

Molecules

Supporting Information

1-Hydroxyanthraquinones containing aryl substituents as potent and selective anticancer agents

Nafisa S. Sirazhetdinova ¹, Victor A. Savelyev ¹, Tatyana S. Frolova ^{2,3},
Dmitry S. Baev ¹, Olga S. Oleshko ³, Teresa Sarojan ³, Lyubov S. Klimenko ⁴,
Ivan V. Chernikov ⁵, Andrey G. Pokrovskii ³, Elvira E. Shults ^{1*}

¹Laboratory of Medicinal Chemistry, N.N. Vorozhtsov Novosibirsk Institute of Organic Chemistry, Siberian Branch of the Russian Academy of Sciences, Lavrentyev Ave, 9, 630090 Novosibirsk, Russian Federation

²The Federal Research Center Institute of Cytology and Genetics, Acad. Lavrentyev Ave., 10, 630090, Novosibirsk, Russia

³Novosibirsk State University, Pirogova Str. 1, 630090 Novosibirsk, Russian Federation

⁴Yugra State University, 628012, Khanty-Mansiysk, Russian Federation

⁵ Institute of Chemical Biology and Fundamental Medicine Siberian Branch of the Russian Academy of Sciences, Lavrentyev Ave, 9, 630090 Novosibirsk, Russian Federation

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✉ Elvira E. Shults

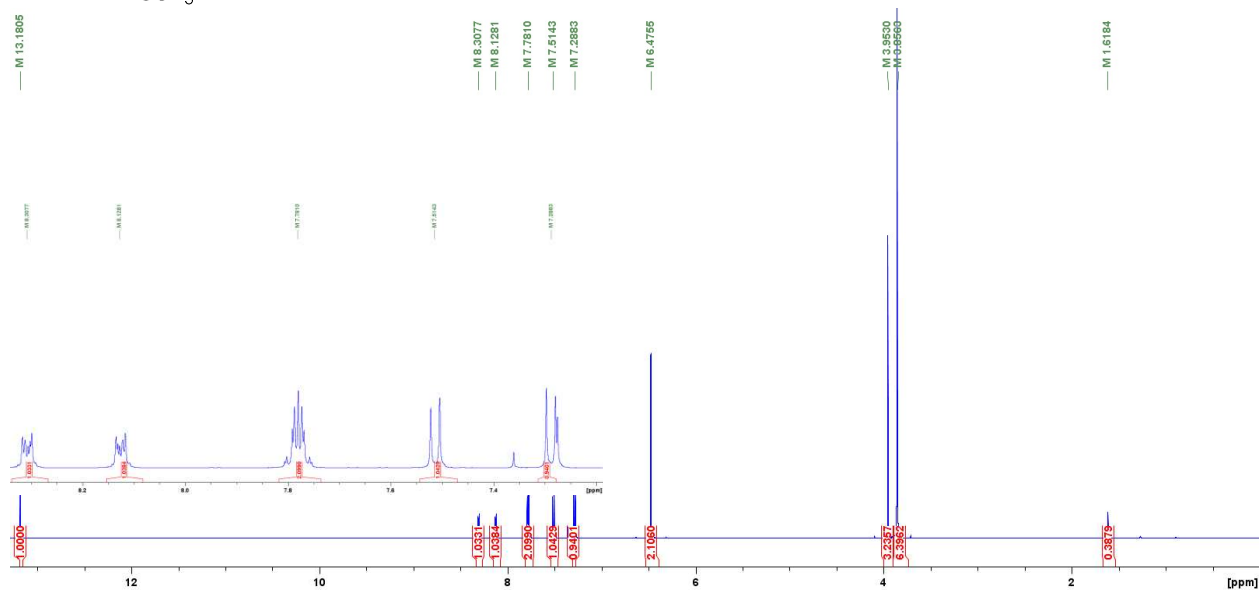
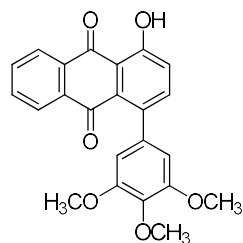
schultz@nioch.nsc.ru

¹ Laboratory of Medicinal Chemistry, Novosibirsk Institute of Organic Chemistry, Siberian Branch of the Russian Academy of Sciences, Lavrentyev Ave, 9, 630090 Novosibirsk, Russia;

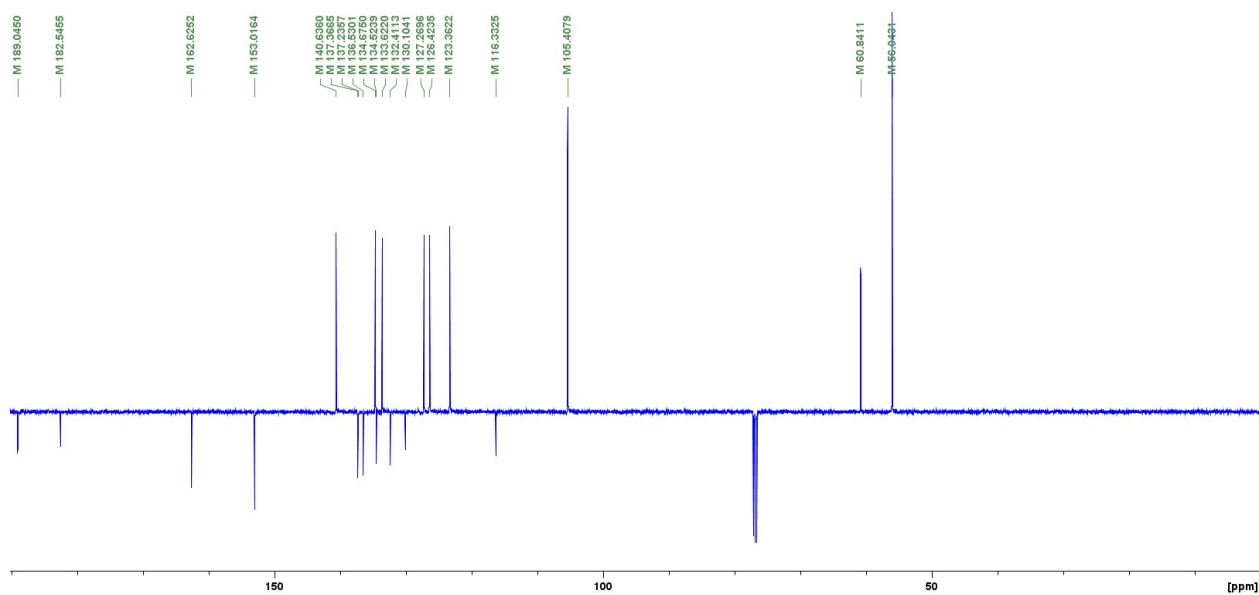
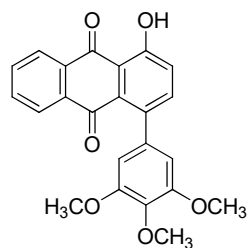
¹H and ¹³C NMR spectra

1-Hydroxy-4-(3,4,5-trimethoxyphenyl)anthracene-9,10-dione (5)

¹H NMR (CDCl₃, 500 MHz)

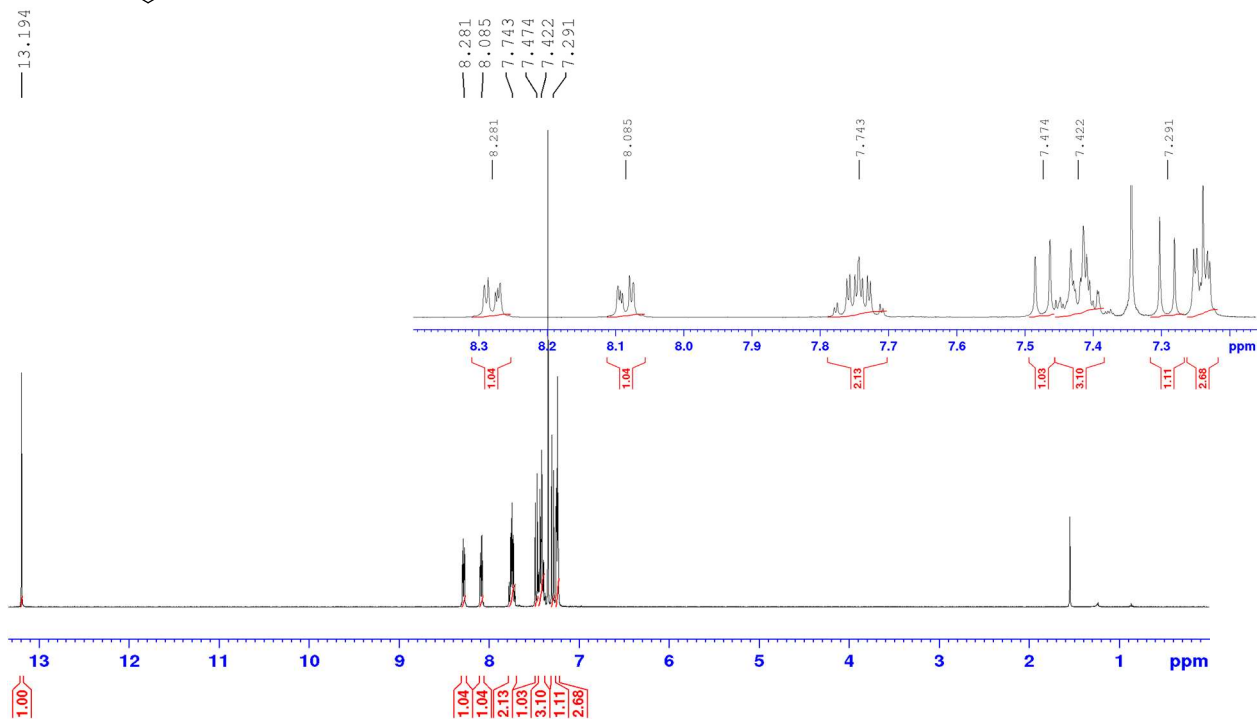
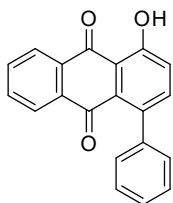


¹³C NMR (CDCl₃, 125 MHz)

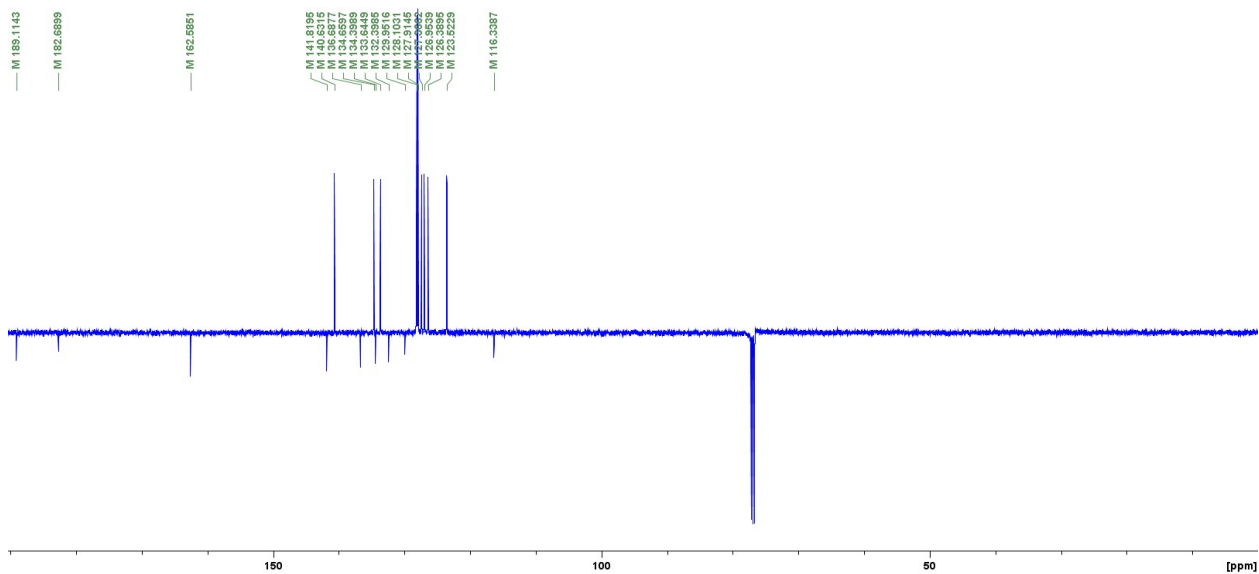
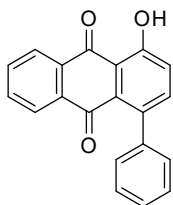


1-Hydroxy-4-phenylanthracene-9,10-dione (13)

^1H NMR (CDCl_3 , 400 MHz)

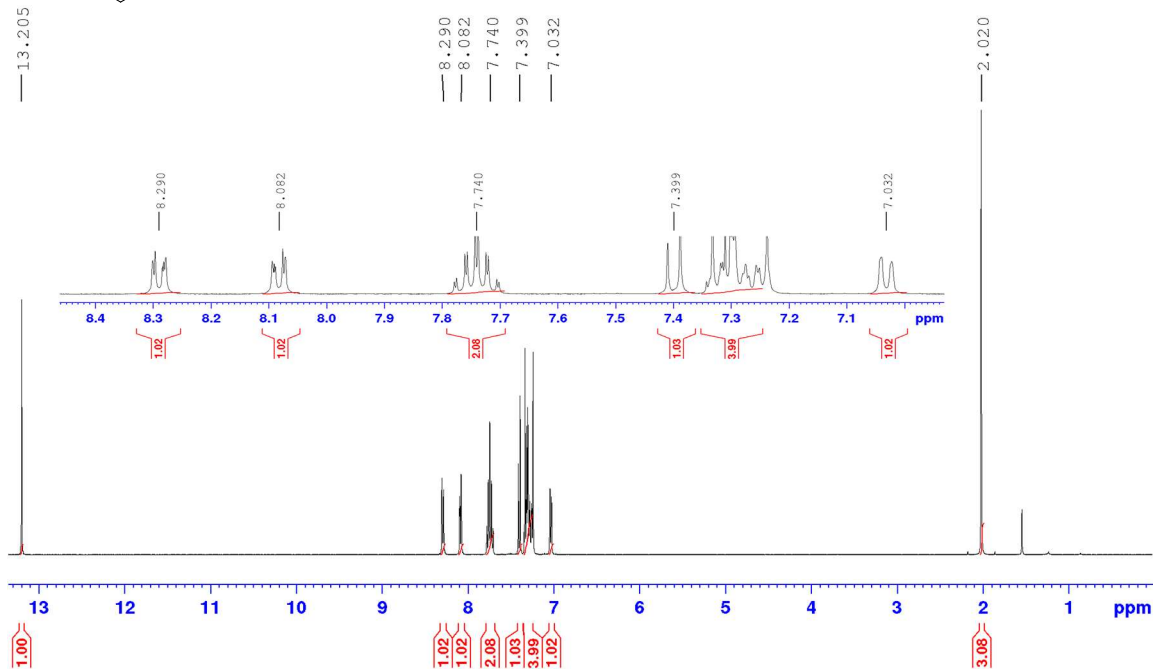
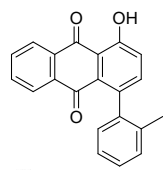


^{13}C NMR (CDCl_3 , 125 MHz)

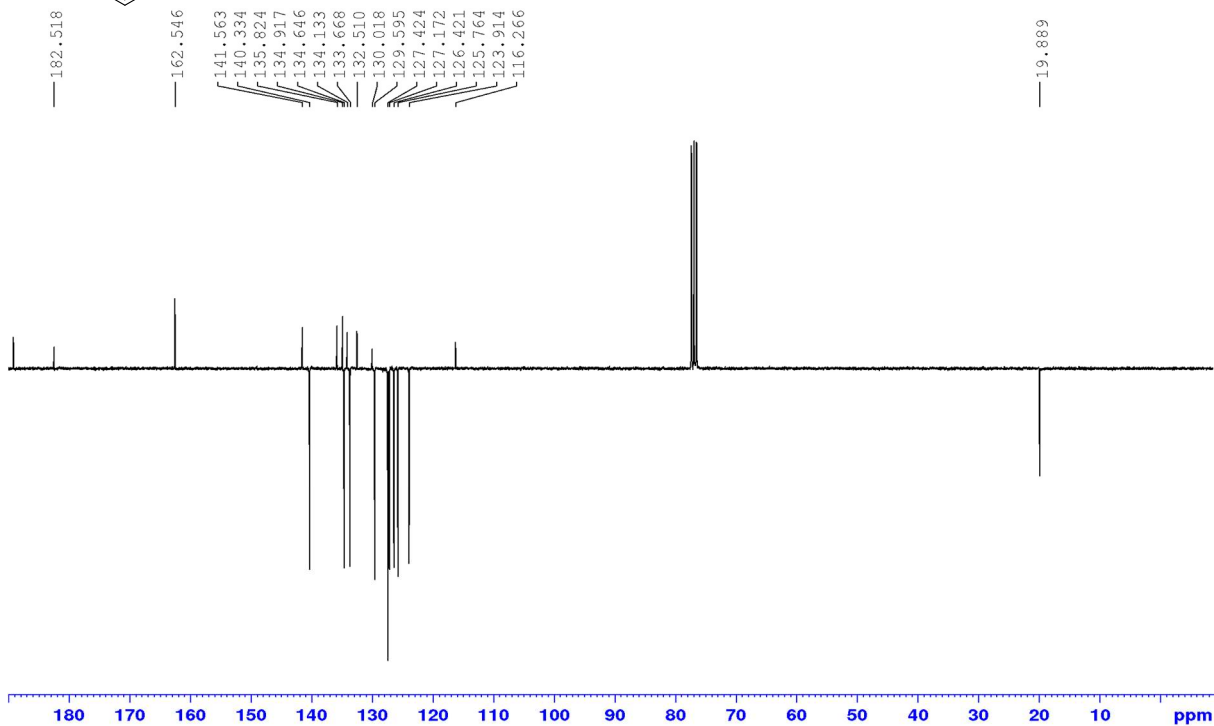
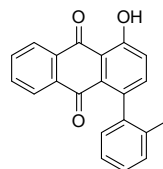


1-Hydroxy-4-(o-tolyl)anthracene-9,10-dione (14)

^1H NMR (CDCl_3 , 400 MHz)

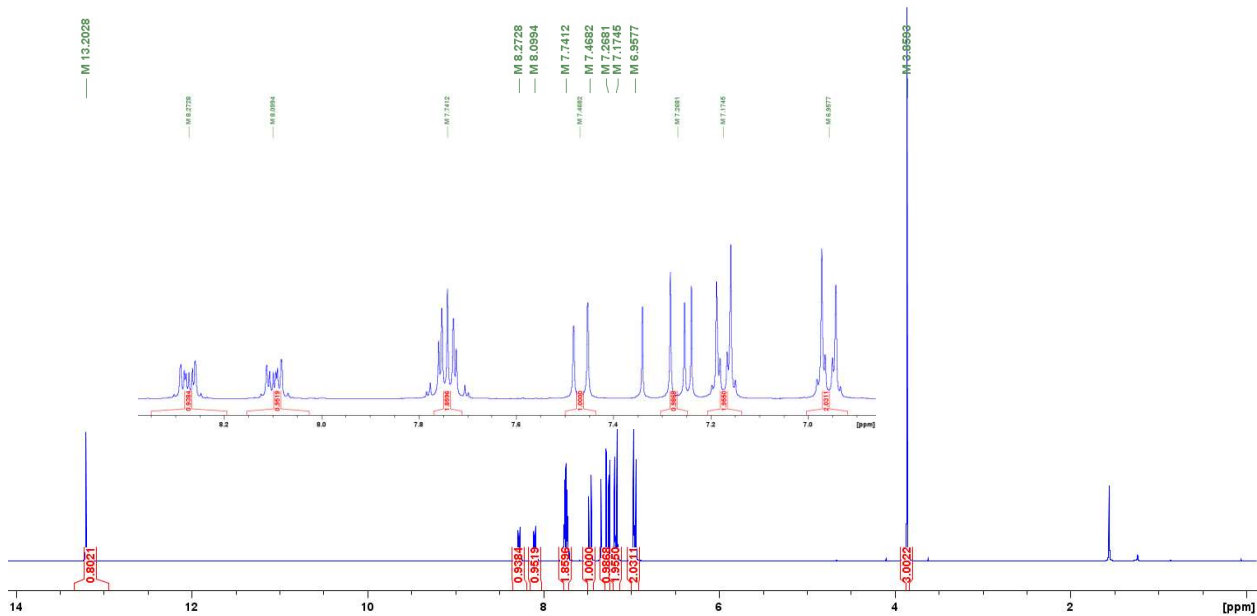
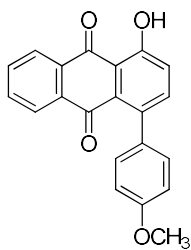


^{13}C NMR (CDCl_3 , 75 MHz)

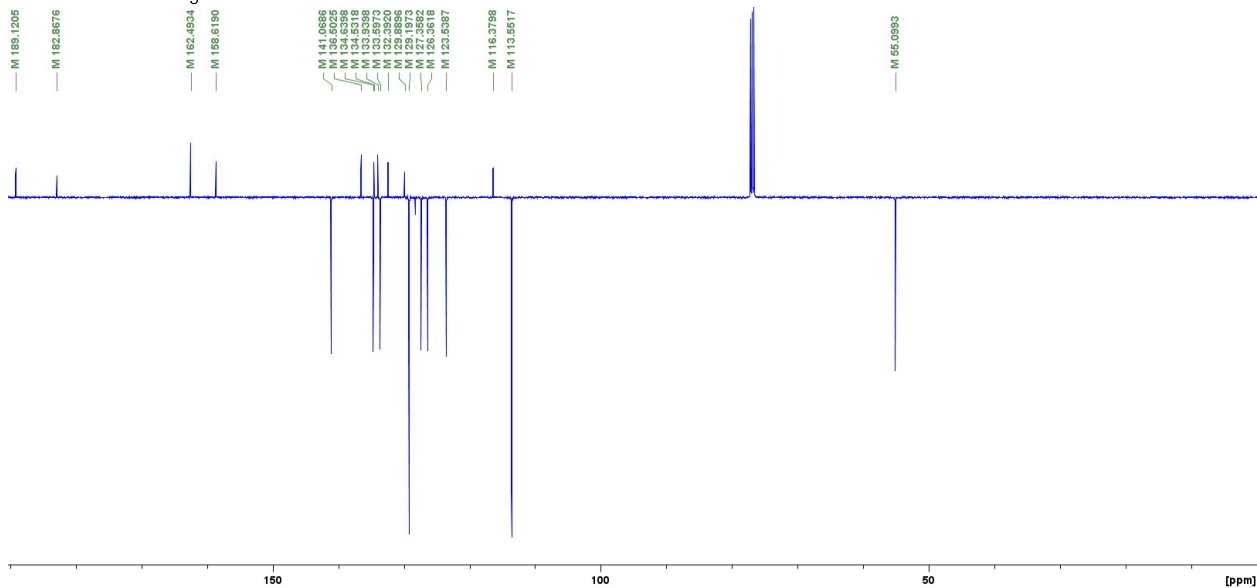
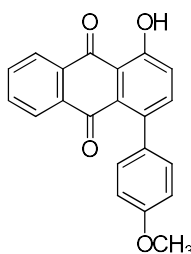


1-Hydroxy-4-(4-methoxyphenyl)anthracene-9,10-dione (15)

¹H NMR (CDCl₃, 300 MHz)

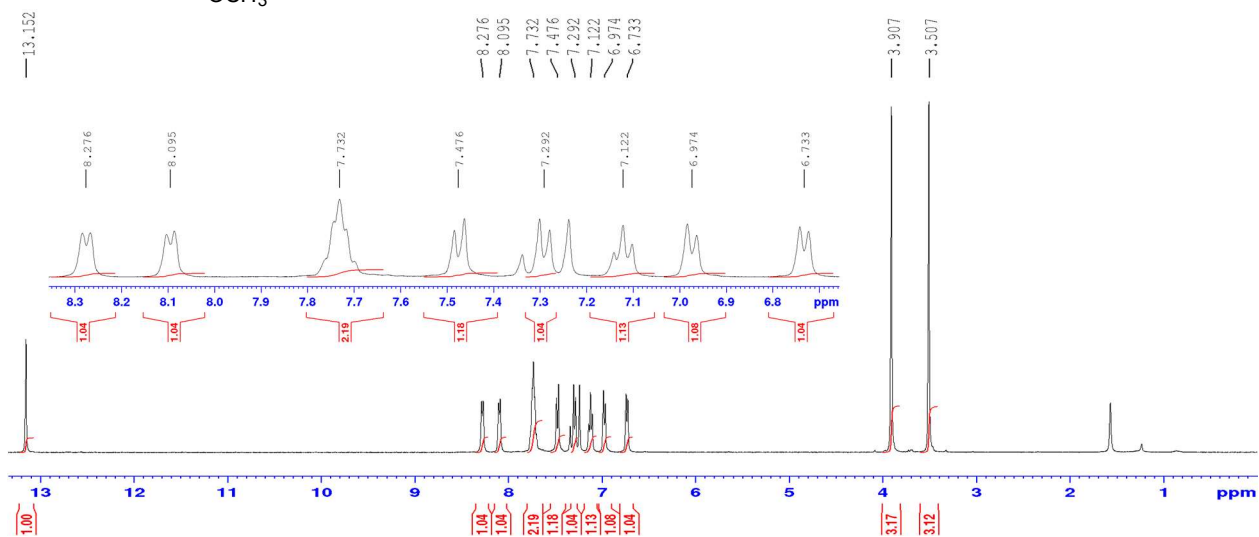
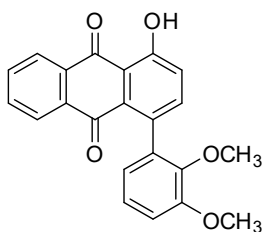


¹³C NMR (CDCl₃, 125 MHz)

