Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information

Visible light enabled [4+2] annulation reactions for anthracenone-furans from 2,3-dibromonaphthoquinone and phenylbenzofurans

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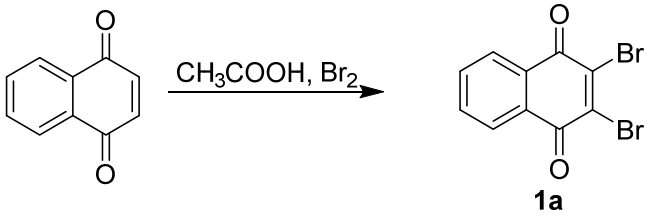
Contents

1. General information

All the commercially available coumarins are purified before use. All solvents are dried before use. Thin-layer chromatography (TLC) was performed with silica gel GF254 plates. Column chromatography was performed on silica gel (300 ~ 400 mesh) with petroleum ether/ethyl acetate for the gradient elution. All melting points were measured without correction. Nuclear magnetic resonance (NMR) spectra were recorded on a Bruker Avance III HD 600 spectrometer at 600 MHz (^{1}H NMR) and 151 MHz (^{13}C NMR) respectively. The chemical shifts are reported relative to $CHCl_3$ (δ = 7.26 for ^{1}H NMR and δ = 77.16 for ^{13}C NMR). The infrared spectra were recorded on a Nicolet iS 50 FT-IR spectrometer. Mass spectra (ESI-MS) were obtained on an Agilent 1240/6460 LC-MS system. HRMS spectra were obtained on Thermo Fisher HRMS, Q Exactive instrument.

2. Synthesis of starting materials

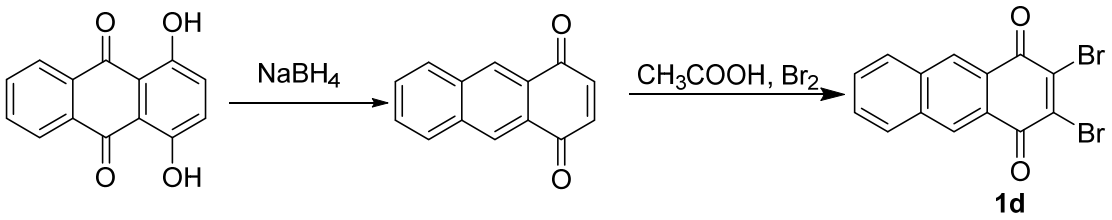
2,3-Dibromoquinones (**1a**, **1d**, **1e**) was synthesized as described[1] in supporting information of ref 1.



1a

2,3-Dibromonaphthalene-1,4-dione (**1a**)[1]: To a solution of naphthalene-1,4-dione (5.0g, 31.5 mmol) in glacial acetic acid, liquid bromine (3.25 mL, 63 mmol, 2eq) was added dropwise. The resulting solution was stirred at room temperature for 30 min and then heated to 110 °C. After 8 h reaction at this temperature, the mixture was poured into 200 mL ice-water, the precipitate was formed, filtered and washed with water and dried under vacuum. The pure product was gained as yellow solid (9.42g, 94%) with m.p. 216-218 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.19 (dd, J = 5.7, 3.3 Hz, 2H), 7.79

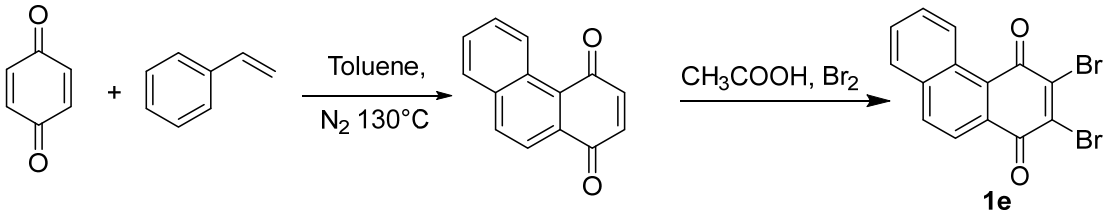
(dd, J = 5.8, 3.3 Hz, 2H). The spectral data agree with the literature value.



1d

1,4-Antraquinone[2]: Quinizarin (1g, 4.16 mmol) was dissolved in methanol (20 mL) at 0 °C. Sodium borohydride (0.96g, 25.4 mmol) was added carefully. The reaction was stirred for 90 min at 0°. An aq. solution of hydrochloric acid (6M, 18 mL) was added and the precipitate was filtered off and washed with water to afford 1,4-antraquinone as a brown solid (0.769g, 89%) with m.p. 214–216 °C.^{1}H NMR (500 MHz, $CDCl_3$) δ 8.60 (s, 2H), 8.10 – 7.98 (m, 2H), 7.73 – 7.64 (m, 2H), 7.06 (s, 2H). The spectral data agree with the literature value.

2,3-Dibromoanthracene-1,4-dione (**1d**) was synthesized as described above. Deep yellow to red solid, m.p. 289-290 °C. (lit[3] 293°C).^{1}H NMR (500 MHz, $CDCl_3$) δ 8.74 (s, 2H), 8.10 (dd, J = 6.1, 3.3 Hz, 2H), 7.75 (dd, J = 6.3, 3.2 Hz, 2H).

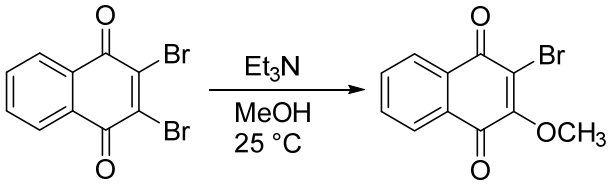


1e

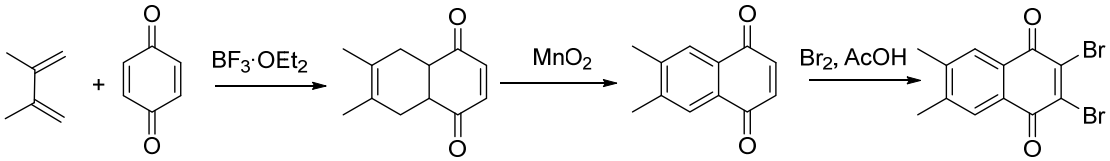
1,4-Phenanthrenedione[4]: In a sealed tube, *p*-benzoquinone (1 g, 9.2 mmol), styrene (1.435 g, 13.8mmol), and toluene (2 ml) were refluxed to 120 °C under N_2 for 27 h. After cooling to rt, the toluene was stripped, and small amounts of *p*-benzoquinone were sublimed under vacuum from the flask heated to its neck in hot water. The solid residue was flash chromatographed on silica gel using petroleum ether/CH_2Cl_2 (3:1) as eluent. After concentration in vacuo, *p*-benzoquinone sublimed from the eluted product (0.815 g, 42%) as an orange solid with m.p. 147-148 °C (lit[4] 146–148 °C). ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.55 (d, J = 8.8 Hz, 1H), 8.20 – 8.15 (m, 2H), 7.90 (d, J = 8.1 Hz, 1H), 7.74 (ddd, J = 8.6, 6.8, 1.4 Hz, 1H), 7.65 (ddd, J = 8.0, 6.9, 1.0 Hz, 1H), 6.98 (d,

J = 10.1 Hz, 1H), 6.94 (d, *J* = 10.2 Hz, 1H). The spectral data agree with the literature value.

2,3-Dibromophenanthrene-1,4-dione (**1e**) was synthesized as **1a**. Yellow solid, m.p. 156-158 °C. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 9.46 (d, *J* = 8.9 Hz, 1H), 8.25 (d, *J* = 8.5 Hz, 1H), 8.20 (d, *J* = 8.5 Hz, 1H), 7.93 (d, *J* = 8.2 Hz, 1H), 7.78 (ddd, *J* = 8.6, 6.9, 1.3 Hz, 1H), 7.72 – 7.67 (m, 1H).



2-Bromo-3-methoxynaphthoquninone (**1c**) was synthesized as similar procedure for 2-chloro-3-methoxynaphthoquninone[5]: 2,3-dibromo quinone (0.315 g, 1.00 mmol) and Et_3N (0.15 mL, 1.10 mmol) were dissolved in MeOH (10 mL) at 25 °C. After 5 h, the solid was filtered off and washed with cold H_2O (20 mL) to afford 2-Bromo-3-methoxynaphthoquninone (**1c**) (195 mg, 73%) as a green solid with m.p.163-165 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.17 – 8.13 (m, 1H), 8.11 – 8.06 (m, 1H), 7.76 – 7.72 (m, 2H), 4.31 (s, 3H).

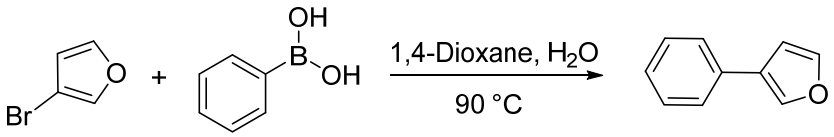


6,7-Dimethyl-4a,5,8,8a-tetrahydronaphthalene-1,4-dione[6]: To a stirred solution of 1,4-benzoquinone (0.2 g, 1.85 mmol) and $BF_3 \cdot OEt_2$ (0.02 mL, 0.185 mmol) in toluene was added 2,3-dimethyl-1,3-butadiene (0.252 mL, 2.22 mmol) dropwise at -16 °C over 10 min. After addition completion the reaction was allowed to warm to rt over 80 min. Upon completion the mixture was washed twice with brine and the organics dried over Na_2SO_4, filtered and solvent condensed under vacuum. The product was recrystallized from toluene to yield yellow crystals.

6,7-Dimethylnaphthalene-1,4-dione[6]: To a stirred solution of 6,7-Dimethyl-4a,5,8,8a-tetrahydronaphthalene-1,4-dione (0.266 g, 1.4 mmol) in toluene (10mL) was added portion wise activated MnO_2(1.3 g, 15.4 mmol) and refluxed for 2 h. The reaction mixture was cooled and filtered through Celite by washing with EtOH. The solvent was condensed and crude material purified by column chromatography to yield a yellow solid (0.172 g, 66%).

2,3-dibromo-6,7-dimethylnaphthalene-1,4-dione was synthesized as **1a**. Yellow solid, m.p.235-236 °C.

Phenylbenzofurans were synthesized as described in the literature[7] we previously reported.



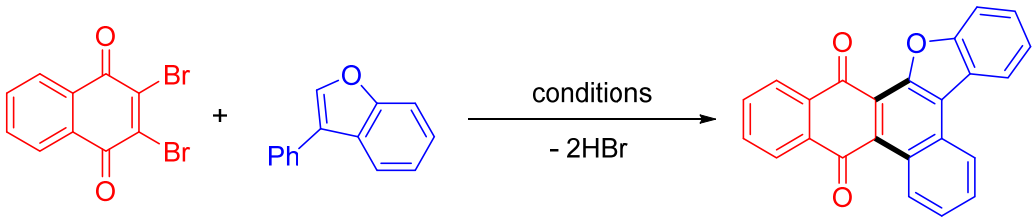
3-Phenylfuran was synthesized as a literature procedure[8] (PCT Int. Appl., 2012119046): To a solution of phenylboronic acid (0.3 g, 2.46 mmol) in dioxane (3.0 mL) and water (0.06 mL) was added 3-bromofuran (0.326 g, 2.25 mmol), H_3PO_4 (0.86 g, 4.05 mmol) and $Pd(PPh_3)_4$ (0.012g, 0.01 mmol) with stirring for 4h at 90 °C in an oil bath maintained with an inert atmosphere of nitrogen. The reaction mixture was concentrated under reduced pressure to give the residue, which was purified by silica gel column chromatography eluting with 1% ethyl acetate in petroleum ether to give 3-phenylfuran as a white solid (0.261, 82%) with m.p. 54-56 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.75 – 7.73 (m, 1H), 7.51 (t, *J* = 1.6 Hz, 1H), 7.49 (ddd, *J* = 4.1, 2.6, 1.3 Hz, 2H), 7.41 – 7.37 (m, 2H), 7.30 – 7.26 (m, 1H), 6.72 (dd, *J* = 1.8, 0.9 Hz, 1H). The spectral data agree with the literature value.

3. Typical procedure

In a 12 mL glass vial, 2,3-dibromo-1,4-naphthoquinone (31.5mg, 0.1 mmol), 3-phenylbenzofuran (25.2 mg, 0.13 mmol) and 4CzIPN (3.9 mg, 0.005 mmol) in 10 mL distilled benzene was dissolved. The solution was then ultrasonicated, purged with N_2 for10 minutes and sealed. The solution was then irradiated by 50 W blue LED until TLC showed the complete consumption of 2,3-dibromo-1,4-naphthoqunone. The solvent was removed in vacuum and the residue was put on silica gel chromatography with PE/DCM as eluent. The product is yielded as a red solid (32.1 mg, 92%).

4. Tables of reaction data

Table S1 Optimizing conditions for **3a**. [a]

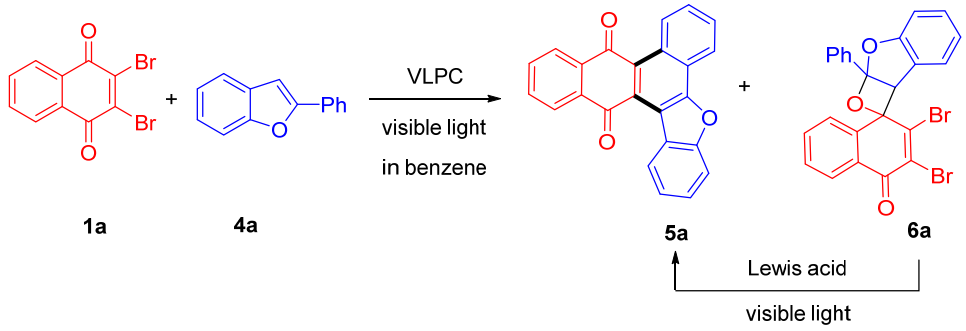


1a **2a** **3a**

Entry	VLPC, 5%	Solvent	Light Source	Time, h	Yield, % [b]
1	No PC	Benzene	24W Blue led	168	51
2	Butanedione, 30%	Benzene	24W Blue led	75	54
3	Rose Bengal, 2%	Benzene	24W Blue led	65	60
4	TXO, 2%	Benzene	24W Blue led	56	69
5	TXO, 5%	Benzene	24W Blue led	53	75
6	4CzIPN, 2%	Benzene	24W Blue led	51	79
7	4CzIPN	Benzene	24W Blue led	49	88
8	4CzIPN	DCE	24W Blue led	56	52
9	4CzIPN	1,4-Dioxane	24W Blue led	39	57
10	4CzIPN	MeCN	24W Blue led	48	19
11	4CzIPN	Benzene(0.02 M)	24W Blue led	76	67(1) [c]
12	4CzIPN	Benzene	24W Blue led	38	87(2) [d]
13	4CzIPN	Benzene	470-475 nm 3W	118	70
14	4CzIPN	Benzene	460-465 nm 3W	79	79
16	4CzIPN	Benzene	450-455 nm 3W	74	85
17	4CzIPN	Benzene	50W Blue Led	10	92
18	4CzIPN	Benzene	Light Off	126	NR
19	4CzIPN	Benzene	No Light, reflux	156	NR
20	4CzIPN	Benzene (0.02 M)	50W Blue Led	23	82
21	TXO	Benzene	50W Blue Led	13	80
22	4CzIPN (2%)	Benzene	50W Blue Led	12	84

[a.] Reagents and conditions: 0.1 mmol **1a** (31.5 mg), 0.13 mmol **2a** (25.2 mg) and 0.005 mmol VLPC in 10 mL distilled benzene was ultra-sonicated and purged with N_2 for 10 minutes and then irradiated under blue LED. TXO: Thioxanthen-9-one. 4CzIPN: 2,4,5,6-tetrakis(carbazol-9-yl)-1,3-dicyanobenze [b.] Isolated yield. [c.] Average of two parallel runs. [d.] Pyridine (2.2 eq) was added.

Table S2 Lewis acid promoted one-pot reaction for **5a**.



Entry	PC, 5%	Light Source	Additive	Time, h	Yield, % [b]
1	4CzIPN	24 W Blue led	N/A	29	46 [a]
2	4CzIPN	24 W Blue led	N/A	101	54
3	4CzIPN	50 W Blue led	/	13	54
4	4CzIPN	50 W Blue led	$SnCl_4$	8	69
5	4CzIPN	50 W Blue led	$FeCl_3.6H_2O$	28	63
6	4CzIPN	50 W Blue led	$FeCl_2.4H_2O$	25	64
7	4CzIPN	50 W Blue led	$BF_3.Et_2O$	16	55
8	4CzIPN	50 W Blue led	$Ni(OTf)_2$	10	57
9	4CzIPN	50 W Blue led	AgOTf	11	59

[a.] Reagents and conditions: 0.1 mmol **1a** (31.5 mg), 0.13 mmol **2b** (25.2 mg), 0.005 mmol 4CzIPN and 0.01 mmol LA in 10 mL distilled benzene was ultrasonicated and purged with N_2 for 10 minutes and then irradiated under blue LED (24W*2). [b.] Isolated yield. [c.] Oxetane **6a** was obtained in 17% yield.

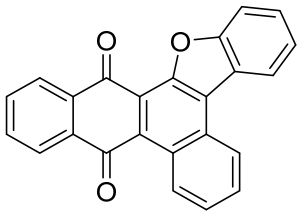
Table S3 Competitive absorption of annulated products to 4CzIPN.

Product	Time, h	Yield, %	λ_{max}, nm	ε, $mol^{-1}.L.cm^{-1}$
3a	10	92	446	9360
3k	15	92	464	7760
3u	22	71	462	8160
3s	22	44	450	11300
3t	24	53	409, 537	24000, 14200
3l	38	50	478	10000

When the UV absorption of annulated product is near 4CzIPN (471 nm) with a large extinction coefficient, the yield is reduced with a longer reaction time needed.

5. The spectral data

All the known compounds' spectral data (^{1}H NMR, ^{13}C NMR, IR, MS) agree with the reported references. The new compounds were characterized by ^{1}H NMR, ^{13}C NMR, IR and HRMS except no clear ^{13}C NMR signals for **3i**, **3j**, **5d**, **5e**, **7a** and **7b** could be acquired for poor solubility in organic solvent.



3a

Tetrapheno[6,5-*b*]benzofuran-5,15-dione

Yellow solid, m.p. 221-223 ℃ (DCM/PE =4/1).

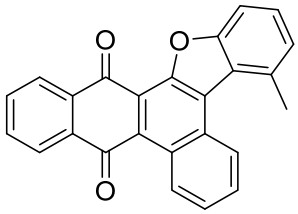
^{1}H NMR (500 MHz, $CDCl_3$) δ 9.67 (d, *J* = 8.8 Hz, 1H), 8.60 (d, *J* = 8.2 Hz, 1H), 8.38 (d, *J* = 7.9 Hz, 1H), 8.30 – 8.22 (m, 2H), 7.87 (d, *J* = 8.3 Hz, 1H), 7.83 – 7.74 (m, 3H), 7.71 – 7.66 (m, 1H), 7.60 (t, *J* = 7.8 Hz, 1H), 7.49 (t, *J* = 7.6 Hz, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 186.0, 183.1, 158.3, 150.1, 134.9, 134.2, 133.7, 132.8, 132.1, 130.1, 129.7, 129.1, 128.5, 128.1, 127.8, 127.2, 126.4, 125.4, 124.1, 123.6, 123.0, 122.9, 121.8, 113.1.

IR(KBr) υ_{max}: 3064, 3030, 1673, 1654, 1572, 1451, 1341, 1292, 1239, 1213, 752, 741, 677 cm^{-1}.

HRMS: (ESI) calcd for $C_{24}H_{13}O_3^+$ $[M+H]^+$ 349.08592; found 349.08572.

UV(in PhH) λ_{max} = 446 nm, ε_{max} = 9360 $mol^{-1}.L.cm^{-1}$.



3b

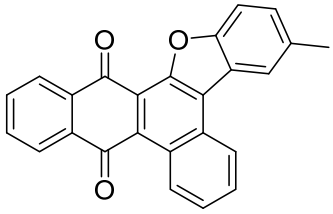
10-Methyltetrapheno[6,5-*b*]benzofuran-5,15-dione

Yellow solid, m.p. 218-220 ℃ (DCM/PE =3/1).

^{1}H NMR (500 MHz, $CDCl_3$) δ 9.67 (d, *J* = 8.5 Hz, 1H), 8.99 (d, *J* = 8.2 Hz, 1H), 8.31 – 8.27 (m, 2H), 7.84 – 7.79 (m, 2H), 7.78 – 7.69 (m, 3H), 7.50 (t, *J* = 7.8 Hz, 1H), 7.29 (d, *J* = 7.4 Hz, 1H), 3.15 (s, 3H).

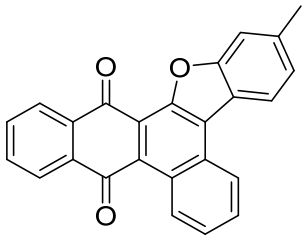
^{13}C NMR (126 MHz, $CDCl_3$) δ 185.9, 183.2, 159.0, 150.4, 135.0, 134.2, 133.7, 133.3, 133.0, 131.8, 130.0, 129.7, 128.7, 128.6, 128.2(2C), 127.6, 127.4, 127.2, 126.5, 126.3, 122.8, 121.4, 110.8, 26.2.

IR(KBr) υ_{max}: 3126, 3077, 3054, 2958, 2858, 1677, 1659, 1613, 1593, 1442, 1336, 1287, 1258, 1238, 1212, 1191, 1129, 1057, 1025, 974, 771, 753, 697, 678 cm^{-1}.
HRMS: (ESI) calcd for $C_{25}H_{15}O_3^+$ $[M+H]^+$ 363.10157; found 363.10110.
UV(in PhH) λ_{max} = 458 nm, ε_{max} = 11760 $mol^{-1}.L.cm^{-1}$.



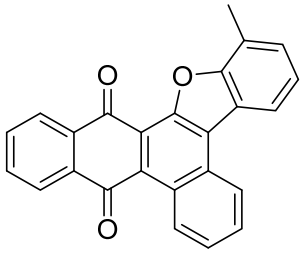
3c

11-Methyltetrapheno[6,5-*b*]benzofuran-5,15-dione
Yellow solid, m.p. 245-247 ℃ (DCM/PE =3/1).
^{1}H NMR (500 MHz, $CDCl_3$) δ 9.51 (d, *J* = 8.8 Hz, 1H), 8.36 (d, *J* = 8.2 Hz, 1H), 8.19 (ddd, *J* = 6.3, 2.8, 1.3 Hz, 2H), 7.93 (s, 1H), 7.78 – 7.72 (m, 2H), 7.62 (dd, *J* = 7.6, 5.2 Hz, 2H), 7.55 – 7.50 (m, 1H), 7.28 (d, *J* = 8.4 Hz, 1H), 2.51 (s, 3H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 185.7, 182.8, 156.6, 150.0, 134.8, 134.0, 133.5(2C), 132.7, 131.8, 129.9, 129.7, 129.4, 128.5, 127.8, 127.6, 127.1, 126.3, 125.1, 123.4, 122.74, 122.71, 121.5, 112.4, 21.7.
IR(KBr) υ_{max}: 3075, 3005, 2958, 2923, 2856, 1671, 1654, 1618, 1571, 1458, 1384, 1330, 1289, 1246, 1080, 1058, 1026, 968, 751, 725 cm^{-1}.
HRMS: (ESI) calcd for $C_{25}H_{15}O_3^+$ $[M+H]^+$ 363.10157; found 363.10117.
UV(in PhH) λ_{max} = 450 nm, ε_{max} = 10960 $mol^{-1}.L.cm^{-1}$.



3d

12-Methyltetrapheno[6,5-*b*]benzofuran-5,15-dione
Yellow solid, m.p. 241-243 ℃ (DCM/PE =4/1).
^{1}H NMR (500 MHz, $CDCl_3$) δ 9.75 (d, *J* = 8.7 Hz, 1H), 8.66 (d, *J* = 8.0 Hz, 1H), 8.32 – 8.27 (m, 3H), 7.85 – 7.77 (m, 3H), 7.77 – 7.72 (m, 1H), 7.69 (s, 1H), 7.34 (d, *J* = 7.8 Hz, 1H), 2.60 (s, 3H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 186.1, 183.4, 159.0, 150.1, 139.6, 135.1, 134.2, 133.6, 132.9, 132.0, 130.2, 129.6, 128.6, 128.1, 128.0, 127.2, 126.4, 125.8, 125.7, 123.8, 122.6, 122.0, 120.6, 113.3, 22.3.
IR(KBr) υ_{max}: 3124, 3065, 3036, 2921, 2854, 1674, 1654, 1626, 1594, 1569, 1440, 1341, 1316, 1292, 1250, 1228, 1212, 1170, 1114, 1058, 1027, 973, 752 cm^{-1}.
HRMS: (ESI) calcd for $C_{25}H_{15}O_3^+$ $[M+H]^+$ 363.10157; found 363.10126.
UV(in PhH) λ_{max} = 456 nm, ε_{max} = 10480 $mol^{-1}.L.cm^{-1}$.



3e

13-Methyltetrapheno[6,5-*b*]benzofuran-5,15-dione

Yellow solid, m.p. 240-242 °C (DCM/PE =4/1).

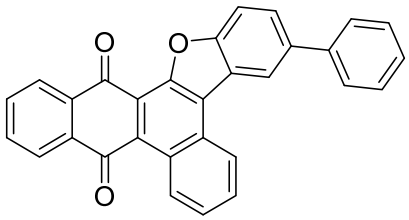
^{1}H NMR (500 MHz, $CDCl_3$) δ 9.65 (d, *J* = 8.8 Hz, 1H), 8.54 (d, *J* = 8.1 Hz, 1H), 8.28 – 8.22 (m, 2H), 8.13 (dt, *J* = 7.5, 3.8 Hz, 1H), 7.81 – 7.75 (m, 2H), 7.71 (dd, *J* = 11.0, 4.0 Hz, 1H), 7.65 (ddd, *J* = 8.2, 6.8, 1.2 Hz, 1H), 7.37 – 7.32 (m, 2H), 2.74 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 185.9, 182.9, 157.3, 149.9, 134.9, 134.0, 133.6, 132.8, 132.1, 130.1, 129.5, 129.4, 128.7, 127.9, 127.8, 127.2, 126.3, 125.8, 124.0, 123.6, 123.2, 122.3, 121.8, 120.4, 15.5.

IR(KBr) υ_{max}: 3061, 2958, 2923, 2854, 1655, 1571, 1341, 1293, 1272, 1181, 1059, 968, 786, 748, 737, 729, 697, 679 cm^{-1}.

HRMS: (ESI) calcd for $C_{25}H_{15}O_3^+$ $[M+H]^+$ 363.10157; found 363.10114.

UV(in PhH) λ_{max} = 450 nm, ε_{max} = 12080 $mol^{-1}.L.cm^{-1}$.



3f

11-Phenyltetrapheno[6,5-*b*]benzofuran-5,15-dione

Yellow solid, m.p. 293-295 °C (DCM/PE =5/1).

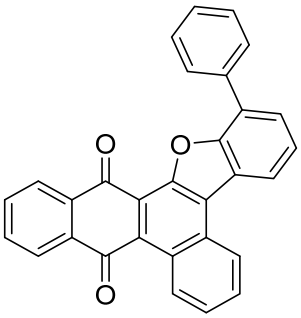
^{1}H NMR (500 MHz, $CDCl_3$) δ 9.70 (d, *J* = 8.8 Hz, 1H), 8.68 (d, *J* = 8.2 Hz, 1H), 8.52 (s, 1H), 8.27 (dd, *J* = 8.2, 6.4 Hz, 2H), 7.91 (d, *J* = 8.6 Hz, 1H), 7.83 – 7.76 (m, 4H), 7.71 (dd, *J* = 12.8, 7.4 Hz, 3H), 7.54 (t, *J* = 7.6 Hz, 2H), 7.44 (t, *J* = 7.4 Hz, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 186.0, 183.1, 157.9, 150.6, 141.2, 137.9, 135.0, 134.2, 133.7, 132.8, 132.2, 130.2, 129.9, 129.3, 129.1(2C), 128.22, 128.18, 127.9, 127.8(2C), 127.6, 127.2, 126.5, 125.4, 123.7, 123.5, 121.9, 121.5, 113.2.

IR(KBr) υ_{max}: 3058, 3027, 1671, 1655, 1648, 1637, 1570, 1460, 1384, 1330, 1304, 1294, 1271, 1162, 1140, 1115, 1058, 1036, 970, 747, 728, 692 cm^{-1}.

HRMS: (ESI) calcd for $C_{30}H_{17}O_3^+$ $[M+H]^+$ 425.11722; found 425.11670.

UV(in PhH) λ_{max} = 446 nm, ε_{max} = 11280 $mol^{-1}.L.cm^{-1}$.



3g

13-Phenyltetrapheno[6,5-*b*]benzofuran-5,15-dione

Yellow solid, m.p. 270-272 °C (DCM/PE =6/1).

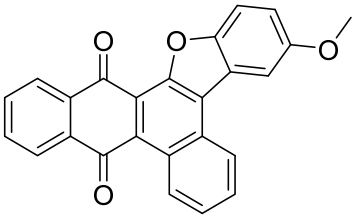
^{1}H NMR (500 MHz, $CDCl_3$) δ 9.78 (d, *J* = 8.7 Hz, 1H), 8.75 (d, *J* = 8.1 Hz, 1H), 8.44 (d, *J* = 7.7 Hz, 1H), 8.33 – 8.21 (m, 4H), 7.86 (t, *J* = 7.6 Hz, 2H), 7.83 – 7.74 (m, 3H), 7.69 (t, *J* = 7.8 Hz, 2H), 7.62 (t, *J* = 7.7 Hz, 1H), 7.52 (t, *J* = 7.4 Hz, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 186.1, 182.7, 155.6, 150.1, 135.6, 135.0, 134.1, 133.6, 132.8, 132.2, 130.3, 129.8, 129.2, 129.1(2C), 129.0(2C), 128.5, 128.1, 128.0, 127.7, 127.2, 126.6, 126.5, 125.3, 124.7, 123.9, 123.7, 122.01, 121.99.

IR(KBr) υ_{max}: 3059, 3030, 1674, 1657, 1594, 1574, 1442, 1404, 1346, 1336, 1294, 1246, 1213, 1152, 1115, 1059, 1025, 973, 752, 738, 690, 681 cm^{-1}.

HRMS: (ESI) calcd for $C_{30}H_{17}O_3^+$ $[M+H]^+$ 425.11722; found 425.11673.

UV(in PhH) λ_{max} = 452 nm, ε_{max} = 7760 $mol^{-1}.L.cm^{-1}$.



3h

11-Methoxytetrapheno[6,5-*b*]benzofuran-5,15-dione

Yellow solid, m.p. 242-244 °C (DCM/PE =3/1).

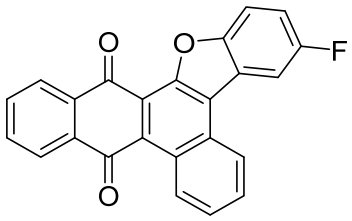
^{1}H NMR (500 MHz, $CDCl_3$) δ 9.67 (d, *J* = 8.8 Hz, 1H), 8.51 (d, *J* = 8.2 Hz, 1H), 8.29 – 8.24 (m, 2H), 7.84 – 7.73 (m, 5H), 7.71 – 7.66 (m, 1H), 7.18 (dd, *J* = 9.0, 2.3 Hz, 1H), 3.99 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 186.0, 183.1, 156.7, 153.3, 150.8, 135.0, 134.2, 133.7, 132.8, 132.1, 130.2, 129.7, 129.0, 127.9, 127.7, 127.2, 126.4, 125.4, 123.4, 123.3, 121.9, 116.9, 113.5, 105.7, 56.3.

IR(KBr) υ_{max}: 3110, 3077, 3001, 2962, 2932, 1678, 1655, 1593, 1571, 1475, 1467, 1458, 1330, 1297, 1236, 1188, 1172, 1061, 970, 832, 749, 726 cm^{-1}.

HRMS: (ESI) calcd for $C_{25}H_{15}O_4^+$ $[M+H]^+$ 379.09648; found 379.09616.

UV(in PhH) λ_{max} = 448 nm, ε_{max} = 10480 $mol^{-1}.L.cm^{-1}$.



3i

11-Fluorotetrapheno[6,5-*b*]benzofuran-5,15-dione

Yellow solid, m.p. >302 °C (DCM/PE =6/1).

^{1}H NMR (500 MHz, $CDCl_3$) δ 9.78 (d, *J* = 8.8 Hz, 1H), 8.61 (d, *J* = 8.2 Hz, 1H), 8.32 (d, *J* = 7.0 Hz, 2H), 8.14 (d, *J* = 8.6 Hz, 1H), 7.89 (dd, *J* = 13.3, 5.2 Hz, 2H), 7.82 (td, *J* = 14.2, 7.1 Hz, 3H), 7.42 – 7.35 (m, 1H).

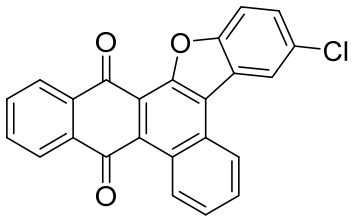
This compound is difficult to solute and no clear ^{13}CNMR signal in solvent could be obtained.

^{19}F NMR (471 MHz, $CDCl_3$) δ -118.13 – -118.25 (m).

IR(KBr) υ_{max}: 3093, 3063, 1673, 1654, 1593, 1571, 1470, 1458, 1333, 1301, 1293, 1231, 1174, 1156, 1127, 1057, 971, 839, 798, 750, 727 cm^{-1}.

HRMS: (ESI) calcd for $C_{24}H_{12}FO_3^+$ $[M+H]^+$ 367.07650; found 367.07648.

UV(in PhH) λ_{max} = 442 nm, ε_{max} = 9120 $mol^{-1}.L.cm^{-1}$.



3j

11-Chlorotetrapheno[6,5-*b*]benzofuran-5,15-dione

Yellow solid, m.p. >302 °C (DCM/PE =6/1).

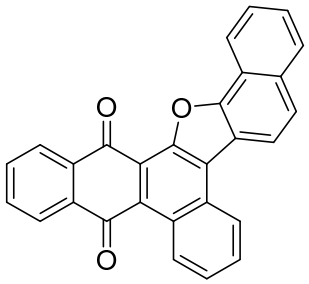
^{1}H NMR (500 MHz, $CDCl_3$) δ 9.76 (d, *J* = 8.8 Hz, 1H), 8.62 (d, *J* = 8.2 Hz, 1H), 8.43 (s, 1H), 8.31 (d, *J* = 7.1 Hz, 2H), 7.95 – 7.74 (m, 5H), 7.60 (d, *J* = 8.3 Hz, 1H).

This compound is difficult to solute and no clear ^{13}CNMR signal in solvent could be obtained.

IR(KBr) υ_{max}: 3106, 3065, 1672, 1655, 1571, 1456, 1333, 1294, 1241, 1145, 1115, 1057, 817, 753 cm^{-1}.

HRMS: (ESI) calcd for $C_{24}H_{12}ClO_3^+$ $[M+H]^+$ 383.04695; found 383.04648.

UV(in PhH) λ_{max} = 444 nm, ε_{max} = 8960 $mol^{-1}.L.cm^{-1}$.



3k

Naphtho[1,2-*b*]tetrapheno[5,6-*d*]furan-11,16-dione

Red solid, m.p. 274-276 °C (DCM/PE=6/1).

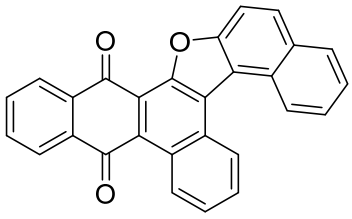
^{1}H NMR (500 MHz, $CDCl_3$) δ 9.70 (d, *J* = 8.8 Hz, 1H), 8.70 – 8.63 (m, 2H), 8.31 (d, *J* = 8.7 Hz, 1H), 8.26 (t, *J* = 8.3 Hz, 2H), 7.95 (d, *J* = 8.0 Hz, 1H), 7.83 – 7.76 (m, 3H), 7.74 (d, *J* = 7.7 Hz, 1H), 7.70 (d, *J* = 7.7 Hz, 1H), 7.67 (d, *J* = 8.4 Hz, 1H), 7.62 (t, *J* = 7.4 Hz, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 186.0, 183.2, 155.3, 150.9, 149.5, 135.1, 134.2, 133.6, 133.2, 132.8, 132.6, 132.0, 130.2, 129.5, 128.4, 128.21, 128.19, 127.6, 127.3, 127.2, 126.5, 126.3, 124.9, 123.9, 122.0, 121.4, 119.8, 118.4.

IR(KBr) υ_{max}: 3114, 3065, 3032, 1671, 1651, 1577, 1569, 1336, 1292, 1245, 1214, 1058, 804, 752, 737, 726 cm^{-1}.

HRMS: (ESI) calcd for $C_{28}H_{15}O_3^+$ $[M+H]^+$ 399.10157; found 399.10132.

UV(in PhH) λ_{max} = 464 nm, ε_{max} = 7760 $mol^{-1}.L.cm^{-1}$.



3l

Naphtho[2,1-*b*]tetrapheno[5,6-*d*]furan-11,16-dione

Dark red solid, m.p. 268-270 °C (DCM/PE=5/1).

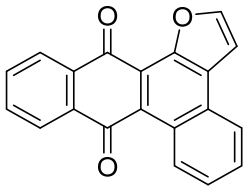
^{1}H NMR (500 MHz, $CDCl_3$) δ 9.69 (d, *J* = 8.5 Hz, 1H), 9.08 (d, *J* = 8.1 Hz, 1H), 8.98 (d, *J* = 8.4 Hz, 1H), 8.30 (dd, *J* = 5.7, 3.2 Hz, 2H), 8.06 (dd, *J* = 8.3, 4.2 Hz, 2H), 7.99 (d, *J* = 8.9 Hz, 1H), 7.80 (tdd, *J* = 7.1, 5.7, 3.9 Hz, 4H), 7.76 – 7.71 (m, 1H), 7.60 (t, *J* = 7.5 Hz, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 185.7, 183.4, 158.1, 150.0, 135.0, 134.3, 133.7, 133.0, 131.6, 131.5, 131.4, 130.2, 129.9, 129.0, 128.5, 128.5, 128.4, 128.2, 127.6, 127.2, 127.1, 126.5, 125.6, 125.4, 125.3, 121.5, 117.7, 113.3.

IR(KBr) υ_{max}: 3089, 3054, 1671, 1649, 1585, 1567, 1349, 1320, 1304, 1293, 1253, 1060, 999, 973, 801, 758, 736 cm^{-1}.

HRMS: (ESI) calcd for $C_{28}H_{15}O_3^+$ $[M+H]^+$ 399.10157; found 399.10117.

UV(in PhH) λ_{max} = 478 nm, ε_{max} = 10000 $mol^{-1}.L.cm^{-1}$.



3m

tetrapheno[6,5-b]furan-8,13-dione

Yellow solid, m.p. 250-252 °C (DCM/PE =3/1).

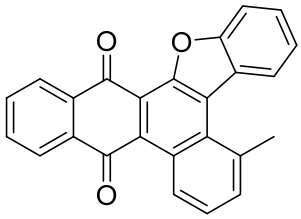
^{1}H NMR (500 MHz, $CDCl_3$) δ 9.74 – 9.69 (m, 1H), 8.31 – 8.24 (m, 2H), 8.19 – 8.15 (m, 1H), 8.14 (d, *J* = 2.1 Hz, 1H), 7.80 (td, *J* = 7.5, 1.7 Hz, 1H), 7.77 (td, *J* = 7.1, 1.4 Hz, 1H), 7.75 – 7.70 (m, 2H), 7.35 (d, *J* = 2.0 Hz, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 186.2, 183.5, 150.0, 148.1, 135.0, 134.3, 133.6, 132.6, 131.3, 130.8, 130.0, 129.2, 128.4, 128.0, 127.2, 127.1, 126.4, 123.9, 122.2, 105.7.

IR(KBr) υ_{max}: 3167, 3140, 3118, 3067, 1671, 1655, 1579, 1511, 1443, 1345, 1328, 1295, 1238, 1180, 1050, 961, 753, 728 cm^{-1}.

HRMS: (ESI) calcd for $C_{20}H_{11}O_3^+$ $[M+H]^+$ 299.07027; found 299.07010.

UV(in PhH) λ_{max} = 434 nm, ε_{max} = 6900 $mol^{-1}.L.cm^{-1}$.



3n

9-Methyltetrapheno[6,5-*b*]benzofuran-5,15-dione

Yellow solid, m.p. 214-216 °C (DCM/PE =3/1).

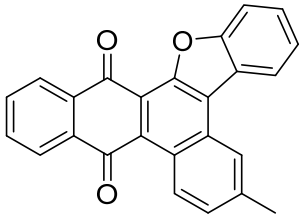
^{1}H NMR (500 MHz, $CDCl_3$) δ 9.47 – 9.42 (m, 1H), 8.30 – 8.22 (m, 3H), 7.85 (d, *J* = 8.3 Hz, 1H), 7.81 – 7.75 (m, 2H), 7.60 (dd, *J* = 6.7, 3.5 Hz, 2H), 7.58 – 7.53 (m, 1H), 7.43 – 7.39 (m, 1H), 3.06 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 186.1, 182.9, 158.2, 151.2, 135.1, 134.2, 133.6, 133.3, 132.9, 132.5, 132.3, 130.5, 129.1, 128.0, 127.6, 127.4, 127.2, 126.4, 126.2, 125.3, 123.7, 123.1, 121.3, 112.8, 24.9.

IR(KBr) υ_{max}: 3134, 3059, 2962, 2928, 1670, 1571, 1450, 1336, 1320, 1277, 1238, 1221, 1079, 963, 952, 771, 747, 724, 701 cm^{-1}.

HRMS: (ESI) calcd for $C_{25}H_{15}O_3^+$ $[M+H]^+$ 363.10157; found 363.10104.

UV(in PhH) λ_{max} = 467 nm, ε_{max} = 8400 $mol^{-1}.L.cm^{-1}$.



3o

8-Methyltetrapheno[6,5-b]benzofuran-5,15-dione

Yellow solid, m.p. 269-270 °C (DCM/PE =3/1).

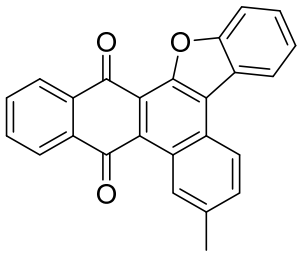
^{1}H NMR (500 MHz, $CDCl_3$) δ 9.61 (d, *J* = 9.0 Hz, 1H), 8.45 (d, *J* = 7.9 Hz, 1H), 8.43 (s, 1H), 8.28 (ddd, *J* = 9.2, 6.6, 2.2 Hz, 2H), 7.90 (d, *J* = 8.3 Hz, 1H), 7.83 – 7.77 (m, 2H), 7.62 (t, *J* = 7.7 Hz, 1H), 7.58 – 7.55 (m, 1H), 7.52 (t, *J* = 7.5 Hz, 1H), 2.67 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 186.2, 183.2, 158.3, 150.5, 140.4, 135.0, 134.1, 133.7, 132.9, 132.6, 130.4, 130.0, 129.2, 128.4, 127.2, 126.4, 126.1, 124.8, 124.0, 123.12, 123.07, 123.05, 121.2, 113.1, 22.3.

IR (KBr) υ_{max}: 3069, 3026, 2921, 2854, 1673, 1655, 1619, 1592, 1574, 1461, 1342, 1325, 1300, 1287, 1244, 1219, 1202, 1184, 1125, 1110, 1056, 1019, 797, 743 cm^{-1}.

HRMS: (ESI) calcd for $C_{25}H_{15}O_3^+$ $[M+H]^+$ 363.10157; found 363.10107.

UV(in PhH) λ_{max} = 446 nm, ε_{max} = 7160 $mol^{-1}.L.cm^{-1}$.



3p

7-Methyltetrapheno[6,5-*b*]benzofuran-5,15-dione

Yellow solid, m.p. 251-253 °C (DCM/PE =3/1).

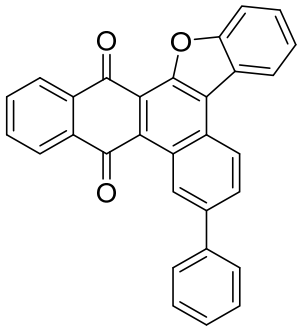
^{1}H NMR (500 MHz, $CDCl_3$) δ 9.49 (s, 1H), 8.51 (d, *J* = 8.4 Hz, 1H), 8.37 (d, *J* = 7.9 Hz, 1H), 8.29 – 8.24 (m, 2H), 7.87 (d, *J* = 8.3 Hz, 1H), 7.83 – 7.76 (m, 2H), 7.62 – 7.57 (m, 2H), 7.49 (t, *J* = 7.5 Hz, 1H), 2.61 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 186.1, 183.3, 158.4, 149.8, 138.2, 135.0, 134.2, 133.6, 132.8, 131.9, 130.3, 129.1, 128.5(2C), 128.2, 127.1, 126.4, 125.4, 124.0, 123.4, 123.04, 122.99, 121.8, 113.1, 22.5.

IR(KBr) υ_{max}: 3075, 3061, 2940, 2913, 1675, 1654, 1615, 1572, 1457, 1341, 1290, 1242, 1214, 1145, 1122, 1110, 1059, 968, 755, 748, 724 cm^{-1}.

HRMS: (ESI) calcd for $C_{25}H_{15}O_3^+$ $[M+H]^+$ 363.10157; found 363.10107.

UV(in PhH) λ_{max} = 457 nm, ε_{max} = 7440 $mol^{-1}.L.cm^{-1}$.



3q

7-Phenyltetrapheno[6,5-*b*]benzofuran-5,15-dione

Yellow solid, m.p. >302 °C (DCM/PE =5/1).

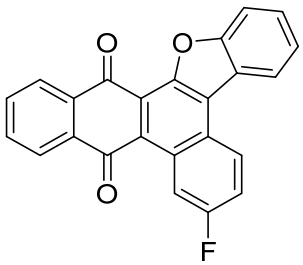
^{1}H NMR (500 MHz, $CDCl_3$) δ 10.06 (s, 1H), 8.73 (d, *J* = 8.6 Hz, 1H), 8.45 (d, *J* = 7.8 Hz, 1H), 8.29 (d, *J* = 7.1 Hz, 2H), 8.09 (dd, *J* = 8.6, 1.5 Hz, 1H), 7.91 (d, *J* = 8.3 Hz, 1H), 7.86 (d, *J* = 7.4 Hz, 2H), 7.83 – 7.77 (m, 2H), 7.63 (t, *J* = 7.7 Hz, 1H), 7.58 – 7.51 (m, 3H), 7.45 (t, *J* = 7.3 Hz, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 186.1, 183.3, 158.9, 158.5, 150.3, 140.8, 140.7, 135.0, 134.3, 133.7, 132.8, 131.2, 129.3, 129.21(2C), 129.15, 128.7, 128.5, 128.1, 128.0, 127.8(2C), 127.2, 126.5, 125.5, 124.2, 123.1, 123.0, 122.3, 113.2.

IR(KBr) υ_{max}: 3140, 3091, 3067, 3030, 1672, 1655, 1616, 1573, 1453, 1345, 1289, 1267, 1147, 1127, 1109, 1056, 970, 759, 751, 679 cm^{-1}.

