Supporting information

Design of MgO@EDTA@Ag Nanocatalyst for Sustainable Synthesis of Xanthene and Rhodamine B degradation

The Electronic Supplementary Information (ESI) includes the Powder X-ray Diffraction (PXRD) data of MgO and recycled MgO@EDTA@Ag, Scanning Electron Microscopy (SEM) data of the recycled nanocatalyst MgO@EDTA@Ag, calculations involving green chemistry matrices, as well as the ^{1}H Nuclear Magnetic Resonance (NMR) and ^{13}C NMR spectra, along with mass spectrometry results for all compounds.

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1. General Remarks

Chemicals and solvents were sourced from Sigma Aldrich, BLD Pharma, and SRL. The ^{1}H and ^{13}C NMR spectra were recorded using a Jeol spectrometer operating at 400 MHz and 100 MHz, respectively, with trimethyl silane (TMS) as an internal standard. Chemical shifts were reported in δ units and coupling constant (J) in hertz (Hz). XRD patterns were collected using a Shimadzu spectrometer within a 2θ range of 10-90°, employing Cu Kα radiation and FTIR was recorded using a Shimadzu spectrometer in the Department of Chemistry, University of Delhi, Delhi, India. Field Emission Scanning electron microscopy (FESEM), elemental mapping, and energy dispersive X-ray spectroscopy were performed on Zeiss Gemini SEM 500 Thermal field emission type with acceleration voltage 0.02 - 30 kV at USIC (University Science Instrument Centre), University of Delhi, Delhi, India. BET surface area analysis was conducted using a quanta chrome instrument, ASI-CI-11 at the University Science Instrument Centre, University of Delhi, India. Transmission Electron Microscopy was performed using Tecnai (HR-TEM) in a Sophisticated Analytical Instrumentation Facility (SAIF), AIIMS, New Delhi, India.

2. PXRD and SEM images of MgO and recycled MgO@EDTA@Ag

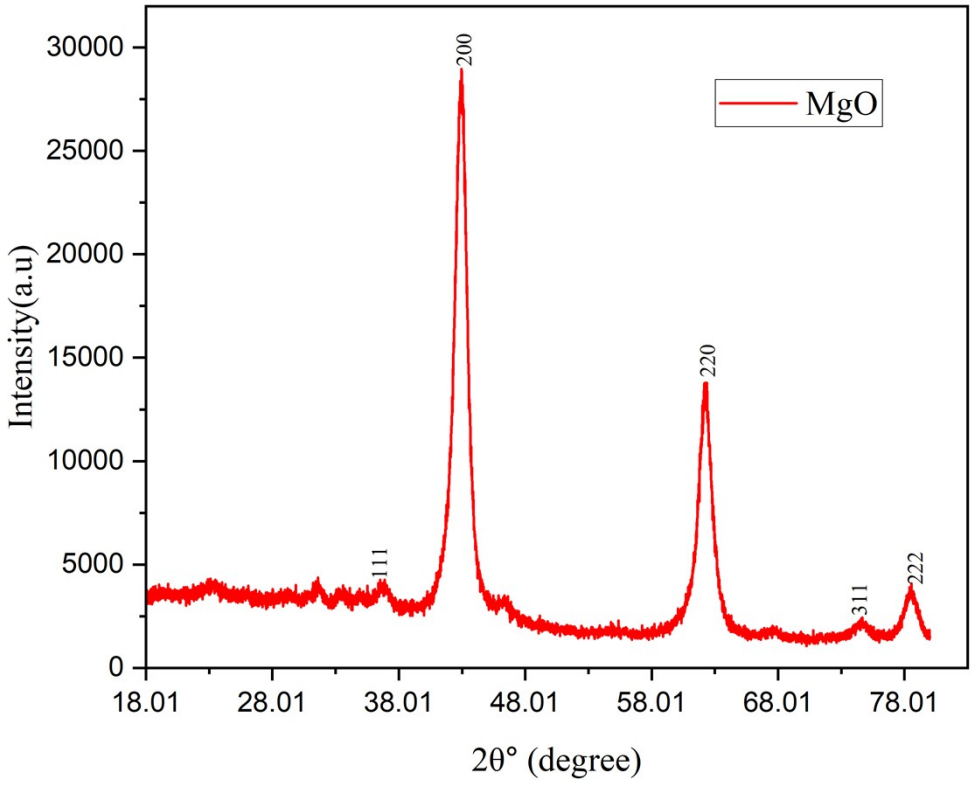


Figure S1: XRD data of MgO

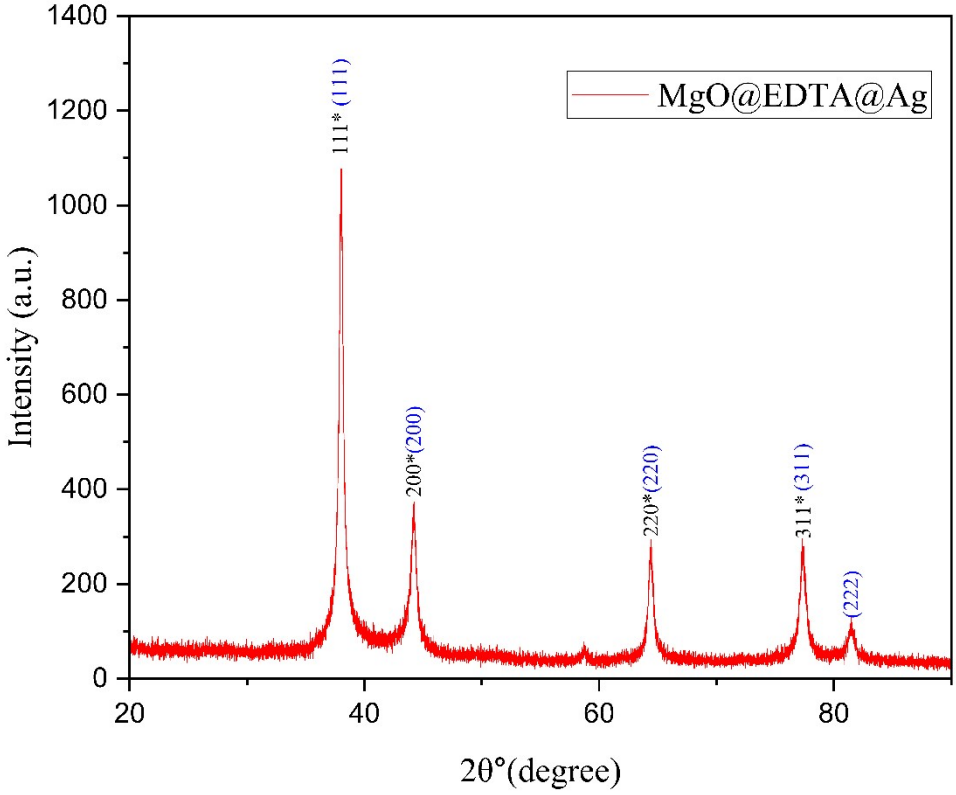


Figure S2: XRD data of recycled MgO@EDTA@Ag

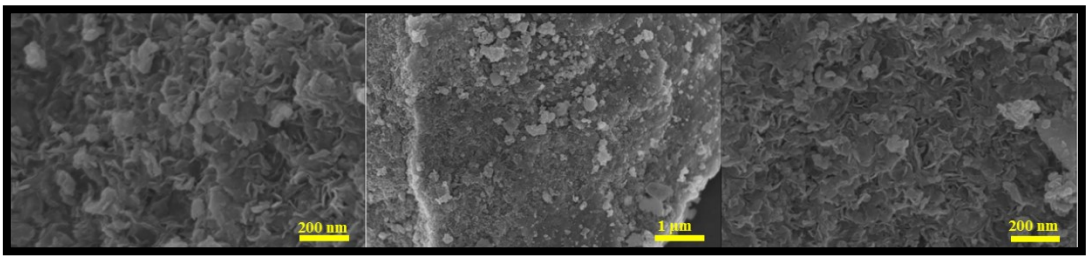


Figure S3: FESEM data of recycled MgO@EDTA@Ag

Element	Mass	ISTD	Tune Mode	Conc.	Units	RSD(%)	CPS	Ratio	Det.	Time(sec)	Rep
Ag	107		He	1.1	ppb	4.7	29880006.6		Analog	0.1002	3
Ag	109		He	1.1	ppb	2.7	28501238.0		Analog	0.1002	3

Element	Mass	ISTD	Tune Mode	Conc.	Units	RSD(%)	CPS	Ratio	Det.	Time(sec)	Rep
Mg	24		He	10969.1	ppb	5.0	28565013.8		Analog	0.1002	3

Figure S4: ICP data of recycled MgO@EDTA@Ag

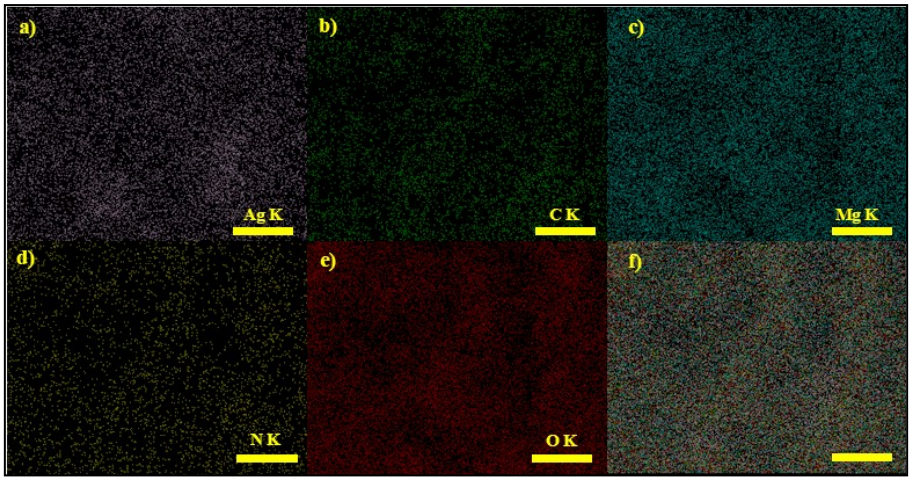


Figure S5: Elemental Mapping of recycled MgO@EDTA@Ag

3. Spectroscopic Data

3,3,6,6-tetramethyl-9-phenyl-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione(**3a**): Orange-yellow crystalline solid; 90% (157 mg); Rf- 0.4 (10% ethyl acetate: hexane); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 – 7.05 (m, 5H), 5.56 (s, 1H), 2.53 – 2.29 (m, 8H), 1.26 (s, 6H), 1.12 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 190.60, 189.53, 138.13, 128.32, 126.86, 125.95, 115.68, 47.13, 46.52, 32.82, 31.50, 29.77, 27.48. HRMS (m/z): calculated for $C_{23}H_{26}O_3$, 350.18; found, 351.19 ($M+H^+$).

9-(3,4-dimethoxyphenyl)-3,3,6,6-tetramethyl-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione (**3b**) : yellow crystalline solid; 66% (130 mg); Rf- 0.17 (10% ethyl acetate: hexane); ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.78 – 6.74 (m, 1H), 6.63 (s, 2H), 5.49 (s, 1H), 3.83 (s, 3H), 3.75 (s, 3H), 2.42 – 2.32 (m, 8H), 1.22 (s, 7H), 1.10 (s, 7H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 190.52, 189.46, 147.10, 130.52, 118.96, 115.85, 110.96, 110.52, 55.92, 55.74, 47.17, 46.48, 32.38, 31.31, 29.98, 27.14. HRMS (m/z): calculated for $C_{25}H_{30}O_5$, 410.21; found, 411.21 ($M+H^+$).

3,3,6,6-tetramethyl-9-(m-tolyl)-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione(**3c**): yellow crystalline solid; 61% (112 mg); Rf- 0.6 (10% ethyl acetate: hexane); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.91 (d, *J* = 9.0 Hz, 1H), 7.43 – 7.32 (m, 1H), 7.15 (t, *J* = 7.9 Hz, 1H), 6.97 (d, *J* = 7.5 Hz, 1H), 6.91 (s, 1H), 5.51 (s, 1H), 2.40 (q, *J* = 15.1, 13.2 Hz, 8H), 2.29 (s, 3H), 1.17 (d, *J* = 55.8 Hz, 13H).^{13}C NMR (101 MHz, CHLOROFORM-*D*) δ 190.54, 189.58, 171.76, 138.10, 137.64, 134.55, 130.77, 128.18, 127.77, 126.71, 123.91, 115.74, 47.16, 46.51, 32.73, 31.52, 29.76, 27.41, 21.82, 21.36; HRMS (m/z): calculated for $C_{24}H_{28}O_3$, 364.20; found, 365.21 $(M+H)^+$.

9-(3-chlorophenyl)-3,3,6,6-tetramethyl-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione(**3d**): yellow solid, 39% (75 mg); Rf- 0.31 (10% ethyl acetate: hexane); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.16 (dt, *J* = 16.2, 7.9 Hz, 2H), 7.05 (s, 1H), 6.96 (d, *J* = 7.4 Hz, 1H), 5.47 (s, 1H), 2.38 (t, *J* = 22.5 Hz, 8H), 1.15 (d, *J* = 52.7 Hz, 12H).^{13}C NMR (101 MHz, CHLOROFORM-D) δ 190.75, 189.56, 140.55, 134.29, 129.49, 127.30, 126.15, 125.06, 115.20, 47.12, 46.50, 32.75, 31.55, 29.66, 27.48. HRMS (m/z): calculated for $C_{23}H_{25}ClO_3$, 384.15; found, 385.15 $(M+H)^+$

3,3,6,6-tetramethyl-9-(4-nitrophenyl)-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione (**3e**): Yellow solid, 91% (180 mg); Rf- 0.80 (10% ethyl acetate: hexane), ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 (d, *J* = 8.6 Hz, 2H), 7.22 – 7.17 (m, 2H), 5.47 (s, 1H), 2.36 (h, *J* = 18.2 Hz, 8H), 1.12 (d, *J* = 47.0 Hz, 12H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 191.09, 189.72, 146.64, 146.18, 127.74, 123.62, 114.99, 53.57, 47.05, 46.47, 33.33, 31.56, 29.64, 27.53; HRMS (m/z): calculated for $C_{23}H_{25}NO_5$, 395.17; found, 396.18 $(M+H)^+$.

9-(4-chlorophenyl)-3,3,6,6-tetramethyl-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione (**3f**): Brown solid, 77% (192.5 mg); Rf- 0.2 (10% ethyl acetate: hexane), ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.21 (d, *J* = 8.6 Hz, 2H), 7.00 (d, *J* = 7.8 Hz, 2H), 5.46 (s, 1H), 2.48 – 2.26 (m, 8H), 1.14 (d, *J* = 47.4 Hz, 12H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 190.77, 189.57, 136.83, 131.67, 128.32, 115.43, 47.14, 46.52, 32.50, 31.53, 29.69, 27.51. HRMS (m/z): calculated for $C_{23}H_{25}ClO_3$,384.15; found, 385.15 $(M+H)^+$.

9-(4-bromophenyl)-3,3,6,6-tetramethyl-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione(**3g**): Yellow solid, 78% (167 mg); Rf- 0.45 (10% ethyl acetate: hexane), ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 (d, *J* = 8.4 Hz, 2H), 6.94 (d, *J* = 8.5 Hz, 2H), 5.43 (s, 1H), 2.37 (dd, *J* = 25.8, 18.2 Hz, 8H), 1.14 (d, *J* = 46.6 Hz, 12H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 190.73, 189.50, 137.39, 131.37, 128.70, 119.72, 115.35, 47.13, 46.52, 32.57, 31.51, 29.66, 27.51; HRMS (m/z): calculated for $C_{23}H_{25}BrO_3$, 428.09; found 429.1062 $(M+H)^+$.

3,3,6,6-tetramethyl-9-(3-nitrophenyl)-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione(**3h**): Yellow solid, 85% (167 mg); R_f- 0.4 (20% ethyl acetate: hexane), ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 – 7.89 (m, 2H), 7.42 – 7.30 (m, 2H), 5.47 (s, 1H), 2.32 (dt, *J* = 28.6, 18.8 Hz, 6H), 1.13 (d, *J* = 61.2 Hz, 12H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 191.06, 189.59, 148.43, 140.75, 132.89, 129.08, 122.21, 121.01, 114.77, 47.01, 46.43, 32.89, 31.44, 29.63, 27.29; HRMS (m/z): calculated for $C_{23}H_{25}NO_5$, 395.17; found 396.1812 $(M+H)^+$.

9-(3-methoxyphenyl)-3,3,6,6-tetramethyl-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione (**3i**): Yellow solid, 60% (114 mg); R_f- 0.05 (20% ethyl acetate: hexane); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.17 (t, J = 7.9 Hz, 1H), 6.72 – 6.64 (m, 3H), 5.50 (s, 1H), 3.73 (s, 3H), 2.37 (dd, J = 27.6, 11.9 Hz, 8H), 1.09 (s, 12H);^{13}C NMR (101 MHz, $CDCl_3$) δ 190.48, 189.49, 159.66, 139.94, 129.17, 119.32, 115.67, 113.08, 111.18, 55.13, 47.16, 46.51, 32.85, 31.46, 31.01, 29.77, 27.43; HRMS (m/z): calculated for $C_{24}H_{28}O_4$, 380.1989; found 381.20 $(M+H)^+$.

9-(3-bromophenyl)-3,3,6,6-tetramethyl-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione (**3j**): Yellow solid, 64% (137 mg); R_f- 0.25 (10% ethyl acetate: hexane); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 (t, *J* = 7.9 Hz, 1H), 7.32 – 7.24 (m, 1H), 7.16 – 7.08 (m, 1H), 7.00 (d, *J* = 7.0 Hz, 1H), 5.48 (s, 1H), 2.53 – 2.25 (m, 8H), 1.15 (d, *J* = 52.2 Hz, 12H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 190.76, 189.57, 140.85, 130.24, 129.80, 129.03, 125.52, 122.57, 115.16, 47.13, 46.51, 32.71, 31.54, 29.77, 29.67, 29.31, 27.46; HRMS (m/z): calculated for $C_{23}H_{25}BrO_3$,428.10; found, 431.1054 $(M+H)^+$.

9-phenyl-9H-xanthene-1,8-diol (**5k**): Orange solid, 65%,94 mg; Rf- 0.25 (40% ethyl acetate: hexane) ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.27 (s, 2H), 9.22 (s, 2H), 7.28 (t, *J* = 7.5 Hz, 2H), 7.18 (t, *J* = 7.3 Hz, 1H), 7.00 (d, *J* = 7.4 Hz, 2H), 6.48 (d, *J* = 8.3 Hz, 2H), 6.31 (d, *J* = 2.2 Hz, 2H), 6.17 (d, *J* = 10.5 Hz, 2H), 5.85 (s, 1H).; 13C NMR (101 MHz, DMSO) δ 156.51, 155.77,

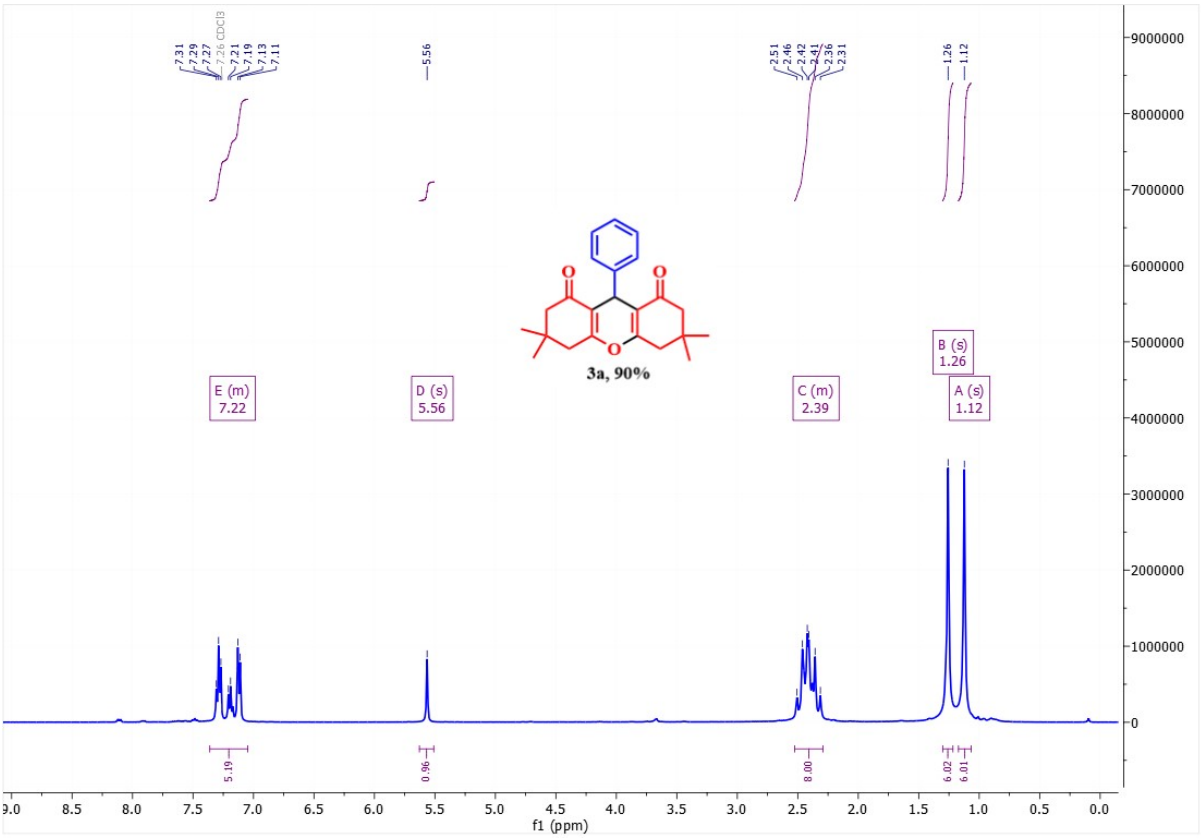
145.76, 130.55, 129.22, 128.22, 125.77, 121.86, 105.84, 102.77, 41.78. HRMS (m/z): calculated for $C_{19}H_{13}O_3$, 289.0883 ; found, 289.0878 $(M+H)^+$.

