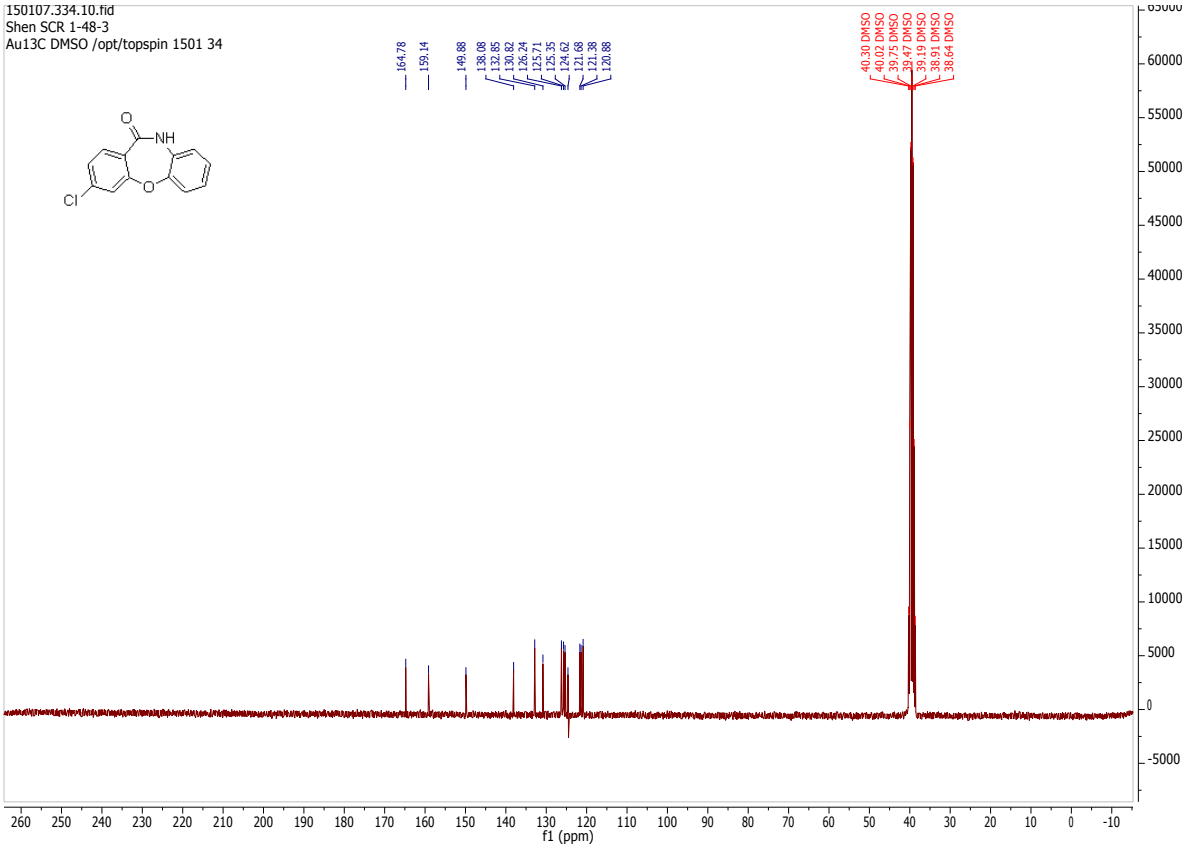



150108.311.11.fid
Shen SCR1-48-2
Au19F DMSO /opt/topspin 1501 11
-104.43
-104.46
-104.49
-104.51
f1 (ppm)

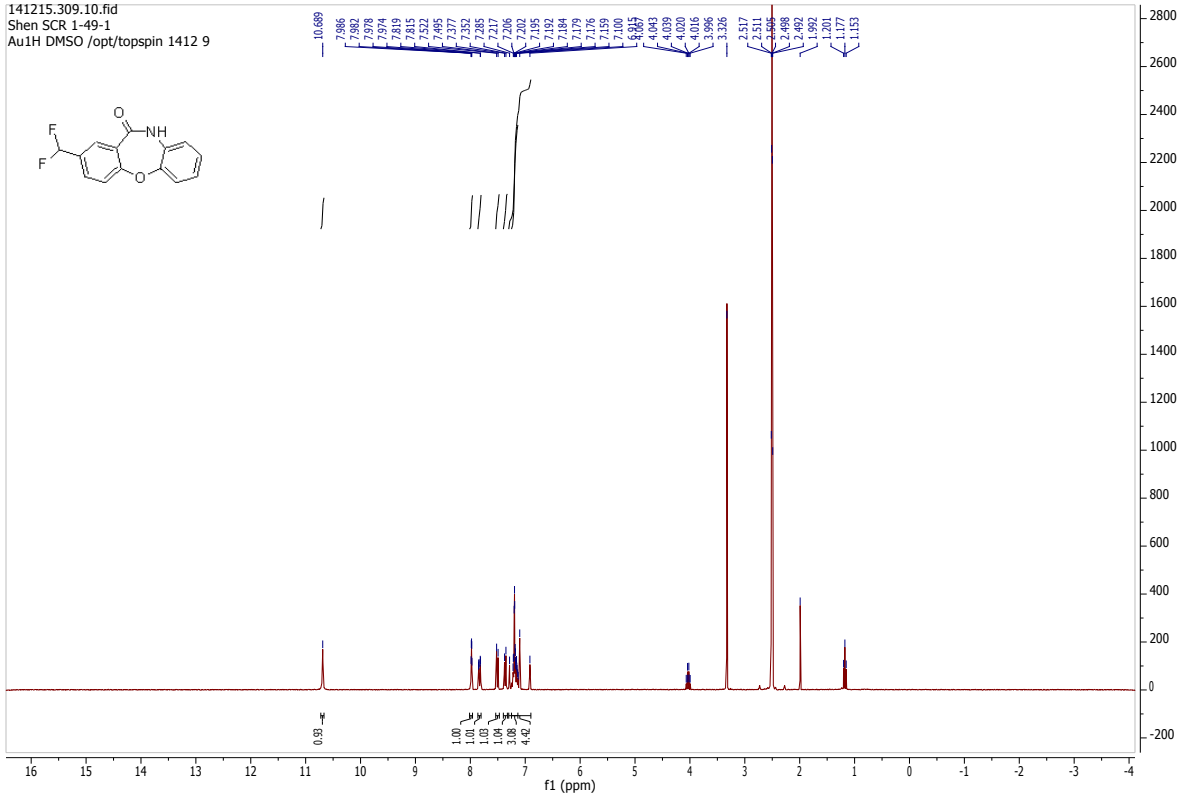

150109.356.10.fid
Shen SCR1-48-2
Au13C DMSO /opt/topspin 1501 56
166.67
164.78
163.32
160.05
159.89
149.82
133.61
133.47
130.90
126.22
125.28
122.39
122.34
121.64
121.31
113.06
112.78
108.35
108.03
40.29 DMSO
40.02 DMSO
39.74 DMSO
39.46 DMSO
39.18 DMSO
38.91 DMSO
38.63 DMSO
f1 (ppm)

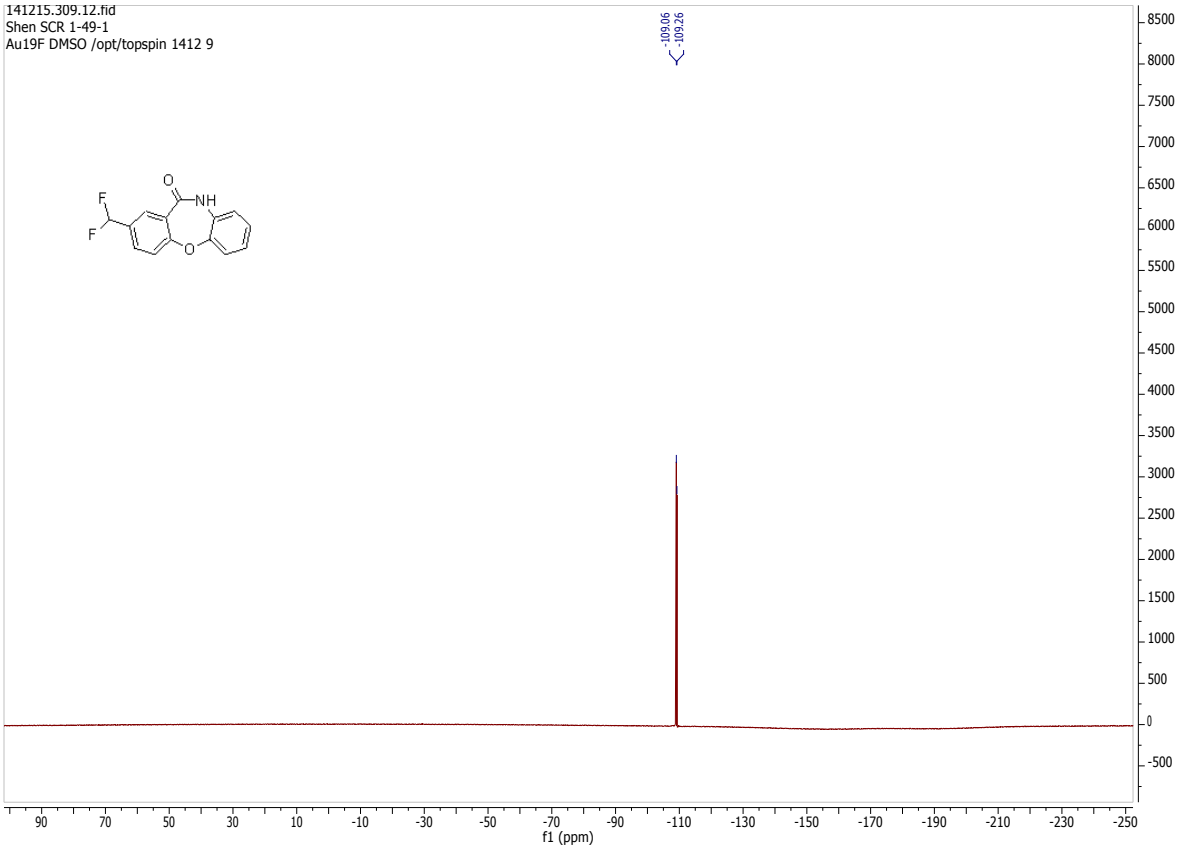
3-chlorodibenzo[b,f][1,4]oxazepin-11(10H)-one (3i)

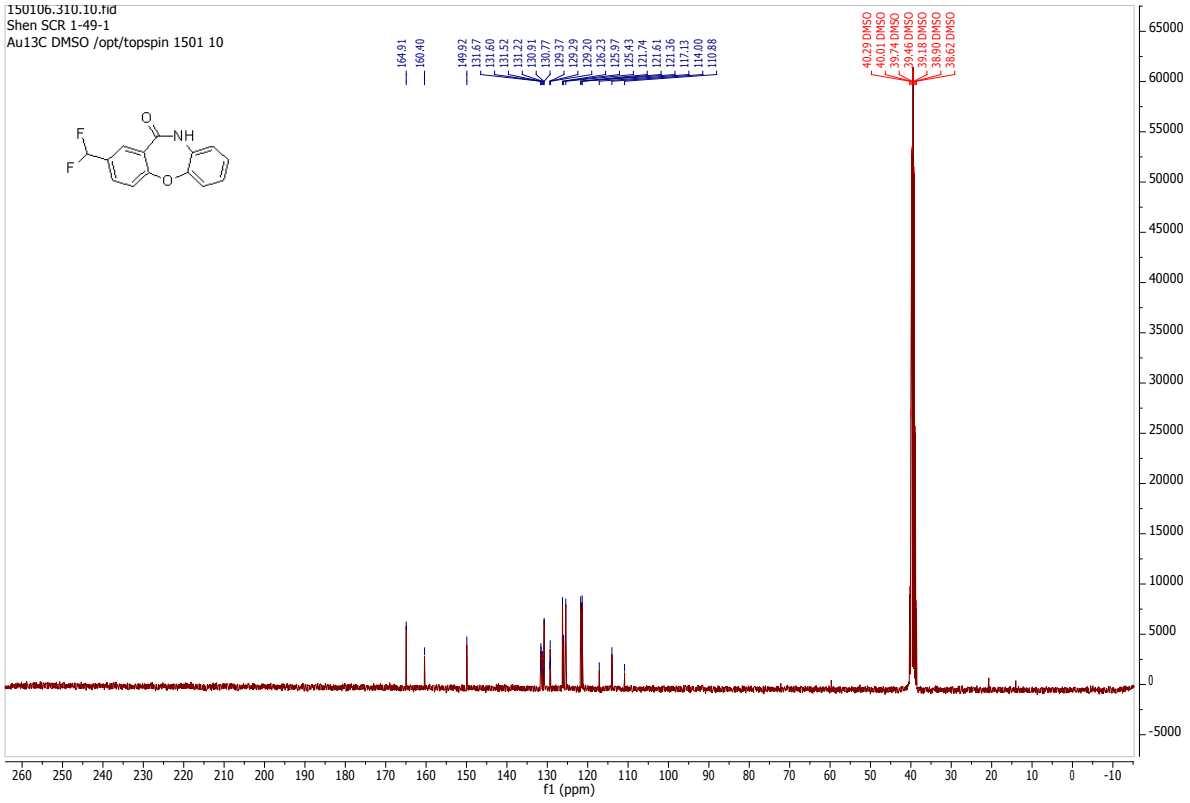




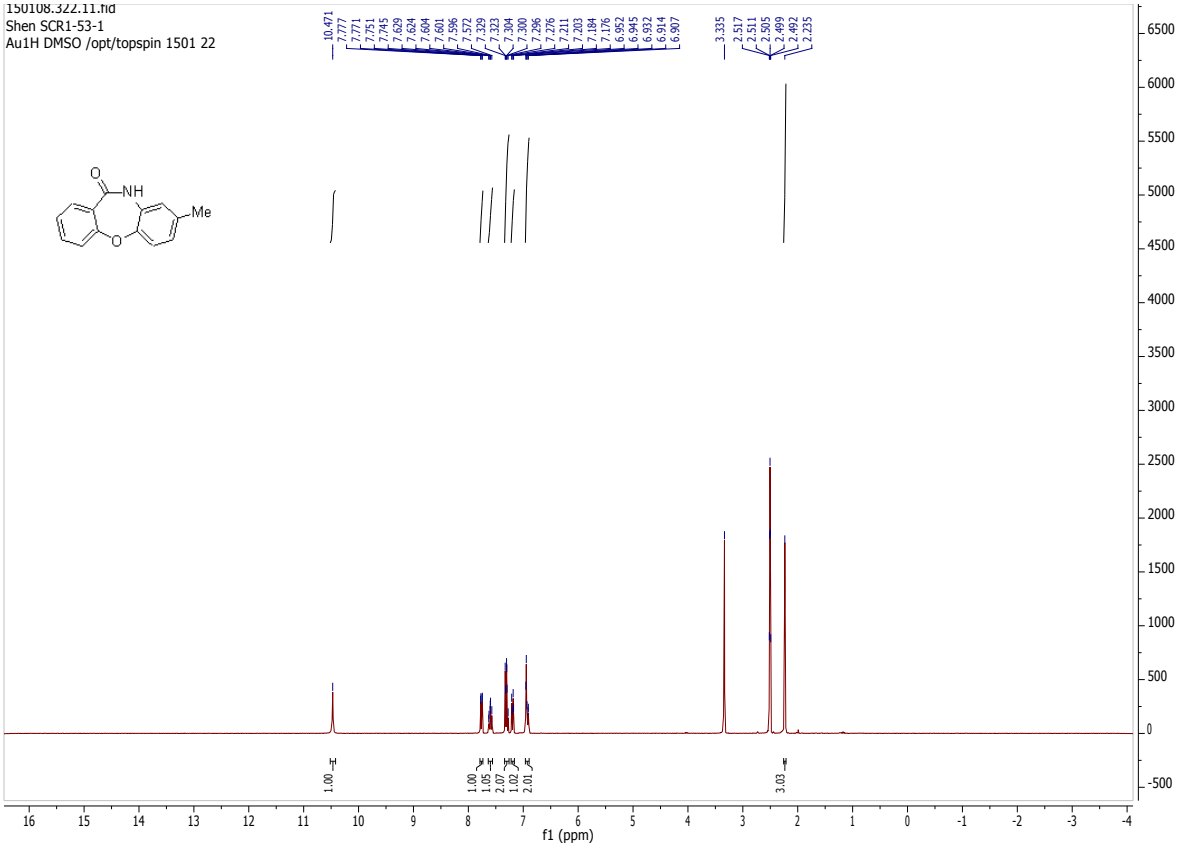
2-(difluoromethyl)dibenzo[b,f][1,4]oxazepin-11(10H)-one (3j)

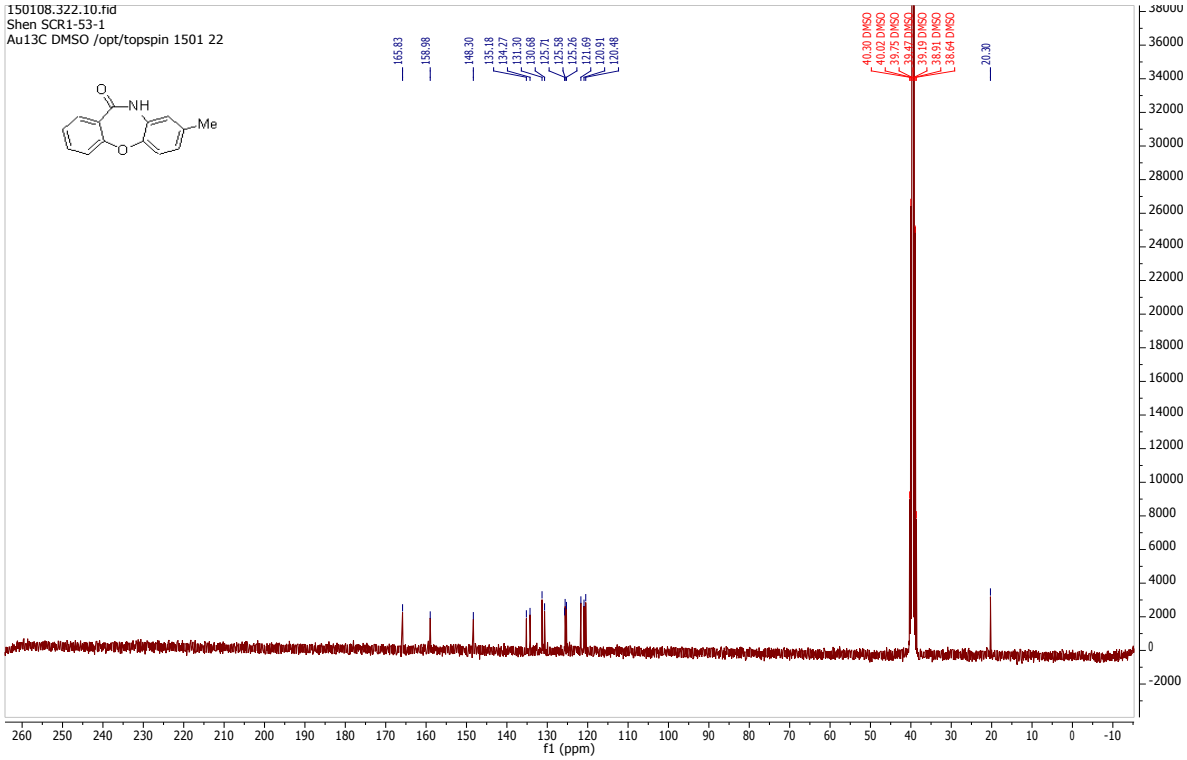




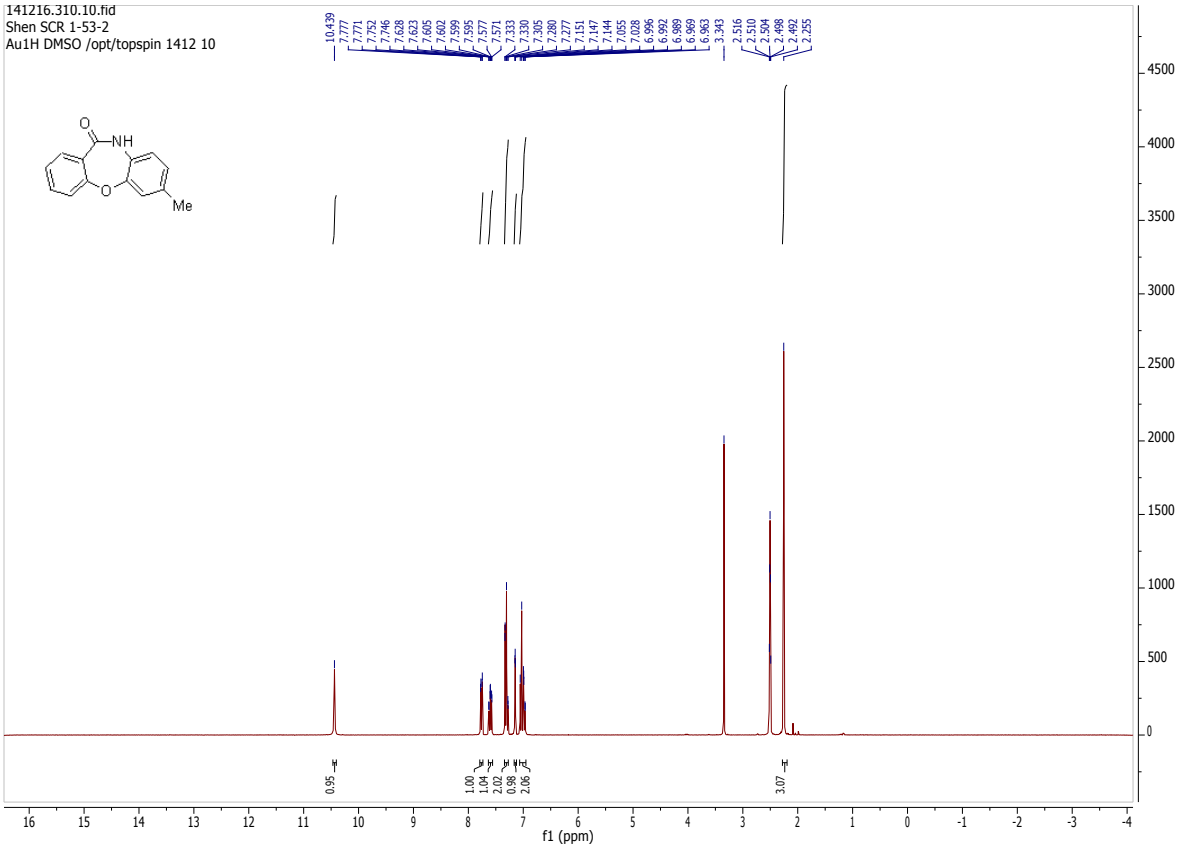


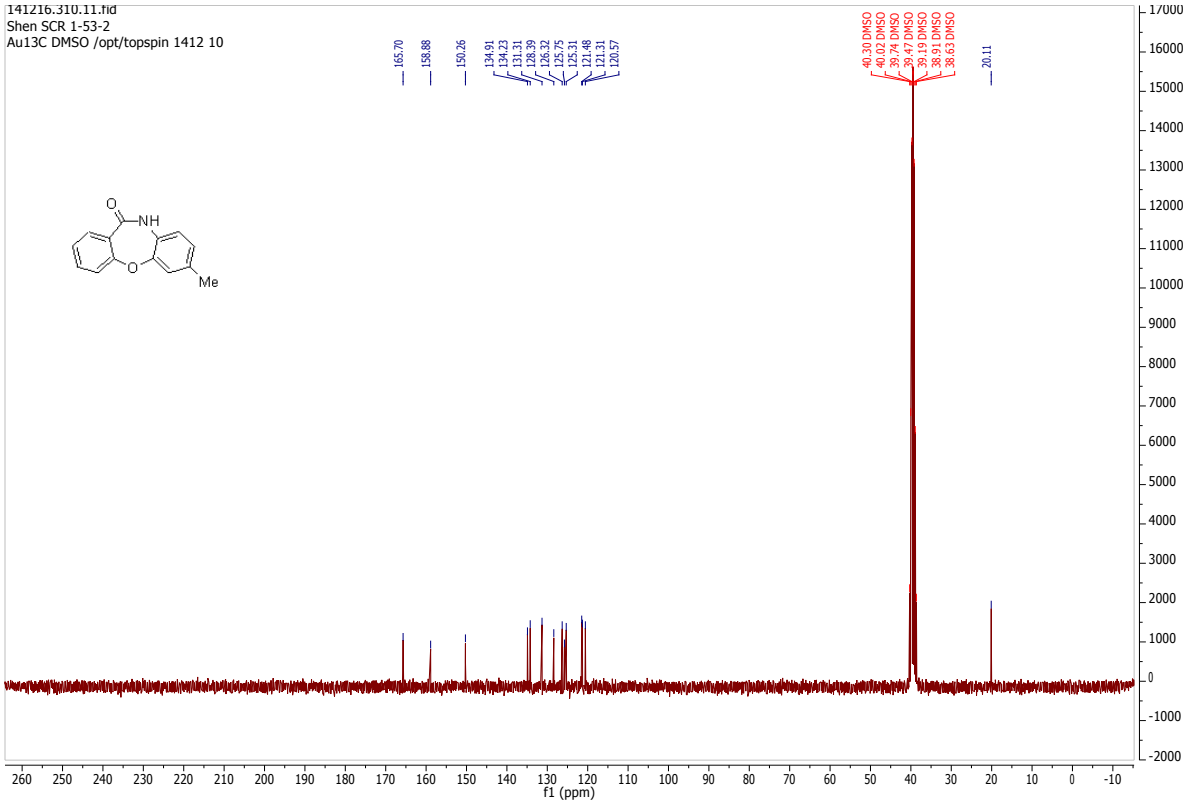
8-methyldibenzo[b,f][1,4]oxazepin-11(10H)-one[4] (3l)



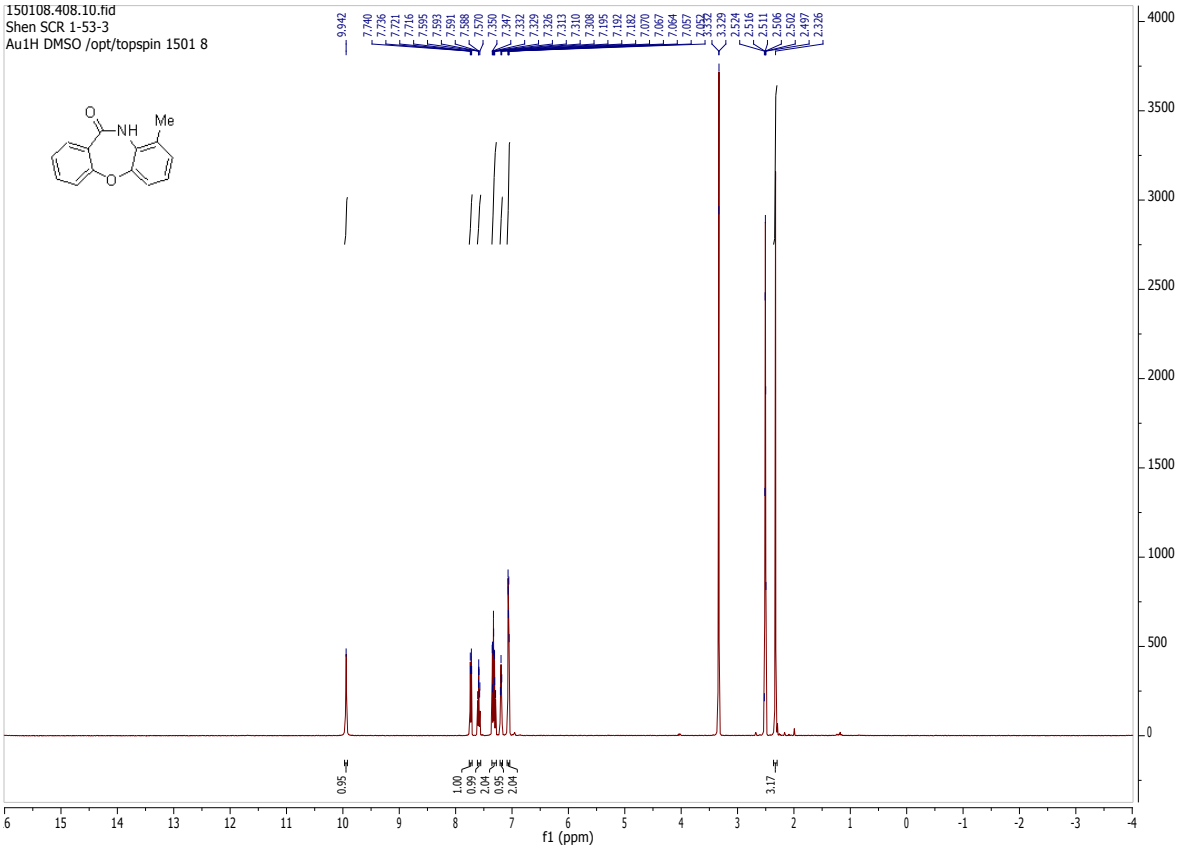


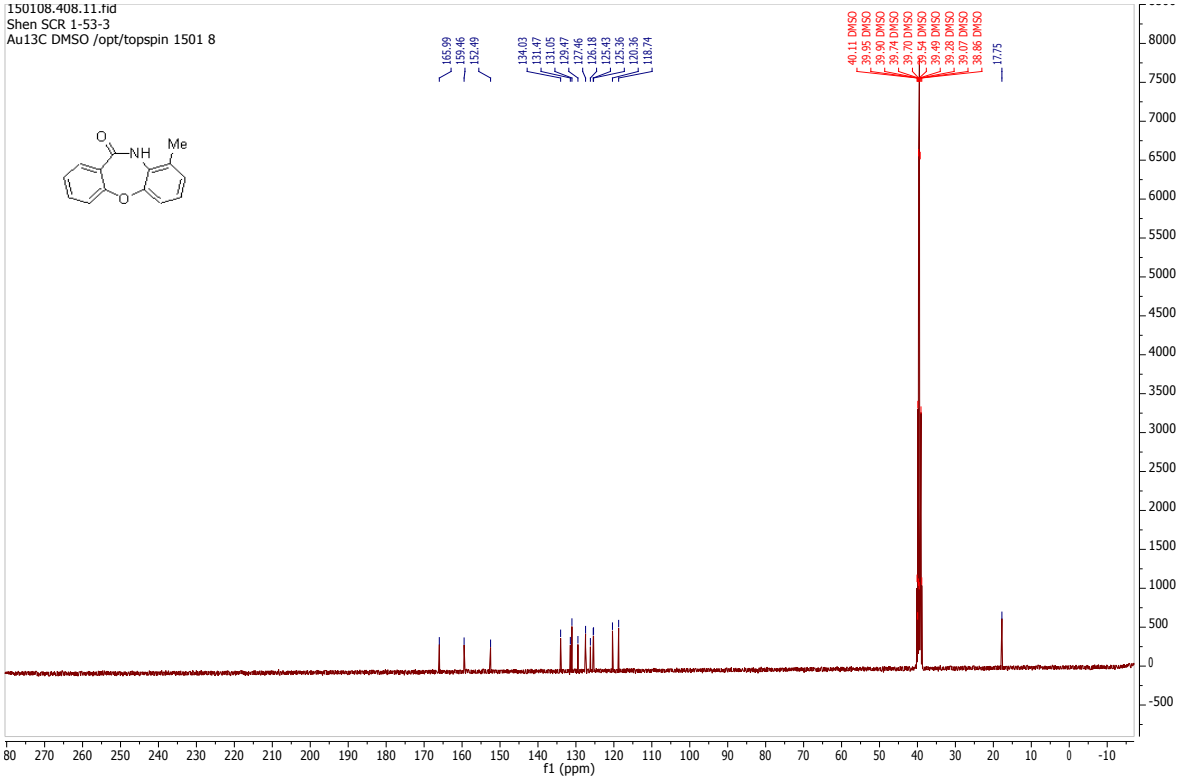
7-methyldibenzo[b,f][1,4]oxazepin-11(10H)-one[5] (3m)



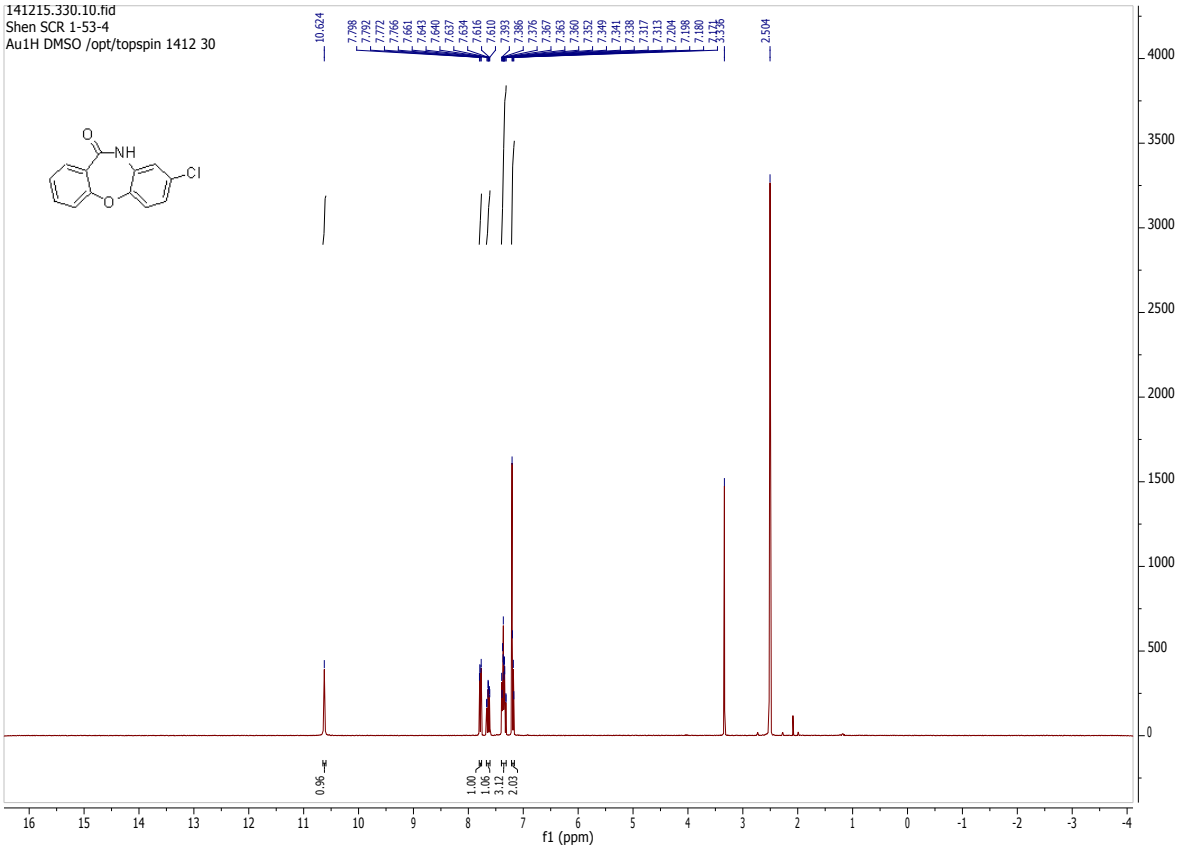


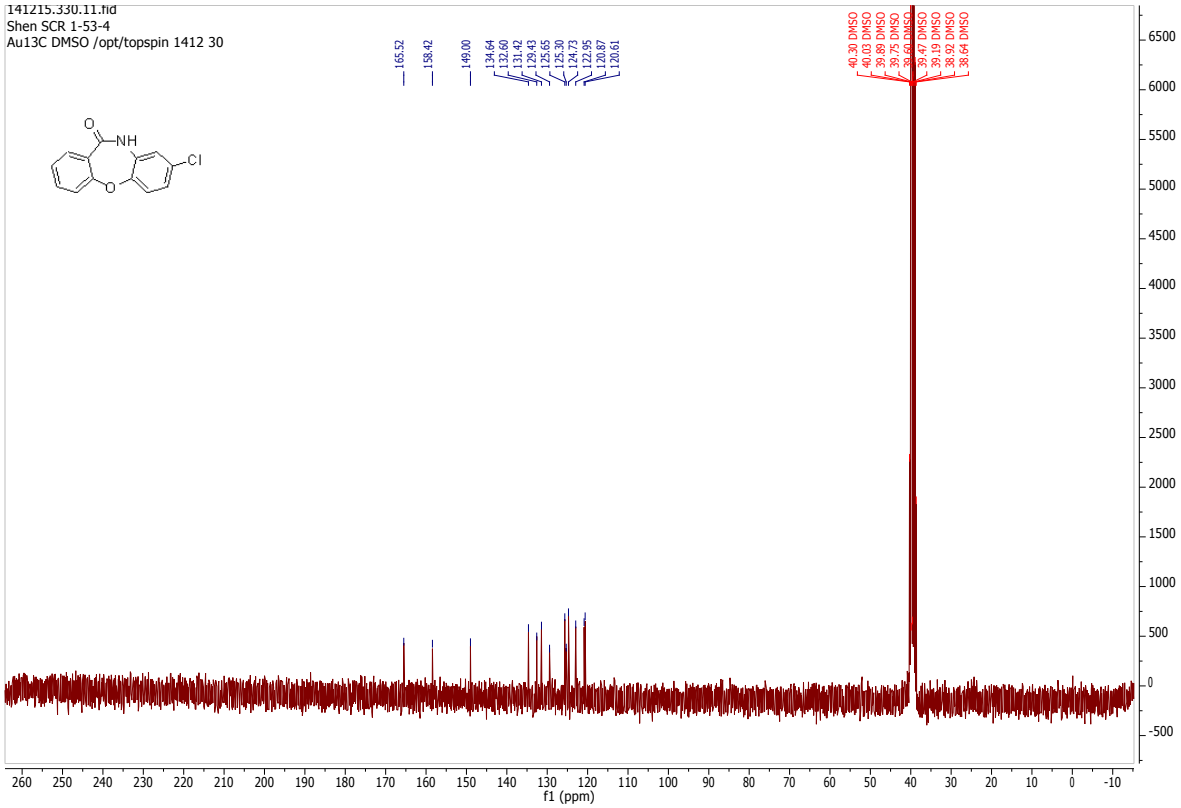
9-methyldibenzo[b,f][1,4]oxazepin-11(10H)-one (3n)



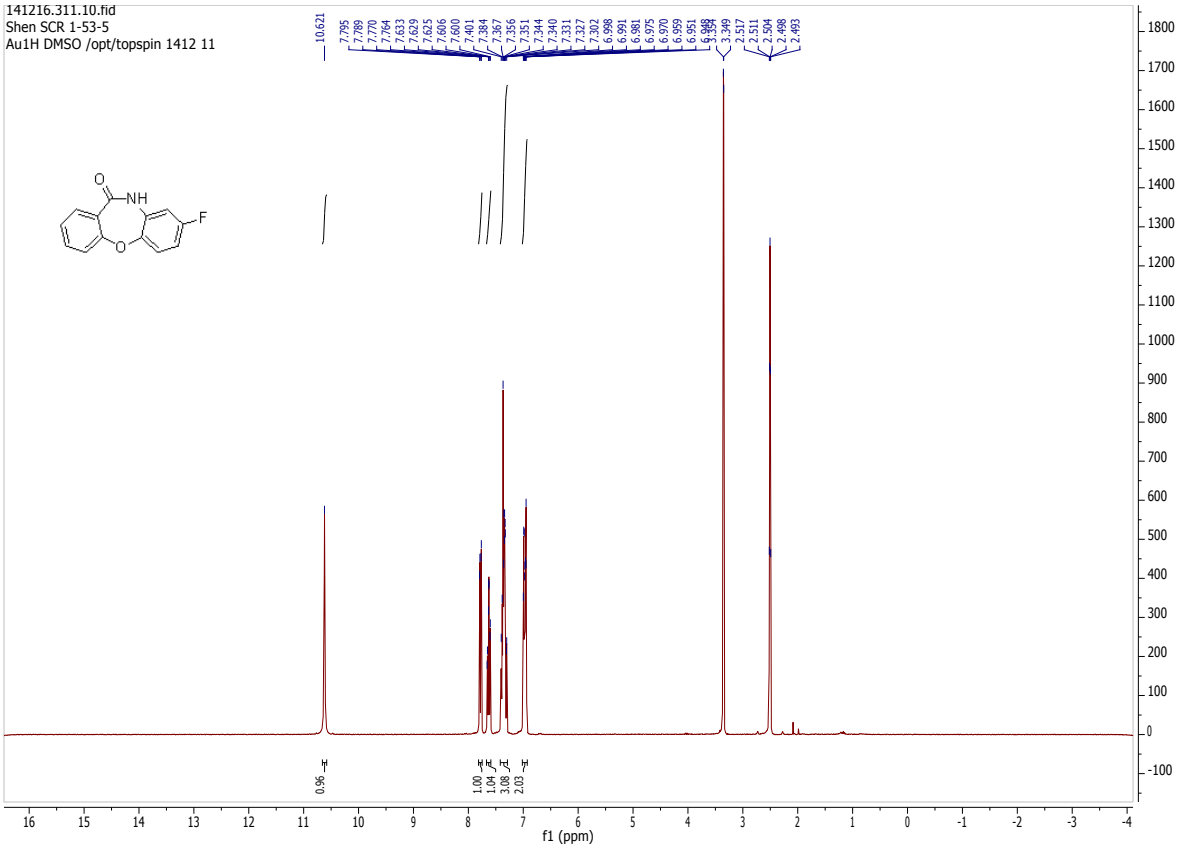


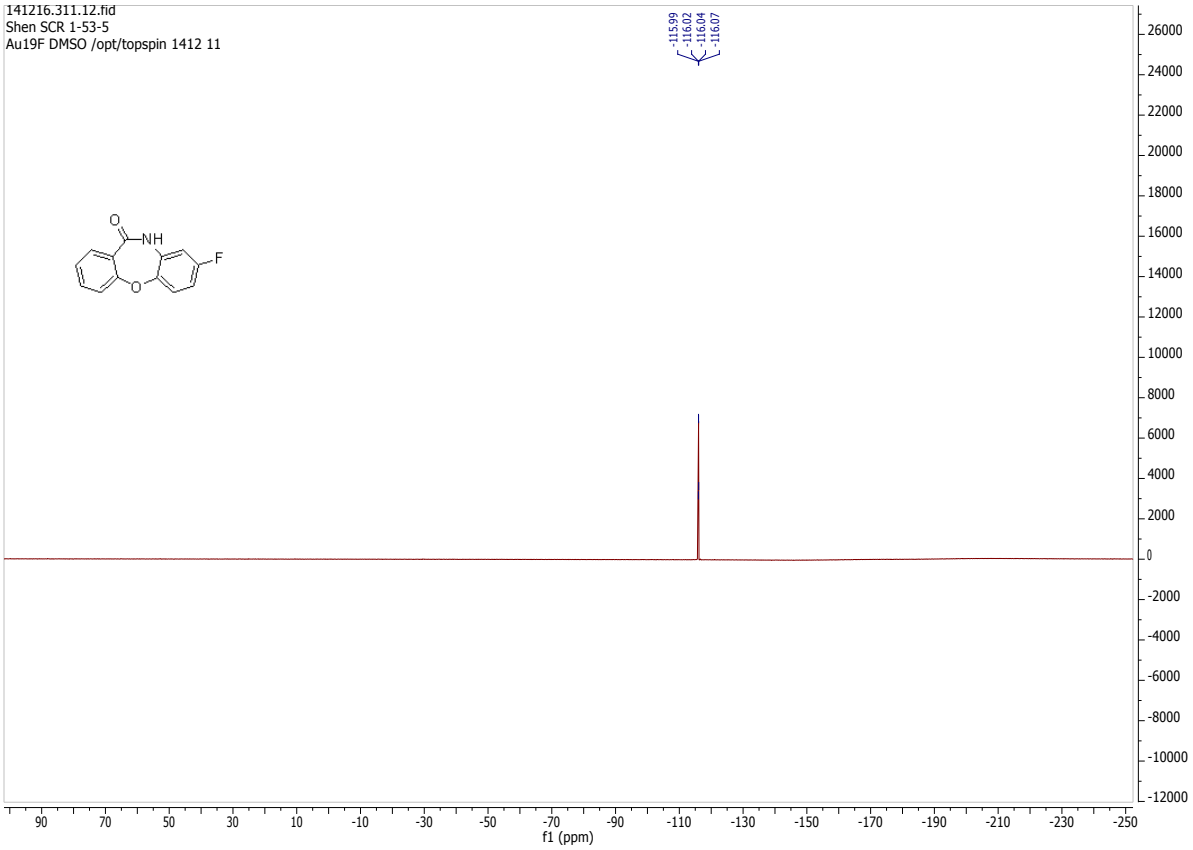
8-chlorodibenzo[b,f][1,4]oxazepin-11(10H)-one[6] (3o)

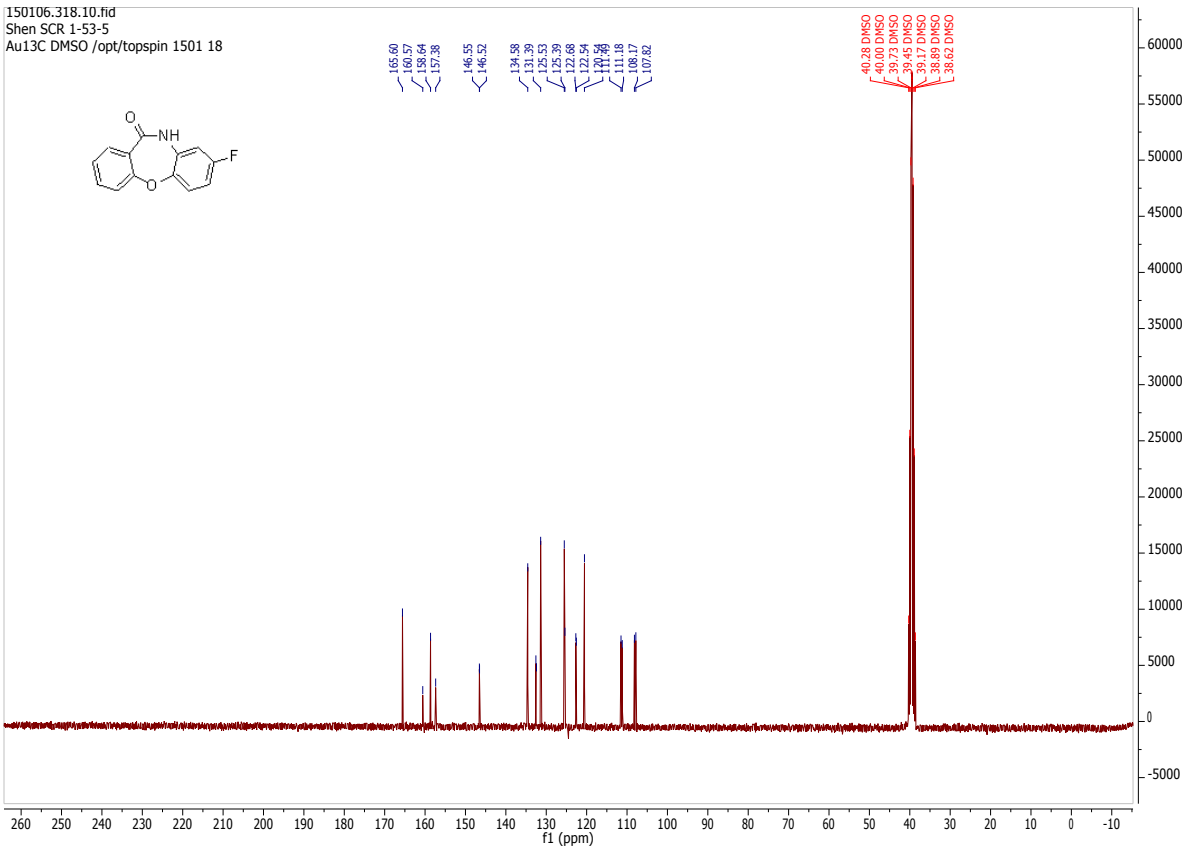




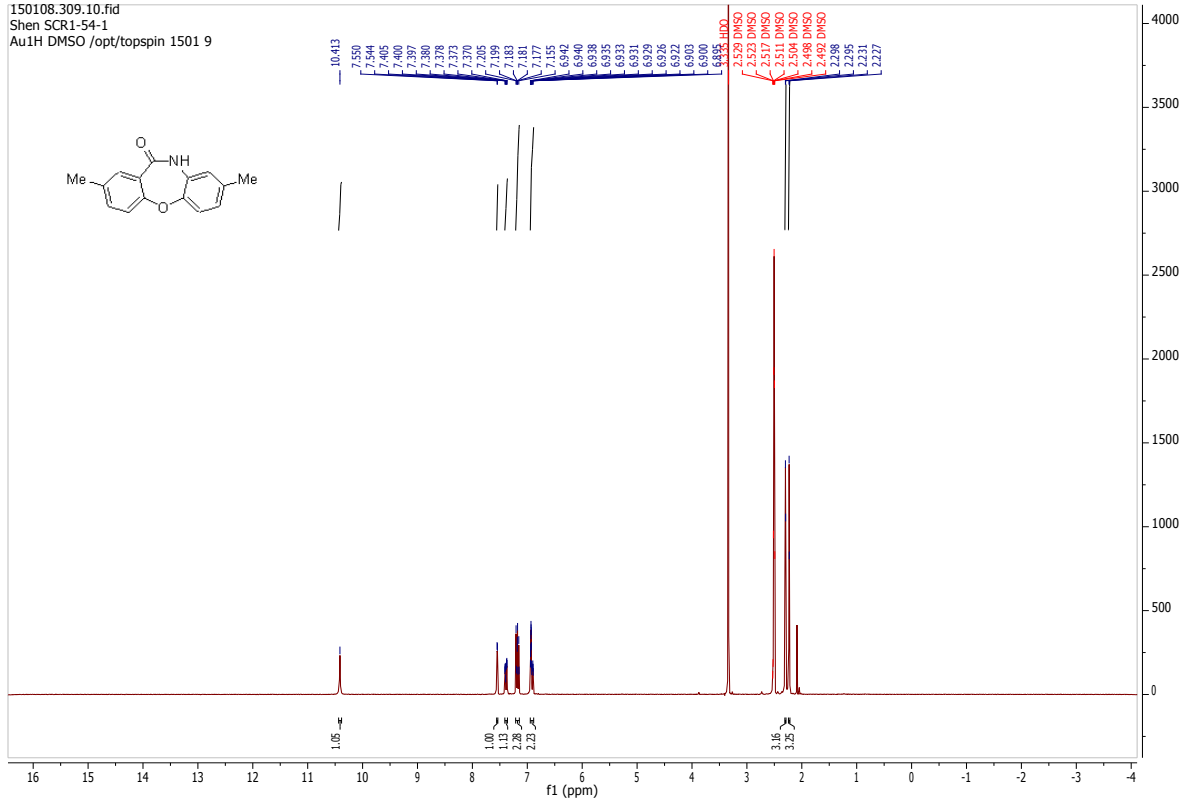
8-fluorodibenzo[b,f][1,4]oxazepin-11(10H)-one (3p)

