Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Asymmetric Difluorocarbonylation Reactions of Non-active Imines Catalyzed by $Bi(OAc)_3$/Chiral Phosphoric Acid

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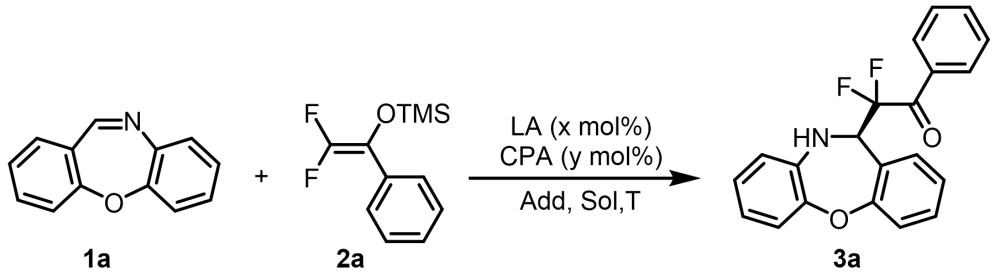
Table of Contents

1. General information

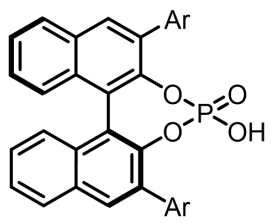
Unless otherwise noted, commercially available reagents were used without further purification. Proton (^{1}H NMR) and carbon (^{13}C NMR) were recorded on a Bruker - DPX 400 spectrometer. Fluorine(^{19}F NMR) were recorded on a Varian NMR 400 spectrometer. Chemical shifts are reported in parts per million (ppm) on the delta (δ) scale, and the residual solvent peak was used as an internal reference, for ^{1}H NMR: $CDCl_3$ = 7.26 ppm; $(CD_3)_2CO$ = 2.05 ppm; for ^{13}C NMR: $CDCl_3$ = 77.16 ppm; $(CD_3)_2CO$ = 206.26 ppm. Analytical TLC was performed on precoated silica gel GF254 plates. Flash column chromatography was performed using 200-300 mesh silica gel.The following abbreviations were used to designate the multiplicities: s = singlet; d = doublet; t = triplet; q = quartet; m = multiplet; br = broad. All first-order splitting patterns were assigned on the basis of the appearance of the multiplet. Splitting patterns that could not be easily interpreted are designated as multiplet (m) or broad (br). HPLC analysis was performed using Chiralcel columns purchased. Mass spectra were obtained using electrospray ionization (ESI) mass spectrometer. Seven-membered cyclic Imines[1] and enol silyl ethers[2] were prepared as previously described. All other reagents were obtained commercially unless otherwise noted.

2. Optimization of the Reaction Conditions

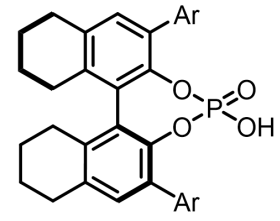
Table S1. Detailed Reaction Optimization[a]



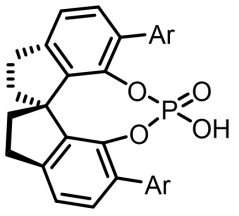
1a + **2a** → **3a**



(*S*)-**4a**: Ar= 2,4,6-^{i}Pr$_3$C$_6$H$_2$
(*S*)-**4b**: Ar= 9-anthryl
(*S*)-**4c**: Ar= 1-naphthyl
(*S*)-**4d**: Ar= phenanthrenyl
(*S*)-**4e**: Ar= 3,5-(CF$_3$)$_2$C$_6$H$_3$
(*S*)-**4f**: Ar= 2-naphthyl
(*S*)-**4g**: Ar= 3,5-^{t}Bu$_2$-4-OMeC$_6$H$_2$
(*S*)-**4h**: Ar= 4-(2-naphthyl)C$_6$H$_4$
(*S*)-**4i**: Ar= 3,5-Me$_2$C$_6$H$_3$



(*S*)-**5j**: Ar= 2,4,6-^{i}Pr$_3$C$_6$H$_2$
(*S*)-**5k**: Ar= 9-anthryl
(*S*)-**5l**: Ar= 4-Ph-C$_6$H$_4$
(*S*)-**5m**: Ar= phenanthrenyl
(*R*)-**5n**: Ar= 1-pyrenyl
(*S*)-**5o**: Ar= 1-naphthyl



(*S*)-**6p**: Ar= 2,4,6-^{i}Pr$_3$C$_6$H$_2$
(*S*)-**6q**: Ar= 3,5-(CF$_3$)$_2$C$_6$H$_3$
(*R*)-**6r**: Ar= 1-pyrenyl
(*S*)-**6s**: Ar= 9-anthryl
(*S*)-**6t**: Ar= phenanthreny
(*S*)-**6u**: Ar= 3,5-Ph$_2$C$_6$H$_3$

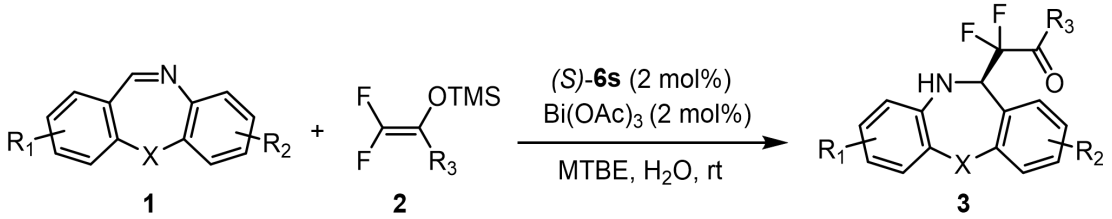
Entry	LA	CPA	Solvent	x/%	y/%	Add	Time/h	Yield[b]/%	e.r.[c]/%
1	--	**4a**	DCM	--	2	--	24	20	66:34
2	Bi(OAc)$_3$	**4a**	DCM	2	2	--	24	32	68:32
3	Bi(OAc)$_3$	**4b**	DCM	2	2	--	24	35	69:31
4	Bi(OAc)$_3$	**4c**	DCM	2	2	--	24	26	59:41
5	Bi(OAc)$_3$	**4d**	DCM	2	2	--	24	33	63:37

6	$Bi(OAc)_3$	**4e**	DCM	2	2	--	24	42	65:35
7	$Bi(OAc)_3$	**4f**	DCM	2	2	--	24	15	50:50
8	$Bi(OAc)_3$	**4g**	DCM	2	2	--	24	10	64:36
9	$Bi(OAc)_3$	**4h**	DCM	2	2	--	24	36	54:46
10	$Bi(OAc)_3$	**4i**	DCM	2	2	--	24	22	52:48
11	$Bi(OAc)_3$	**5j**	DCM	2	2	--	24	52	69:31
12	$Bi(OAc)_3$	**5k**	DCM	2	2	--	24	41	67:33
13	$Bi(OAc)_3$	**5l**	DCM	2	2	--	24	21	53:47
14	$Bi(OAc)_3$	**5m**	DCM	2	2	--	24	61	59:41
15	$Bi(OAc)_3$	**5n**	DCM	2	2	--	24	50	60:40
16	$Bi(OAc)_3$	**5o**	DCM	2	2	--	24	11	50:50
17	$Bi(OAc)_3$	**6p**	DCM	2	2	--	24	57	72:28
18	$Bi(OAc)_3$	**6q**	DCM	2	2	--	24	53	74:26
19	$Bi(OAc)_3$	**6r**	DCM	2	2	--	24	43	76:24
20	$Bi(OAc)_3$	**6s**	DCM	2	2	--	24	58	84:16
21	$Bi(OAc)_3$	**6t**	DCM	2	2	--	24	39	76:24
22	$Bi(OAc)_3$	**6u**	DCM	2	2	--	24	47	77:23
23	$Bi(OAc)_3$	**6s**	$CHCl_3$	2	2	--	24	40	89:11
24	$Bi(OAc)_3$	**6s**	CCl_4	2	2	--	24	53	92:8
25	$Bi(OAc)_3$	**6s**	DCE	2	2	--	24	57	90:10
26	$Bi(OAc)_3$	**6s**	toluene	2	2	--	24	50	91:9
27	$Bi(OAc)_3$	**6s**	CH_3CN	2	2	--	24	47	88:12
28	$Bi(OAc)_3$	**6s**	THF	2	2	--	24	42	93:7
29	$Bi(OAc)_3$	**6s**	dioxane	2	2	--	24	10	94:6
30	$Bi(OAc)_3$	**6s**	DIPE	2	2	--	24	24	95:5
31	$Bi(OAc)_3$	**6s**	MTBE	2	2	--	24	30	95:5
32	$Bi(OAc)_3$	**6s**	Et_2O	2	2	--	24	45	94:6
33	$Bi(OAc)_3$	**6s**	DME	2	2	--	24	66	86:14
34[d]	$Bi(OAc)_3$	**6s**	MTBE	2	2	3Å MS	24	8	84:16
35[d]	$Bi(OAc)_3$	**6s**	MTBE	2	2	4Å MS	24	7	72:28
36[d]	$Bi(OAc)_3$	**6s**	MTBE	2	2	5Å MS	24	5	61:39
37[e]	$Bi(OAc)_3$	**6s**	MTBE	2	2	HFIP	24	19	92:8
38[e]	$Bi(OAc)_3$	**6s**	MTBE	2	2	H_2O	24	65	96:4
39[f]	$Bi(OAc)_3$	**6s**	MTBE	2	2	H_2O	24	75	95:5
40[g]	$Bi(OAc)_3$	**6s**	MTBE	2	2	H_2O	24	98	97:3
41[h]	$Bi(OAc)_3$	**6s**	MTBE	2	2	H_2O	24	83	94:6
42[i]	$Bi(OAc)_3$	**6s**	MTBE	2	2	H_2O	24	80	93:7
43[g]	$Bi(OAc)_3$	**6s**	MTBE	5	5	H_2O	24	93	94:6
44[g,j]	$Bi(OAc)_3$	**6s**	MTBE	2	2	H_2O	24	66	94:6
45[g]	BiF_3	**6s**	MTBE	2	2	H_2O	48	73	95:5
46[g]	$BiCl_3$	**6s**	MTBE	2	2	H_2O	48	65	94:6
47[g]	$Bi(OTf)_3$	**6s**	MTBE	2	2	H_2O	48	80	75:25
48[g]	$Bi(OH)_3$	**6s**	MTBE	2	2	H_2O	48	70	92:8
49[g]	$Cu(OAc)_2$	**6s**	MTBE	2	2	H_2O	48	65	92:8
50[g]	$In(OAc)_3$	**6s**	MTBE	2	2	H_2O	48	61	93:7
51[g]	$Sc(OAc)_3$	**6s**	MTBE	2	2	H_2O	48	80	94:6

[a] The reactions were carried out with **1a** (0.1 mmol), **2a** (0.15 mmol) in 1 mL dry solvent at room temperature. [b] Yield of isolated products. [c] Determined by HPLC analysis. [d] The Add was 40 mg. [e] The add was 1 equiv. [f] The add was 2 equivalent. [g] The add was 5 equivalent. [h] The add was 10 equivalent. [i] The add was 20 equivalent. [j] The reaction was

performed at 0 ℃.

3. General procedure for Asymmetric Mukaiyama-Mannich Reaction of Difluoroenoxysilanes with Seven-Membered Cyclic Imines

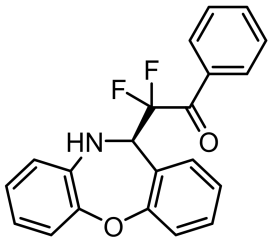


1 **2** **3**

To a 10 mL Schlenk flask equipped with a stirring bar was added **1** (0.1 mmol), Difluoroenoxysilanes **2** (0.15 mmol), $Bi(OAc)_3$ (2 mol%), chiral phosphoric acid catalyst (*S*)-**6s** (2 mol%), H_2O (5 equiv.) and dry MTBE (1.0 mL). The reaction was stirred at room temperature until completed. Then, the crude mixture was direct purified by flash chromatography to afford the product **3**.

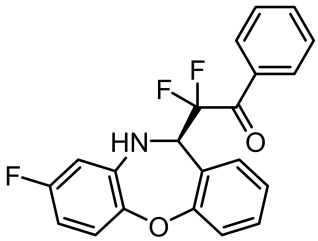
4. Characterization data of products 3

(*R*)-2-(10,11-dihydrodibenzo[*b,f*][1,4]oxazepin-11-yl)-2,2-difluoro-1-phenylethan-1-one (3a)



White solid, m.p. 89-90 °C, 34.4 mg, 98% yield, 97:3 e.r.; $[\alpha]_D^{27}$ = -14.5 (c = 1.0, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, *J* = 7.5 Hz, 2H), 7.53 (t, *J* = 7.4 Hz, 1H), 7.37 (t, *J* = 7.8 Hz, 2H), 7.33 - 7.27 (m, 1H), 7.24 - 7.18 (m, 2H), 7.11 - 7.02 (m, 2H), 6.84 (td, *J* = 7.8, 1.4 Hz, 1H), 6.68 (td, *J* = 7.8, 1.5 Hz, 1H), 6.59 (dd, *J* = 7.9, 1.4 Hz, 1H), 5.14 (dd, *J* = 19.0, 8.8 Hz, 1H), 4.31 (br, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 190.87 (dd, *J* = 30.9, 29.4 Hz), 158.1, 144.6, 136.6, 134.5, 132.60 (t, *J* = 2.4 Hz), 131.82 (d, *J* = 1.2 Hz), 130.9, 130.26 (t, *J* = 3.4 Hz), 128.6, 124.9, 124.2, 124.0, 121.69 (d, *J* = 5.0 Hz), 119.9, 118.6, 117.52 (d, *J* = 3.5 Hz), 114.9 , 60.82 (dd, *J* = 26.5, 24.1 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -101.94 (dd, *J* = 281.0, 8.8 Hz), -109.00 (dd, *J* = 280.9, 19.0 Hz); HRMS (ESI): *m/z* calcd for $C_{21}H_{15}F_2NNaO_2$ $[M+Na]^+$: 374.0963; found: 374.0956; HPLC: Daicel Chiralpak AD, *n*-hexane/*i*-PrOH = 3:1, Flow rate = 1.0 mL/min, λ = 210 nm, t_R = 9.4 min (major) and t_R = 11.9 min (minor).

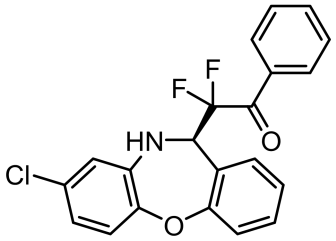
(*R*)-2,2-difluoro-2-(8-fluoro-10,11-dihydrodibenzo[*b,f*][1,4]oxazepin-11-yl)-1-phenylethan-1-one (3b)



White solid, m.p. 94-95 °C, 35.0 mg, 95% yield, 96:4 e.r.; $[\alpha]_D^{27}$ = -17.6 (c = 1.0, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (d, *J* = 7.7 Hz, 2H), 7.58 (t, *J* = 7.4 Hz, 1H), 7.41 (t, *J* = 7.8 Hz, 2H), 7.34 (td, *J* = 7.8, 1.5 Hz, 1H), 7.26 - 7.21 (m, 2H), 7.10 (td, *J* = 7.5, 0.7 Hz, 1H), 7.00 (dd, *J* = 8.7, 5.6 Hz, 1H), 6.34 (ddd, *J* = 12.9, 9.2, 2.9 Hz, 2H), 5.14 (dd, *J* = 19.2, 8.2 Hz, 1H), 4.46 (br, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 190.64 (dd, *J* = 30.9, 29.6 Hz), 160.9, 158.35 (d, *J* = 39.9 Hz), 140.63 (d, *J* = 2.4 Hz), 137.87 (d, *J* = 10.8 Hz), 134.6, 131.97 (d, *J* = 1.1 Hz), 130.54 (dd, *J* = 48.1, 44.6 Hz), 128.7, 124.6, 123.9, 122.67 (d, *J* = 10.2 Hz), 121.6, 119.9, 117.29 (d, *J* = 3.9 Hz), 114.7, 105.77 (d, *J* = 23.1 Hz), 104.68 (d, *J* = 26.6 Hz), 60.57 (dd, *J* = 27.2, 24.3 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -102.13 (dd, *J* = 282.4, 8.2 Hz), -109.24 (dd, *J* = 282.3, 19.1 Hz), -118.72; HRMS (ESI): *m/z* calcd for $C_{21}H_{14}F_3NNaO_2$ $[M+Na]^+$: 392.0869; found:

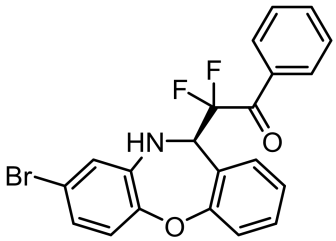
392.0866; HPLC: Daicel Chiralpak IA, *n*-hexane/*i*-PrOH = 5:1, Flow rate = 1.0 mL/min, λ = 210 nm, t_R = 10.2 min (major) and t_R = 15.3 min (minor).

(*R*)-2-(8-chloro-10,11-dihydrodibenzo[*b,f*][1,4]oxazepin-11-yl)-2,2-difluoro-1-phenylethan-1-one (3c)



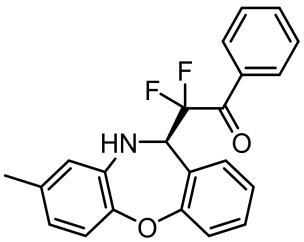
White solid, m.p. 90-91 °C,35.8 mg, 93% yield, 89:11 e.r.; $[\alpha]_D^{27}$ = -24.9 (c = 1.0, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 8.00 (d, *J* = 7.6 Hz, 2H), 7.57 (t, *J* = 7.4 Hz, 1H), 7.40 (t, *J* = 7.9 Hz, 2H), 7.33 (td, *J* = 7.8, 1.6 Hz, 1H), 7.25 - 7.18 (m, 2H), 7.08 (td, *J* = 7.5, 1.1 Hz, 1H), 6.98 (d, *J* = 8.5 Hz, 1H), 6.64 - 6.57 (m, 2H), 5.12 (dd, *J* = 18.8, 6.3 Hz, 1H), 4.46 (br, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 190.59 (dd, *J* = 32.2, 28.1 Hz), 157.8, 143.0, 137.7, 134.6, 132.5, 132.0, 130.51 (dd, *J* = 47.3, 43.9 Hz), 129.6, 128.7, 124.5, 123.8, 122.23 (d, *J* = 123.2 Hz), 112.0, 119.4, 117.9, 117.34 (d, *J* = 3.3 Hz), 114.7, 60.60 (dd, *J* = 26.9, 24.2 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -101.99 (dd, *J* = 283.4, 8.3 Hz), -109.08 (dd, *J* = 283.4, 19.1 Hz); HRMS (ESI): *m/z* calcd for $C_{21}H_{14}ClF_2NNaO_2$ $[M+Na]^+$: 408.0573; found: 408.0570; HPLC: Daicel Chiralpak IA, *n*-hexane/*i*-PrOH = 5:1, Flow rate = 1.0 mL/min, λ = 210 nm, t_R = 10.9 min (major) and t_R = 12.4 min (minor).

(*R*)-2-(8-bromo-10,11-dihydrodibenzo[*b,f*][1,4]oxazepin-11-yl)-2,2-difluoro-1-phenylethan-1-one (3d)



White solid, m.p. 89-90 °C,37.3 mg, 87% yield, 90:10 e.r.; $[\alpha]_D^{27}$ = -21.8 (c = 1.0, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 8.01 (d, *J* = 8.0 Hz, 2H), 7.59 (t, *J* = 7.3 Hz, 1H), 7.42 (t, *J* = 7.8 Hz, 2H), 7.37 - 7.32 (m, 1H), 7.21 (t, *J* = 8.2 Hz, 2H), 7.10 (t, *J* = 7.3 Hz, 1H), 6.94 (d, *J* = 8.3 Hz, 1H), 6.76 (dt, *J* = 6.5, 2.1 Hz, 2H), 5.13 (dd, *J* = 19.3, 8.4 Hz, 1H), 4.25 (br, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 190.59 (dd, *J* = 30.8, 29.8 Hz), 157.7, 143.4, 138.1, 134.7, 132.4, 132.0, 131.2, 130.30 (t, *J* = 3.4 Hz), 128.7, 124.6, 123.8, 123.2, 122.4, 121.6, 120.7, 117.1, 114.7, 60.55 (dd, *J* = 27.0, 24.1 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -101.95 (dd, *J* = 283.8, 8.4 Hz), -109.16 (dd, *J* = 283.8, 19.3 Hz); HRMS (ESI): *m/z* calcd for $C_{21}H_{14}BrF_2NNaO_2$ $[M+Na]^+$: 452.0068; found: 452.0069; HPLC: Daicel Chiralpak IA, *n*-hexane/*i*-PrOH = 5:1, Flow rate = 1.0 mL/min, λ = 210 nm, t_R = 11.5 min (major) and t_R = 12.3 min (minor).

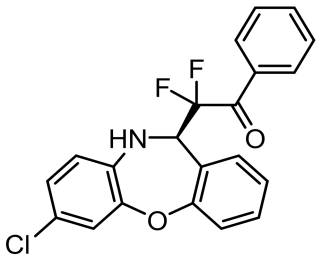
(*R*)-2,2-difluoro-2-(8-methyl-10,11-dihydrodibenzo[*b,f*][1,4]oxazepin-11-yl)-1-phenylethan-1-one (3e)



Yellow solid, m.p. 104-105 °C,32.9 mg, 90% yield, 90:10 e.r.; $[\alpha]_D^{27}$ = -12.6 (c = 1.0, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, *J* = 7.6 Hz, 2H), 7.57 (t, *J* = 7.4 Hz, 1H), 7.41 (t, *J* = 7.8 Hz, 2H), 7.32 (td, *J* = 7.9, 1.6 Hz, 1H), 7.22 (t, *J* = 7.0 Hz, 2H), 7.10 - 7.03 (m, 1H), 6.91 (d, *J* = 1.1 Hz, 1H), 6.67 (dd, *J* =

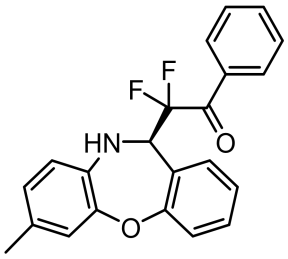
8.0, 1.2 Hz, 1H), 6.52 (d, *J* = 8.0 Hz, 1H), 5.15 (dd, *J* = 19.0, 9.0 Hz, 1H), 4.26 (br, 1H), 2.21 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 190.99 (dd, *J* = 32.4, 27.9 Hz), 158.1, 144.7, 134.4, 133.9, 132.8, 131.8, 130.8, 130.28 (t, *J* = 3.4 Hz), 123.0, 128.6, 125.4, 124.02 (d, *J* = 5.6 Hz), 122.1, 121.7, 118.8, 117.65 (d, *J* = 3.0 Hz), 115.0, 61.36 - 60.49 (m), 20.4; ^{19}F NMR (376 MHz, $CDCl_3$) δ -101.74 (dd, *J* = 281.4, 8.9 Hz), -109.17 (dd, *J* = 281.4, 19.0 Hz); HRMS (ESI): *m/z* calcd for $C_{22}H_{17}F_2NNaO_2$ $[M+Na]^+$: 388.1120; found: 388.1117; HPLC: Daicel Chiralpak AD, *n*-hexane/*i*-PrOH = 3:1, Flow rate = 1.0 mL/min, λ = 210 nm, t_R = 9.5 min (major) and t_R = 12.0 min (minor).

(*R*)-2-(7-chloro-10,11-dihydrodibenzo[*b,f*][1,4]oxazepin-11-yl)-2,2-difluoro-1-phenylethan-1-one (3f)



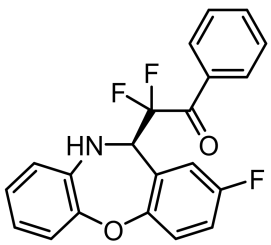
Yellow oil, 38.1 mg, 99% yield, 99:1 e.r.; $[\alpha]_D^{27}$ = -9.7 (c = 1.0, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (d, *J* = 7.7 Hz, 2H), 7.61 (t, *J* = 7.4 Hz, 1H), 7.44 (t, *J* = 7.8 Hz, 2H), 7.37 (td, *J* = 8.0, 1.6 Hz, 1H), 7.24 (t, *J* = 8.1 Hz, 2H), 7.16 - 7.08 (m, 2H), 6.85 (dd, *J* = 8.5, 2.4 Hz, 1H), 6.55 (d, *J* = 8.5 Hz, 1H), 5.16 (dd, *J* = 19.0, 8.7 Hz, 1H), 4.46 (br, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 190.68 (dd, *J* = 33.1, 27.5 Hz), 157.6, 144.6, 135.4, 134.6, 132.5, 131.9, 131.1, 130.28 (t, *J* = 3.2 Hz), 128.7, 124.7, 124.5, 123.80 (d, *J* = 7.1 Hz), 121.77 (d, *J* = 22.1 Hz), 120.1, 119.3, 117.43 (d, *J* = 2.8 Hz), 114.8, 60.70 (dd, *J* = 26.3, 24.4 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -101.79 (dd, *J* = 283.6, 8.7 Hz), -108.96 (dd, *J* = 283.5, 19.0 Hz); HRMS (ESI): *m/z* calcd for $C_{21}H_{14}ClF_2NNaO_2$ $[M+Na]^+$: 408.0573; found: 408.0572; HPLC: Daicel Chiralpak AD, *n*-hexane/*i*-PrOH = 3:1, Flow rate = 1.0 mL/min, λ = 210 nm, t_R = 8.8 min (major) and t_R = 12.0 min (minor).

(*R*)-2,2-difluoro-2-(7-methyl-10,11-dihydrodibenzo[*b,f*][1,4]oxazepin-11-yl)-1-phenylethan-1-one (3g)



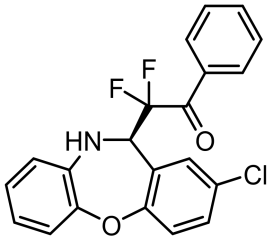
Yellow solid, m.p. 101-102 °C,31.8 mg, 87% yield, 83:17 e.r.; $[\alpha]_D^{27}$ = -36.2 (c = 1.0, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (d, *J* = 7.8 Hz, 2H), 7.57 (t, *J* = 7.4 Hz, 1H), 7.41 (t, *J* = 7.8 Hz, 2H), 7.32 (td, *J* = 7.9, 1.5 Hz, 1H), 7.21 (t, *J* = 6.6 Hz, 2H), 7.06 (dd, *J* = 11.1, 4.5 Hz, 1H), 6.97 (d, *J* = 8.1 Hz, 1H), 6.50 (dd, *J* = 8.0, 1.7 Hz, 1H), 6.42 (d, *J* = 1.5 Hz, 1H), 5.15 (dd, *J* = 19.0, 8.9 Hz, 1H), 4.61 - 3.79 (br, 1H), 2.17 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 190.97 (dd, *J* = 33.4, 26.9 Hz), 158.3, 142.7, 136.2, 134.5, 134.4, 132.8, 131.78 (d, *J* = 1.2 Hz), 130.9, 130.28 (t, *J* = 3.5 Hz), 128.64 (s), 124.2 - 124.0 (m), 121.54 (d, *J* = 15.8 Hz), 120.6, 120.2, 119.1, 117.6, 115.0, 60.88 (dd, *J* = 26.5, 24.1 Hz), 20.8; ^{19}F NMR (376 MHz, $CDCl_3$) δ -102.07 (dd, *J* = 280.6, 8.9 Hz), -109.12 (dd, *J* = 280.5, 19.0 Hz); HRMS (ESI): *m/z* calcd for $C_{22}H_{17}F_2NNaO_2$ $[M+Na]^+$: 388.1120; found: 388.1116; HPLC: Daicel Chiralpak AD, *n*-hexane/*i*-PrOH = 9:1, Flow rate = 1.0 mL/min, λ = 210 nm, t_R = 9 min (major) and t_R = 9.4 min (minor).

(*R*)-2,2-difluoro-2-(2-fluoro-10,11-dihydrodibenzo[*b,f*][1,4]oxazepin-11-yl)-1-phenylethan-1-one (3h)



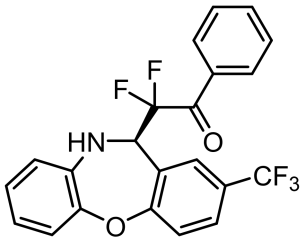
White solid, m.p. 104-105 °C, 34.3 mg, 93% yield, 96:4 e.r.; $[\alpha]_D^{27}$ = -30.6 (c = 1.0, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 8.06 (d, *J* = 7.5 Hz, 2H), 7.61 (t, *J* = 7.4 Hz, 1H), 7.44 (t, *J* = 7.9 Hz, 2H), 7.29 - 7.22 (m, 2H), 7.10 - 7.02 (m, 2H), 6.88 (td, *J* = 7.7, 1.4 Hz, 1H), 6.72 (td, *J* = 7.9, 1.5 Hz, 1H), 6.59 (dd, *J* = 7.9, 1.5 Hz, 1H), 5.56 (dt, *J* = 22.4, 5.4 Hz, 1H), 4.46 (d, *J* = 6.0 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 189.89 (dd, *J* = 31.9, 29.6 Hz), 161.8, 159.3, 158.88 (d, *J* = 5.4 Hz), 143.5, 135.9, 134.8, 132.13 (t, *J* = 2.6 Hz), 130.5 - 130.2 (m), 128.8, 125.3, 123.18 (d, *J* = 13.3 Hz), 121.6, 121.14 (d, *J* = 3.5 Hz), 120.2, 118.6, 114.85 (d, *J* = 27.0 Hz), 112.10 (d, *J* = 16.4 Hz), 52.18 (dd, *J* = 28.7, 23.3 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -99.74 (dd, *J* = 296.1, 8.3 Hz), -110.89 (dd, *J* = 291.2, 22.4 Hz), -111.85 (s); HRMS (ESI): *m/z* calcd for $C_{21}H_{14}F_3NNaO_2$ $[M+Na]^+$: 392.0869; found: 392.0866; HPLC: Daicel Chiralpak AD, *n*-hexane/*i*-PrOH =3:1, Flow rate = 1.0 mL/min, λ = 210 nm, t_R = 8.5 min (minor) and t_R = 9.1 min (major).

(*R*)-2-(2-chloro-10,11-dihydrodibenzo[*b,f*][1,4]oxazepin-11-yl)-2,2-difluoro-1-phenylethan-1-one (3i)



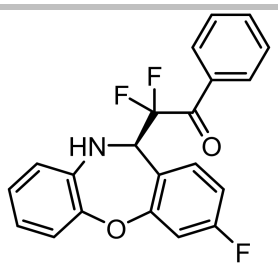
Colorless oil, 37.4 mg, 97% yield, 97:3 e.r.; $[\alpha]_D^{27}$ = -25.8 (c = 1.0, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 8.07 - 7.99 (m, 2H), 7.65 - 7.55 (m, 1H), 7.48 - 7.39 (m, 2H), 7.29 (dd, *J* = 8.6, 2.6 Hz, 1H), 7.24 (d, *J* = 2.4 Hz, 1H), 7.16 (d, *J* = 8.6 Hz, 1H), 7.06 (dd, *J* = 8.0, 1.5 Hz, 1H), 6.87 (td, *J* = 7.7, 1.5 Hz, 1H), 6.77 - 6.67 (m, 1H), 6.61 (dd, *J* = 7.9, 1.5 Hz, 1H), 5.12 (dd, *J* = 19.8, 7.6 Hz, 1H), 4.37 (br, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 190.37 (dd, *J* = 32.7, 27.7 Hz), 156.6, 144.5, 136.2, 134.7, 131.4, 130.7, 130.33 (t, *J* = 3.2 Hz), 129.0, 128.8, 125.6, 125.1, 123.1, 121.6, 120.4, 118.9, 117.23 (d, *J* = 4.7 Hz), 114.6, 60.27 (dd, *J* = 26.6, 23.9 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -100.62 (dd, *J* = 286.6, 7.5 Hz), -109.75 (dd, *J* = 286.6, 19.8 Hz); HRMS (ESI): *m/z* calcd for $C_{21}H_{14}ClF_2NNaO_2$ $[M+Na]^+$: 408.0573; found: 408.0571; HPLC: Daicel Chiralpak AD, *n*-hexane/*i*-PrOH = 3:1, Flow rate = 1.0 mL/min, λ = 210 nm, t_R = 8.1 min (major) and t_R = 21.1 min (minor).

(*R*)-2,2-difluoro-1-phenyl-2-(2-(trifluoromethyl)-10,11-dihydrodibenzo[*b,f*][1,4]oxazepin-11-yl)ethan-1-one (3j)



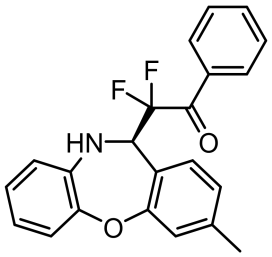
Yellow solid, m.p. 115-116 °C, 41.5 mg, 99% yield, 98:2 e.r.; $[\alpha]_D^{27}$ = -49.2 (c = 1.0, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 8.02 (d, *J* = 7.6 Hz, 2H), 7.65 - 7.57 (m, 2H), 7.53 (s, 1H), 7.43 (t, *J* = 7.8 Hz, 2H), 7.33 (d, *J* = 8.5 Hz, 1H), 7.10 (dd, *J* = 8.0, 1.3 Hz, 1H), 6.89 (td, *J* = 7.8, 1.4 Hz, 1H), 6.76 (td, *J* = 7.9, 1.5 Hz, 1H), 6.63 (dd, *J* = 7.9, 1.4 Hz, 1H), 5.22 (dd, *J* = 19.9, 7.7 Hz, 1H), 4.47 (br, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 190.23 (dd, *J* = 33.3, 27.1 Hz), 160.2, 144.4, 135.9, 134.8, 132.3, 130.31 (t, *J* = 3.1 Hz), 129.3, 128.8, 127.87 (dd, *J* = 6.9, 3.4 Hz), 125.89 (d, *J* = 33.1 Hz), 125.1, 124.1, 122.4, 121.6, 120.7, 119.9, 119.2, 117.22 (d, *J* = 5.3 Hz), 60.76 (dd, *J* = 26.0, 23.2 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -61.94 (s), -99.75 (dd, *J* = 290.1, 7.8 Hz), -109.41 (dd, *J* = 290.6, 19.9 Hz); HRMS (ESI): *m/z* calcd for $C_{22}H_{14}F_5NNaO_2$ $[M+Na]^+$: 442.0837; found: 442.0836; HPLC: Daicel Chiralpak AD, *n*-hexane/*i*-PrOH = 3:1, Flow rate = 1.0 mL/min, λ = 210 nm, t_R = 5.8 min (major) and t_R = 10.4 min (minor).

(*R*)-2,2-difluoro-2-(7-fluoro-10,11-dihydrodibenzo[*b,f*][1,4]oxazepin-11-yl)-1-phenylethan-1-one (3k)



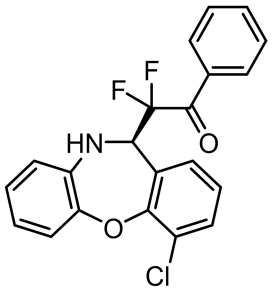
Yellow solid, m.p. 84-85 °C, 35.1 mg, 95% yield, 96:4 e.r.; $[\alpha]_D^{27}$ = -19.1 (c = 1.0, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 8.00 (d, *J* = 7.6 Hz, 2H), 7.58 (td, *J* = 7.7, 0.9 Hz, 1H), 7.41 (t, *J* = 7.2 Hz, 2H), 7.19 (t, *J* = 7.4 Hz, 1H), 7.06 (d, *J* = 8.0 Hz, 1H), 6.95 (d, *J* = 9.3 Hz, 1H), 6.87 (t, *J* = 7.6 Hz, 1H), 6.79 (td, *J* = 8.4, 2.3 Hz, 1H), 6.75 - 6.67 (m, 1H), 6.61 (d, *J* = 7.9 Hz, 1H), 5.13 (dd, *J* = 19.1, 8.5 Hz, 1H), 4.40 (br, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 190.74 (dd, *J* = 31.1, 29.5 Hz), 164.9, 162.4, 158.97 (d, *J* = 11.2 Hz), 144.4, 136.4, 134.6, 132.99 (dd, *J* = 9.9, 1.3 Hz), 132.5, 130.30 (t, *J* = 3.5 Hz), 128.7, 125.1, 121.7, 120.2, 119.9, 118.8, 111.20 (d, *J* = 21.3 Hz), 109.35 (d, *J* = 23.3 Hz), 60.35 (dd, *J* = 26.4, 23.9 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -101.56 (dd, *J* = 284.2, 8.7 Hz), -109.24 (dd, *J* = 284.1, 19.2 Hz), -109.95; HRMS (ESI): *m/z* calcd for $C_{21}H_{14}F_3NNaO_2$ $[M+Na]^+$: 392.0869; found: 392.0868; HPLC: Daicel Chiralpak AD, *n*-hexane/*i*-PrOH = 3:1, Flow rate = 1.0 mL/min, λ = 210 nm, t_R = 9.4 min (major) and t_R = 10.0 min (minor).

(*R*)-2,2-difluoro-2-(3-methyl-10,11-dihydrodibenzo[*b,f*][1,4]oxazepin-11-yl)-1-phenylethan-1-one (3l)



White solid, m.p. 91-92 °C, 32.9 mg, 90% yield, 94:6 e.r.; $[\alpha]_D^{27}$ = -33.4 (c = 1.0, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 8.01 (d, *J* = 7.5 Hz, 2H), 7.61 - 7.52 (m, 1H), 7.41 (t, *J* = 7.8 Hz, 2H), 7.16 - 7.04 (m, 3H), 6.94 - 6.81 (m, 2H), 6.69 (td, *J* = 7.8, 1.5 Hz, 1H), 6.61 (dd, *J* = 7.9, 1.5 Hz, 1H), 5.12 (dd, *J* = 19.1, 8.7 Hz, 1H), 4.07 (br, 1H), 2.33 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 191.01 (dd, *J* = 30.9, 29.4 Hz), 157.9, 144.7, 141.4, 136.8, 134.4, 132.69 (t, *J* = 2.4 Hz), 131.62 (d, *J* = 1.2 Hz), 130.31 (t, *J* = 3.4 Hz), 128.6, 124.92 (d, *J* = 15.5 Hz), 121.92 (d, *J* = 42.4 Hz), 120.7, 120.1, 119.8, 118.6, 117.5, 114.9, 60.57 (dd, *J* = 26.6, 24.0 Hz), 21.2; ^{19}F NMR (376 MHz, $CDCl_3$) δ -102.02 (dd, *J* = 280.5, 8.7 Hz), -109.36 (dd, *J* = 280.6, 19.2 Hz); HRMS (ESI): *m/z* calcd for $C_{22}H_{17}F_2NNaO_2$ $[M+Na]^+$: 388.1120; found: 388.1120; HPLC: Daicel Chiralpak AD, *n*-hexane/*i*-PrOH = 3:1, Flow rate = 1.0 mL/min, λ = 210 nm, t_R = 10.8 min (minor) and t_R = 11.8 min (major).

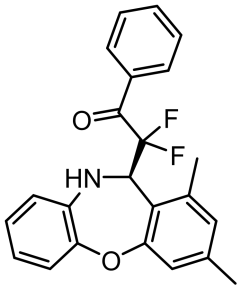
(*R*)-2-(4-chloro-10,11-dihydrodibenzo[*b,f*][1,4]oxazepin-11-yl)-2,2-difluoro-1-phenylethan-1-one (3m)



White solid, m.p. 114-115 °C, 35.4 mg, 92% yield, 95:5 e.r.; $[\alpha]_D^{27}$ =-41.2 (c = 1.0, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 8.05 (d, *J* = 7.5 Hz, 2H), 7.63 - 7.56 (m, 1H), 7.42 (ddd, *J* = 6.9, 5.6, 4.9 Hz, 3H), 7.29 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.19 - 7.13 (m, 1H), 7.02 (t, *J* = 7.8 Hz, 1H), 6.90 (td, *J* = 7.9, 1.5 Hz, 1H), 6.72 (td, *J* = 7.9, 1.5 Hz, 1H), 6.61 (dd, *J* = 8.0, 1.5 Hz, 1H), 5.24 (dt, *J* = 19.8, 6.8 Hz, 1H), 4.37 (d, *J* = 5.8 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 190.52 (dd, *J* = 31.0, 29.4 Hz), 153.8, 143.7, 136.6, 134.7, 132.5, 131.5, 130.31 (t, *J* = 3.5 Hz), 130.01 (d, *J* = 1.4 Hz), 128.7, 126.93 (d, *J* = 61.9 Hz), 125.5, 124.8, 122.6,

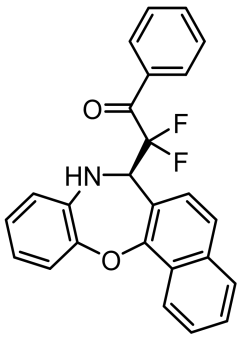
119.8, 118.4, 117.27 (d, *J* = 4.6 Hz), 114.7, 60.16 (dd, *J* = 27.4, 23.9 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -101.73 (dd, *J* = 282.8, 7.7 Hz), -109.85 (dd, *J* = 282.8, 19.8 Hz); HRMS (ESI): *m/z* calcd for $C_{21}H_{14}ClF_2NNaO_2$ $[M+Na]^+$: 408.0573; found: 408.0577; HPLC: Daicel Chiralpak AD, *n*-hexane/*i*-PrOH = 3:1, Flow rate = 1.0 mL/min, λ = 210 nm, t_R = 7.6 min (major) and t_R = 9.0 min (minor).

(*R*)-2-(1,3-dimethyl-10,11-dihydrodibenzo[*b,f*][1,4]oxazepin-11-yl)-2,2-difluoro-1-phenylethan-1-one (3n)



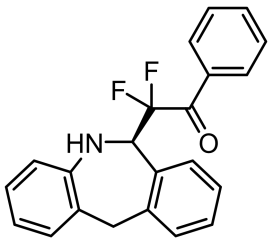
White solid, m.p. 141-142 °C, 32.2 mg, 85% yield, 84:16 e.r.; $[\alpha]_D^{27}$ = -14.3 (c = 1.0, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (d, *J* = 7.9 Hz, 2H), 7.54 (t, *J* = 7.4 Hz, 1H), 7.38 (t, *J* = 7.5 Hz, 2H), 7.01 (d, *J* = 7.9 Hz, 1H), 6.90 (s, 1H), 6.83 (t, *J* = 7.6 Hz, 2H), 6.62 (t, *J* = 7.6 Hz, 1H), 6.53 (d, *J* = 7.9 Hz, 1H), 5.39 (dd, *J* = 20.1, 6.9 Hz, 1H), 4.42 (br, 1H), 2.36 (s, 3H), 2.27 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 191.30 (dd, *J* = 31.2, 29.3 Hz), 158.5, 144.0, 140.7, 138.5, 137.1, 134.2, 132.9, 130.48 - 130.32 (m), 128.5, 128.0, 125.1, 121.6, 120.6, 119.63 (d, *J* = 99.0 Hz), 118.2, 117.4, 115.6, 55.51 (dd, *J* = 28.2, 26.0 Hz), 21.1, 20.3; ^{19}F NMR (377 MHz, $CDCl_3$) δ -116.57 (s); ^{19}F NMR (376 MHz, $CDCl_3$) δ -100.95 (dd, *J* = 275.9, 6.9 Hz), -108.78 (dd, *J* = 275.9, 20.1 Hz); HRMS (ESI): *m/z* calcd for $C_{23}H_{19}F_2NNaO_2$ $[M+Na]^+$: 402.1276; found: 402.1273; HPLC: Daicel Chiralpak AD, *n*-hexane/*i*-PrOH = 3:1, Flow rate = 1.0 mL/min, λ = 210 nm, t_R = 8.8 min (minor) and t_R = 12.7 min (major).

(*R*)-2-(7,8-dihydrobenzo[b]naphtho[2,1-f][1,4]oxazepin-7-yl)-2,2-difluoro-1-phenylethan-1-one (3o)



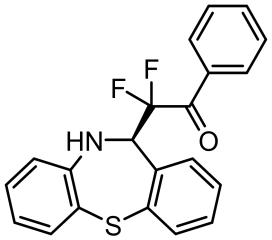
Yellow solid, m.p. 106-107 °C, 38.9 mg, 97% yield, 97:3 e.r.; $[\alpha]_D^{27}$ = -84.5 (c = 1.0, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.53 (d, *J* = 8.3 Hz, 1H), 8.01 (d, *J* = 7.6 Hz, 2H), 7.81 (d, *J* = 7.8 Hz, 1H), 7.62 - 7.50 (m, 4H), 7.41 - 7.27 (m, 4H), 6.88 (td, *J* = 7.7, 1.4 Hz, 1H), 6.73 (td, *J* = 7.7, 1.5 Hz, 1H), 6.65 (dd, *J* = 7.9, 1.5 Hz, 1H), 5.31 (dd, *J* = 19.2, 8.5 Hz, 1H), 4.49 (br, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 190.84 (dd, *J* = 31.1, 29.7 Hz), 154.1, 144.5, 137.1, 135.1, 134.5, 132.6, 131.5, 130.28 (t, *J* = 3.4 Hz), 128.55 (d, *J* = 12.1 Hz), 127.7, 127.38 (d, *J* = 18.3 Hz), 126.6, 125.0, 123.8, 122.6, 121.8, 120.4, 119.7, 118.9, 118.7, 115.2, 60.80 (dd, *J* = 26.5, 23.9 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -101.81 (dd, *J* = 283.0, 8.5 Hz), -108.81 (dd, *J* = 283.0, 19.2 Hz); HRMS (ESI): *m/z* calcd for $C_{25}H_{17}F_2NNaO_2$ $[M+Na]^+$: 424.1120; found: 424.1118; HPLC: Daicel Chiralpak AD, *n*-hexane/*i*-PrOH = 19:1, Flow rate = 1.0 mL/min, λ = 210 nm, t_R = 12.3 min (major) and t_R = 17.3 min (minor).

(*R*)-2-(6,11-dihydro-5H-dibenzo[*b,e*]azepin-6-yl)-2,2-difluoro-1-phenylethan-1-one (3p)



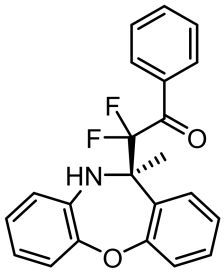
Yellow solid, m.p. 129-130 °C, 27.9 mg, 80% yield, 68:32 e.r.; $[\alpha]_D^{27}$ = -21.4 (c = 1.0, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 8.02 (d, *J* = 7.8 Hz, 2H), 7.59 (t, *J* = 7.4 Hz, 1H), 7.44 (t, *J* = 7.8 Hz, 2H), 7.21 (dd, *J* = 10.5, 2.9 Hz, 2H), 7.16 - 7.10 (m, 2H), 7.08 - 6.96 (m, 2H), 6.81 - 6.67 (m, 2H), 5.41 (dd, *J* = 20.3, 5.9 Hz, 1H), 4.60 (d, *J* = 13.8 Hz, 1H), 4.23 (br, 1H), 3.50 (d, *J* = 13.8 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 191.33 (dd, *J* = 32.3, 29.3 Hz), 143.3, 142.0, 134.5, 132.9, 132.3, 132.2, 130.48 - 130.00 (m), 129.3, 128.9, 128.8, 128.3, 127.6, 126.6, 121.3, 120.0, 117.32 (d, *J* = 8.8 Hz), 114.7, 62.55 (dd, *J* = 25.9, 21.6 Hz), 39.42 (d, *J* = 4.7 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -100.65 (dd, *J* = 283.3, 5.8 Hz), -113.24 (dd, *J* = 283.3, 20.4 Hz); HRMS (ESI): *m/z* calcd for $C_{22}H_{17}F_2NNaO$ $[M+Na]^+$: 372.1170; found: 372.1167; HPLC: Daicel Chiralpak AD, *n*-hexane/*i*-PrOH = 3:1, Flow rate = 1.0 mL/min, λ = 210 nm, t_R = 7.3 min (major) and t_R = 10.5 min (minor).

(*R*)-2-(10,11-dihydrodibenzo[*b,f*][1,4]thiazepin-11-yl)-2,2-difluoro-1-phenylethan-1-one (3q)



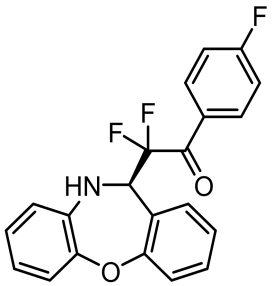
Yellow solid, m.p. 99-100 °C, 34.9 mg, 95% yield, 94:6 e.r.; $[\alpha]_D^{27}$ = -34.4 (c = 1.0, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 8.08 (d, *J* = 8.0 Hz, 2H), 7.63 (dd, *J* = 10.8, 4.0 Hz, 1H), 7.58 - 7.54 (m, 1H), 7.52 - 7.45 (m, 3H), 7.32 - 7.23 (m, 2H), 7.19 (d, *J* = 7.7 Hz, 1H), 6.94 (t, *J* = 7.6 Hz, 1H), 6.78 - 6.63 (m, 2H), 6.53 (d, *J* = 8.0 Hz, 1H), 4.07 (br, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 189.16 (dd, *J* = 33.0, 24.5 Hz), 144.5, 138.2, 136.8, 134.6, 132.5, 132.3, 130.11 (t, *J* = 3.2 Hz), 129.1, 128.9, 128.8, 128.6, 127.32 (t, *J* = 3.1 Hz), 120.83 (d, *J* = 11.5 Hz), 120.5, 120.2, 117.9, 115.3, 58.65 (dd, *J* = 25.9, 21.7 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -102.10 (d, *J* = 279.9 Hz), -110.99 (dd, *J* = 279.9, 19.5 Hz); HRMS (ESI): *m/z* calcd for $C_{21}H_{15}F_2NNaOS$ $[M+Na]^+$: 390.0735; found: 390.0729; HPLC: Daicel Chiralpak IA, *n*-hexane/*i*-PrOH = 5:1, Flow rate = 1.0 mL/min, λ = 210 nm, t_R = 7.6 min (minor) and t_R = 8.0 min (major).

(*R*)-2,2-difluoro-2-(11-methyl-10,11-dihydrodibenzo[*b,f*][1,4]oxazepin-11-yl)-1-phenylethan-1-one (3r)



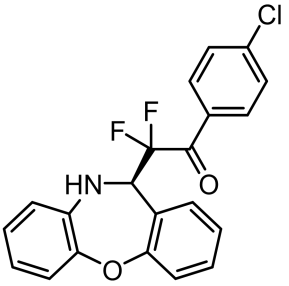
White solid, m.p. 120-121 °C, 30.3 mg, 83% yield, 79:21 e.r.; $[\alpha]_D^{27}$ = -12.1 (c = 1.0, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 7.86 (d, *J* = 7.8 Hz, 2H), 7.48 (t, *J* = 7.4 Hz, 1H), 7.41 (d, *J* = 7.9 Hz, 1H), 7.34 - 7.24 (m, 3H), 7.15 - 7.07 (m, 2H), 7.03 (dd, *J* = 7.9, 1.1 Hz, 1H), 6.90 (dd, *J* = 10.7, 4.3 Hz, 1H), 6.78 (td, *J* = 7.7, 1.2 Hz, 1H), 6.71 (d, *J* = 7.7 Hz, 1H), 4.02 (br, 1H), 1.98 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 190.38 (dd, *J* = 34.6, 25.9 Hz), 156.9, 148.6, 136.9, 133.9, 133.7, 130.3, 130.2, 130.21 (d, *J* = 6.3 Hz), 128.2, 127.1, 125.0, 124.1, 122.1, 121.8, 120.8, 120.4, 118.3, 64.14 (t, *J* = 23.5 Hz), 25.5; ^{19}F NMR (376 MHz, $CDCl_3$) δ -102.31 (d, *J* = 272.4 Hz), -105.12 (d, *J* = 272.4 Hz); HRMS (ESI): *m/z* calcd for $C_{22}H_{17}F_2NNaO_2$ $[M+Na]^+$: 388.1120; found: 388.1113; HPLC: Daicel Chiralpak AD, *n*-hexane/*i*-PrOH = 3:1, Flow rate = 1.0 mL/min, λ = 210 nm, t_R = 6.2 min (minor) and t_R = 10.7 min (major).

(*R*)-2-(10,11-dihydrodibenzo[*b,f*][1,4]oxazepin-11-yl)-2,2-difluoro-1-(4-fluorophenyl)ethan-1-one (3s)



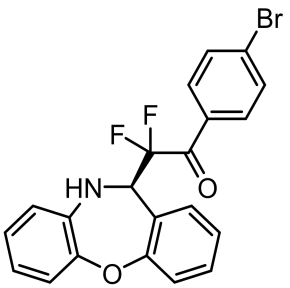
Colorless oil, 35.1 mg, 95% yield, 97:3 e.r.; $[\alpha]_D^{27}$ = -24.1 (c = 1.0, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 8.10 (dd, *J* = 7.8, 5.8 Hz, 2H), 7.42 - 7.35 (m, 1H), 7.33 - 7.25 (m, 3H), 7.18 - 7.08 (m, 4H), 6.97 - 6.88 (m, 1H), 6.80 - 6.72 (m, 1H), 6.66 (dd, *J* = 7.9, 1.3 Hz, 1H), 5.17 (dd, *J* = 18.6, 9.0 Hz, 1H), 4.46 (br, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 189.30 (dd, *J* = 33.4, 26.8 Hz), 166.47 (d, *J* = 257.8 Hz), 158.1, 144.5, 136.6, 133.27 (dt, *J* = 9.6, 3.7 Hz), 131.9, 131.1, 129.10 (d, *J* = 2.6 Hz), 124.66 (d, *J* = 61.6 Hz), 123.9, 121.73 (d, *J* = 5.0 Hz), 120.2, 112.0, 118.5, 117.59 (d, *J* = 3.2 Hz), 115.94 (d, *J* = 22.0 Hz), 115.0, 61.02 (dd, *J* = 26.5, 24.7 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -102.04 (s), -102.08 (dd, *J* = 279.4, 9.0 Hz), -108.53 (dd, *J* = 279.4, 18.6 Hz); HRMS (ESI): *m/z* calcd for $C_{21}H_{14}F_3NNaO_2$ $[M+Na]^+$: 392.0869; found: 392.0866; HPLC: Daicel Chiralpak AD, *n*-hexane/*i*-PrOH = 3:1, Flow rate = 1.0 mL/min, λ = 210 nm, t_R = 8.7 min (major) and t_R = 10.8 min (minor).

(*R*)-1-(4-chlorophenyl)-2-(10,11-dihydrodibenzo[*b,f*][1,4]oxazepin-11-yl)-2,2-difluoroethan-1-one (3t)



White solid, m.p. 107-108 °C, 38.1 mg, 99% yield, 97:3 e.r.; $[\alpha]_D^{27}$ = -27.2 (c = 1.0, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 7.92 (d, *J* = 8.4 Hz, 2H), 7.39 - 7.29 (m, 3H), 7.26 - 7.18 (m, 2H), 7.11 - 7.03 (m, 2H), 6.85 (dd, *J* = 10.5, 4.5 Hz, 1H), 6.74 - 6.65 (m, 1H), 6.64 - 6.55 (m, 1H), 5.08 (dd, *J* = 18.1, 9.0 Hz, 1H), 4.39 (br, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 189.81 (dd, *J* = 32.4, 27.8 Hz), 158.1, 144.5, 141.1, 136.5, 131.8, 131.68 (t, *J* = 3.6 Hz), 131.1, 131.0, 129.0, 125.0, 124.4, 123.8, 121.73 (d, *J* = 5.7 Hz), 120.0, 118.5, 117.55 (d, *J* = 2.4 Hz), 114.9, 61.42 - 60.69 (m); ^{19}F NMR (376 MHz, $CDCl_3$) δ -102.31 (dd, *J* = 278.7, 9.2 Hz), -108.48 (dd, *J* = 278.7, 18.2 Hz); HRMS (ESI): *m/z* calcd for $C_{21}H_{14}ClF_2NNaO_2$ $[M+Na]^+$: 408.0573; found: 408.0574; HPLC: Daicel Chiralpak AD, *n*-hexane/*i*-PrOH = 3:1, Flow rate = 1.0 mL/min, λ = 210 nm, t_R = 8.9 min (major) and t_R = 11.7 min (minor).

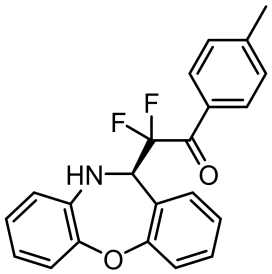
(*R*)-1-(4-bromophenyl)-2-(10,11-dihydrodibenzo[*b,f*][1,4]oxazepin-11-yl)-2,2-difluoroethan-1-one (3u)



White solid, m.p. 122-123 °C, 41.6 mg, 97% yield, 97:3 e.r.; $[\alpha]_D^{27}$ = -26.2 (c = 1.0, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 8.00 (d, *J* = 7.9 Hz, 2H), 7.60 - 7.53 (m, 1H), 7.41 (t, *J* = 7.8 Hz, 2H), 7.36 - 7.29 (m, 1H), 7.22 - 7.20 (m, 1H), 7.08 (ddd, *J* = 5.5, 3.5, 1.2 Hz, 2H), 6.92 - 6.81 (m, 1H), 6.76 - 6.66 (m, 1H), 6.61 (dd, *J* = 7.9, 1.1 Hz, 1H), 5.16 (dd, *J* = 19.1, 8.7 Hz, 1H), 4.39 (br, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 189.97 (dd, *J* = 22.5, 8.5 Hz), 158.1, 144.6, 136.5, 134.5, 132.11 - 131.55 (m), 131.4, 131.04 (d, *J* = 17.7 Hz), 130.3, 130.1, 128.7, 125.0, 124.4, 123.8, 121.75 (d, *J* = 5.4 Hz), 120.0, 118.5, 114.9, 61.09

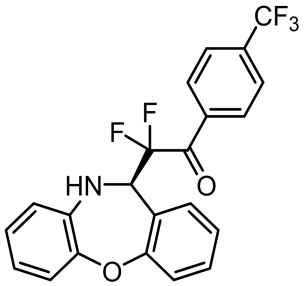
(dd, *J* = 26.4, 24.9 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -102.35 (dd, *J* = 278.7, 9.2 Hz), -108.54 (dd, *J* = 278.7, 18.3 Hz); HRMS (ESI): *m/z* calcd for $C_{21}H_{14}BrF_2NNaO_2$ $[M+Na]^+$: 452.0068; found: 452.0063; HPLC: Daicel Chiralpak AD, *n*-hexane/*i*-PrOH = 3:1, Flow rate = 1.0 mL/min, λ = 210 nm, t_R = 9.9 min (major) and t_R = 12.9 min (minor).

(*R*)-2-(10,11-dihydrodibenzo[*b,f*][1,4]oxazepin-11-yl)-2,2-difluoro-1-(p-tolyl)ethan-1-one (3v)



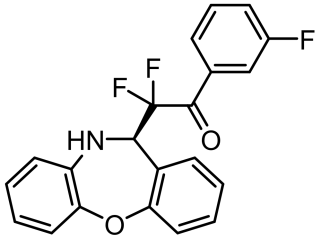
White solid, m.p. 127-128 °C, 36.1 mg, 99% yield, 96:4 e.r.; $[\alpha]_D^{27}$ = -41.4 (c = 1.0, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 (d, *J* = 7.7 Hz, 2H), 7.32 (t, *J* = 7.7 Hz, 1H), 7.25 - 7.18 (m, 4H), 7.07 (ddd, *J* = 11.4, 6.2, 1.5 Hz, 2H), 6.85 (dd, *J* = 10.7, 4.4 Hz, 1H), 6.69 (dd, *J* = 10.7, 4.5 Hz, 1H), 6.60 (d, *J* = 7.9 Hz, 1H), 5.15 (dd, *J* = 19.5, 8.4 Hz, 1H), 4.41 (br, 1H), 2.39 (d, *J* = 16.5 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 190.36 (dd, *J* = 30.5, 29.6 Hz), 158.1, 145.8, 144.6, 136.7, 131.9, 130.9, 130.45 (t, *J* = 3.4 Hz), 130.0, 129.4, 124.8, 124.10 (d, *J* = 13.3 Hz), 121.69 (d, *J* = 4.1 Hz), 120.2, 119.9, 118.6, 117.6, 114.9, 60.74 (dd, *J* = 26.6, 23.8 Hz), 21.93 ; ^{19}F NMR (376 MHz, $CDCl_3$) δ -101.66 (dd, *J* = 281.9, 8.4 Hz), -109.34 (dd, *J* = 281.9, 19.5 Hz); HRMS (ESI): *m/z* calcd for $C_{22}H_{17}F_2NNaO_2$ $[M+Na]^+$: 388.1120; found: 388.1112; HPLC: Daicel Chiralpak AD, *n*-hexane/*i*-PrOH = 3:1, Flow rate = 1.0 mL/min, λ = 210 nm, t_R = 9.5 min (major) and t_R = 14.3 min (minor).

(*R*)-2-(10,11-dihydrodibenzo[*b,f*][1,4]oxazepin-11-yl)-2,2-difluoro-1-(4-(trifluoromethyl)phenyl)ethan-1-one (3w)



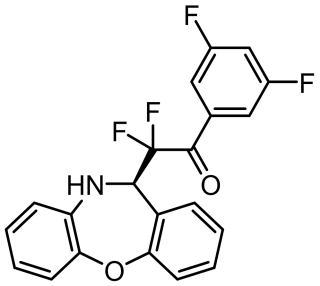
Yellow solid, m.p. 114-115 °C, 38.9 mg, 93% yield, 97:3 e.r.; $[\alpha]_D^{27}$ = -33.9 (c = 1.0, $CHCl_3$); ^{1}H NMR (400 MHz, Acetone) δ 8.25 (s, 2H), 7.91 (d, *J* = 7.8 Hz, 1H), 7.67 (t, *J* = 8.1 Hz, 1H), 7.44 - 7.34 (m, 2H), 7.22 - 7.12 (m, 2H), 6.92 (dd, *J* = 7.9, 1.1 Hz, 1H), 6.85 - 6.78 (m, 1H), 6.73 (dd, *J* = 8.0, 1.5 Hz, 1H), 6.55 (td, *J* = 7.9, 1.6 Hz, 1H), 6.19 (d, *J* = 7.5 Hz, 1H), 5.23 - 5.04 (m, 1H); ^{13}C NMR (101 MHz, Acetone) δ 190.19 (t, *J* = 28.7 Hz), 159.1, 144.5, 138.3, 135.0, 134.3, 132.7, 132.1, 131.2, 131.23 - 130.74 (m), 130.5, 127.52 (dd, *J* = 8.0, 4.0 Hz), 125.9, 125.7, 123.3, 122.05 (d, *J* = 6.7 Hz), 119.38 (d, *J* = 15.4 Hz), 118.7, 116.7, 62.77 (dd, *J* = 28.6, 26.9 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -58.19 (s), -98.71 (dd, *J* = 255.3, 12.4 Hz), -100.14 (dd, *J* = 255.4, 13.7 Hz); HRMS (ESI): *m/z* calcd for $C_{22}H_{14}F_5NNaO_2$ $[M+Na]^+$: 442.0837; found: 442.0831; HPLC: Daicel Chiralpak AD, *n*-hexane/*i*-PrOH = 3:1, Flow rate = 1.0 mL/min, λ = 210 nm, t_R = 6.6 min (major) and t_R = 8.7 min (minor).

(*R*)-2-(10,11-dihydrodibenzo[*b,f*][1,4]oxazepin-11-yl)-2,2-difluoro-1-(3-fluorophenyl)ethan-1-one (3x)



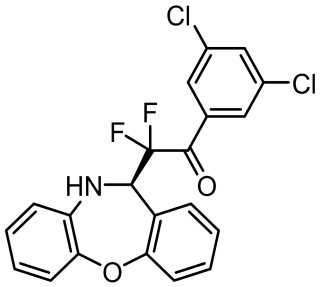
White solid, m.p. 121-122 °C, 35.8 mg, 97% yield, 96:4 e.r.; $[\alpha]_D^{27}$ = -20.1 (c = 1.0, $CHCl_3$); ^1H NMR (400 MHz, Acetone) δ 7.83 (d, *J* = 7.8 Hz, 1H), 7.67 (d, *J* = 9.8 Hz, 1H), 7.49 (td, *J* = 8.0, 5.7 Hz, 1H), 7.43 - 7.34 (m, 3H), 7.20 (d, *J* = 7.7 Hz, 1H), 7.17 - 7.10 (m, 1H), 6.98 (dd, *J* = 7.9, 1.0 Hz, 1H), 6.87 - 6.80 (m, 1H), 6.76 (dd, *J* = 8.0, 1.5 Hz, 1H), 6.59 (td, *J* = 8.0, 1.6 Hz, 1H), 6.08 (d, *J* = 7.3 Hz, 1H), 5.15 (ddd, *J* = 14.7, 12.5, 7.4 Hz, 1H); ^{13}C NMR (101 MHz, Acetone) δ 190.13 (dd, *J* = 32.6, 24.9 Hz), 163.14 (d, *J* = 245.5 Hz), 159.1, 144.6, 138.40 (d, *J* = 5.5 Hz), 136.11 (d, *J* = 6.5 Hz), 132.7, 132.0, 131.46 (d, *J* = 7.8 Hz), 126.83 (dd, *J* = 6.9, 3.4 Hz), 125.8, 125.4, 122.09 (d, *J* = 8.5 Hz), 121.71 (d, *J* = 21.4 Hz), 119.5, 119.2, 118.80 (d, *J* = 5.1 Hz), 117.34 (t, *J* = 3.6 Hz), 117.16 - 117.04 (m), 116.6, 62.46 (dd, *J* = 32.3, 21.9 Hz); ^{19}F NMR (376 MHz, Acetone) δ 73.32 (dd, *J* = 257.1, 12.4 Hz), 71.55 (dd, *J* = 257.1, 14.8 Hz), 63.97 (s); HRMS (ESI): *m/z* calcd for $C_{21}H_{14}F_3NNaO_2$ $[M+Na]^+$: 392.0869; found: 392.0865; HPLC: Daicel Chiralpak AD, *n*-hexane/*i*-PrOH = 3:1, Flow rate = 1.0 mL/min, λ = 210 nm, t_R = 8.1 min (major) and t_R = 9.7 min (minor).

(*R*)-1-(3,5-difluorophenyl)-2-(10,11-dihydrodibenzo[*b,f*][1,4]oxazepin-11-yl)-2,2-difluoroethan-1-one (3y)



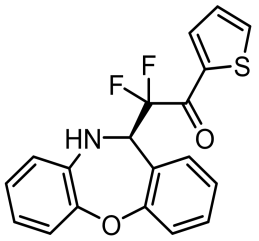
White solid, m.p. 99-100 °C, 36.8 mg, 95% yield, 96:4 e.r.; $[\alpha]_D^{27}$ = -23.9 (c = 1.0, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 7.53 (d, *J* = 6.4 Hz, 2H), 7.37 (ddd, *J* = 9.5, 3.6, 1.8 Hz, 1H), 7.29 - 7.21 (m, 2H), 7.17 - 7.10 (m, 1H), 7.10 - 7.06 (m, 1H), 7.06 - 6.98 (m, 1H), 6.90 (ddd, *J* = 9.3, 3.4, 1.7 Hz, 1H), 6.72 (ddd, *J* = 9.3, 3.5, 1.7 Hz, 1H), 6.67 - 6.58 (m, 1H), 5.07 (dd, *J* = 16.6, 9.8 Hz, 1H), 4.43 (br, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 188.53 (dd, *J* = 29.7, 26.8 Hz), 163.95 (d, *J* = 11.8 Hz), 161.45 (d, *J* = 12.1 Hz), 158.1, 144.5, 136.4, 131.8, 131.3, 125.1, 124.6, 123.7, 121.76 (d, *J* = 6.1 Hz), 120.1, 118.4, 117.4, 114.8, 113.59 - 112.68 (m), 109.73 (t, *J* = 25.3 Hz), 61.41 (t, *J* = 26.0 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -102.68 (dd, *J* = 276.9, 9.8 Hz), -107.68 (dd, *J* = 277.1, 17.0 Hz), -107.69 -107.93 (m); HRMS (ESI): *m/z* calcd for $C_{21}H_{13}F_4NNaO_2$ $[M+Na]^+$: 410.0775; found: 410.0769; HPLC: Daicel Chiralpak AD, *n*-hexane/*i*-PrOH = 3:1, Flow rate = 1.0 mL/min, λ = 210 nm, t_R = 6.4 min (major) and t_R = 7.4 min (minor).

(*R*)-1-(3,5-dichlorophenyl)-2-(10,11-dihydrodibenzo[*b,f*][1,4]oxazepin-11-yl)-2,2-difluoroethan-1-one (3z)



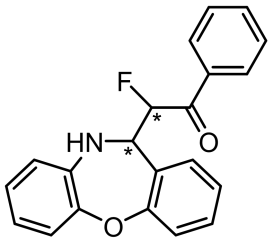
Yellow oil, 42.2 mg, 96% yield,97:3 e.r.; $[\alpha]_D^{27}$ = -31.8(c = 1.0, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 7.88 - 7.77 (m, 2H), 7.50 (t, *J* = 1.8 Hz, 1H), 7.34 (ddd, *J* = 8.5, 7.8, 2.1 Hz, 2H), 7.21 (dd, *J* = 16.7, 7.8 Hz, 2H), 7.11 (td, *J* = 7.5, 1.0 Hz, 1H), 7.04 (dd, *J* = 8.0, 1.3 Hz, 1H), 6.88 (td, *J* = 7.9, 1.4 Hz, 1H), 6.69 (td, *J* = 7.9, 1.4 Hz, 1H), 6.61 (dd, *J* = 7.9, 1.2 Hz, 1H), 5.02 (dd, *J* = 16.7, 10.0 Hz, 1H), 4.39 (br, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 188.76 (dd, *J* = 19.3, 11.1 Hz), 158.1, 144.4, 136.3, 135.5, 135.0, 134.3, 133.9, 131.8, 131.4, 131.2, 128.59 (t, *J* = 3.7 Hz), 125.2, 124.7, 123.7, 121.77 (d, *J* = 5.1 Hz), 120.2, 118.4, 61.52 (t, *J* = 26.0 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -102.52 (dd, *J* = 276.1, 9.9 Hz), -107.41 (dd, *J* = 276.1, 16.7 Hz); HRMS (ESI): *m/z* calcd for $C_{21}H_{13}Cl_2F_2NNaO_2$ $[M+Na]^+$: 442.0184; found: 442.0178; HPLC: Daicel Chiralpak IC, *n*-hexane/*i*-PrOH = 19:1, Flow rate = 1.0 mL/min, λ = 210 nm, t_R = 5.9 min (minor) and t_R = 6.8 min (major).