9-(m-tolyl)-9H-xanthene-1,8-diol(**5l**): Orange solid, 61%, 92 mg; Rf- 0.28(40% ethyl acetate:hexane) ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.99 (d, J = 12.6 Hz, 3H), 7.09 (t, J = 7.5 Hz, 1H), 6.92 (d, J = 7.5 Hz, 1H), 6.80 – 6.69 (m, 2H), 6.42 (d, J = 8.3 Hz, 2H), 6.25 (d, J = 2.2 Hz, 2H), 6.09 (d, J = 10.5 Hz, 2H), 5.76 (s, 1H), 2.21 (s, 3H). ^{13}C NMR (101 MHz, DMSO) δ 156.60, 155.79, 145.96, 136.96, 130.59, 129.96, 128.02, 126.36, 121.88, 105.85, 102.84, 79.61, 41.73, 21.59, -7.02. HRMS (m/z): calculated for $C_{20}H_{16}O_3$, 304.10; found, 306.129 $(M+H)^+$.

9-(3-chlorophenyl)-9H-xanthene-1,8-diol (**5m**): Orange solid, 68%, 100 mg; Rf- 0.21 (40% ethyl acetate:hexane) ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.10 (s, 1H), 9.03 (s, 1H), 7.26 (d, J = 8.4 Hz, 2H), 6.93 (d, J = 8.3 Hz, 2H), 6.38 (d, J = 8.3 Hz, 2H), 6.26 (s, 2H), 6.10 (dd, J = 8.3, 2.2 Hz, 2H), 5.75 (s, 1H). 13C NMR (101 MHz, DMSO) δ 156.84, 155.83, 145.12, 130.98, 130.46, 130.18, 128.09, 121.24, 105.99, 102.89. HRMS (m/z): calculated for $C_{19}H_{13}O_3Cl$, 324.05; found, 324.05 $(M+H)^+$.

9-(4-nitrophenyl)-9H-xanthene-1,8-diol (**5n**): Orange solid, 70%, 117 mg; Rf- 0.18 (50% ethyl acetate:hexane) ^{1}H NMR (400 MHz, MeOD) δ 7.97 (d, J = 8.7 Hz, 2H), 7.12 (d, J = 8.7 Hz, 2H), 6.40 (d, J = 8.3 Hz, 2H), 6.21 (d, J = 2.2 Hz, 2H), 6.17 (d, J = 2.1 Hz, 1H), 6.15 (s, 1H), 6.10 (dd, J = 8.3, 2.3 Hz, 2H), 5.92 (s, 1H). ^{13}C NMR (101 MHz, MeOD) δ 158.14, 156.55, 155.58, 154.20, 145.87, 130.35, 129.66, 122.50, 120.75, 106.36, 105.71, 102.15, 42.45. HRMS (m/z):

9-(4-bromophenyl)-9H-xanthene-1,8-diol(**5o**): Orange solid, 67%, 123 mg; Rf- 0.23 (50% ethyl acetate:hexane) ^{1}H NMR (400 MHz, MeOD) δ 7.23 (d, J = 8.4 Hz, 2H), 6.82 (d, J = 8.4 Hz, 2H), 6.38 (d, J = 8.3 Hz, 2H), 6.19 (d, J = 2.4 Hz, 2H), 6.18 – 6.13 (m, 2H), 6.10 – 6.06 (m, 2H), 5.77 (s, 1H). ^{13}C NMR (101 MHz, MeOD) δ 156.24, 155.45, 144.80, 130.81, 130.29, 130.27, 121.66, 118.53, 106.31, 105.52, 102.07, 41.65. HRMS (m/z):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7.29
7.27
7.26 CDCl3
7.21
7.19
7.13
7.11
5.56
2.51
2.46
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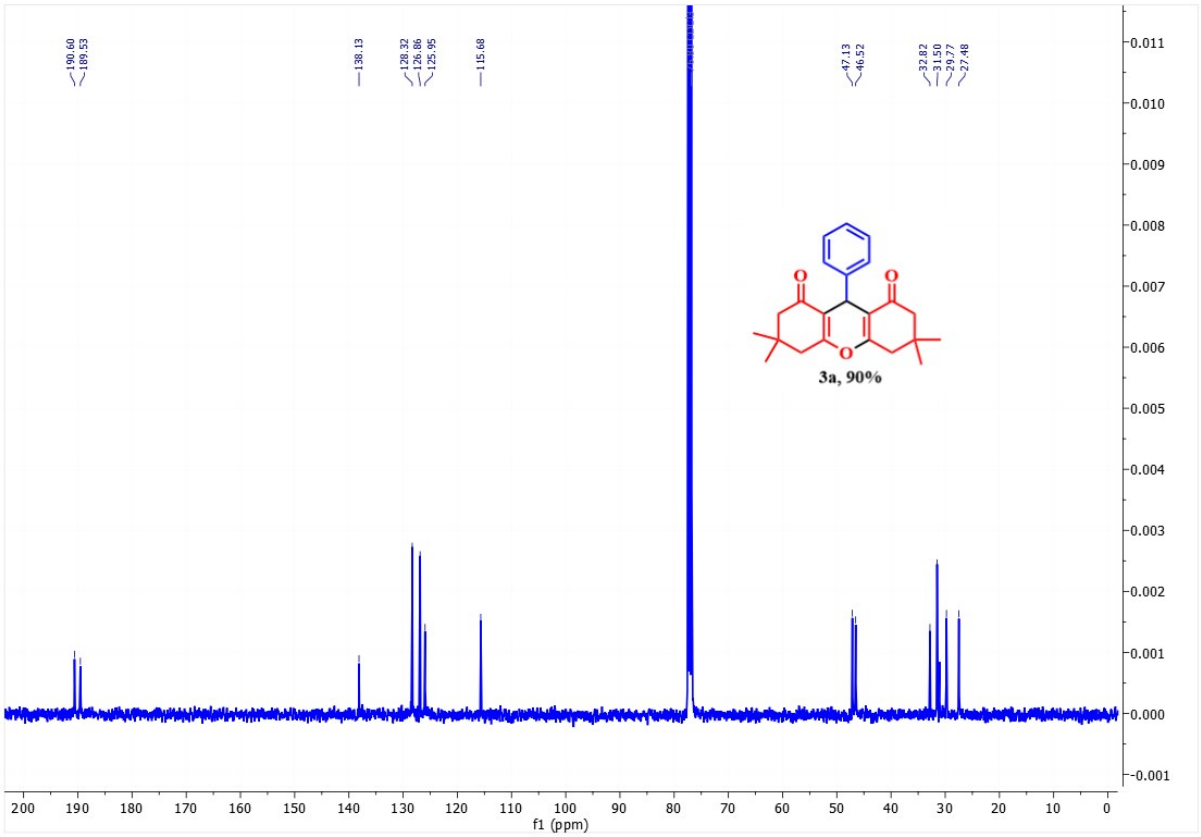
2.41
2.36
2.31
1.26
1.12
E (m)
7.22
D (s)
5.56
C (m)
2.39
B (s)
1.26
A (s)
1.12
5.19
0.96
8.00
6.02
6.01
f1 (ppm)

3a, 90%


190.60
189.53
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128.32
126.86
125.95
115.68
47.13
46.52
32.82
31.50
29.77
27.48
f1 (ppm)

3a, 90%

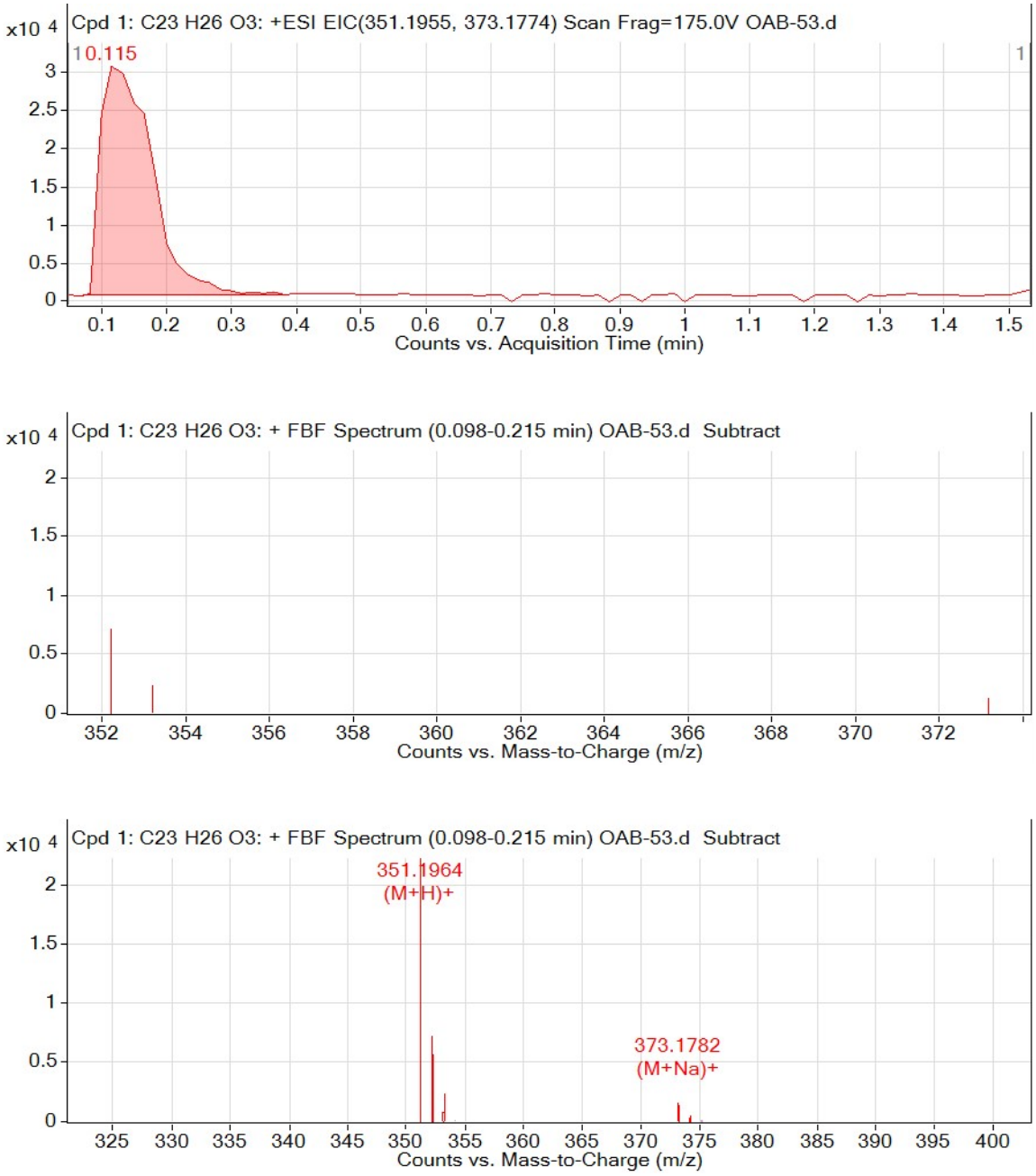
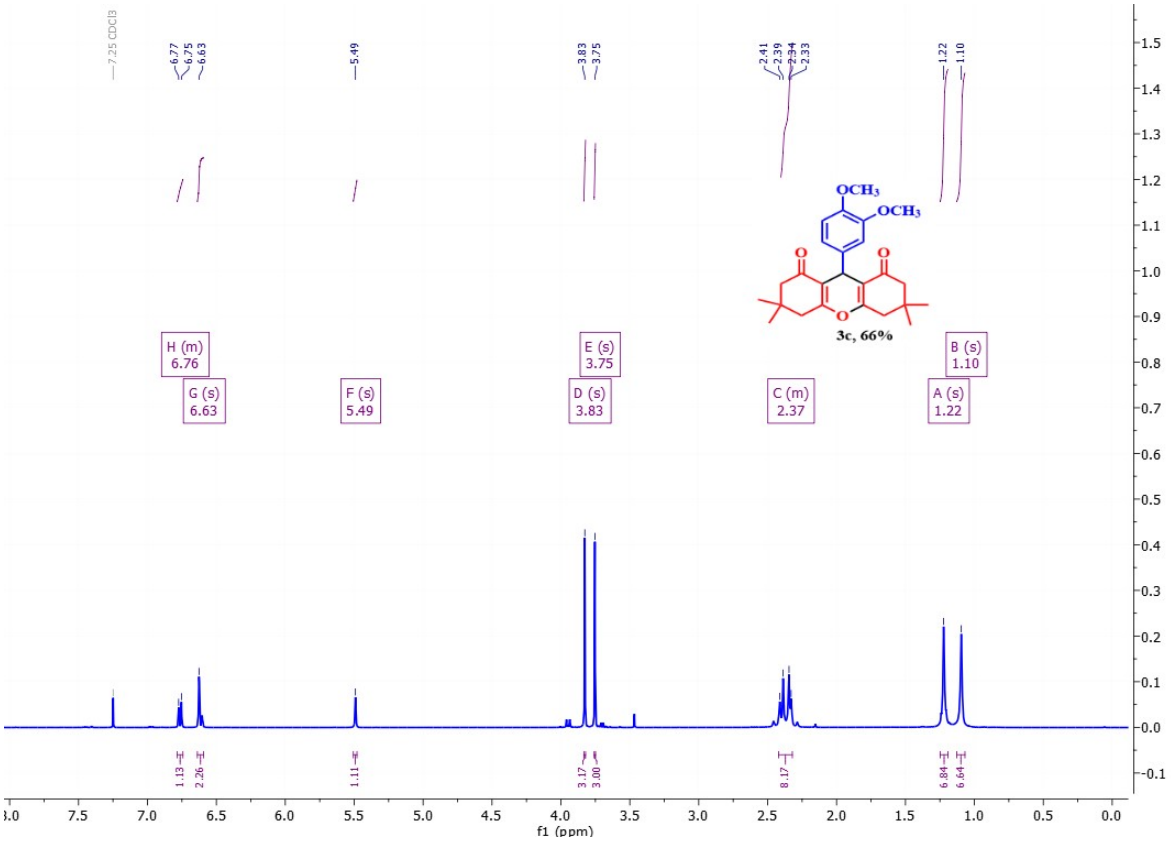


Figure S5: ^{1}H NMR, ^{13}C NMR and HRMS of *3,3,6,6-tetramethyl-9-phenyl-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione* (**3a**)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6.75
6.63
5.49
3.83
3.75
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2.39
2.34
2.33
1.22
1.10
OCH3
OCH3
O
O
O
3c, 66%
H (m)
6.76
G (s)
6.63
F (s)
5.49
E (s)
3.75
D (s)
3.83
C (m)
2.37
B (s)
1.10
A (s)
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1.13
2.26
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3.17
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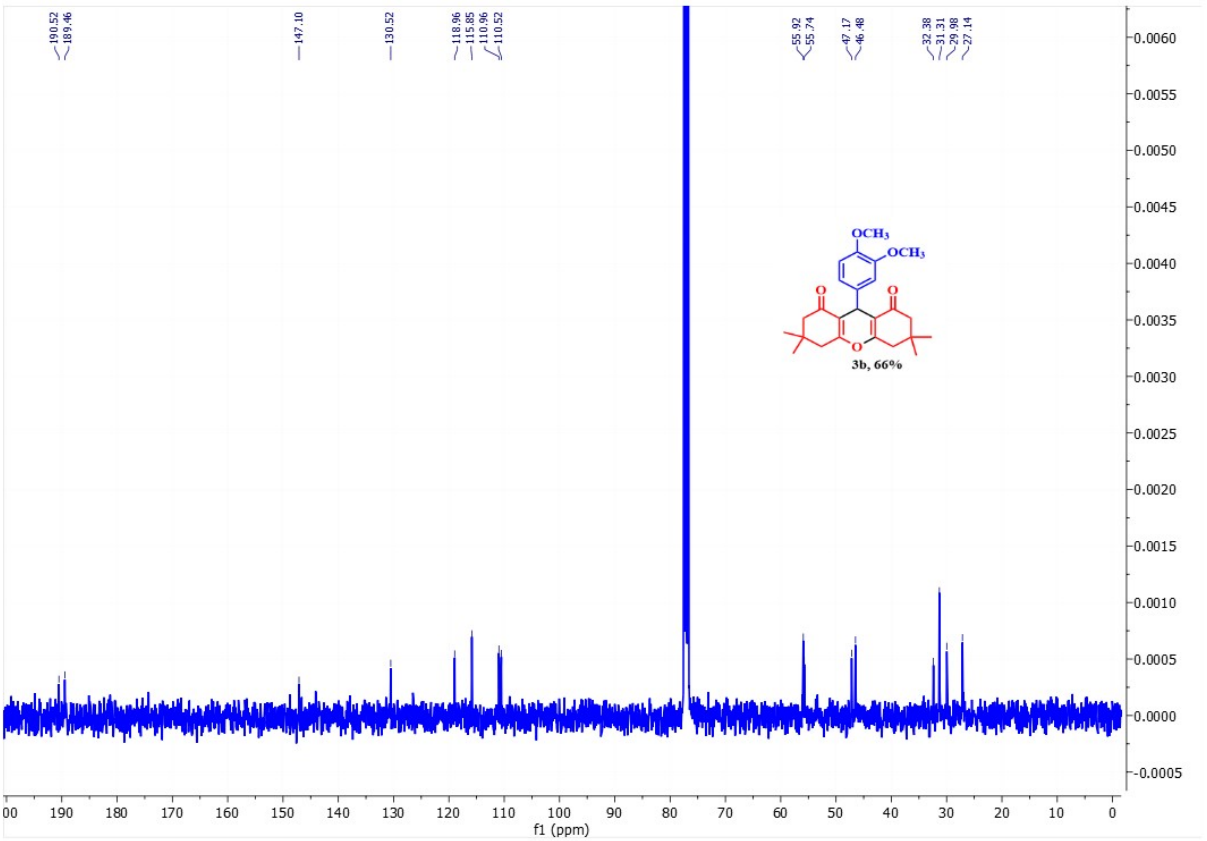
6.64
f1 (ppm)



Cpd	Name	Formula	CAS	RT	Mass	Mass (Tgt)	Diff (Tgt, ppm)	Score	Algorithm
1		C25 H30 O5		0.837	410.2129	410.2093	8.74	91.51	FBF

Compound Details

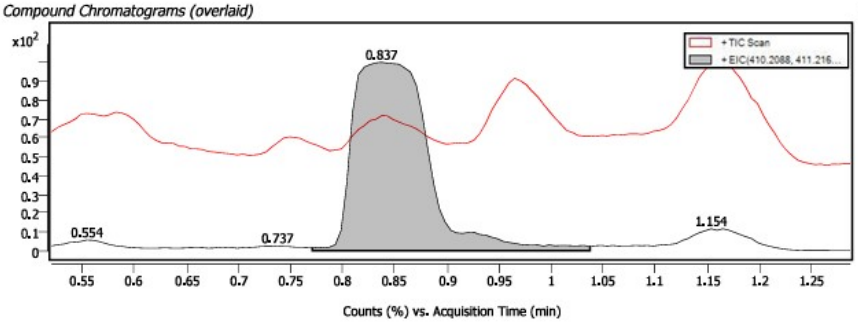
Cpd 1: C25 H30 O5

Name	Formula	RT	RI	Mass	Diff (Tgt, ppm)	CAS	ID Source	Score	Algorithm
	C25 H30 O5	0.837		410.2129	8.74		FBF	91.51	FBF

Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M+H)+ (M+Na)+	411.2183 433.2028	91.51				

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)