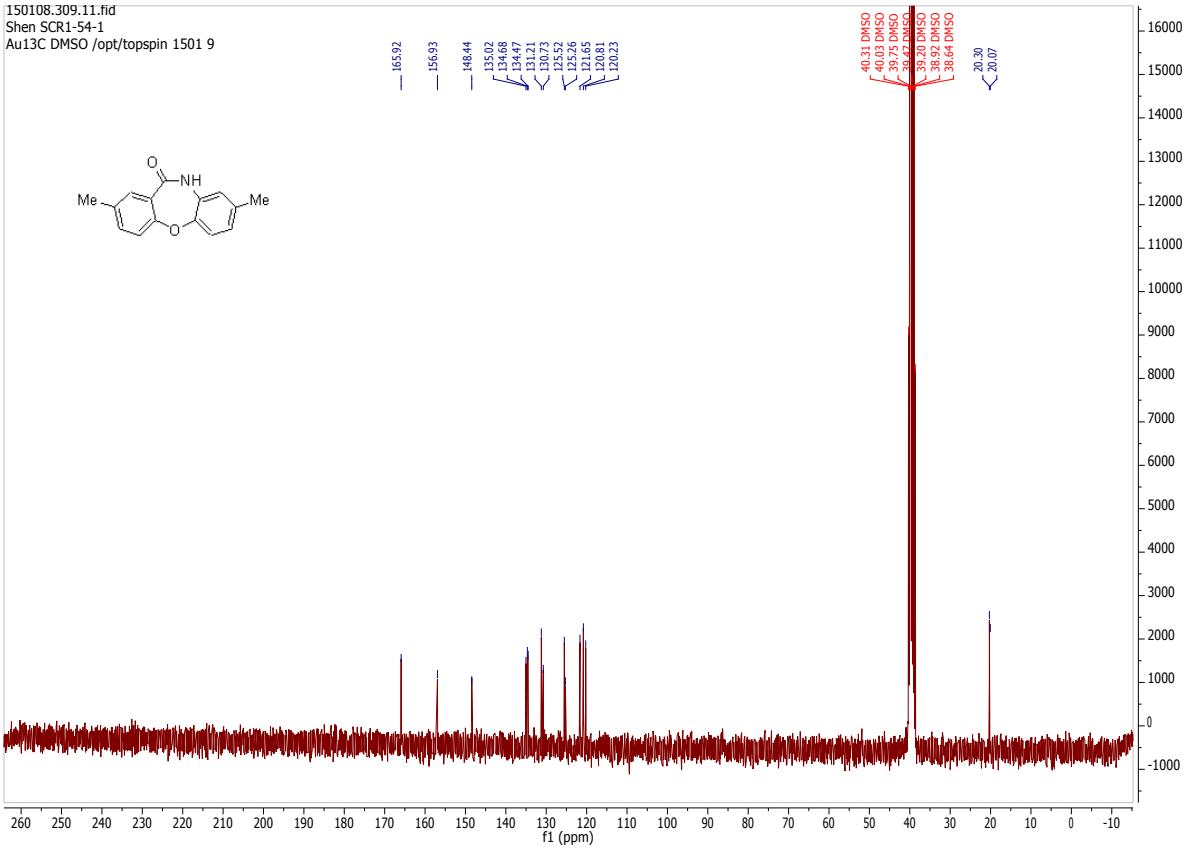



141216.311.12.fid
Shen SCR 1-53-5
Au19F DMSO /opt/topspin 1412 11
-115.99
-116.02
-116.04
-116.07
O
NH
F
O
f1 (ppm)

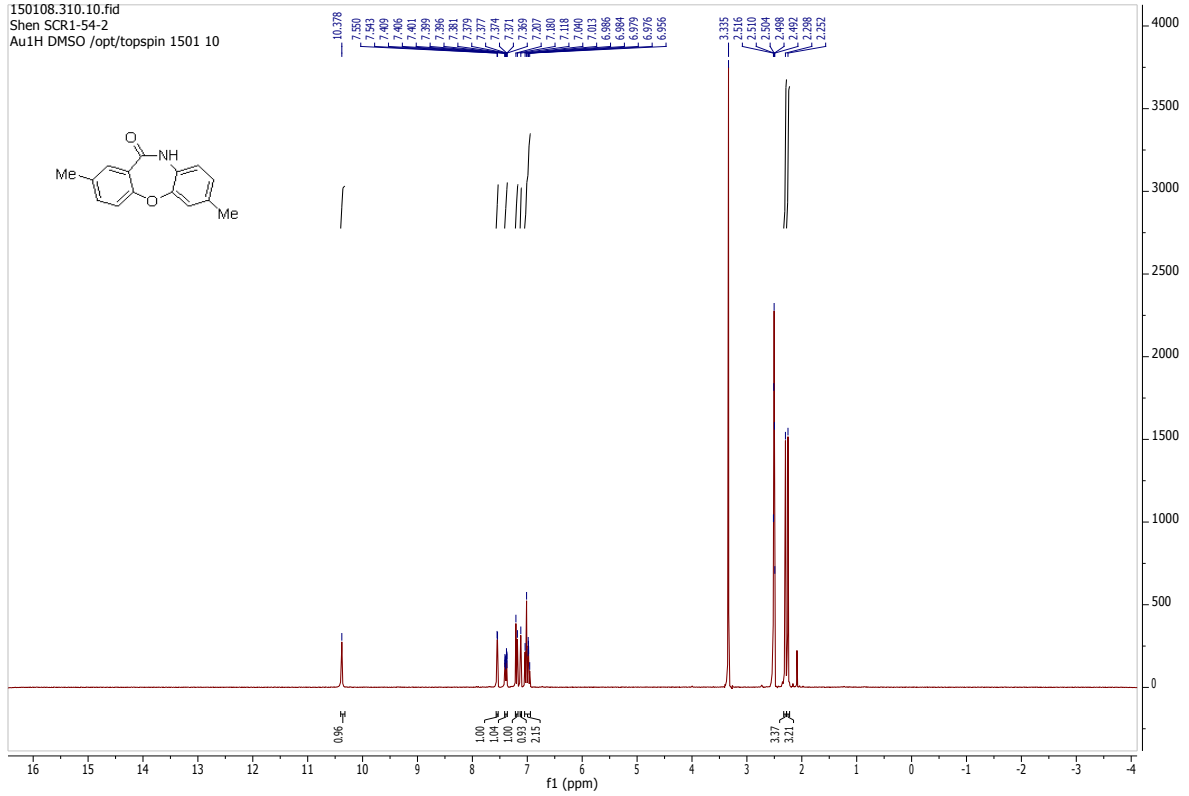

150106.318.10.fid
Shen SCR 1-53-5
Au13C DMSO /opt/topspin 1501 18
165.60
160.57
158.64
157.38
146.55
146.52
134.58
131.39
125.53
125.39
122.68
122.54
111.18
108.17
107.82
40.28 DMSO
40.00 DMSO
39.73 DMSO
39.45 DMSO
39.17 DMSO
38.89 DMSO
38.62 DMSO
O
NH
F
O
f1 (ppm)

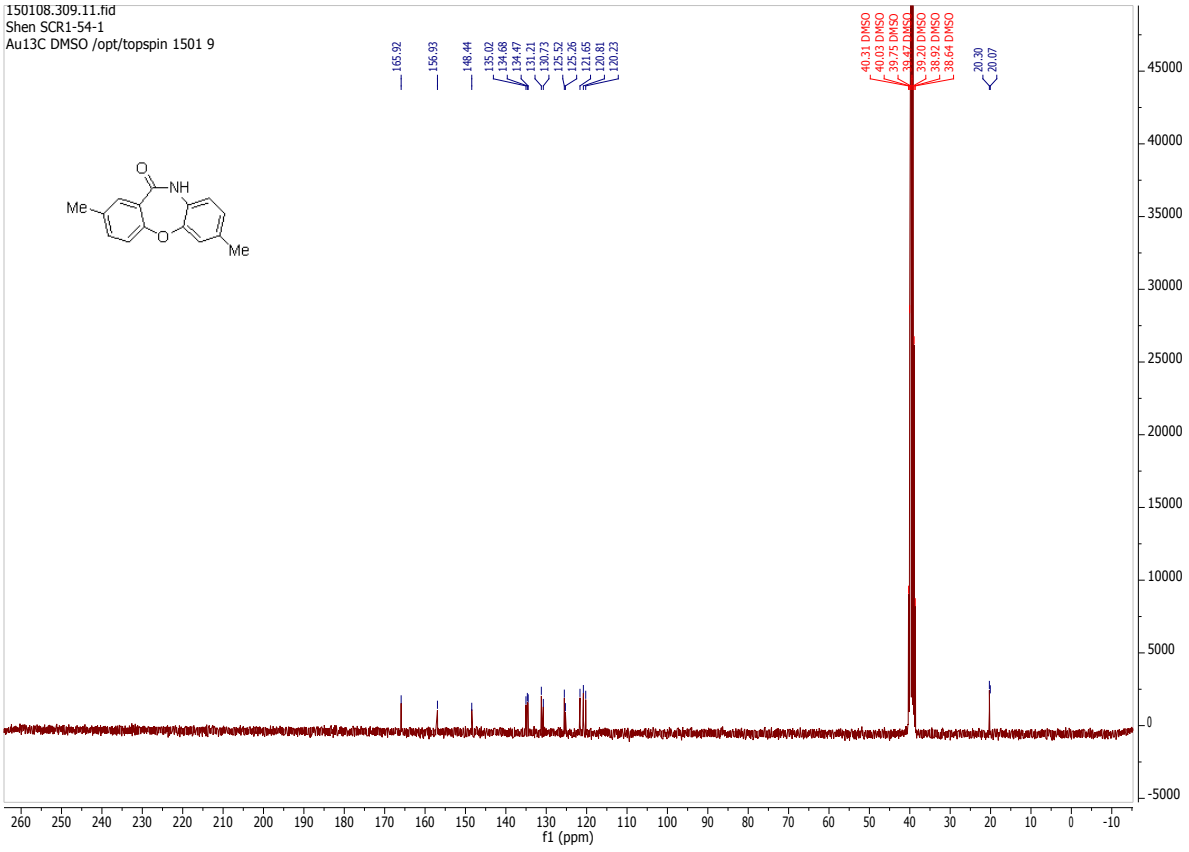
2,8-dimethyldibenzo[b,f][1,4]oxazepin-11(10H)-one (3r)



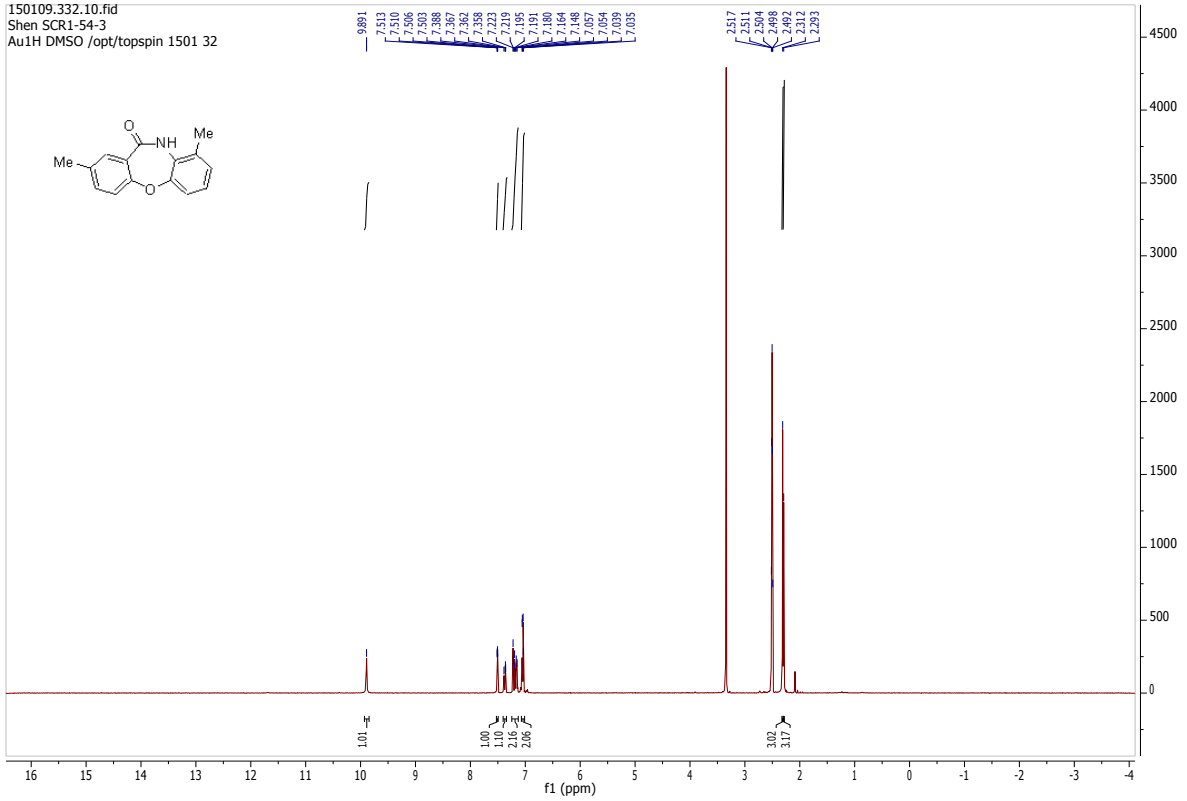


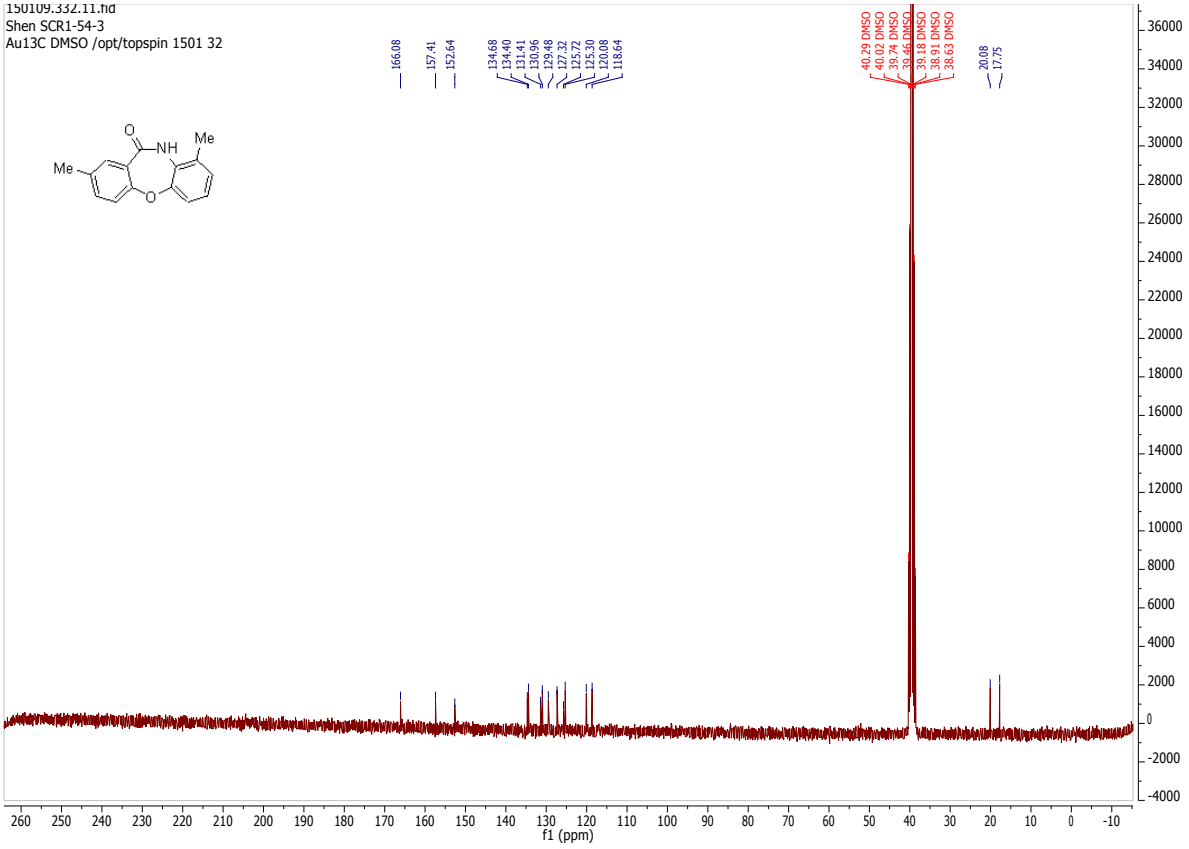
2,7-dimethyldibenzo[b,f][1,4]oxazepin-11(10H)-one (3s)



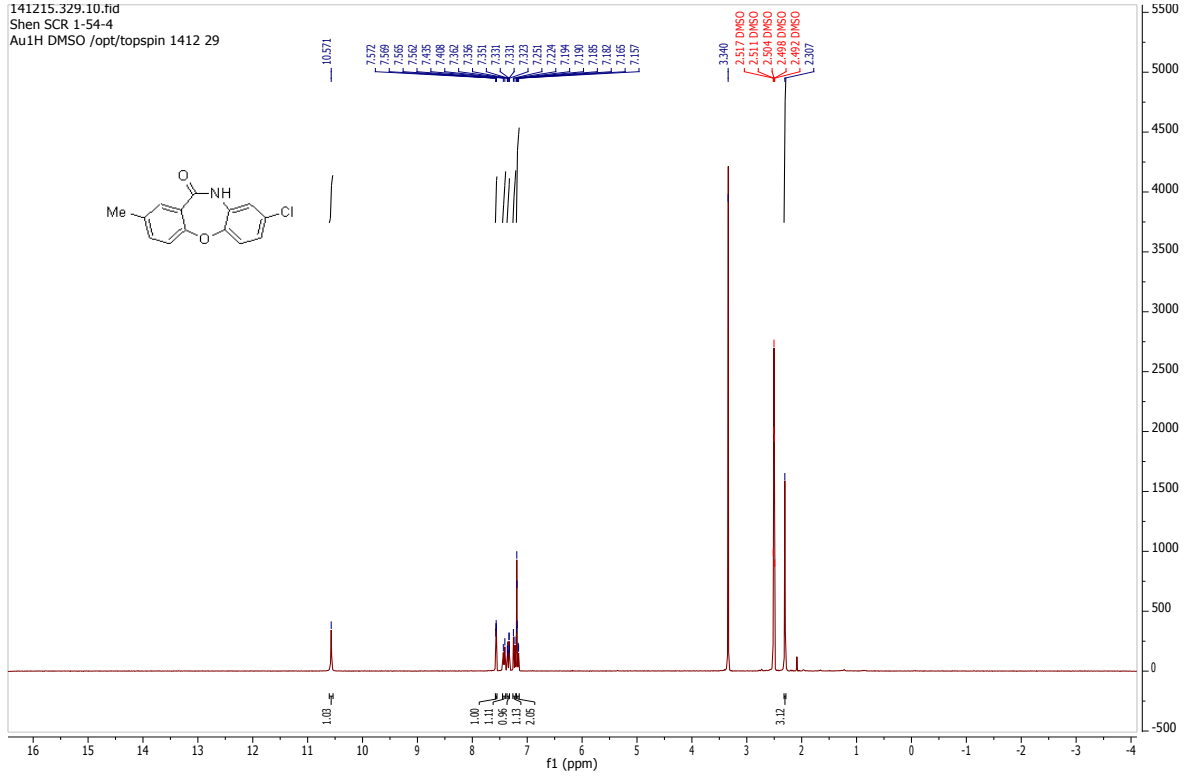


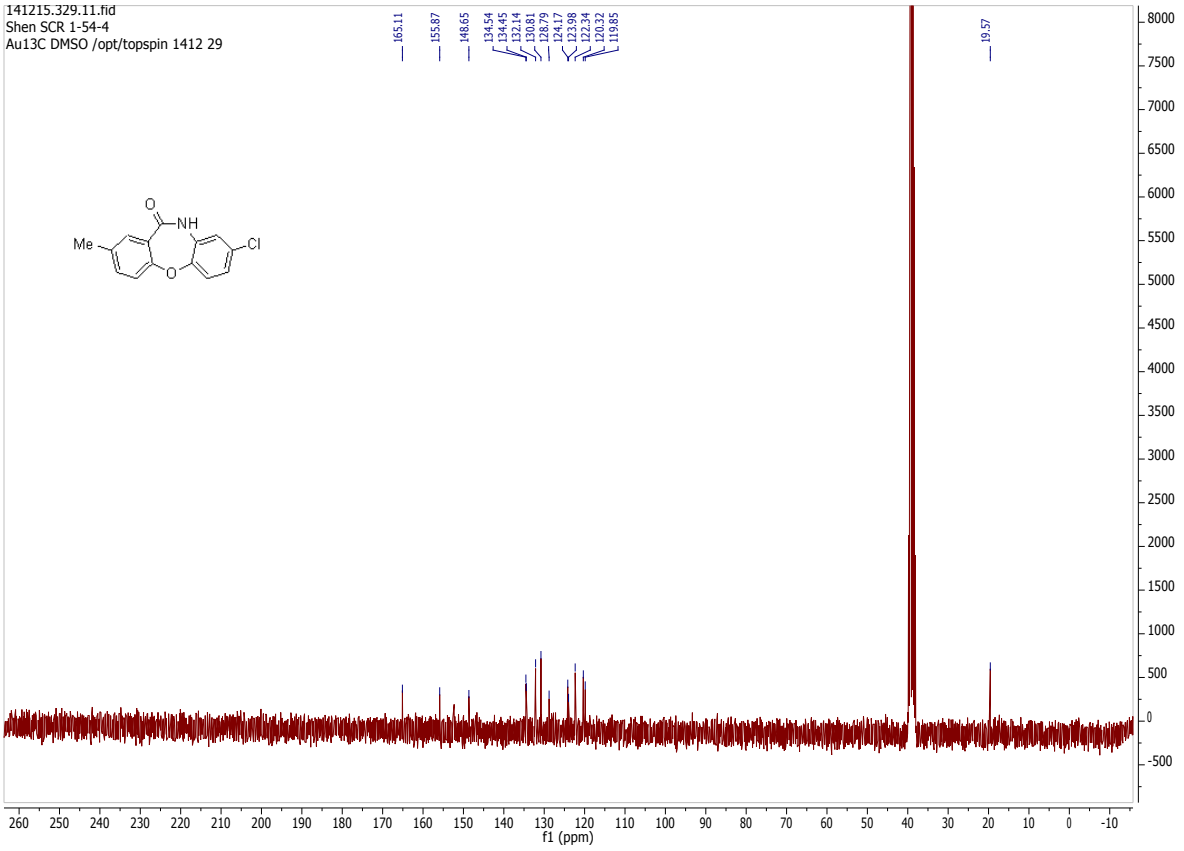
2,9-dimethyldibenzo[b,f][1,4]oxazepin-11(10H)-one (3t)



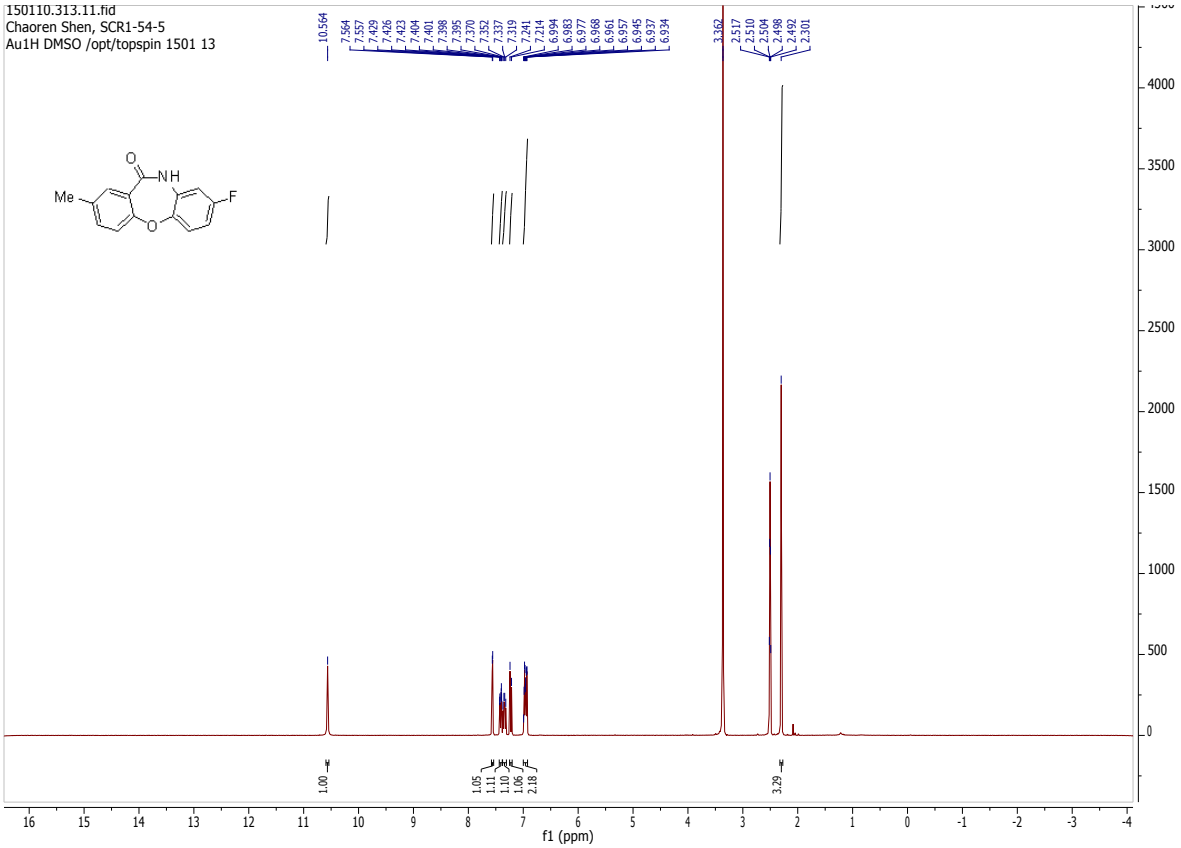


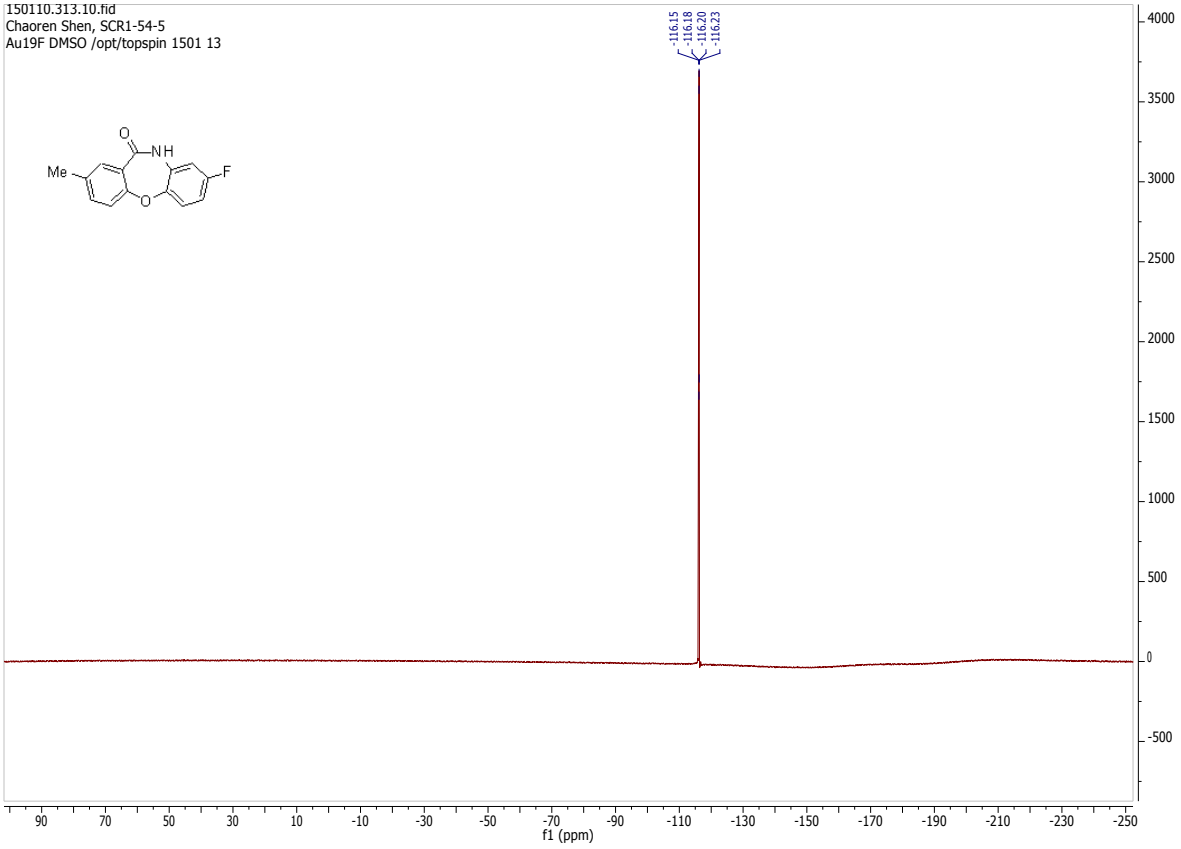
8-chloro-2-methyldibenzo[b,f][1,4]oxazepin-11(10H)-one (3u)

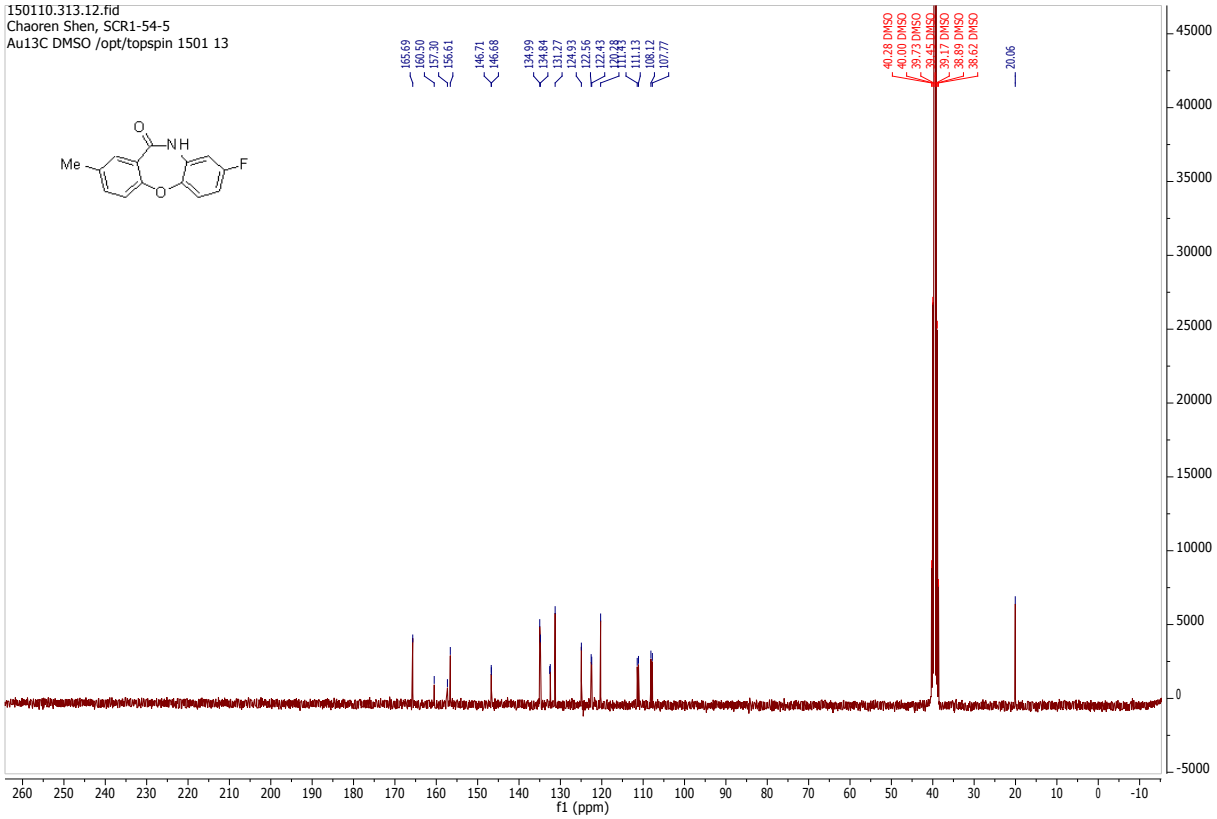




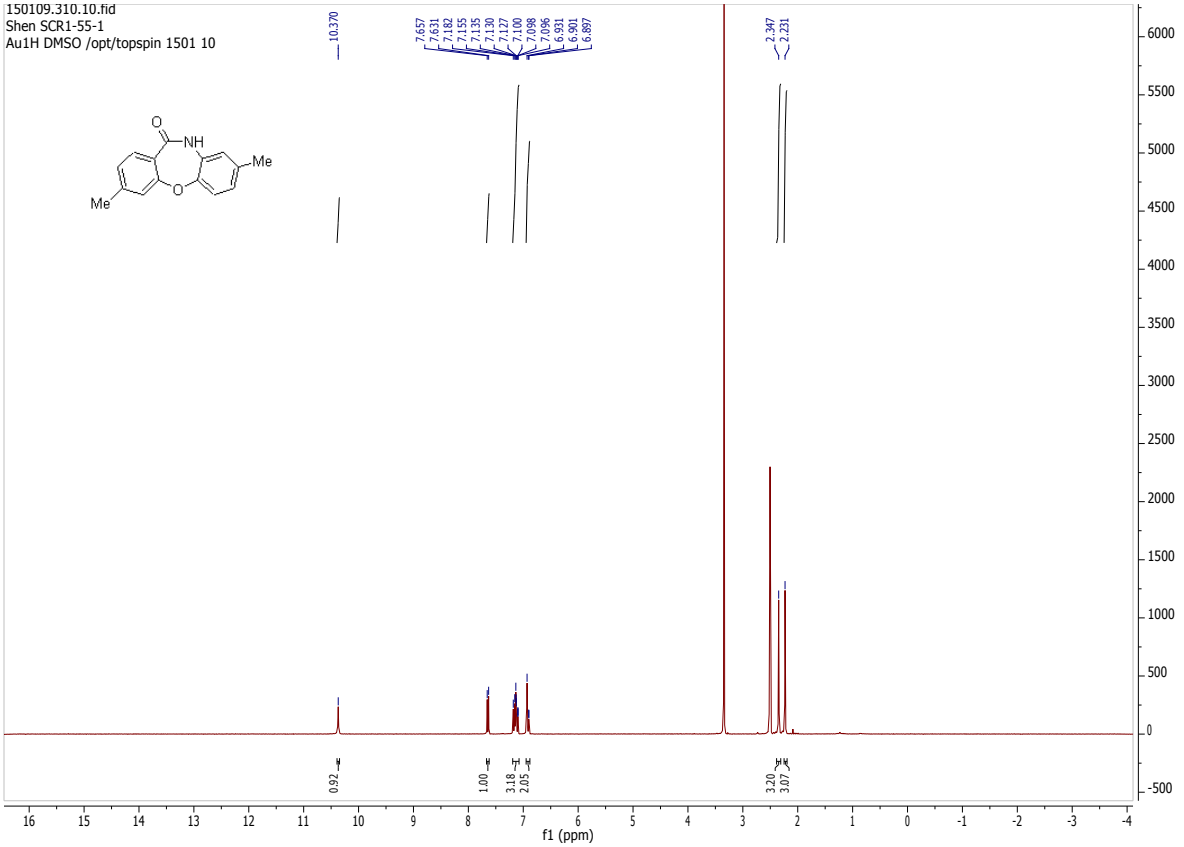
8-fluoro-2-methyldibenzo[b,f][1,4]oxazepin-11(10H)-one (3v)

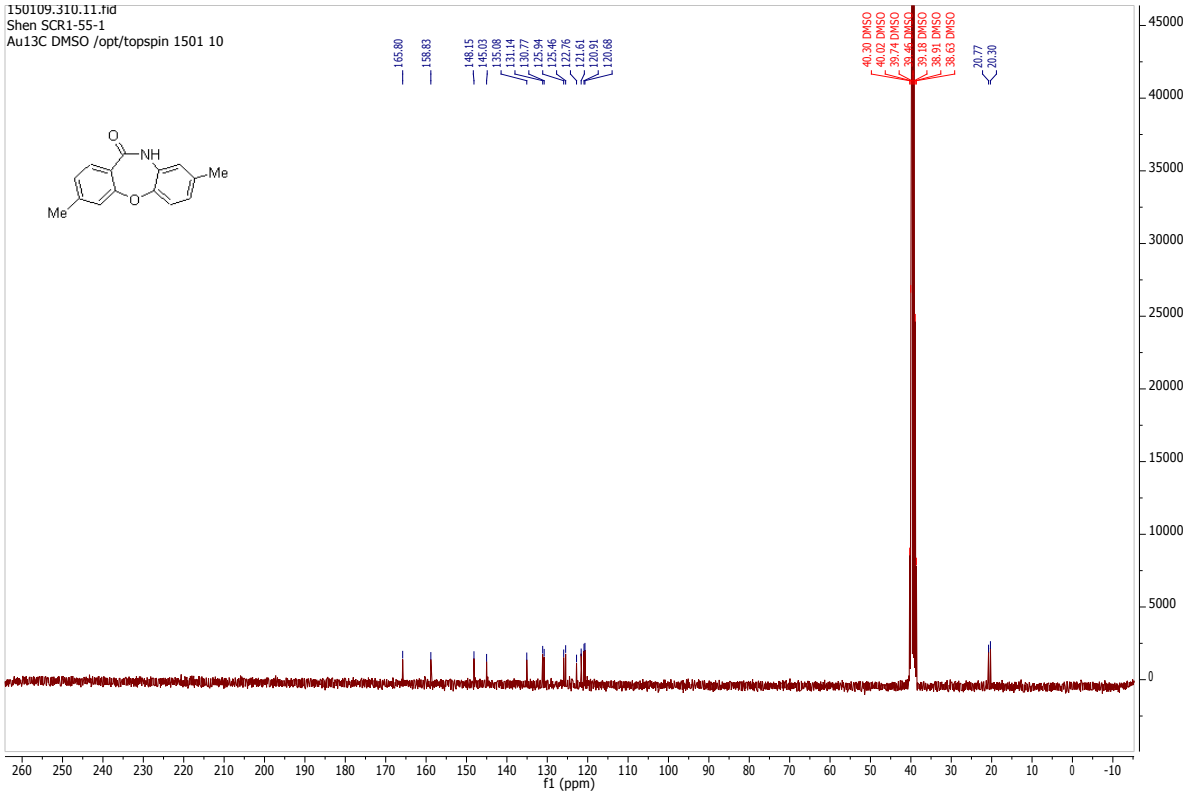

150110.313.11.fid
Chaoren Shen, SCR1-54-5
Au1H DMSO /opt/topspin 1501 13
10.564
7.564
7.557
7.429
7.426
7.423
7.404
7.401
7.398
7.395
7.370
7.352
7.337
7.319
7.241
7.214
6.994
6.983
6.977
6.968
6.961
6.957
6.945
6.937
6.934
3.362
2.517
2.510
2.504
2.498
2.492
2.301
O
NH
Me
F
O
1.00
1.05
1.11
1.10
1.06
2.18
3.29
f1 (ppm)


150110.313.10.fid
Chaoren Shen, SCR1-54-5
Au19F DMSO /opt/topspin 1501 13
-116.15
-116.18
-116.20
-116.23
O
NH
Me
F
O
f1 (ppm)

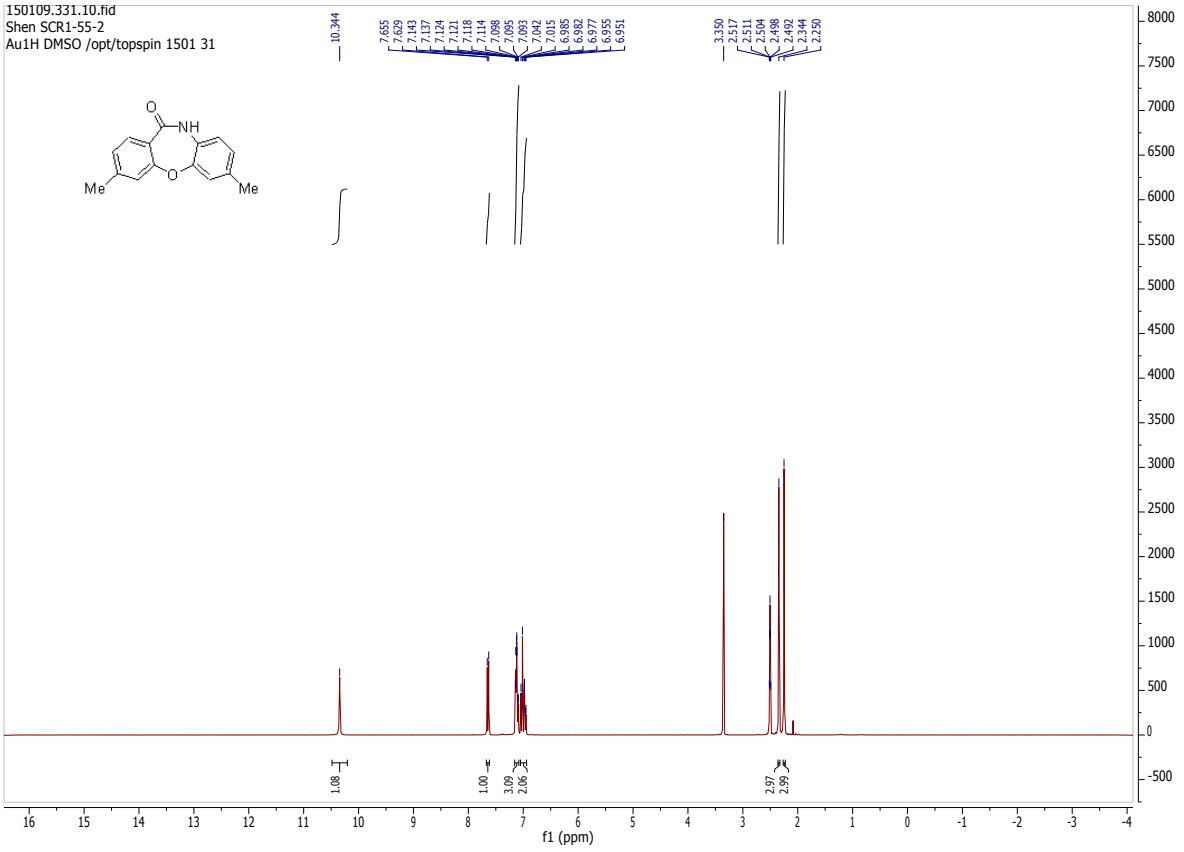


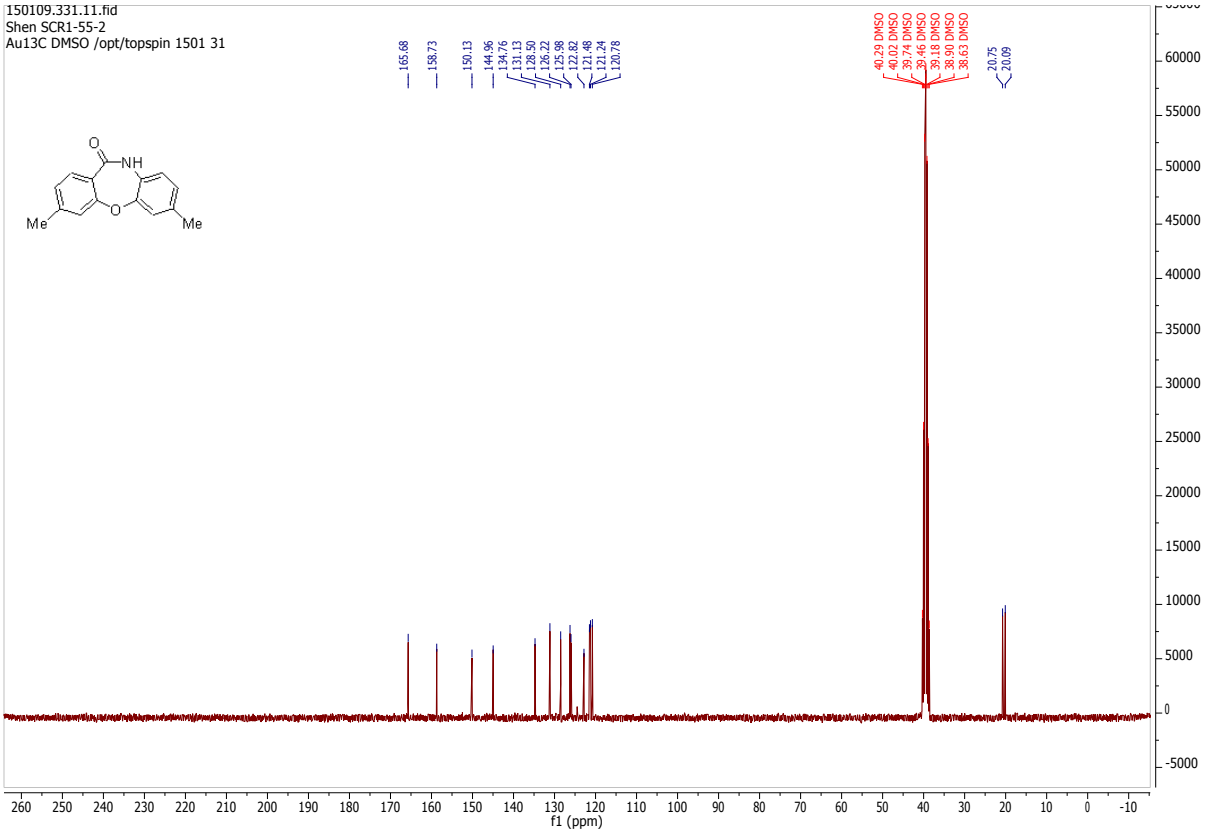
3,8-dimethyldibenzo[b,f][1,4]oxazepin-11(10H)-one (3w)



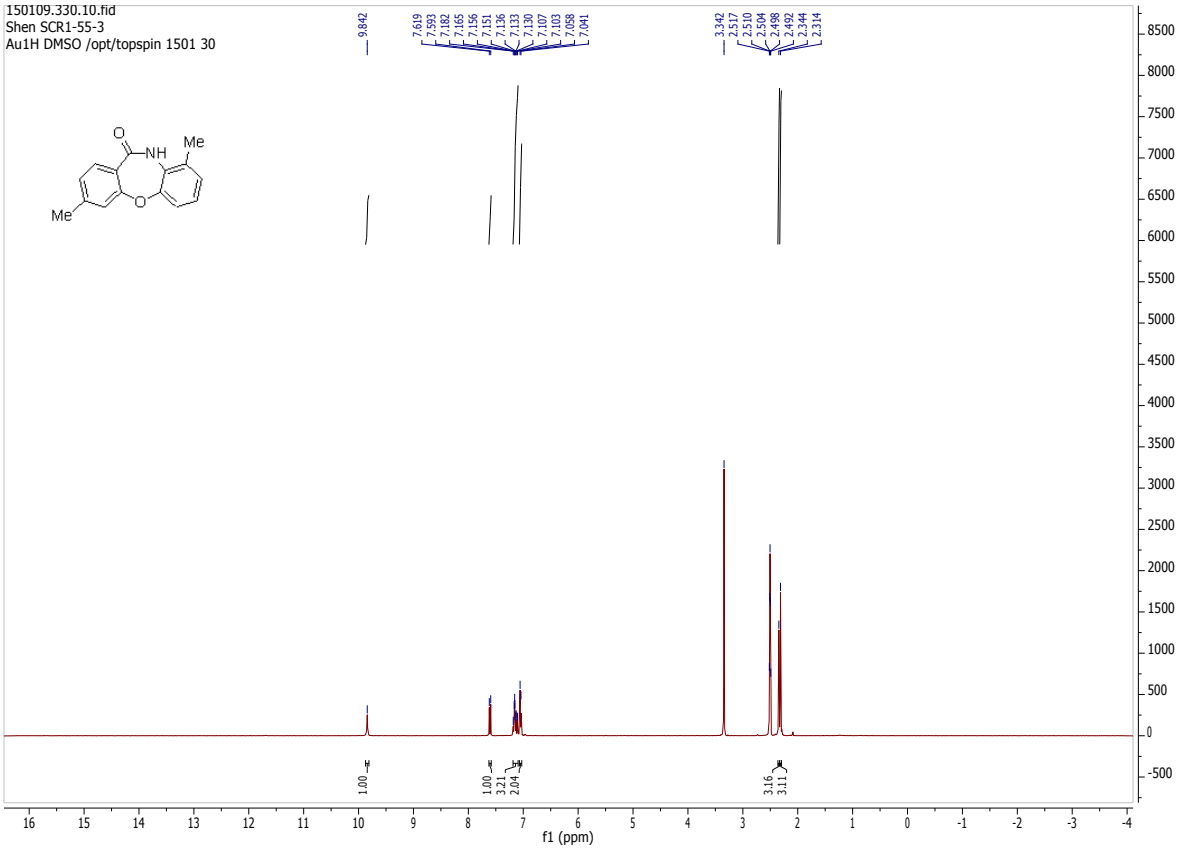


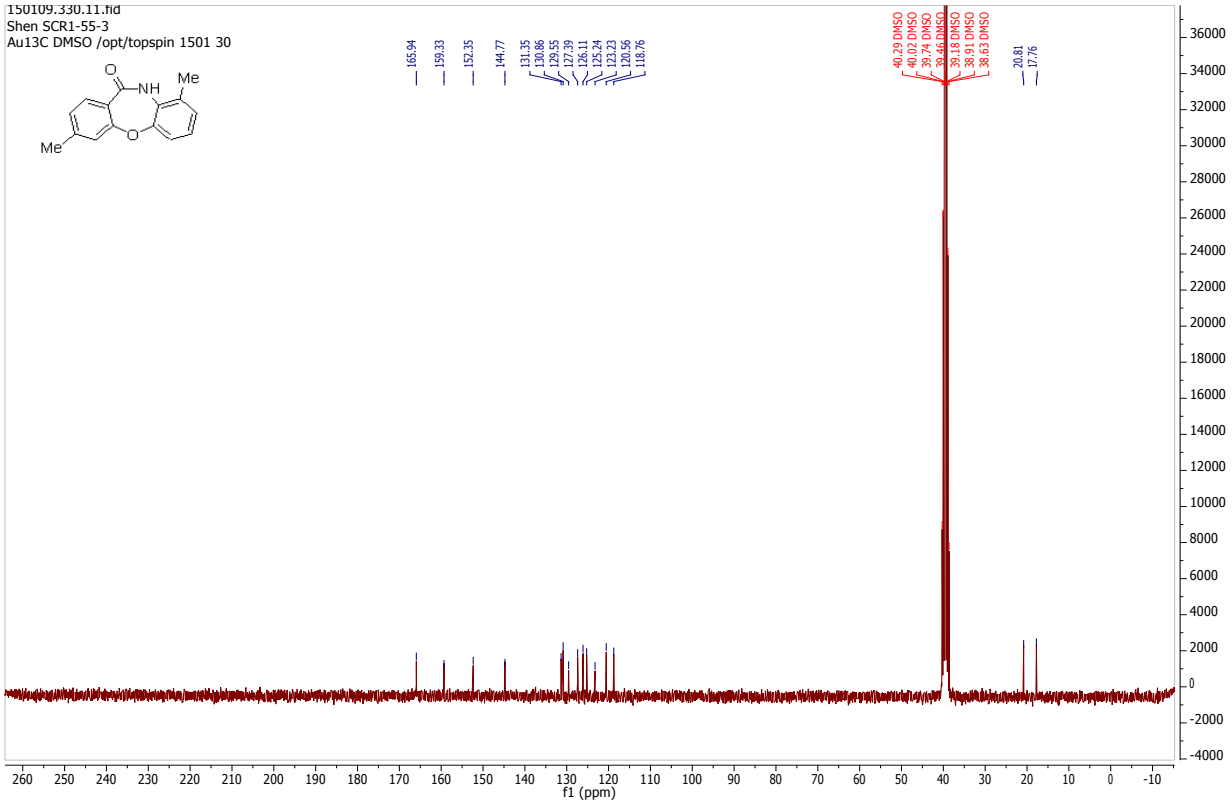
3,7-dimethyldibenzo[b,f][1,4]oxazepin-11(10H)-one (3x)