HRMS: (ESI) calcd for $C_{30}H_{17}O_3^+$ $[M+H]^+$ 425.11722; found 425.11682.

UV(in PhH) λ_{max} = 465 nm, ε_{max} = 6320 $mol^{-1}.L.cm^{-1}$.



3r

7-Fluorotetrapheno[6,5-b]benzofuran-5,15-dione.

Yellow solid, m.p. 286-288 °C (DCM/PE =5/1).

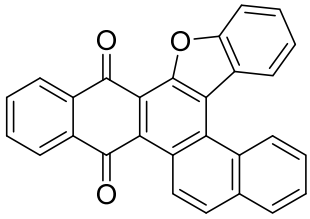
^{1}H NMR (500 MHz, $CDCl_3$) δ 9.59 (dd, *J* = 12.9, 2.0 Hz, 1H), 8.68 (dd, *J* = 8.9, 6.0 Hz, 1H), 8.39 (d, *J* = 7.8 Hz, 1H), 8.34 – 8.24 (m, 2H), 7.90 (d, *J* = 8.3 Hz, 1H), 7.87 – 7.77 (m, 2H), 7.68 – 7.58 (m, 2H), 7.53 (t, *J* = 7.5 Hz, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 185.7, 183.1, 162.4 (d, *J* = 246.9 Hz), 158.6, 149.8, 134.8, 134.4, 133.9, 132.8, 129.3 (d, *J* = 10.6 Hz), 129.1, 129.0, 128.0, 127.9, 127.4, 126.5, 126.0, 125.7 (d, *J* = 9.0 Hz), 124.3, 122.9, 122.7 (d, *J* = 3.5 Hz), 119.9 (d, *J* = 25.7 Hz), 114.4 (d, *J* = 25.5 Hz), 113.3.

^{19}F NMR (471 MHz, $CDCl_3$) δ -110.69 (dt, *J* = 13.0, 6.6 Hz).

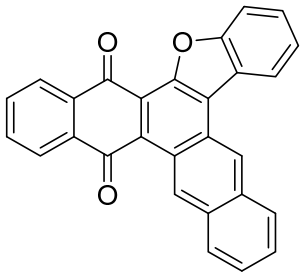
IR(KBr) υ_{max}: 3128, 3079, 3054, 1669, 1595, 1573, 1456, 1435, 1409, 1341, 1325, 1297, 1282, 1246, 1222, 1195, 1160, 1139, 1113, 1056, 1026, 971, 880, 812, 733, 721, 675 cm^{-1}.

HRMS: (ESI) calcd for $C_{24}H_{12}FO_3^+$ $[M+H]^+$ 367.07650; found 367.07632.
UV(in PhH) λ_{max} = 450 nm, ε_{max} = 8880 $mol^{-1}.L.cm^{-1}$.



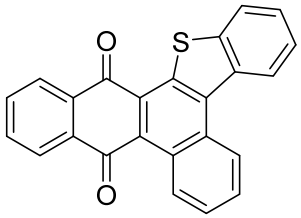
3s

Benzo[3,4]tetrapheno[6,5-b]benzofuran-10,15-dione.
Yellow solid, m.p. 244-246 °C (DCM/PE =3/1).
^{1}H NMR (500 MHz, $CDCl_3$) δ 9.49 (d, *J* = 9.4 Hz, 1H), 9.14 (d, *J* = 8.2 Hz, 1H), 8.60 (d, *J* = 8.0 Hz, 1H), 8.36 – 8.28 (m, 2H), 7.99 (d, *J* = 7.7 Hz, 1H), 7.95 (d, *J* = 9.4 Hz, 1H), 7.92 (d, *J* = 8.3 Hz, 1H), 7.85 – 7.79 (m, 2H), 7.77 (t, *J* = 7.0 Hz, 1H), 7.69 (dd, *J* = 11.1, 4.0 Hz, 1H), 7.63 (dd, *J* = 11.4, 4.1 Hz, 1H), 7.41 (t, *J* = 7.3 Hz, 1H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 186.3, 183.0, 158.8, 152.4, 135.3, 134.2, 133.8, 133.4, 133.2, 132.6, 129.28, 129.26, 128.9, 128.6, 128.5, 128.3, 128.1, 127.8, 127.4, 126.5, 126.0, 125.6(2C), 124.1, 123.5, 123.0, 120.5, 113.1.
IR(KBr) υ_{max}: 3136, 3067, 3042, 1674, 1655, 1616, 1453, 1296, 1269, 1256, 1243, 1212, 1158, 1064, 1025, 755, 743, 712, 658 cm^{-1}.
HRMS: (ESI) calcd for $C_{28}H_{15}O_3^+$ $[M+H]^+$ 399.10157; found 399.10144.
UV(in PhH) λ_{max} = 450 nm, ε_{max} =11300 $mol^{-1}.L.cm^{-1}$.



3t

Pentapheno[6,7-b]benzofuran-6,11-dione
Purple solid, m.p. >302 °C (DCM/PE =4/1).
^{1}H NMR (500 MHz, $CDCl_3$) δ 10.39 (s, 1H), 9.08 (s, 1H), 8.57 (d, *J* = 7.8 Hz, 1H), 8.31 (dd, *J* = 7.5, 1.2 Hz, 1H), 8.28 (dd, *J* = 7.4, 1.4 Hz, 1H), 8.16 (d, *J* = 8.4 Hz, 1H), 8.08 (d, *J* = 8.3 Hz, 1H), 7.91 (d, *J* = 8.2 Hz, 1H), 7.86 – 7.78 (m, 2H), 7.62 (t, *J* = 7.8 Hz, 2H), 7.56 (dd, *J* = 15.2, 7.4 Hz, 2H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 185.9, 183.0, 158.0, 149.0, 134.7, 134.1, 133.6, 133.0, 132.58, 132.56, 131.5, 130.1, 129.6, 128.8, 128.2, 128.14, 128.11, 127.5, 127.0, 126.3, 126.2, 125.3, 124.4, 124.1, 123.2, 122.7, 121.7, 113.0.
IR(KBr) υ_{max}: 3102, 3073, 3048, 1670, 1651, 1591, 1552, 1469, 1449, 1340, 1332, 1307, 1290, 1255, 1228, 1211, 1181, 1158, 1146, 1132, 1106, 1049, 1020, 745, 737 cm^{-1}.
HRMS: (ESI) calcd for $C_{28}H_{15}O_3^+$ $[M+H]^+$ 399.10157; found 399.10120.
UV(in PhH) λ_{max} = 537 nm, ε_{max} =14200 $mol^{-1}.L.cm^{-1}$.



3u

Benzo[b]tetrapheno[5,6-d]thiophene-5,15-dione

Yellow solid, m.p. 244-246 °C (DCM/PE =3/1).

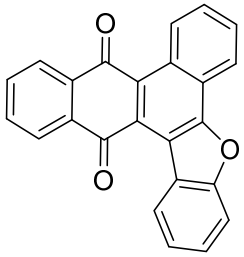
^{1}H NMR (500 MHz, $CDCl_3$) δ 9.64 (d, *J* = 8.2 Hz, 1H), 9.00 (d, *J* = 8.4 Hz, 1H), 8.77 (d, *J* = 7.6 Hz, 1H), 8.28 – 8.22 (m, 2H), 8.06 – 8.00 (m, 1H), 7.82 – 7.74 (m, 3H), 7.73 – 7.68 (m, 1H), 7.58 – 7.51 (m, 2H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 185.8, 184.3, 145.7, 136.3, 134.91, 134.85, 134.4, 134.0, 133.7, 133.3, 132.0, 130.1, 129.8, 129.2, 129.1, 128.2, 128.0, 127.3, 127.1, 126.7, 125.8, 125.3, 123.8, 123.3.

IR(KBr) υ_{max}: 3130, 3063, 1658, 1591, 1528, 1430, 1405, 1333, 1310, 1291, 1272, 1221, 1210, 1148, 1099, 1083, 1068, 1058, 1043, 1014, 782, 754, 718, 658 cm^{-1}.

HRMS: (ESI) calcd for $C_{24}H_{13}O_2S^+$ $[M+H]^+$ 365.06308; found 365.06287.

UV(in PhH) λ_{max} = 462 nm, ε_{max} = 8160 $mol^{-1}.L.cm^{-1}$.



5a

Tetrapheno[5,6-b]benzofuran-10,15-dione

Yellow solid, m.p. 216-218 °C (DCM/PE =2/1).

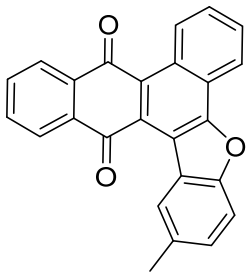
^{1}H NMR (500 MHz, $CDCl_3$) δ 9.75 – 9.70 (m, 1H), 9.30 – 9.23 (m, 1H), 8.65 – 8.60 (m, 1H), 8.36 – 8.27 (m, 2H), 7.89 – 7.79 (m, 4H), 7.77 (d, *J* = 8.1 Hz, 1H), 7.64 – 7.58 (m, 1H), 7.57 – 7.50 (m, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 186.0, 185.1, 157.1, 156.4, 134.6, 134.0, 133.4, 132.9, 132.0, 130.3, 129.8, 129.5, 129.0, 128.0, 127.5, 127.4, 126.9, 126.4, 124.1, 123.8(2C), 121.5, 116.5, 111.5.

IR(KBr) υ_{max}: 3116, 3052, 3016, 1676, 1655, 1594, 1453, 1347, 1294, 1277, 1244, 1203, 1110, 1086, 1062, 1048, 1021, 1005, 795, 760, 746, 716, 681 cm^{-1}.

HRMS: (ESI) calcd for $C_{24}H_{13}O_3^+$ $[M+H]^+$ 349.08592; found 349.08557.

UV(in PhH) λ_{max} = 445 nm, ε_{max} = 5920 $mol^{-1}.L.cm^{-1}$.



5b

2-Methyltetrapheno[5,6-b]benzofuran-10,15-dione

Yellow solid, m.p. 230-232 °C (DCM/PE =3/1).

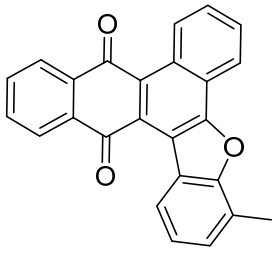
^{1}H NMR (500 MHz, $CDCl_3$) δ 9.60 (dd, *J* = 7.3, 2.1 Hz, 1H), 8.88 (s, 1H), 8.44 (dd, *J* = 6.8, 2.6 Hz, 1H), 8.28 – 8.20 (m, 2H), 7.82 – 7.76 (m, 2H), 7.72 (ddt, *J* = 9.5, 6.8, 3.5 Hz, 2H), 7.52 (d, *J* = 8.3 Hz, 1H), 7.33 (d, *J* = 7.4 Hz, 1H), 2.59 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 186.1, 185.3, 156.8, 155.5, 134.7, 134.0, 133.4, 133.3, 133.0, 132.1, 130.3, 129.7, 129.5, 129.2, 129.0, 127.34, 127.29, 126.9, 126.4, 124.0, 123.9, 121.6, 116.5, 110.9, 22.0.

IR(KBr) υ_{max}: 3120, 3069, 3020, 2926, 1672, 1660, 1591, 1344, 1319, 1298, 1203, 1116, 800, 755, 683 cm^{-1}.

HRMS: (ESI) calcd for $C_{25}H_{15}O_3^+$ $[M+H]^+$ 363.10157; found 363.10107.

UV(in PhH) λ_{max} = 450 nm, ε_{max} =8240 $mol^{-1}.L.cm^{-1}$.



5c

4-Methyltetrapheno[5,6-b]benzofuran-10,15-dione

Yellow solid, m.p. 206-208 °C (DCM/PE =3/1).

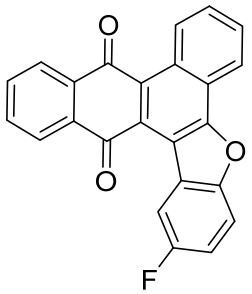
^{1}H NMR (500 MHz, $CDCl_3$) δ 9.62 – 9.58 (m, 1H), 8.95 – 8.90 (m, 1H), 8.49 – 8.44 (m, 1H), 8.26 – 8.20 (m, 2H), 7.81 – 7.74 (m, 2H), 7.74 – 7.67 (m, 2H), 7.35 – 7.30 (m, 2H), 2.65 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 186.1, 185.2, 156.3, 156.0, 134.7, 134.0, 133.4, 133.0, 132.1, 130.3, 129.7, 129.5, 129.1, 128.9, 127.3, 126.9, 126.4, 124.9, 123.9, 123.7, 123.6, 121.53, 121.51, 116.9, 15.3.

IR(KBr) υ_{max}: 3140, 3067, 3022, 2923, 1675, 1657, 1592, 1435, 1343, 1300, 1249, 1196, 1110, 1058, 798, 756, 745 cm^{-1}.

HRMS: (ESI) calcd for $C_{25}H_{15}O_3^+$ $[M+H]^+$ 363.10157; found 363.10101.

UV(in PhH) λ_{max} = 459 nm, ε_{max} =9240 $mol^{-1}.L.cm^{-1}$.



5d

2-Fluorotetrapheno[5,6-b]benzofuran-10,15-dione

Yellow solid, m.p. 256-258 °C (DCM/PE =4/1)

^{1}H NMR (500 MHz, $CDCl_3$) δ 9.68 (dd, *J* = 7.3, 1.8 Hz, 1H), 8.96 (dd, *J* = 10.4, 2.7 Hz, 1H), 8.57 – 8.51 (m, 1H), 8.34 – 8.25 (m, 2H), 7.85 – 7.77 (m, 4H), 7.66 (dd, *J* = 8.9, 4.4 Hz, 1H), 7.31 (td, *J* = 8.6, 2.8 Hz, 1H).

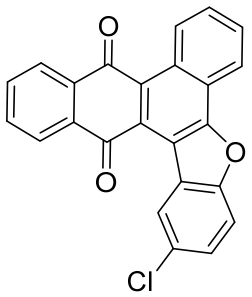
This compound is difficult to solute and no clear ^{13}CNMR signal in solvent could be obtained.

^{19}F NMR (471 MHz, $CDCl_3$) δ -118.68 (td, *J* = 8.9, 4.4 Hz).

IR(KBr) υ_{max}: 3138, 3071, 1671, 1658, 1591, 1572, 1462, 1449, 1419, 1346, 1300, 1258, 1243, 1171, 1160, 1108, 1098, 1088, 1009, 811, 770, 759, 686 cm^{-1}.

HRMS: (ESI) calcd for $C_{24}H_{12}FO_3^+$ $[M+H]^+$ 367.07650; found 367.07605.

UV(in PhH) λ_{max} = 439 nm, ε_{max} =7750 mol^{-1}.L.cm^{-1}.



5e

2-Chlorotetrapheno[5,6-b]benzofuran-10,15-dione

Yellow solid, m.p. 262-264 °C (DCM/PE =3/1)

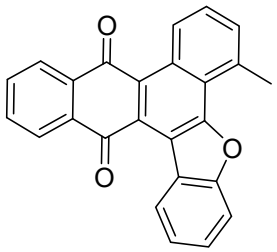
^{1}H NMR (500 MHz, $CDCl_3$) δ 9.63 (s, 1H), 9.18 (s, 1H), 8.47 (s, 1H), 8.33 – 8.16 (m, 2H), 7.88 – 7.72 (m, 4H), 7.60 (d, *J* = 7.5 Hz, 1H), 7.55 – 7.48 (m, 1H).

This compound is difficult to solute and no clear ^{13}CNMR signal in solvent could be obtained.

IR(KBr) υ_{max}: 3138, 3081, 1674, 1656, 1590, 1448, 1346, 1315, 1298, 1254, 1243, 1113, 1087, 1076, 1047, 1007, 802, 760, 700, 686 cm^{-1}.

HRMS: (ESI) calcd for $C_{24}H_{12}ClO_3^+$ $[M+H]^+$ 383.04695; found 383.04642.

UV(in PhH) λ_{max} = 440 nm, ε_{max} =7120 mol^{-1}.L.cm^{-1}.



5f

6-Methyltetrapheno[5,6-b]benzofuran-10,15-dione

Yellow solid, m.p. 202-204 ° (DCM/PE=3/1).

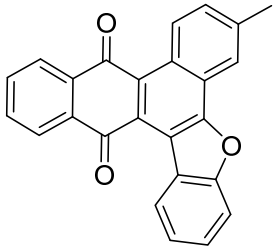
^{1}H NMR (500 MHz, $CDCl_3$) δ 9.41 (d, *J* = 8.8 Hz, 1H), 9.13 (d, *J* = 8.1 Hz, 1H), 8.25 (d, *J* = 6.9 Hz, 1H), 8.22 (d, *J* = 7.0 Hz, 1H), 7.81 – 7.75 (m, 2H), 7.67 (d, *J* = 8.1 Hz, 1H), 7.59 (t, *J* = 7.8 Hz, 1H), 7.54 (t, *J* = 7.6 Hz, 1H), 7.49 (d, *J* = 6.9 Hz, 1H), 7.46 (t, *J* = 7.7 Hz, 1H), 3.11 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 186.3, 185.3, 157.5, 156.8, 135.1, 134.3, 134.0, 133.4, 133.0, 131.74, 131.71, 131.5, 129.1, 128.4, 127.8, 127.3, 127.2, 127.0, 126.4, 123.9, 123.7, 123.2, 117.2, 111.4, 24.2.

IR(KBr) υ_{max}: 3128, 3063, 2918, 2849, 1738, 1673, 1650, 1455, 1338, 1290, 1245, 772, 739, 716 cm^{-1}.

HRMS: (ESI) calcd for $C_{25}H_{15}O_3^+$ $[M+H]^+$ 363.10157; found 363.10132.

UV(in PhH) λ_{max} = 457 nm, ε_{max} =9280 $mol^{-1}.L.cm^{-1}$.



5g

7-Methyltetrapheno[5,6-b]benzofuran-10,15-dione

Yellow solid, m.p. 252-254 °C (DCM/PE=3/1).

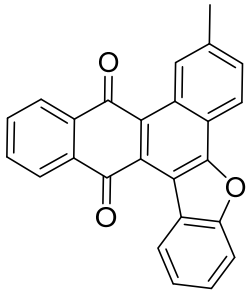
^{1}H NMR (500 MHz, $CDCl_3$) δ 9.55 (d, *J* = 9.0 Hz, 1H), 9.22 (d, *J* = 8.0 Hz, 1H), 8.33 – 8.28 (m, 2H), 8.28 – 8.25 (m, 1H), 7.83 – 7.76 (m, 2H), 7.71 (d, *J* = 8.1 Hz, 1H), 7.62 – 7.55 (m, 2H), 7.49 (t, *J* = 7.6 Hz, 1H), 2.63 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 186.3, 185.4, 157.2, 156.2, 139.8, 134.8, 134.0, 133.4, 133.1, 132.2, 131.4, 129.4, 128.7, 128.0, 127.7, 127.6, 127.0, 126.5, 124.31, 124.29, 123.8, 120.7, 116.8, 111.5, 22.0.

IR(KBr) υ_{max}: 3122, 3059, 3024, 2919, 2856, 1668, 1630, 1457, 1347, 1291, 1268, 1249, 1203, 1181, 1163, 1113, 1089, 1061, 1040, 1013, 788, 757, 721 cm^{-1}.

HRMS: (ESI) calcd for $C_{25}H_{15}O_3^+$ $[M+H]^+$ 363.10157; found 363.10126.

UV(in PhH) λ_{max} = 449 nm, ε_{max} =9200 $mol^{-1}.L.cm^{-1}$.



5h

8-Methyltetrapheno[5,6-b]benzofuran-10,15-dione

Yellow solid, m.p. 298-298°C (DCM/PE=3/1).

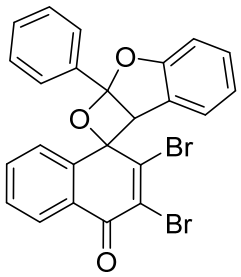
^{1}H NMR (500 MHz, $CDCl_3$) δ 9.45 (s, 1H), 9.17 (dd, *J* = 8.1, 0.8 Hz, 1H), 8.40 (d, *J* = 8.4 Hz, 1H), 8.29 – 8.23 (m, 2H), 7.82 – 7.75 (m, 2H), 7.68 (d, *J* = 8.1 Hz, 1H), 7.59 – 7.53 (m, 2H), 7.50 – 7.45 (m, 1H), 2.63 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 186.3, 185.5, 157.2, 156.8, 140.4, 134.9, 134.1, 133.4, 133.1, 132.3, 131.3, 130.9, 128.6, 127.9, 127.5, 127.0, 126.9, 126.5, 124.3, 123.8, 122.2, 121.5, 116.1, 111.5, 22.8.

IR(KBr) υ_{max}: 3108, 3057, 3016, 2917, 1672, 1655, 1593, 1449, 1348, 1293, 1246, 1206, 1109, 1087, 816, 744, 720 cm^{-1}.

HRMS: (ESI) calcd for $C_{25}H_{15}O_3^+$ $[M+H]^+$ 363.10157; found 363.10107.

UV(in PhH) λ_{max} = 459 nm, ε_{max} =9500 $mol^{-1}.L.cm^{-1}$.



6a

2,3-Dibromo-7a'-phenyl-2a',7a'-dihydro-4H-spiro[naphthalene-1,2'-oxeto[2,3-b]benzofuran]-4-one

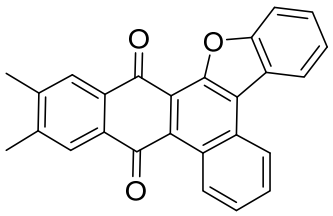
White solid, m.p. 154-156 °C (DCM/PE =2/1).

^{1}H NMR (500 MHz, DMSO) δ 7.90 (dd, *J* = 7.7, 1.2 Hz, 1H), 7.77 – 7.73 (m, 1H), 7.59 (d, *J* = 1.6 Hz, 1H), 7.57 (d, *J* = 1.2 Hz, 1H), 7.53 – 7.45 (m, 3H), 7.40 (td, *J* = 7.5, 1.1 Hz, 1H), 7.34 (td, *J* = 7.6, 1.4 Hz, 1H), 7.13 – 7.08 (m, 1H), 6.92 (d, *J* = 8.0 Hz, 1H), 6.73 (d, *J* = 7.3 Hz, 1H), 6.60 (t, *J* = 7.4 Hz, 1H), 5.36 (s, 1H).

^{13}C NMR (126 MHz, DMSO) δ 175.4, 160.7, 151.4, 138.8, 137.1, 132.5, 130.1, 129.4, 129.2, 129.1, 128.3(2C), 127.3, 127.2, 127.1, 125.8, 124.9(2C), 123.7, 122.0, 115.8, 109.2, 88.4, 60.1.

IR(KBr) υ_{max}: 3067, 3038, 3001, 1666, 1593, 1555, 1475, 1463, 1451, 1337, 1269, 1235, 1129, 974, 954, 941, 914, 880, 764, 750 cm^{-1}.

HRMS: (ESI) calcd for $C_{24}H_{15}Br_2O_3^+$ $[M+H]^+$ 508.93825; found 508.93781.



7a

2,3-Dimethyltetrapheno[6,5-b]benzofuran-5,15-dione.

Yellow blocks, m.p. 266-268 °C (DCM/PE = 4/1).

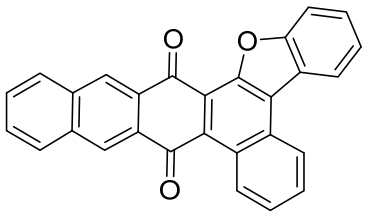
^{1}H NMR (500 MHz, $CDCl_3$) δ 9.74 (d, *J* = 8.6 Hz, 1H), 8.71 – 8.65 (m, 1H), 8.44 (d, *J* = 7.9 Hz, 1H), 8.00 (s, 2H), 7.91 (d, *J* = 8.3 Hz, 1H), 7.81 (ddd, *J* = 8.2, 6.8, 1.3 Hz, 1H), 7.73 (ddd, *J* = 8.4, 6.8, 1.4 Hz, 1H), 7.62 (ddd, *J* = 8.3, 7.2, 1.2 Hz, 1H), 7.52 (td, *J* = 7.5, 7.1, 1.0 Hz, 1H), 2.45 (s, 6H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 186.3, 183.3, 158.3, 150.2, 144.1, 143.5, 132.9, 132.1, 130.8, 130.2, 129.6, 129.3, 128.4, 128.1, 127.9, 127.3(2C), 125.2, 124.0, 123.6, 123.05, 122.98, 122.0, 113.1, 20.5, 20.4.

IR(KBr) υ_{max}: 3097, 3061, 2983, 2942, 1738, 1667, 1638, 1600, 1451, 1340, 1321, 1306, 782, 766, 746 cm^{-1}.

HRMS: (ESI) calcd for $C_{26}H_{17}O_3^+$ $[M+H]^+$ 377.11722; found 377.11667.

UV (in PhH) λ_{max} = 448 nm, ε_{max} = 8000 $mol^{-1}.L.cm^{-1}$.



8a

Benzo[3,4]tetraceno[1,2-b]benzofuran-9,16-dione

Yellow solid, m.p. >302 °C (DCM/PE =5/1).

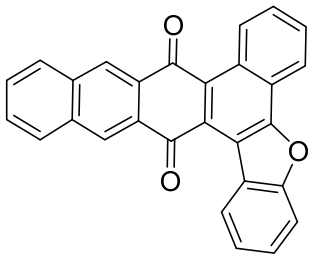
^{1}H NMR (500 MHz, $CDCl_3$) δ 9.85 (d, *J* = 8.6 Hz, 1H), 8.82 (d, *J* = 5.4 Hz, 2H), 8.75 (d, *J* = 7.7 Hz, 1H), 8.49 (d, *J* = 7.7 Hz, 1H), 8.13 (d, *J* = 8.5 Hz, 2H), 7.96 (d, *J* = 8.3 Hz, 1H), 7.88 (dd, *J* = 7.6, 6.3 Hz, 1H), 7.80 (dd, *J* = 8.6, 7.0 Hz, 1H), 7.73 – 7.68 (m, 2H), 7.66 (t, *J* = 7.8 Hz, 1H), 7.56 (t, *J* = 7.5 Hz, 1H).

This compound is difficult to solute and no clear ^{13}CNMR signal in solvent could be obtained.

IR(KBr) υ_{max}: 3126, 3091, 3059, 1672, 1614, 1570, 1453, 1438, 1403, 1338, 1318, 1288, 1245, 1209, 1180, 1162, 1142, 1054, 1044, 974, 842, 782, 769, 746 cm^{-1}.

HRMS: (ESI) calcd for $C_{28}H_{15}O_3^+$ $[M+H]^+$ 399.10157; found 399.10114.

UV(in PhH) λ_{max} = 435 nm, ε_{max} = 13280 $mol^{-1}.L.cm^{-1}$.



8b

Benzo[3,4]tetraceno[2,1-b]benzofuran-10,17-dione

Yellow solid, m.p. >302 °C (DCM/PE =5/1).

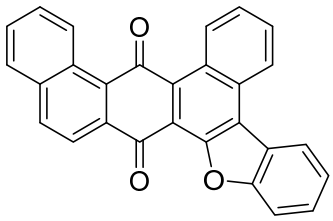
^{1}H NMR (500 MHz, $CDCl_3$) δ 9.81 (dd, *J* = 7.7, 1.6 Hz, 1H), 9.30 (d, *J* = 7.9 Hz, 1H), 8.87 (s, 1H), 8.82 (s, 1H), 8.64 (dd, *J* = 7.1, 2.1 Hz, 1H), 8.13 (dd, *J* = 5.2, 3.6 Hz, 2H), 7.89 – 7.81 (m, 2H), 7.78 (d, *J* = 8.1 Hz, 1H), 7.74 – 7.67 (m, 2H), 7.62 (t, *J* = 7.4 Hz, 1H), 7.55 (t, *J* = 7.5 Hz, 1H).

This compound is difficult to solute and no clear ^{13}CNMR signal in solvent could be obtained.

IR(KBr) υ_{max}: 3134, 3052, 1671, 1619, 1460, 1452, 1425, 1403, 1367, 1343, 1296, 1250, 1217, 1198, 1186, 1131, 1077, 1055, 1025, 1017, 769, 736, 618 cm^{-1}.

HRMS: (ESI) calcd for $C_{28}H_{15}O_3^+$ $[M+H]^+$ 399.10157; found 399.10114.

UV(in PhH) λ_{max} = 428 nm, ε_{max} =11440 $mol^{-1}.L.cm^{-1}$.



9a

Benzo[10,11]tetrapheno[6,5-b]benzofuran-7,17-dione

Yellow solid, m.p. >302 °C (DCM/PE =4/1).

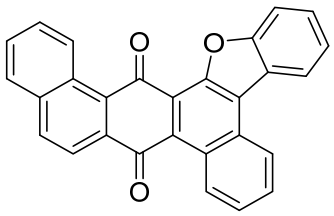
^{1}H NMR (500 MHz, $CDCl_3$) δ 9.66 (d, *J* = 8.7 Hz, 1H), 9.61 (d, *J* = 8.7 Hz, 1H), 8.68 (d, *J* = 8.2 Hz, 1H), 8.44 (d, *J* = 7.8 Hz, 1H), 8.32 (d, *J* = 8.5 Hz, 1H), 8.19 (d, *J* = 8.5 Hz, 1H), 7.93 (t, *J* = 8.3 Hz, 2H), 7.84 – 7.72 (m, 3H), 7.67 (t, *J* = 7.6 Hz, 1H), 7.63 (t, *J* = 7.8 Hz, 1H), 7.52 (t, *J* = 7.5 Hz, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 186.7, 186.1, 158.3, 150.0, 136.4, 135.3, 135.1, 131.9, 129.97, 129.96, 129.66, 129.62, 129.0(2C), 128.8, 128.7, 128.5, 128.2, 127.9, 127.4, 125.5, 124.1, 123.8, 123.6, 123.2, 123.1, 122.7, 113.1.

IR(KBr) υ_{max}: 3079, 3059, 3038, 1668, 1615, 1569, 1454, 1342, 1298, 1235, 1209, 1169, 1146, 1122, 1074, 1057, 772, 744, 724 cm^{-1}.

HRMS: (ESI) calcd for $C_{28}H_{15}O_3^+$ $[M+H]^+$ 399.10157; found 399.10098.

UV(in PhH) λ_{max} = 428 nm, ε_{max} =10350 $mol^{-1}.L.cm^{-1}$.



9a'

Benzo[8,9]tetrapheno[6,5-b]benzofuran-7,17-dione

Yellow solid, m.p. >302 °C (DCM/PE =4/1).

^{1}H NMR (500 MHz, $CDCl_3$) δ 9.35 (d, *J* = 8.7 Hz, 1H), 9.25 (d, *J* = 8.6 Hz, 1H), 8.71 (d, *J* = 8.2 Hz, 1H), 8.45 (d, *J* = 7.8 Hz, 1H), 8.35 (d, *J* = 8.5 Hz, 1H), 8.17 (d, *J* = 8.5 Hz, 1H), 7.94 (t, *J* = 8.1 Hz, 2H), 7.86 (t, *J* = 7.5 Hz, 1H), 7.80 – 7.74 (m, 2H), 7.68 (t, *J* = 7.4 Hz, 1H), 7.63 (t, *J* = 7.7 Hz, 1H), 7.54 (t, *J* = 7.5 Hz, 1H).

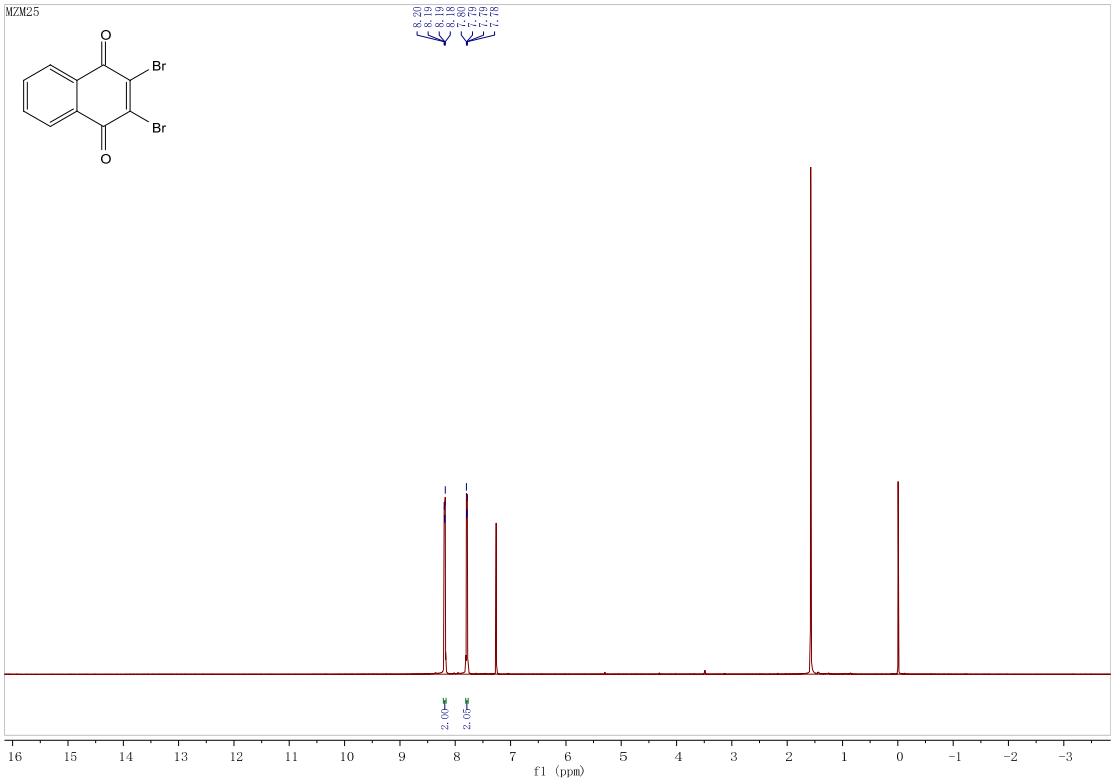
^{13}C NMR (126 MHz, $CDCl_3$) δ 189.6, 183.5, 158.2, 149.6, 136.7, 134.4, 133.1, 133.0, 132.6, 132.3, 130.0, 129.8, 129.6, 129.5, 128.98, 128.96, 128.32, 128.30, 127.6, 127.2, 124.4, 124.2, 123.9, 123.2, 122.9, 121.8, 120.1, 113.2.

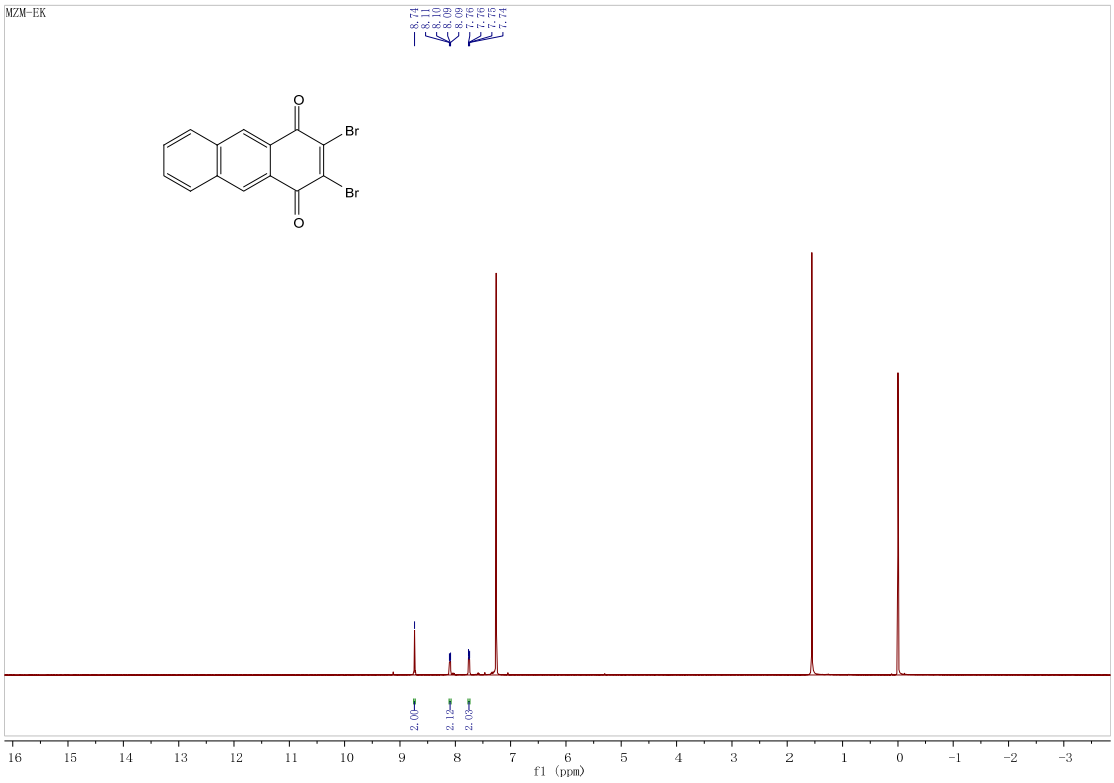
IR(KBr) υ_{max}: 3091, 3075, 1675, 1654, 1615, 1455, 1345, 1325, 1293, 1217, 1203, 1190, 1170, 1164, 1149, 1117, 1110, 1100, 1044, 1035, 978, 767, 739, 725 cm^{-1}.

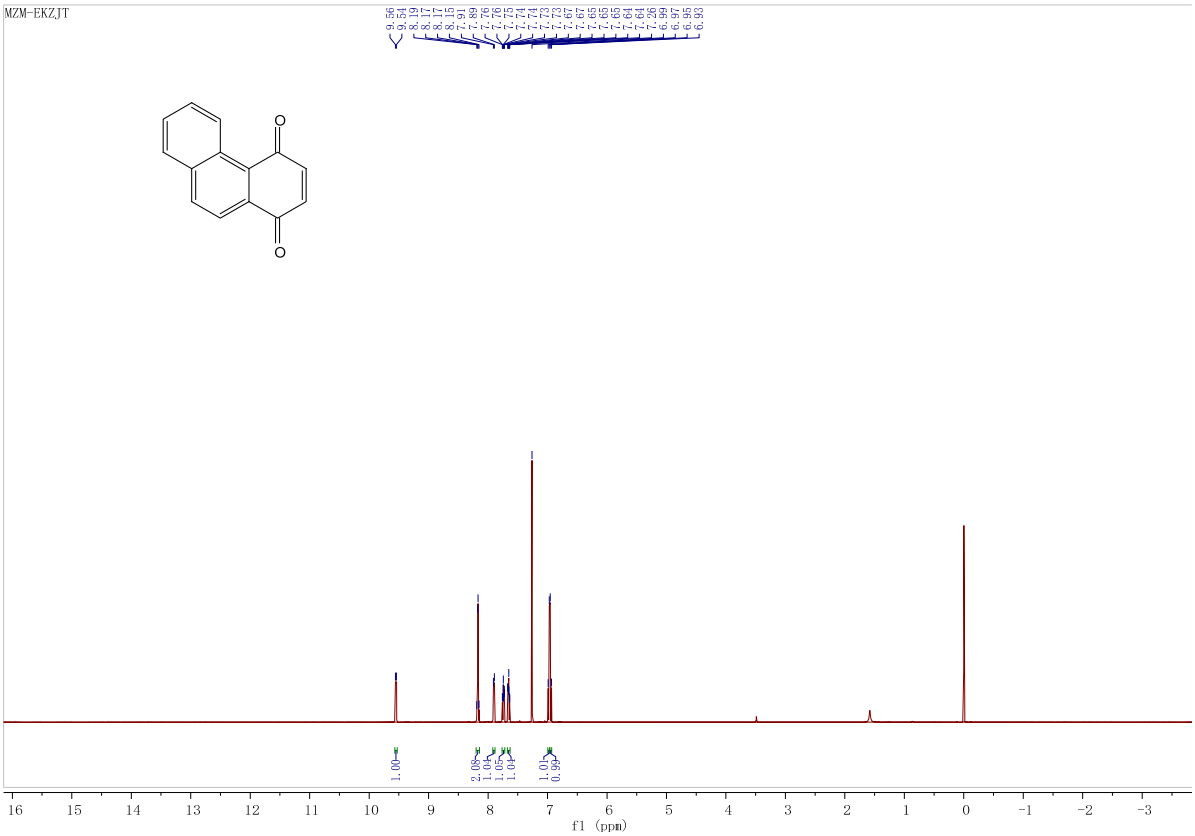
HRMS: (ESI) calcd for $C_{28}H_{15}O_3^+$ $[M+H]^+$ 399.10157; found 399.10098.

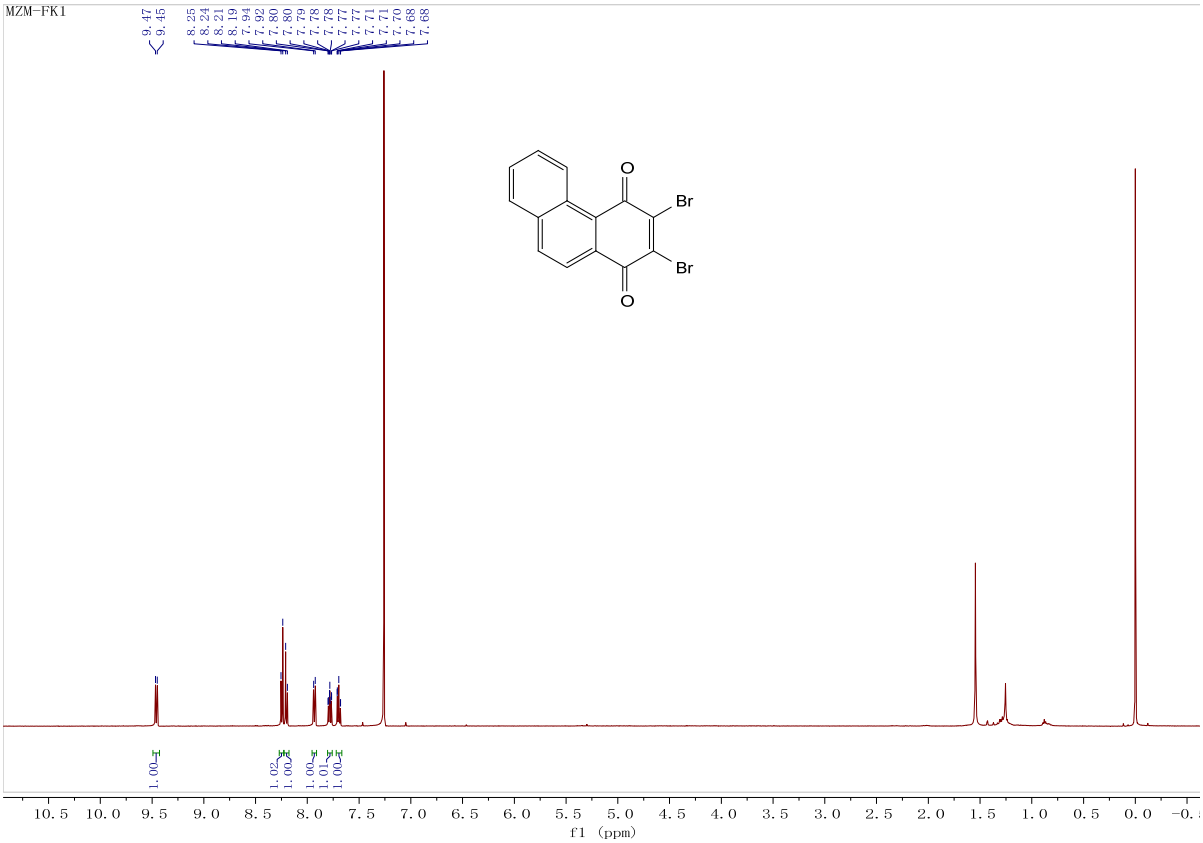
UV(in PhH) λ_{max} = 454 nm, ε_{max} =10200 $mol^{-1}.L.cm^{-1}$.