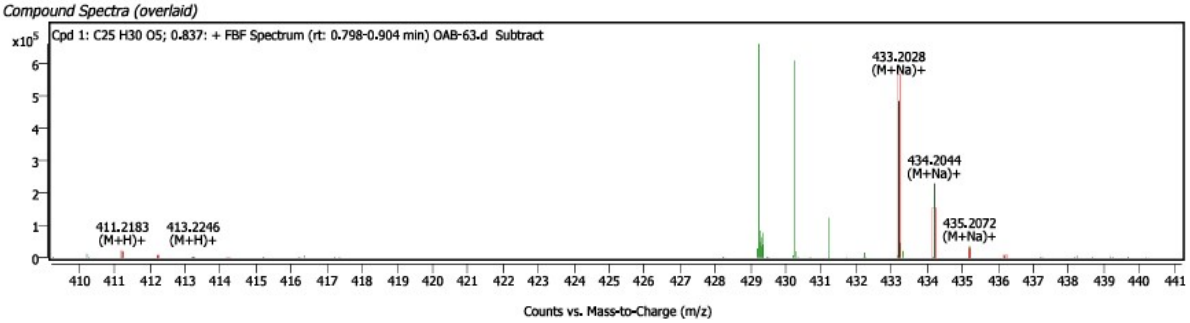
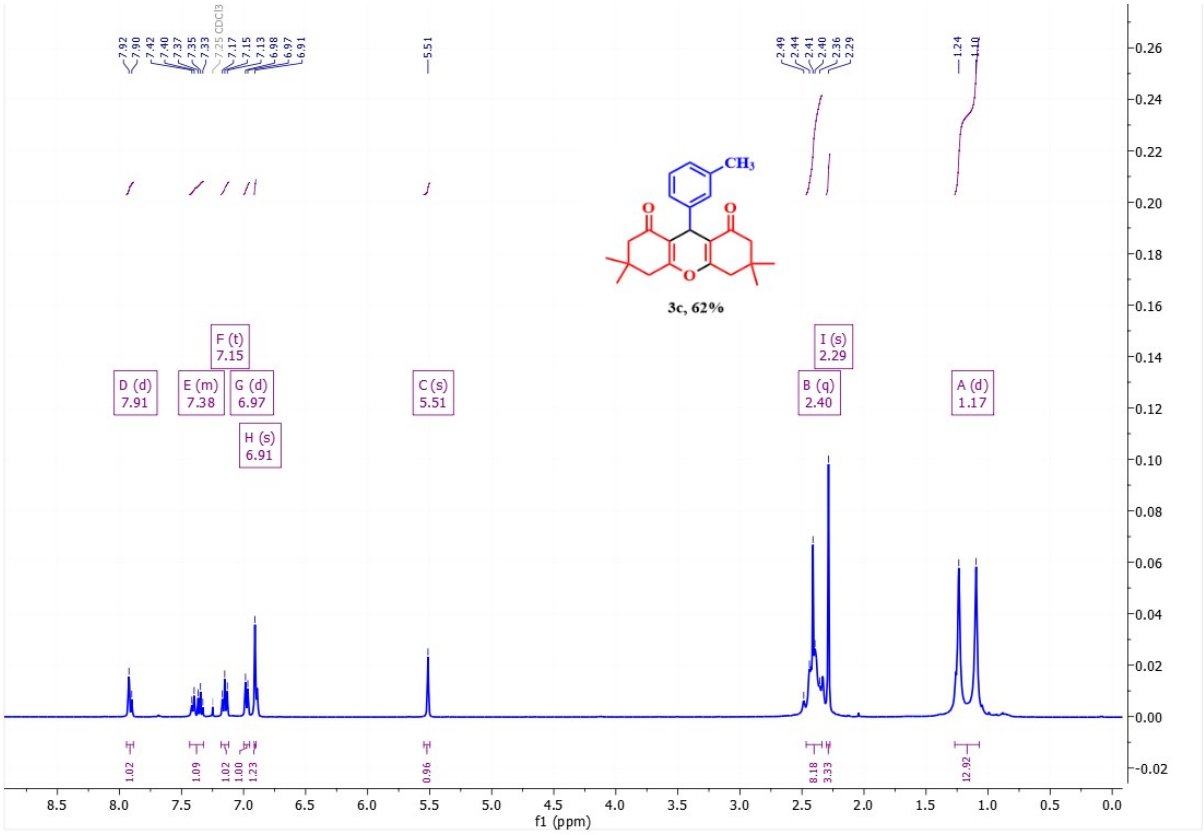
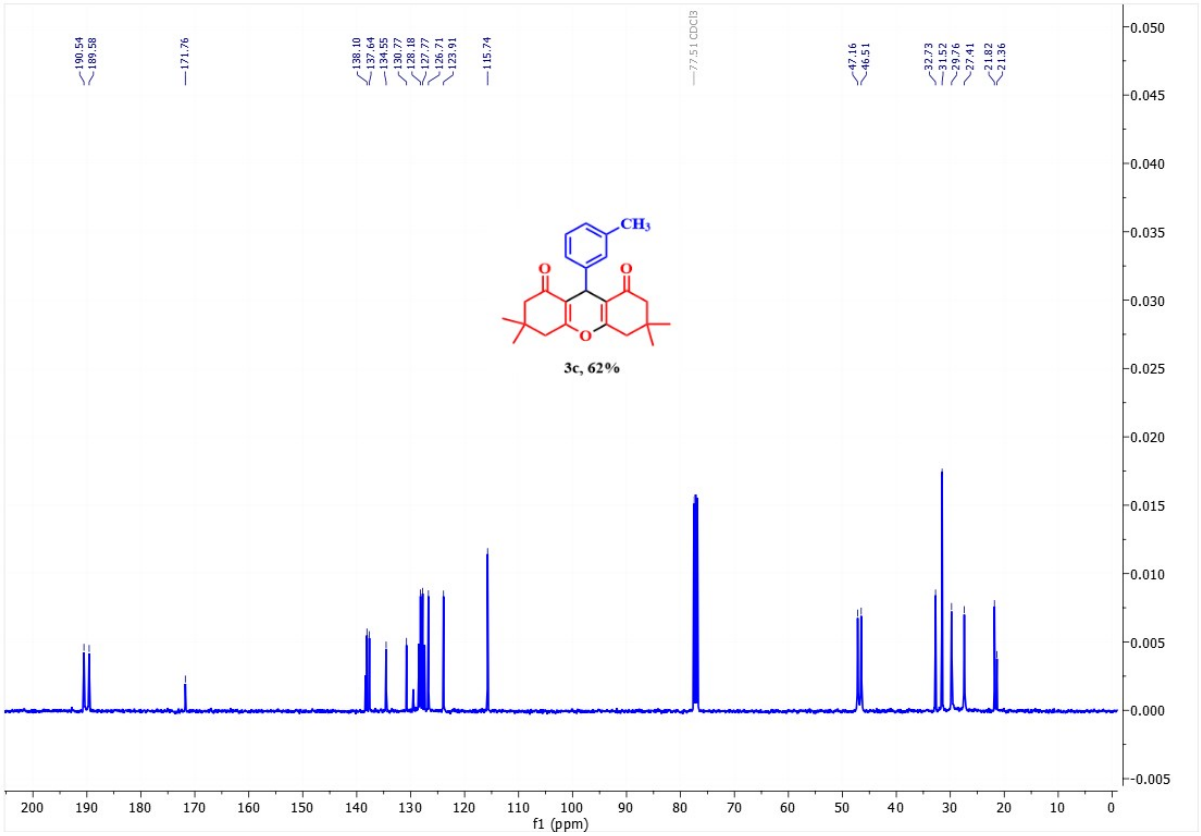


Figure S6: ^{1}H NMR, ^{13}C NMR and HRMS of *9-(3,4-dimethoxyphenyl)-3,3,6,6-tetramethyl-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione* (**3b**)





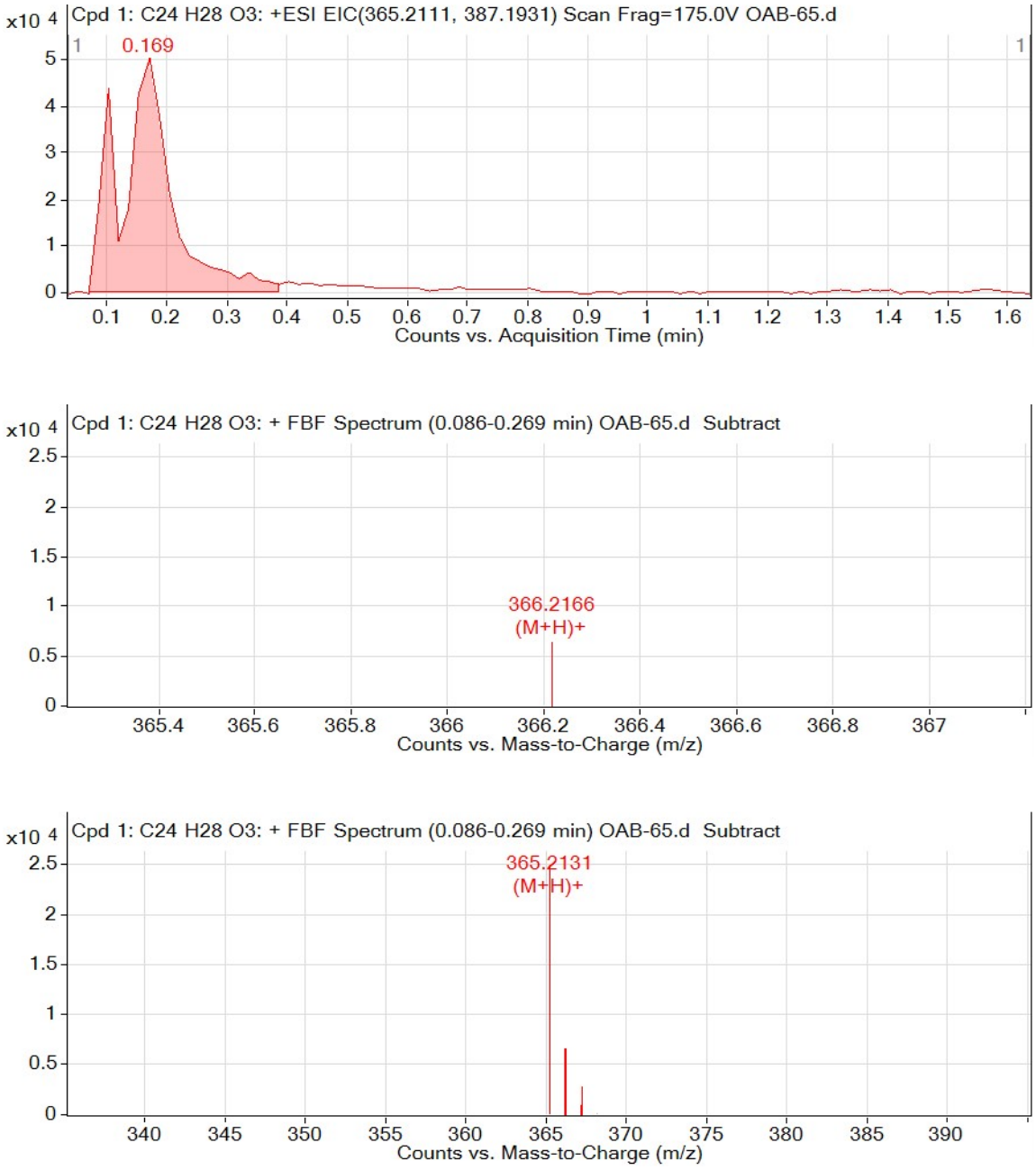
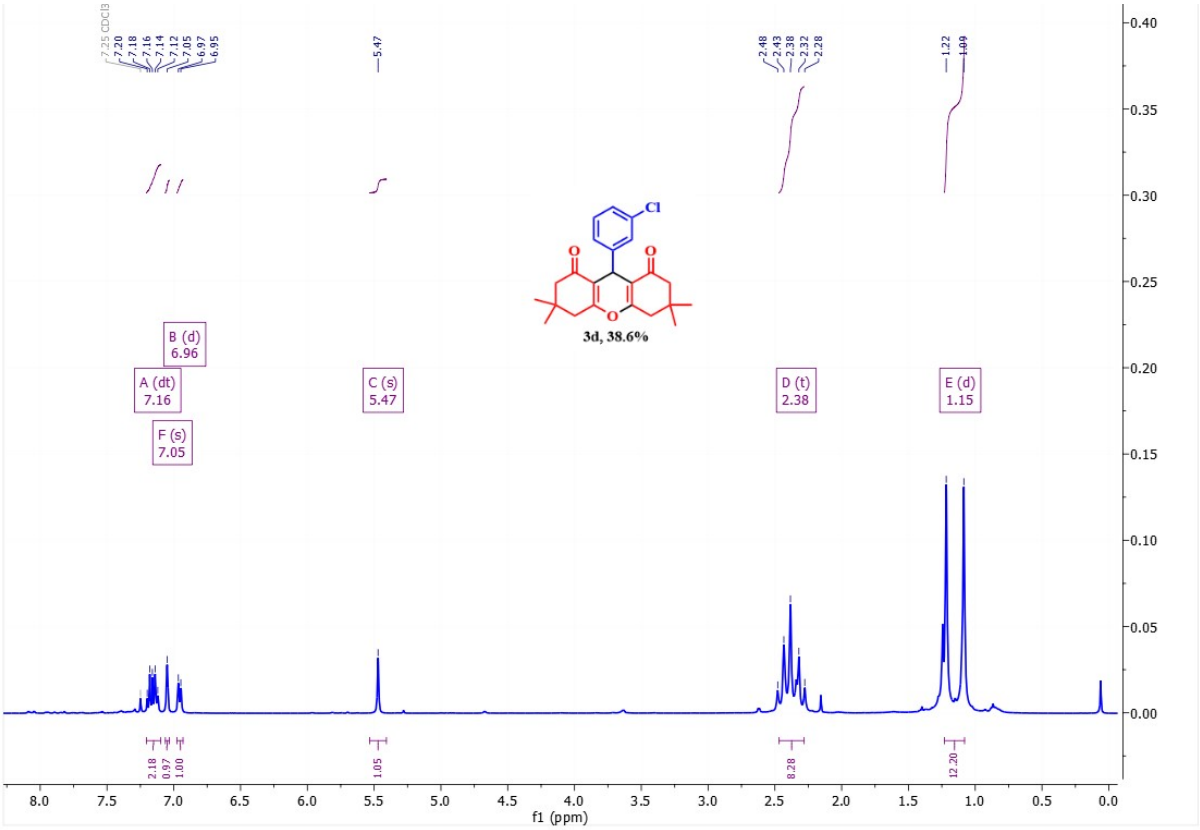


Figure S7: ^{1}H NMR, ^{13}C NMR and HRMS of *3,3,6,6-tetramethyl-9-(m-tolyl)-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione*(**3c**)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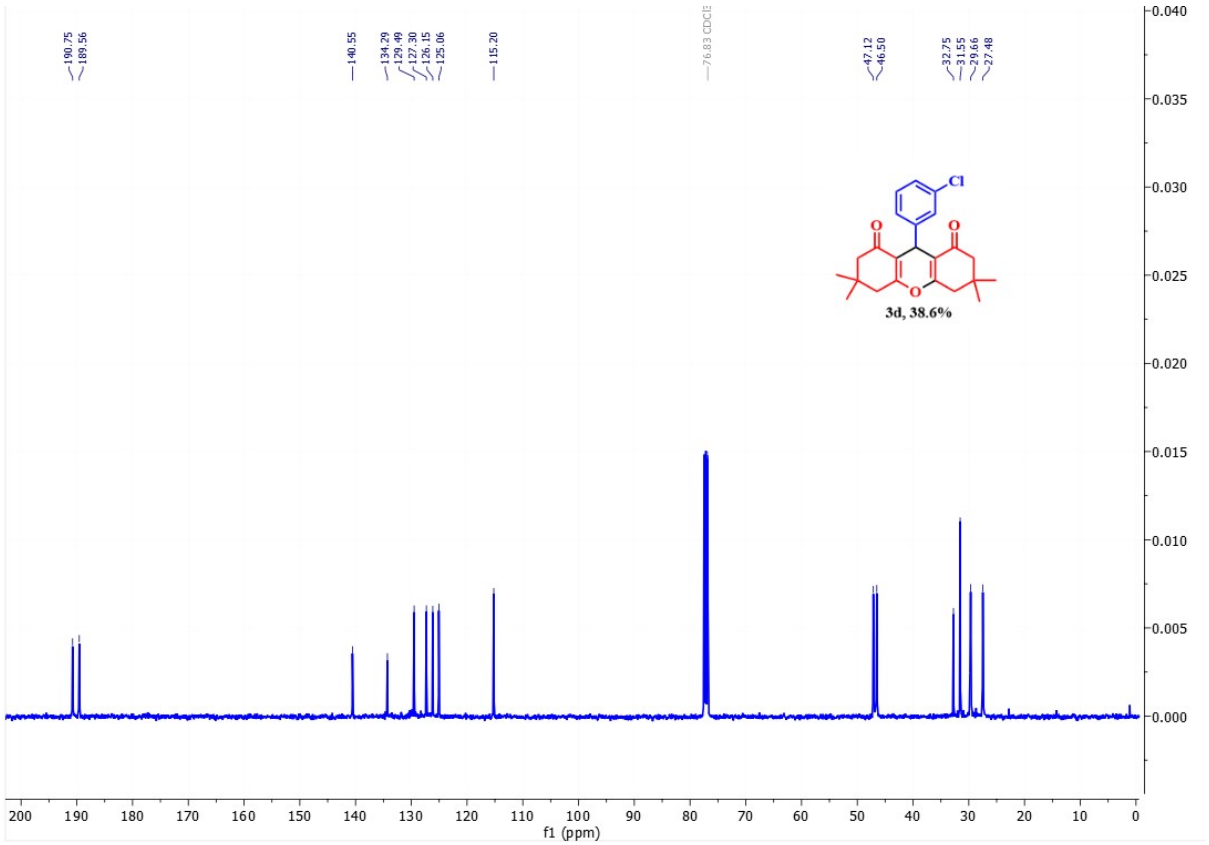
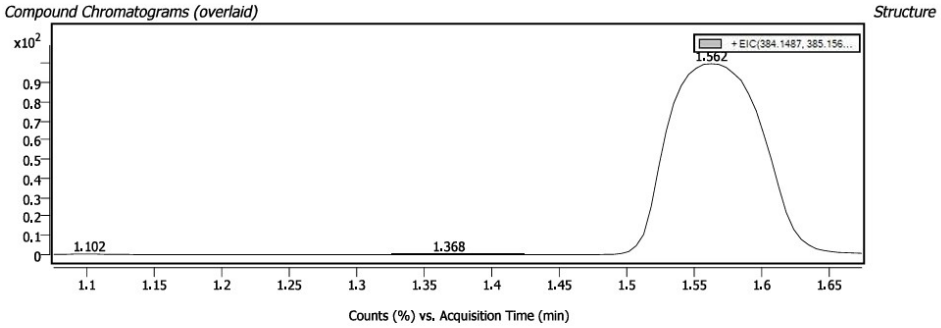
7.20
7.18
7.16
7.14
7.12
7.05
6.97
6.95
5.47
2.48
2.43
2.38
2.32
2.28
1.22
1.09
Cl
O
O
O
3d, 38.6%
B (d)
6.96
A (dt)
7.16
F (s)
7.05
C (s)
5.47
D (t)
2.38
E (d)
1.15
2.18
0.97
1.00
1.05
8.28
12.20
f1 (ppm)



Name	Formula	RT	RI	Mass	Diff (Tgt, ppm)	CAS	ID Source	Score	Algorithm
	C23 H25 Cl O3	1.368		384.1510	4.74		FBF	89.84	FBF

Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M+H)+ (M+Na)+	385.1582 407.1406	89.84				