(*R*)-2-(10,11-dihydrodibenzo[*b,f*][1,4]oxazepin-11-yl)-2,2-difluoro-1-(thiophen-2-yl)ethan-1-one (3aa)



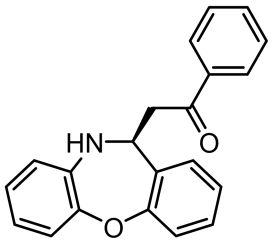
Yellow solid, m.p. 144-145 °C, 24.9 mg, 70% yield, 83:17 e.r.; $[\alpha]_D^{27}$ = -15.9 (c = 1.0, $CHCl_3$); ^1H NMR (400 MHz, Acetone) δ 8.05 - 7.96 (m, 1H), 7.89 (dd, *J* = 3.7, 1.4 Hz, 1H), 7.34 (ddd, *J* = 14.2, 7.7, 4.0 Hz, 2H), 7.21 - 7.07 (m, 3H), 7.00 (dd, *J* = 8.0, 1.3 Hz, 1H), 6.85 - 6.79 (m, 1H), 6.75 (dd, *J* = 8.0, 1.6 Hz, 1H), 6.63 - 6.56 (m, 1H), 6.06 (d, *J* = 7.1 Hz, 1H), 5.09 (ddd, *J* = 14.7, 13.4, 7.2 Hz, 1H); ^{13}C NMR (101 MHz, Acetone) δ 183.83 (dd, *J* = 30.9, 28.2 Hz), 159.1, 144.5, 140.3, 138.5, 137.8, 136.92 (t, *J* = 5.9 Hz), 132.7, 131.8, 129.7, 125.8, 125.6, 125.2, 122.05 (t, *J* = 6.3 Hz), 121.6, 119.3, 119.1, 118.9, 62.30 (t, *J* = 26.5 Hz); ^{19}F NMR (376 MHz, Acetone) δ 71.10 (dd, *J* = 253.2, 13.2 Hz), 69.64 (dd, *J* = 253.2, 14.8 Hz); HRMS (ESI): *m/z* calcd for $C_{19}H_{13}F_2NNaO_2S$ $[M+Na]^+$: 380.0527; found: 380.0525; HPLC: Daicel Chiralpak AD, *n*-hexane/*i*-PrOH = 3:1, Flow rate = 1.0 mL/min, λ = 210 nm, t_R = 11.3 min (major) and t_R = 13.5 min (minor).

(*S*)-2-((*R*)-10,11-dihydrodibenzo[*b,f*][1,4]oxazepin-11-yl)-2-fluoro-1-phenylethan-1-one (3ab)



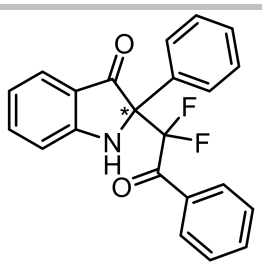
Yellow solid, m.p. 104-105 °C, 33.0 mg, 99% yield, 97:3 e.r.; $[\alpha]_D^{27}$ = -13.8 (c = 1.0, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 7.80 - 7.76 (m, 2H), 7.46 (t, *J* = 7.4 Hz, 1H), 7.32 (t, *J* = 7.8 Hz, 2H), 7.17 - 7.06 (m, 2H), 7.02 - 6.98 (m, 2H), 6.90 (dtd, *J* = 29.2, 7.6, 1.3 Hz, 2H), 6.77 - 6.68 (m, 2H), 6.56 (dd, *J* = 50.1, 8.6 Hz, 1H), 4.63 (dd, *J* = 14.0, 8.6 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.77 (d, *J* = 17.3 Hz), 157.8, 143.5, 136.6, 135.3, 133.9, 130.6, 129.9, 128.79 - 128.42 (m), 127.36 (d, *J* = 6.1 Hz), 125.3, 124.9, 122.1, 121.3, 119.7, 119.1, 90.8, 89.0, 61.18 (d, *J* = 23.1 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -189.06 (dd, *J* = 50.1, 13.9 Hz); HRMS (ESI): *m/z* calcd for $C_{21}H_{16}FNNaO_2$ $[M+Na]^+$: 356.1057; found: 356.1053; HPLC: Daicel Chiralpak AD, *n*-hexane/*i*-PrOH = 3:1, Flow rate = 1.0 mL/min, λ = 210 nm, t_R = 11.2 min (minor) and t_R = 12.4 min (major).

***(S)*-2-(10,11-dihydrodibenzo[*b,f*][1,4]oxazepin-11-yl)-1-phenylethan-1-one (3ac)**



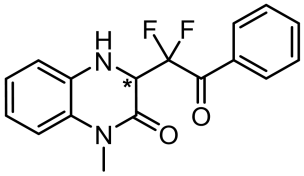
Yellow oil, 20.5 mg, 65% yield, 71:29 e.r.; $[\alpha]_D^{27}$ = -13.8 (c = 1.0, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 7.98 - 7.89 (m, 2H), 7.57 - 7.49 (m, 1H), 7.41 (t, *J* = 7.7 Hz, 2H), 7.29 - 7.19 (m, 3H), 7.14 - 7.04 (m, 2H), 6.86 - 6.77 (m, 1H), 6.71 - 6.62 (m, 1H), 6.56 (dd, *J* = 7.9, 1.5 Hz, 1H), 4.96 (dd, *J* = 9.7, 3.3 Hz, 1H), 4.64 (br, 1H), 4.15 (dd, *J* = 18.1, 9.7 Hz, 1H), 3.46 (dd, *J* = 18.1, 3.4 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 199.2, 157.2, 143.8, 137.1, 136.7, 133.6, 132.6, 129.4, 128.7, 128.5, 128.2, 124.9, 124.6, 121.8, 121.4, 119.3, 119.2, 54.6, 44.3; HRMS (ESI): *m/z* calcd for $C_{21}H_{17}NNaO_2$ $[M+Na]^+$: 338.1151; found: 338.1146; HPLC: Daicel Chiralpak AD, *n*-hexane/*i*-PrOH = 3:1, Flow rate = 1.0 mL/min, λ = 210 nm, t_R = 11.9 min (major) and t_R = 12.7 min (minor).

2-(1,1-difluoro-2-oxo-2-phenylethyl)-2-phenylindolin-3-one (7)



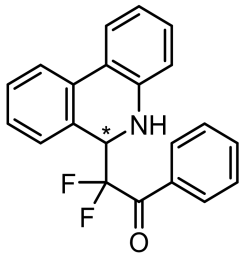
Yellow oil, 35.6 mg, 98% yield, 96:4 e.r.; $[\alpha]_D^{27}$ = -36.1 (c = 1.0, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 7.91 (dd, *J* = 23.6, 7.4 Hz, 4H), 7.65 - 7.53 (m, 2H), 7.39 (qdd, *J* = 7.6, 6.5, 2.0 Hz, 6H), 6.94 (d, *J* = 8.2 Hz, 1H), 6.84 (t, *J* = 7.4 Hz, 1H), 5.90 (s, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.7, 188.44 (dd, *J* = 33.0, 30.3 Hz), 159.6, 137.6, 134.7, 132.51 (d, *J* = 2.4 Hz), 132.27 - 131.89 (m), 130.30 (dd, *J* = 4.1, 2.5 Hz), 129.0, 128.65 (d, *J* = 13.2 Hz), 126.34 (d, *J* = 195.8 Hz), 120.70 (d, *J* = 1.8 Hz), 120.0, 119.6, 116.94 (d, *J* = 3.3 Hz), 114.3, 112.3, 70.94 (dd, *J* = 24.9, 22.0 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -102.76 (d, *J* = 300.5 Hz), -104.35 (d, *J* = 300.5 Hz); HRMS (ESI): *m/z* calcd for $C_{22}H_{15}F_2NNaO_2$ $[M+Na]^+$: 386.0963; found: 386.0953; HPLC: HPLC: Daicel Chiralpak AD, *n*-hexane/*i*-PrOH = 3:1, Flow rate = 1.0 mL/min, λ = 210 nm, t_R = 13.0 min (major) and t_R = 16.6 min (minor).

3-(1,1-difluoro-2-oxo-2-phenylethyl)-1-methyl-3,4-dihydroquinoxalin-2(*1H*)-one (8)



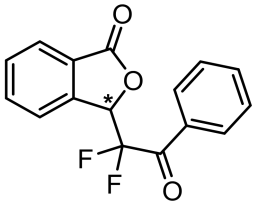
Yellow oil, 29.4 mg, 93% yield, 92:8 e.r.; $[\alpha]_D^{27}$ = 6.8 (c = 1.0, $CHCl_3$); ^1H NMR (400 MHz, Acetone) δ 7.98 (d, *J* = 7.6 Hz, 2H), 7.75 - 7.66 (m, 1H), 7.56 (dd, *J* = 10.8, 4.8 Hz, 2H), 7.02 (d, *J* = 8.1 Hz, 1H), 6.98 - 6.87 (m, 2H), 6.85 - 6.75 (m, 1H), 6.18 (s, 1H), 5.10 (ddd, *J* = 20.6, 6.7, 2.6 Hz, 1H), 3.32 (s, 3H); ^{13}C NMR (101 MHz, Acetone) δ 189.48 (dd, *J* = 28.4, 25.4 Hz), 161.20 (d, *J* = 7.4 Hz), 134.8, 134.5, 134.2, 130.44 (dd, *J* = 4.1, 2.5 Hz), 129.5, 128.1, 124.7, 121.0, 119.7, 118.42 (d, *J* = 11.2 Hz), 115.8, 115.19 (d, *J* = 66.3 Hz), 60.69 (t, *J* = 23.6 Hz); ^{19}F NMR (376 MHz, Acetone) δ 70.76 (dd, *J* = 264.5, 6.7 Hz), 61.91 (dd, *J* = 264.5, 20.6 Hz); HRMS (ESI): *m/z* calcd for $C_{17}H_{14}F_2N_2NaO_2$ $[M+Na]^+$: 339.0916; found: 339.0908; HPLC: Daicel Chiralpak AS, *n*-hexane/*i*-PrOH = 19:1, Flow rate = 1.0 mL/min, λ = 210 nm, t_R = 10.1 min (minor) and t_R = 23.6 min (major).

2-(5,6-dihydrophenanthridin-6-yl)-2,2-difluoro-1-phenylethan-1-one (9)



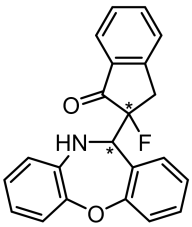
Yellow oil, 26.8 mg, 80% yield, 59:41 e.r.; $[\alpha]_D^{27}$ = 7.3 (c = 1.0, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 7.86 - 7.81 (m, 2H), 7.78 (d, *J* = 7.9 Hz, 1H), 7.65 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.59 - 7.52 (m, 1H), 7.43 - 7.32 (m, 3H), 7.22 (dd, *J* = 10.4, 4.1 Hz, 2H), 7.08 (td, *J* = 7.9, 1.4 Hz, 1H), 6.80 (td, *J* = 7.7, 1.1 Hz, 1H), 6.61 (dd, *J* = 7.9, 0.9 Hz, 1H), 5.24 (dd, *J* = 17.7, 9.5 Hz, 1H), 4.68 (br, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 191.02 (dd, *J* = 31.9, 28.4 Hz), 142.5, 134.5, 133.1, 132.7, 130.22 (t, *J* = 3.5 Hz), 129.53 (d, *J* = 1.9 Hz), 129.36 (d, *J* = 2.7 Hz), 128.6, 127.1, 125.7, 123.2, 122.7, 120.3, 119.9, 119.1, 117.2, 114.8, 57.12 (dd, *J* = 25.0, 23.3 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -105.50 (dd, *J* = 286.9, 9.5 Hz), -110.95 (dd, *J* = 286.8, 17.8 Hz); HRMS (ESI): *m/z* calcd for $C_{21}H_{15}F_2NNaO$ $[M+Na]^+$: 358.1014; found: 358.1013; HPLC: Daicel Chiralpak AD, *n*-hexane/*i*-PrOH = 3:1, Flow rate = 1.0 mL/min, λ = 210 nm, t_R = 8.6 min (major) and t_R = 9.7 min (minor).

3-(1,1-difluoro-2-oxo-2-phenylethyl)isobenzofuran-1(3*H*)-one (10)



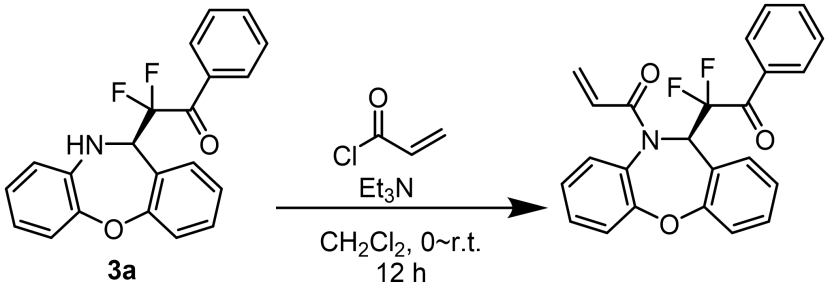
White solid, m.p. 107-108 °C, 12.4 mg, 43% yield, 60:40 e.r.; $[\alpha]_D^{27}$ = 5.1 (c = 1.0, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 8.10 - 8.06 (m, 2H), 7.97 (d, *J* = 7.6 Hz, 1H), 7.77 - 7.73 (m, 1H), 7.70 - 7.62 (m, 3H), 7.51 (t, *J* = 7.8 Hz, 2H), 6.14 (dd, *J* = 13.7, 7.2 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 188.00 (dd, *J* = 30.5, 27.7 Hz), 169.1, 142.3, 135.1, 134.7, 130.7, 130.49 - 130.13 (m), 129.0, 126.2, 124.30 (d, *J* = 1.6 Hz), 117.5, 114.87 (d, *J* = 6.8 Hz), 112.3, 100.1; ^{19}F NMR (376 MHz, $CDCl_3$) δ -107.44 (dd, *J* = 298.2, 7.1 Hz), -112.68 (dd, *J* = 298.2, 13.8 Hz); HRMS (ESI): *m/z* calcd for $C_{16}H_{10}F_2NaO_3$ $[M+Na]^+$: 311.0490; found: 311.0481; HPLC: Daicel Chiralpak OD, *n*-hexane/*i*-PrOH = 5:1, Flow rate = 1.0 mL/min, λ = 210 nm, t_R = 7.8 min (major) and t_R = 8.3 min (minor).

(*S*)-2-((*R*)-10,11-dihydrodibenzo[*b,f*][1,4]oxazepin-11-yl)-2-fluoro-2,3-dihydro-1H-inden-1-one (11)



Yellow oil, 23.1 mg, 67% yield, 64:36 e.r.; $[\alpha]_D^{27}$ = 7.2 (c = 1.0, $CHCl_3$); ^1H NMR (400 MHz, Acetone) δ 7.60 (td, *J* = 7.6, 1.1 Hz, 1H), 7.48 (t, *J* = 8.1 Hz, 2H), 7.31 (t, *J* = 7.3 Hz, 1H), 7.16 - 7.02 (m, 3H), 7.02 - 6.97 (m, 1H), 6.96 - 6.87 (m, 3H), 6.68 - 6.59 (m, 1H), 5.88 (d, *J* = 5.6 Hz, 1H), 5.02 (dd, *J* = 15.1, 5.9 Hz, 1H), 4.28 (dd, *J* = 18.1, 11.6 Hz, 1H), 3.19 (dd, *J* = 24.1, 18.1 Hz, 1H); ^{13}C NMR (101 MHz, Acetone) δ 200.81 (d, *J* = 17.9 Hz), 158.3, 152.50 (d, *J* = 4.7 Hz), 145.4, 139.7, 136.9, 135.2, 132.5, 131.0, 128.7, 127.4, 126.45 (d, *J* = 7.5 Hz), 126.0, 124.9, 124.6, 121.95 (d, *J* = 18.7 Hz), 119.5, 119.3, 102.7, 100.8, 62.81 (d, *J* = 26.1 Hz), 36.24 (d, *J* = 24.2 Hz); ^{19}F NMR (376 MHz, Acetone) δ 24.34 (s); HRMS (ESI): *m/z* calcd for $C_{22}H_{16}FNNaO_2$ $[M+Na]^+$: 368.1057; found: 368.1049; HPLC: Daicel Chiralpak AD, *n*-hexane/*i*-PrOH = 3:1, Flow rate = 1.0 mL/min, λ = 210 nm, t_R = 12.0 min (major) and t_R = 15.8 min (minor).

5. Transformations of products

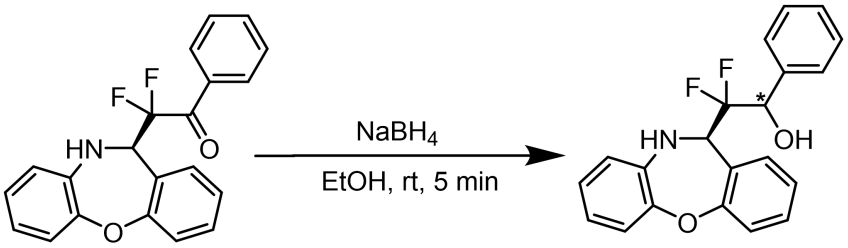


3a

(*R*)-1-(11-(1,1-difluoro-2-oxo-2-phenylethyl)dibenzo[*b,f*][1,4]oxazepin-10(11*H*)-yl)prop-2-en-1-one (12)

To a stirred solution of compound **3a** (35.1 mg, 0.1 mmol) in dry DCM (1 mL) was added triehylamine (16.7 uL, 0.12 mmol) and Acryloyl chloride (9.7 uL, 0.12 mmol) at 0 ˚C. After 12 h, the reaction was quenched by addition of a saturated aqueous solution of $NaHCO_3$ (2 mL) and aqueous layer was extracted with EtOAc (10 mL) for three times. The combined organic layer was washed with brine (5 mL) and dried over Na_2SO_4. After filtered and evaporation, the crude mixture was purified by flash column chromatography (ethyl acetate/petroleum ether = 1/10, v/v) to afford the colorless oil **12** (37.7 mg, 93% yield, 96:4 e.r.); $[\alpha]_D^{27}$ = -22.7 (c = 1.0, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 8.00 - 7.91 (m, 2H), 7.61 (ddd, *J* = 7.4, 4.2, 1.1 Hz, 1H), 7.50 - 7.40 (m, 2H), 7.36 - 7.18 (m, 6H), 7.08 - 6.97 (m, 3H), 6.51 - 6.39 (m, 1H), 6.27 - 6.13 (m, 1H), 5.65 (ddd, *J* = 10.3, 4.1, 1.7 Hz, 1H); ^{113}C NMR (101 MHz, $CDCl_3$) δ 188.28 (dd, *J* = 31.0, 27.2 Hz), 165.4, 154.3, 152.6, 134.6, 132.2, 131.8, 130.6, 130.30 - 129.91 (m), 129.8, 129.4, 128.9, 127.4, 124.2, 122.7, 121.6, 121.3, 119.3, 119.1, 116.72 (d, *J* = 4.9 Hz), 114.1, 58.09 (dd, *J*

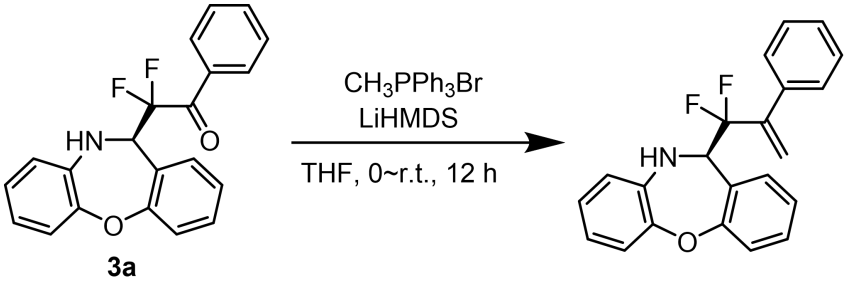
= 25.8, 22.3 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -98.93 (dd, *J* = 285.3, 14.8 Hz), -102.50 (dd, *J* = 285.4, 12.9 Hz); HRMS (ESI): *m/z* calcd for $C_{24}H_{17}F_2NNaO_3$ [M+Na]$^+$: 428.1069; found: 428.1056; HPLC: Daicel Chiralpak IA, *n*-hexane/*i*-PrOH = 3:1, Flow rate = 1.0 mL/min, λ = 210 nm, t_R = 7.8 min (major) and t_R = 14.5 min (minor).



3a

2-((*R*)-10,11-dihydrodibenzo[*b,f*][1,4]oxazepin-11-yl)-2,2-difluoro-1-phenylethan-1-ol (13)[3]

To a 5 mL flask, compound **3a** (35.1 mg, 0.1 mmol) in dry EtOH (1 mL) was added $NaBH_4$ (11.7 mg, 0.3 mmol) in one portion at room temperature. The resulting mixture was stirred at the same temperature until the complete consumption of **3a** as indicated by TLC analysis (about 5 min). After quenching with saturated aqueous NH_4Cl (5.0 mL), the solution was extracted with CH_2Cl_2 (3 × 10 mL) and dried over Na_2SO_4. After filtered and evaporation, the reaction mixture was purified by silica gel column chromatography (ethyl acetate/petroleum ether = 1/3, v/v) to afford the colorless oil **13** (35 mg, 99% yield, dr = 1.3:1, 96:4 e.r. / 99:1 e.r.); $[\alpha]_D^{27}$ = -14.3 (c = 1.0, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 - 7.29 (m, 14H), 7.24 (d, *J* = 0.5 Hz, 2H), 7.19 - 7.03 (m, 4H), 6.96 (td, *J* = 7.7, 1.2 Hz, 1H), 6.90 - 6.85 (m, 1H), 6.84 - 6.78 (m, 1H), 6.78 - 6.70 (m, 2H), 6.59 (dd, *J* = 7.9, 1.2 Hz, 1H), 5.21 - 5.01 (m, 2H), 5.00 - 4.91 (m, 2H), 3.33 (br, 4H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.0, 157.6, 146.7, 144.7, 136.64 (d, *J* = 5.9 Hz), 136.27 (d, *J* = 4.7 Hz), 131.1, 130.6, 130.46 (d, *J* = 2.8 Hz), 128.93 (d, *J* = 4.1 Hz), 128.43 (d, *J* = 8.5 Hz), 128.00 (d, *J* = 12.9 Hz), 126.37 (d, *J* = 2.6 Hz), 125.4, 125.1, 124.6, 124.32 (d, *J* = 16.2 Hz), 121.8, 121.68 (d, *J* = 3.0 Hz), 121.6, 121.5, 121.1, 120.9, 120.3, 119.6, 119.3, 73.67 (ddd, *J* = 30.7, 24.6, 10.6 Hz), 60.76 - 59.80 (m).; ^{19}F NMR (376 MHz, $CDCl_3$) δ -111.10 (ddd, *J* = 254.1, 15.2, 4.9 Hz), -113.61 (ddd, *J* = 256.9, 19.5, 3.9 Hz), -116.34 (ddd, *J* = 256.9, 19.5, 6.0 Hz), -120.34 (ddd, *J* = 254.3, 18.2, 12.6 Hz); HRMS (ESI): *m/z* calcd for $C_{21}H_{17}F_2NNaO_2$ [M+Na]$^+$: 376.1120; found: 376.1108; HPLC: Daicel Chiralpak OJ , *n*-hexane/*i*-PrOH = 3:2, Flow rate = 1.0 mL/min, λ = 210 nm, t_R = 10.2 min (major) and t_R = 13.9 min (minor), t_R = 20.9 min (minor) and t_R = 28.4 min (major).



3a

(*R*)-11-(1,1-difluoro-2-phenylallyl)-10,11-dihydrodibenzo[*b,f*][1,4]oxazepine (14)[4]

To a stirred suspension of methyltriphenylphosphonium bromide (80.0 mg, 0.225 mmol) in dry THF (2.0 mL) under an argon atmosphere, LiHMDS (225 μL, 0.225 mmol, 1 M in THF) was added slowly at 0 °C. After the mixture stirred for 30 min, the compound **3a** (52.7 mg, 0.15 mmol) was added, and then the mixture was gradually warmed to room temperature and stirred until full conversion. The reaction was quenched by addition of water at 0 °C and aqueous layer was extracted with EtOAc (5 mL) for three times. The combined organic layer was washed with brine (5 mL) and dried over Na_2SO_4. After filtered and evaporation, the crude mixture was purified by silica gel column chromatography (ethyl acetate/petroleum ether = 1/15, v/v) to afford the yellow oil **14** (29.7 mg, 85% yield, 96:4 e.r.); $[\alpha]_D^{27}$ = -11.1 (c = 1.0, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 - 7.32 (m, 5H), 7.29 - 7.24 (m, 1H), 7.15 (d, *J* = 7.9 Hz, 1H), 7.08 (dd, *J* = 8.0, 1.3 Hz, 1H), 6.96 (q, *J* = 7.6 Hz, 2H), 6.85 (td, *J* = 7.8, 1.4 Hz, 1H), 6.71 (td, *J* = 7.9, 1.4 Hz, 1H), 6.57 (dd, *J* = 7.9, 1.4 Hz, 1H), 5.71 (s, 1H), 5.49 (s, 1H), 4.63 (t, *J* = 14.1 Hz, 1H), 4.06 (s, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.6, 144.5, 142.97 (t, *J* = 21.9 Hz), 136.8, 136.6, 131.1, 130.3, 128.7, 128.7, 128.4, 125.1, 124.3, 123.5, 121.7, 121.5, 120.94 (t, *J* = 9.0 Hz), 119.9, 119.2, 118.9, 61.96 (t, *J* = 27.6 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -100.71 (dd, *J* = 247.1, 13.8 Hz), -102.11 (dd, *J* = 247.1, 14.5 Hz); HRMS (ESI): *m/z* calcd for $C_{22}H_{17}F_2NNaO$ [M+Na]$^+$: 372.1170; found: 372.1163;

HPLC: Daicel Chiralpak AS, *n*-hexane/*i*-PrOH = 3:1, Flow rate = 1.0 mL/min, λ = 210 nm, t_R = 5.7 min (major) and t_R = 6.7 min (minor).

6. Crystal structure data of 3k

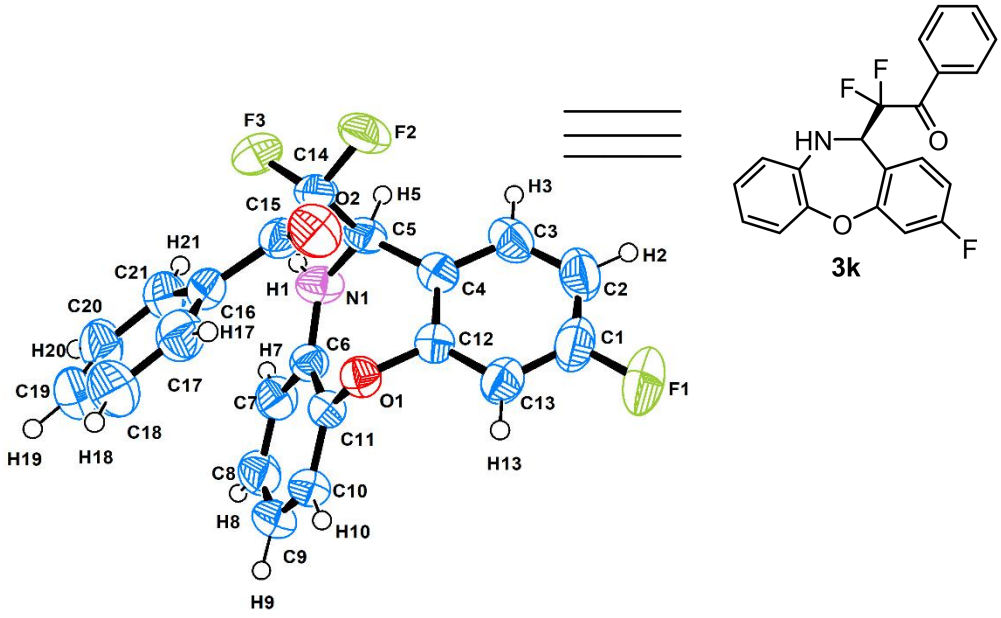


Figure S1. ORTEP diagram of **3k** (CCDC: 2086556). Thermal ellipsoids are shown at the 50% probability level.

Method of crystallization: A solution of **3k** in n-hexane/CH_2Cl_2 (3:1) was added to a 10 mL vial. The vial was closed with parafilm and poked a few of holes with a needle on the parafilm to slowly evaporation of solvent.

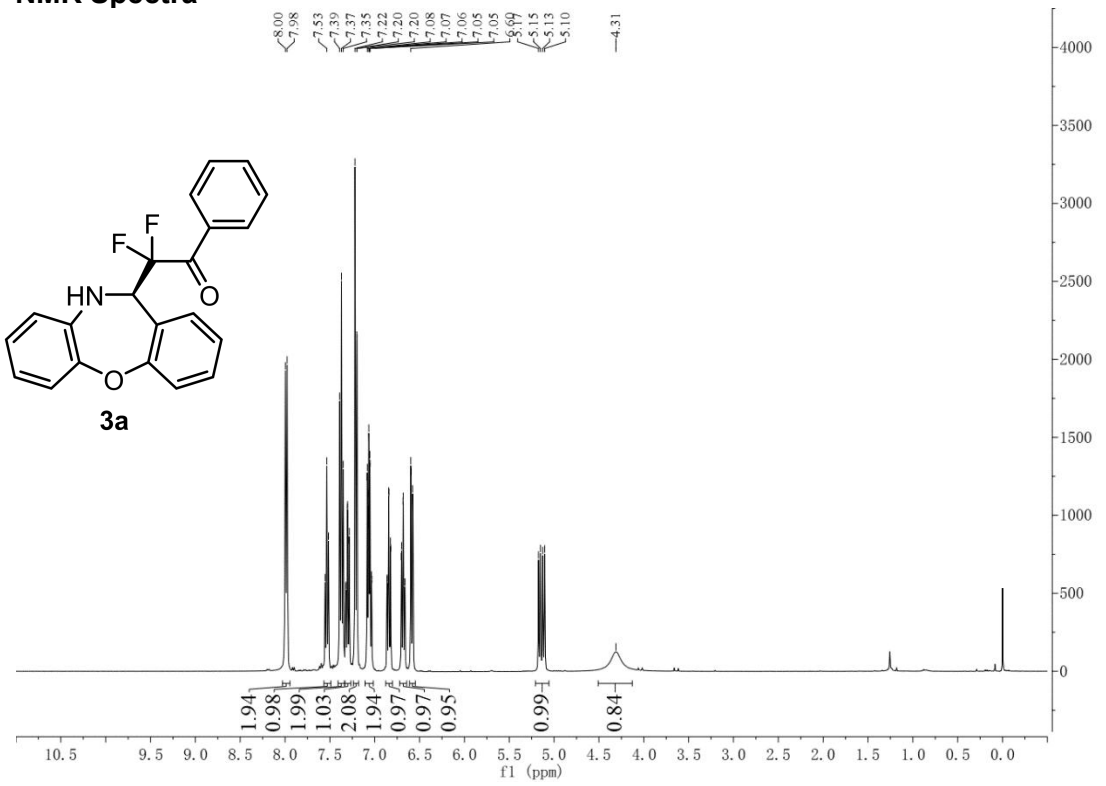
The X-ray intensity data was measured on a Rigaku 007HF XtaLAB P200 single crystal diffractometer.

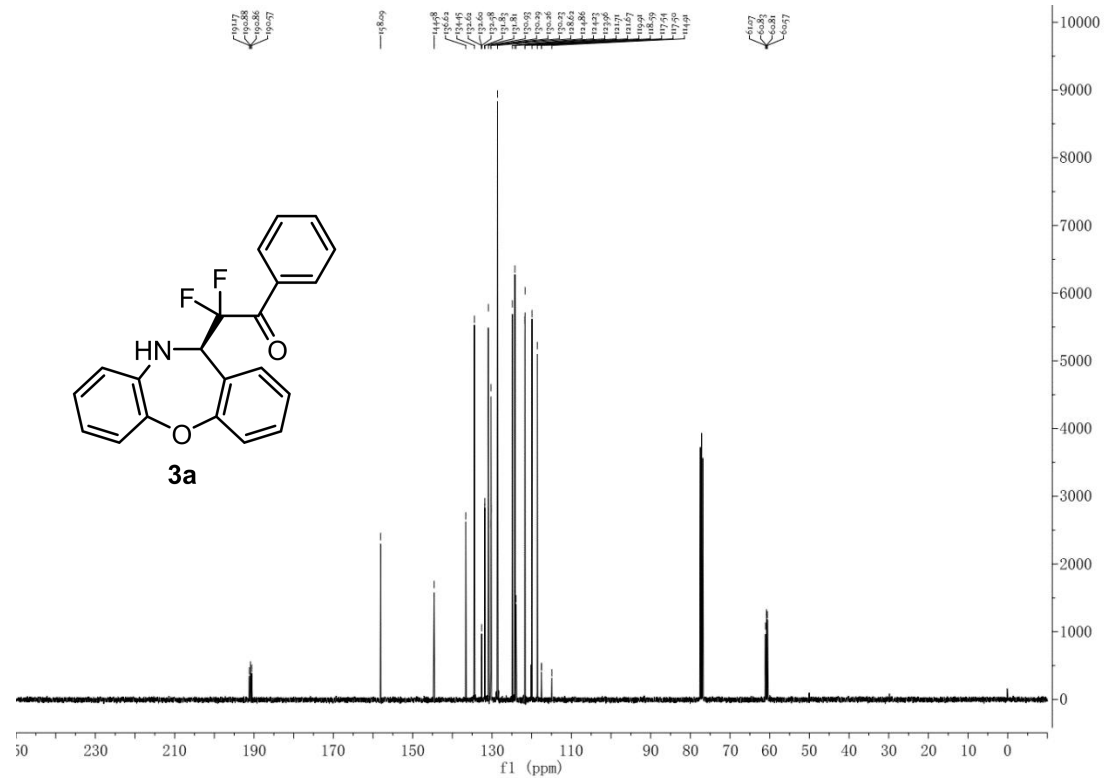
Identification code	**3k:** 2086556
Empirical formula	$C_{21}H_{14}F_3NO_2$
Formula weight	369.33
Temperature/K	293.15
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	9.41501(4)
b/Å	11.47864(6)
c/Å	16.21315(9)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	1752.179(16)
Z	4
ρ_{calc}g/cm^3	1.400
μ/mm^{-1}	0.952
F(000)	760.0
Crystal size/mm^3	0.23 × 0.21 × 0.17
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	9.44 to 158.144
Index ranges	-11 ≤ h ≤ 11, -11 ≤ k ≤ 14, -20 ≤ l ≤ 18
Reflections collected	21558

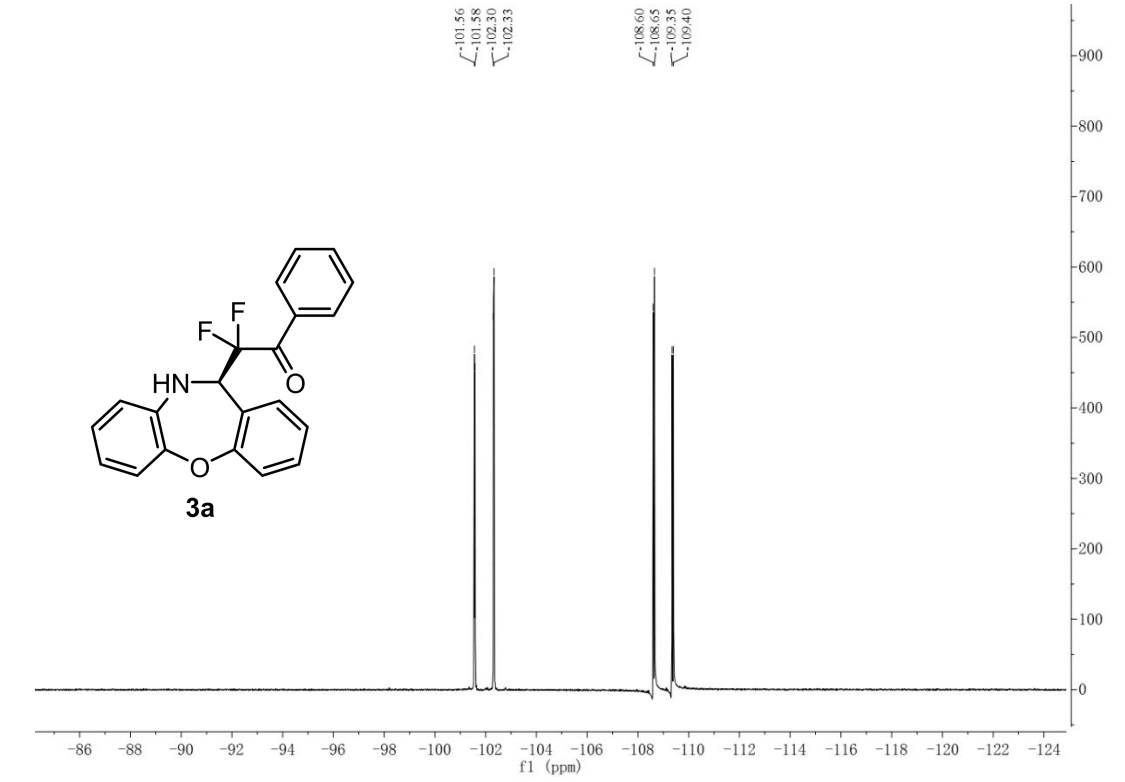
Independent reflections	3730 [R_{int} = 0.0236, R_{sigma} = 0.0137]
Data/restraints/parameters	3730/0/245
Goodness-of-fit on F^2	1.064
Final R indexes [I>=2σ (I)]	R_1 = 0.0266, wR_2 = 0.0738
Final R indexes [all data]	R_1 = 0.0270, wR_2 = 0.0742
Largest diff. peak/hole / e $Å^{-3}$	0.14/-0.10
Flack parameter	-0.05(3)

7. NMR and HPLC spectra

NMR Spectra



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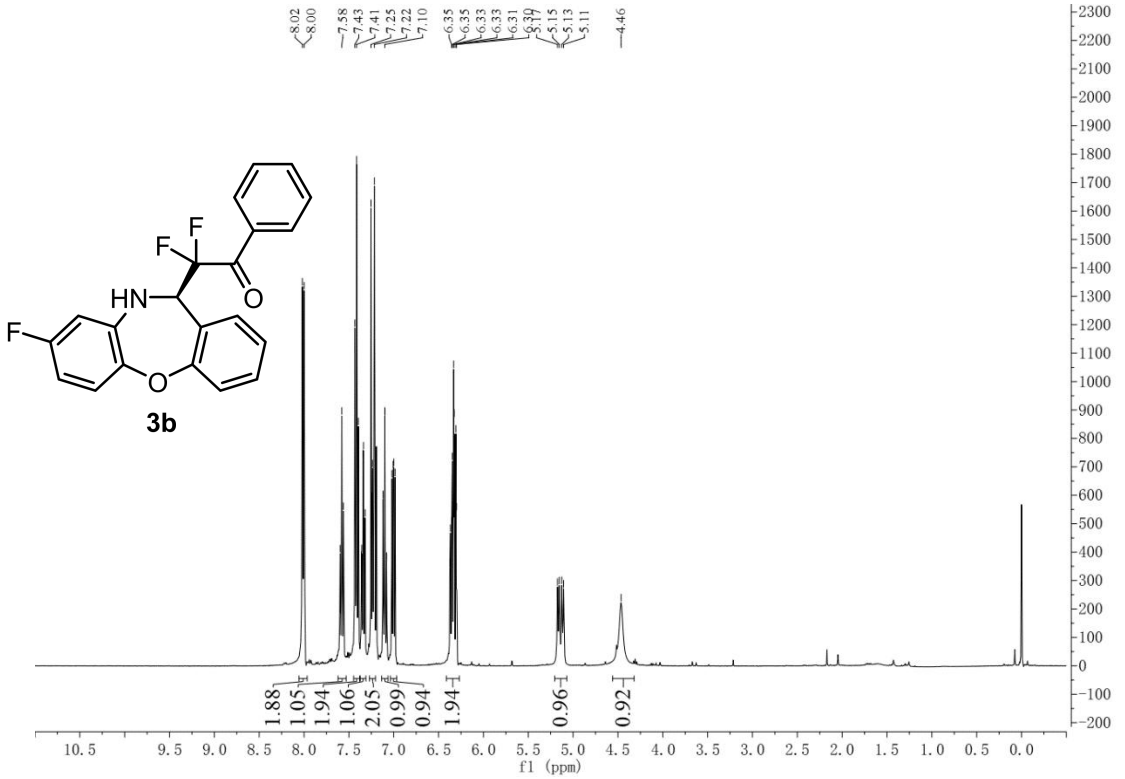
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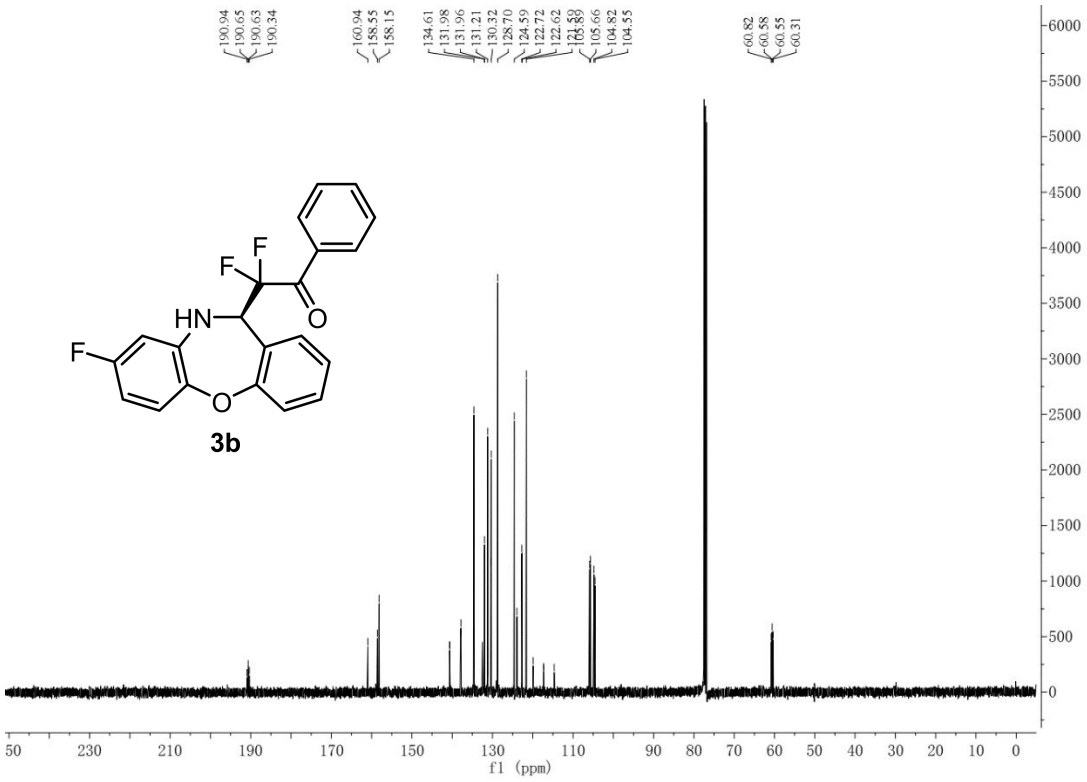
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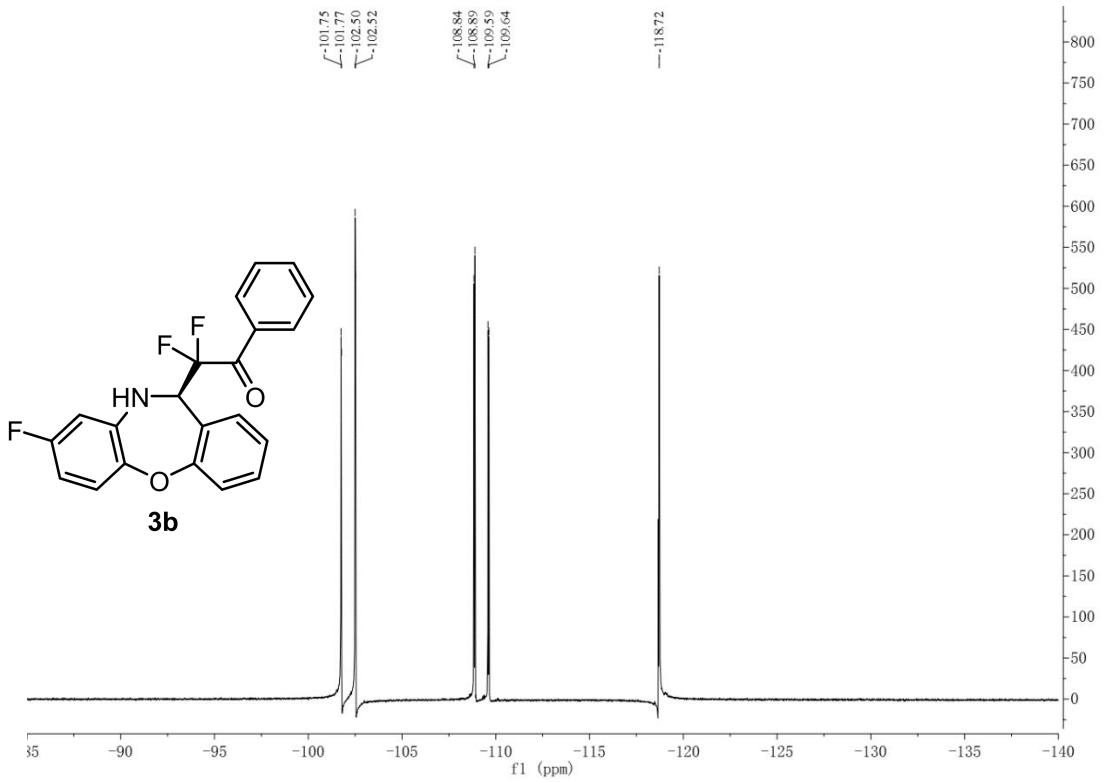
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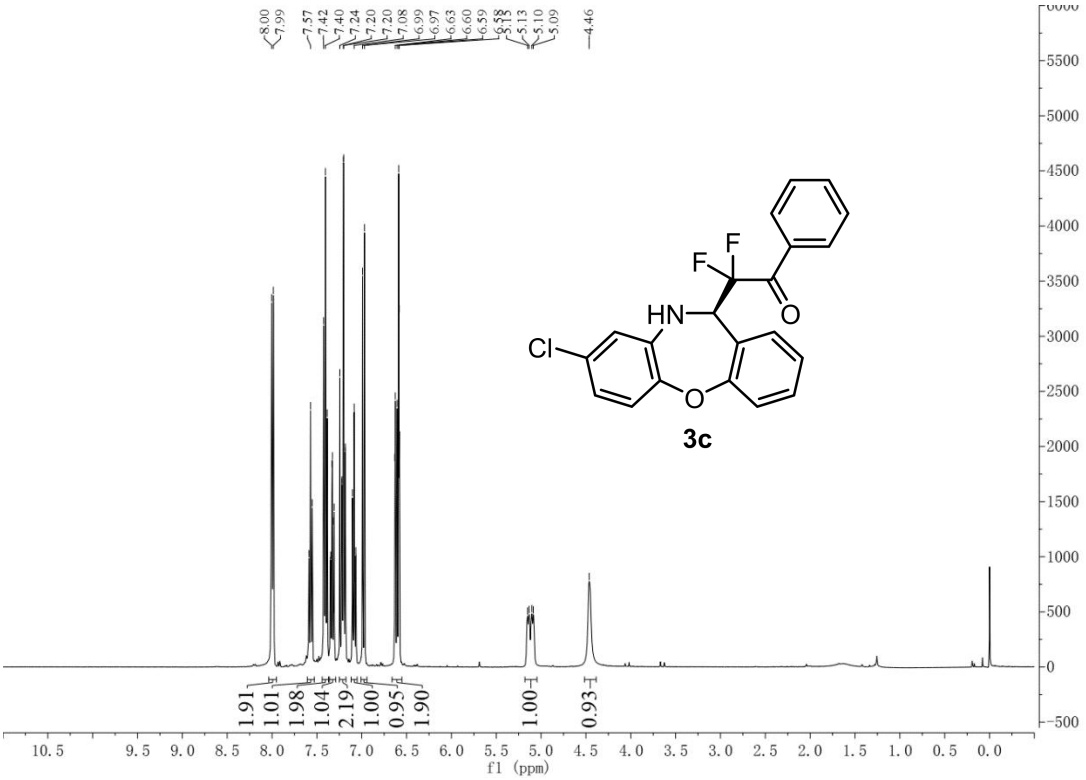
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Cl
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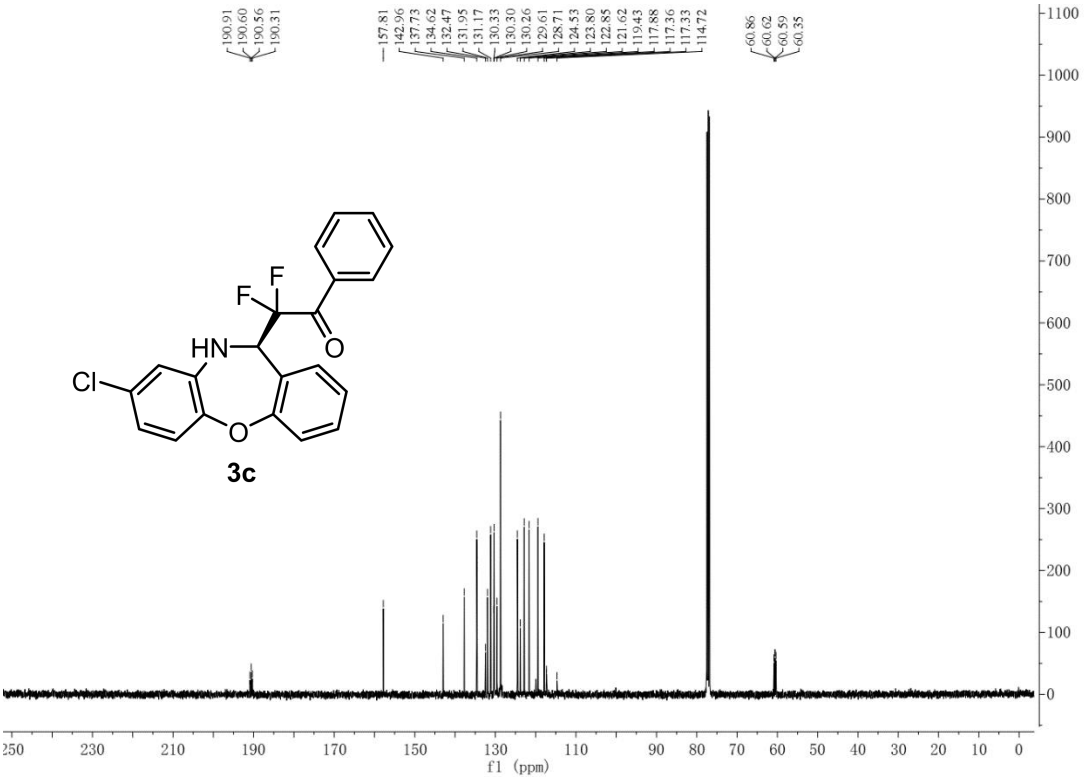
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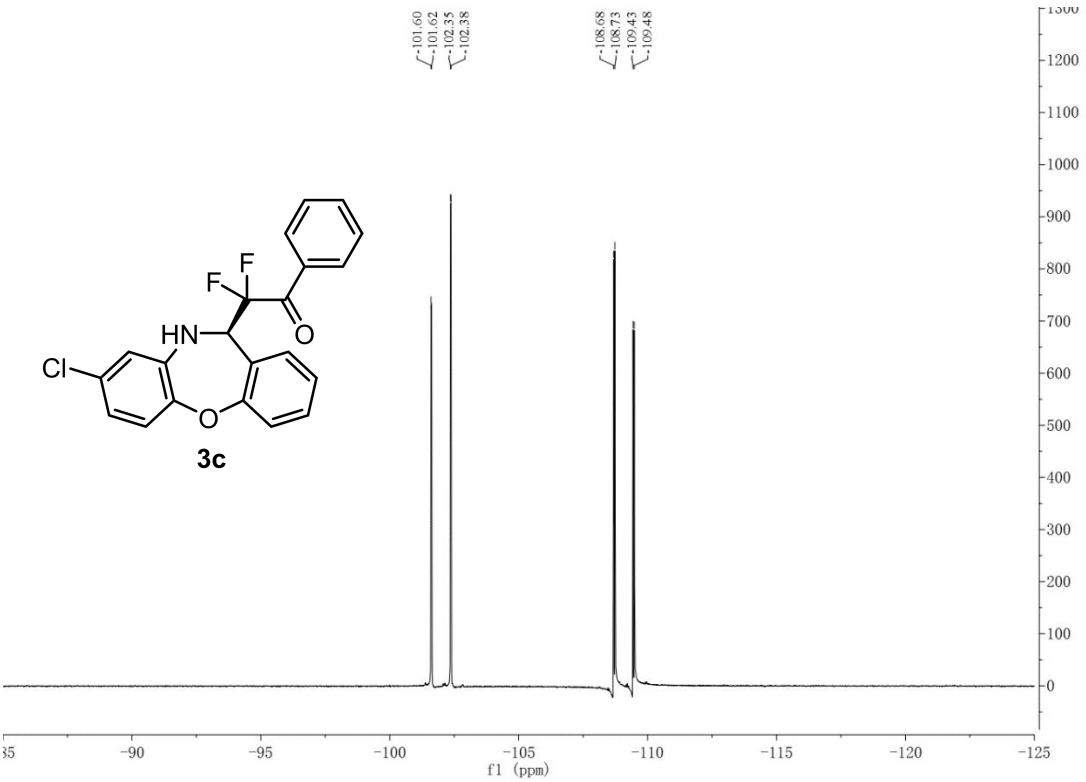
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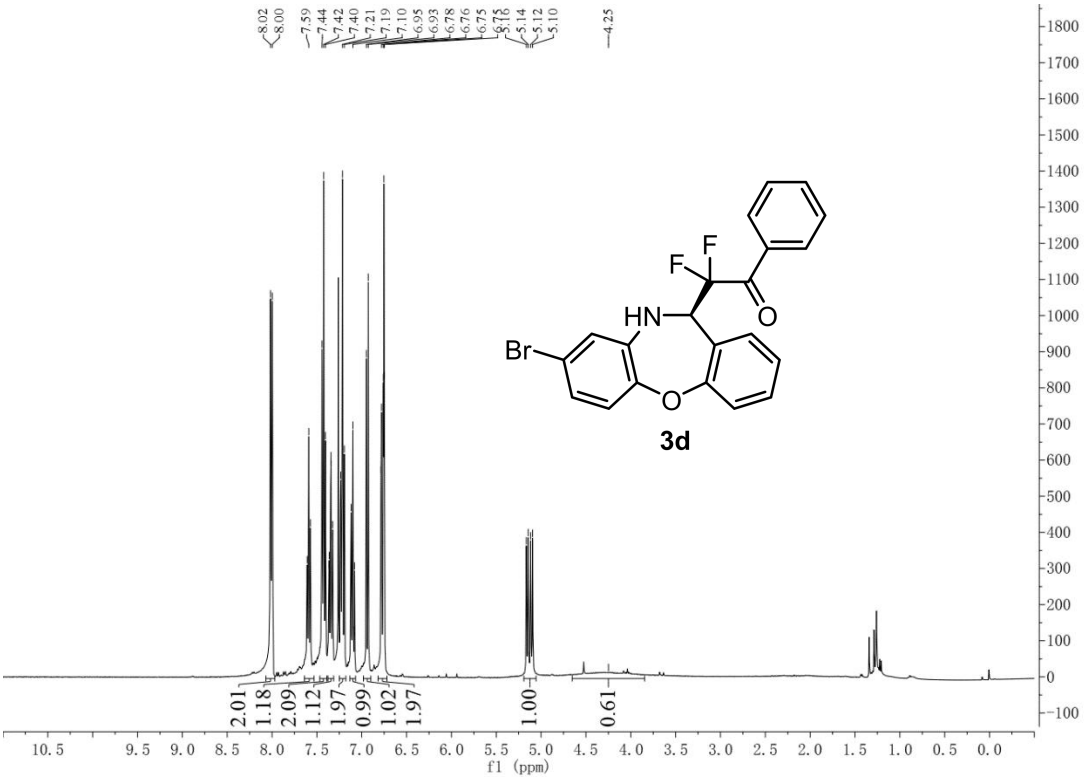
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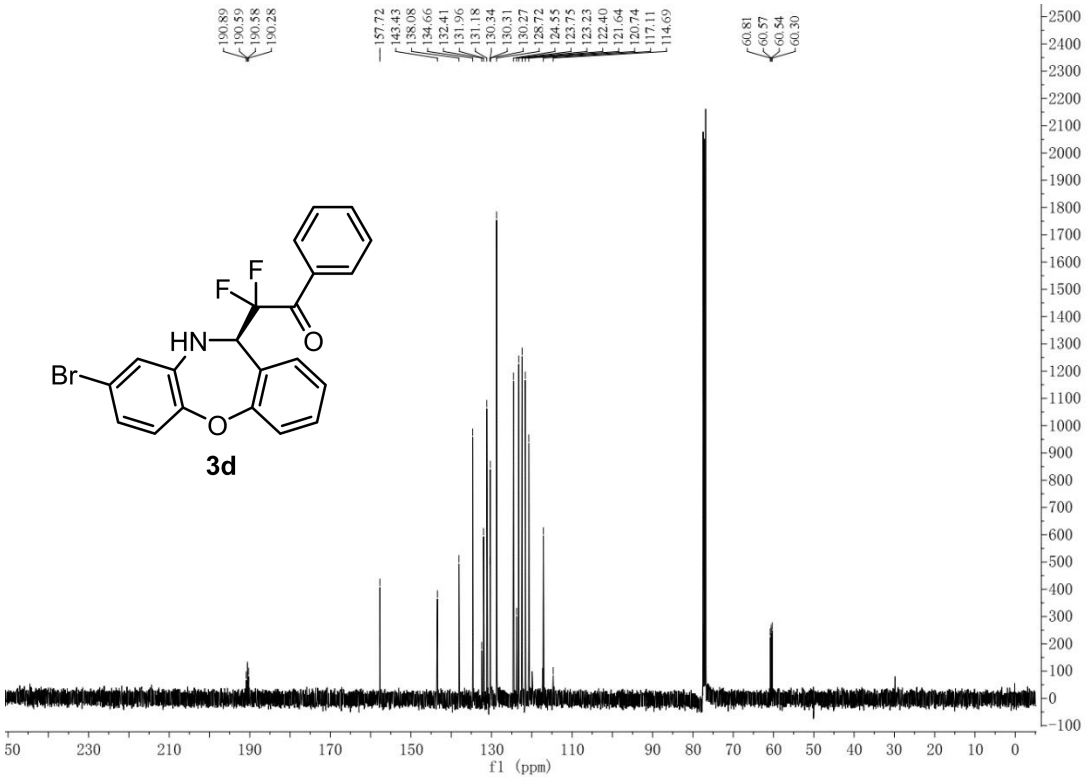
3d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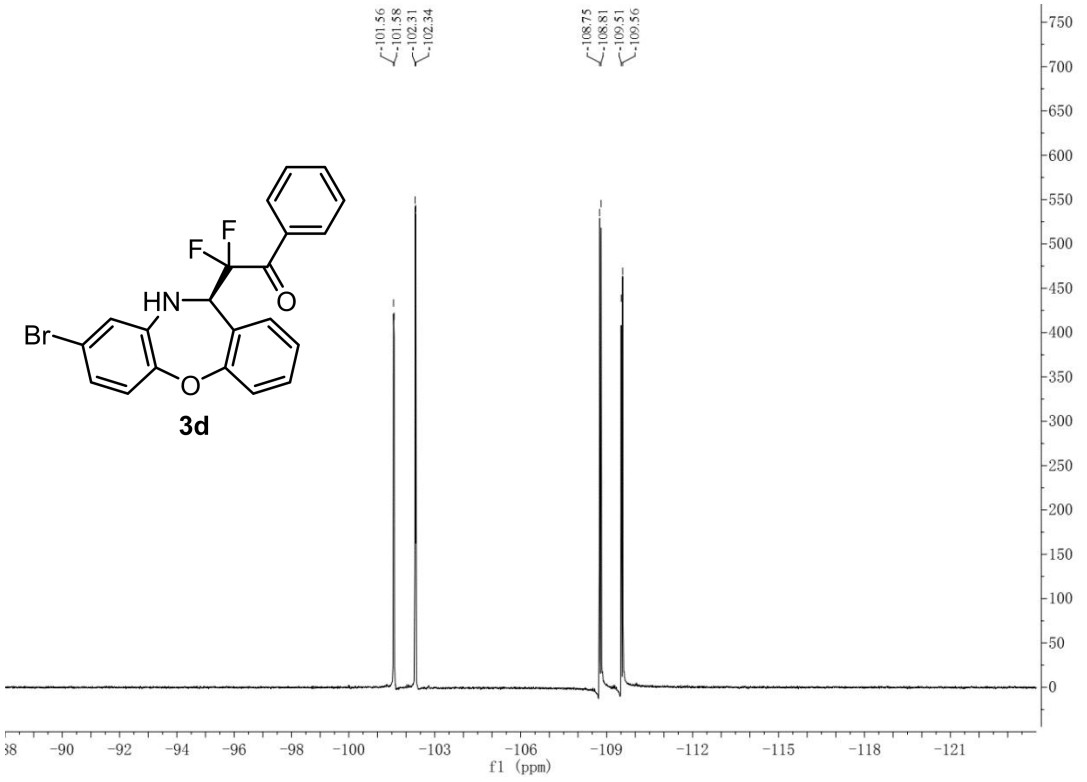
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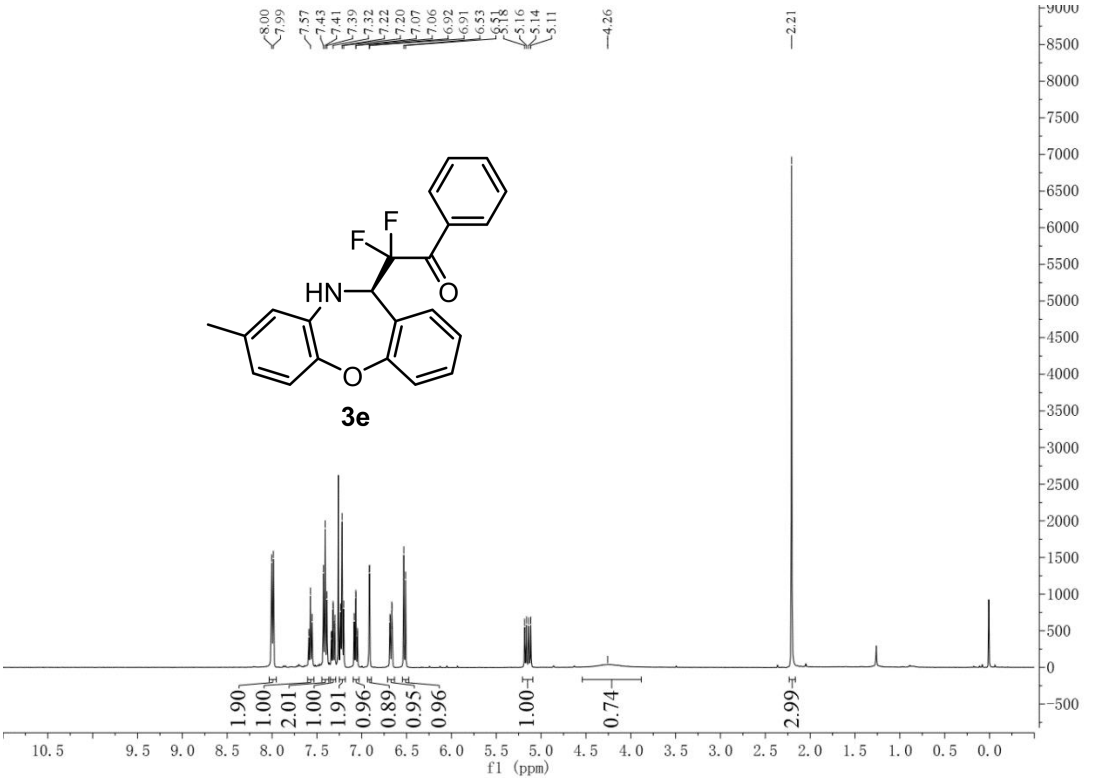
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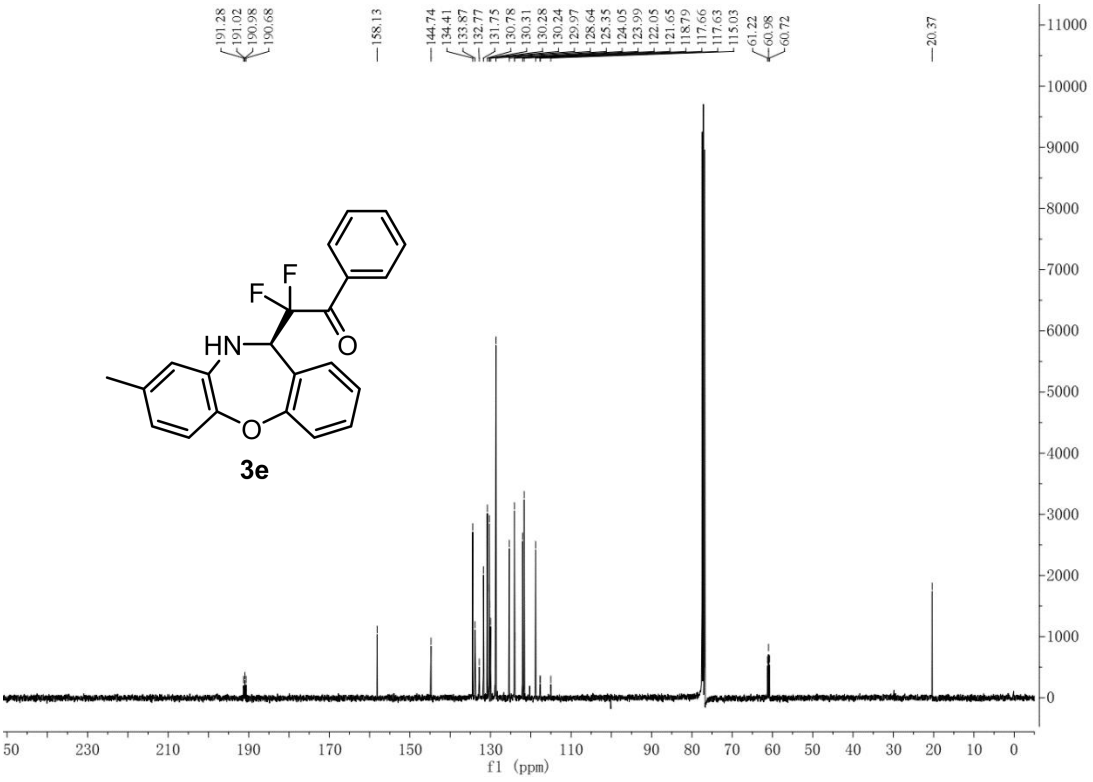
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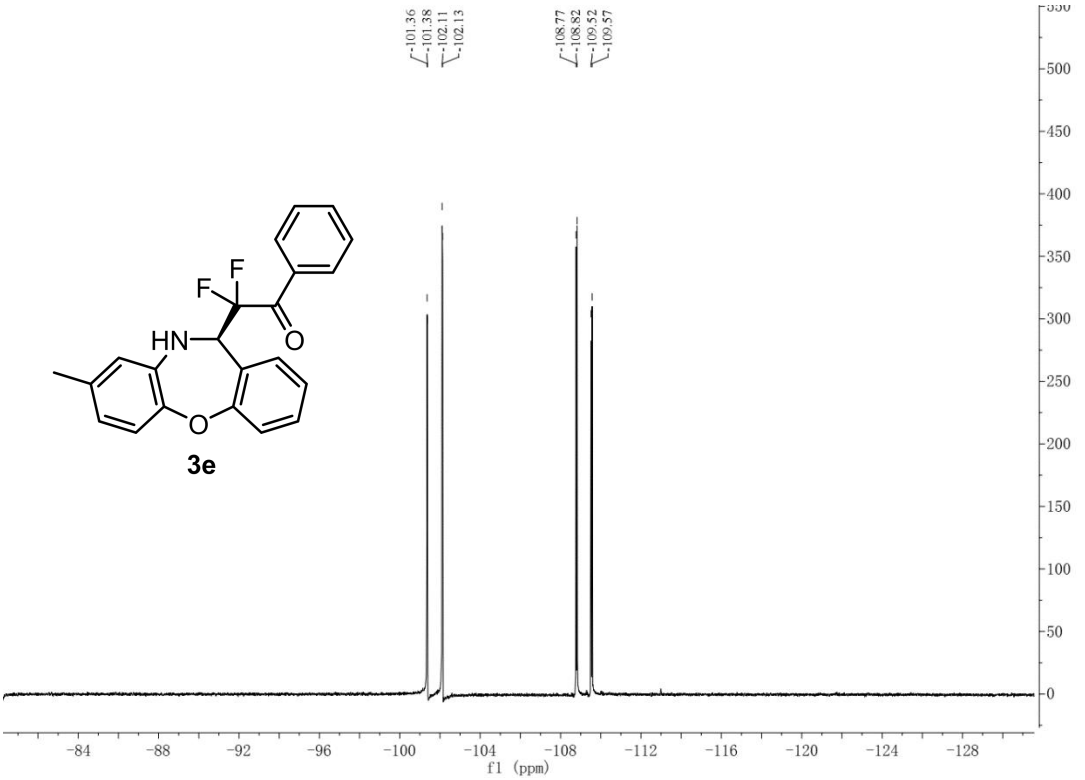
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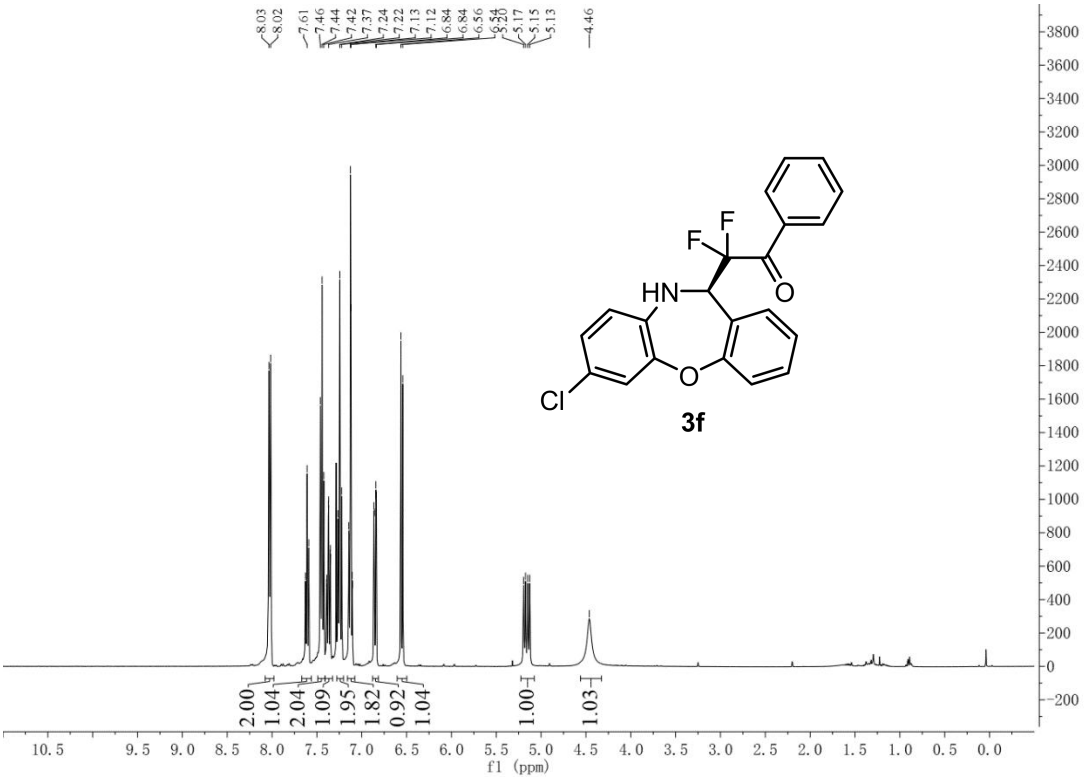
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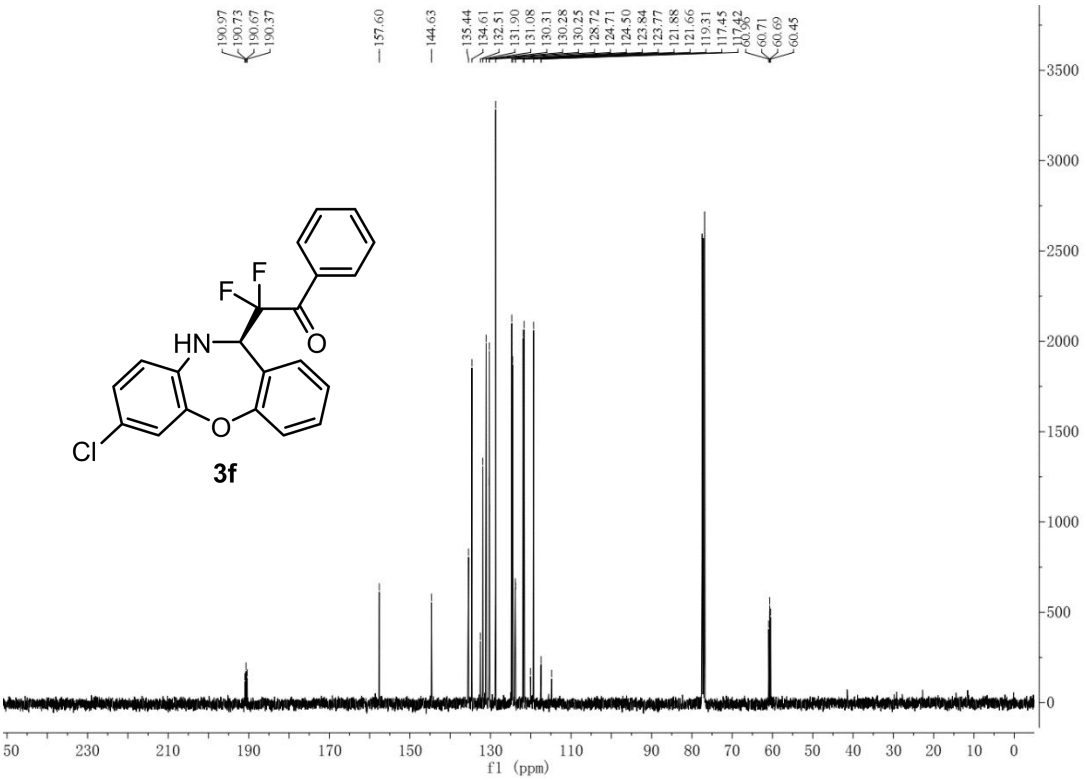
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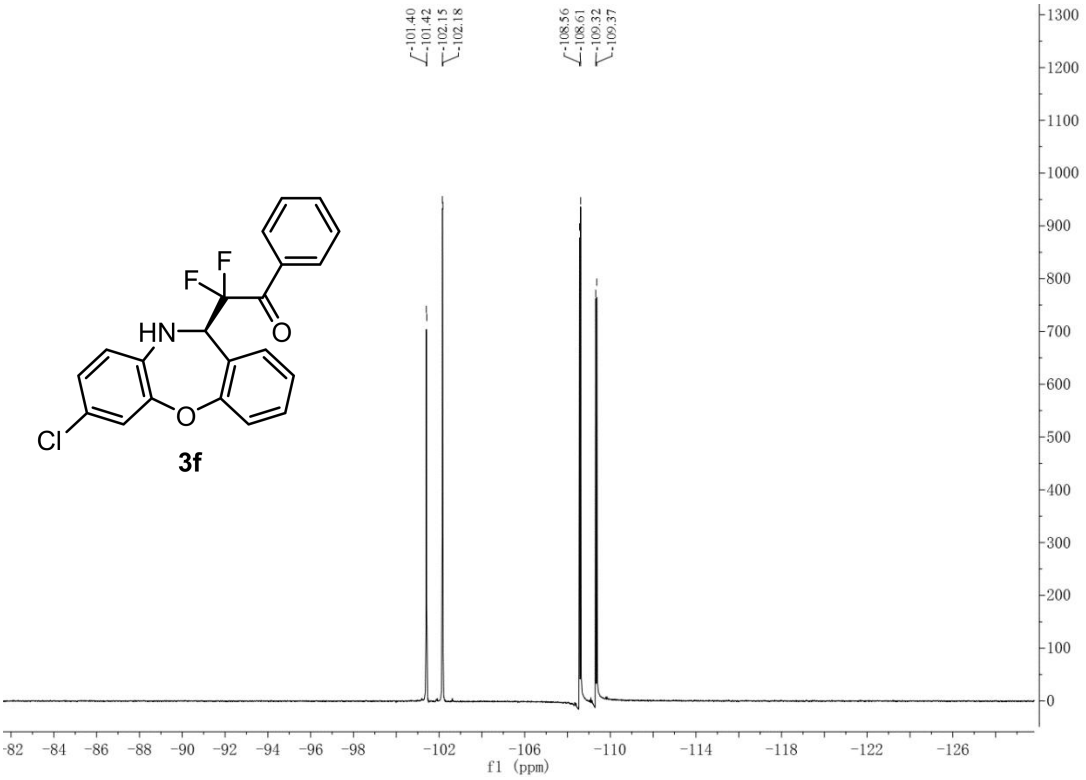
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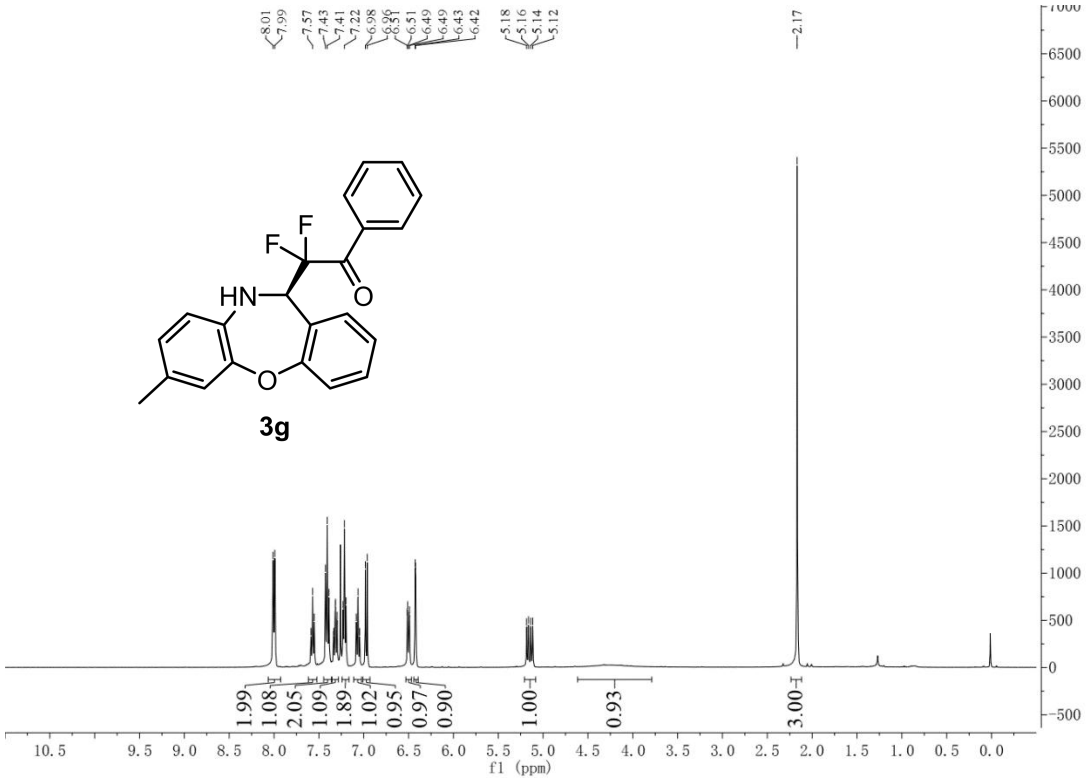
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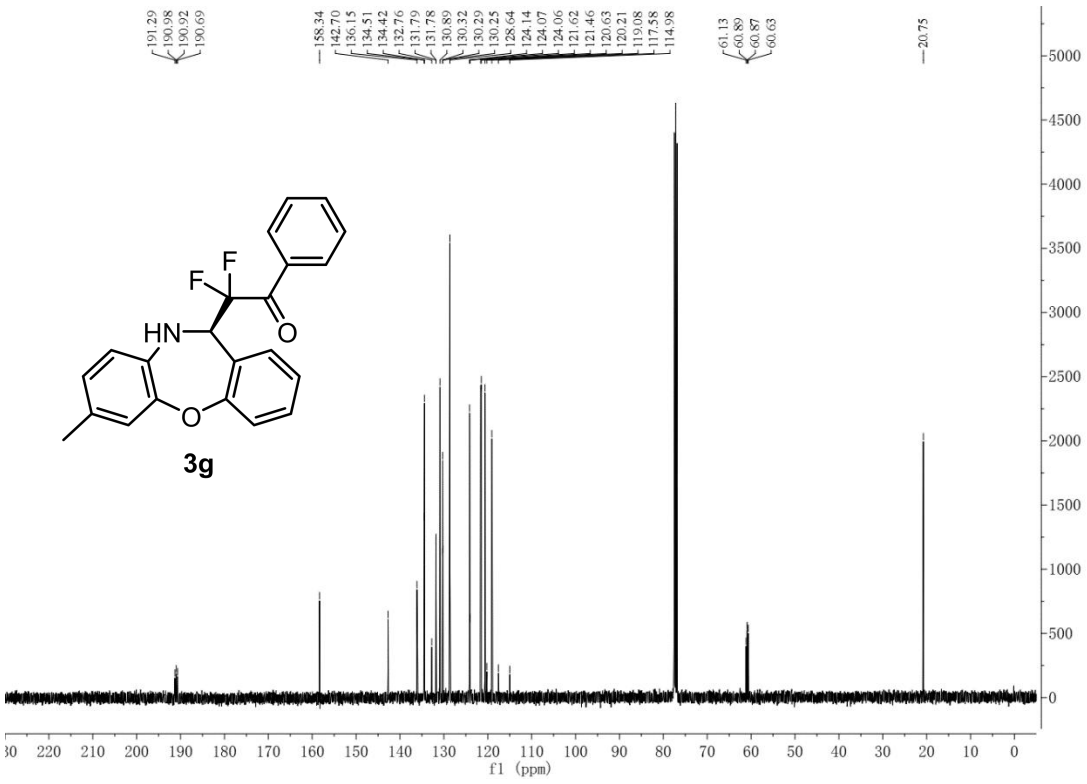
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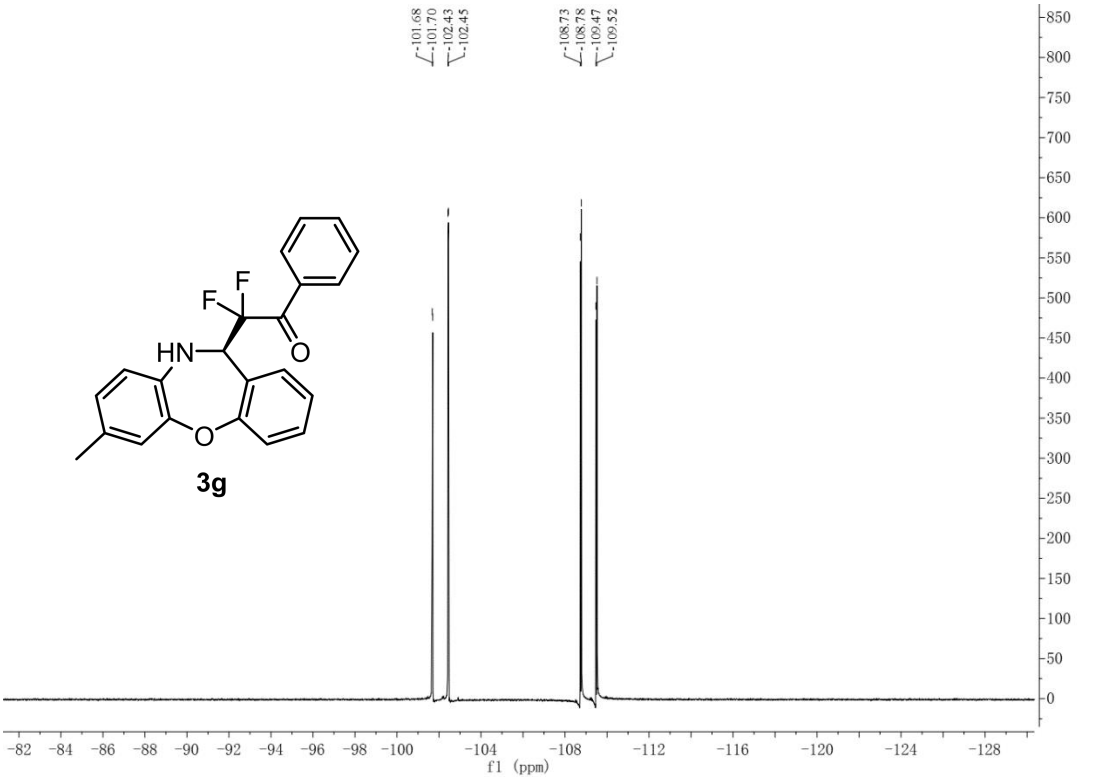
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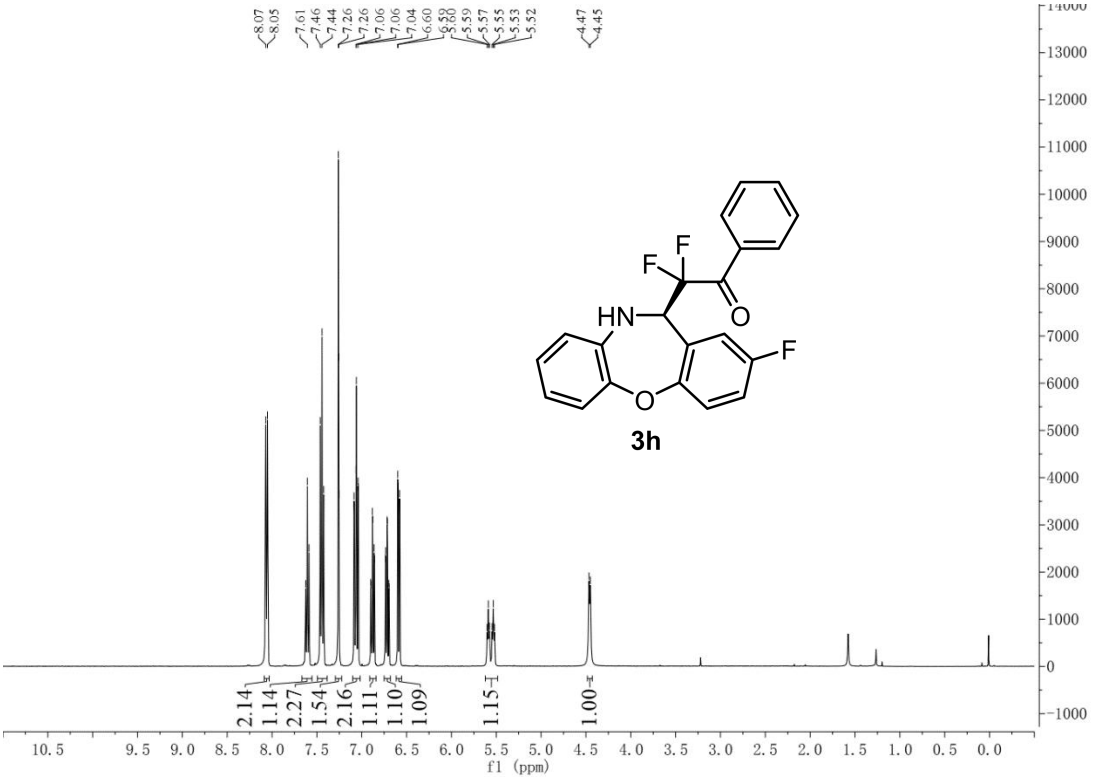
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1.15
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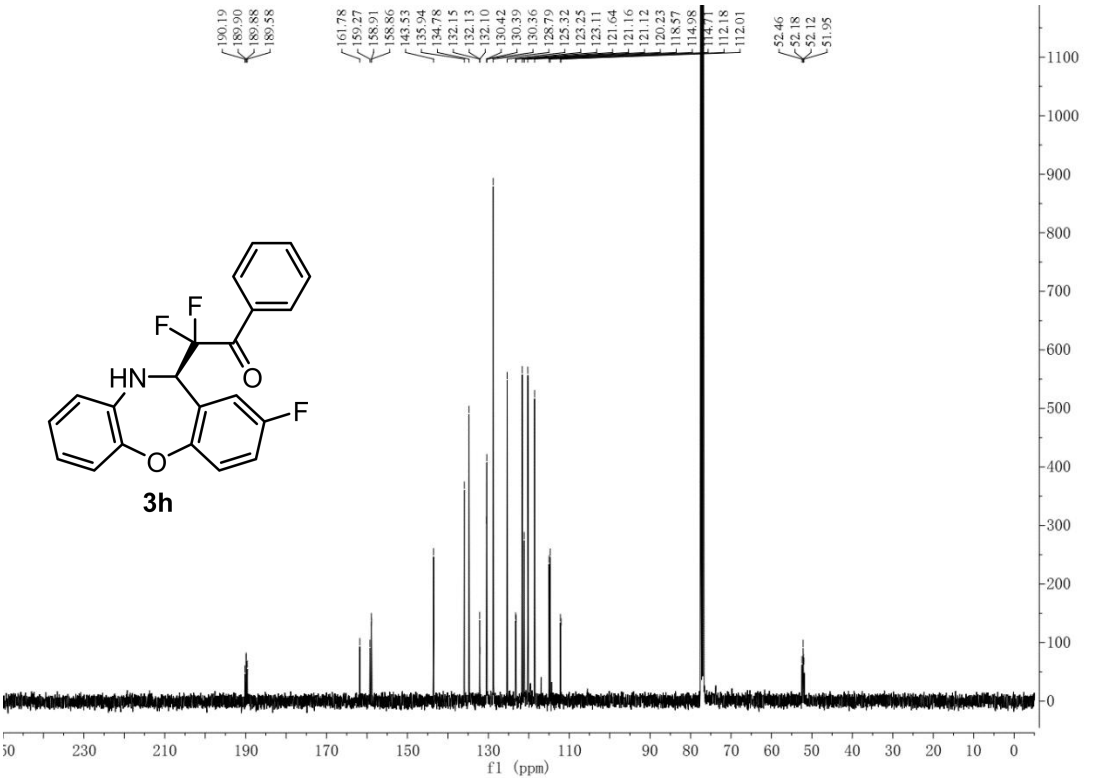
f1 (ppm)