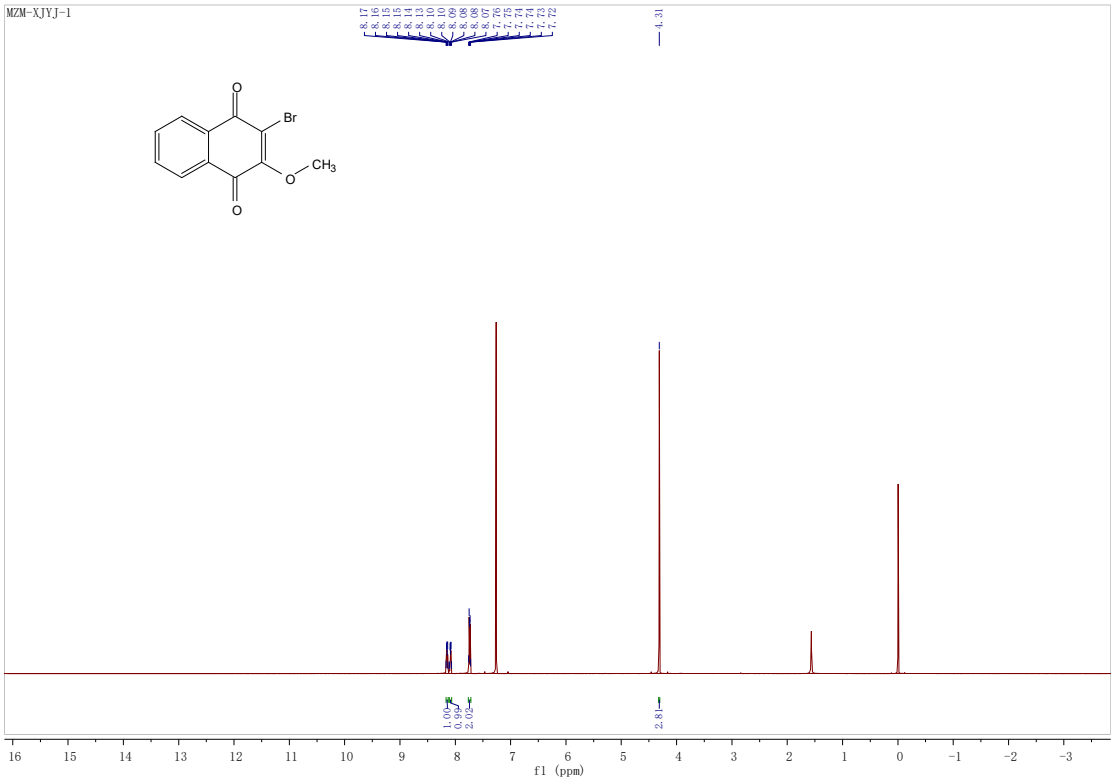
6. The NMR and HRMS Charts

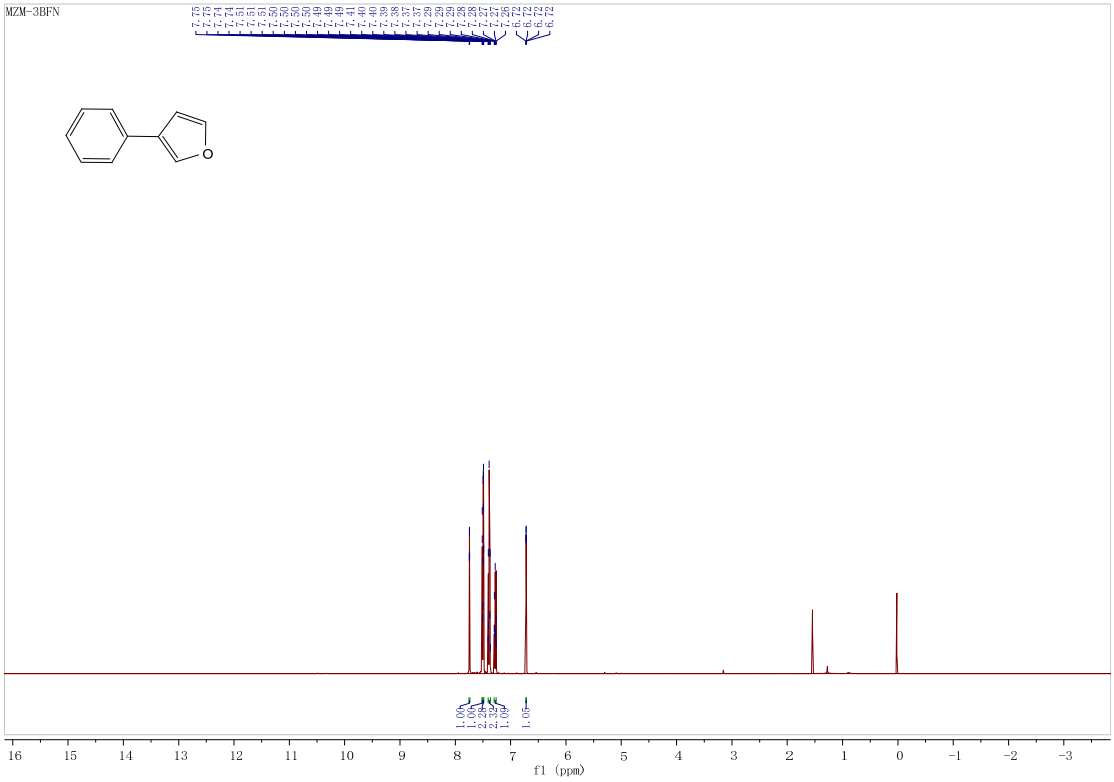


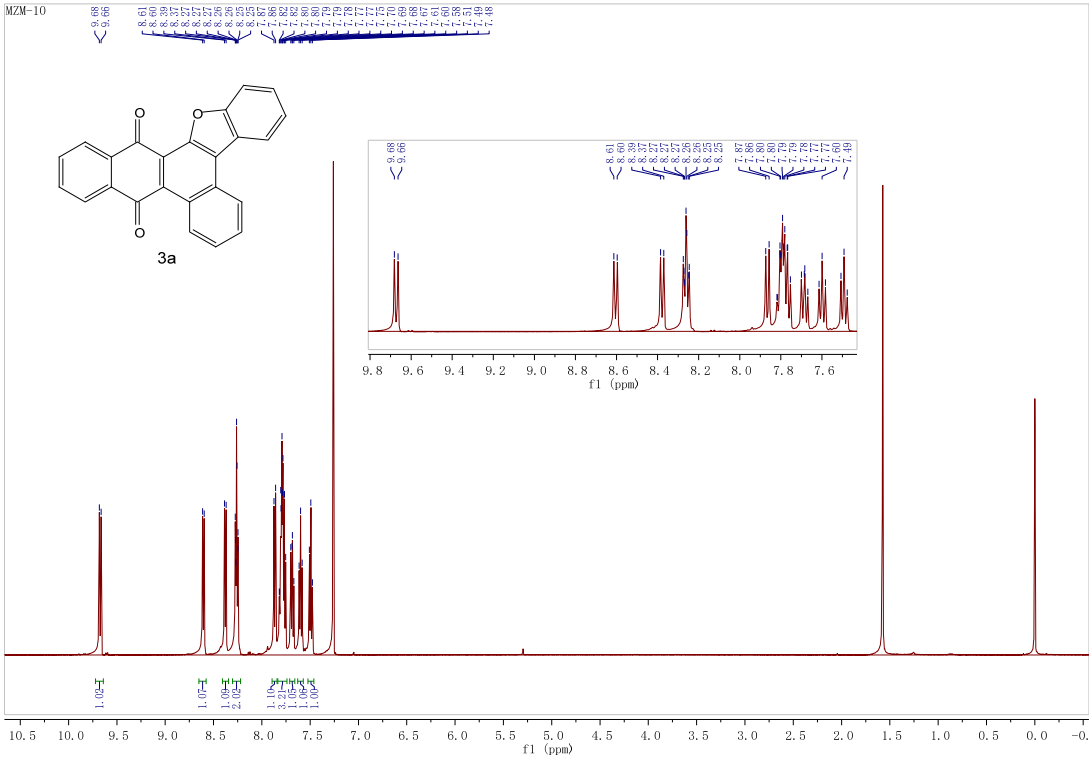


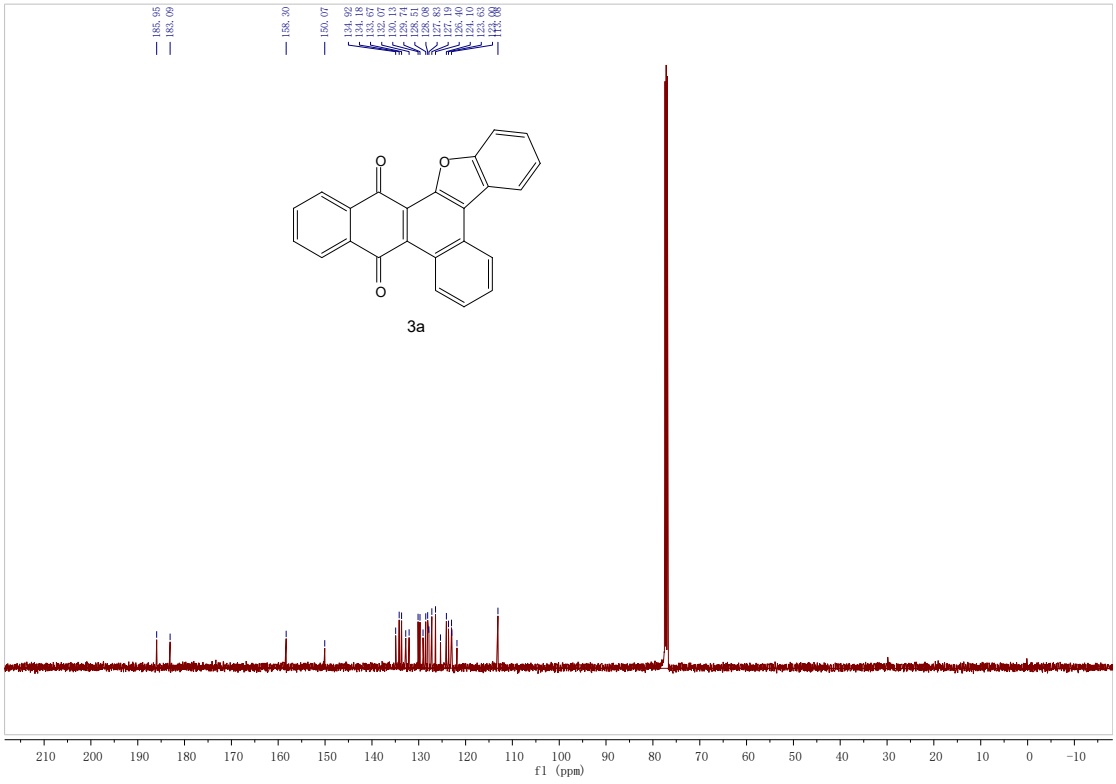

MZM-EKZJT
9.56
9.54
8.19
8.17
8.17
8.17
8.15
7.91
7.89
7.76
7.76
7.75
7.74
7.74
7.73
7.73
7.67
7.67
7.65
7.65
7.64
7.64
7.26
6.99
6.97
6.95
6.93
O
O
1.00
2.08
1.04
1.05
1.04
1.01
0.99
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)

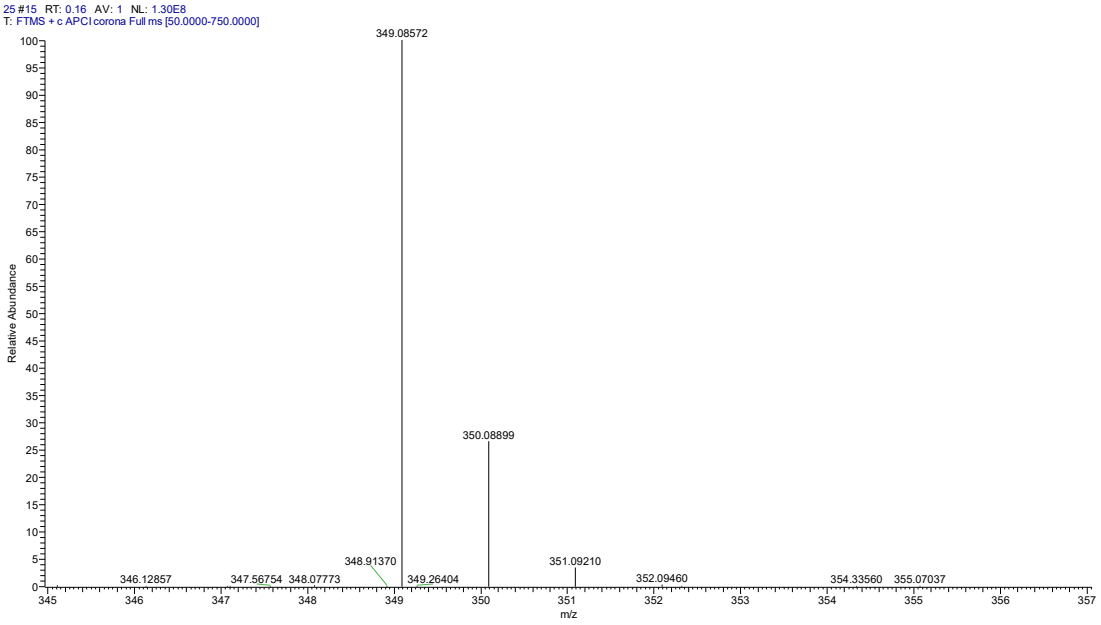

MZM-FK1
9.47
9.45
8.25
8.24
8.21
8.19
7.94
7.92
7.80
7.80
7.79
7.78
7.78
7.77
7.77
7.71
7.71
7.70
7.68
7.68
O
Br
Br
O
1.00
1.02
1.00
1.00
1.01
1.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

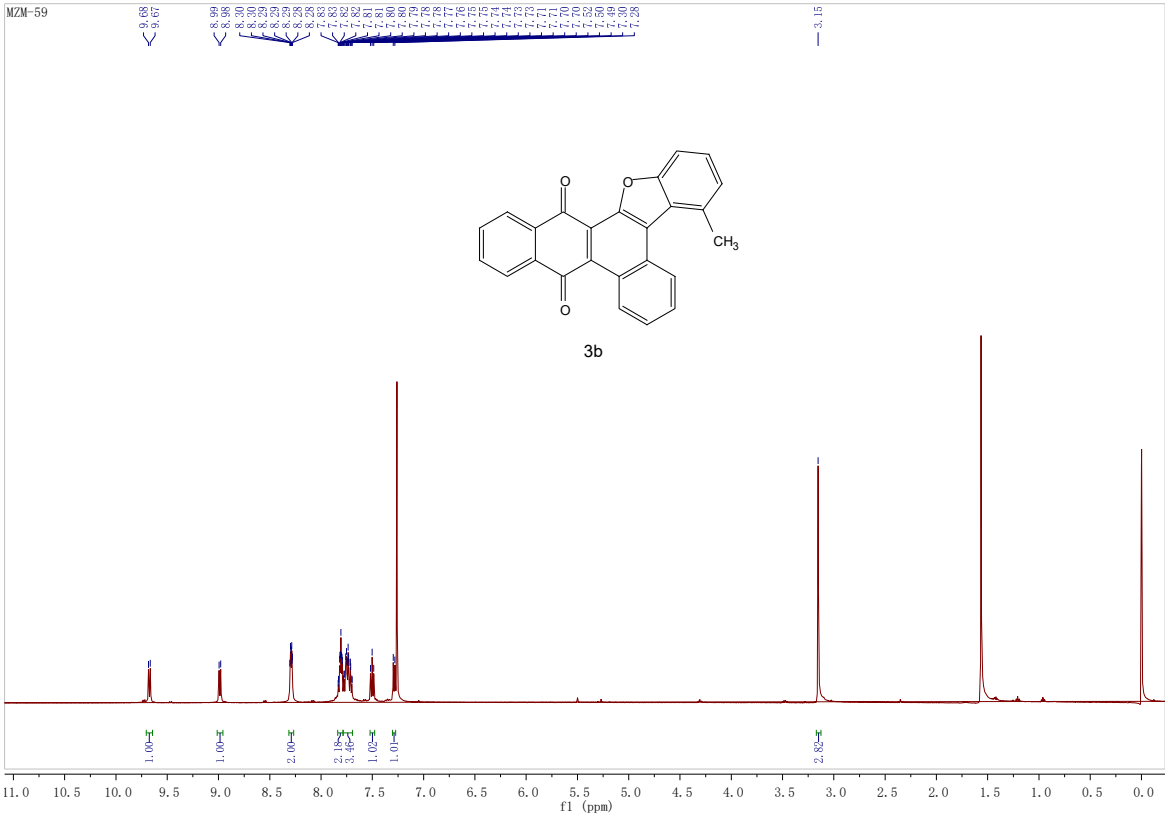

MZM-XJYJ-1
O
Br
O
CH3
O
f1 (ppm)

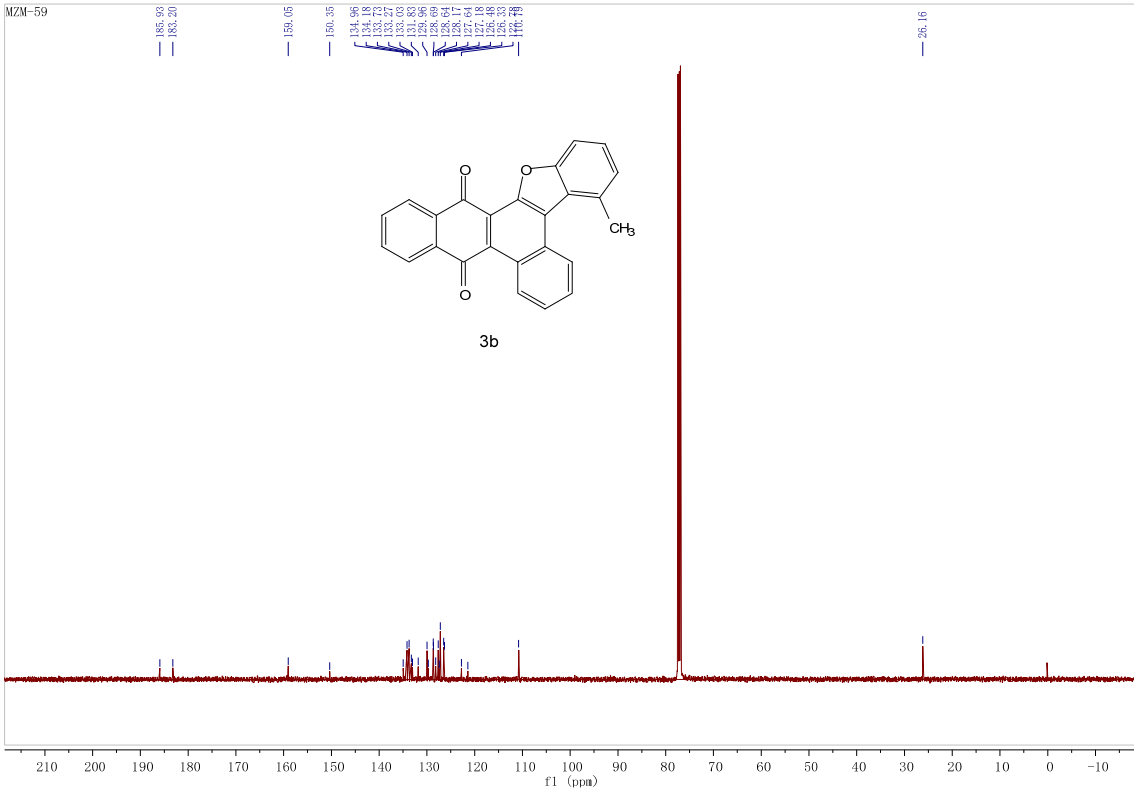

MZM-3BFN
O
f1 (ppm)

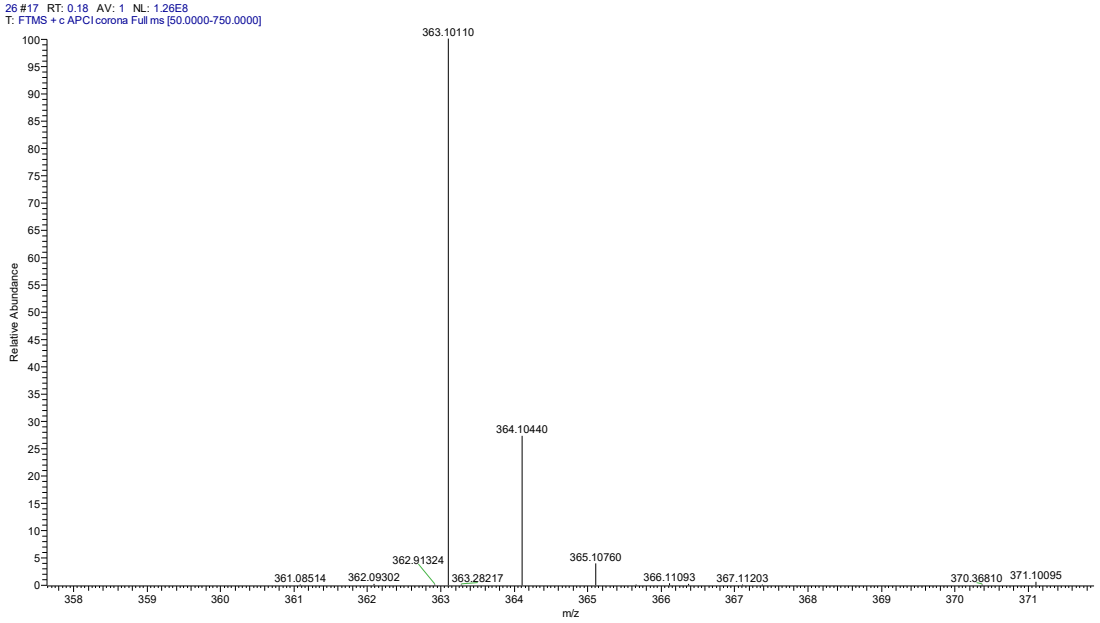

MZM-10
3a
f1 (ppm)

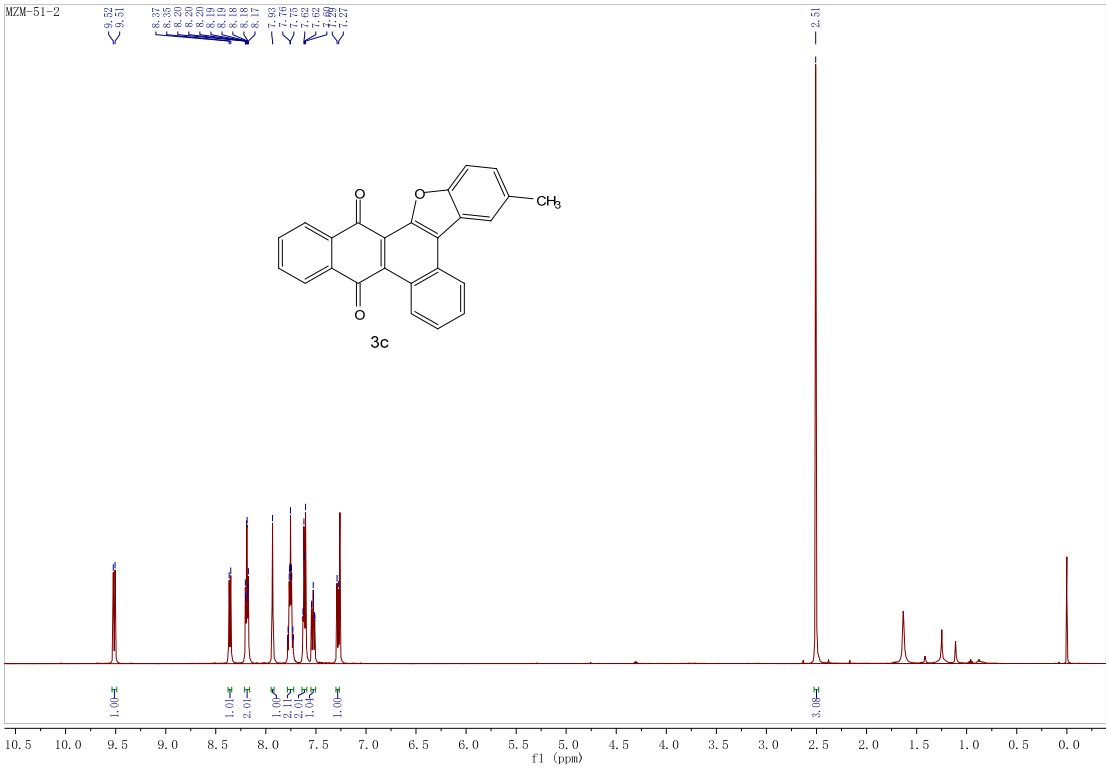

3a
f1 (ppm)

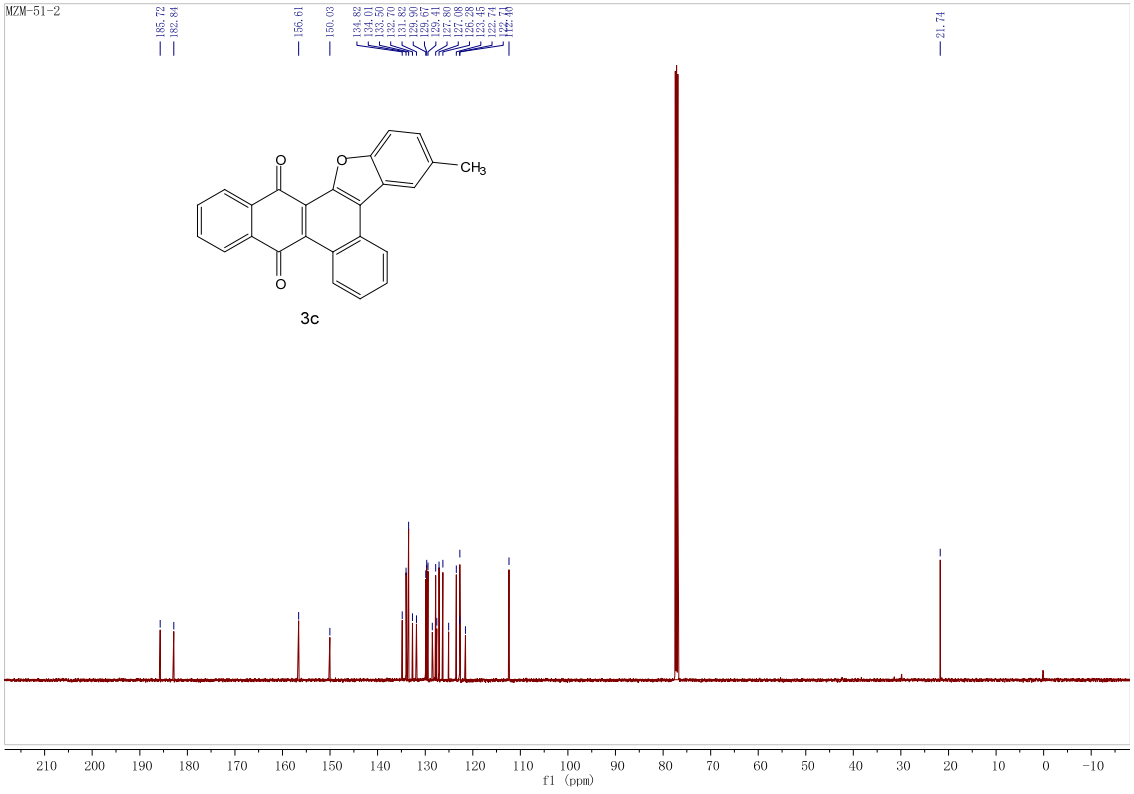

25 #15 RT: 0.16 AV: 1 NL: 1.30E8
T: FTMS + c APCI corona Full ms [50.0000-750.0000]
Relative Abundance
m/z
349.08572
350.08899
348.91370
351.09210
346.12857
347.56754
348.07773
349.26404
352.09460
354.33560
355.07037

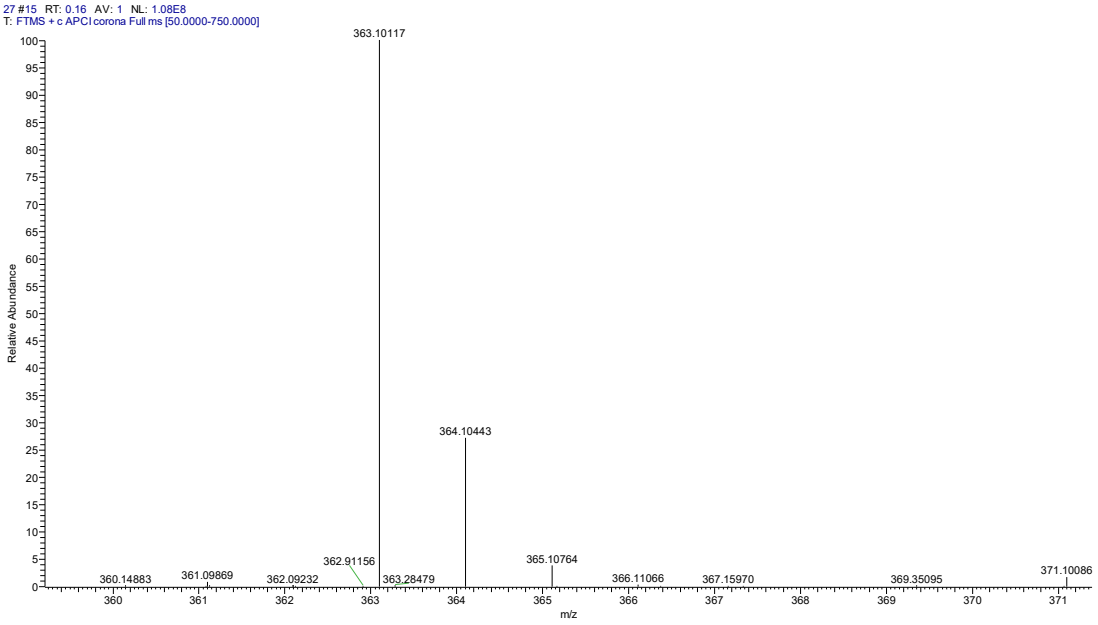

MZM-59
O
O
O
CH3
3b
f1 (ppm)

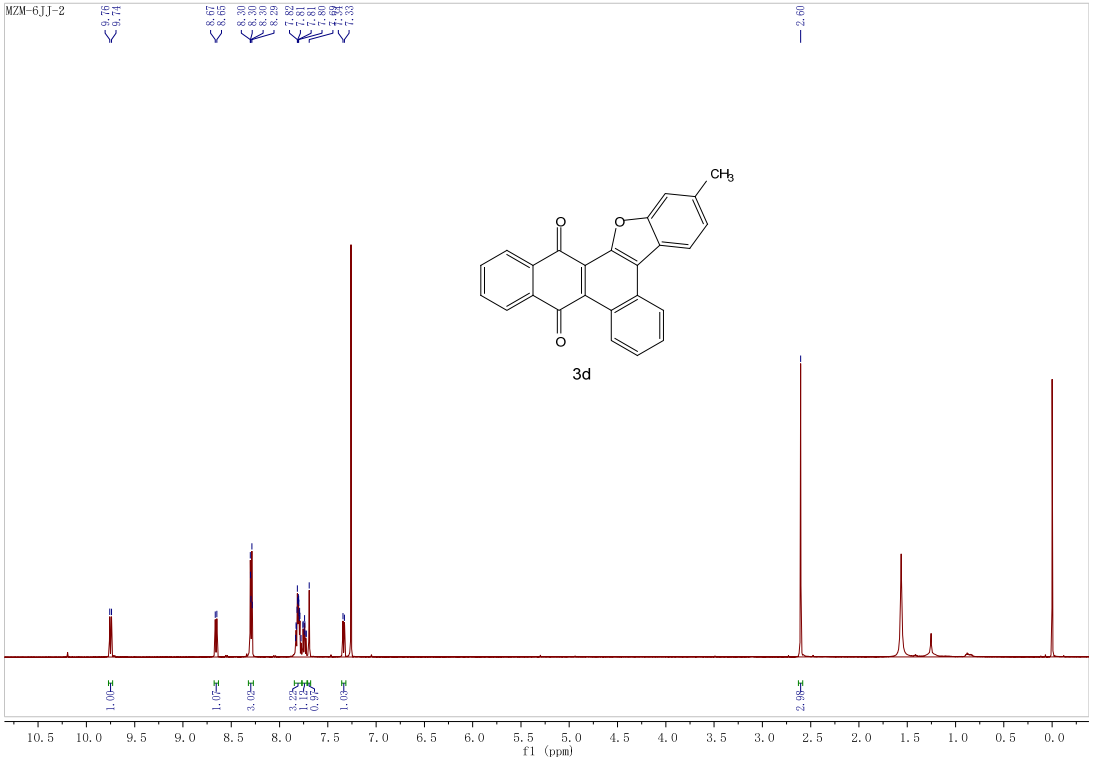

MZM-59
185.93
183.20
159.05
150.35
134.96
134.18
133.73
133.27
133.03
131.83
129.96
129.69
128.64
128.17
127.64
127.18
126.48
126.33
122.78
110.19
26.16
O
O
O
CH3
3b
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


26 #17 RT: 0.18 AV: 1 NL: 1.26E8
T: FTMS + c APCI corona Full ms [50.0000-750.0000]
363.10110
364.10440
365.10760
362.91324
361.08514
362.09302
363.28217
366.11093
367.11203
370.36810
371.10095
Relative Abundance
m/z


MZM-51-2
9.52
9.51
8.37
8.35
8.20
8.20
8.19
8.19
8.18
8.18
8.17
7.93
7.78
7.75
7.62
7.60
7.59
7.27
2.51
O
O
O
CH3
3c
1.00
1.01
2.01
1.00
2.11
2.01
1.04
1.00
3.08
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


MZM-51-2
185.72
182.84
156.61
150.03
134.82
134.01
133.50
132.79
131.82
128.90
128.67
128.41
127.80
127.08
126.28
123.45
122.74
122.40
21.74
O
O
O
CH3
3c
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


27 #15 RT: 0.16 AV: 1 NL: 1.08E8
T: FTMS + c APCI corona Full ms [50.0000-750.0000]
Relative Abundance
m/z
363.10117
364.10443
362.91156
365.10764
360.14883
361.09869
362.09232
363.28479
366.11066
367.15970
369.35095
371.10086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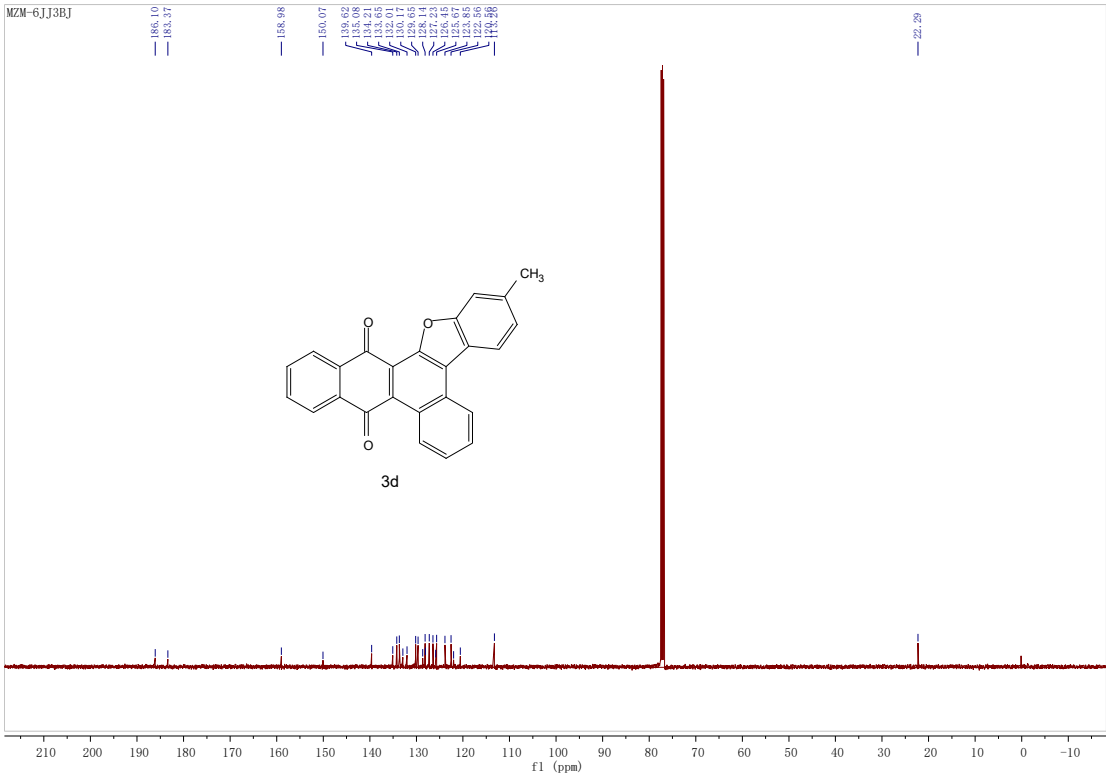
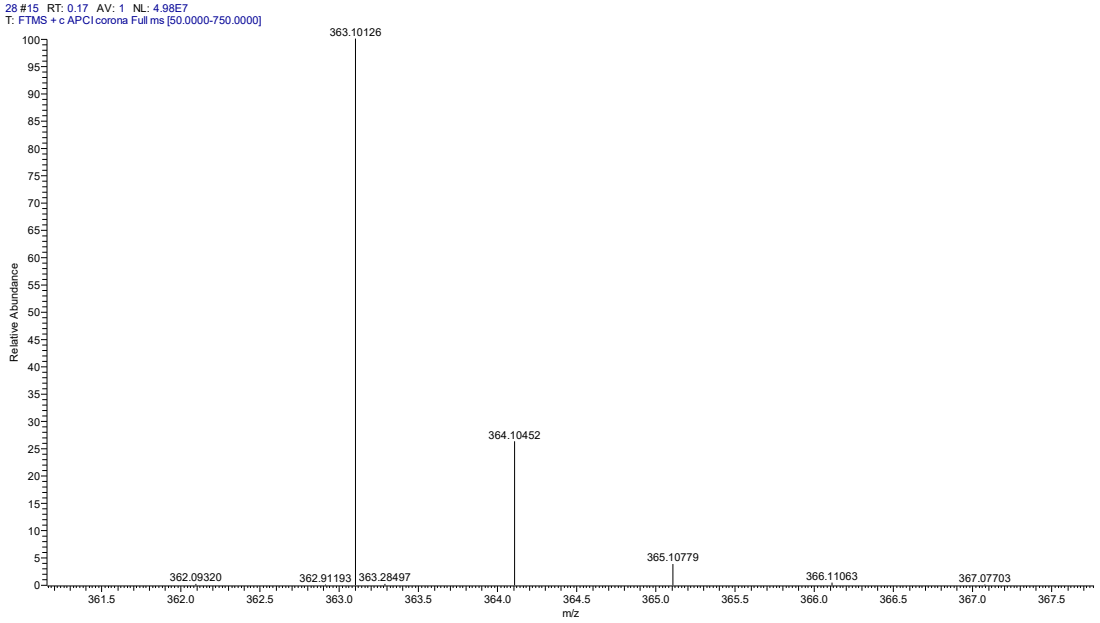
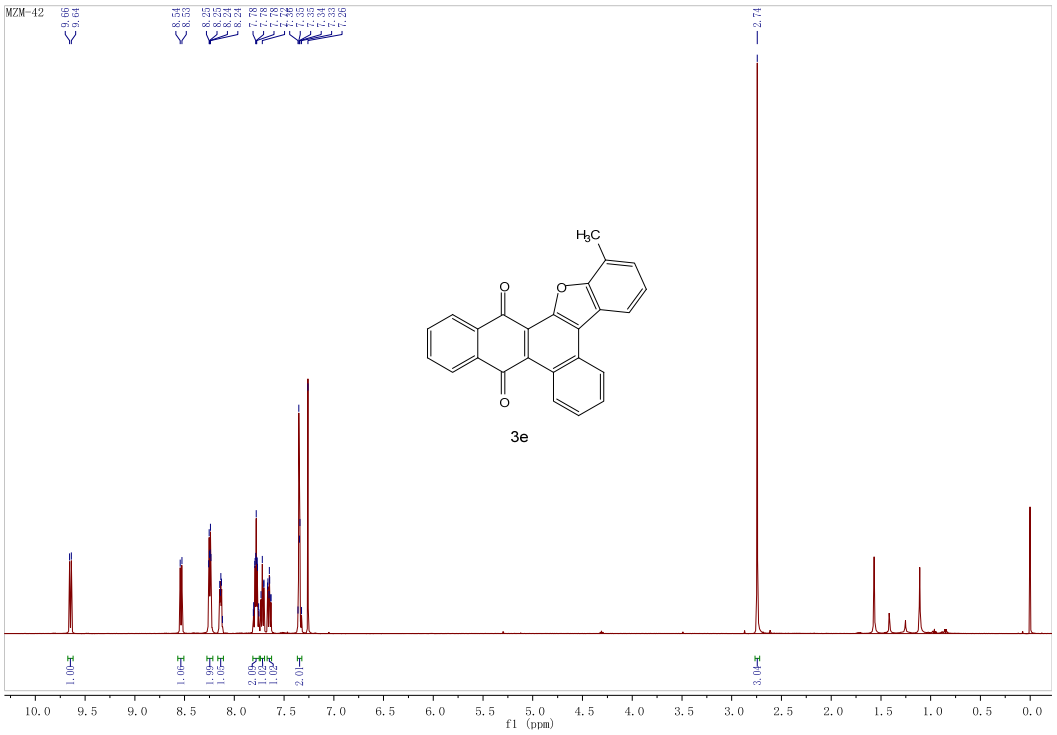
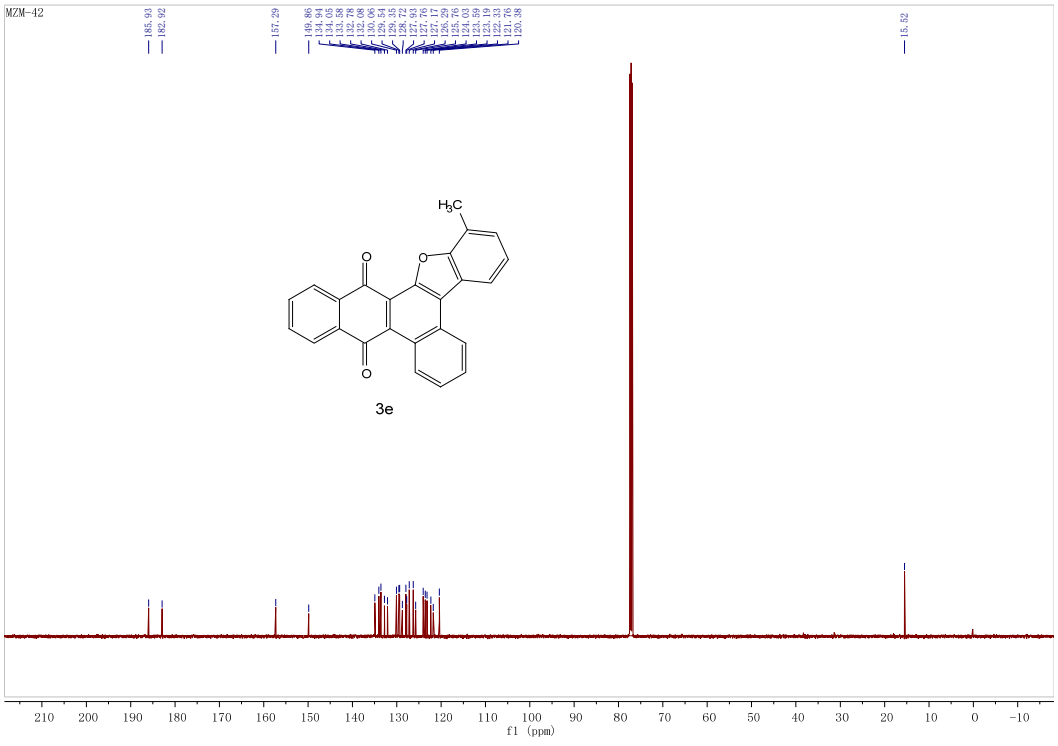
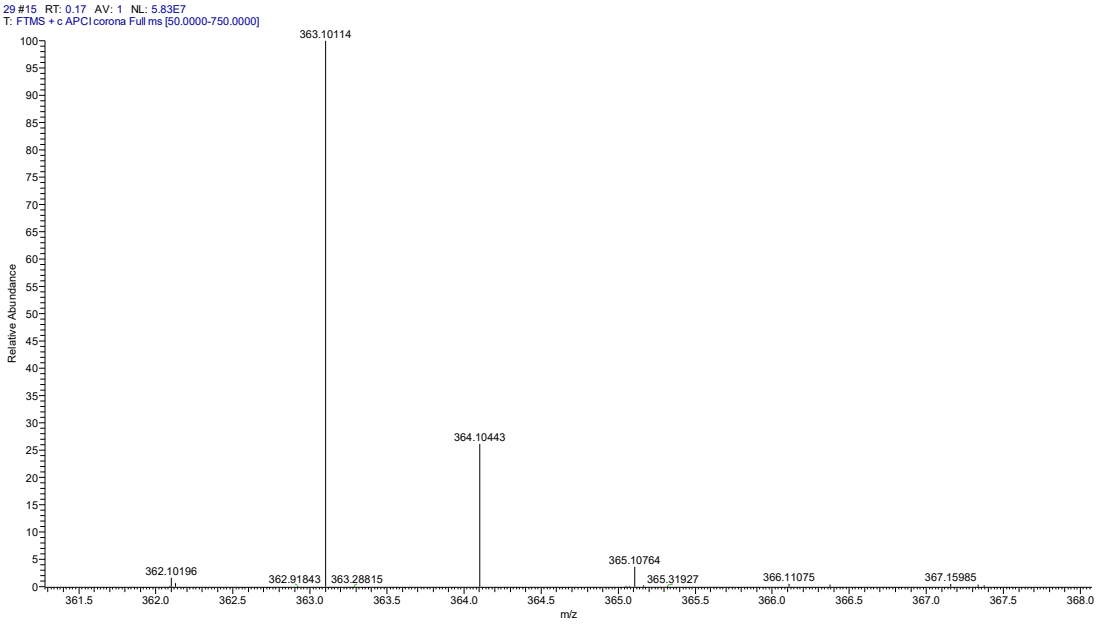
9.76
9.74
8.67
8.65
8.30
8.30
8.29
7.82
7.81
7.80
7.69
7.33
2.60
CH3
O
O
O
3d
1.00
1.07
3.02
3.22
1.15
0.97
1.00
2.98
f1 (ppm)

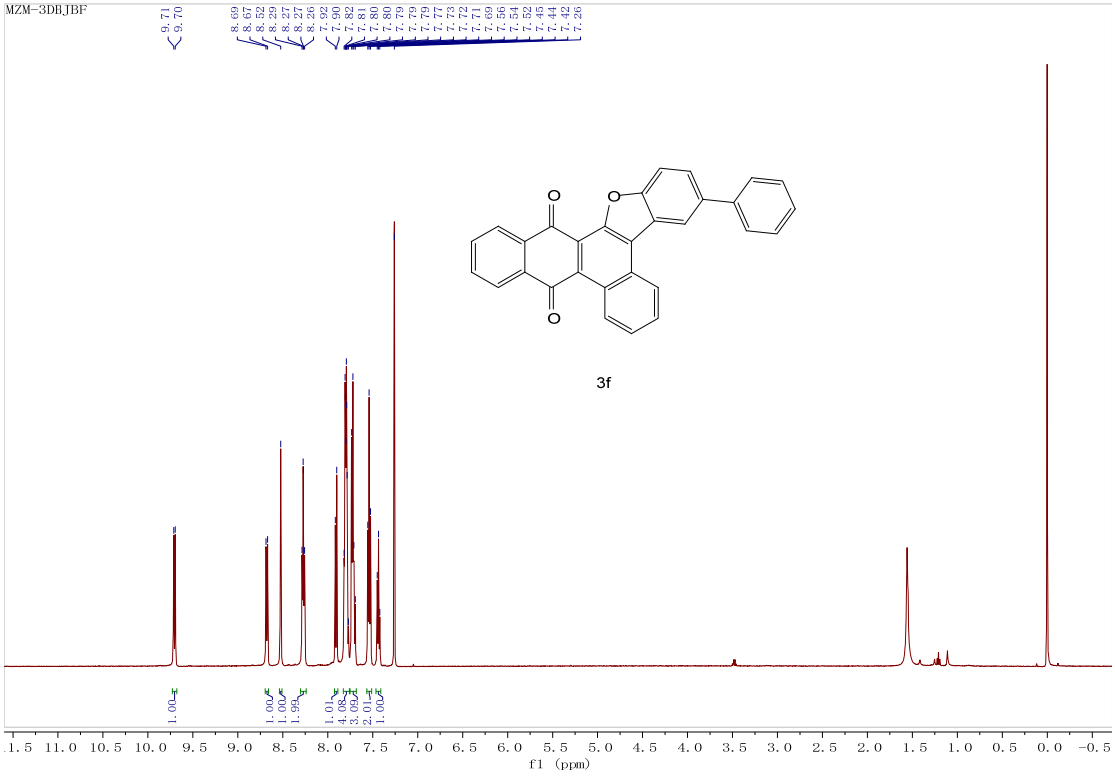

MZM-6JJ3BJ
186.10
183.37
158.98
150.07
139.62
135.08
134.21
133.65
132.01
130.17
129.65
128.14
127.23
126.45
125.67
123.85
122.55
120.46
112.26
22.29
O
O
O
CH3
3d
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)