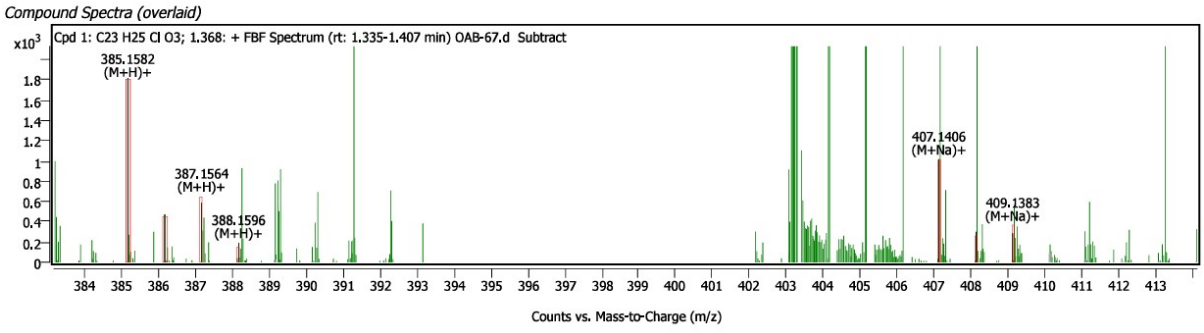
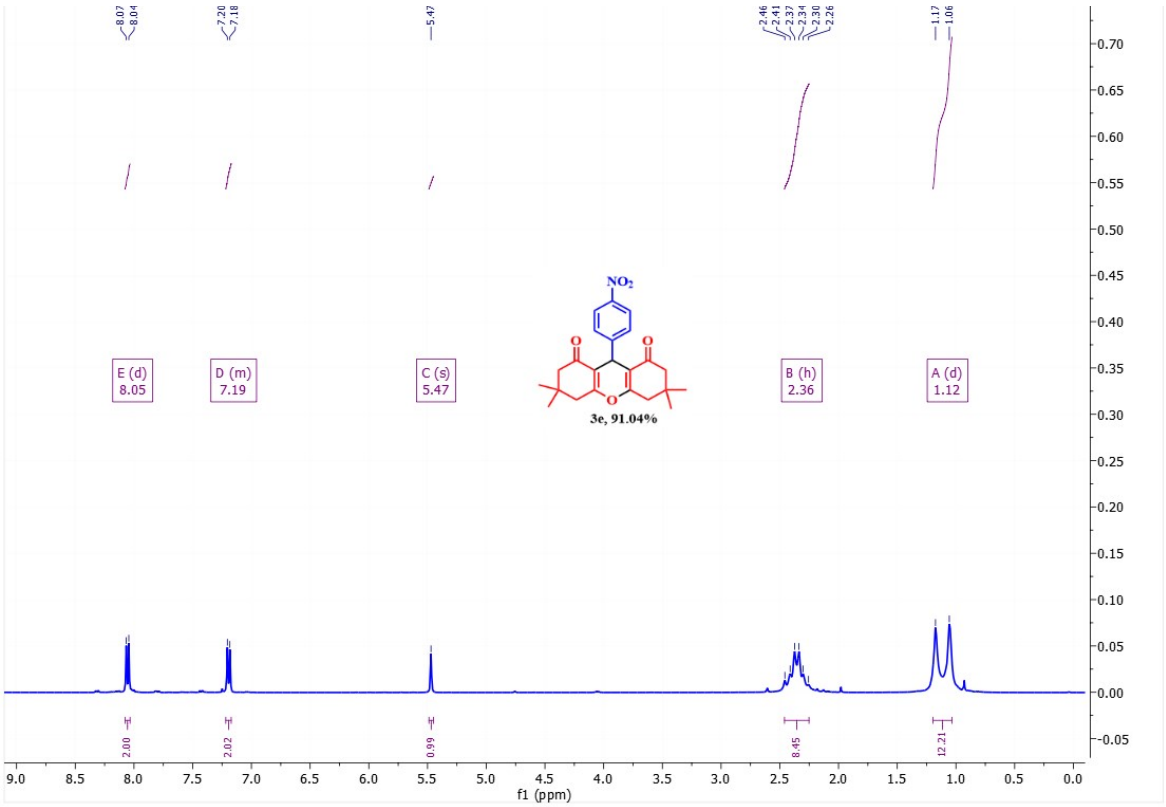
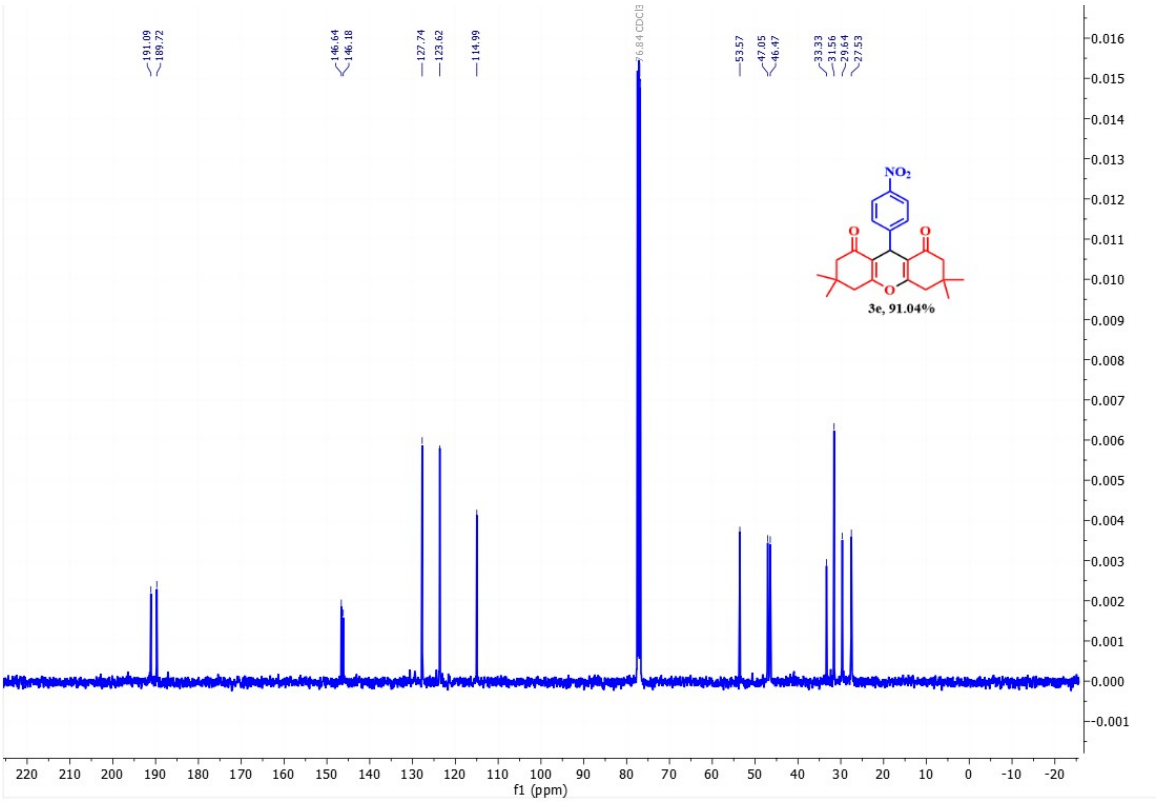


Figure S8: ^{1}H NMR, ^{13}C NMR and HRMS of *9-(3-chlorophenyl)-3,3,6,6-tetramethyl-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione*(**3d**)


8.07
8.04
7.20
7.18
5.47
2.46
2.41
2.37
2.34
2.30
2.26
1.17
1.06
E (d)
8.05
D (m)
7.19
C (s)
5.47
B (h)
2.36
A (d)
1.12
NO2
O
O
O
3e, 91.04%
2.00
2.02
0.99
8.45
12.21
f1 (ppm)


191.09
189.72
146.64
146.18
127.74
123.62
114.99
76.84 CDCl3
53.57
47.05
46.47
33.33
31.56
29.64
27.53
NO2
O
O
O
3e, 91.04%
f1 (ppm)

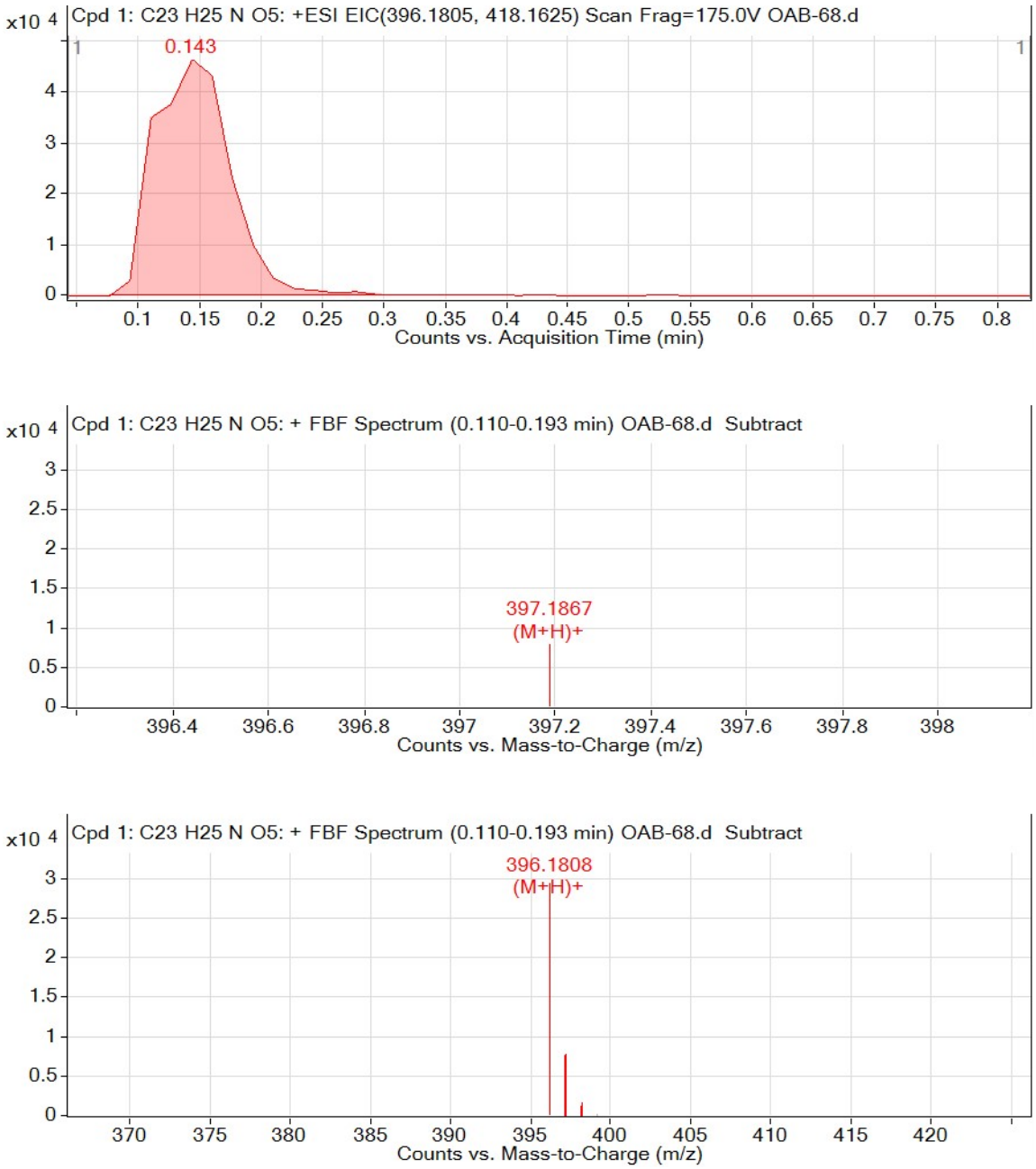
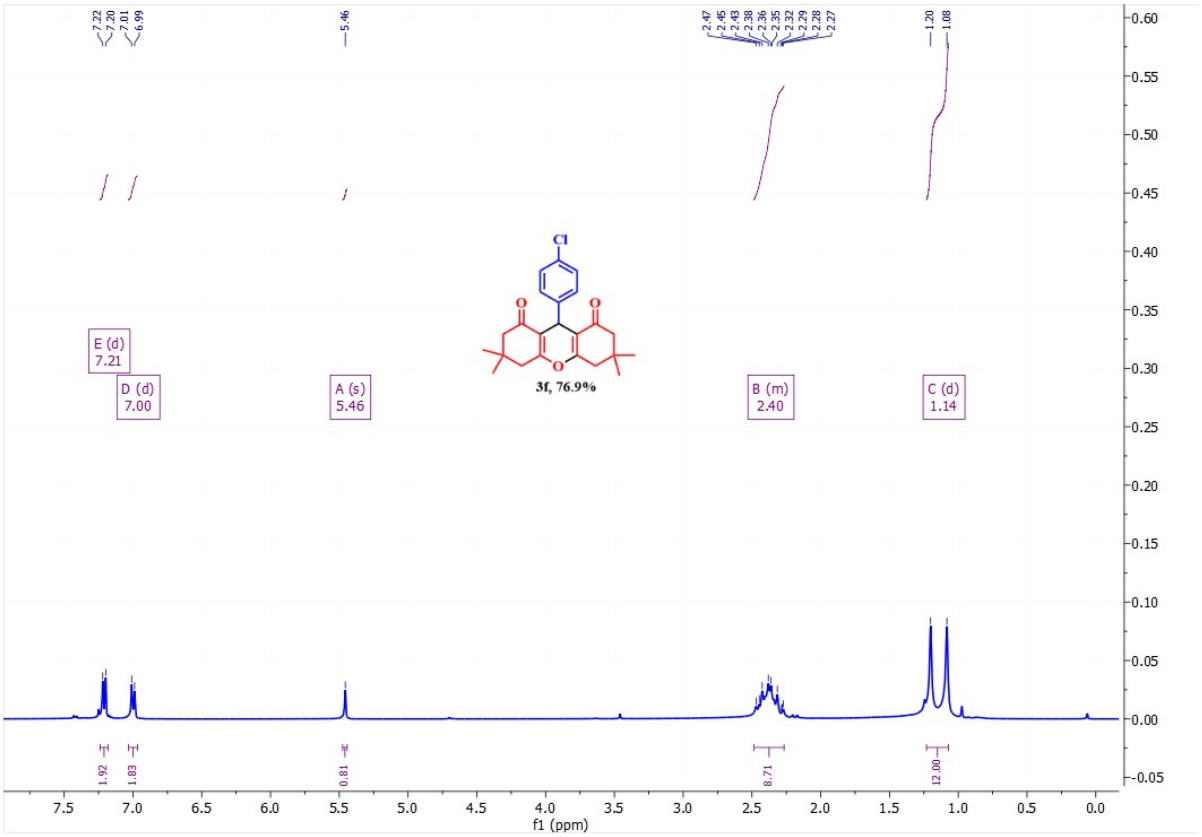
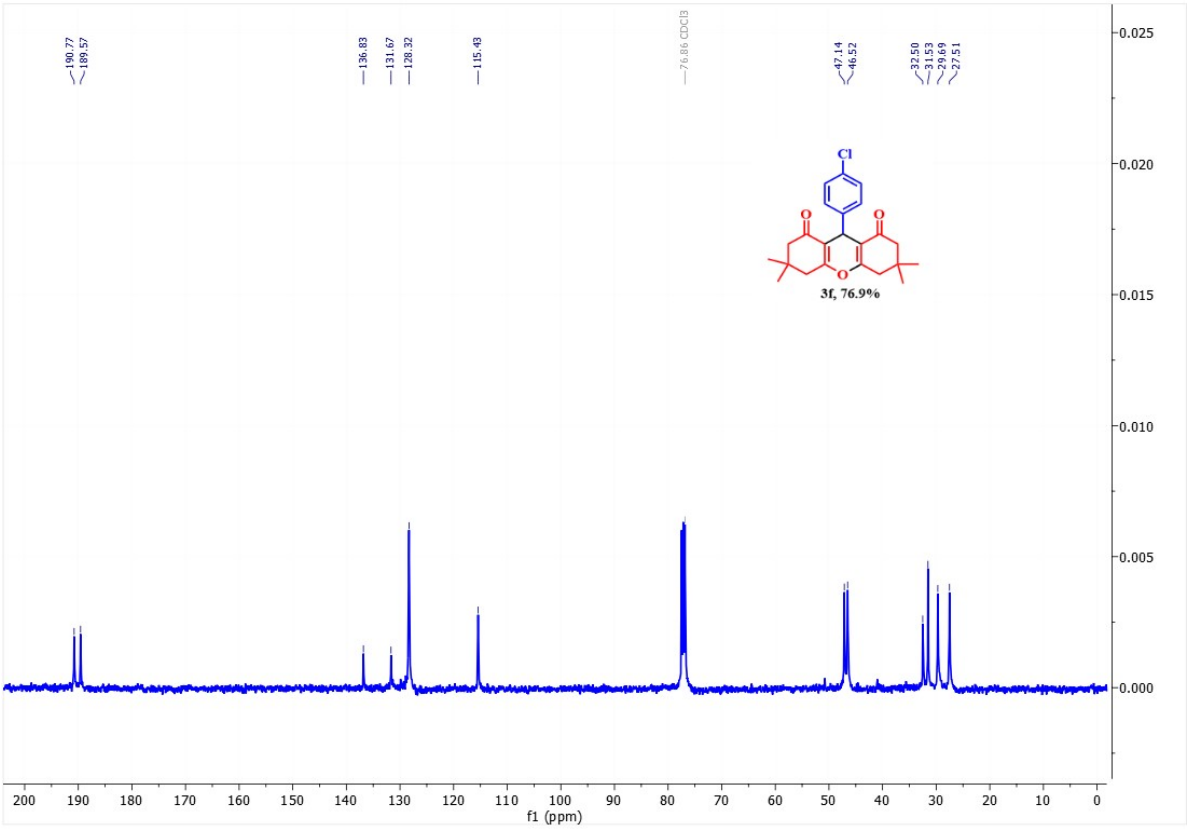


Figure S9: ^{1}H NMR, ^{13}C NMR and HRMS of *3,3,6,6-tetramethyl-9-(4-nitrophenyl)-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione* (**3e**)


7.22
7.20
7.01
6.99
5.46
2.47
2.45
2.43
2.38
2.36
2.35
2.32
2.29
2.28
2.27
1.20
1.08
Cl
O
O
O
3f, 76.9%
E (d)
7.21
D (d)
7.00
A (s)
5.46
B (m)
2.40
C (d)
1.14
1.92
1.83
0.81
8.71
12.00
f1 (ppm)


190.77
189.57
136.83
131.67
128.32
115.43
76.86 CDCl3
47.14
46.52
32.50
31.53
29.69
27.51
Cl
O
O
O
3f, 76.9%
f1 (ppm)