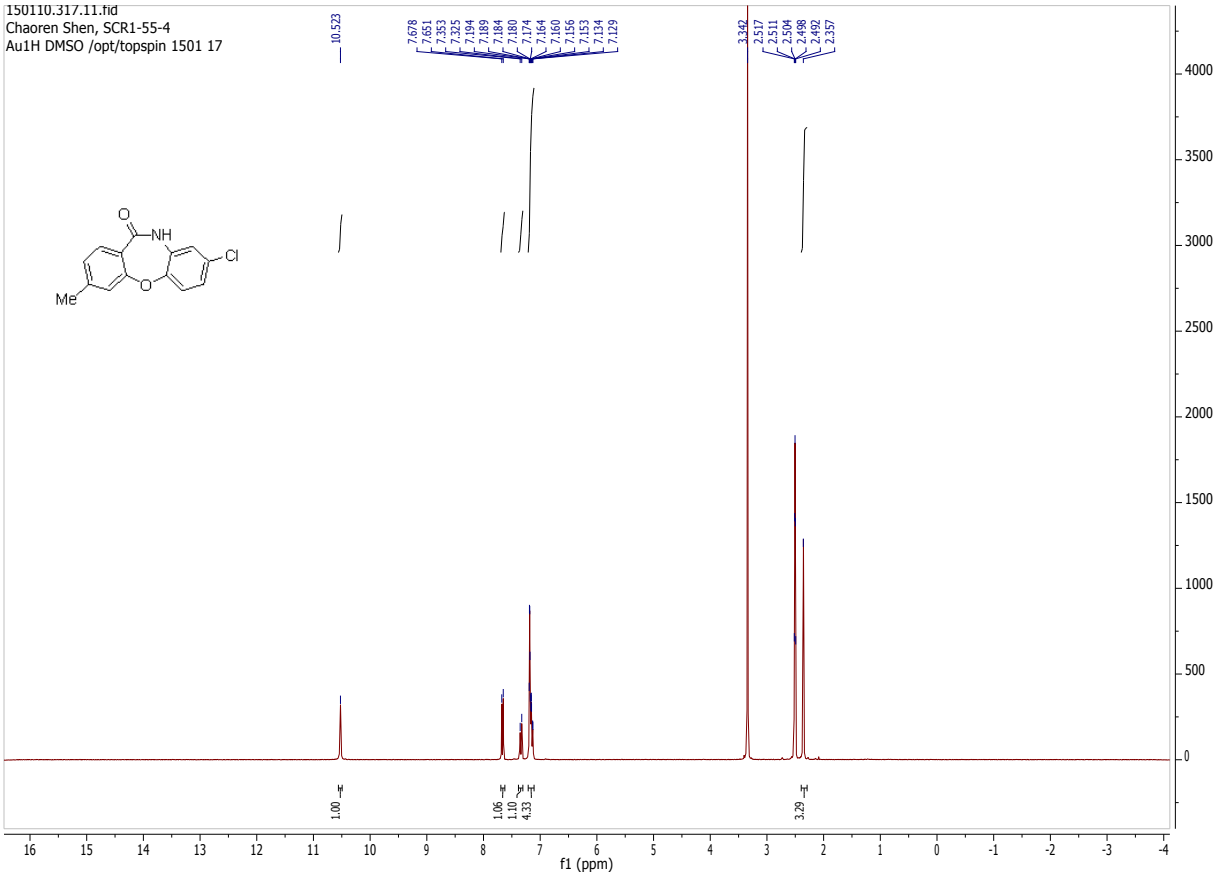


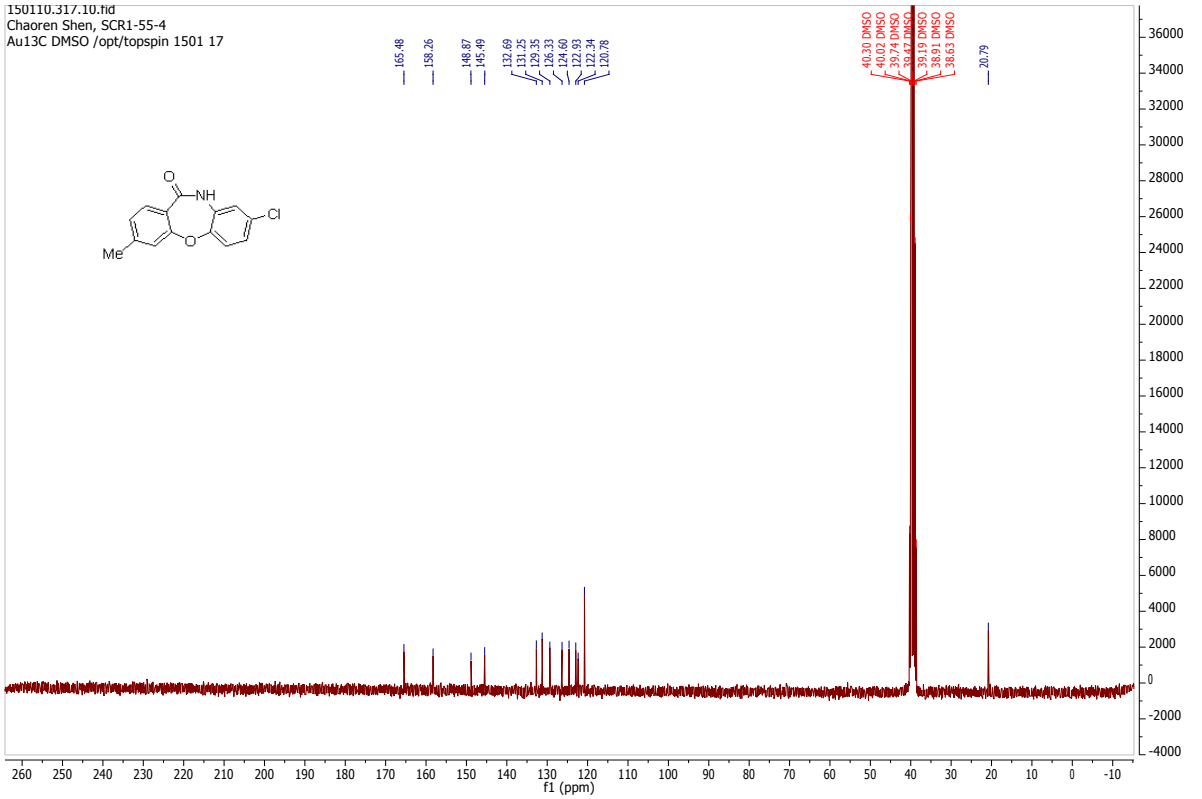
3,9-dimethyldibenzo[b,f][1,4]oxazepin-11(10H)-one (3y)



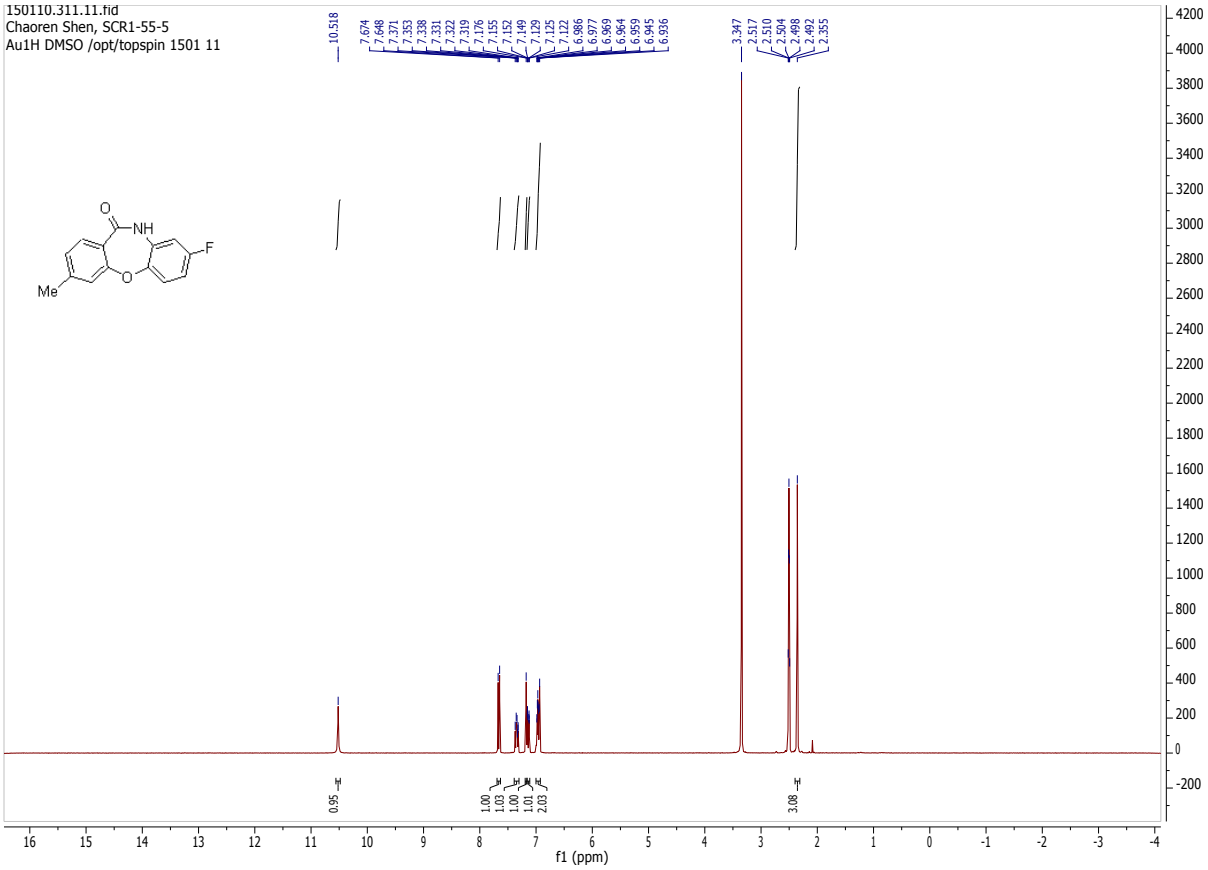


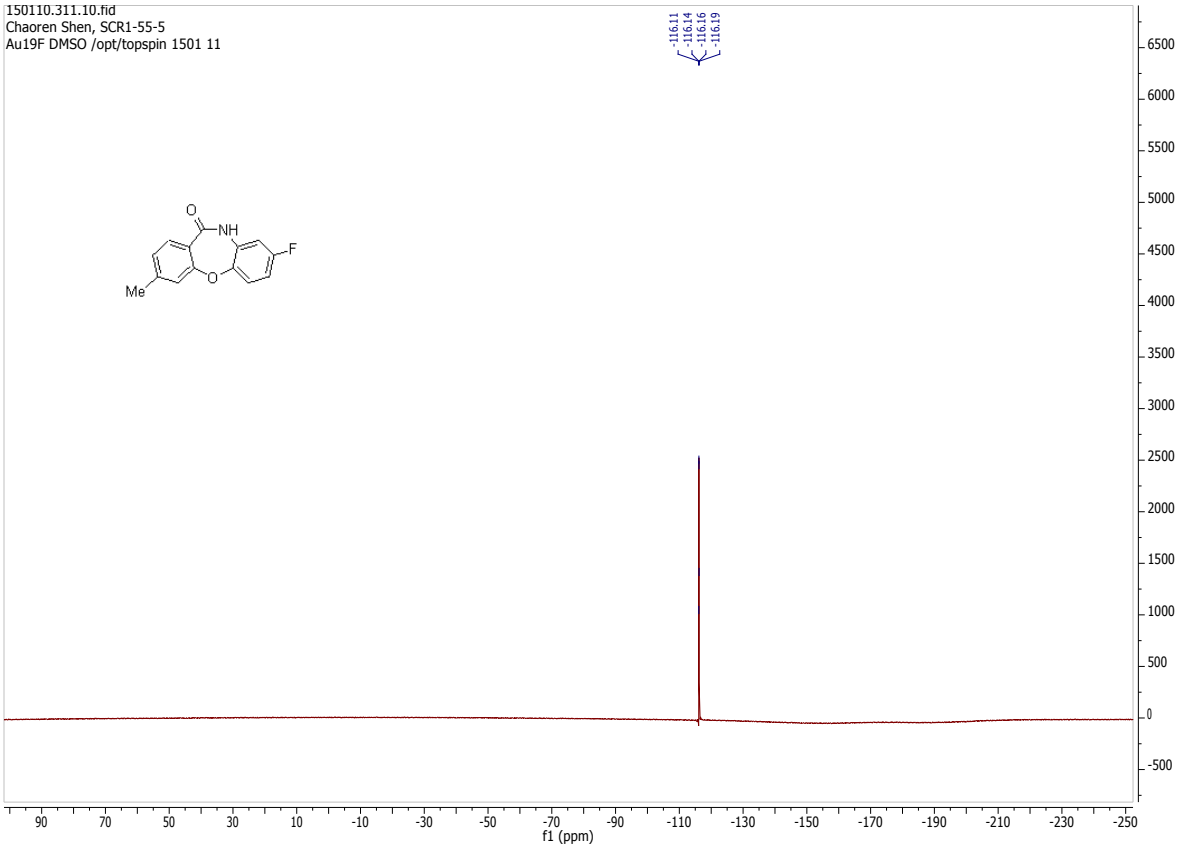
8-chloro-3-methyldibenzo[b,f][1,4]oxazepin-11(10H)-one (3z)

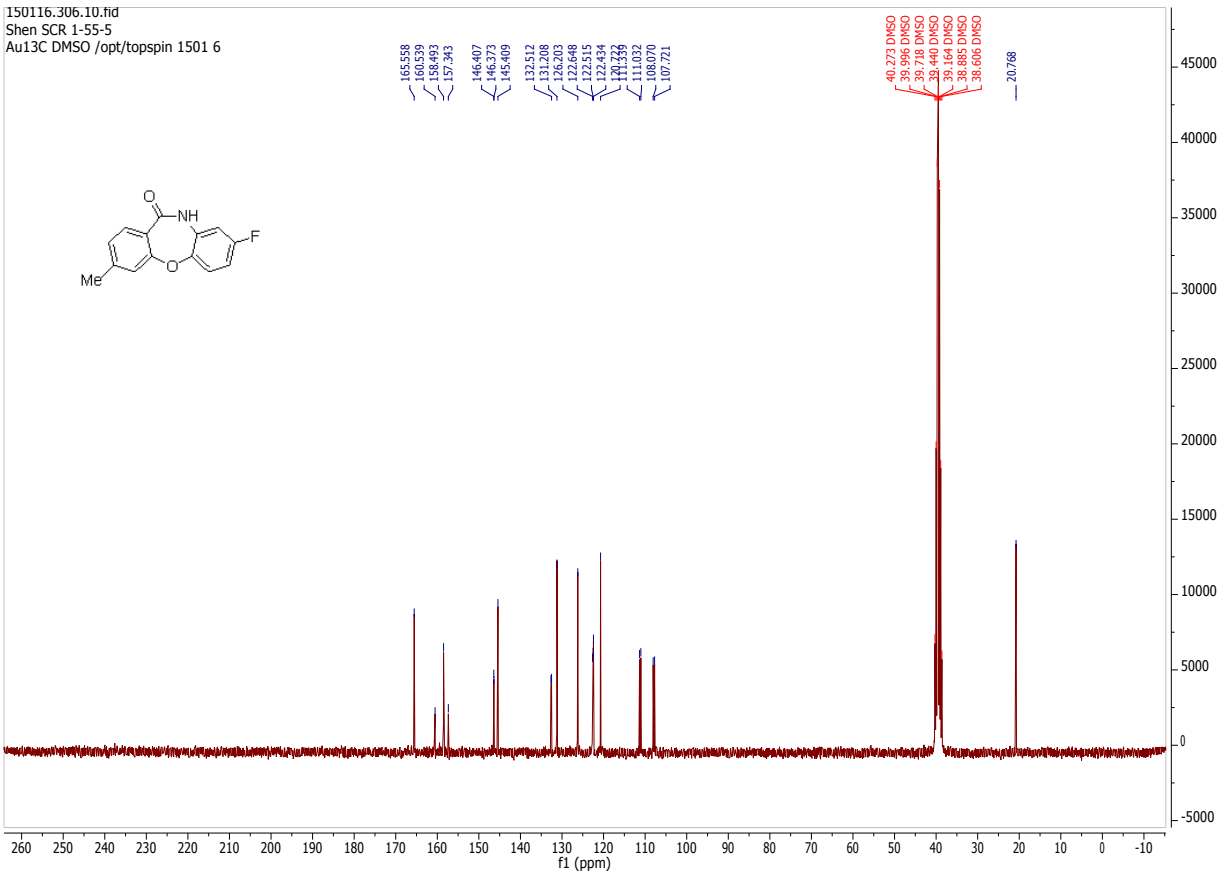




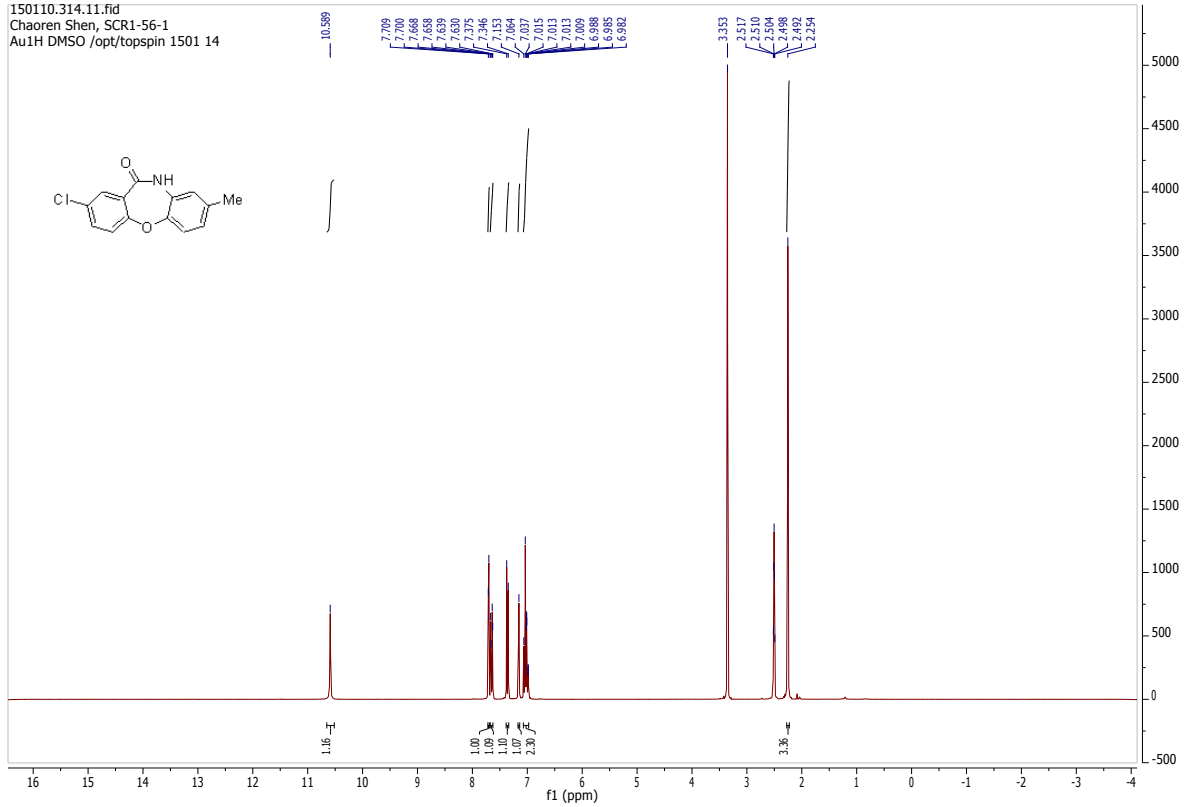
8-fluoro-3-methyldibenzo[b,f][1,4]oxazepin-11(10H)-one (3aa)

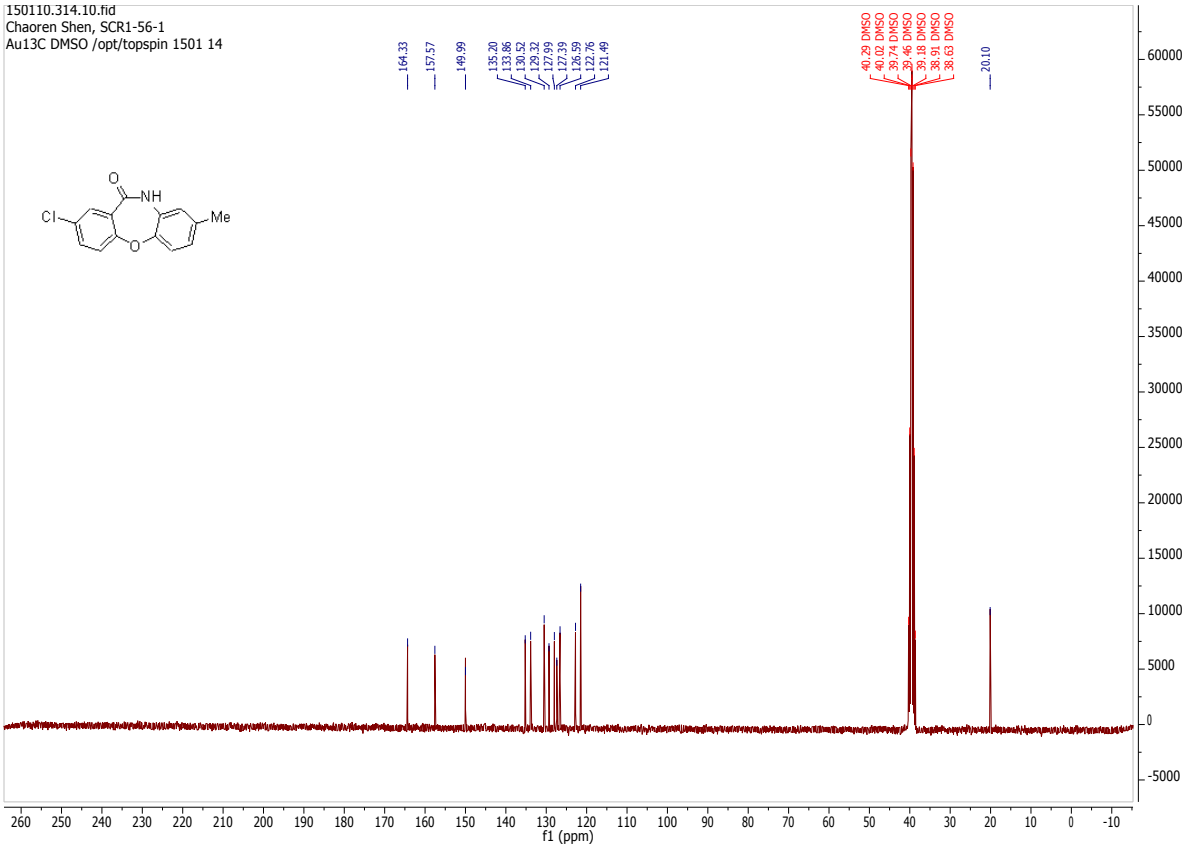



150110.311.10.fid
Chaoren Shen, SCR1-55-5
Au19F DMSO /opt/topspin 1501 11
-116.11
-116.14
-116.16
-116.19
O
NH
F
Me
O
f1 (ppm)

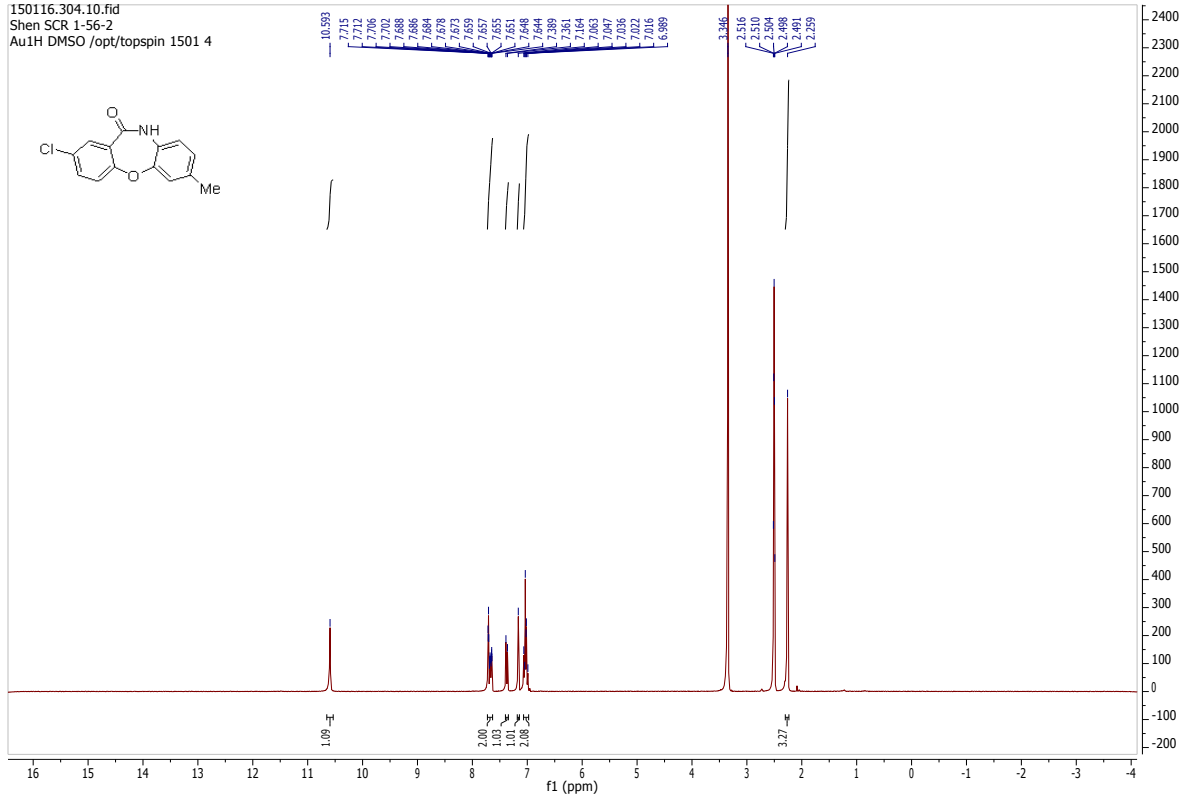

150116.306.10.fid
Shen SCR 1-55-5
Au13C DMSO /opt/topspin 1501 6
165.558
160.539
158.493
157.343
146.407
146.373
145.409
132.512
131.208
126.203
122.648
122.515
122.434
111.032
108.070
107.721
40.273 DMSO
39.996 DMSO
39.718 DMSO
39.440 DMSO
39.164 DMSO
38.885 DMSO
38.606 DMSO
20.768
O
NH
F
Me
O
f1 (ppm)

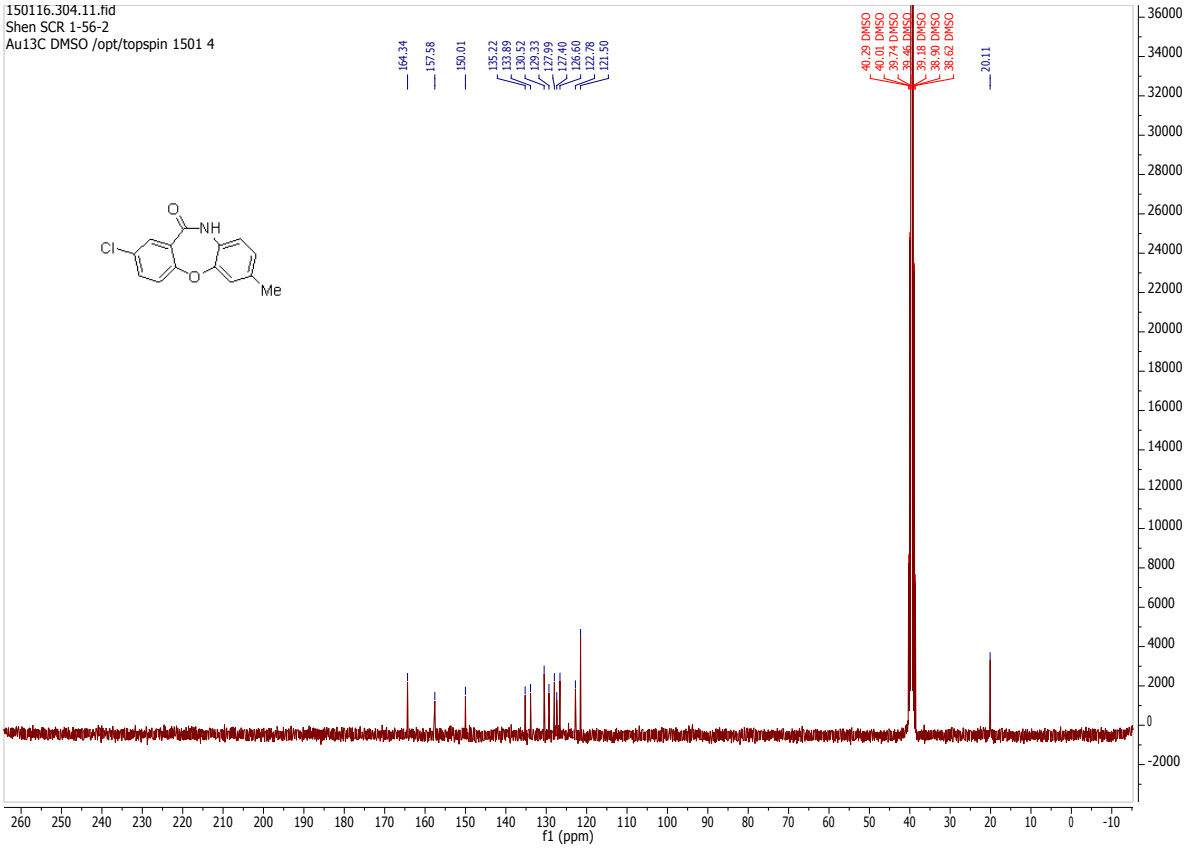
2-chloro-8-methyldibenzo[b,f][1,4]oxazepin-11(10H)-one (3ab)



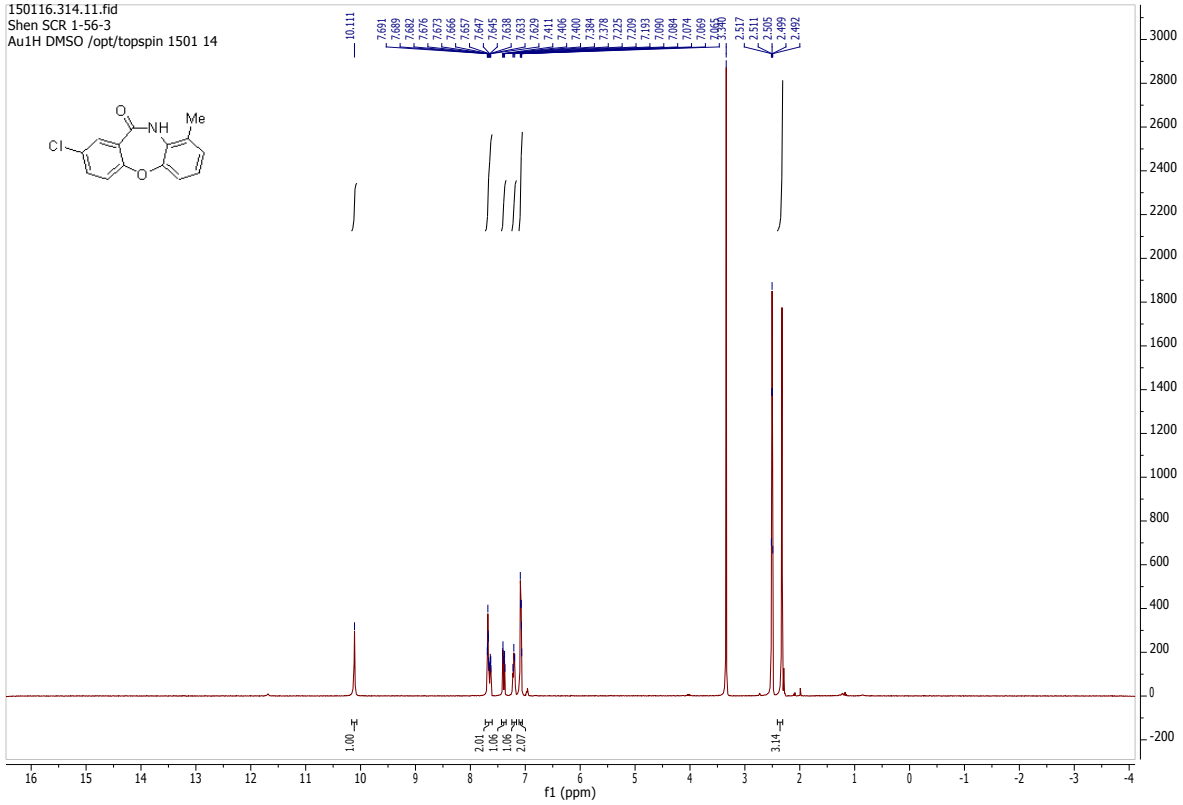


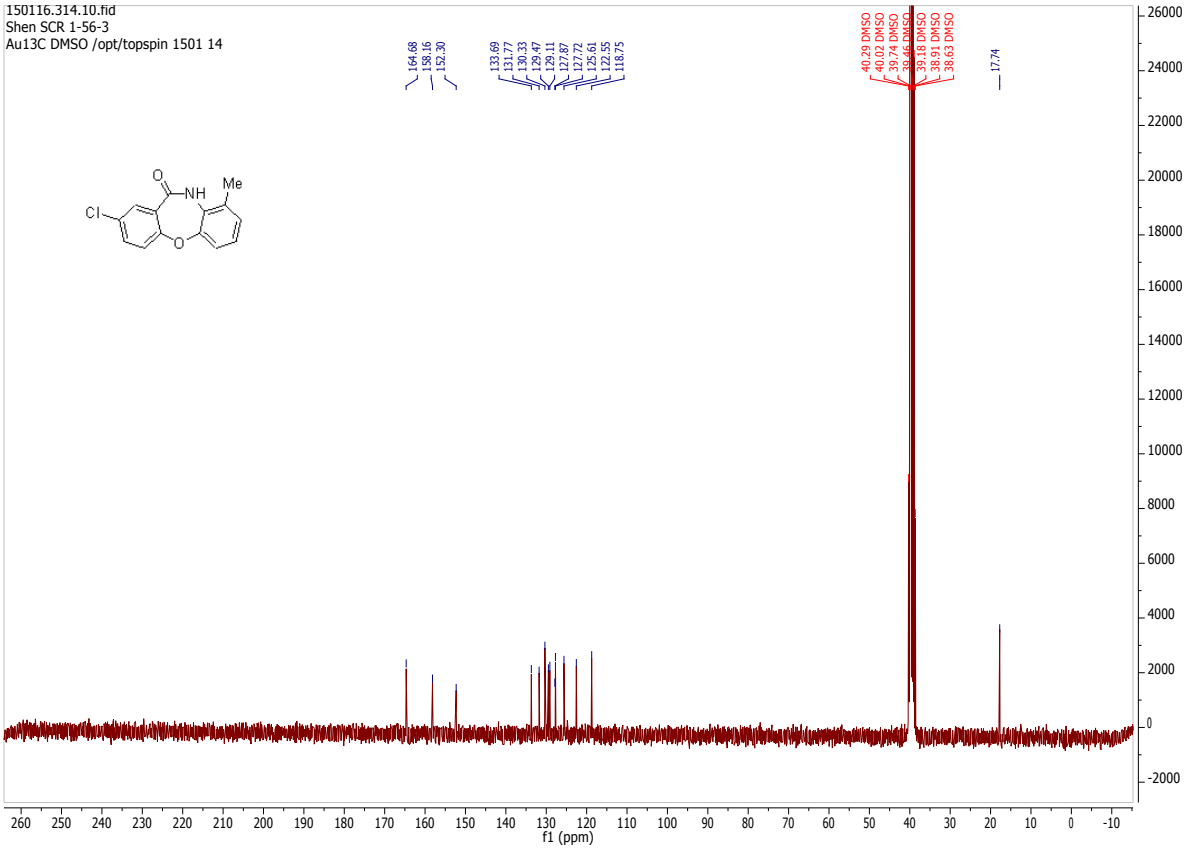
2-chloro-7-methyldibenzo[b,f][1,4]oxazepin-11(10H)-one (3ac)



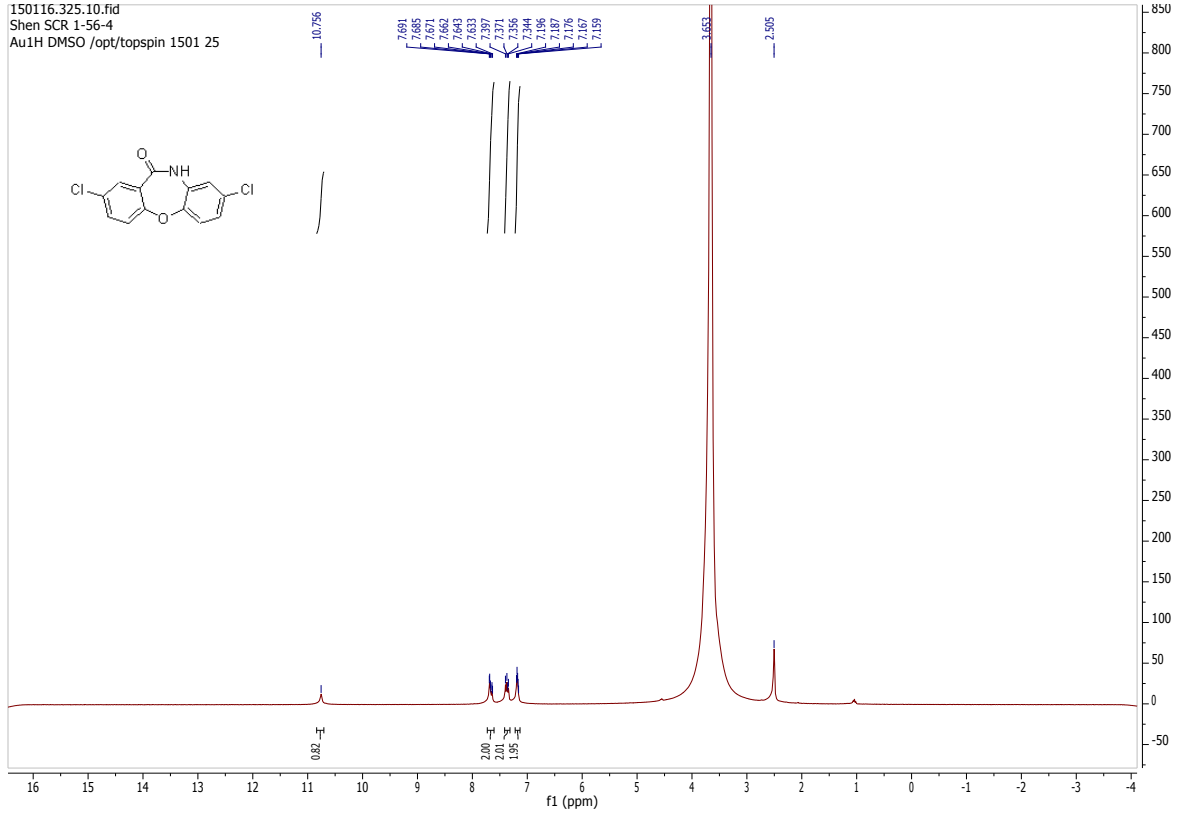


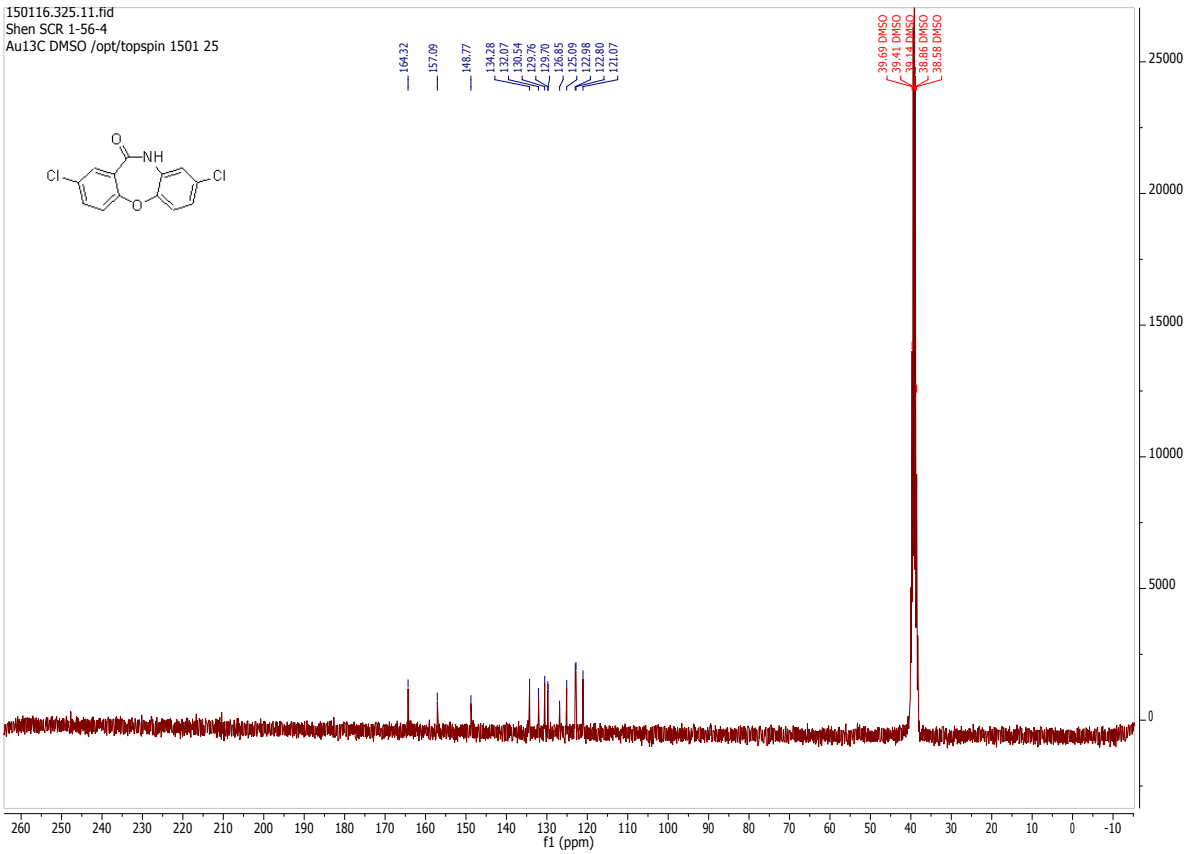
2-chloro-9-methyldibenzo[b,f][1,4]oxazepin-11(10H)-one (3ad)



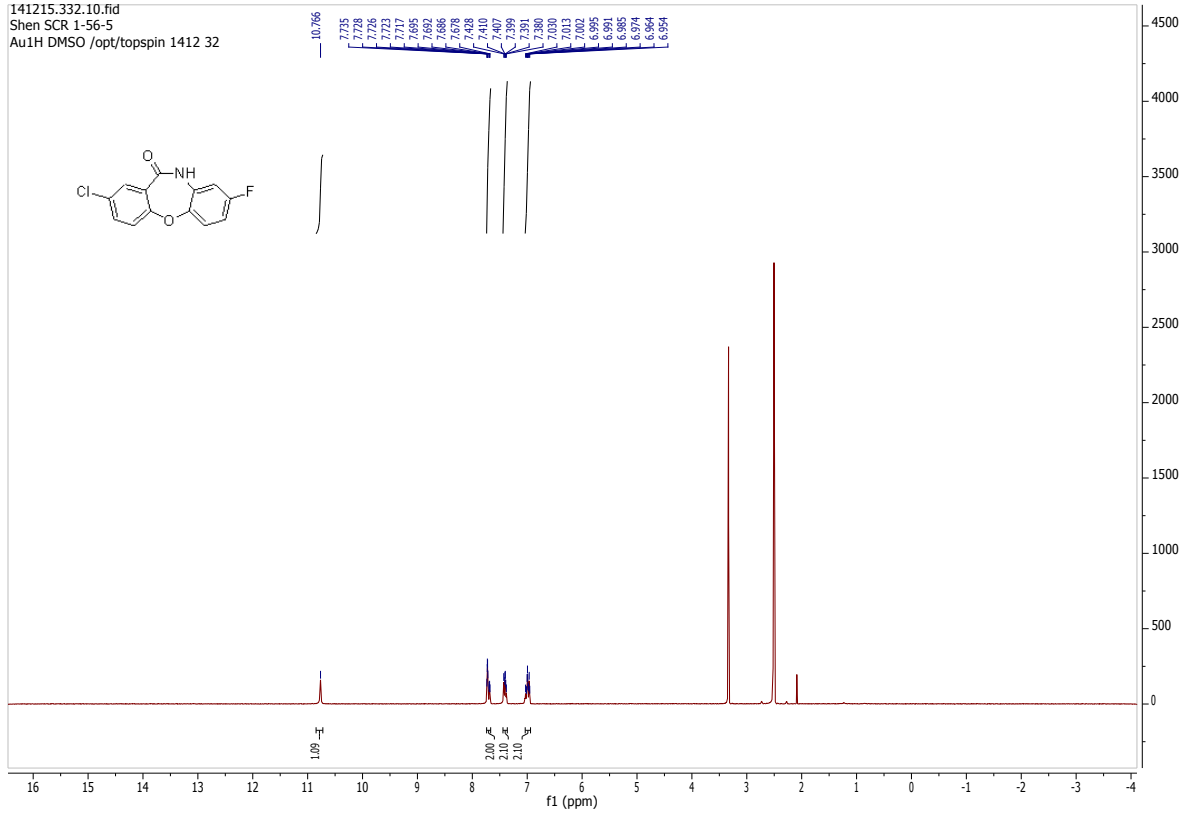


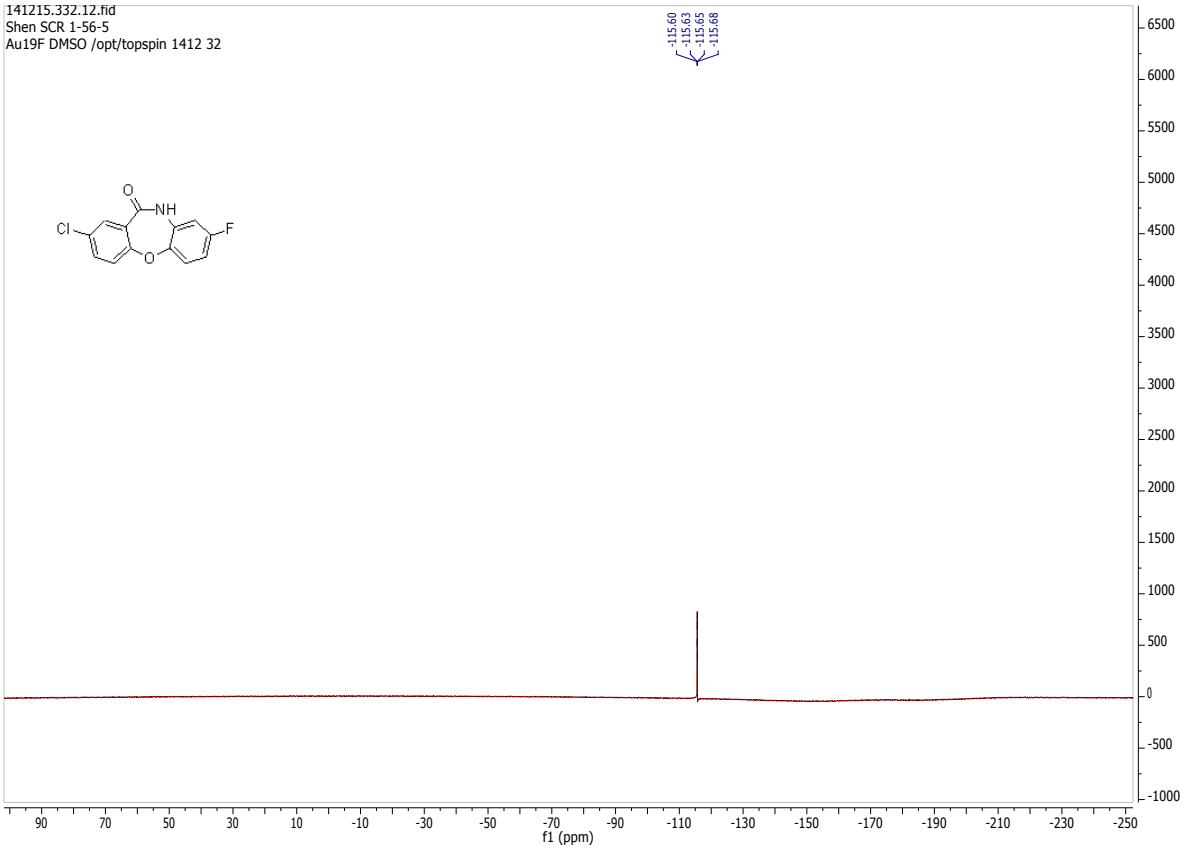
2,8-dichlorodibenzo[b,f][1,4]oxazepin-11(10H)-one (3ae)

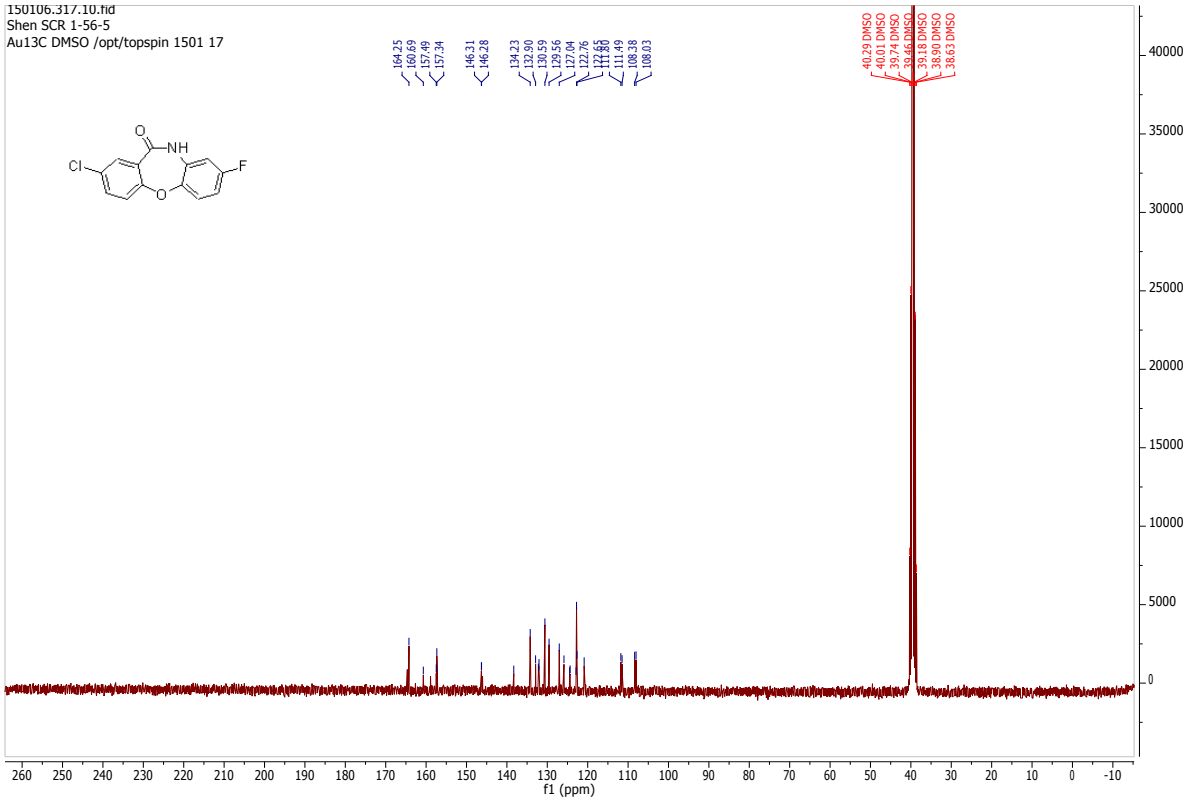




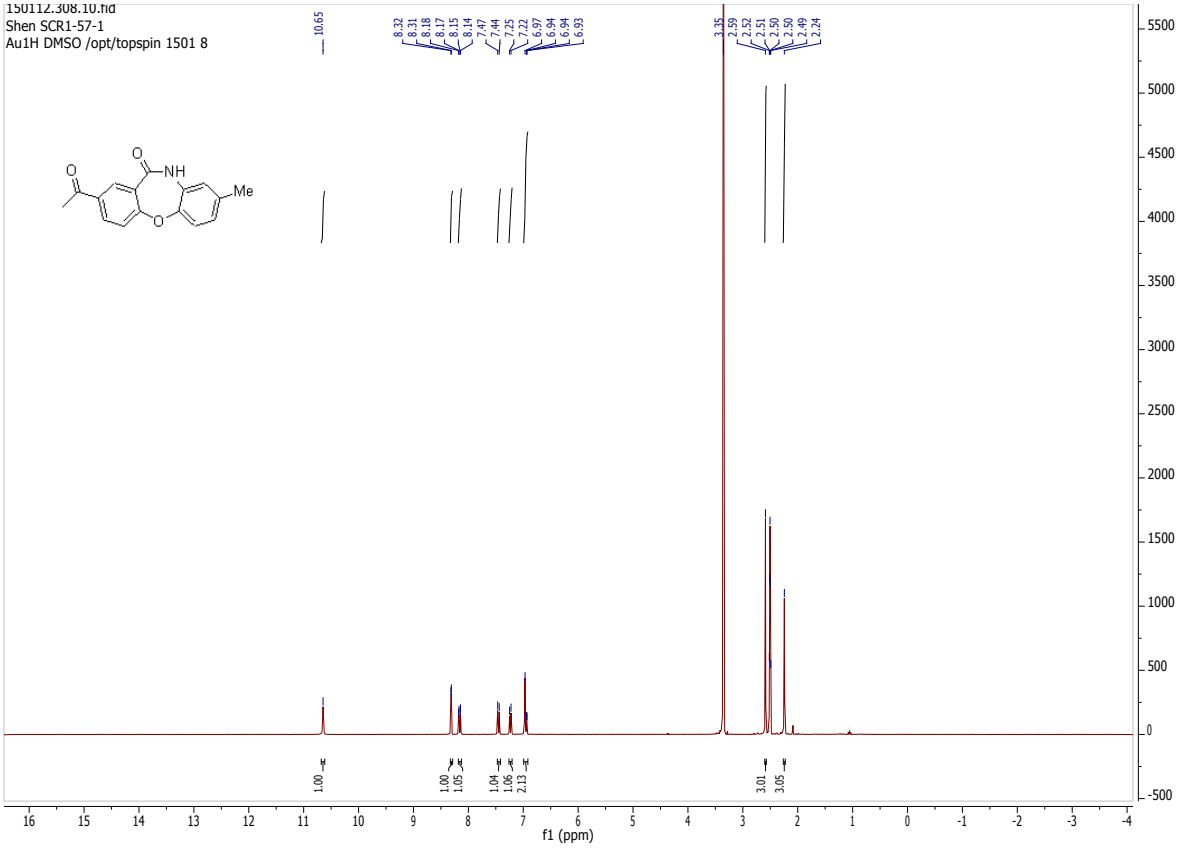
2-chloro-8-fluorodibenzo[b,f][1,4]oxazepin-11(10H)-one (3af)