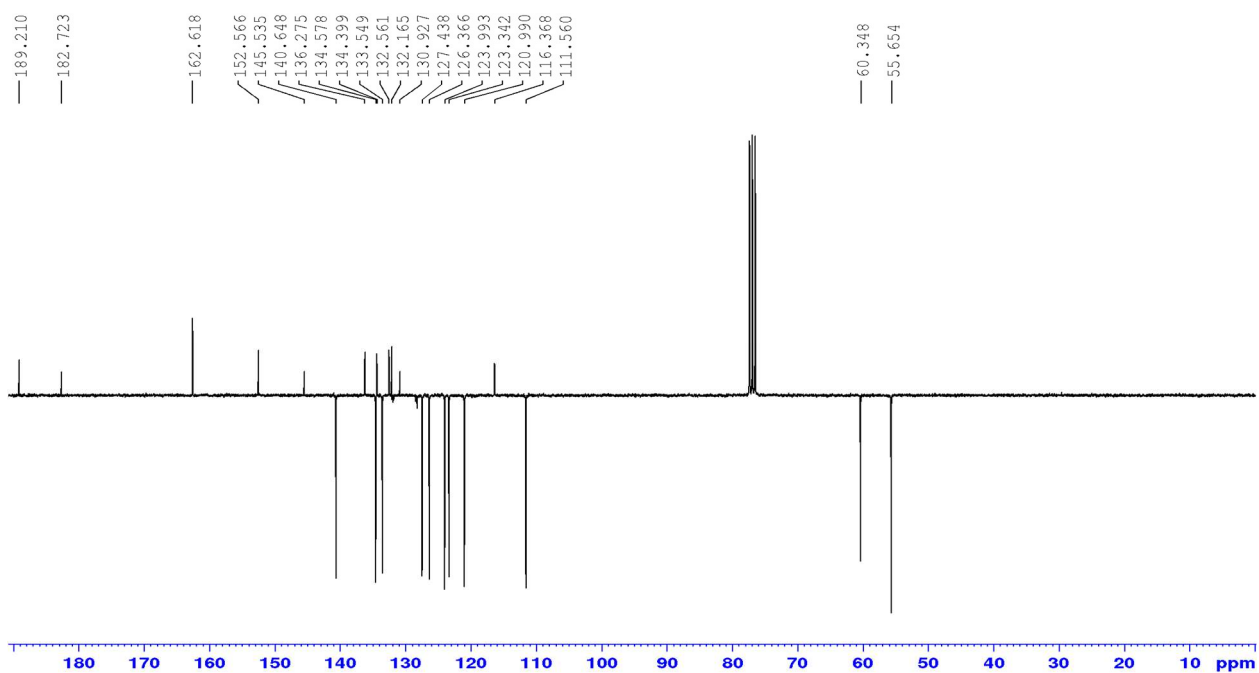


1-(2,3-Dimethoxyphenyl)-4-hydroxyanthracene-9,10-dione (16)

¹H NMR (CDCl₃, 400 MHz)

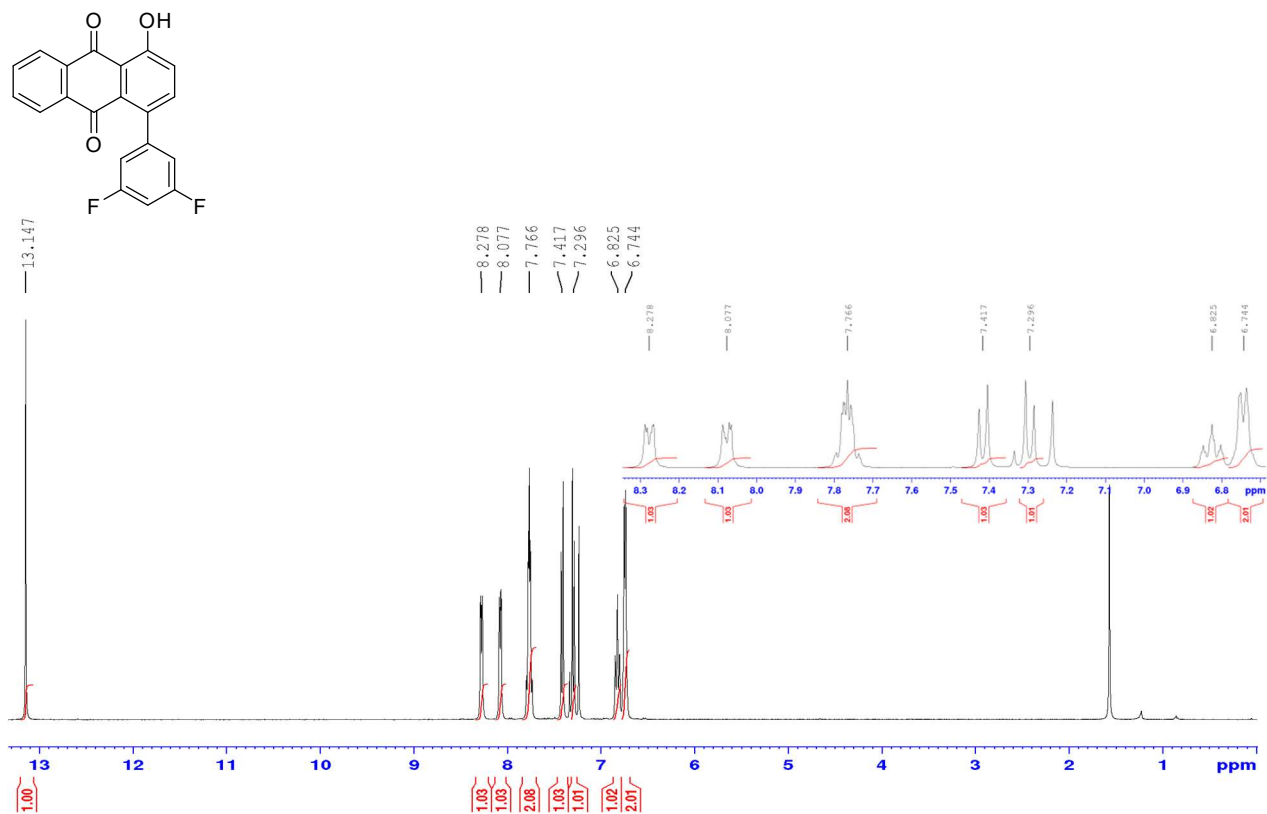


¹³C NMR (CDCl₃, 75 MHz)

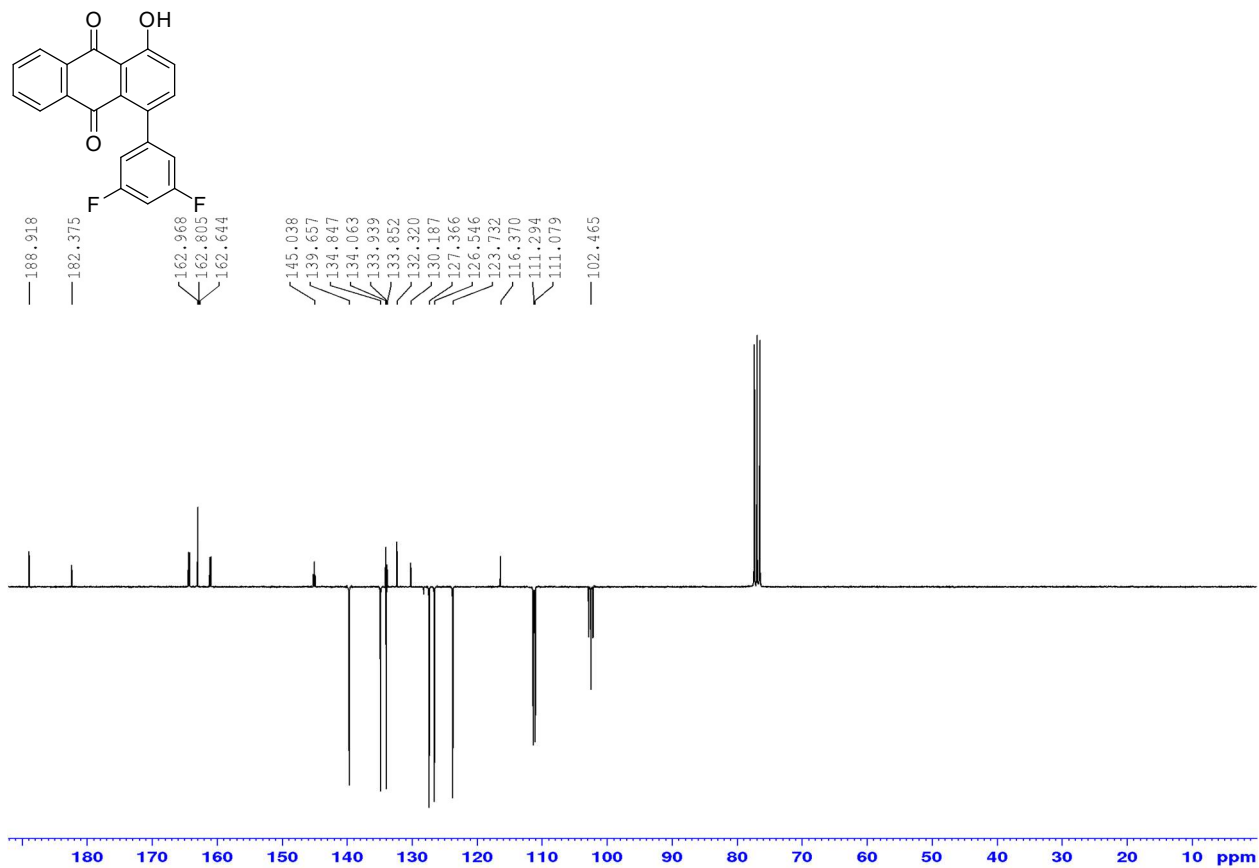


1-(3,5-Difluorophenyl)-4-hydroxyanthracene-9,10-dione (17)

^1H NMR (CDCl_3 , 400 MHz)

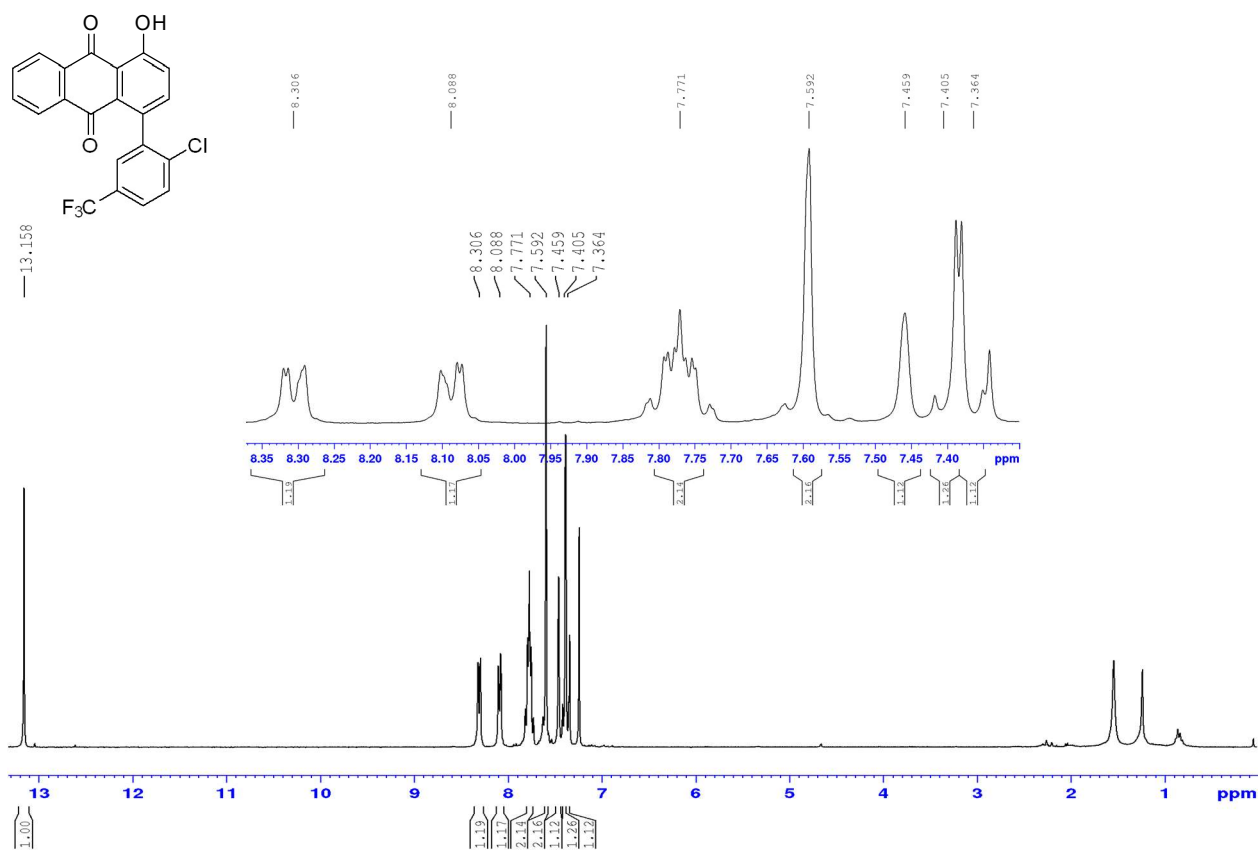


^{13}C NMR (CDCl_3 , 75 MHz)

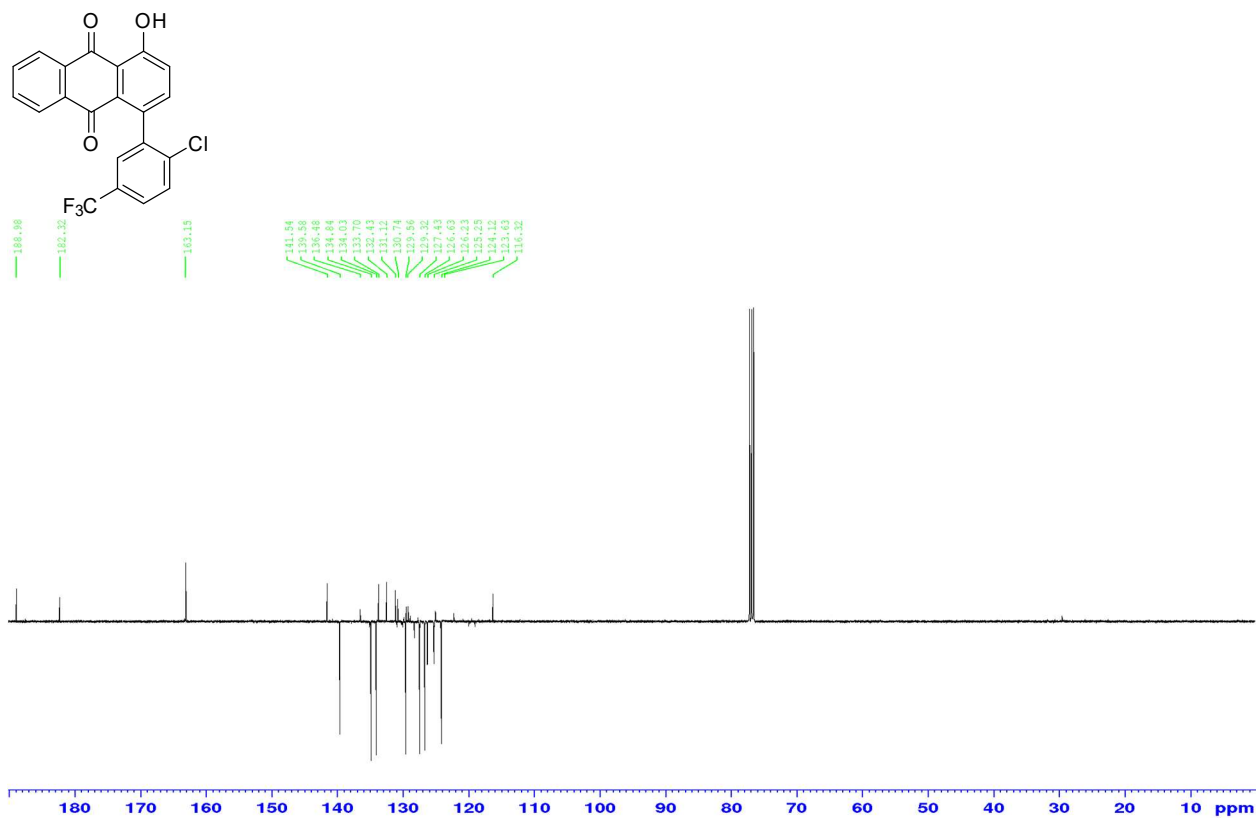


1-(2-Chloro-5-(trifluoromethyl)phenyl)-4-hydroxyanthracene-9,10-dione (18)

$^1\text{H NMR}$ (CDCl_3 , 300 MHz)

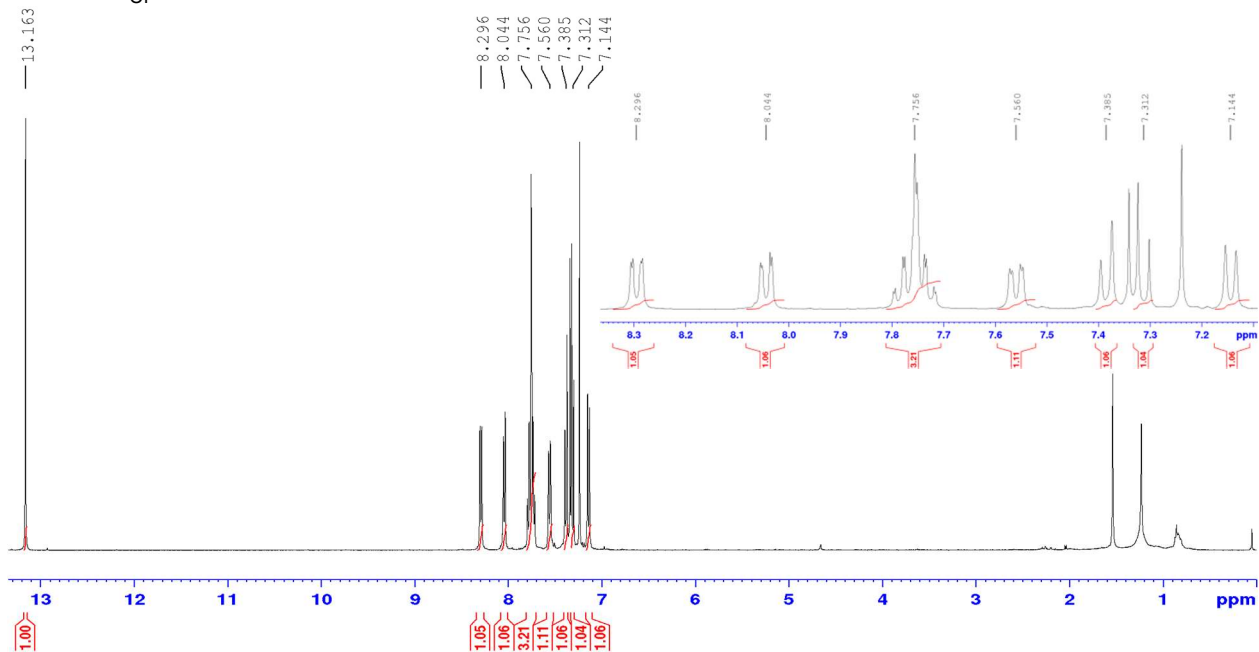
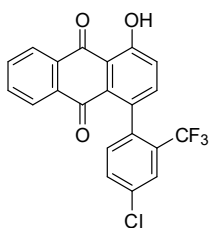


$^{13}\text{C NMR}$ (CDCl_3 , 100 MHz)

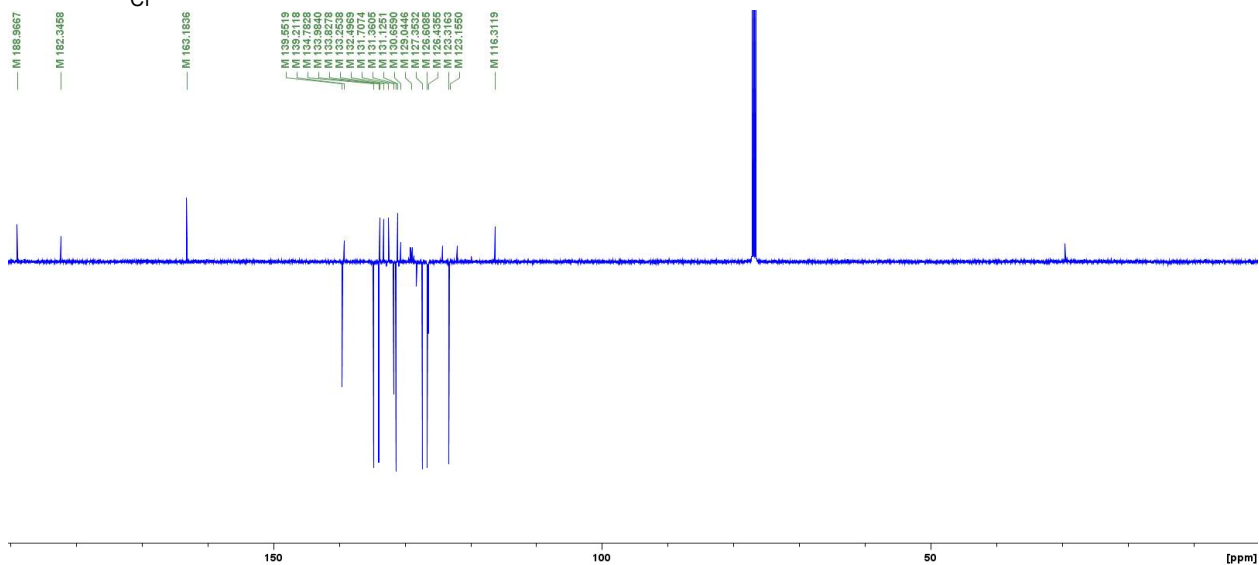
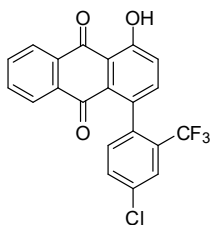


1-(4-Chloro-2-(trifluoromethyl)phenyl)-4-hydroxyanthracene-9,10-dione (19)

^1H NMR (CDCl_3 , 400 MHz)

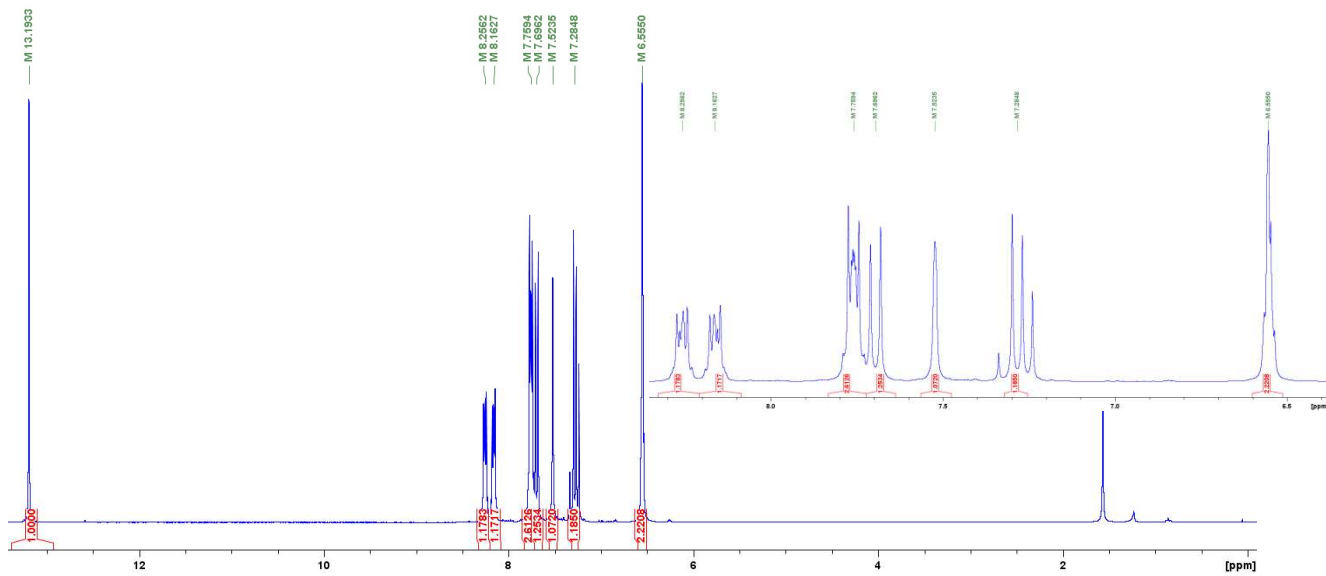
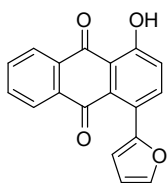


^{13}C NMR (CDCl_3 , 125 MHz)

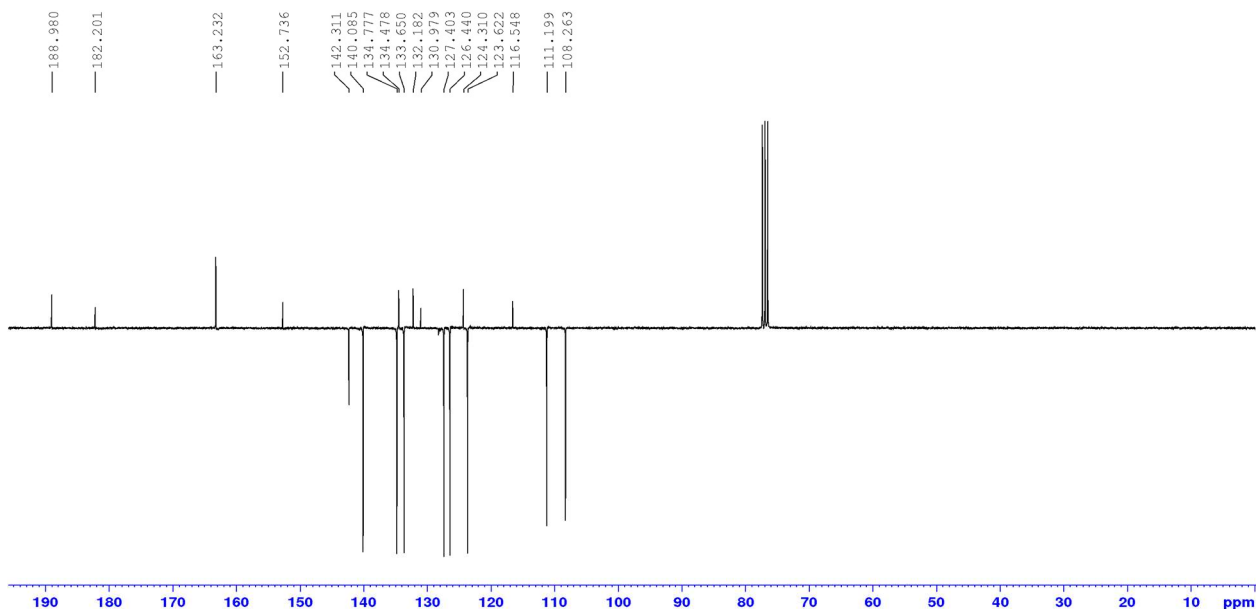


1-(Furan-2-yl)-4-hydroxyanthracene-9,10-dione (22)

^1H NMR (CDCl_3 , 300 MHz)