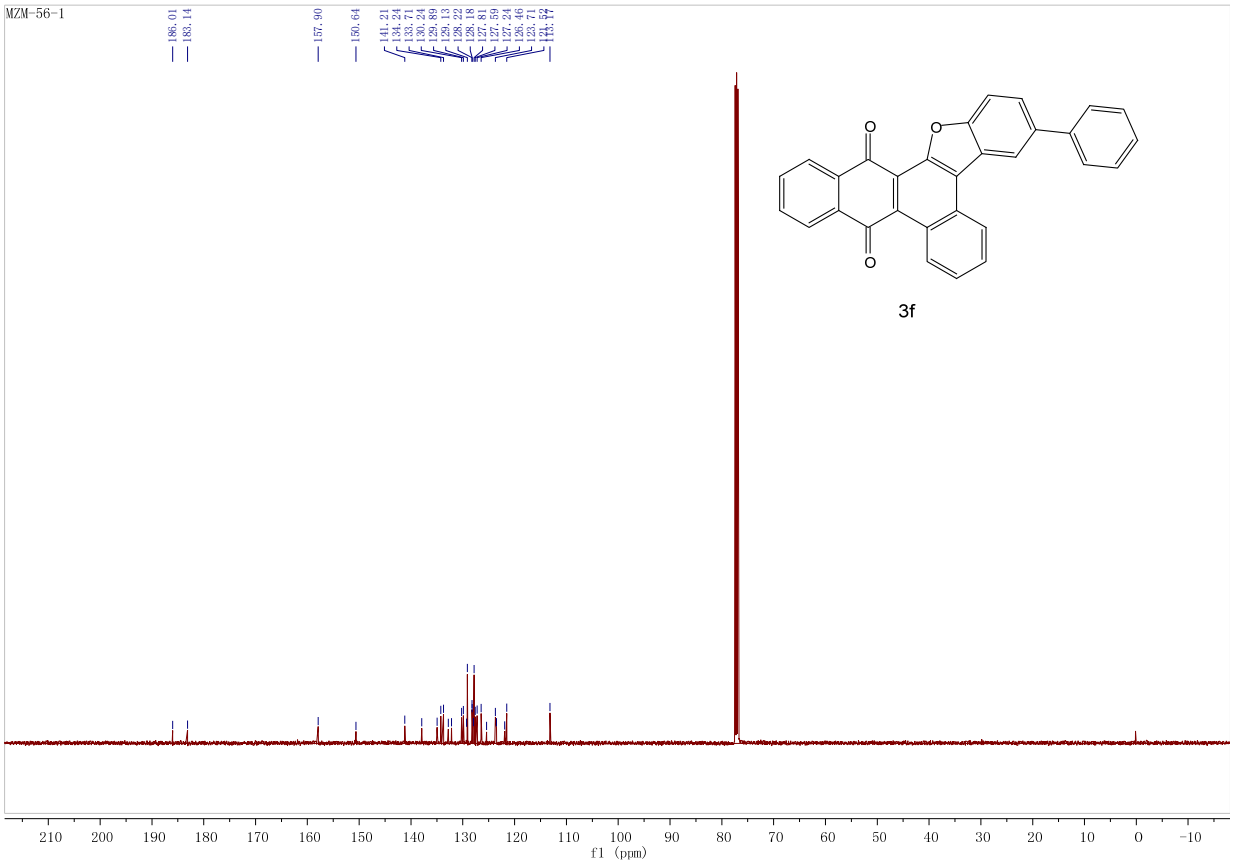

28 #15 RT: 0.17 AV: 1 NL: 4.98E7
T: FTMS + c APCI corona Full ms [50.0000-750.0000]
363.10126
364.10452
365.10779
362.09320
362.91193
363.28497
366.11063
367.07703
Relative Abundance
m/z
361.5 362.0 362.5 363.0 363.5 364.0 364.5 365.0 365.5 366.0 366.5 367.0 367.5

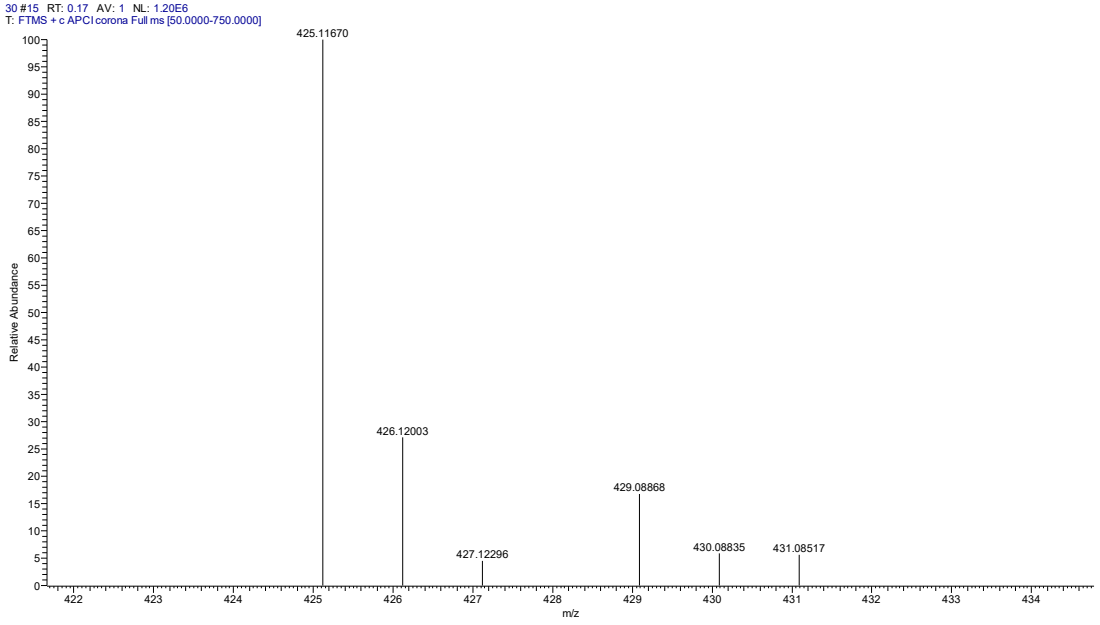

MZM-42
9.66
9.64
8.54
8.53
8.25
8.25
8.24
8.24
7.78
7.78
7.78
7.78
7.35
7.34
7.33
7.26
2.74
H3C
O
O
O
3e
1.00
1.00
1.99
1.05
2.09
1.02
1.02
2.01
3.04
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

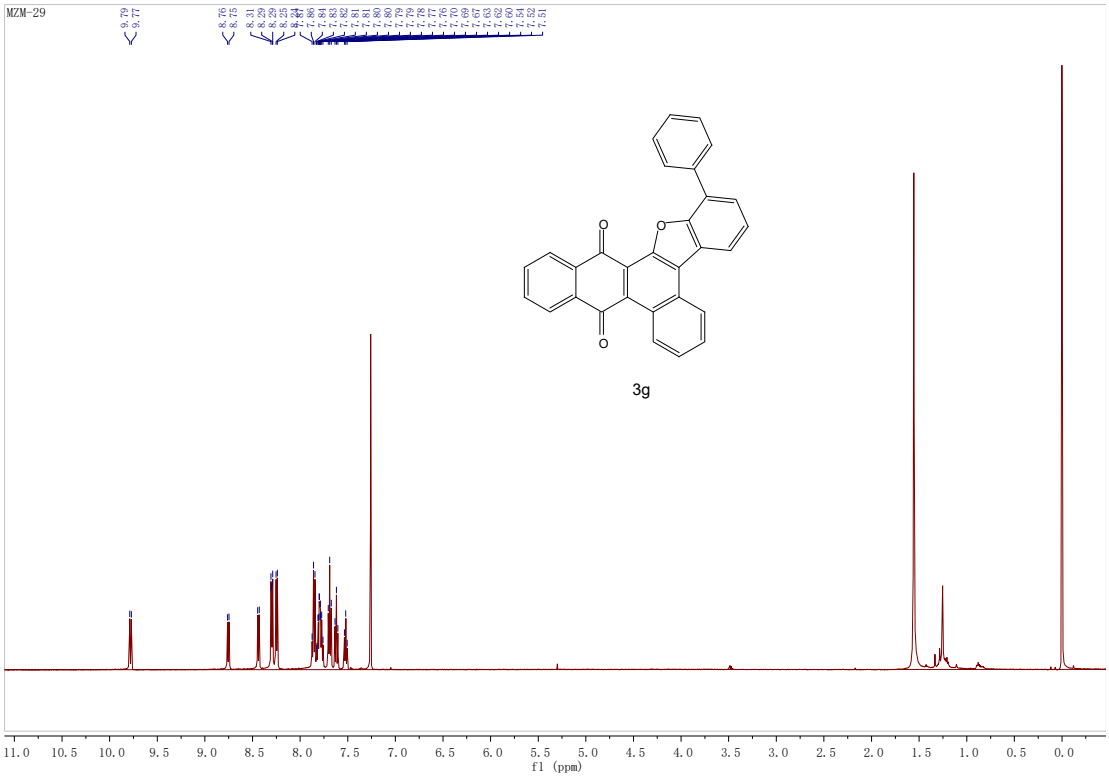

MZM-42
185.93
182.92
157.29
149.86
134.94
134.05
133.38
132.78
132.08
130.06
129.54
129.35
128.72
127.93
127.76
127.17
126.29
125.76
124.03
123.89
123.19
122.33
121.76
120.98
15.52
H3C
O
O
O
3e
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

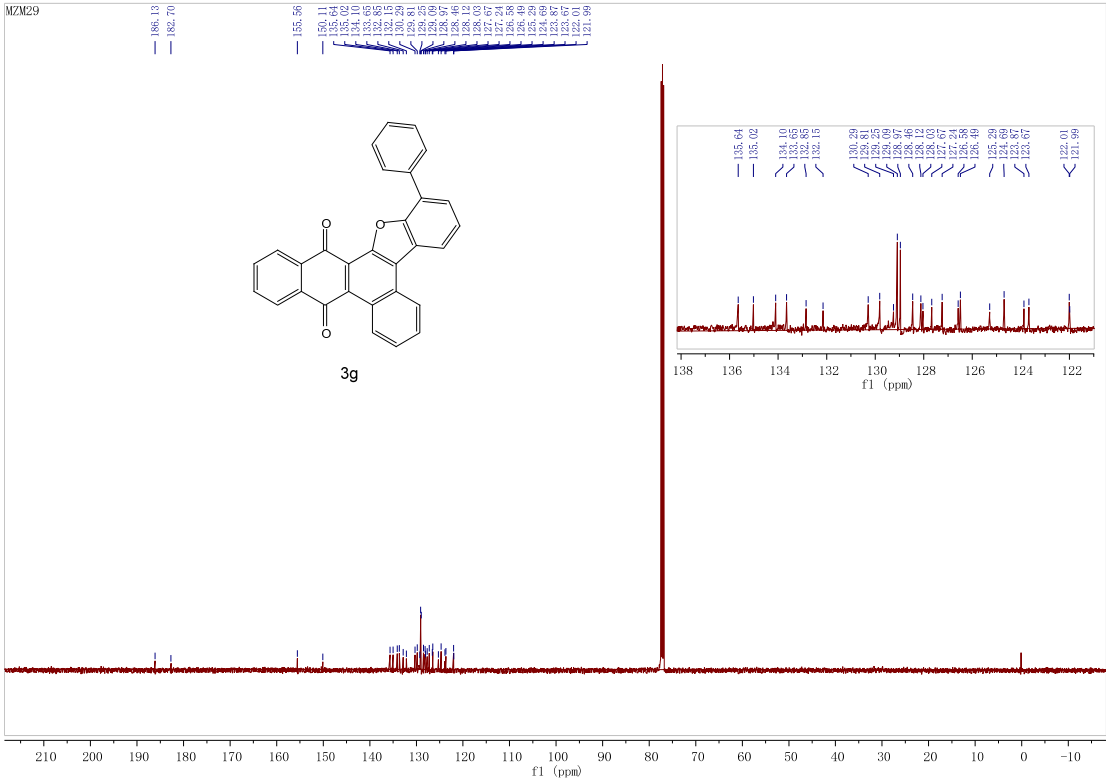

29 #15 RT: 0.17 AV: 1 NL: 5.83E7
T: FTMS + c APCI corona Full ms [50.0000-750.0000]
363.10114
364.10443
365.10764
362.10196
362.91843
363.28815
365.31927
366.11075
367.15985
Relative Abundance
m/z

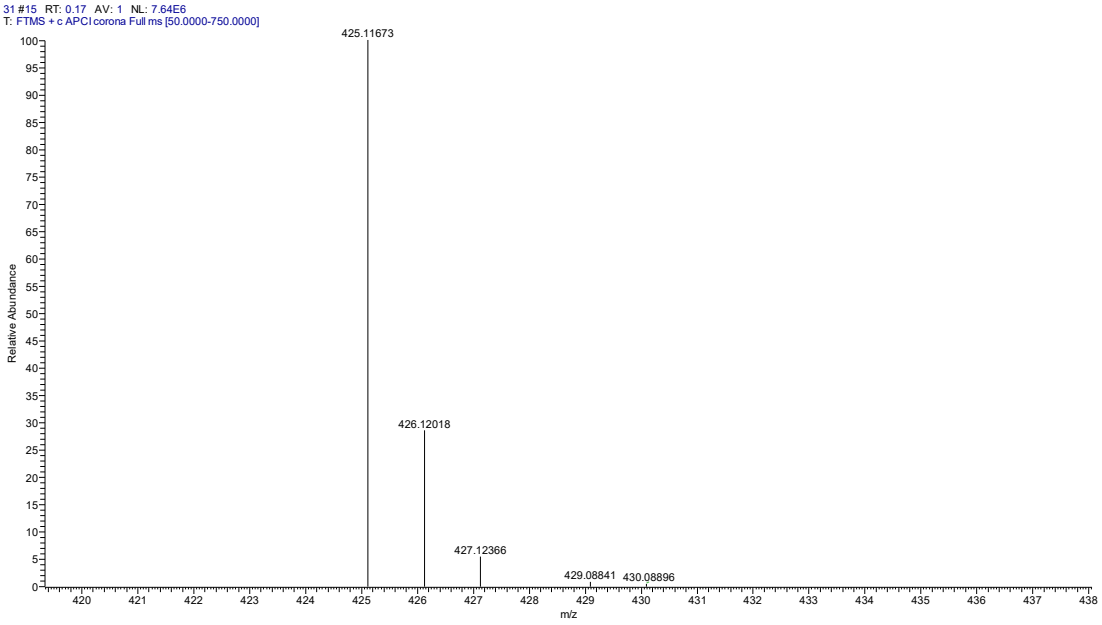

MZM-3DB_JBF
3f
f1 (ppm)

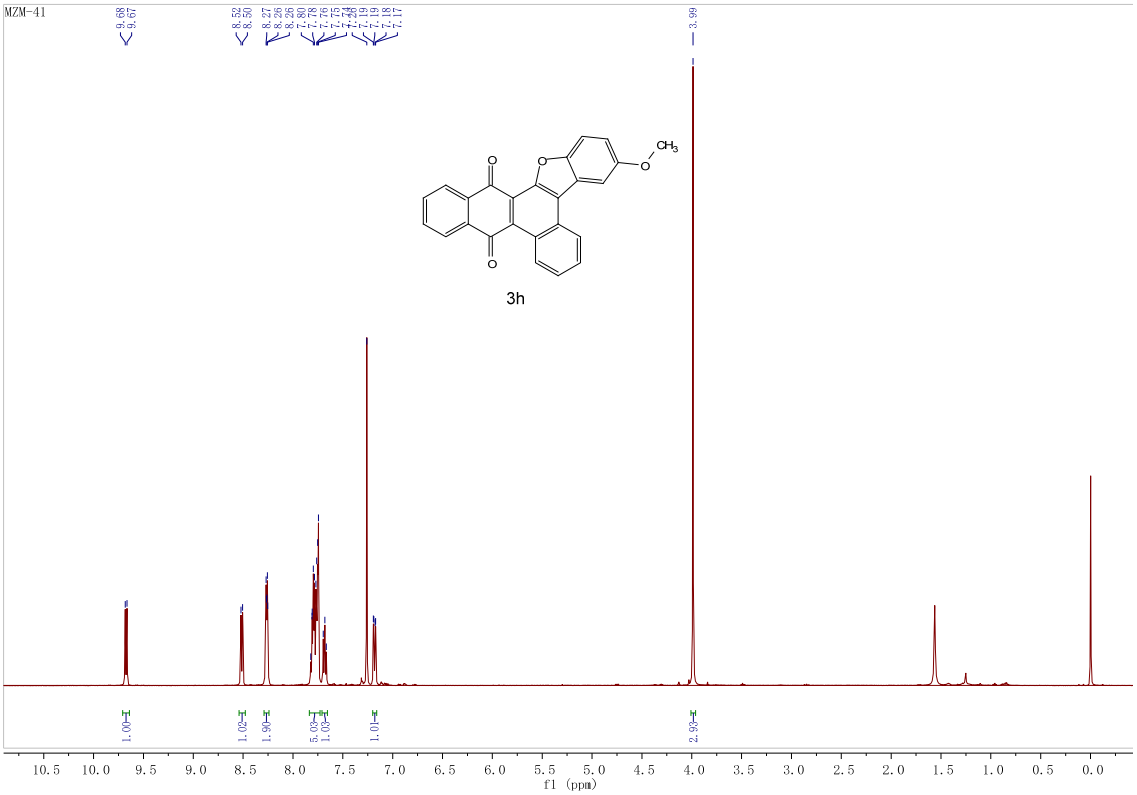

MZM-56-1
186.01
183.14
157.90
150.64
141.21
134.24
133.71
132.24
129.89
129.13
128.22
128.18
127.81
127.59
127.24
126.46
123.71
121.52
115.17
O
O
O
3f
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

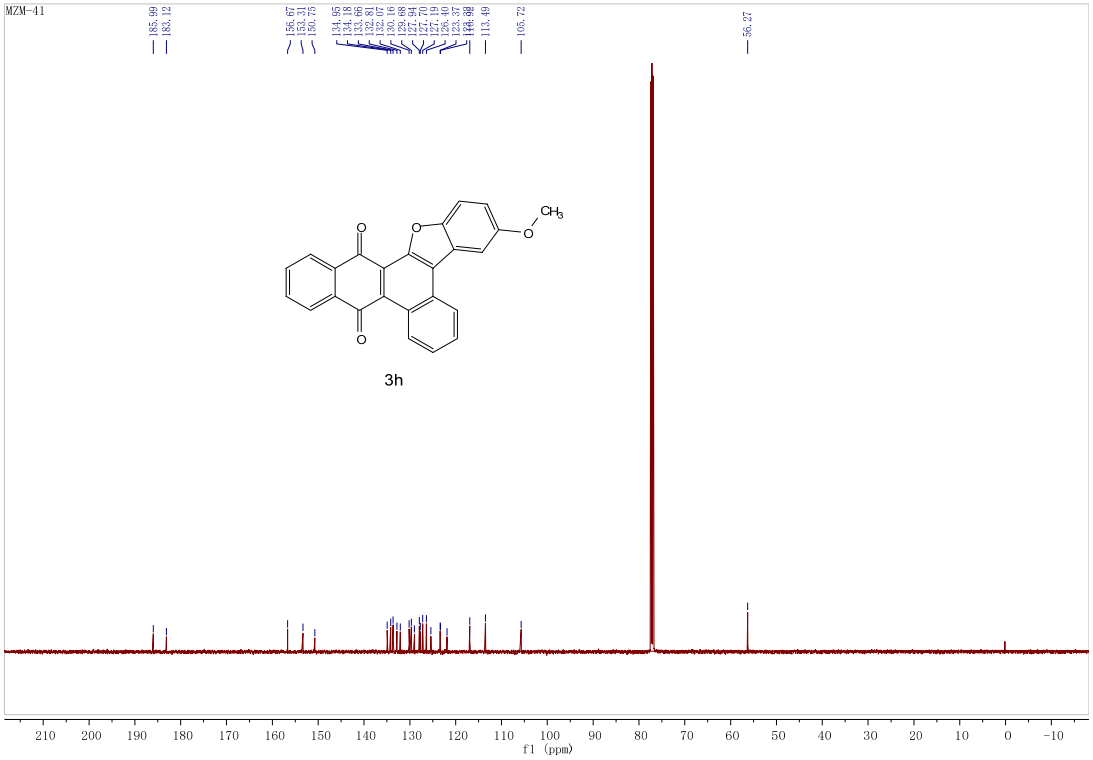

30 #15 RT: 0.17 AV: 1 NL: 1.20E6
T: FTMS + c APCI corona Full ms [50.0000-750.0000]
425.11670
426.12003
427.12296
429.08868
430.08835
431.08517
Relative Abundance
m/z
422
423
424
425
426
427
428
429
430
431
432
433
434

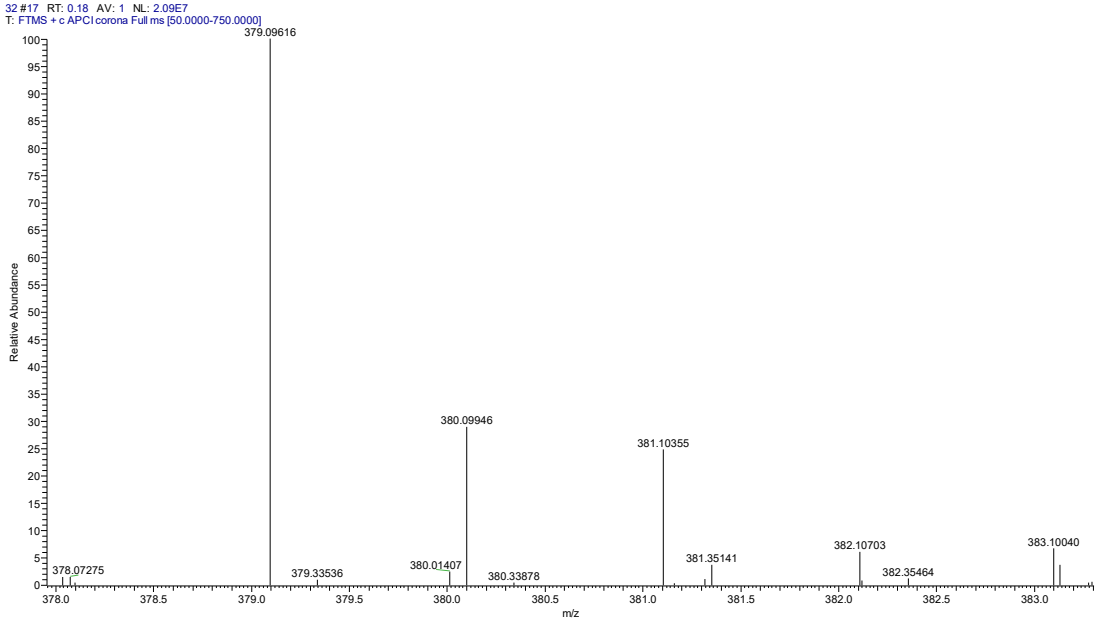

MZM-29
3g
f1 (ppm)

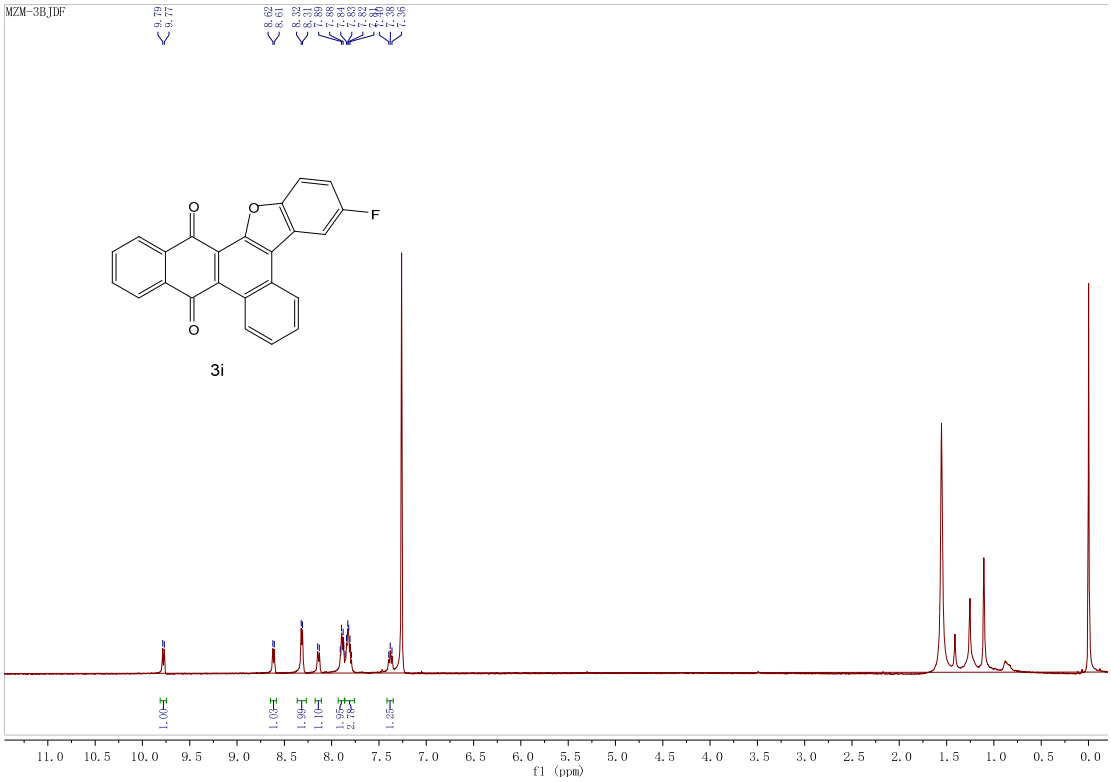

MZM29
3g
f1 (ppm)
f1 (ppm)

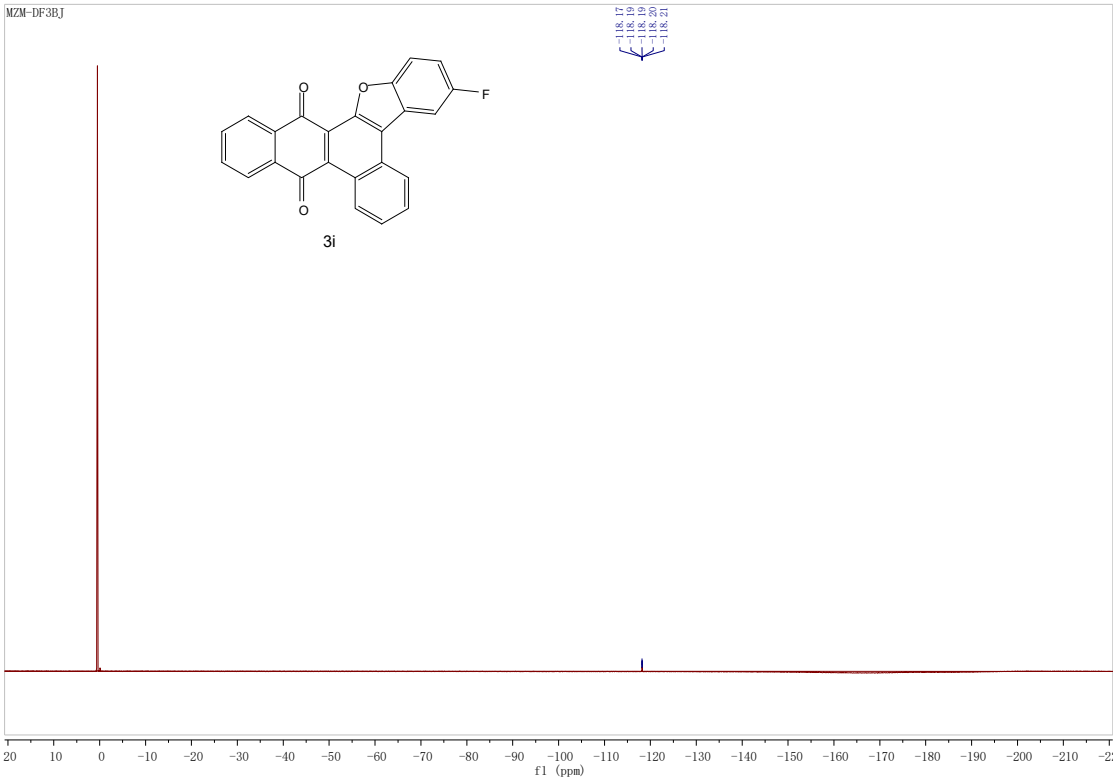

31 #15 RT: 0.17 AV: 1 NL: 7.64E6
T: FTMS + c APCI corona Full ms [50.0000-750.0000]
425.11673
426.12018
427.12366
429.08841
430.08896
Relative Abundance
m/z

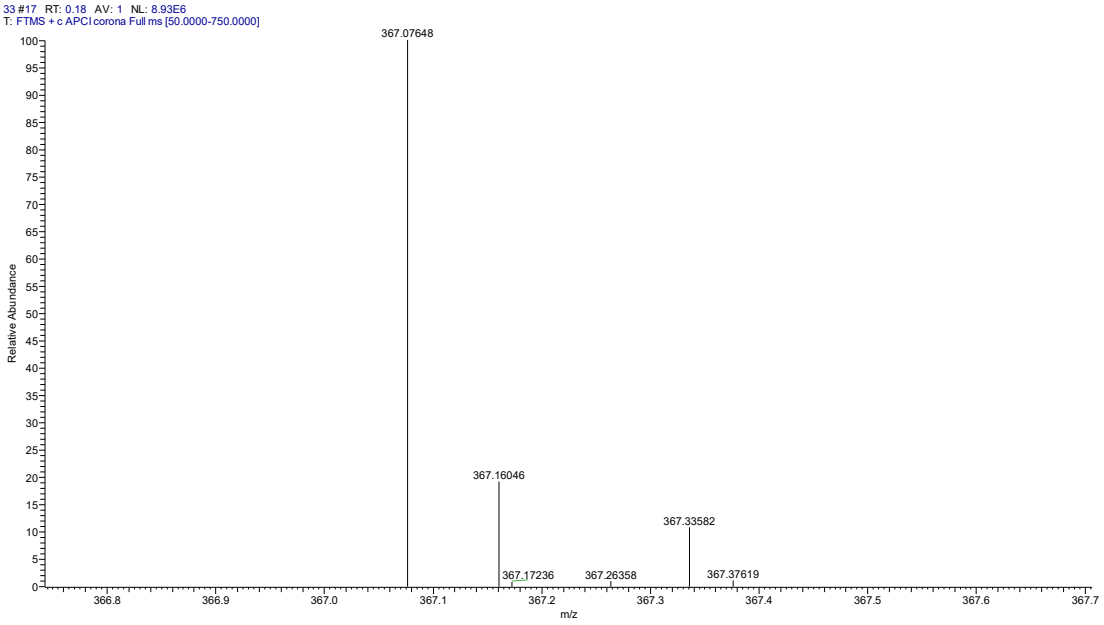

MZM-41
3h
f1 (ppm)

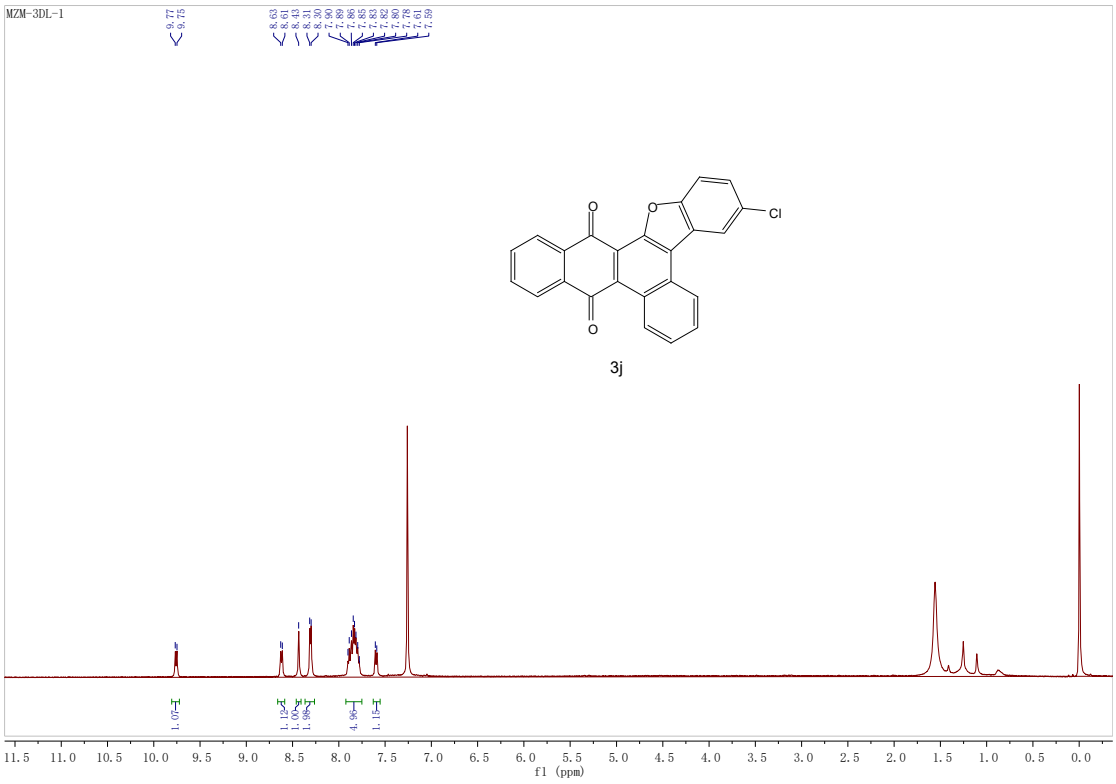

MZM-41
185.99
183.12
156.67
153.31
150.75
134.95
134.18
133.66
132.81
132.17
130.16
129.88
127.94
127.70
127.19
126.40
123.37
113.49
105.72
56.27
O
O
O
O
CH3
3h
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


32 #17 RT: 0.18 AV: 1 NL: 2.09E7
T: FTMS + c APCI corona Full ms [50.0000-750.0000]
379.09616
380.09946
381.10355
382.10703
383.10040
381.35141
382.35464
378.07275
379.33536
380.01407
380.33878
Relative Abundance
m/z
100
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
378.0
378.5
379.0
379.5
380.0
380.5
381.0
381.5
382.0
382.5
383.0

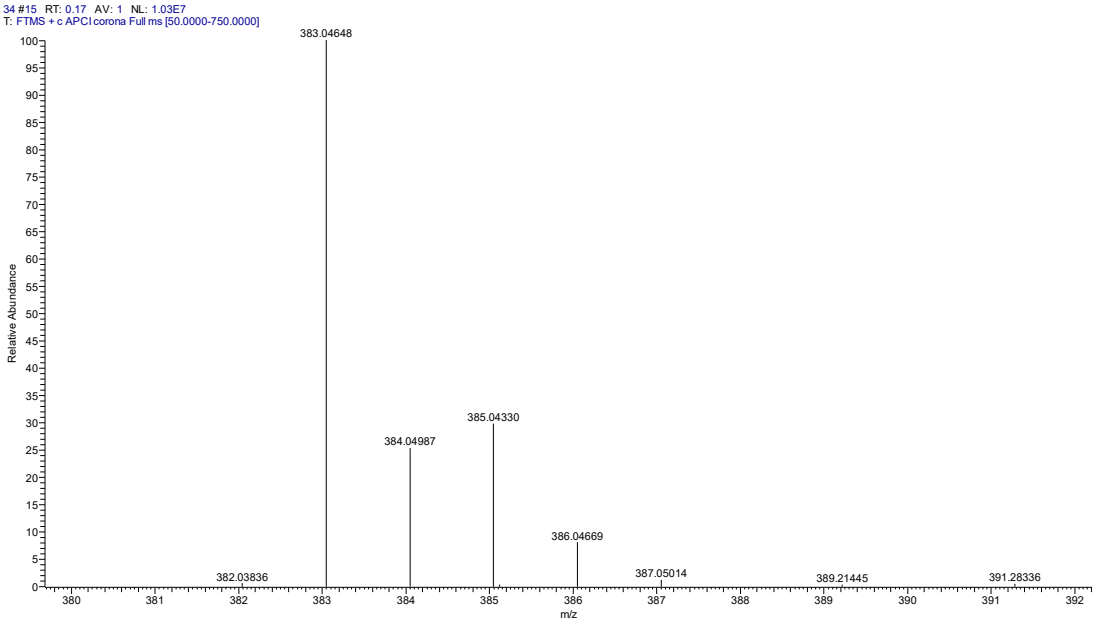

MZM-3B.1DF
9.79
9.77
8.62
8.61
8.32
8.31
7.89
7.88
7.84
7.83
7.82
7.81
7.38
7.36
O
O
O
F
3i
1.00
1.05
1.90
1.10
1.95
2.76
1.25
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

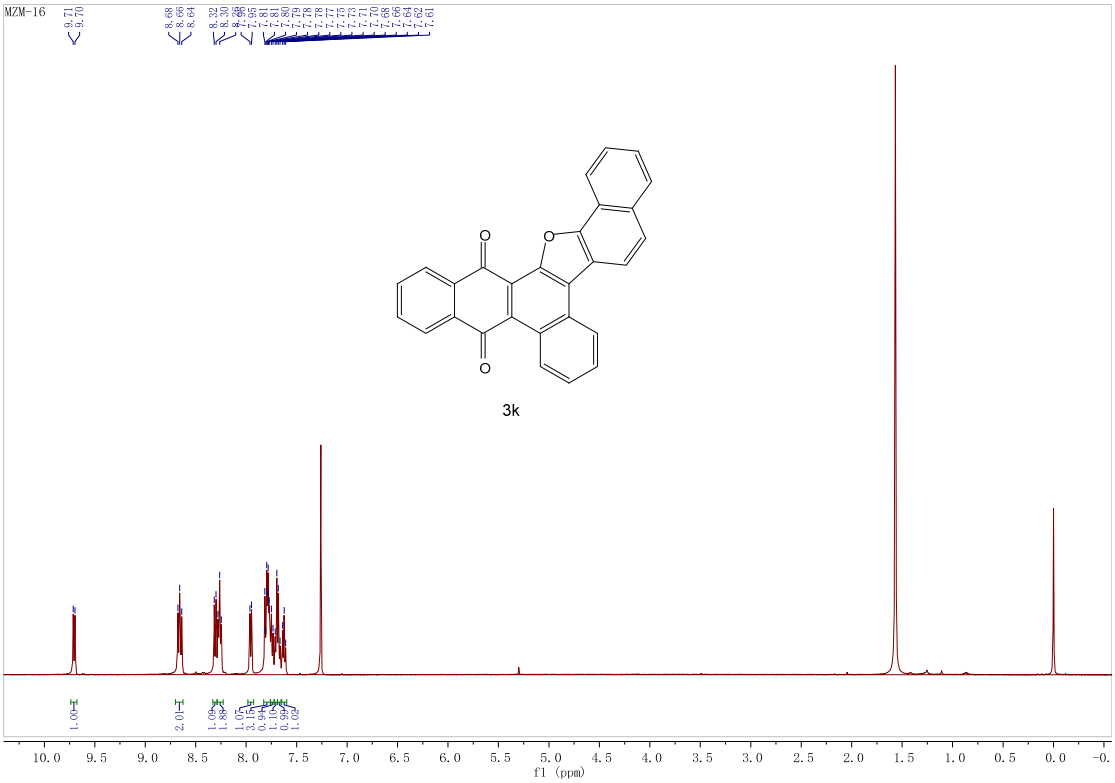

MZM-DF3BJ
-118.17
-118.18
-118.19
-118.20
-118.21
O
O
O
F
3i
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

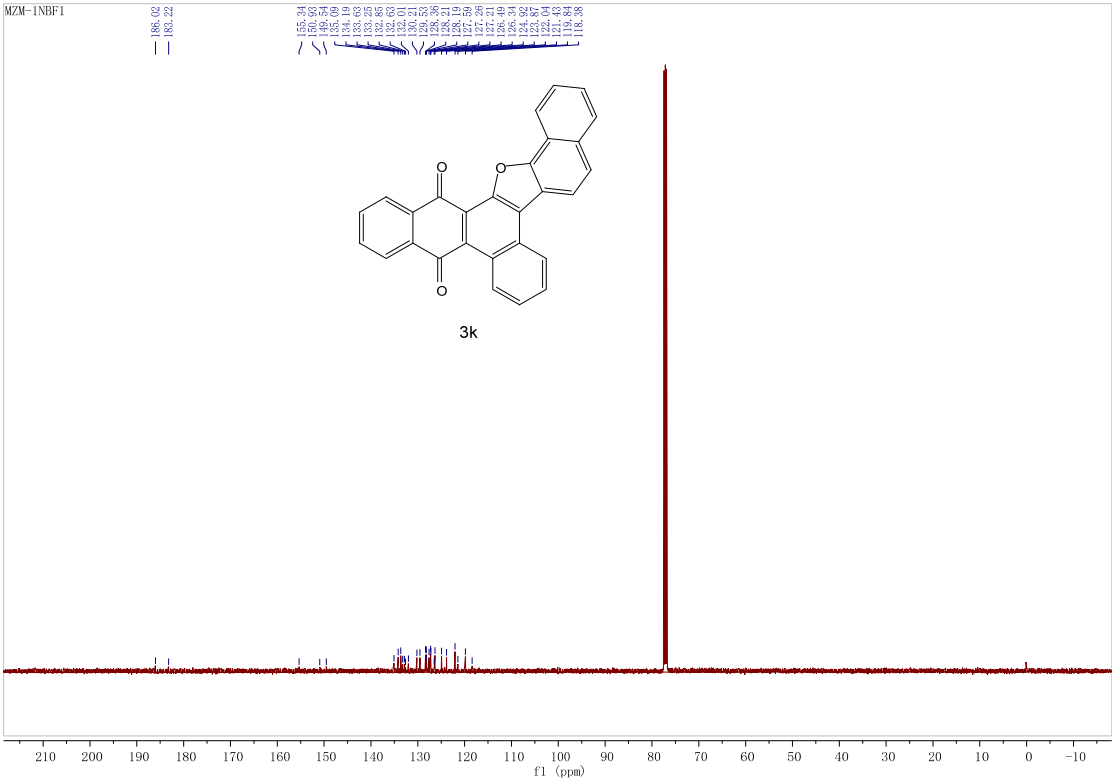

33 #17 RT: 0.18 AV: 1 NL: 8.93E6
T: FTMS + c APCI corona Full ms [50.0000-750.0000]
367.07648
367.16046
367.33582
367.17236
367.26358
367.37619
Relative Abundance
m/z

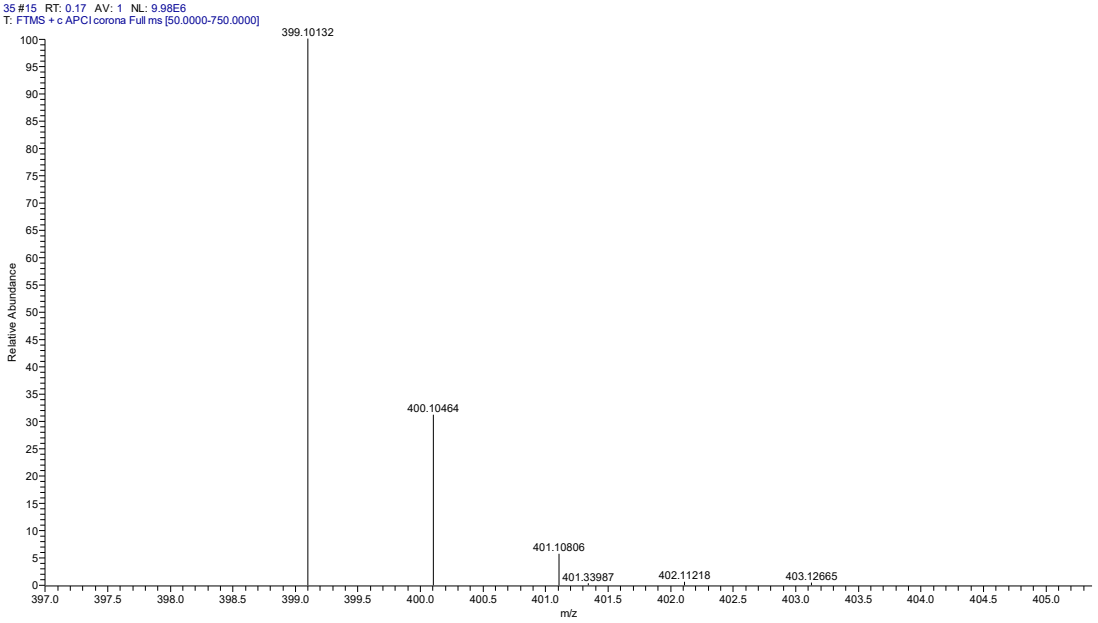

MZM-3DL-1
O
O
O
Cl
f1 (ppm)

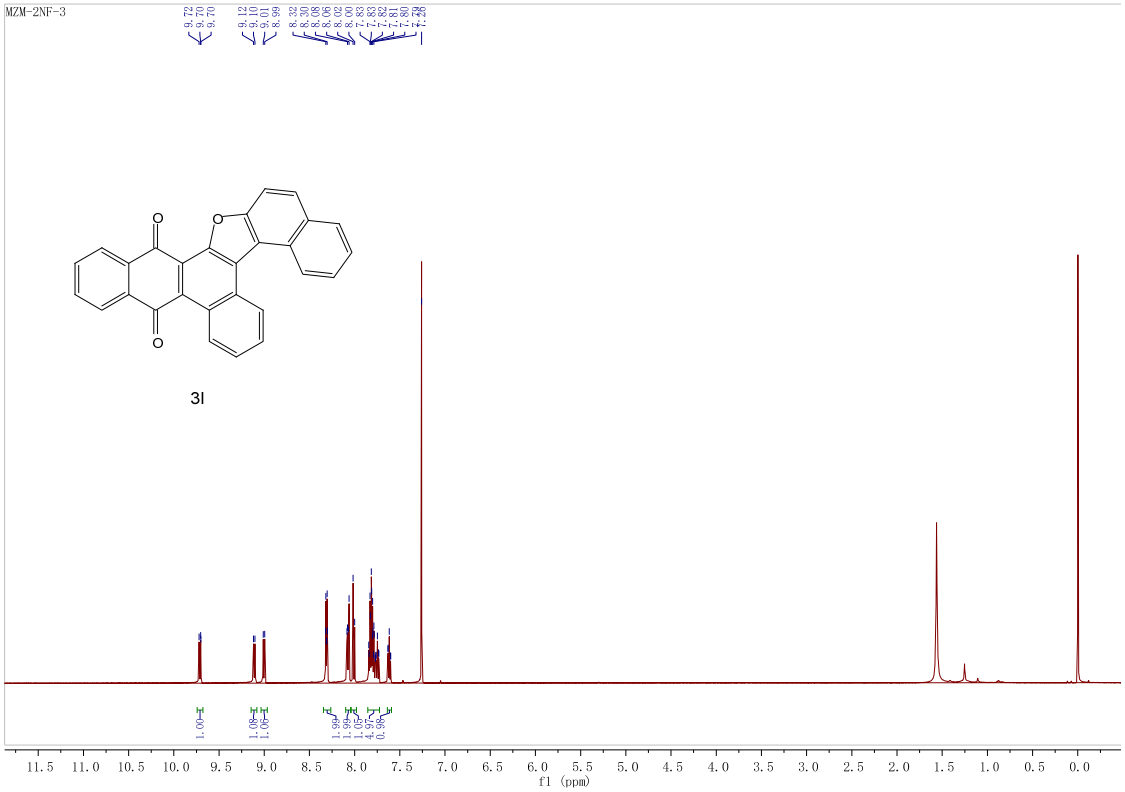
3j

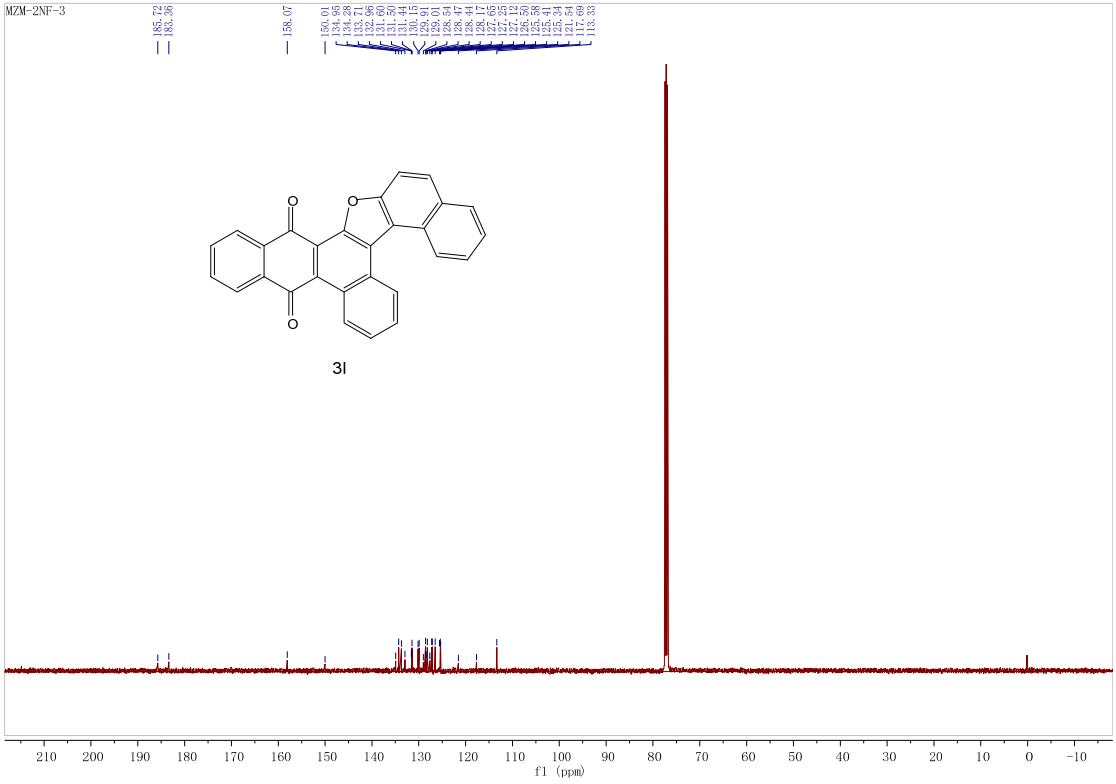

34 #15 RT: 0.17 AV: 1 NL: 1.03E7
T: FTMS + c APCI corona Full ms [50.0000-750.0000]
383.04648
385.04330
384.04987
386.04669
382.03836
387.05014
389.21445
391.28336
Relative Abundance
m/z