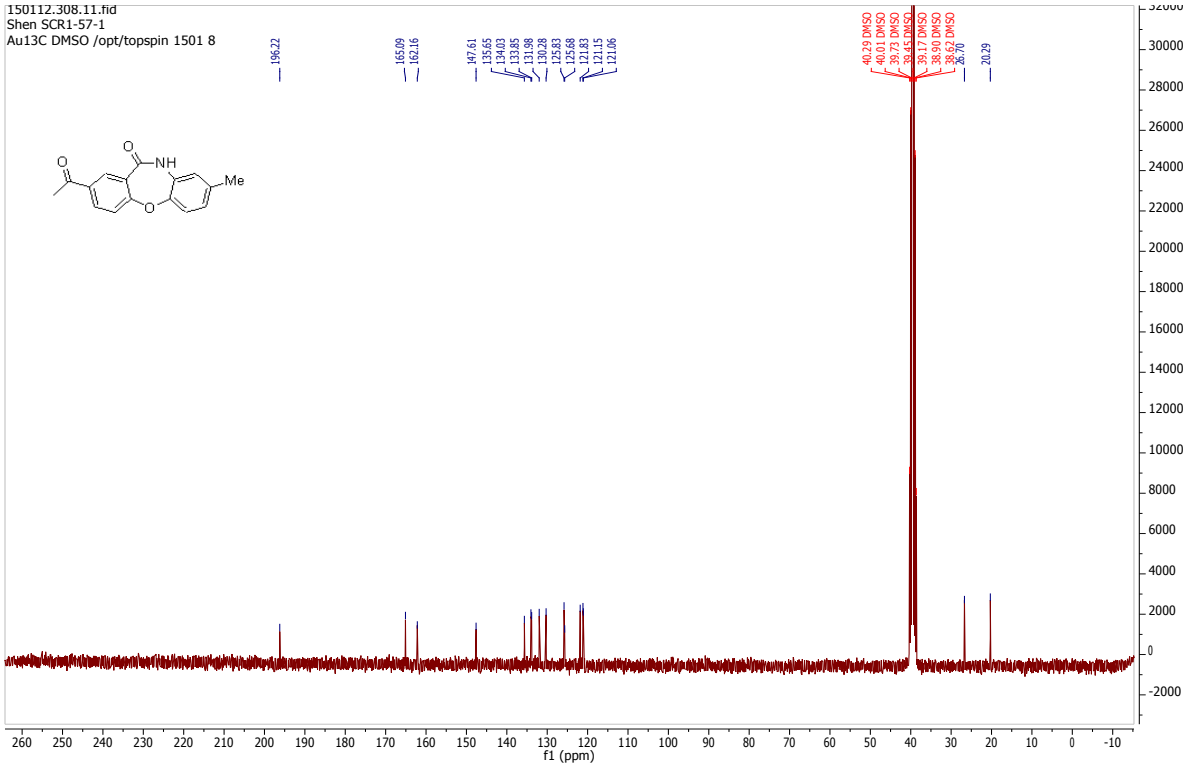




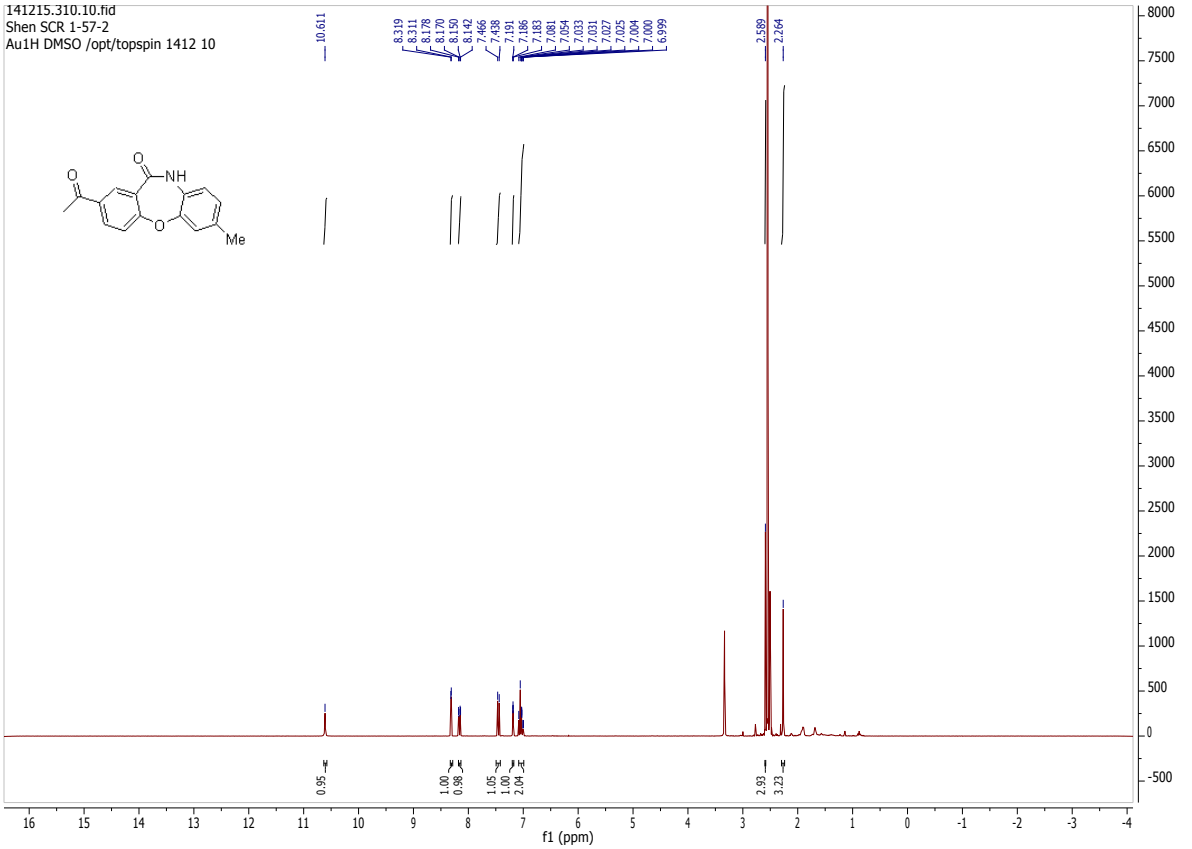


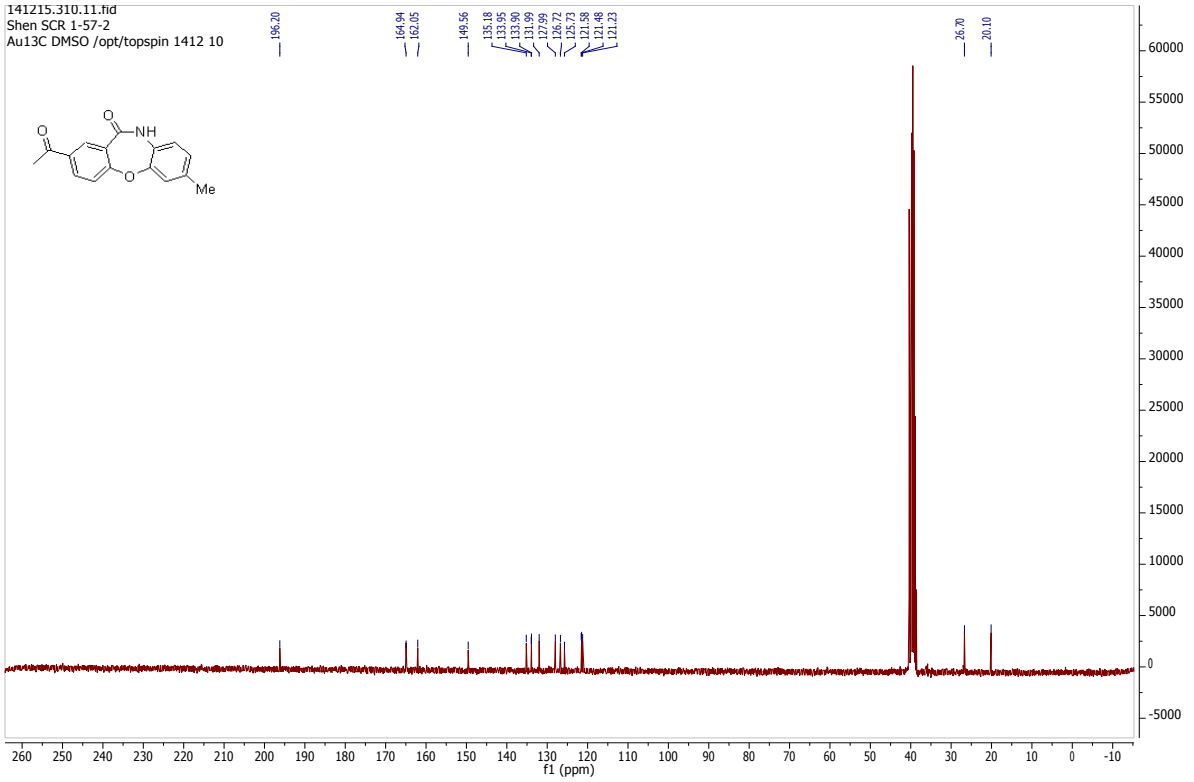
2-acetyl-8-methyldibenzo[b,f][1,4]oxazepin-11(10H)-one (3ag)



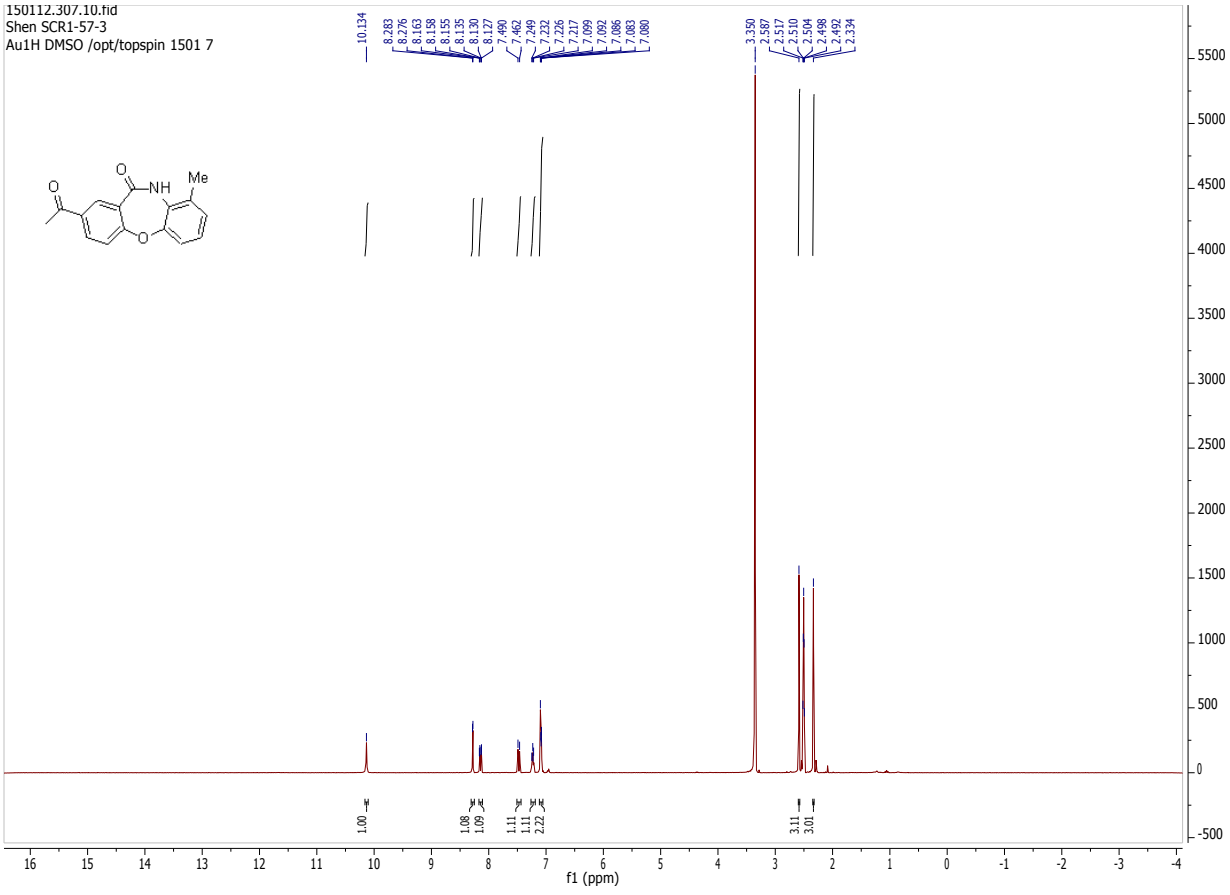


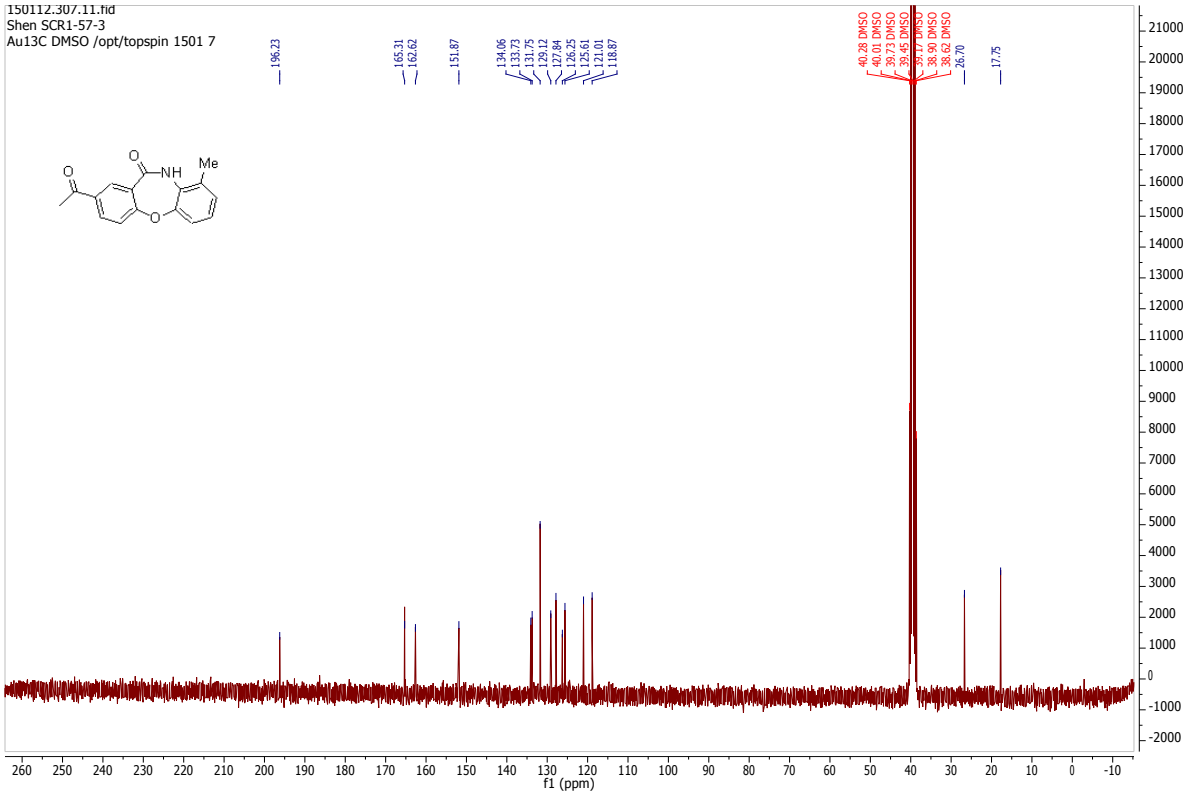
2-acetyl-7-methyldibenzo[b,f][1,4]oxazepin-11(10H)-one (3ah)



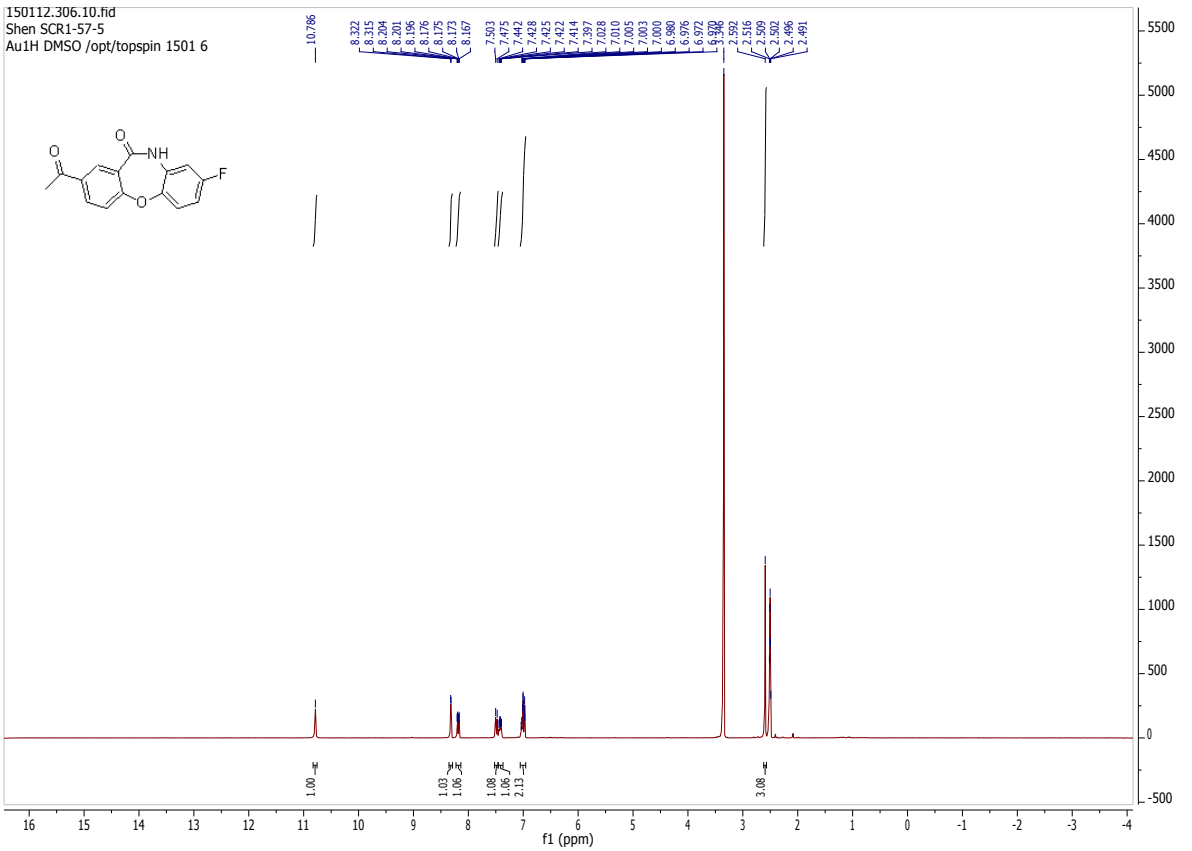


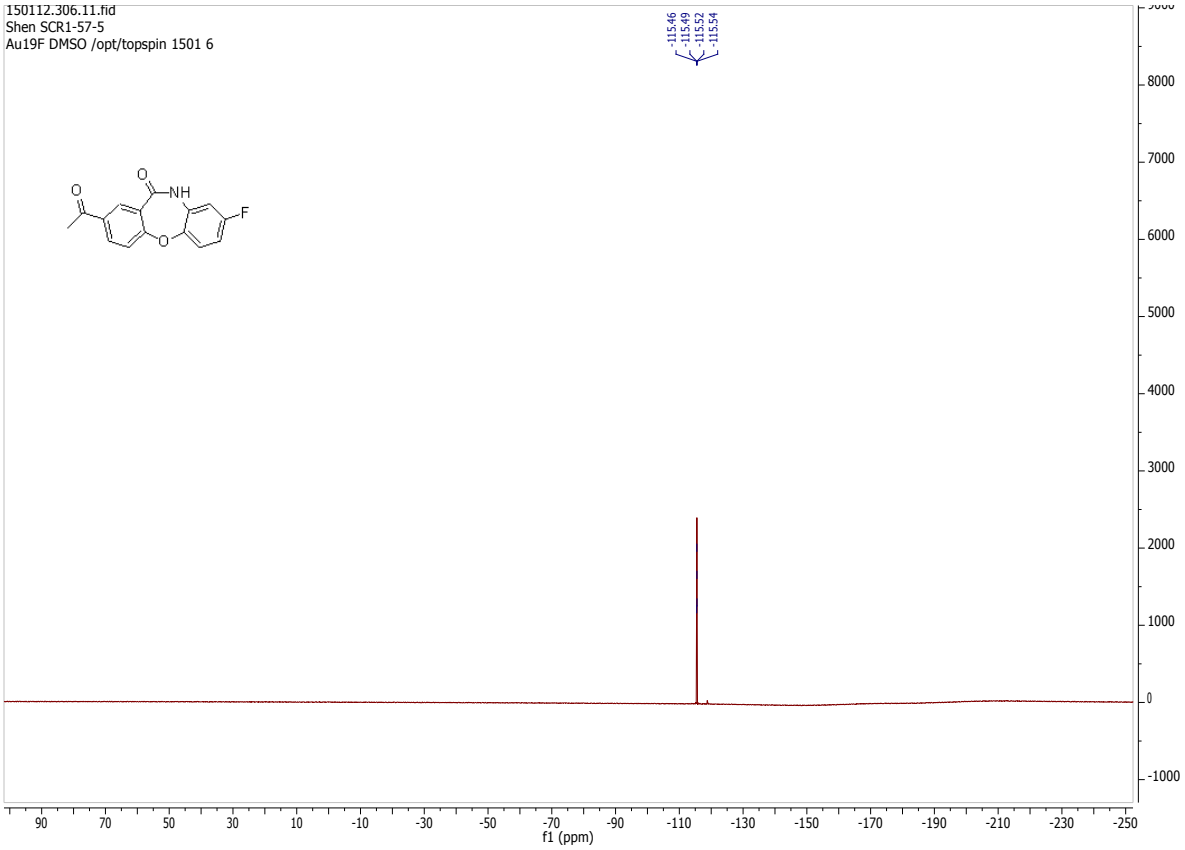
2-acetyl-9-methyldibenzo[b,f][1,4]oxazepin-11(10H)-one) (3ai)

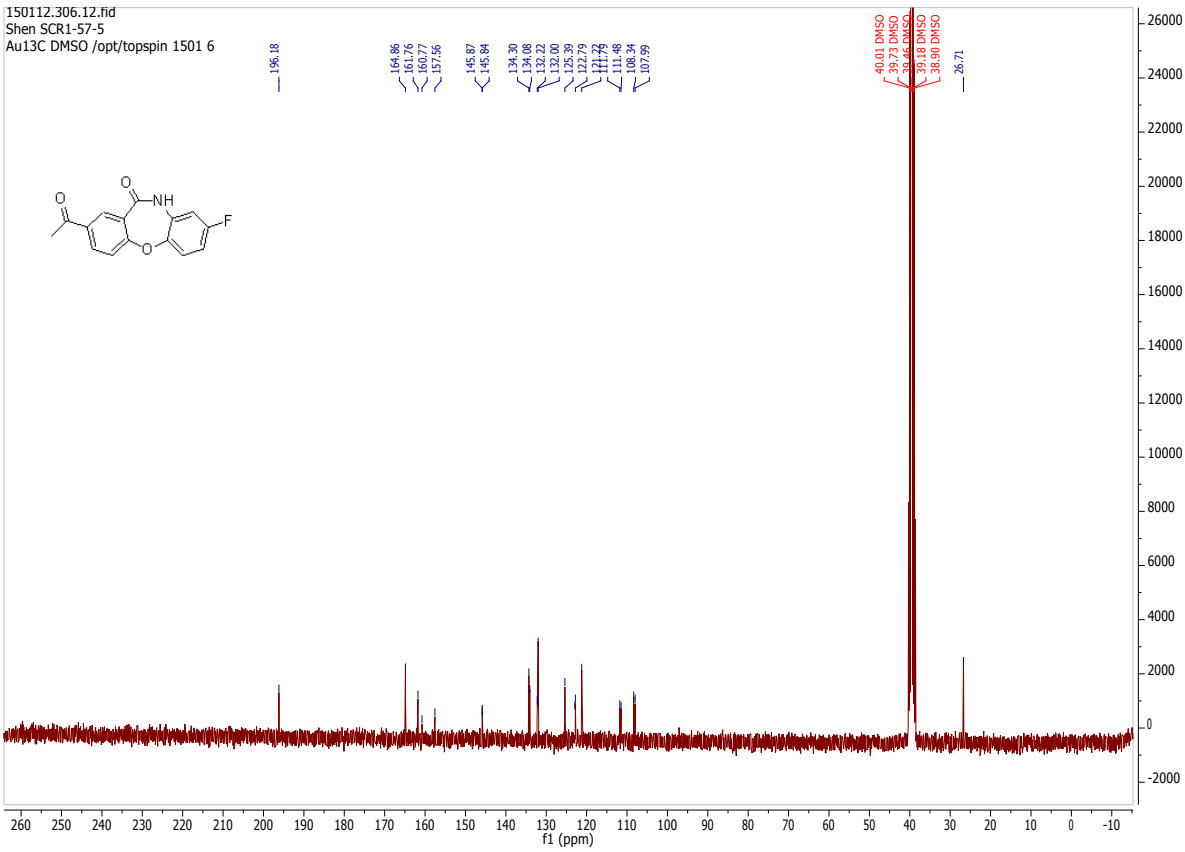




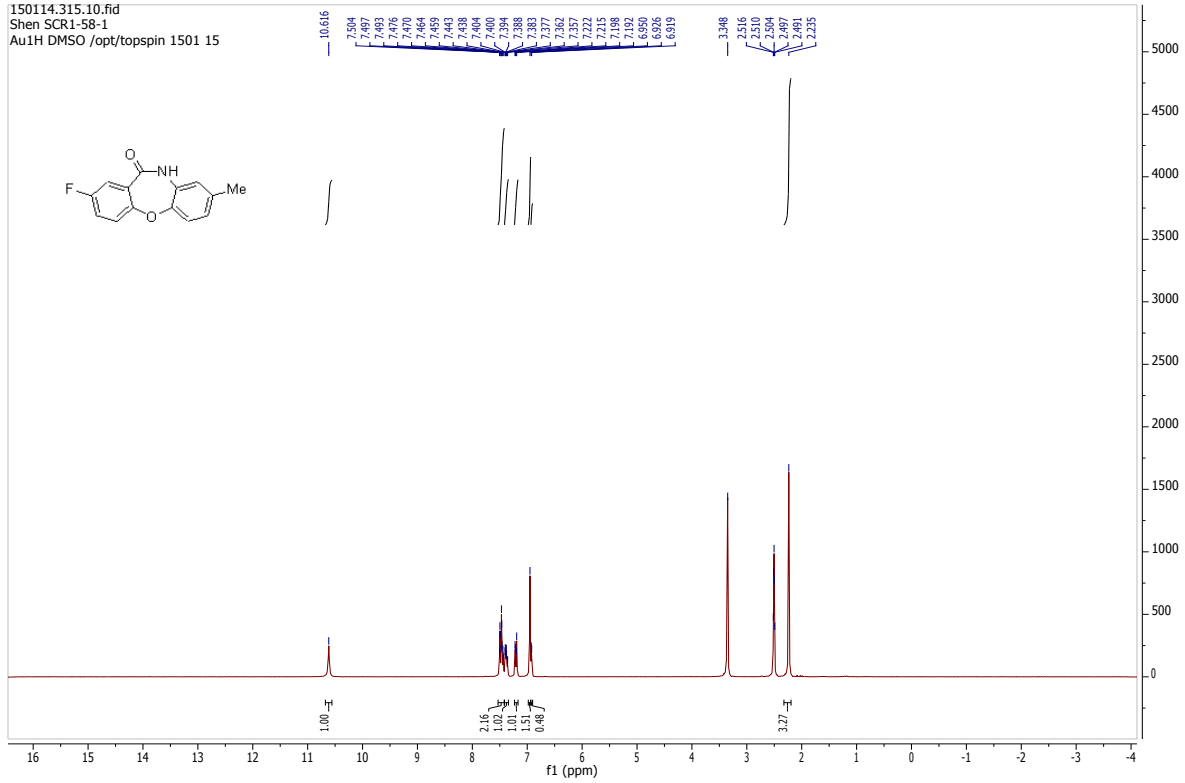
2-acetyl-8-fluorodibenzo[b,f][1,4]oxazepin-11(10H)-one (3ak)

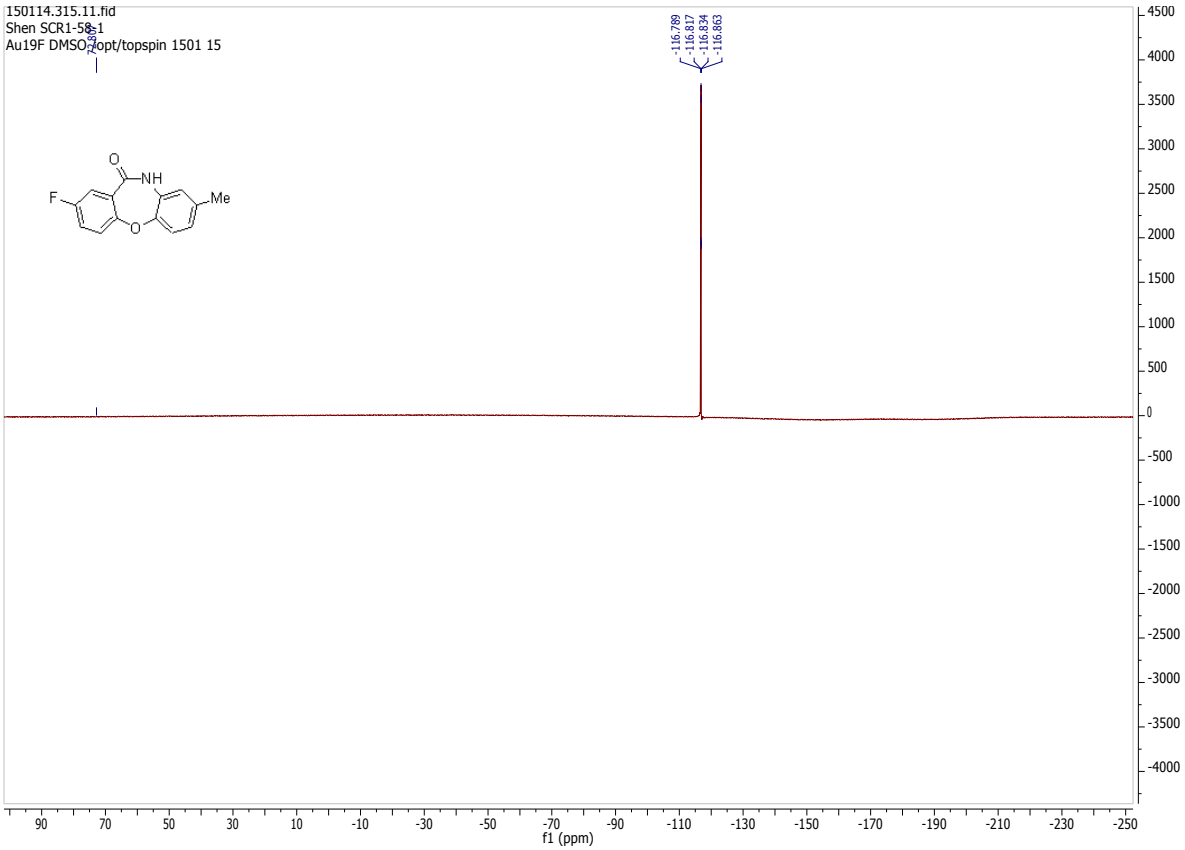


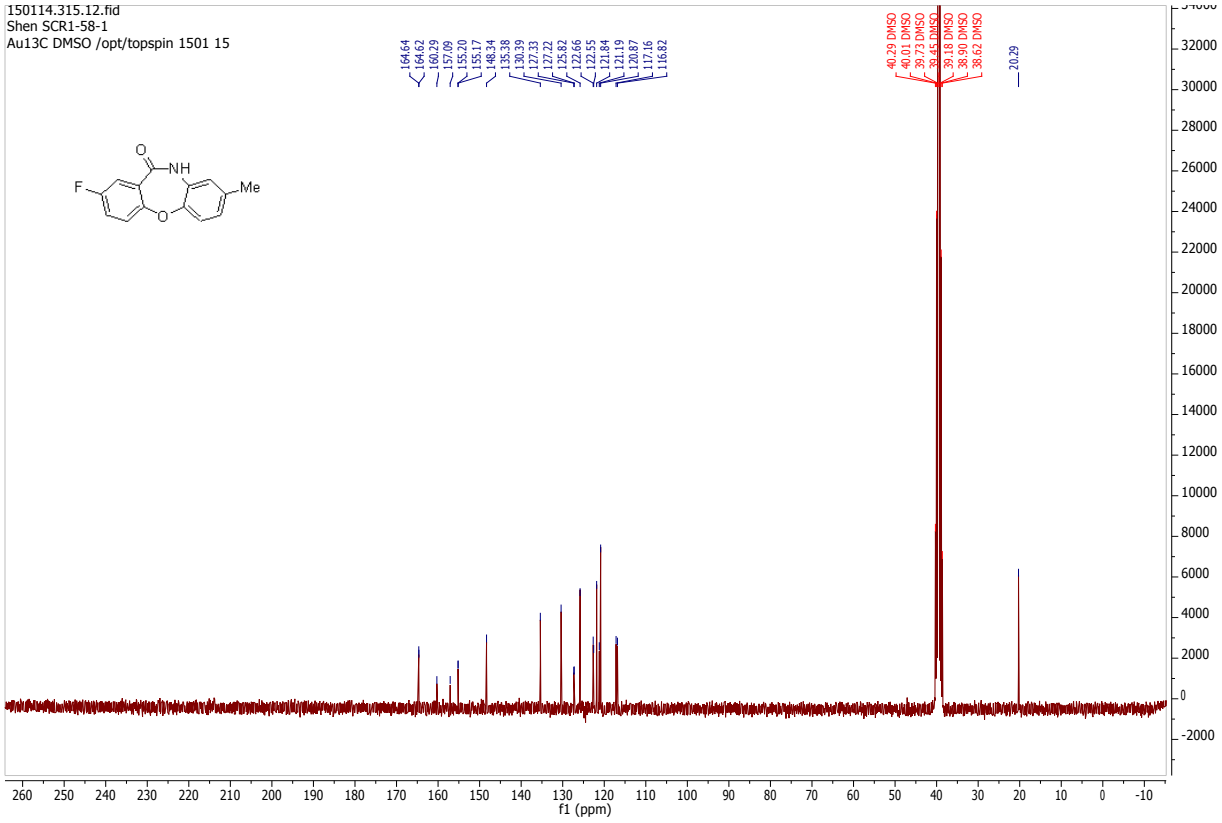

150112.306.11.fid
Shen SCR1-57-5
Au19F DMSO /opt/topspin 1501 6
-115.46
-115.49
-115.52
-115.54
O
NH
O
F
O
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
90 70 50 30 10 -10 -30 -50 -70 -90 -110 -130 -150 -170 -190 -210 -230 -250
f1 (ppm)


150112.306.12.fid
Shen SCR1-57-5
Au13C DMSO /opt/topspin 1501 6
196.18
164.86
161.76
160.77
157.56
145.87
145.84
134.30
134.08
132.22
132.00
125.39
122.79
121.22
111.79
111.48
108.34
107.99
40.01 DMSO
39.73 DMSO
39.46 DMSO
39.18 DMSO
38.90 DMSO
26.71
O
NH
O
F
O
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
260 250 240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

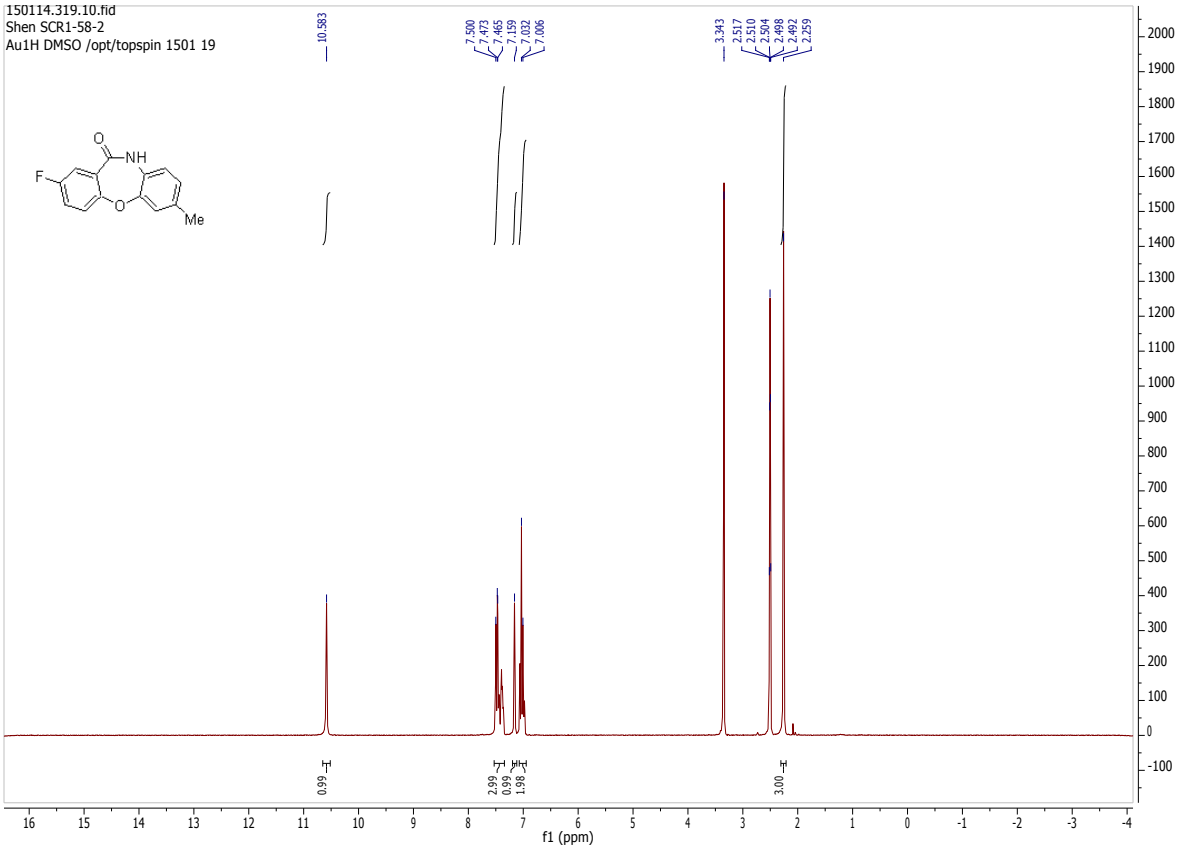
2-fluoro-8-methyldibenzo[b,f][1,4]oxazepin-11(10H)-one (3al)

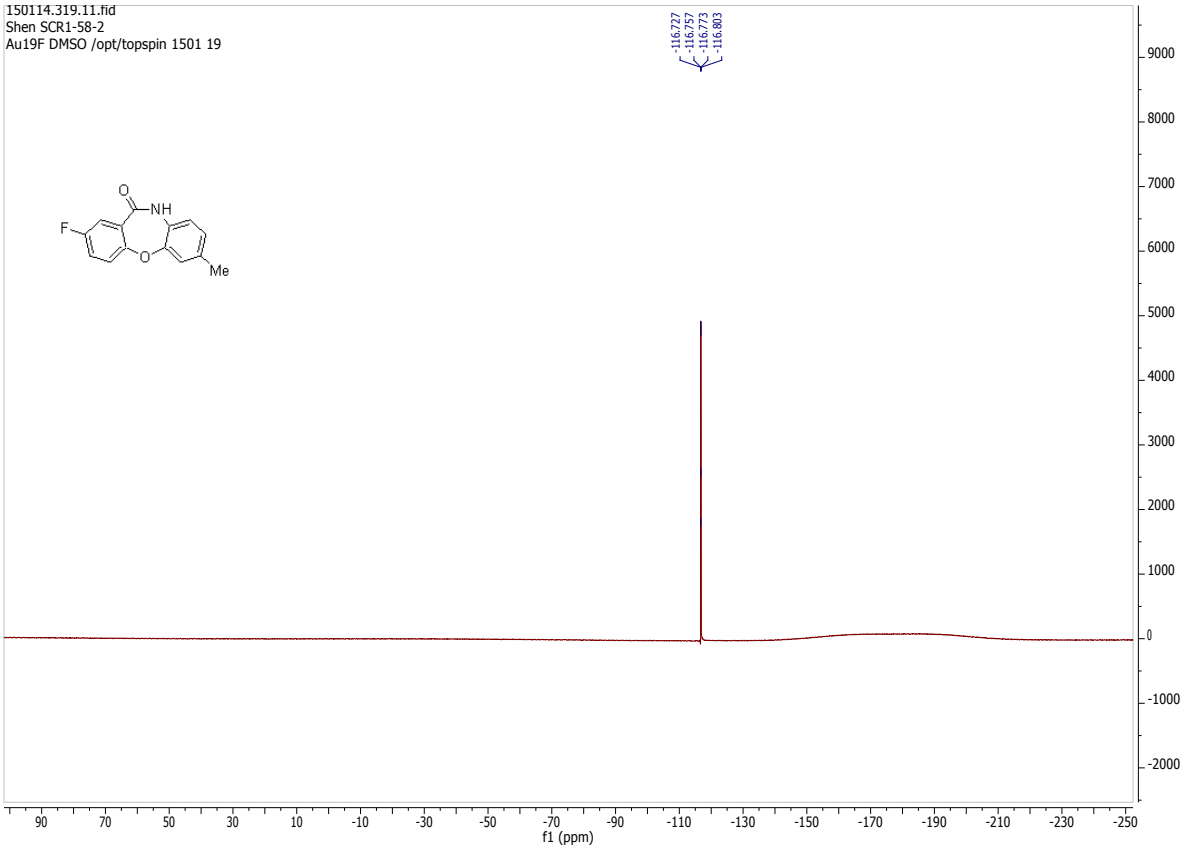


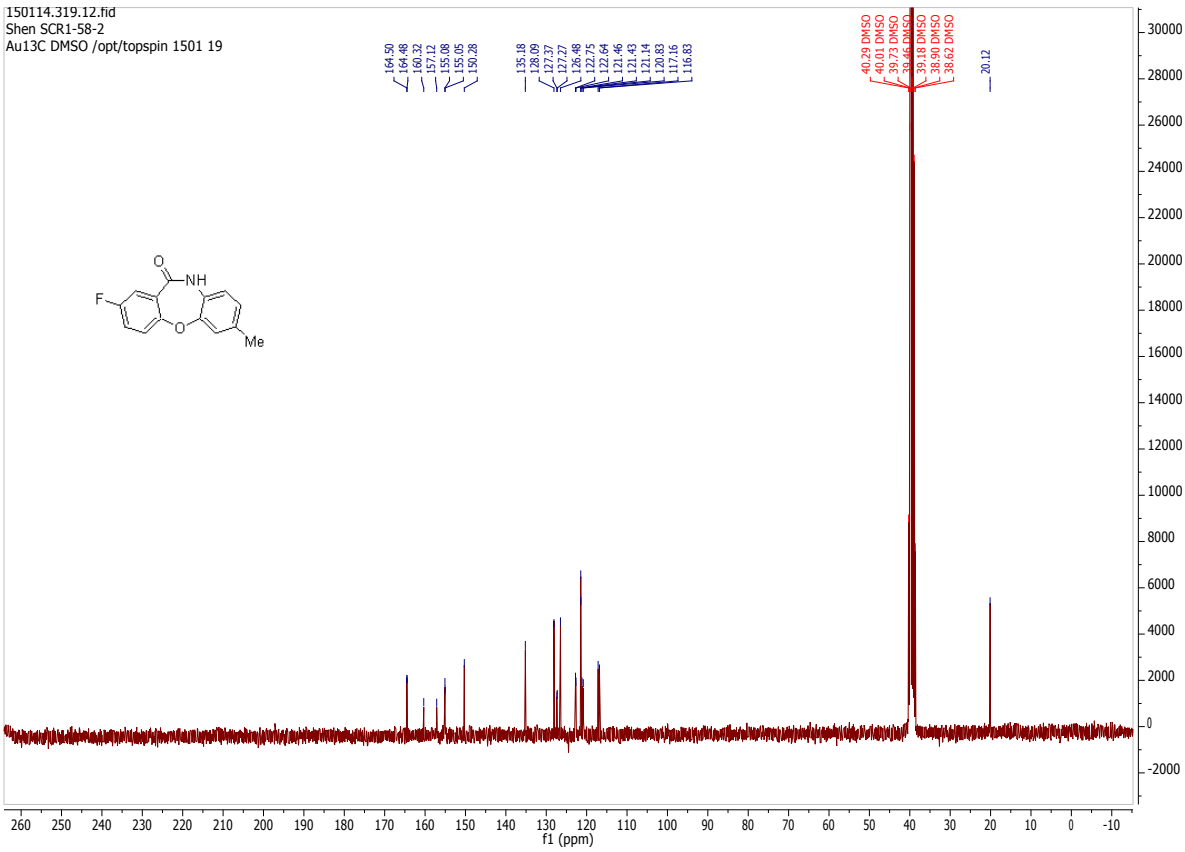




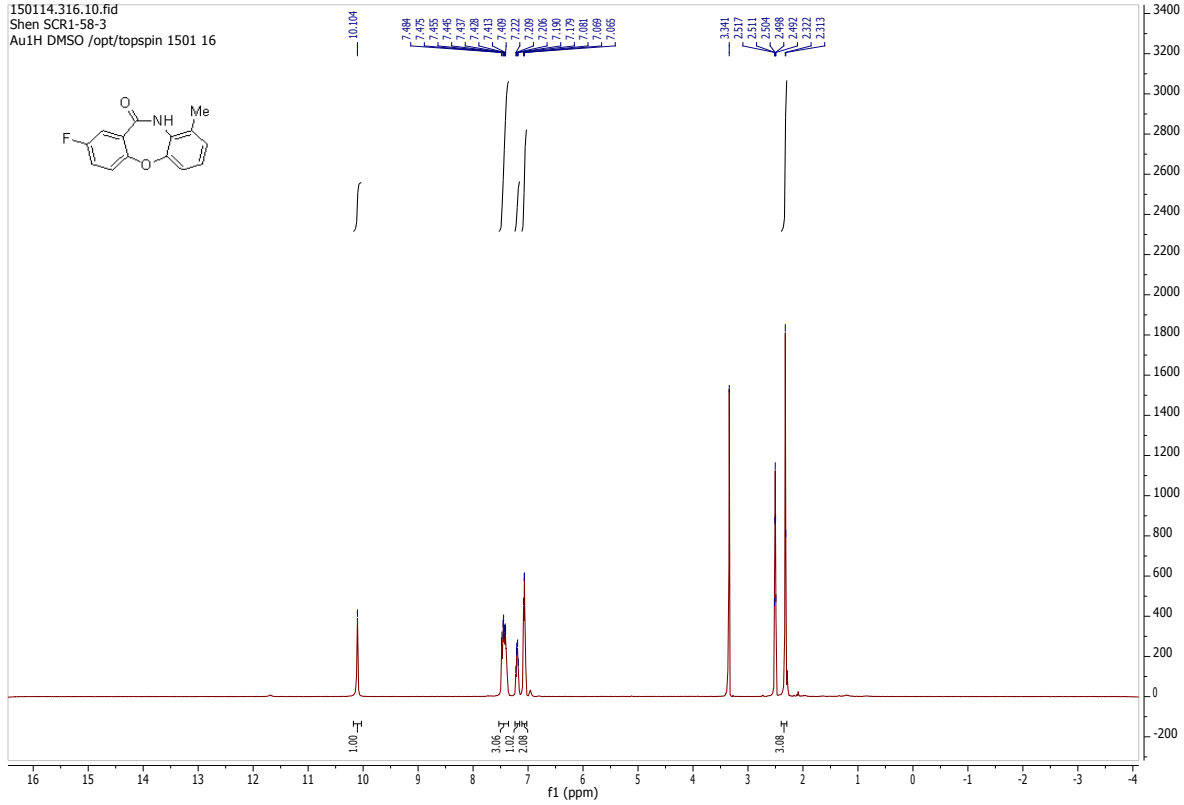
2-fluoro-7-methyldibenzo[b,f][1,4]oxazepin-11(10H)-one (3am)