3h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158.91
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135.94
134.78
132.15
132.13
132.10
130.42
130.39
130.36
128.79
125.32
123.25
123.11
121.64
121.16
121.12
120.23
118.57
114.98
114.71
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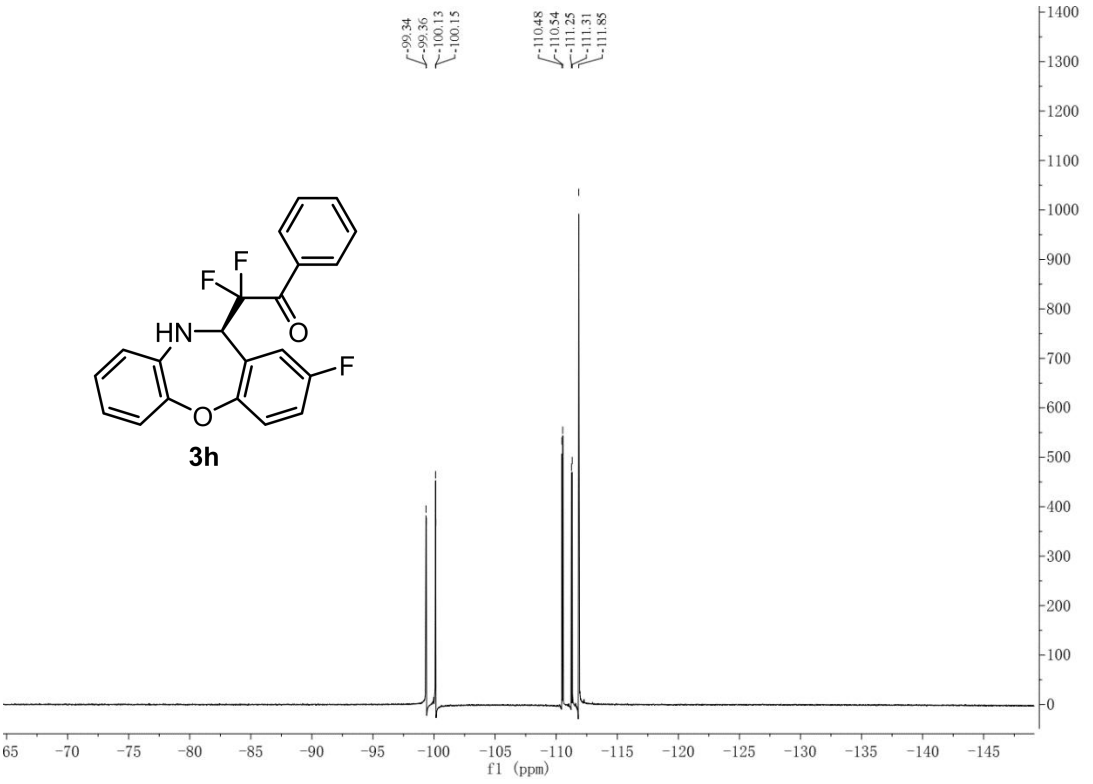
52.18
52.12
51.95
F
F
HN
O
F
O
3h
f1 (ppm)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-100.13
-100.15
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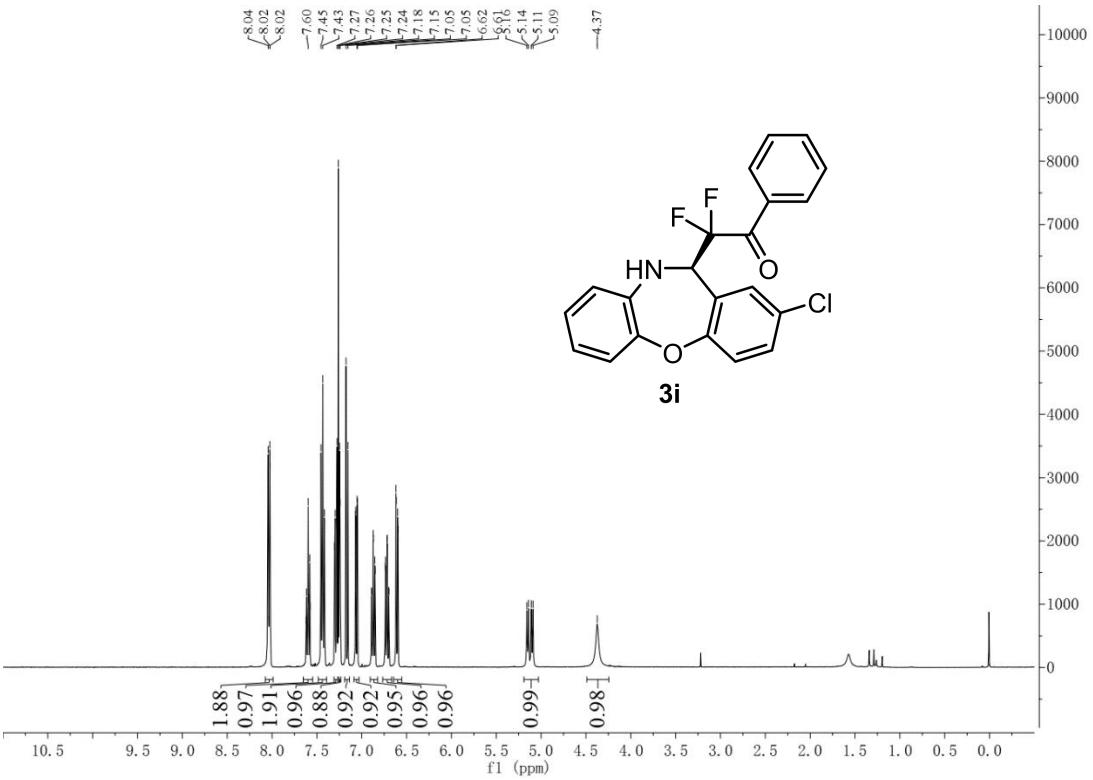
-111.25
-111.31
-111.85
F
F
HN
O
F
O
3h
f1 (ppm)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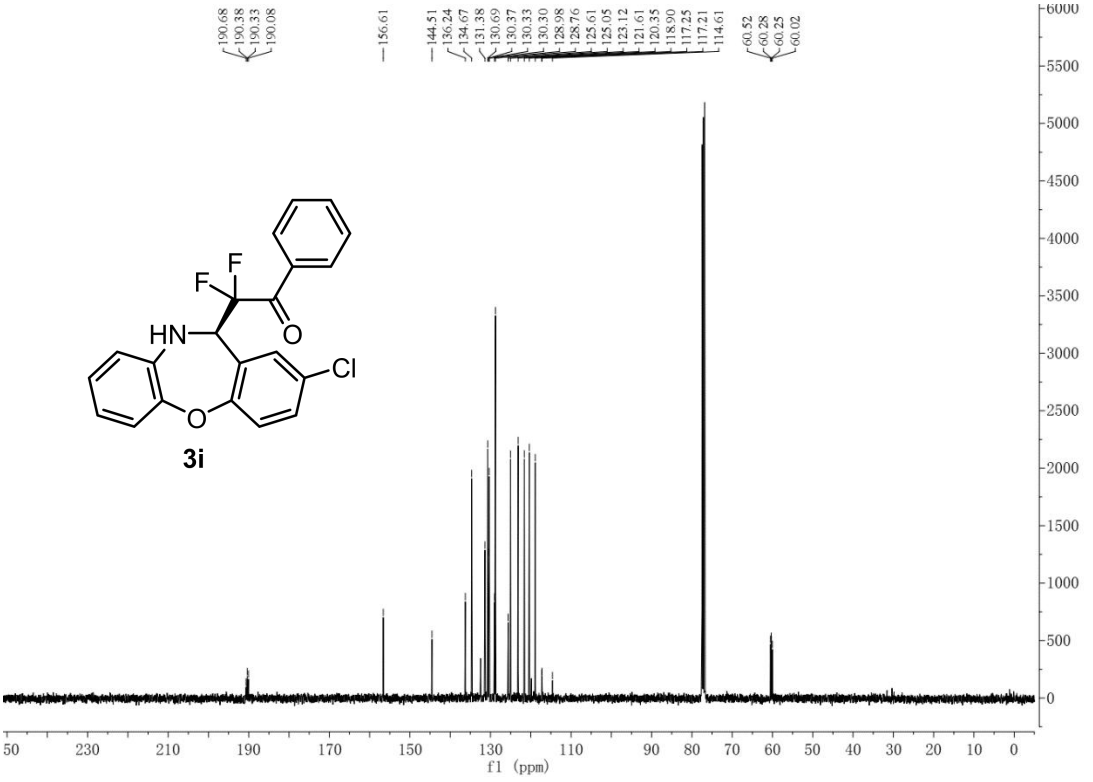
8.02
8.02
7.60
7.45
7.43
7.27
7.26
7.25
7.24
7.18
7.15
7.05
7.05
6.62
6.61
5.16
5.14
5.11
5.09
4.37
F
F
HN
O
Cl
O
3i
1.88
0.97
1.91
0.96
0.88
0.92
0.92
0.95
0.96
0.96
0.99
0.98
f1 (ppm)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134.67
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130.37
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130.30
128.98
128.76
125.61
125.05
123.12
121.61
120.35
118.90
117.25
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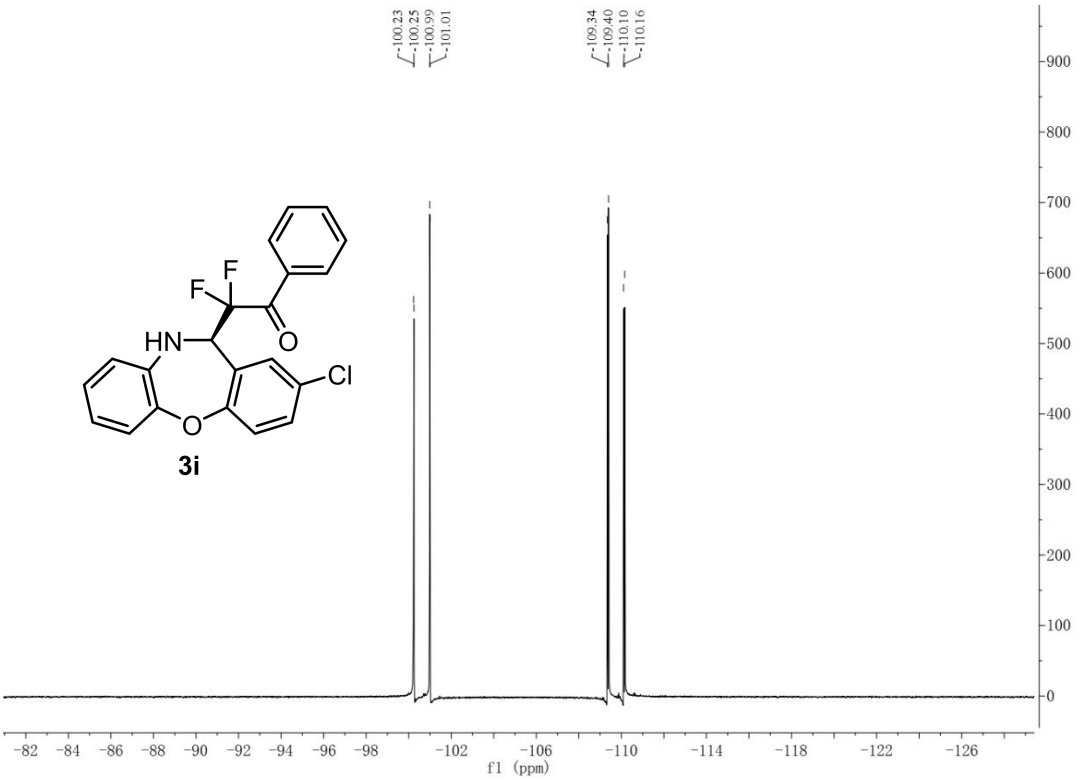
60.28
60.25
60.02
F
F
HN
O
Cl
O
3i
f1 (ppm)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-100.99
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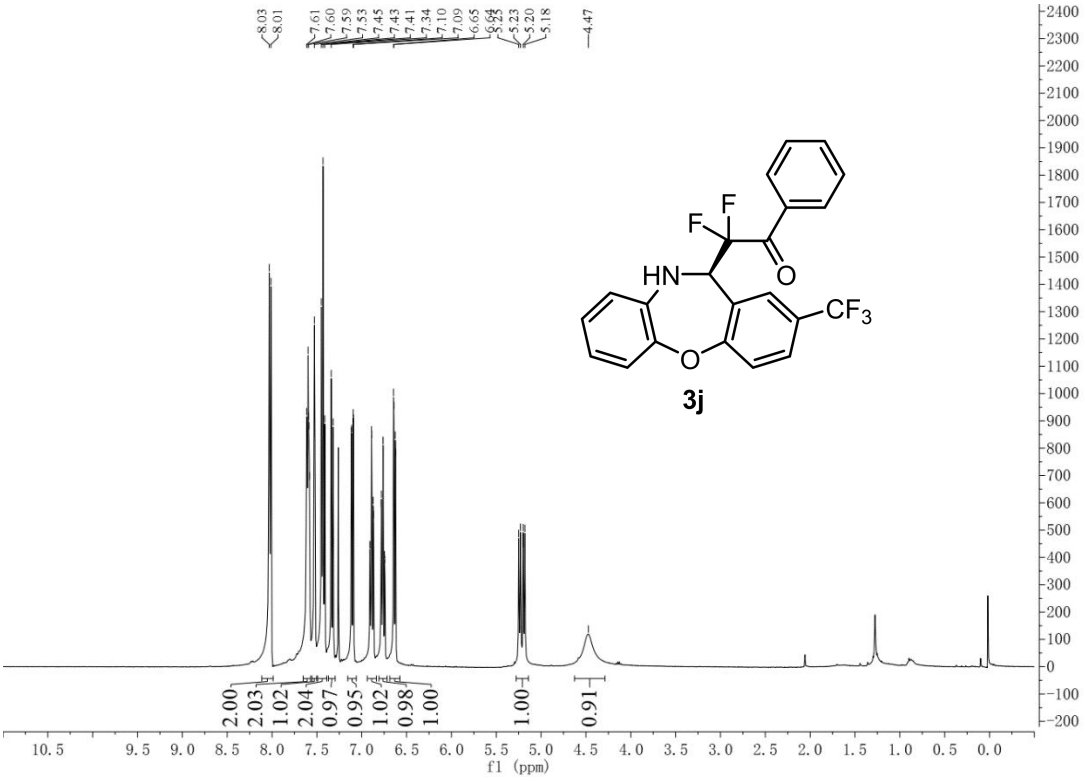
-110.10
-110.16
F
F
HN
O
Cl
O
f1 (ppm)

3i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8.01
7.61
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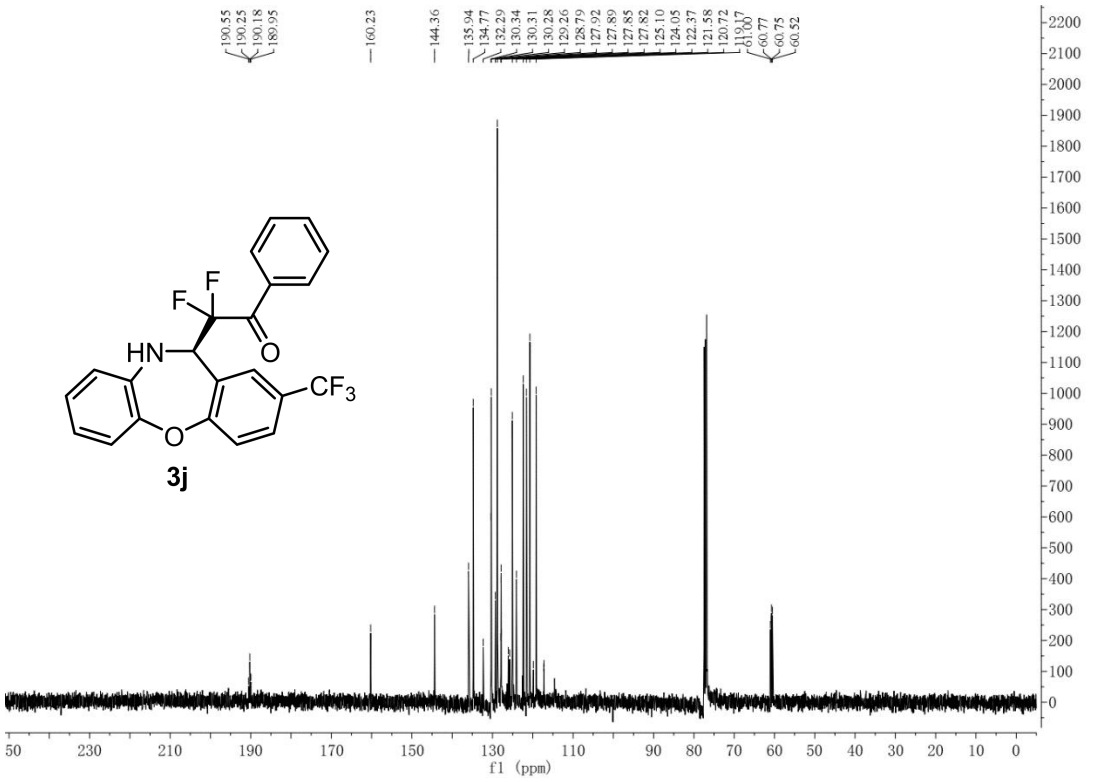
7.59
7.53
7.45
7.43
7.41
7.34
7.10
7.09
6.65
5.23
5.20
5.18
4.47
F
F
HN
O
CF3
O
2.00
2.03
1.02
2.04
0.97
0.95
1.02
0.98
1.00
1.00
0.91
f1 (ppm)

3j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134.77
132.29
130.34
130.31
130.28
129.26
128.79
127.92
127.89
127.85
127.82
125.10
124.05
122.37
121.58
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61.00
60.77
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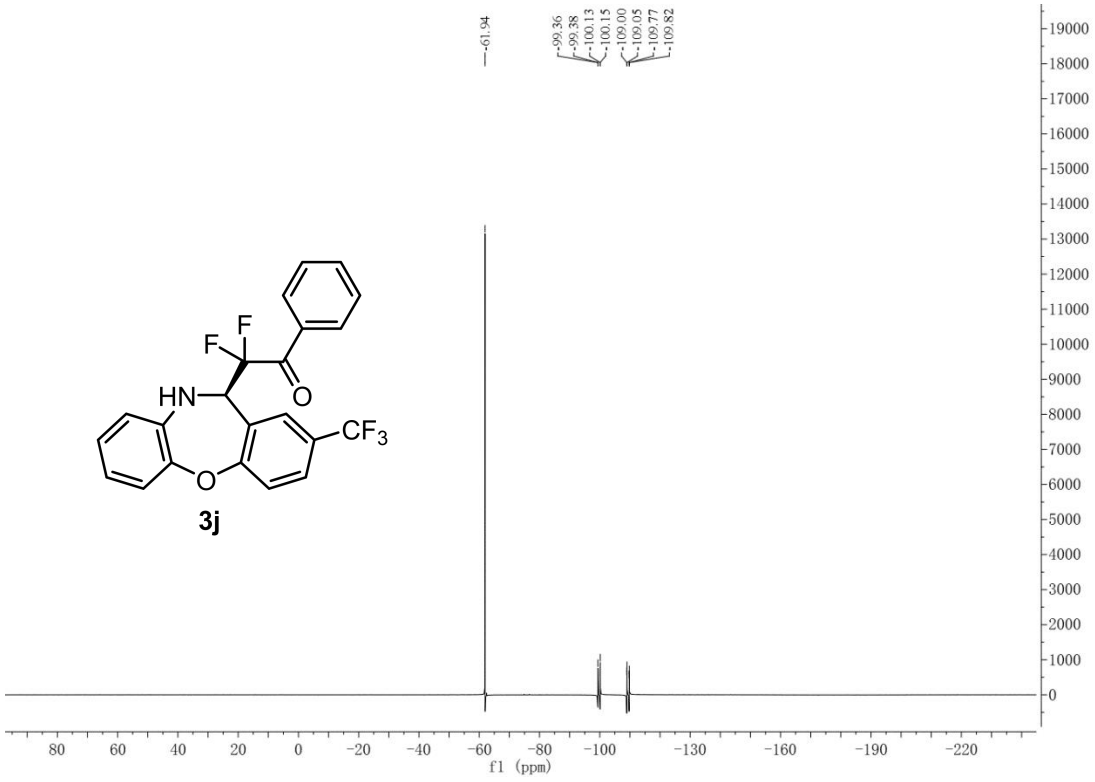
60.52
F
F
HN
O
CF3
O
3j
f1 (ppm)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-100.13
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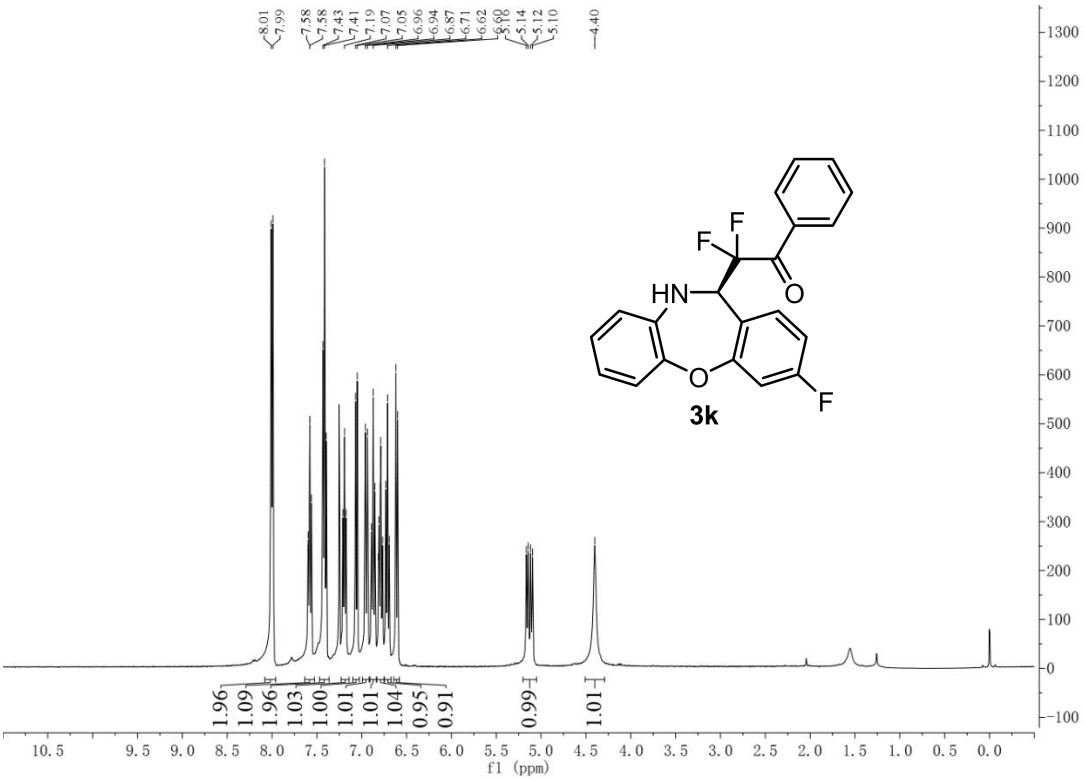
-109.00
-109.05
-109.77
-109.82
F
F
HN
O
CF3
O
3j
f1 (ppm)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7.99
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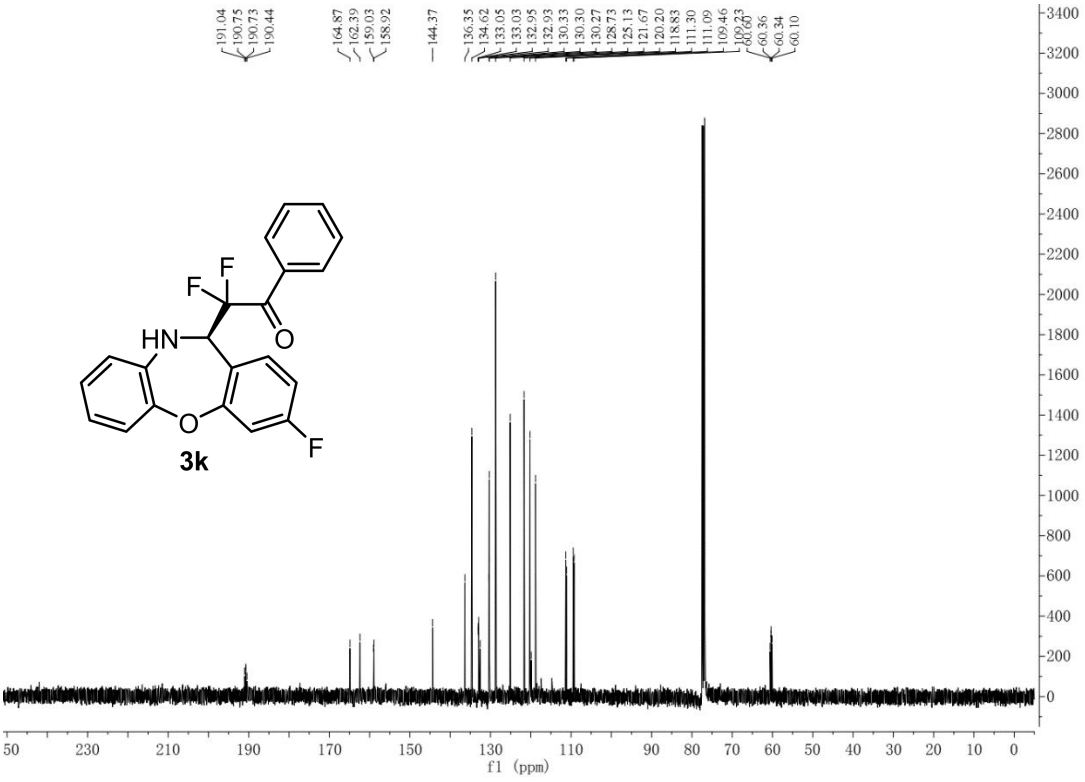
7.58
7.43
7.41
7.19
7.07
7.05
6.96
6.94
6.87
6.71
6.62
6.60
5.18
5.14
5.12
5.10
4.40
F
F
HN
O
O
F
3k
1.96
1.09
1.96
1.03
1.00
1.01
1.01
1.04
0.95
0.91
0.99
1.01
f1 (ppm)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162.39
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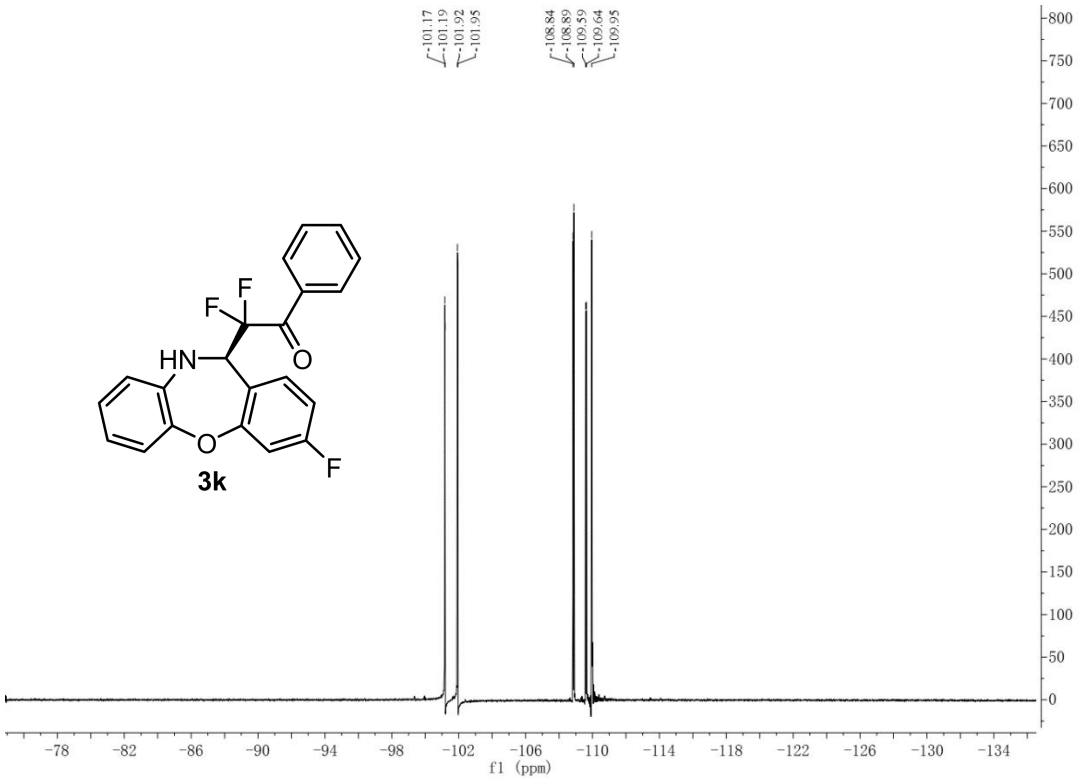
158.92
144.37
136.35
134.62
133.05
133.03
132.95
132.93
130.33
130.30
130.27
128.73
125.13
121.67
120.20
118.83
111.30
111.09
109.46
109.23
60.68
60.36
60.34
60.10
F
F
HN
O
O
F
3k
f1 (ppm)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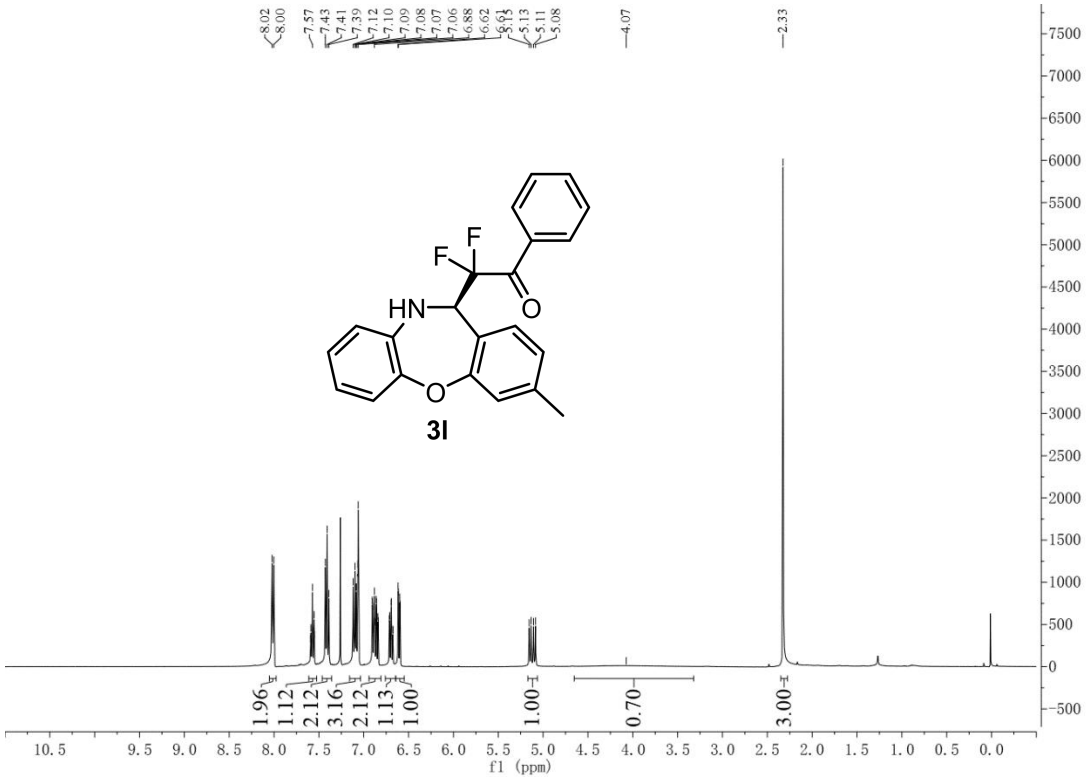
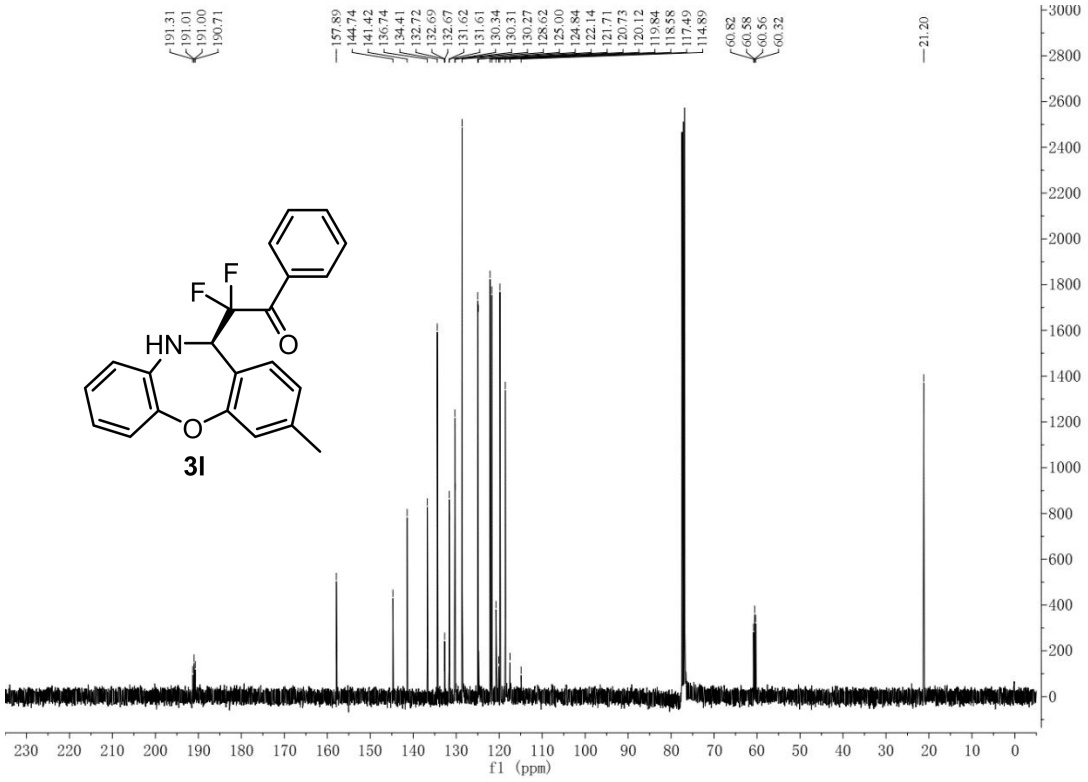
-101.19
-101.92
-101.95
-108.84
-108.89
-109.59
-109.64
-109.95
F
F
HN
O
O
F
3k
f1 (ppm)