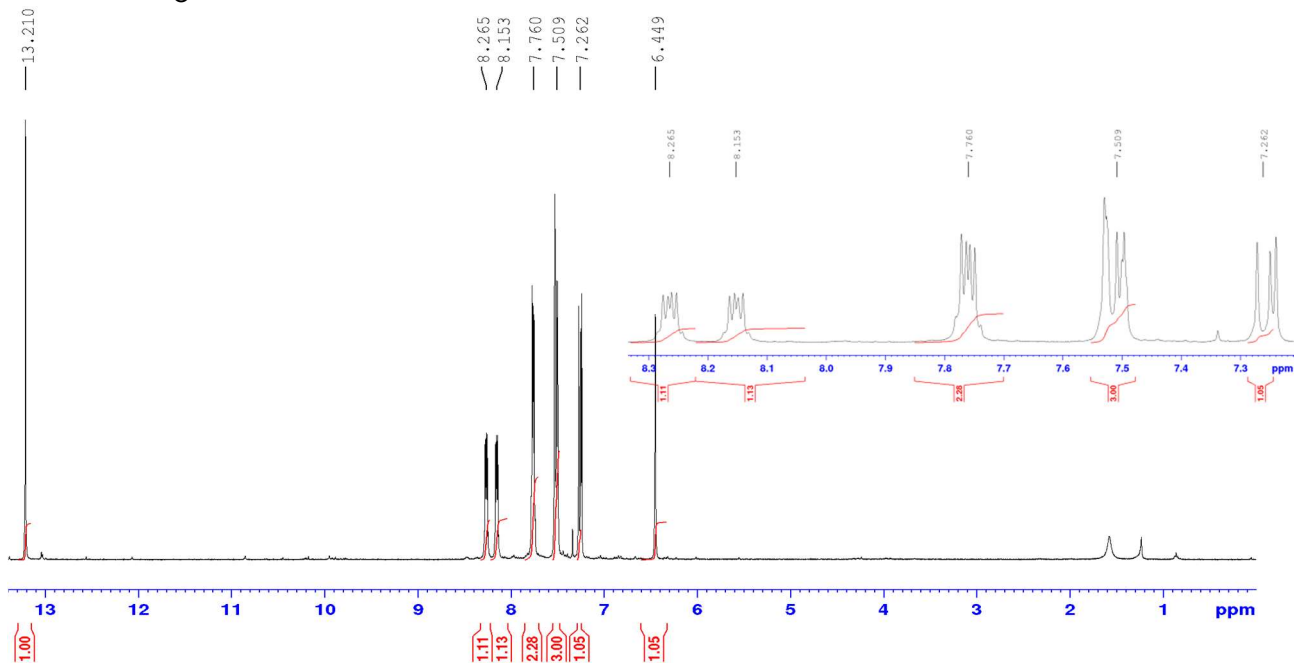
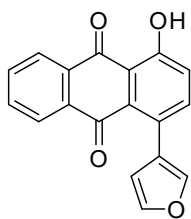


^{13}C NMR (CDCl_3 , 75 MHz)

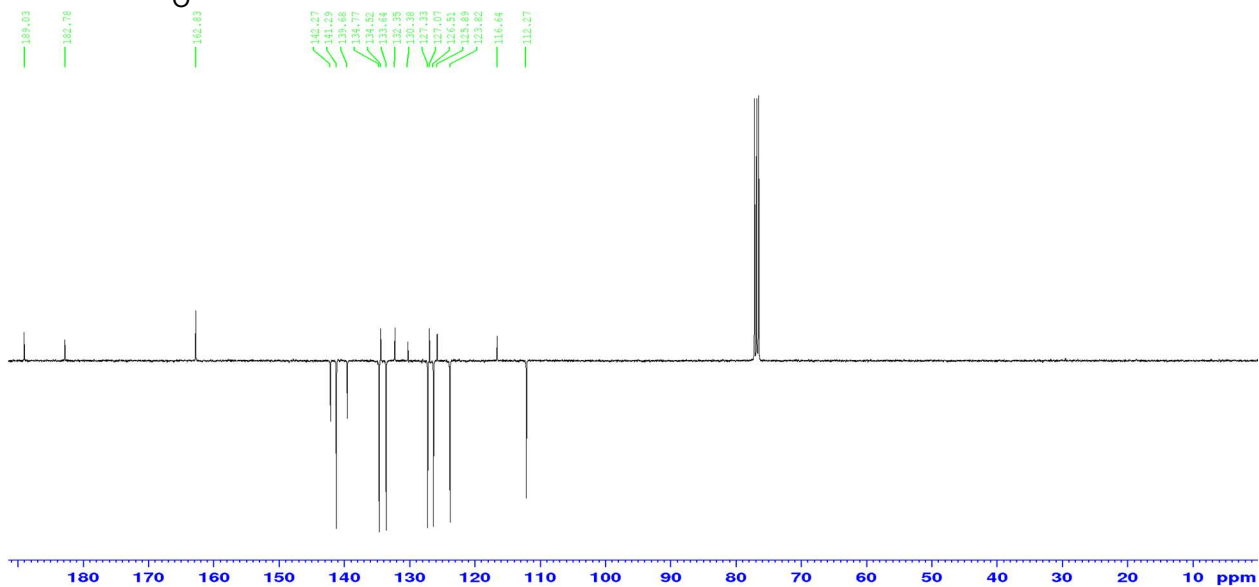
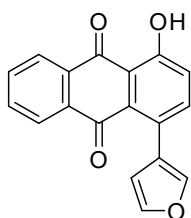


1-(Furan-3-yl)-4-hydroxyanthracene-9,10-dione (23)

¹H NMR (CDCl₃, 400 MHz)

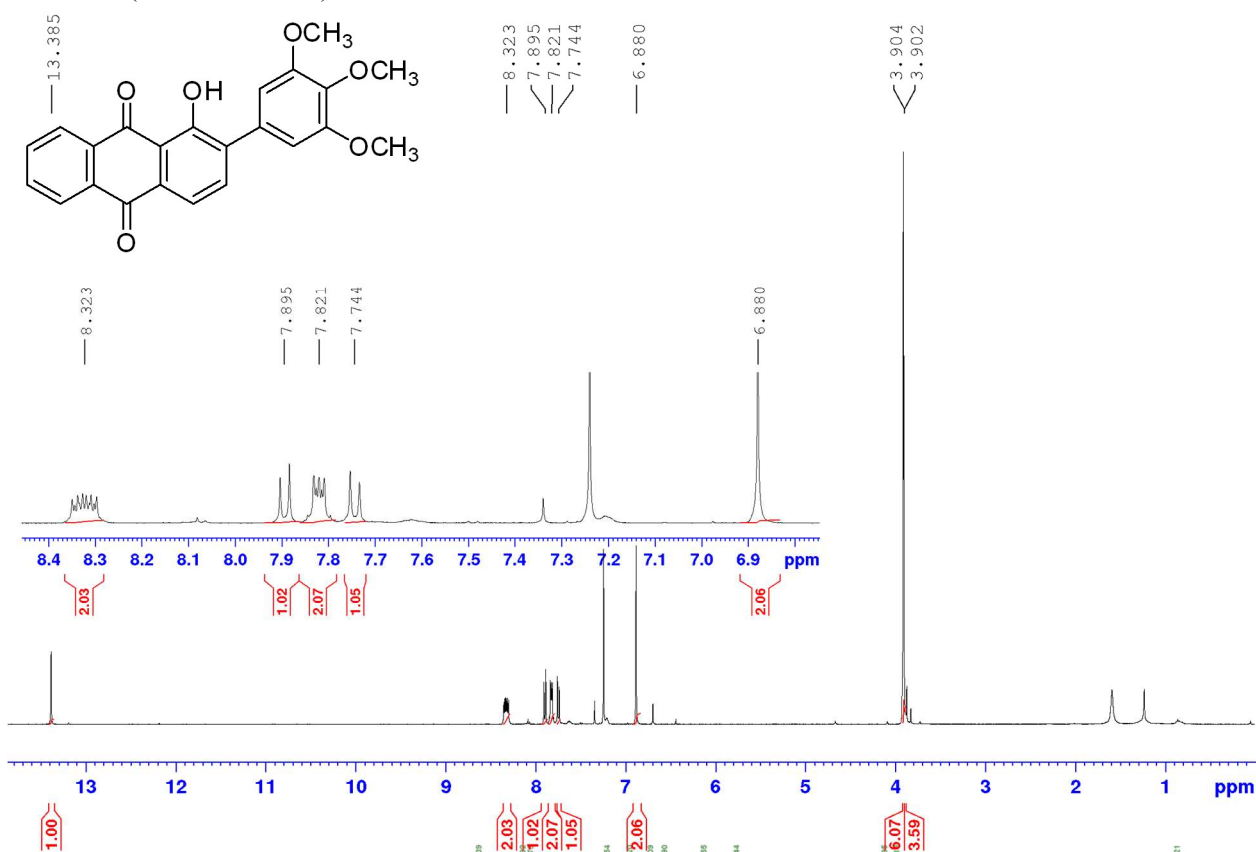


¹³C NMR (CDCl₃, 100 MHz)

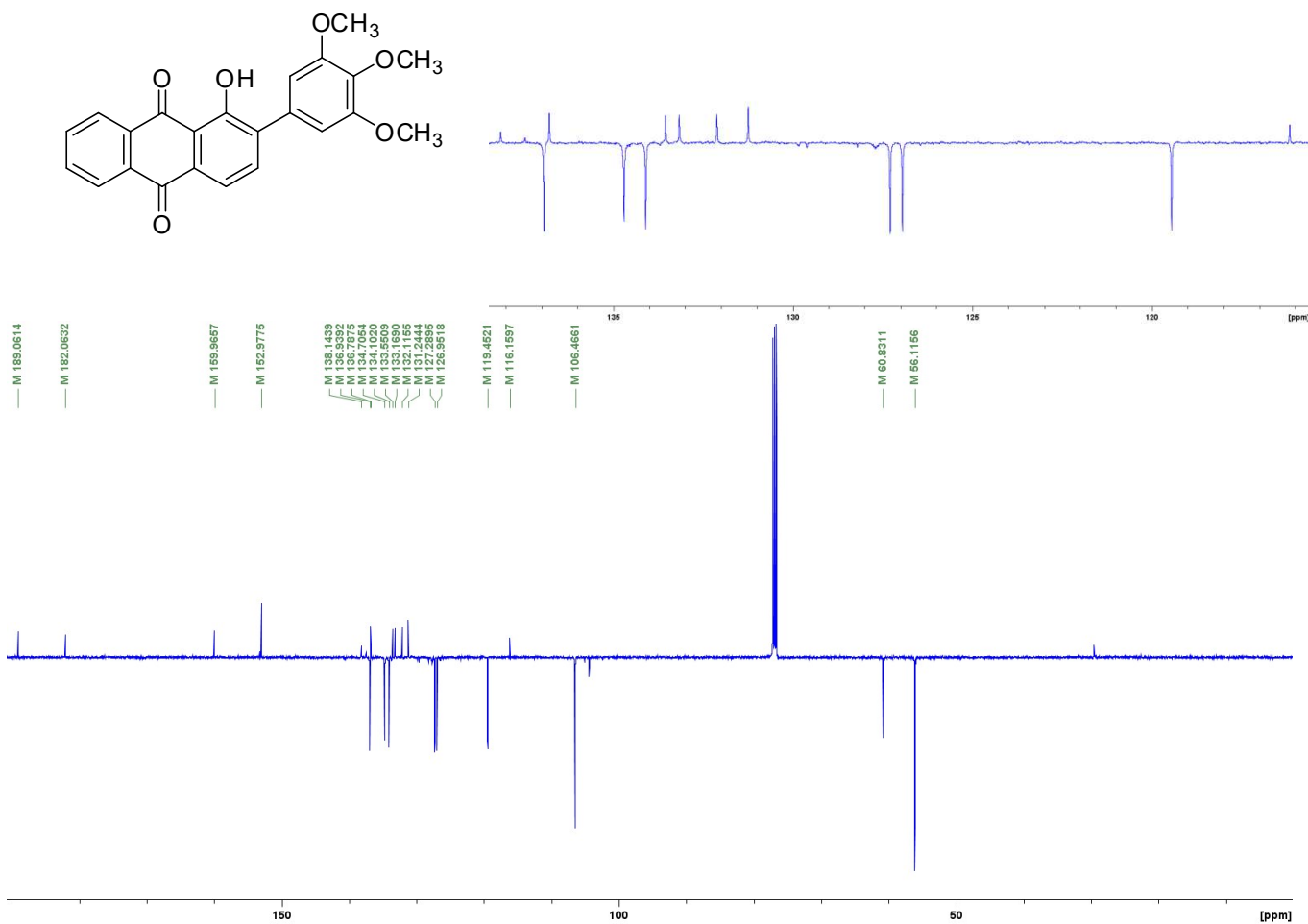


1-Hydroxy-2-(3,4,5-trimethoxyphenyl)anthracene-9,10-dione (24)

¹H NMR (CDCl₃, 400 MHz)

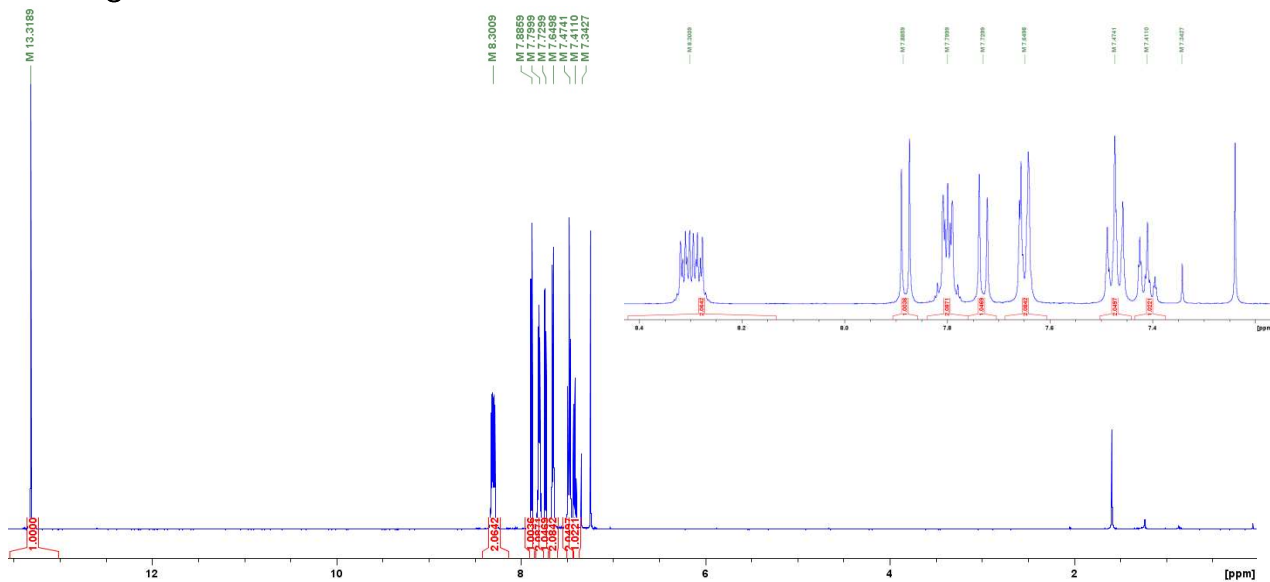
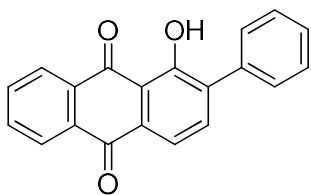


¹³C NMR (CDCl₃, 125 MHz)

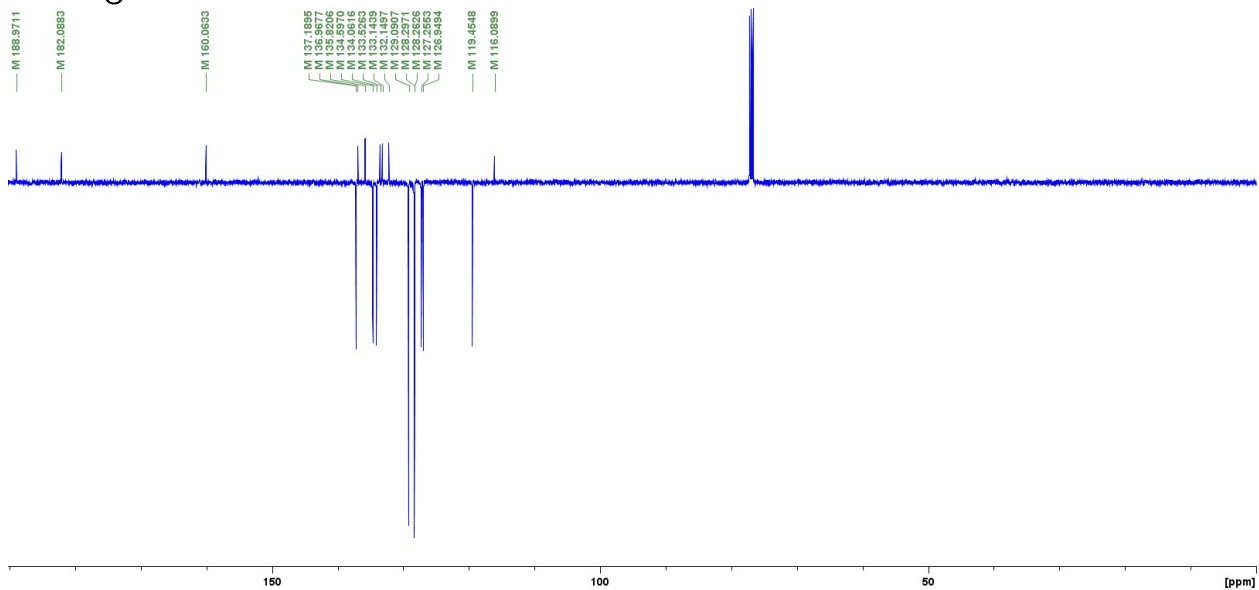
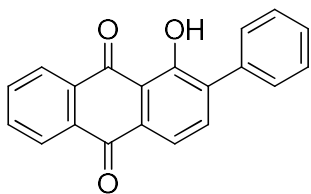


1-Hydroxy-2-phenylanthracene-9,10-dione (25)

^1H NMR (CDCl_3 , 500 MHz)

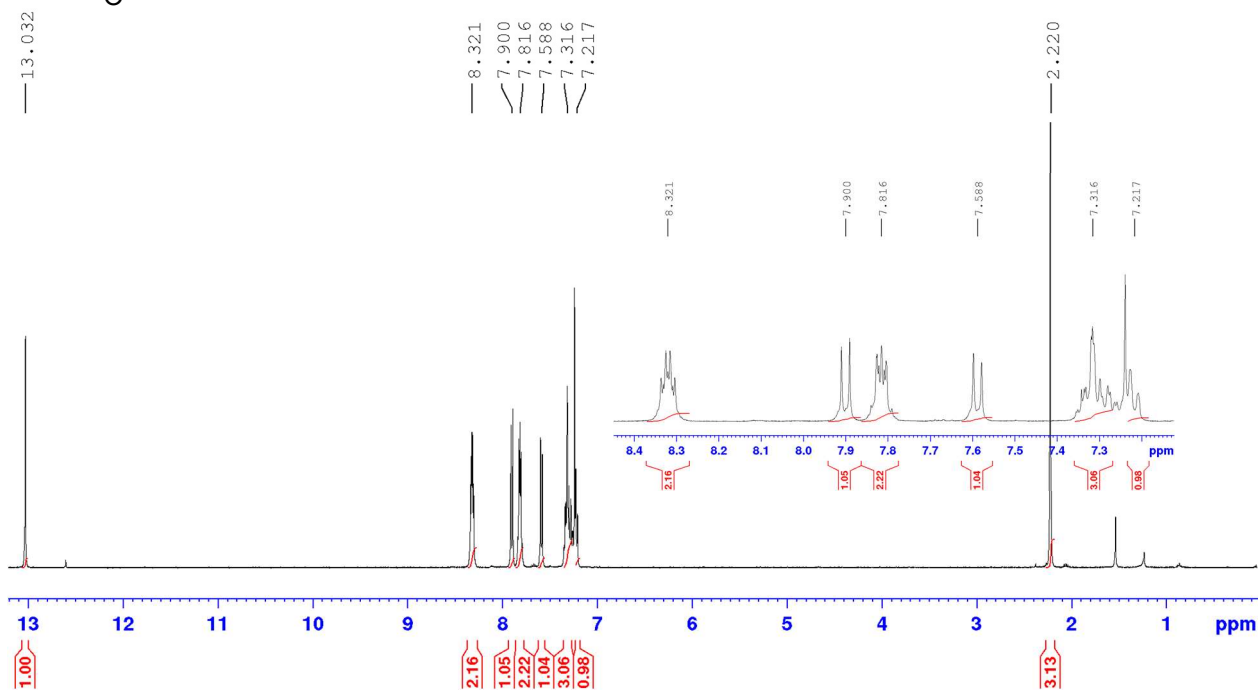
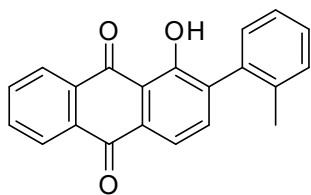


^{13}C NMR (CDCl_3 , 125 MHz)

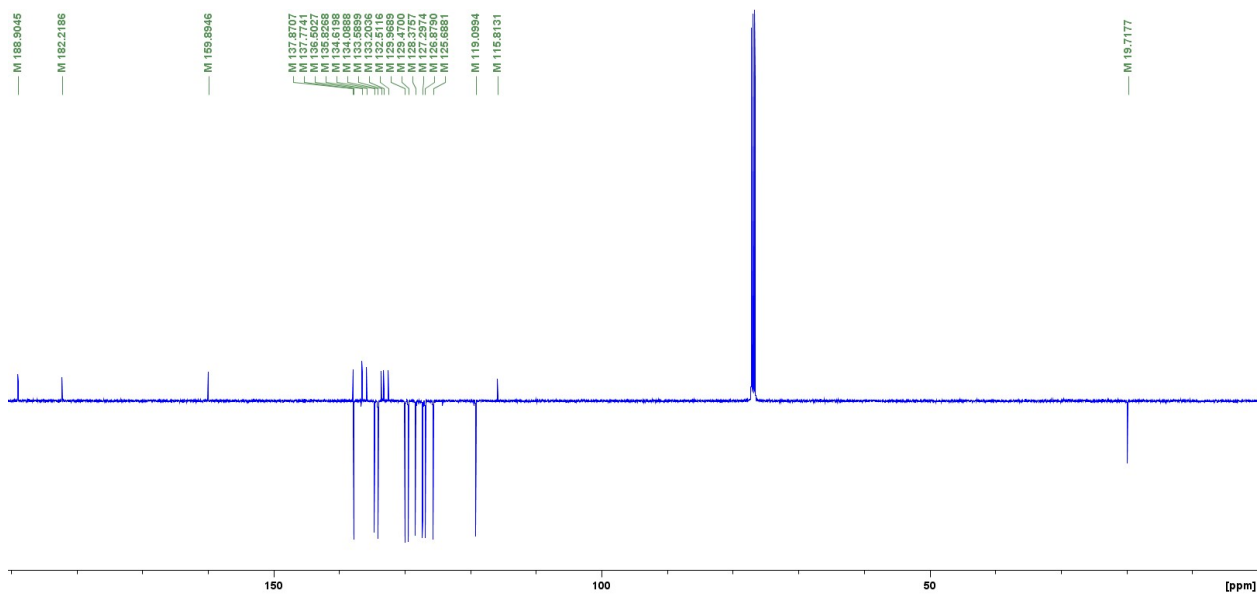
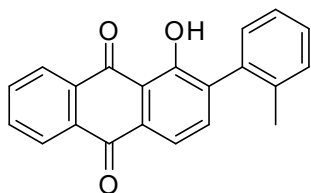


1-Hydroxy-2-(o-tolyl)anthracene-9,10-dione (26)

¹H NMR (CDCl₃, 400 MHz)

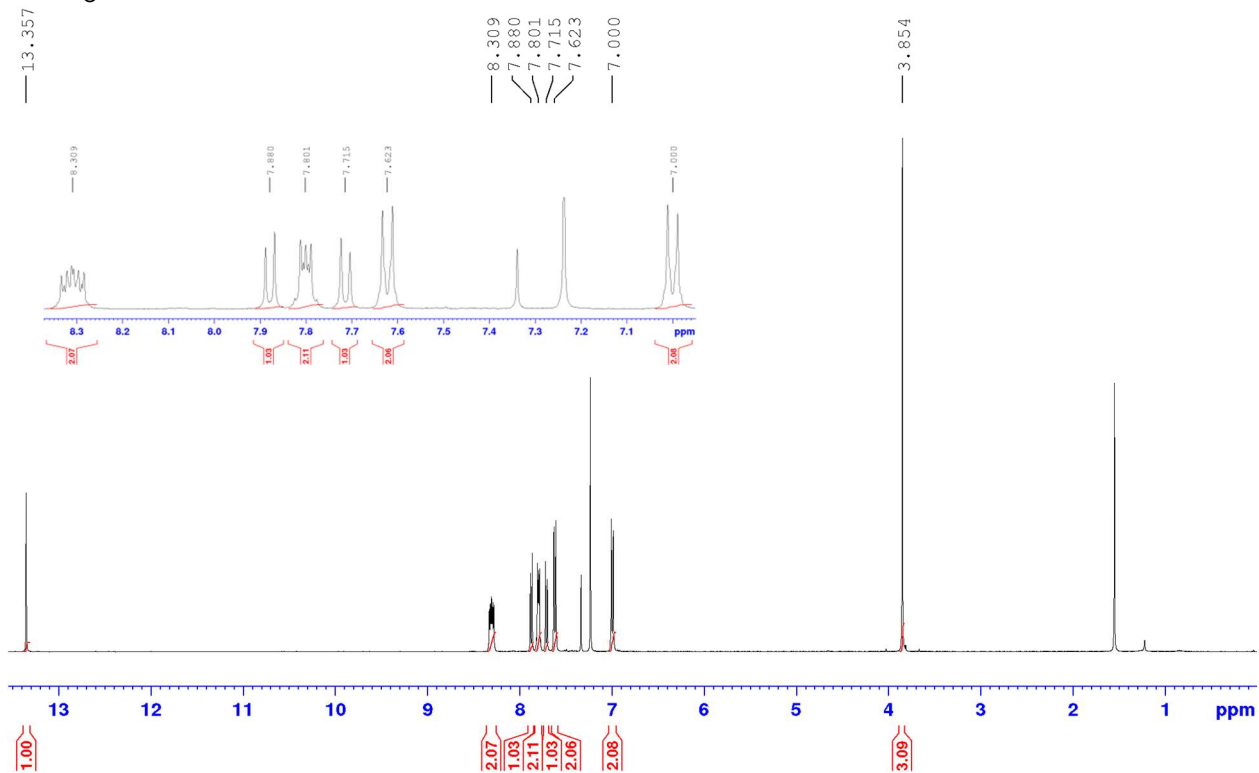
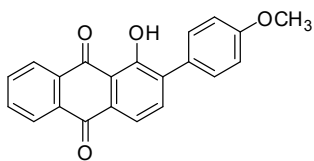