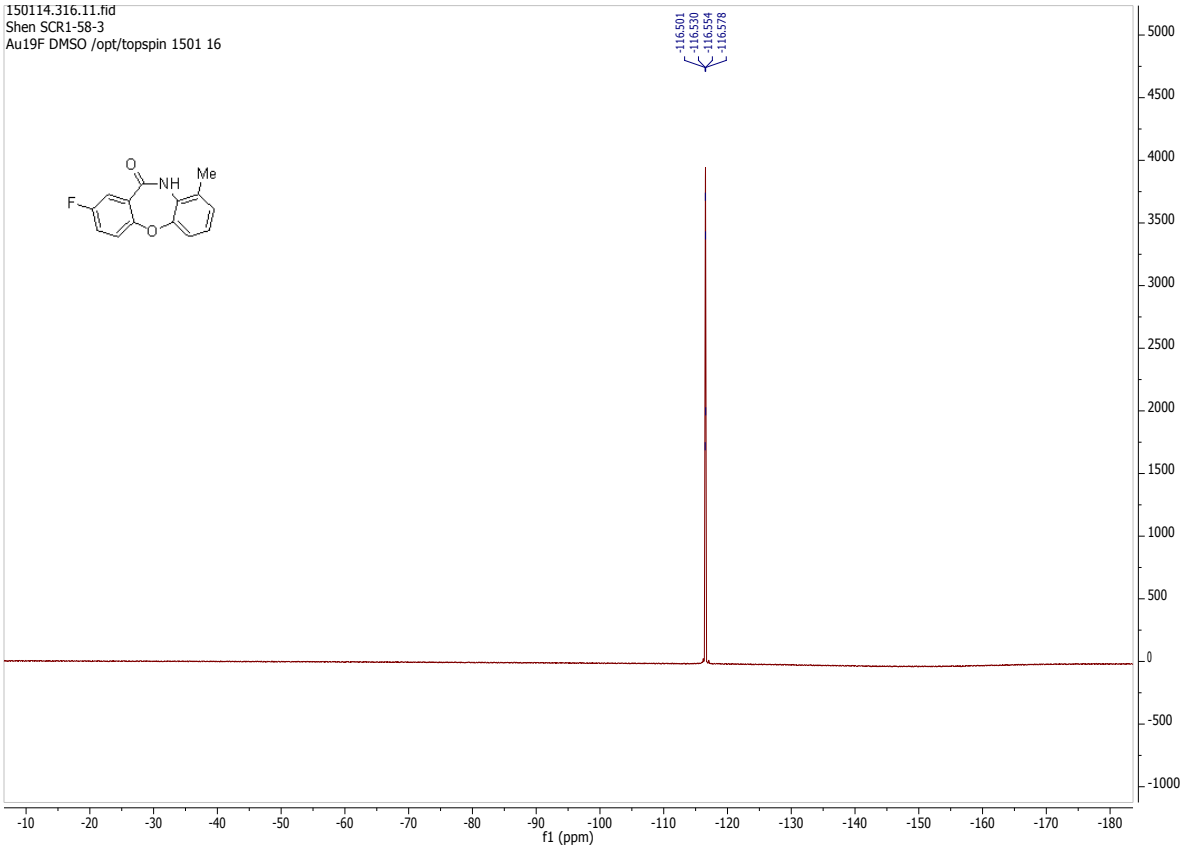


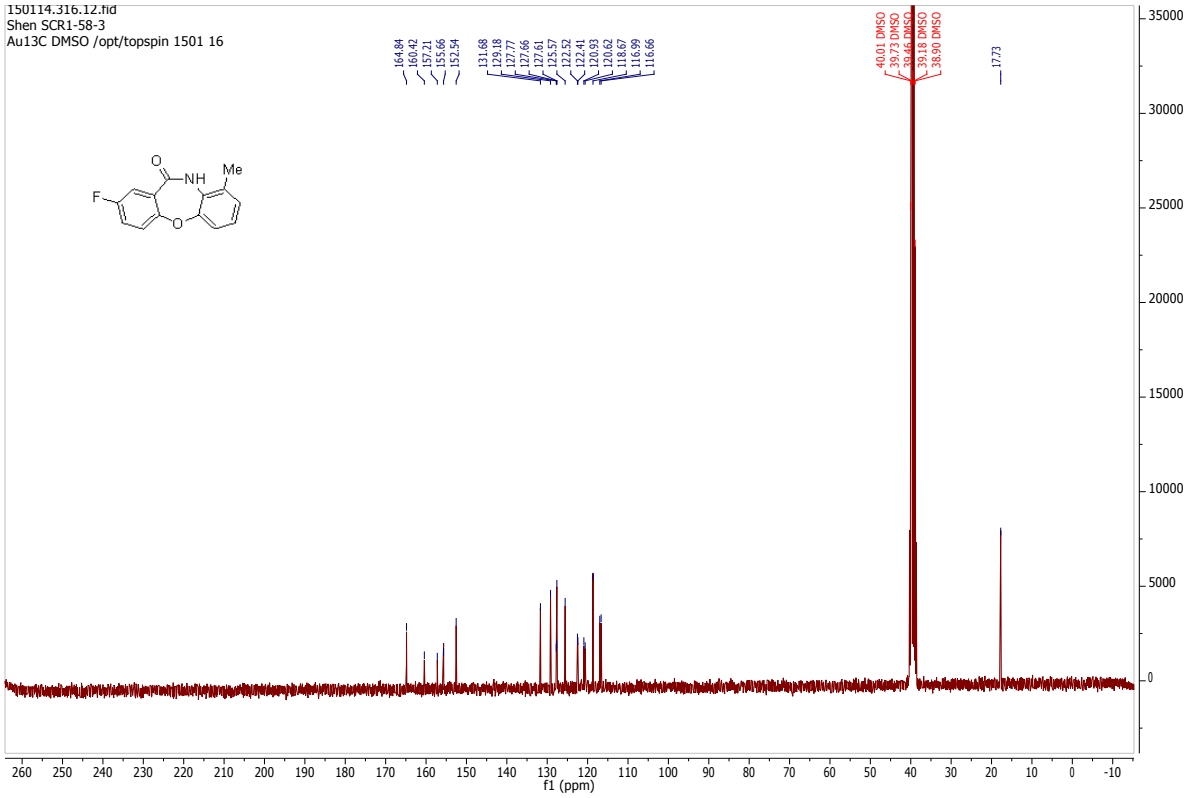

150114.319.11.fid
Shen SCR1-58-2
Au19F DMSO /opt/topspin 1501 19
-116.727
-116.757
-116.773
-116.803
O
NH
F
O
Me
f1 (ppm)


150114.319.12.fid
Shen SCR1-58-2
Au13C DMSO /opt/topspin 1501 19
164.50
164.48
160.32
157.12
155.08
155.05
150.28
135.18
128.09
127.37
127.27
126.48
122.75
122.64
121.46
121.43
121.14
120.83
117.16
116.83
40.29 DMSO
40.01 DMSO
39.73 DMSO
39.46 DMSO
39.18 DMSO
38.90 DMSO
38.62 DMSO
20.12
O
NH
F
O
Me
f1 (ppm)

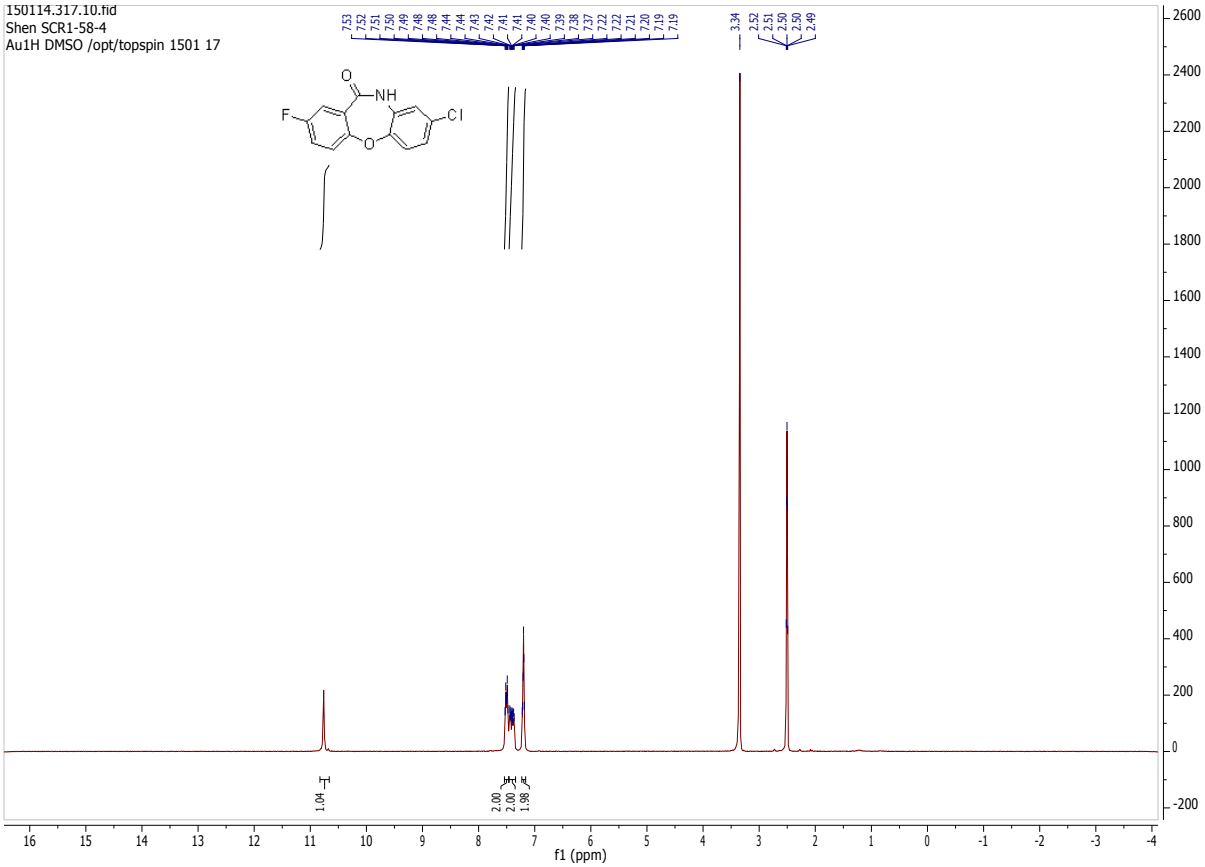
2-fluoro-9-methyldibenzo[b,f][1,4]oxazepin-11(10H)-one (3an)

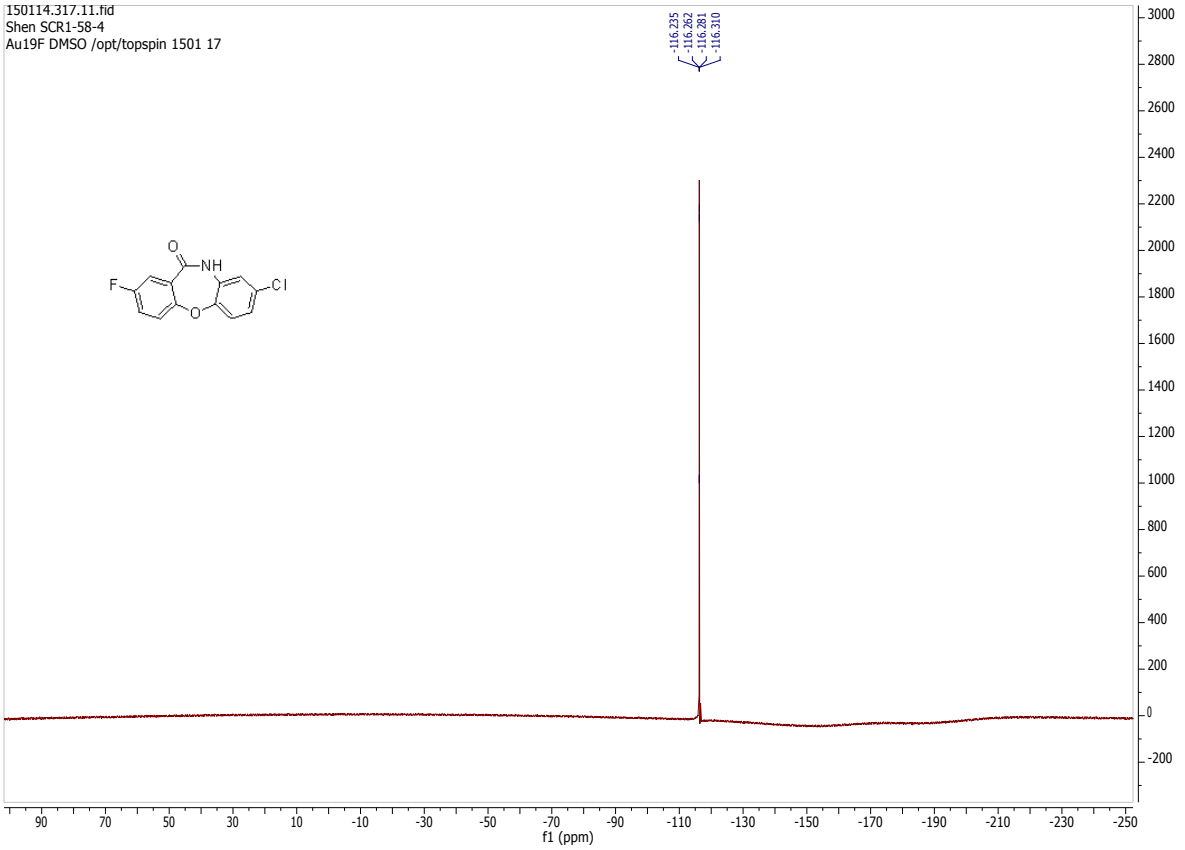


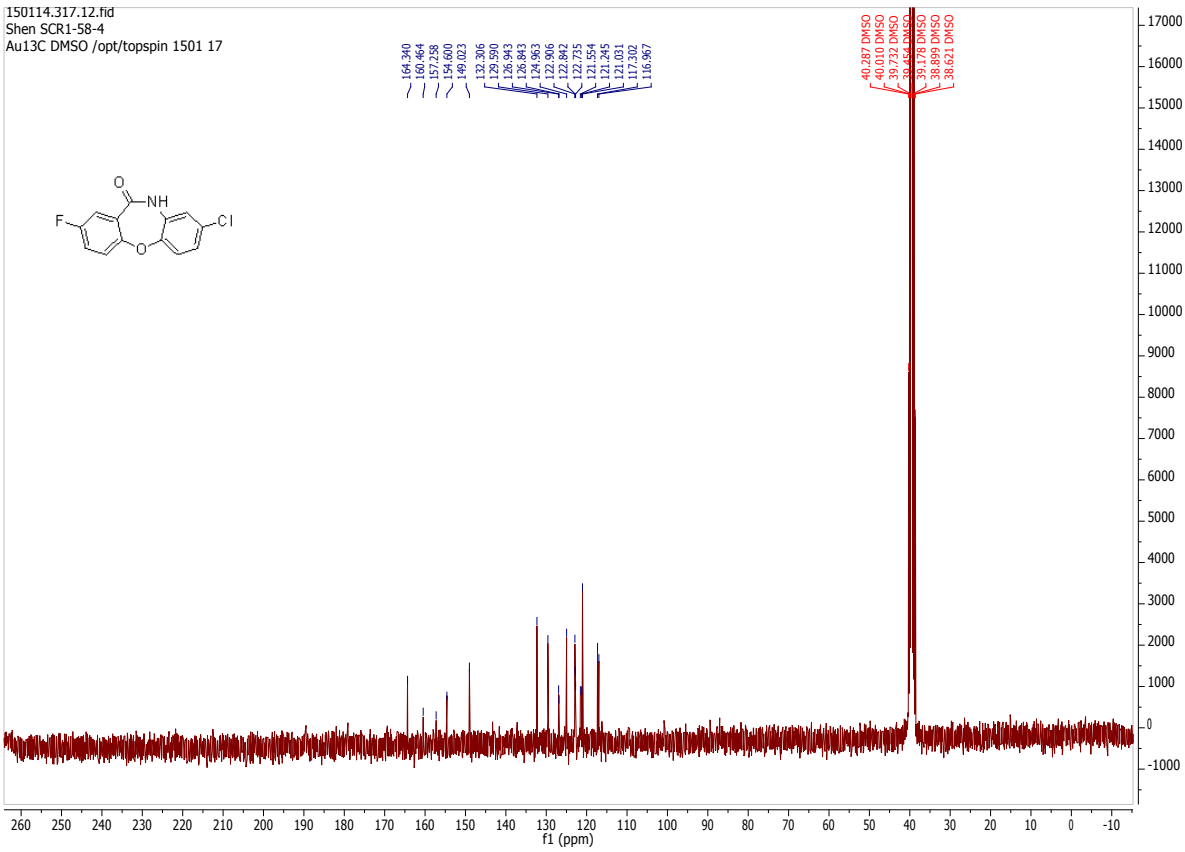




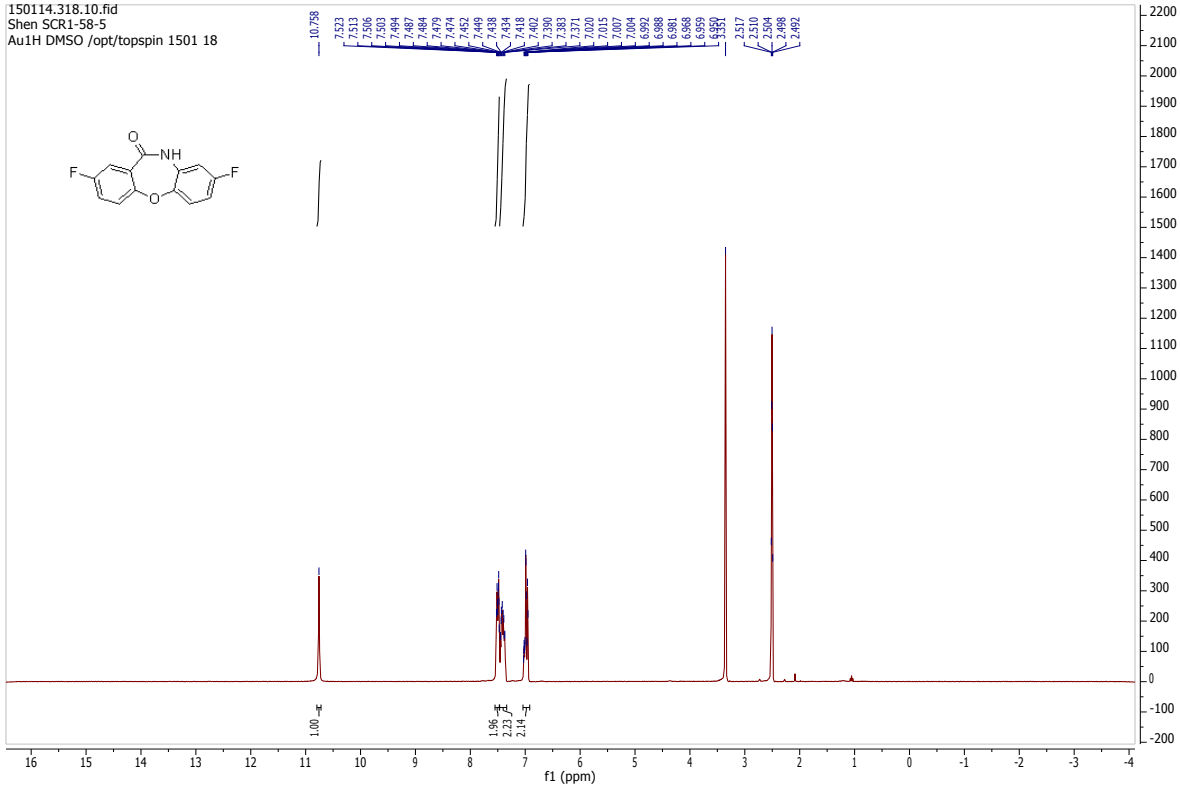
8-chloro-2-fluorodibenzo[b,f][1,4]oxazepin-11(10H)-one (3ao)

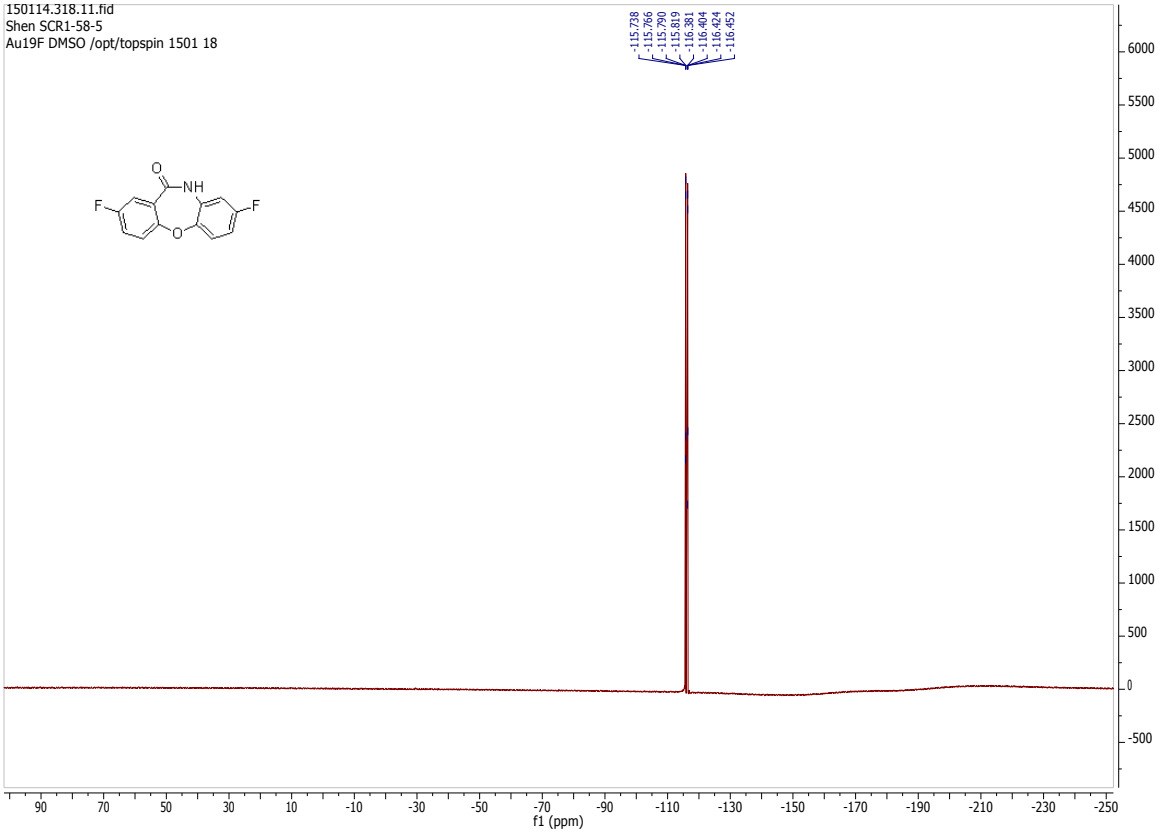


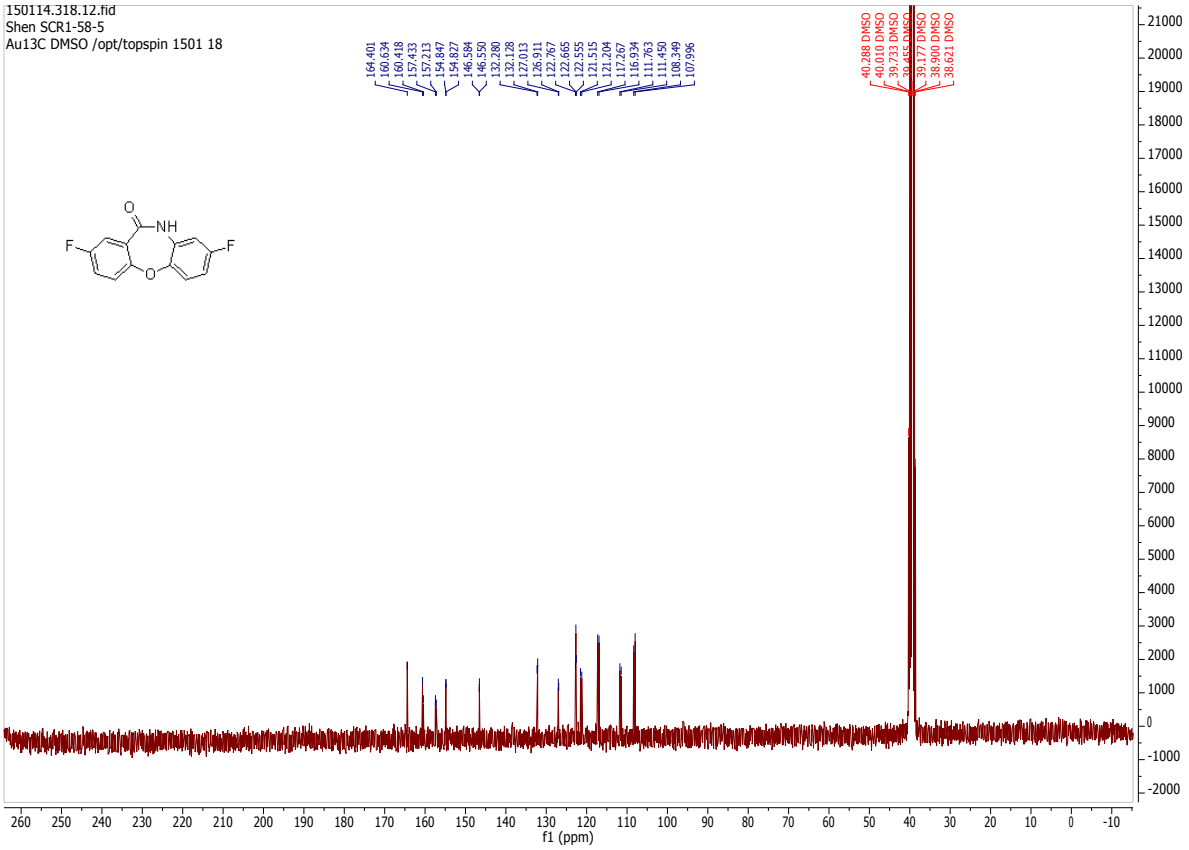

150114.317.11.fid
Shen SCR1-58-4
Au19F DMSO /opt/topspin 1501 17
-116.235
-116.262
-116.281
-116.310
O
NH
F
Cl
O
f1 (ppm)

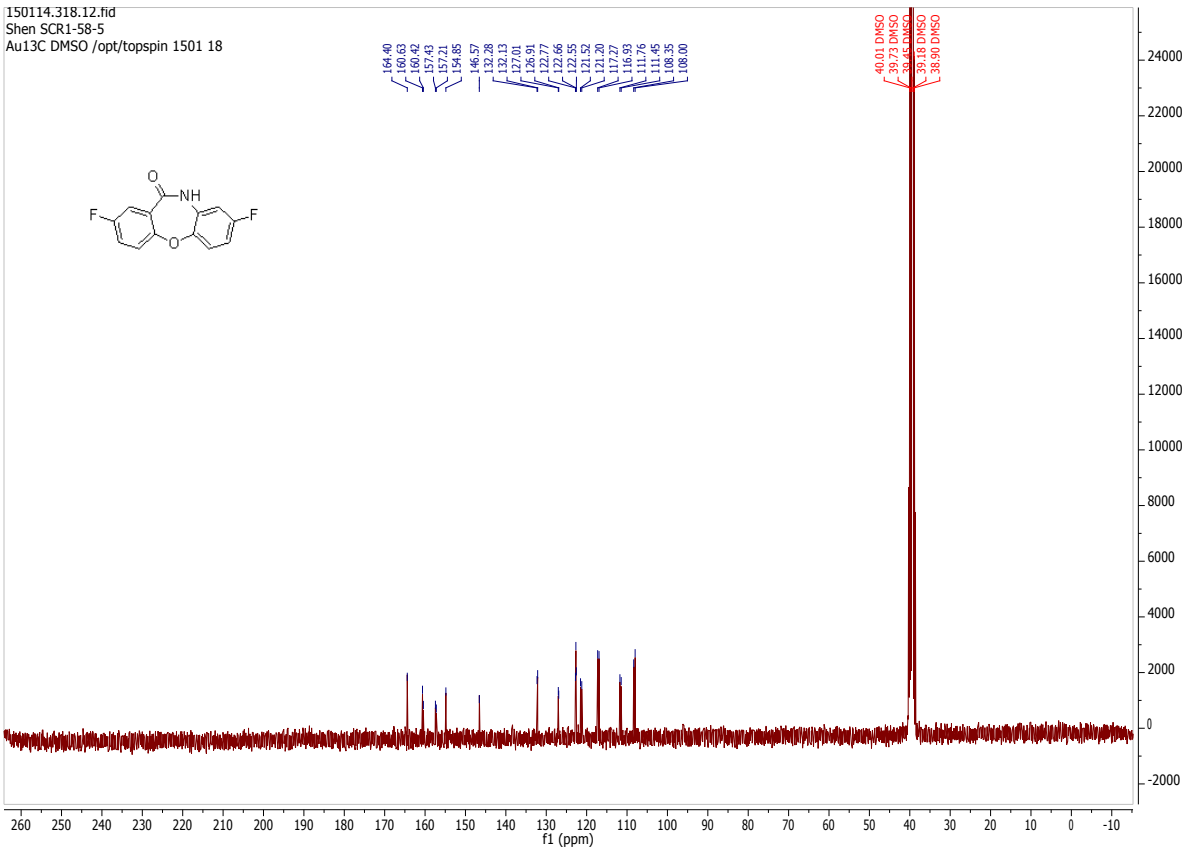

150114.317.12.fid
Shen SCR1-58-4
Au13C DMSO /opt/topspin 1501 17
164.340
160.464
157.258
154.600
149.023
132.306
129.590
126.943
126.843
124.963
122.906
122.842
122.735
121.554
121.245
121.031
117.302
116.967
40.287 DMSO
40.010 DMSO
39.732 DMSO
39.454 DMSO
39.178 DMSO
38.899 DMSO
38.621 DMSO
O
NH
F
Cl
O
f1 (ppm)

2,8-difluorodibenzo[b,f][1,4]oxazepin-11(10H)-one (3ap)

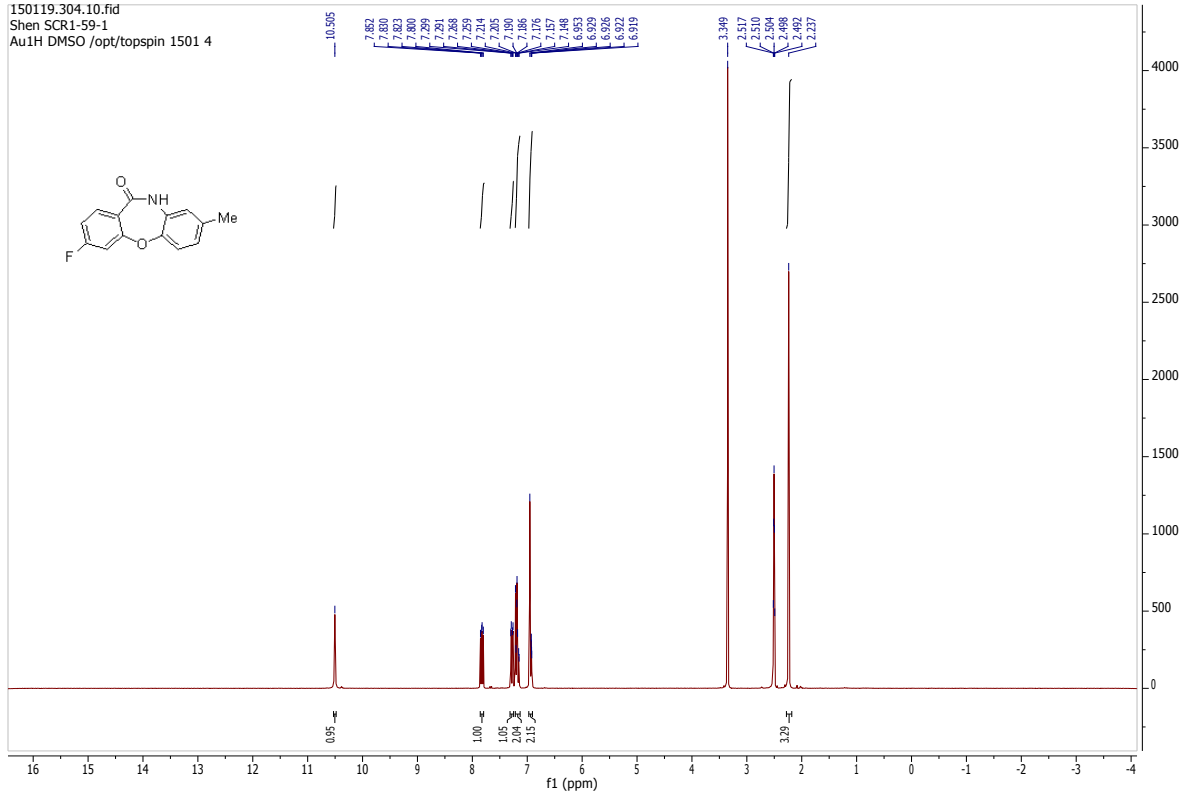


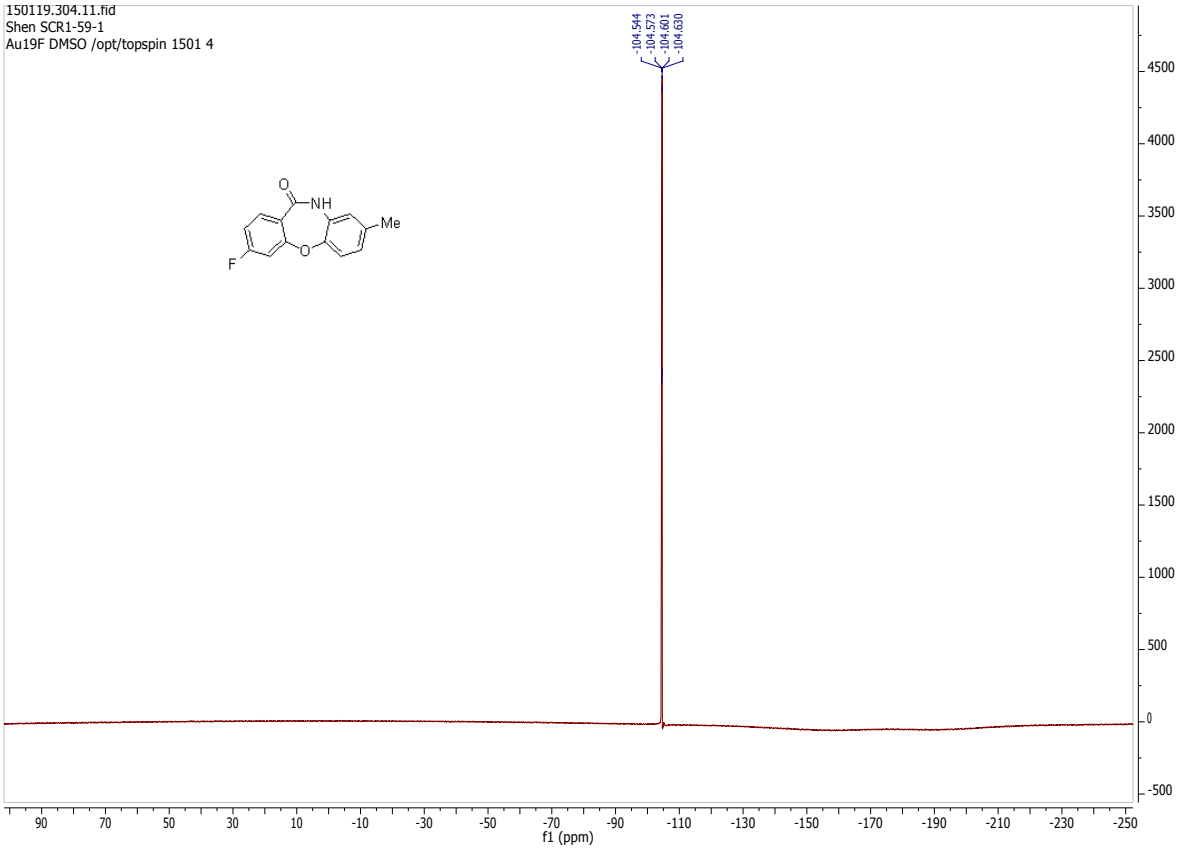



150114.318.12.fid
Shen SCR1-58-5
Au13C DMSO /opt/topspin 1501 18
164.401
160.634
160.418
157.433
157.213
154.847
154.827
146.584
146.550
132.280
132.128
127.013
126.911
122.767
122.665
122.555
121.515
121.204
117.267
116.934
111.763
111.450
108.349
107.996
40.288 DMSO
40.010 DMSO
39.733 DMSO
39.455 DMSO
39.177 DMSO
38.900 DMSO
38.6221 DMSO
O
NH
F
F
O
f1 (ppm)

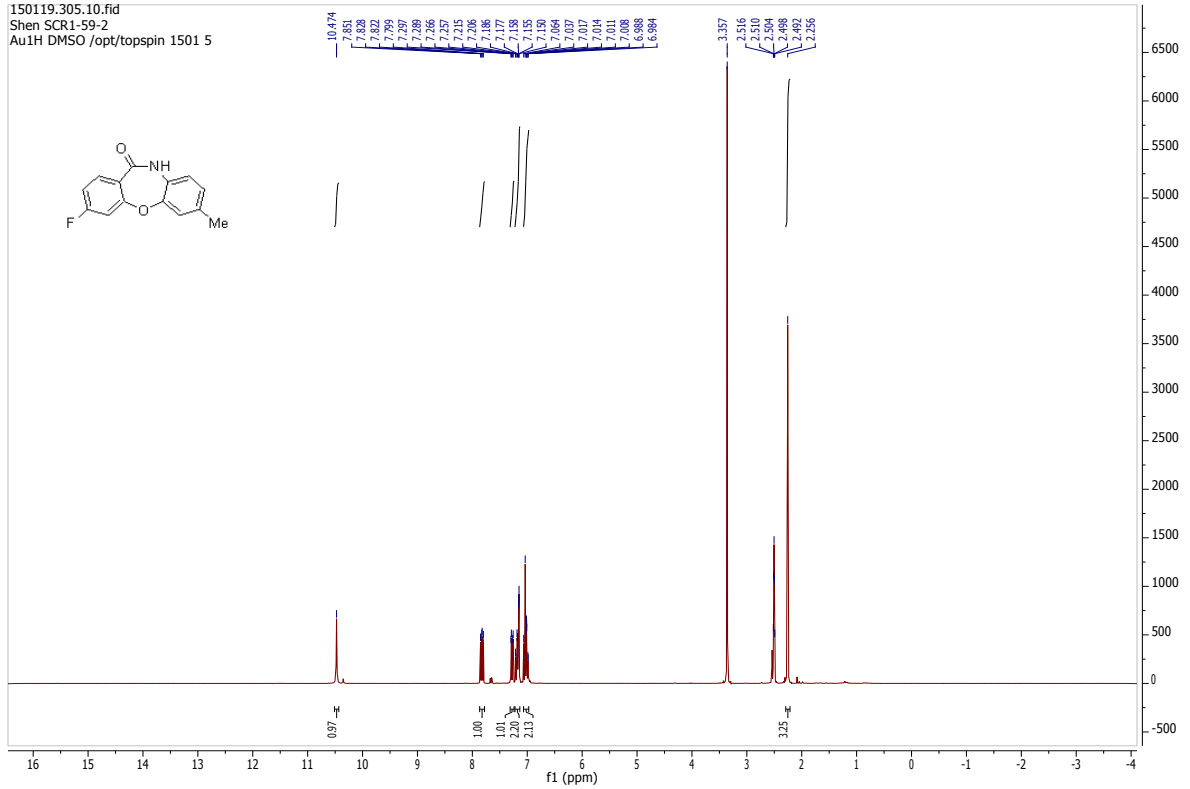

150114.318.12.fid
Shen SCR1-58-5
Au13C DMSO /opt/topspin 1501 18
164.40
160.63
160.42
157.43
157.21
154.85
146.57
132.28
132.13
127.01
126.91
122.77
122.66
122.55
121.52
121.20
117.27
116.93
111.76
111.45
108.35
108.00
40.01 DMSO
39.73 DMSO
39.45 DMSO
39.18 DMSO
38.90 DMSO
O
NH
F
F
O
f1 (ppm)

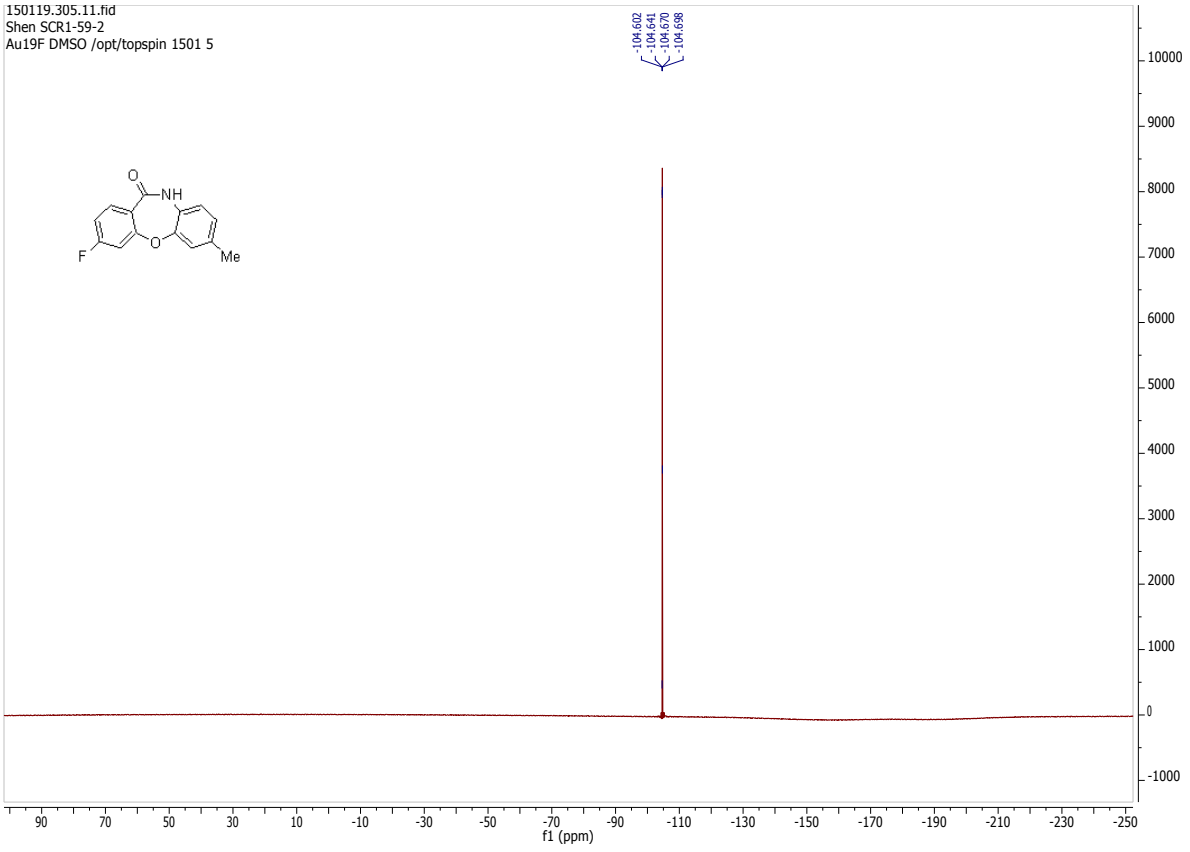
3-fluoro-8-methyldibenzo[b,f][1,4]oxazepin-11(10H)-one (3aq)



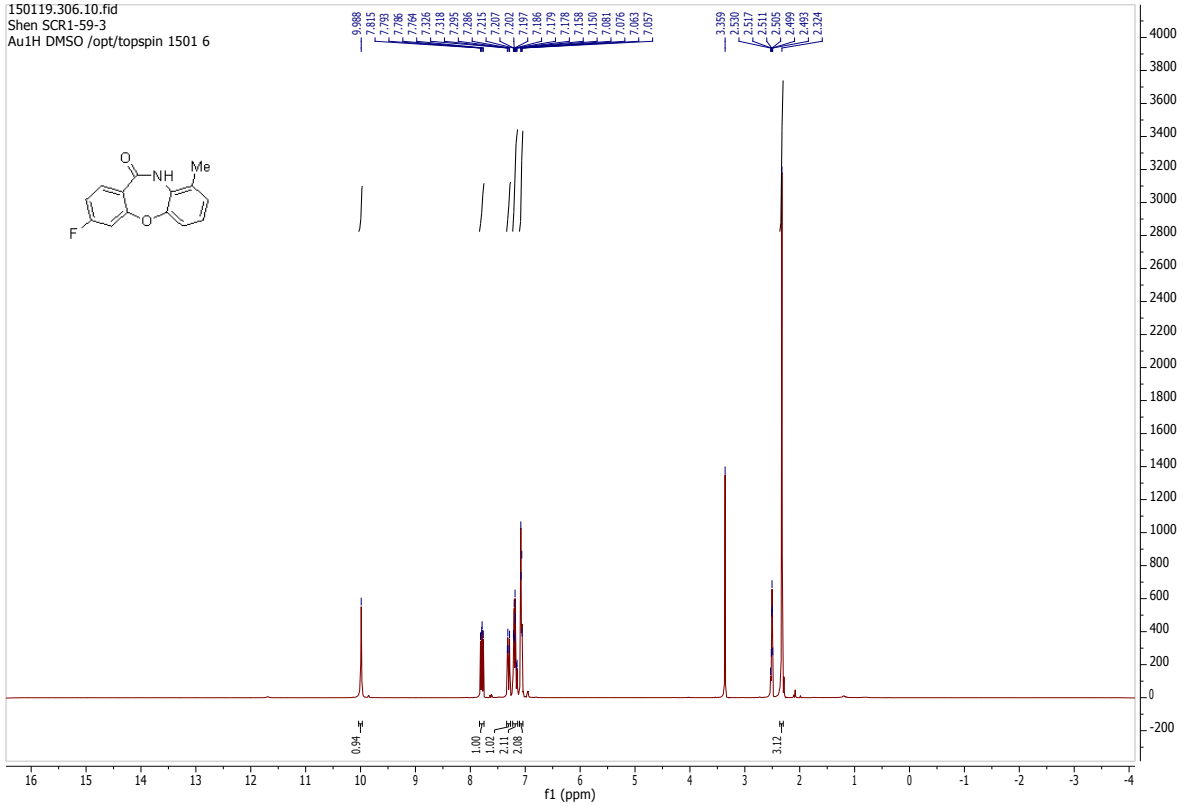


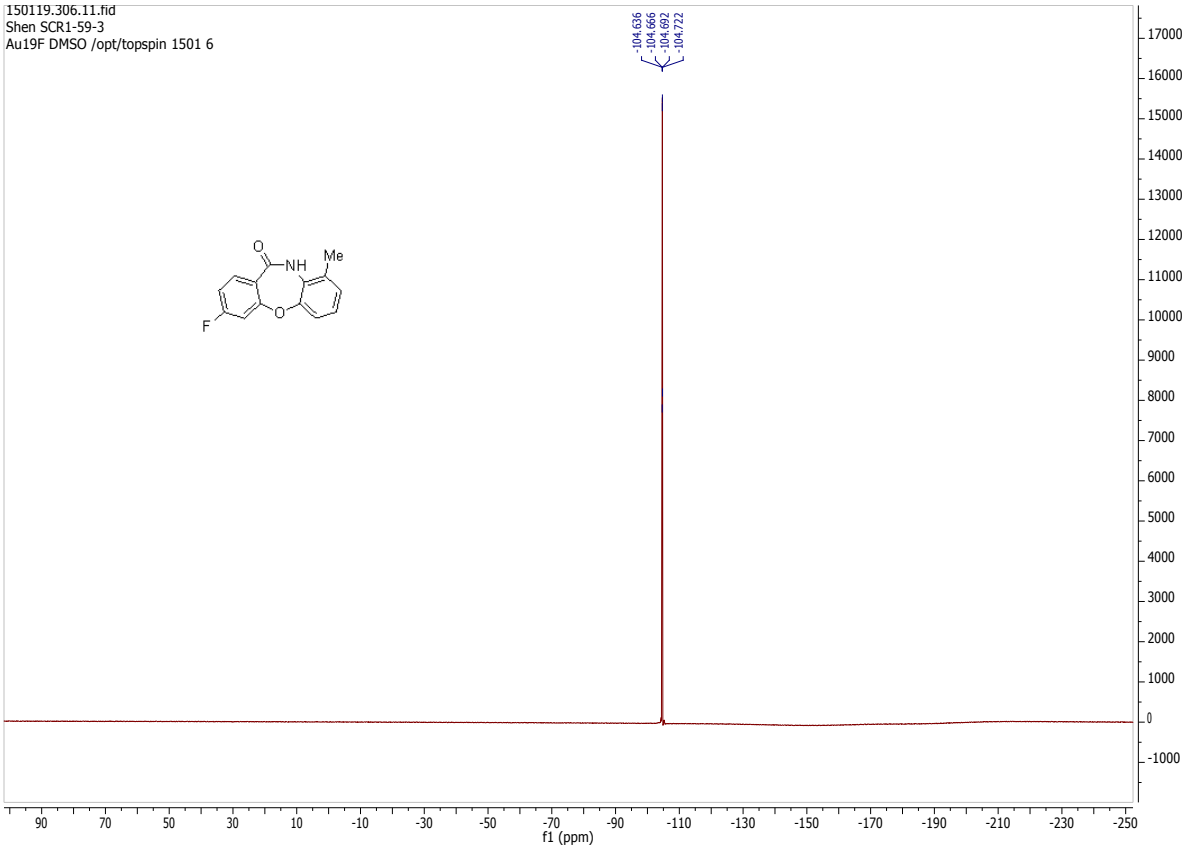
3-fluoro-7-methyldibenzo[b,f][1,4]oxazepin-11(10H)-one (3ar)

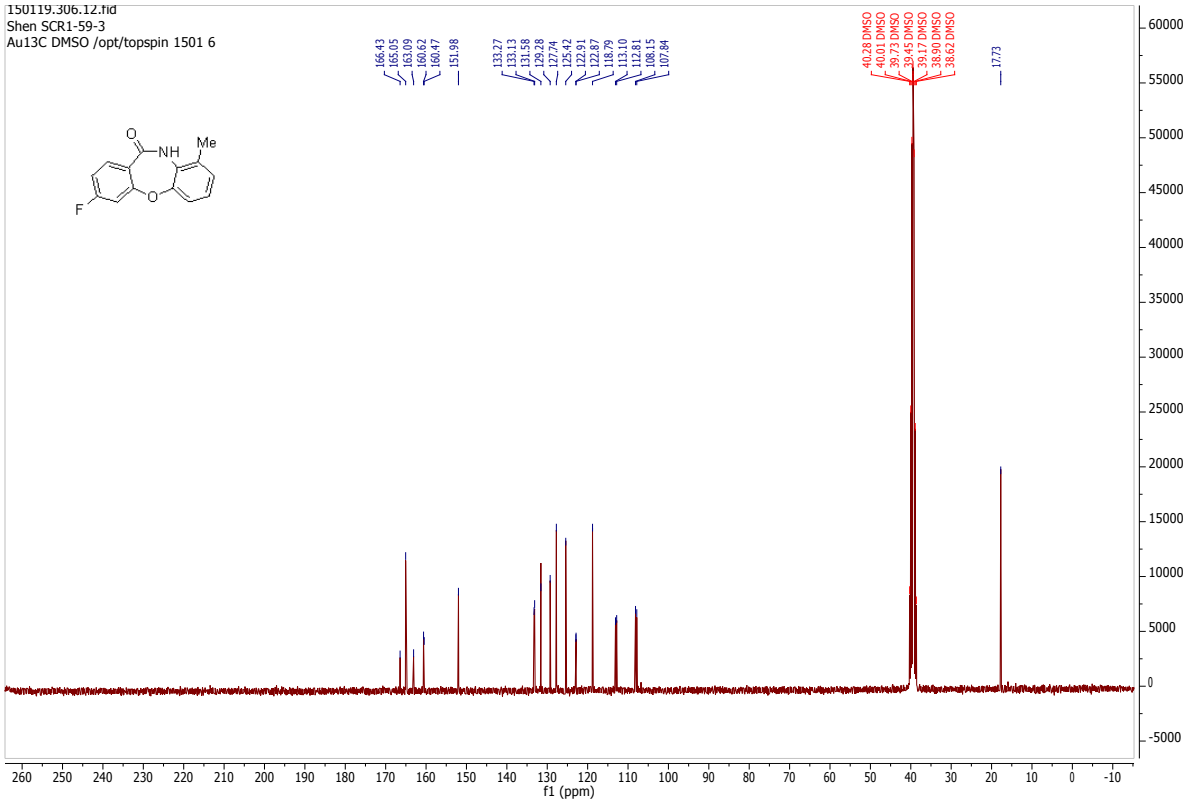




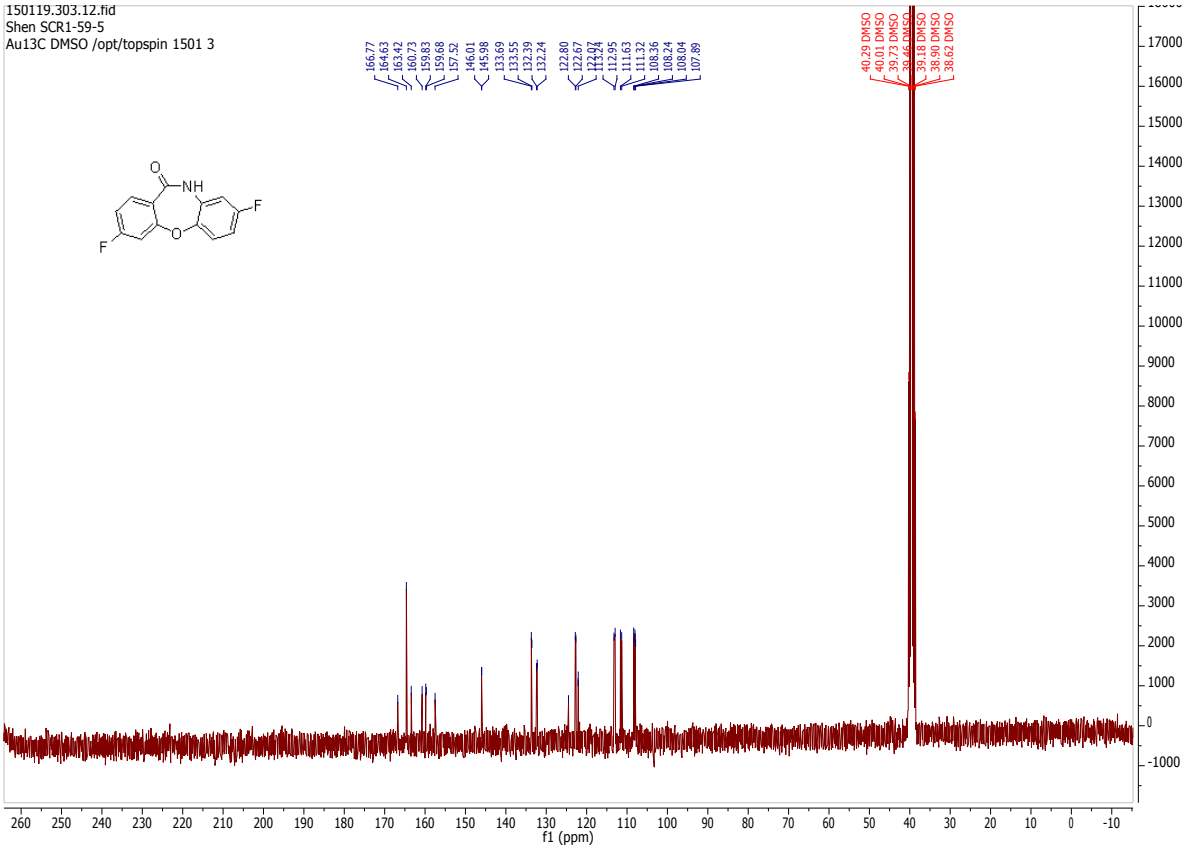
3-fluoro-9-methyldibenzo[b,f][1,4]oxazepin-11(10H)-one (3as)