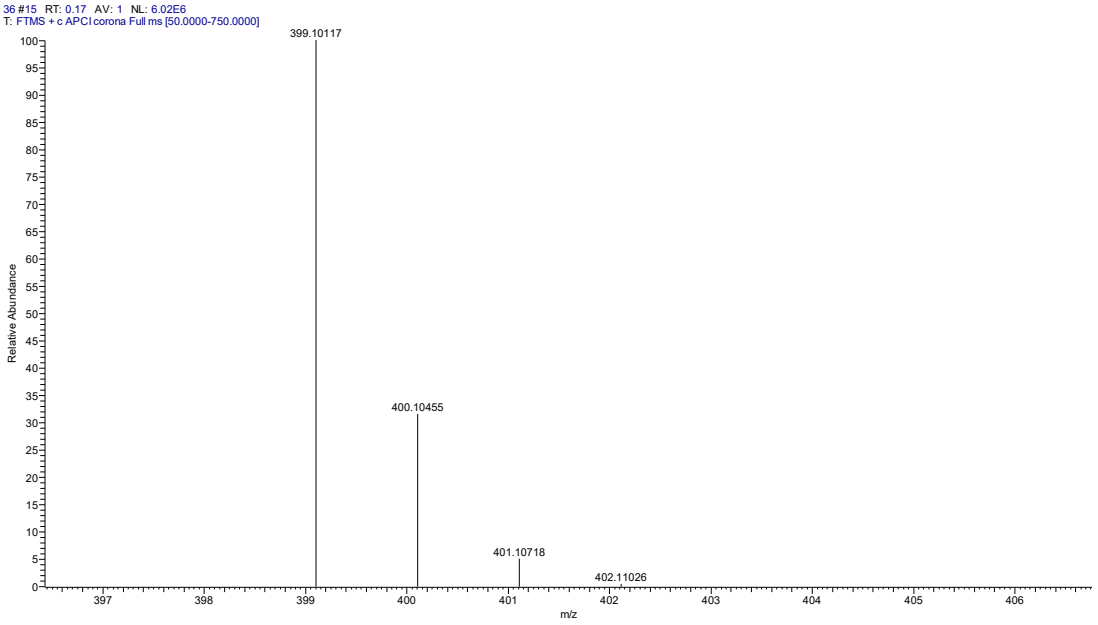

MZM-16
3k
f1 (ppm)

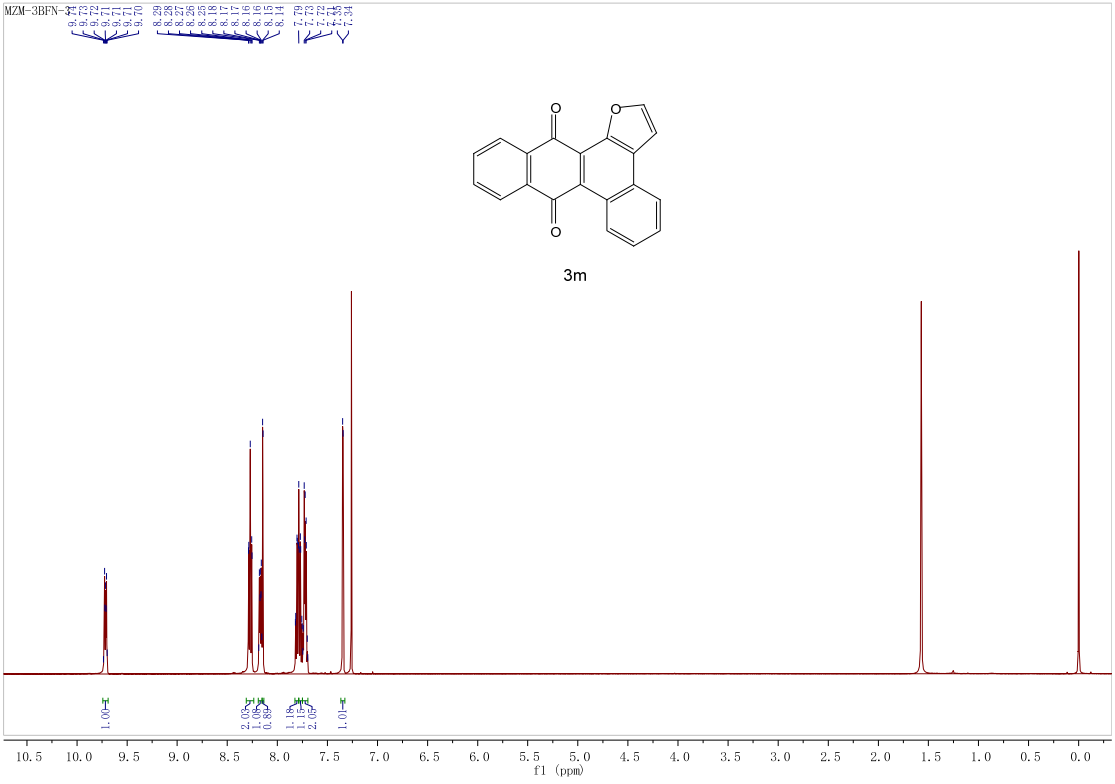

MZM-1NBF1
186.02
183.22
155.34
150.93
145.54
135.09
134.19
133.63
133.25
132.85
132.63
132.01
130.21
129.53
128.36
128.21
128.19
127.59
127.26
127.21
126.49
126.34
124.92
123.87
122.04
121.43
119.84
118.38
O
O
O
3k
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

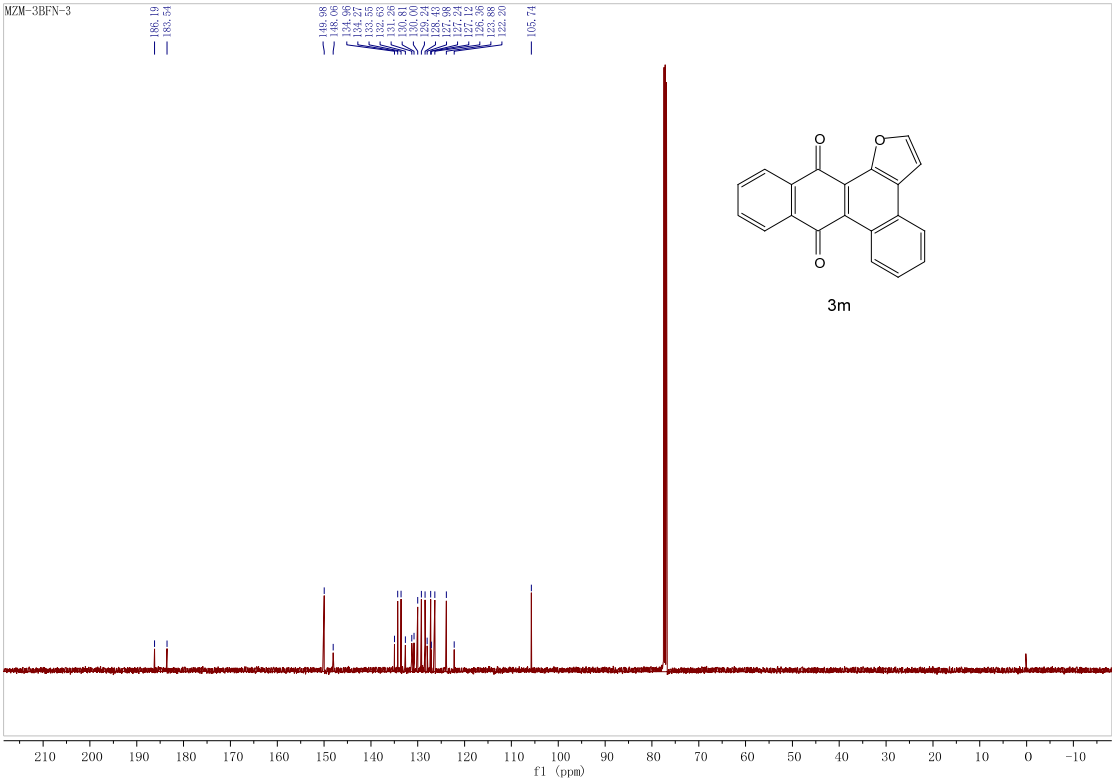

35 #15 RT: 0.17 AV: 1 NL: 9.98E6
T: FTMS + c APCI corona Full ms [50.0000-750.0000]
399.10132
400.10464
401.10806
401.33987
402.11218
403.12665
Relative Abundance
m/z
397.0 397.5 398.0 398.5 399.0 399.5 400.0 400.5 401.0 401.5 402.0 402.5 403.0 403.5 404.0 404.5 405.0

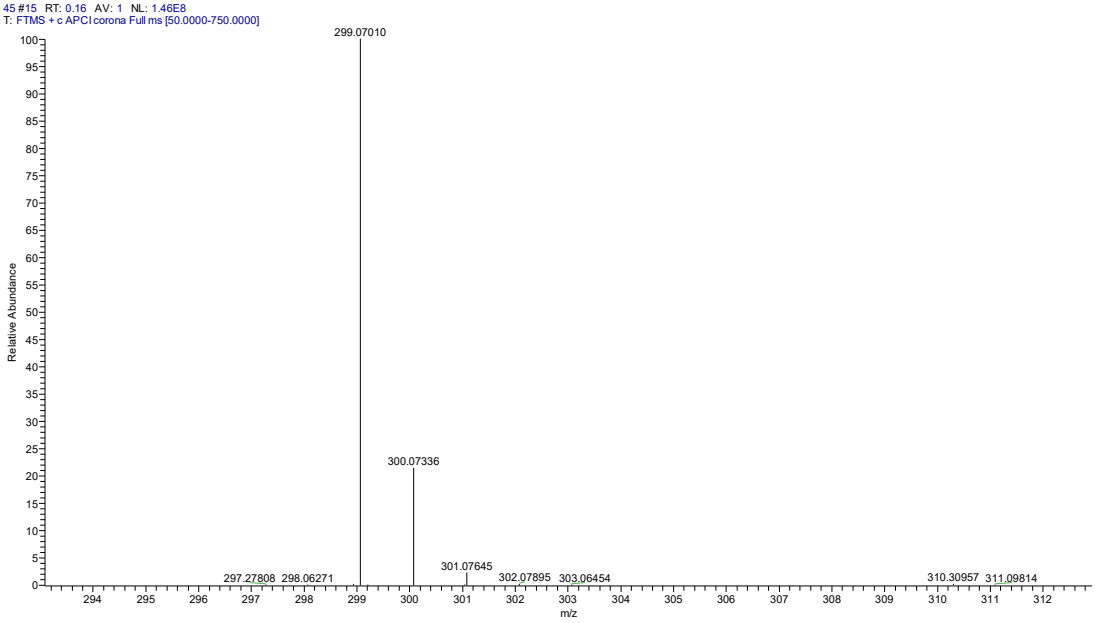

MZM-2NF-3
9.72
9.70
9.70
9.12
9.10
9.01
8.99
8.32
8.30
8.08
8.06
8.02
8.00
7.83
7.82
7.81
7.80
7.28
7.26
O
O
O
3l
1.00
1.08
1.08
1.99
1.99
1.05
4.97
0.98
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

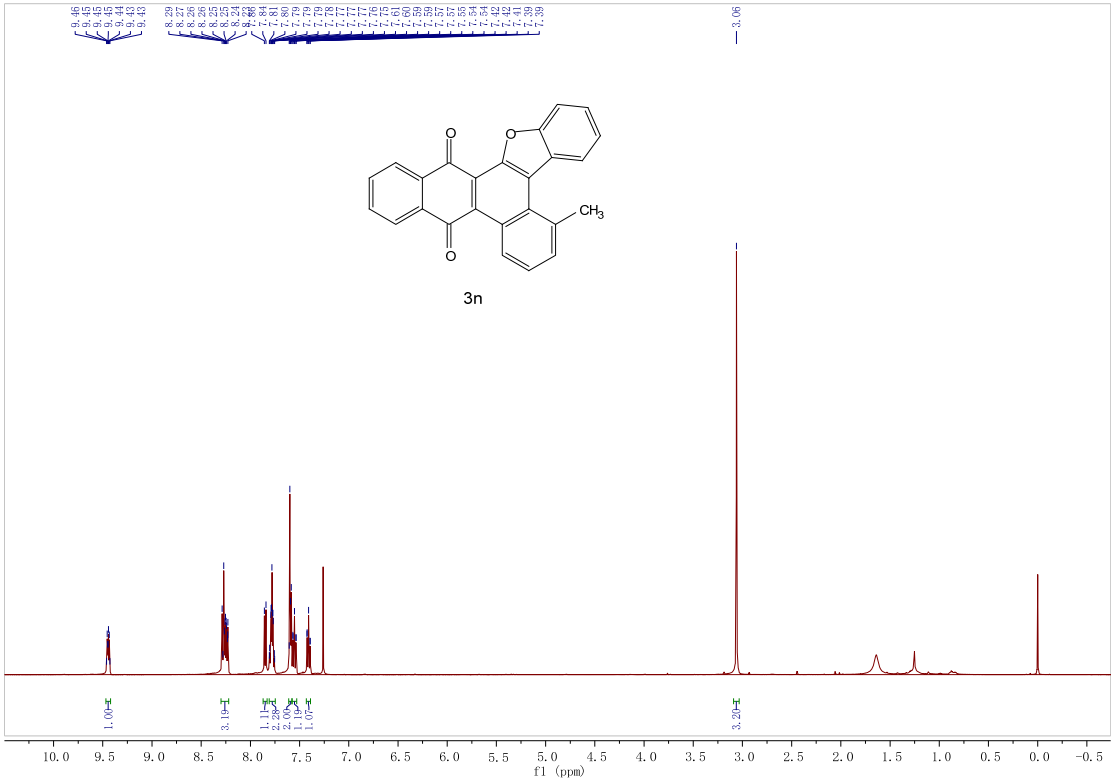

MZM-2NF-3
185.72
183.98
158.07
150.01
134.45
134.28
133.71
132.96
131.60
131.50
131.44
130.15
129.91
129.01
128.54
128.47
128.44
128.17
127.65
127.25
127.12
126.50
125.88
125.41
125.34
121.54
117.69
113.33
O
O
O
3l
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

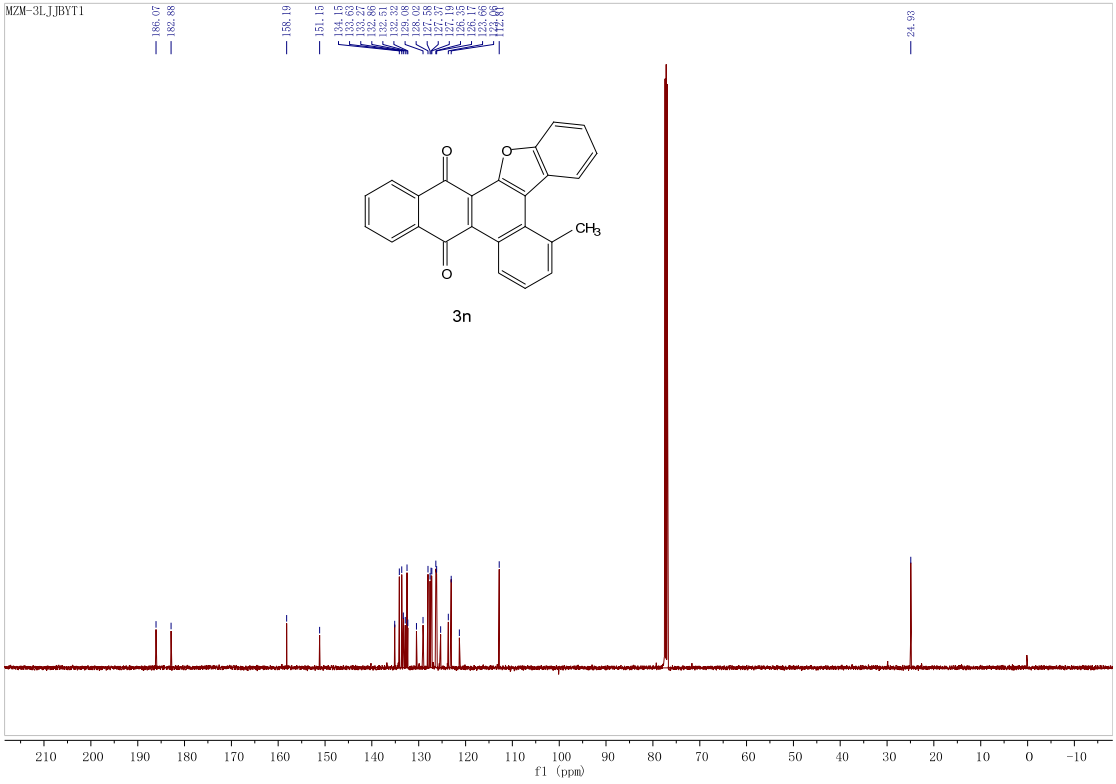

36 #15 RT: 0.17 AV: 1 NL: 6.02E6
T: FTMS + c APCI corona Full ms [50.0000-750.0000]
399.10117
400.10455
401.10718
402.11026
Relative Abundance
m/z

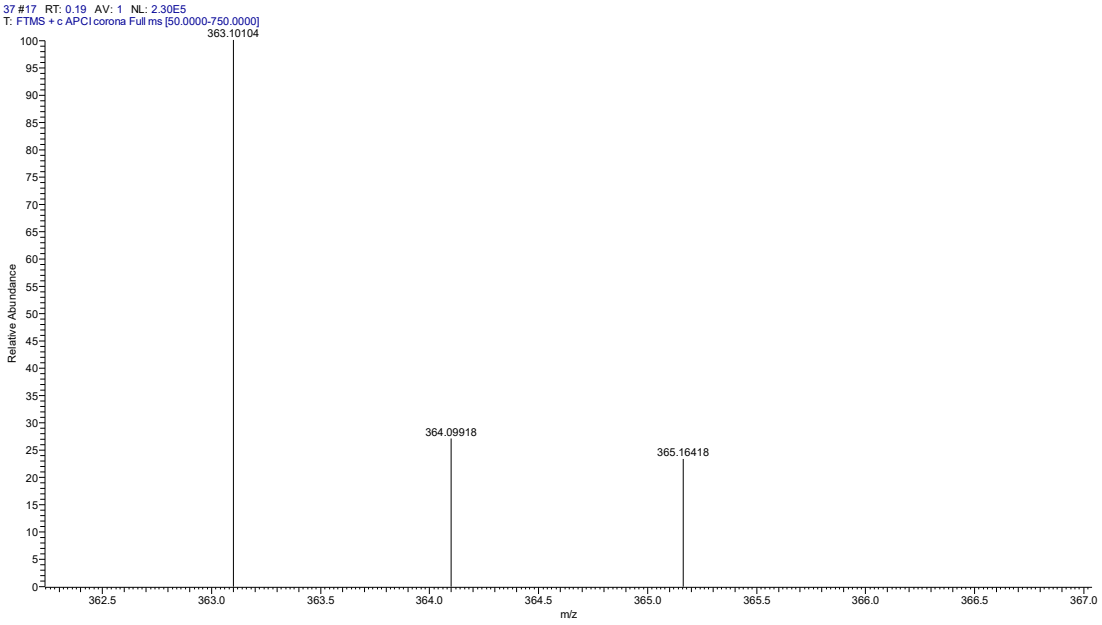

MZM-3BFN-3
3m
f1 (ppm)

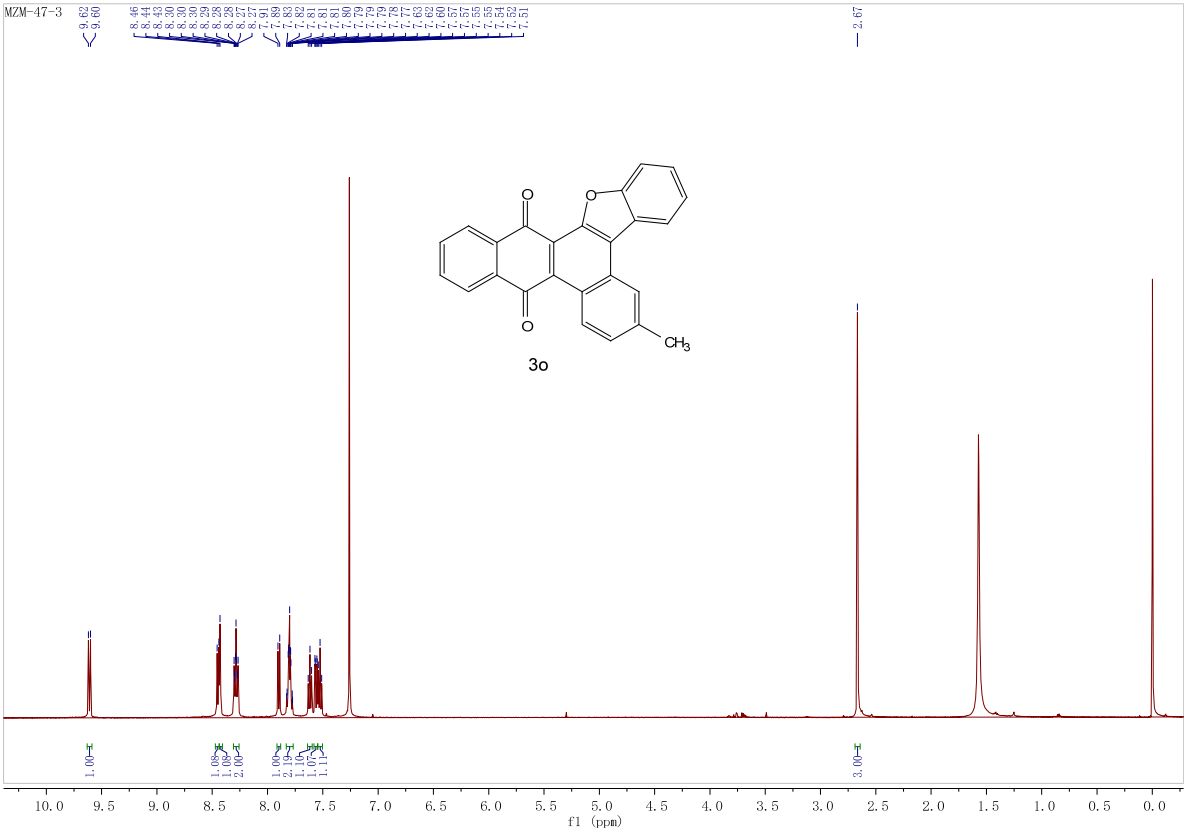

MZM-3BFN-3
186.19
183.54
149.98
148.96
134.96
134.27
133.55
131.63
131.26
130.81
130.00
129.24
128.48
127.94
127.24
127.12
126.36
126.08
122.96
122.20
105.74
O
O
O
3m
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

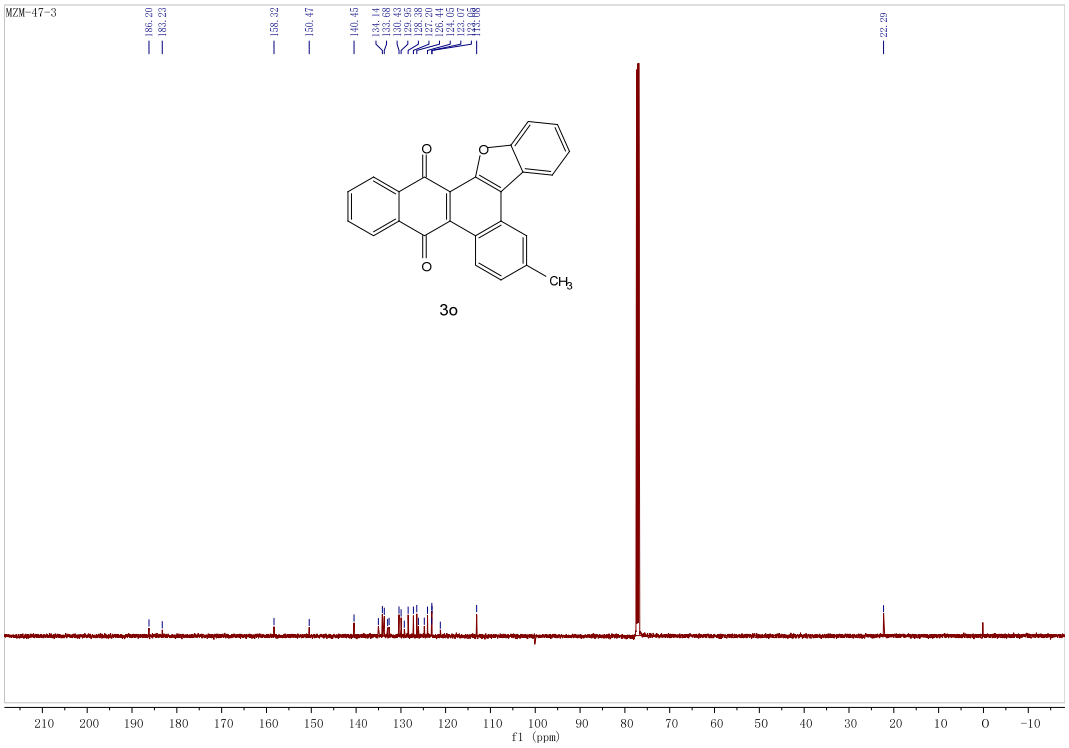

45 #15 RT: 0.16 AV: 1 NL: 1.46E8
T: FTMS + c APCI corona Full ms [50.0000-750.0000]
299.07010
300.07336
301.07645
297.27808
298.06271
302.07895
303.06454
310.30957
311.09814
Relative Abundance
m/z
294 295 296 297 298 299 300 301 302 303 304 305 306 307 308 309 310 311 312

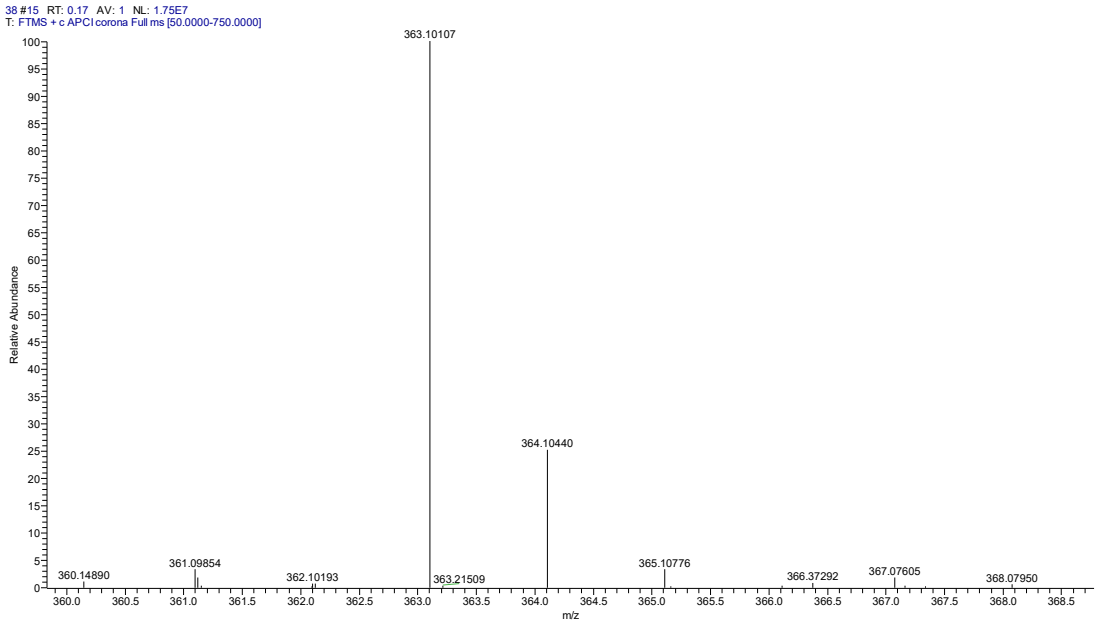

O
O
O
CH3
3n
f1 (ppm)

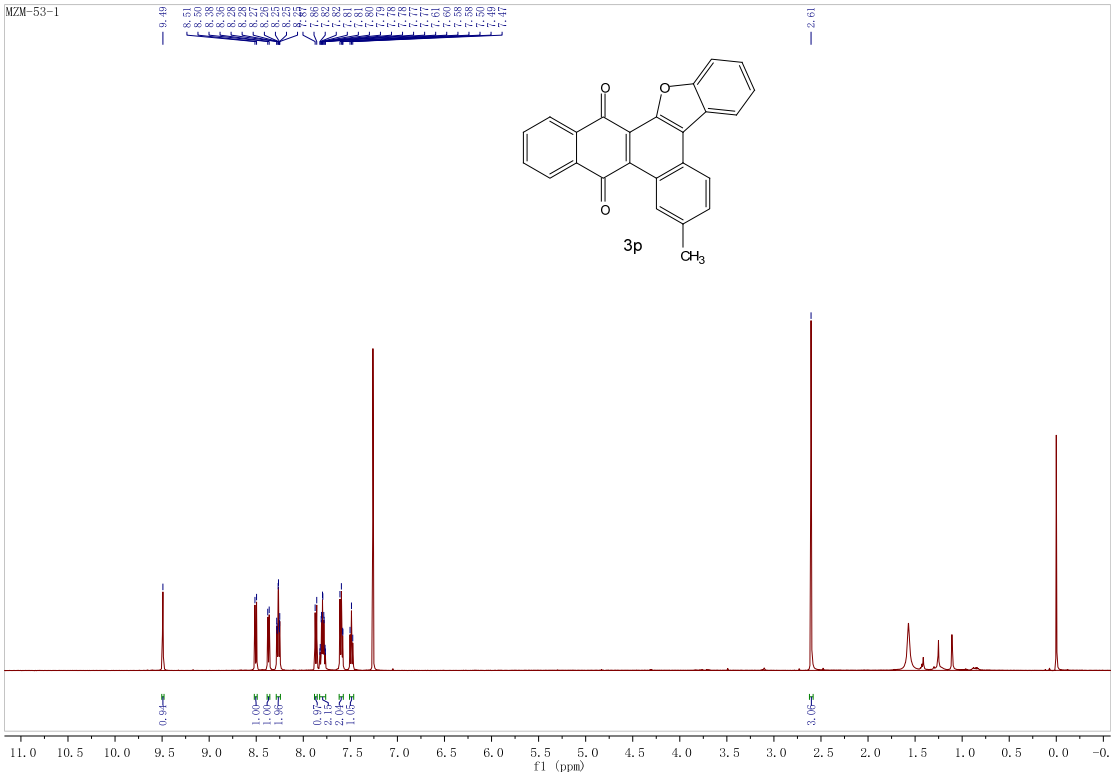

MZM-3L_JJBYT1
O
O
O
CH3
3n
f1 (ppm)

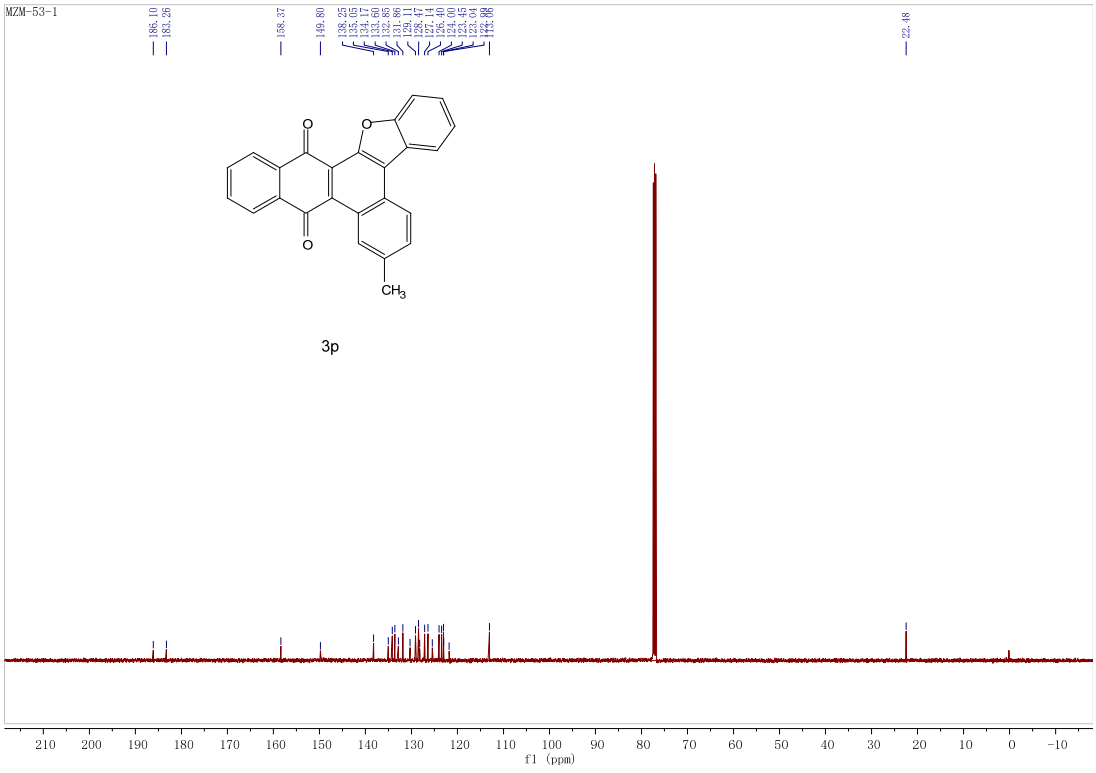

37 #17 RT: 0.19 AV: 1 NL: 2.30E5
T: FTMS + c APCI corona Full ms [50.0000-750.0000]
363.10104
364.09918
365.16418
Relative Abundance
m/z

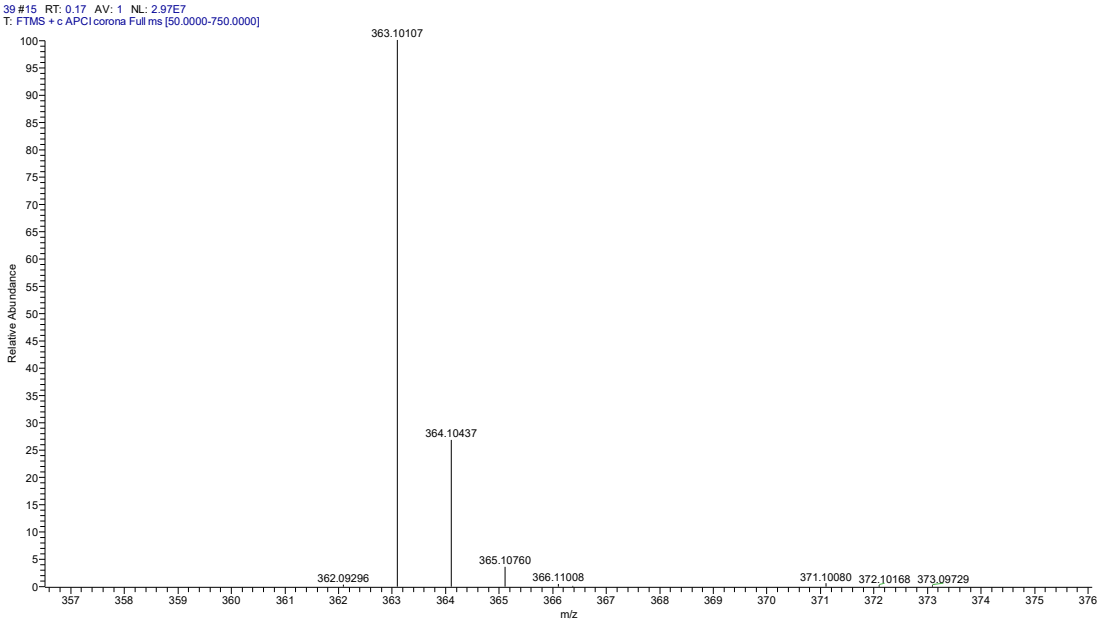

MZM-47-3
3o
f1 (ppm)

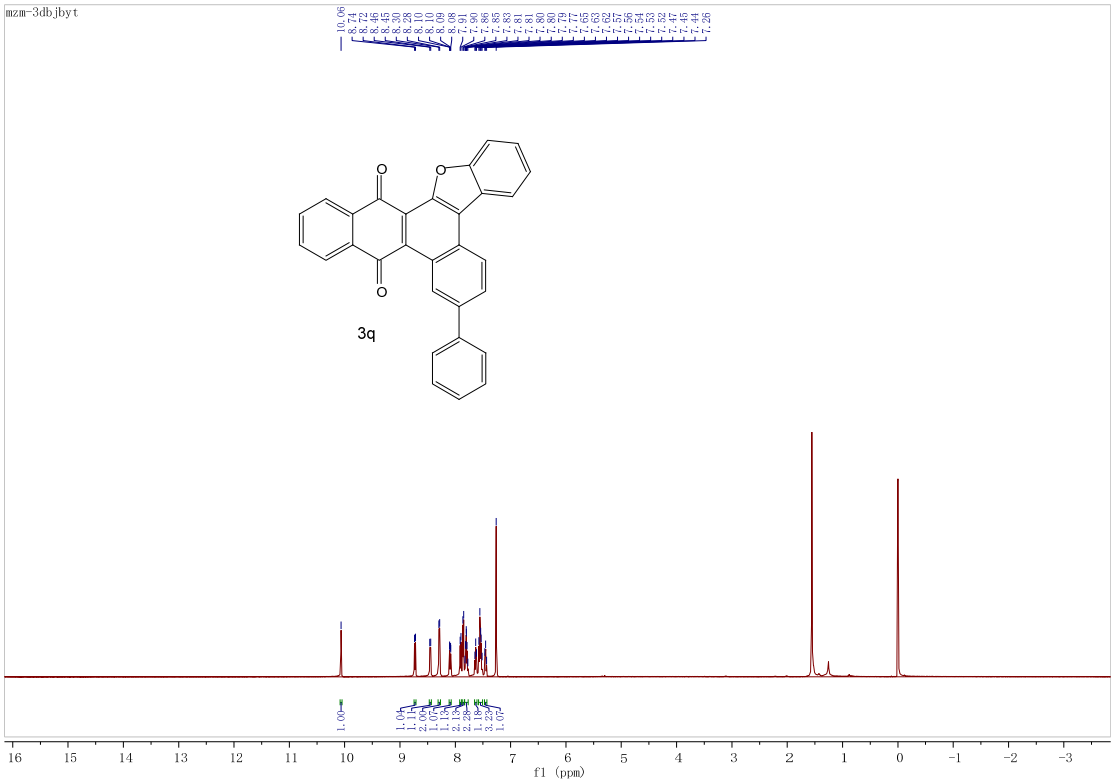

MZM-47-3
186.20
183.23
158.32
150.47
140.45
134.14
133.68
130.43
129.45
128.38
127.20
126.44
124.05
123.15
122.29
O
O
O
CH3
3o
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

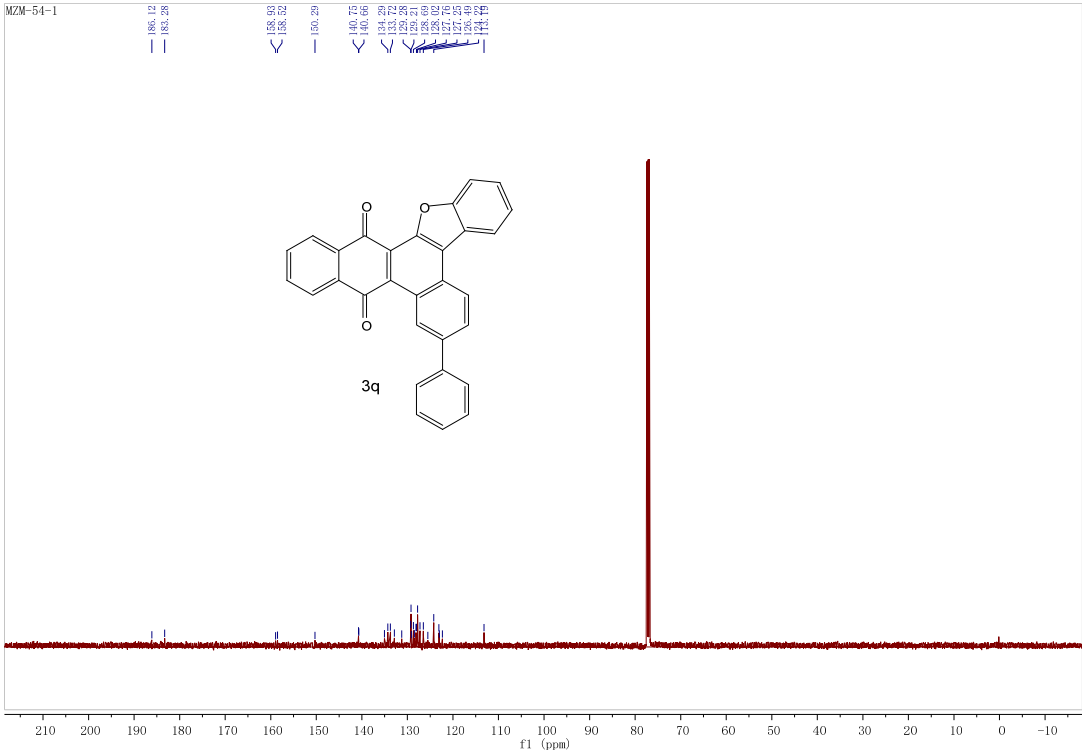

38 #15 RT: 0.17 AV: 1 NL: 1.75E7
T: FTMS + c APCI corona Full ms [50.0000-750.0000]
363.10107
364.10440
361.09854
365.10776
360.14890
362.10193
363.21509
366.37292
367.07605
368.07950
Relative Abundance
m/z

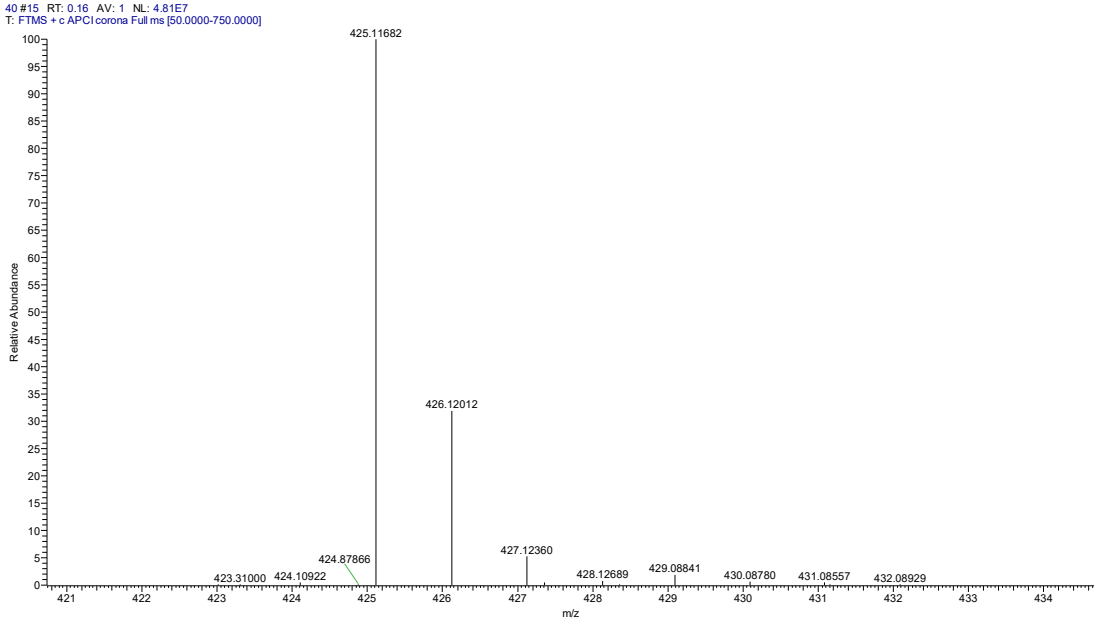

MZM-53-1
3p
f1 (ppm)