¹³C NMR (CDCl₃, 125 MHz)

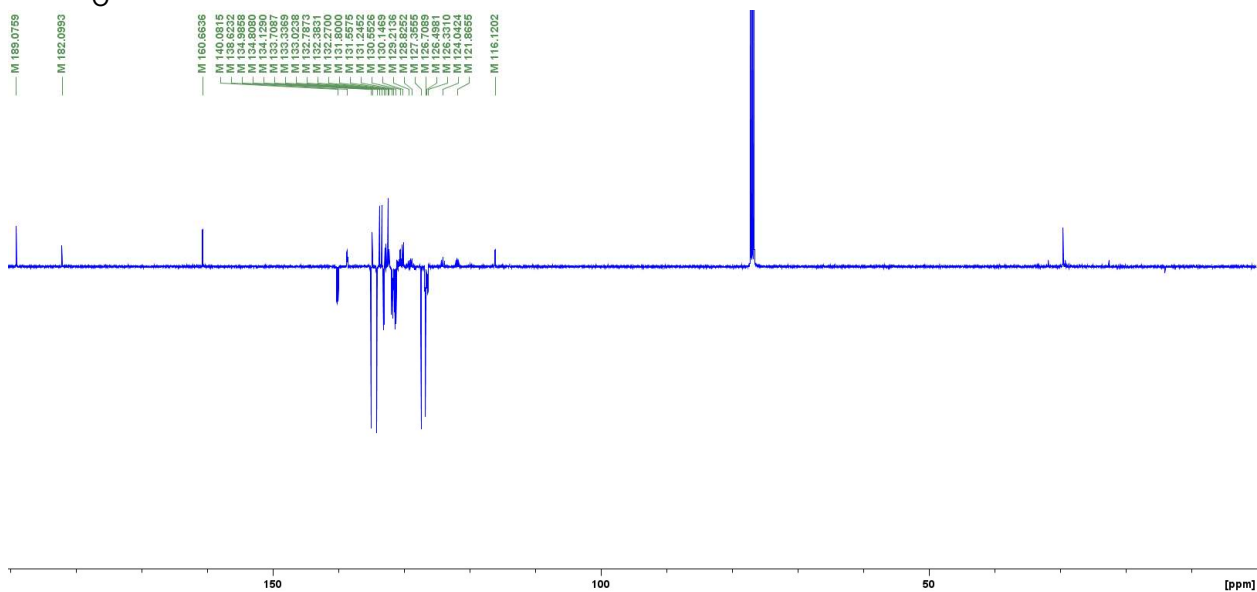
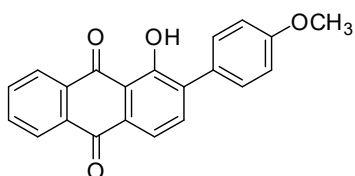


1-Hydroxy-2-(4-methoxyphenyl)anthracene-9,10-dione (27)

^1H NMR (CDCl_3 , 400 MHz)

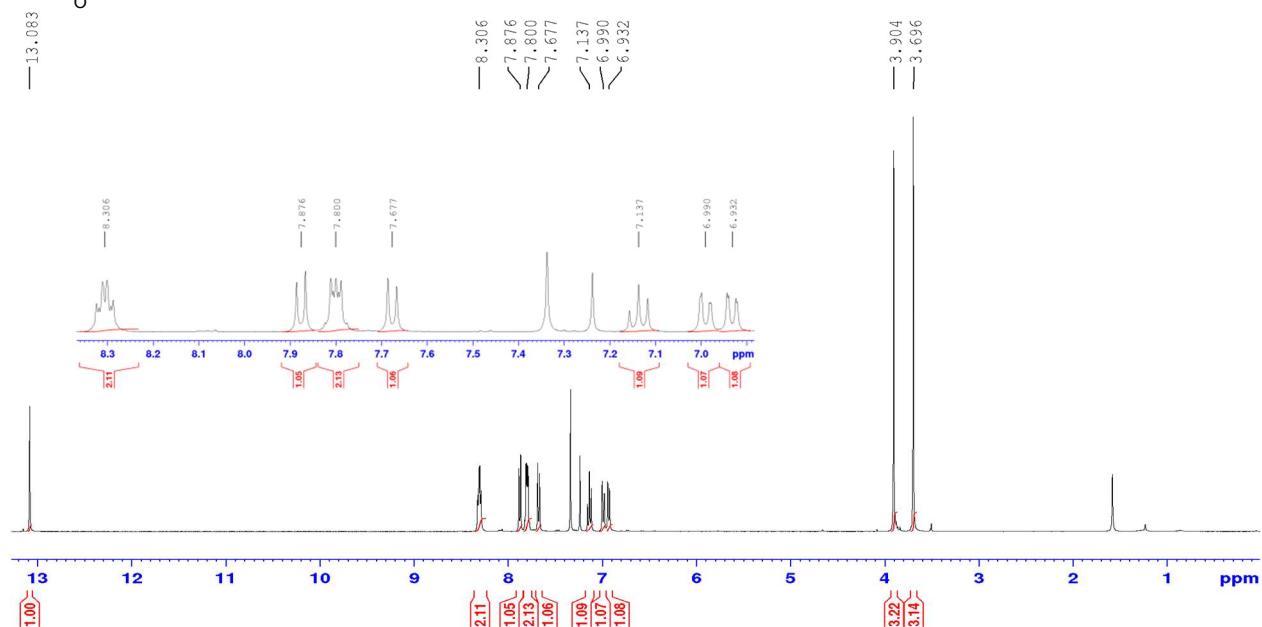
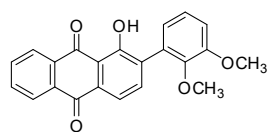


^{13}C NMR (CDCl_3 , 125 MHz)

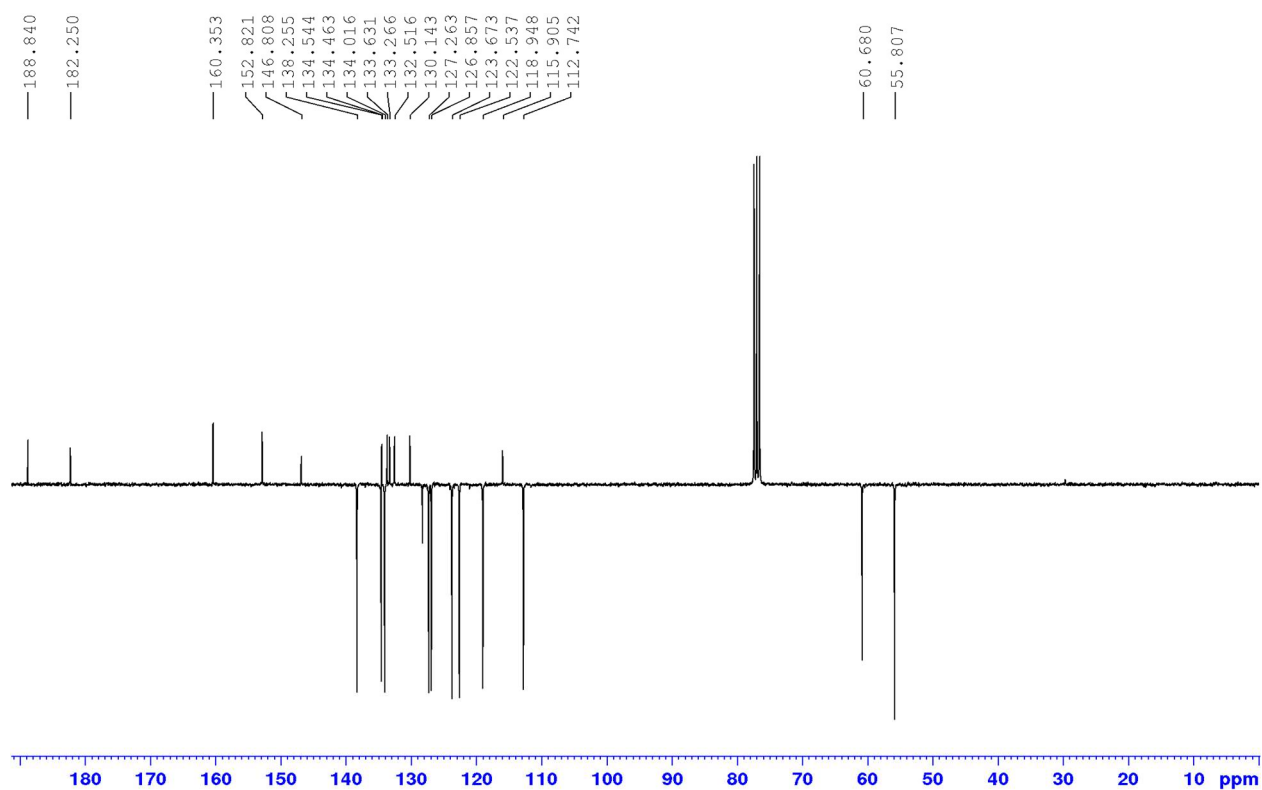
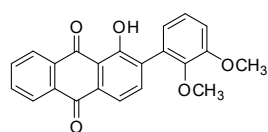


2-(2,3-Dimethoxyphenyl)-1-hydroxyanthracene-9,10-dione (28)

^1H NMR (CDCl_3 , 400 MHz)

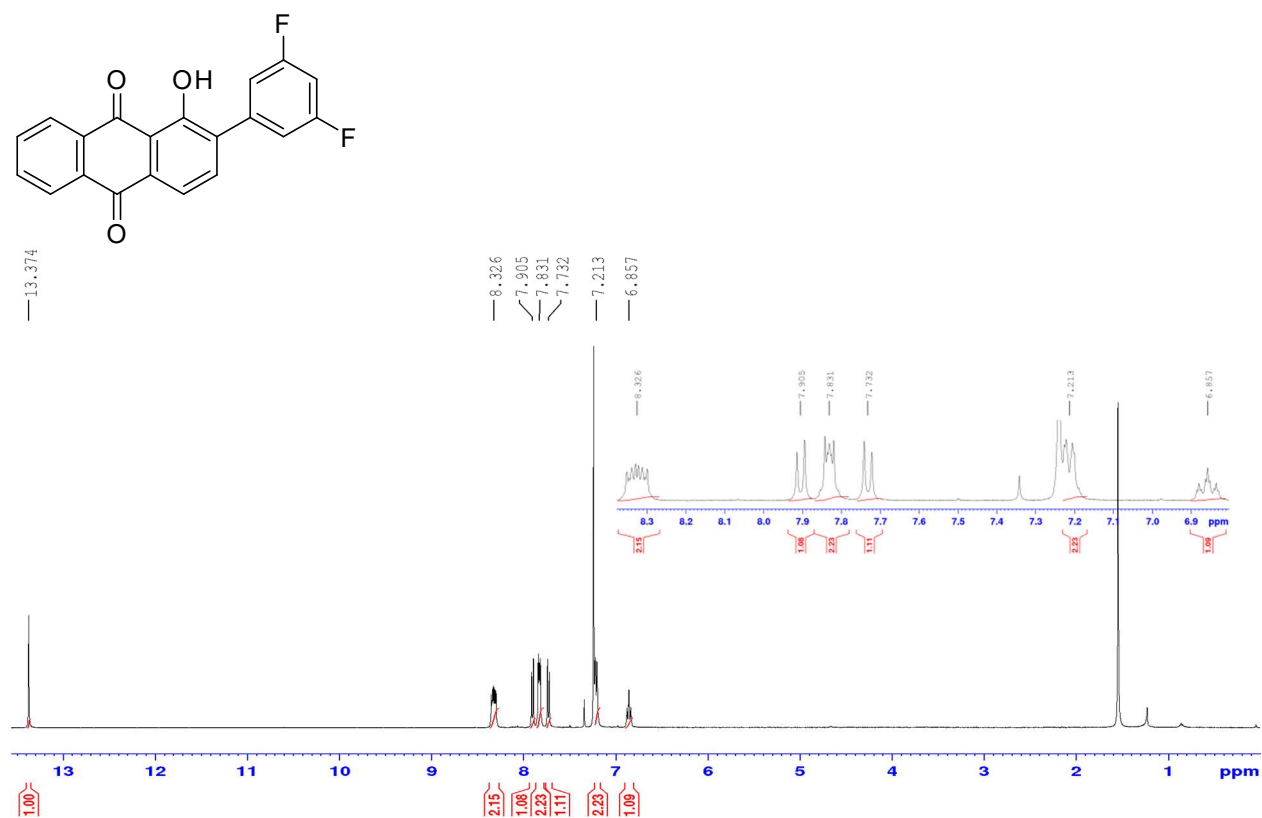


^{13}C NMR (CDCl_3 , 75 MHz)

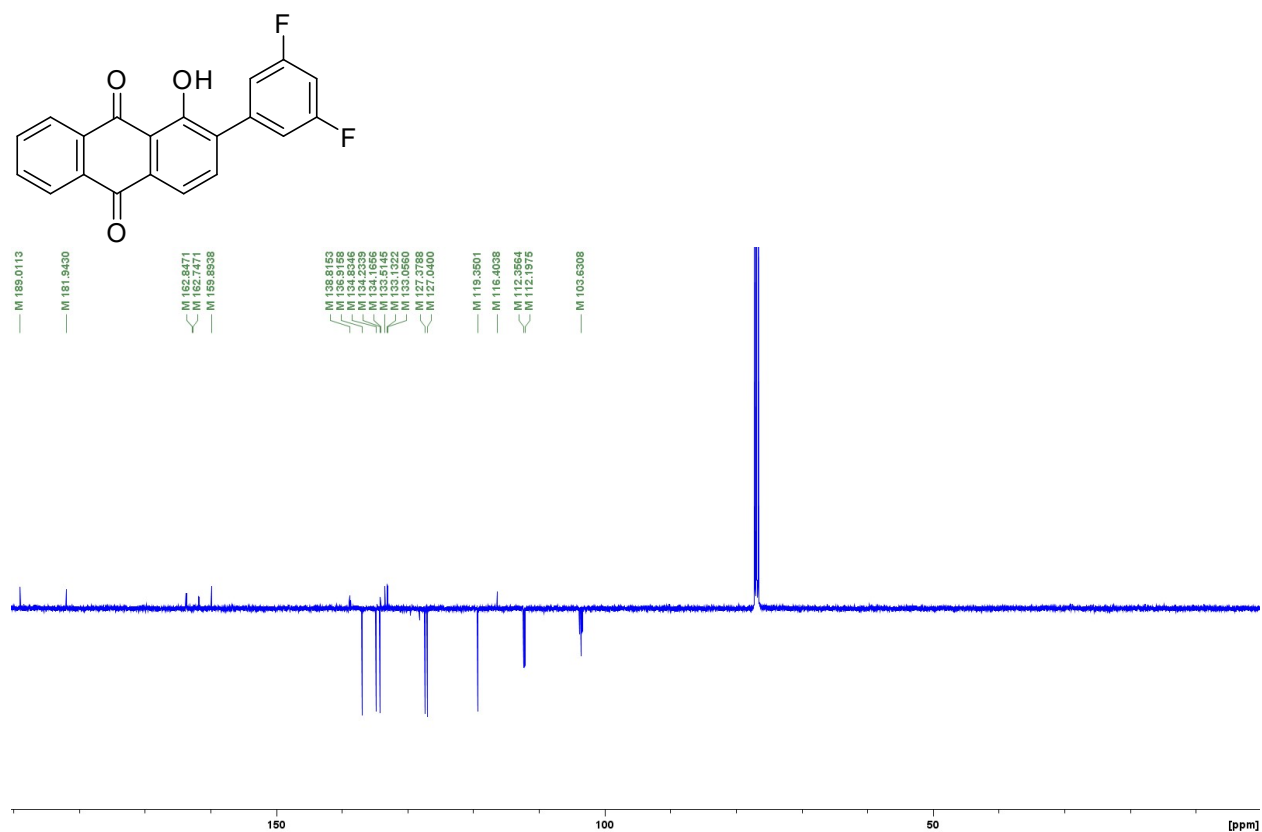


2-(3,5-Difluorophenyl)-1-hydroxyanthracene-9,10-dione (29)

$^1\text{H NMR}$ (CDCl_3 , 400 MHz)

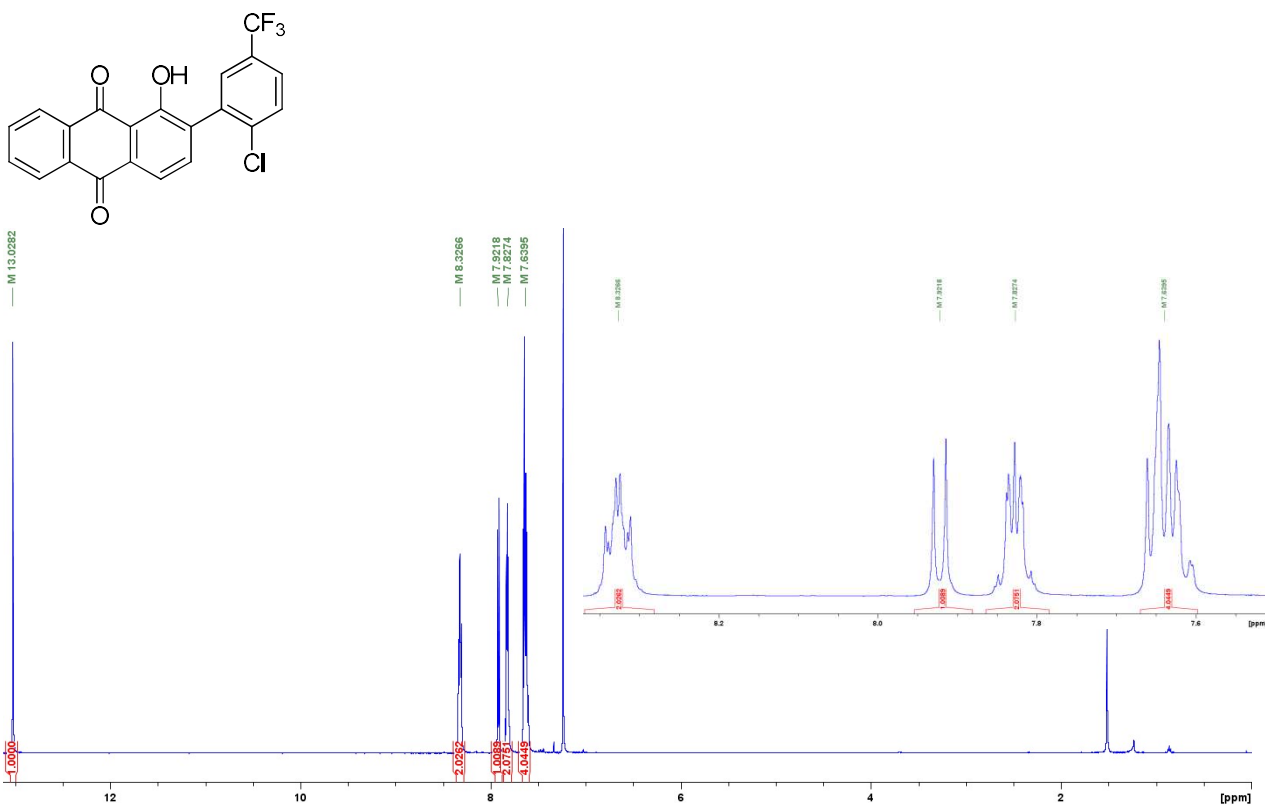


$^{13}\text{C NMR}$ (CDCl_3 , 125 MHz)

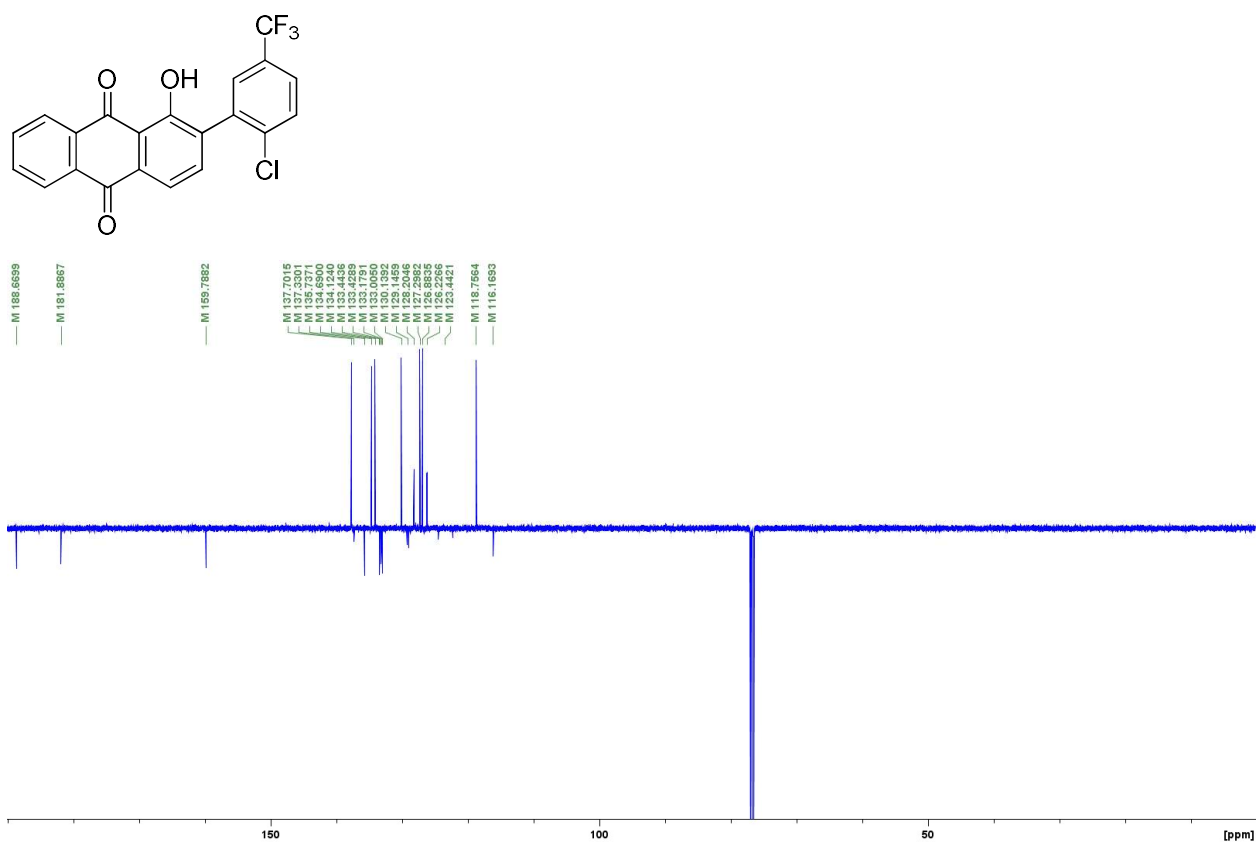


2-(2-Chloro-5-(trifluoromethyl)phenyl)-1-hydroxyanthracene-9,10-dione (30)

¹H NMR (CDCl₃, 500 MHz)

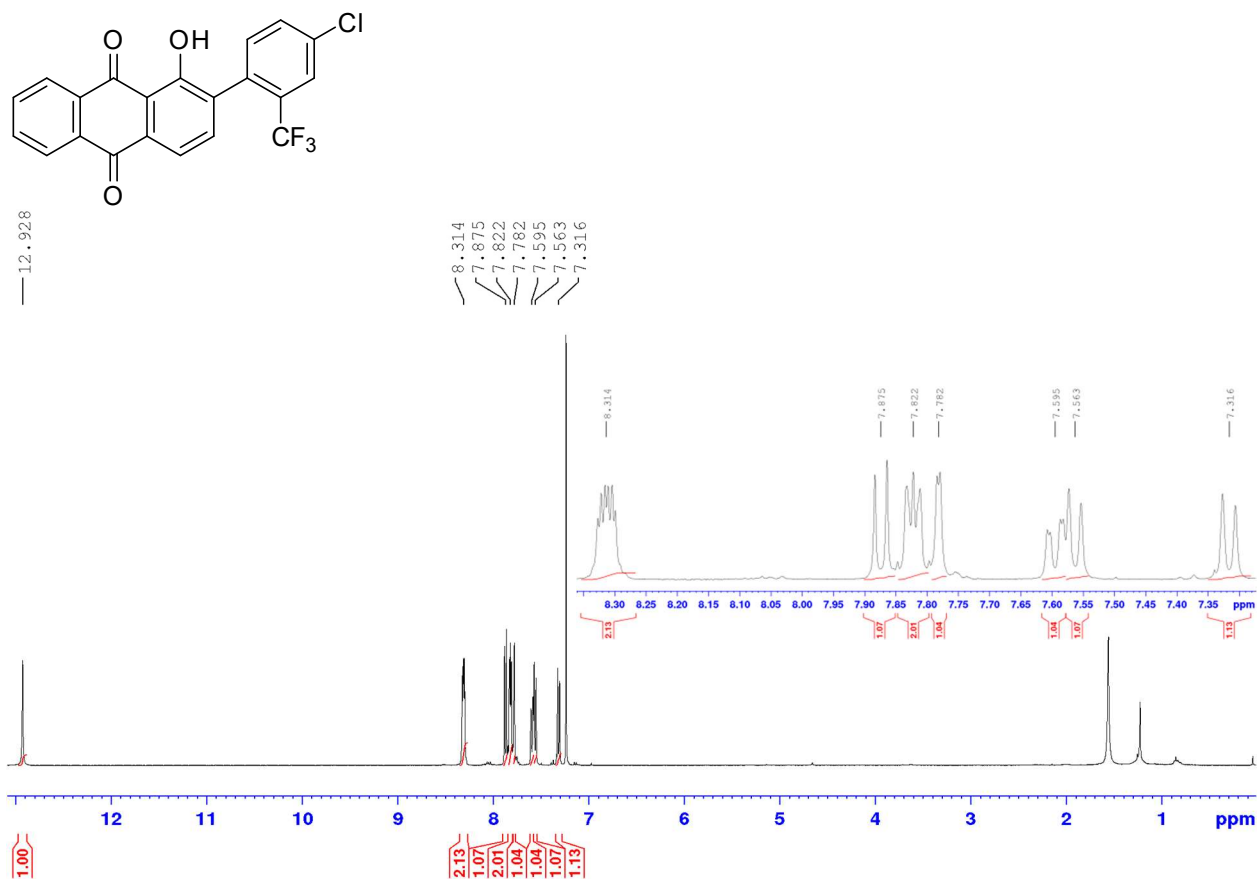


¹³C NMR (CDCl₃, 125 MHz)