8.02
8.00
7.57
7.43
7.41
7.39
7.12
7.10
7.09
7.08
7.07
7.06
6.88
6.62
6.61
5.13
5.11
5.08
4.07
2.33
F
F
HN
O
O
3l
1.96
1.12
2.12
3.16
2.12
1.13
1.00
1.00
0.70
3.00
f1 (ppm)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141.42
136.74
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132.72
132.69
132.67
131.62
131.61
130.34
130.31
130.27
128.62
125.00
124.84
122.14
121.71
120.73
120.12
119.84
118.58
117.49
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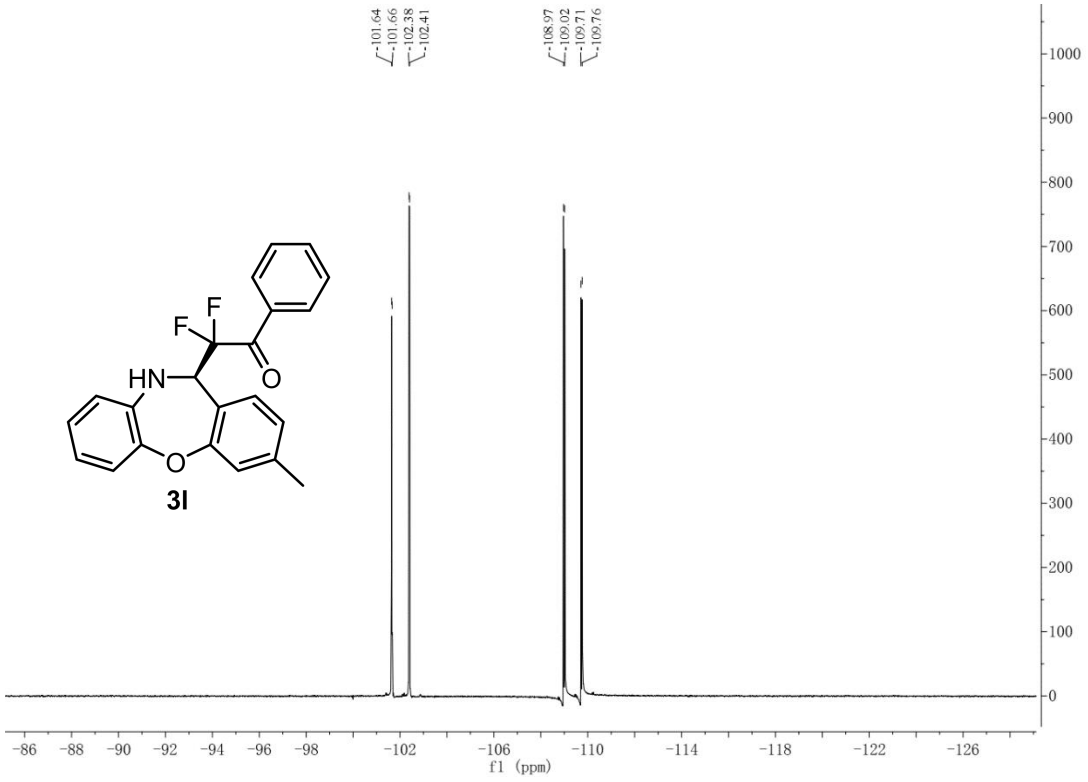
60.58
60.56
60.32
21.20
F
F
HN
O
O
3l
f1 (ppm)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102.41
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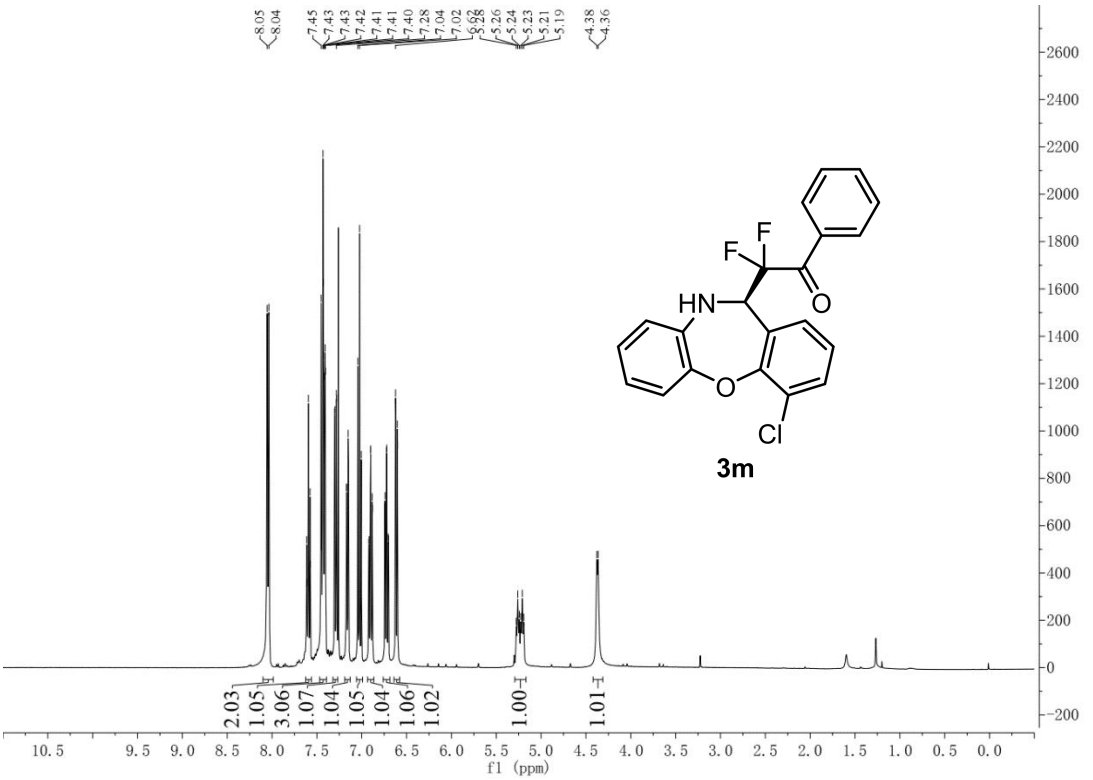
109.02
109.71
109.76
F
F
HN
O
O
3l
f1 (ppm)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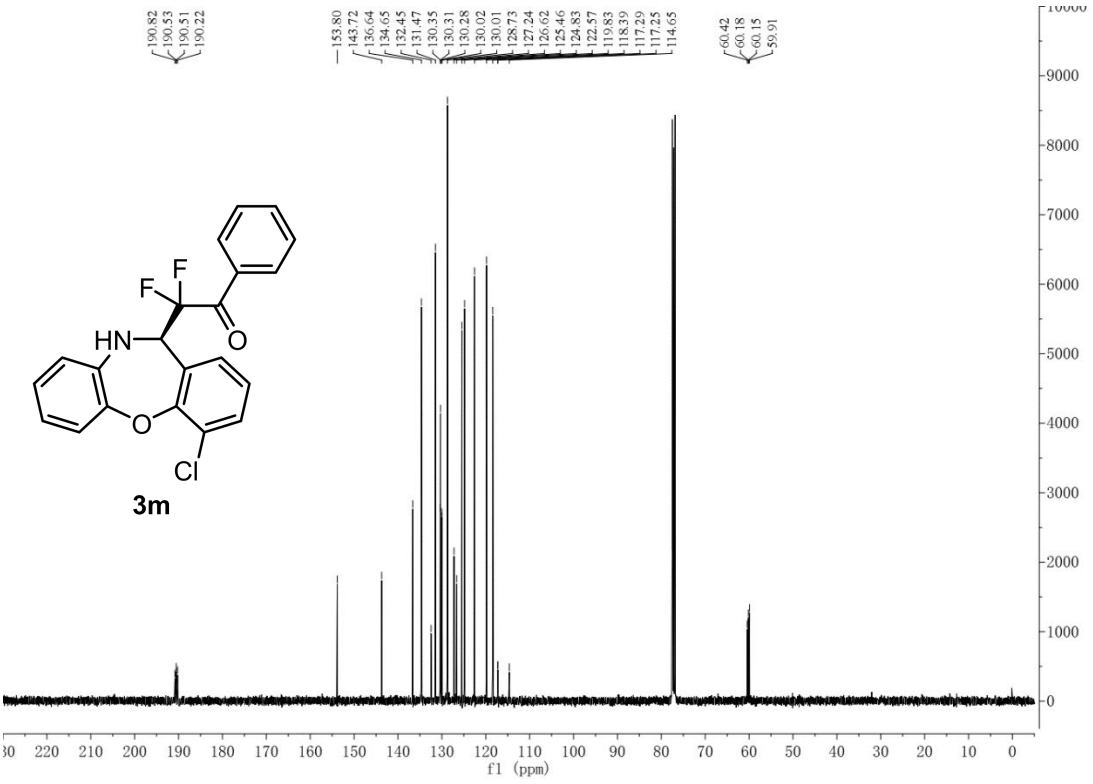
8.04
7.45
7.43
7.43
7.42
7.41
7.41
7.40
7.28
7.04
7.02
6.62
5.28
5.26
5.24
5.23
5.21
5.19
4.38
4.36
F
F
HN
O
O
Cl
3m
2.03
1.05
3.06
1.07
1.04
1.05
1.04
1.06
1.02
1.00
1.01
f1 (ppm)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134.65
132.45
131.47
130.35
130.31
130.28
130.02
130.01
128.73
127.24
126.62
125.46
124.83
122.57
119.83
118.39
117.29
117.25
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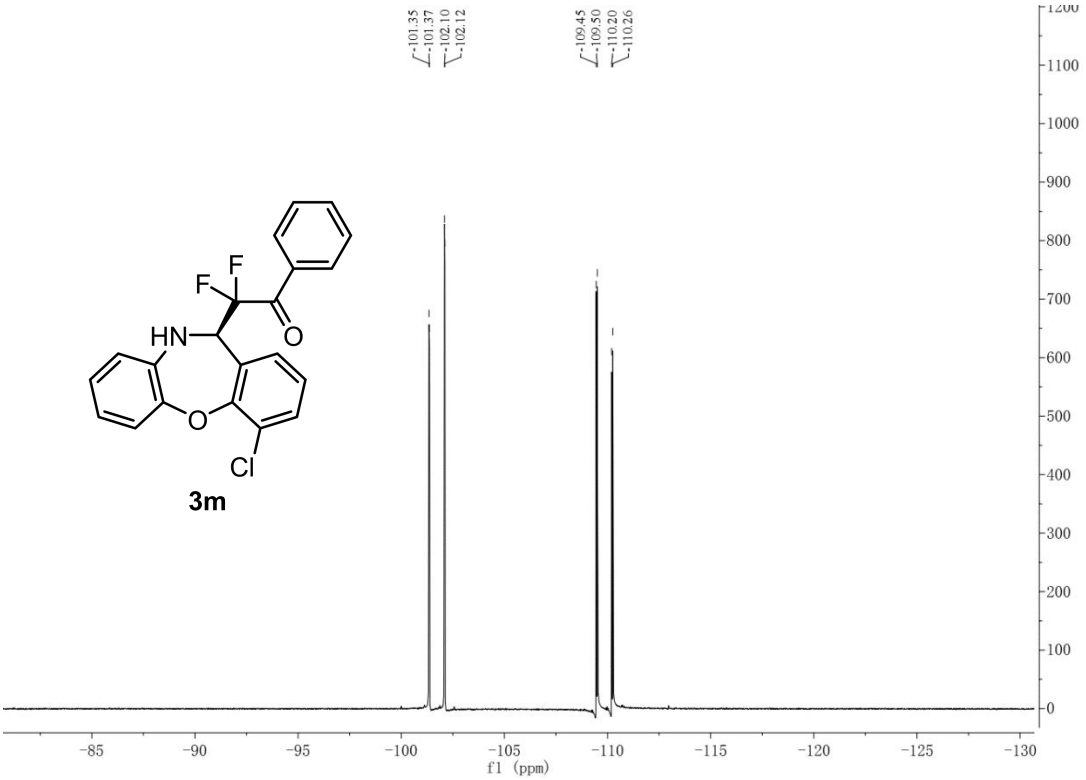
F
F
HN
O
O
Cl
3m
f1 (ppm)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-101.37
-102.10
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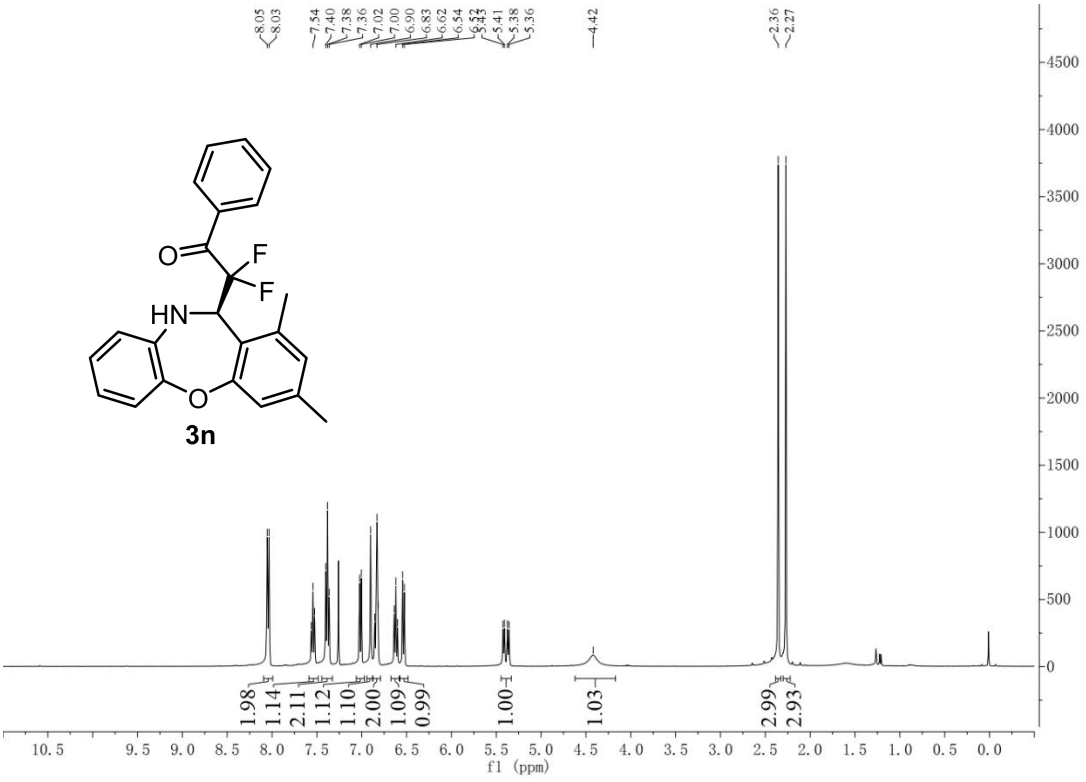
-109.50
-110.20
-110.26
F
F
HN
O
O
Cl
3m
f1 (ppm)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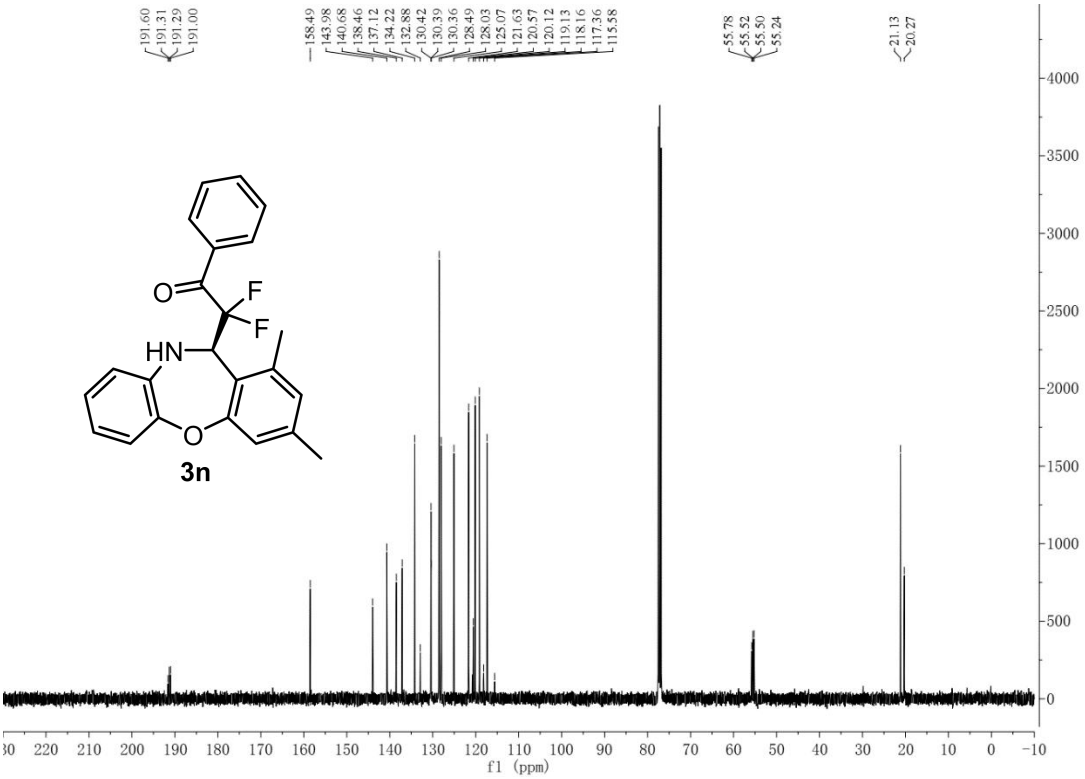
8.03
7.54
7.40
7.38
7.36
7.02
7.00
6.90
6.83
6.62
6.54
6.52
5.43
5.41
5.38
5.36
4.42
2.36
2.27
O
F
F
HN
O
3n
1.98
1.14
2.11
1.12
1.10
2.00
1.09
0.99
1.00
1.03
2.99
2.93
f1 (ppm)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128.03
125.07
121.63
120.57
120.12
119.13
118.16
117.36
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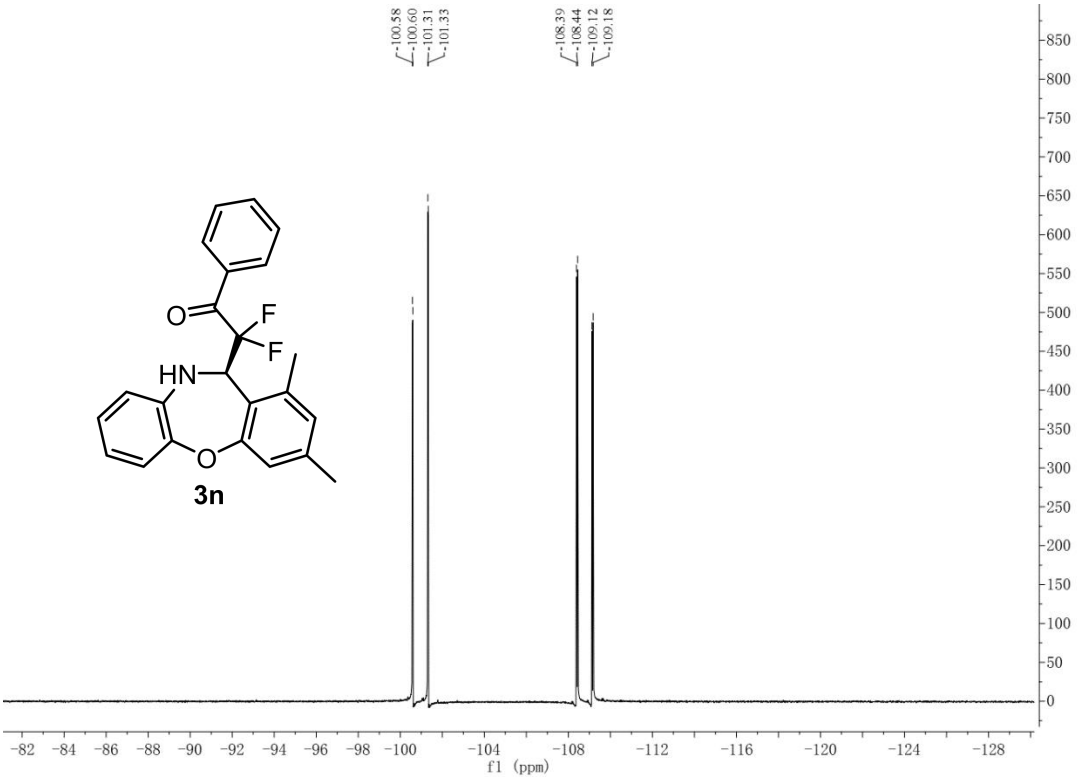
55.50
55.24
21.13
20.27
O
F
F
HN
O
3n
f1 (ppm)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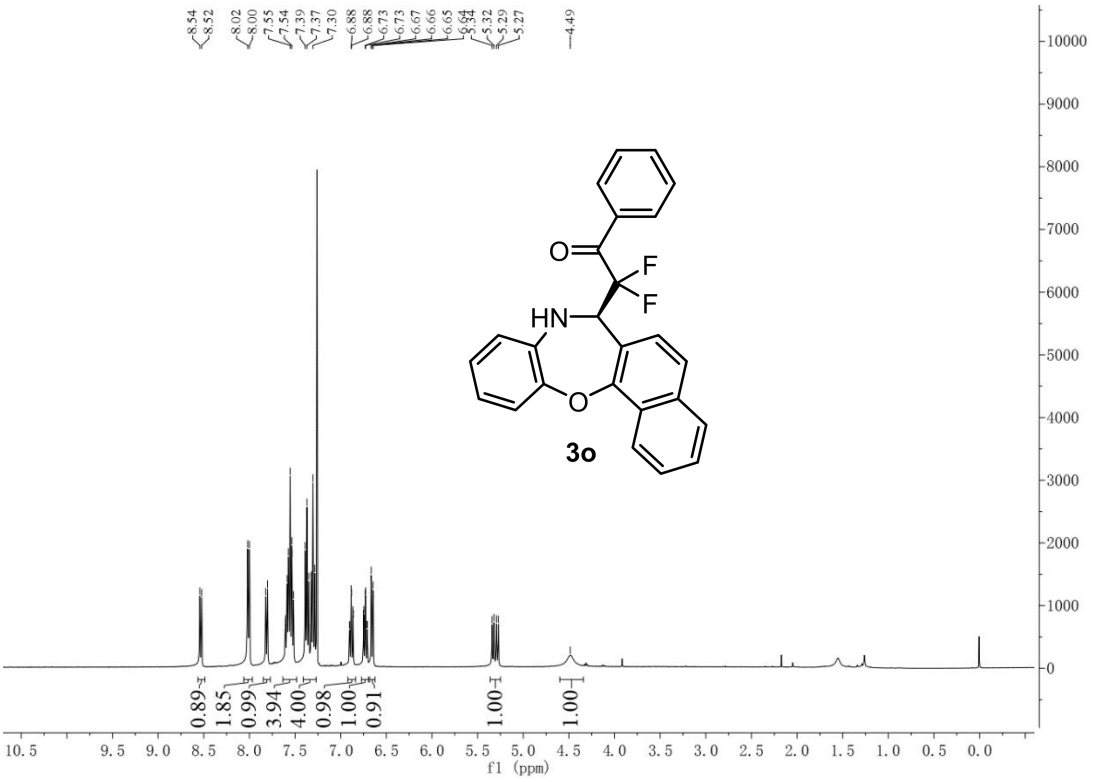
-109.18
O
F
F
HN
O
3n
f1 (ppm)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7.37
7.30
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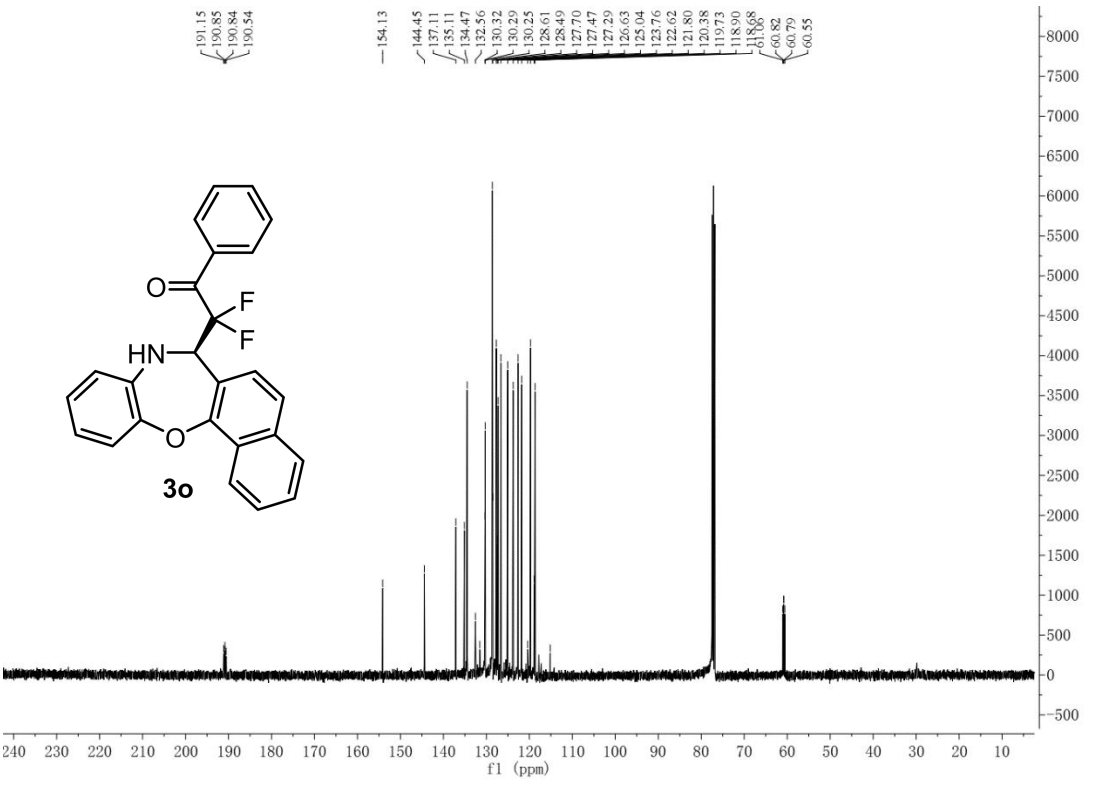
6.73
6.67
6.66
6.65
5.44
5.32
5.29
5.27
4.49
O
F
F
HN
O
3o
0.89
1.85
0.99
3.94
4.00
0.98
1.00
0.91
1.00
1.00
f1 (ppm)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127.47
127.29
126.63
125.04
123.76
122.62
121.80
120.38
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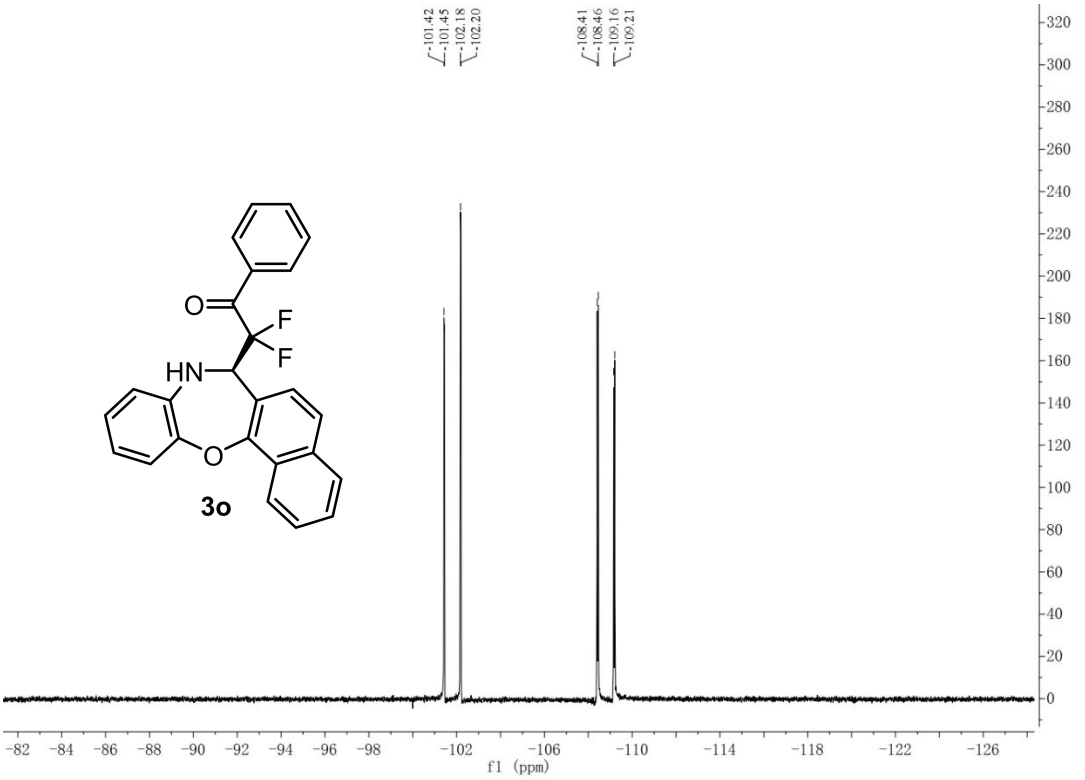
60.55
O
F
F
HN
O
3o
f1 (ppm)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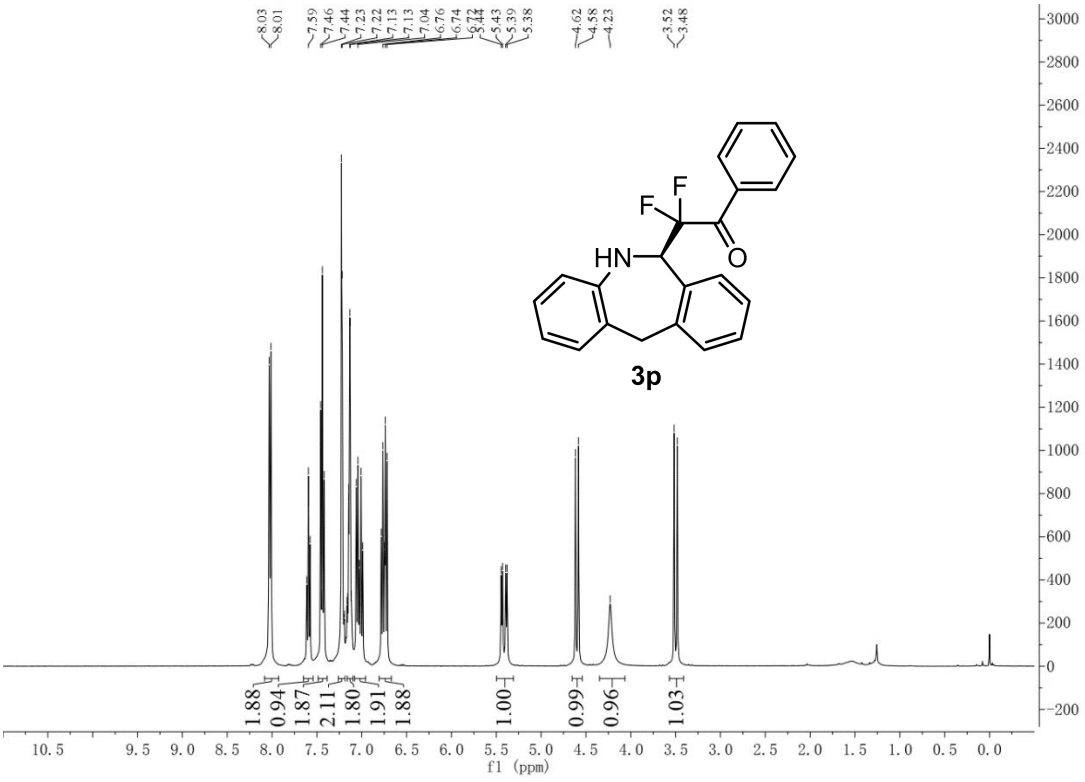
O
F
F
HN
O
3o
f1 (ppm)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7.13
7.04
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6.74
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5.43
5.39
5.38
4.62
4.58
4.23
3.52
3.48
F
F
HN
O
3p
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0.99
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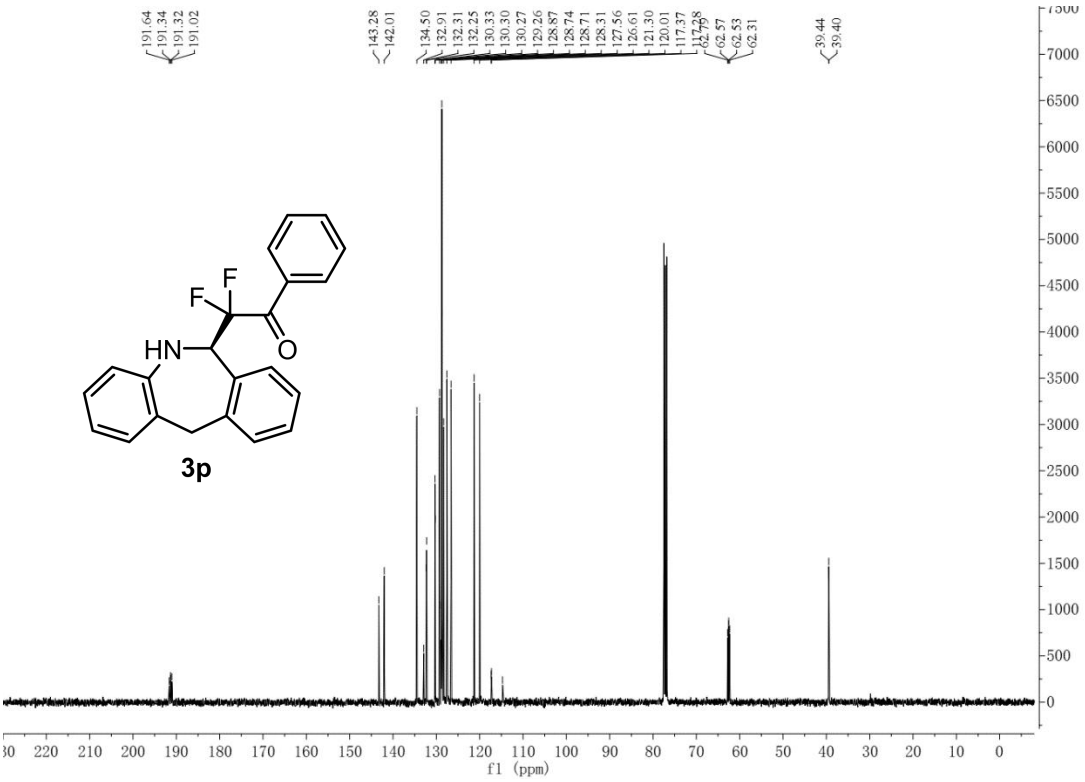
1.03
f1 (ppm)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128.87
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128.31
127.56
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120.01
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F
F
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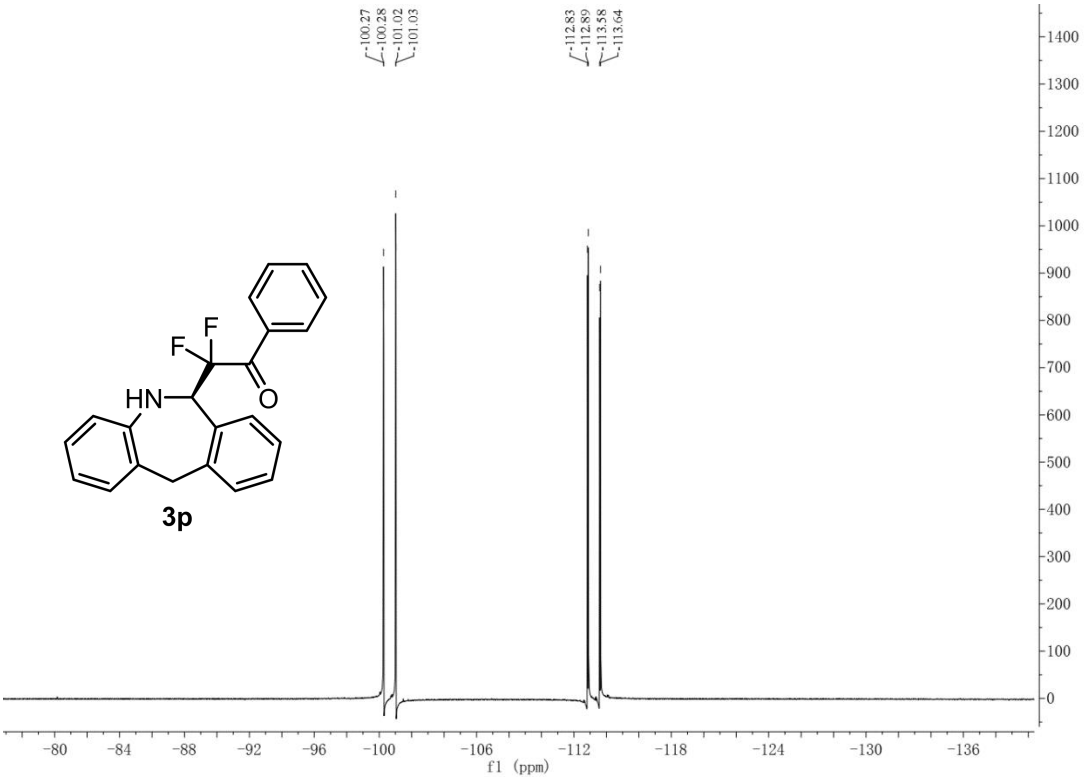
O
3p
f1 (ppm)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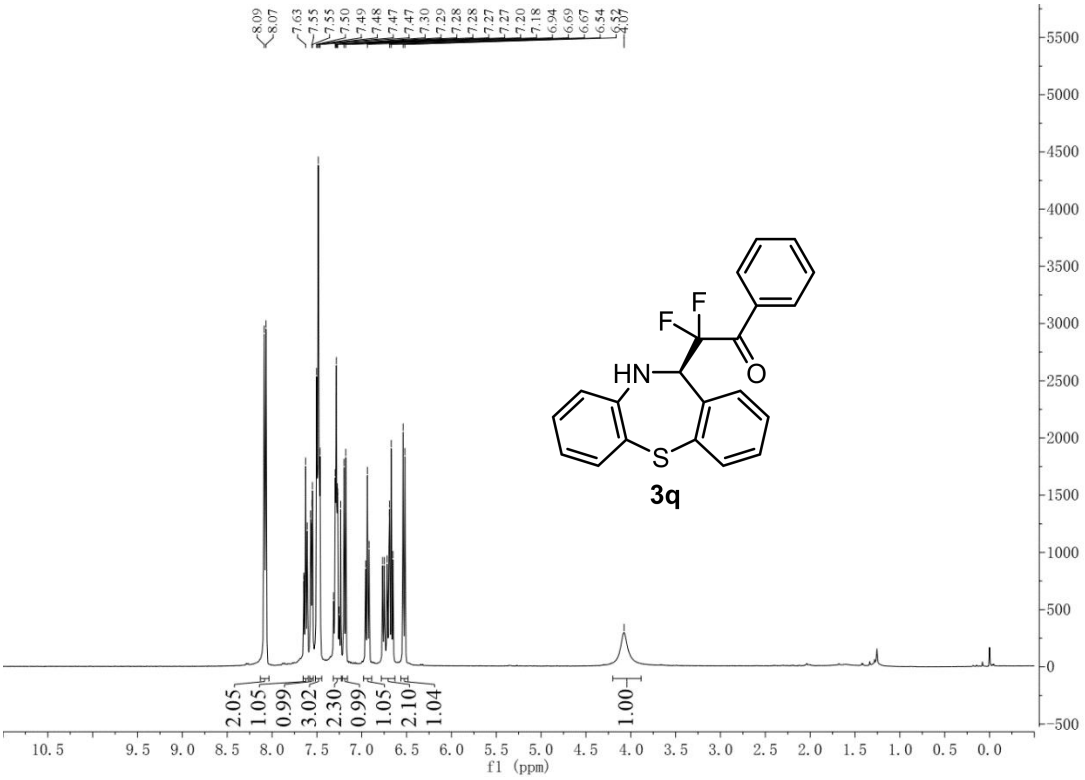
-113.64
F
F
HN
O
3p
f1 (ppm)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7.47
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7.28
7.28
7.27
7.27
7.20
7.18
6.94
6.69
6.67
6.54
6.52
4.07
F
F
HN
O
S
3q
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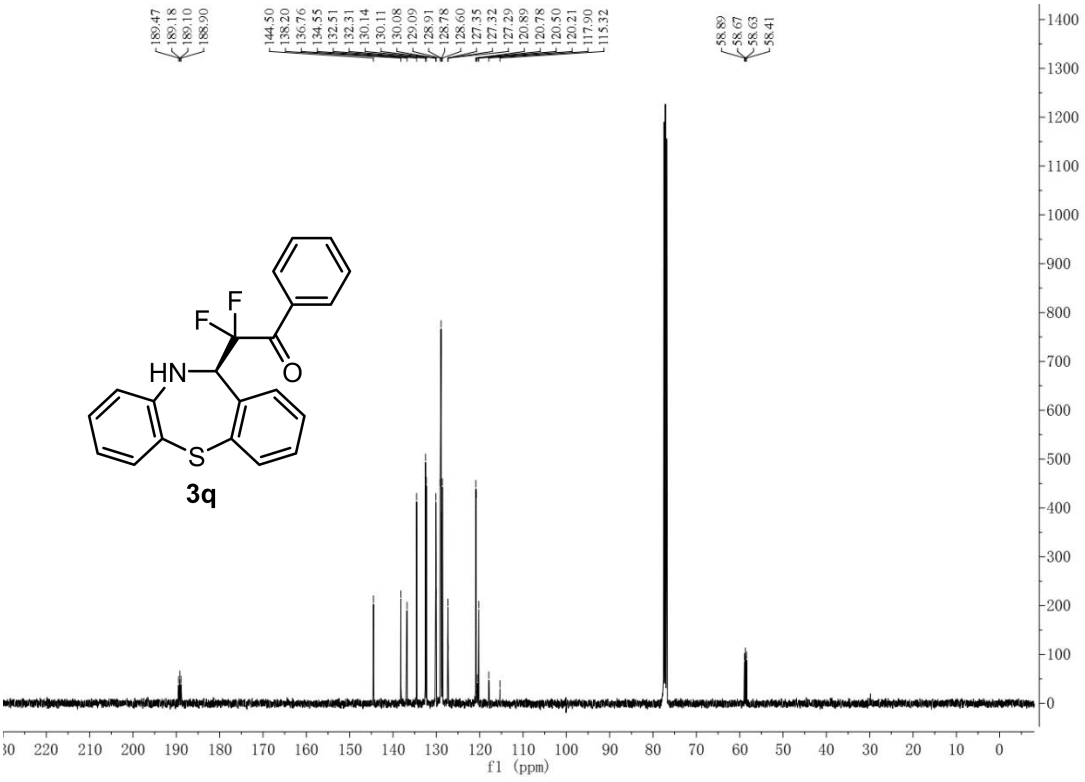
3.02
2.30
0.99
1.05
2.10
1.04
1.00
f1 (ppm)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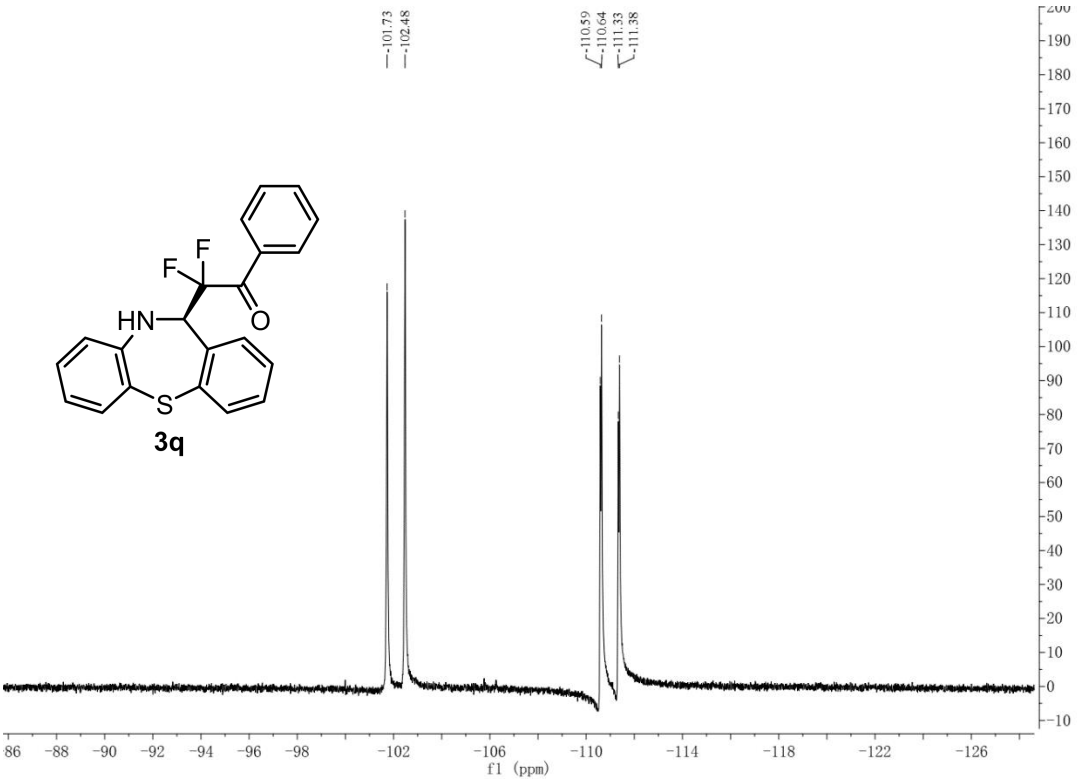
F
F
HN
O
S
3q
f1 (ppm)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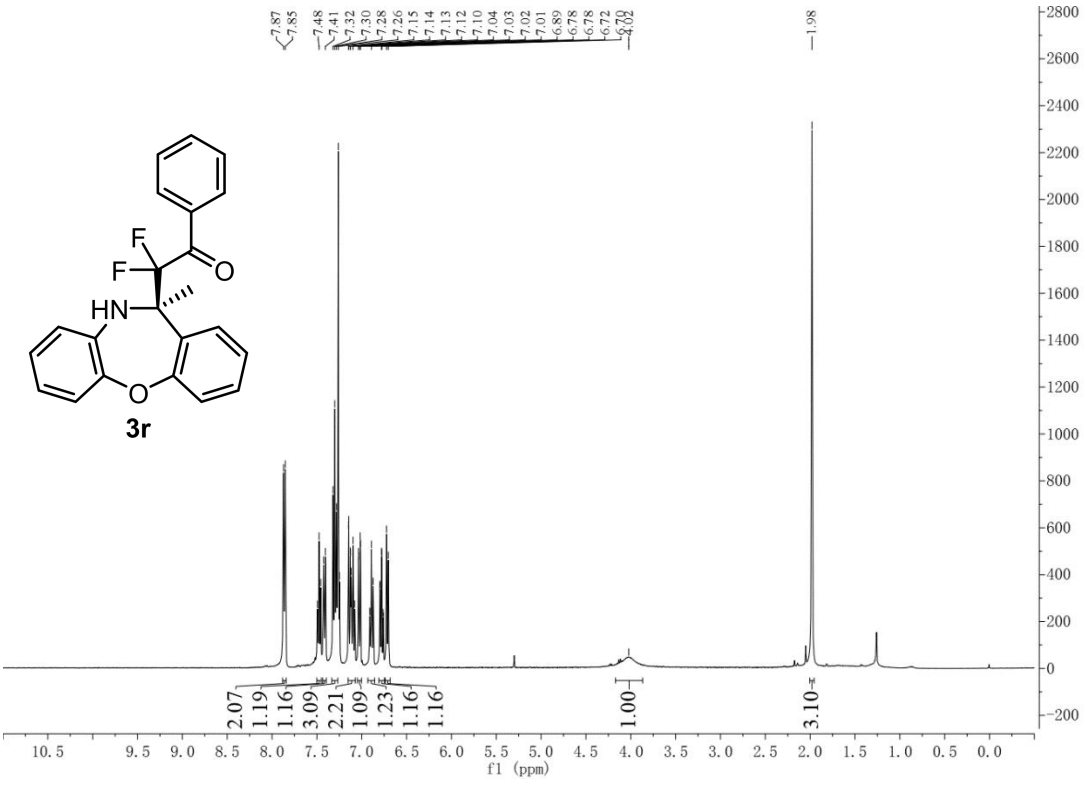
-110.64
-111.33
-111.38
F
F
HN
O
S
3q
f1 (ppm)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7.13
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7.10
7.04
7.03
7.02
7.01
6.89
6.78
6.78
6.72
6.70
4.02
1.98
F
F
HN
O
O
3r
2.07
1.19
1.16
3.09
2.21
1.09
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1.00
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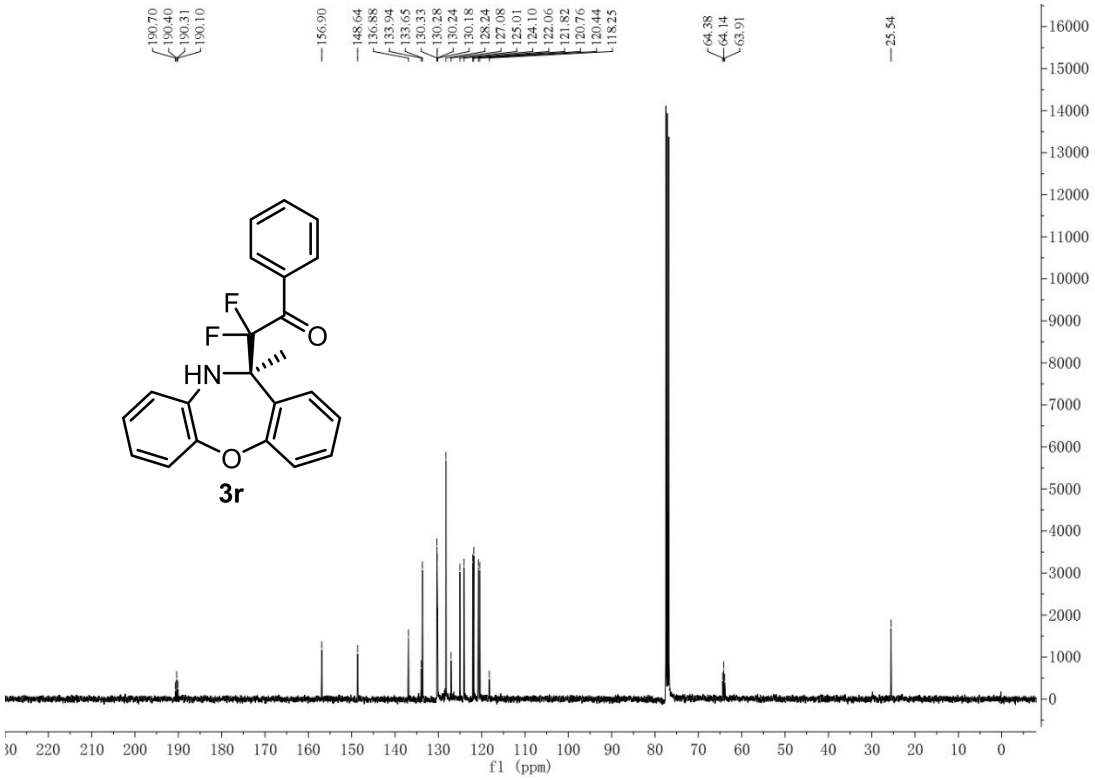
f1 (ppm)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128.24
127.08
125.01
124.10
122.06
121.82
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63.91
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F
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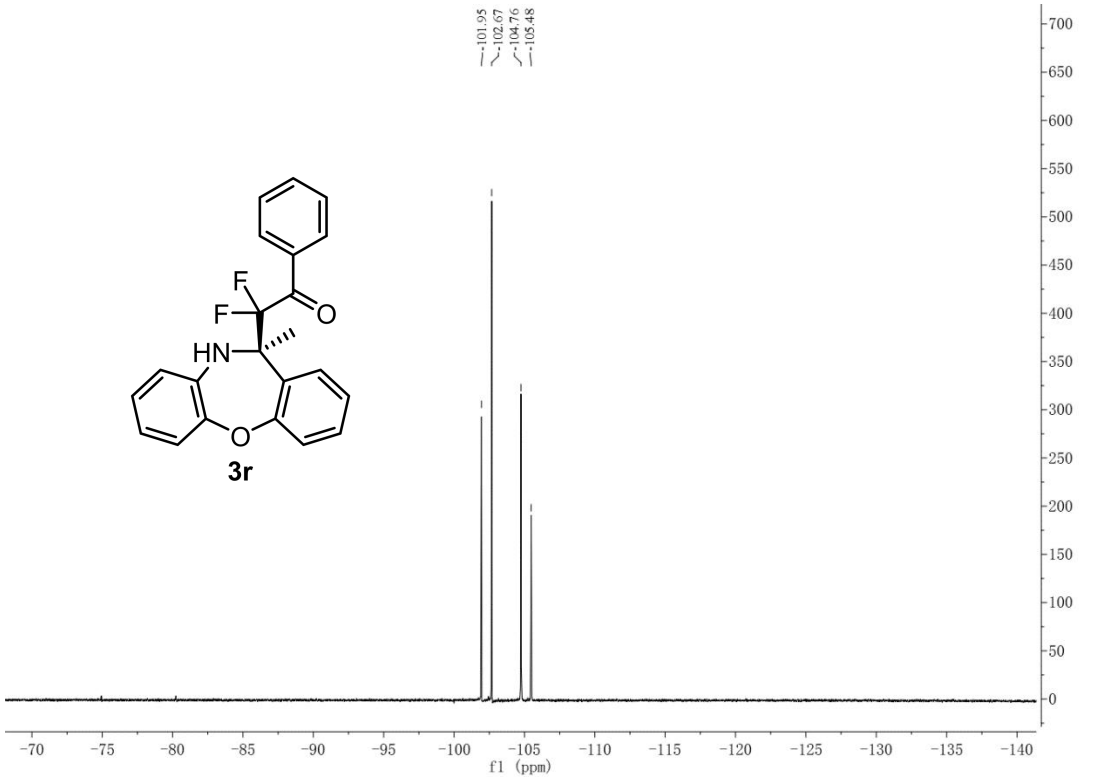
HN
O
3r
f1 (ppm)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O
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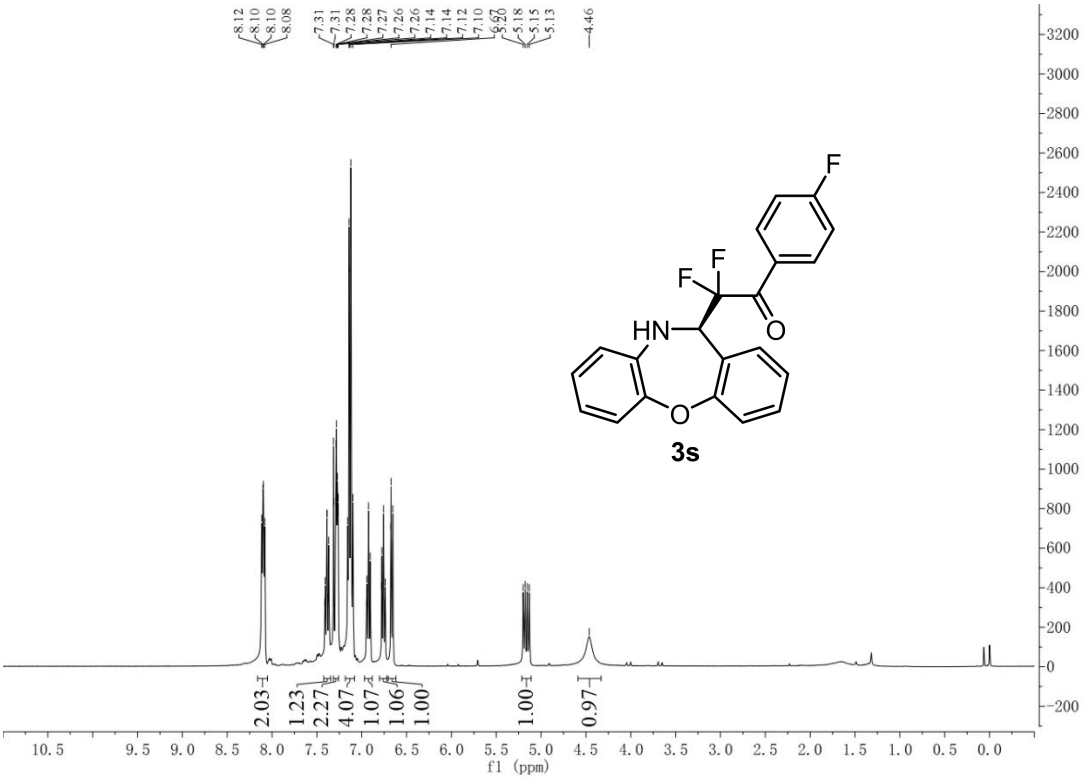
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7.14
7.14
7.12
7.10
5.18
5.15
5.13
4.46
F
F
F
HN
O
O
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2.27
4.07
1.07
1.06
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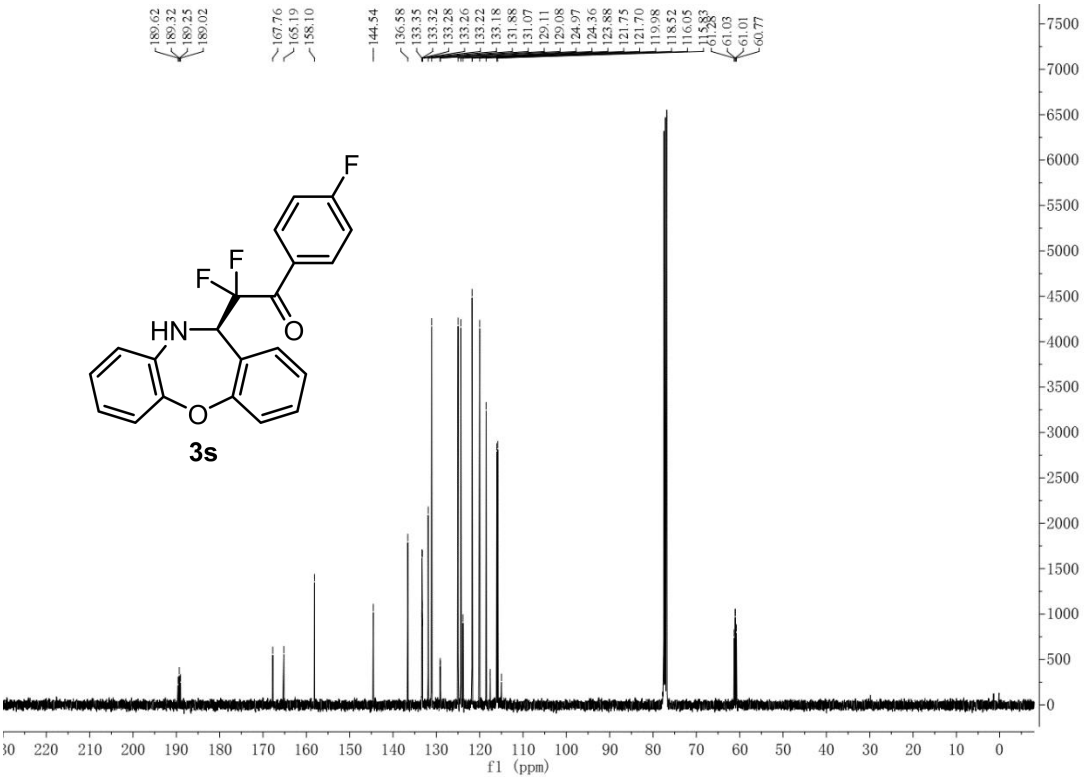
f1 (ppm)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131.88
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129.11
129.08
124.97
124.36
123.88
121.75
121.70
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61.03
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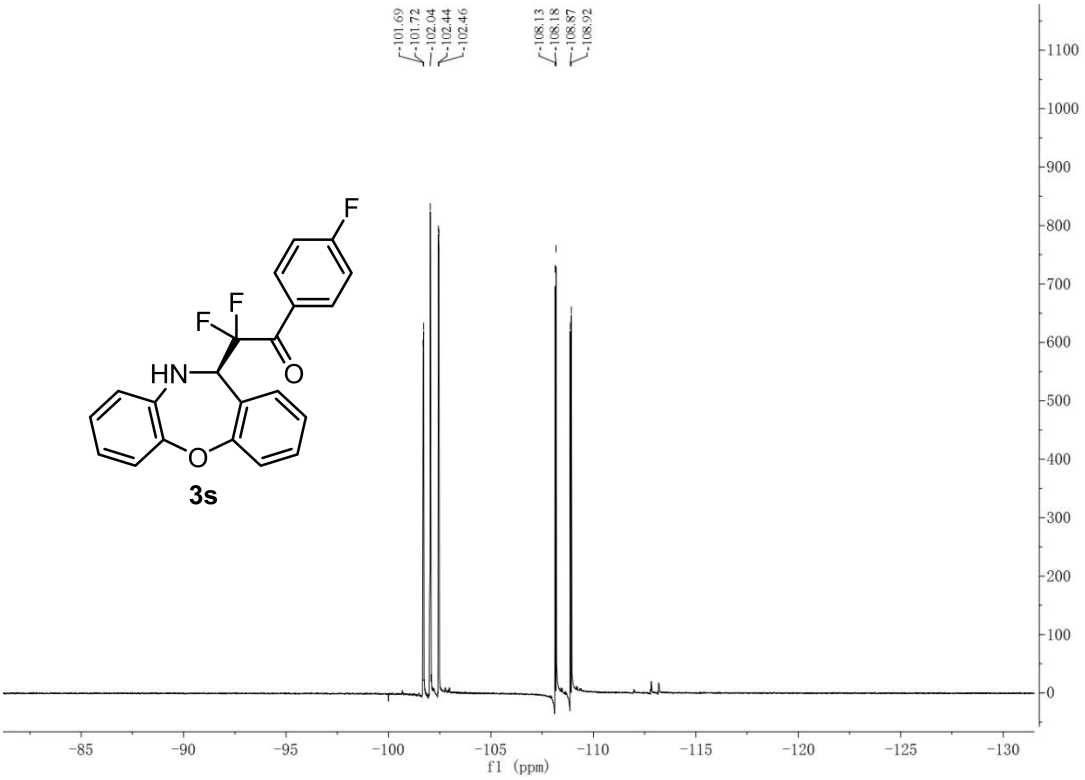
F
F
HN
O
O
3s
f1 (ppm)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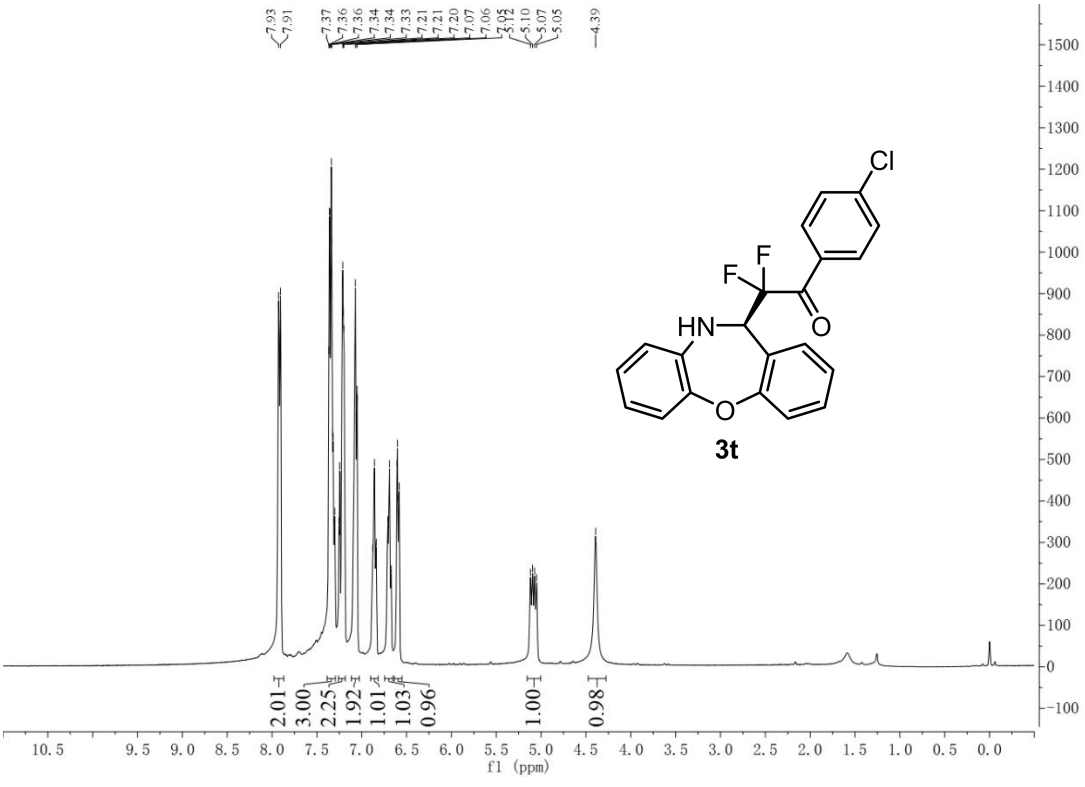
F
F
HN
O
O
3s
f1 (ppm)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7.34
7.33
7.21
7.21
7.20
7.07
7.06
5.10
5.07
5.05
4.39
Cl
F
F
HN
O
O
3t
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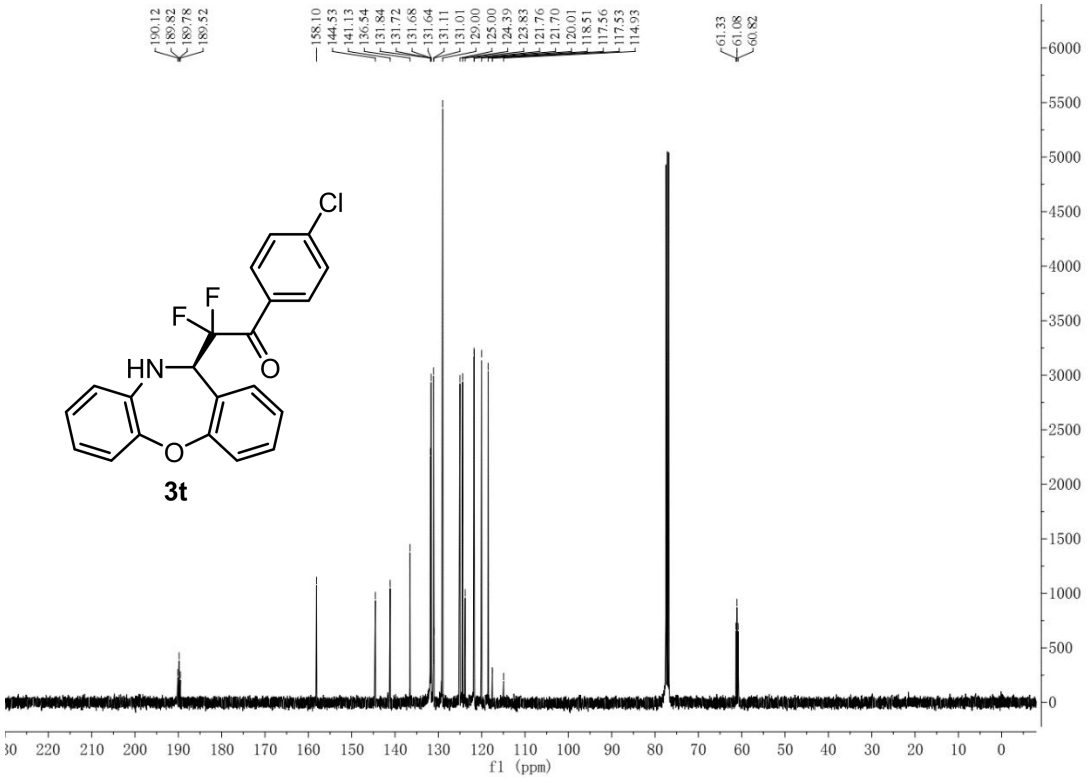
3.00
2.25
1.92
1.01
1.03
0.96
1.00
0.98
f1 (ppm)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129.00
125.00
124.39
123.83
121.76
121.70
120.01
118.51
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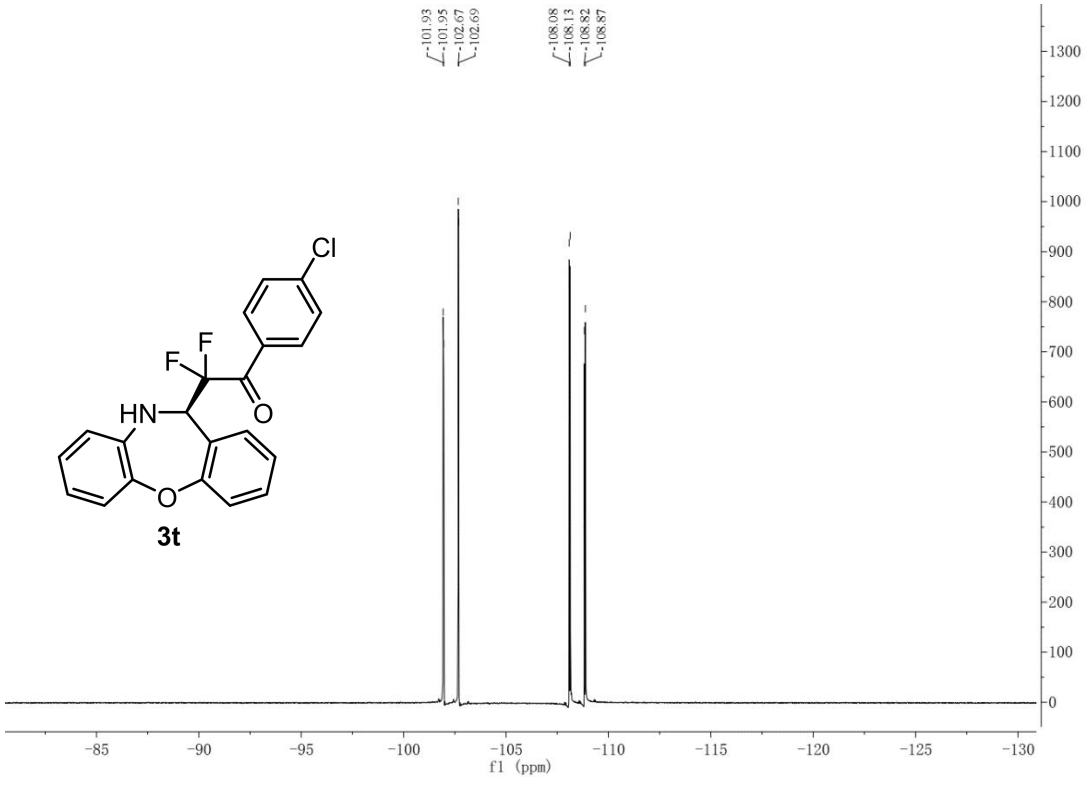
61.33
61.08
60.82
Cl
F
F
HN
O
O
3t
f1 (ppm)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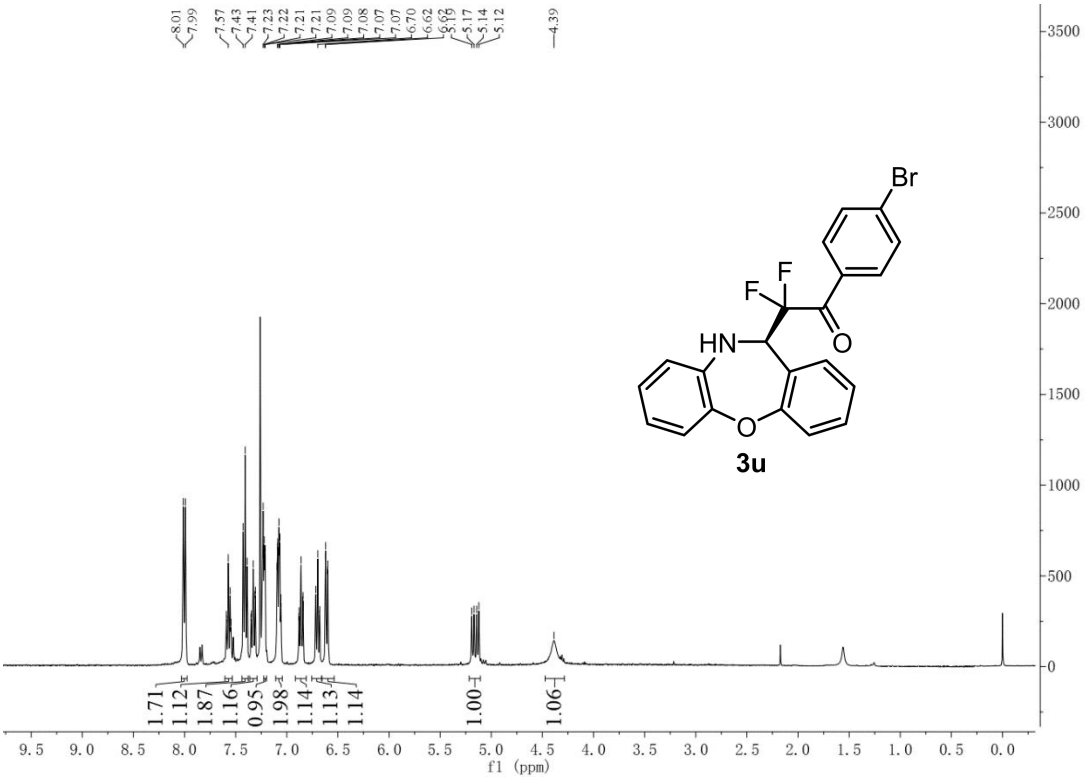
Cl
F
F
HN
O
O
3t
f1 (ppm)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7.22
7.21
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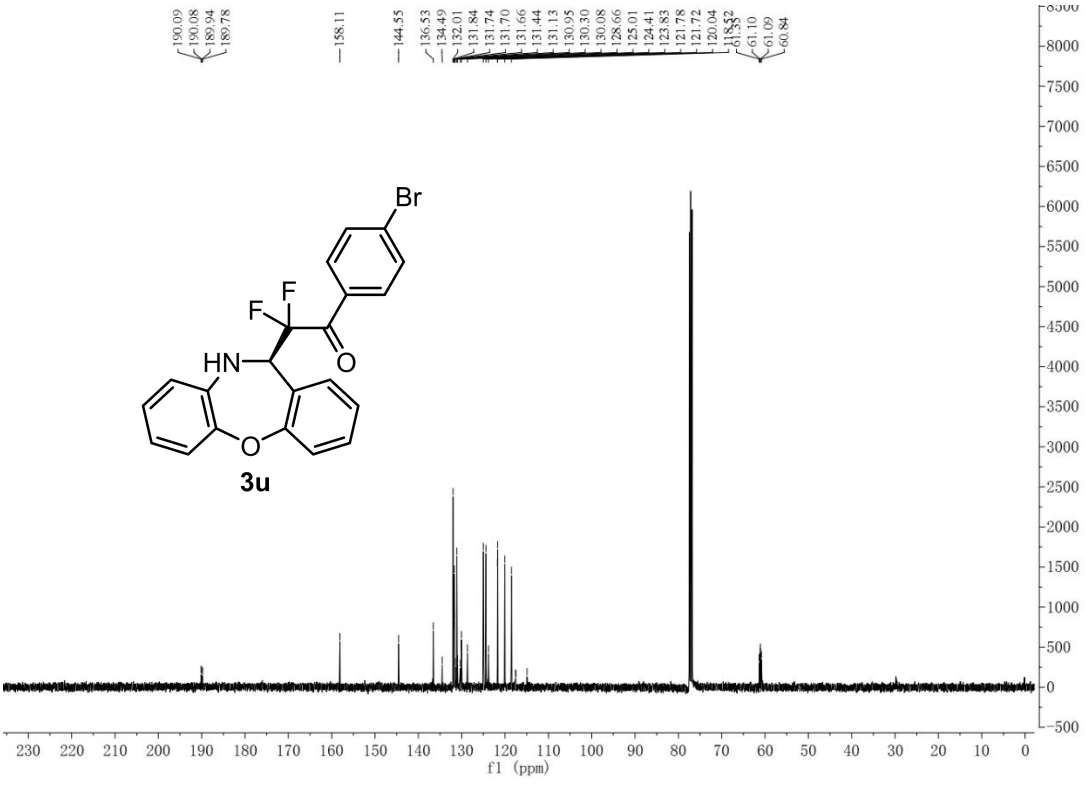
7.09
7.09
7.08
7.07
7.07
6.70
6.62
6.62
5.19
5.17
5.14
5.12
4.39
Br
F
F
HN
O
O
3u
1.71
1.12
1.87
1.16
0.95
1.98
1.14
1.13
1.14
1.00
1.06
f1 (ppm)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131.13
130.95
130.30
130.08
128.66
125.01
124.41
123.83
121.78
121.72
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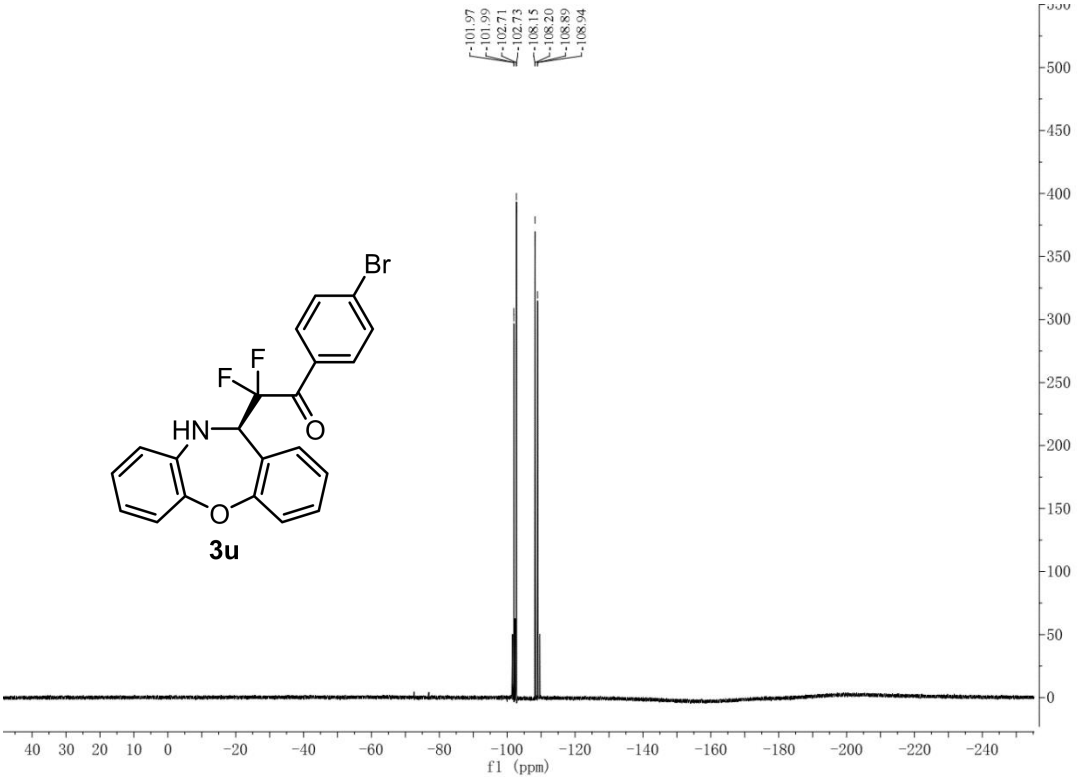
61.33
61.10
61.09
60.84
Br
F
F
HN
O
O
3u
f1 (ppm)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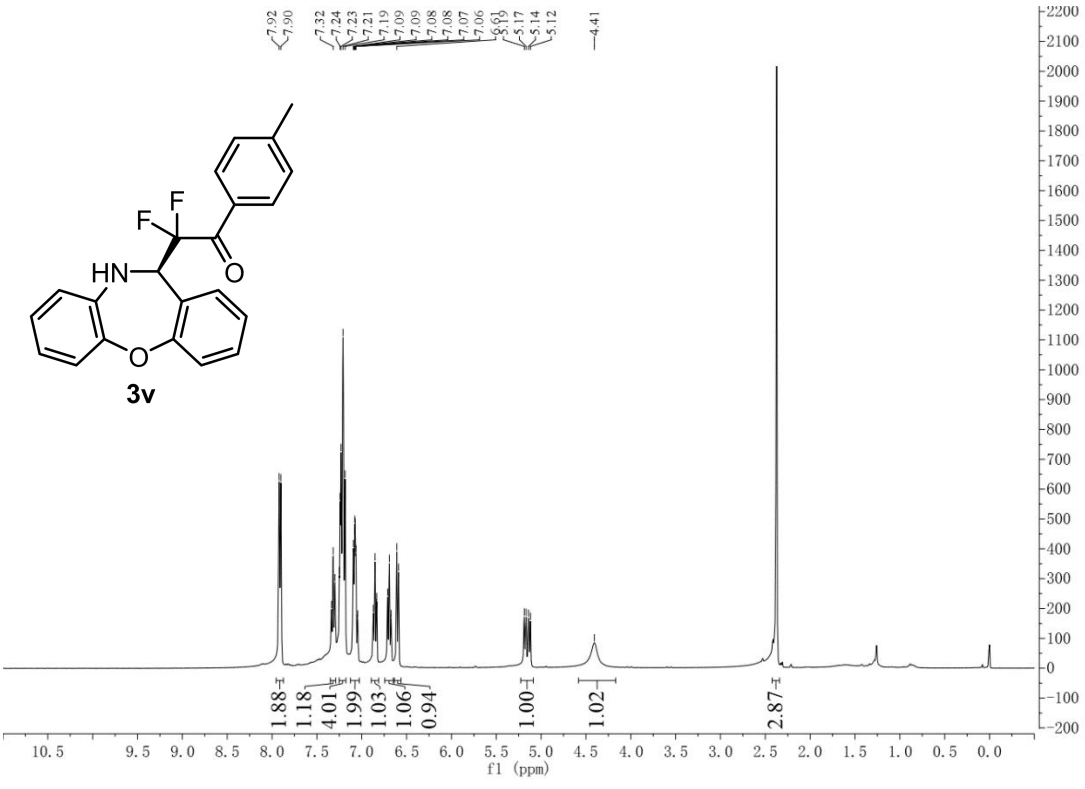
Br
F
F
HN
O
O
3u
f1 (ppm)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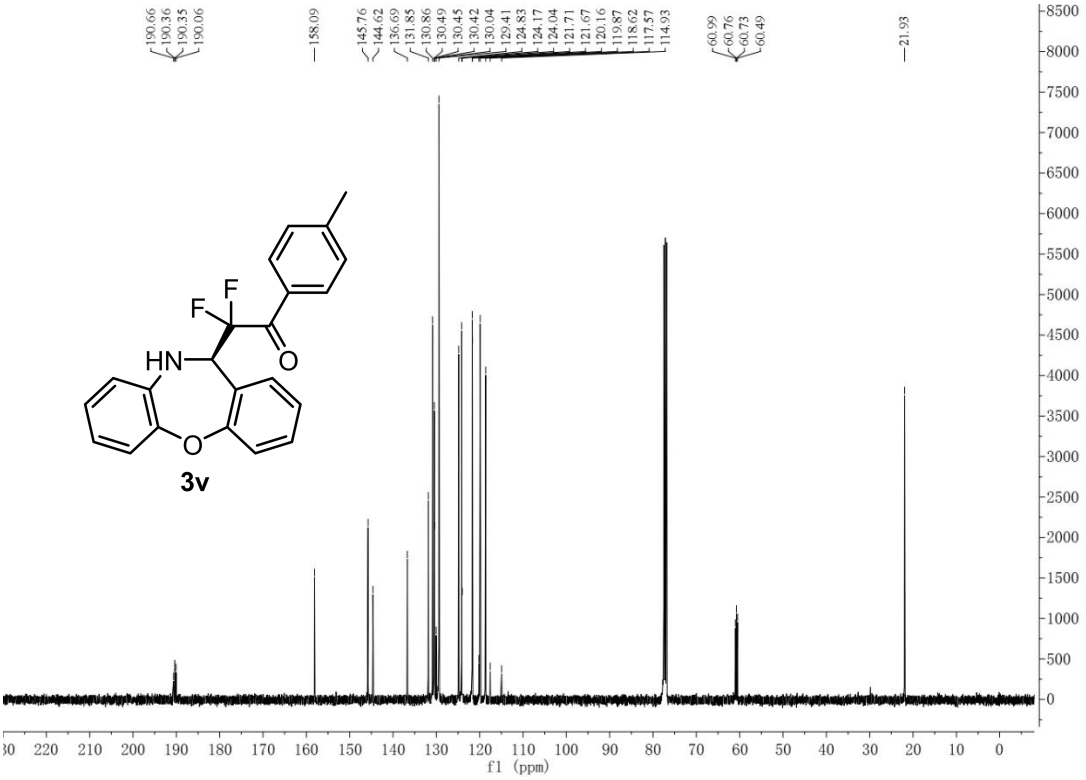
7.09
7.09
7.08
7.08
7.07
7.06
6.63
5.19
5.17
5.14
5.12
4.41
F
F
HN
O
O
3v
1.88
1.18
4.01
1.99
1.03
1.06
0.94
1.00
1.02
2.87
f1 (ppm)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124.04
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120.16
119.87
118.62
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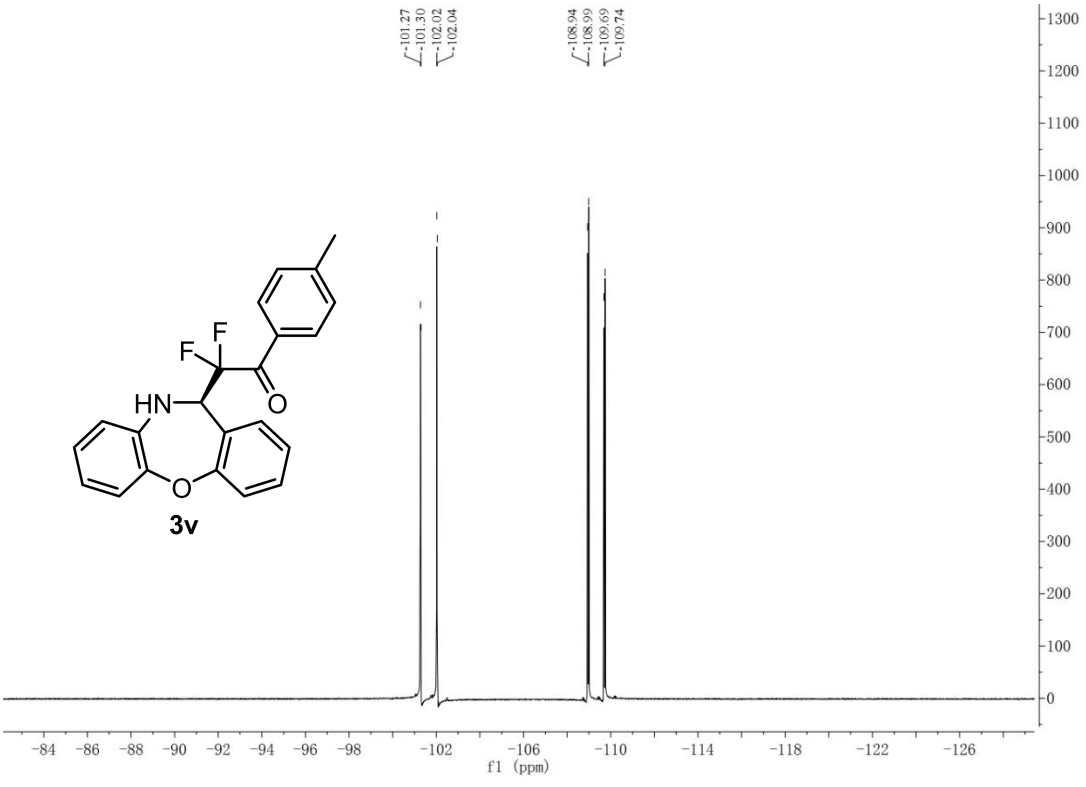
60.76
60.73
60.49
21.93
F
F
HN
O
O
3v
f1 (ppm)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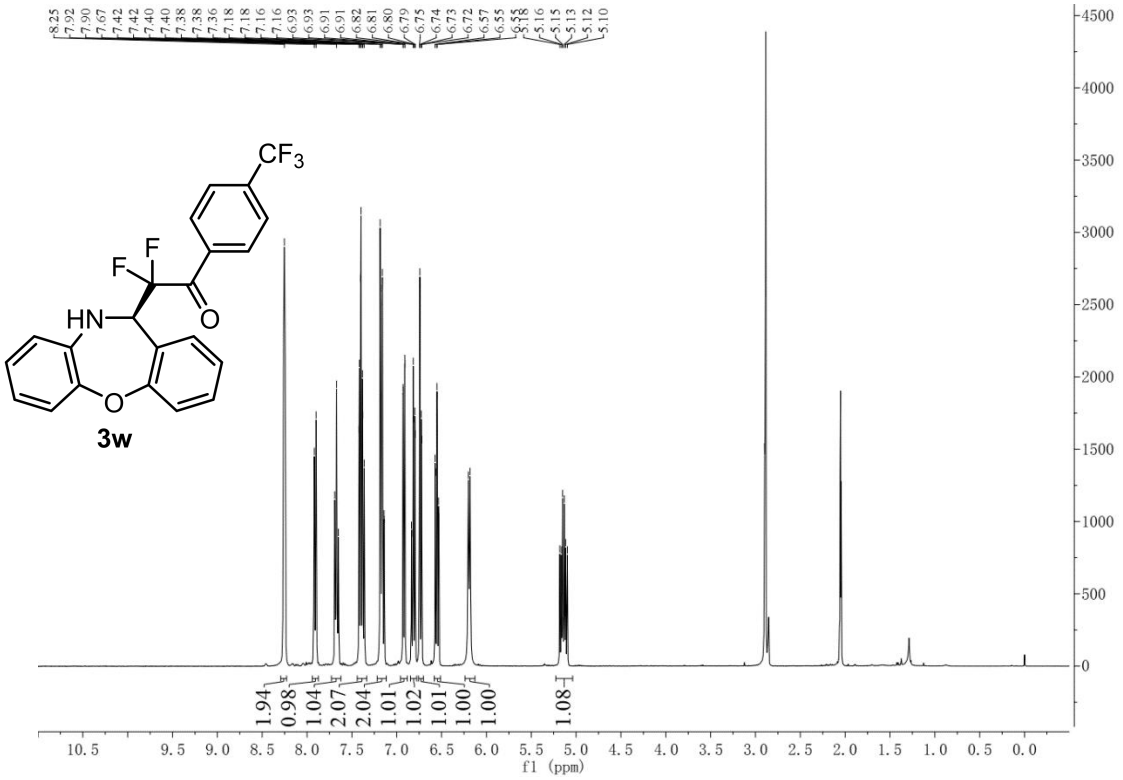
109.74
F
F
HN
O
O
3v
f1 (ppm)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7.18
7.16
7.16
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6.93
6.91
6.91
6.82
6.81
6.80
6.79
6.75
6.74
6.73
6.72
6.57
6.55
5.18
5.16
5.15
5.13
5.12
5.10
CF3
F
F
HN
O
O
3w
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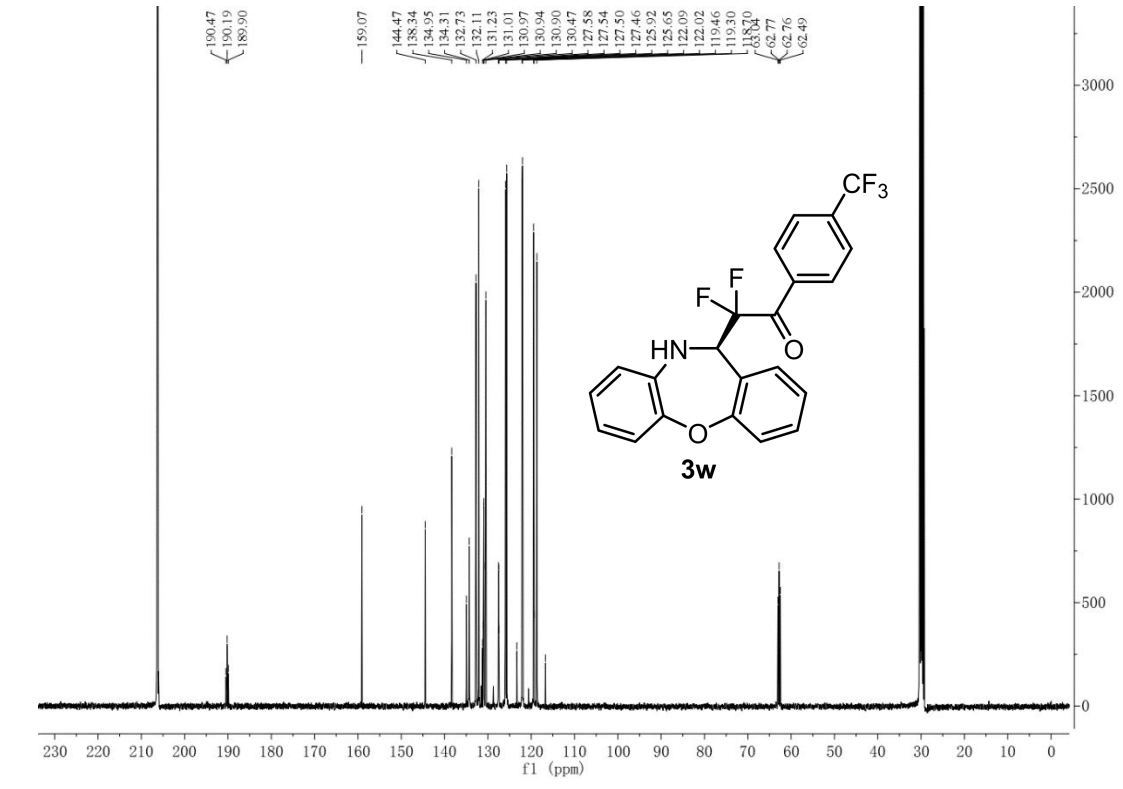
1.04
2.07
2.04
1.01
1.02
1.01
1.00
1.00
1.08
f1 (ppm)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130.90
130.47
127.58
127.54
127.50
127.46
125.92
125.65
122.09
122.02
119.46
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62.49
CF3
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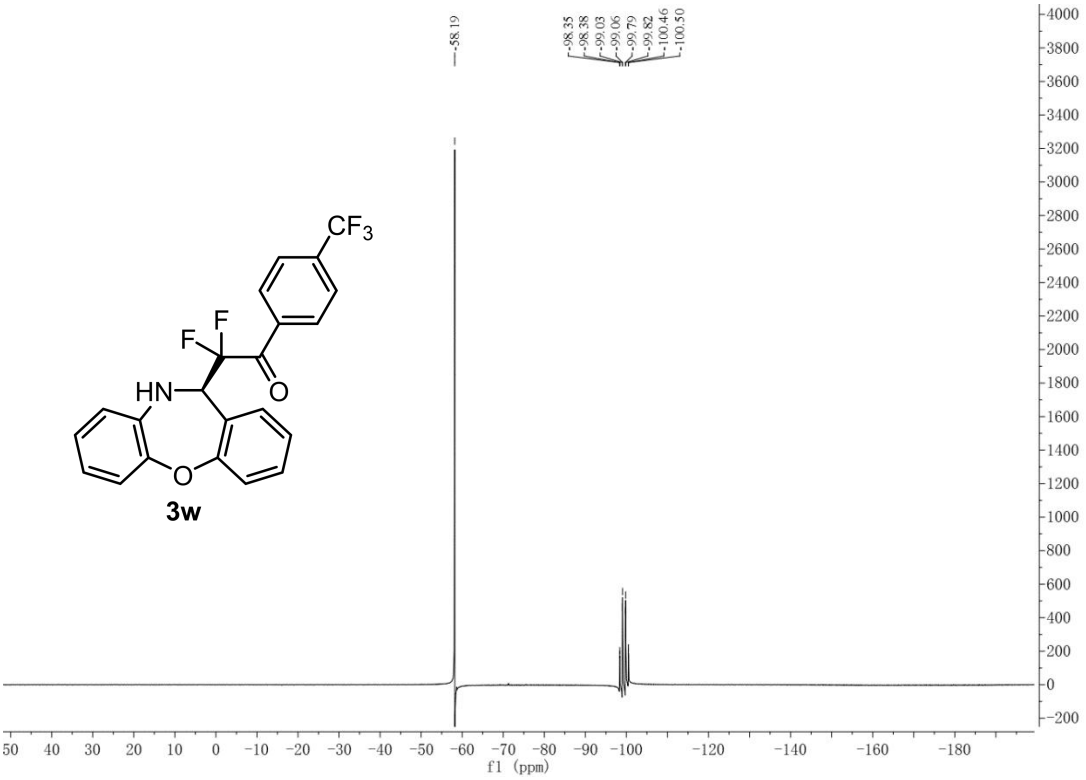
F
HN
O
O
3w
f1 (ppm)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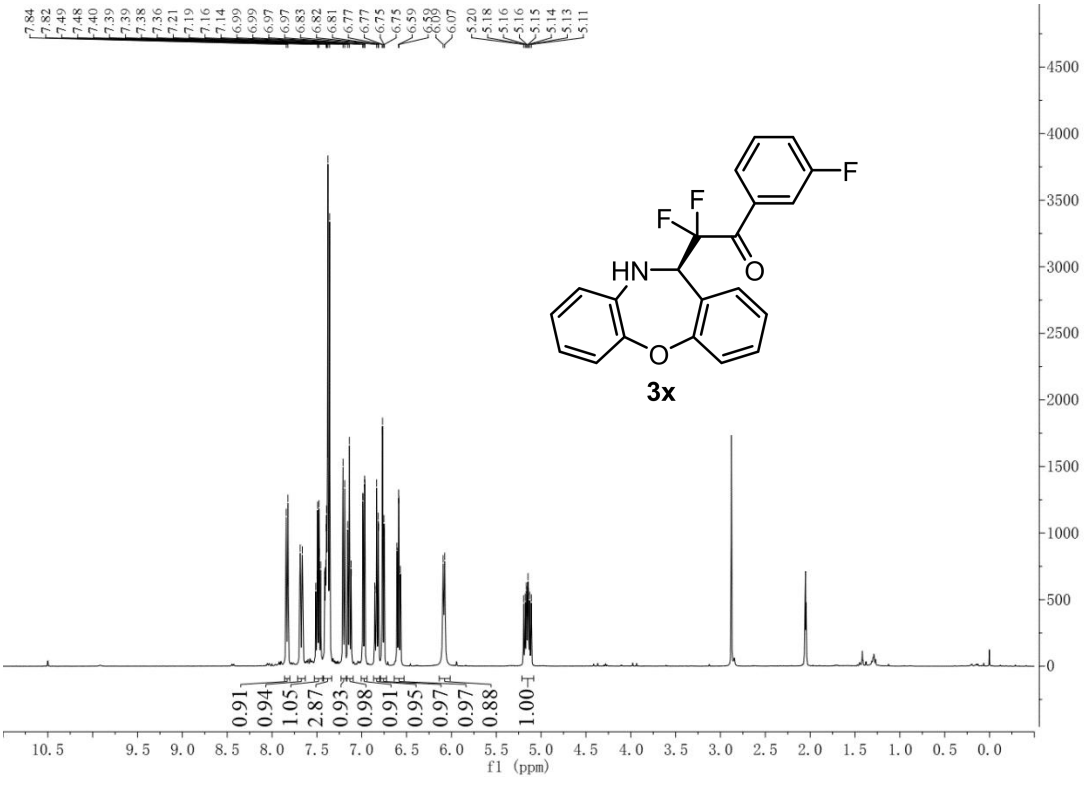
-100.50
CF3
F
F
HN
O
O
3w
f1 (ppm)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6.97
6.83
6.82
6.81
6.77
6.77
6.75
6.75
6.59
6.58
6.09
6.07
5.20
5.18
5.16
5.16
5.15
5.14
5.13
5.11
F
F
F
HN
O
O
3x
0.91
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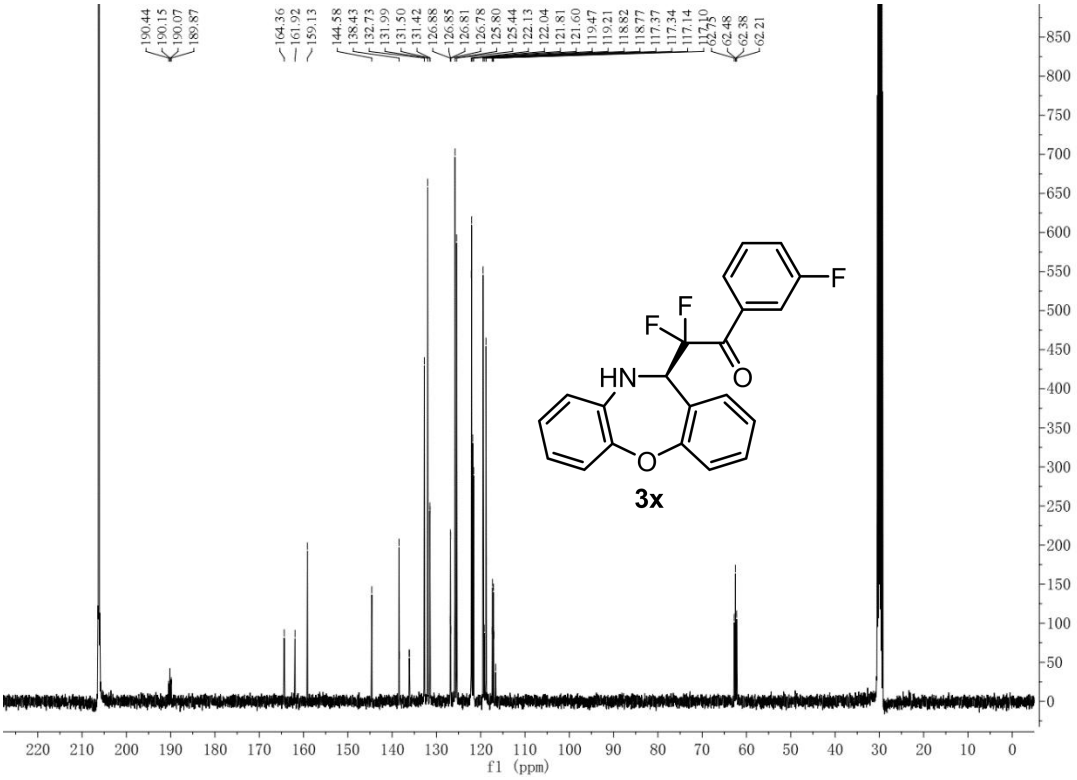
0.98
0.91
0.95
0.97
0.97
0.88
1.00
f1 (ppm)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121.60
119.47
119.21
118.82
118.77
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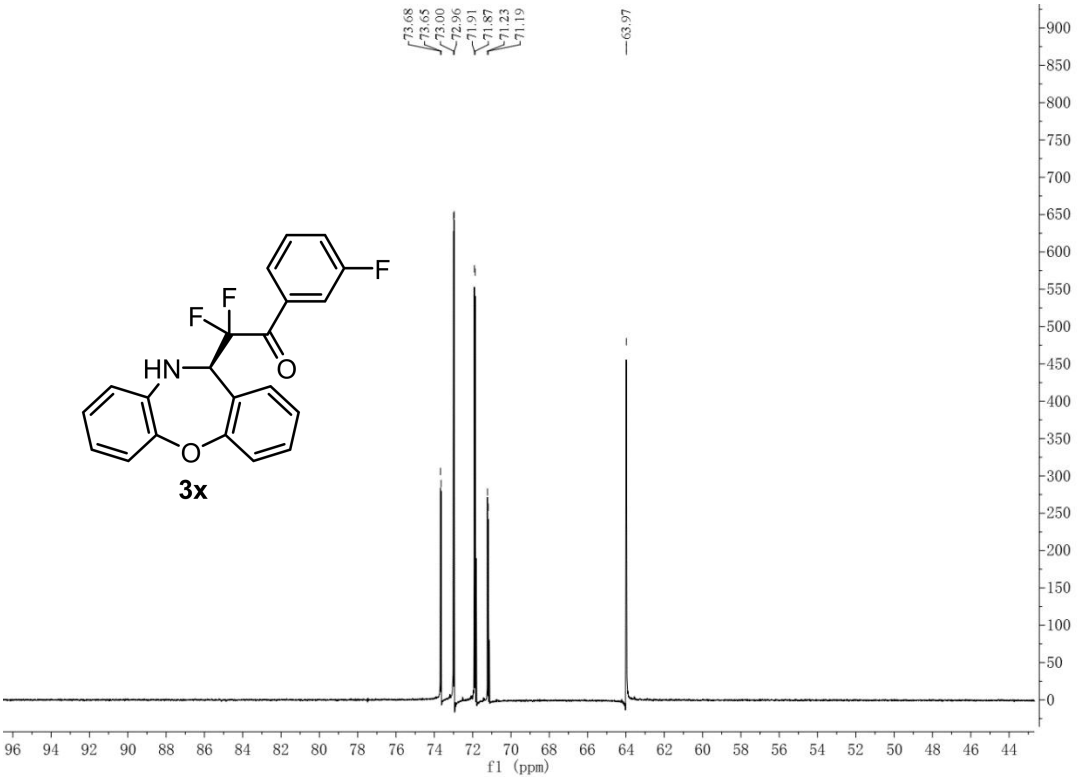
117.14
62.48
62.38
62.21
F
F
F
HN
O
O
3x
f1 (ppm)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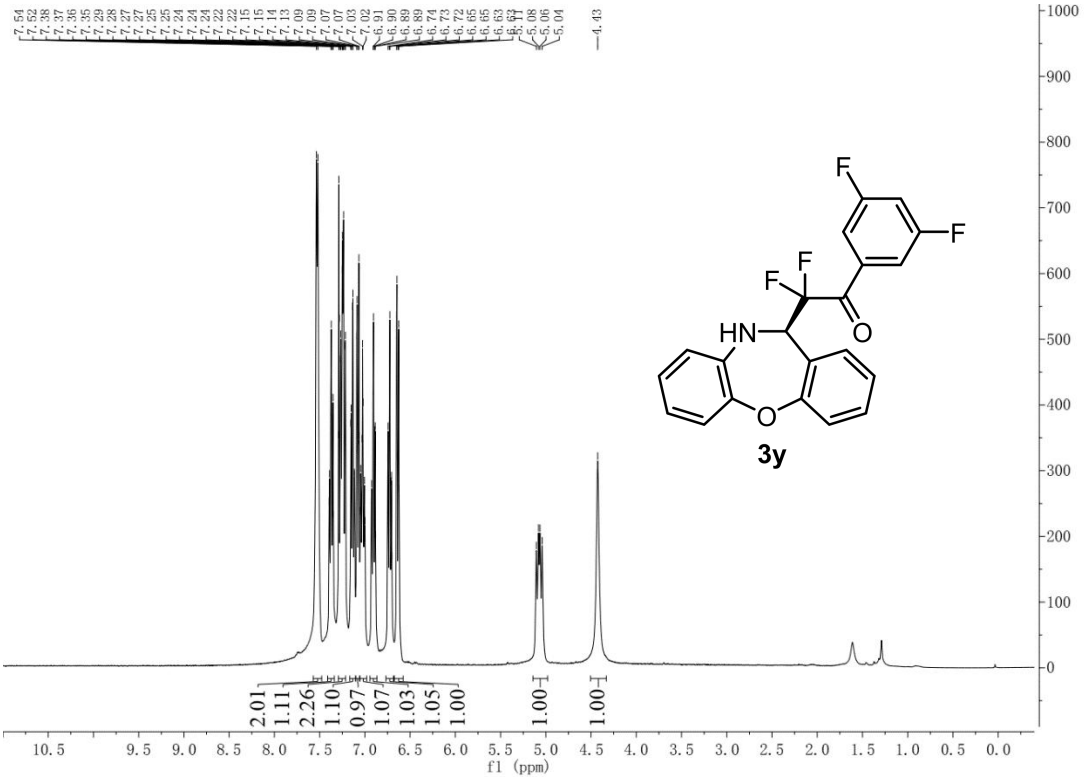
63.97
F
F
F
HN
O
O
3x
f1 (ppm)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7.22
7.15
7.15
7.14
7.13
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7.09
7.07
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7.03
7.02
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6.73
6.72
6.65
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6.62
5.08
5.06
5.04
4.43
F
F
F
HN
O
O
3y
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1.03
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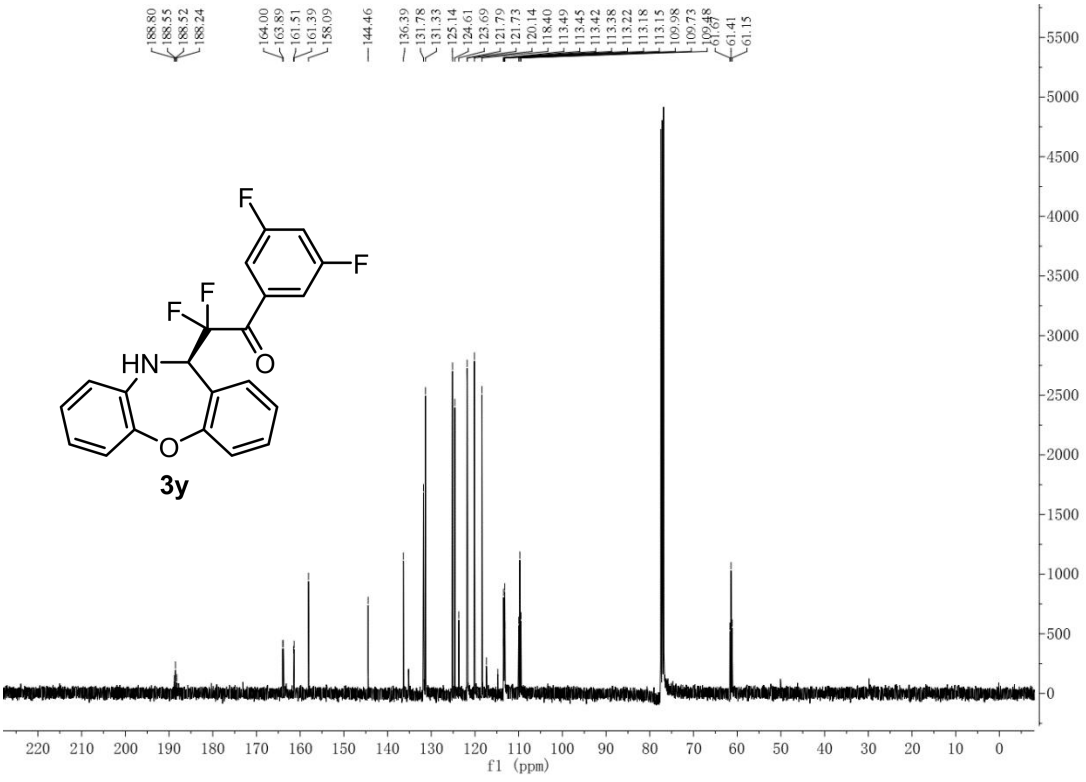
1.00
1.00
1.00
f1 (ppm)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113.38
113.22
113.18
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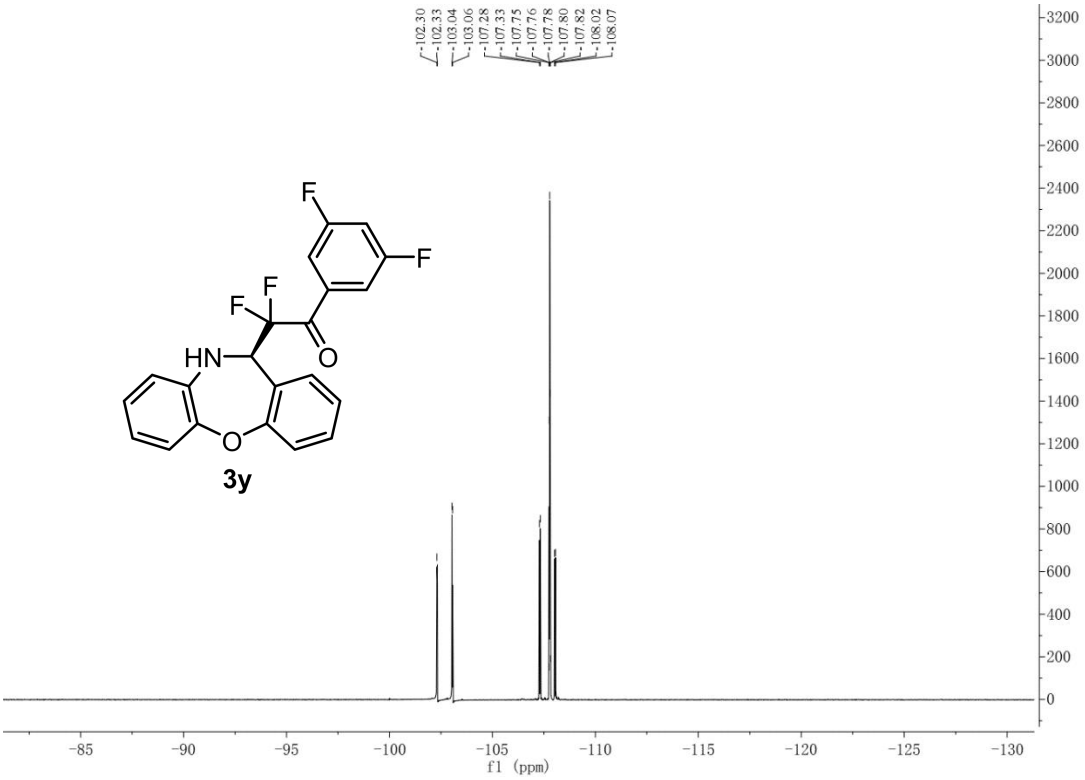
F
F
HN
O
O
3y
f1 (ppm)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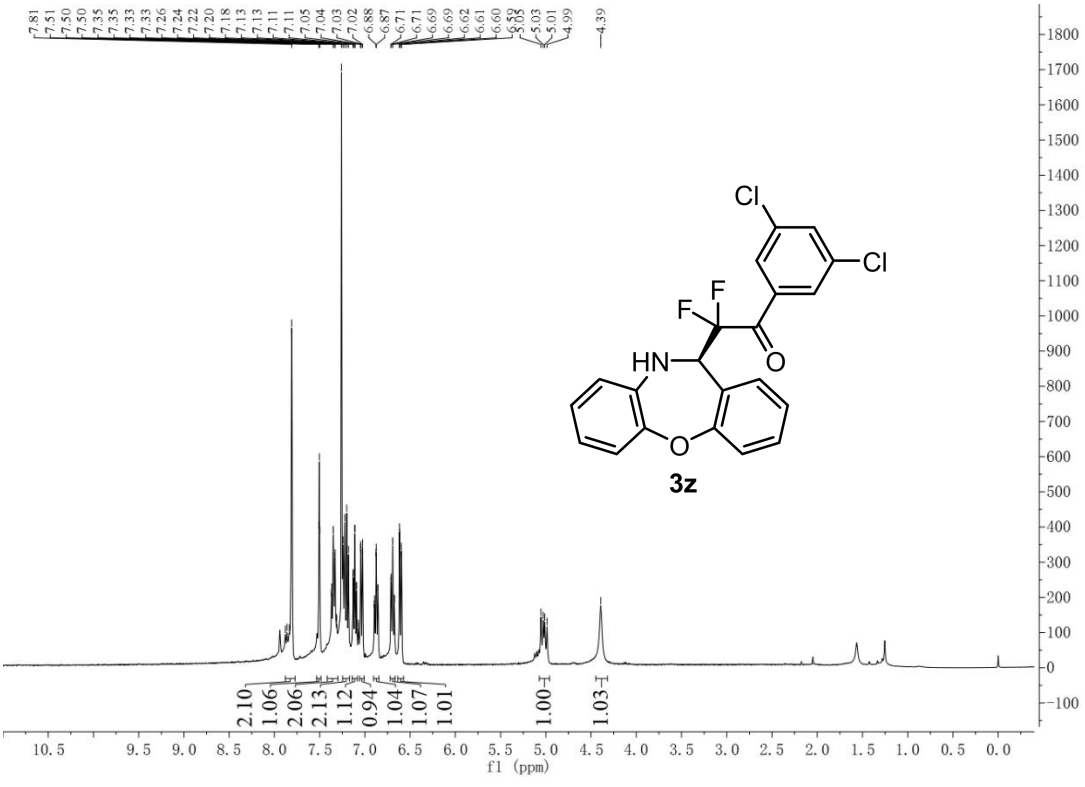
F
F
F
HN
O
O
3y
f1 (ppm)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7.13
7.13
7.11
7.11
7.05
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7.03
7.02
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6.87
6.71
6.71
6.69
6.69
6.62
6.61
6.60
5.03
5.01
4.99
4.39
Cl
Cl
F
F
HN
O
O
3z
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2.06
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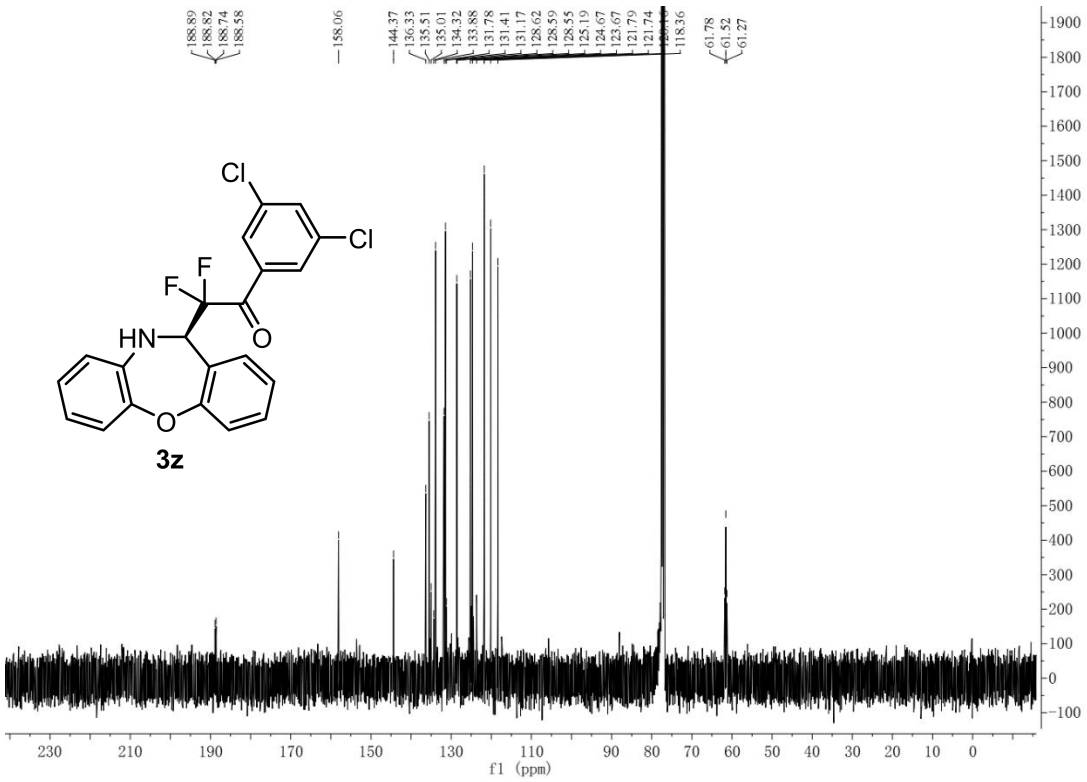
1.12
0.94
1.04
1.07
1.01
1.00
1.03
f1 (ppm)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128.62
128.59
128.55
125.19
124.67
123.67
121.79
121.74
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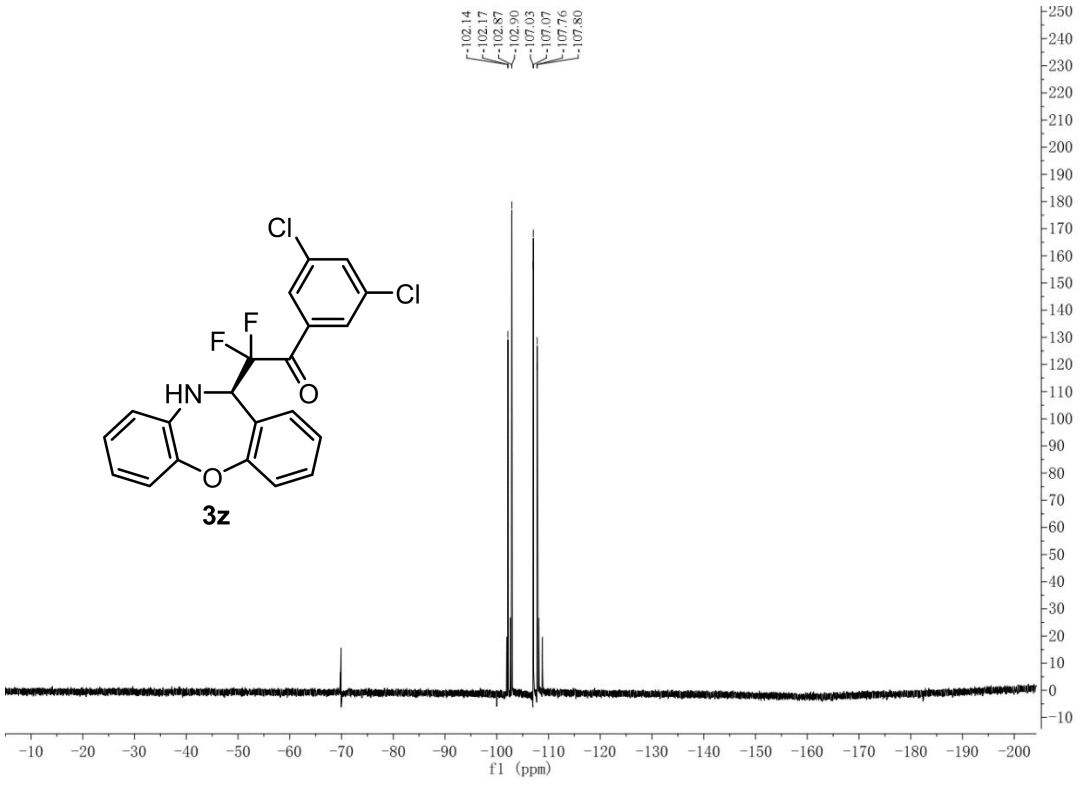
61.78
61.52
61.27
Cl
Cl
F
F
HN
O
O
3z
f1 (ppm)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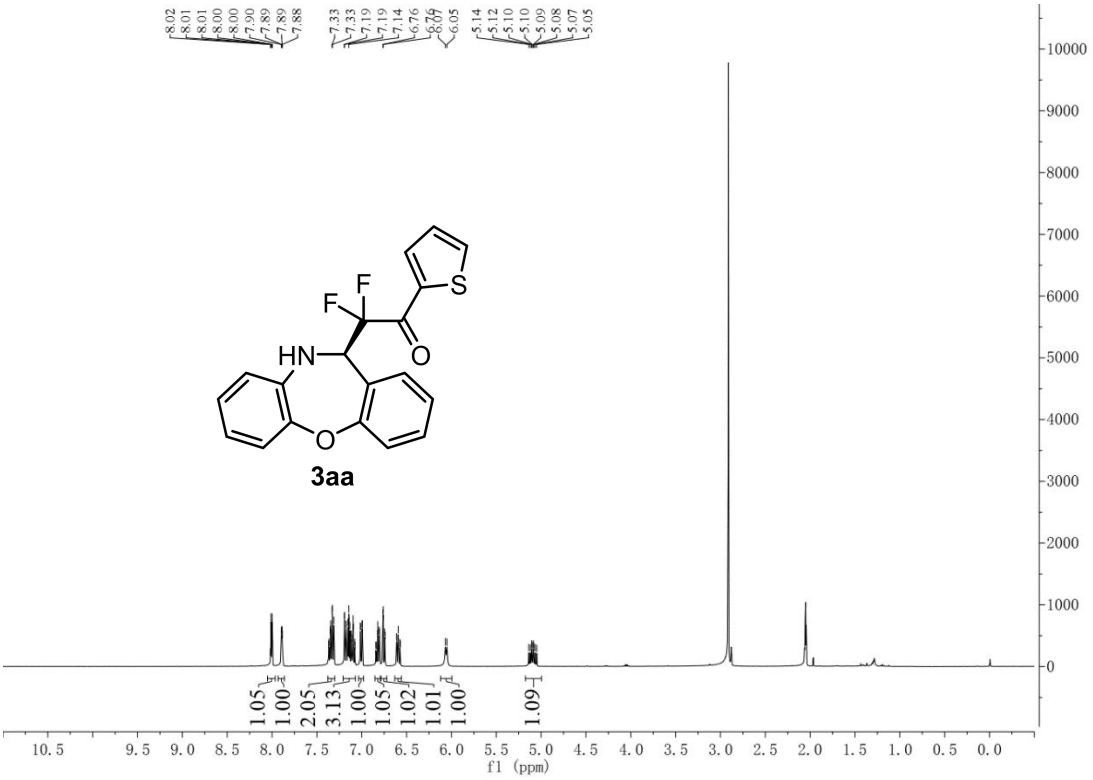
107.76
107.80
Cl
Cl
F
F
HN
O
O
3z
f1 (ppm)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6.76
6.07
6.05
5.14
5.12
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5.09
5.08
5.07
5.05
F
F
S
HN
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O
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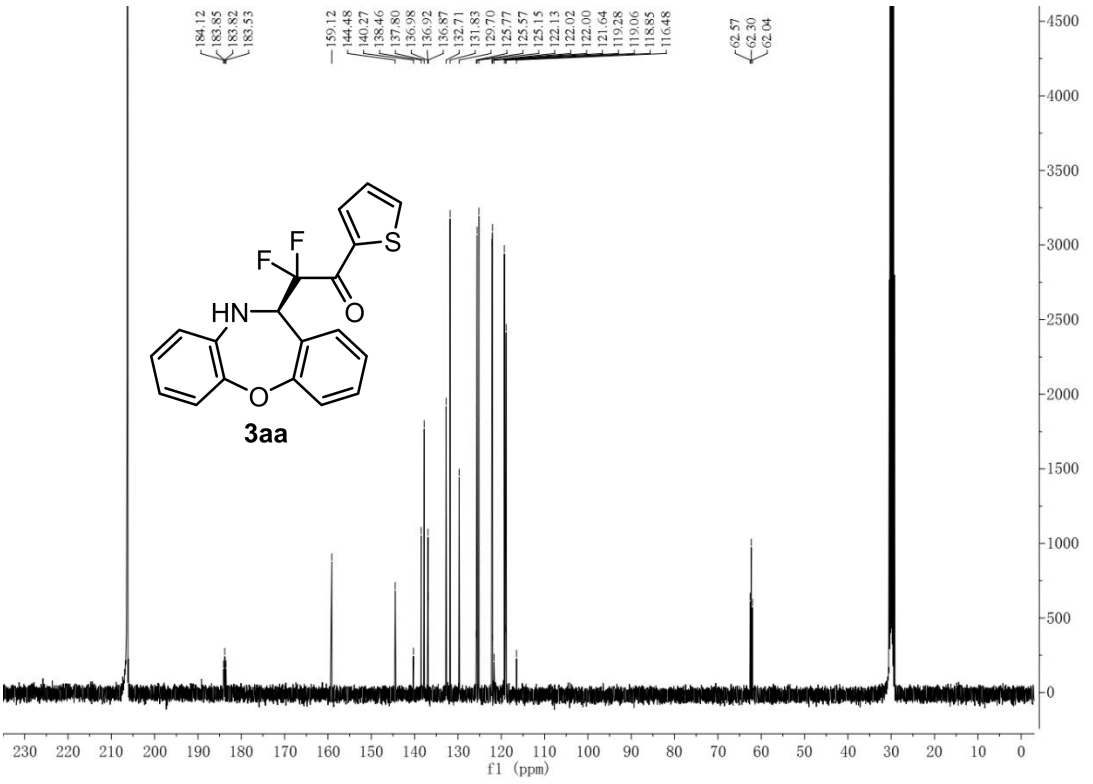
1.01
1.00
1.09
f1 (ppm)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125.15
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122.02
122.00
121.64
119.28
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116.48
62.57
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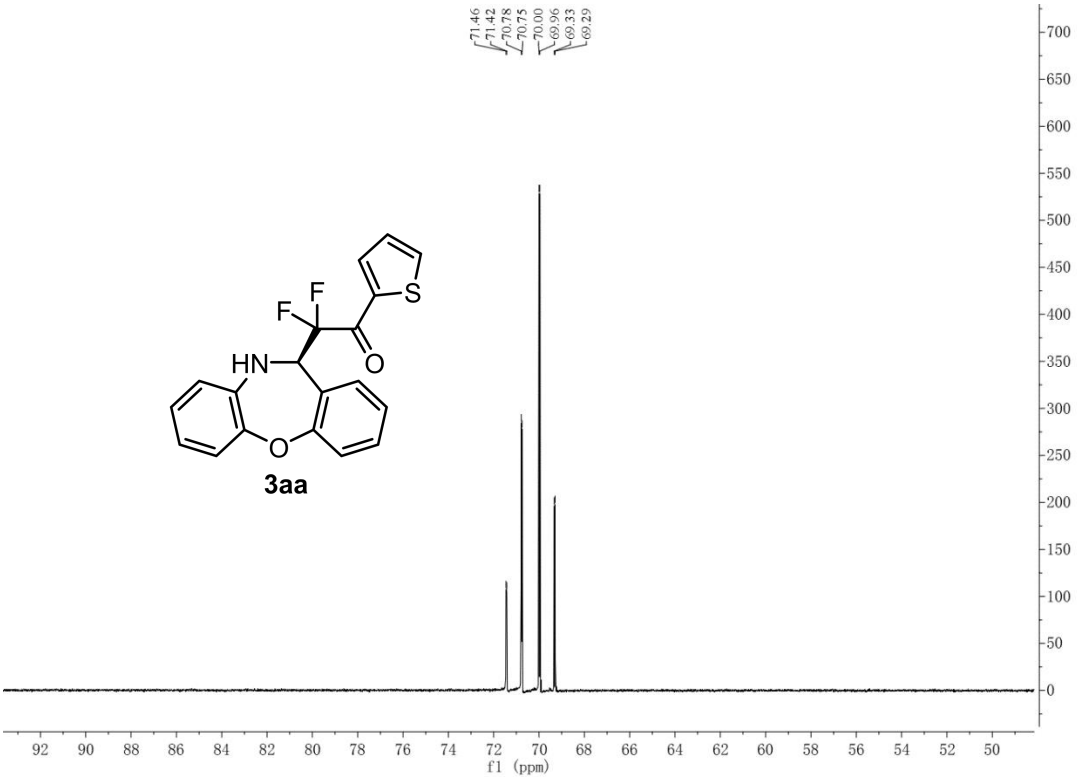
62.04
F
F
S
HN
O
O
3aa
f1 (ppm)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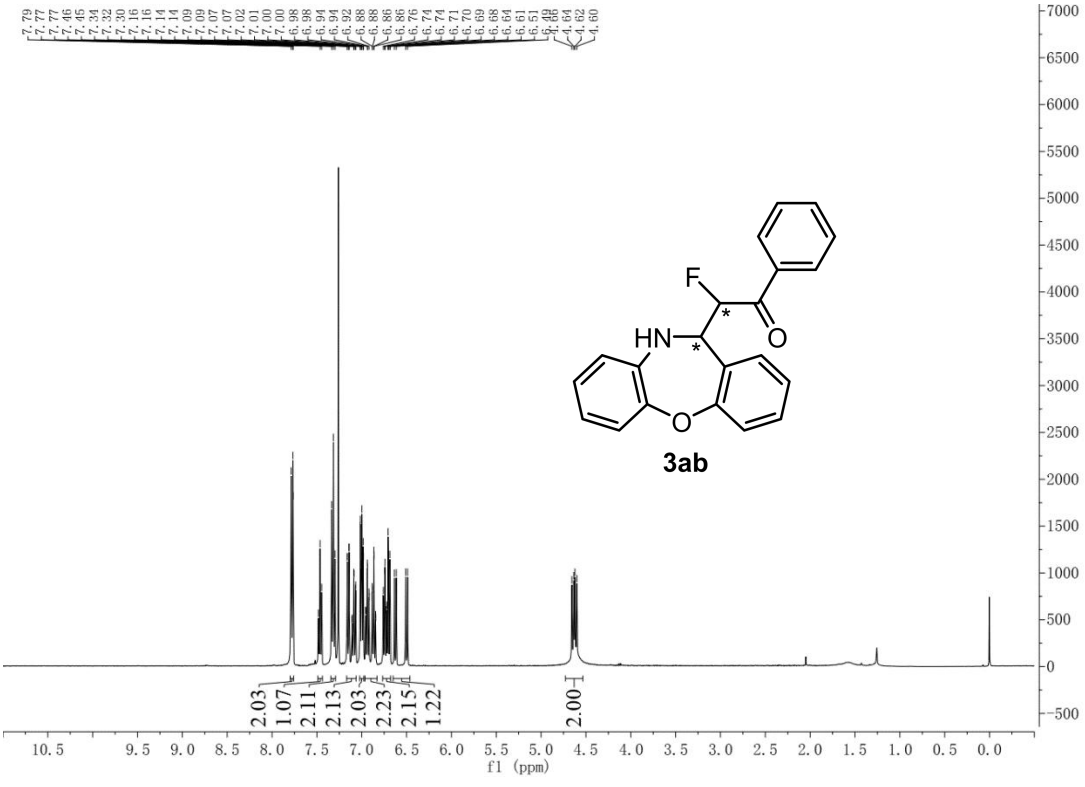
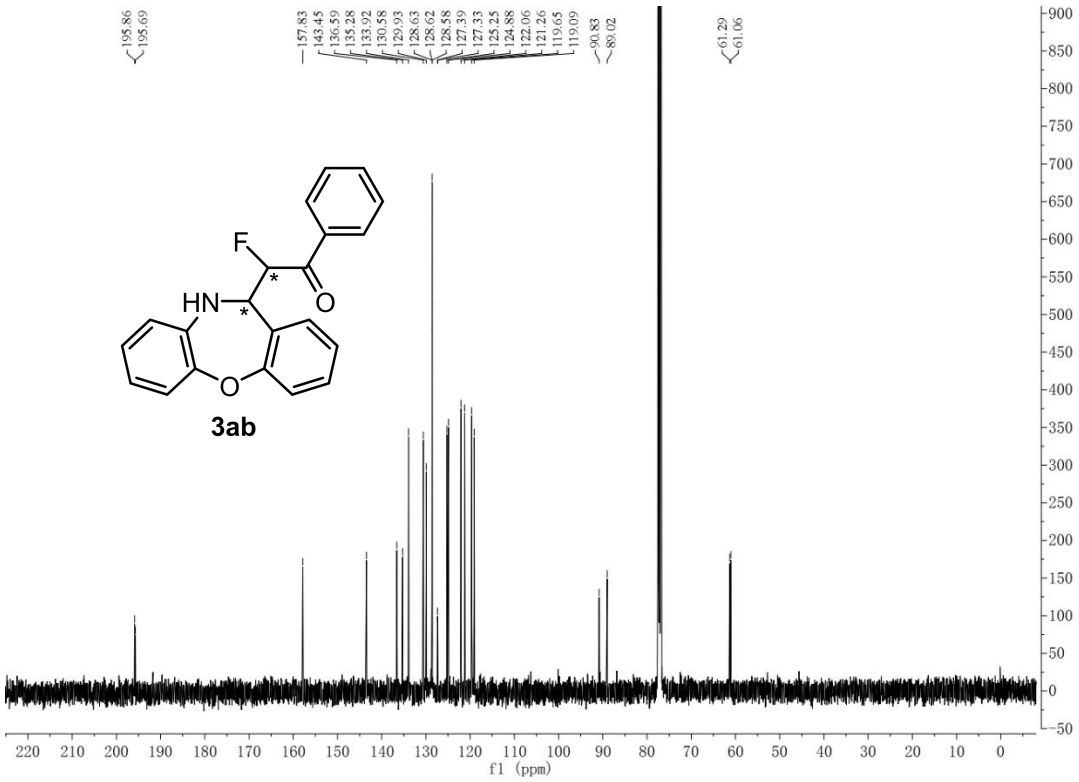
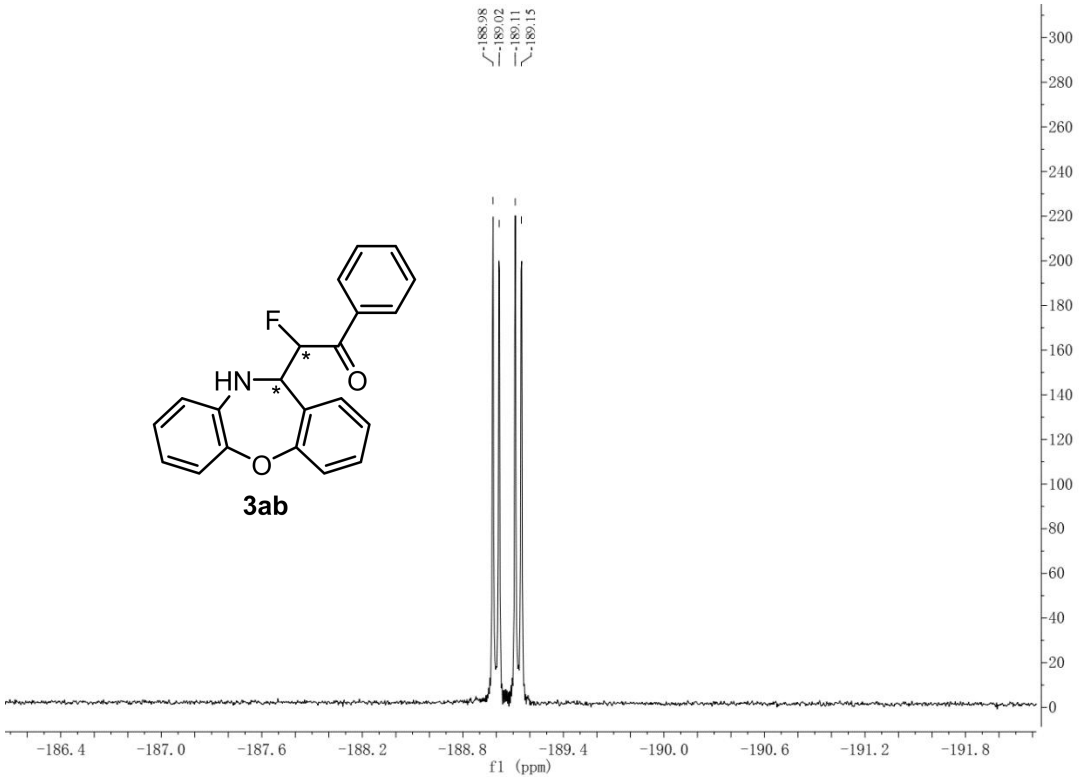
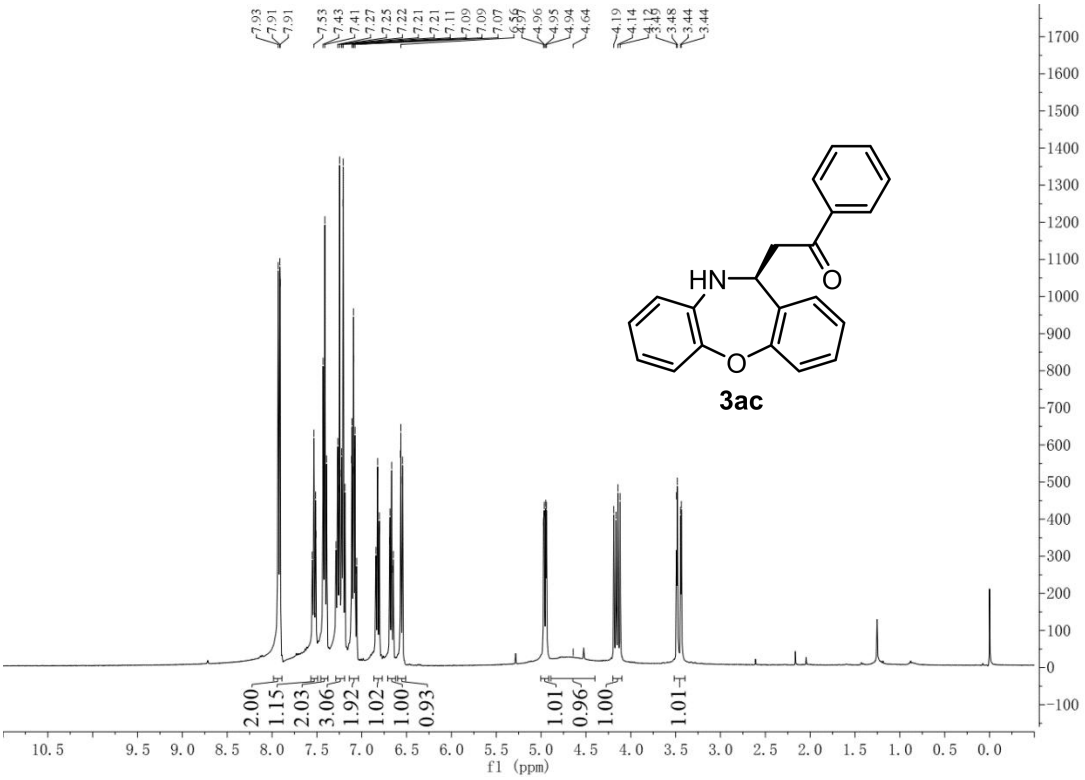
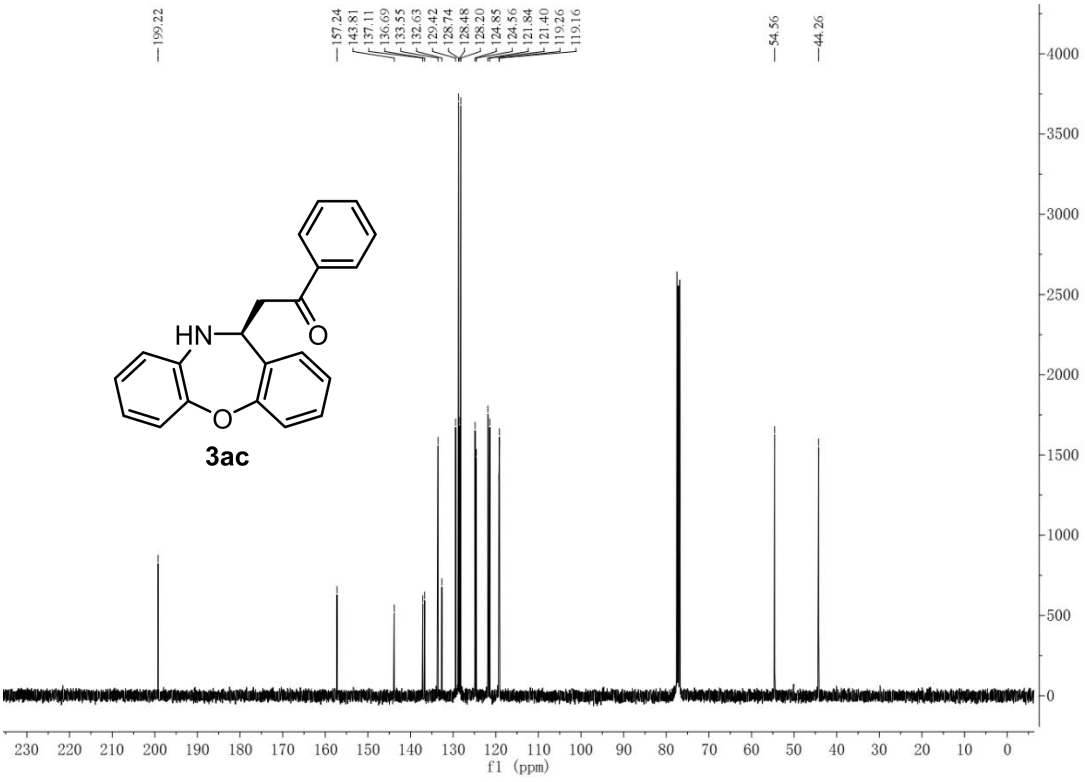
70.75
70.00
69.96
69.33
69.29
F
F
S
HN
O
O
3aa
f1 (ppm)