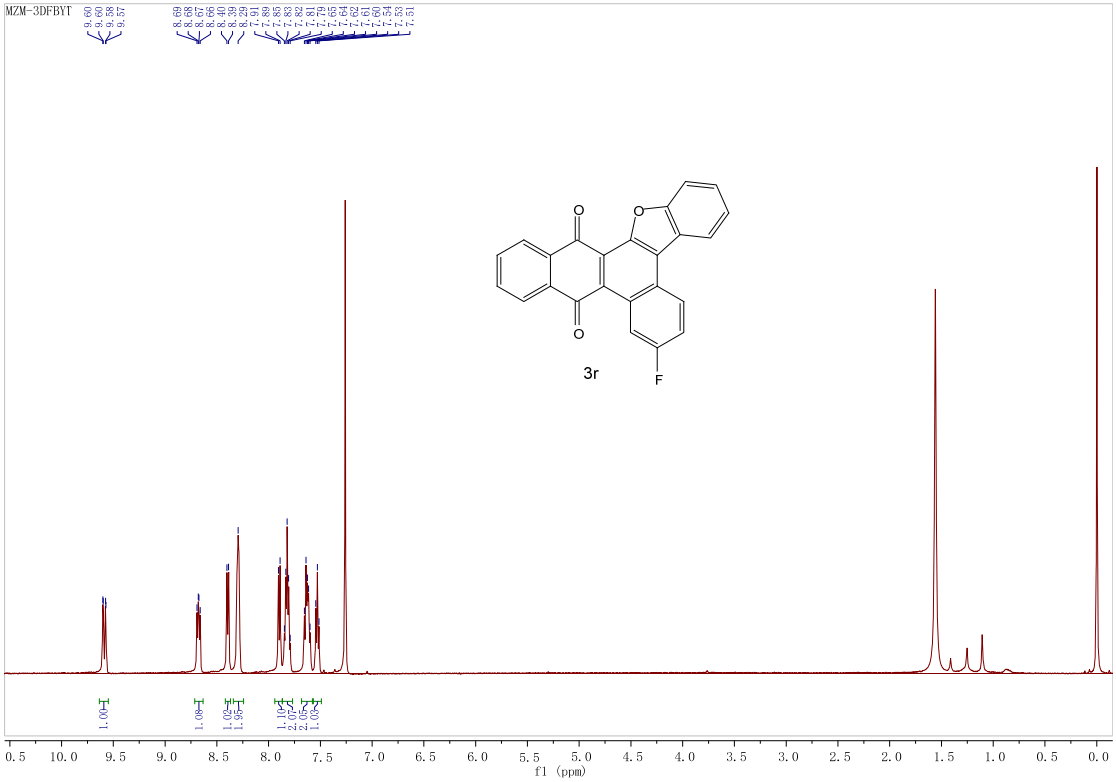

MZM-53-1
3p
f1 (ppm)

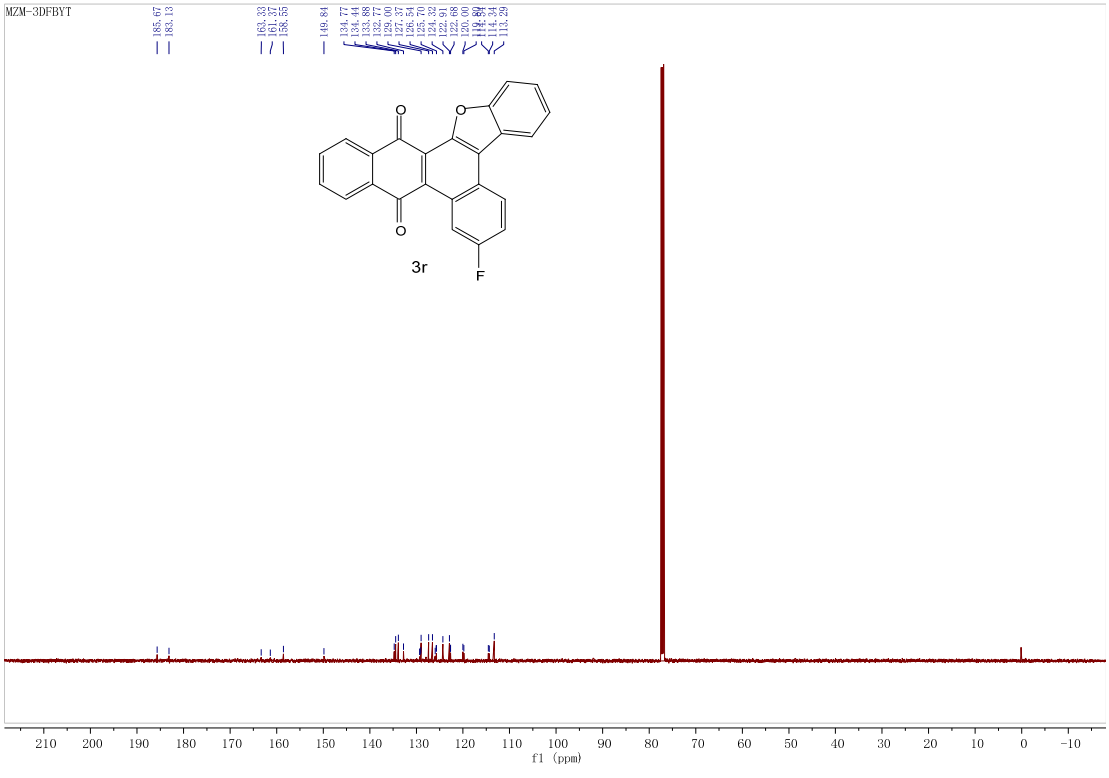

39 #15 RT: 0.17 AV: 1 NL: 2.97E7
T: FTMS + c APCI corona Full ms [50.0000-750.0000]
363.10107
364.10437
365.10760
362.09296
366.11008
371.10080
372.10168
373.09729
Relative Abundance
m/z

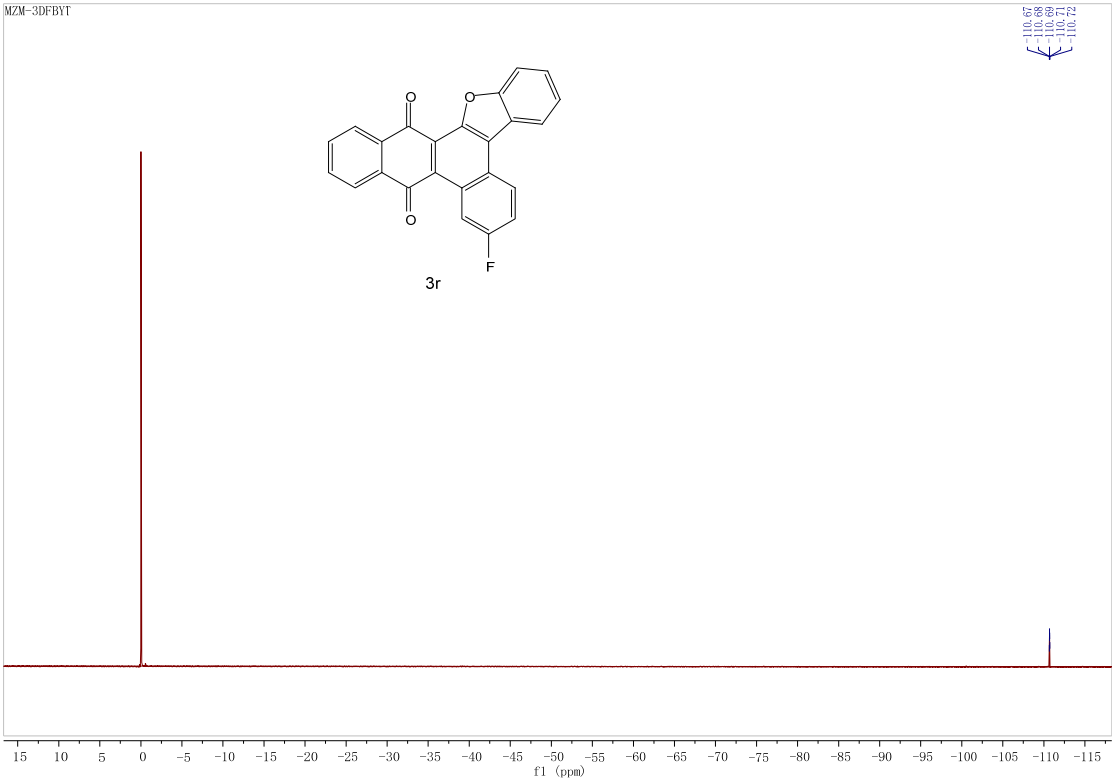

mzm-3db.jbyt
3q
f1 (ppm)

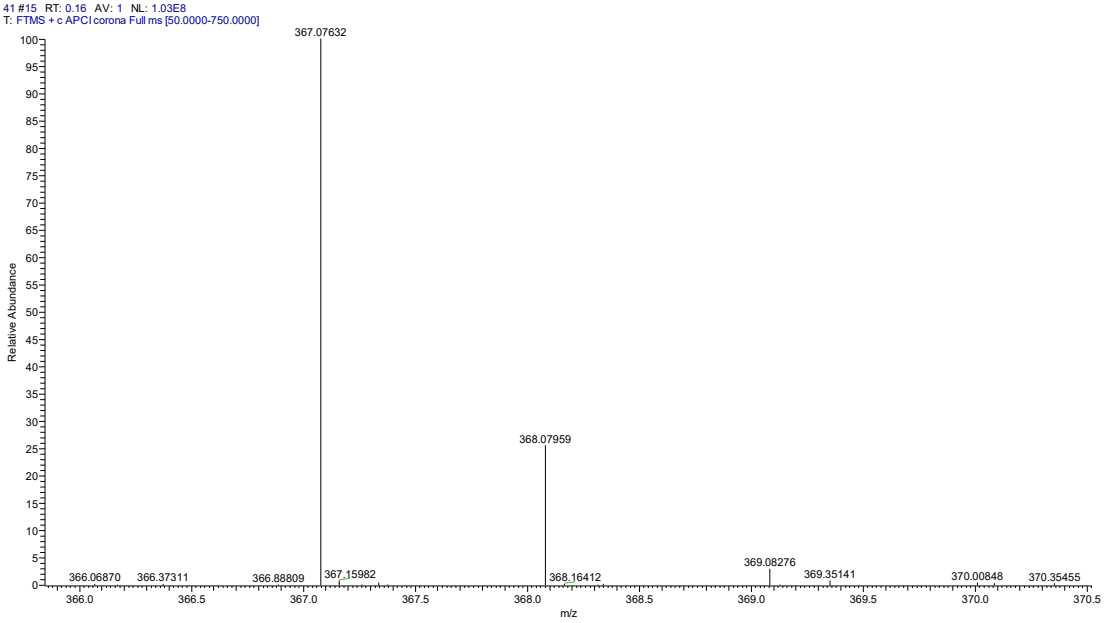

MZM-54-1
186.12
183.28
158.93
138.32
150.29
140.75
140.66
134.29
133.72
129.28
129.21
128.69
128.03
127.76
127.25
125.49
124.97
114.19
O
O
O
3q
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

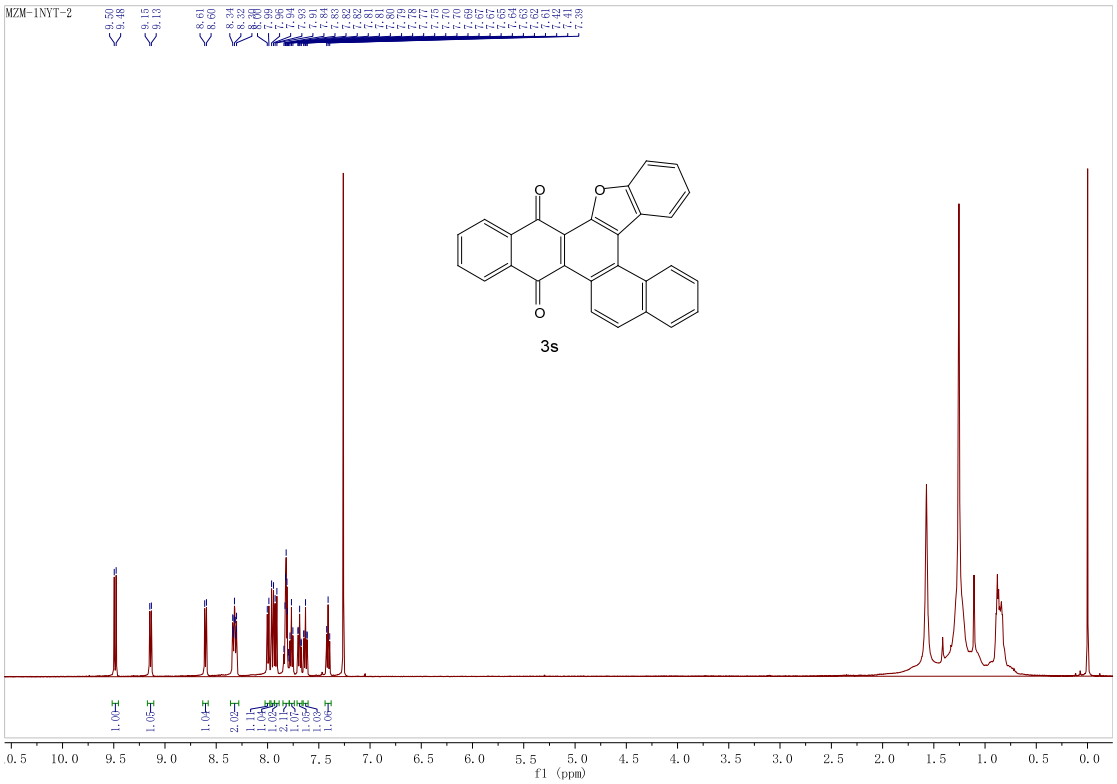

40 #15 RT: 0.16 AV: 1 NL: 4.81E7
T: FTMS + c APCI corona Full ms [50.0000-750.0000]
425.11682
426.12012
427.12360
424.87866
423.31000
424.10922
428.12689
429.08841
430.08780
431.08557
432.08929
Relative Abundance
m/z
421 422 423 424 425 426 427 428 429 430 431 432 433 434

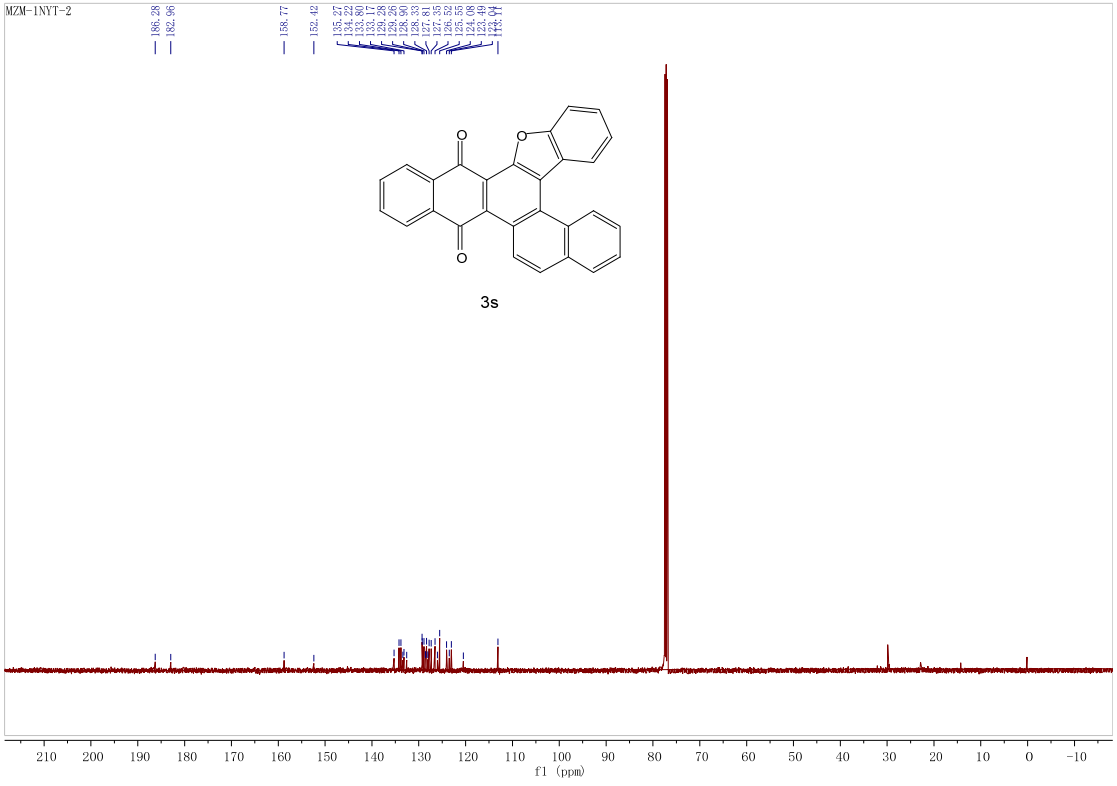

MZM-3DFBYT
3r
F
f1 (ppm)

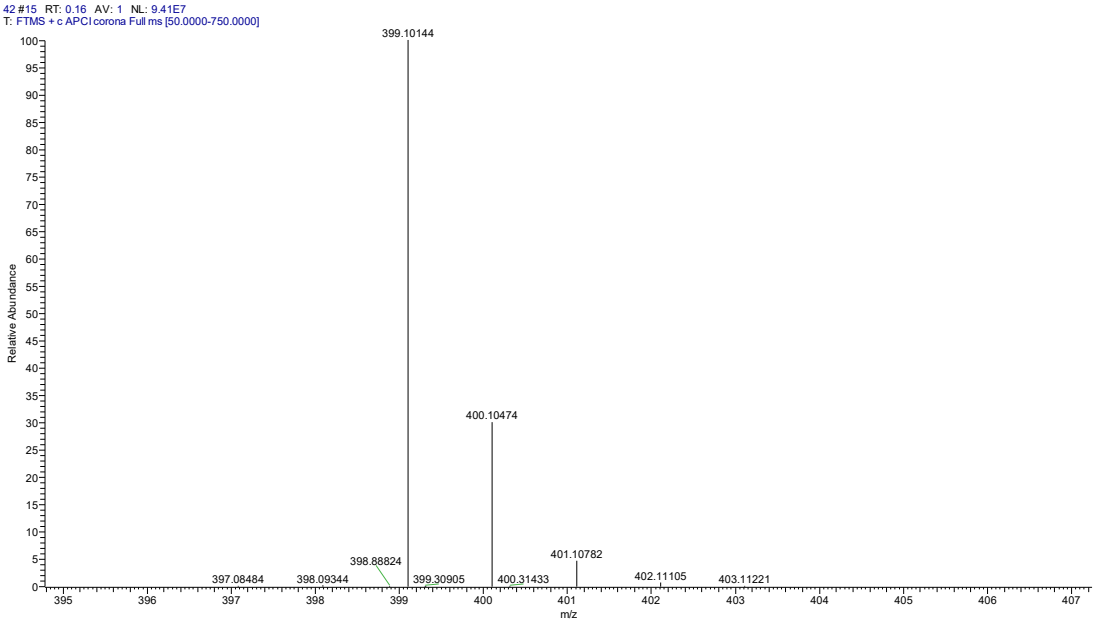

MZM-3DFBYT
3r
F
f1 (ppm)

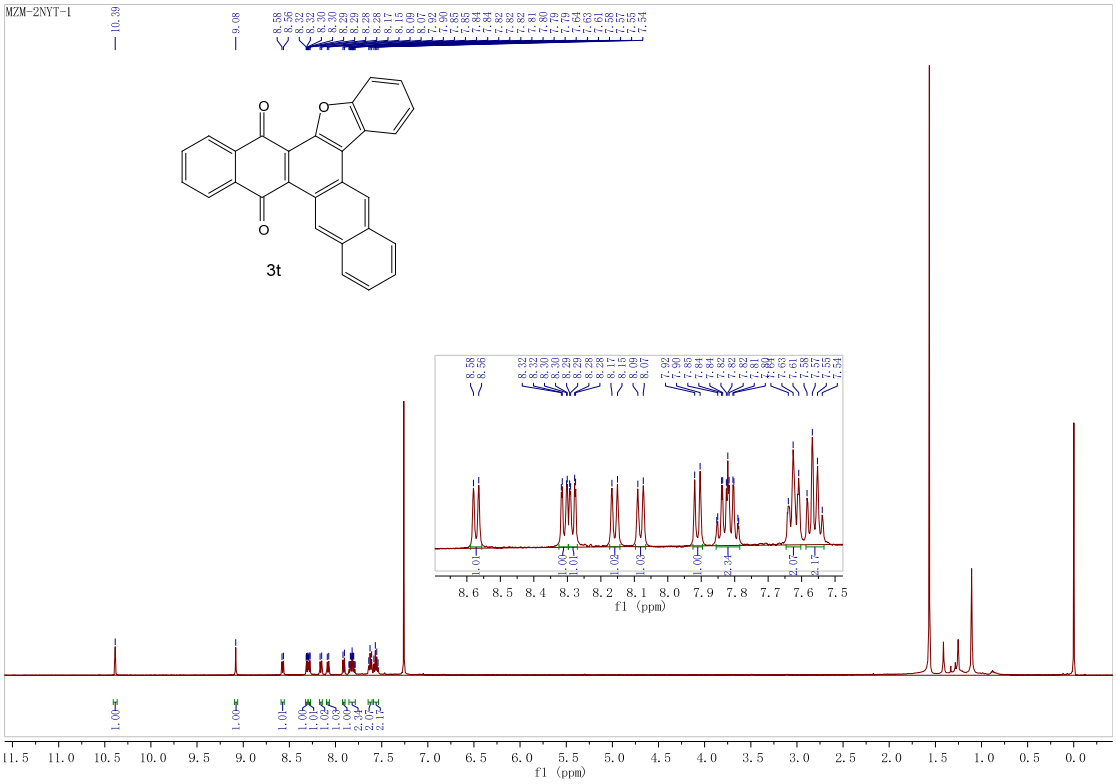

MZM-3DFBYT
-110.67
-110.68
-110.69
-110.71
-110.72
O
O
O
F
3r
15 10 5 0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -100 -105 -110 -115
f1 (ppm)

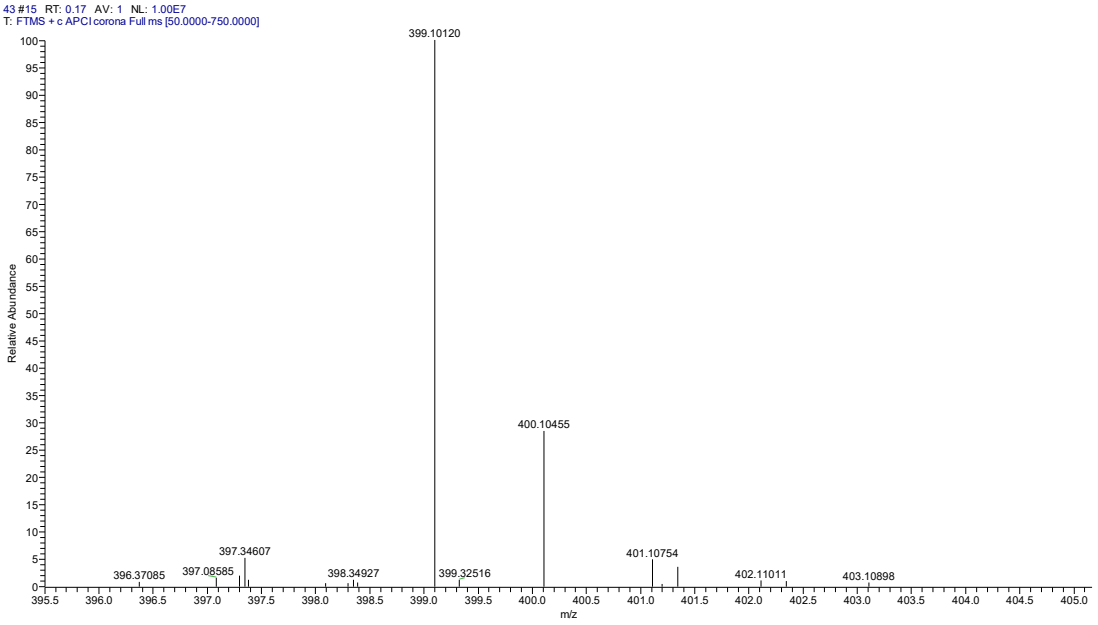

41 #15 RT: 0.16 AV: 1 NL: 1.03E8
T: FTMS + c APCI corona Full ms [50.0000-750.0000]
Relative Abundance
m/z
367.07632
368.07959
369.08276
366.06870
366.37311
366.88809
367.15982
368.16412
369.35141
370.00848
370.35455
366.0 366.5 367.0 367.5 368.0 368.5 369.0 369.5 370.0 370.5

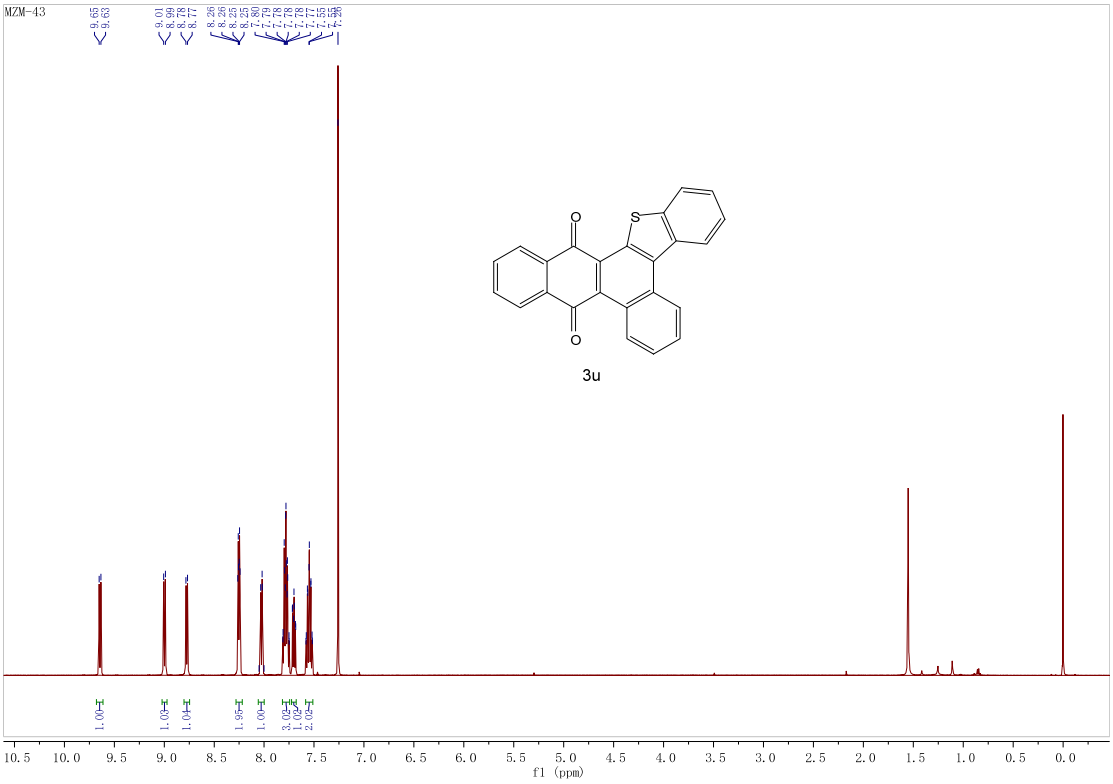

MZM-1NYT-2
3s
f1 (ppm)

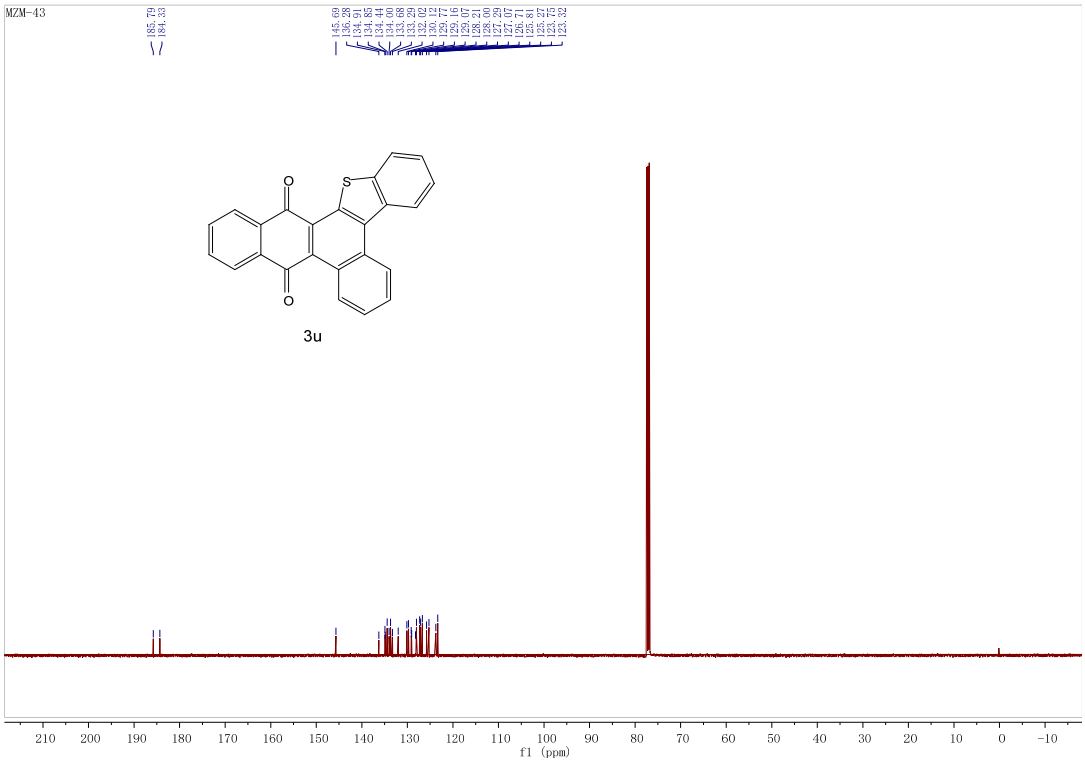

MZM-1NYT-2
3s
f1 (ppm)

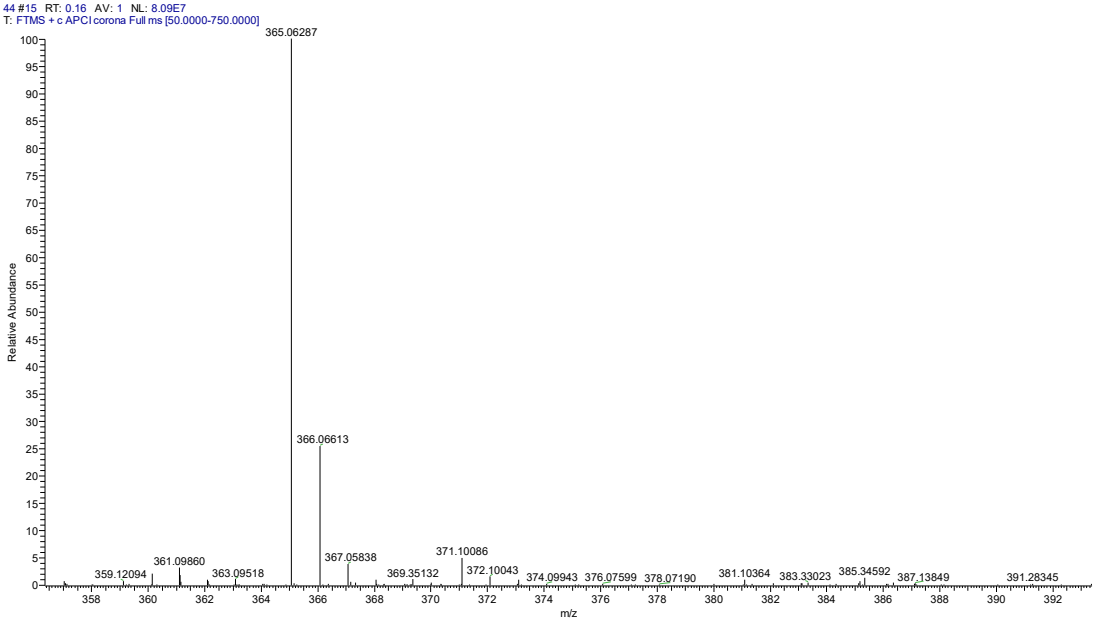

42 #15 RT: 0.16 AV: 1 NL: 9.41E7
T: FTMS + c APCI corona Full ms [50.0000-750.0000]
399.10144
400.10474
401.10782
398.88824
397.08484
398.09344
399.30905
400.31433
402.11105
403.11221
Relative Abundance
m/z

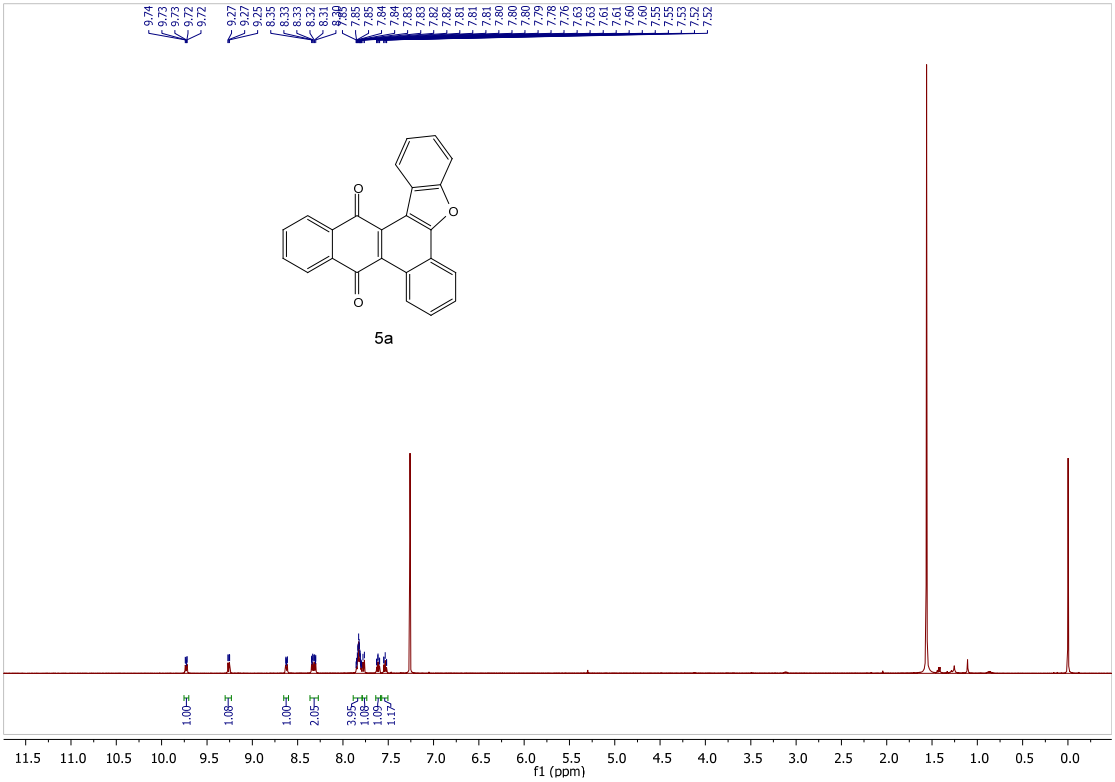

MZM-2NYT-1
3t
f1 (ppm)

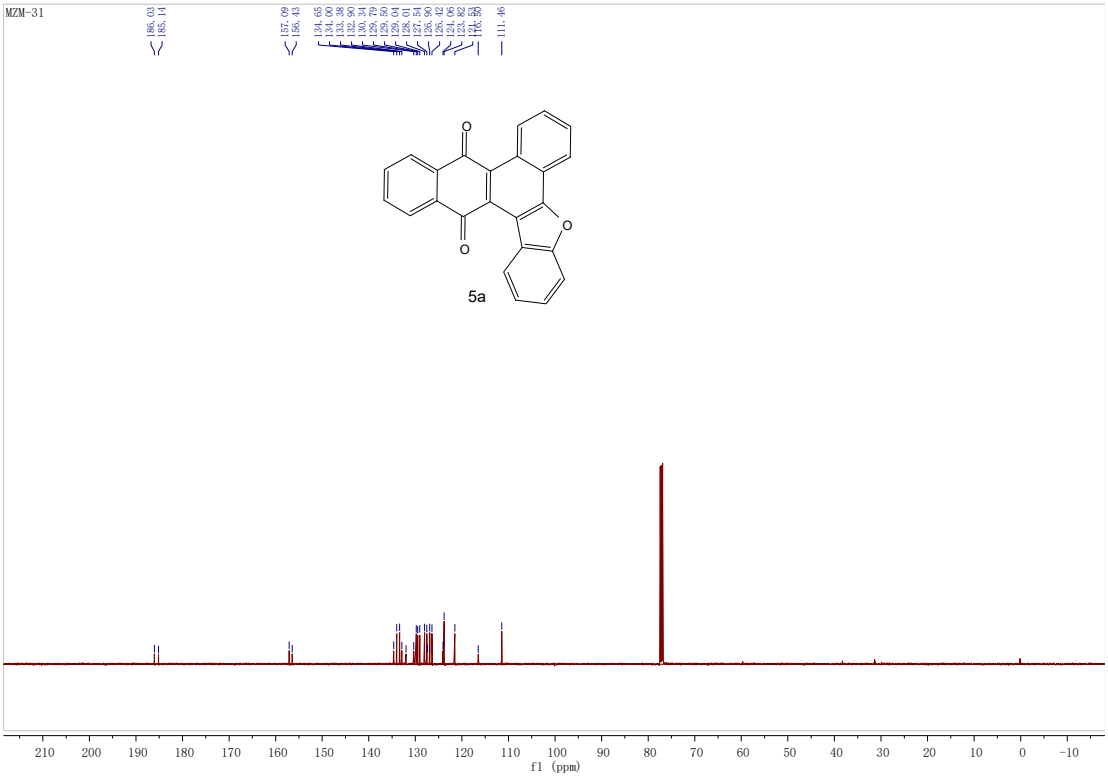

43 #15 RT: 0.17 AV: 1 NL: 1.00E7
T: FTMS + c APCI corona Full ms [50.0000-750.0000]
399.10120
400.10455
397.34607
396.37085
397.08585
398.34927
399.32516
401.10754
402.11011
403.10898
Relative Abundance
m/z

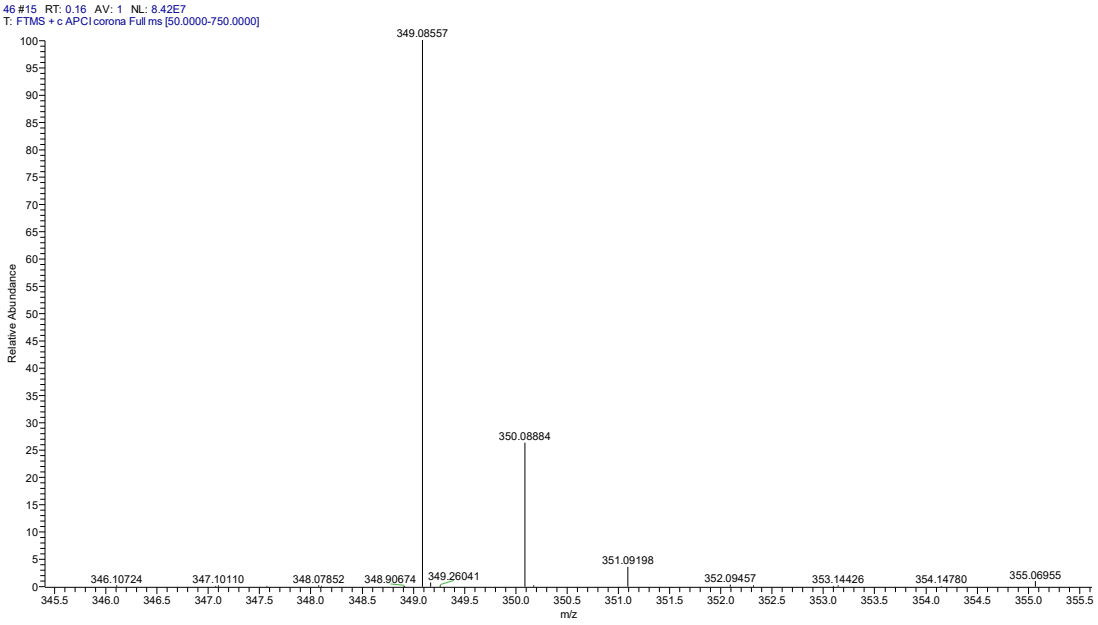

MZM-43
O
S
O
3u
f1 (ppm)

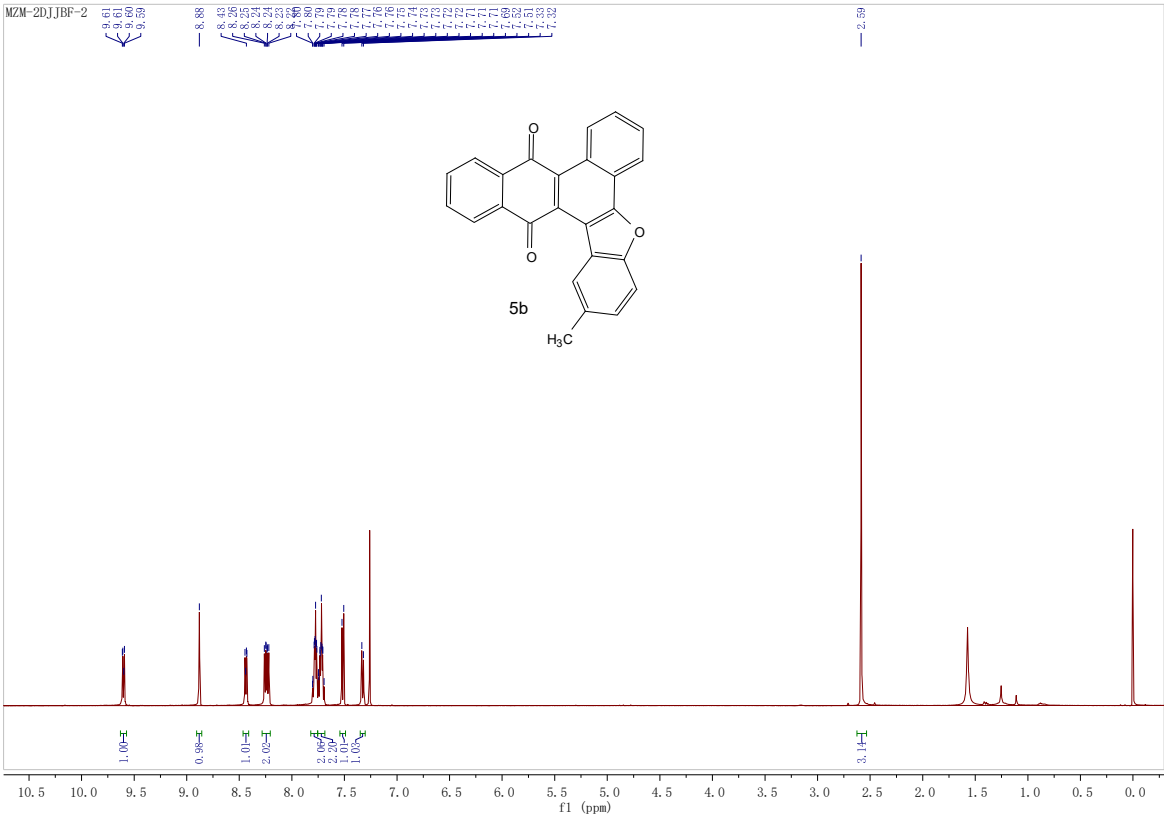

MZM-43
185.79
184.33
145.69
136.28
134.91
134.85
134.44
134.00
133.68
133.29
132.72
132.12
129.77
129.16
128.97
128.71
128.00
127.29
127.07
126.71
125.81
125.27
123.75
123.32
O
S
O
3u
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)

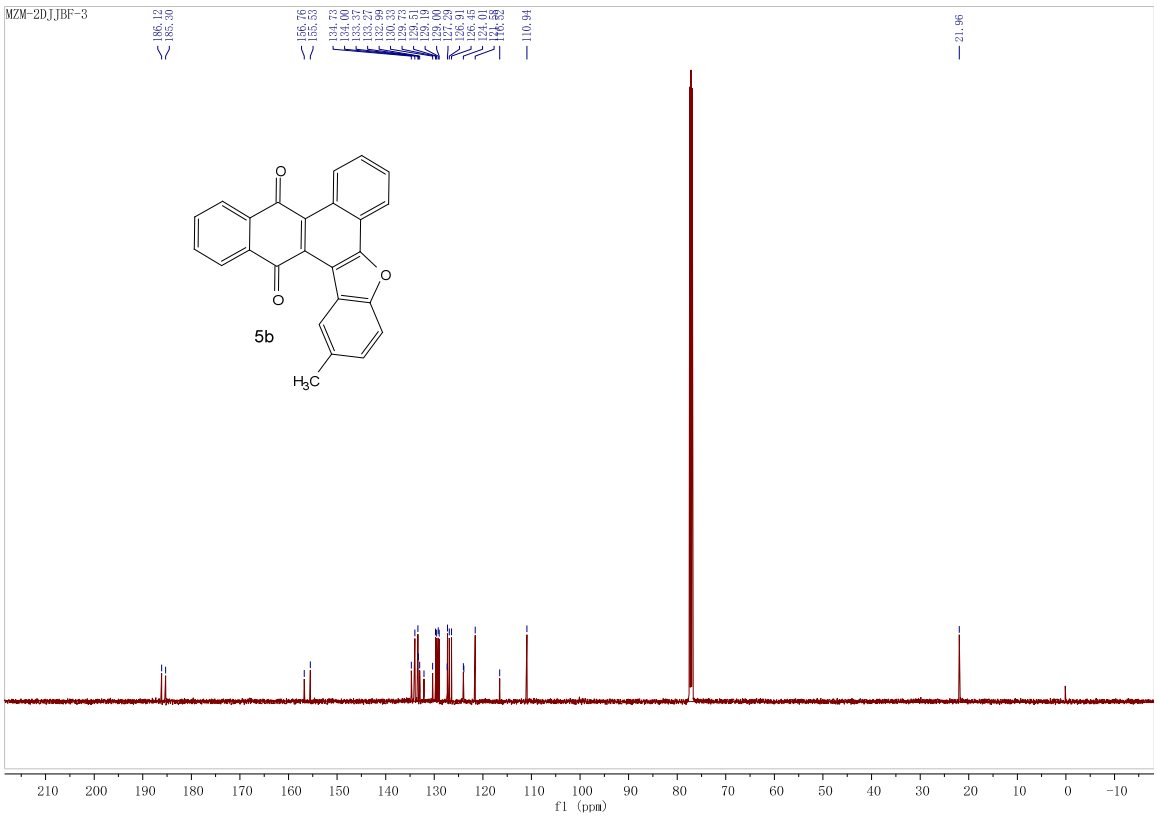

44 #15 RT: 0.16 AV: 1 NL: 8.09E7
T: FTMS + c APCI corona Full ms [50.0000-750.0000]
Relative Abundance
m/z
365.06287
366.06613
367.05838
371.10086
372.10043
359.12094
361.09860
363.09518
369.35132
374.09943
376.07599
378.07190
381.10364
383.33023
385.34592
387.13849
391.28345