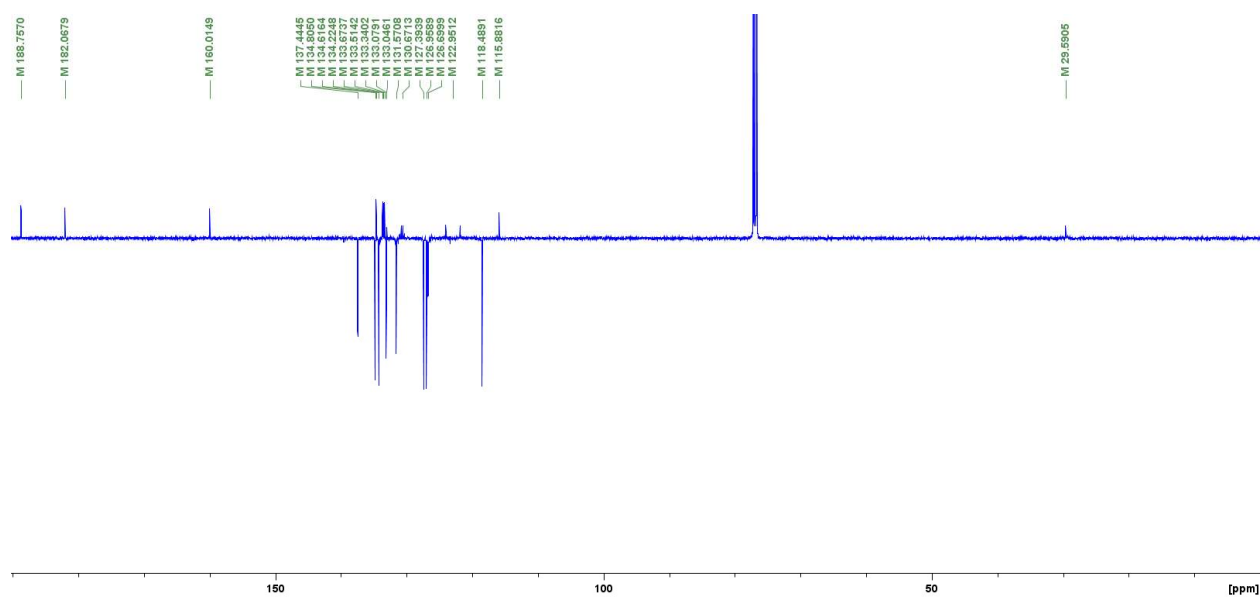


2-(4-Chloro-2-(trifluoromethyl)phenyl)-1-hydroxyanthracene-9,10-dione (31)

^1H NMR (CDCl_3 , 400 MHz)

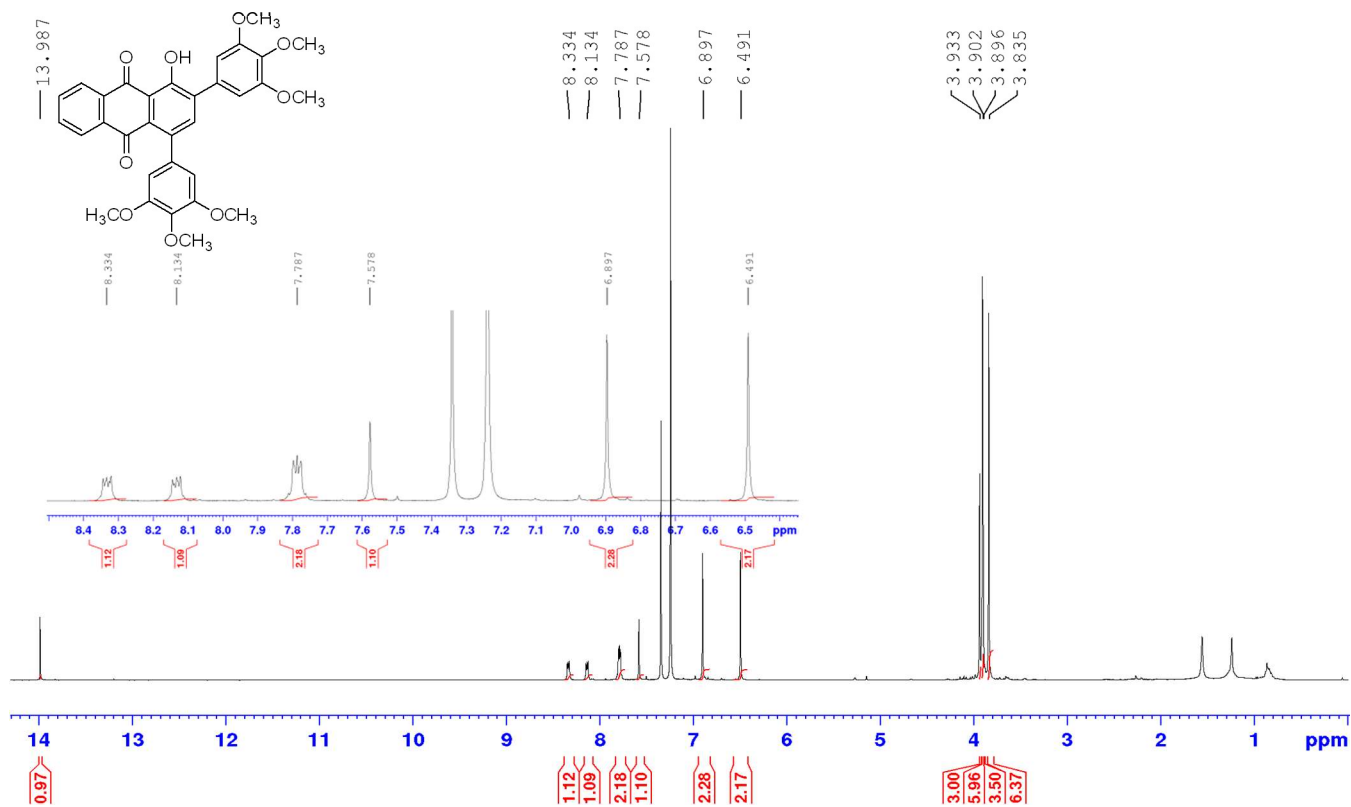


^{13}C NMR (CDCl_3 , 125 MHz)

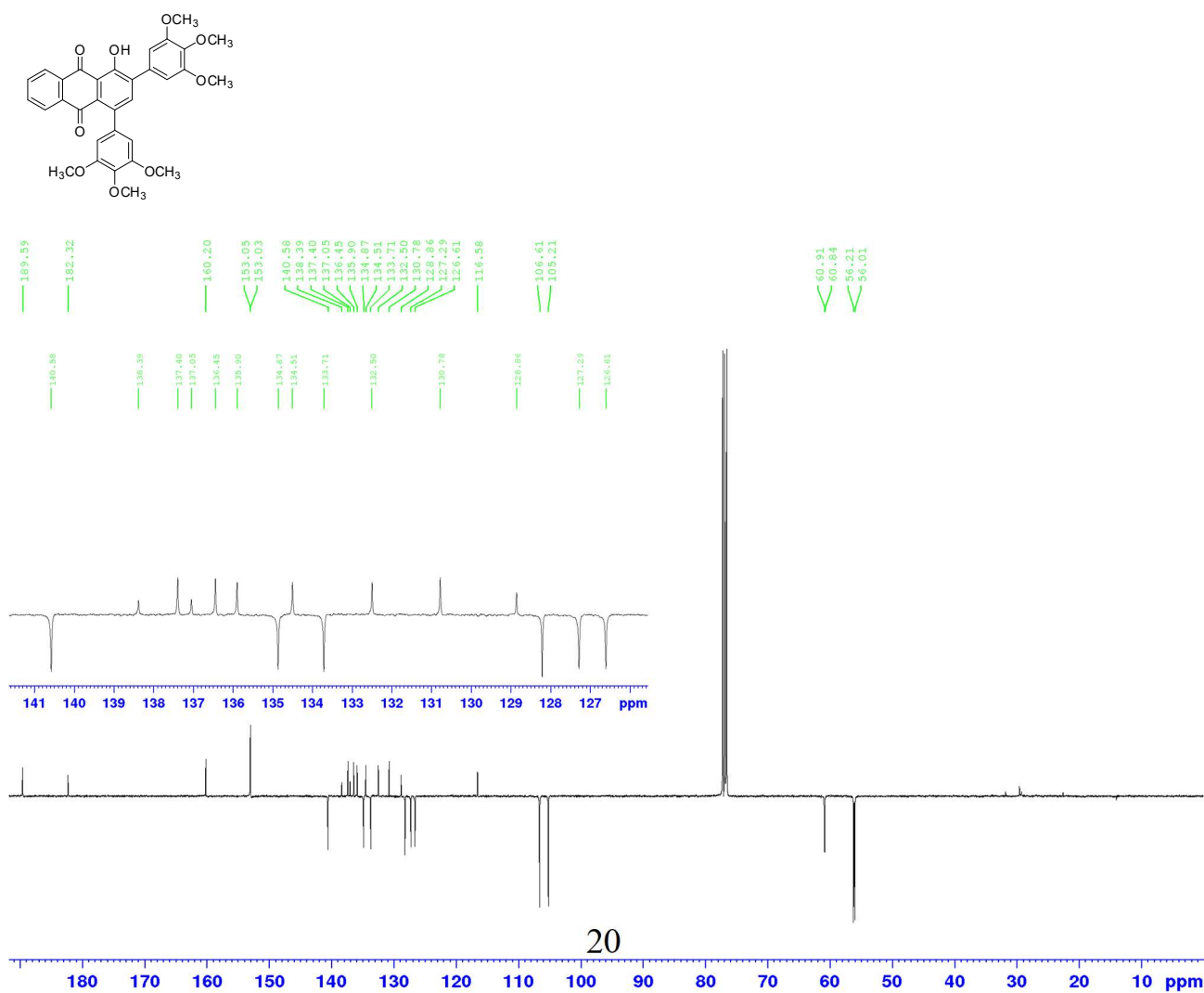


1-Hydroxy-2,4-di-(3,4,5-trimethoxyphenyl)anthracene-9,10-dione (32)

¹H NMR (CDCl₃, 400 MHz)

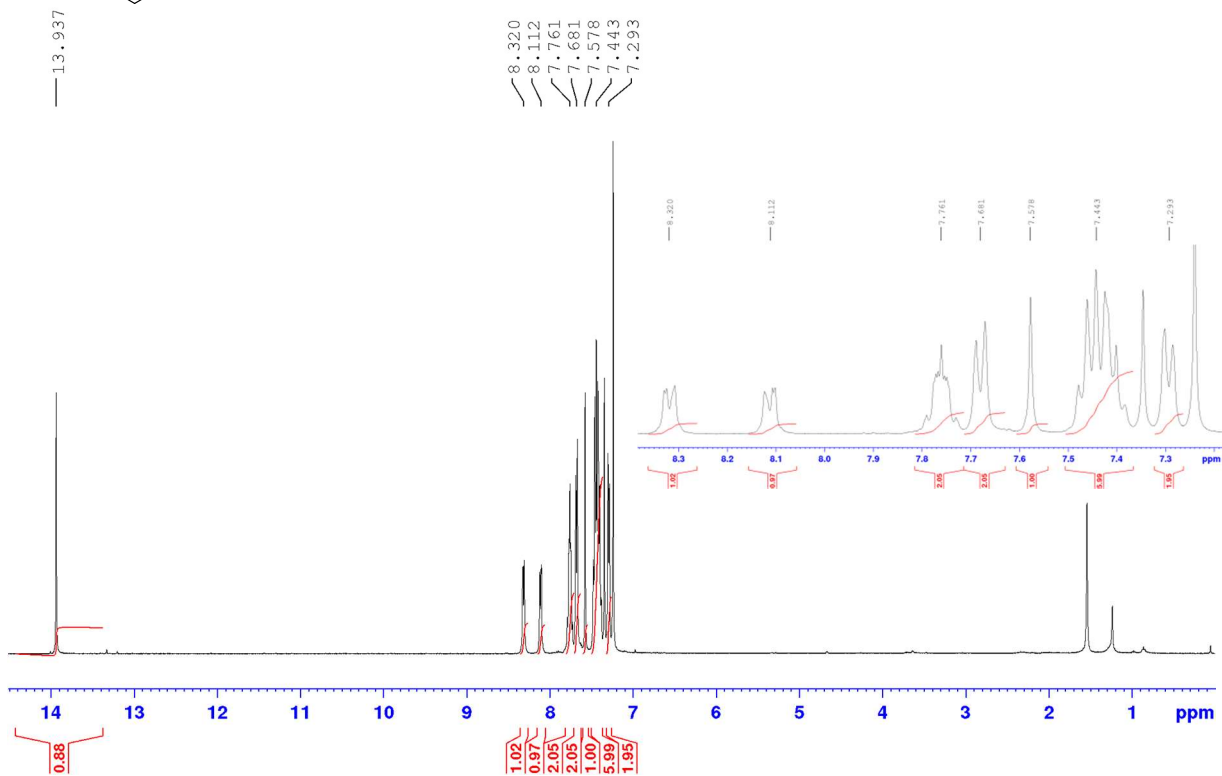
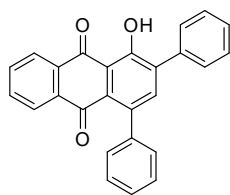


¹³C NMR (CDCl₃, 100 MHz)

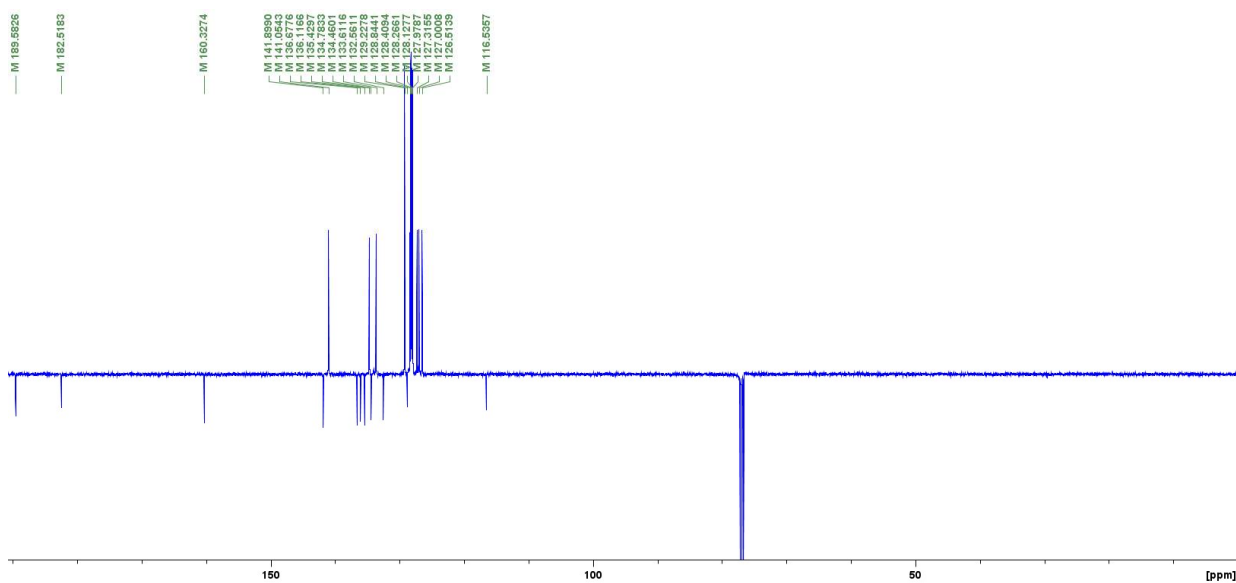
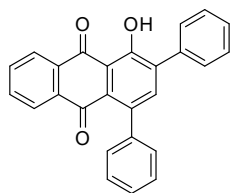


1-Hydroxy-2,4-diphenylanthracene-9,10-dione (33)

^1H NMR (CDCl_3 , 400 MHz)

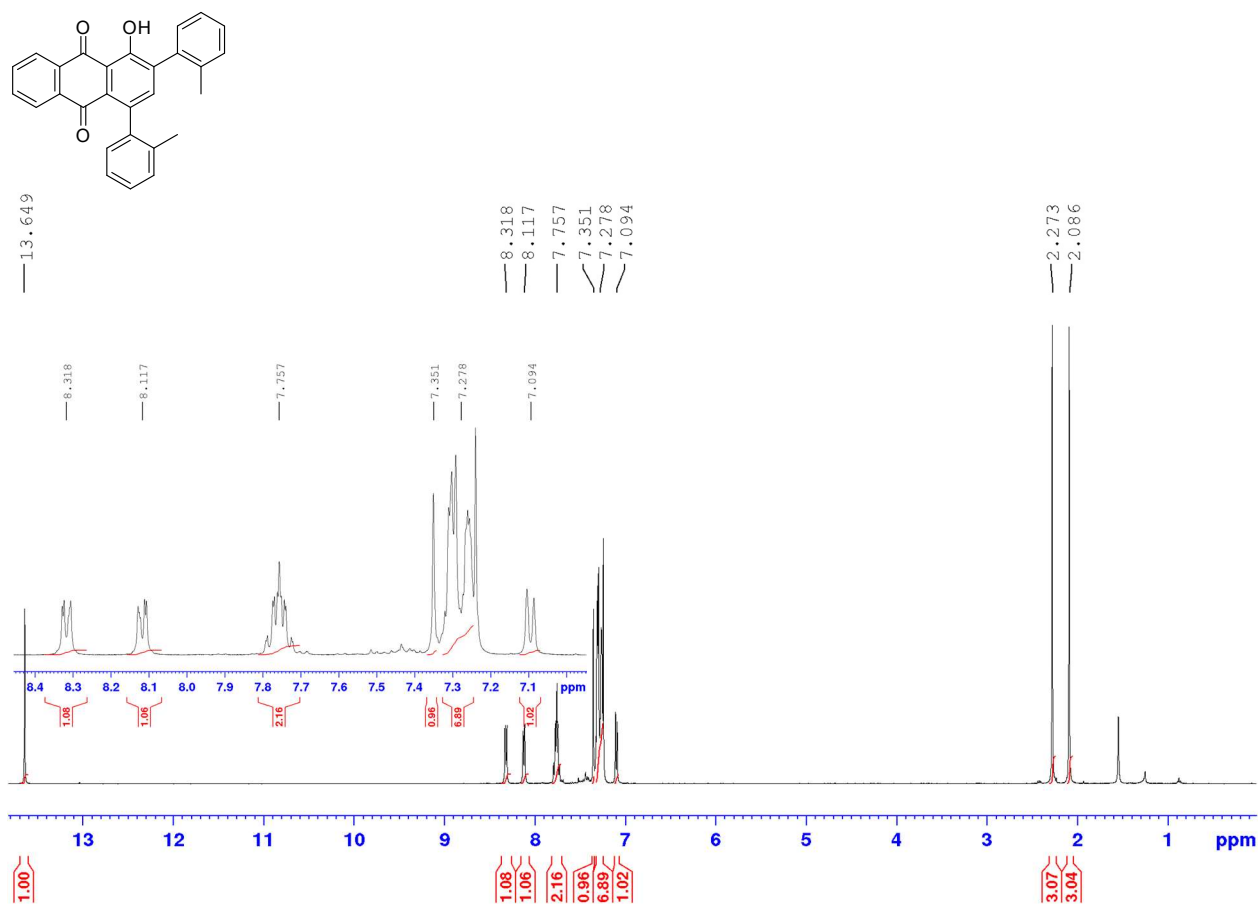


^{13}C NMR (CDCl_3 , 125 MHz)

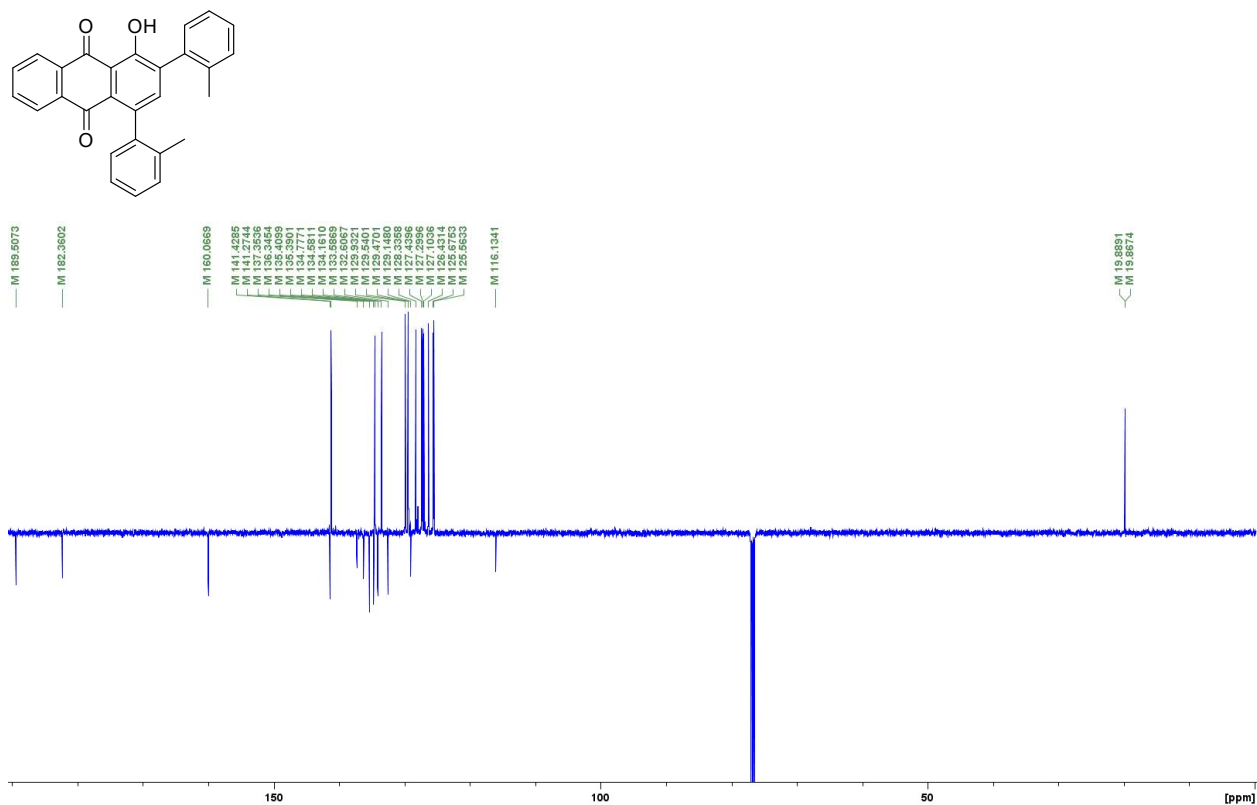


1-Hydroxy-2,4-di-(*o*-tolyl)anthracene-9,10-dione (34)

^1H NMR (CDCl_3 , 400 MHz)

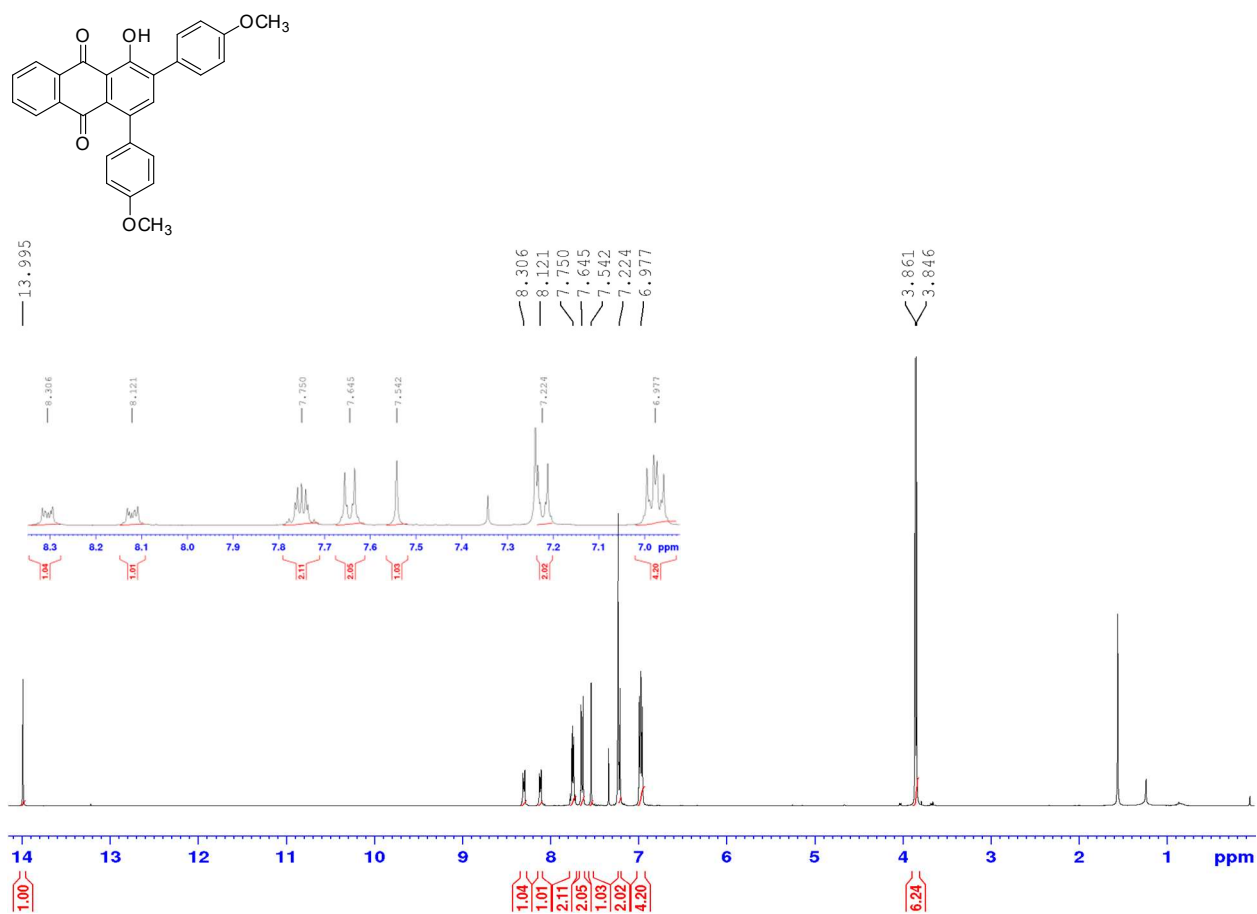


^{13}C NMR (CDCl_3 , 125 MHz)