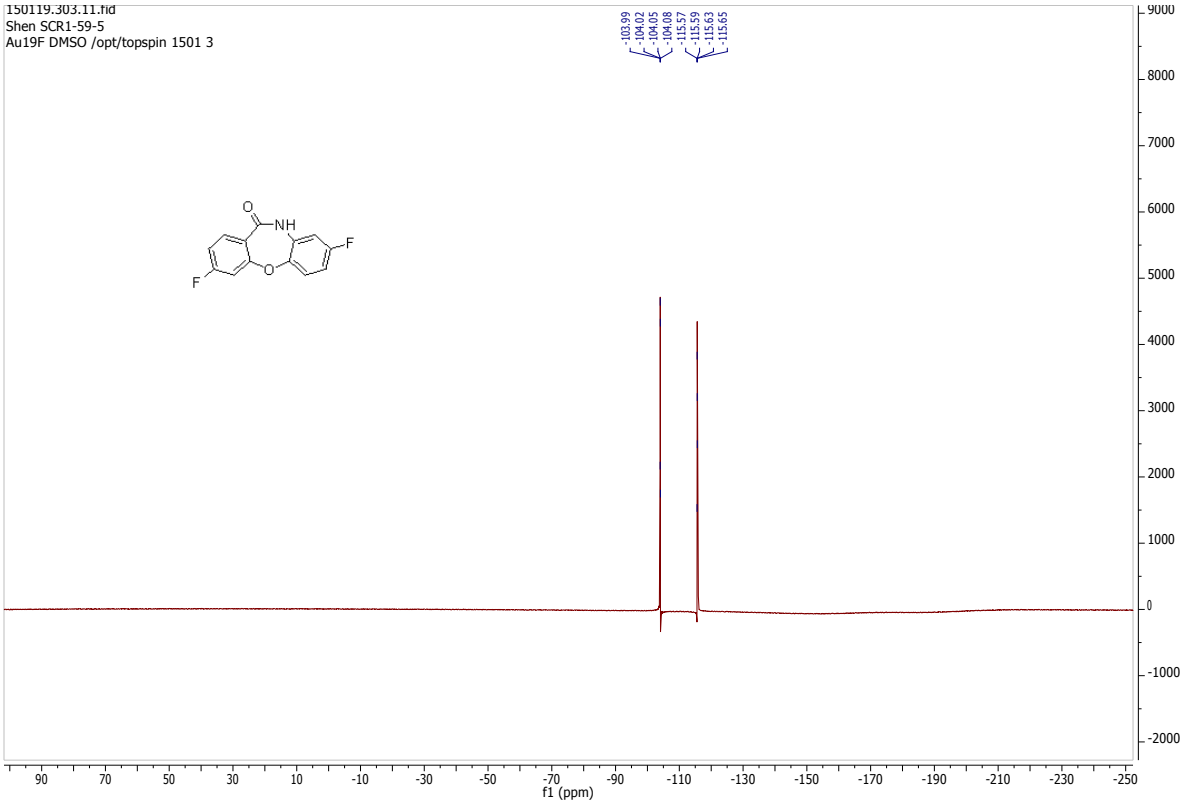




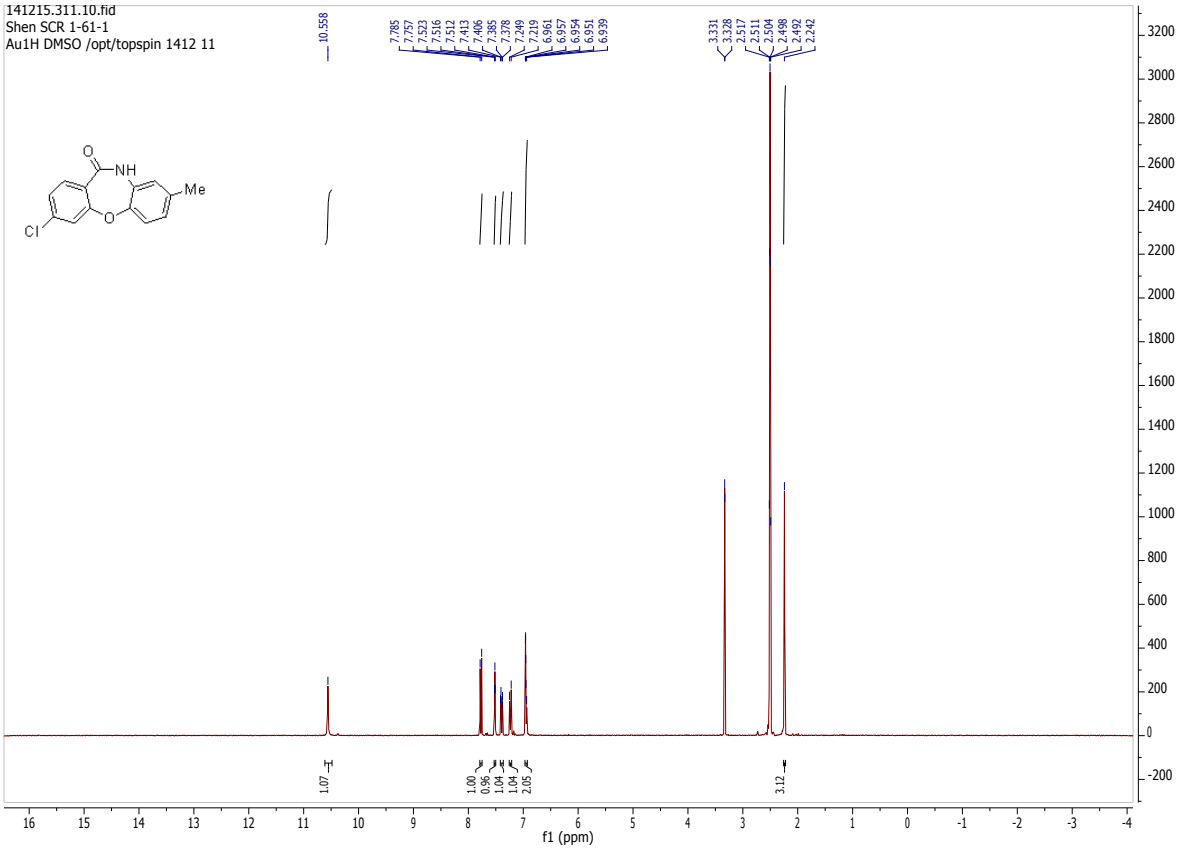


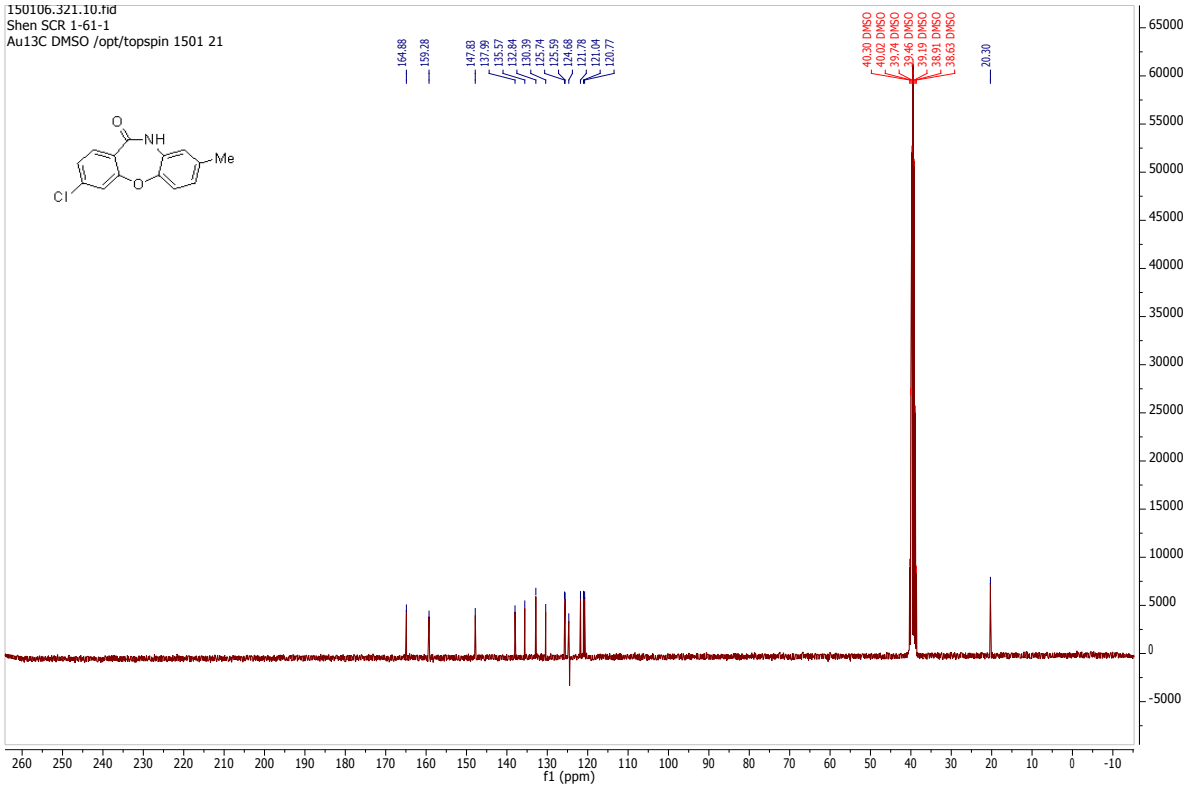
3,8-difluorodibenzo[b,f][1,4]oxazepin-11(10H)-one (3au)



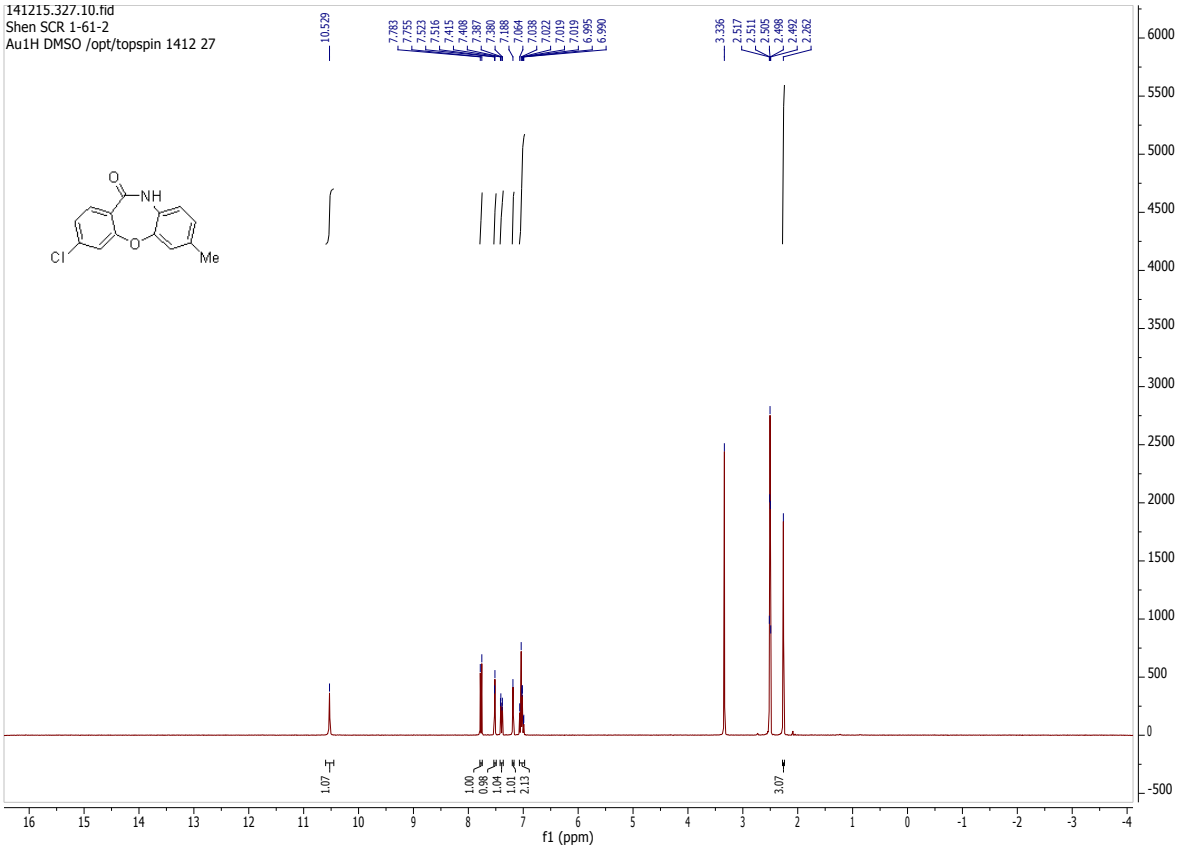


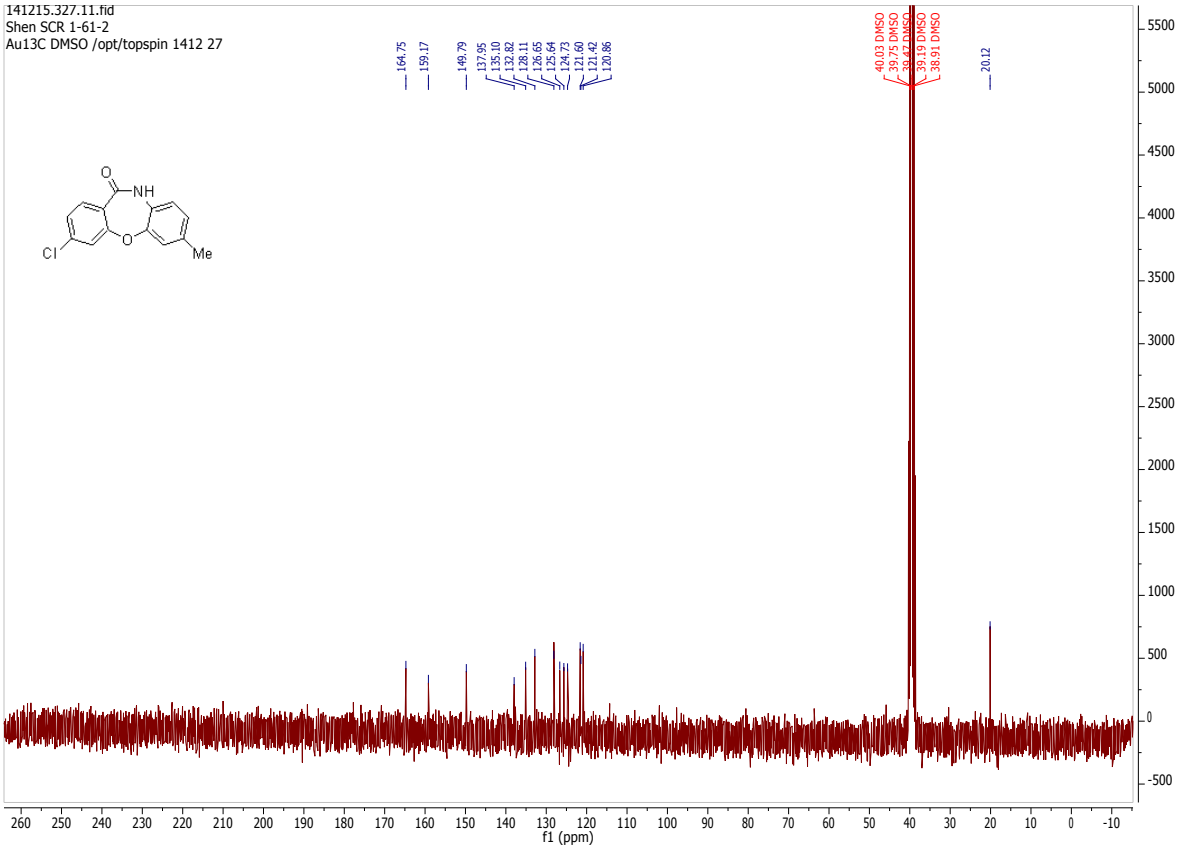
3-chloro-8-methyldibenzo[b,f][1,4]oxazepin-11(10H)-one (3av)

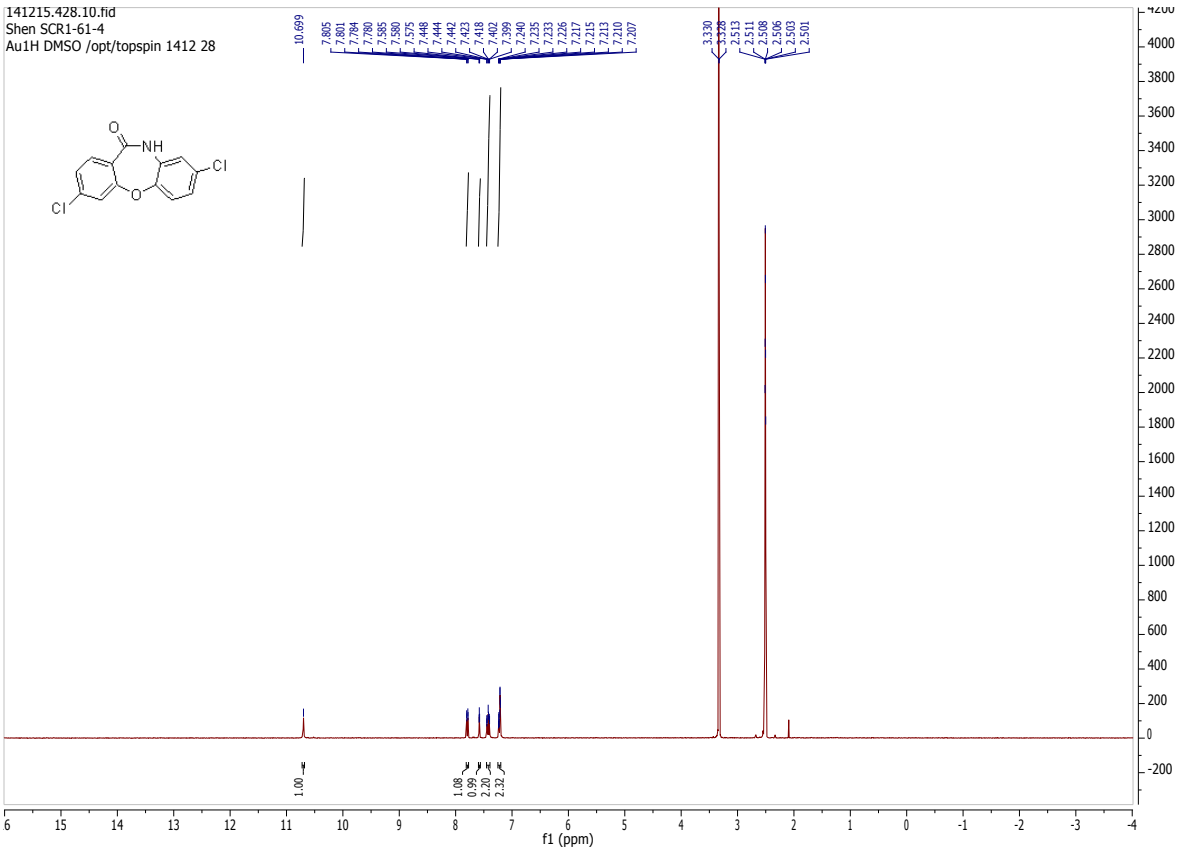


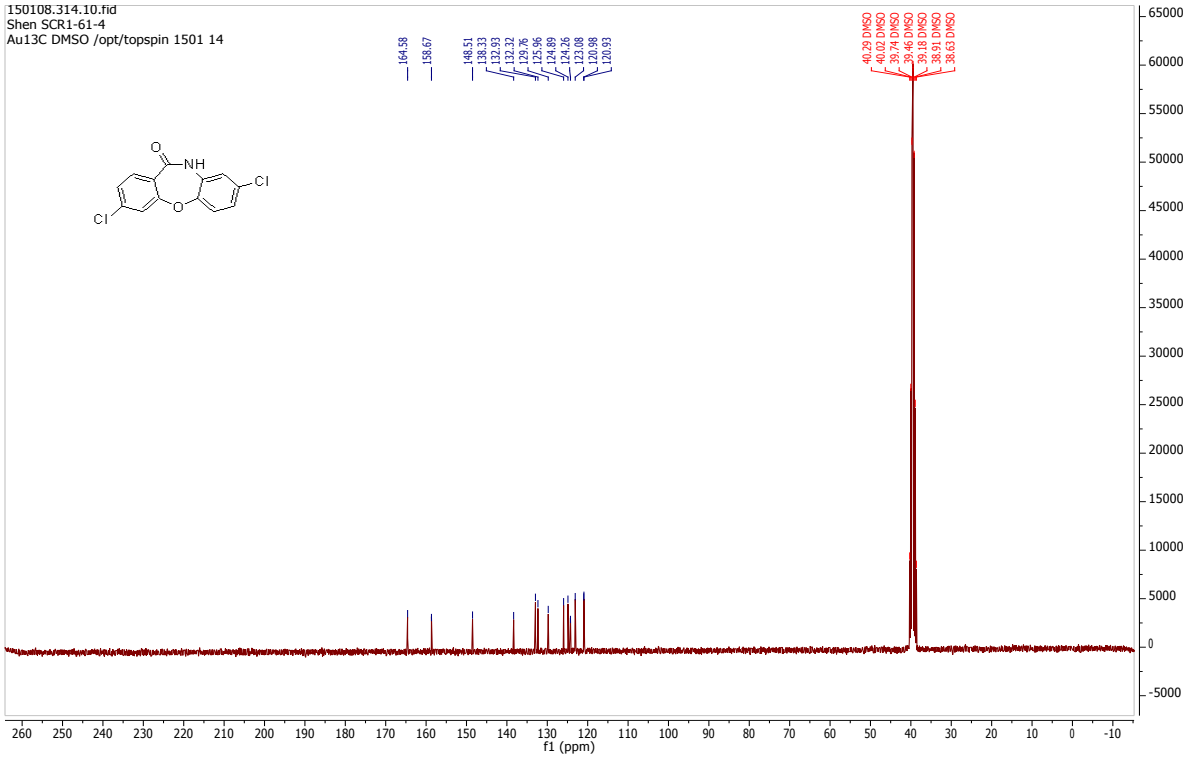


3-chloro-8-methyldibenzo[b,f][1,4]oxazepin-11(10H)-one (3ay)

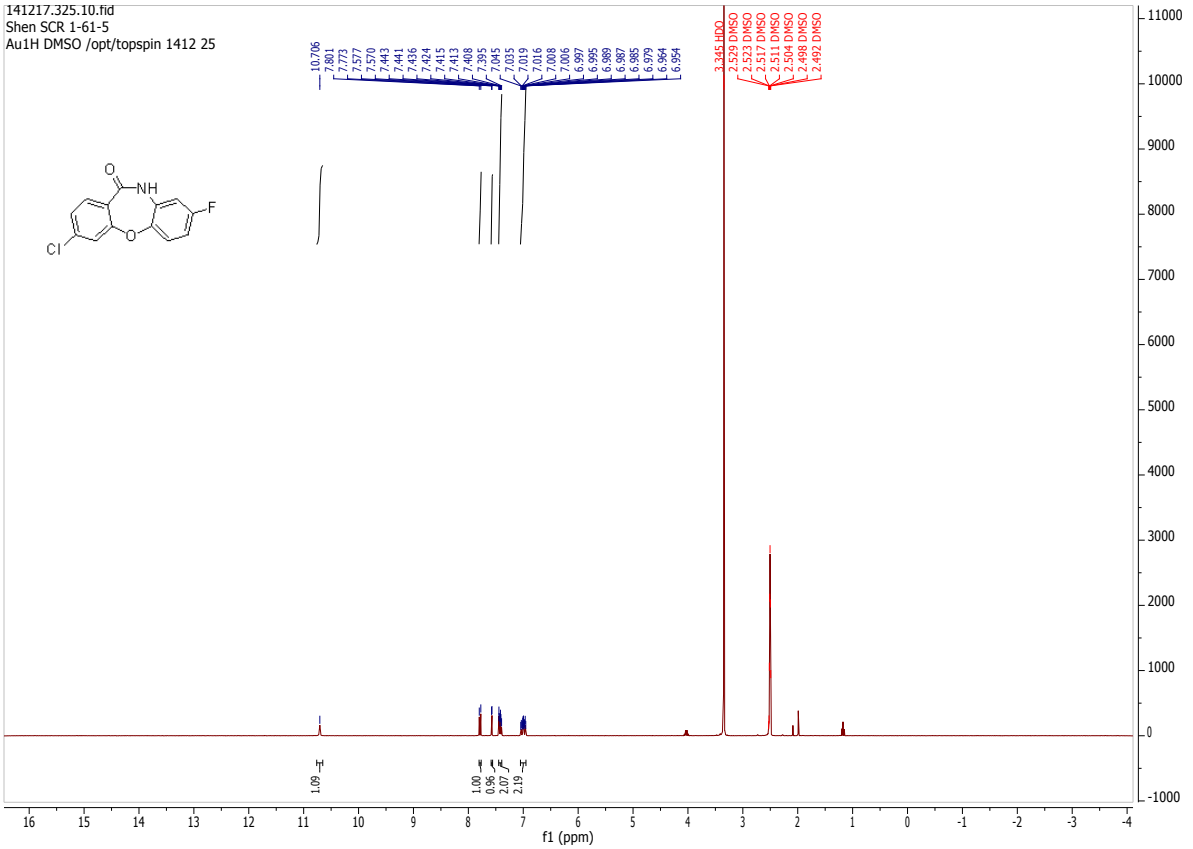


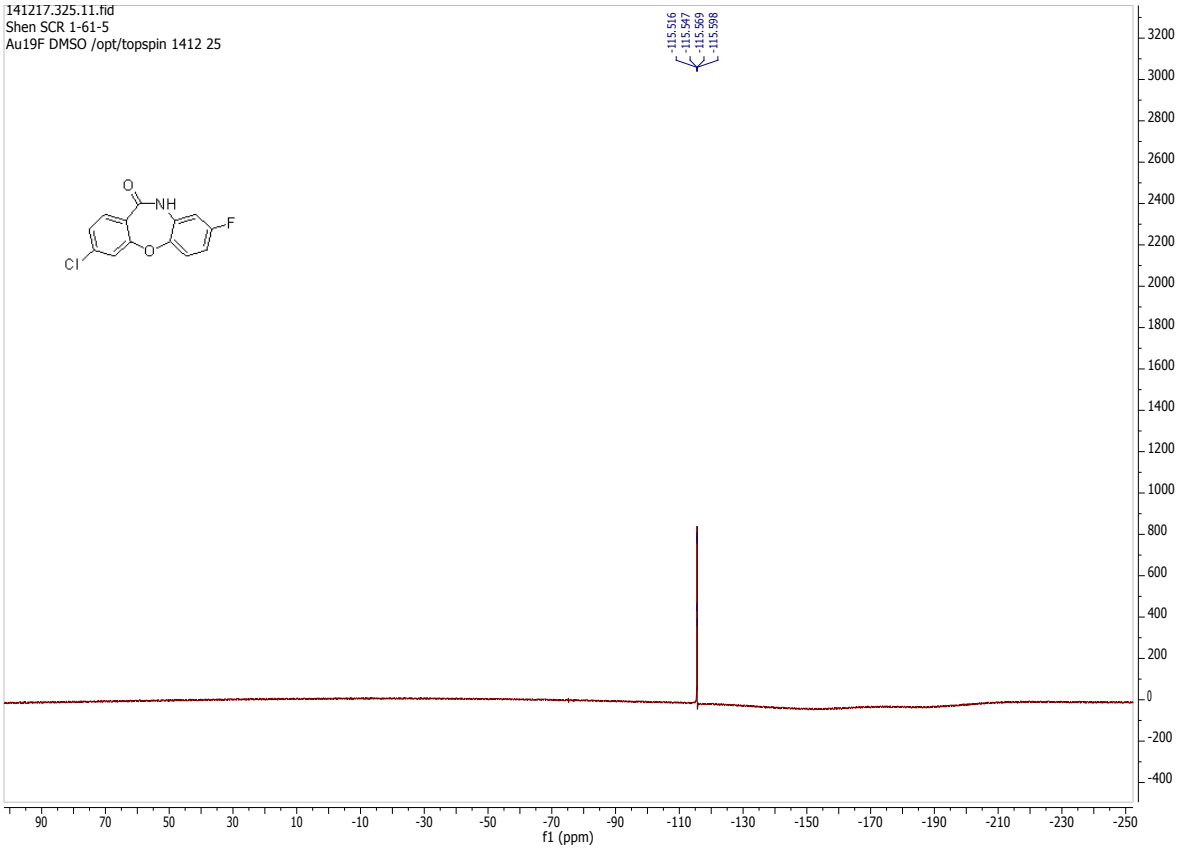

141215.327.11.fid
Shen SCR 1-61-2
Au13C DMSO /opt/topspin 1412 27
164.75
159.17
149.79
137.95
135.10
132.82
128.11
126.65
125.64
124.73
121.60
121.42
120.86
40.03 DMSO
39.75 DMSO
39.47 DMSO
39.19 DMSO
38.91 DMSO
20.12
O
NH
Cl
O
Me
f1 (ppm)

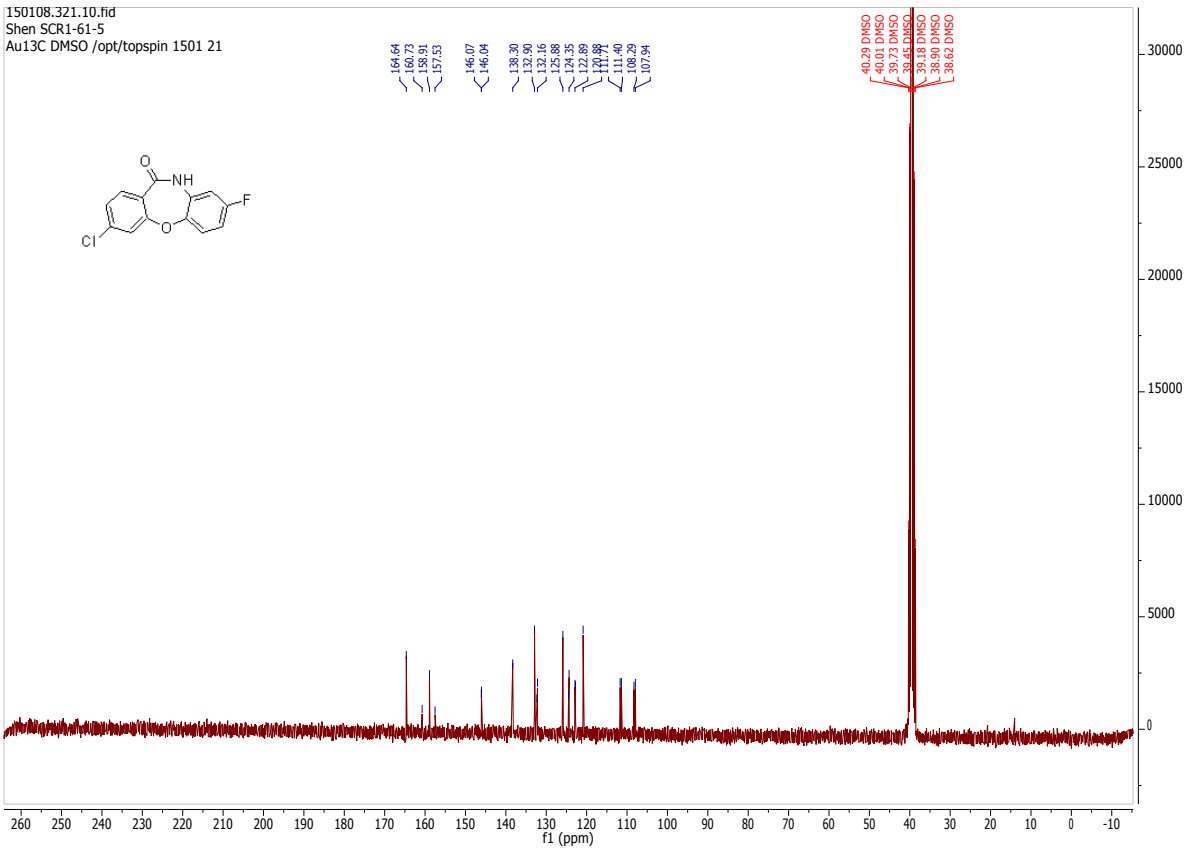

141215.428.10.fid
Shen SCR1-61-4
Au1H DMSO /opt/topspin 1412 28
10.699
7.805
7.801
7.784
7.780
7.585
7.580
7.575
7.448
7.444
7.442
7.423
7.418
7.402
7.399
7.240
7.235
7.233
7.226
7.217
7.215
7.213
7.210
7.207
3.330
3.328
2.513
2.511
2.508
2.506
2.503
2.501
1.00
1.08
0.99
2.20
2.32
O
NH
Cl
Cl
O
f1 (ppm)



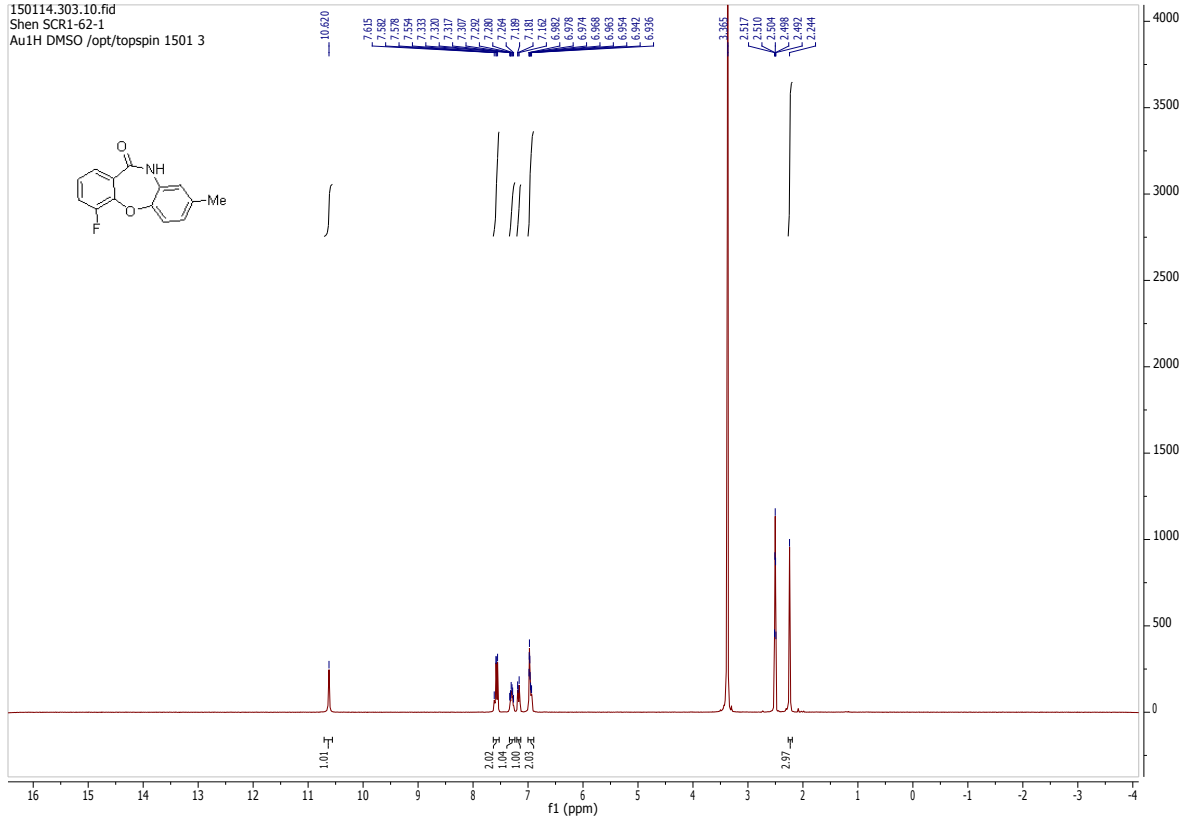
3-chloro-8-fluorodibenzo[b,f][1,4]oxazepin-11(10H)-one (3az)

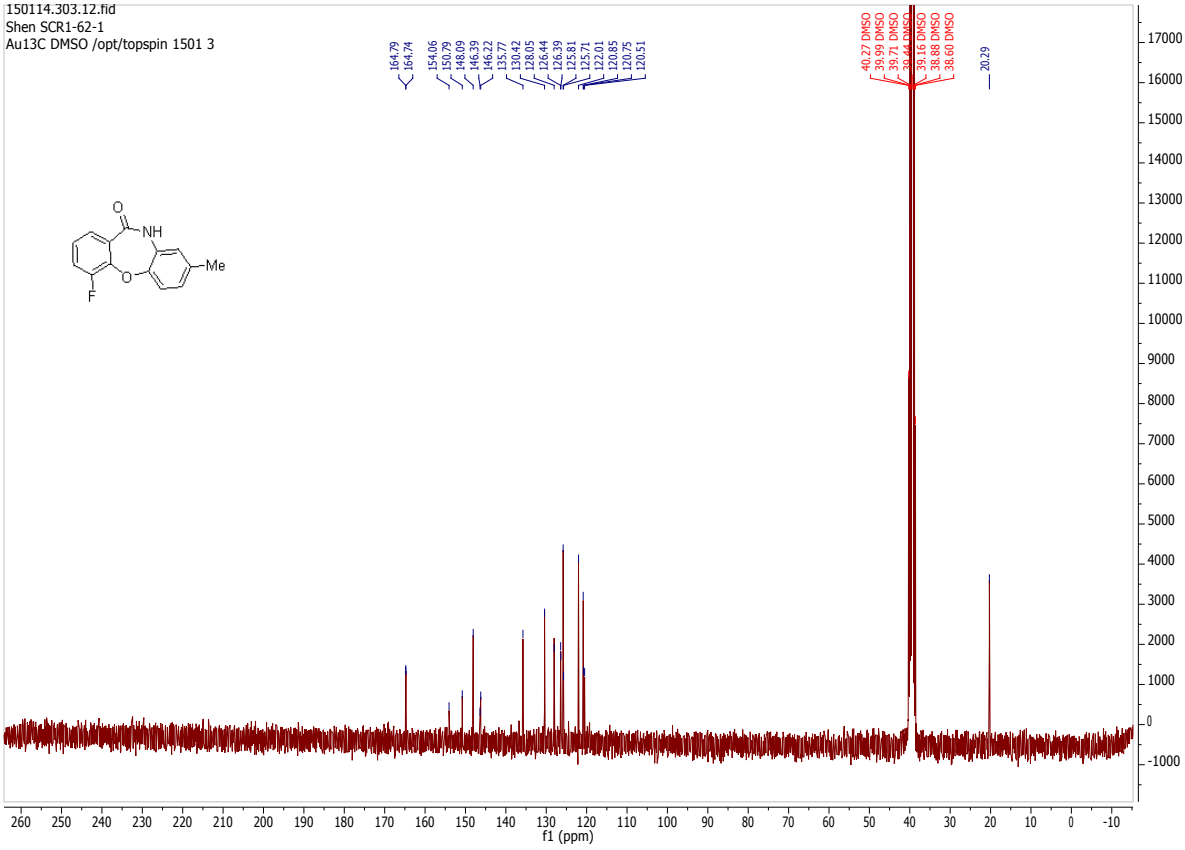


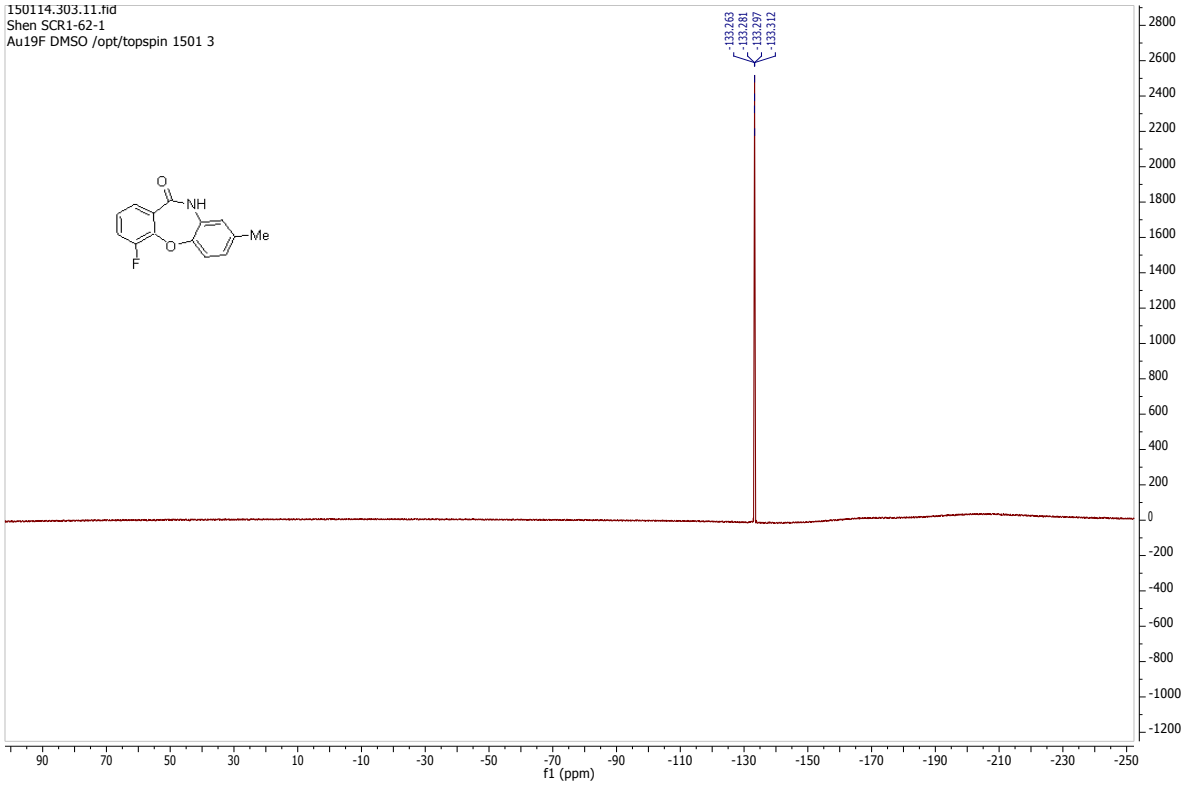

141217.325.11.fid
Shen SCR 1-61-5
Au19F DMSO /opt/topspin 1412 25
-115.516
-115.547
-115.569
-115.598
O
NH
F
Cl
O
f1 (ppm)


150108.321.10.fid
Shen SCR1-61-5
Au13C DMSO /opt/topspin 1501 21
164.64
160.73
158.91
157.53
146.07
146.04
138.30
132.90
132.16
125.88
124.35
122.89
120.88
111.71
111.40
108.29
107.94
40.29 DMSO
40.01 DMSO
39.73 DMSO
39.45 DMSO
39.18 DMSO
38.90 DMSO
38.62 DMSO
O
NH
F
Cl
O
f1 (ppm)

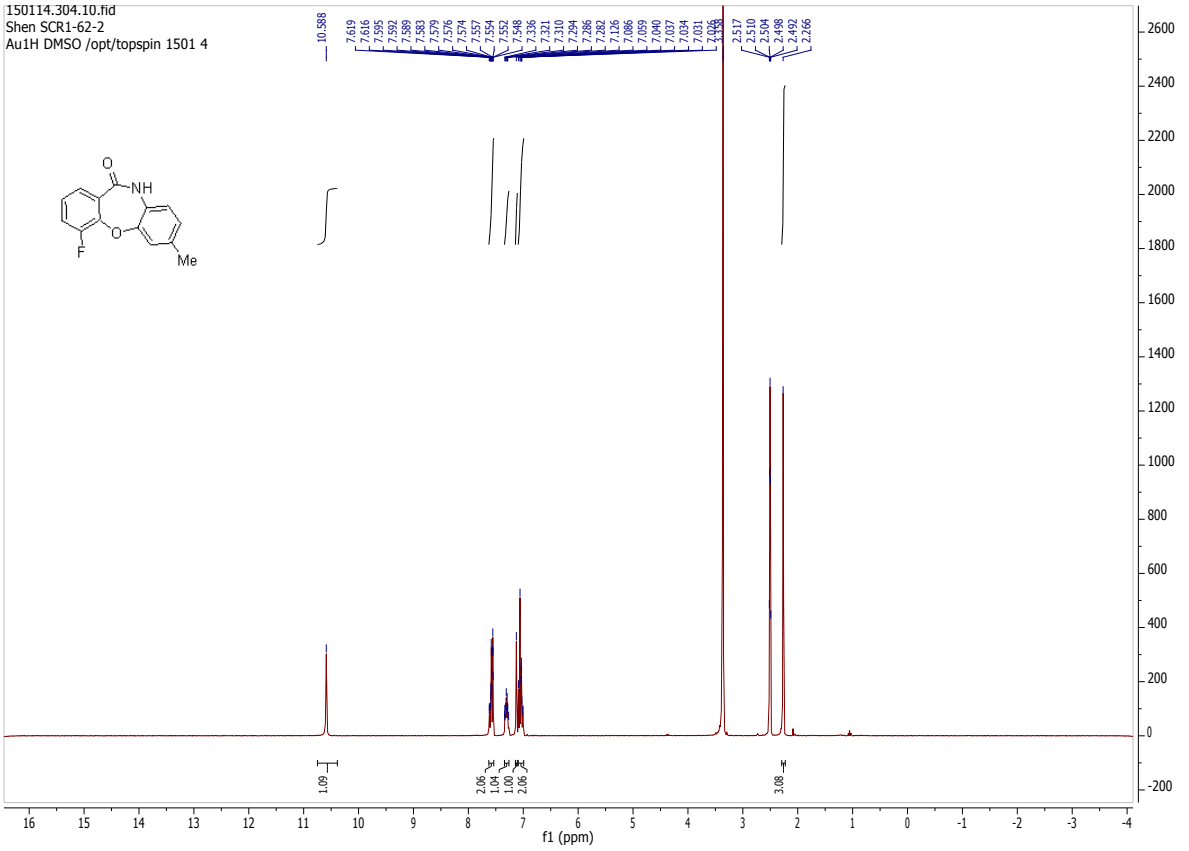
4-fluoro-8-methyldibenzo[b,f][1,4]oxazepin-11(10H)-one (3ba)

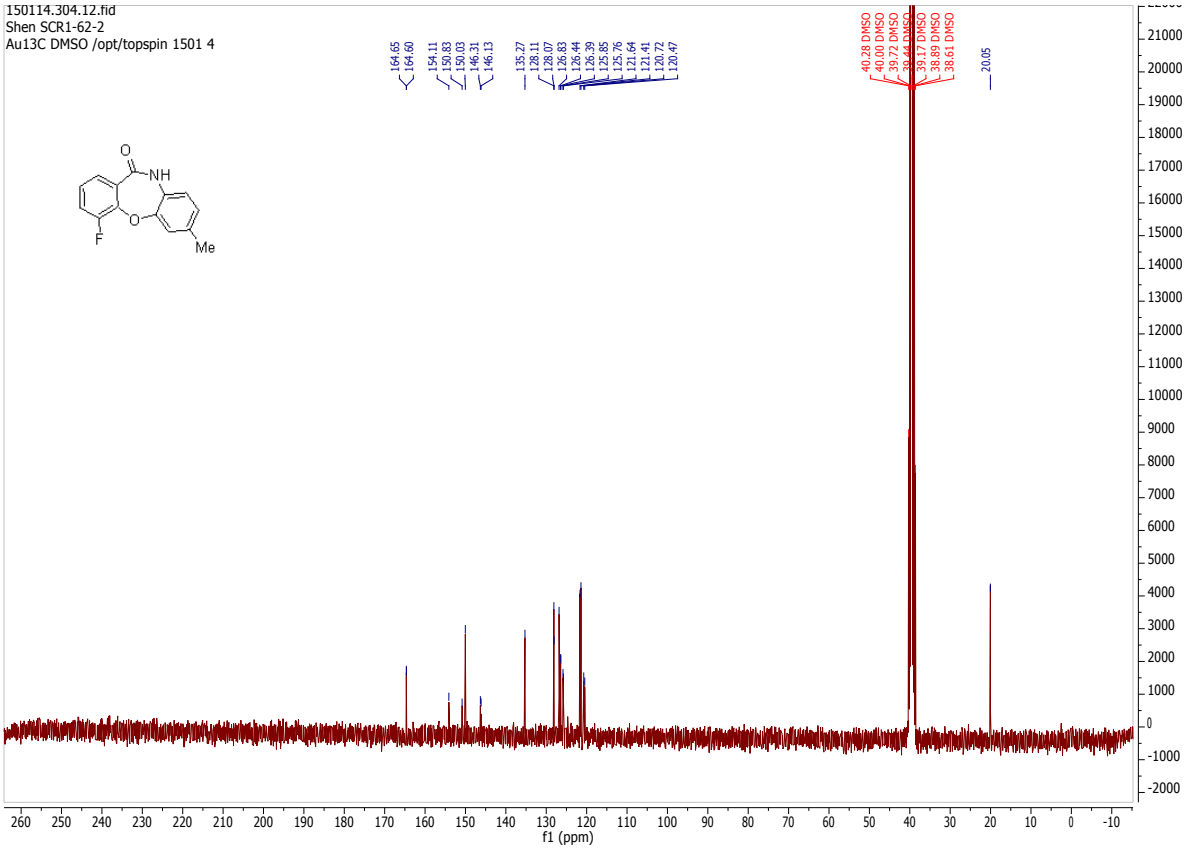


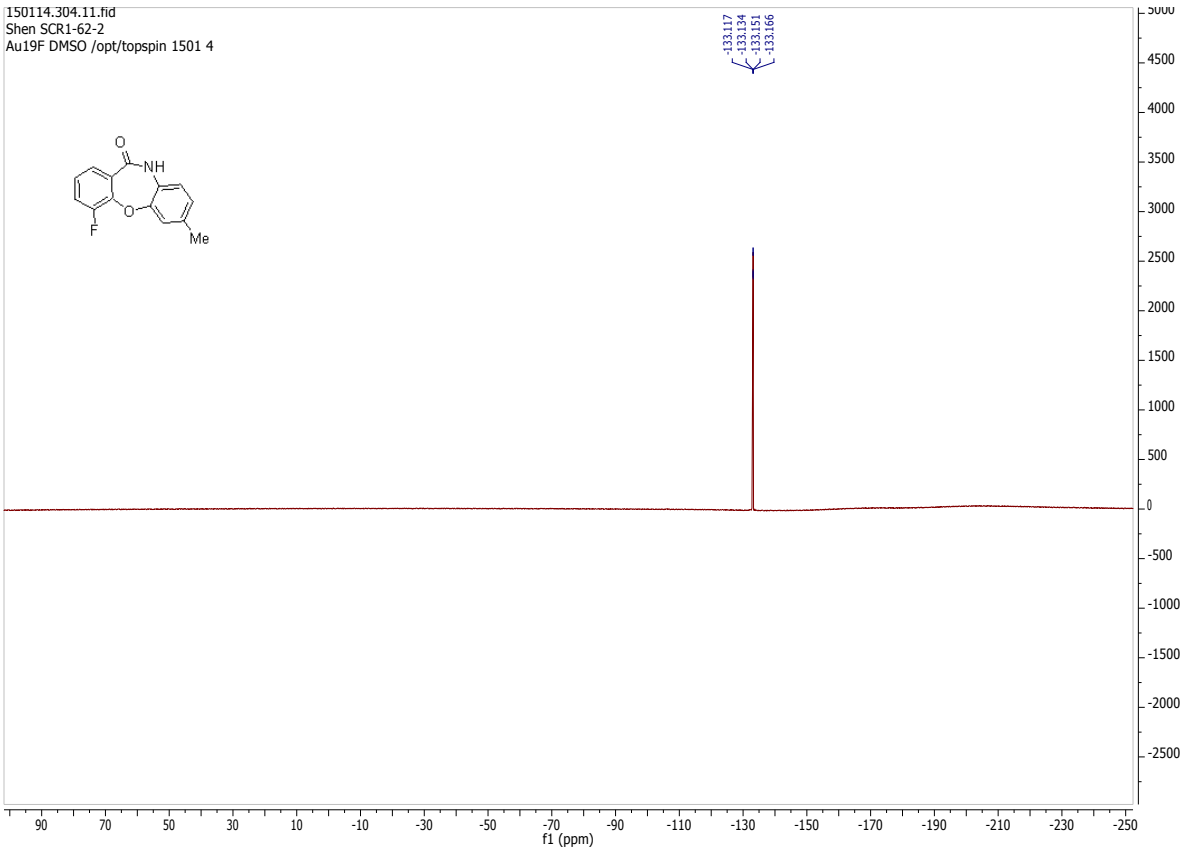




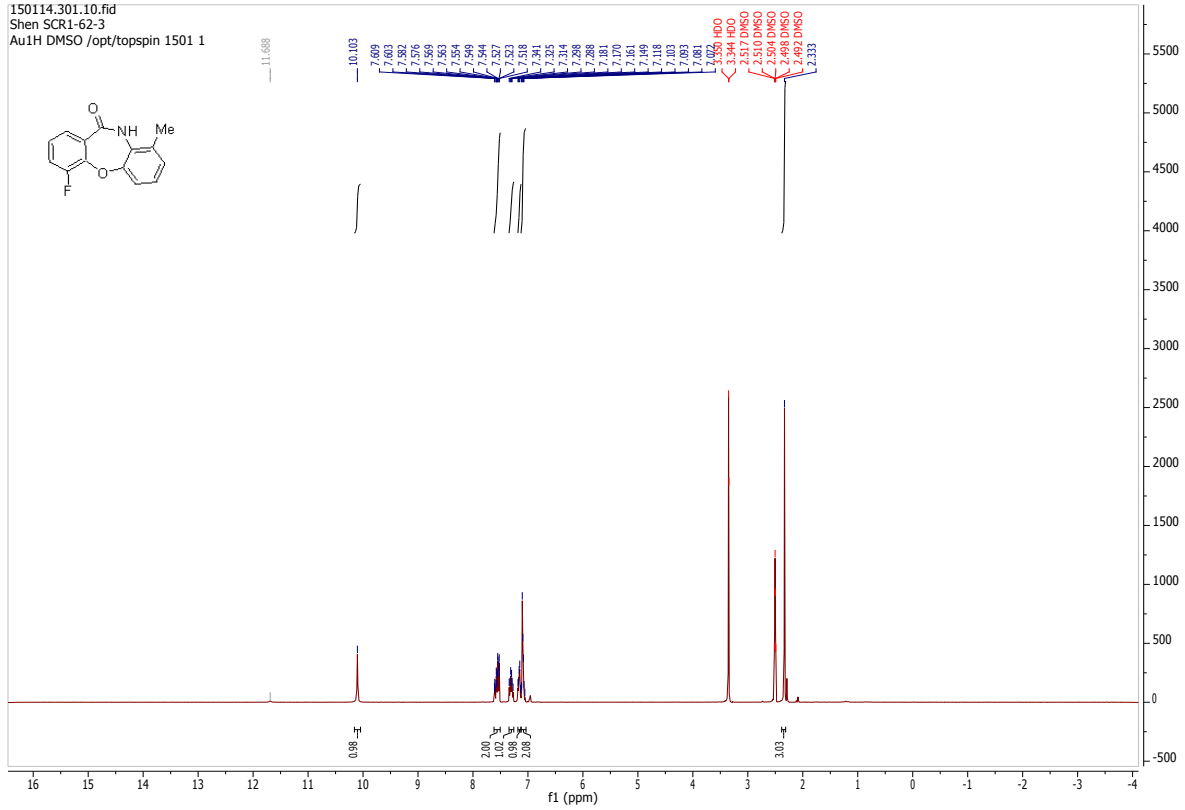
4-fluoro-7-methyldibenzo[b,f][1,4]oxazepin-11(10H)-one (3bb)