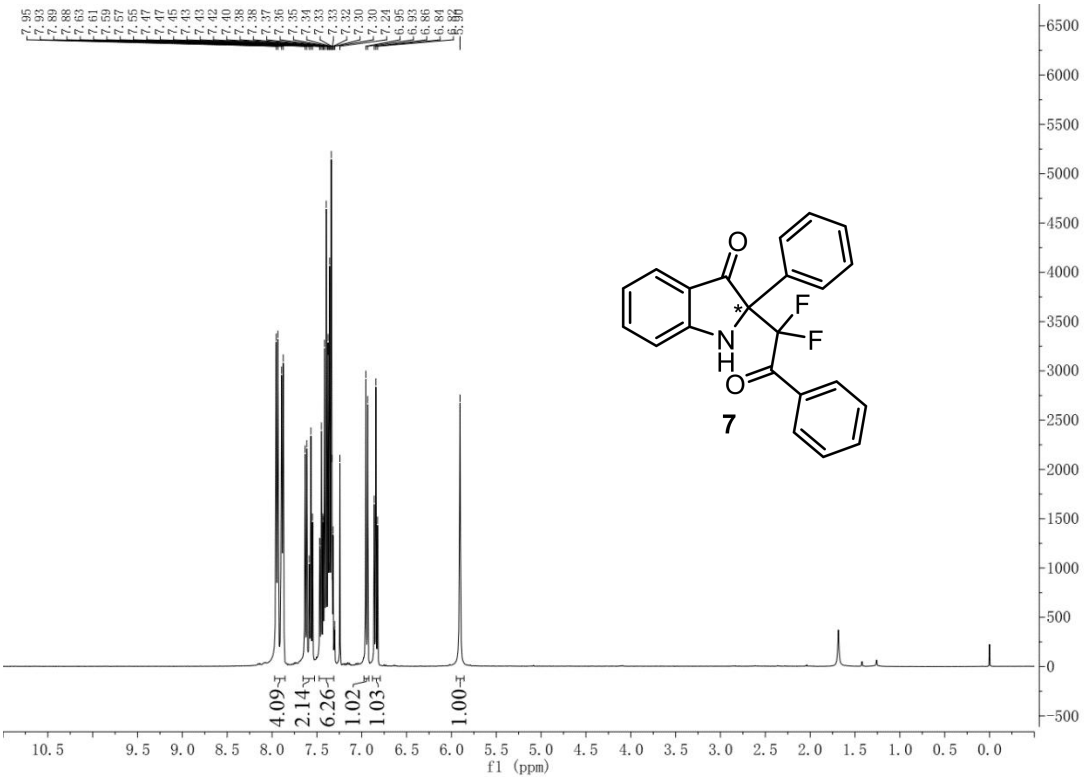

F
HN
O
O
3ab
2.03
1.07
2.11
2.13
2.03
2.23
2.15
1.22
2.00
f1 (ppm)

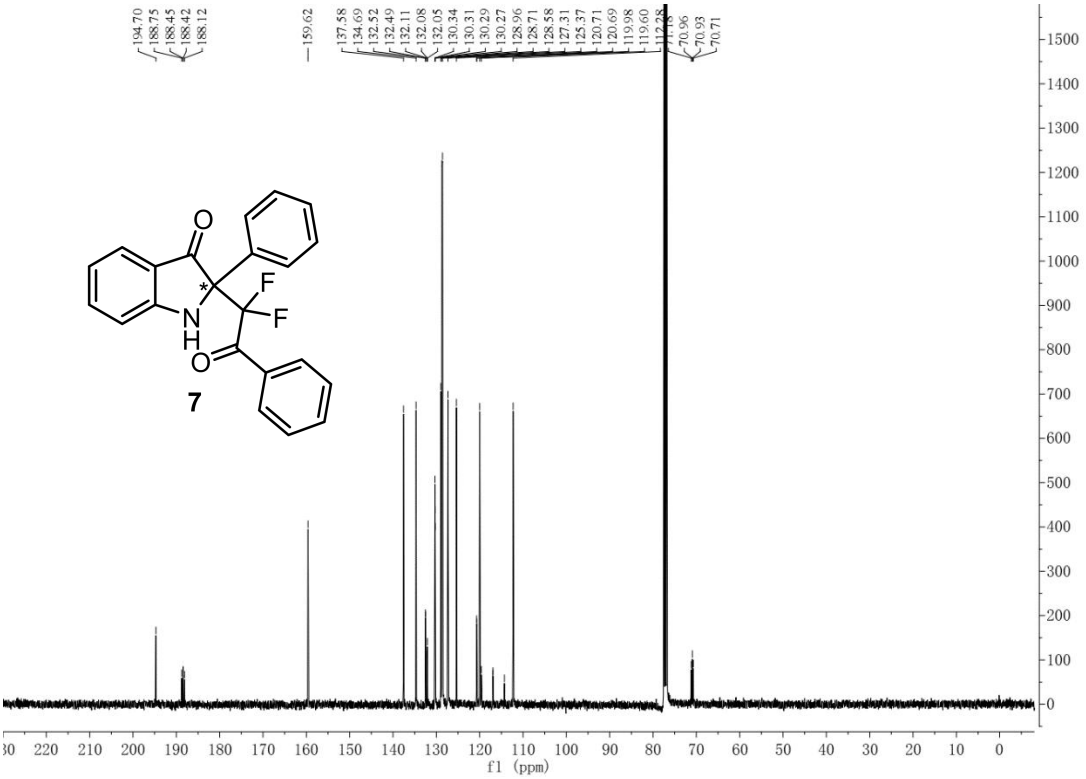

195.86
195.69
157.83
143.45
136.59
135.28
133.92
130.58
129.93
128.63
128.62
128.58
127.39
127.33
125.25
124.88
122.06
121.26
119.65
119.09
90.83
89.02
61.29
61.06
F
HN
O
O
3ab
f1 (ppm)

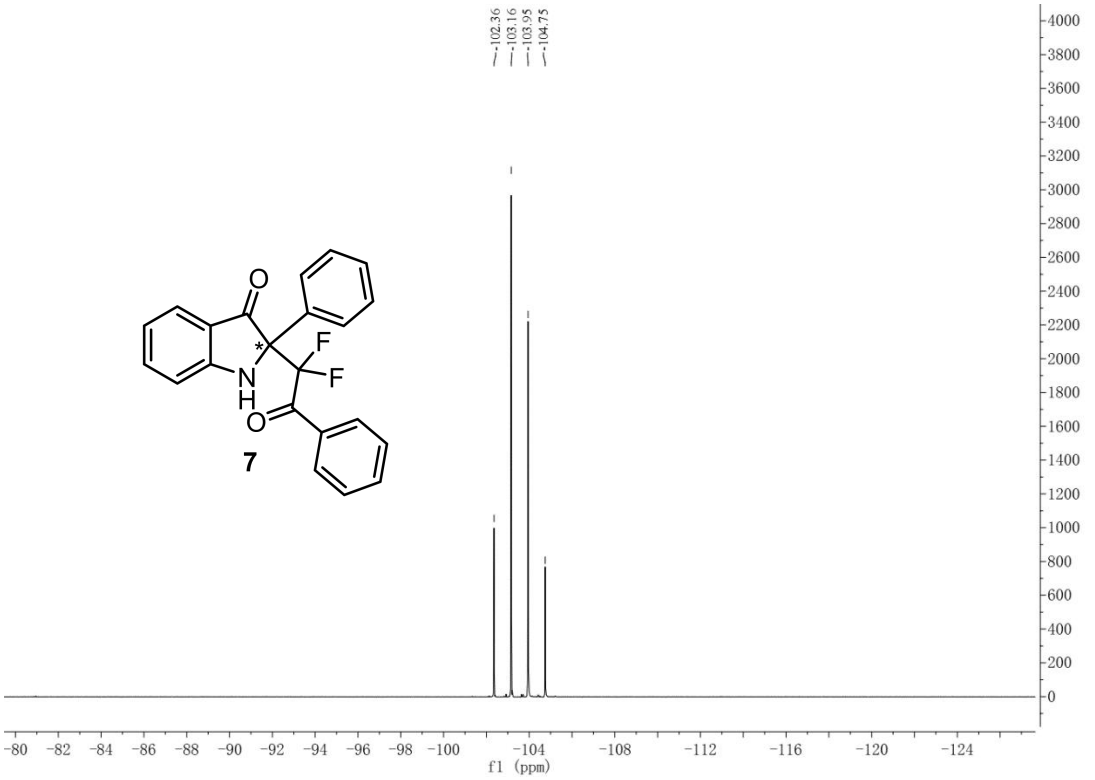

188.98
189.02
189.11
189.15
F
HN
O
O
3ab
f1 (ppm)

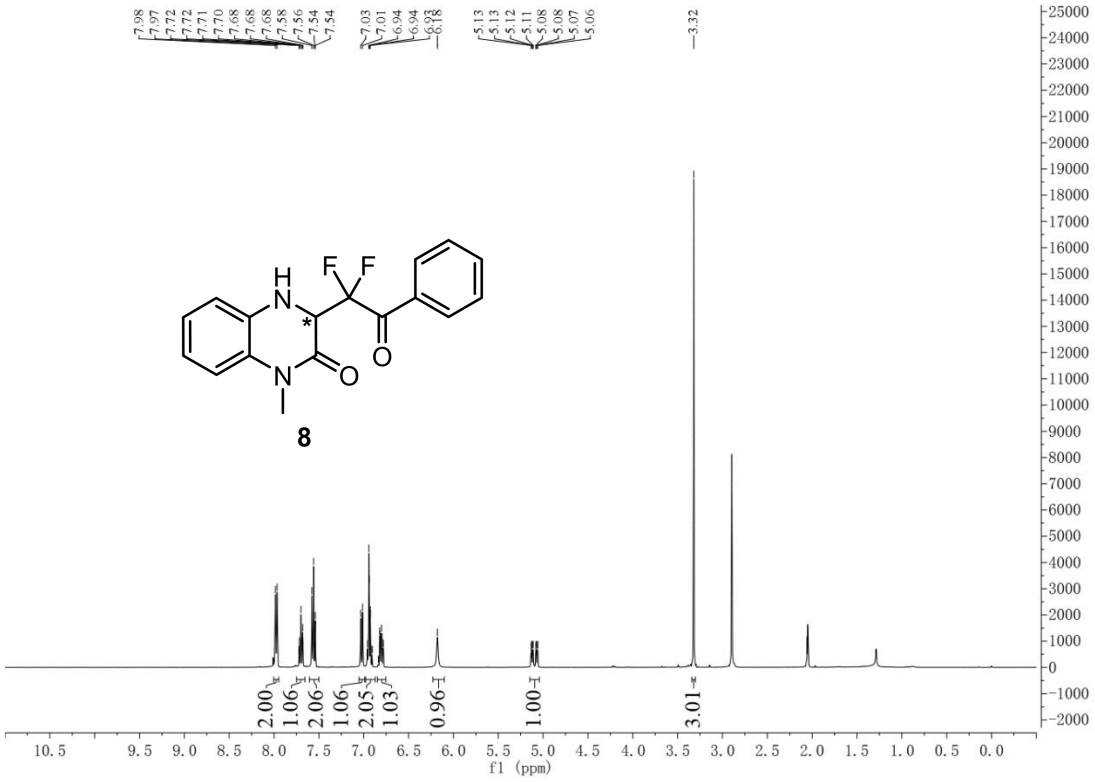

7.93
7.91
7.91
7.53
7.43
7.41
7.27
7.25
7.22
7.21
7.21
7.11
7.09
7.09
7.07
6.56
4.97
4.96
4.95
4.94
4.64
4.19
4.14
3.48
3.44
3.44
HN
O
O
3ac
2.00
1.15
2.03
3.06
1.92
1.02
1.00
0.93
1.01
0.96
1.00
1.01
f1 (ppm)

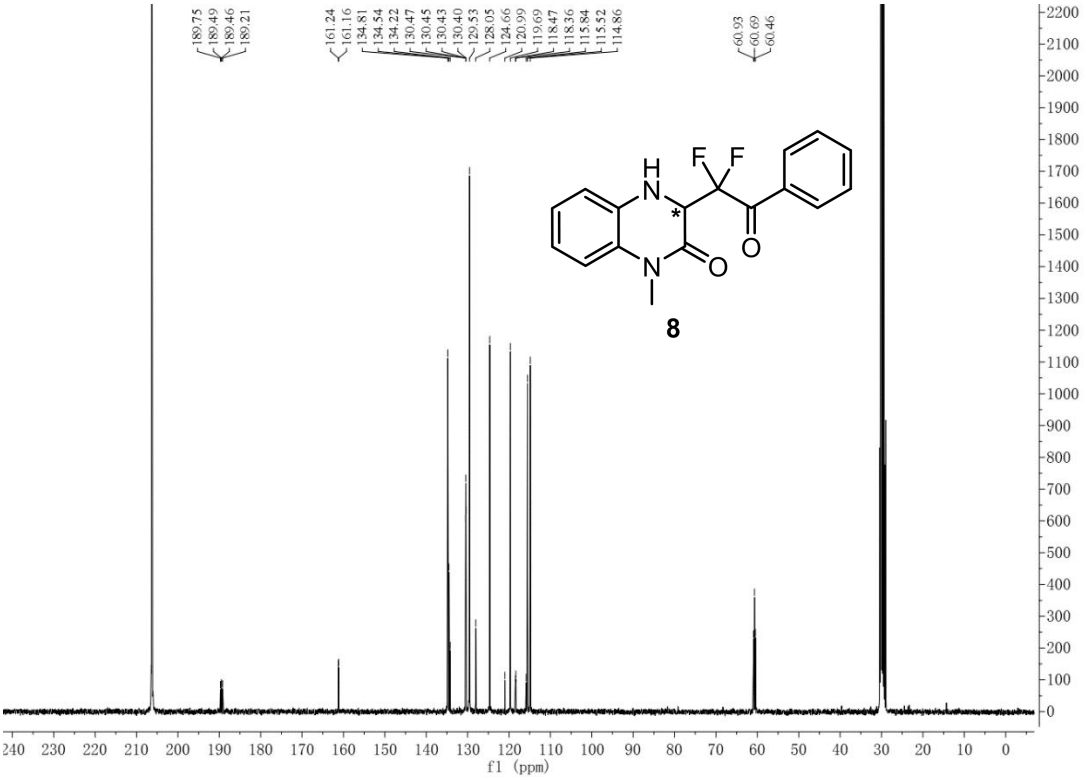

199.22
157.24
143.81
137.11
136.69
133.55
132.63
129.42
128.74
128.48
128.20
124.85
124.56
121.84
121.40
119.26
119.16
54.56
44.26
HN
O
O
3ac
f1 (ppm)