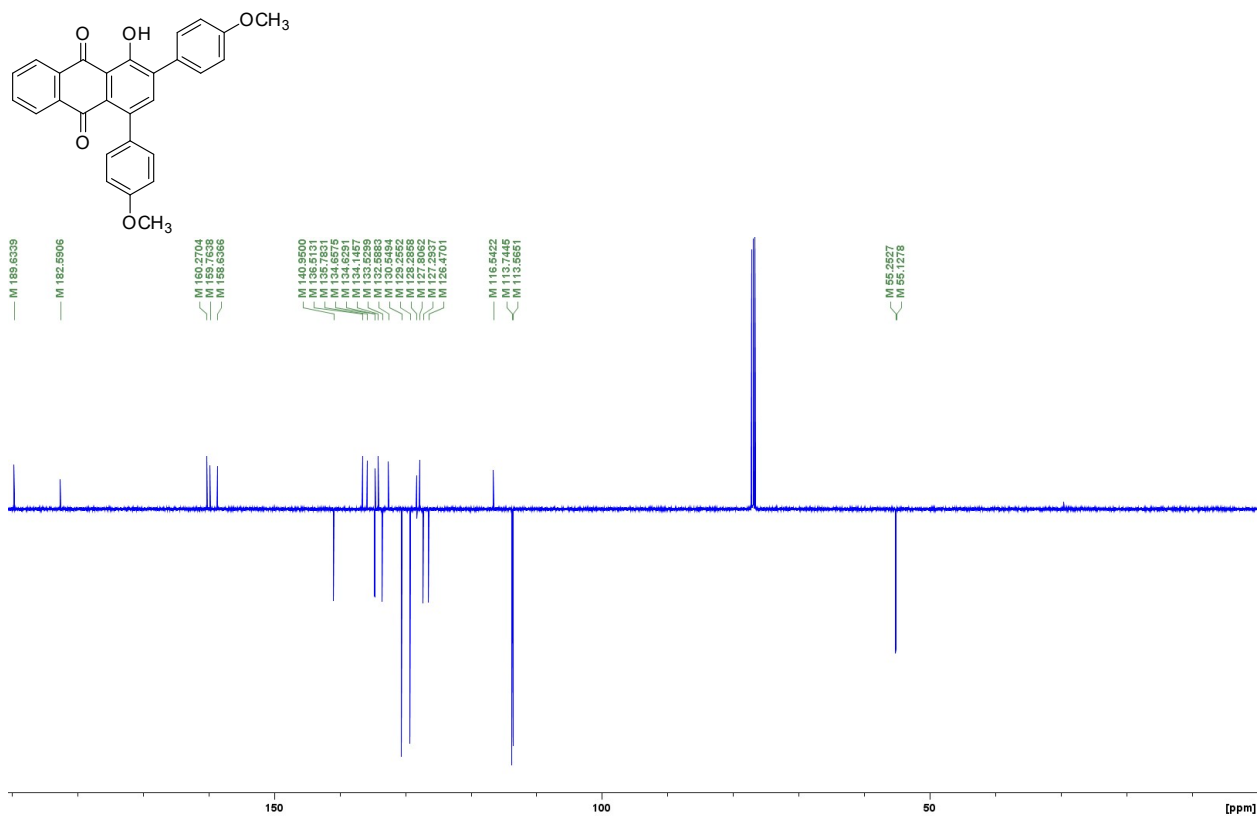


1-Hydroxy-2,4-di-(4-methoxyphenyl)anthracene-9,10-dione (35)

¹H NMR (CDCl₃, 400 MHz)

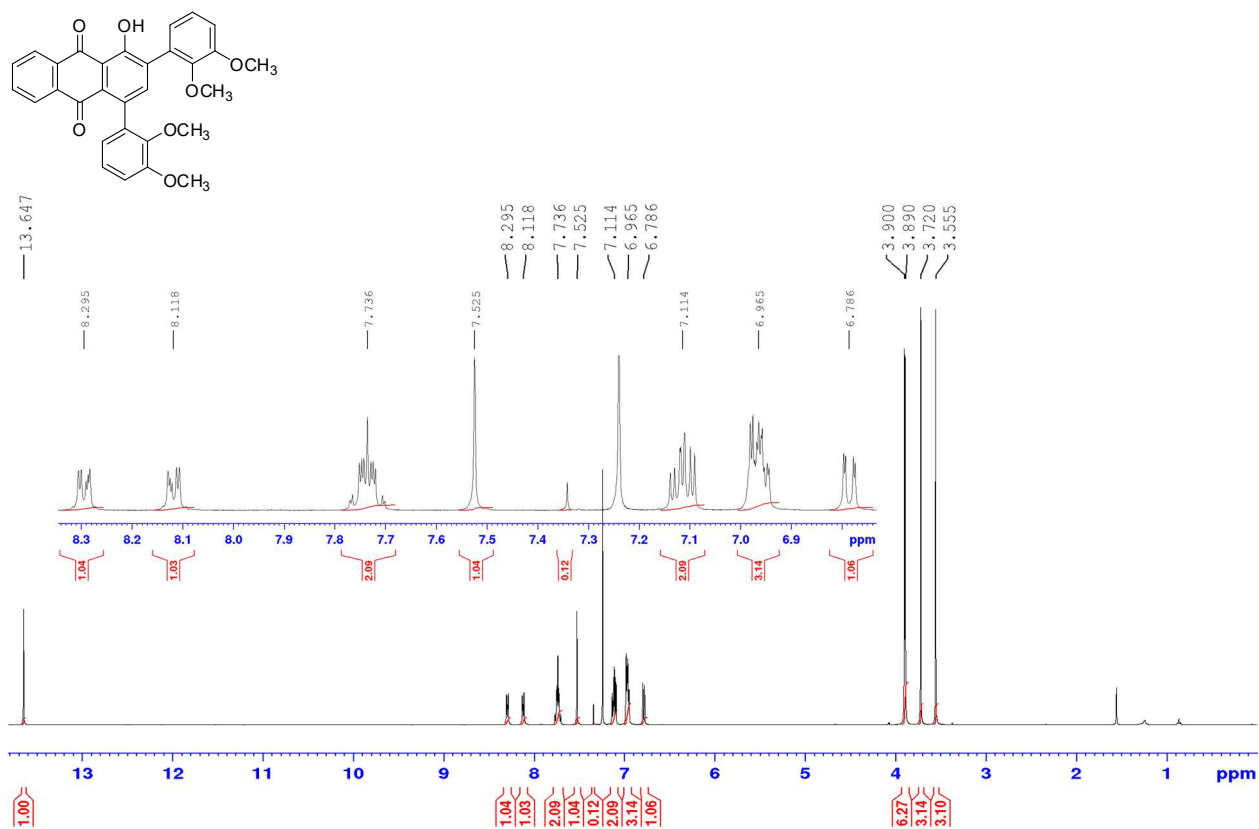


¹³C NMR (CDCl₃, 125 MHz)

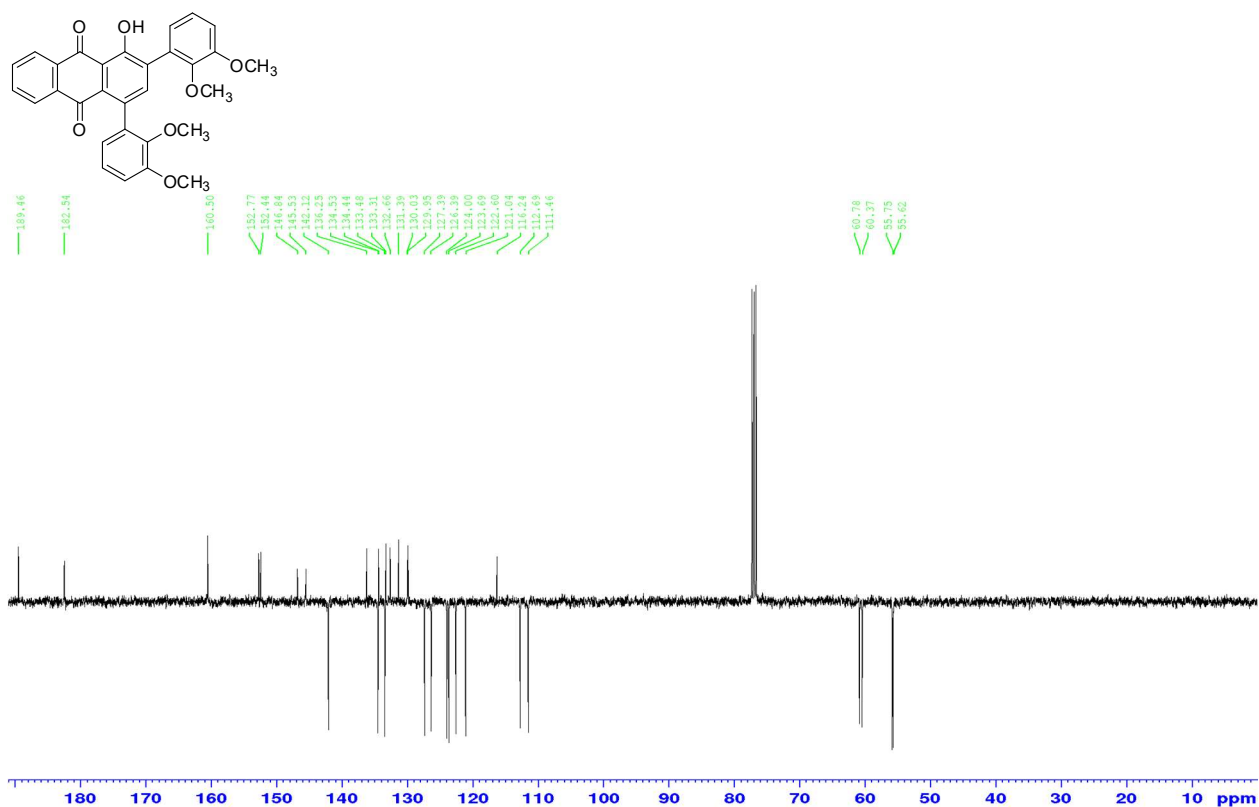


2,4-Di-(2,3-dimethoxyphenyl)-1-hydroxyanthracene-9,10-dione (36)

^1H NMR (CDCl_3 , 400 MHz)

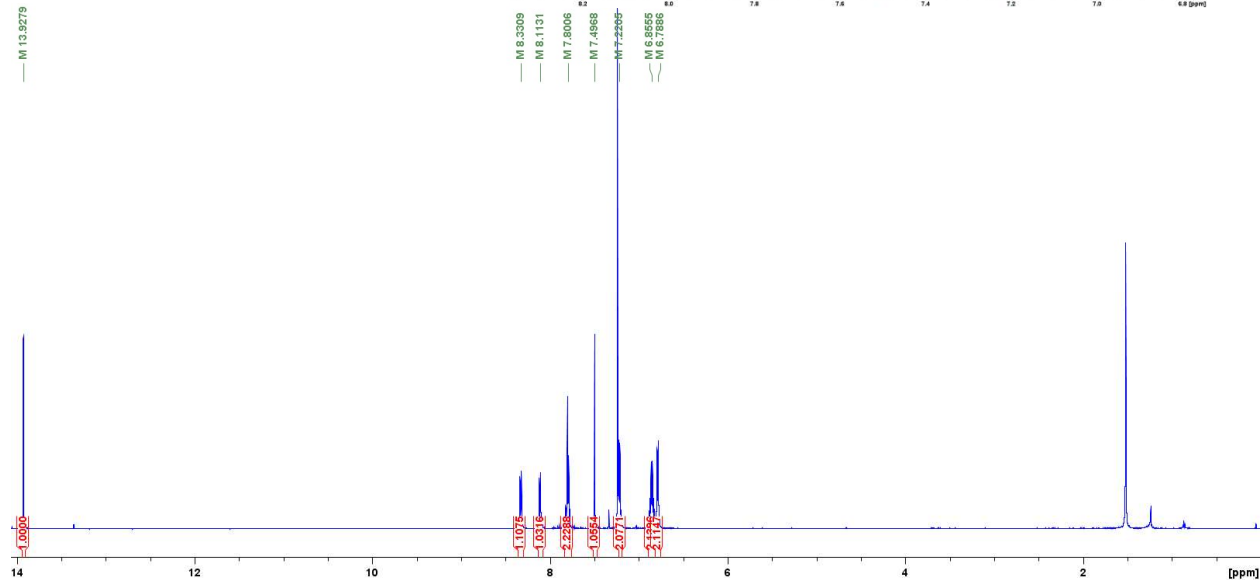
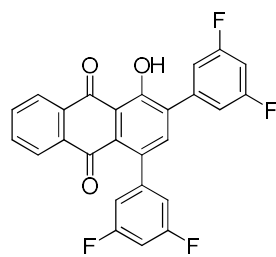


^{13}C NMR (CDCl_3 , 100 MHz)

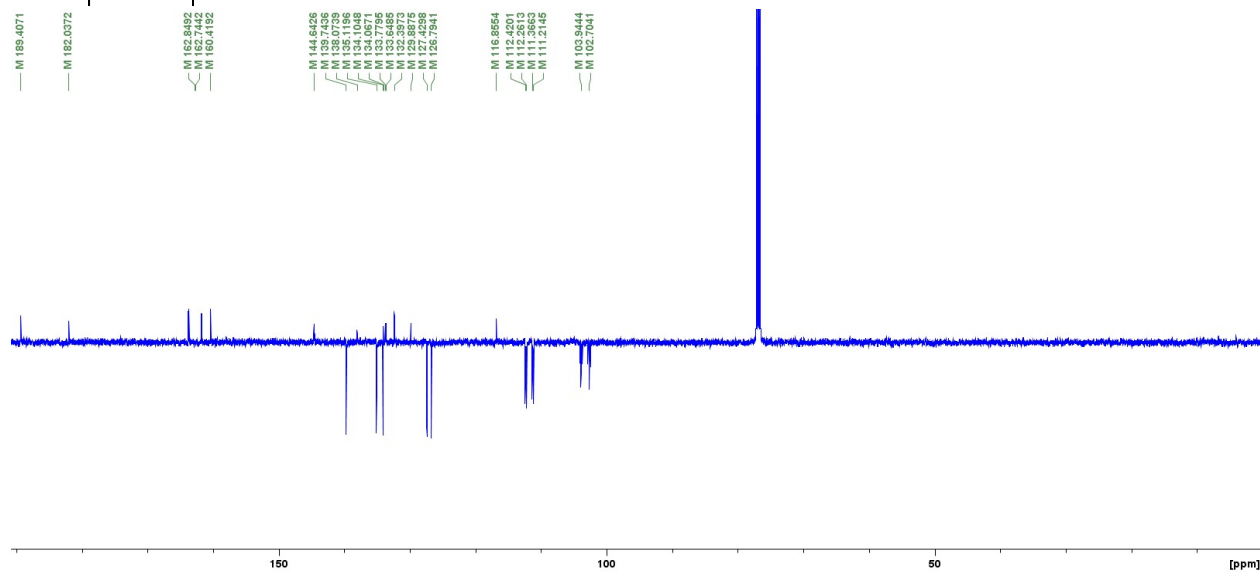
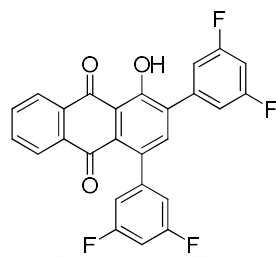


2,4-Di-(3,5-difluorophenyl)-1-hydroxyanthracene-9,10-dione (37)

¹H NMR (CDCl₃, 500 MHz)

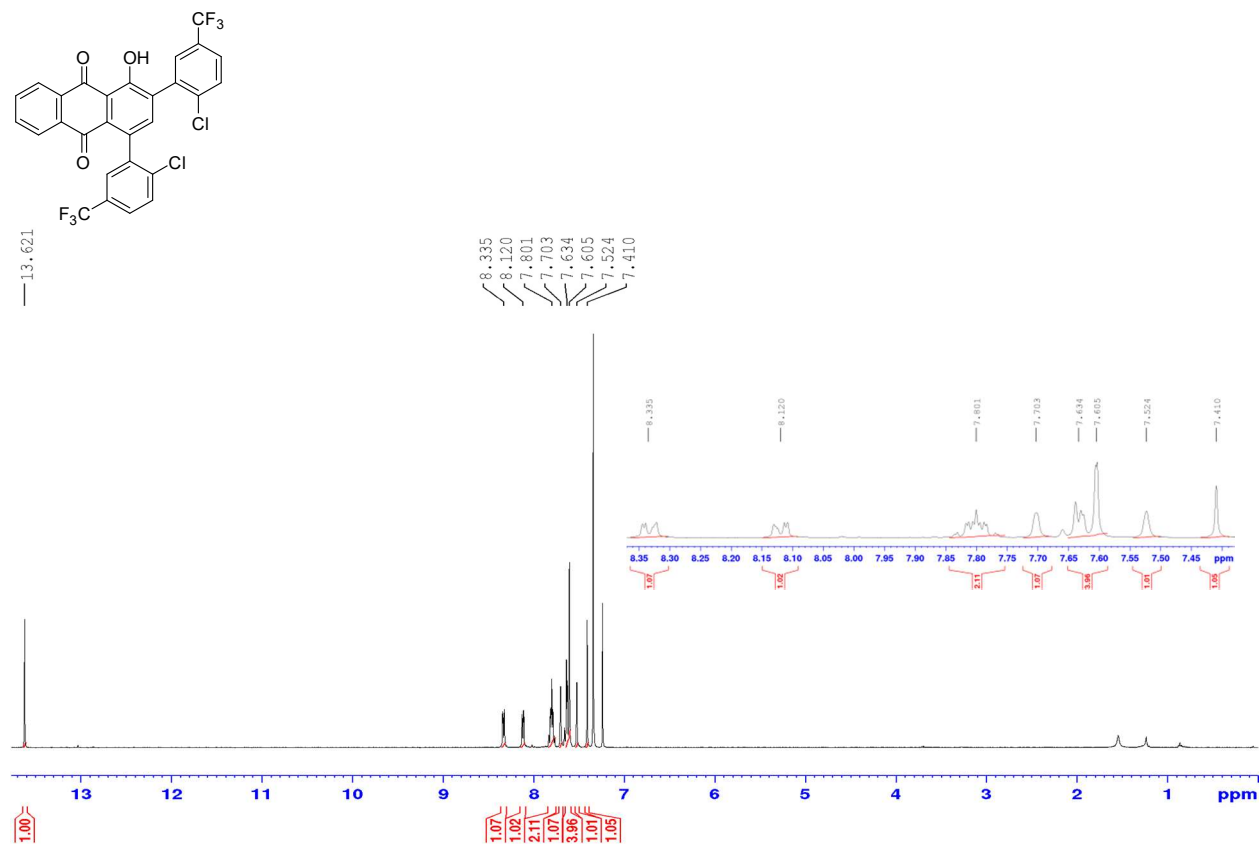


¹³C NMR (CDCl₃, 125 MHz)

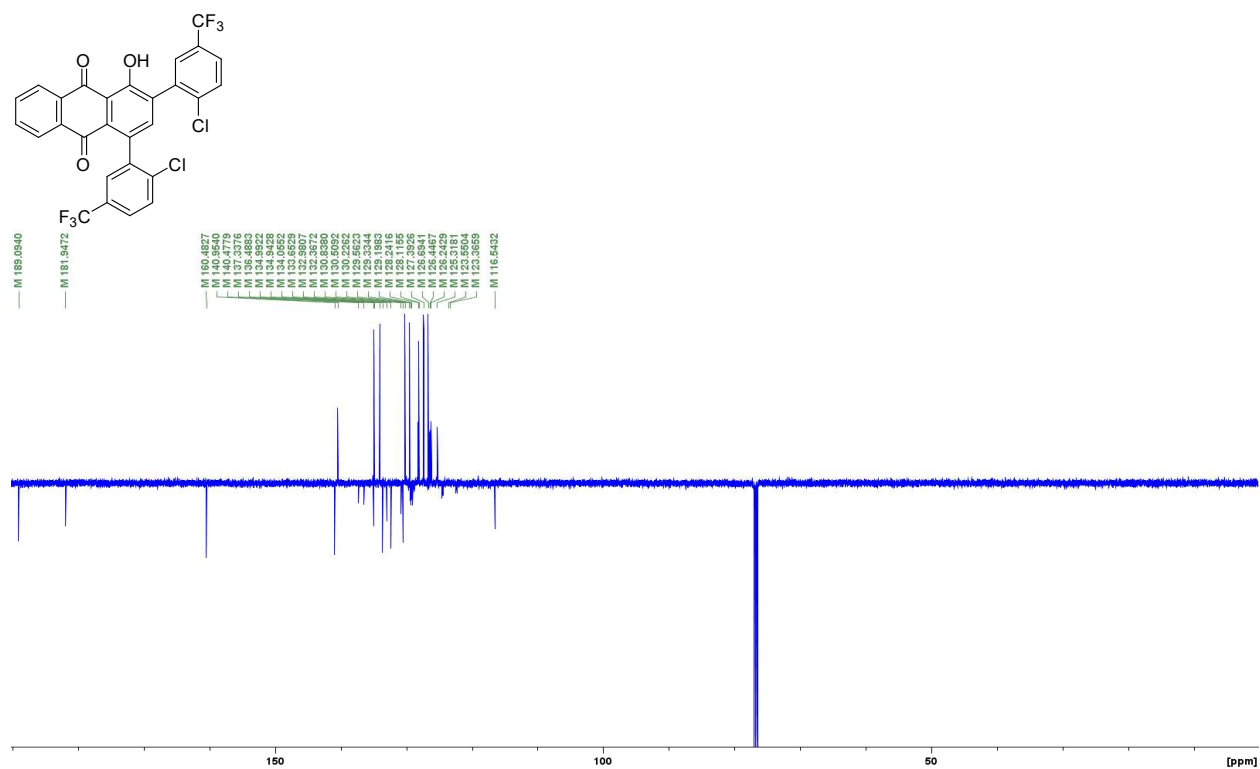


2,4-Di-(2-chloro-5-(trifluoromethyl)phenyl)-1-hydroxyanthracene-9,10-dione (38)

^1H NMR (CDCl_3 , 400 MHz)

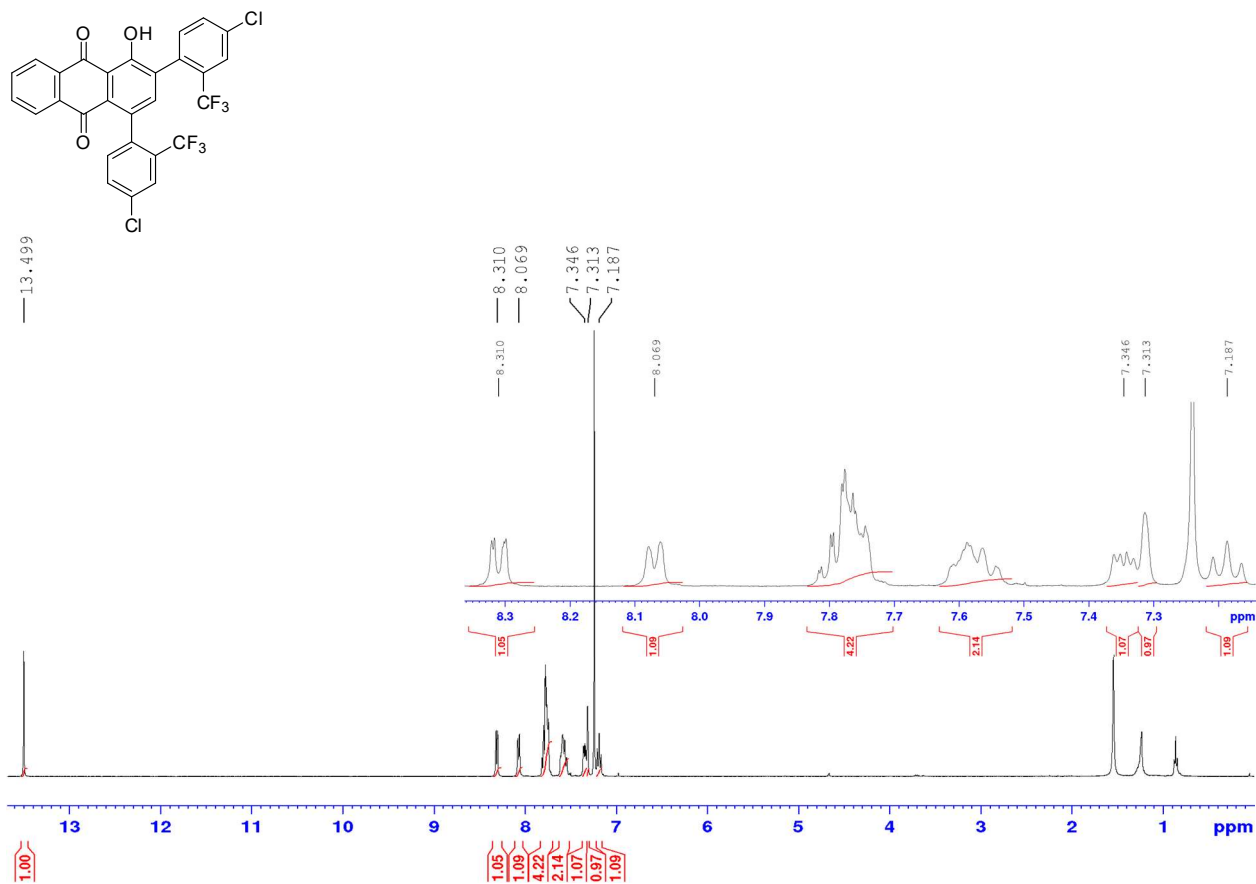


^{13}C NMR (CDCl_3 , 125 MHz)