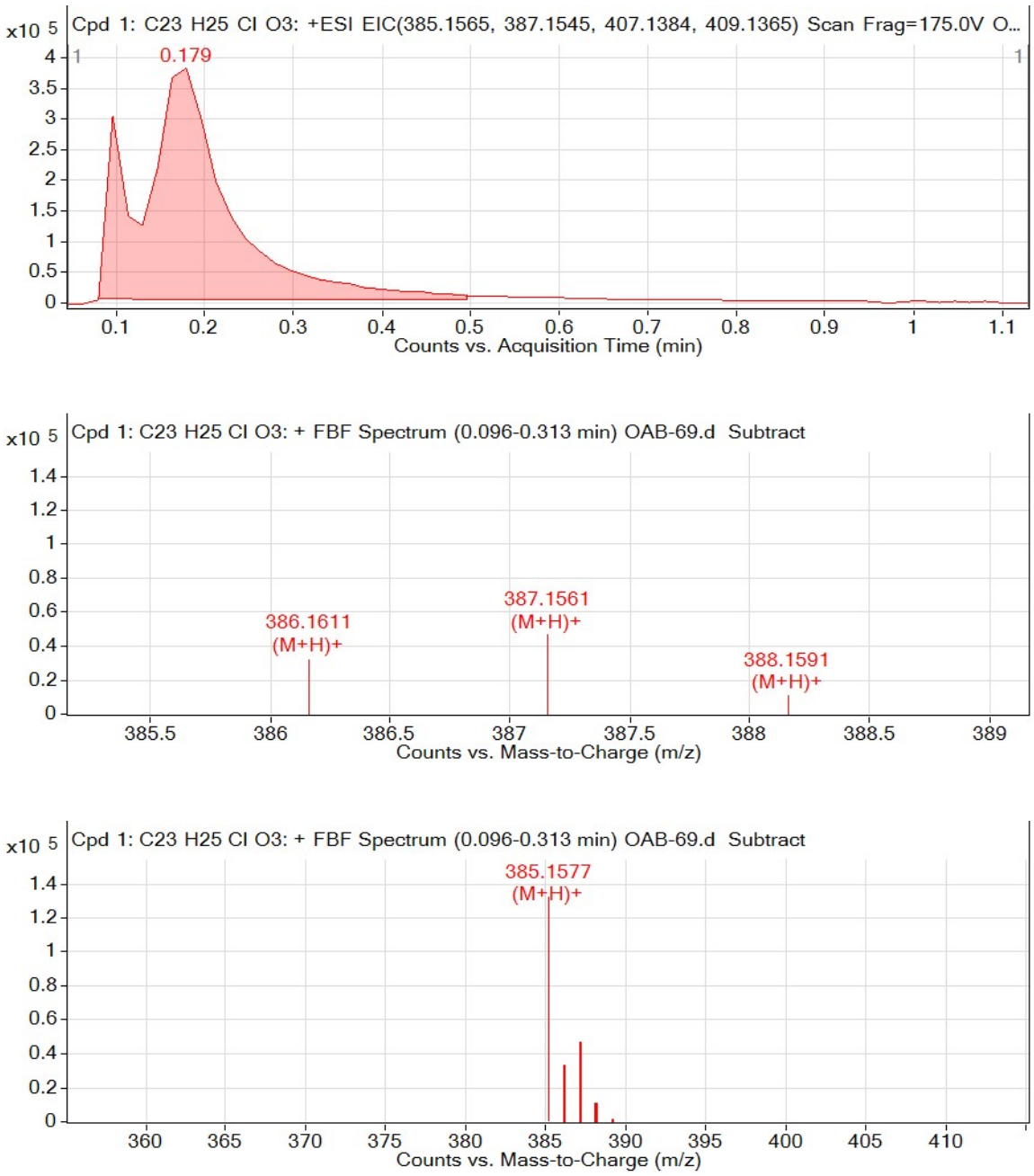
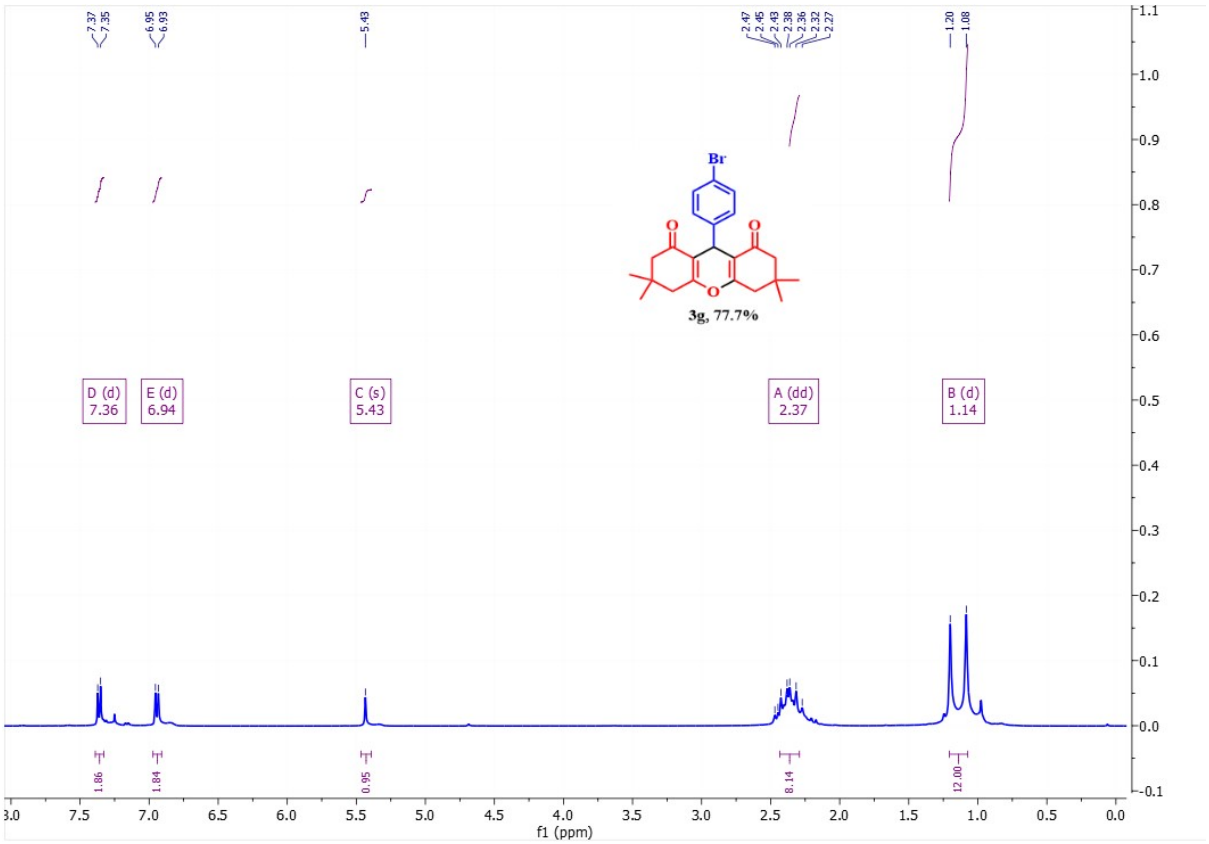
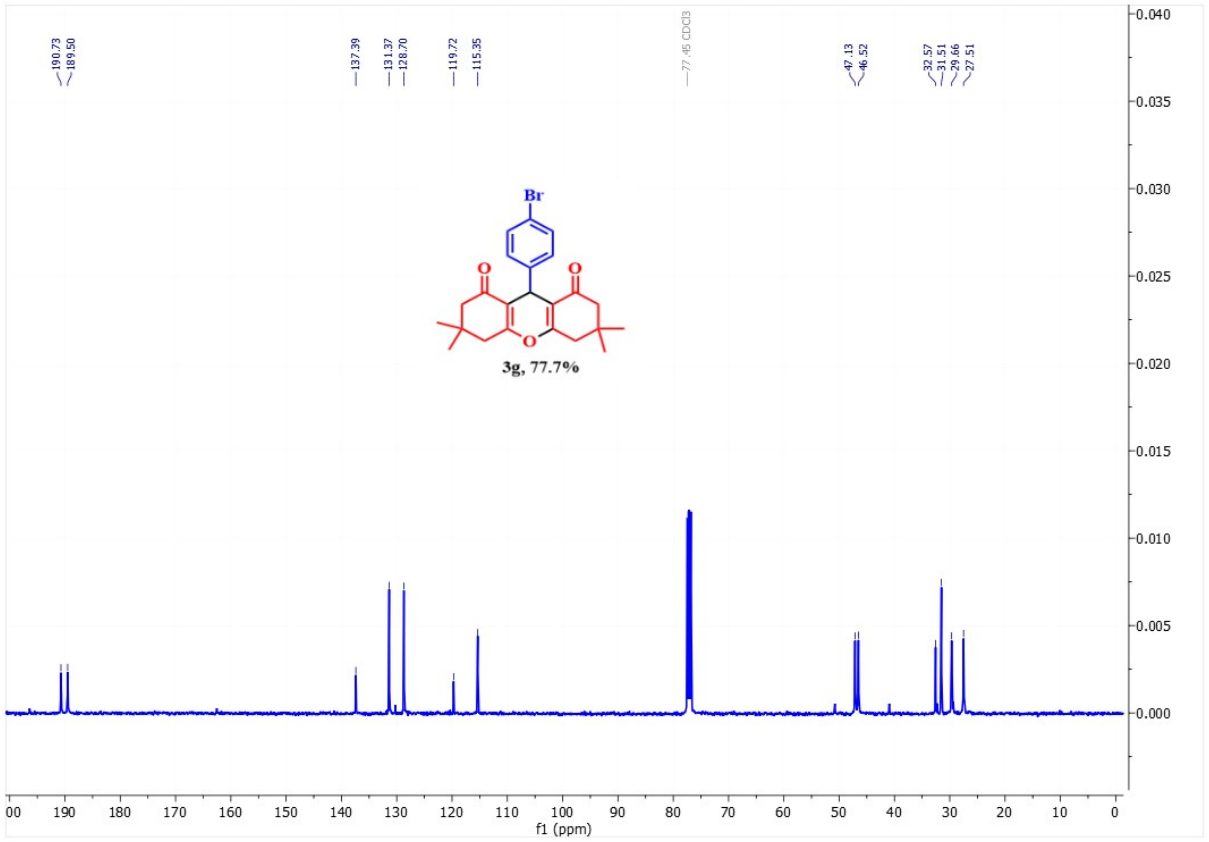


Figure S10: ^{1}H NMR, ^{13}C NMR and HRMS of *9-(4-chlorophenyl)-3,3,6,6-tetramethyl-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione* (**3f**)


7.37
7.35
6.95
6.93
5.43
2.47
2.45
2.43
2.38
2.36
2.32
2.27
1.20
1.08
Br
O
O
O
3g, 77.7%
D (d)
7.36
E (d)
6.94
C (s)
5.43
A (dd)
2.37
B (d)
1.14
1.86
1.84
0.95
8.14
12.00
f1 (ppm)


190.73
189.50
137.39
131.37
128.70
119.72
115.35
77.45 CDCl3
47.13
46.52
32.57
31.51
29.66
27.51
Br
O
O
O
3g, 77.7%
f1 (ppm)

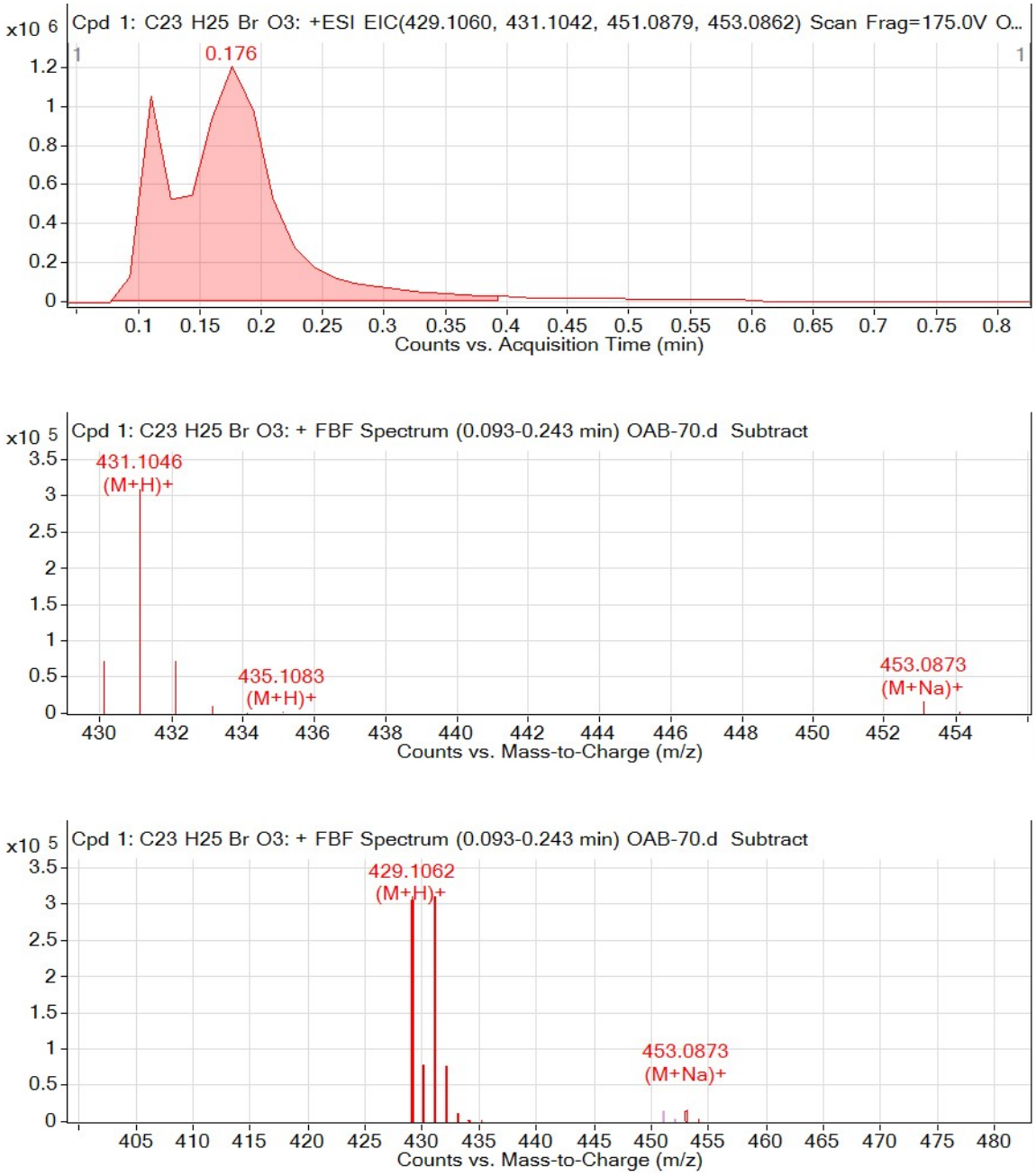
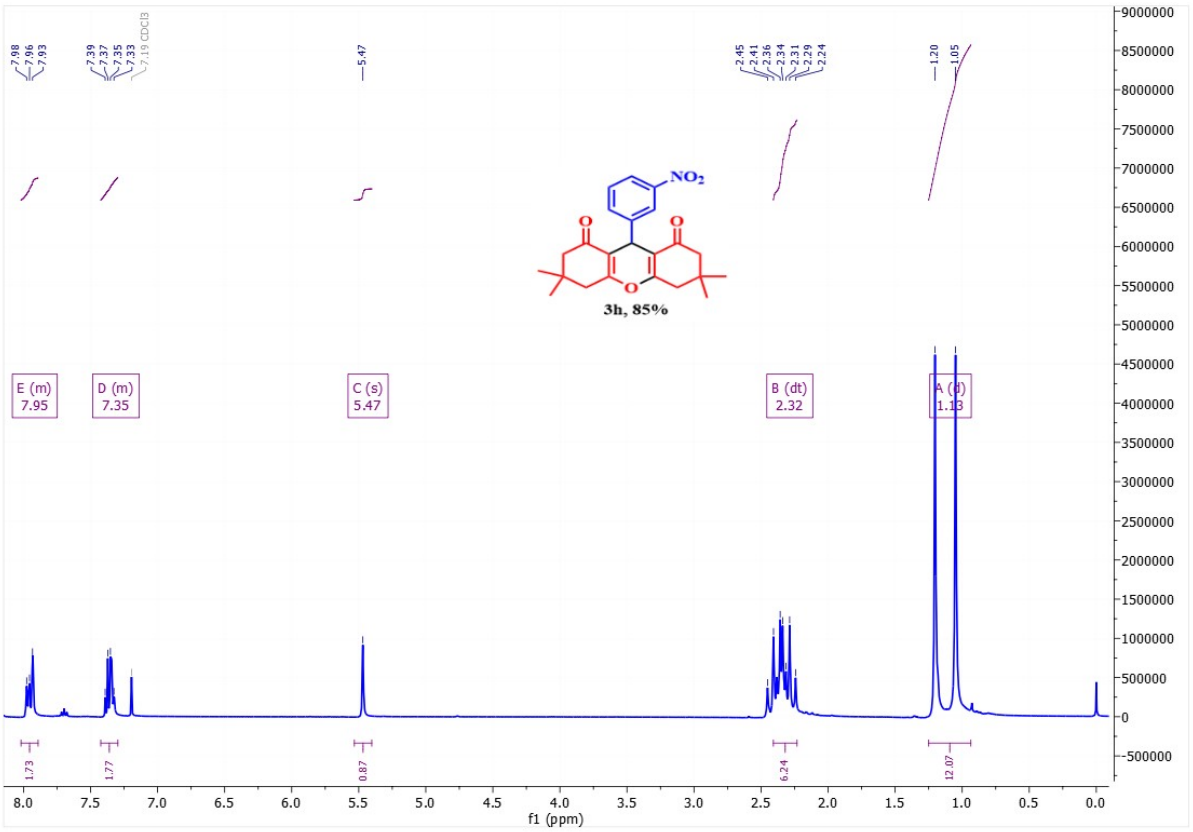
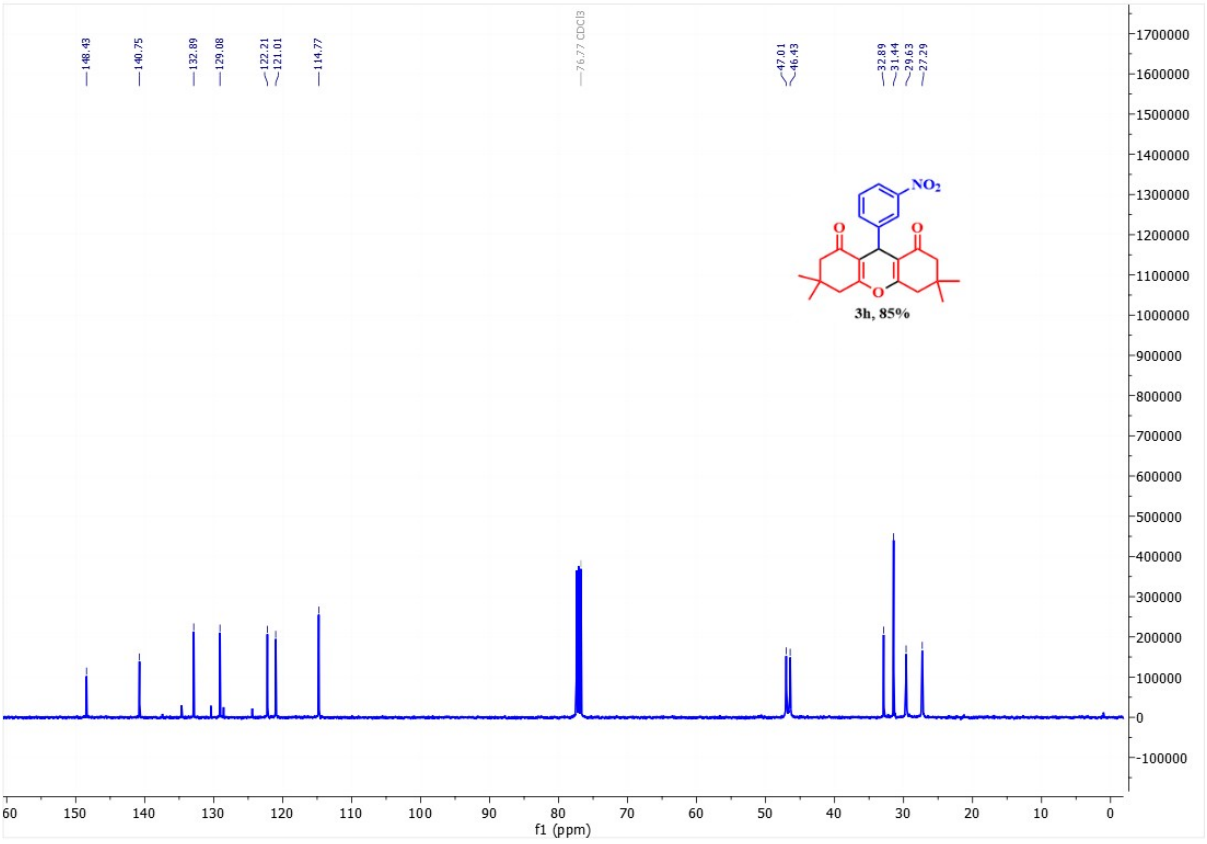


Figure S11: ^{1}H NMR, ^{13}C NMR and HRMS of *9-(4-bromophenyl)-3,3,6,6-tetramethyl-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione*(**3g**)


7.98
7.96
7.93
7.39
7.37
7.35
7.33
7.19 CDCl3
5.47
2.45
2.41
2.36
2.34
2.31
2.29
2.24
1.20
1.05
NO2
O
O
O
3h, 85%
E (m)
7.95
D (m)
7.35
C (s)
5.47
B (dt)
2.32
A (d)
1.13
1.73
1.77
0.87
6.24
12.07
f1 (ppm)


148.43
140.75
132.89
129.08
122.21
121.01
114.77
77.77 CDCl3
47.01
46.43
32.89
31.44
29.63
27.29
NO2
O
O
O
3h, 85%
f1 (ppm)