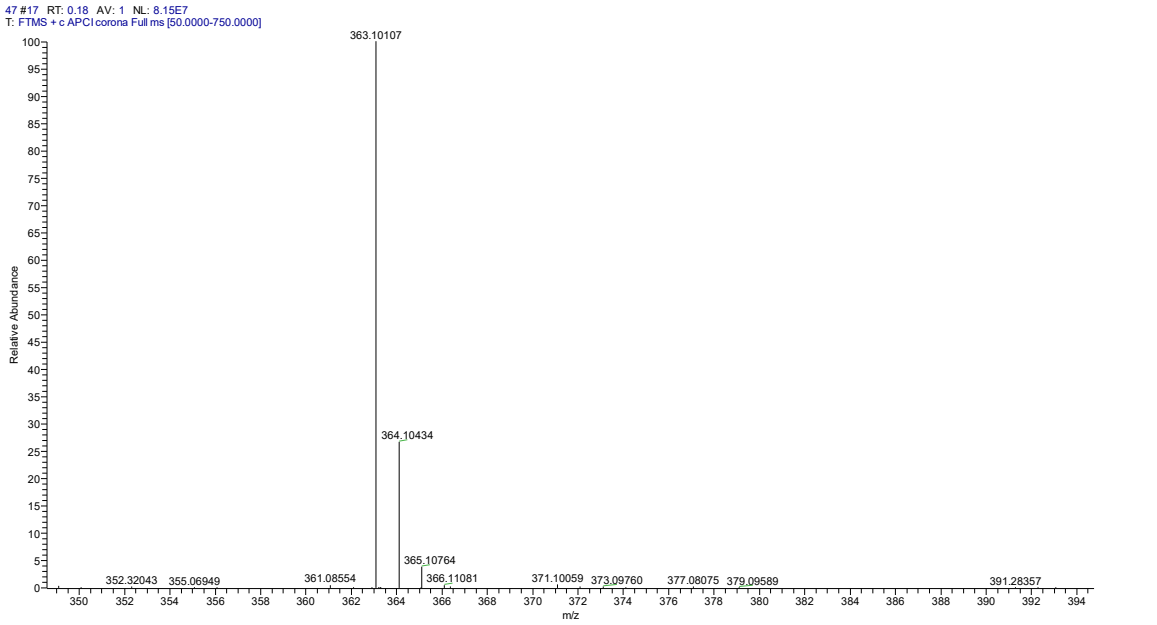

9.74
9.73
9.73
9.72
9.72
9.27
9.27
9.25
8.35
8.33
8.33
8.32
8.31
7.85
7.85
7.85
7.84
7.84
7.83
7.83
7.82
7.82
7.81
7.81
7.81
7.80
7.80
7.80
7.79
7.78
7.76
7.63
7.61
7.61
7.60
7.60
7.55
7.55
7.53
7.52
7.52
O
O
O
5a
1.00
1.08
1.00
2.05
3.95
1.09
1.17
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

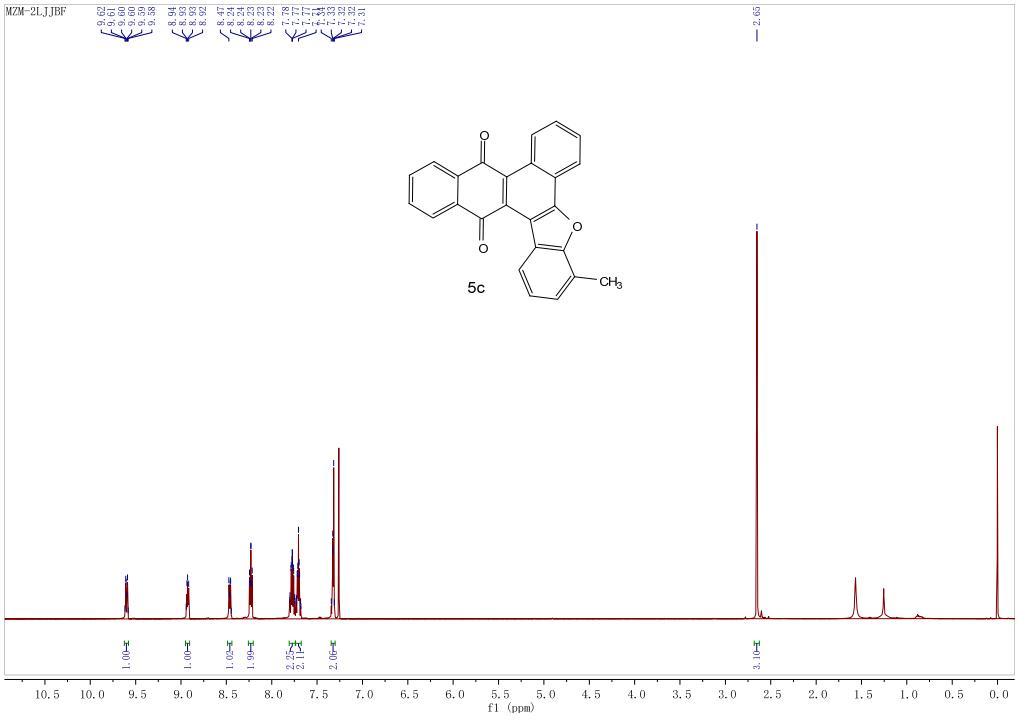

MZM-31
186.03
185.14
157.09
156.43
134.65
134.00
133.38
132.90
132.34
129.79
129.50
129.04
128.01
127.54
126.90
126.42
124.06
123.62
121.53
118.50
111.46
O
O
O
5a
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

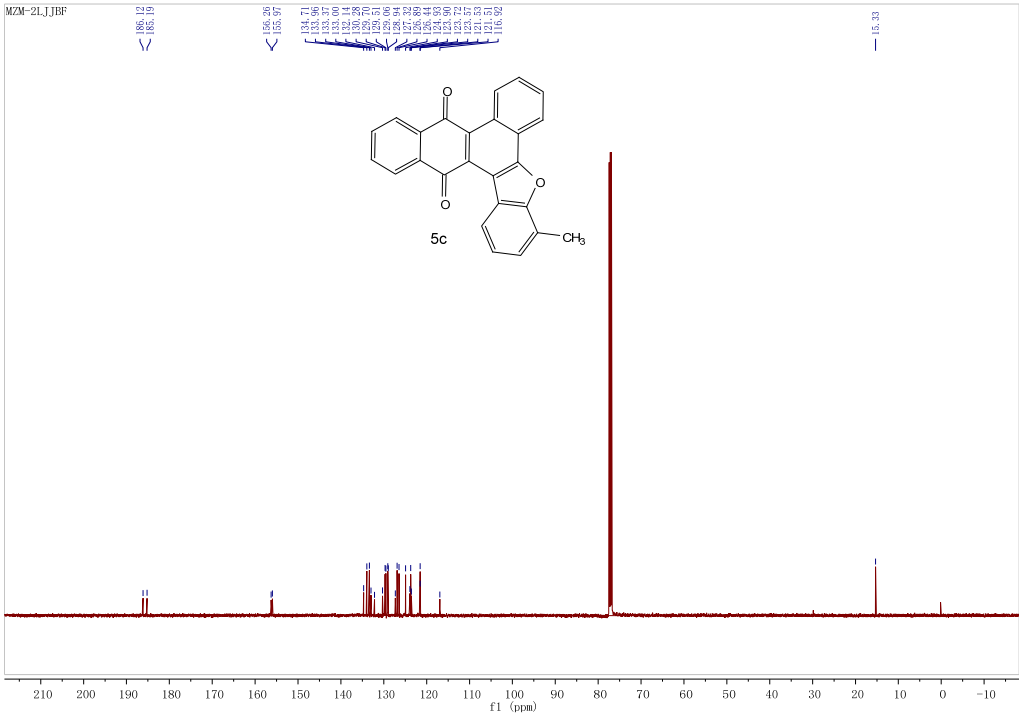

46 #15 RT: 0.16 AV: 1 NL: 8.42E7
T: FTMS + c APCI corona Full ms [50.0000-750.0000]
349.08557
350.08884
351.09198
346.10724
347.10110
348.07852
348.90674
349.26041
352.09457
353.14426
354.14780
355.06955
Relative Abundance
m/z

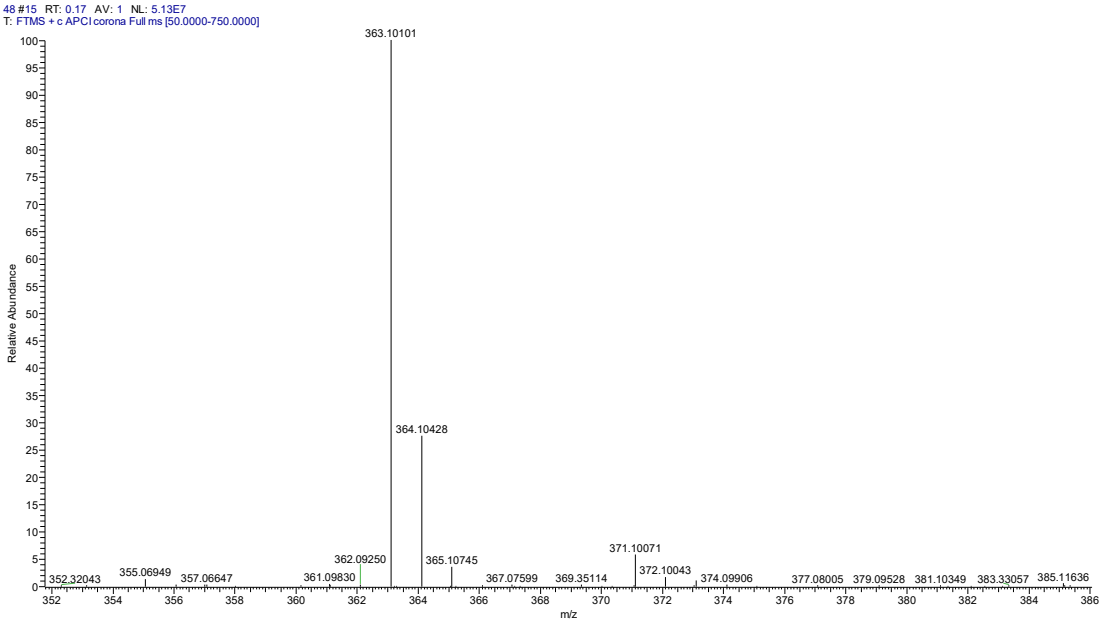

MZM-2DJJBF-2
5b
H3C
f1 (ppm)

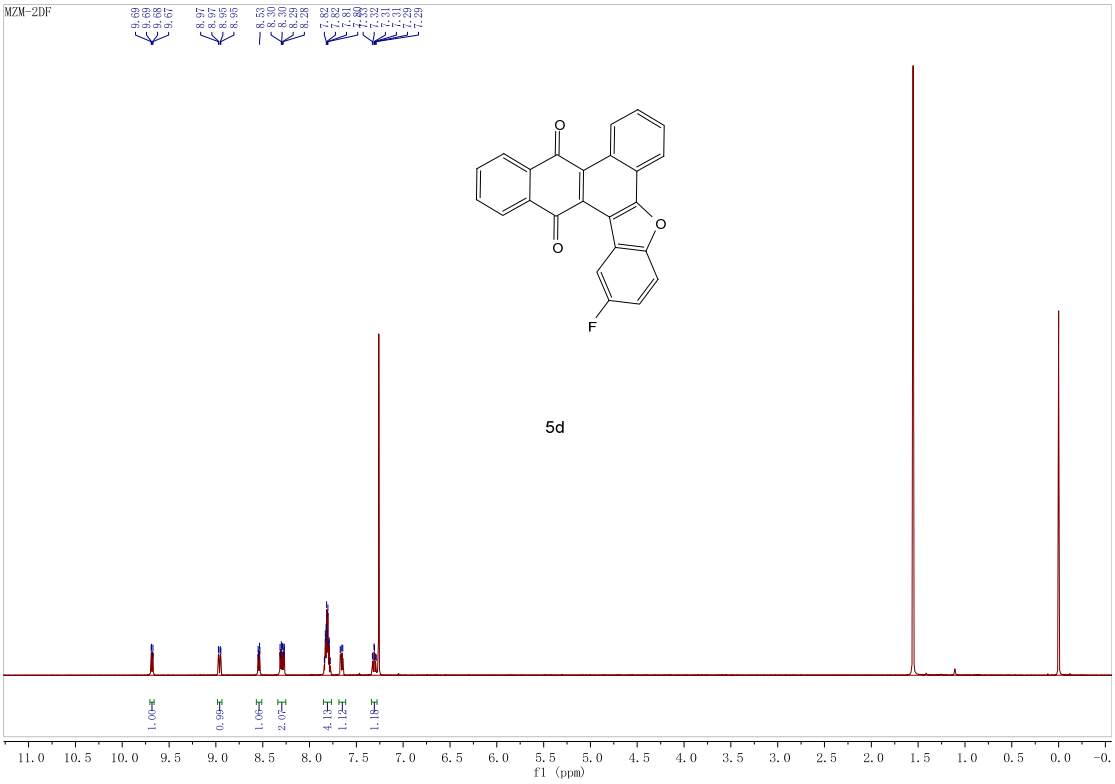

MZM-2DJJBF-3
186.12
185.30
156.76
155.53
134.73
134.00
133.37
133.27
132.99
130.33
129.73
129.61
129.19
129.00
128.93
128.91
126.45
124.01
118.68
116.82
110.94
21.96
O
O
O
5b
H3C
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

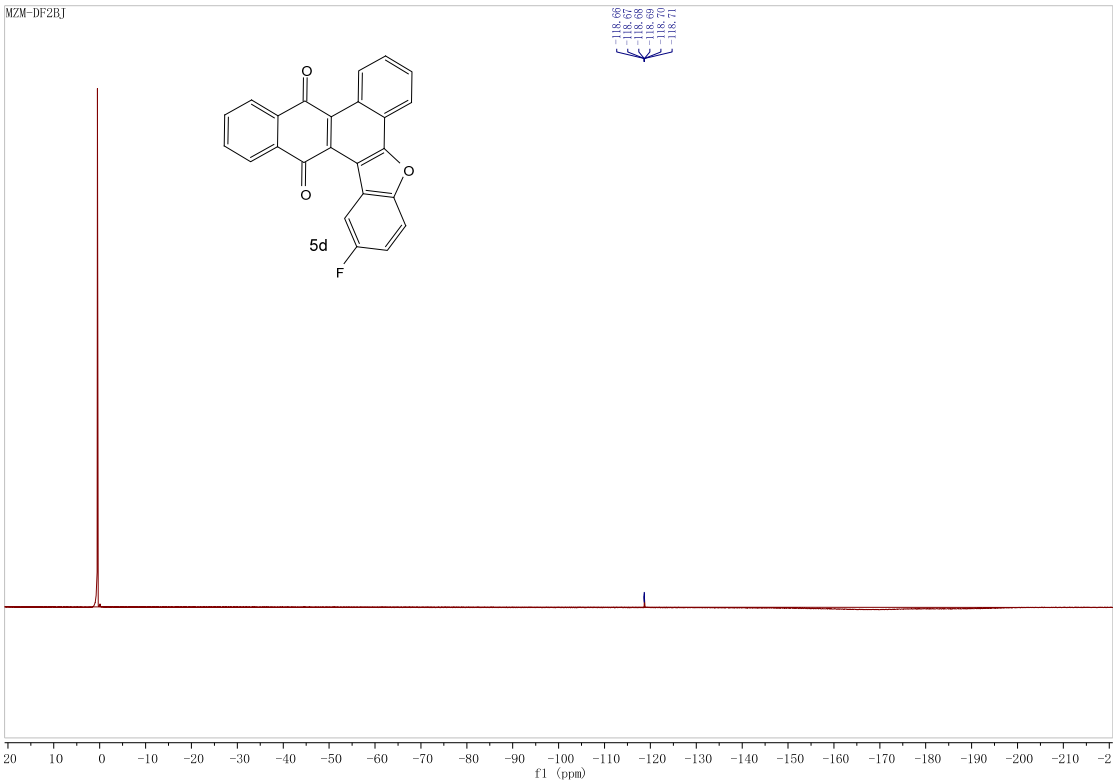

47 #17 RT: 0.18 AV: 1 NL: 8.15E7
T: FTMS + c APCI corona Full ms [50.0000-750.0000]
363.10107
364.10434
365.10764
366.11081
352.32043
355.06949
361.08554
371.10059
373.09760
377.08075
379.09589
391.28357
Relative Abundance
m/z

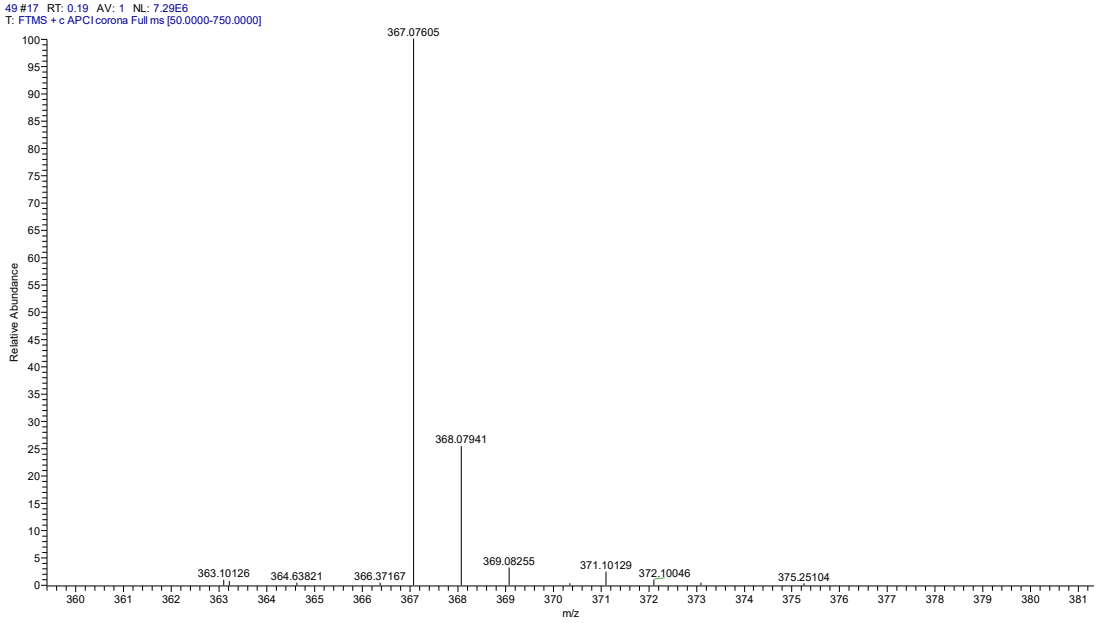

MZM-2L.JJBF
9.62
9.61
9.60
9.59
9.58
8.94
8.93
8.92
8.47
8.24
8.24
8.23
8.23
8.22
7.78
7.77
7.77
7.34
7.33
7.32
7.31
2.65
5c
1.00
1.00
1.02
1.99
2.25
2.11
2.06
3.10
f1 (ppm)

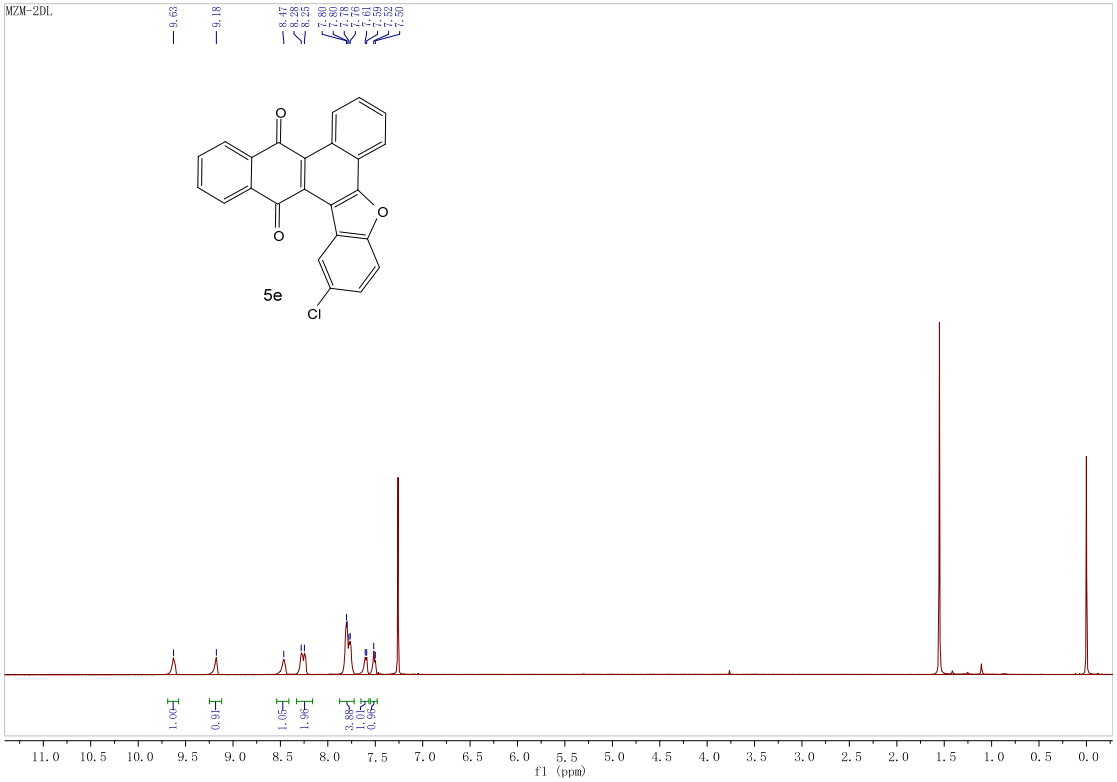

MZM-2L.JJBF
186.12
183.19
156.26
155.97
134.71
133.96
133.37
133.09
132.14
130.28
129.70
129.51
129.06
128.94
127.32
126.89
126.44
124.65
123.96
123.72
121.57
121.53
121.51
116.92
15.33
5c
f1 (ppm)

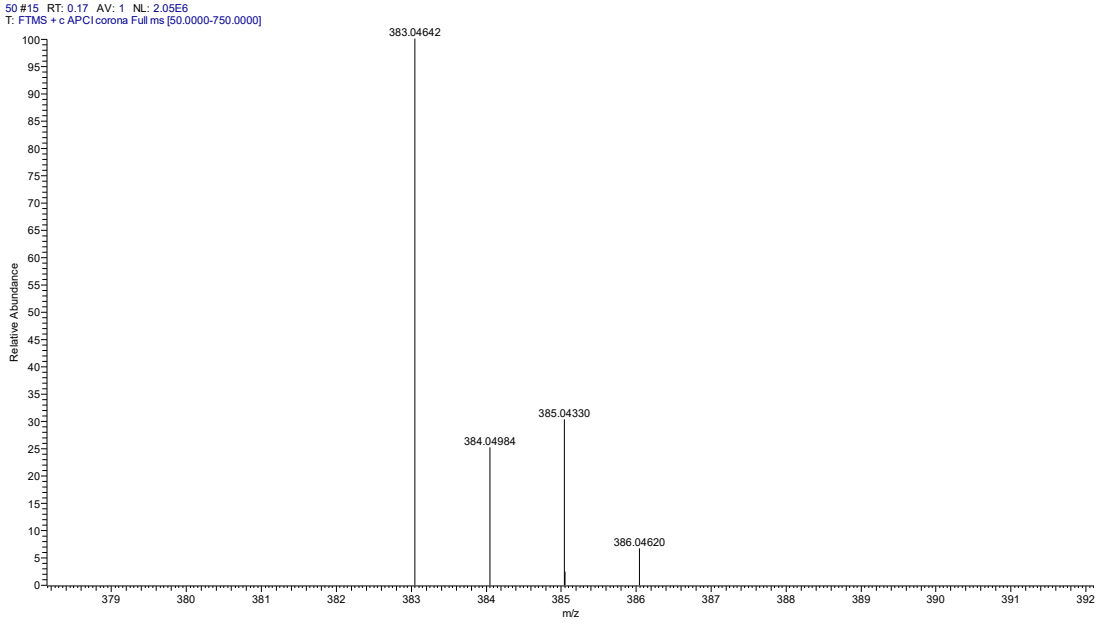

48 #15 RT: 0.17 AV: 1 NL: 5.13E7
T: FTMS + c APCI corona Full ms [50.0000-750.0000]
Relative Abundance
m/z
363.10101
364.10428
362.09250
365.10745
371.10071
372.10043
355.06949
357.06647
352.32043
361.09830
367.07599
369.35114
374.09906
377.08005
379.09528
381.10349
383.33057
385.11636

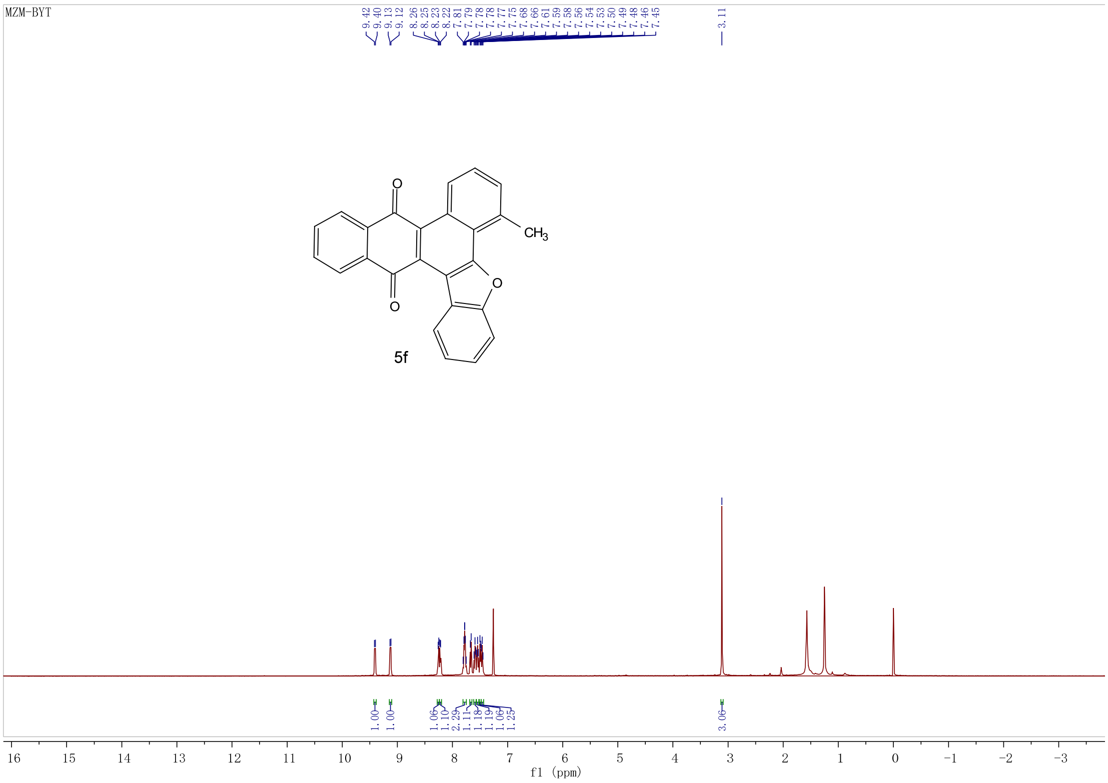

MZM-2DF
O
O
O
F
5d
f1 (ppm)

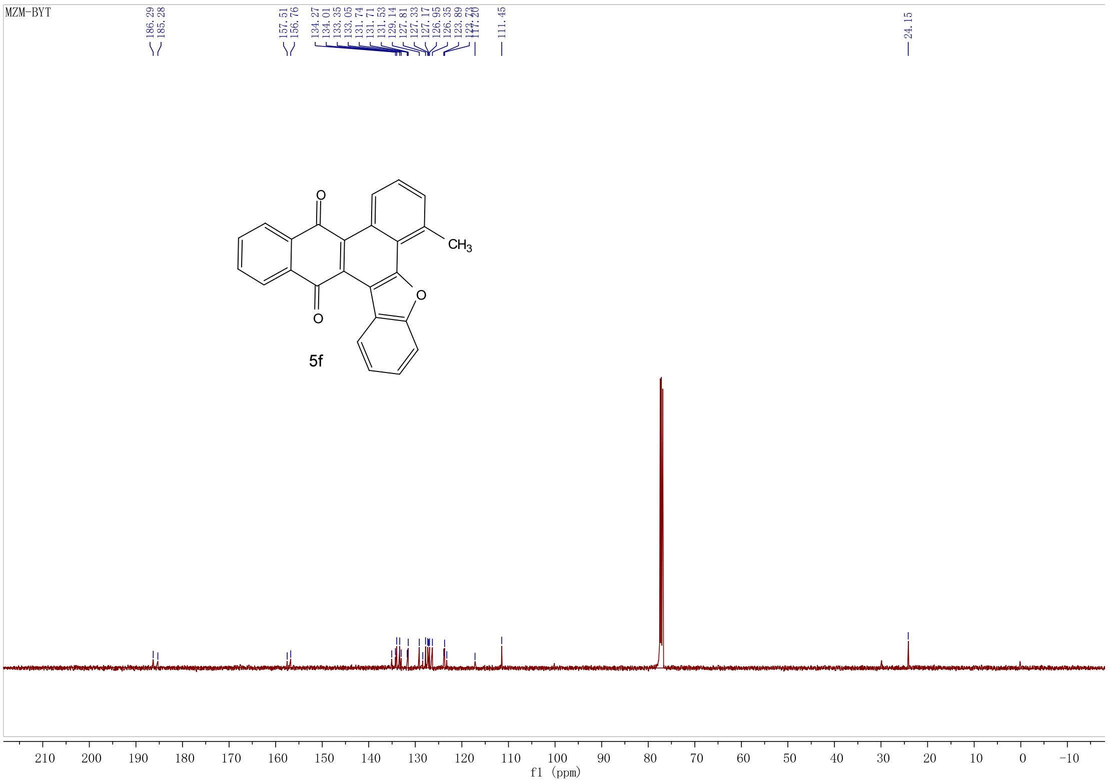

MZM-DF2BJ
-118.66
-118.67
-118.68
-118.69
-118.70
-118.71
O
O
O
5d
F
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -2
f1 (ppm)

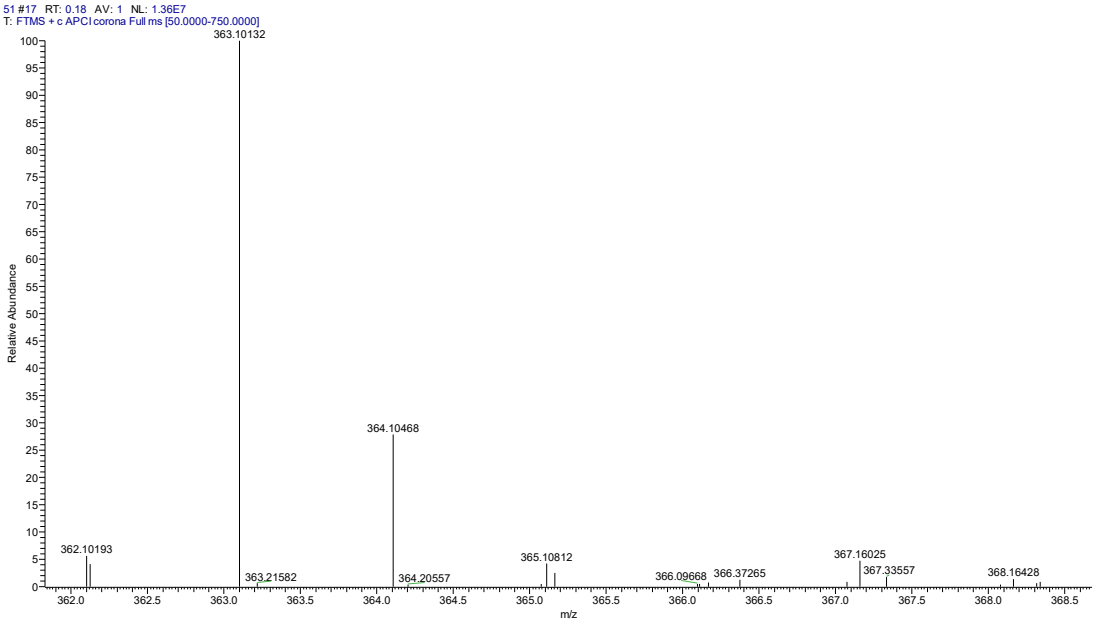

49 #17 RT: 0.19 AV: 1 NL: 7.29E6
T: FTMS + c APCI corona Full ms [50.0000-750.0000]
Relative Abundance
m/z
367.07605
368.07941
369.08255
371.10129
372.10046
375.25104
363.10126
364.63821
366.37167

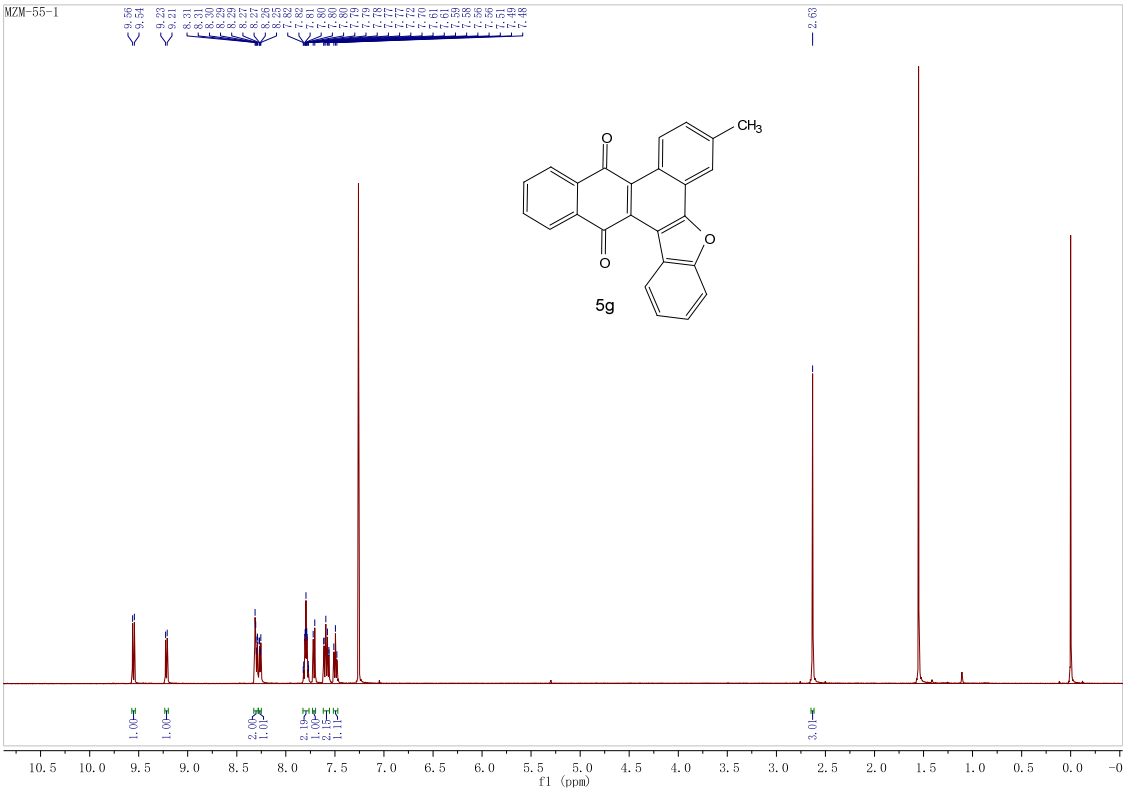

MZM-2DL
9.63
9.18
8.47
8.36
8.25
7.80
7.78
7.76
7.61
7.59
7.52
7.50
O
O
O
Cl
5e
1.00
0.91
1.05
1.96
3.88
1.01
0.96
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

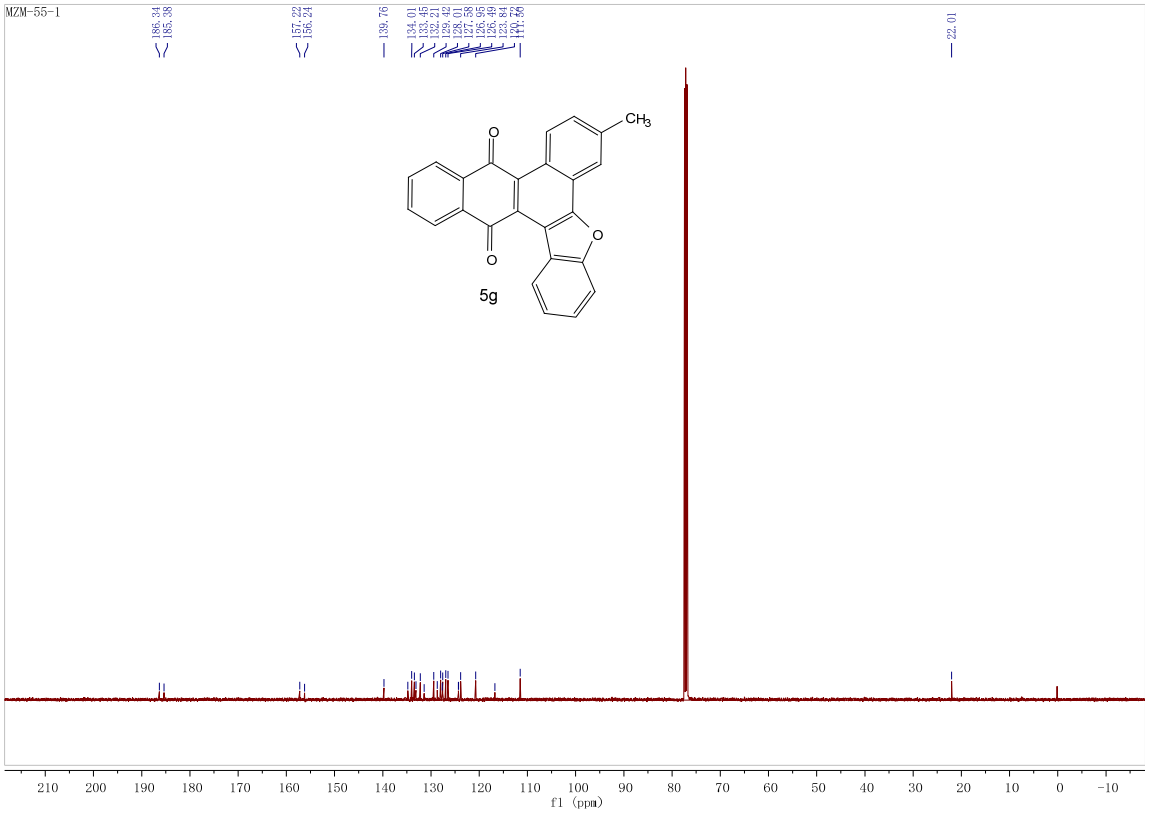

50 #15 RT: 0.17 AV: 1 NL: 2.05E6
T: FTMS + c APCI corona Full ms [50.0000-750.0000]
383.04642
385.04330
384.04984
386.04620
Relative Abundance
m/z
379 380 381 382 383 384 385 386 387 388 389 390 391 392

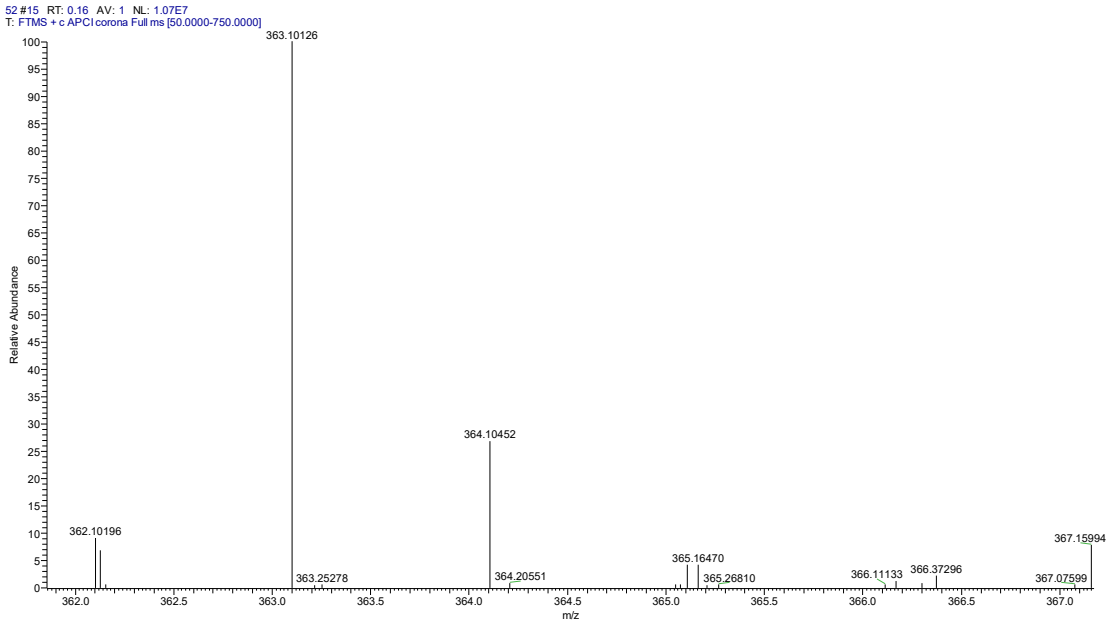

MZM-BYT
9.42
9.40
9.13
9.12
8.26
8.25
8.23
8.22
7.81
7.79
7.78
7.78
7.77
7.75
7.68
7.66
7.61
7.59
7.58
7.56
7.54
7.53
7.50
7.49
7.48
7.46
7.45
3.11
CH3
O
5f
1.00
1.00
1.06
1.10
2.29
1.11
1.18
1.19
1.06
1.25
3.06
f1 (ppm)

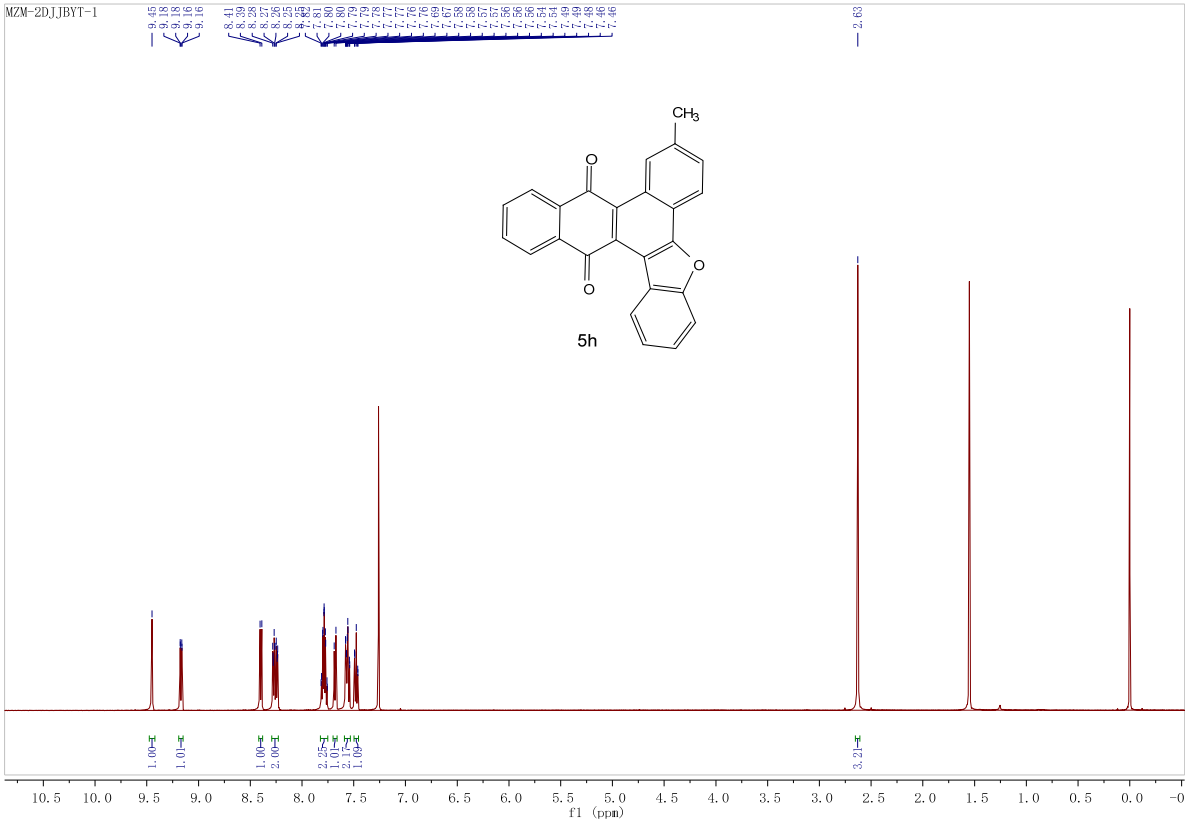

MZM-BYT
186.29
185.28
157.51
156.76
134.27
134.01
133.35
133.05
131.74
131.71
131.53
129.14
127.81
127.33
127.17
126.95
126.35
123.89
123.73
117.20
111.45
24.15
CH3
O
5f
f1 (ppm)

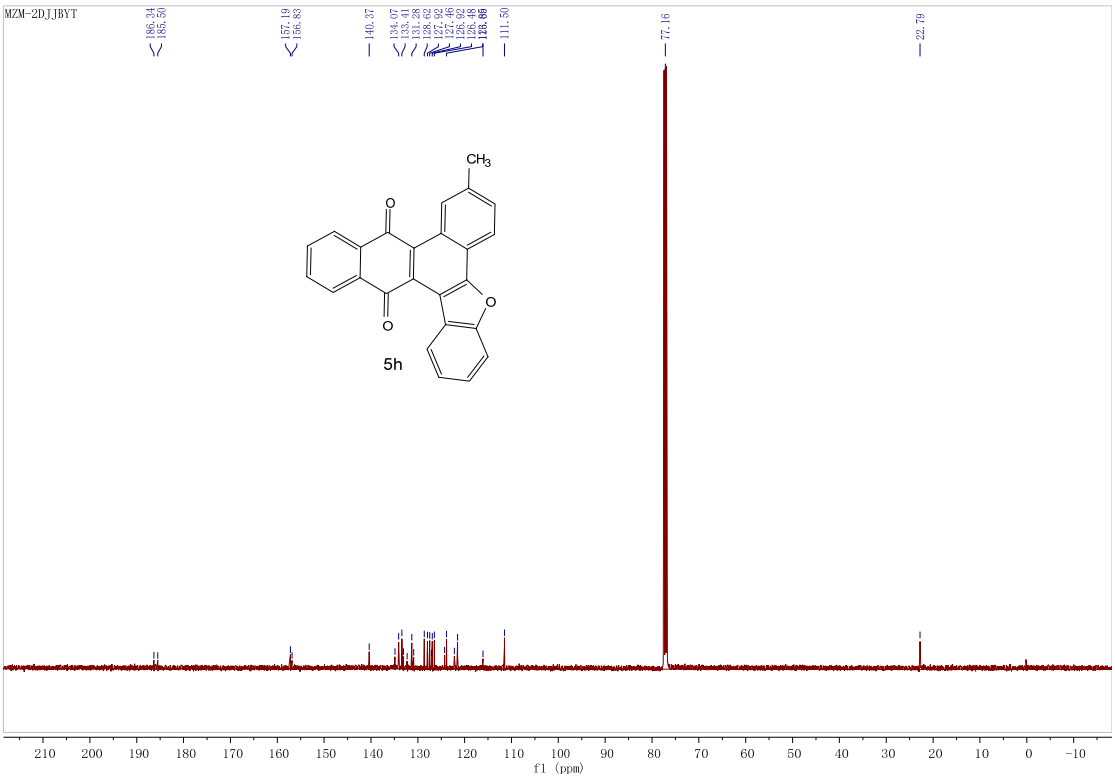

51 #17 RT: 0.18 AV: 1 NL: 1.36E7
T: FTMS + c APCI corona Full ms [50.0000-750.0000]
363.10132
364.10468
362.10193
363.21582
364.20557
365.10812
366.09668
366.37265
367.16025
367.33557
368.16428
Relative Abundance
m/z