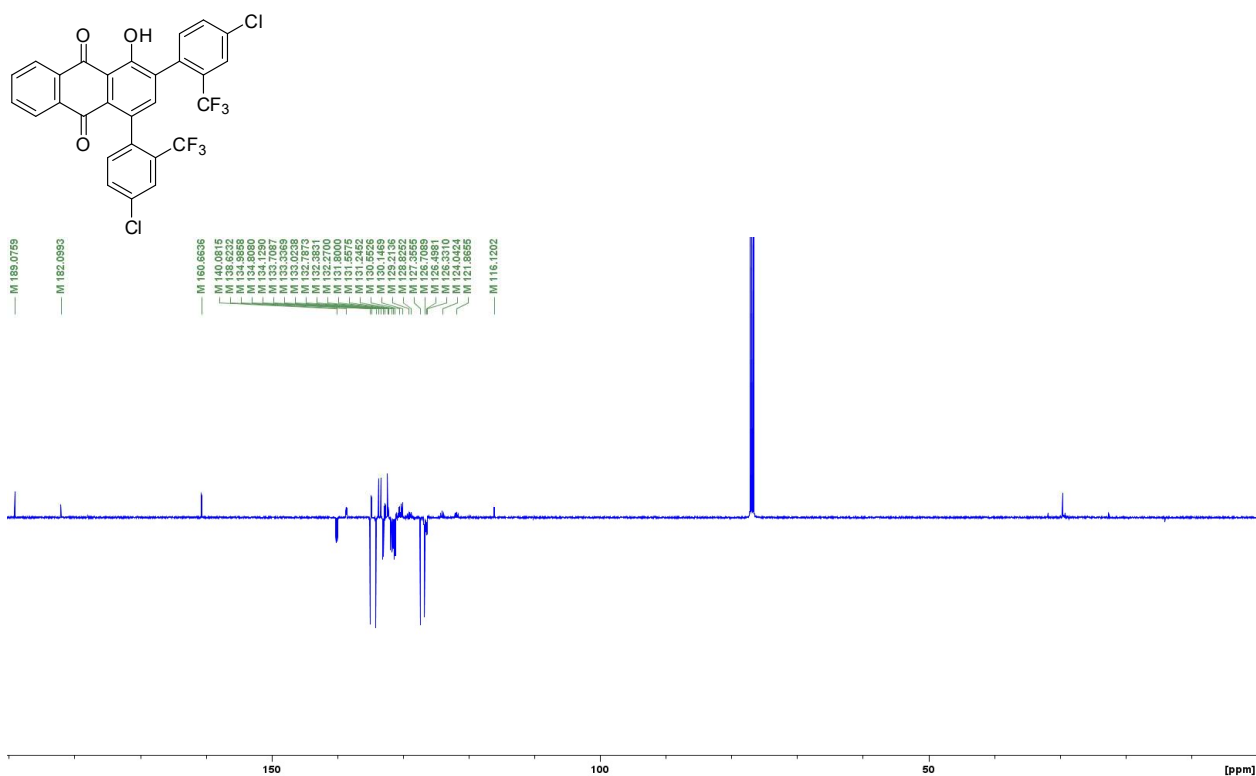


2,4-Di-(4-chloro-2-(trifluoromethyl)phenyl)-1-hydroxyanthracene-9,10-dione (39)

¹H NMR (CDCl₃, 400 MHz)

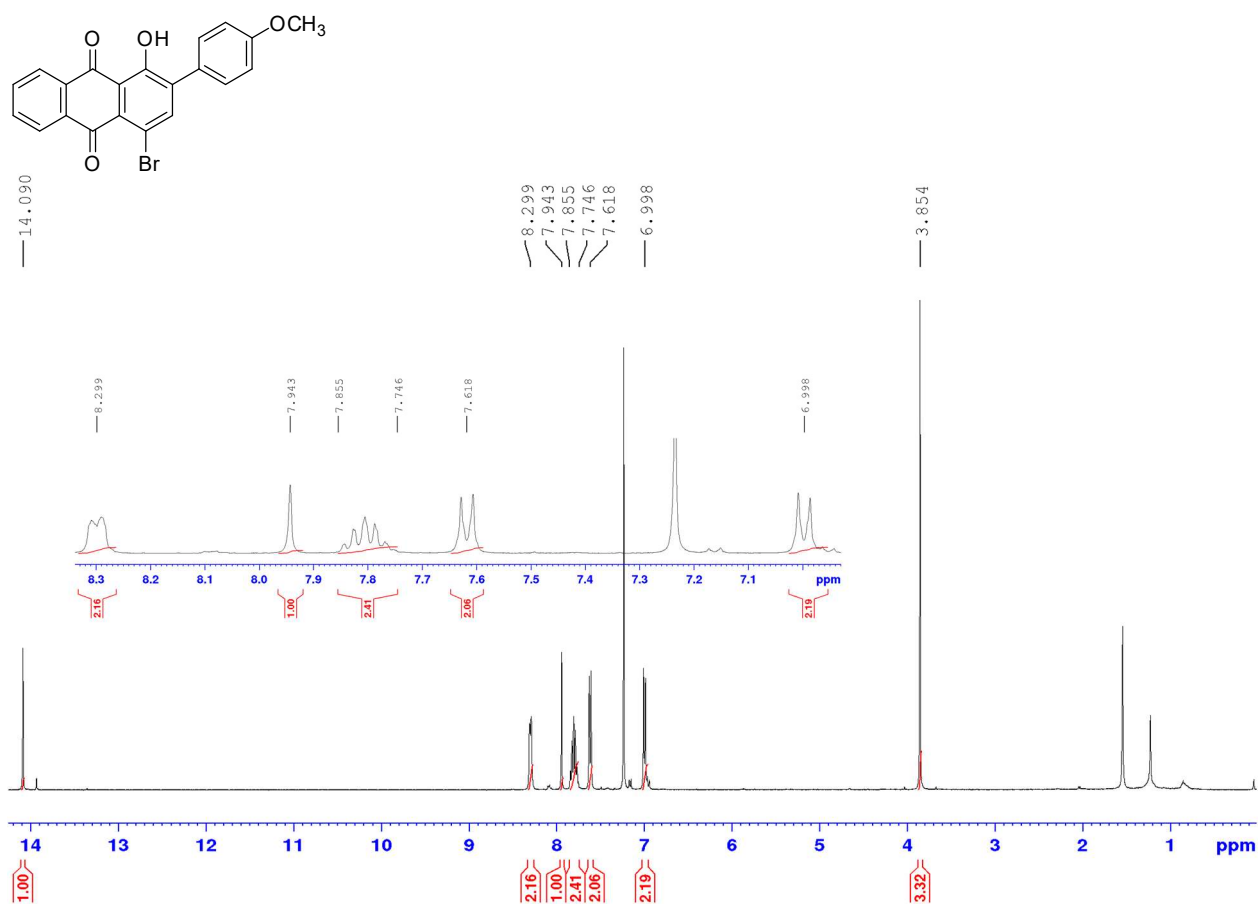


¹³C NMR (CDCl₃, 125 MHz)

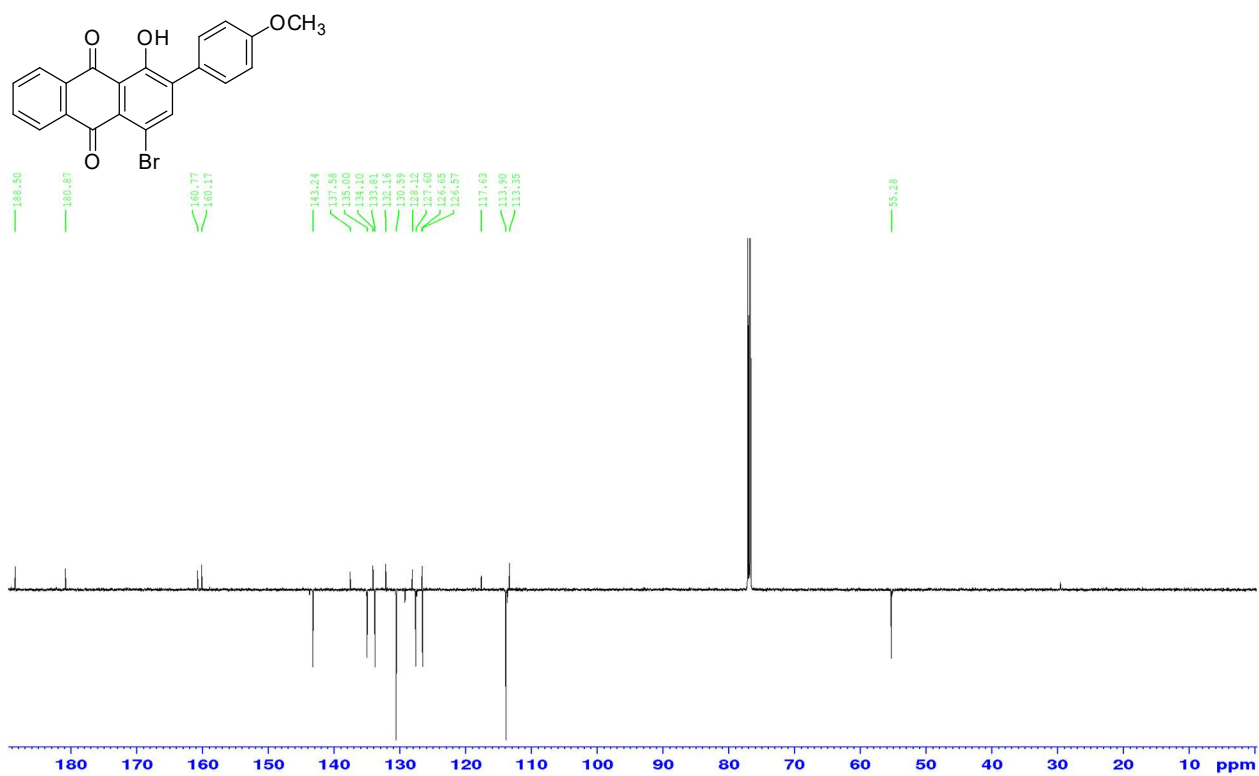


4-bromo-1-hydroxy-2-(4-methoxyphenyl)anthracene-9,10-dione (40)

^1H NMR (CDCl_3 , 400 MHz)

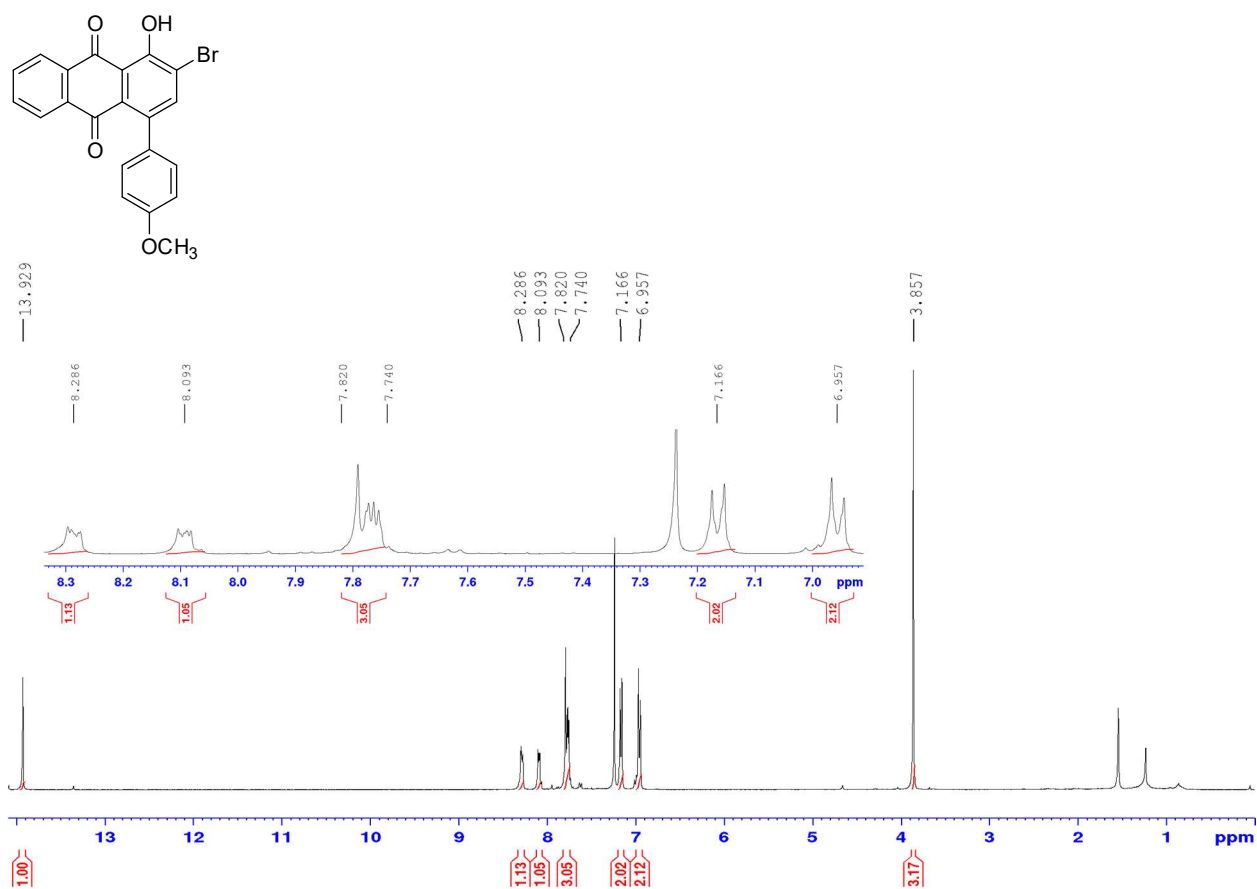


^{13}C NMR (CDCl_3 , 150MHz)

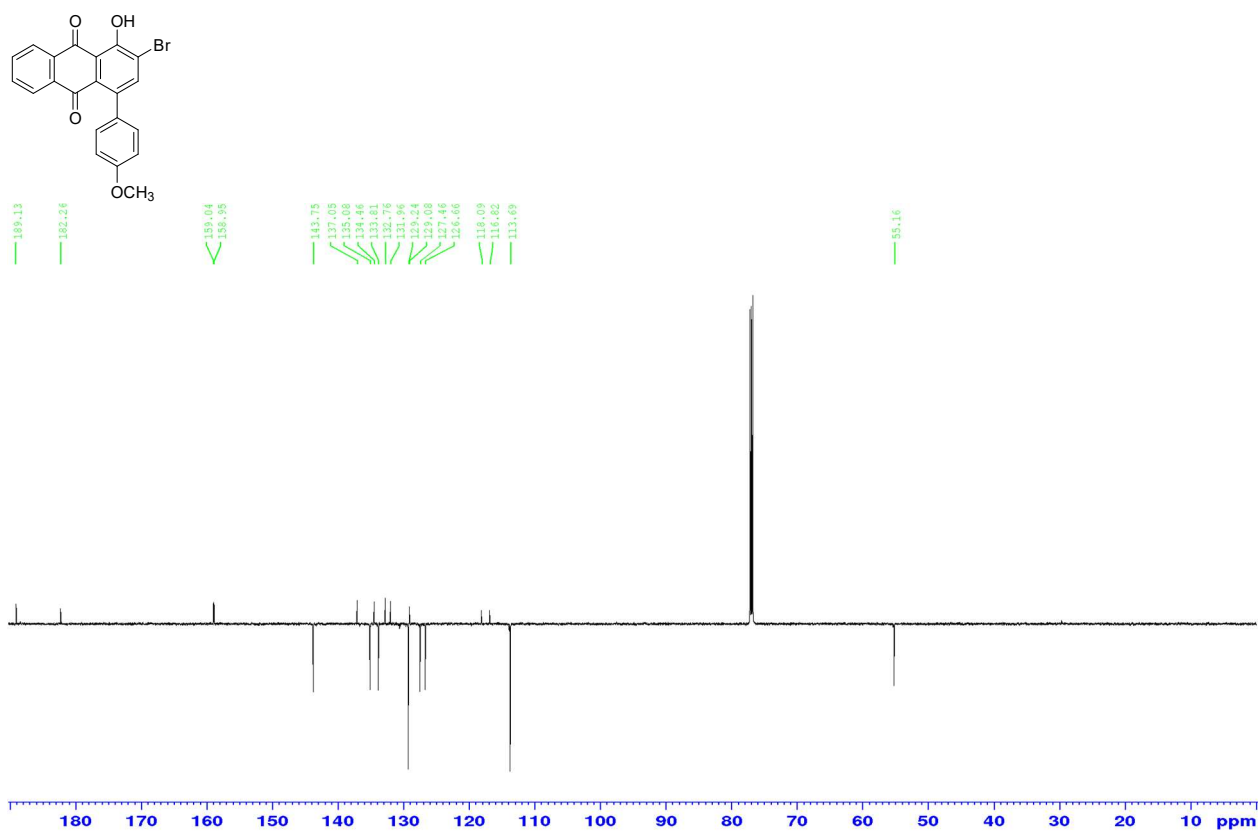


2-bromo-1-hydroxy-4-(4-methoxyphenyl)anthracene-9,10-dione (41)

$^1\text{H NMR}$ (CDCl_3 , 400 MHz)

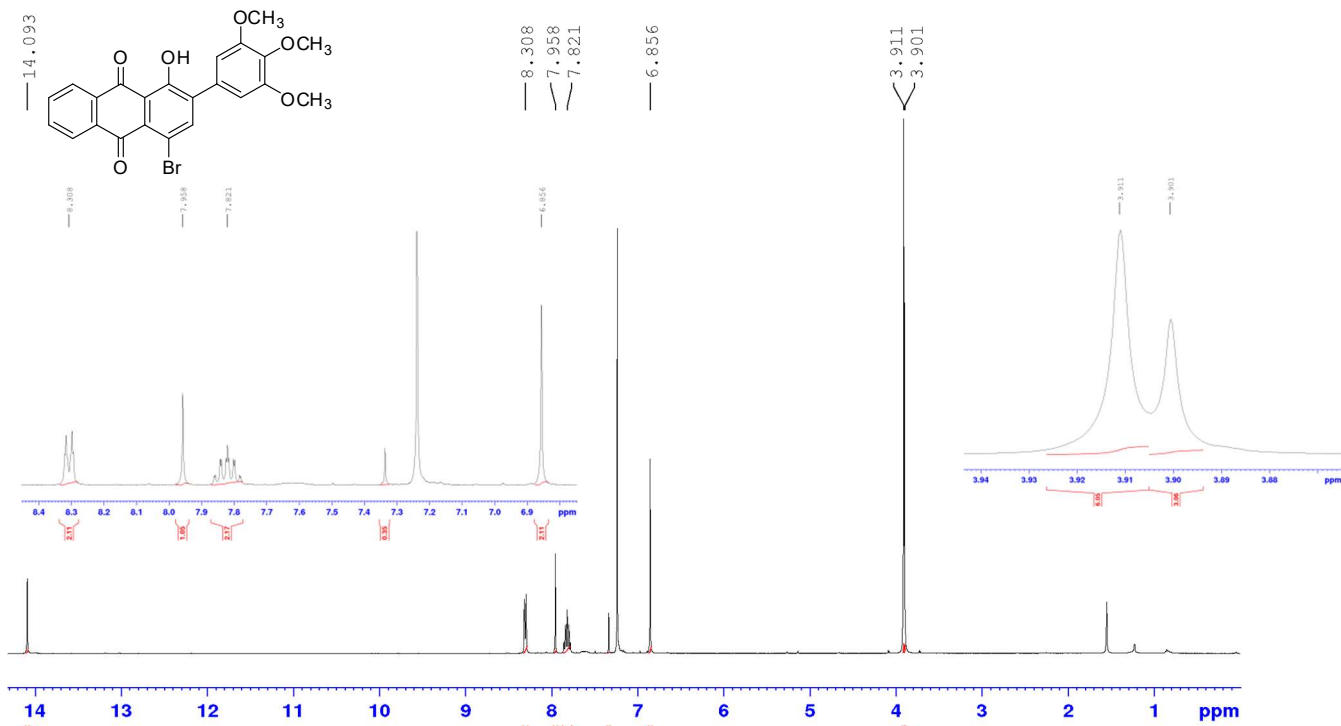


$^{13}\text{C NMR}$ (CDCl_3 , 150MHz)

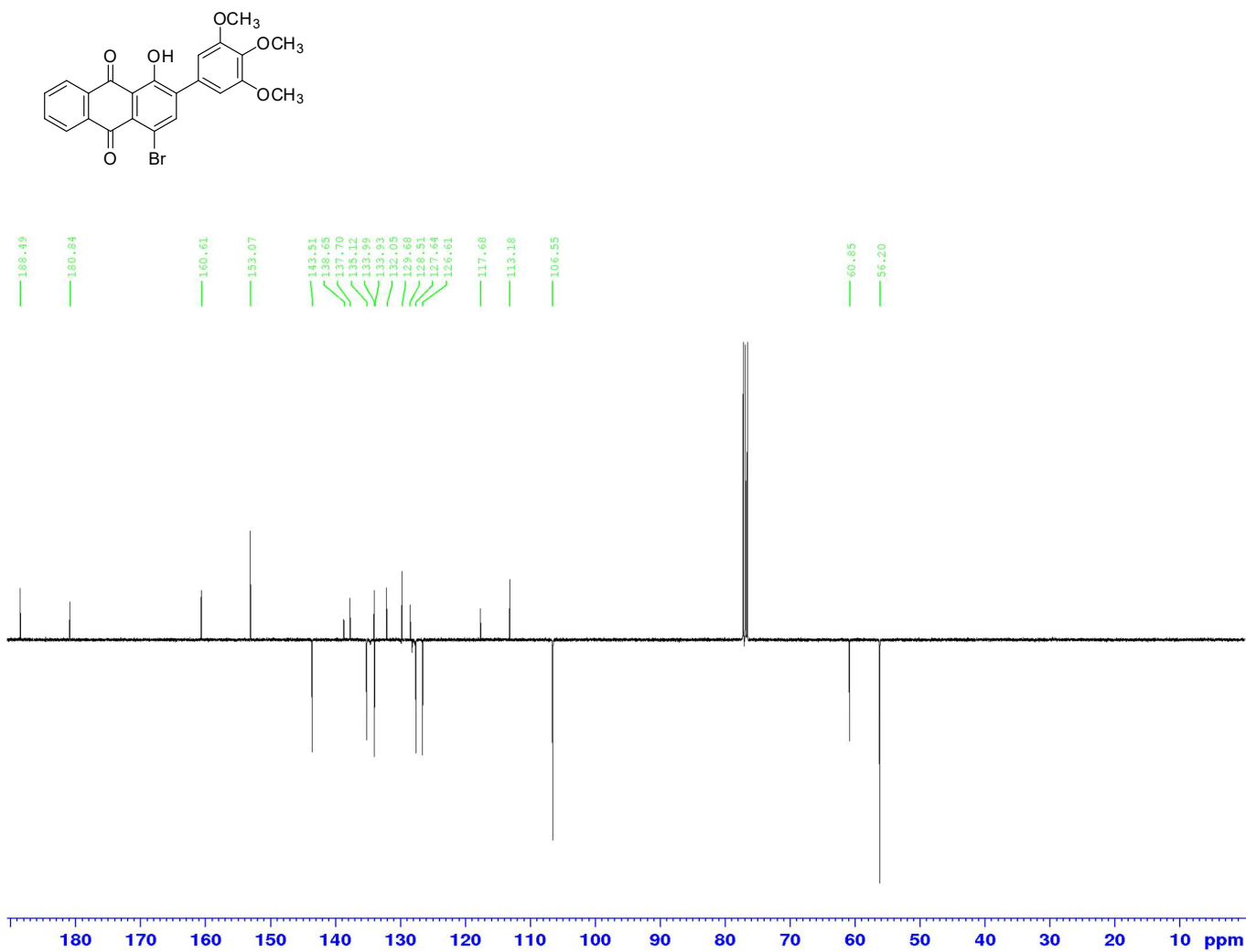


4-Bromo-1-hydroxy-2-(3,4,5-trimethoxyphenyl)anthracene-9,10-dione (42)

^1H NMR (CDCl_3 , 400 MHz)

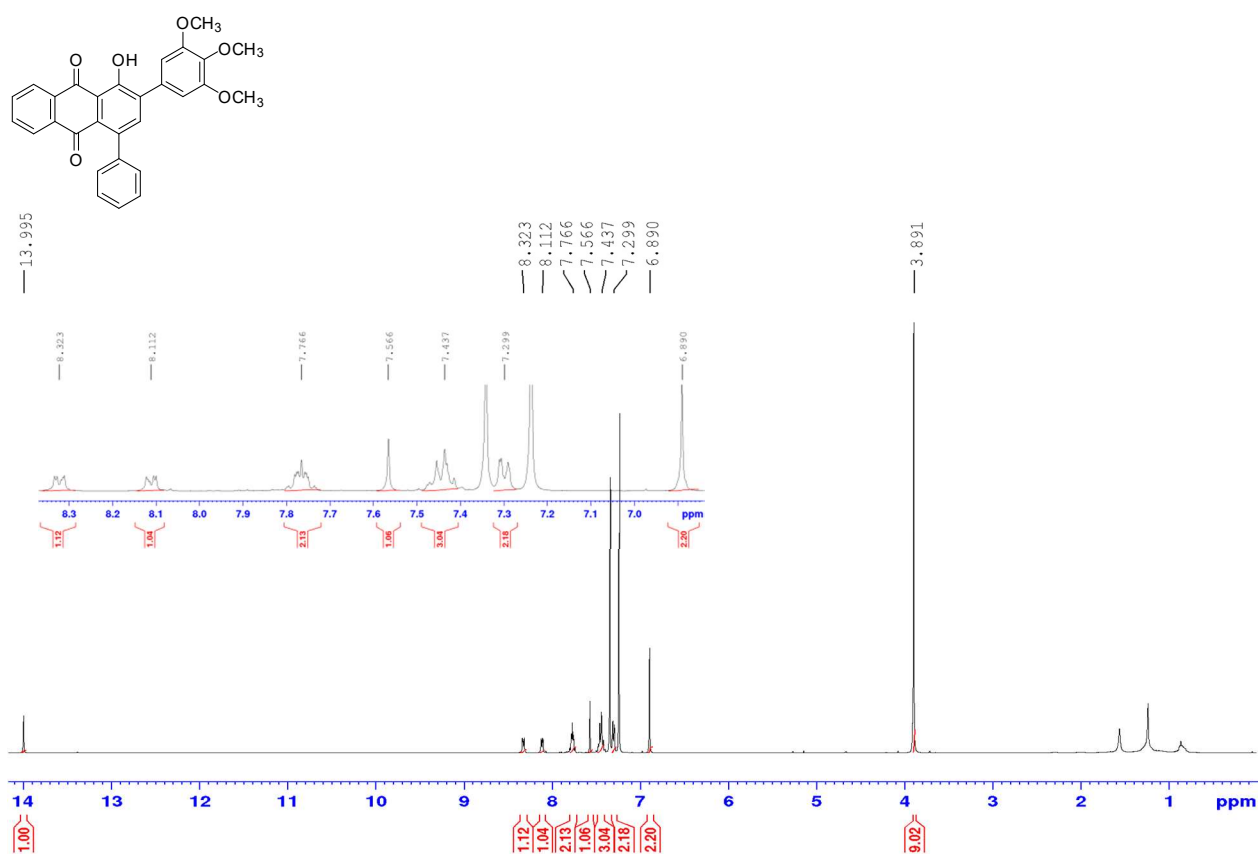


^{13}C NMR (CDCl_3 , 100 MHz)