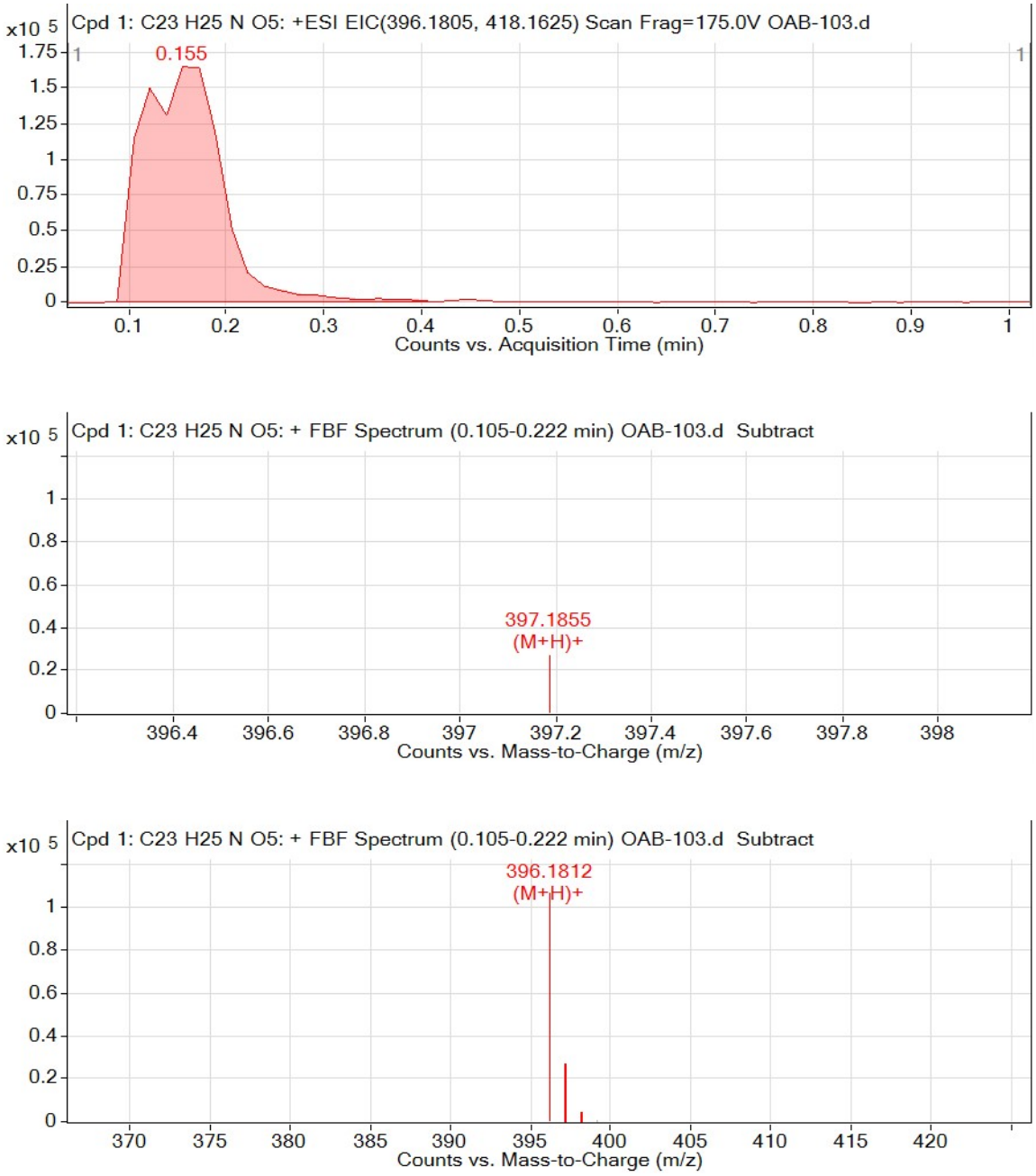
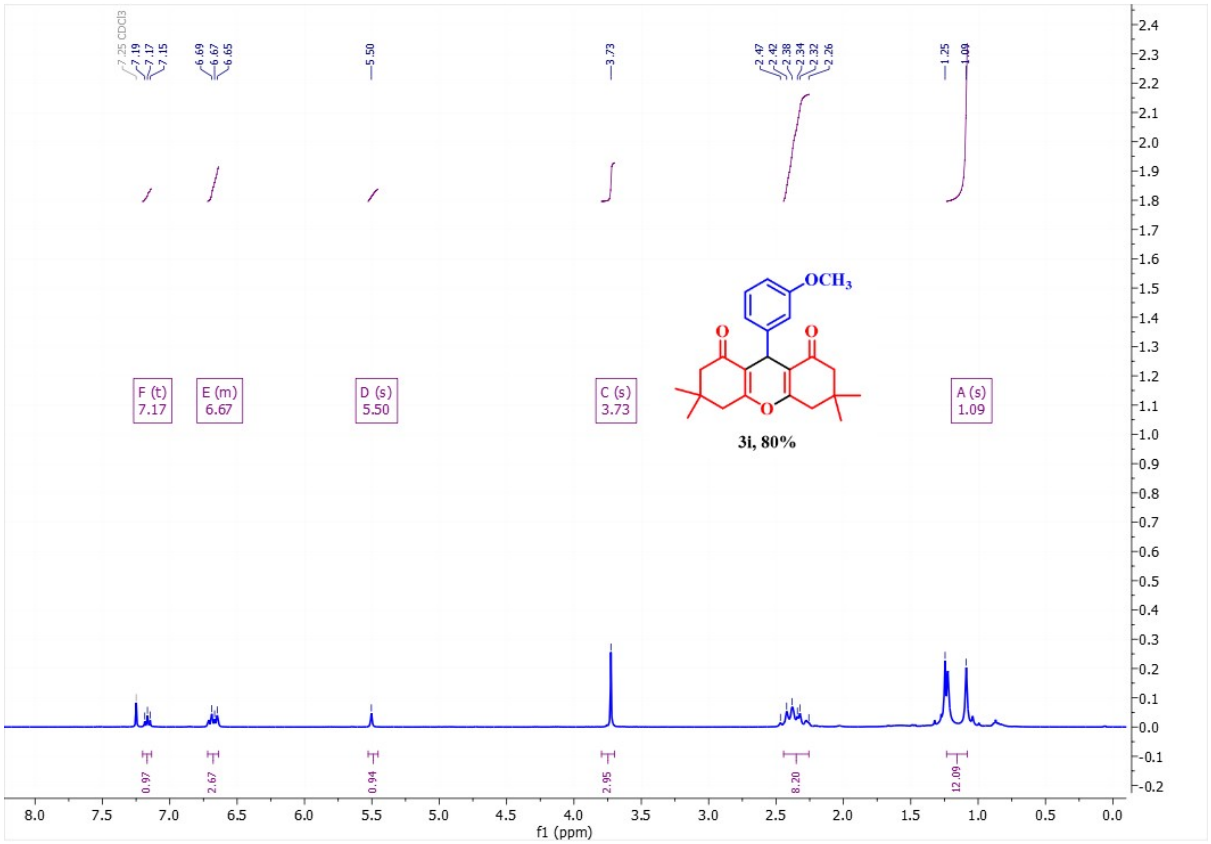
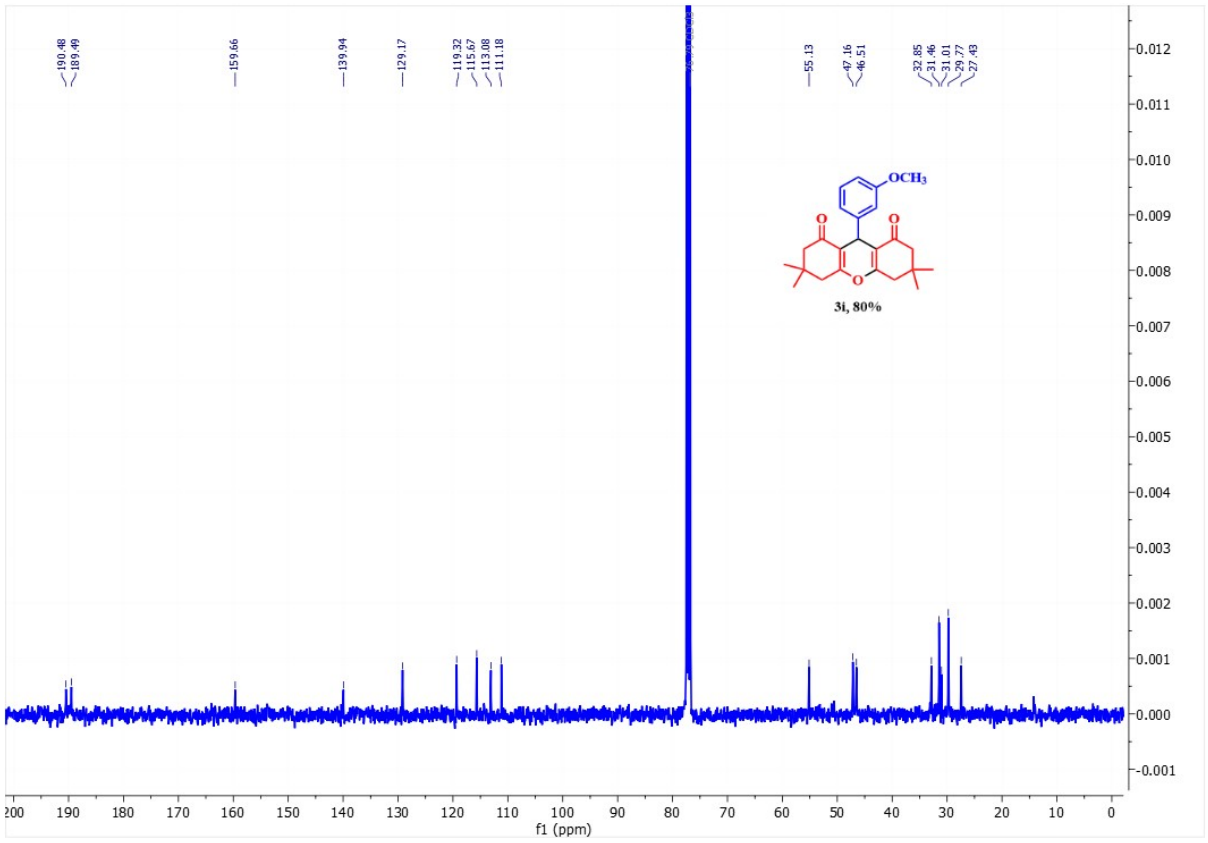


Figure S12: ^{1}H NMR, ^{13}C NMR and HRMS of *3,3,6,6-tetramethyl-9-(3-nitrophenyl)-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione* (**3h**)


7.25 CDCl3
7.19
7.17
7.15
6.69
6.67
6.65
5.50
3.73
2.47
2.42
2.38
2.34
2.32
2.26
1.25
1.09
F (t)
7.17
E (m)
6.67
D (s)
5.50
C (s)
3.73
A (s)
1.09
OCH3
O
O
O
3i, 80%
0.97
2.67
0.94
2.95
8.20
12.09
f1 (ppm)


190.48
189.49
159.66
139.94
129.17
119.32
115.67
113.08
111.18
55.13
47.16
46.51
32.85
31.46
31.01
29.77
27.43
OCH3
O
O
O
3i, 80%
f1 (ppm)

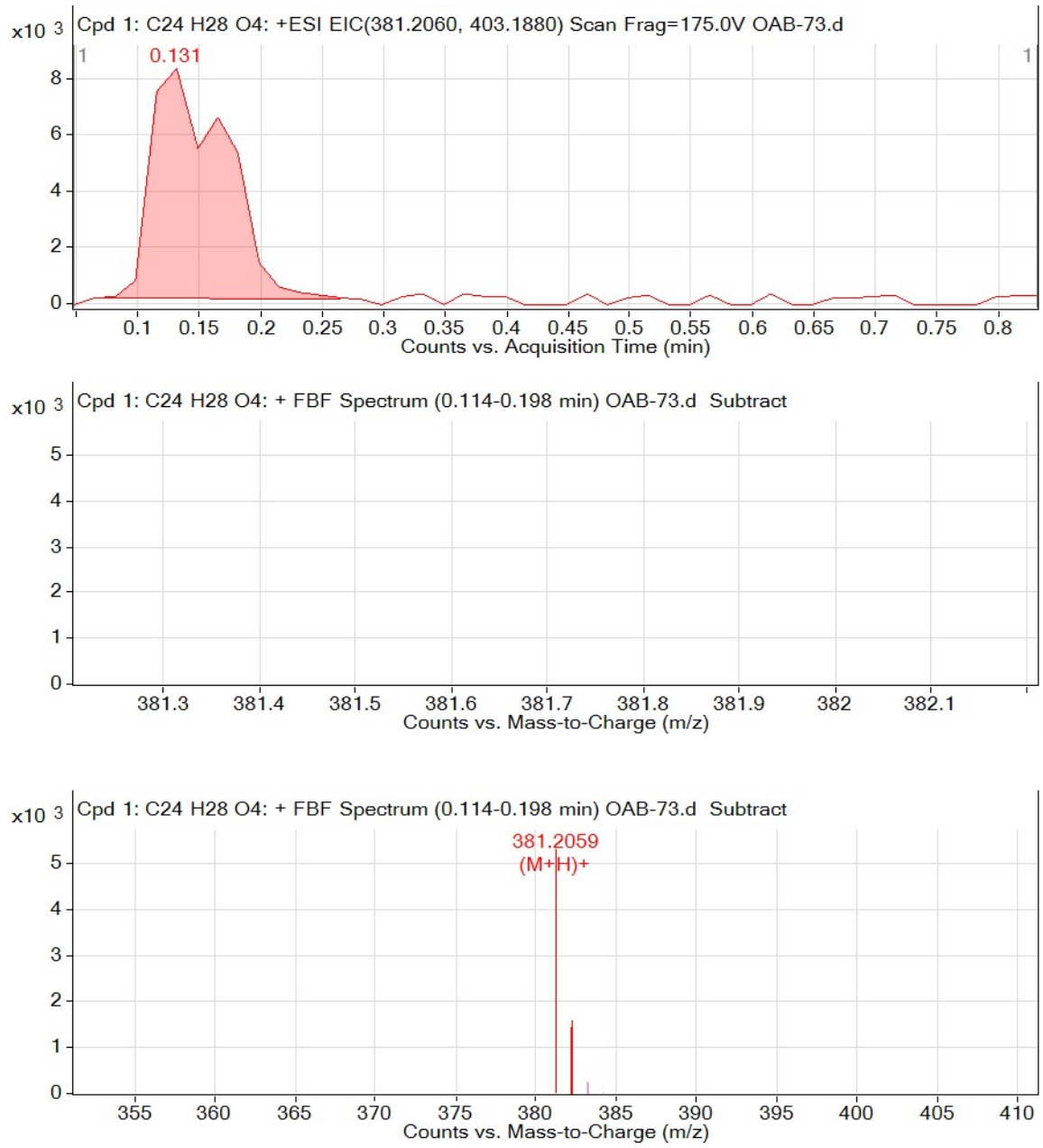
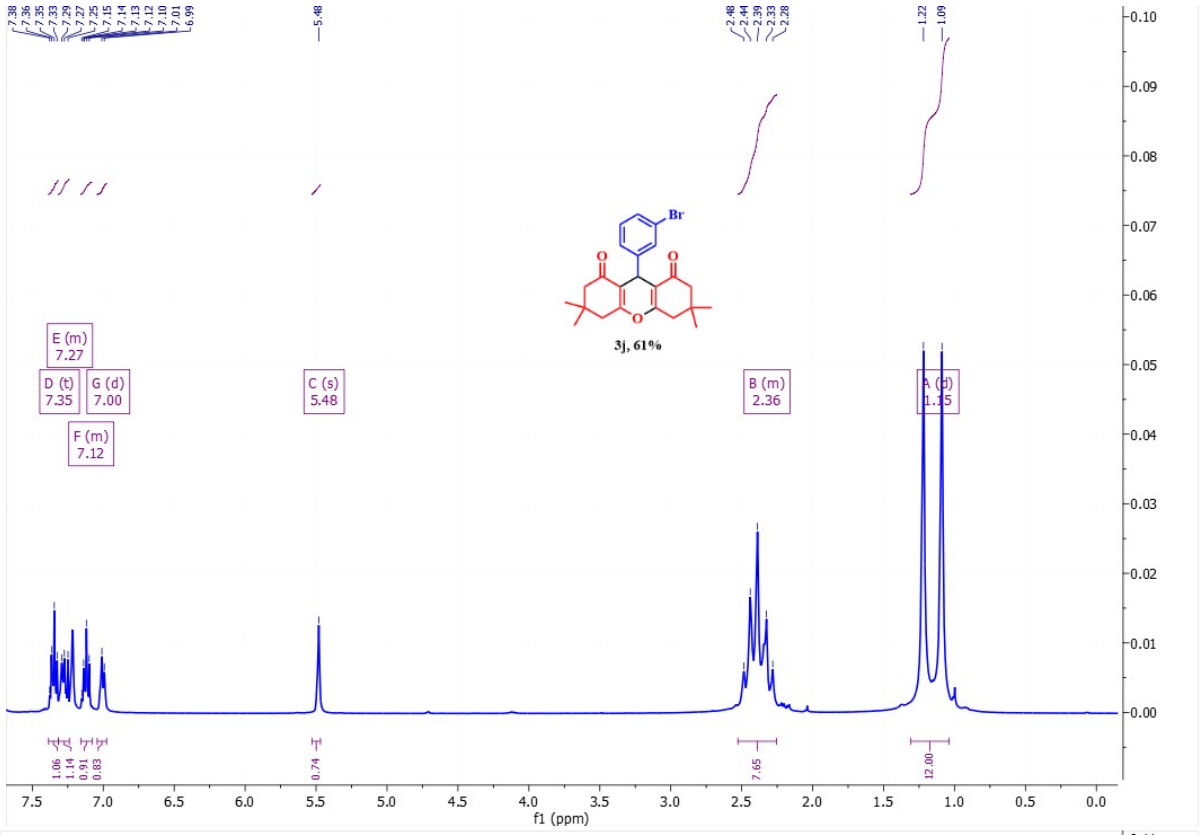
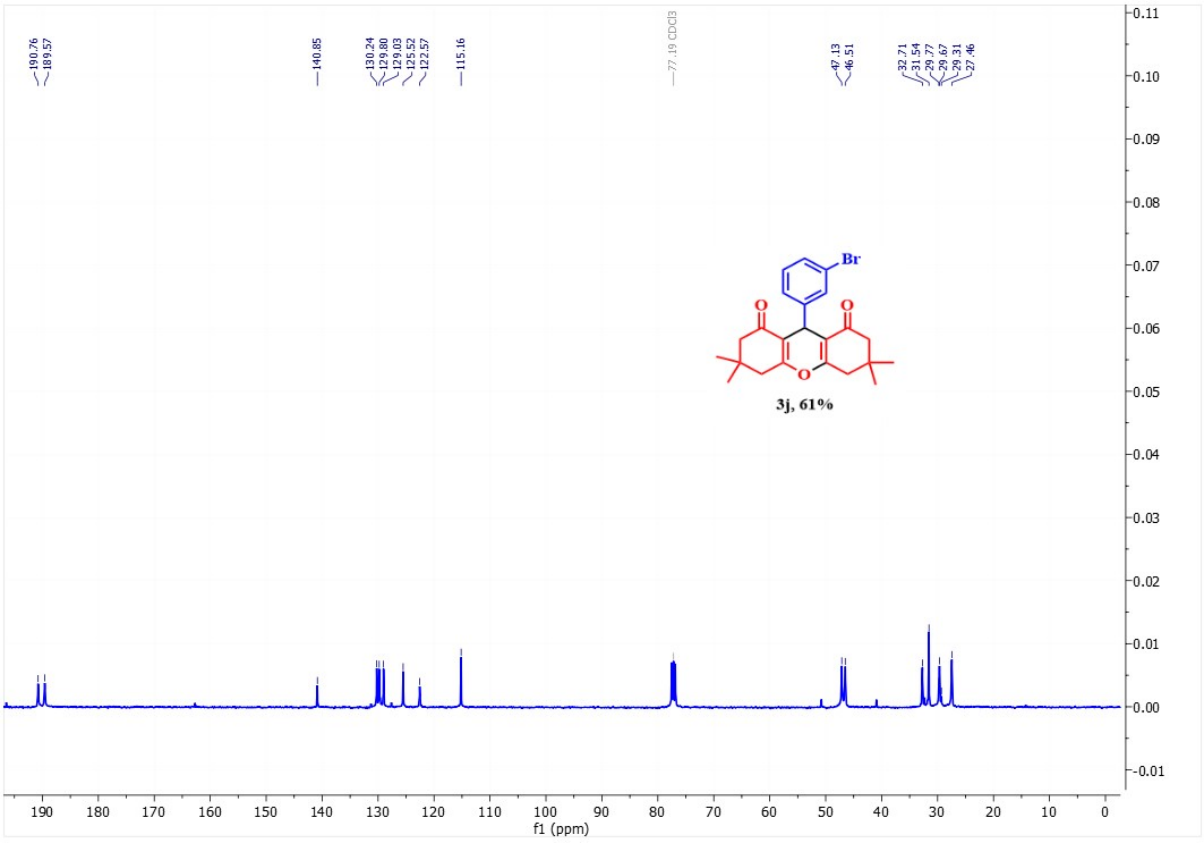


Figure S13: ^{1}H NMR, ^{13}C NMR and HRMS of *9-(3-methoxyphenyl)-3,3,6,6-tetramethyl-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione* (**3i**)


7.38
7.36
7.35
7.33
7.29
7.27
7.25
7.15
7.14
7.13
7.12
7.10
7.01
6.99
5.48
2.48
2.44
2.39
2.33
2.28
1.22
1.09
Br
O
O
O
3j, 61%
E (m)
7.27
D (t)
7.35
G (d)
7.00
F (m)
7.12
C (s)
5.48
B (m)
2.36
A (d)
1.15
1.06
1.14
0.91
0.83
0.74
7.65
12.00
f1 (ppm)


190.76
189.57
140.85
130.24
129.80
129.03
125.52
122.57
115.16
77.19 CDCl3
47.13
46.51
32.71
31.54
29.77
29.67
29.31
27.46
Br
O
O
O
3j, 61%
f1 (ppm)