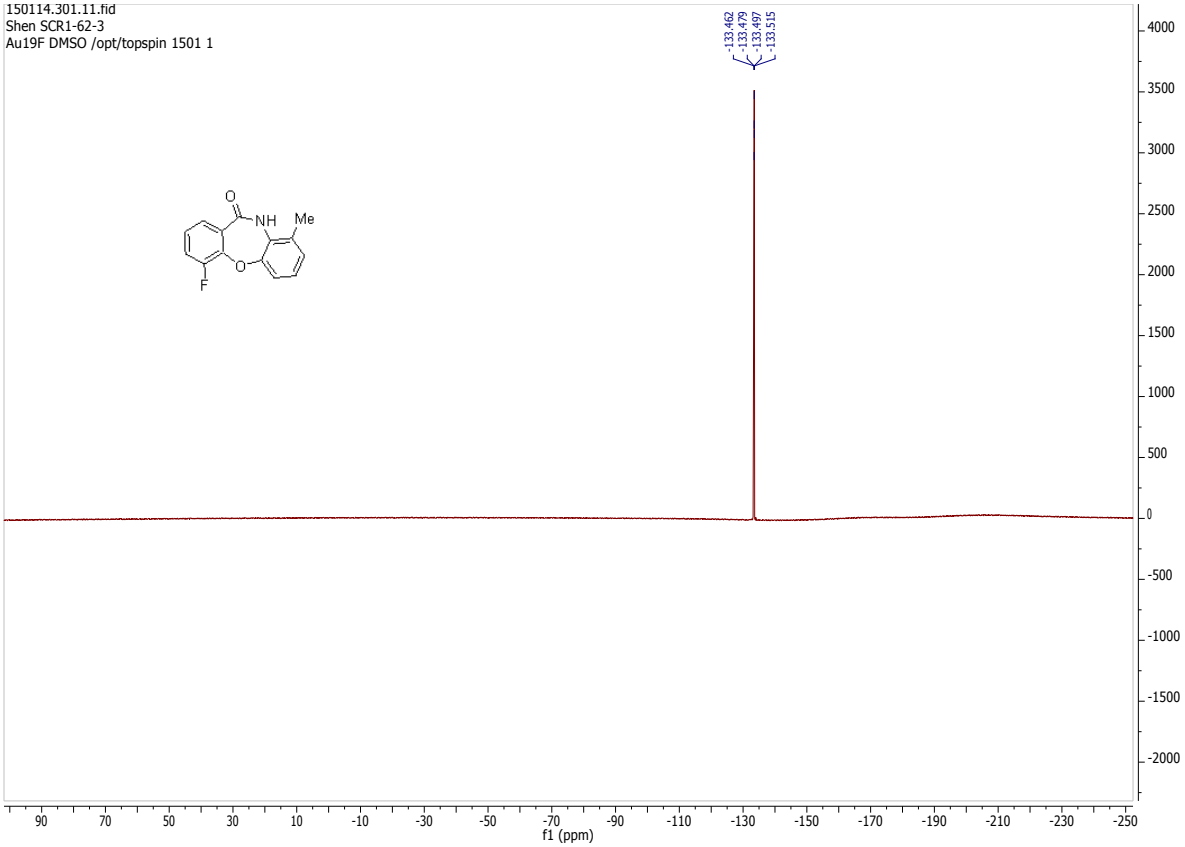


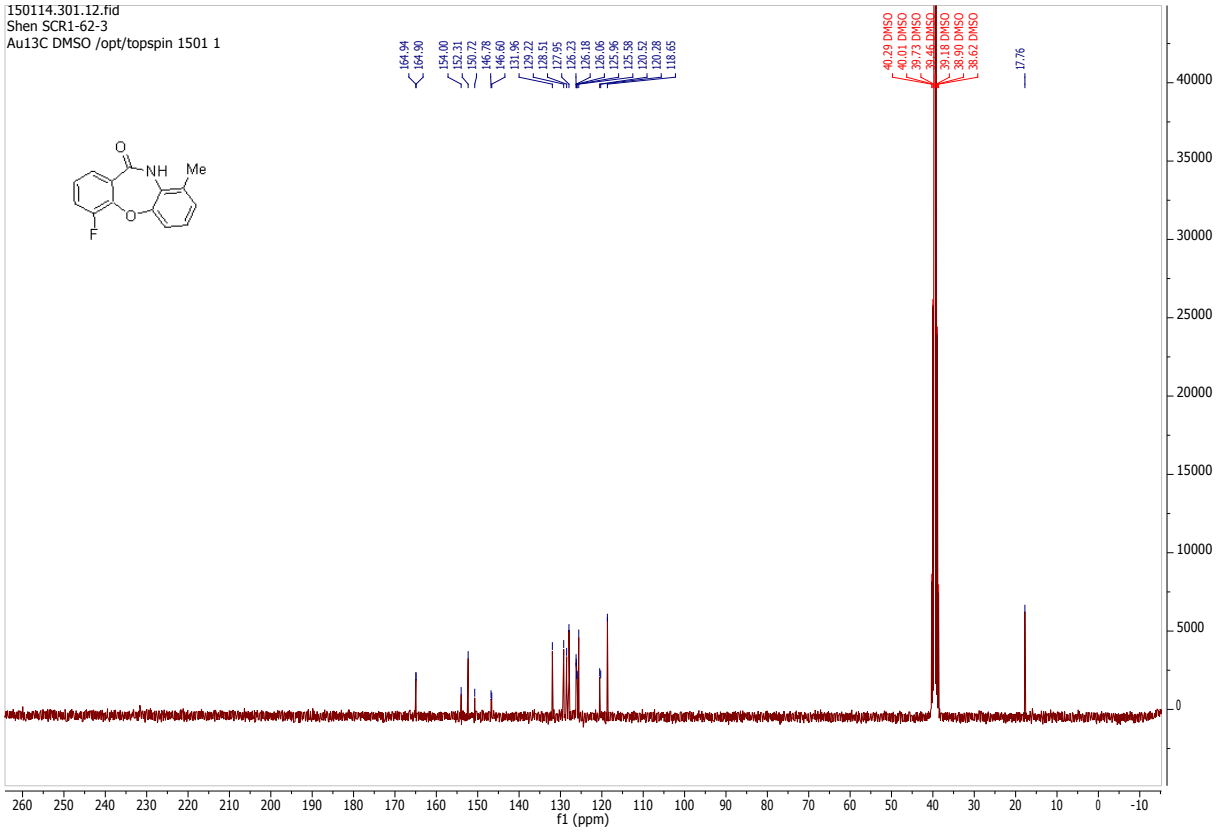

150114.304.12.fid
Shen SCR1-62-2
Au13C DMSO /opt/topspin 1501 4
164.65
164.60
154.11
150.83
150.03
146.31
146.13
135.27
128.11
128.07
126.83
126.44
126.39
125.85
125.76
121.64
121.41
120.72
120.47
40.28 DMSO
40.00 DMSO
39.72 DMSO
39.44 DMSO
39.17 DMSO
38.89 DMSO
38.61 DMSO
20.05
O
NH
O
F
Me
f1 (ppm)


150114.304.11.fid
Shen SCR1-62-2
Au19F DMSO /opt/topspin 1501 4
-133.117
-133.134
-133.151
-133.166
O
NH
O
F
Me
f1 (ppm)

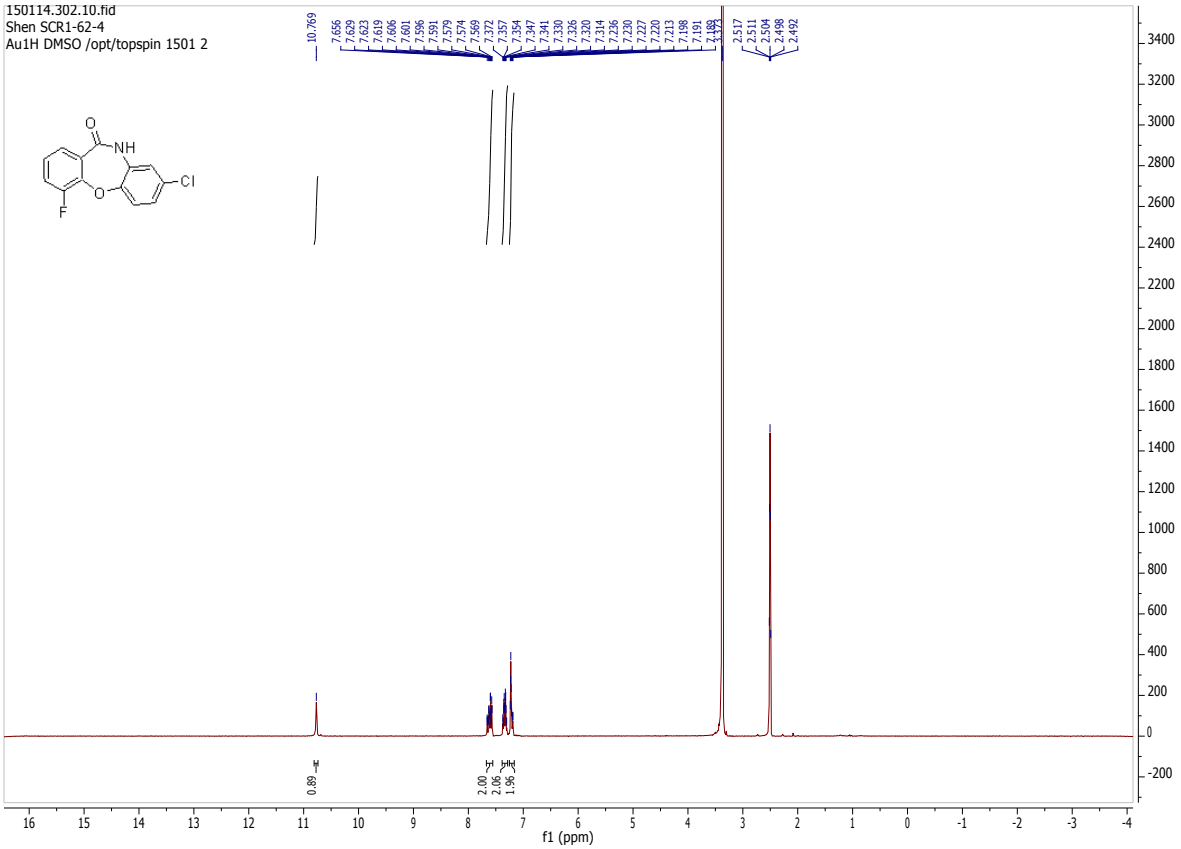
4-fluoro-9-methyldibenzo[b,f][1,4]oxazepin-11(10H)-one (3bc)

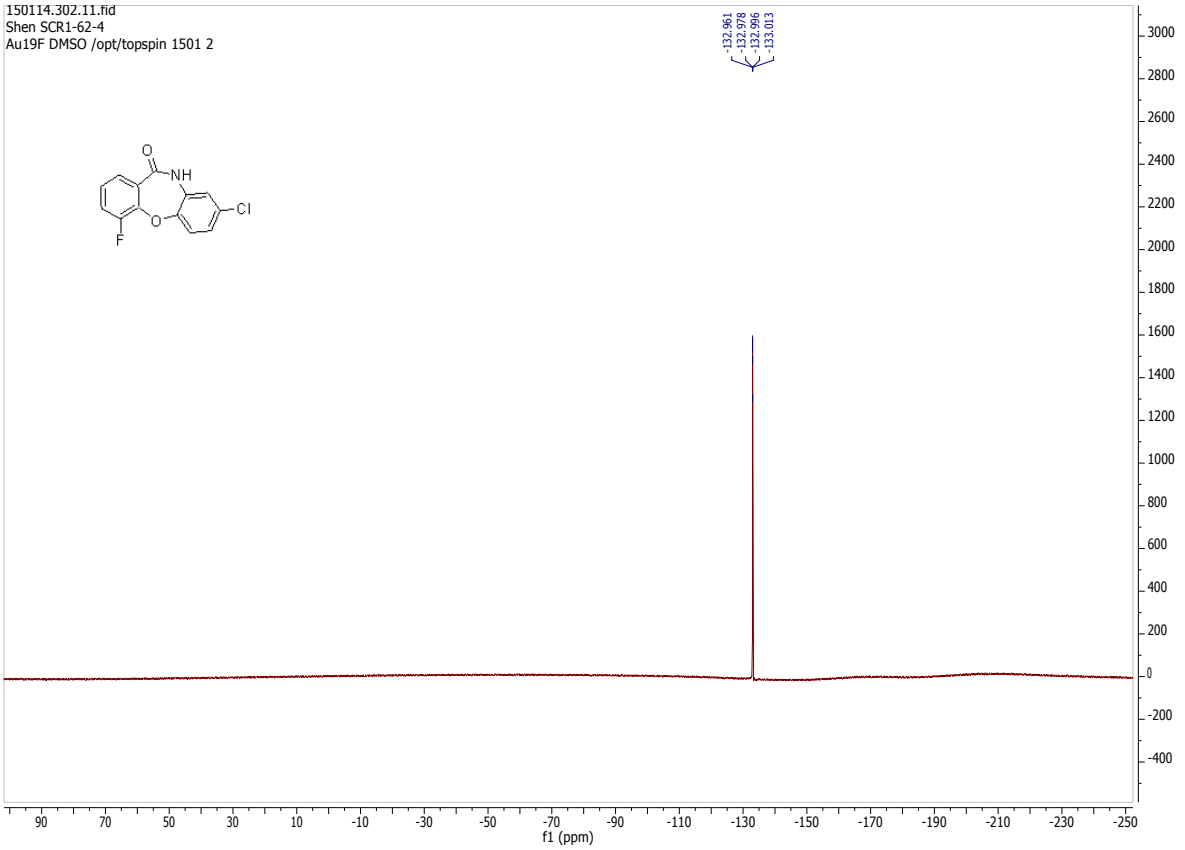


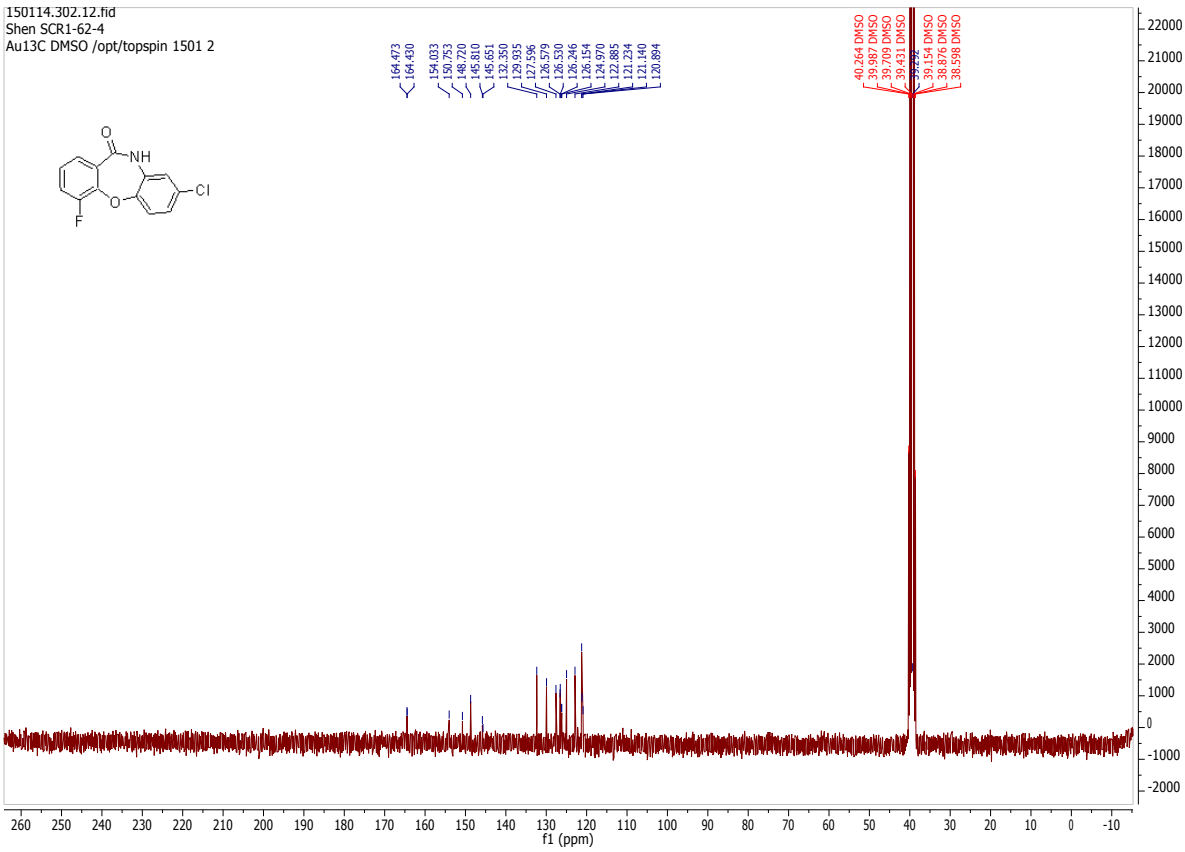




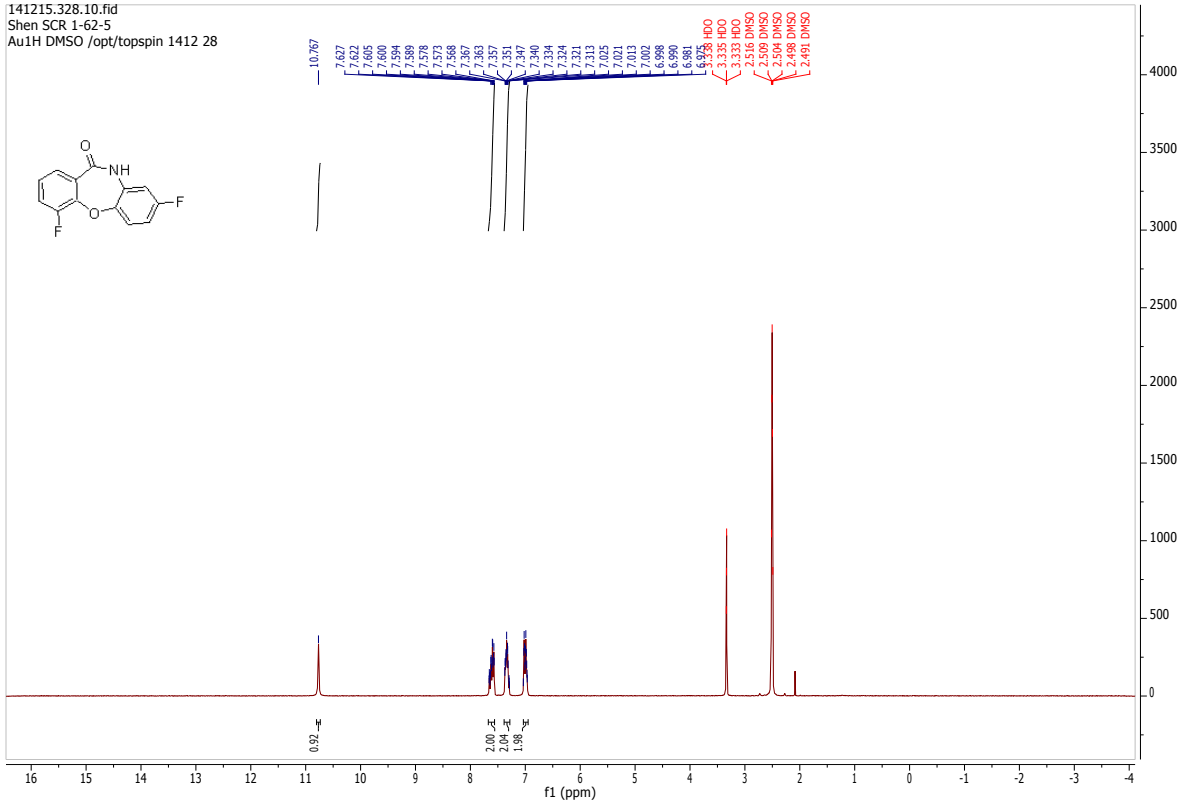
8-chloro-4-fluorodibenzo[b,f][1,4]oxazepin-11(10H)-one (3bd)

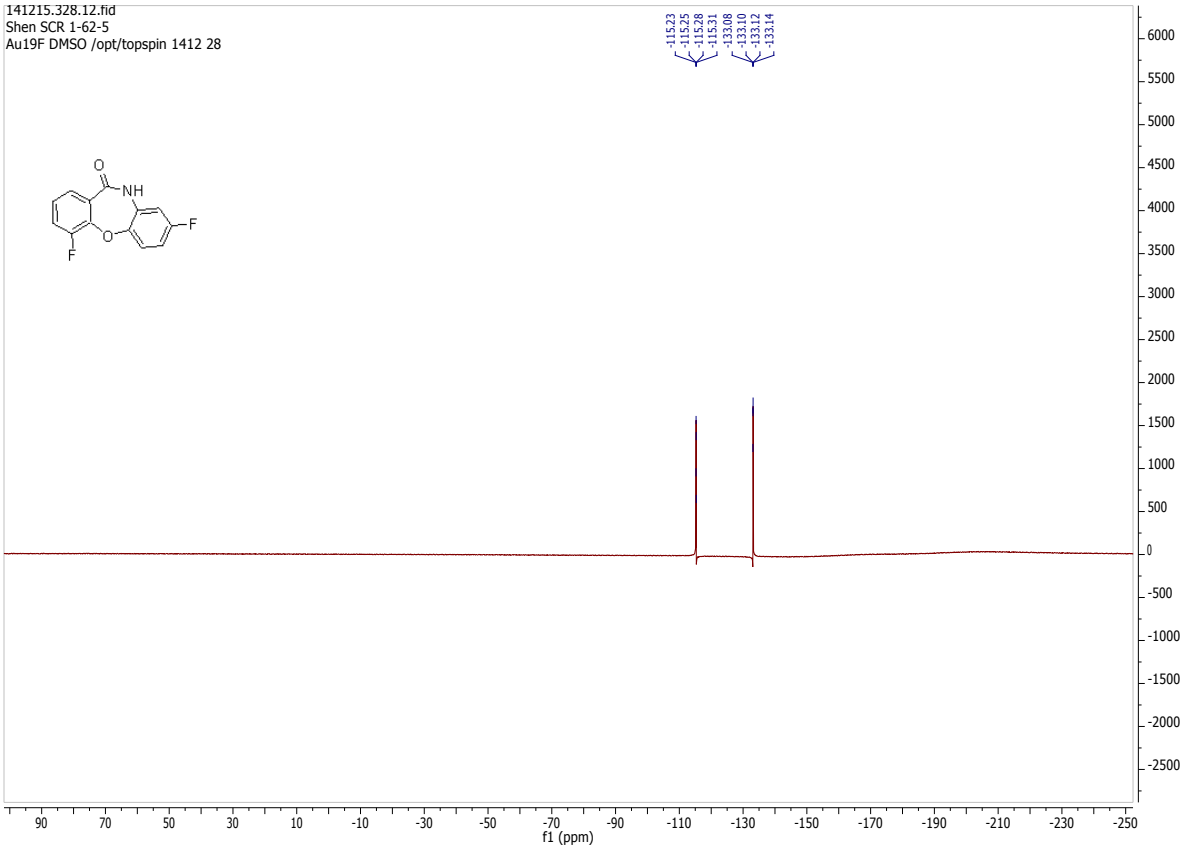


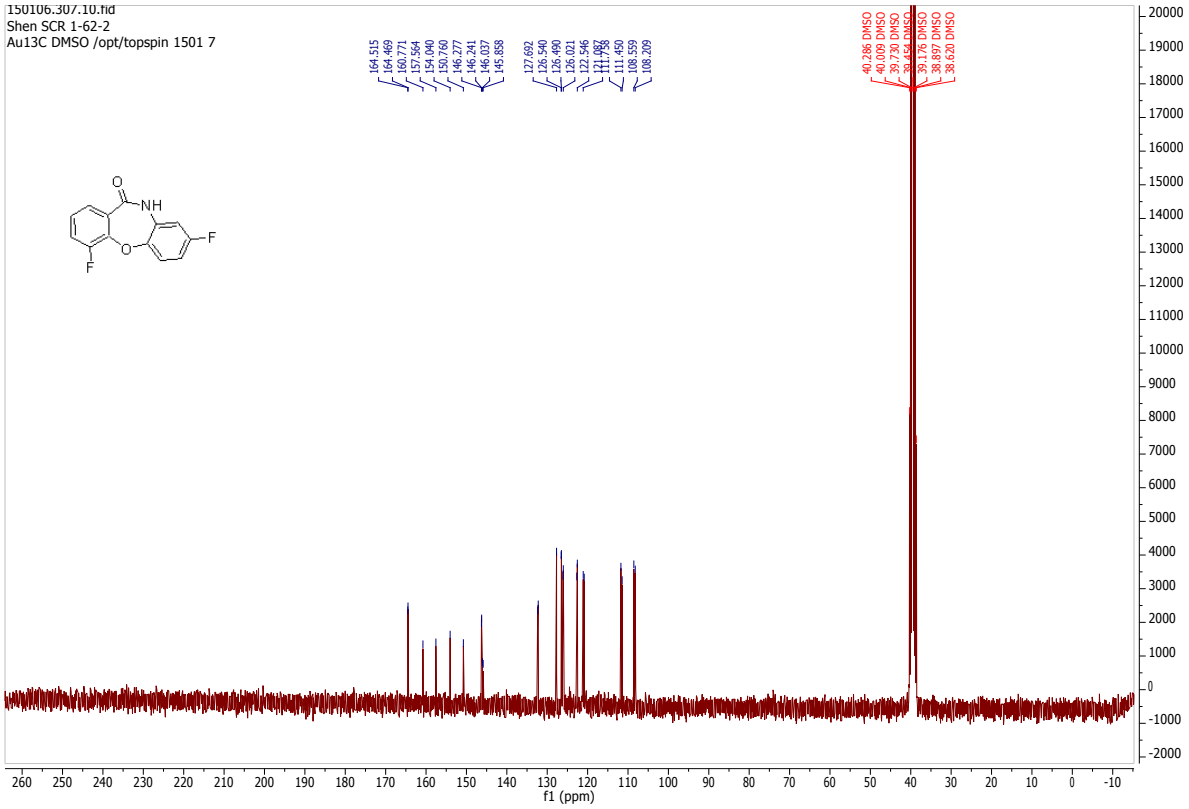

150114.302.11.fid
Shen SCR1-62-4
Au19F DMSO /opt/topspin 1501 2
-132.961
-132.978
-132.996
-133.013
O
NH
Cl
O
F
f1 (ppm)


150114.302.12.fid
Shen SCR1-62-4
Au13C DMSO /opt/topspin 1501 2
164.473
164.430
154.033
150.753
148.720
145.810
145.651
132.350
129.935
127.596
126.579
126.530
126.246
126.154
124.970
122.885
121.234
121.140
120.894
40.264 DMSO
39.987 DMSO
39.709 DMSO
39.431 DMSO
39.154 DMSO
38.876 DMSO
38.598 DMSO
O
NH
Cl
O
F
f1 (ppm)

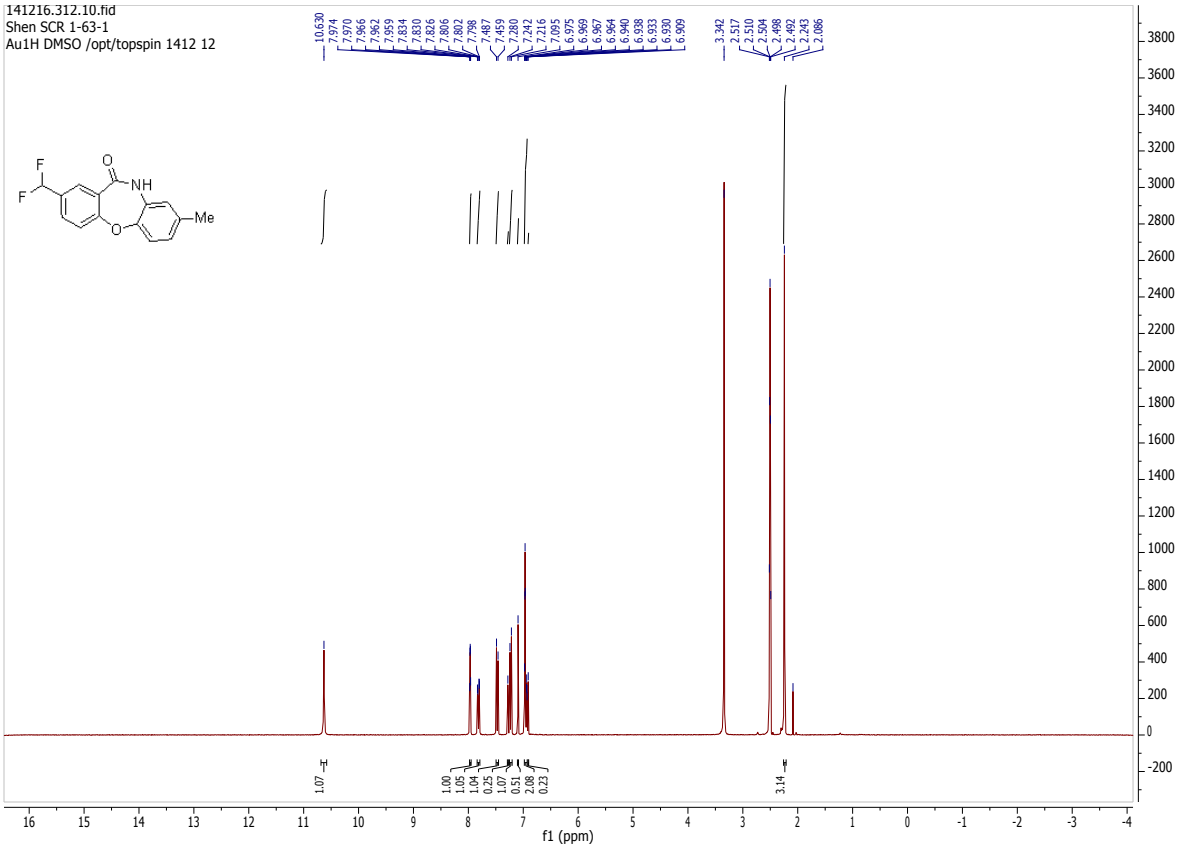
4,8-difluorodibenzo[b,f][1,4]oxazepin-11(10H)-one (3be)

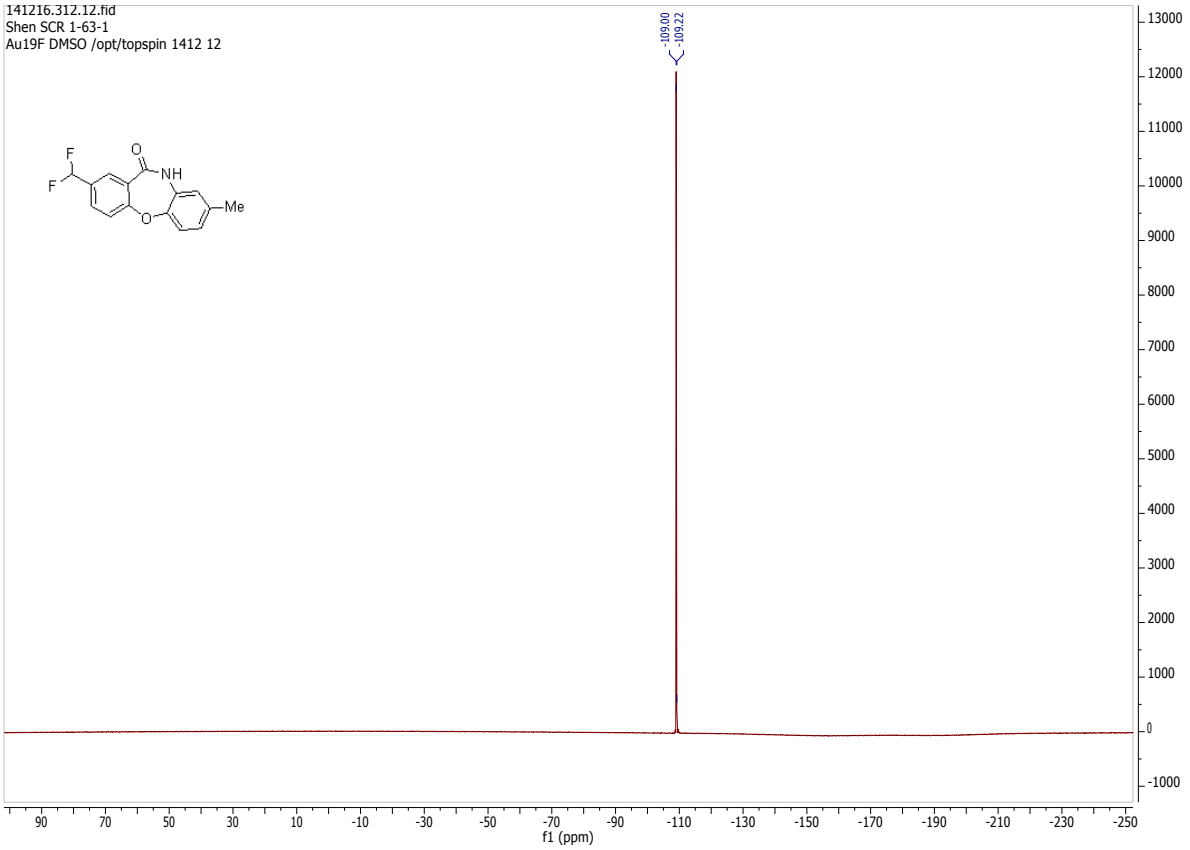


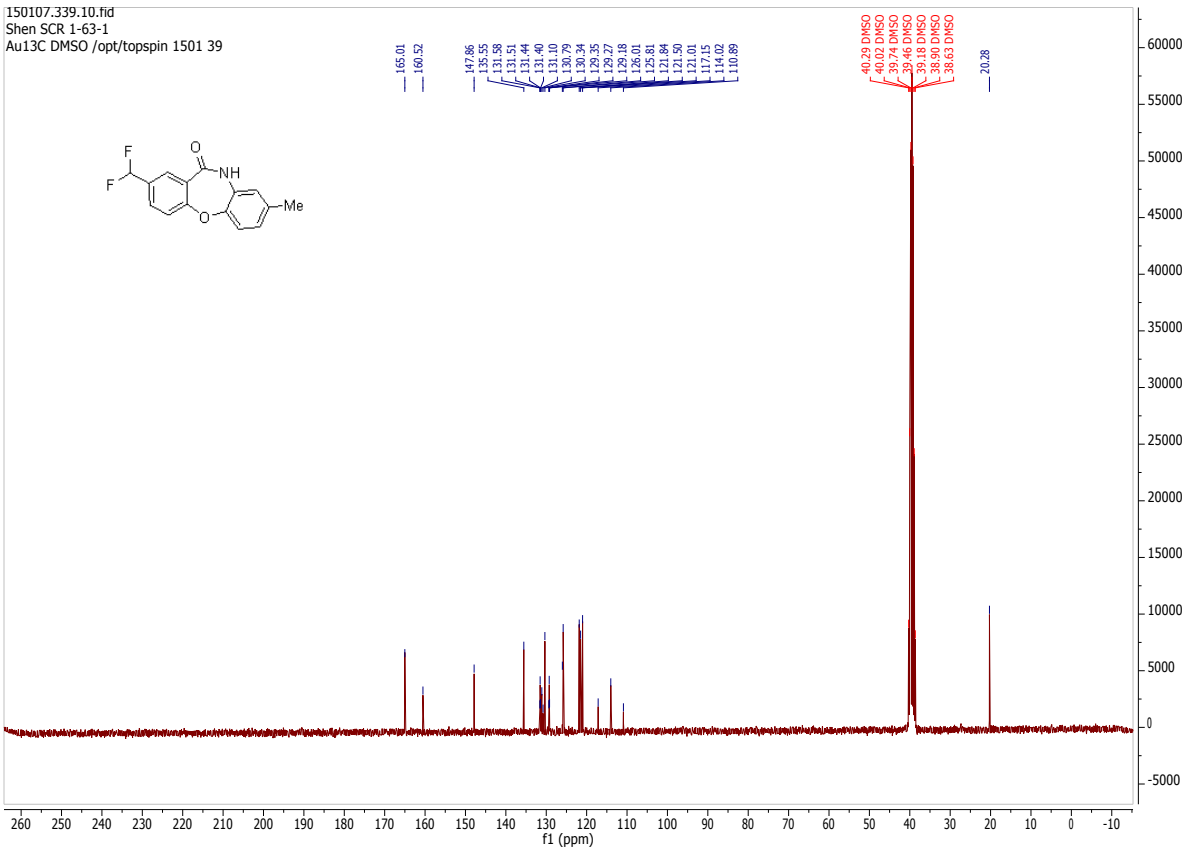




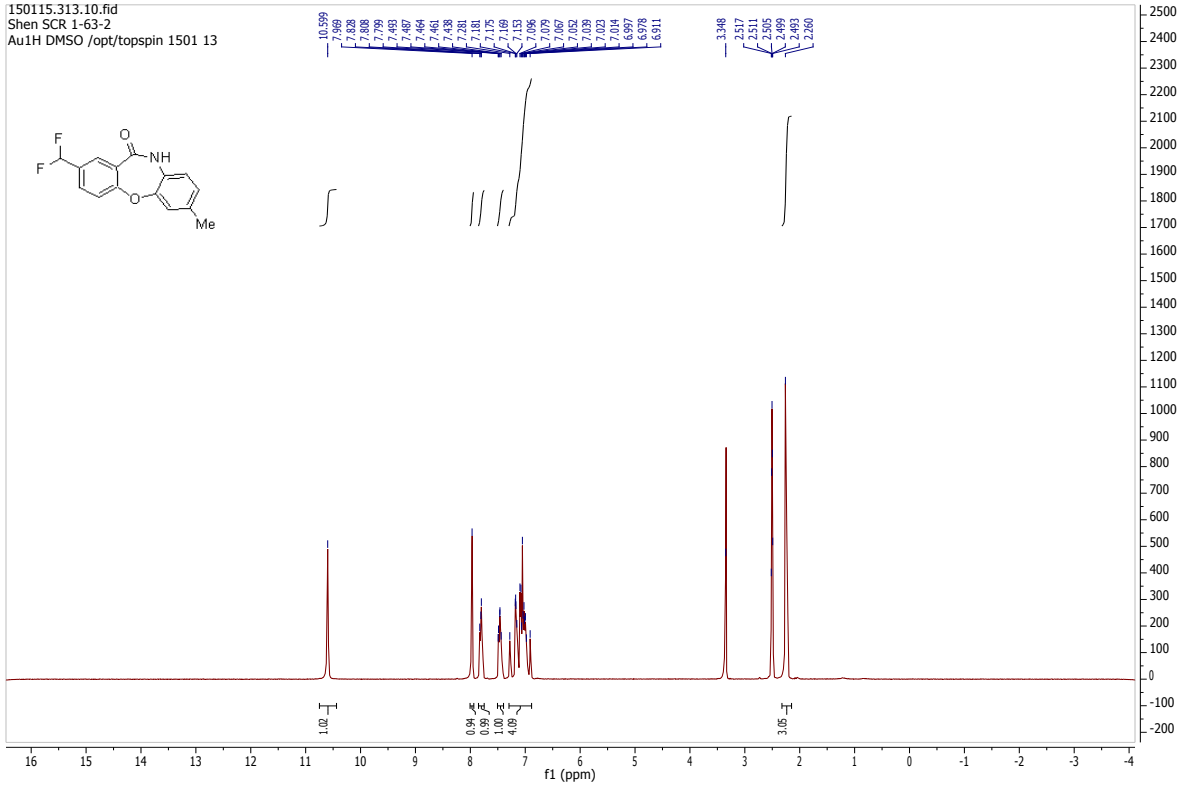
2-(difluoromethyl)-8-methyldibenzo[b,f][1,4]oxazepin-11(10H)-one (3bf)

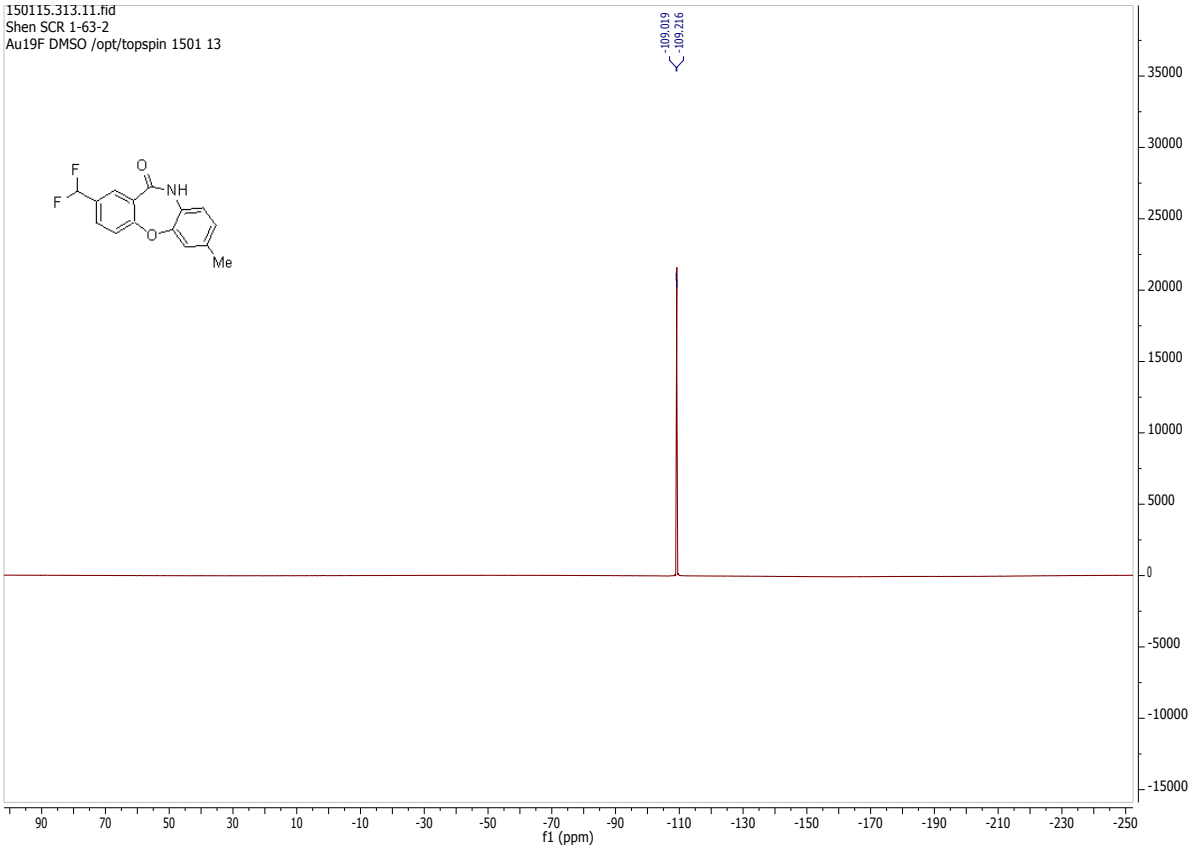


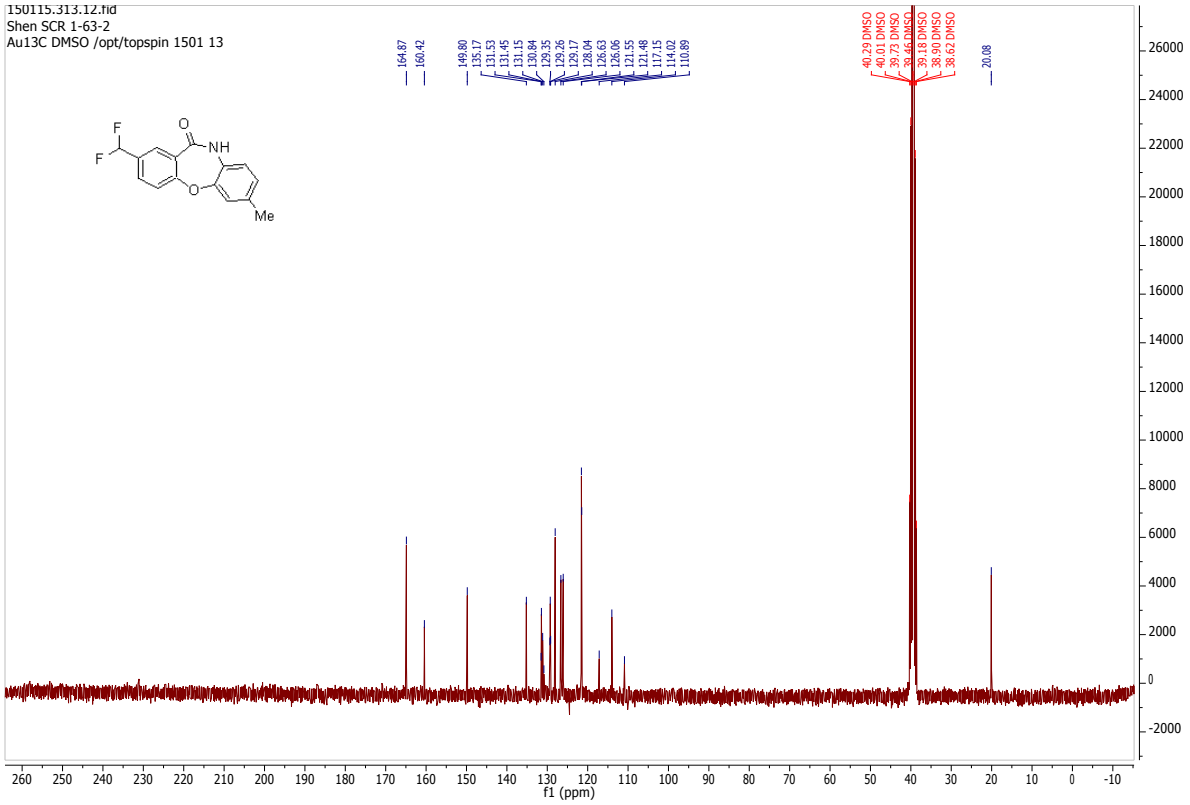

141216.312.12.fid
Shen SCR 1-63-1
Au19F DMSO /opt/topspin 1412 12
-109.00
-109.22
F
F
O
NH
O
Me
f1 (ppm)


150107.339.10.fid
Shen SCR 1-63-1
Au13C DMSO /opt/topspin 1501 39
165.01
160.52
147.86
135.55
131.58
131.51
131.44
131.40
131.10
130.79
130.34
129.35
129.27
129.18
126.01
125.81
121.84
121.50
121.01
117.15
114.02
110.89
40.29 DMSO
40.02 DMSO
39.74 DMSO
39.46 DMSO
39.18 DMSO
38.90 DMSO
38.63 DMSO
20.28
F
F
O
NH
O
Me
f1 (ppm)