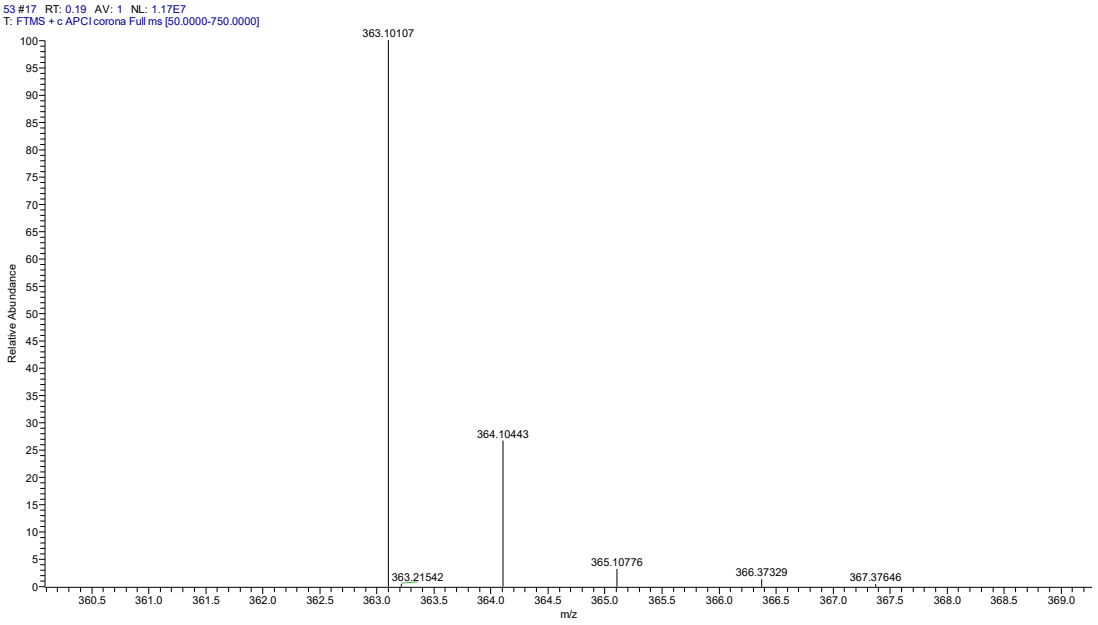

MZM-55-1
CH3
O
O
O
5g
f1 (ppm)

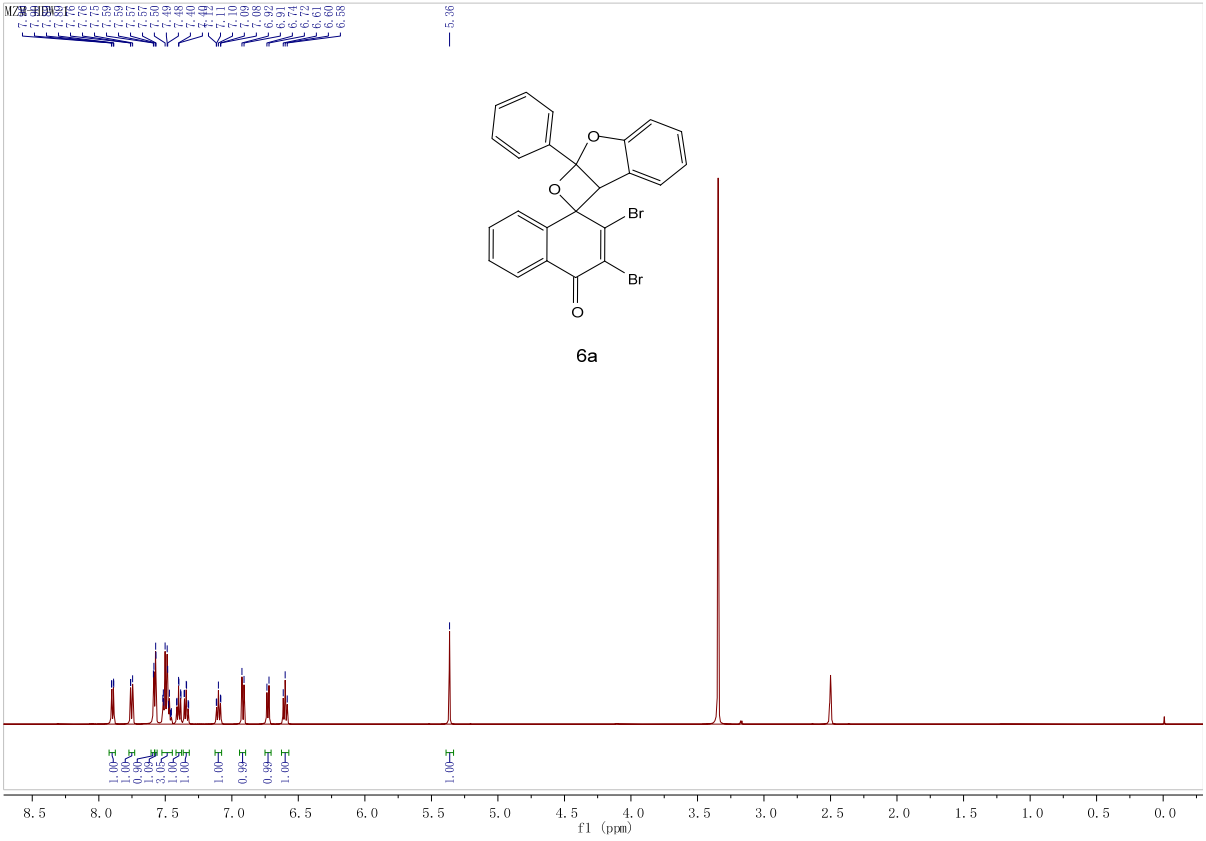

MZM-55-1
186.34
185.38
157.22
156.24
139.76
134.01
133.45
132.21
129.42
128.01
127.58
125.95
125.40
123.84
120.72
111.86
22.01
O
O
O
CH3
5g
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


52 #15 RT: 0.16 AV: 1 NL: 1.07E7
T: FTMS + c APCI corona Full ms [50.0000-750.0000]
363.10126
364.10452
362.10196
363.25278
364.20551
365.16470
365.26810
366.11133
366.37296
367.15994
367.07599
Relative Abundance
m/z
362.0 362.5 363.0 363.5 364.0 364.5 365.0 365.5 366.0 366.5 367.0

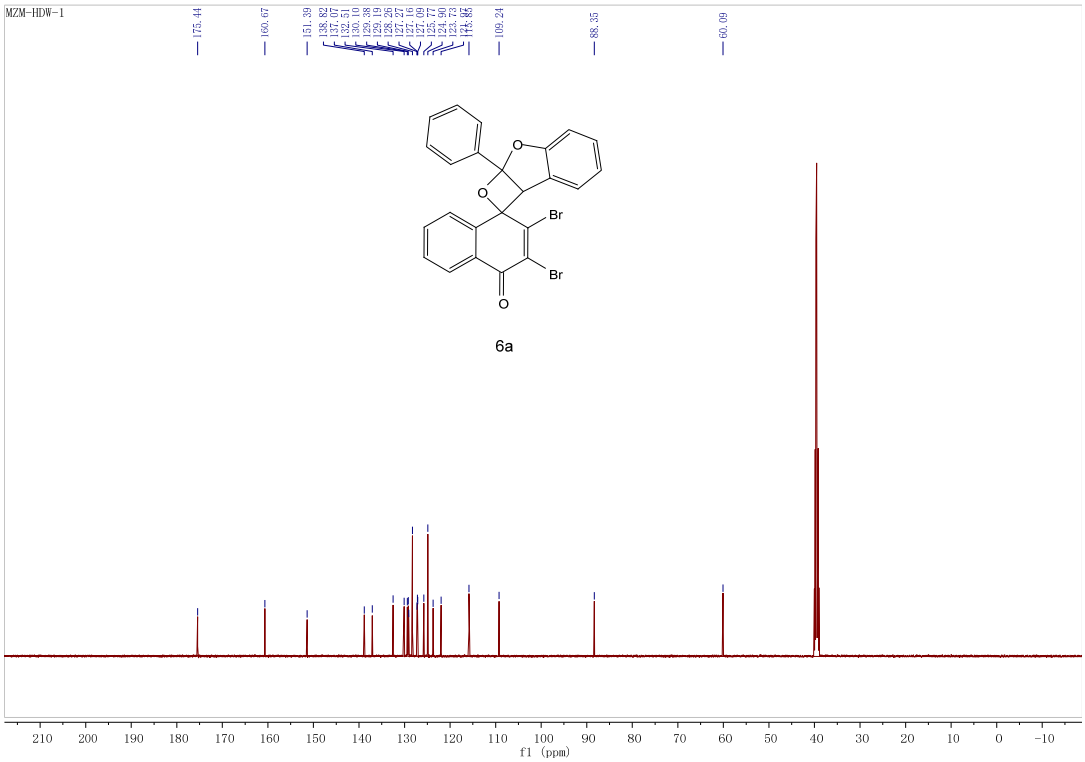

MZM-2DJJBYT-1
9.45
9.18
9.16
8.41
8.39
8.38
8.27
8.26
8.25
7.81
7.80
7.79
7.78
7.77
7.76
7.69
7.67
7.58
7.57
7.56
7.54
7.49
7.48
7.46
2.63
CH3
O
O
O
5h
1.00
1.01
1.00
2.00
2.25
1.01
2.17
1.09
3.21
f1 (ppm)


MZM-2DJJBYT
186.34
185.50
157.19
156.83
140.57
134.07
133.41
133.38
128.62
127.92
127.46
126.92
126.48
111.50
77.16
22.79
CH3
O
O
O
5h
f1 (ppm)

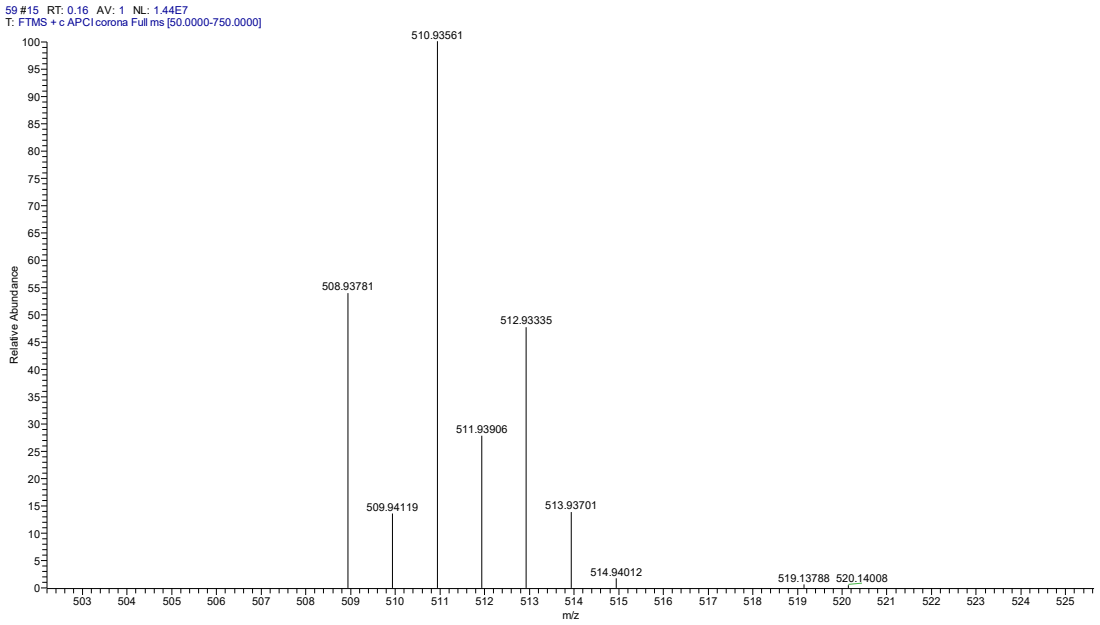

53 #17 RT: 0.19 AV: 1 NL: 1.17E7
T: FTMS + c APCI corona Full ms [50.0000-750.0000]
363.10107
364.10443
365.10776
366.37329
367.37646
363.21542
Relative Abundance
m/z

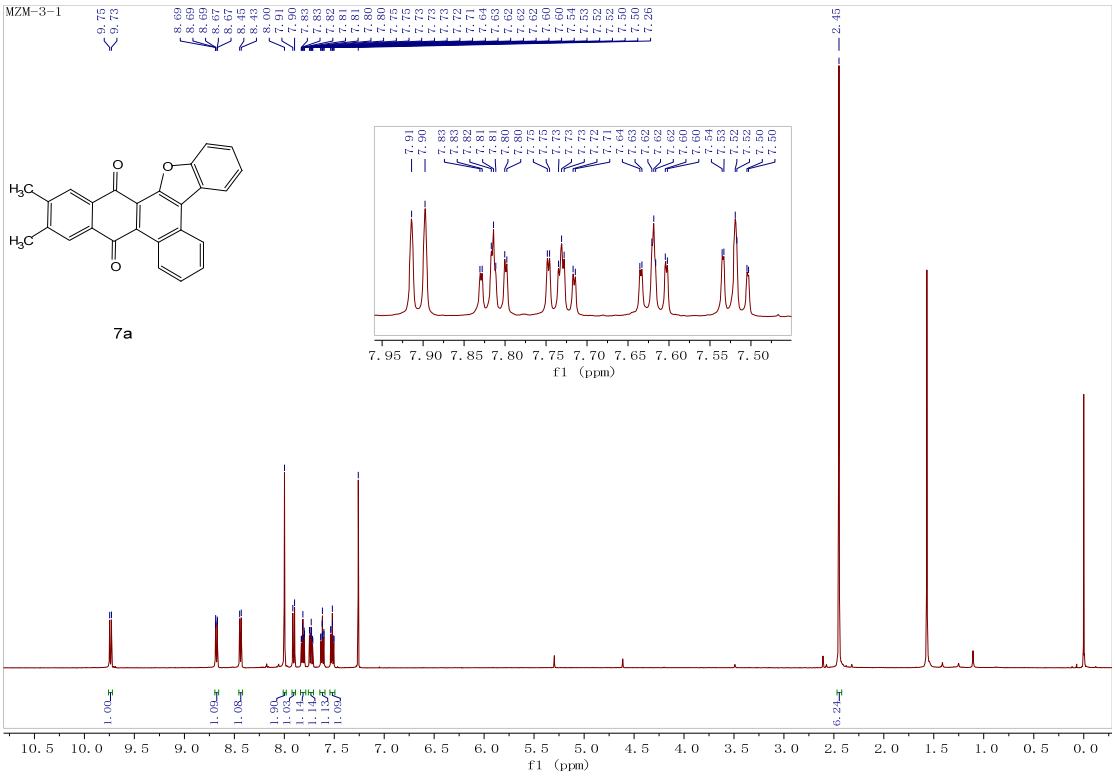

5.36
Br
Br
O
O
O
f1 (ppm)

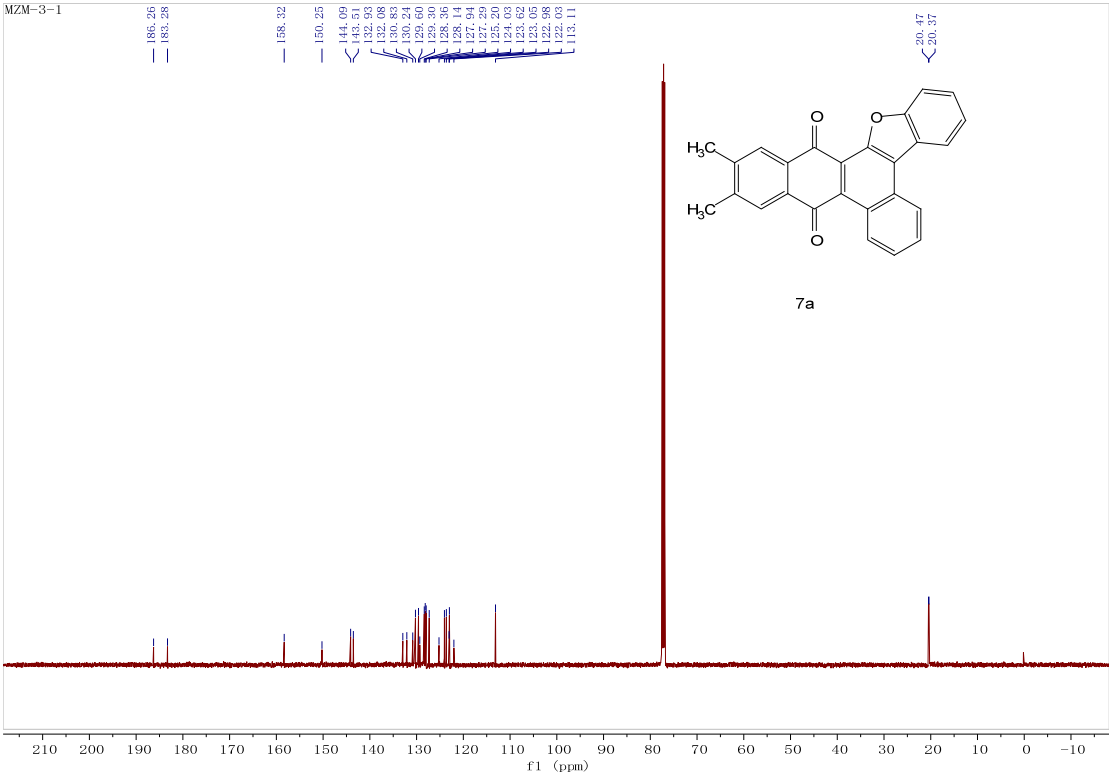
6a

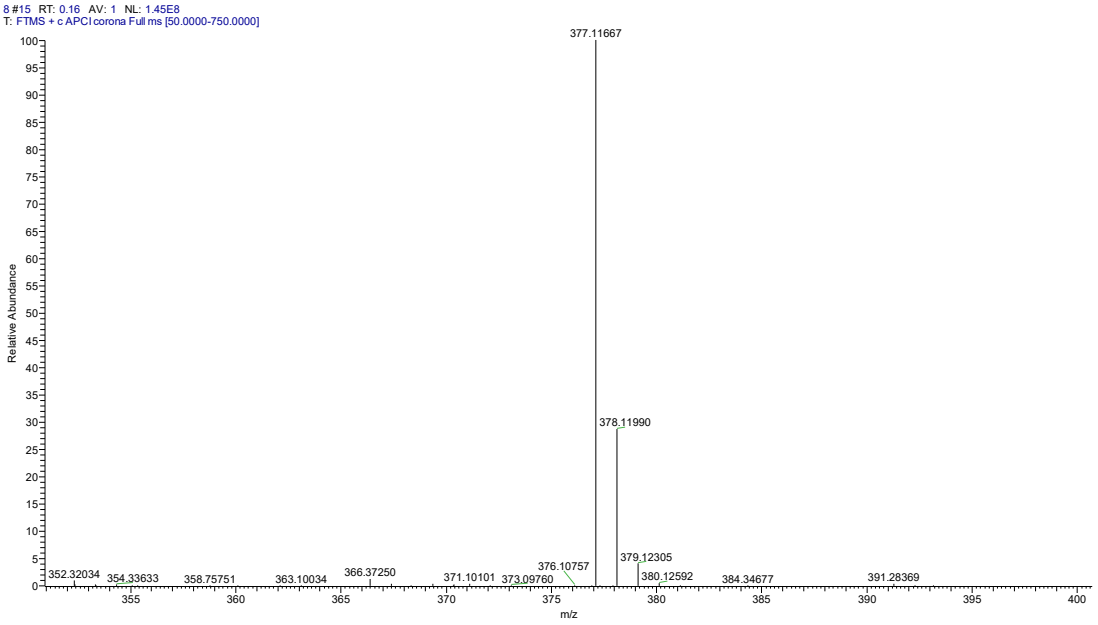

MZM-HDW-1
175.44
160.67
151.39
138.82
137.07
132.51
130.10
129.98
129.31
128.26
127.27
127.16
127.09
125.77
124.90
123.73
123.45
118.85
109.24
88.35
60.09
O
O
Br
Br
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

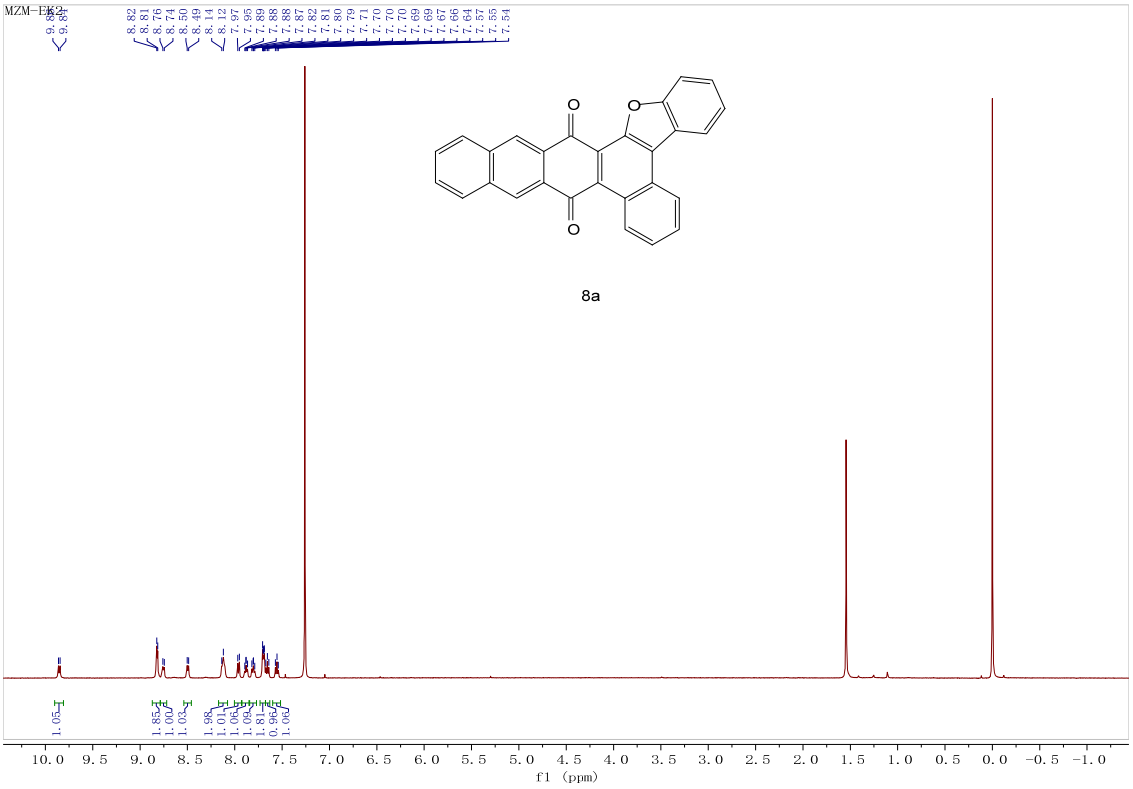
6a

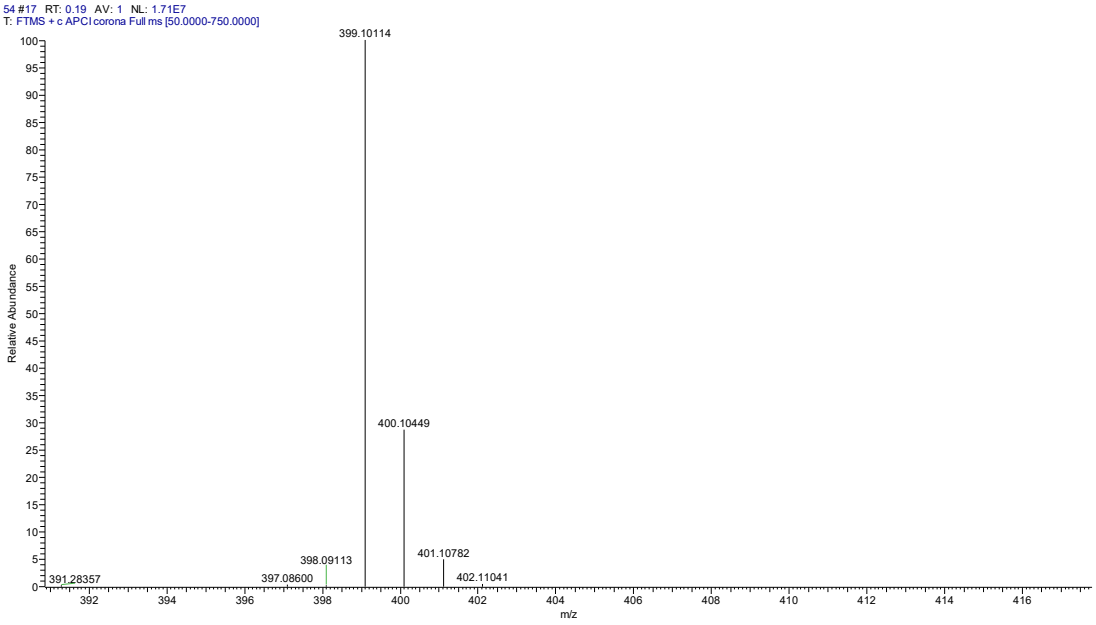

59 #15 RT: 0.16 AV: 1 NL: 1.44E7
T: FTMS + c APCI corona Full ms [50.0000-750.0000]
Relative Abundance
m/z
510.93561
508.93781
512.93335
511.93906
509.94119
513.93701
514.94012
519.13788
520.14008

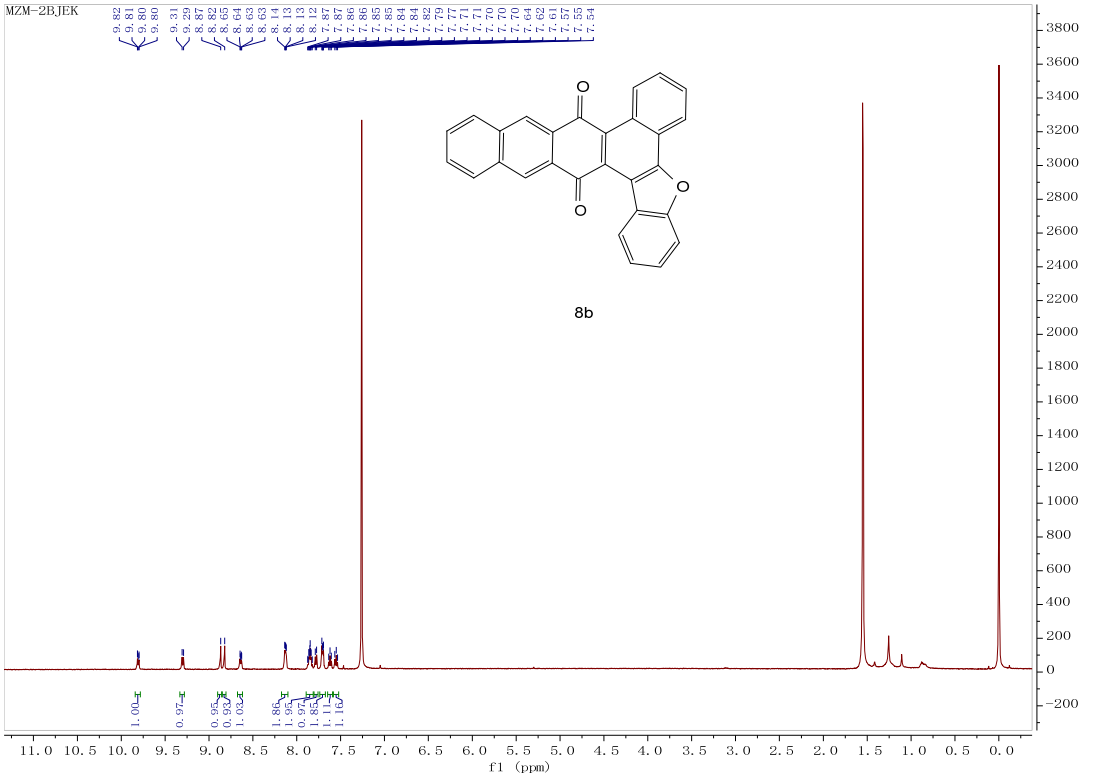

MZM-3-1
7a
f1 (ppm)

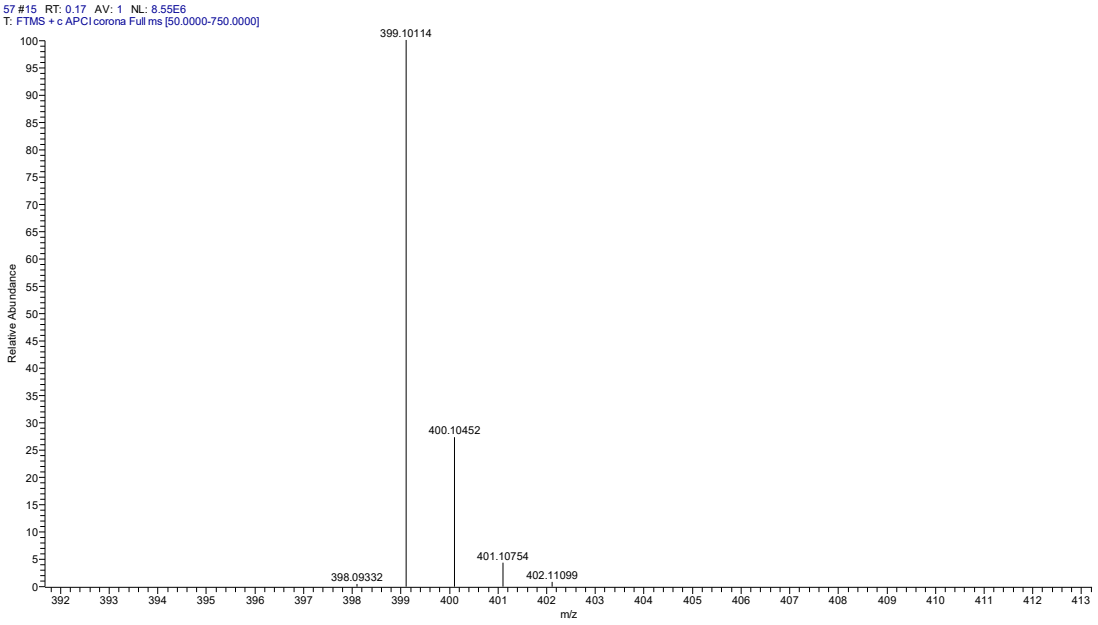

MZM-3-1
7a
f1 (ppm)

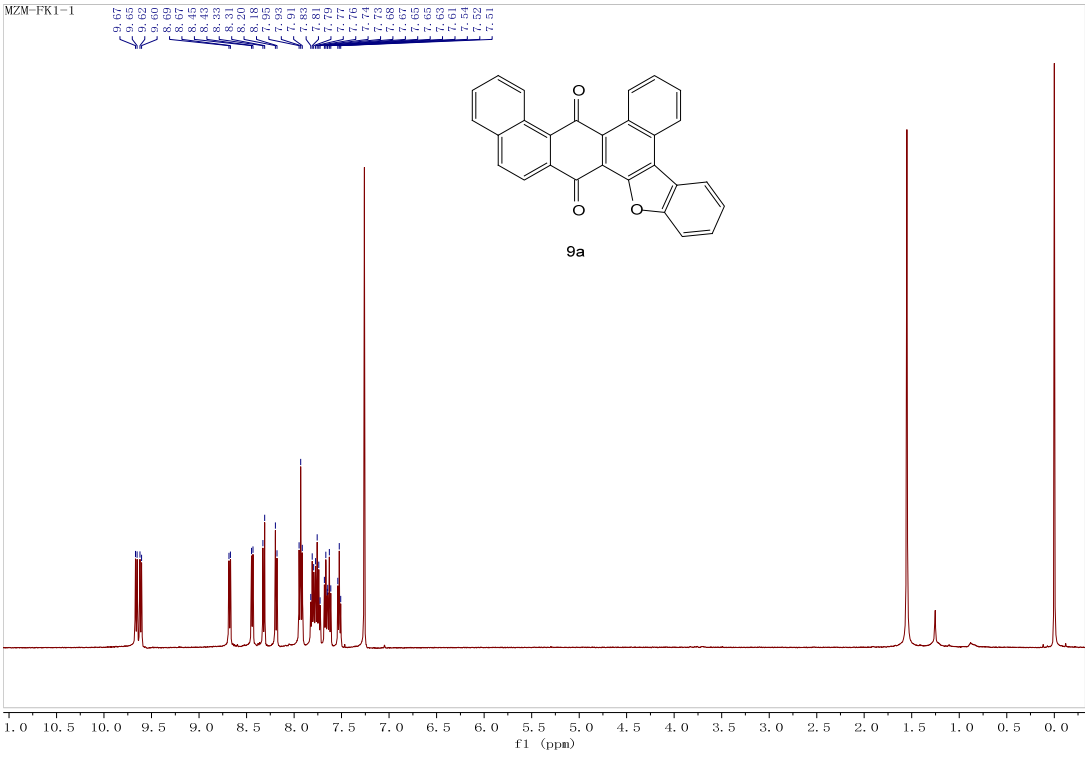

8 #15 RT: 0.16 AV: 1 NL: 1.45E8
T: FTMS + c APCI corona Full ms [50.0000-750.0000]
Relative Abundance
m/z
377.11667
378.11990
379.12305
376.10757
380.12592
352.32034
354.33633
358.75751
363.10034
366.37250
371.10101
373.09760
384.34677
391.28369

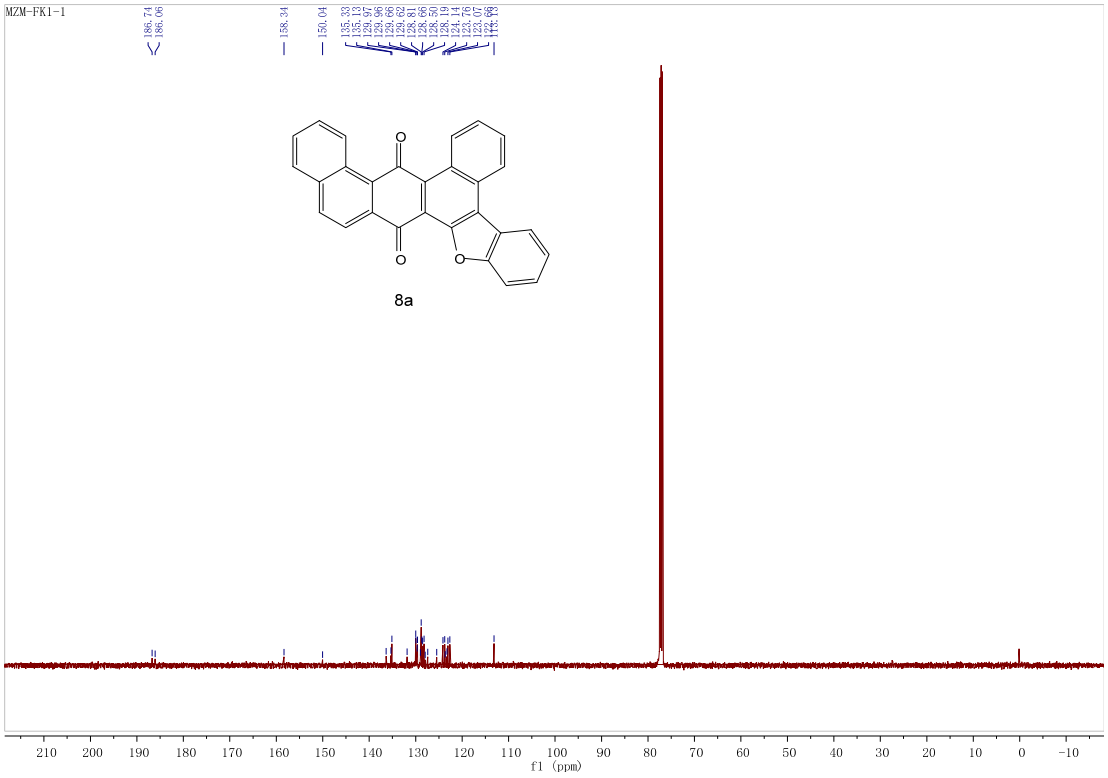

MZM-EK2-
8a
f1 (ppm)

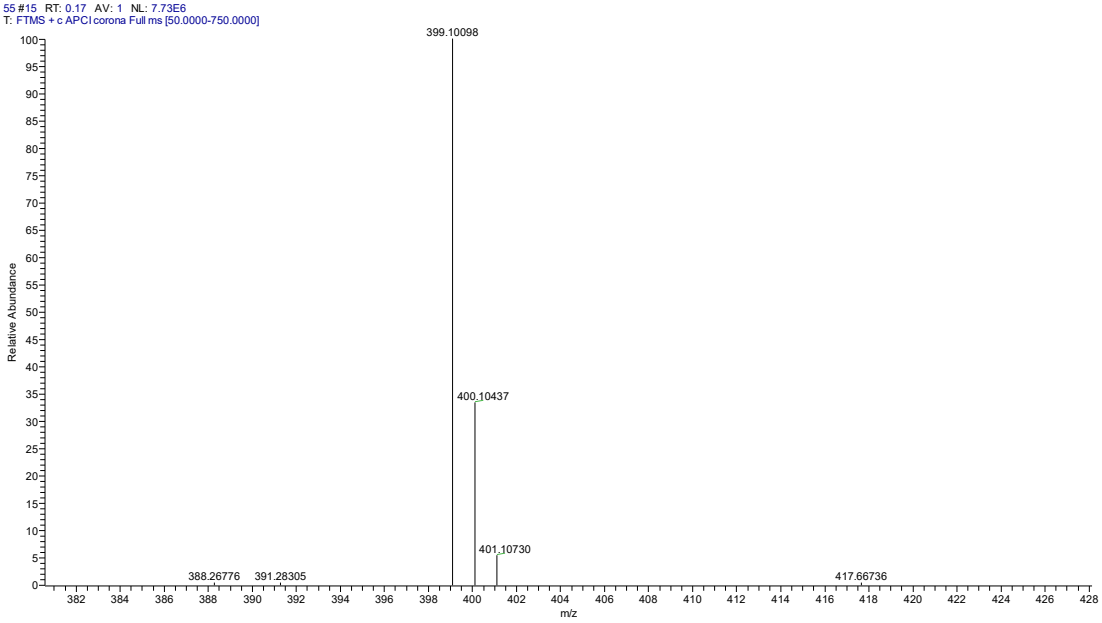

54 #17 RT: 0.19 AV: 1 NL: 1.71E7
T: FTMS + c APCI corona Full ms [50.0000-750.0000]
399.10114
400.10449
401.10782
398.09113
391.28357
397.08600
402.11041
Relative Abundance
m/z

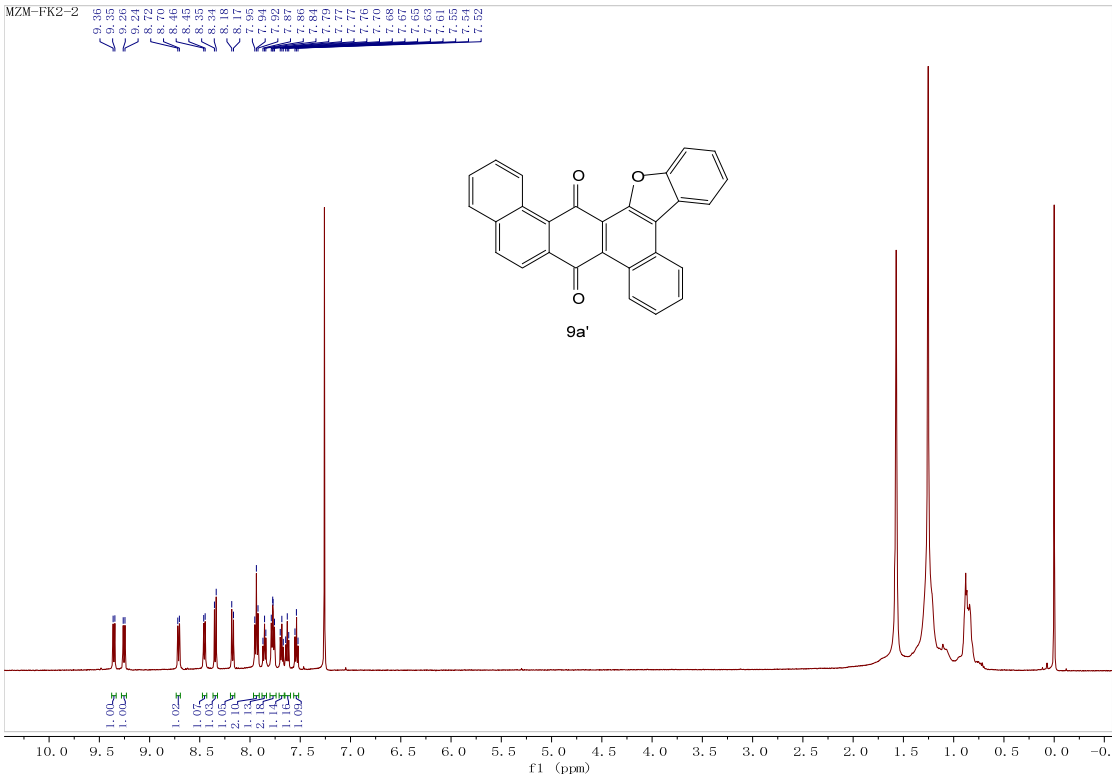

MZM-2BJEK
8b
f1 (ppm)

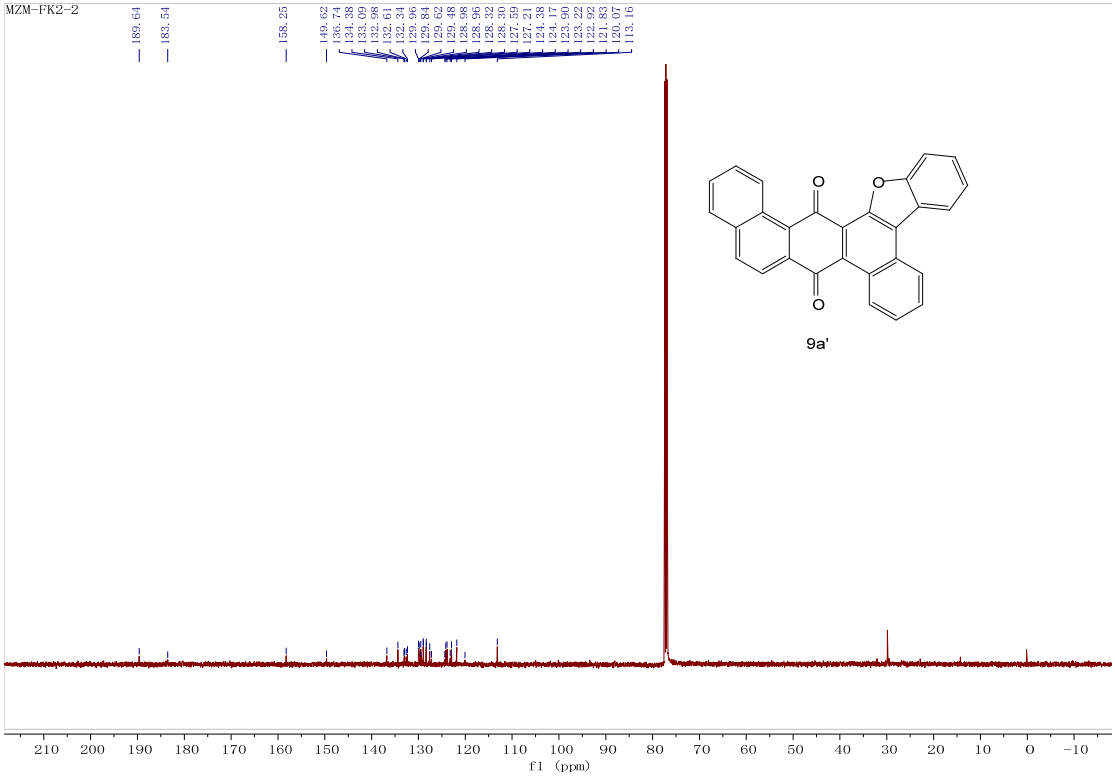

57 #15 RT: 0.17 AV: 1 NL: 8.55E6
T: FTMS + c APCI corona Full ms [50.0000-750.0000]
399.10114
400.10452
401.10754
402.11099
398.09332
Relative Abundance
m/z

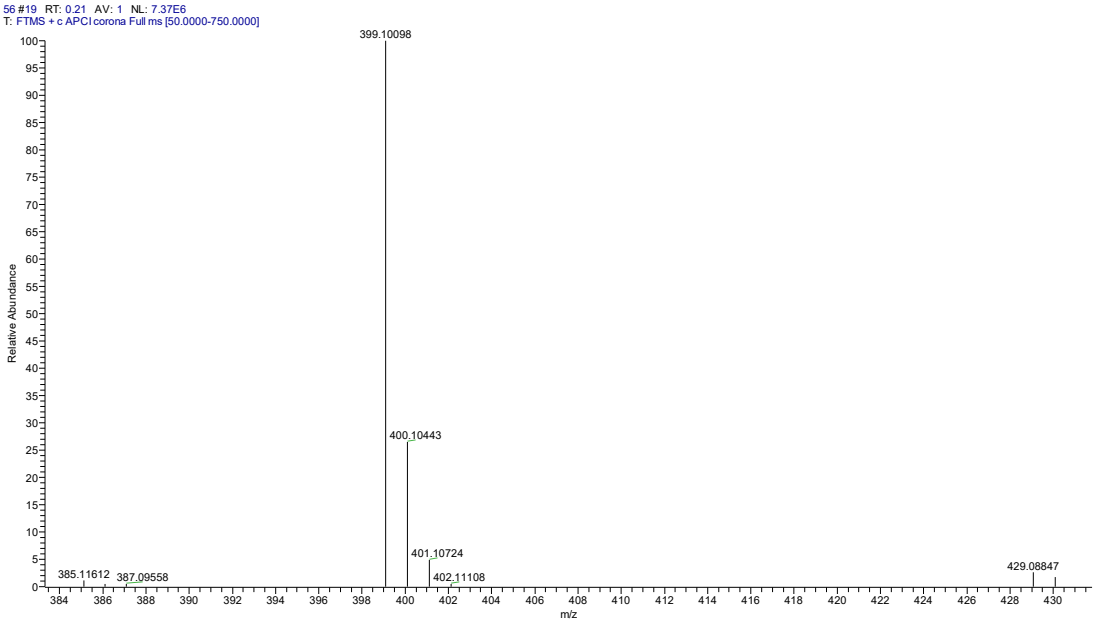

MZM-FK1-1
9.67
9.65
9.62
9.60
8.69
8.67
8.45
8.43
8.33
8.31
8.20
8.18
7.95
7.93
7.91
7.83
7.81
7.79
7.77
7.76
7.74
7.73
7.68
7.67
7.65
7.63
7.61
7.54
7.52
7.51
O
O
O
9a
f1 (ppm)


MZM-FK1-1
186.74
186.06
158.34
150.04
135.33
135.13
129.97
129.96
129.66
129.62
128.81
126.66
126.50
126.19
125.14
123.76
123.07
119.68
114.68
O
O
O
O
8a
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


55 #15 RT: 0.17 AV: 1 NL: 7.73E6
T: FTMS + c APCI corona Full ms [50.0000-750.0000]
399.10098
400.10437
401.10730
388.26776
391.28305
417.66736
Relative Abundance
m/z
382 384 386 388 390 392 394 396 398 400 402 404 406 408 410 412 414 416 418 420 422 424 426 428


MZM-FK2-2
9a'
f1 (ppm)


MZM-FK2-2
9a'
f1 (ppm)


56 #19 RT: 0.21 AV: 1 NL: 7.37E6
T: FTMS + c APCI corona Full ms [50.0000-750.0000]
399.10098
400.10443
401.10724
402.11108
385.11612
387.09558
429.08847
Relative Abundance
m/z

7. References

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