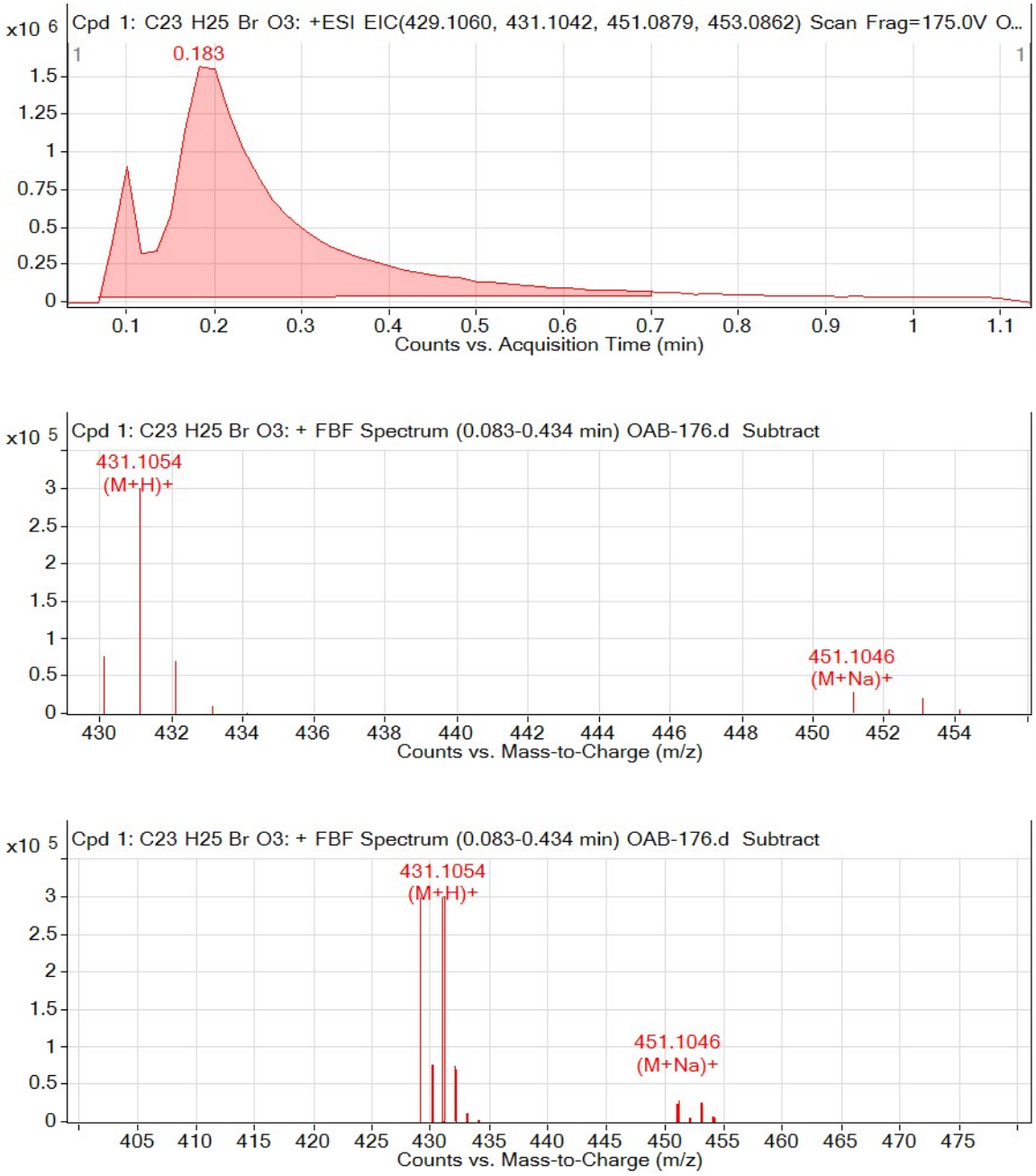
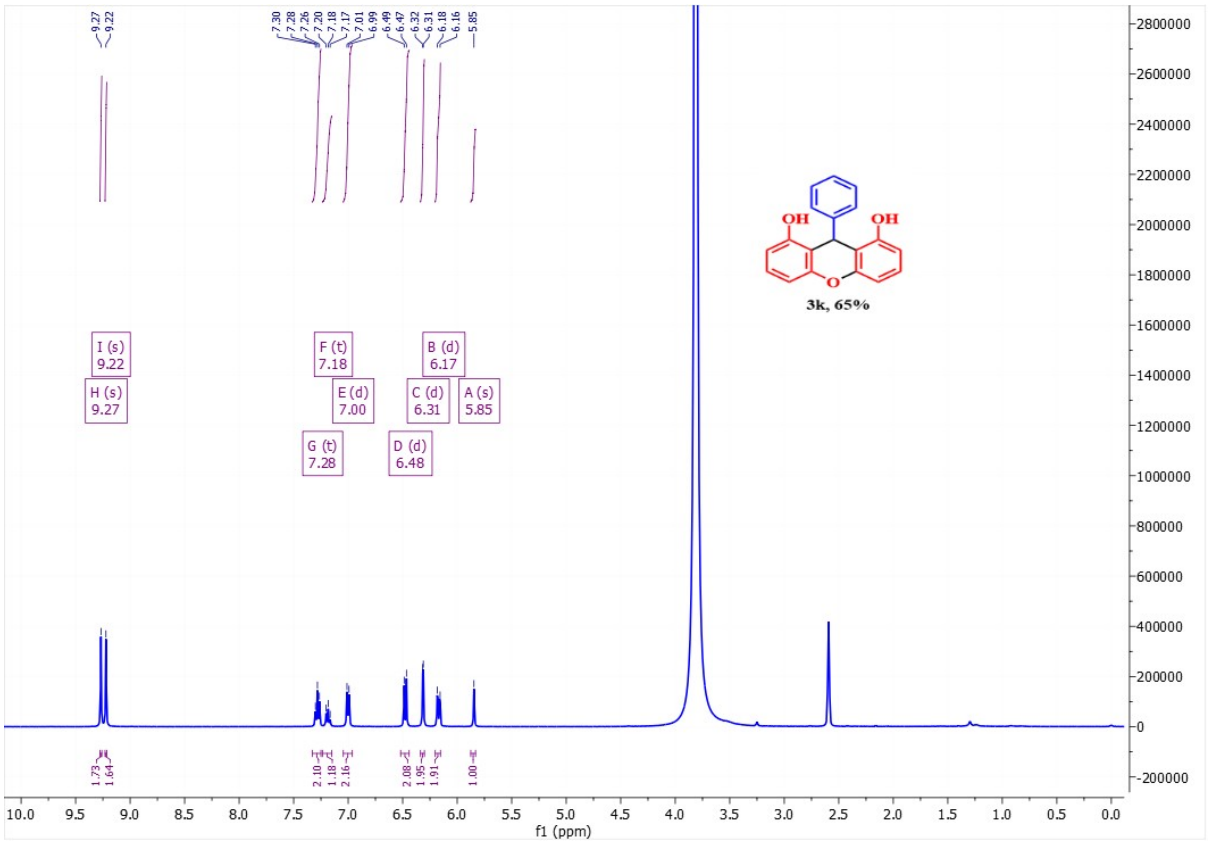
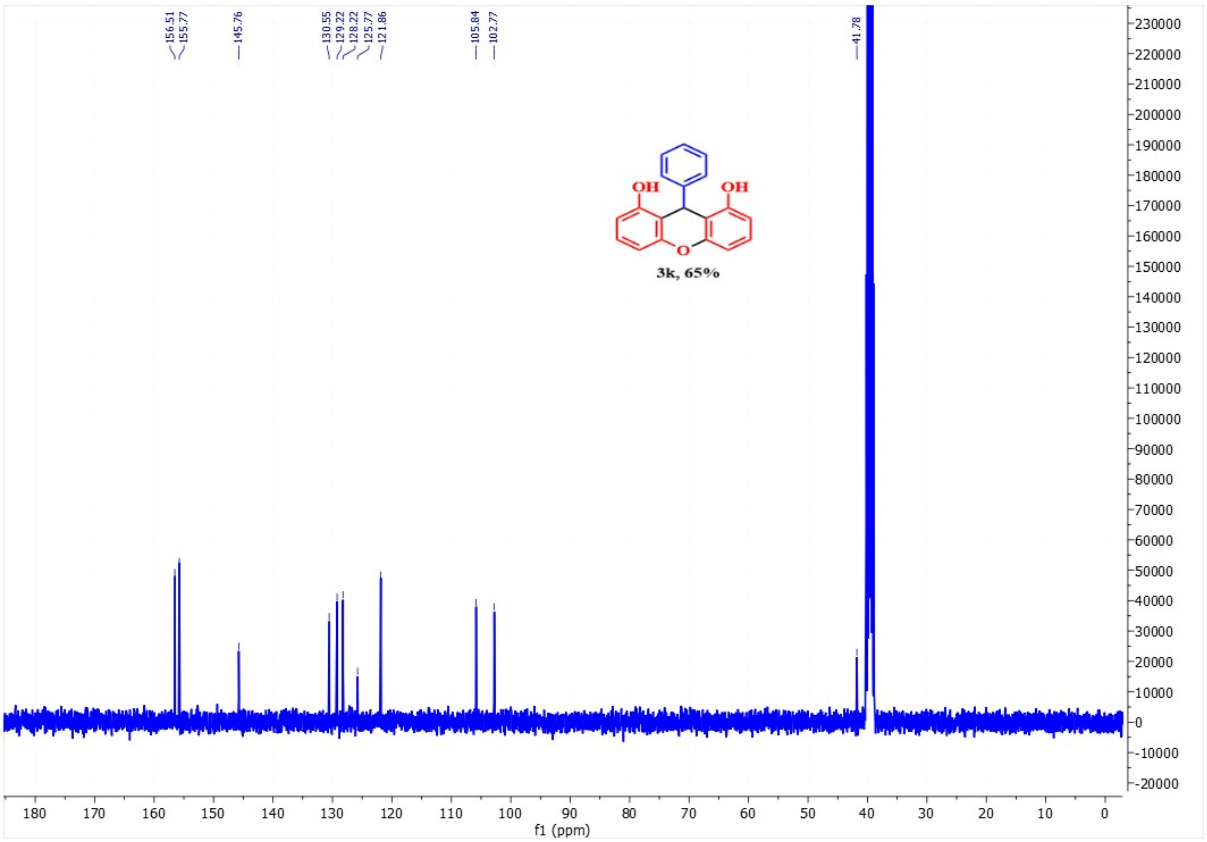


Figure S14: ^{1}H NMR, ^{13}C NMR and HRMS of *9-(3-bromophenyl)-3,3,6,6-tetramethyl-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione* (**3j**)


9.27
9.22
7.30
7.28
7.26
7.20
7.18
7.17
7.01
6.99
6.49
6.47
6.32
6.31
6.18
6.16
5.85
I (s) 9.22
H (s) 9.27
F (t) 7.18
E (d) 7.00
G (t) 7.28
B (d) 6.17
C (d) 6.31
A (s) 5.85
D (d) 6.48
OH
OH
O
3k, 65%
f1 (ppm)


156.51
155.77
145.76
130.55
129.22
128.22
125.77
121.86
105.84
102.77
41.78
OH
OH
O
3k, 65%
f1 (ppm)

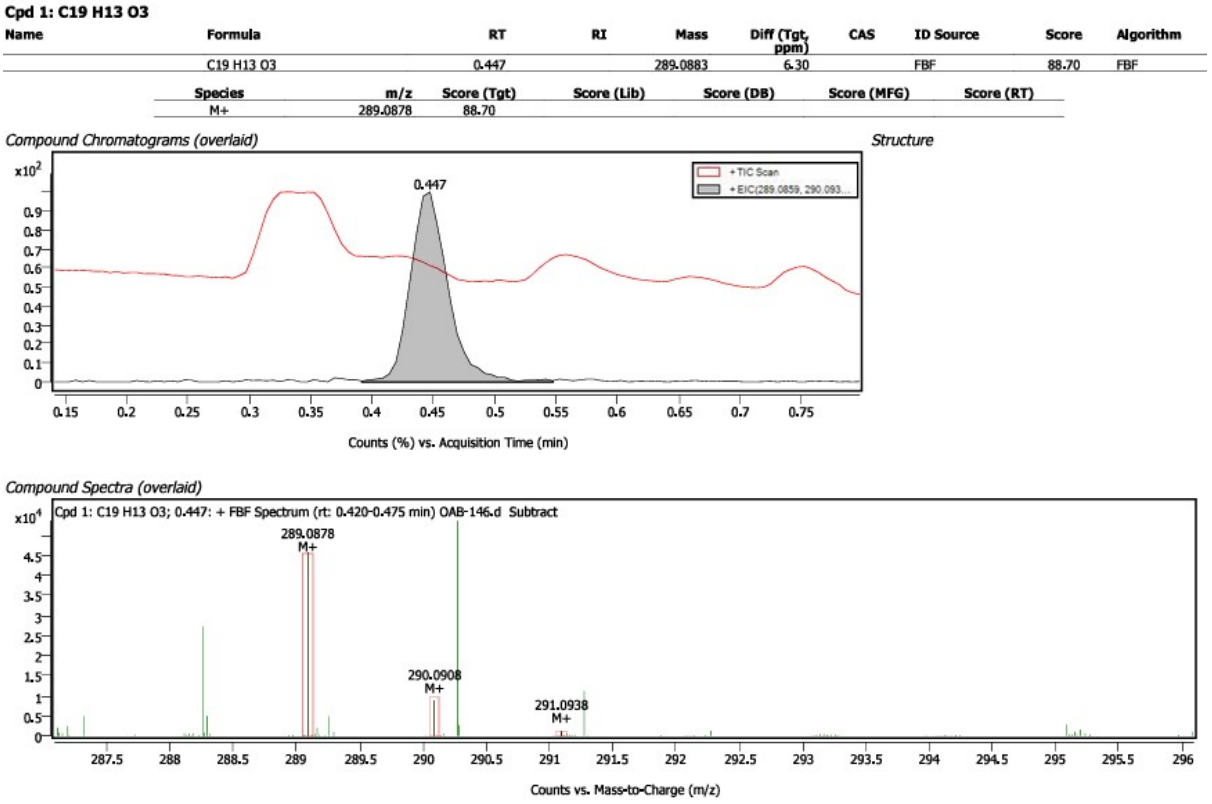
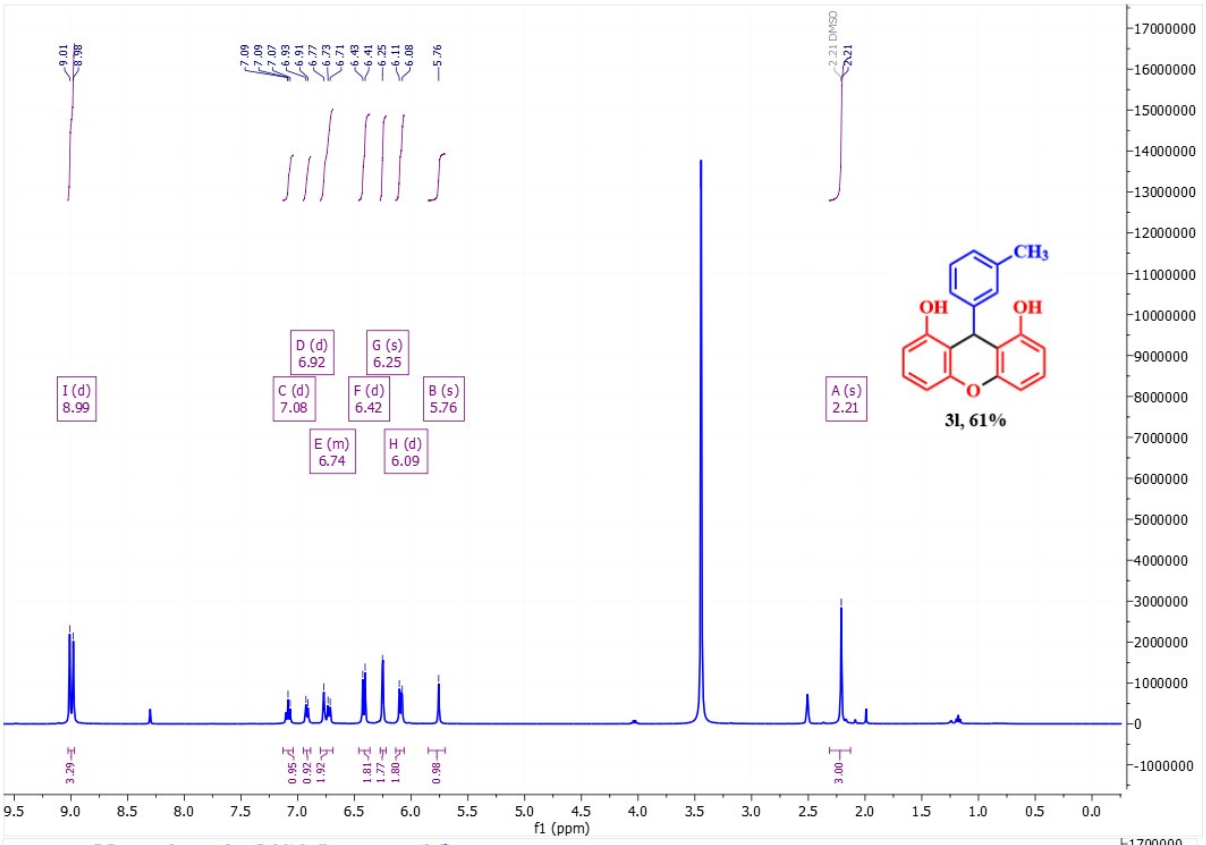
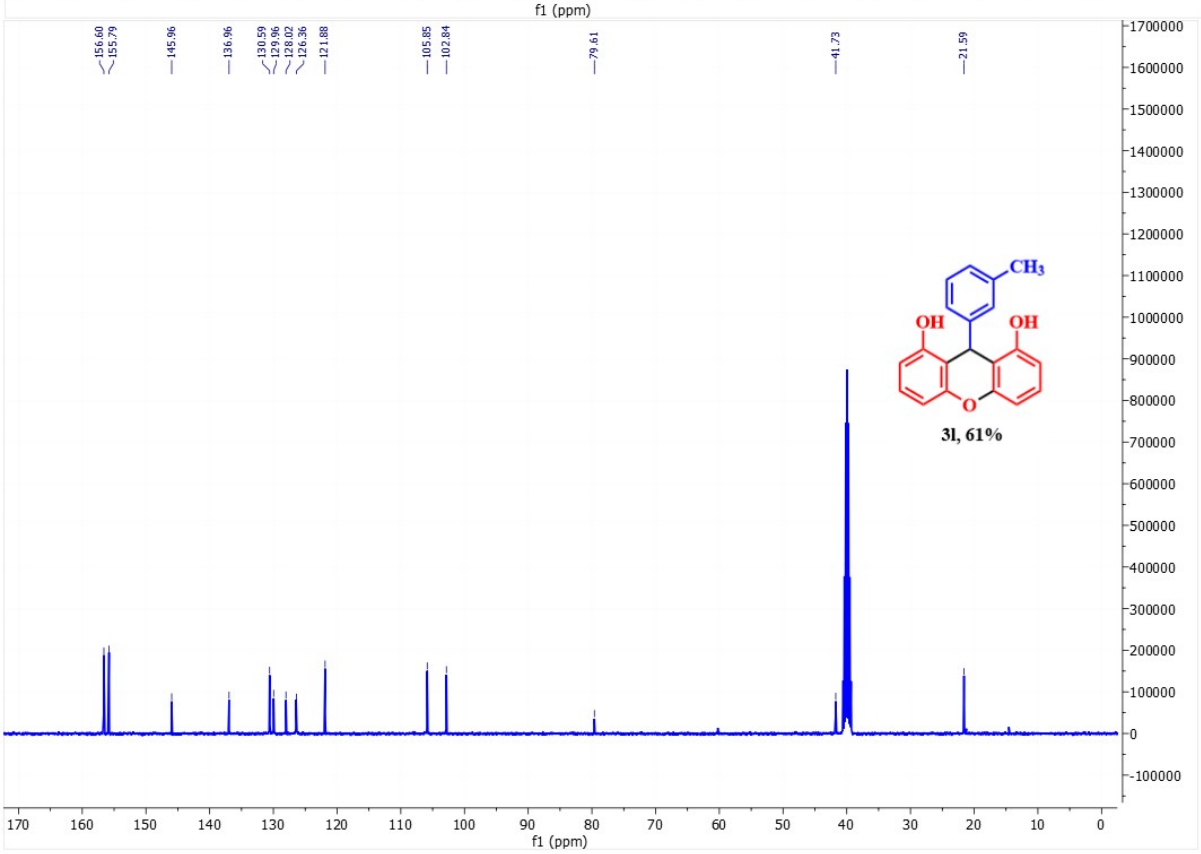


Figure S15: ^{1}H NMR, ^{13}C NMR and HRMS of 9-phenyl-9H-xanthene-1,8-diol (**5k**)


I (d) 8.99
C (d) 7.08
D (d) 6.92
E (m) 6.74
F (d) 6.42
G (s) 6.25
H (d) 6.09
B (s) 5.76
A (s) 2.21
CH3
OH
OH
O
3l, 61%
f1 (ppm)


CH3
OH
OH
O
3l, 61%
f1 (ppm)