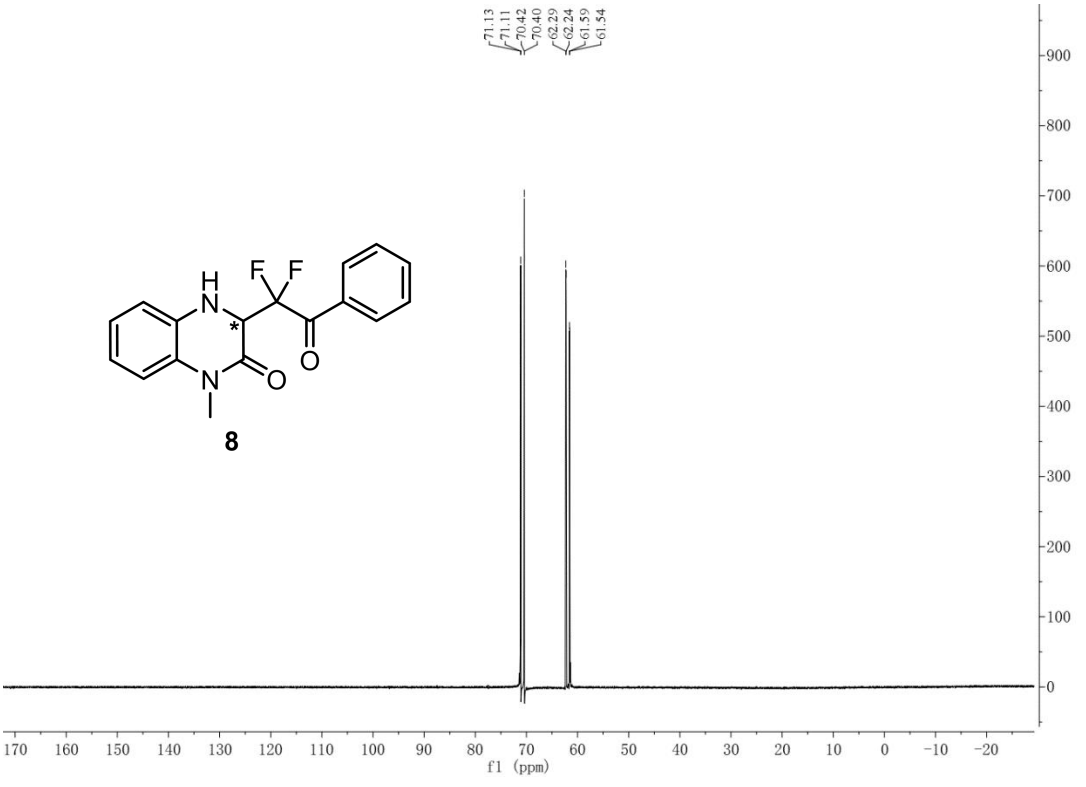

7.95
7.93
7.89
7.88
7.63
7.61
7.59
7.57
7.55
7.47
7.47
7.45
7.43
7.43
7.42
7.40
7.38
7.38
7.37
7.36
7.35
7.34
7.33
7.33
7.32
7.30
7.30
7.24
6.95
6.93
6.86
6.84
4.09
2.14
6.26
1.02
1.03
1.00
O
F
F
N
H
O
*
7
f1 (ppm)

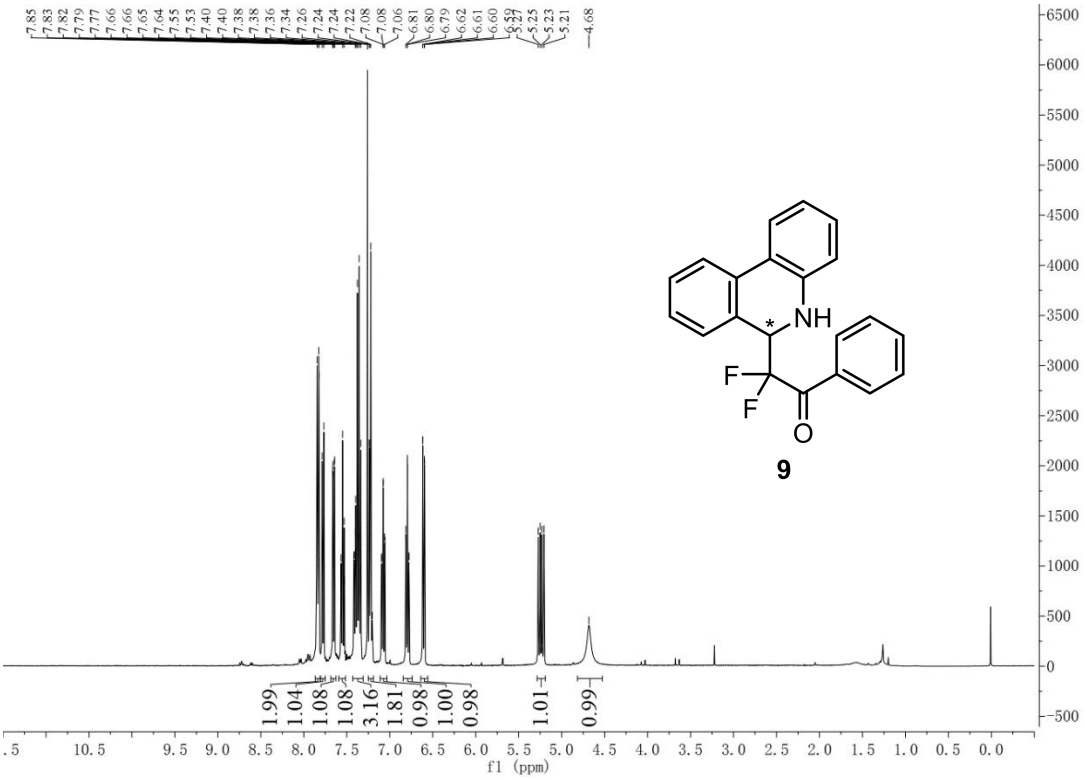

194.70
188.75
188.45
188.42
188.12
159.62
137.58
134.69
132.52
132.49
132.11
132.08
132.05
130.34
130.31
130.29
130.27
128.96
128.71
128.58
127.31
125.37
120.71
120.69
119.98
119.60
70.96
70.93
70.71
O
F
F
N
H
O
*
7
f1 (ppm)

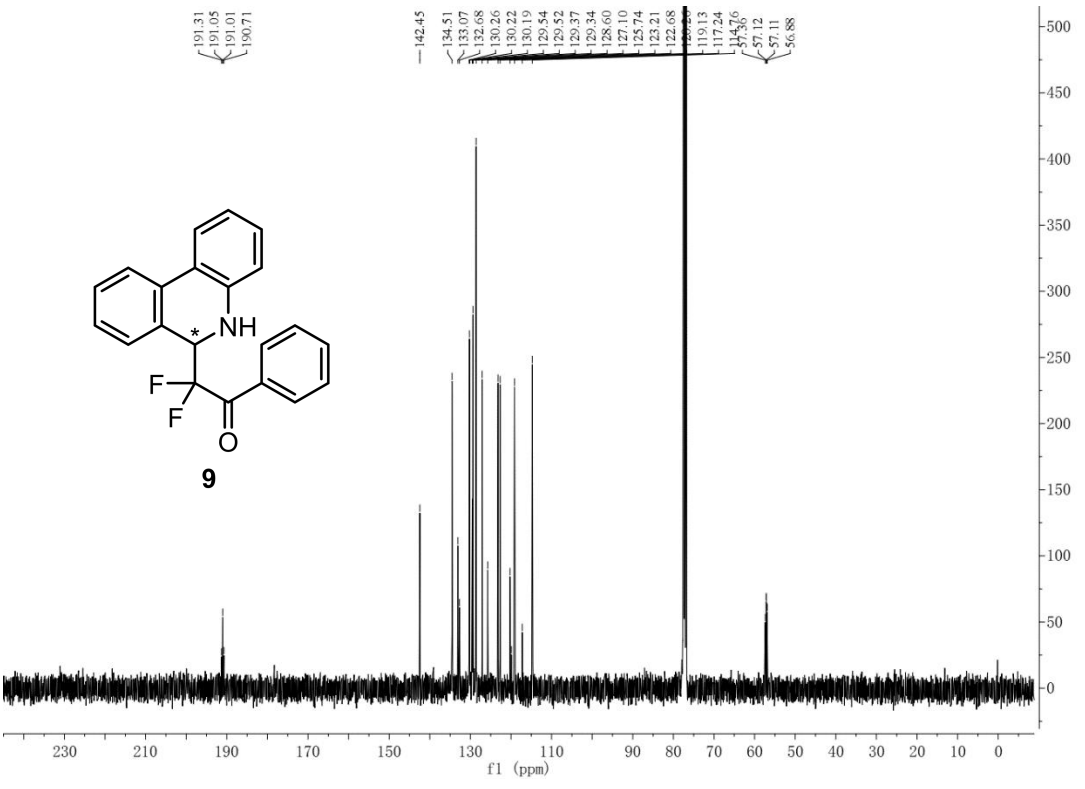

-102.36
-103.16
-103.95
-104.75
O
*
F
F
N
H
O
7
f1 (ppm)

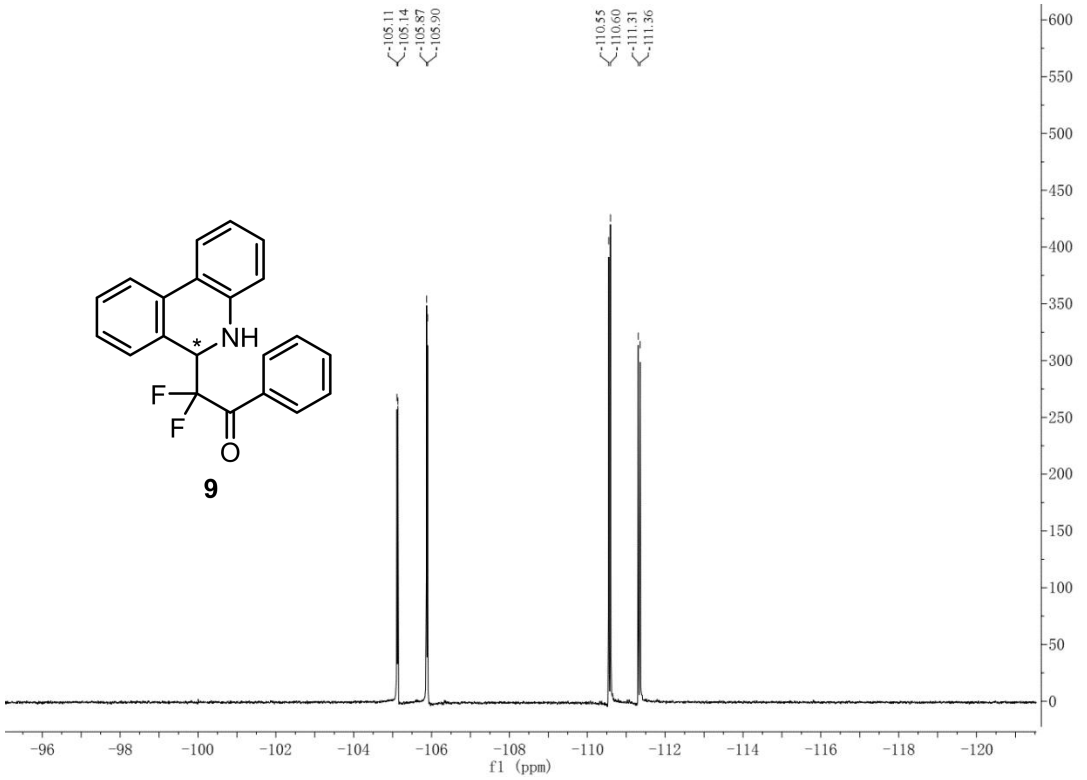

7.98
7.97
7.72
7.72
7.71
7.70
7.68
7.68
7.68
7.58
7.56
7.54
7.54
7.03
7.01
6.94
6.94
6.93
6.18
5.13
5.13
5.12
5.11
5.08
5.08
5.07
5.06
3.32
H
N
*
F
F
O
N
O
8
2.00
1.06
2.06
1.06
2.05
1.03
0.96
1.00
3.01
f1 (ppm)

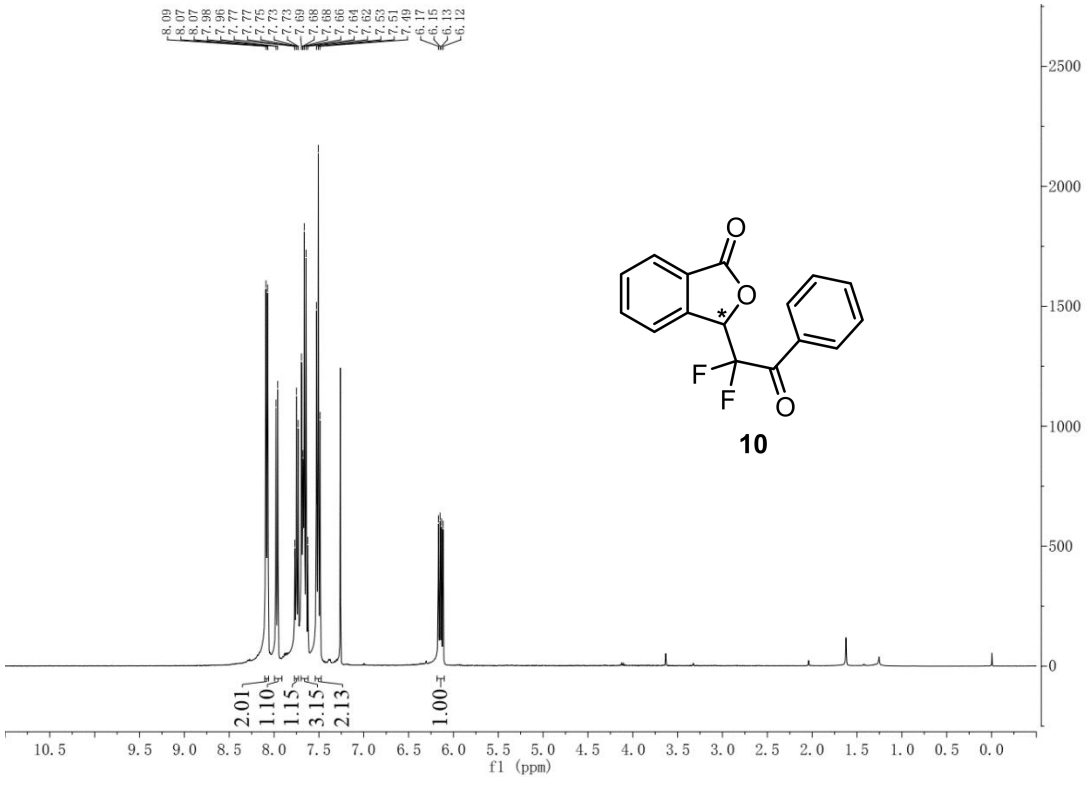

189.75
189.49
189.46
189.21
161.24
161.16
134.81
134.54
134.22
130.47
130.45
130.43
130.40
129.53
128.05
124.66
120.99
119.69
118.47
118.36
115.84
115.52
114.86
60.93
60.69
60.46
F
F
H
N
*
O
N
O
8
f1 (ppm)

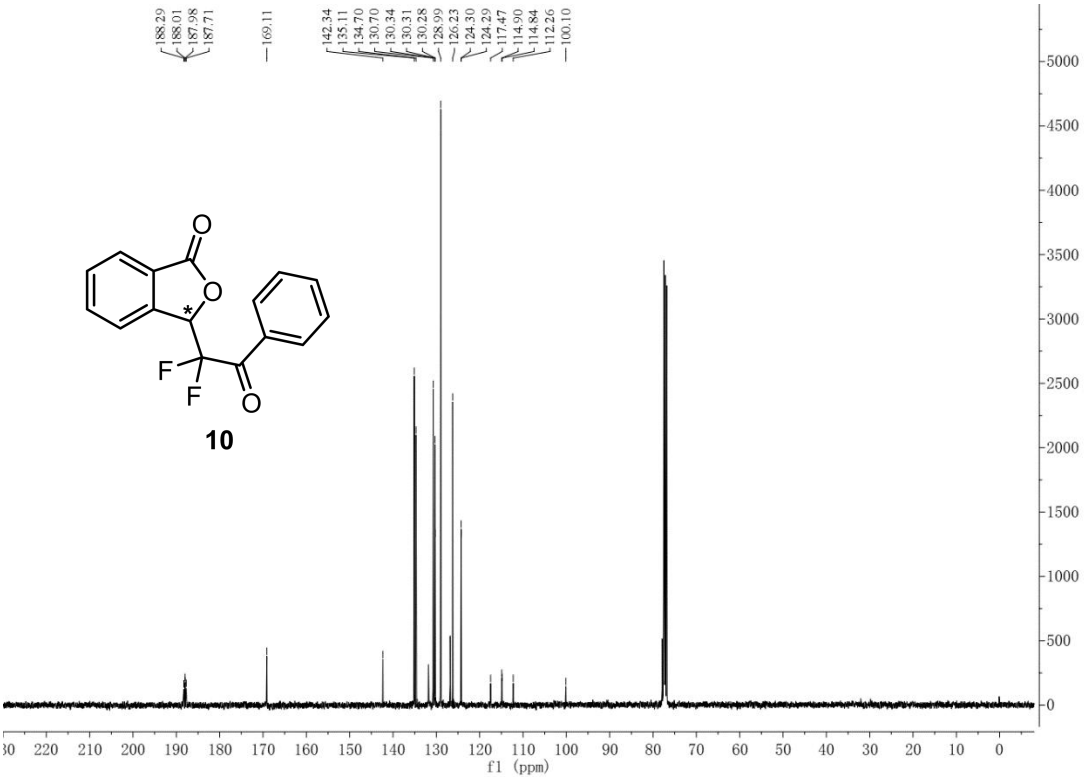

71.13
71.11
70.42
70.40
62.29
62.24
61.59
61.54
F
F
H
N
*
O
N
O
8
f1 (ppm)

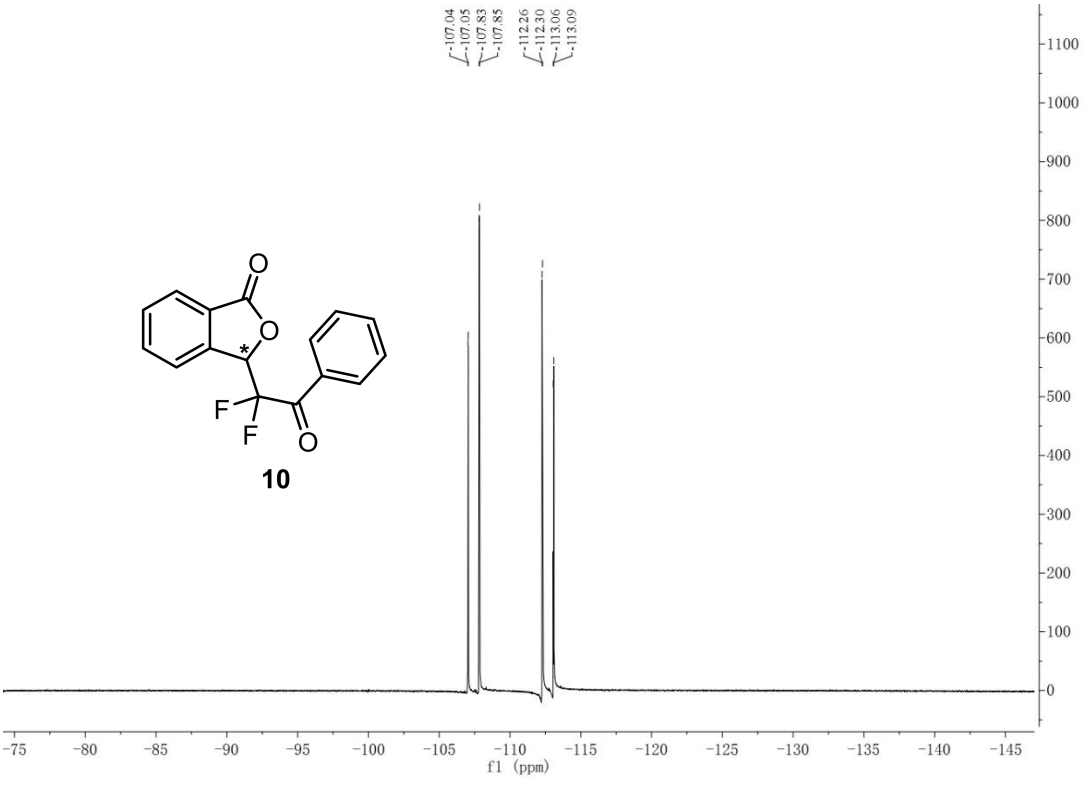

7.85
7.83
7.82
7.79
7.77
7.66
7.66
7.65
7.64
7.55
7.53
7.40
7.40
7.38
7.38
7.36
7.34
7.26
7.24
7.24
7.22
7.08
7.08
7.06
6.81
6.80
6.79
6.62
6.61
6.60
5.25
5.23
5.21
4.68
1.99
1.04
1.08
1.08
3.16
1.81
0.98
1.00
0.98
1.01
0.99
f1 (ppm)
NH
F
F
O
9

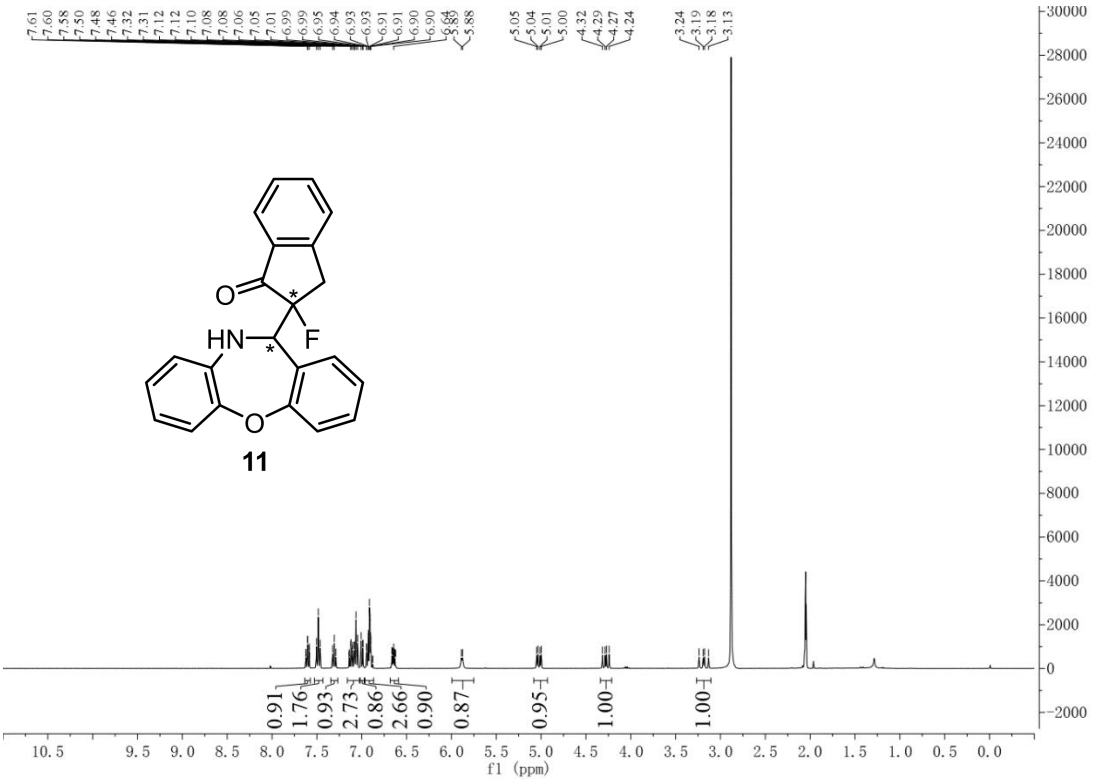

191.31
191.05
191.01
190.71
142.45
134.51
133.07
132.68
130.26
130.22
130.19
129.54
129.52
129.37
129.34
128.60
127.10
125.74
123.21
122.68
119.13
117.24
57.12
57.11
56.88
f1 (ppm)
NH
F
F
O
9

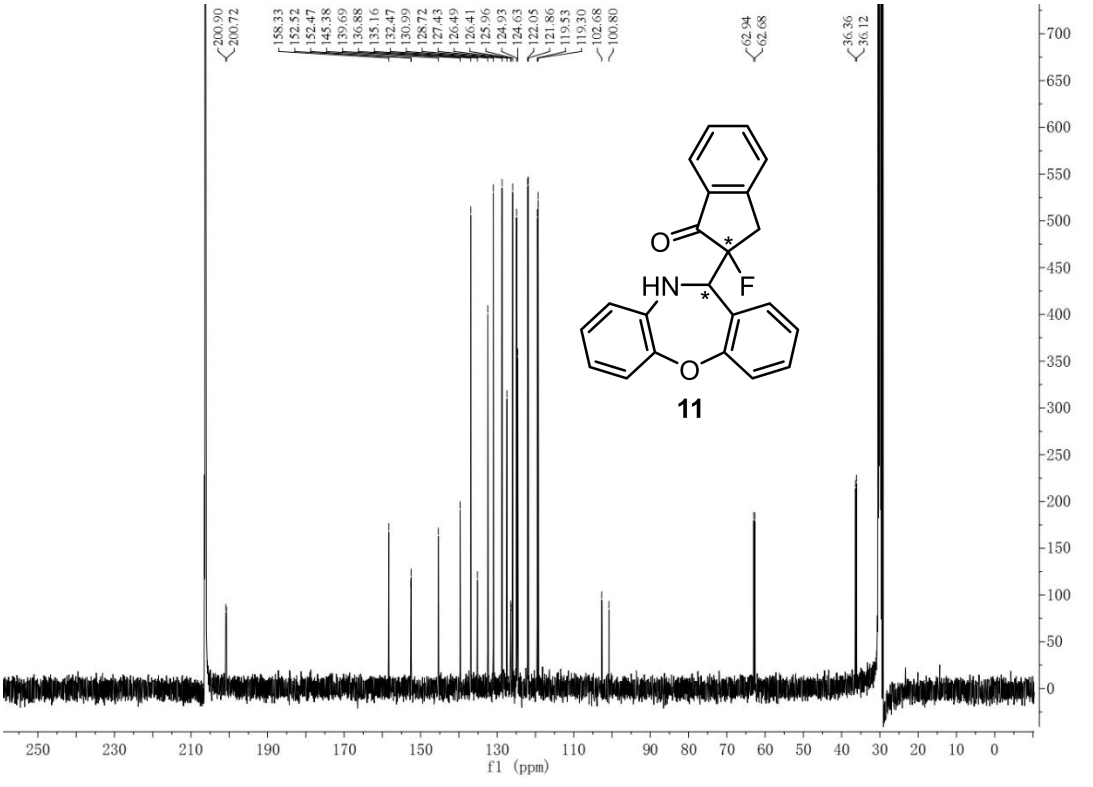

-105.11
-105.14
-105.87
-105.90
-110.55
-110.60
-111.31
-111.36
NH
F
F
O
9
f1 (ppm)

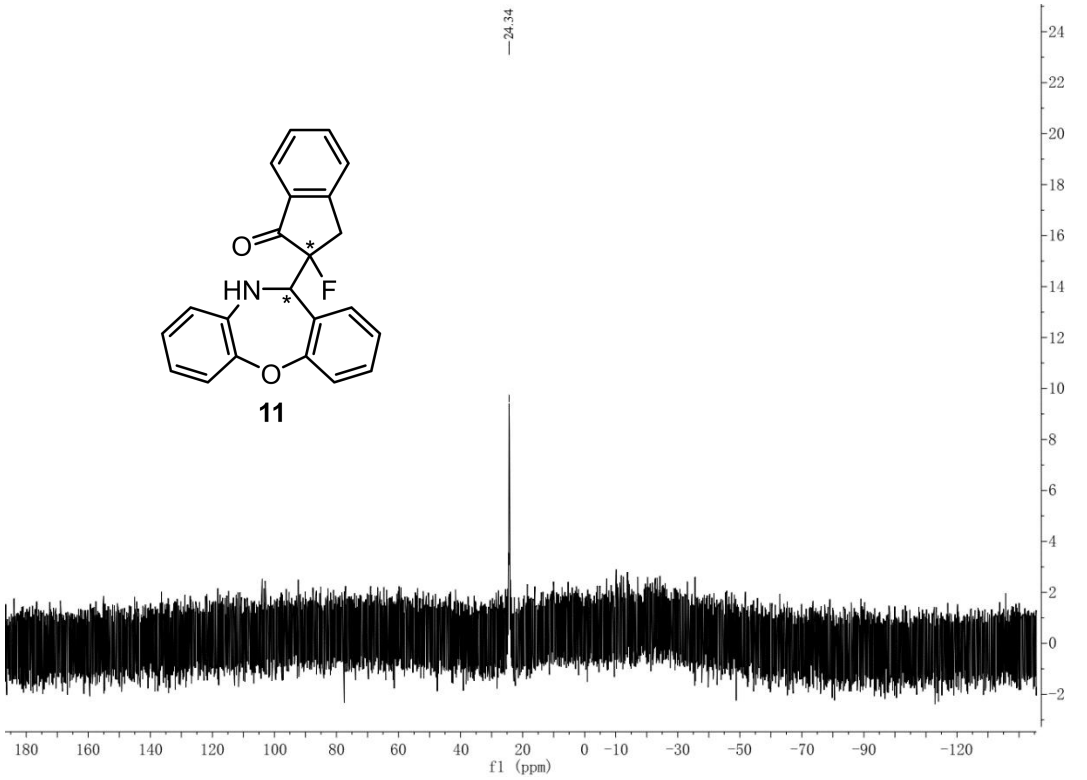

8.09
8.07
8.07
7.98
7.96
7.77
7.77
7.75
7.73
7.73
7.69
7.68
7.68
7.66
7.64
7.62
7.53
7.51
7.49
6.17
6.15
6.13
6.12
O
O
F
F
O
10
2.01
1.10
1.15
3.15
2.13
1.00
f1 (ppm)

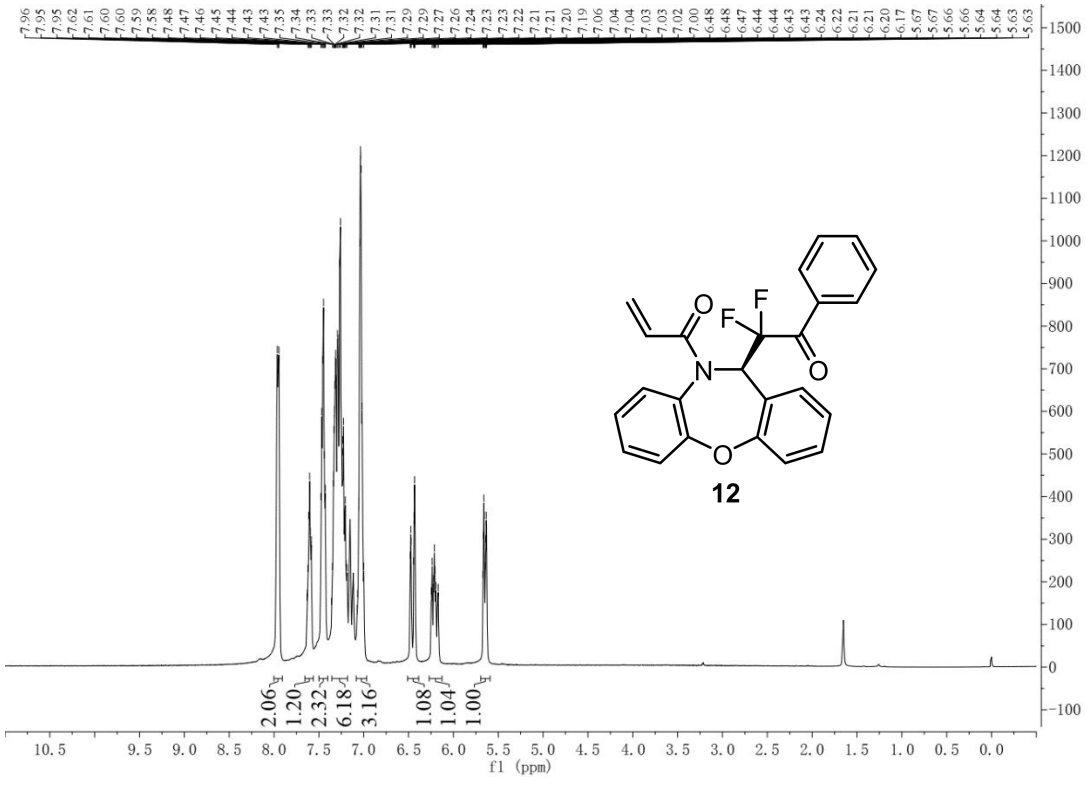

188.29
188.01
187.98
187.71
169.11
142.34
135.11
134.70
130.70
130.34
130.31
130.28
128.99
126.23
124.30
124.29
117.47
114.90
114.84
112.26
100.10
O
O
*
F
F
O
10
f1 (ppm)

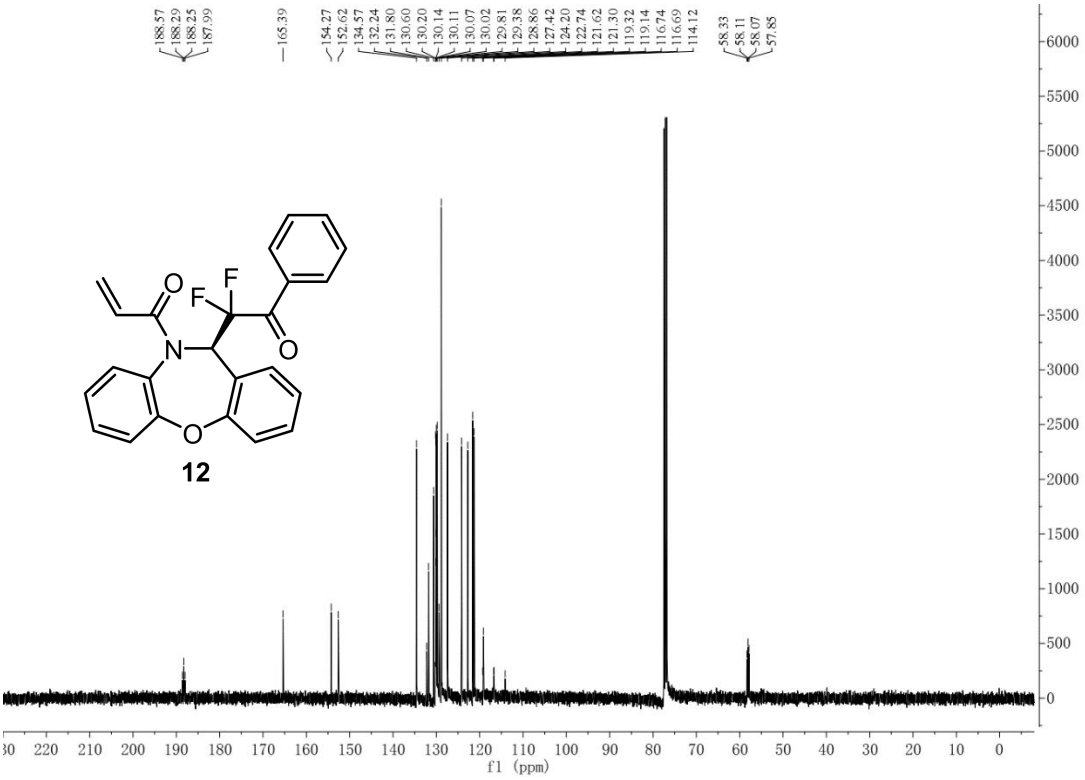

-107.04
-107.05
-107.83
-107.85
-112.26
-112.30
-113.06
-113.09
O
O
*
F
F
O
10
f1 (ppm)

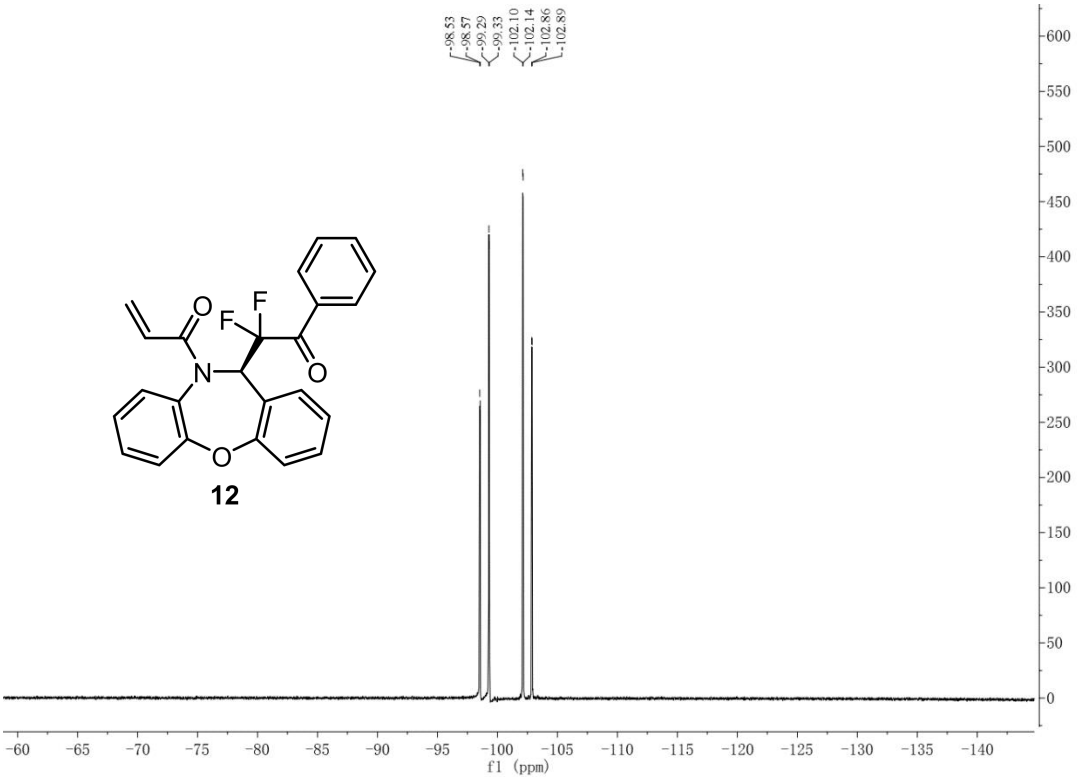

7.61
7.60
7.58
7.50
7.48
7.46
7.32
7.31
7.12
7.12
7.10
7.08
7.08
7.06
7.05
7.01
6.99
6.99
6.95
6.94
6.93
6.93
6.91
6.91
6.90
6.90
6.64
5.88
5.05
5.04
5.01
5.00
4.32
4.29
4.27
4.24
3.24
3.19
3.18
3.13
O
HN
F
O
11
0.91
1.76
0.93
2.73
0.86
2.66
0.90
0.87
0.95
1.00
1.00
f1 (ppm)

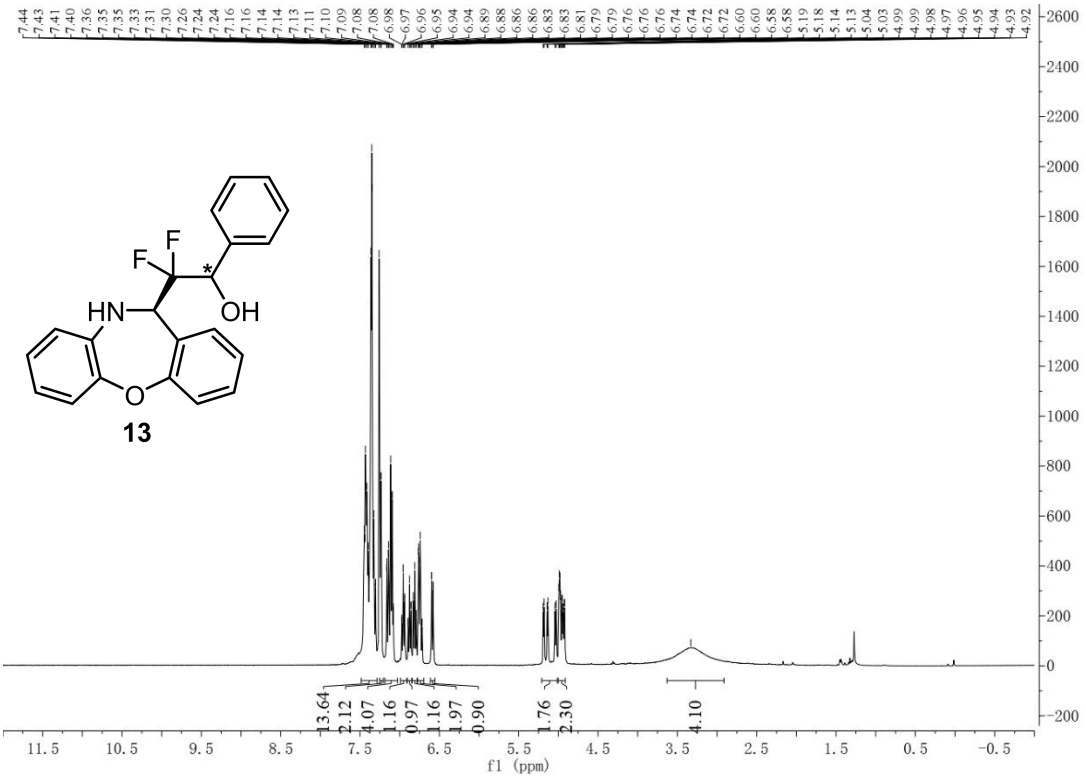

200.90
200.72
158.33
152.52
152.47
145.38
139.69
136.88
135.16
132.47
130.99
128.72
127.43
126.49
126.41
125.96
124.93
124.63
122.05
121.86
119.53
119.30
102.68
100.80
62.94
62.68
36.36
36.12
O
HN
F
O
11
f1 (ppm)

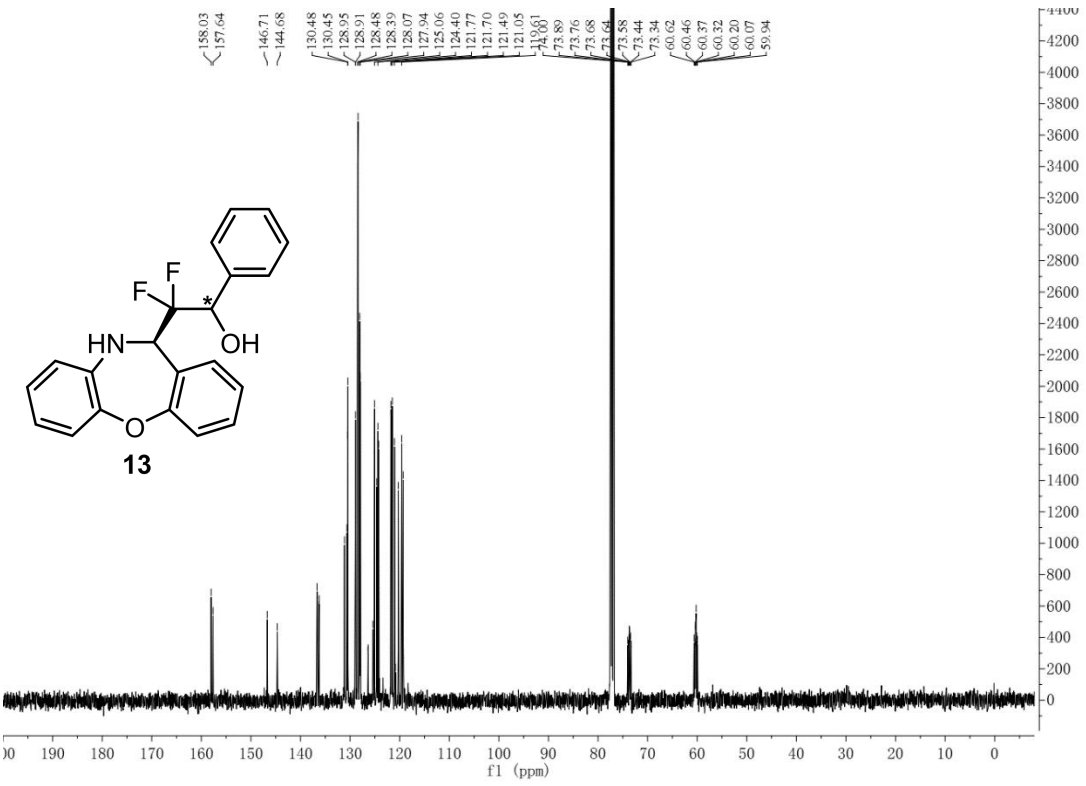

24.34
O
HN
F
O
11
f1 (ppm)

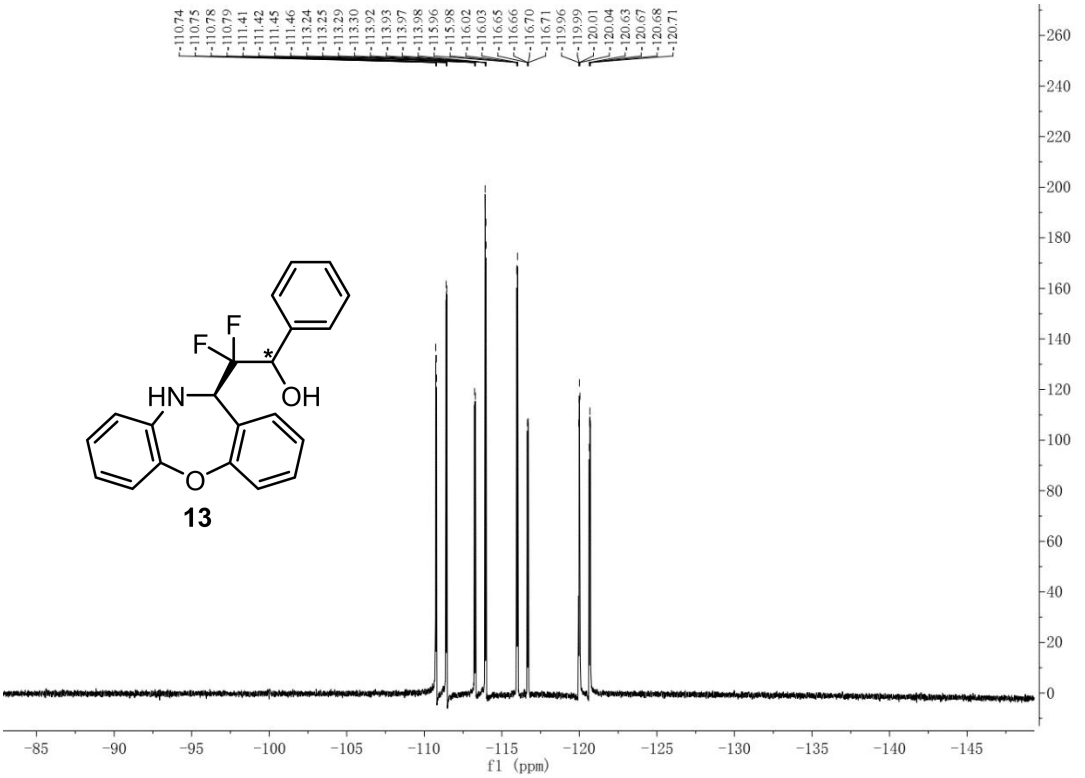

7.96
7.95
7.95
7.62
7.61
7.60
7.60
7.59
7.58
7.48
7.47
7.46
7.45
7.44
7.43
7.43
7.35
7.34
7.33
7.33
7.32
7.32
7.31
7.31
7.29
7.29
7.27
7.26
7.24
7.23
7.23
7.22
7.21
7.21
7.20
7.19
7.06
7.04
7.04
7.03
7.03
7.02
7.00
6.48
6.48
6.47
6.44
6.44
6.43
6.43
6.24
6.22
6.21
6.21
6.20
6.17
5.67
5.67
5.66
5.66
5.64
5.64
5.63
5.63
O
F
F
N
O
O
12
2.06
1.20
2.32
6.18
3.16
1.08
1.04
1.00
f1 (ppm)

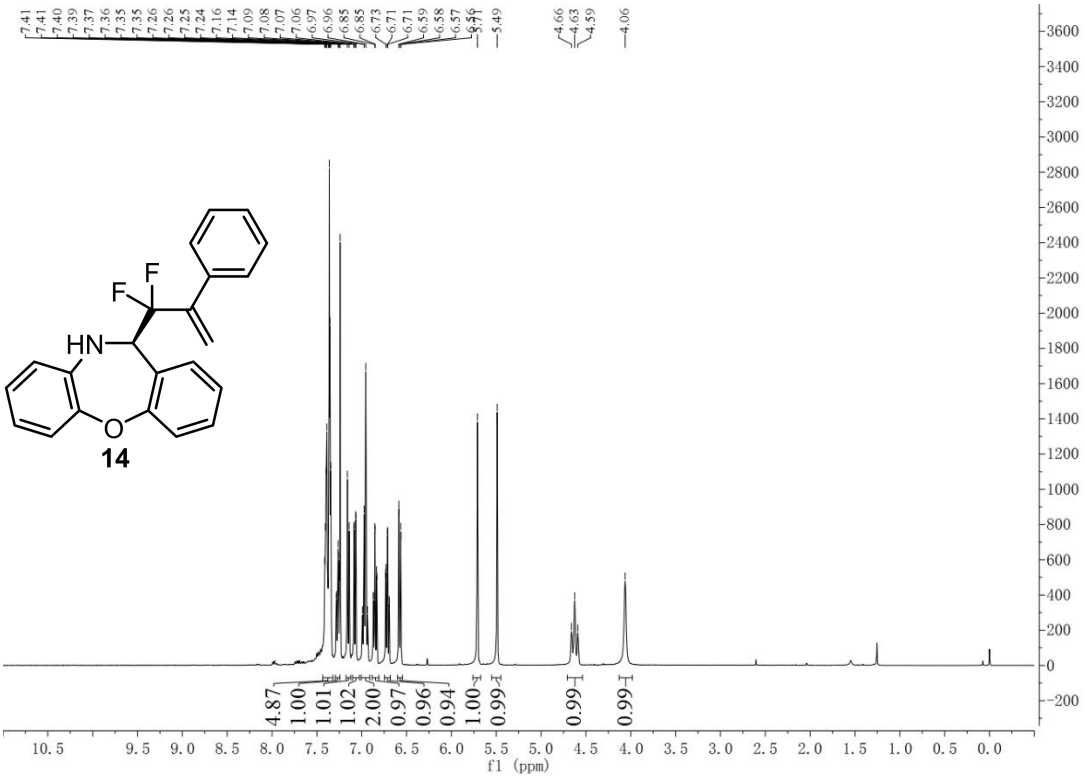

188.57
188.29
188.25
187.99
165.39
154.27
152.62
134.57
132.24
131.80
130.60
130.20
130.14
130.11
130.07
130.02
129.81
129.38
128.86
127.42
124.20
122.74
121.62
121.30
119.32
119.14
116.74
116.69
114.12
58.33
58.11
58.07
57.85
O
F
F
O
N
O
12
f1 (ppm)

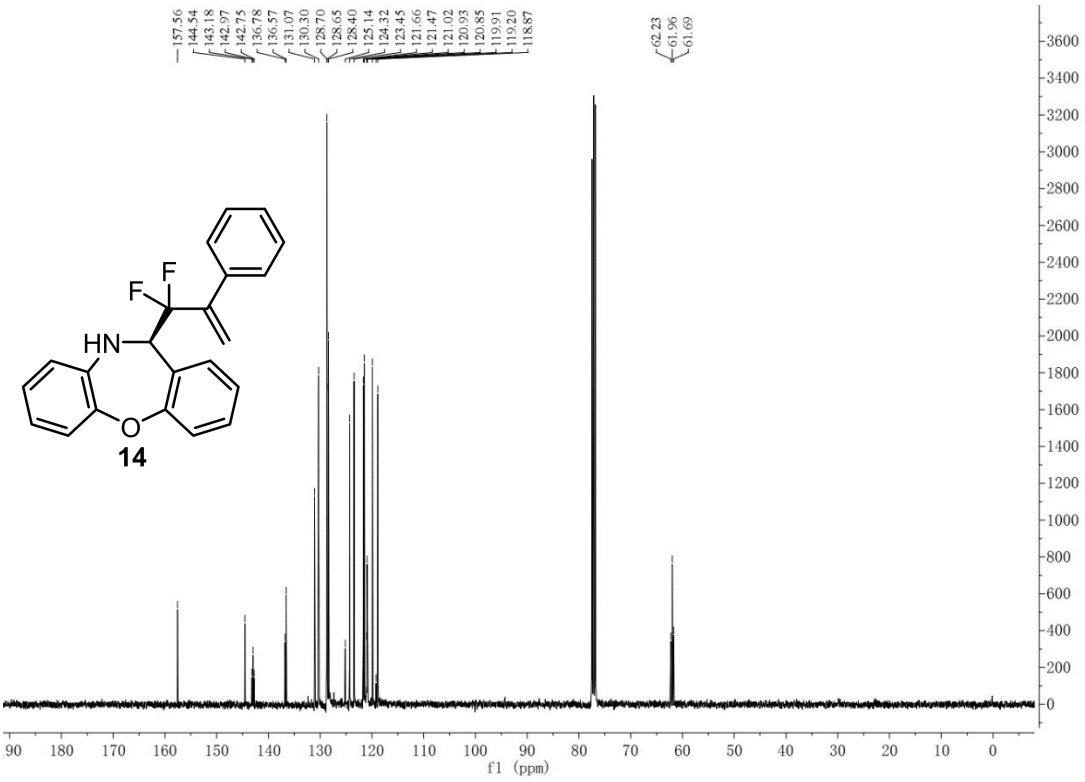

98.53
98.57
99.29
99.33
102.10
102.14
102.86
102.89
O
F
F
O
N
O
12
f1 (ppm)

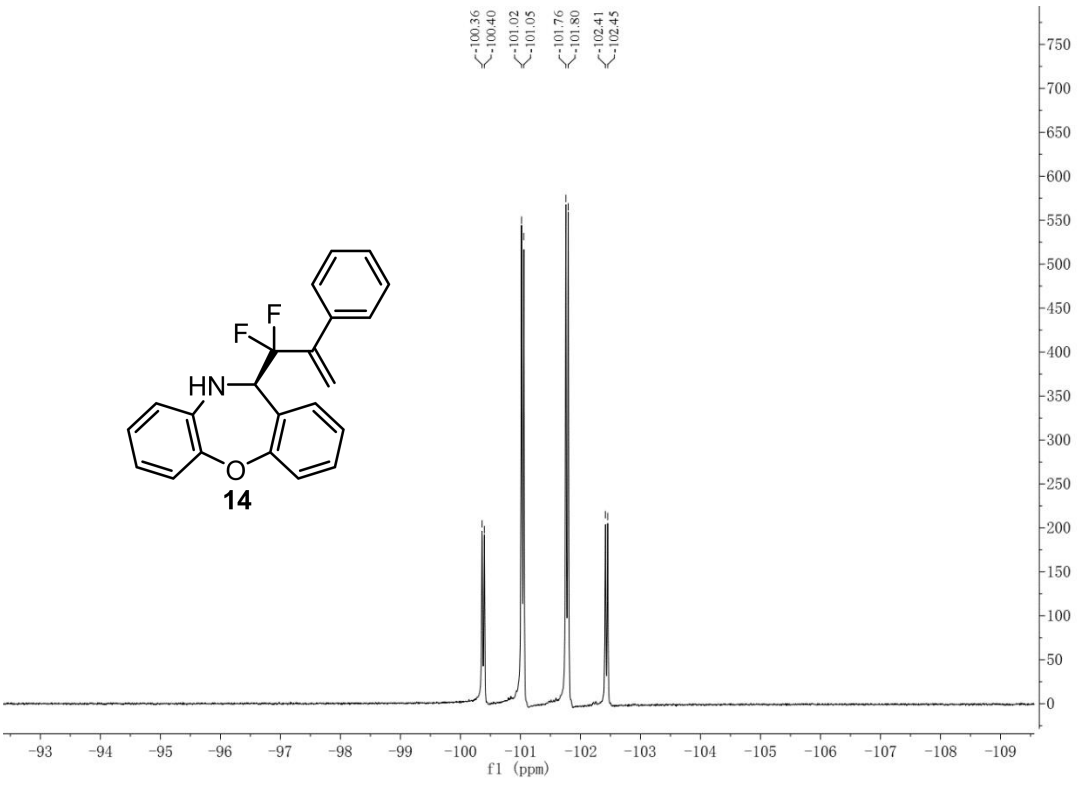

F
F
*
HN
OH
O
13
13.64
2.12
4.07
1.16
0.97
1.16
1.97
0.90
1.76
2.30
4.10
f1 (ppm)


F
F
*
HN
OH
O
13
f1 (ppm)

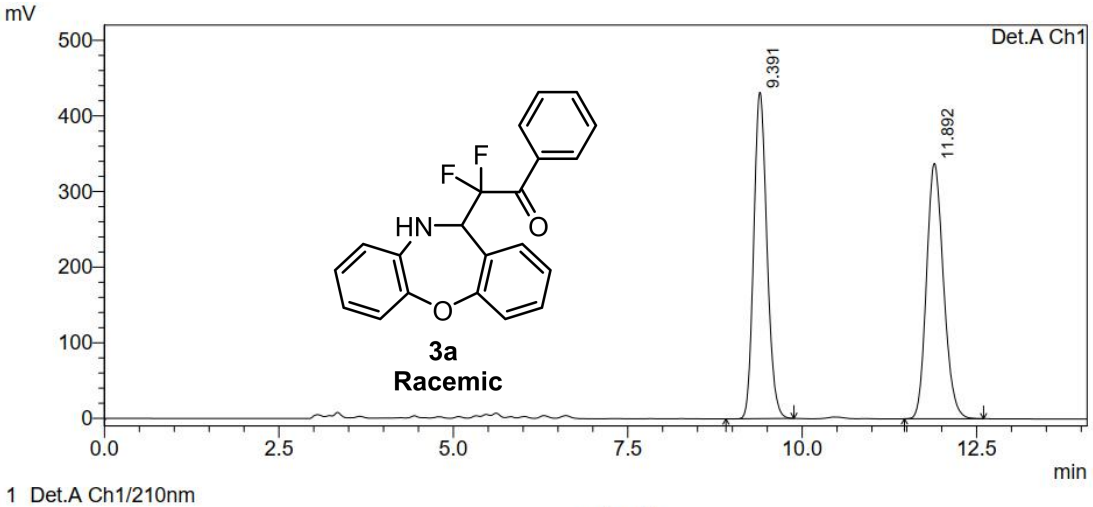

F
F
*
HN
OH
O
13
f1 (ppm)


F
F
HN
O
14
4.87
1.00
1.01
1.02
2.00
0.97
0.96
0.94
1.00
0.99
0.99
0.99
f1 (ppm)


157.56
144.54
143.18
142.97
142.75
136.78
136.57
131.07
130.30
128.70
128.65
128.40
125.14
124.32
123.45
121.66
121.47
121.02
120.93
120.85
119.91
119.20
118.87
62.23
61.96
61.69
F
F
HN
O
14
f1 (ppm)


100.36
100.40
101.02
101.05
101.76
101.80
102.41
102.45
F
F
HN
O
14
f1 (ppm)

HPLC Spectra

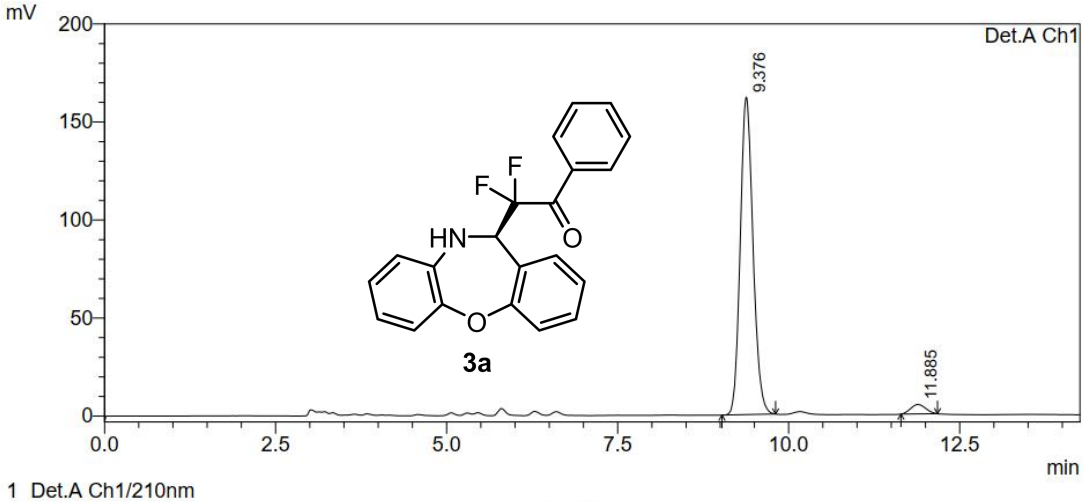


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.391	5675112	431311	49.736	56.098
2	11.892	5735335	337538	50.264	43.902
Total		11410448	768849	100.000	100.000

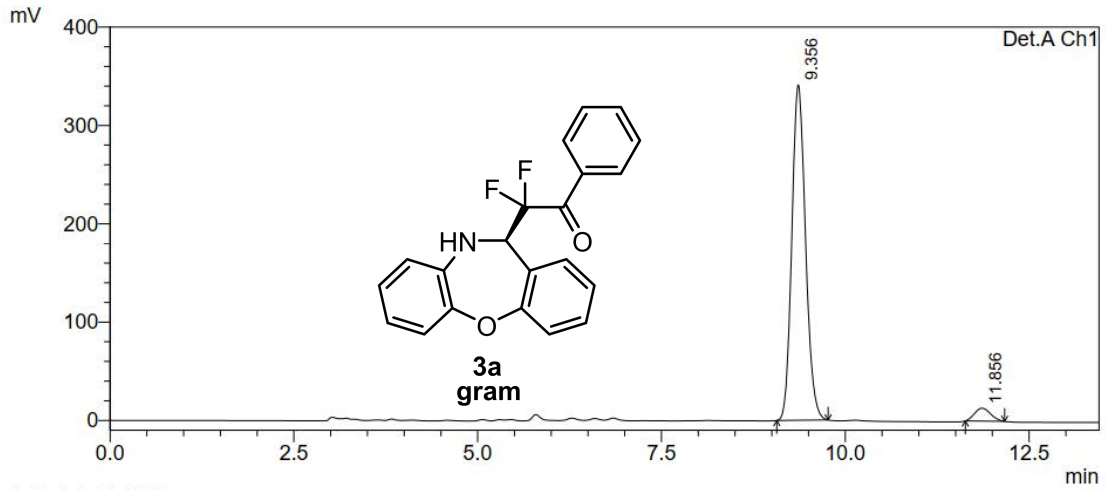


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.376	2103315	161233	96.618	97.087
2	11.885	73618	4838	3.382	2.913
Total		2176933	166071	100.000	100.000

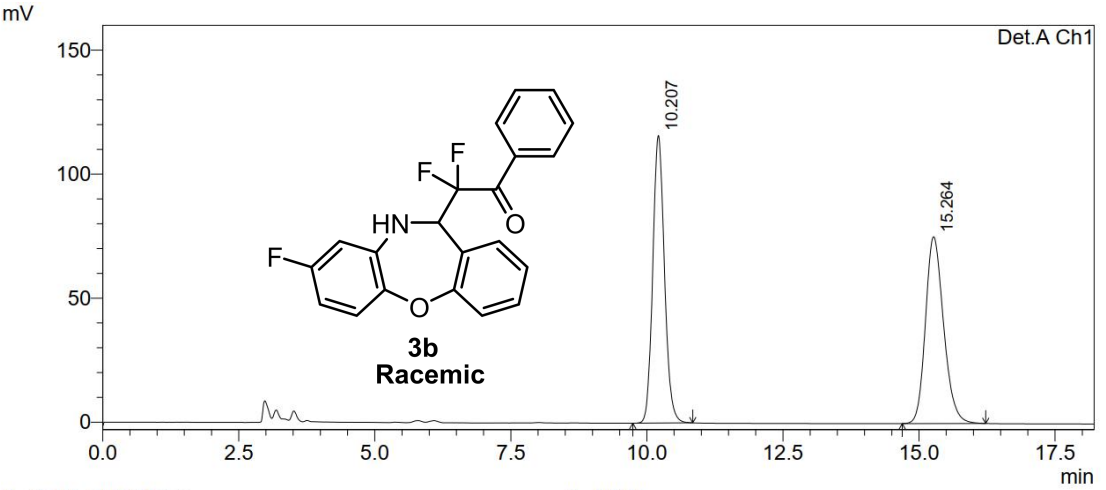


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.356	4437570	340713	95.694	96.278
2	11.856	199688	13172	4.306	3.722
Total		4637258	353884	100.000	100.000

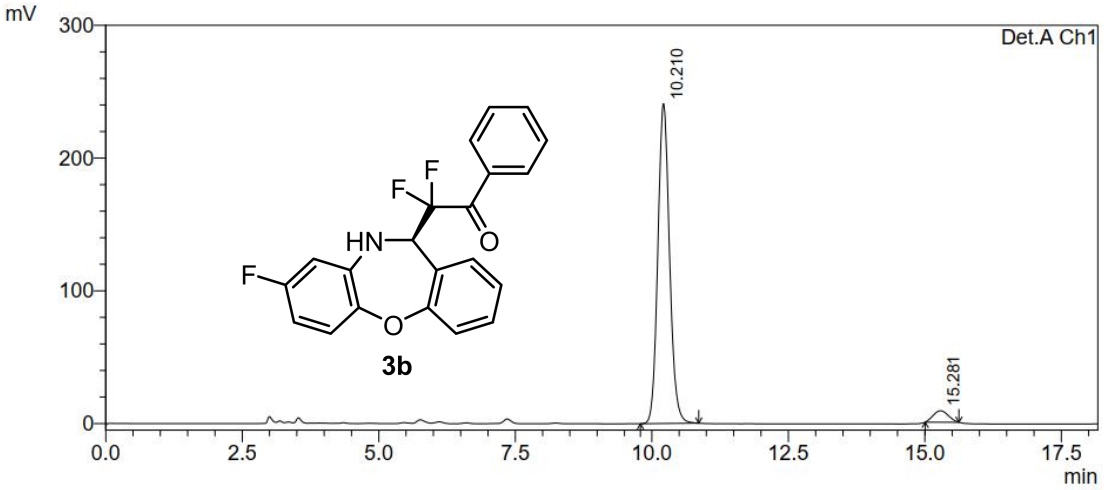


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.207	1736987	115608	49.849	60.556
2	15.264	1747483	75302	50.151	39.444
Total		3484470	190910	100.000	100.000

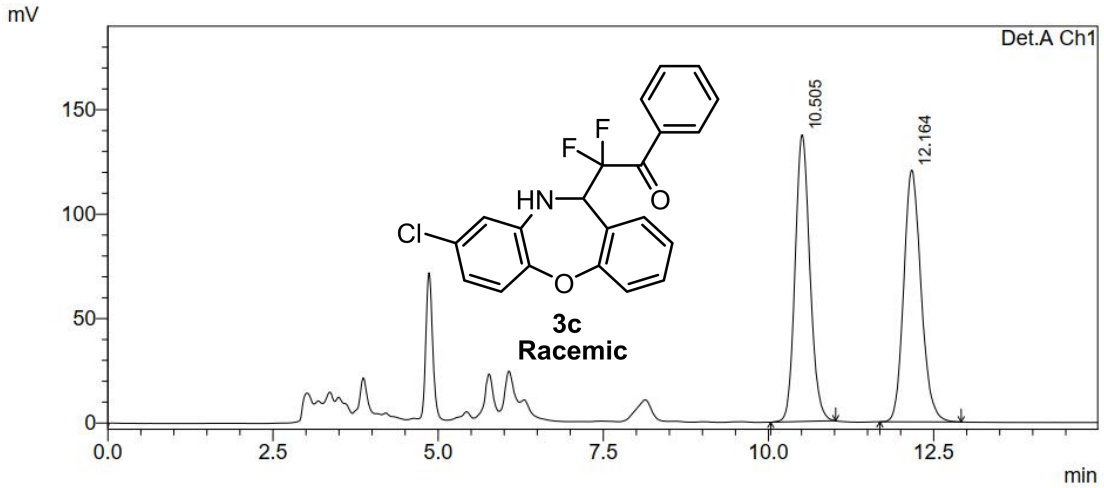


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.210	3592353	240193	95.599	96.524
2	15.281	165368	8649	4.401	3.476
Total		3757721	248842	100.000	100.000

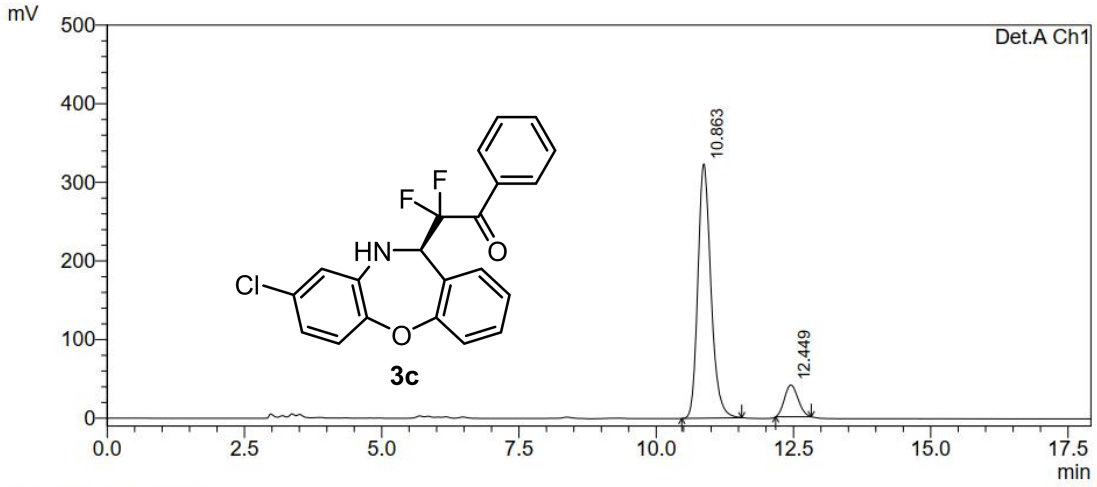


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.505	2139433	137070	49.233	53.281
2	12.164	2206112	120189	50.767	46.719
Total		4345545	257259	100.000	100.000