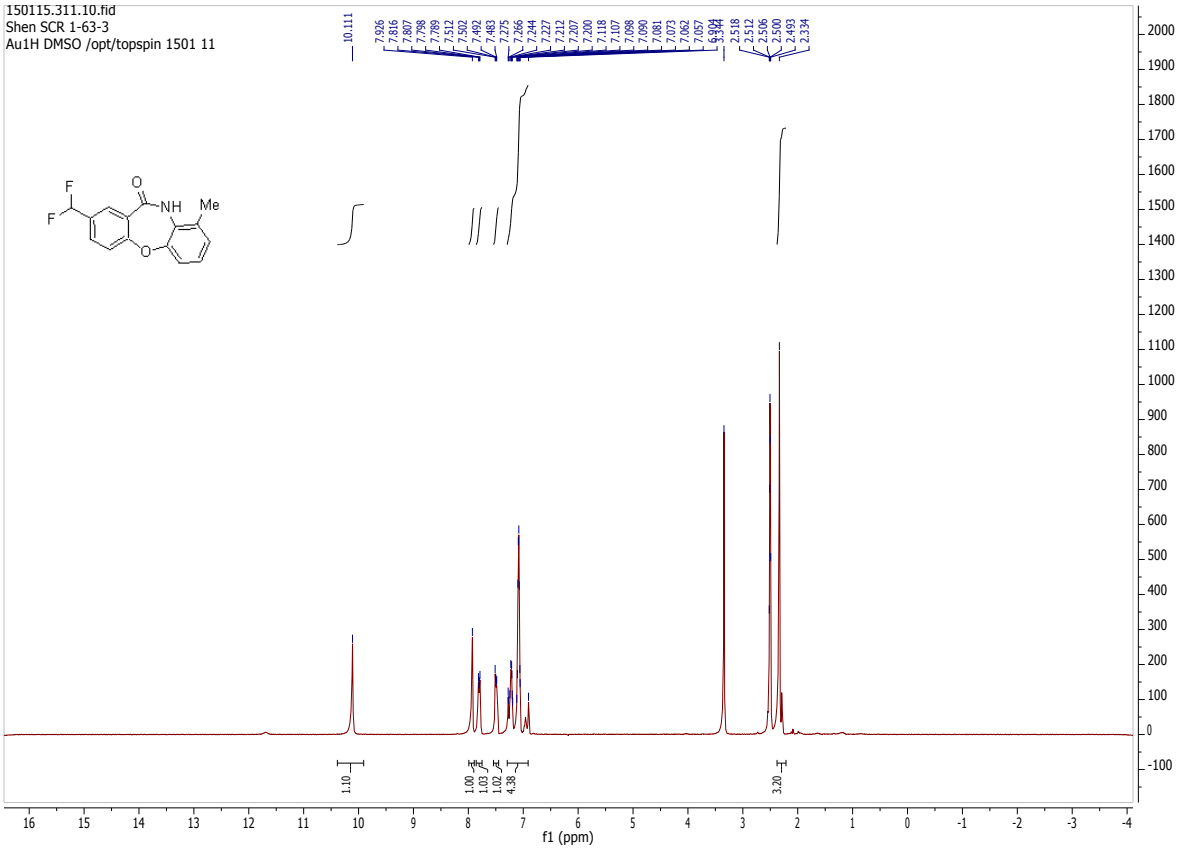
2-(difluoromethyl)-7-methyldibenzo[b,f][1,4]oxazepin-11(10H)-one (3bg)

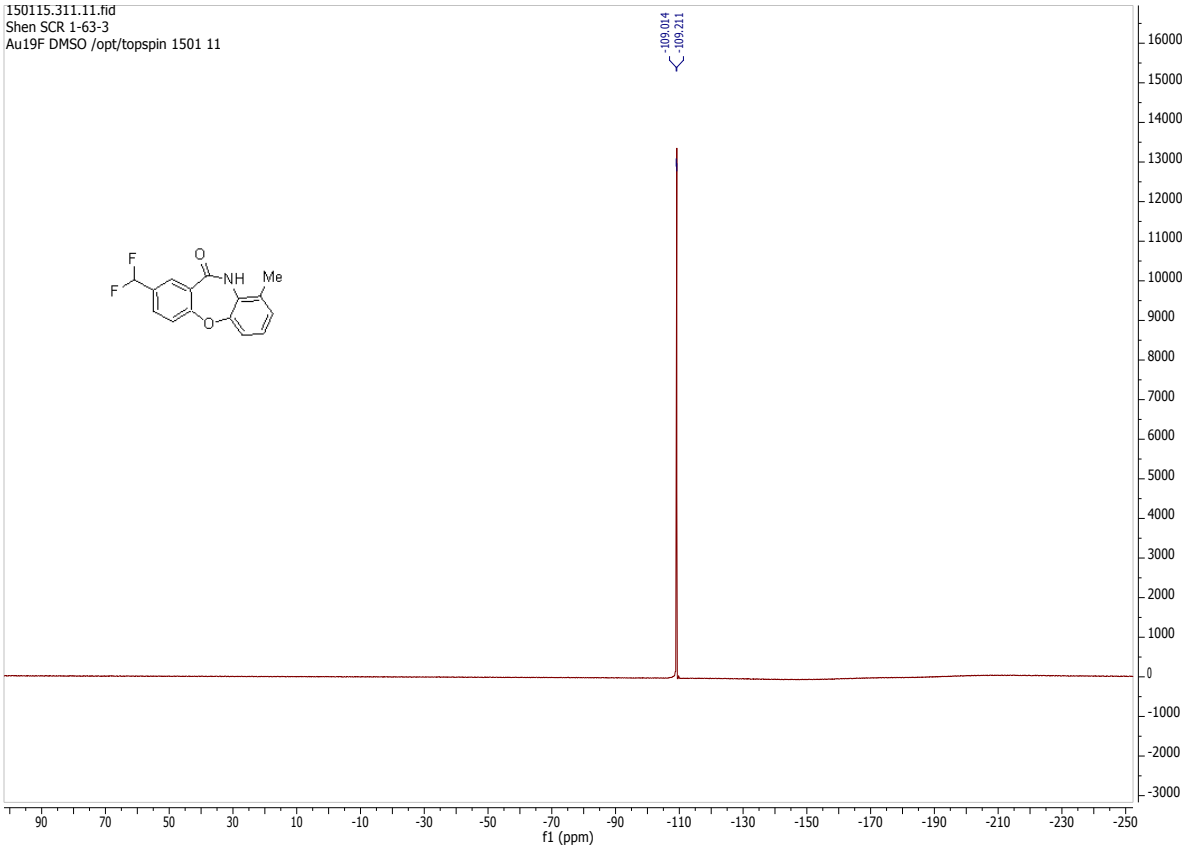


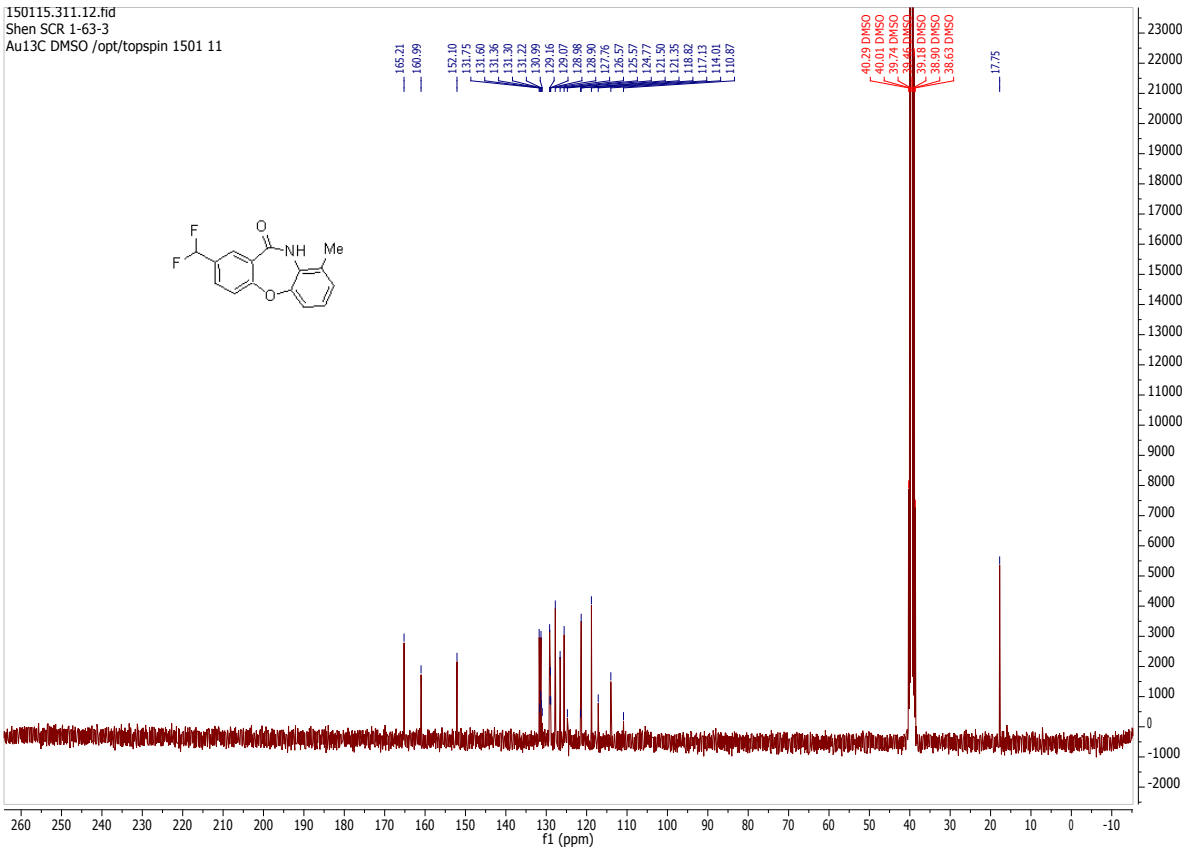




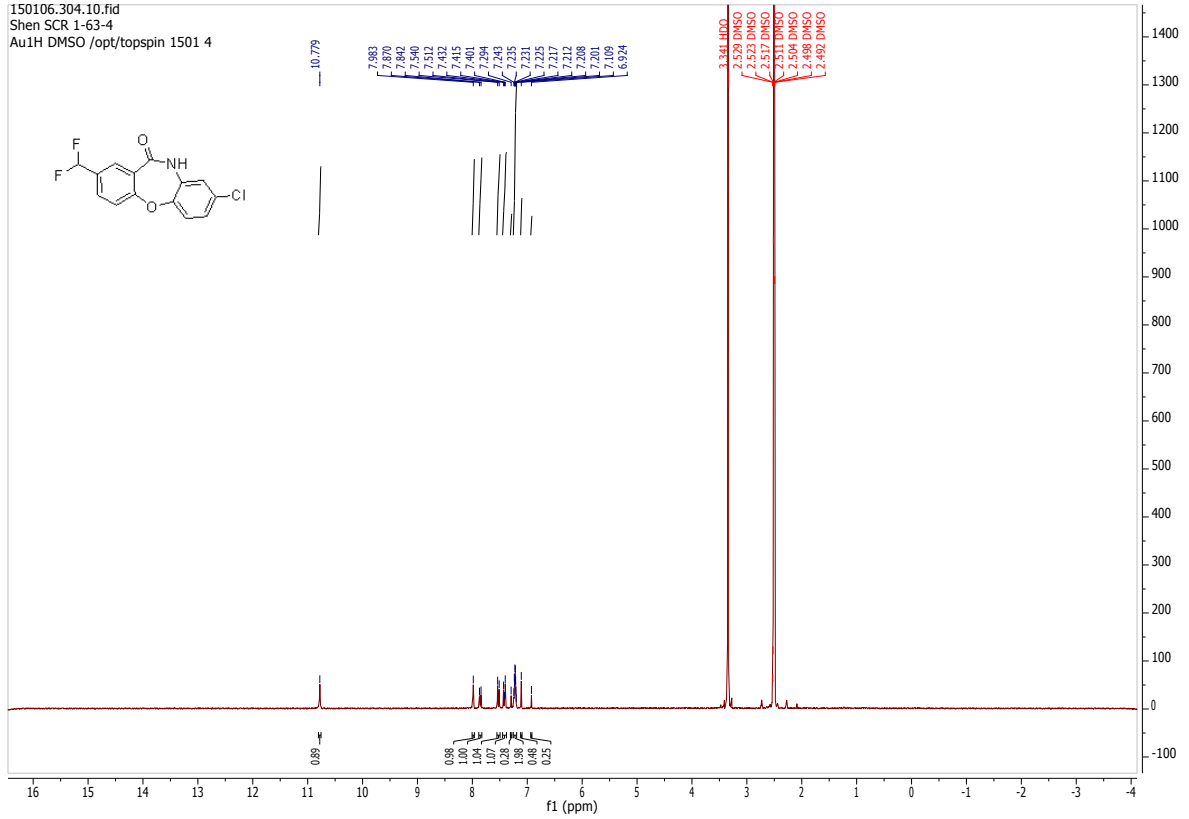
2-(difluoromethyl)-9-methyldibenzo[b,f][1,4]oxazepin-11(10H)-one (3bh)

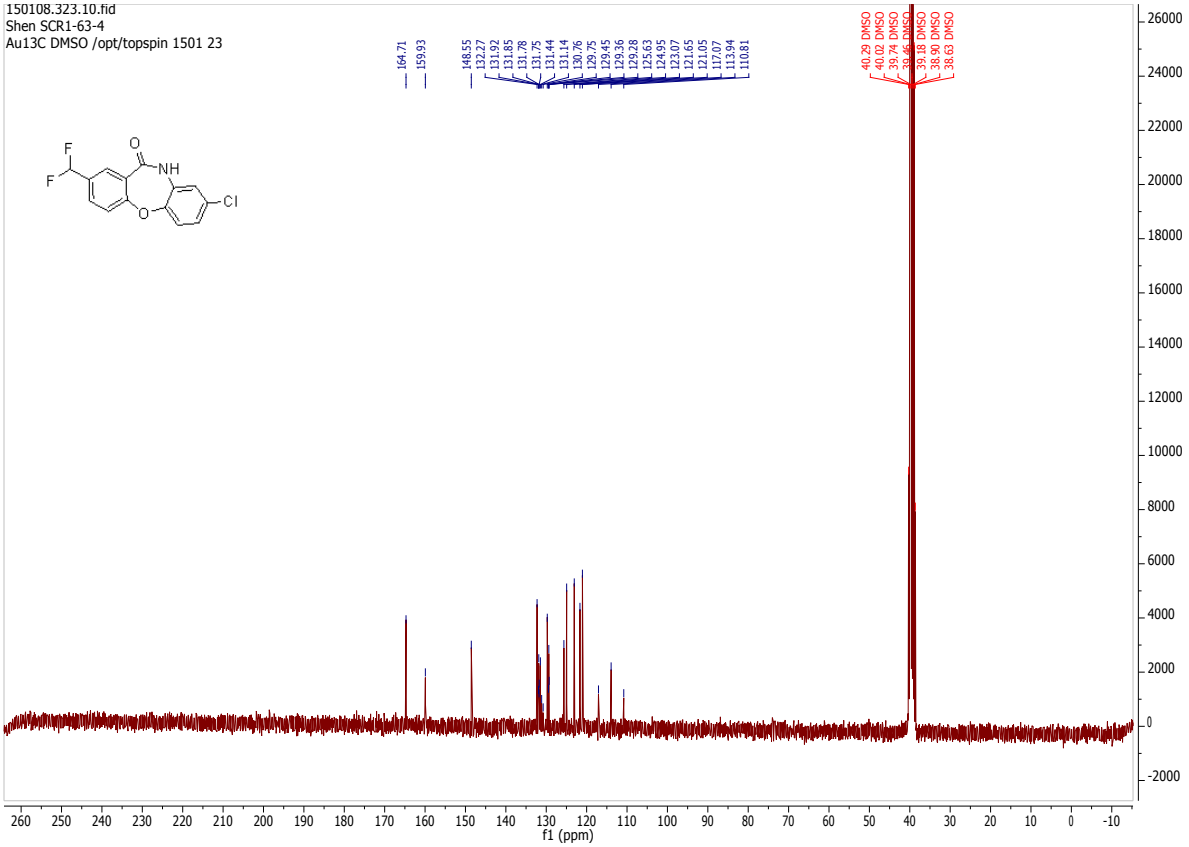


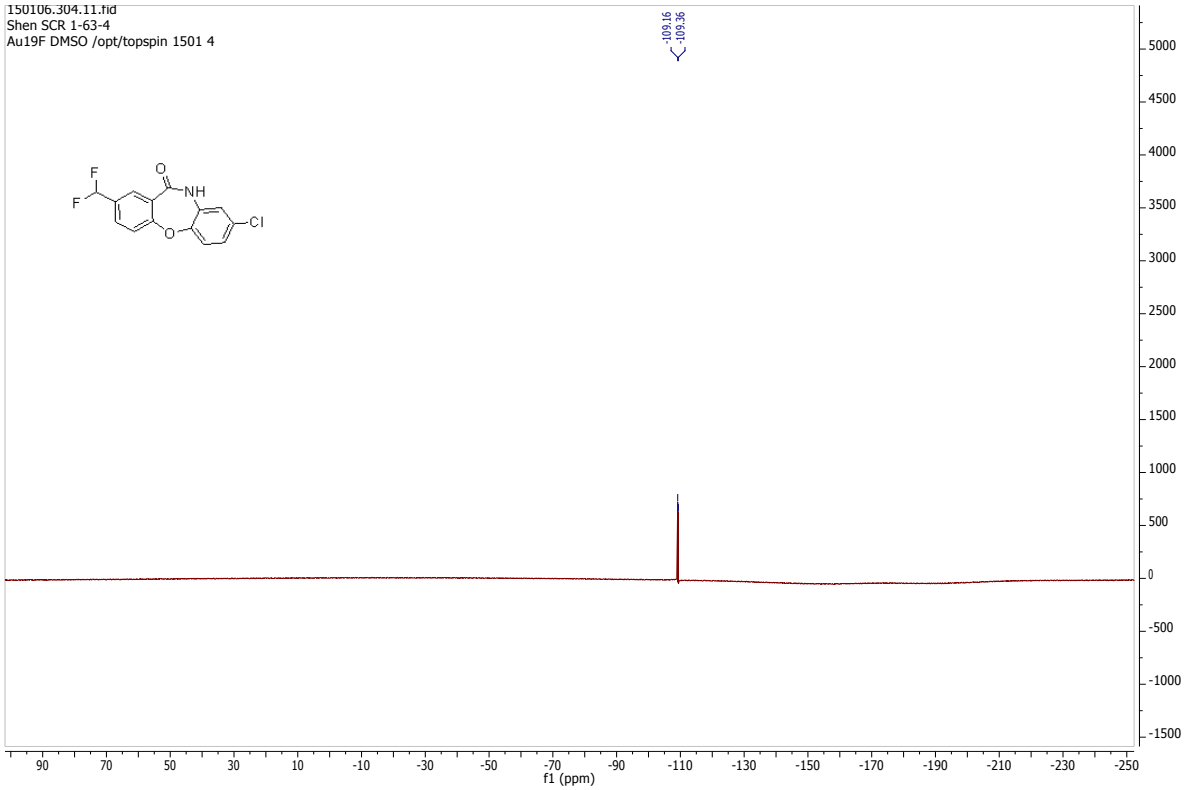

150115.311.11.fid
Shen SCR 1-63-3
Au19F DMSO /opt/topspin 1501 11
-109.014
-109.211
F
F
O
NH
Me
O
f1 (ppm)


150115.311.12.fid
Shen SCR 1-63-3
Au13C DMSO /opt/topspin 1501 11
165.21
160.99
152.10
131.75
131.60
131.36
131.30
131.22
130.99
129.16
129.07
128.98
128.90
127.76
126.57
125.57
124.77
121.50
121.35
118.82
117.13
114.01
110.87
40.29 DMSO
40.01 DMSO
39.74 DMSO
39.46 DMSO
39.18 DMSO
38.90 DMSO
38.63 DMSO
17.75
F
F
O
NH
Me
O
f1 (ppm)

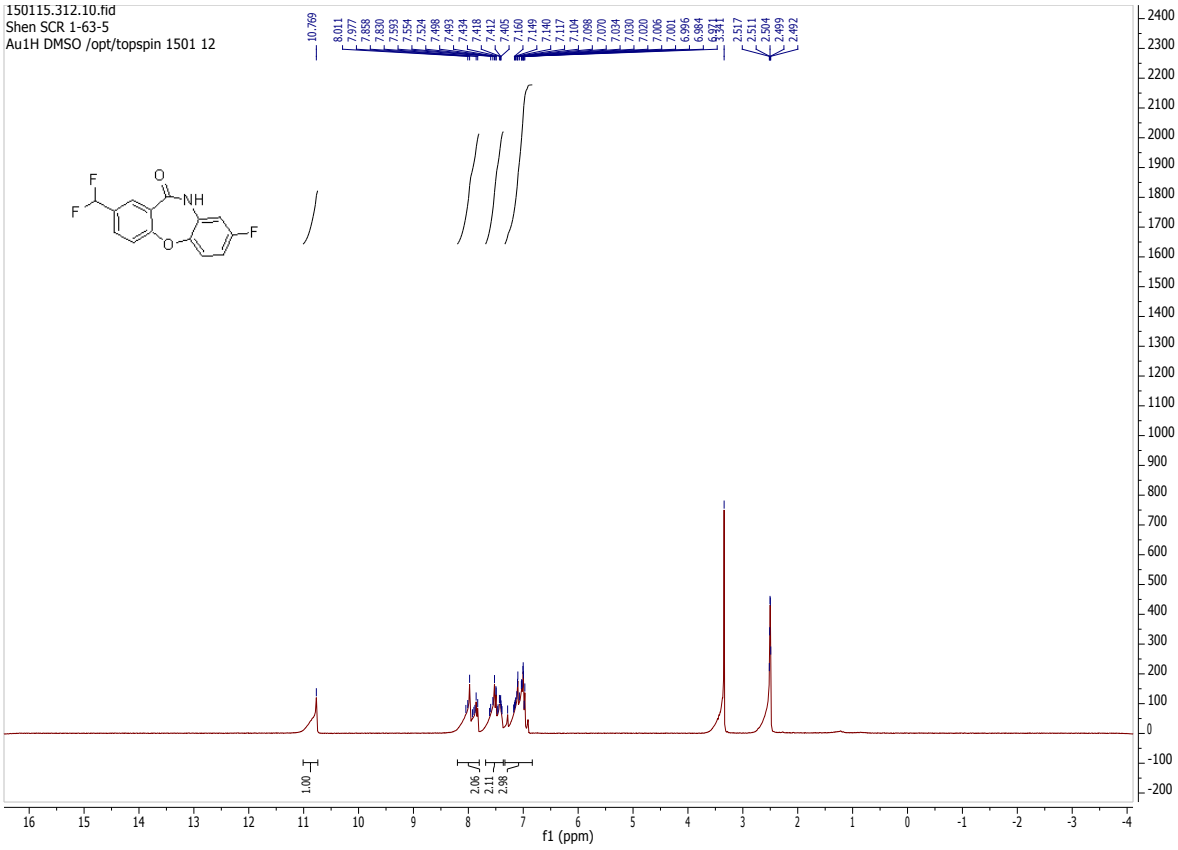
8-chloro-2-(difluoromethyl)dibenzo[b,f][1,4]oxazepin-11(10H)-one (3bi)

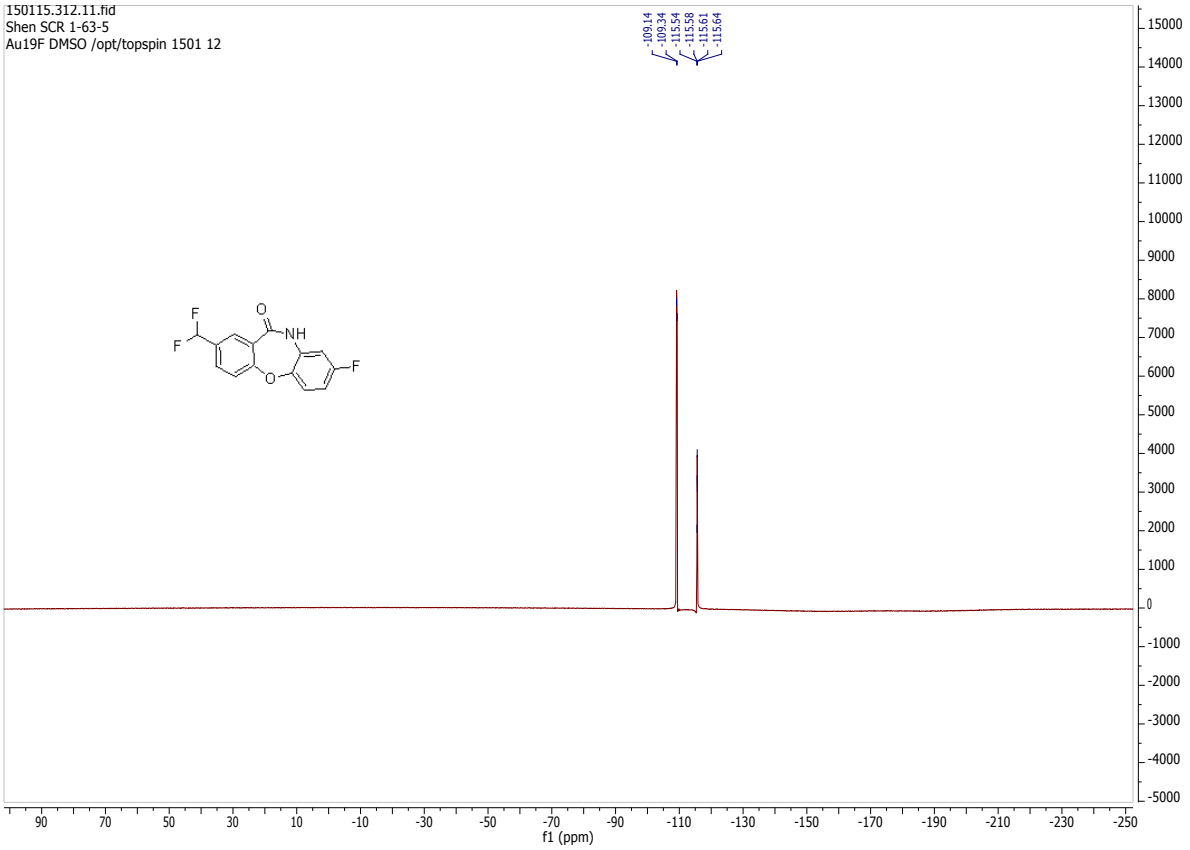


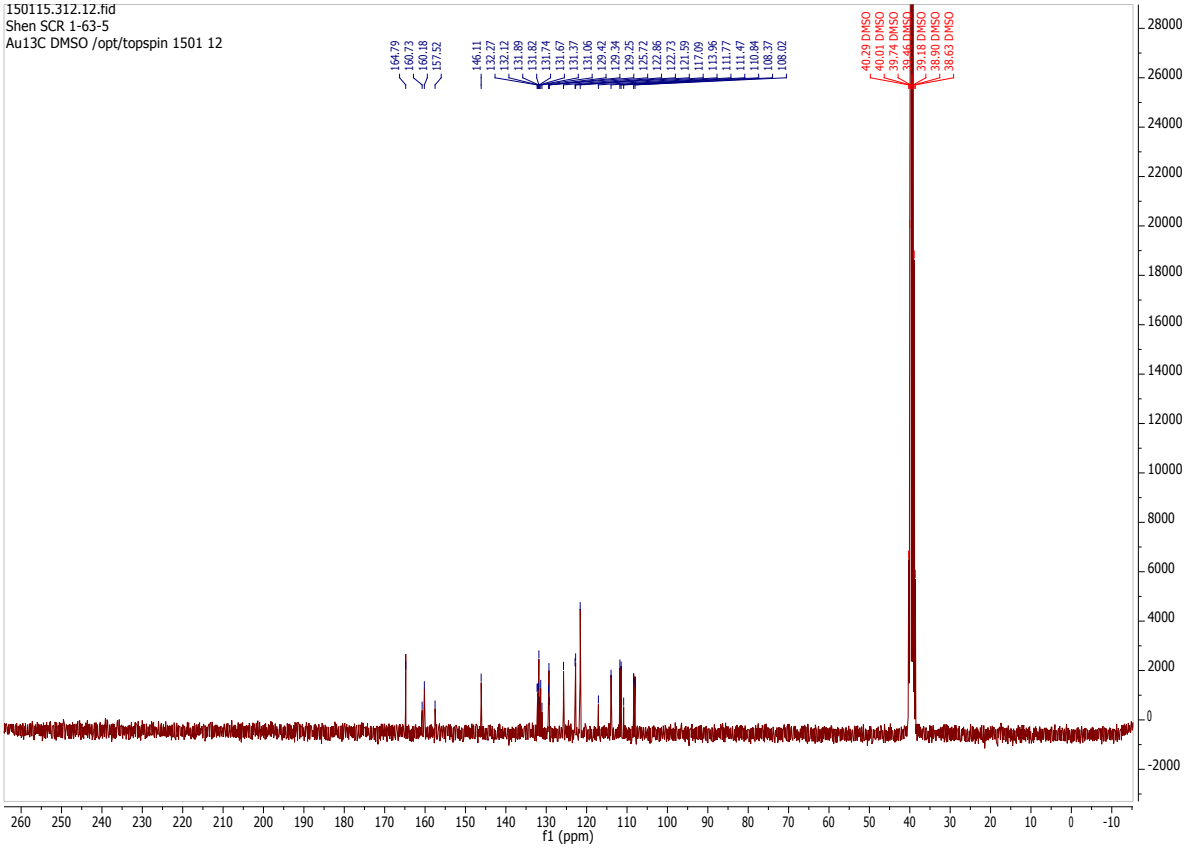




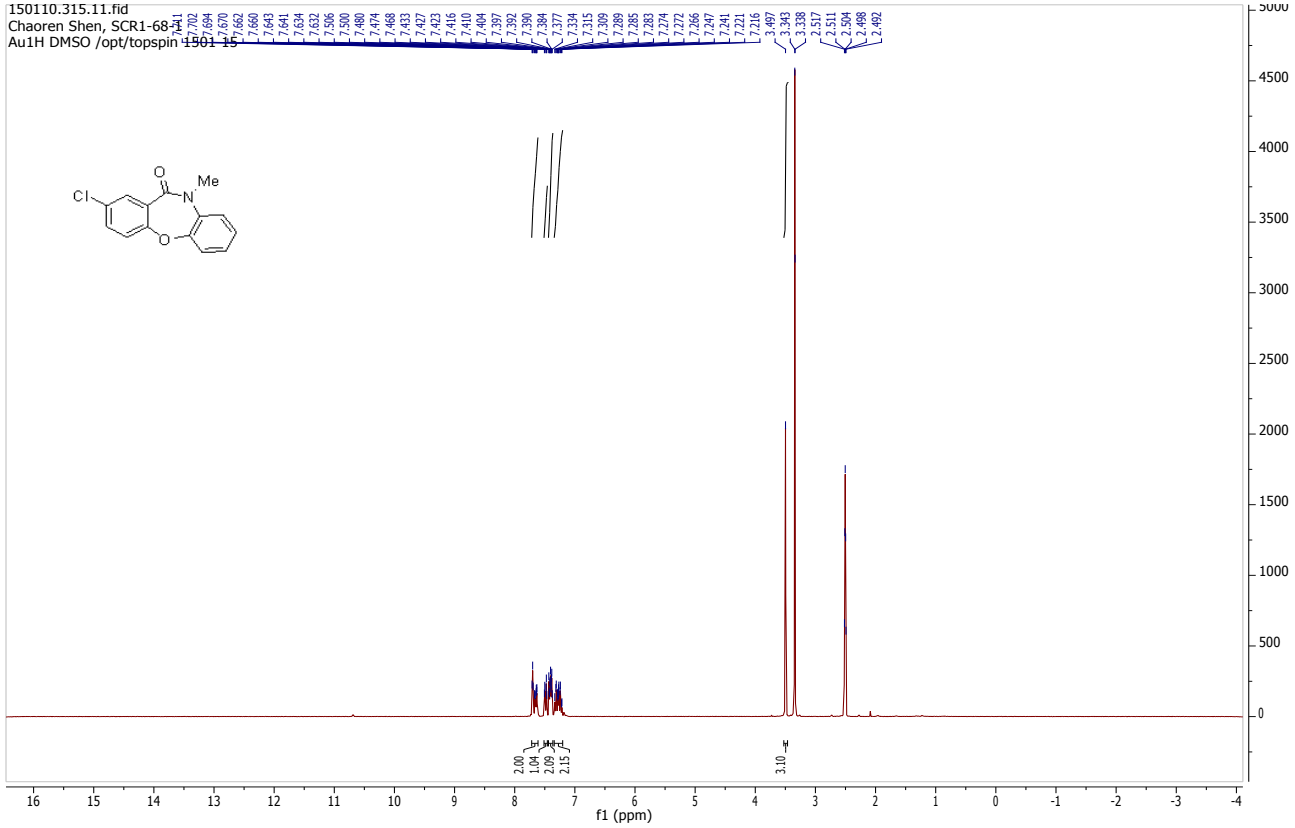
2-(difluoromethyl)-8-fluorodibenzo[b,f][1,4]oxazepin-11(10H)-one (3bj)

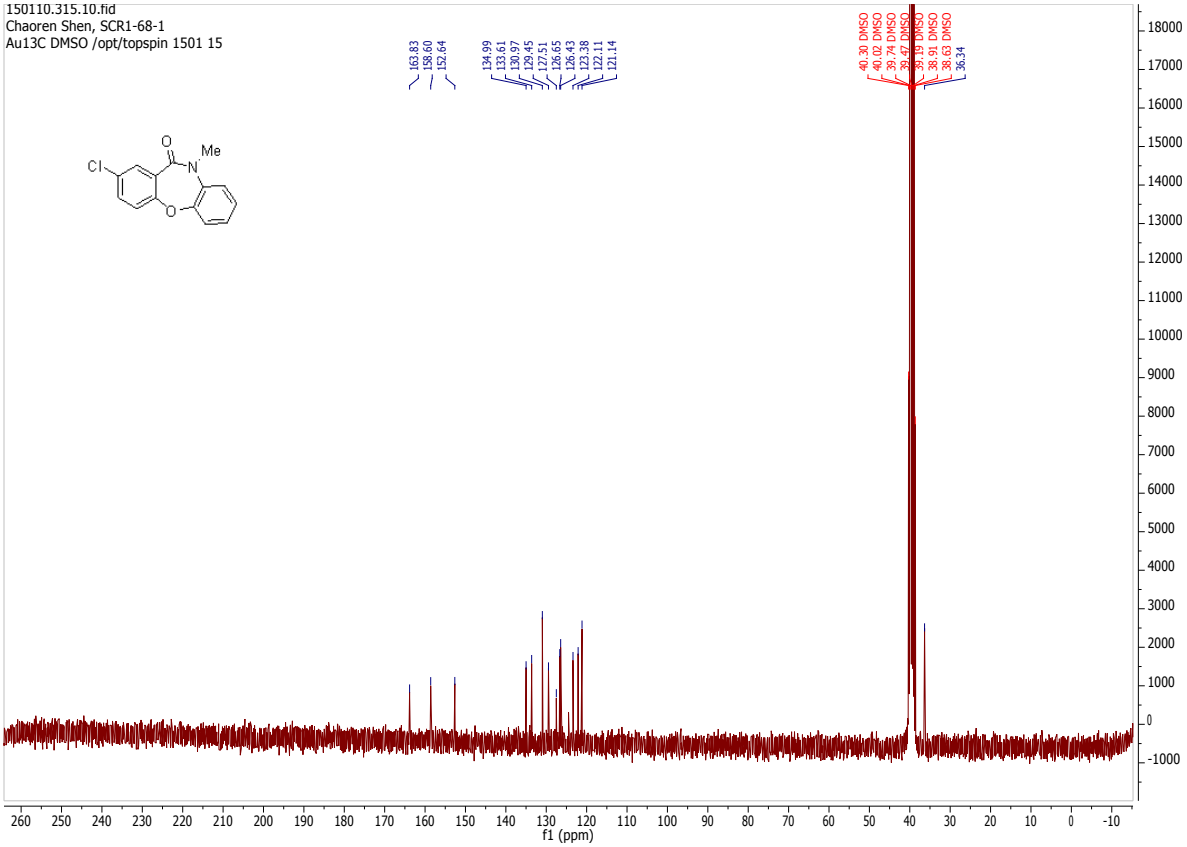



150115.312.11.fid
Shen SCR 1-63-5
Au19F DMSO /opt/topspin 1501 12
-109.14
-109.34
-115.54
-115.58
-115.61
-115.64
F
F
O
NH
O
F
f1 (ppm)

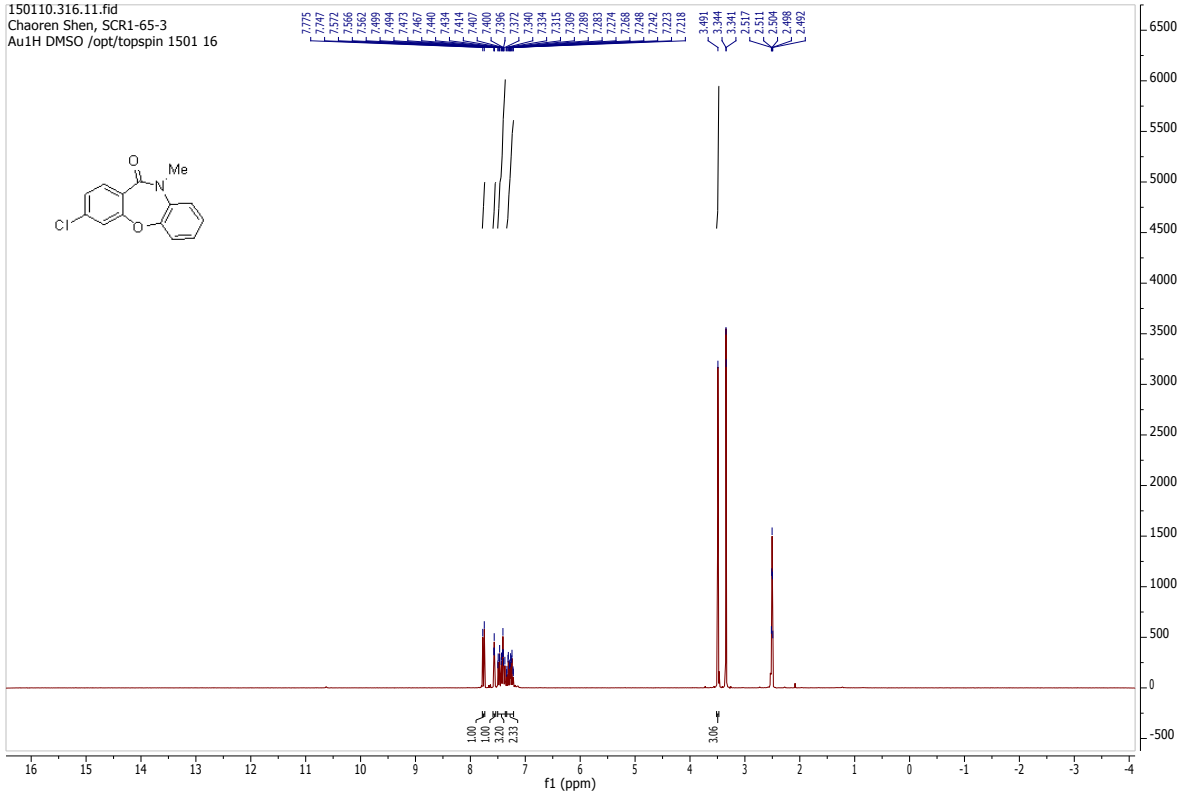

150115.312.12.fid
Shen SCR 1-63-5
Au13C DMSO /opt/topspin 1501 12
164.79
160.73
160.18
157.52
146.11
132.27
132.12
131.89
131.82
131.74
131.67
131.37
131.06
129.42
129.34
129.25
125.72
122.86
122.73
121.59
117.09
113.96
111.77
111.47
110.84
108.37
108.02
40.29 DMSO
40.01 DMSO
39.74 DMSO
39.46 DMSO
39.18 DMSO
38.90 DMSO
38.63 DMSO
f1 (ppm)

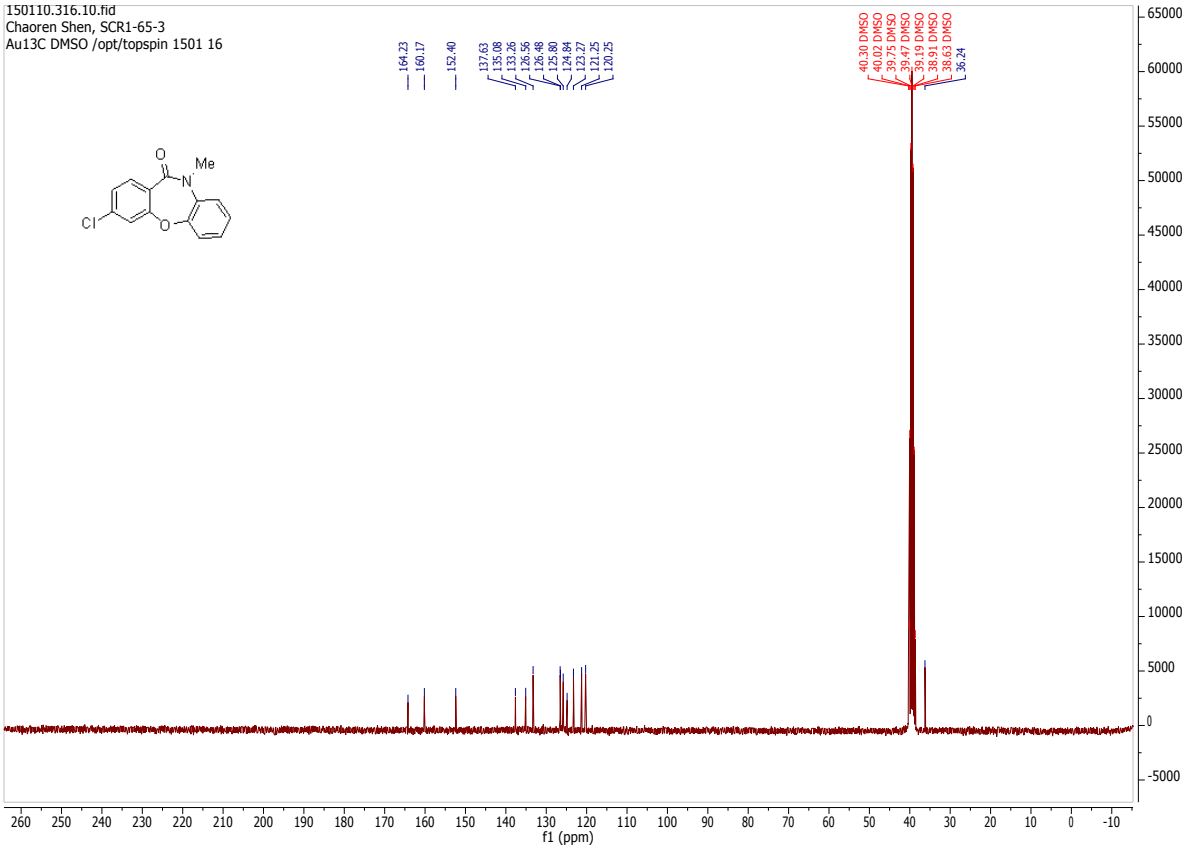
2-chloro-10-methyldibenzo[b,f][1,4]oxazepin-11(10H)-one (5a)



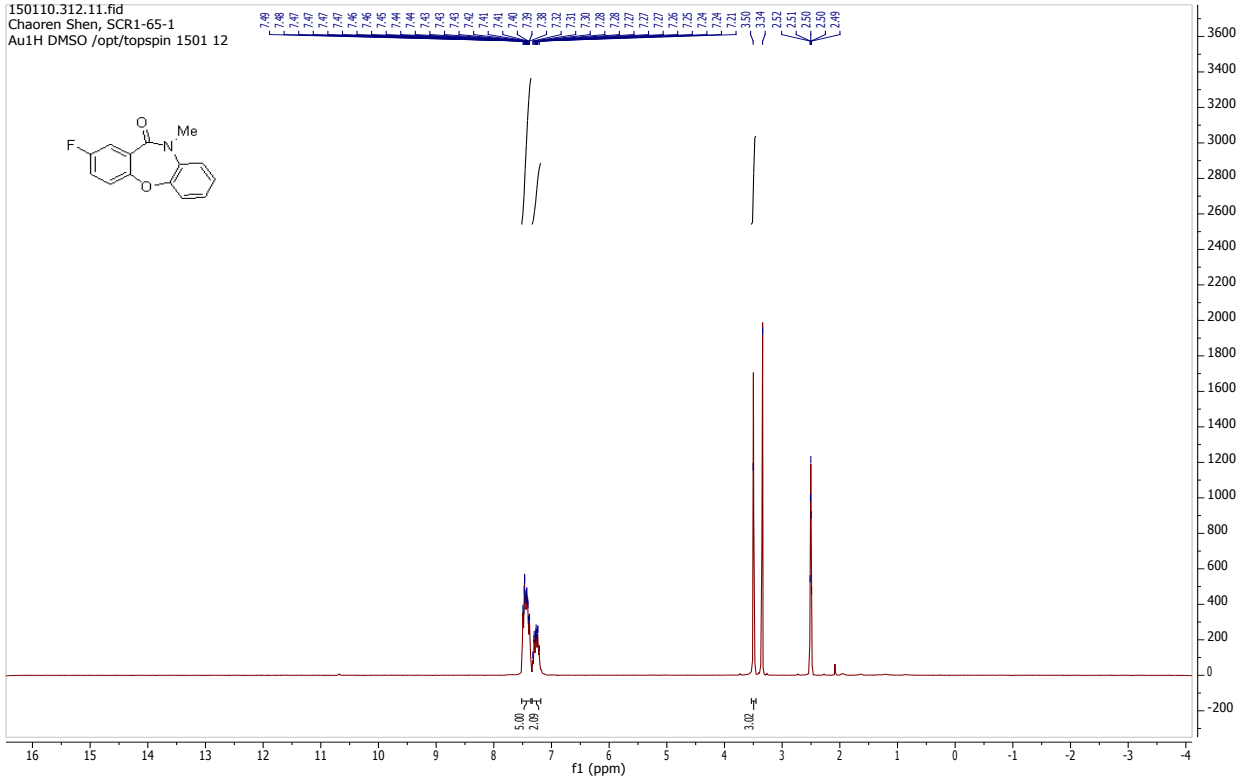


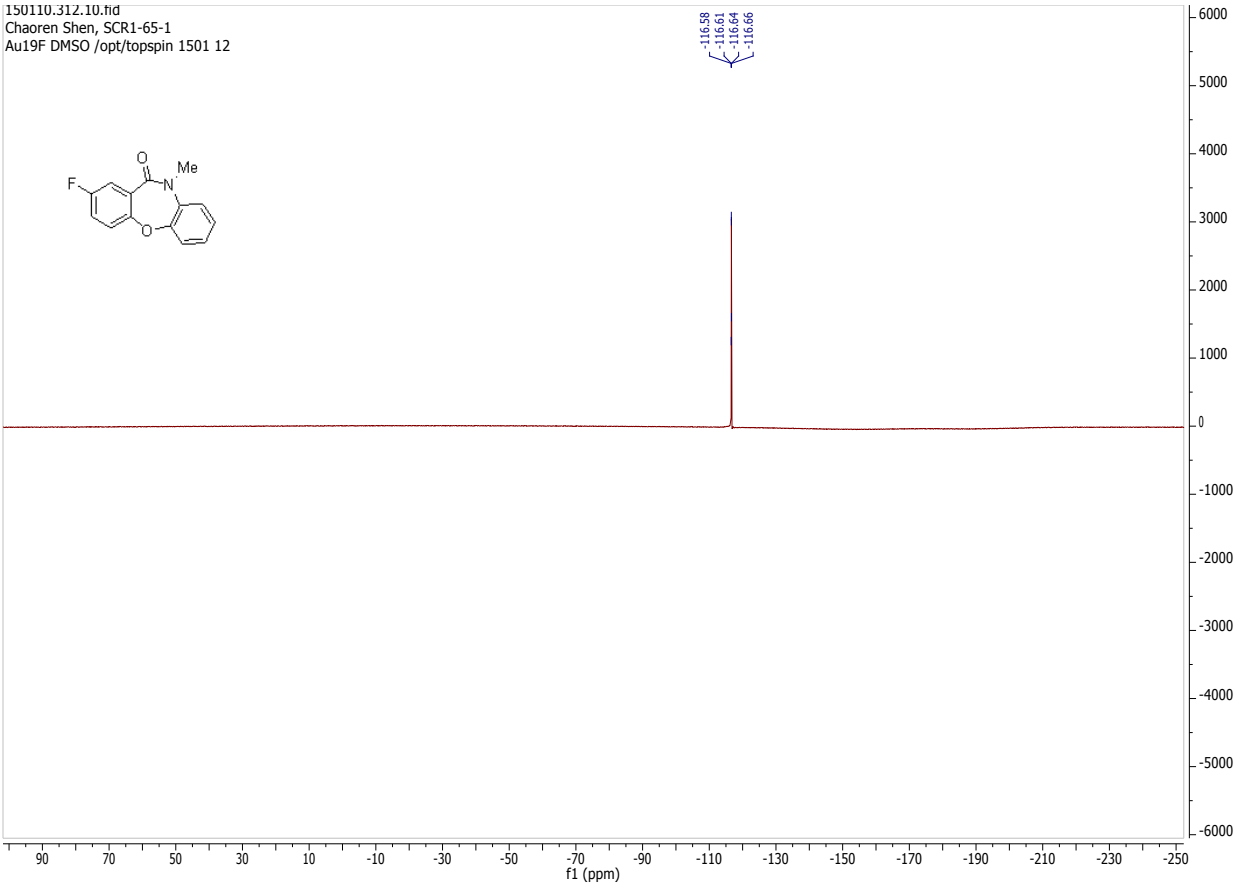
3-chloro-10-methyldibenzo[b,f][1,4]oxazepin-11(10H)-one (5b)

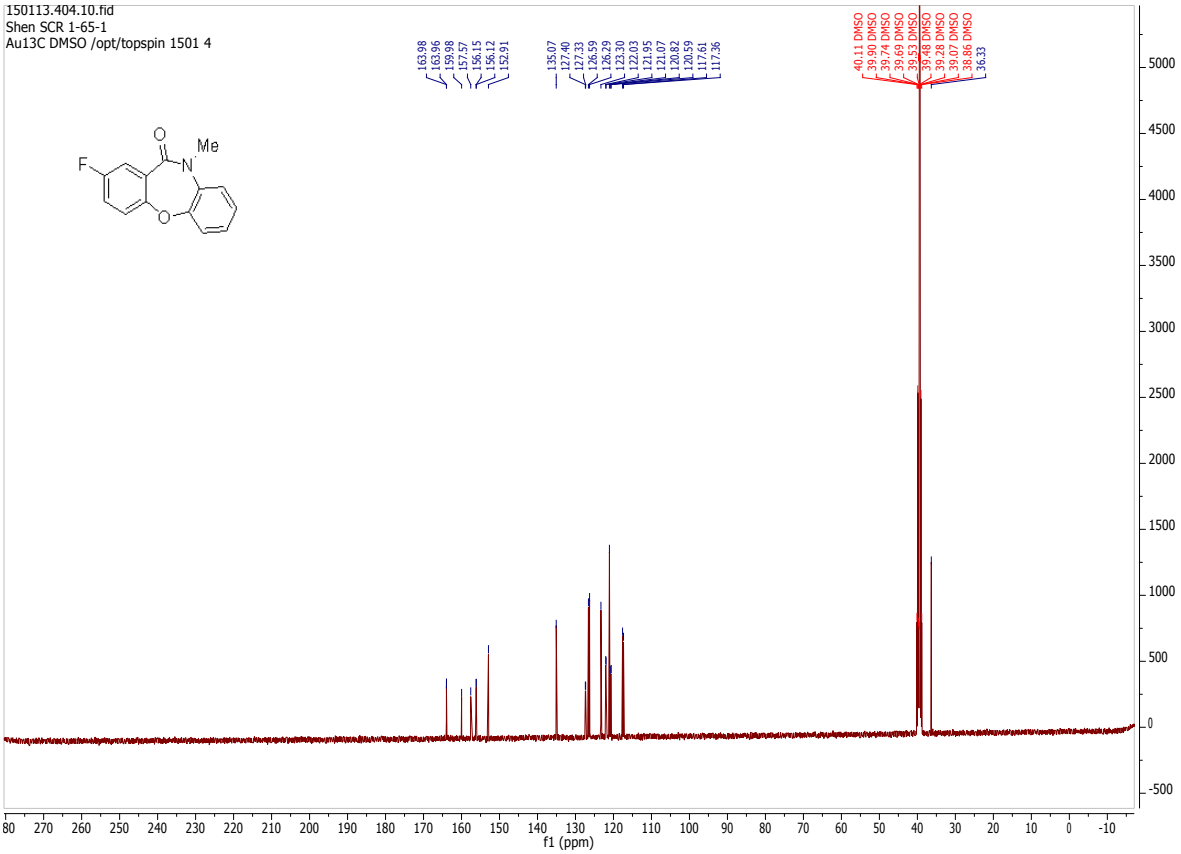




2-fluoro-10-methyldibenzo[b,f][1,4]oxazepin-11(10H)-one (5c)







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