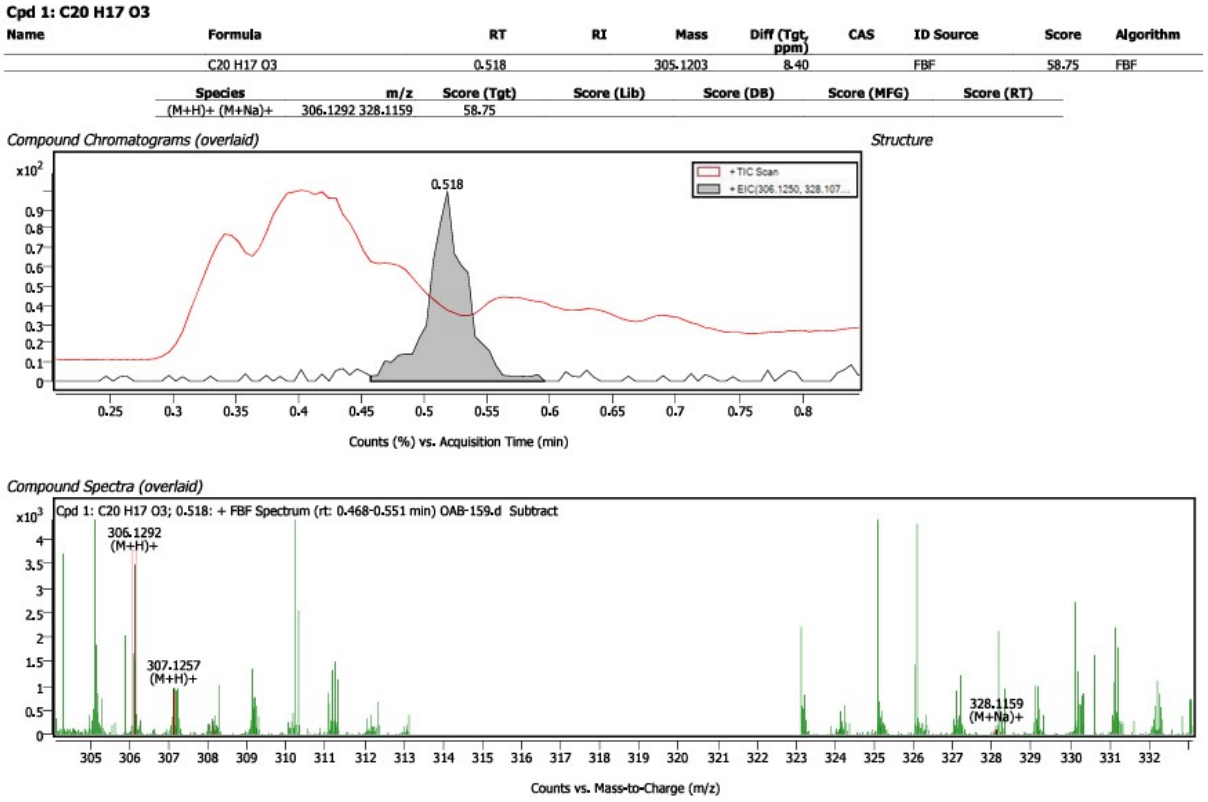
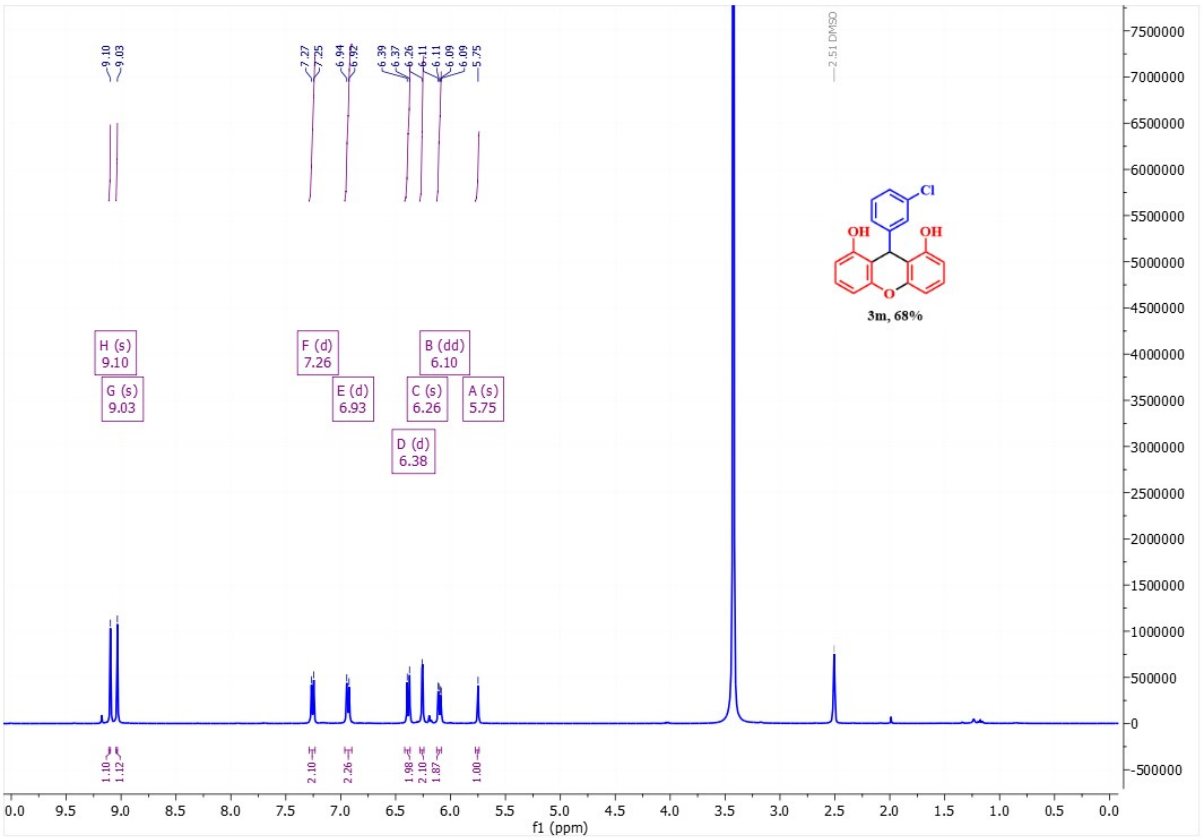
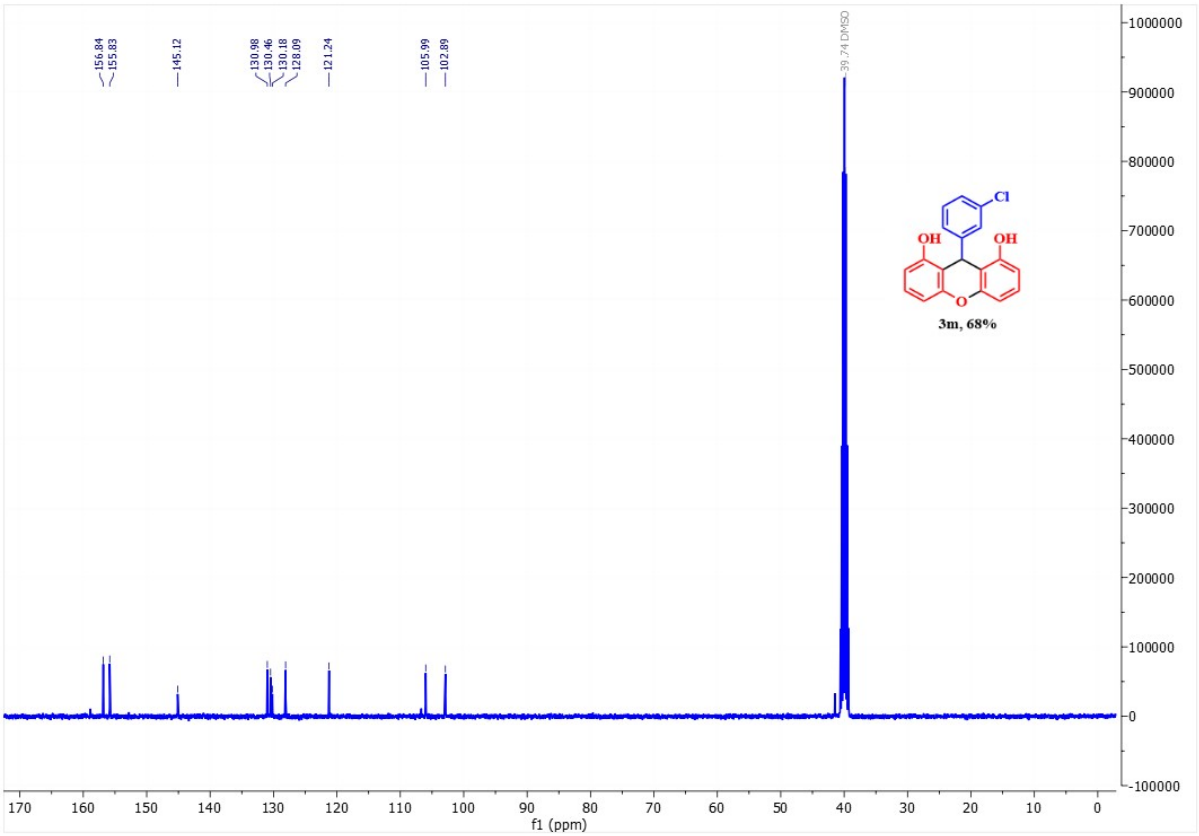


Figure S16: ^{1}H NMR, ^{13}C NMR and HRMS of 9-(m-tolyl)-9H-xanthene-1,8-diol (**5l**)





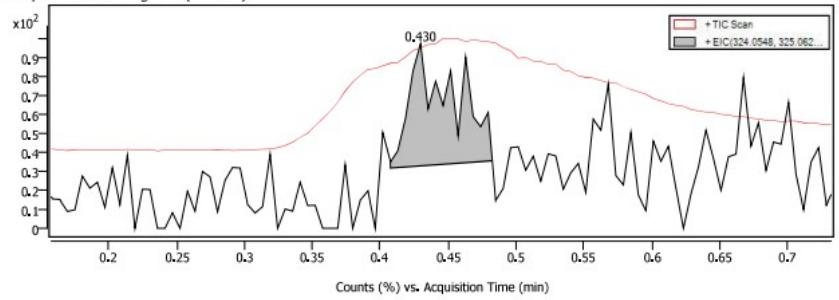
Cpd 1: C19 H13 Cl O3

Name	Formula	RT	RI	Mass	Diff (Tgt, ppm)	CAS	ID Source	Score	Algorithm
	C19 H13 Cl O3	0.430		324.0561	2.32		FBF	56.32	FBF

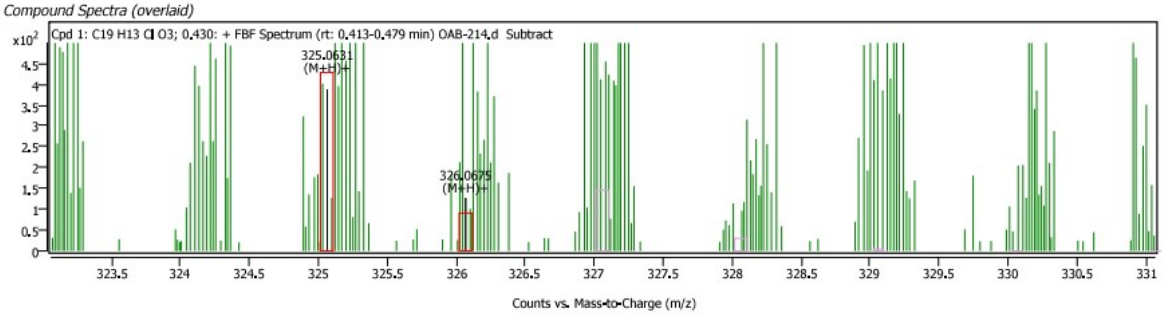
Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M+H)+	325.0631	56.32				

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Compound ID Table

Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
	C19 H13 Cl O3	(M+H)+	0.430		324.0561		FBF	56.32		56.32

Figure S17: ^{1}H NMR, ^{13}C NMR and HRMS of 9-(3-chlorophenyl)-9H-xanthene-1,8-diol (**5m**)

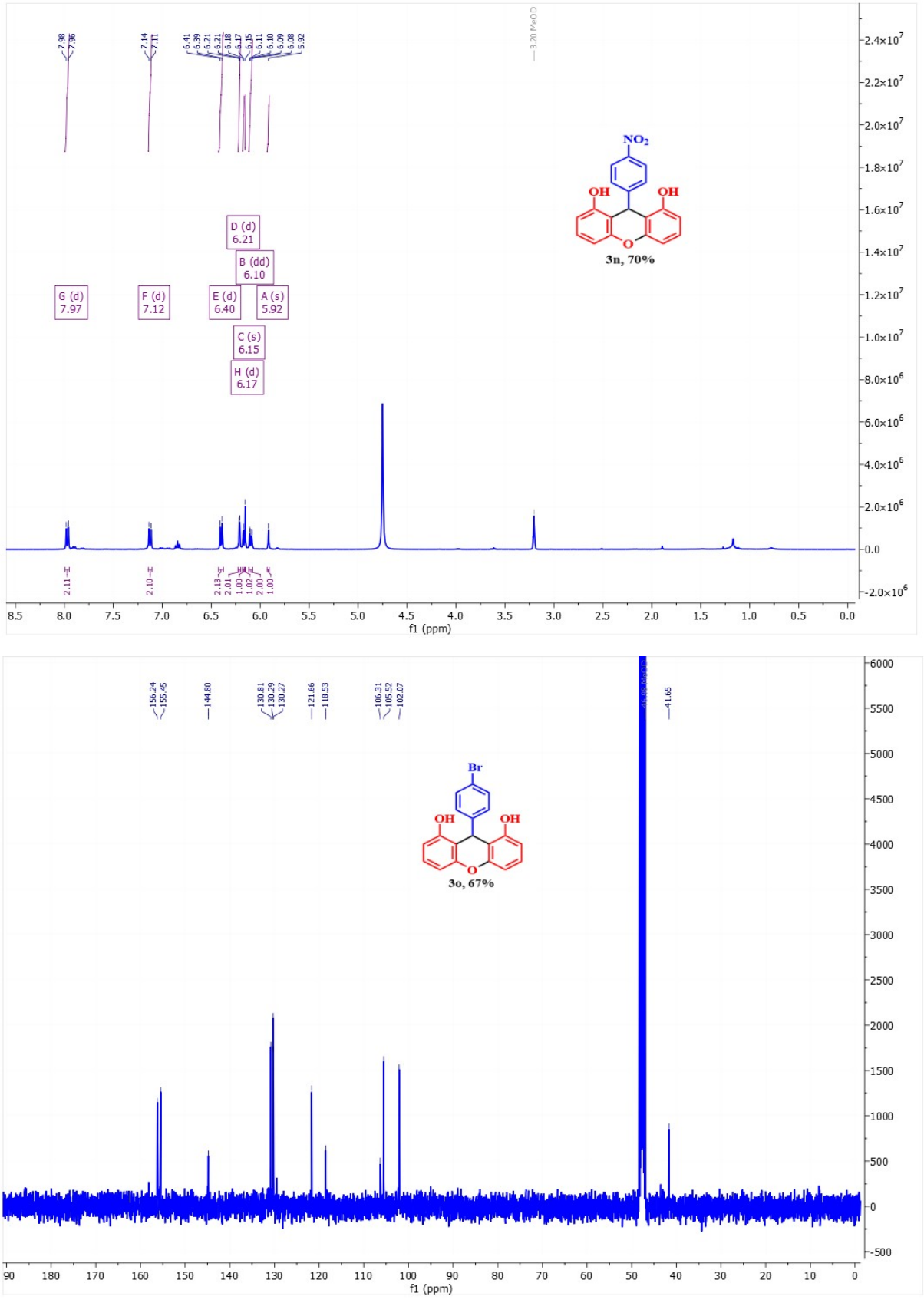
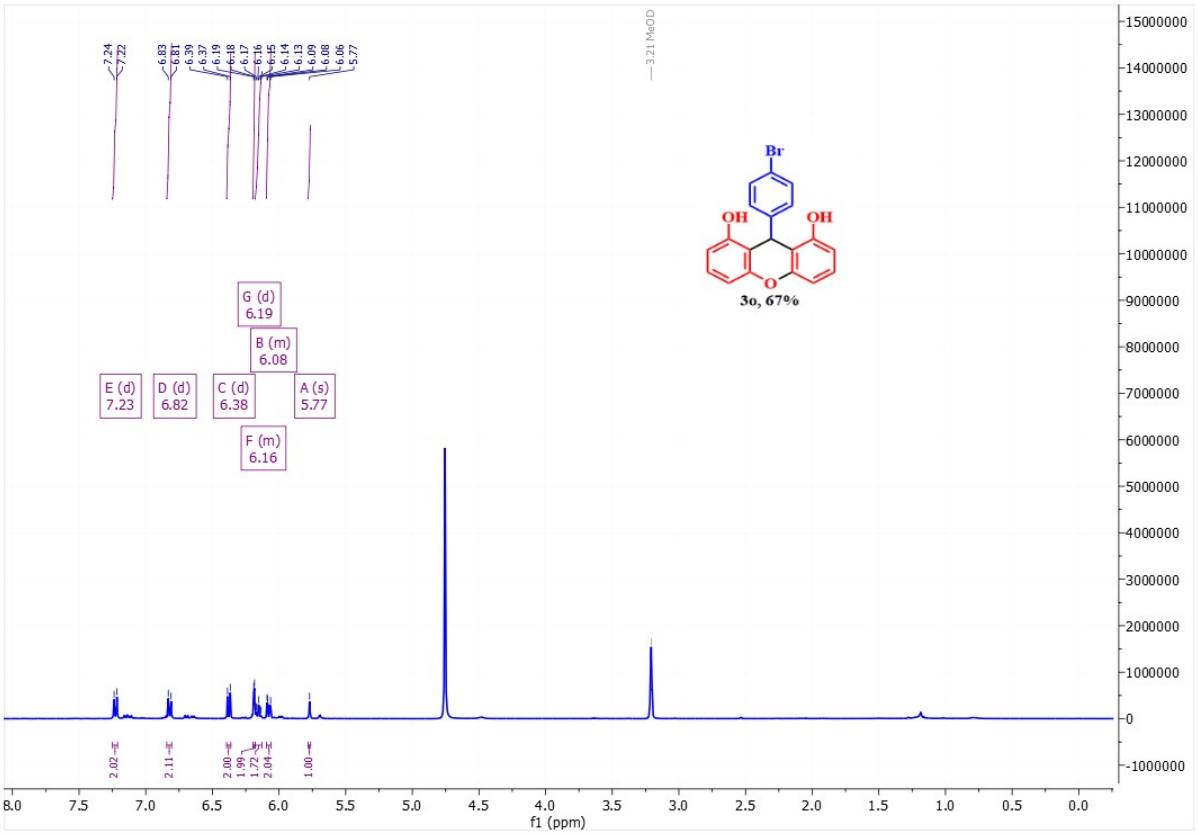


Figure S18: ^{1}H NMR, ^{13}C NMR and HRMS of 9-(4-bromophenyl)-9H-xanthene-1,8-diol (**5n**)


7.24
7.22
6.83
6.81
6.39
6.37
6.19
6.18
6.17
6.16
6.15
6.14
6.13
6.09
6.08
6.06
5.77
3.21 MeOD
Br
OH
OH
O
3o, 67%
G (d)
6.19
B (m)
6.08
E (d)
7.23
D (d)
6.82
C (d)
6.38
A (s)
5.77
F (m)
6.16
2.02
2.11
2.00
1.99
1.72
2.04
1.00
f1 (ppm)

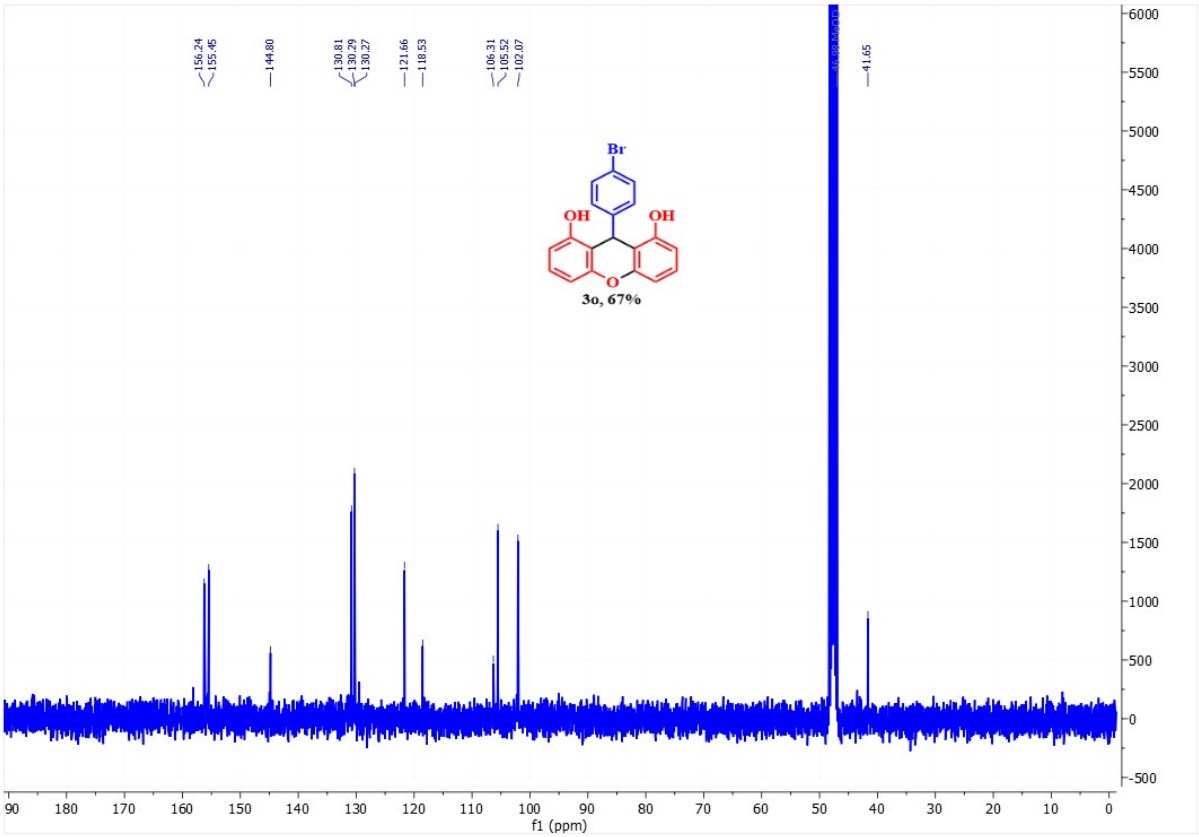

156.24
155.45
144.80
130.81
130.29
130.27
121.66
118.53
106.31
105.52
102.07
41.65
Br
OH
OH
O
3o, 67%
f1 (ppm)

Figure S19: ^{1}H NMR, ^{13}C NMR and HRMS of 9-(4-nitrophenyl)-9H-xanthene-1,8-diol (**5o**)