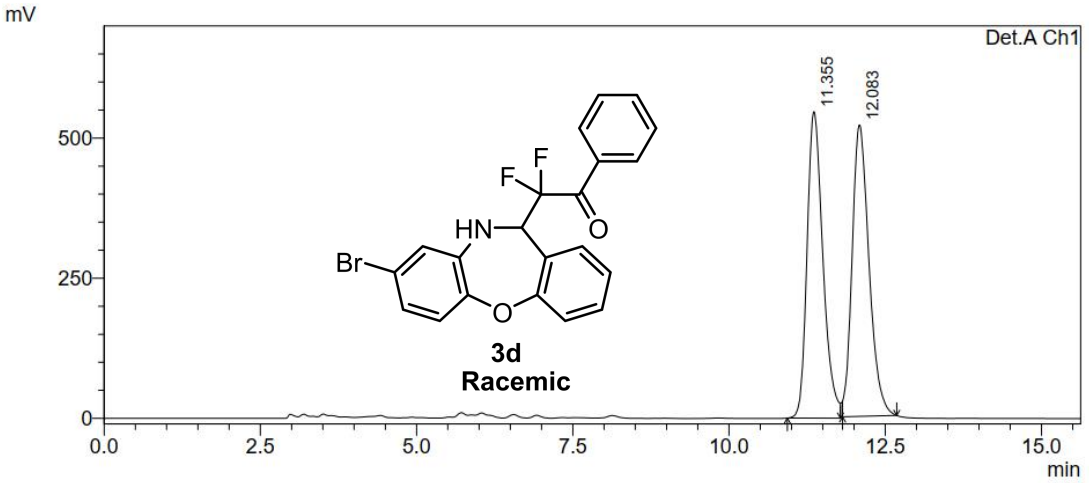


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.863	5356172	323141	88.525	88.909
2	12.449	694310	40310	11.475	11.091
Total		6050482	363450	100.000	100.000

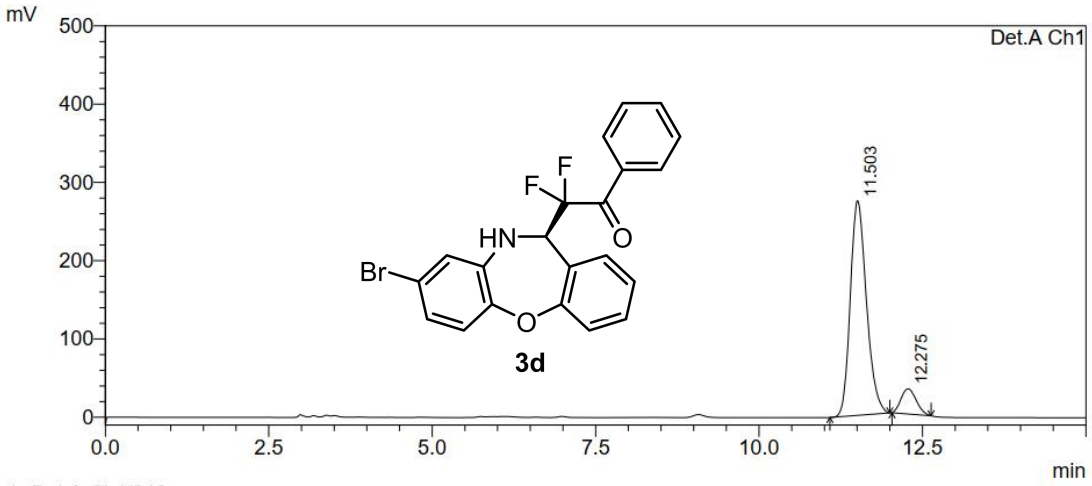


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	11.355	9646938	546119	49.714	51.293
2	12.083	9758099	518587	50.286	48.707
Total		19405037	1064705	100.000	100.000

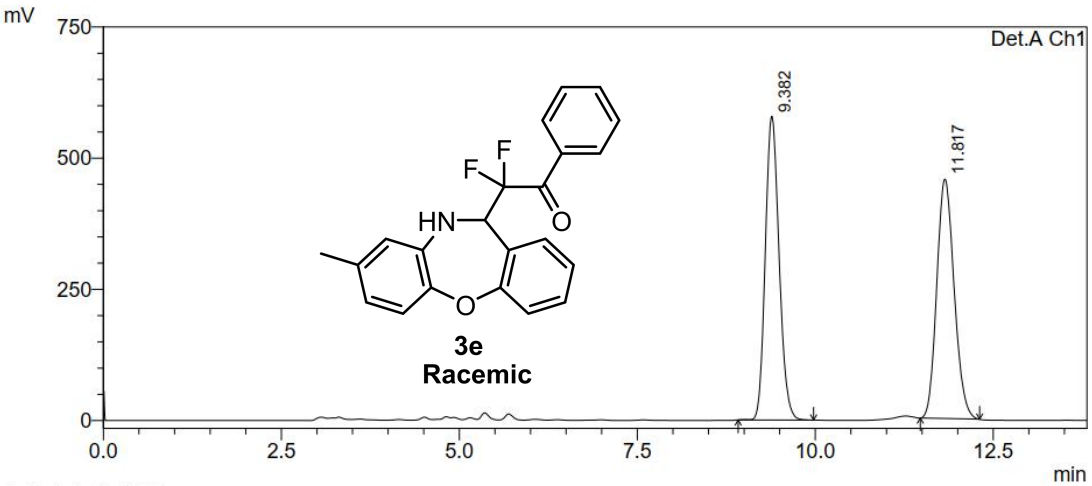


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	11.503	4716523	273828	90.054	89.488
2	12.275	520941	32165	9.946	10.512
Total		5237464	305993	100.000	100.000

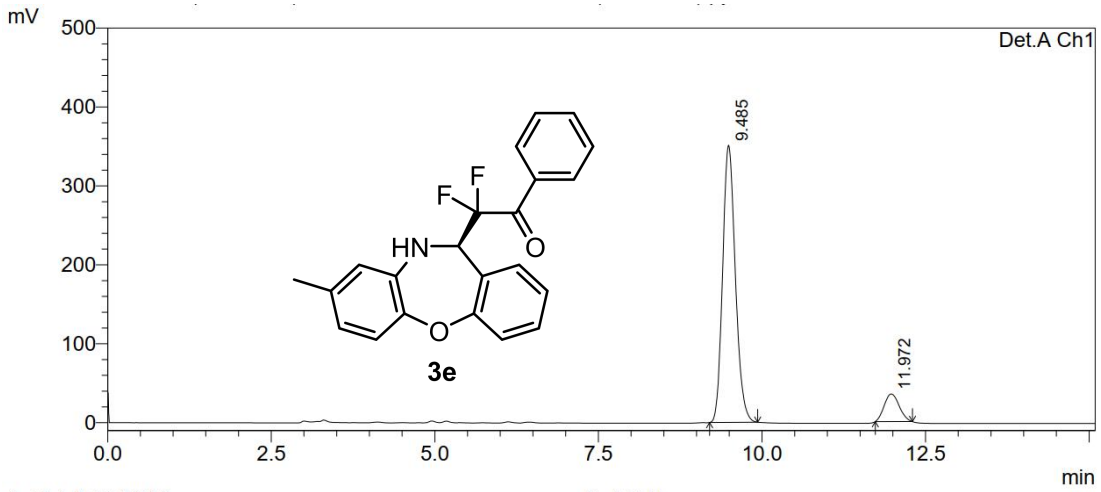


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.382	7795853	578545	50.156	56.052
2	11.817	7747245	453610	49.844	43.948
Total		15543099	1032155	100.000	100.000

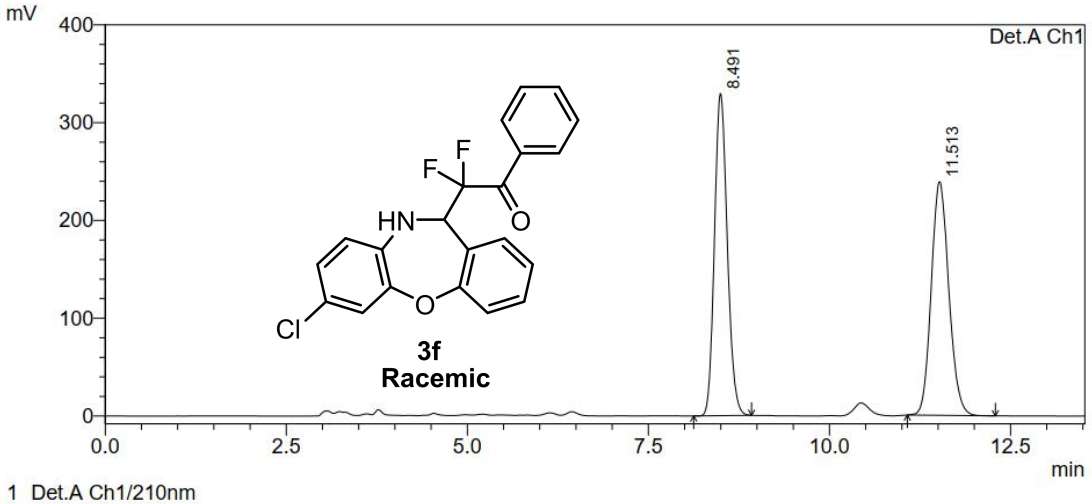


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.485	4756489	350077	89.531	90.875
2	11.972	556202	35151	10.469	9.125
Total		5312691	385228	100.000	100.000

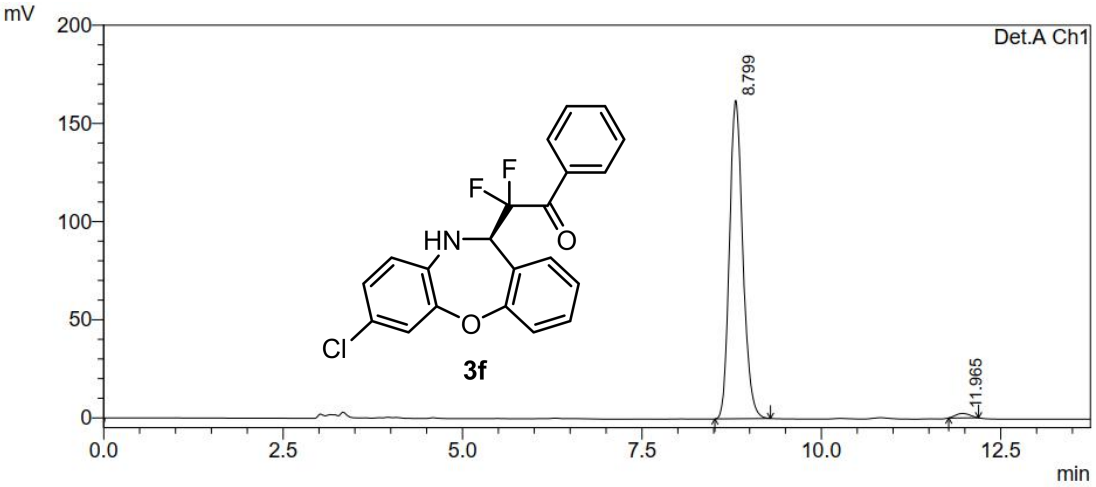


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	8.491	4053982	327622	50.127	57.977
2	11.513	4033361	237471	49.873	42.023
Total		8087343	565093	100.000	100.000

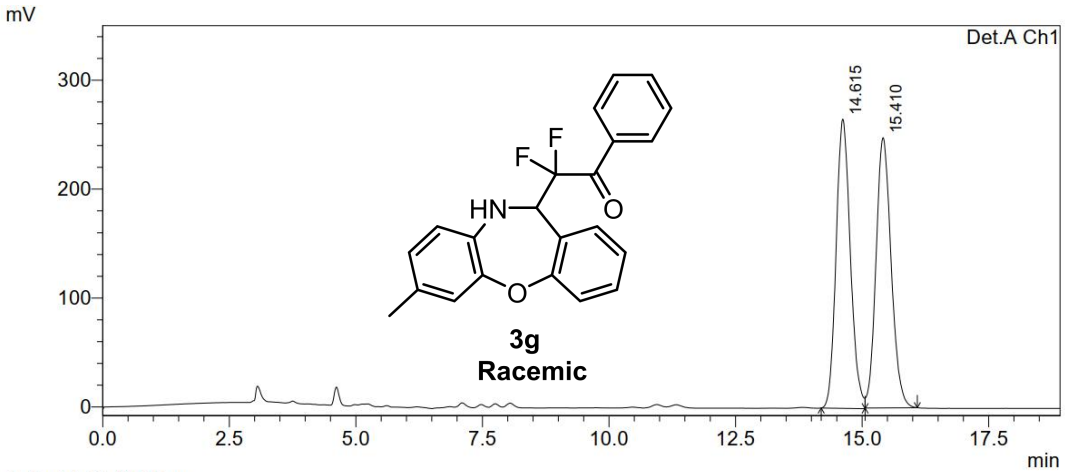


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	8.799	2104335	162074	98.502	98.585
2	11.965	31999	2327	1.498	1.415
Total		2136334	164401	100.000	100.000

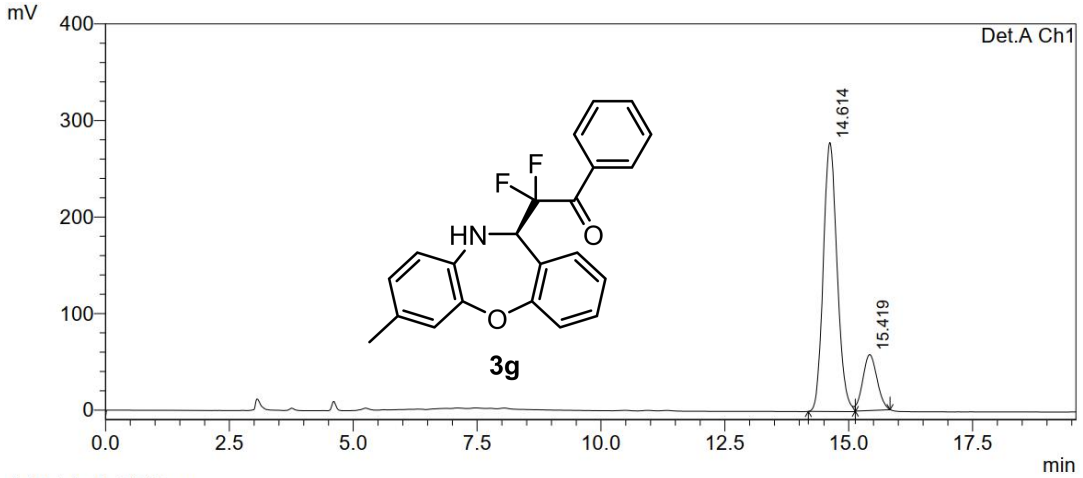


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	14.615	5197016	265355	50.135	51.721
2	15.410	5168990	247693	49.865	48.279
Total		10366005	513047	100.000	100.000

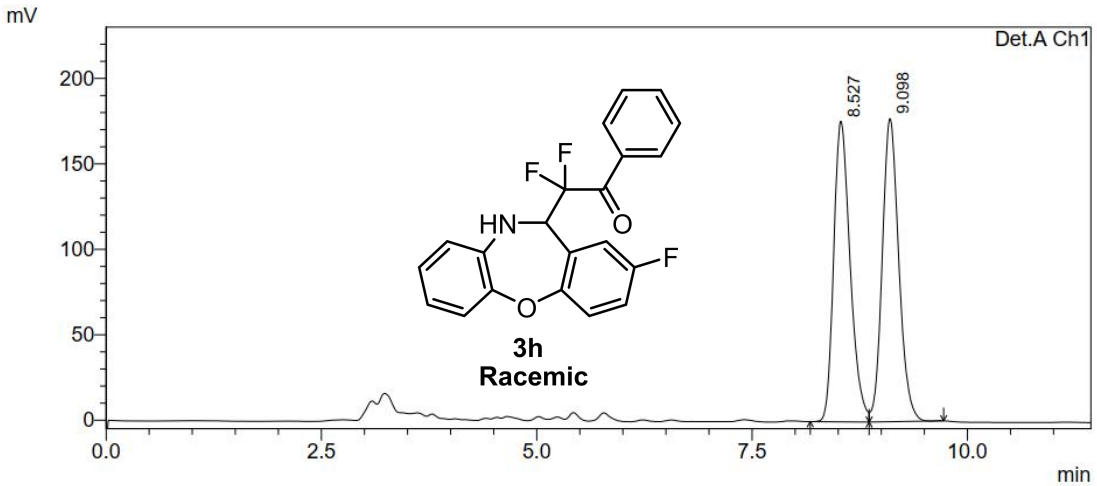


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	14.614	5450771	278240	82.540	82.774
2	15.419	1153046	57904	17.460	17.226
Total		6603817	336144	100.000	100.000

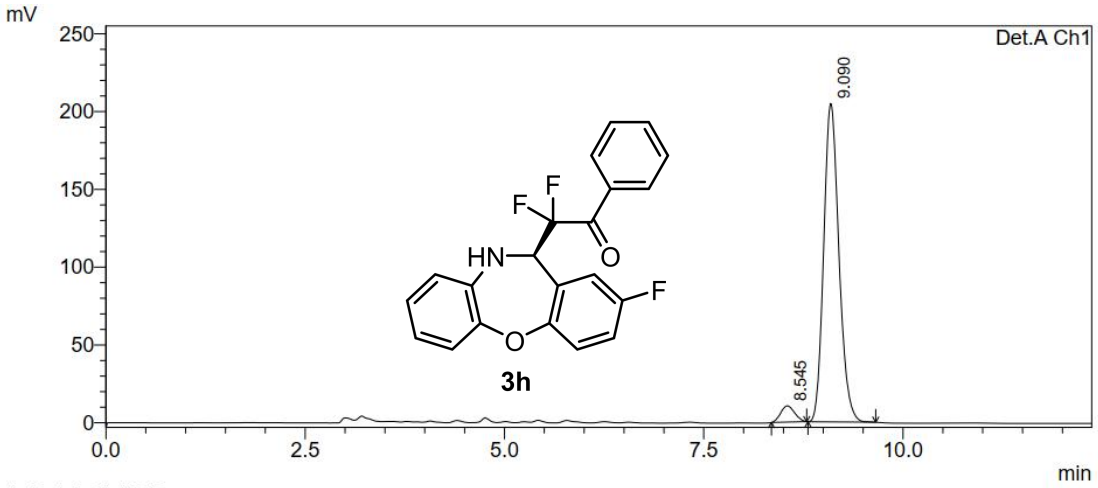


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	8.527	2340388	175201	49.680	49.731
2	9.098	2370548	177095	50.320	50.269
Total		4710936	352296	100.000	100.000

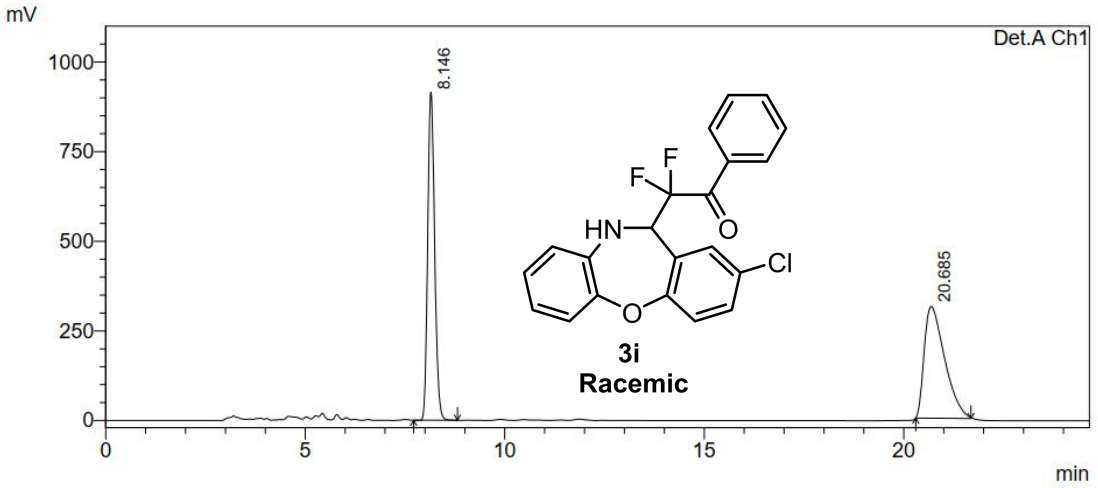


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	8.545	126680	10470	4.452	4.883
2	9.090	2718938	203948	95.548	95.117
Total		2845618	214418	100.000	100.000

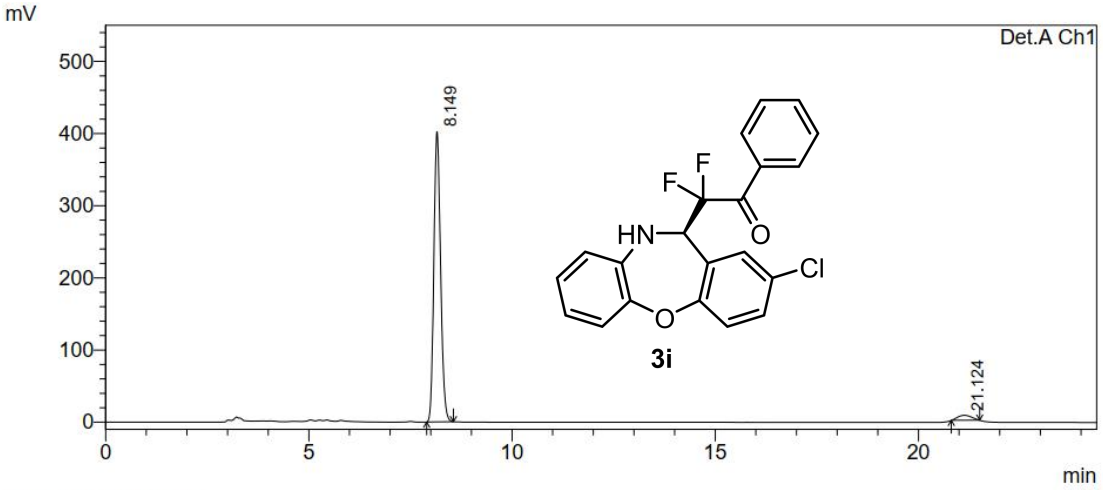


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	8.146	10995059	912713	49.719	74.556
2	20.685	11119370	311486	50.281	25.444
Total		22114428	1224199	100.000	100.000

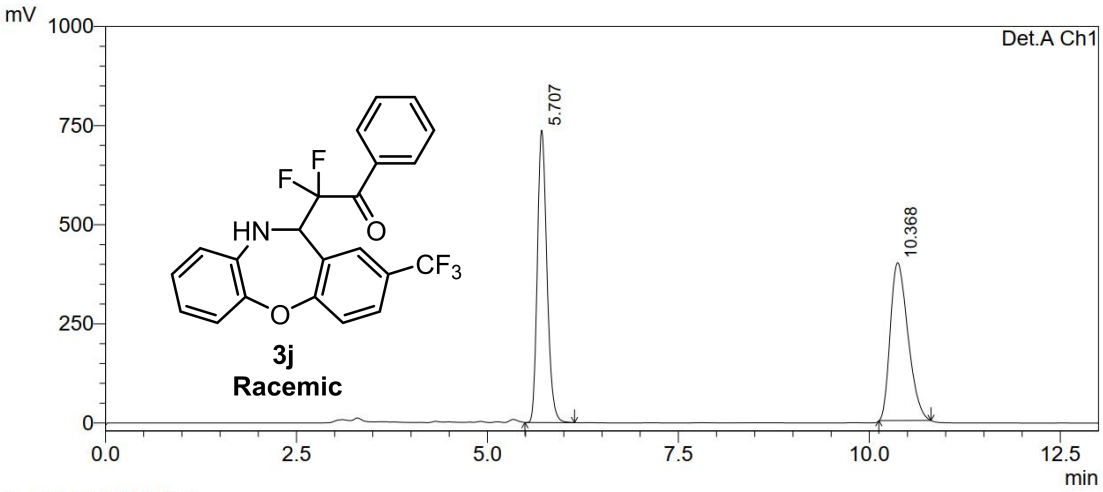


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	8.149	4634566	402105	96.574	98.310
2	21.124	164406	6913	3.426	1.690
Total		4798972	409019	100.000	100.000

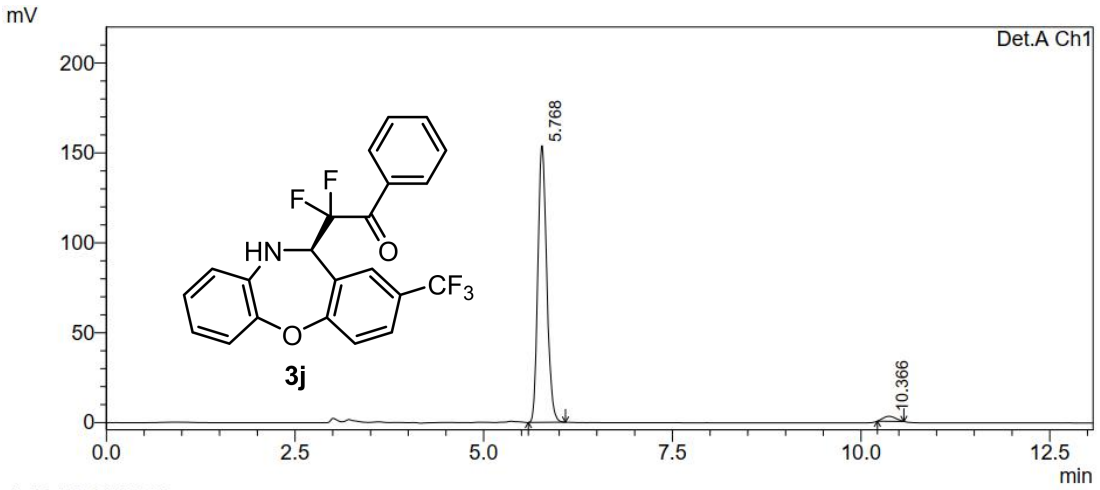


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.707	6427338	731019	49.998	64.765
2	10.368	6427725	397700	50.002	35.235
Total		12855064	1128719	100.000	100.000

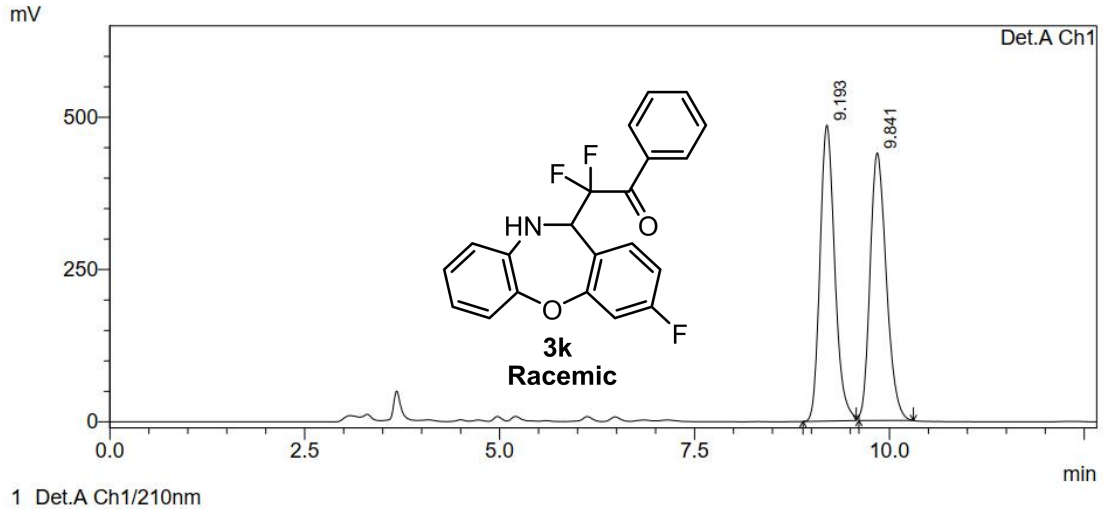


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.768	1249980	153909	97.518	98.248
2	10.366	31820	2744	2.482	1.752
Total		1281800	156653	100.000	100.000

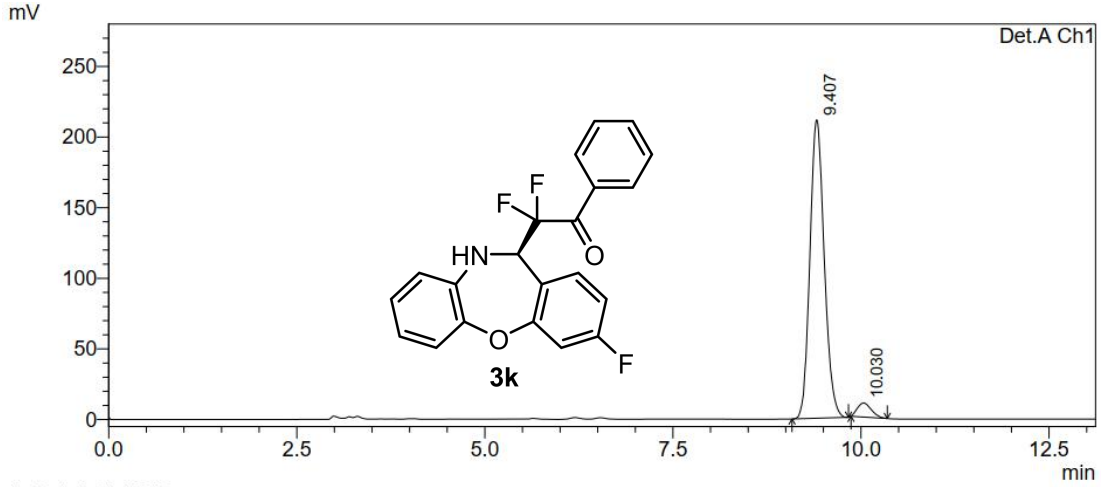


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.193	6398397	483927	50.098	52.874
2	9.841	6373418	431312	49.902	47.126
Total		12771814	915239	100.000	100.000

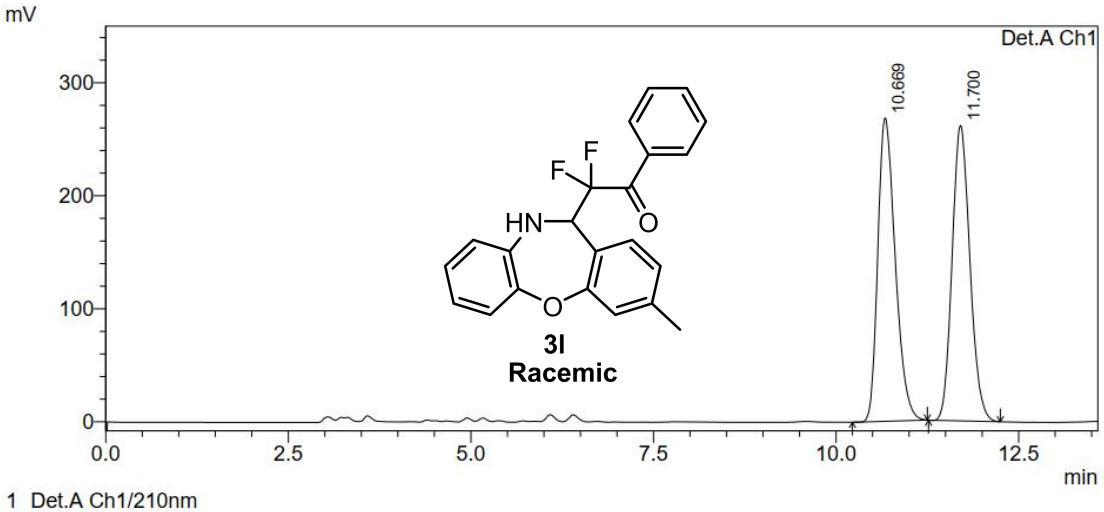


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.407	2798397	211129	95.634	95.520
2	10.030	127759	9901	4.366	4.480
Total		2926156	221030	100.000	100.000

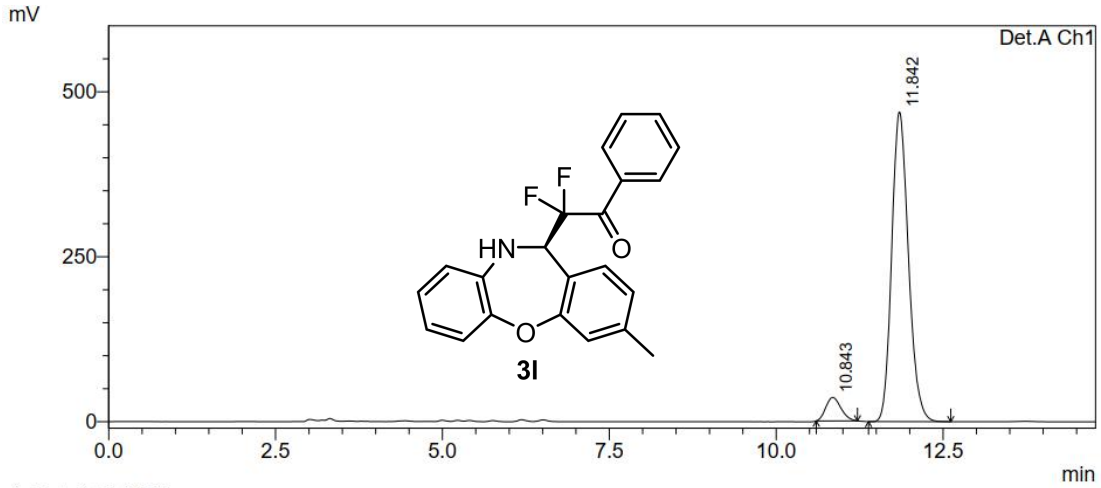


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.669	4463090	267837	50.144	50.689
2	11.700	4437398	260553	49.856	49.311
Total		8900488	528390	100.000	100.000

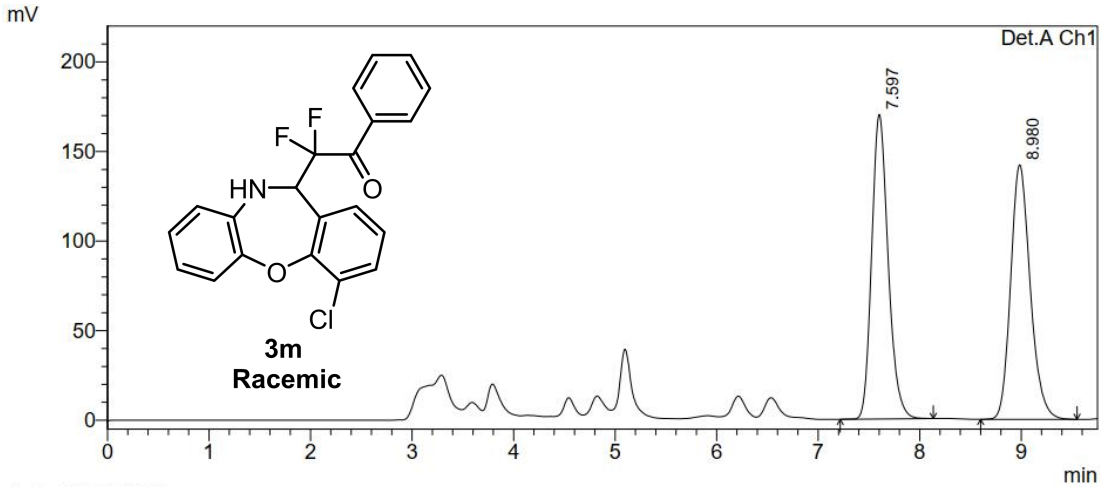


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.843	562228	35607	6.417	7.048
2	11.842	8199472	469582	93.583	92.952
Total		8761700	505189	100.000	100.000

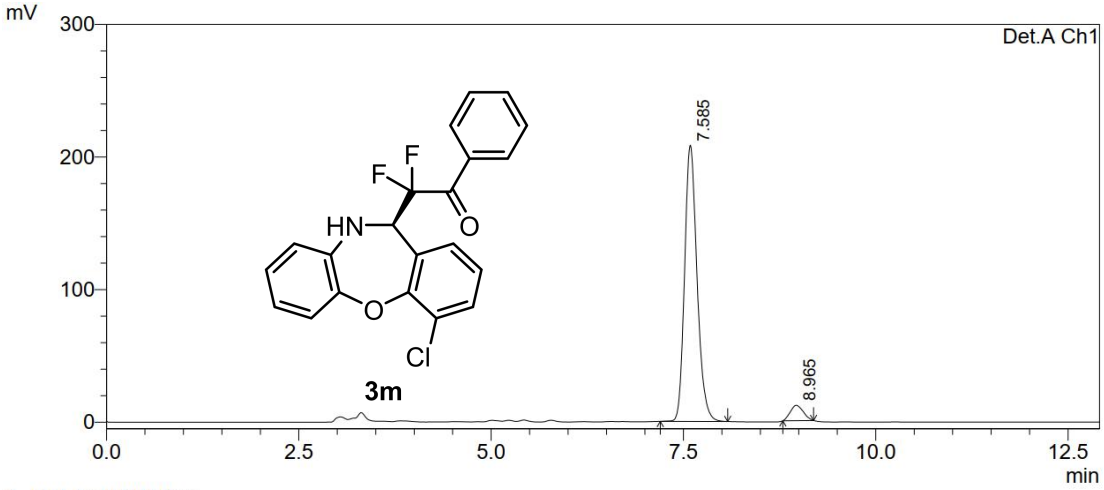


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.597	1914539	169286	50.058	54.426
2	8.980	1910106	141751	49.942	45.574
Total		3824645	311037	100.000	100.000

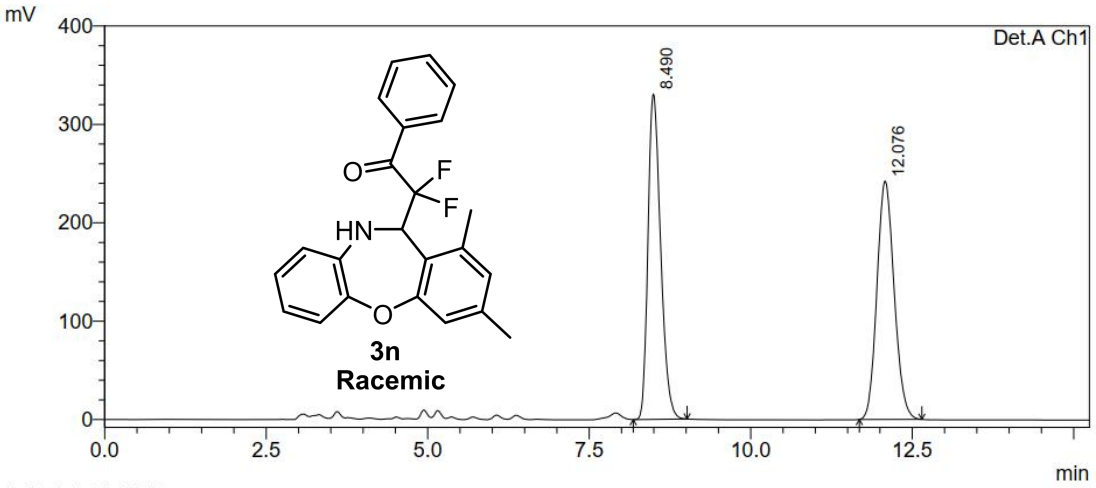


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.585	2340340	208091	94.542	94.752
2	8.965	135114	11525	5.458	5.248
Total		2475454	219617	100.000	100.000

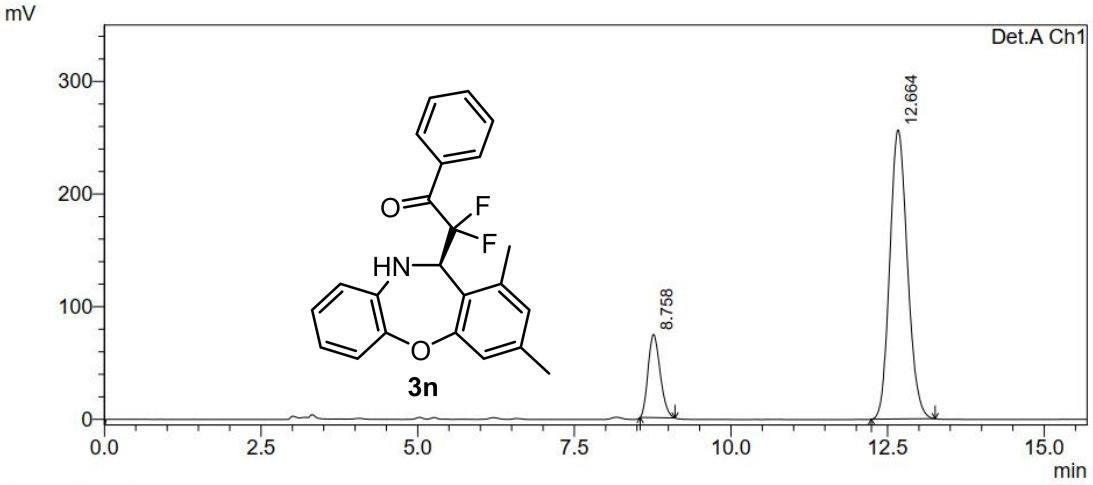


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	8.490	4494885	330358	50.000	57.706
2	12.076	4494957	242126	50.000	42.294
Total		8989842	572484	100.000	100.000

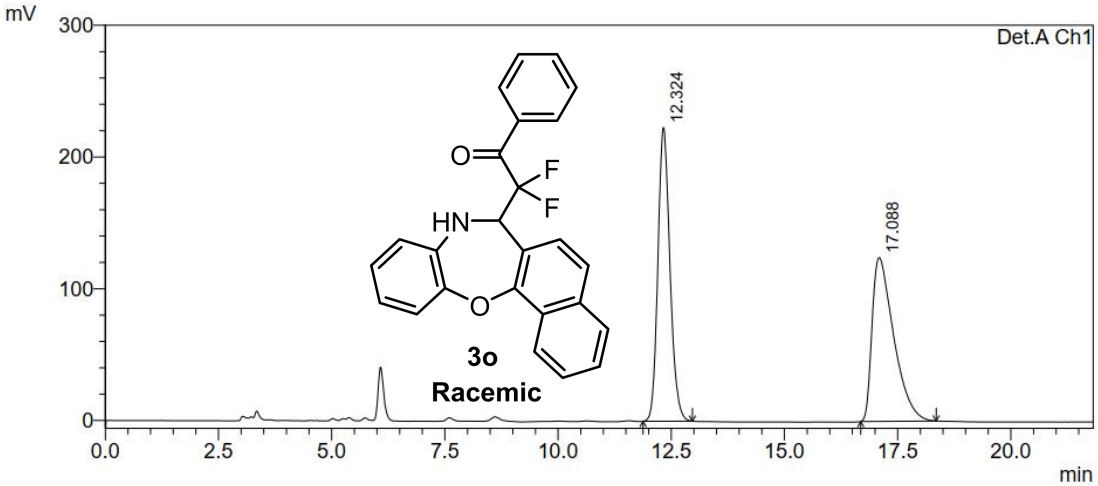


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	8.758	990351	73736	16.470	22.328
2	12.664	5022778	256510	83.530	77.672
Total		6013129	330246	100.000	100.000

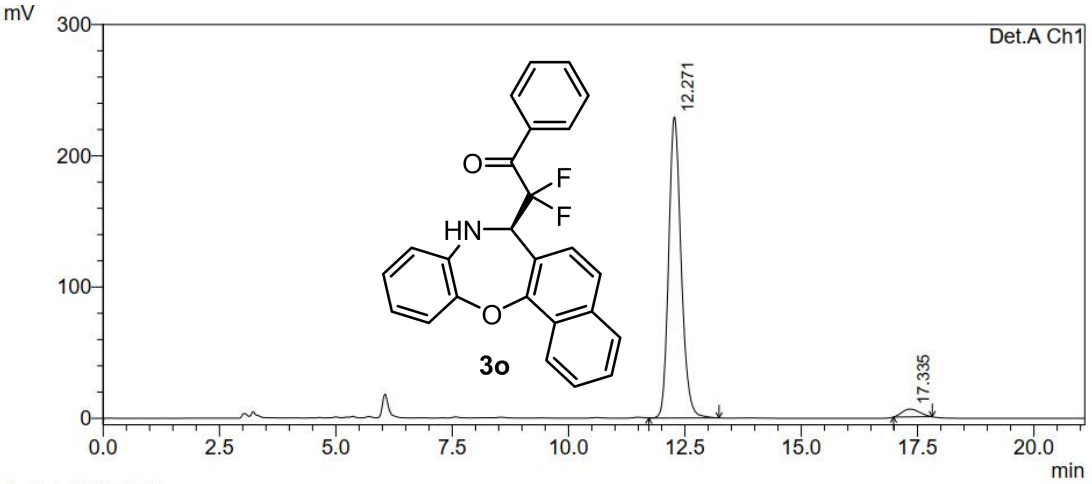


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	12.324	4126400	222921	49.987	64.191
2	17.088	4128534	124355	50.013	35.809
Total		8254934	347276	100.000	100.000

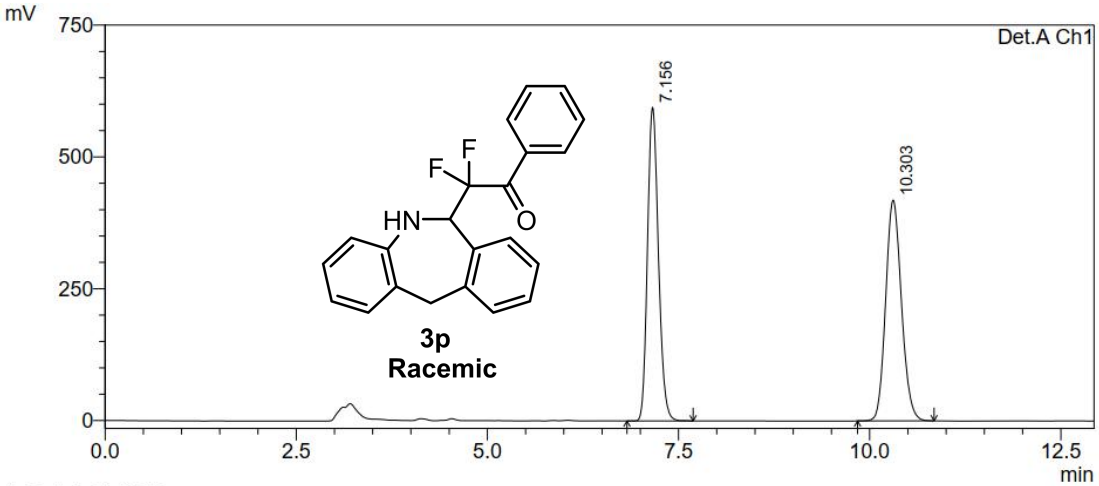


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	12.271	4276822	229235	96.531	97.478
2	17.335	153699	5930	3.469	2.522
Total		4430521	235165	100.000	100.000

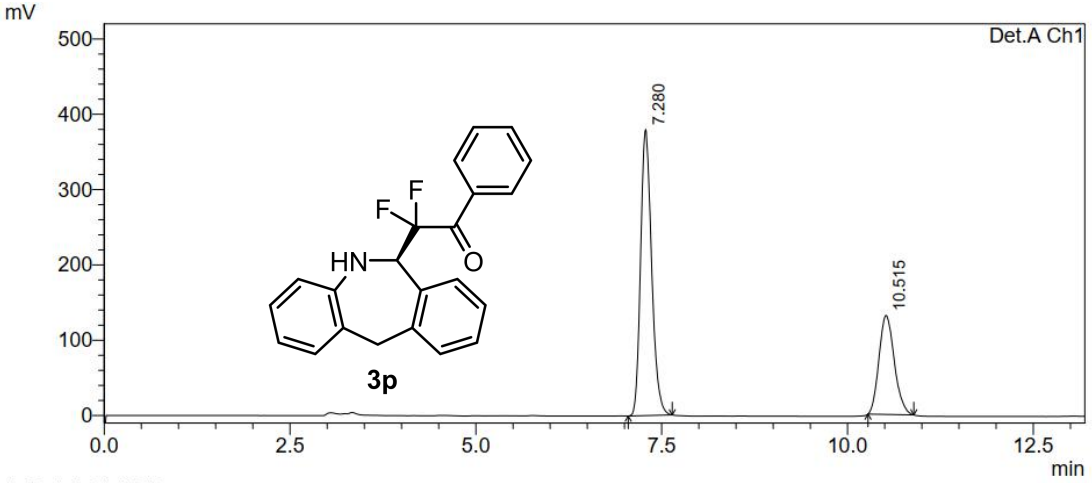


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.156	5906002	591256	49.561	58.554
2	10.303	6010735	418510	50.439	41.446
Total		11916737	1009766	100.000	100.000

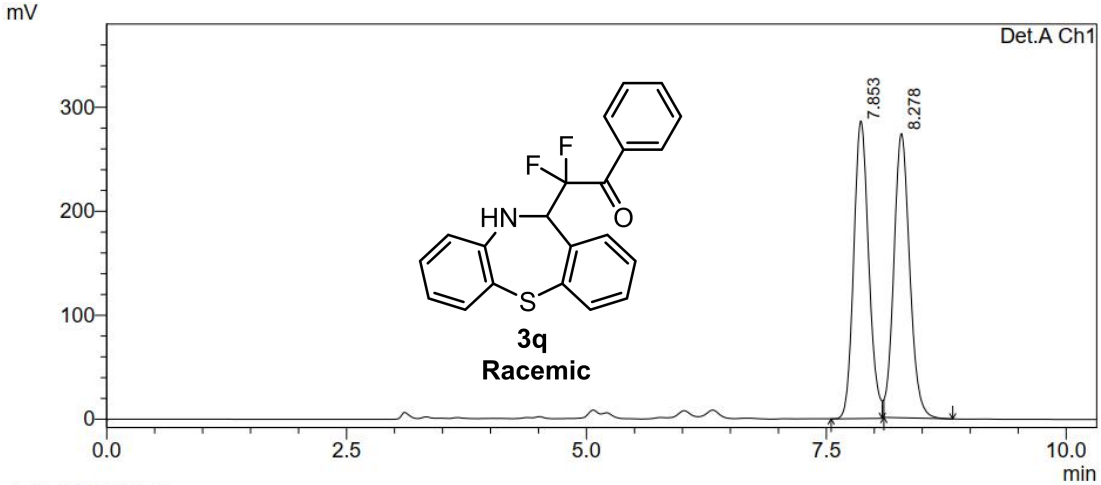


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.280	3916697	379936	67.507	74.315
2	10.515	1885247	131318	32.493	25.685
Total		5801943	511254	100.000	100.000

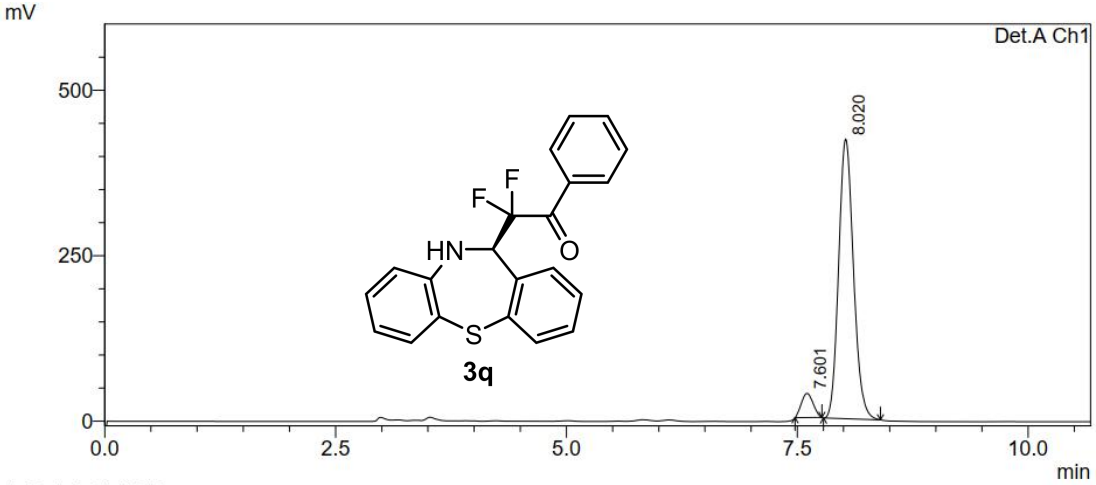


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.853	3111646	285678	49.764	51.150
2	8.278	3141190	272838	50.236	48.850
Total		6252836	558516	100.000	100.000

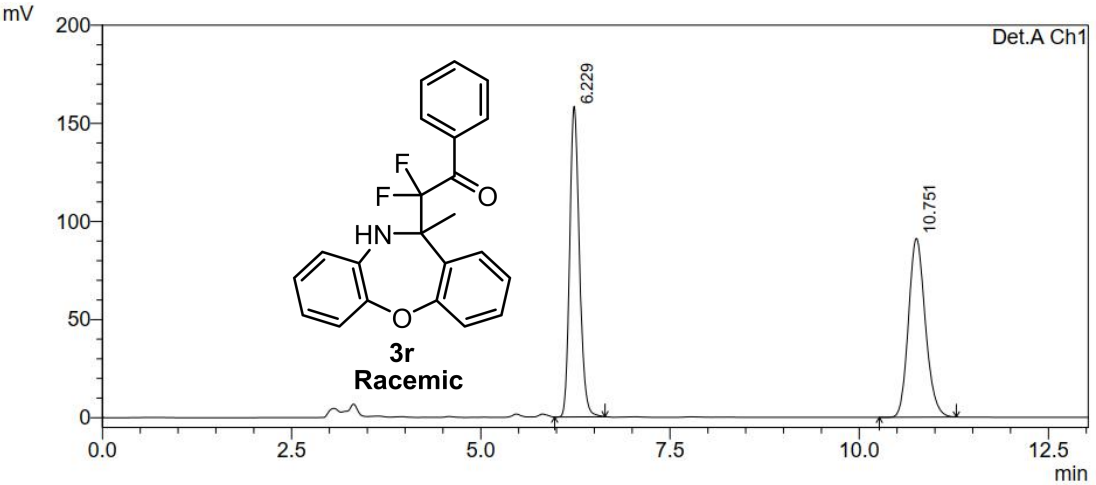


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.601	323408	36537	6.423	7.989
2	8.020	4711700	420799	93.577	92.011
Total		5035109	457336	100.000	100.000

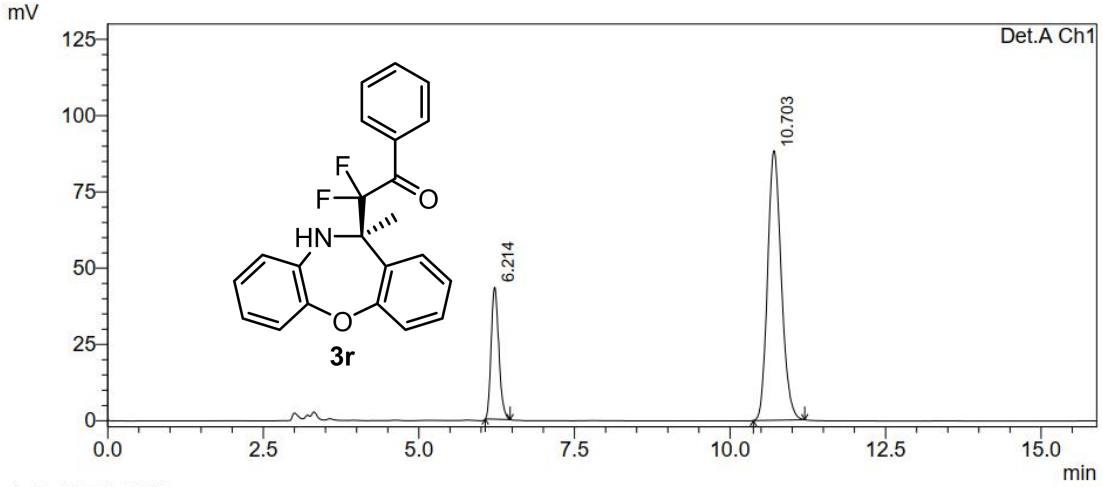


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.229	1413010	158396	50.090	63.552
2	10.751	1407950	90841	49.910	36.448
Total		2820961	249237	100.000	100.000

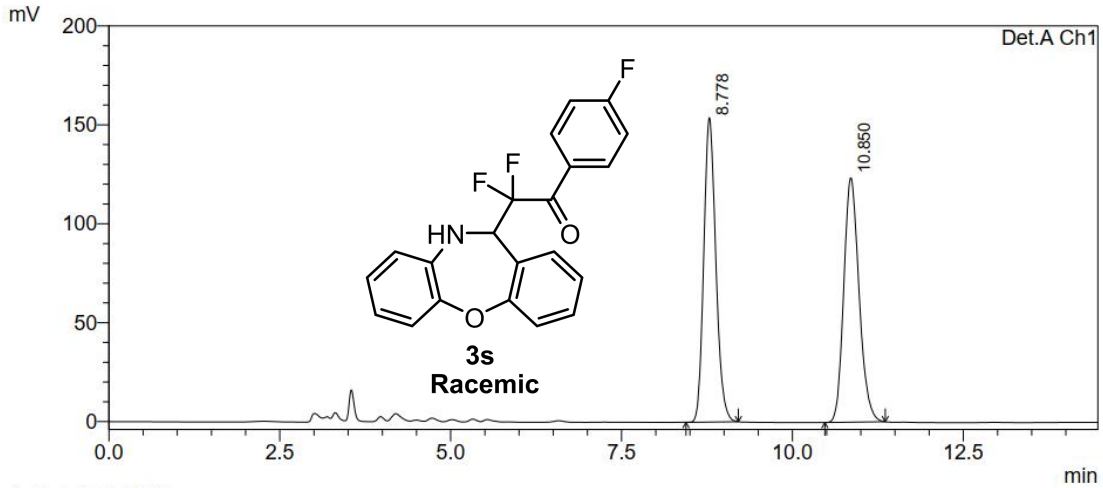


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.214	369390	43280	21.489	32.928
2	10.703	1349580	88156	78.511	67.072
Total		1718970	131435	100.000	100.000

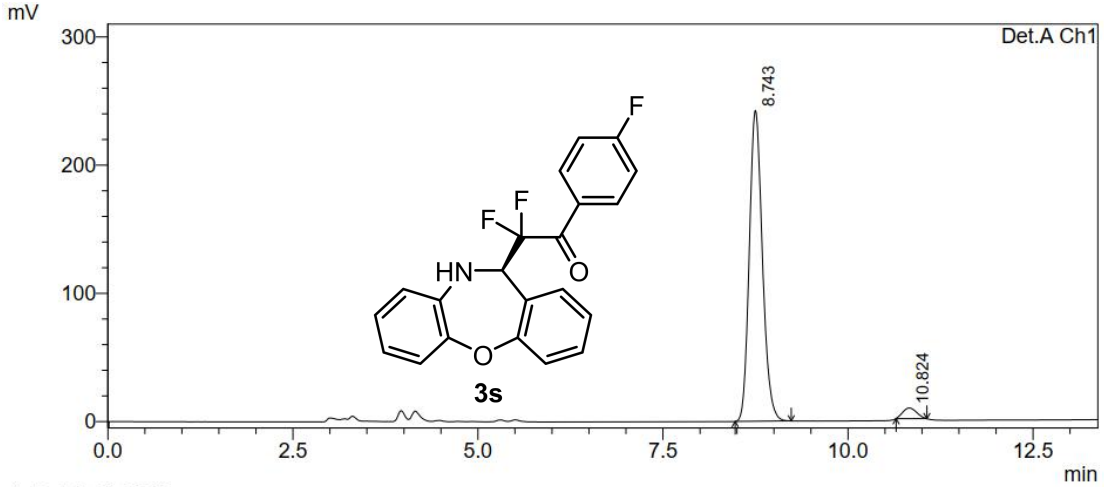


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	8.778	1886873	153628	49.510	55.437
2	10.850	1924245	123493	50.490	44.563
Total		3811118	277121	100.000	100.000

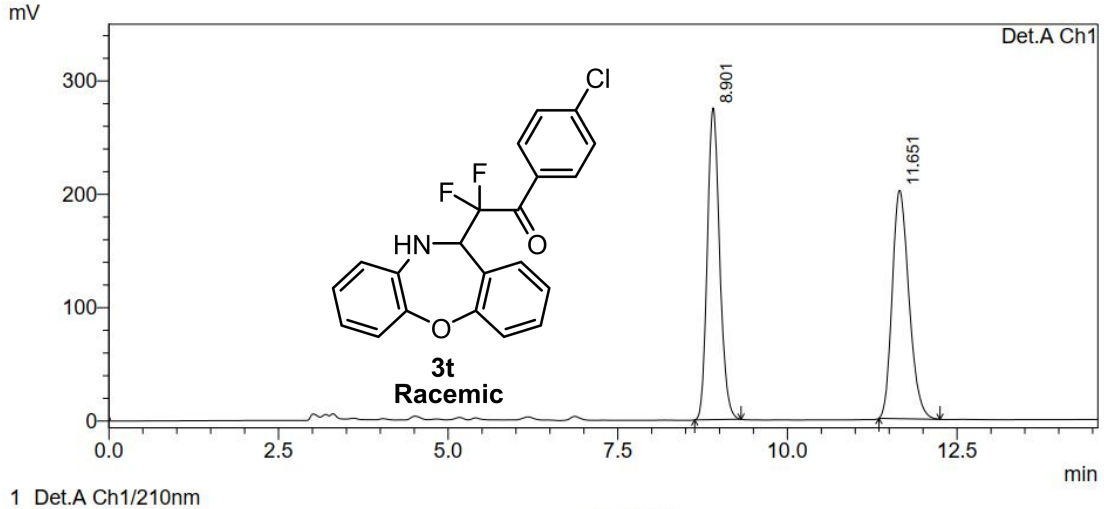


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	8.743	2982909	242058	96.520	96.674
2	10.824	107543	8329	3.480	3.326
Total		3090452	250387	100.000	100.000

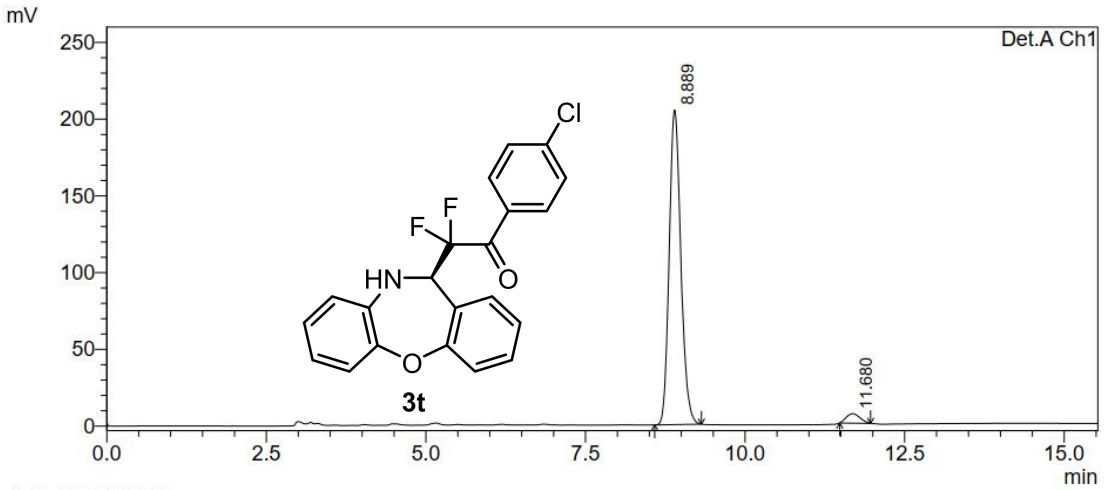


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	8.901	3465855	273670	49.989	57.654
2	11.651	3467445	201007	50.011	42.346
Total		6933300	474676	100.000	100.000

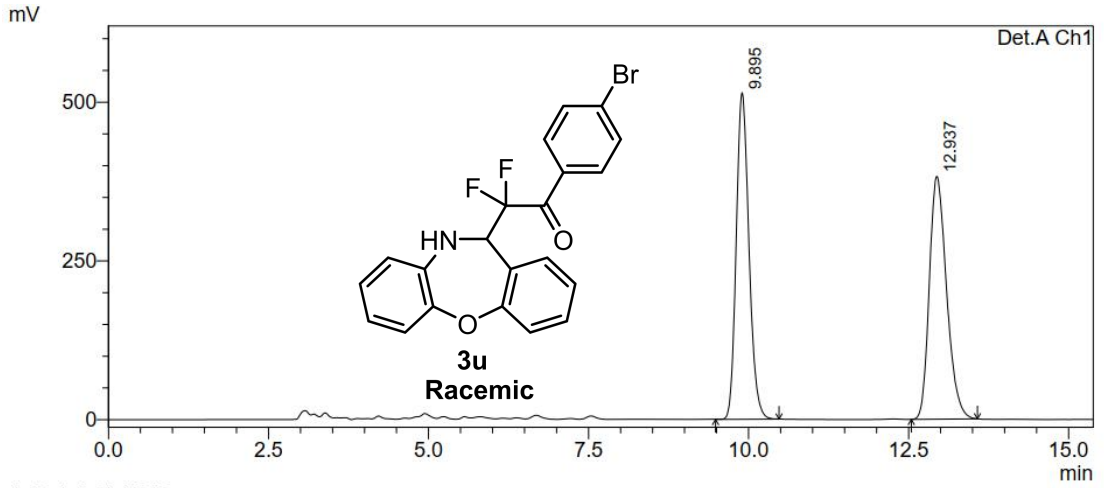


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	8.889	2596424	205014	96.524	97.040
2	11.680	93504	6253	3.476	2.960
Total		2689929	211268	100.000	100.000

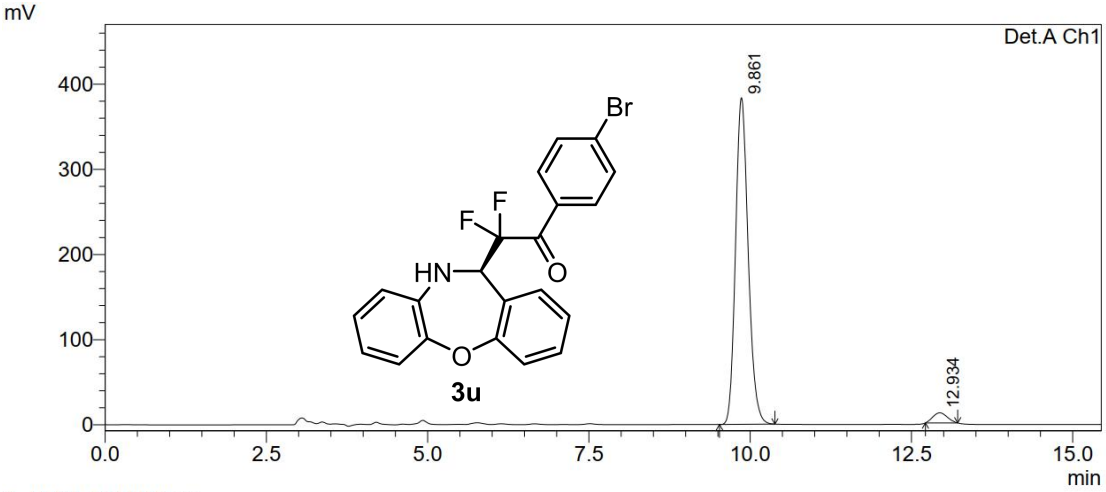


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.895	7114997	513106	49.765	57.317
2	12.937	7182143	382097	50.235	42.683
Total		14297140	895203	100.000	100.000

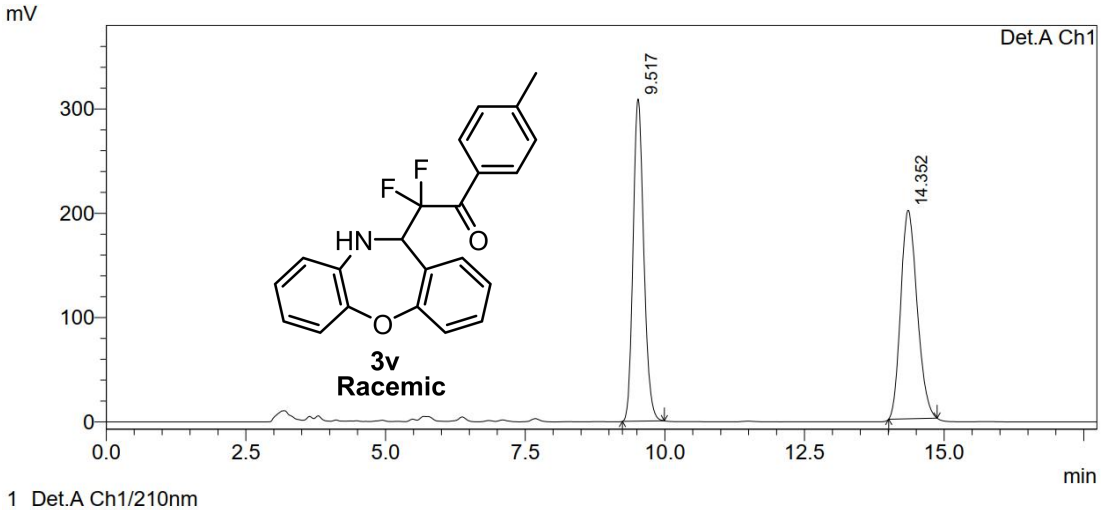


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.861	5237912	383214	96.595	96.985
2	12.934	184635	11913	3.405	3.015
Total		5422548	395127	100.000	100.000

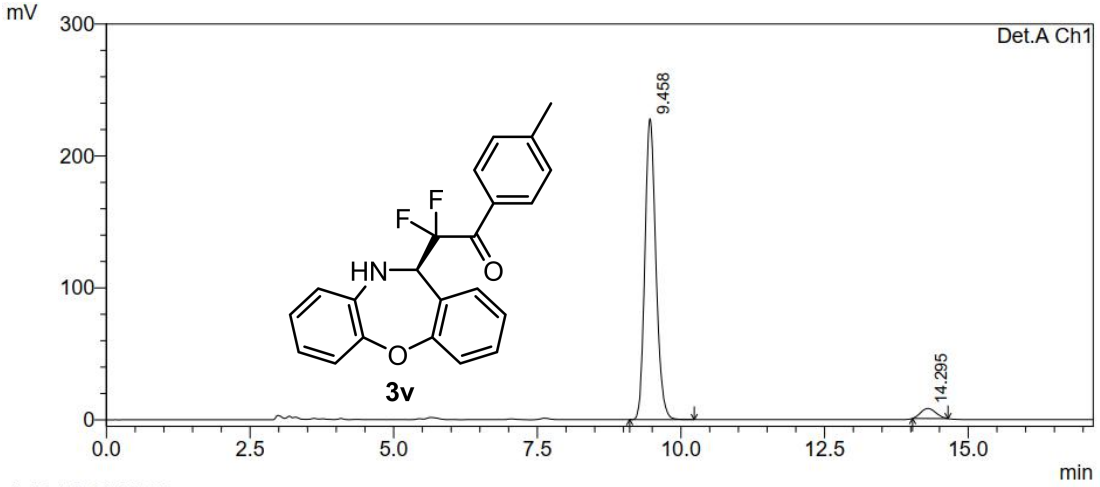


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.517	4113363	308926	50.129	60.719
2	14.352	4092211	199856	49.871	39.281
Total		8205574	508782	100.000	100.000

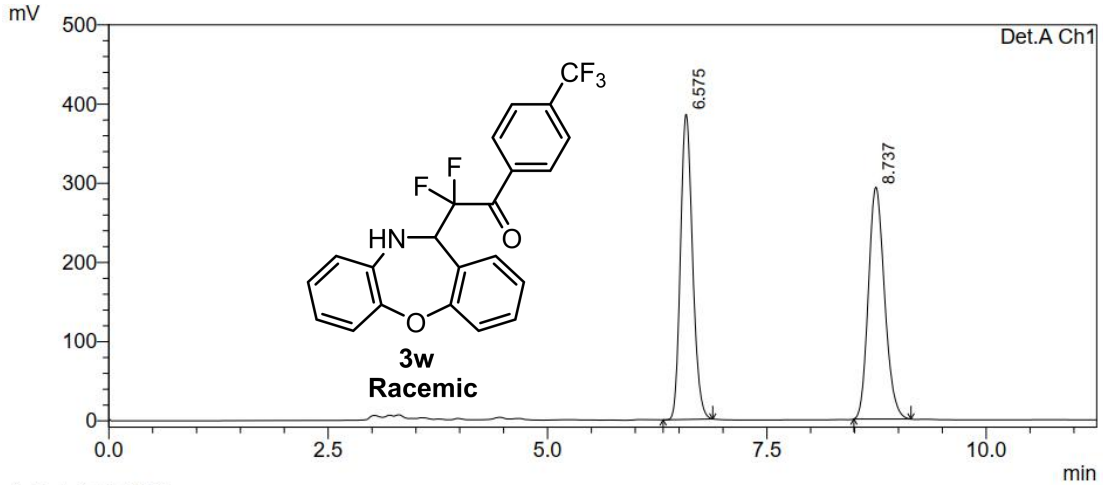


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.458	3029060	228052	95.593	96.752
2	14.295	139655	7655	4.407	3.248
Total		3168715	235707	100.000	100.000

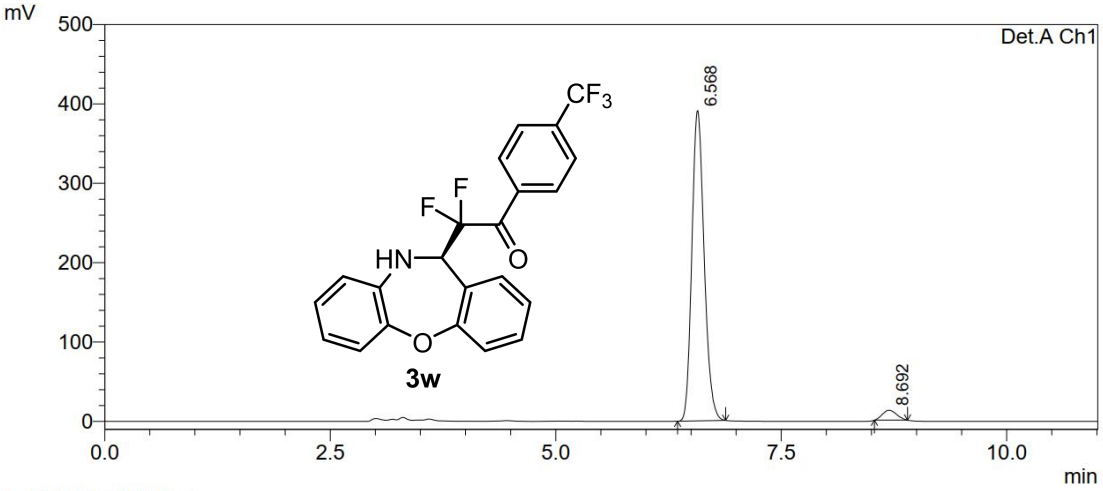


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.575	3688952	385084	49.579	56.875
2	8.737	3751640	291985	50.421	43.125
Total		7440592	677069	100.000	100.000

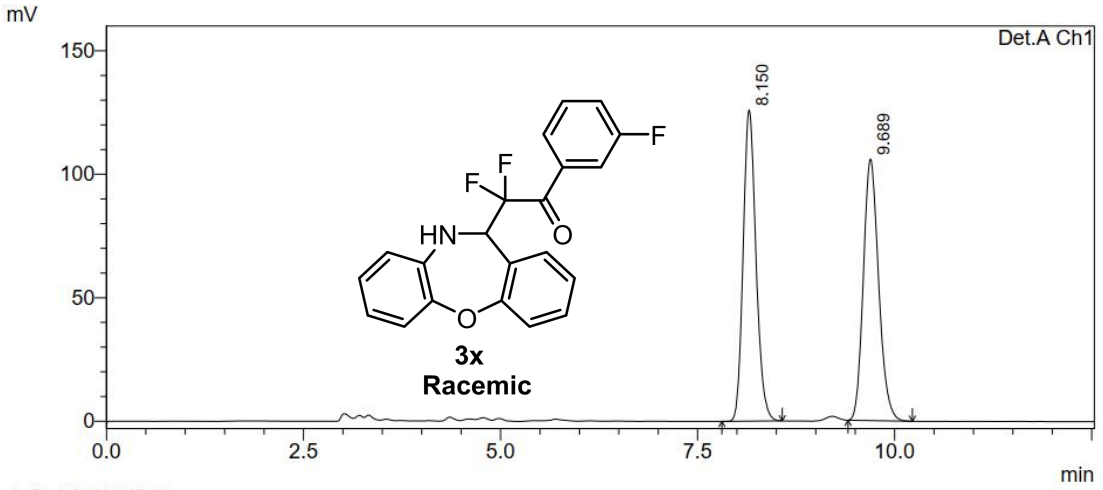


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.568	3714265	391162	96.512	96.924
2	8.692	134221	12413	3.488	3.076
Total		3848486	403576	100.000	100.000

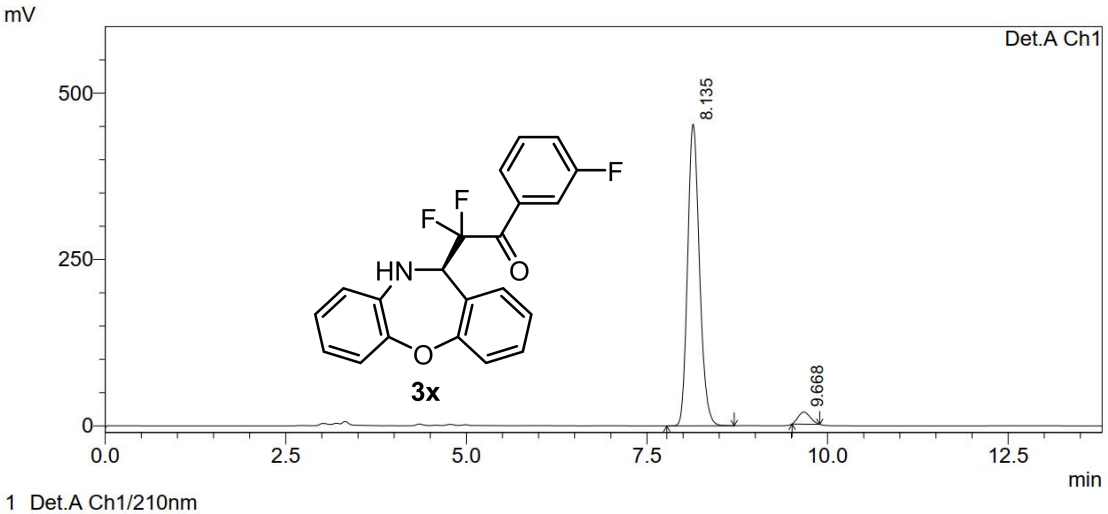


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	8.150	1426957	125938	49.916	54.405
2	9.689	1431788	105545	50.084	45.595
Total		2858745	231483	100.000	100.000

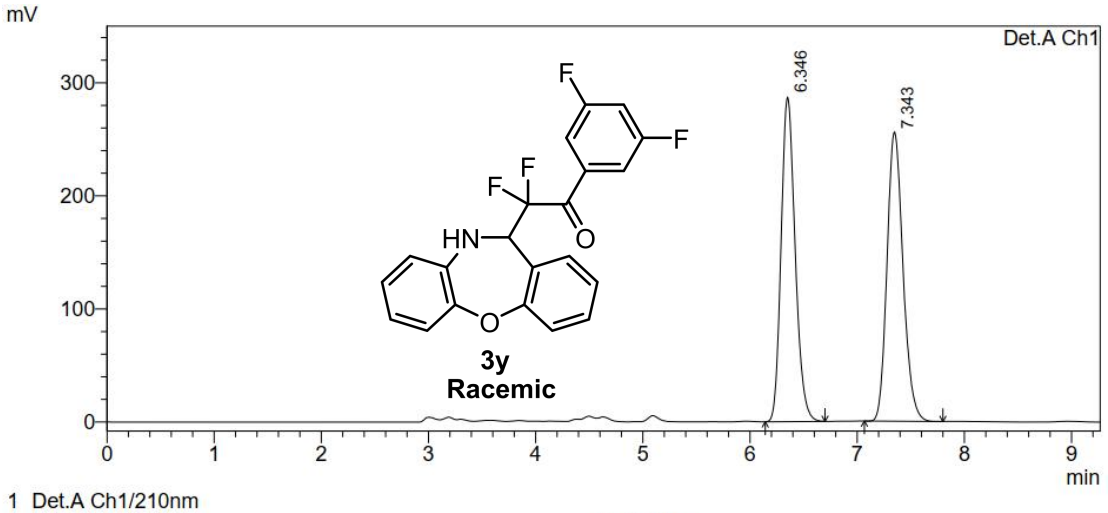


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	8.135	5184965	453325	96.095	96.142
2	9.668	210708	18191	3.905	3.858
Total		5395672	471516	100.000	100.000

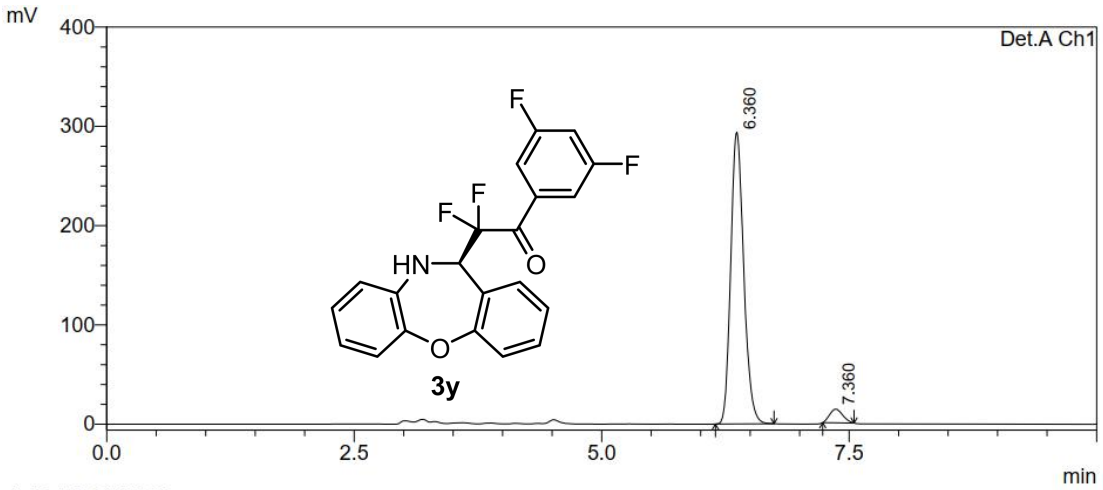


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.346	2615947	287177	49.628	52.888
2	7.343	2655137	255812	50.372	47.112
Total		5271084	542989	100.000	100.000

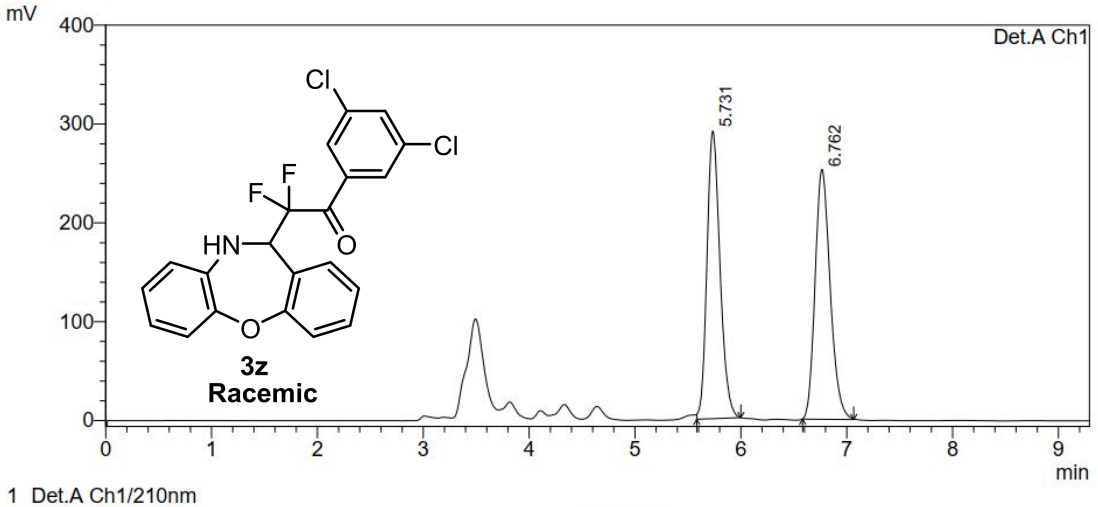


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.360	2680272	293974	95.528	95.538
2	7.360	125487	13729	4.472	4.462
Total		2805759	307703	100.000	100.000

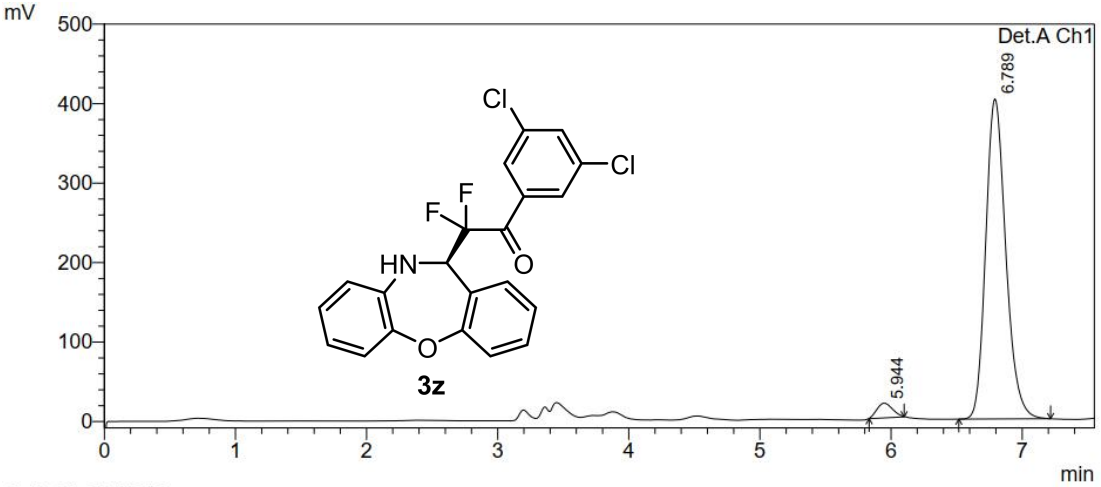


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.731	2488920	288638	49.894	53.395
2	6.762	2499537	251934	50.106	46.605
Total		4988458	540573	100.000	100.000

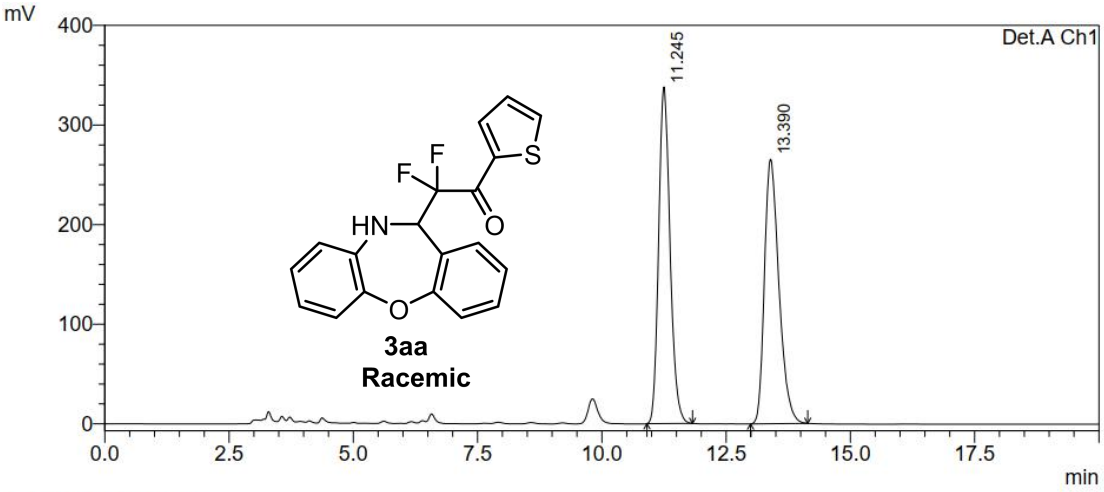


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.944	154654	18501	3.477	4.402
2	6.789	4292844	401754	96.523	95.598
Total		4447498	420255	100.000	100.000

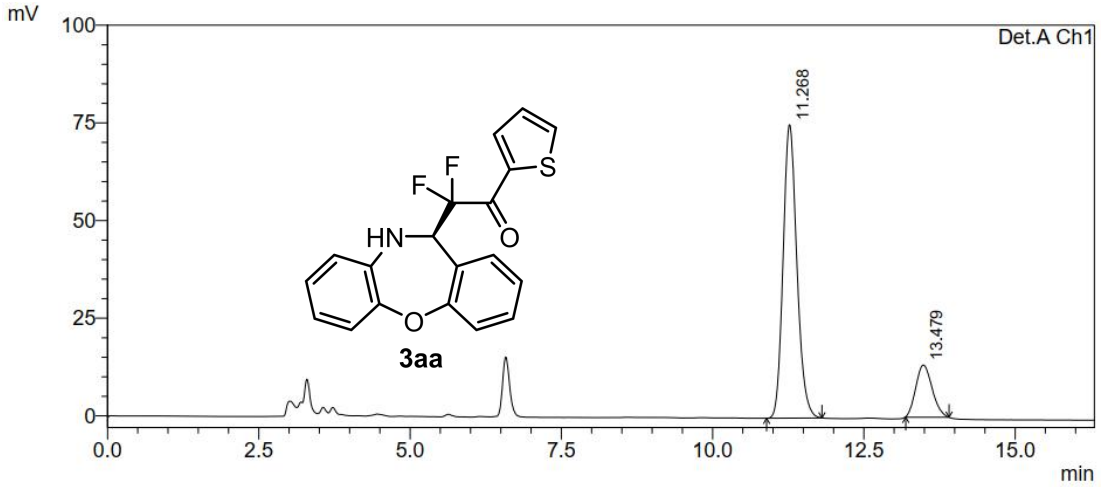


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	11.245	5385154	337341	49.980	55.999
2	13.390	5389564	265062	50.020	44.001
Total		10774718	602402	100.000	100.000

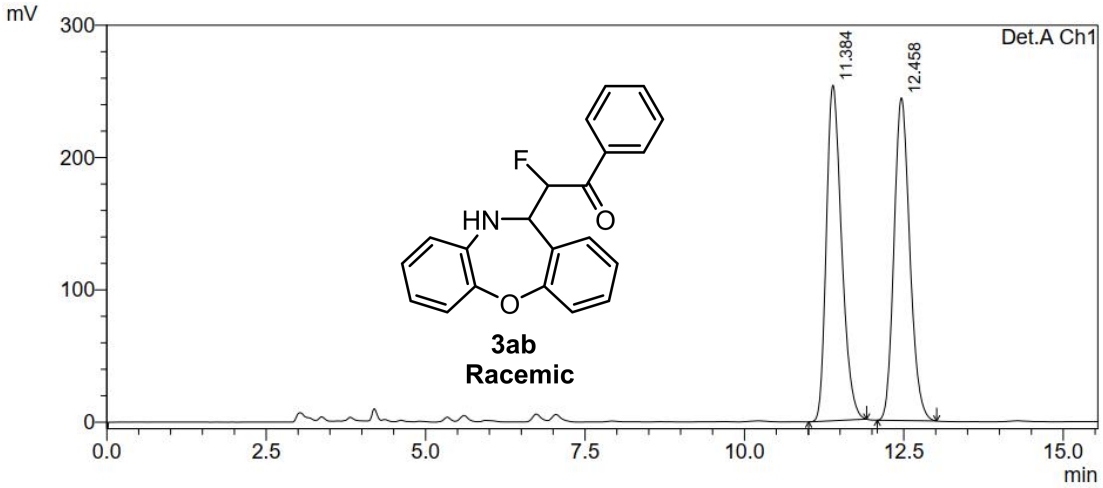


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	11.268	1189769	75096	82.564	84.888
2	13.479	251257	13369	17.436	15.112
Total		1441026	88465	100.000	100.000

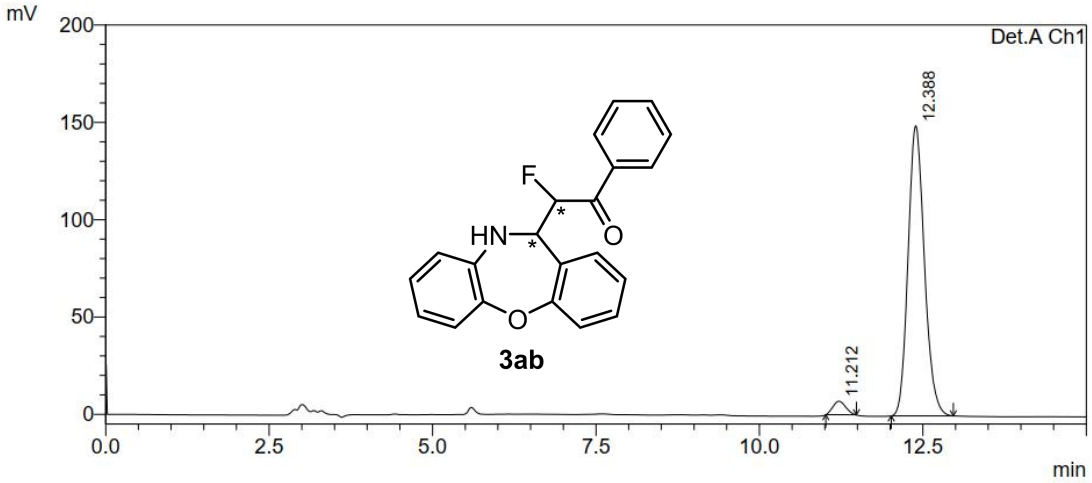


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	11.384	4221597	252953	50.105	50.918
2	12.458	4203837	243833	49.895	49.082
Total		8425434	496786	100.000	100.000

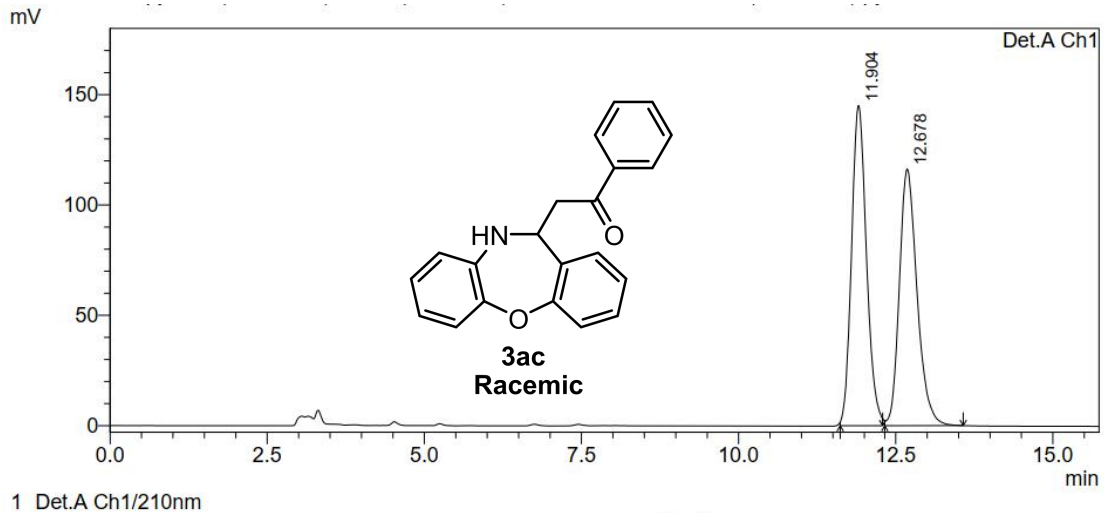


1 Det.A Ch1/21

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	11.212	93930	6918	3.496	4.440
2	12.388	2592952	148889	96.504	95.560
Total		2686882	155807	100.000	100.000

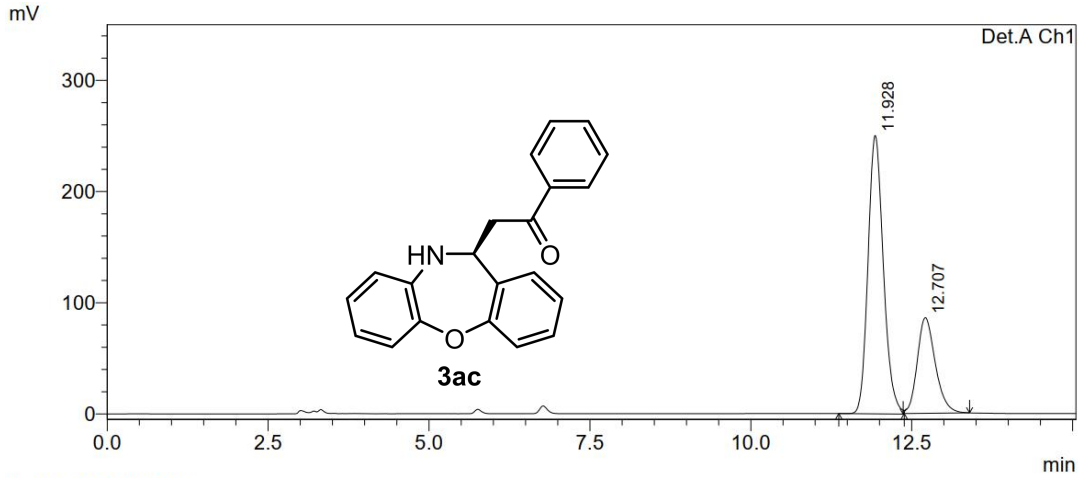


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	11.904	2392710	144960	51.171	55.508
2	12.678	2283227	116193	48.829	44.492
Total		4675937	261153	100.000	100.000

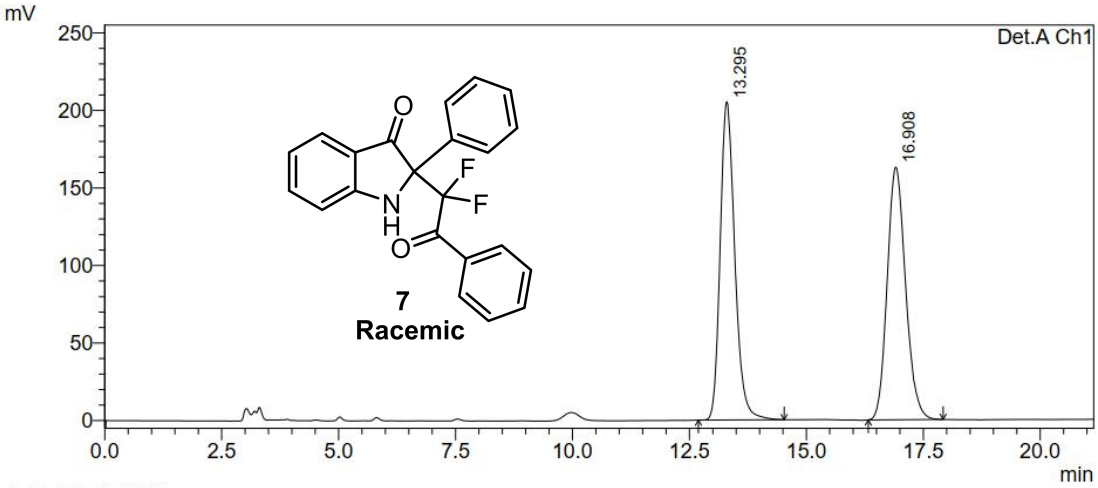


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	11.928	4162423	250117	71.253	74.417
2	12.707	1679356	85984	28.747	25.583
Total		5841778	336101	100.000	100.000

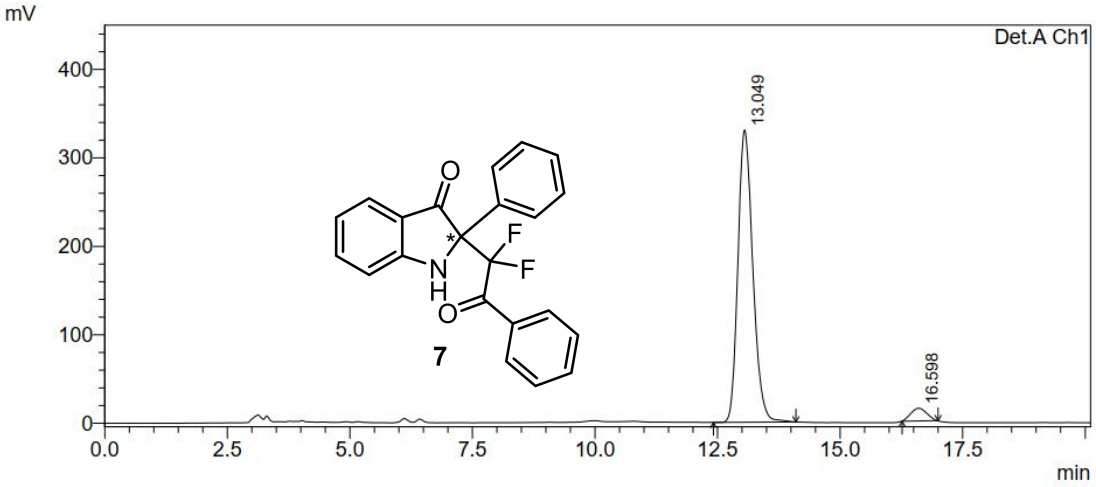


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	13.295	4460347	203748	50.072	55.597
2	16.908	4447515	162727	49.928	44.403
Total		8907862	366475	100.000	100.000

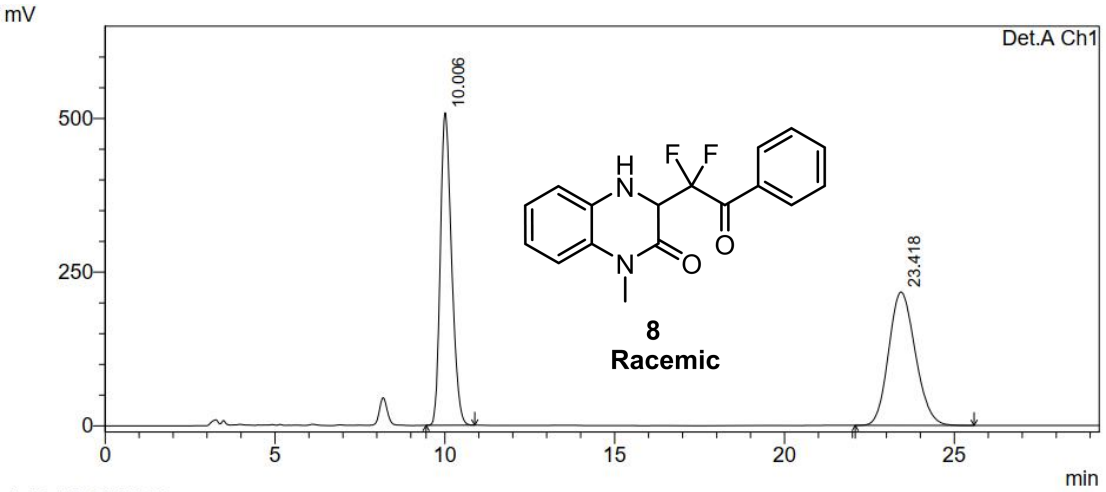


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	13.049	6989048	329856	95.542	95.849
2	16.598	326142	14284	4.458	4.151
Total		7315190	344140	100.000	100.000

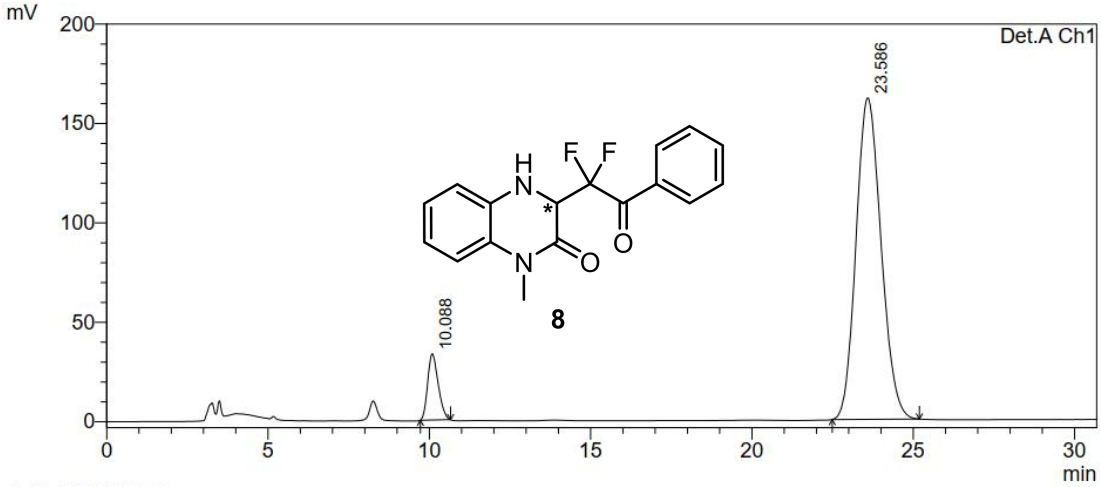


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.006	11731388	507009	49.734	70.071
2	23.418	11857078	216551	50.266	29.929
Total		23588466	723560	100.000	100.000

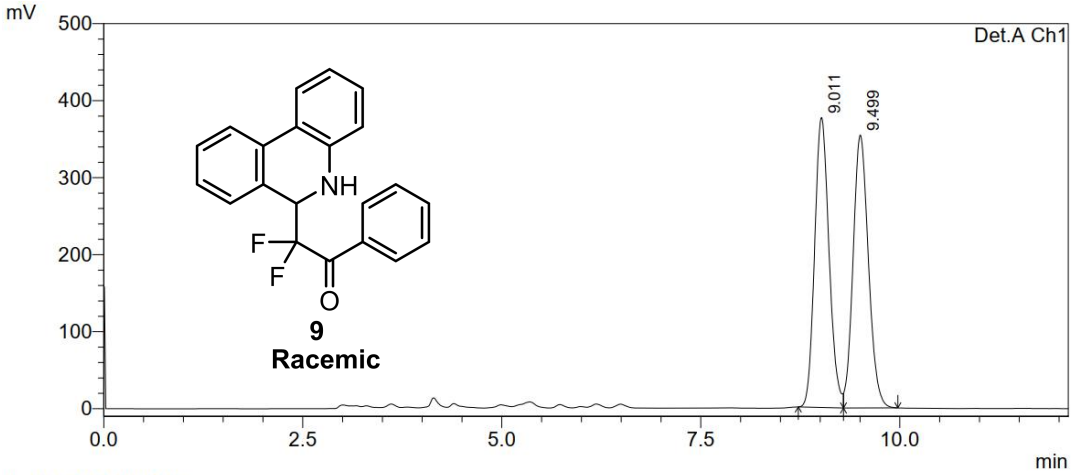


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.088	756098	33153	7.975	17.077
2	23.586	8724445	160984	92.025	82.923
Total		9480543	194137	100.000	100.000

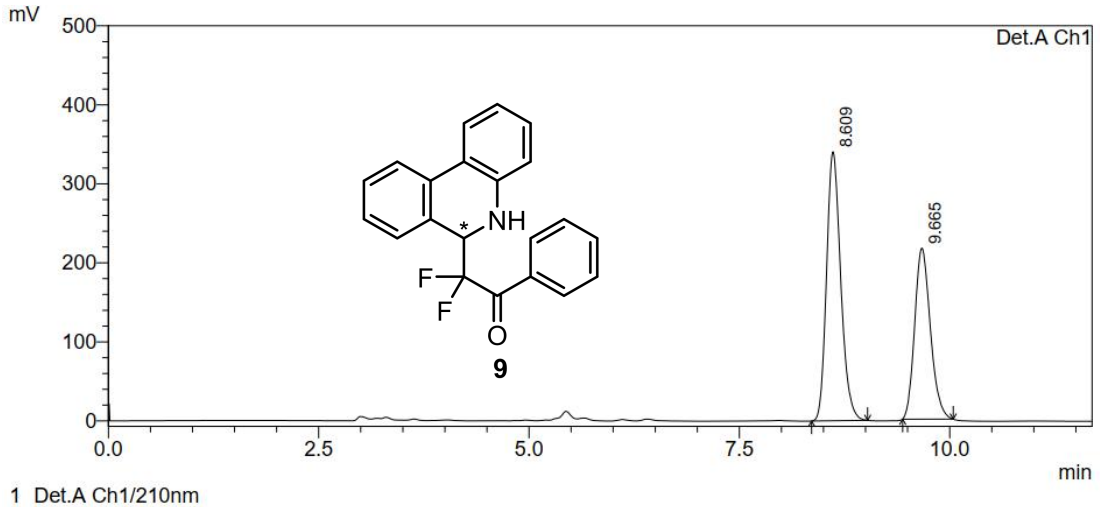


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.011	4743368	375346	49.966	51.458
2	9.499	4749853	354069	50.034	48.542
Total		9493222	729415	100.000	100.000

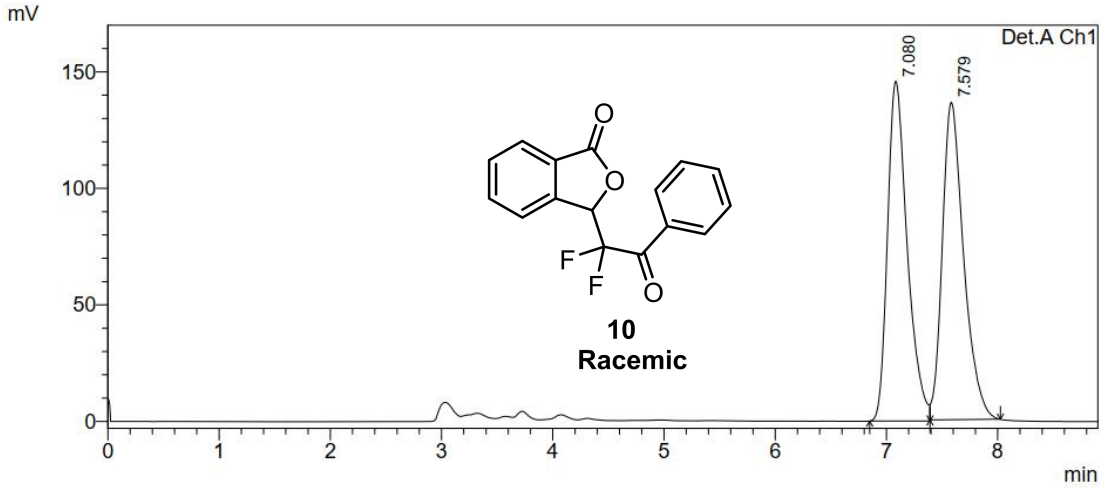


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	8.609	3974123	340345	58.550	61.155
2	9.665	2813498	216187	41.450	38.845
Total		6787622	556532	100.000	100.000

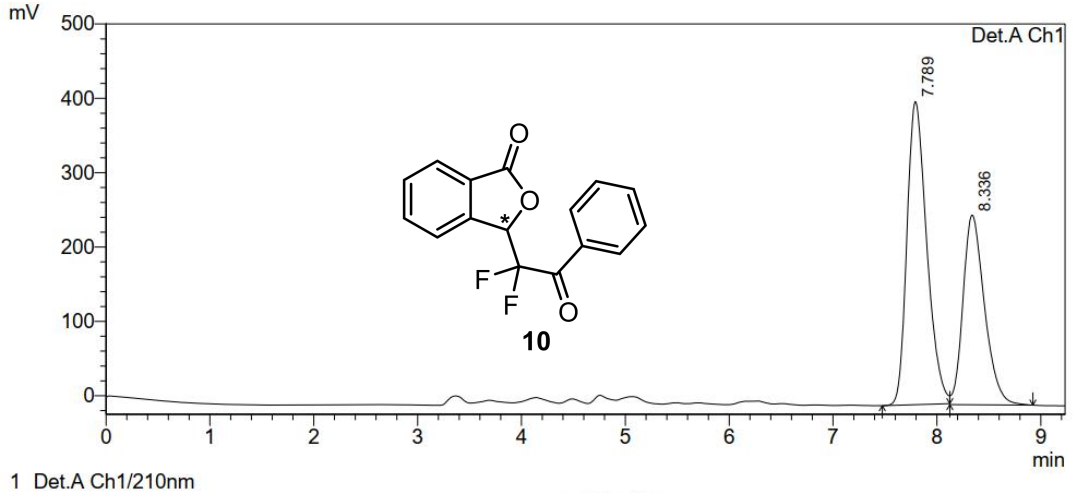


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.080	1800192	145833	49.719	51.766
2	7.579	1820540	135883	50.281	48.234
Total		3620731	281716	100.000	100.000

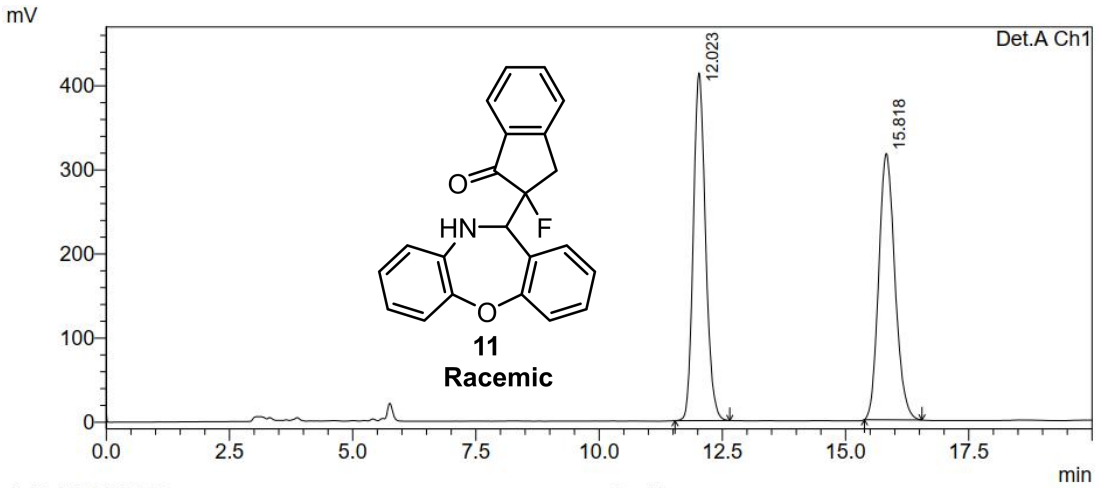


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.789	5416076	406257	59.610	61.460
2	8.336	3669727	254752	40.390	38.540
Total		9085803	661009	100.000	100.000

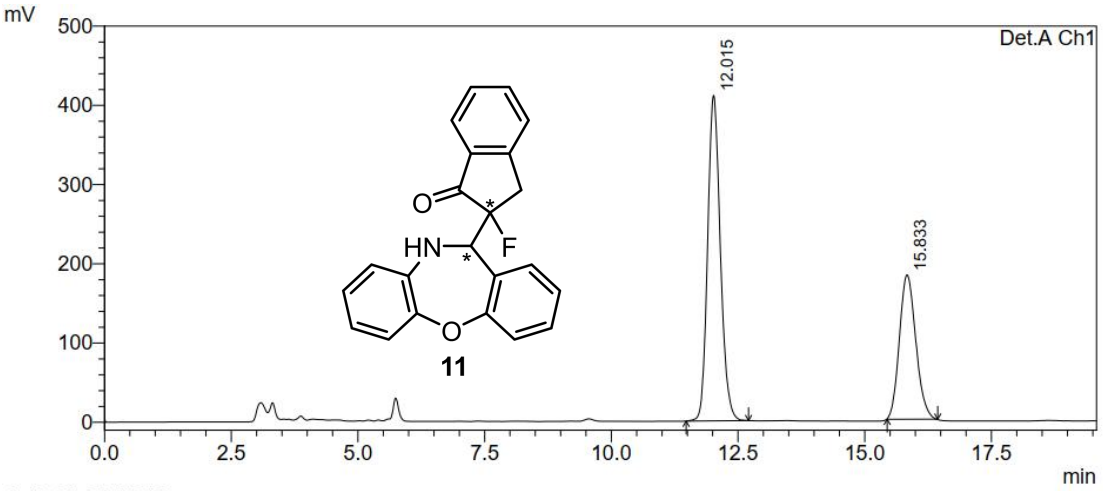


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	12.023	7129331	413395	49.606	56.707
2	15.818	7242451	315607	50.394	43.293
Total		14371782	729002	100.000	100.000

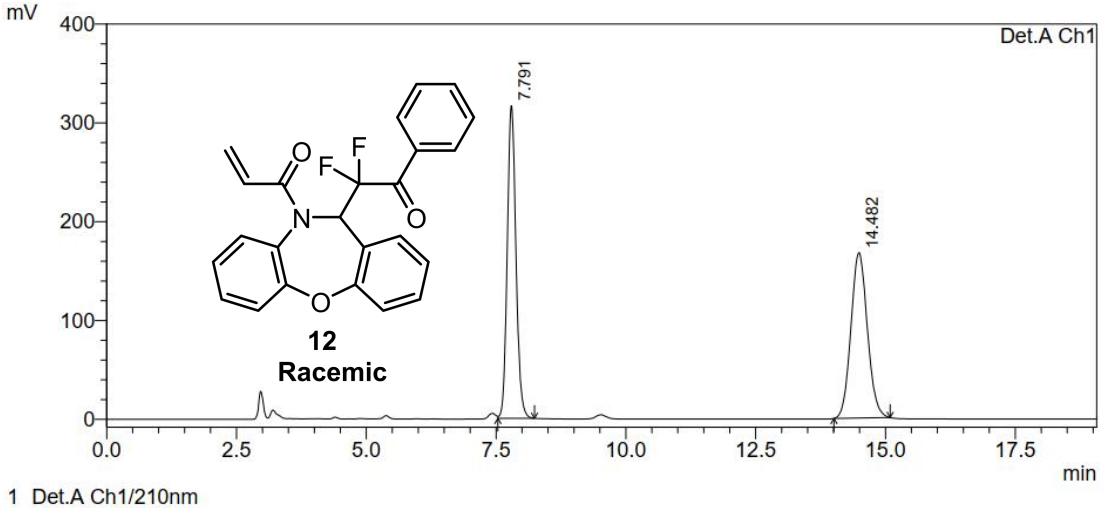


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	12.015	7165080	407926	63.551	69.194
2	15.833	4109478	181613	36.449	30.806
Total		11274559	589539	100.000	100.000

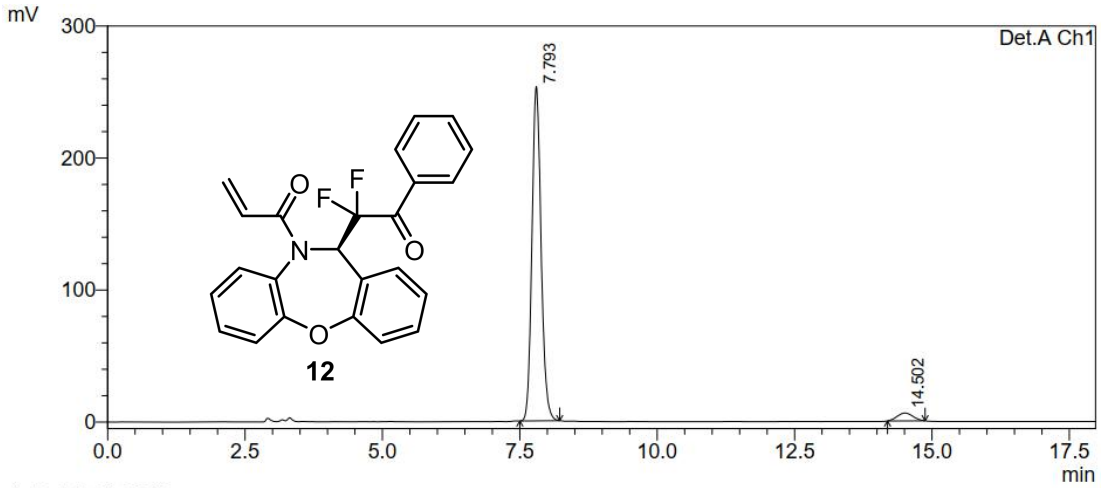


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.791	3682595	316527	50.015	65.514
2	14.482	3680415	166621	49.985	34.486
Total		7363010	483148	100.000	100.000

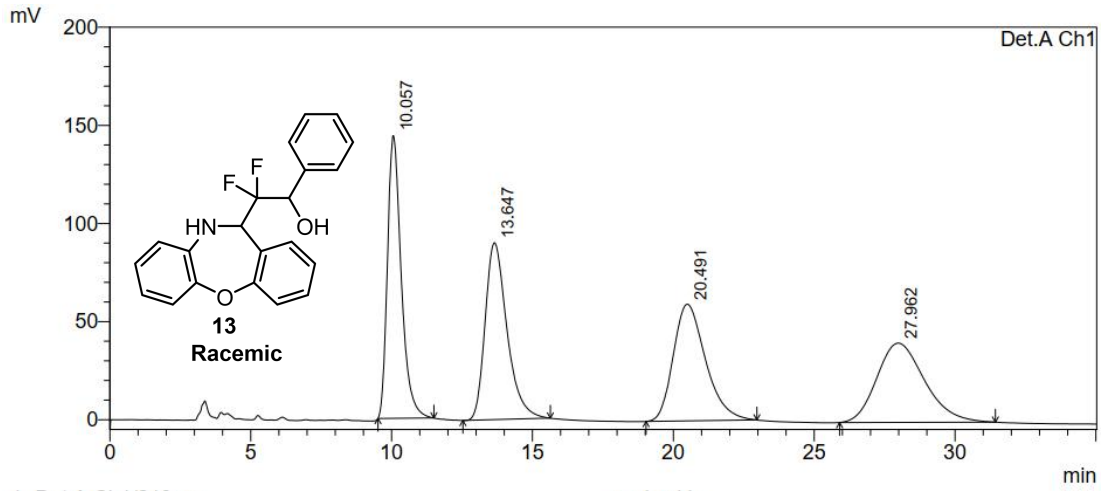


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.793	2935756	252729	96.127	97.687
2	14.502	118276	5984	3.873	2.313
Total		3054032	258713	100.000	100.000

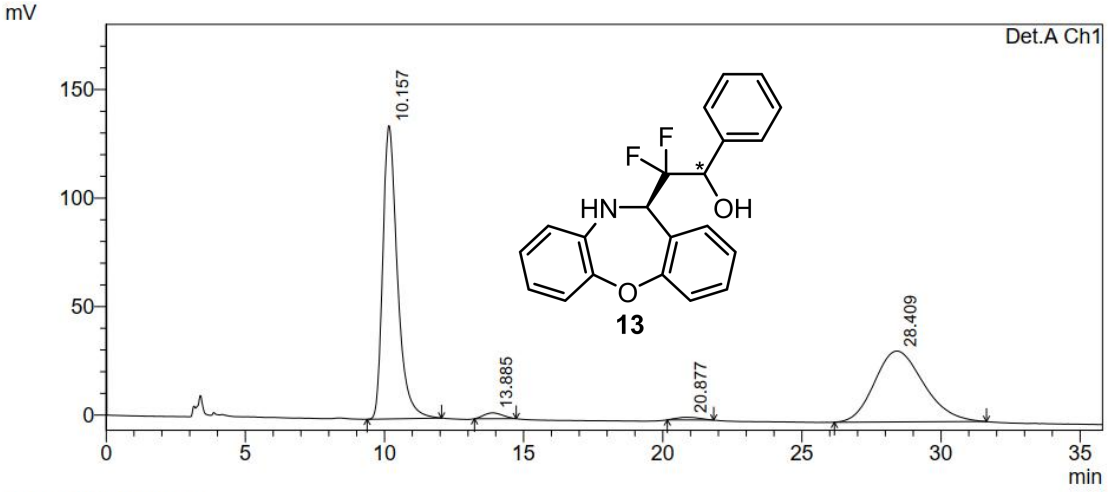


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.057	4904209	143938	25.467	43.135
2	13.647	4861366	90116	25.245	27.006
3	20.491	4738955	59355	24.609	17.787
4	27.962	4752431	40282	24.679	12.072
Total		19256961	333691	100.000	100.000

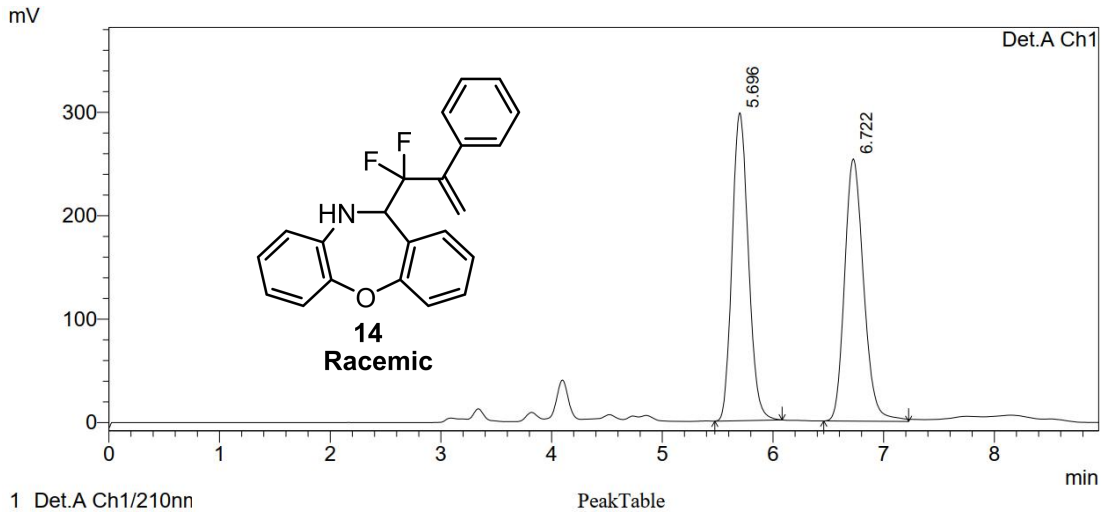


1 Det.A Ch1/210nm

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.157	4944376	135123	54.018	78.741
2	13.885	126298	2684	1.380	1.564
3	20.877	71371	1223	0.780	0.713
4	28.409	4011105	32576	43.822	18.983
Total		9153150	171606	100.000	100.000

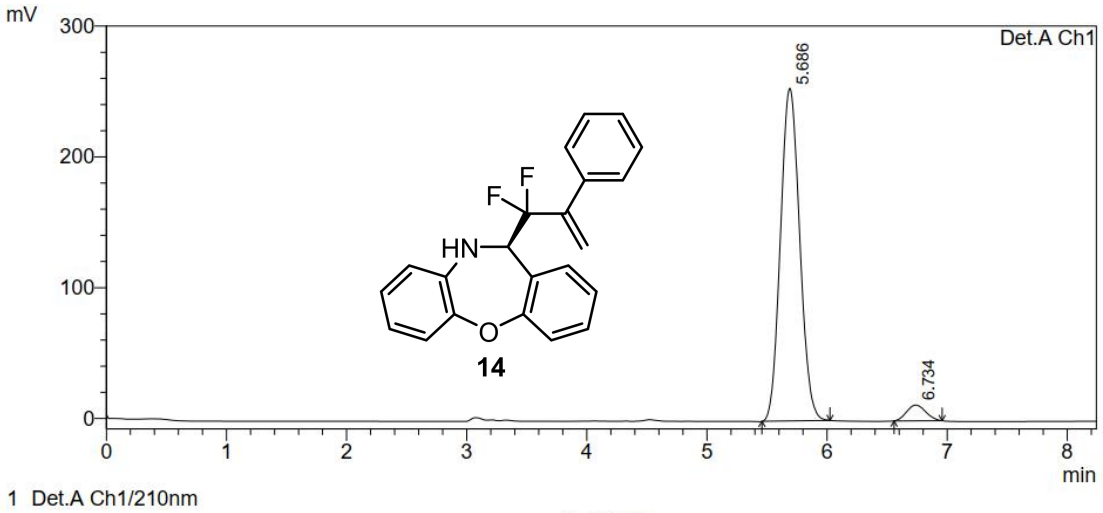


1 Det.A Ch1/210nn

PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.696	3050399	297944	50.056	54.019
2	6.722	3043607	253607	49.944	45.981
Total		6094007	551551	100.000	100.000



PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.686	2826630	254455	95.508	95.471
2	6.734	132950	12070	4.492	4.529
Total		2959579	266526	100.000	100.000

8. Calculation details

Conformational searches were performed using the CREST[5] conformer-rotamer ensemble sampling tool, version 2.7.1 with xtb[6] version 6.2. Conformers were then optimized in Gaussian 16[7] at the B3LYP-D3(BJ) / 6-31G(d)–SDD(Bi). All geometries were verified as stationary points on the potential energy surface and characterized as transition states or minima by frequency calculations. Single point energies were computed at the wB97X-D / 6-311++G(d,p)–SDD(Bi), SMD[8](generic, eps=4.5, epsinf=1.9) level of theory. The weak interaction was performed by the noncovalent interaction (NCI) analysis[9].

SMD / wB97X-D / 6-311++G(d,p)–SDD(Bi) // B3LYP-D3(BJ) / 6-31G(d)–SDD(Bi) calculated Cartesian coordinates and energies. Molecular structures were completed with the aid of the CREST conformational search program.

TS-major

C	-4.60075	3.72285	-2.48954
C	-5.22947	2.48276	-2.60398
C	-4.76947	1.41103	-1.84651
C	-3.6813	1.53563	-0.97585
C	-3.09027	2.79902	-0.83438
C	-3.54021	3.87783	-1.59271
H	-4.94914	4.56315	-3.08261
H	-6.06822	2.32518	-3.27422
H	-2.27984	2.916	-0.12892
H	-3.06179	4.84554	-1.47521
O	-5.39255	0.17927	-1.99857
C	-6.02097	-0.35391	-0.89148
C	-7.3388	-0.76904	-1.09344
C	-5.37014	-0.57899	0.33731
C	-8.0345	-1.42569	-0.08327
H	-7.78951	-0.57035	-2.06005
C	-6.08878	-1.26892	1.32915
C	-7.40299	-1.67929	1.13594

H	-9.05928	-1.74384	-0.25064
H	-5.59239	-1.4999	2.2627
H	-7.92631	-2.20623	1.92779
C	-3.91318	-0.31846	0.54018
H	-3.41571	-1.22771	0.88368
N	-3.15876	0.4007	-0.32258
C	-3.76803	0.74625	2.31075
C	-1.92787	-0.8049	3.1956
C	-2.78274	-1.72979	3.82423
C	-0.54485	-1.0772	3.14907
C	-2.26672	-2.9107	4.35237
H	-3.8433	-1.53168	3.89749
C	-0.04087	-2.26816	3.6629
H	0.12657	-0.3509	2.70645
C	-0.90104	-3.19108	4.26074
H	-2.93782	-3.62139	4.8265
H	1.02046	-2.47979	3.58281
H	-0.5071	-4.12442	4.6507
F	-4.6791	0.37825	3.24448
F	-4.05816	1.98904	1.90093
C	-2.3793	0.42505	2.50305
O	-1.57106	1.04011	1.73927
Bi	-0.88541	-0.18773	-0.20653
C	4.14169	3.54212	2.01252
C	3.31868	2.97099	1.02808
C	3.83681	1.89688	0.28398
C	5.12302	1.41346	0.5084
C	5.89583	1.97222	1.53668
C	5.41542	3.04266	2.28411
H	3.74793	4.37249	2.5903
H	6.01439	3.47695	3.08004
C	7.19773	1.21767	1.68808
H	8.03086	1.76882	1.23002
H	7.46736	1.04699	2.7359
C	5.91257	0.32684	-0.2085
C	6.90792	-0.0902	0.92319
H	7.80466	-0.5774	0.52912
H	6.40143	-0.80032	1.58632
C	6.70788	0.87904	-1.43383
H	6.02557	1.47076	-2.05394
H	7.53886	1.52452	-1.13399
C	7.15375	-0.38393	-2.20601
H	7.27777	-0.20268	-3.27912
H	8.11749	-0.75735	-1.83319
C	4.10209	-1.57588	-0.48874
C	5.26125	-0.89461	-0.83604
C	6.03562	-1.36002	-1.90805
C	5.70068	-2.54395	-2.55864
C	4.56899	-3.25192	-2.14741
C	3.73239	-2.77199	-1.1273
H	6.30138	-2.91138	-3.38633
H	4.29552	-4.17649	-2.64633
O	3.03424	1.26757	-0.66652
O	3.24812	-1.02168	0.46153
P	2.12635	0.01134	-0.14104
O	1.38925	-0.54438	-1.3377
O	1.22133	0.37657	1.01788
C	-0.64081	1.46591	-2.36066
O	-1.10407	0.31512	-2.60384
O	-0.38624	1.77651	-1.14129
C	-0.38928	2.48048	-3.42915
H	-0.50846	2.03594	-4.41765
H	-1.10017	3.3022	-3.29775
H	0.61407	2.89445	-3.30194
C	0.97523	5.73646	-2.67513
C	0.06224	5.631	-1.66022
C	0.35237	4.88275	-0.47859

C	1.6353	4.23238	-0.35525
C	2.5592	4.37253	-1.43736
C	2.24077	5.09365	-2.55968
C	-0.56758	4.79281	0.56883
C	1.94498	3.51923	0.82467
C	0.98954	3.40759	1.86046
C	-0.28848	4.06571	1.72773
C	-1.23844	3.97146	2.79152
H	-2.20069	4.46073	2.66636
C	-0.95406	3.26446	3.92666
C	0.29303	2.5878	4.05006
C	1.22816	2.6527	3.05212
H	-1.52376	5.30435	0.48233
H	0.74151	6.30951	-3.56804
H	-0.90479	6.12302	-1.73173
H	3.53123	3.90033	-1.35733
H	2.96264	5.18462	-3.3666
H	-1.68515	3.19537	4.72752
H	0.49434	1.99786	4.93992
H	2.1578	2.10552	3.14171
C	3.16561	-4.46362	2.79572
C	3.33588	-3.91763	1.55024
C	2.33696	-4.05003	0.53472
C	1.14518	-4.79731	0.86166
C	1.0049	-5.35015	2.17188
C	1.98384	-5.19144	3.11523
C	2.48463	-3.50102	-0.7613
C	0.167	-4.99511	-0.11646
C	0.30278	-4.46839	-1.40227
C	1.46415	-3.67432	-1.72576
C	1.5108	-3.06217	-3.01919
H	2.32811	-2.39037	-3.24477
C	0.5235	-3.27799	-3.94279
C	-0.58138	-4.12709	-3.64541
C	-0.68999	-4.69466	-2.4059
H	3.94242	-4.34873	3.54638
H	4.24695	-3.37937	1.31891
H	0.09875	-5.90601	2.39859
H	1.86862	-5.62257	4.106
H	-0.71842	-5.57749	0.12836
H	0.57481	-2.7893	-4.91136
H	-1.34428	-4.29897	-4.39946
H	-1.54109	-5.32115	-2.15121
C	-2.9498	-2.33514	-2.18913
O	-2.22512	-2.22522	-1.20057
O	-2.84742	-1.59924	-3.2811
H	-2.15346	-0.90104	-3.16561
C	-4.07894	-3.32512	-2.25782
H	-4.06177	-3.85744	-3.2127
H	-4.00885	-4.02539	-1.42542
H	-5.02565	-2.77686	-2.1965

Zero-point correction= 1.047673 (Hartree/Particle)
Thermal correction to Energy= 1.117973
Thermal correction to Enthalpy= 1.118917
Thermal correction to Gibbs Free Energy= 0.941019
sp-E = -4051.67947652 hartree
Vibration= -309.00

TS-minor

C	0.90335	2.58766	3.56238
C	2.20969	2.1042	3.57315
C	2.77999	1.58722	2.41589
C	2.06164	1.54309	1.20267
C	0.76612	2.09526	1.20471
C	0.18464	2.58506	2.36746
H	0.45324	2.96974	4.47336
H	2.80535	2.08201	4.47981

H	0.20747	2.13739	0.27518
H	-0.83114	2.95135	2.33856
O	4.05144	1.03734	2.55791
C	5.02932	1.56125	1.74007
C	6.11955	2.20357	2.31541
C	4.94094	1.37562	0.35651
C	7.14849	2.67277	1.49638
H	6.15056	2.31663	3.39383
C	5.98221	1.85173	-0.4517
C	7.07797	2.50364	0.1118
H	8.0044	3.17126	1.94191
H	5.91721	1.71141	-1.52697
H	7.87623	2.87133	-0.52547
C	3.81221	0.65363	-0.25668
H	3.97397	0.40863	-1.3011
N	2.51375	0.94534	0.00785
C	4.342	-1.36421	0.12271
C	2.90494	-1.77963	2.17123
C	3.91591	-2.13091	3.08163
C	1.62518	-1.45275	2.65003
C	3.64833	-2.14775	4.44669
H	4.90296	-2.39181	2.72355
C	1.37598	-1.43593	4.01735
H	0.83581	-1.20548	1.95305
C	2.38274	-1.78743	4.91898
H	4.43119	-2.42935	5.14499
H	0.39136	-1.15086	4.37543
H	2.18449	-1.7821	5.98755
F	5.49798	-1.39986	0.81204
F	4.58481	-1.751	-1.15049
C	3.11321	-1.76751	0.71486
O	2.10267	-1.84479	-0.06797
Bi	0.96321	-0.26472	-1.25292
C	-2.9858	-4.24493	1.91198
C	-2.58731	-3.46006	0.81418
C	-3.28344	-2.25358	0.601
C	-4.33645	-1.87436	1.42168
C	-4.63332	-2.62364	2.56742
C	-3.96815	-3.82167	2.80875
H	-2.4841	-5.19327	2.07287
H	-4.21017	-4.42859	3.67719
C	-5.70863	-1.93375	3.38033
H	-6.66999	-2.45903	3.29857
H	-5.46308	-1.89022	4.4472
C	-5.36987	-0.77902	1.24155
C	-5.77844	-0.53258	2.72791
H	-6.76011	-0.05795	2.81815
H	-5.03751	0.1307	3.18792
C	-6.59667	-1.33294	0.44389
H	-6.22404	-1.84504	-0.45014
H	-7.17936	-2.05255	1.0258
C	-7.39014	-0.07911	0.03129
H	-7.9701	-0.22332	-0.88663
H	-8.10124	0.21768	0.81485
C	-3.95541	1.28368	0.35429
C	-5.11064	0.51505	0.48441
C	-6.29663	0.95198	-0.12869
C	-6.34958	2.16585	-0.80321
C	-5.20289	2.95609	-0.85786
C	-3.99128	2.5316	-0.29234
H	-7.26755	2.49575	-1.28191
H	-5.22439	3.91851	-1.35967
O	-2.93284	-1.41695	-0.45355
O	-2.738	0.79485	0.83834
P	-1.8998	-0.18116	-0.18471
O	-1.60227	0.45172	-1.51777
O	-0.65332	-0.6469	0.56311

C	2.4842	-1.33325	-3.46121
O	1.52509	-2.03489	-3.08887
O	2.69061	-0.16534	-2.93003
C	3.47419	-1.81322	-4.49199
H	3.10597	-2.71102	-4.99009
H	3.67724	-1.02604	-5.22391
H	4.41483	-2.04017	-3.97751
C	-1.98914	-4.09216	-4.29887
C	-0.76363	-4.3489	-3.74869
C	-0.57499	-4.33639	-2.333
C	-1.67812	-3.9866	-1.47278
C	-2.95023	-3.7726	-2.0915
C	-3.10096	-3.82301	-3.45167
C	0.6557	-4.67572	-1.7689
C	-1.4736	-3.89386	-0.07191
C	-0.2149	-4.23816	0.48291
C	0.85147	-4.67432	-0.38899
C	2.10012	-5.08195	0.17329
H	2.88382	-5.40582	-0.50696
C	2.30685	-5.06284	1.52485
C	1.2805	-4.58616	2.38618
C	0.0775	-4.16834	1.88268
H	1.48161	-4.94133	-2.4227
H	-2.12322	-4.10458	-5.37686
H	0.0963	-4.56906	-4.37472
H	-3.81181	-3.57669	-1.4656
H	-4.08004	-3.65411	-3.89126
H	3.25849	-5.37651	1.94407
H	1.47494	-4.50278	3.4509
H	-0.66385	-3.75543	2.55409
C	-2.77627	4.67231	3.2025
C	-3.14085	3.97037	2.08268
C	-2.49425	4.19156	0.82513
C	-1.47222	5.20897	0.76135
C	-1.11683	5.91159	1.95304
C	-1.74338	5.65053	3.14206
C	-2.83099	3.46741	-0.34087
C	-0.86867	5.49717	-0.46603
C	-1.20004	4.79572	-1.62833
C	-2.18129	3.73894	-1.56379
C	-2.46399	3.00705	-2.75949
H	-3.15546	2.17705	-2.70653
C	-1.84082	3.31529	-3.93848
C	-0.89975	4.38203	-4.0077
C	-0.5894	5.09896	-2.88455
H	-3.27735	4.48106	4.14718
H	-3.92649	3.22632	2.14091
H	-0.33195	6.66119	1.89268
H	-1.46048	6.19052	4.04104
H	-0.12791	6.29256	-0.5172
H	-2.05787	2.73567	-4.83086
H	-0.42597	4.61908	-4.95648
H	0.12917	5.91384	-2.92436
C	2.04871	2.80158	-2.24589
O	1.01269	2.14515	-2.12639
O	3.07121	2.41677	-2.99995
H	2.92635	1.4684	-3.27247
C	2.31619	4.08366	-1.5158
H	2.58604	4.87712	-2.21883
H	1.44732	4.36829	-0.9275
H	3.17448	3.91627	-0.85514

Zero-point correction= 1.047487 (Hartree/Particle)
Thermal correction to Energy= 1.118035
Thermal correction to Enthalpy= 1.118979
Thermal correction to Gibbs Free Energy= 0.940400
sp-E = -4051.67458743 hartree
Vibration= -288.49

9. References

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