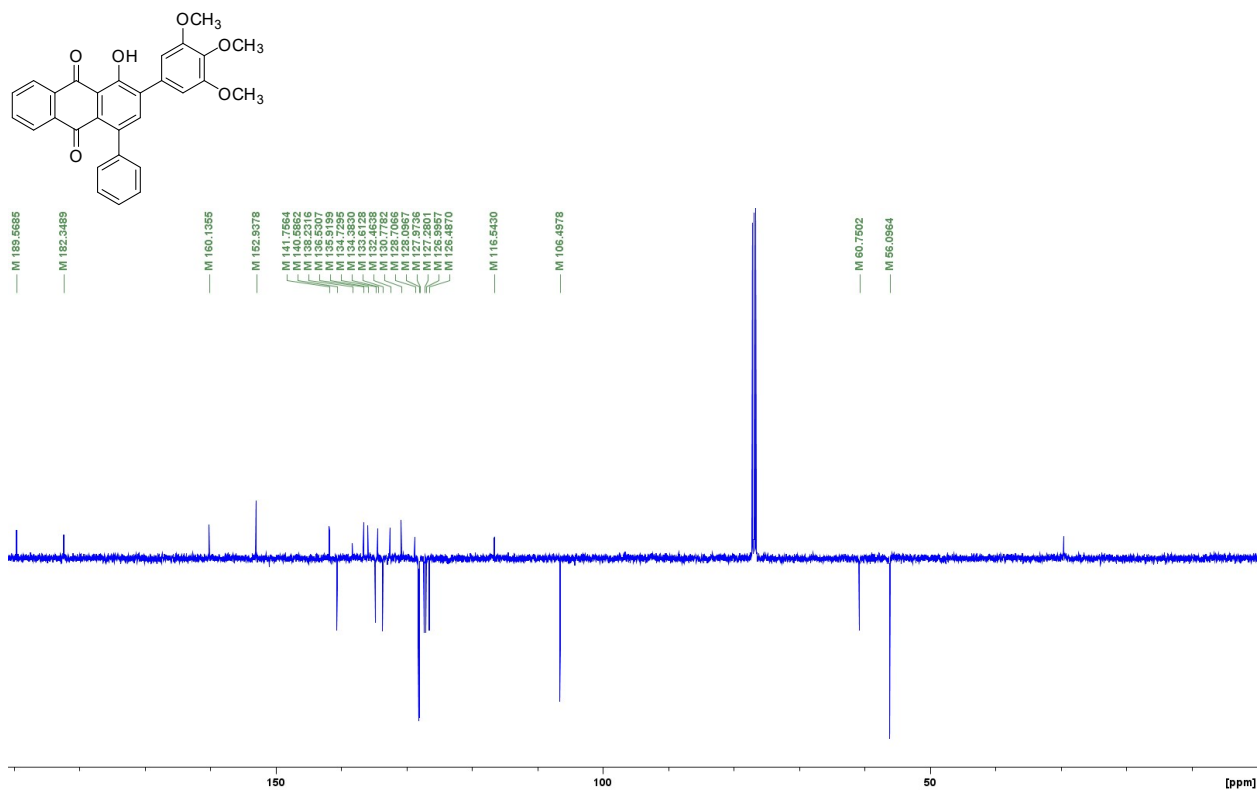


1-Hydroxy-4-phenyl-2-(3,4,5-trimethoxyphenyl)anthracene-9,10-dione (43)

^1H NMR (CDCl_3 , 400 MHz)

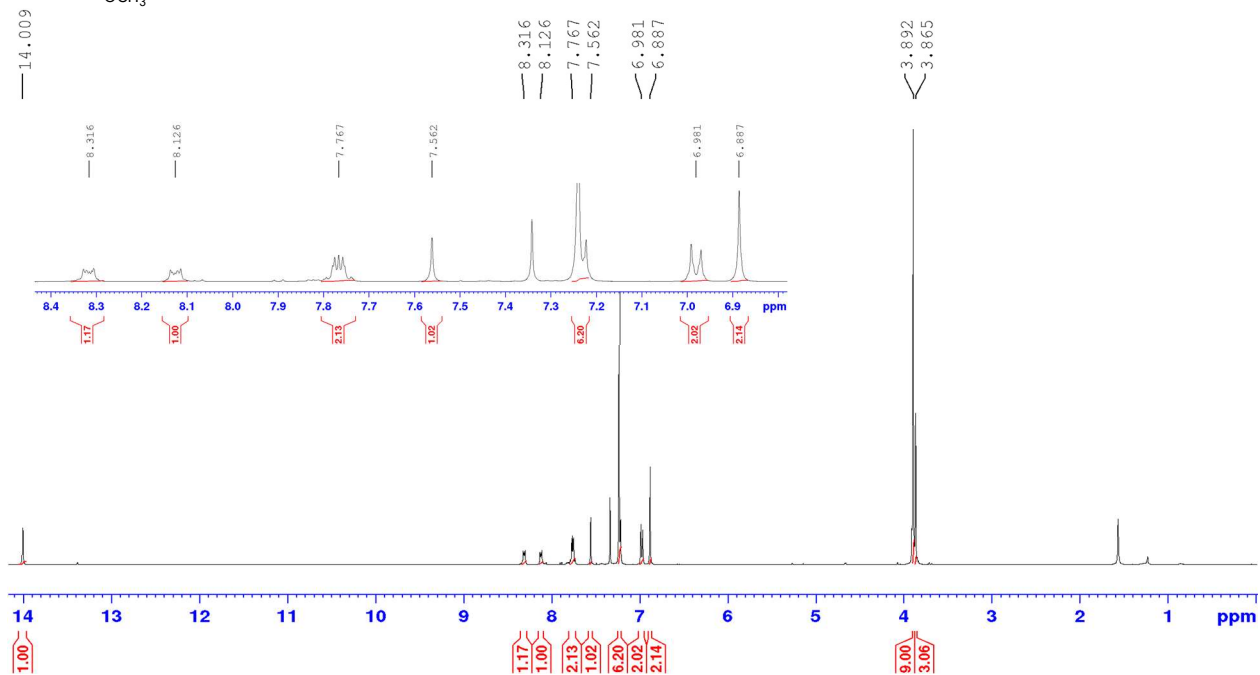
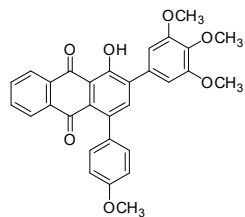


^{13}C NMR (CDCl_3 , 125 MHz)

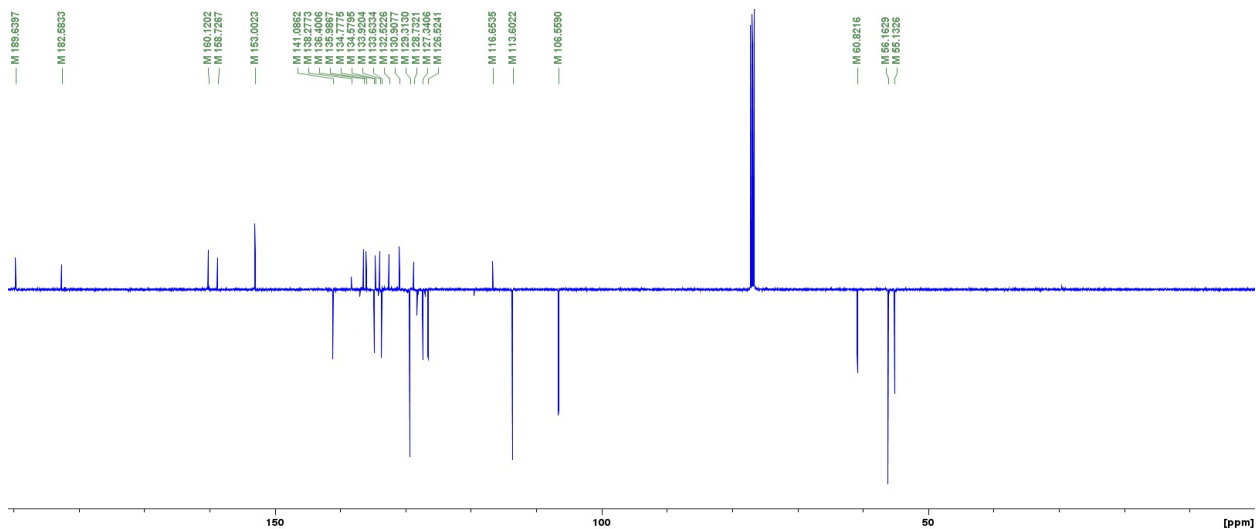


1-Hydroxy-4-(4-methoxyphenyl)-2-(3,4,5-trimethoxyphenyl)anthracene-9,10-dione (44)

¹H NMR (CDCl₃, 400 MHz)

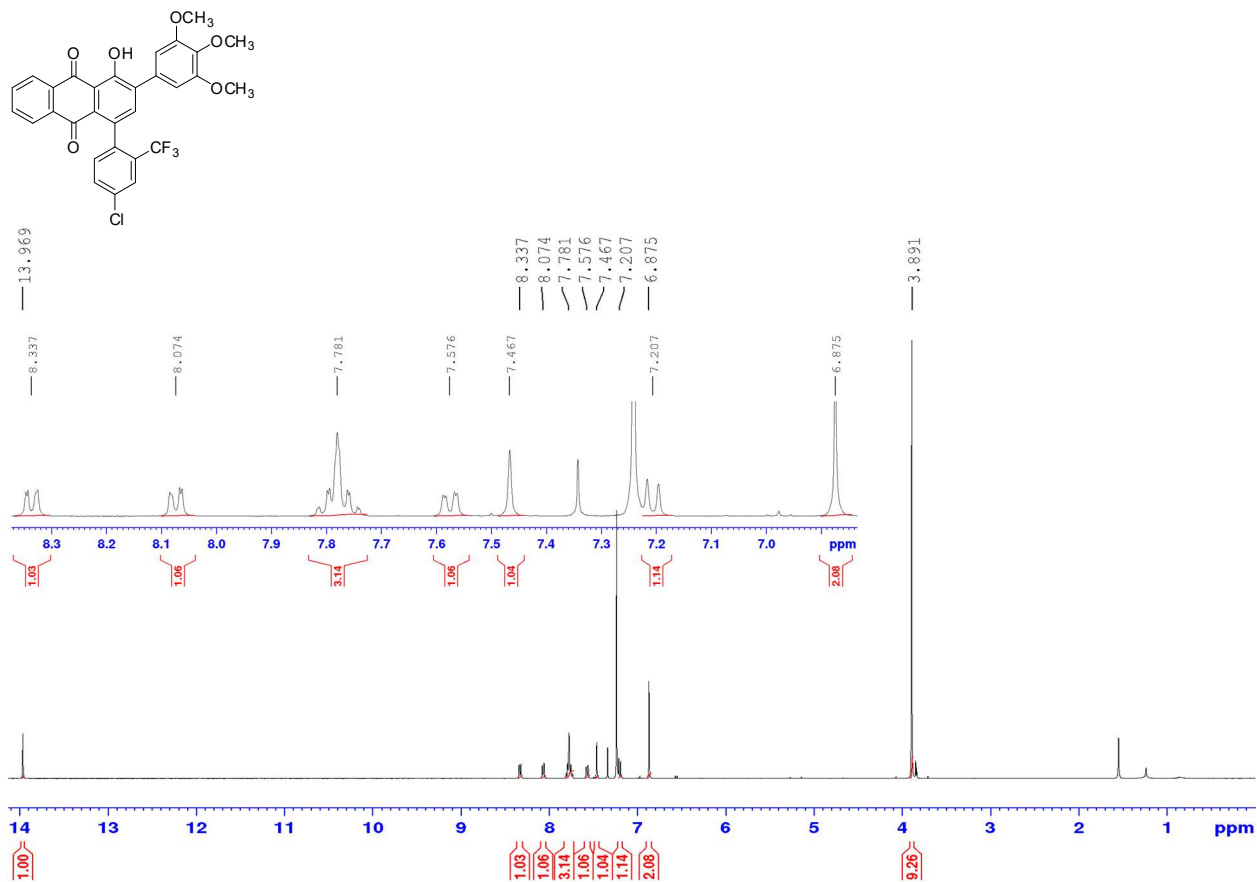


¹³C NMR (CDCl₃, 125 MHz)

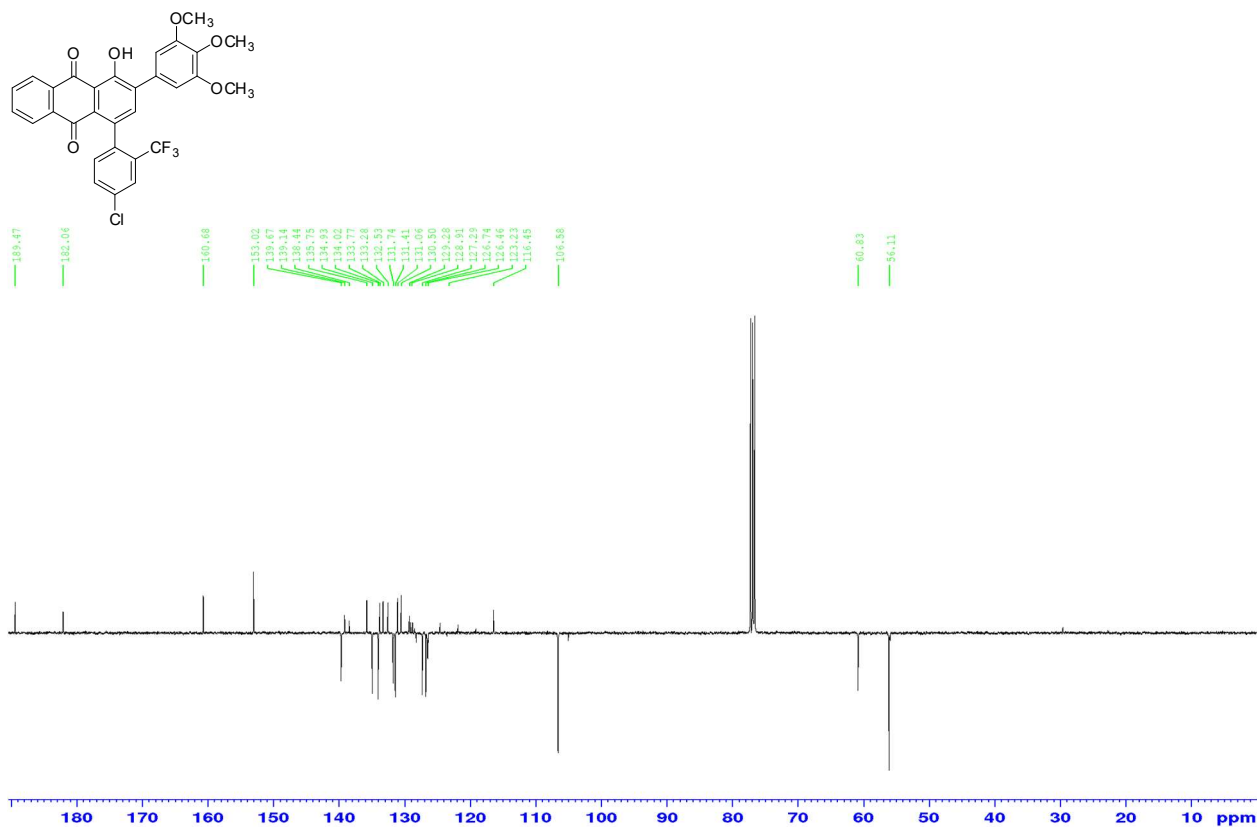


4-(4-Chloro-2-(trifluoromethyl)phenyl)-1-hydroxy-2-(3,4,5-trimethoxyphenyl)anthracene-9,10-dione (45)

¹H NMR (CDCl₃, 400 MHz)



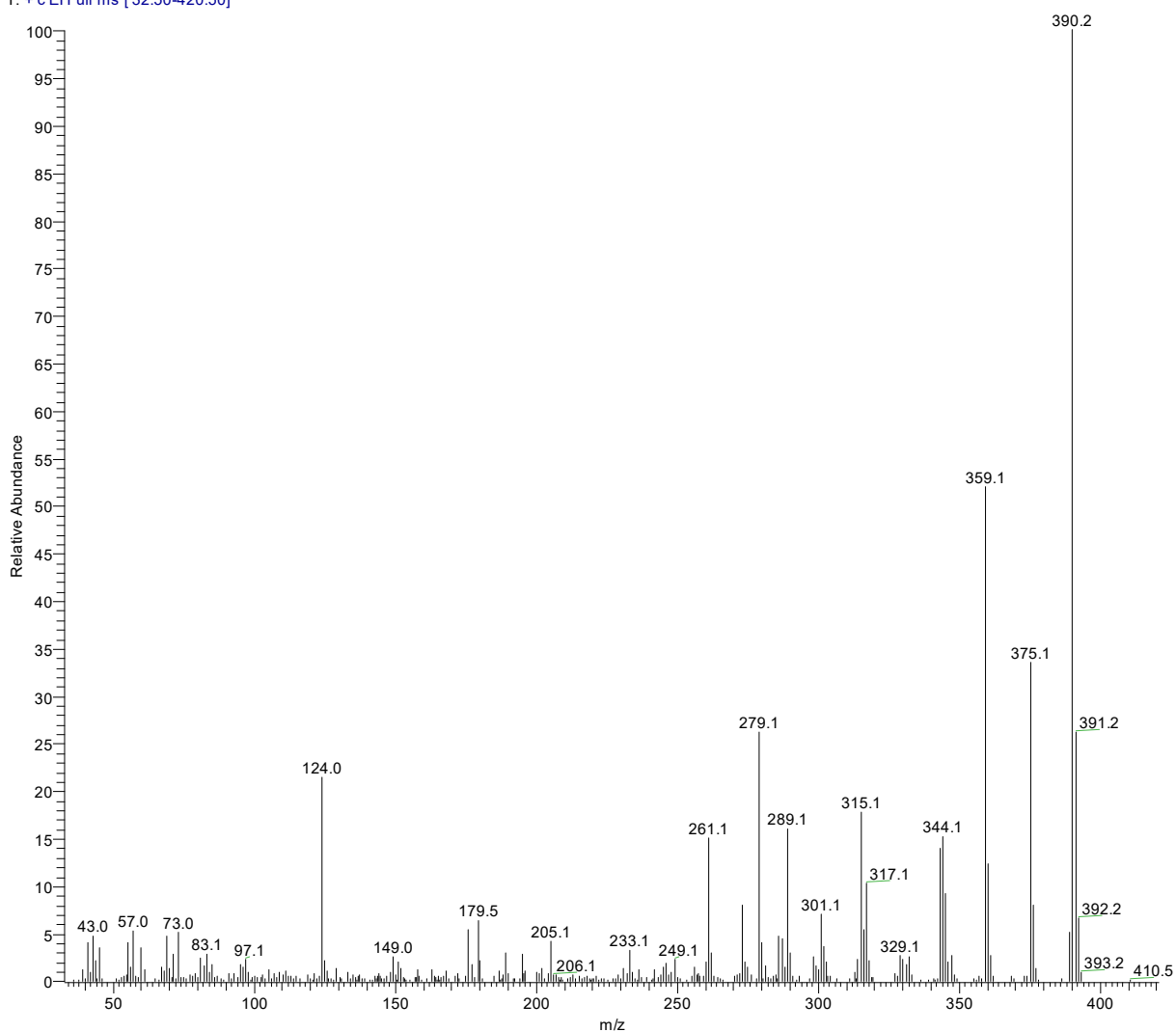
¹³C NMR (CDCl₃, 100MHz)



HR-MS spectra

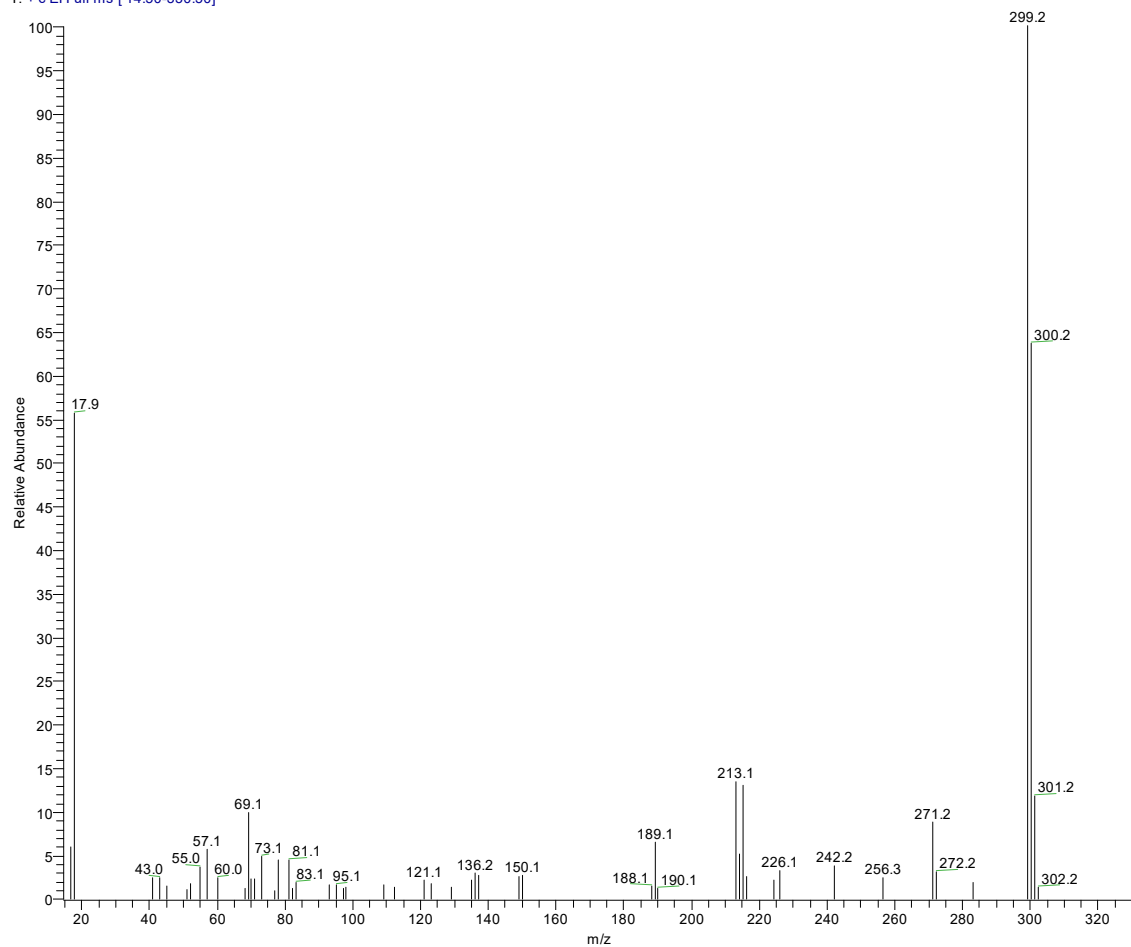
1-Hydroxy-4-(3,4,5-trimethoxyphenyl)anthracene-9,10-dione (5)

C-18-09-kp-II #15 RT: 0.84 AV: 1 NL: 1.86E6
T: + c EI Full ms [32.50-420.50]



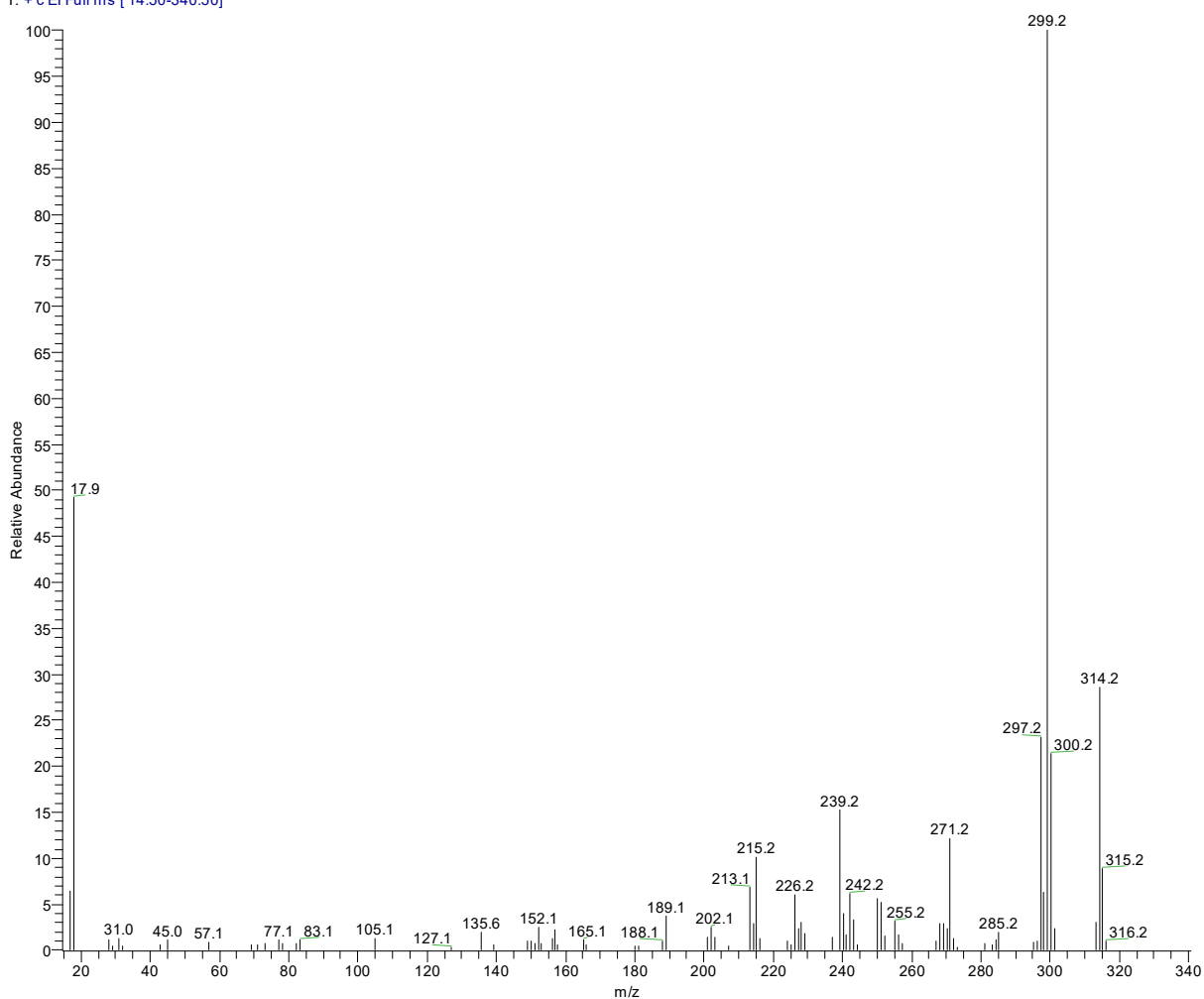
1-Hydroxy-4-phenylanthracene-9,10-dione (13)

HC-58 #2 RT: 0.14 AV: 1 NL: 7.05E5
T: + c EI Full ms [14.50-330.50]



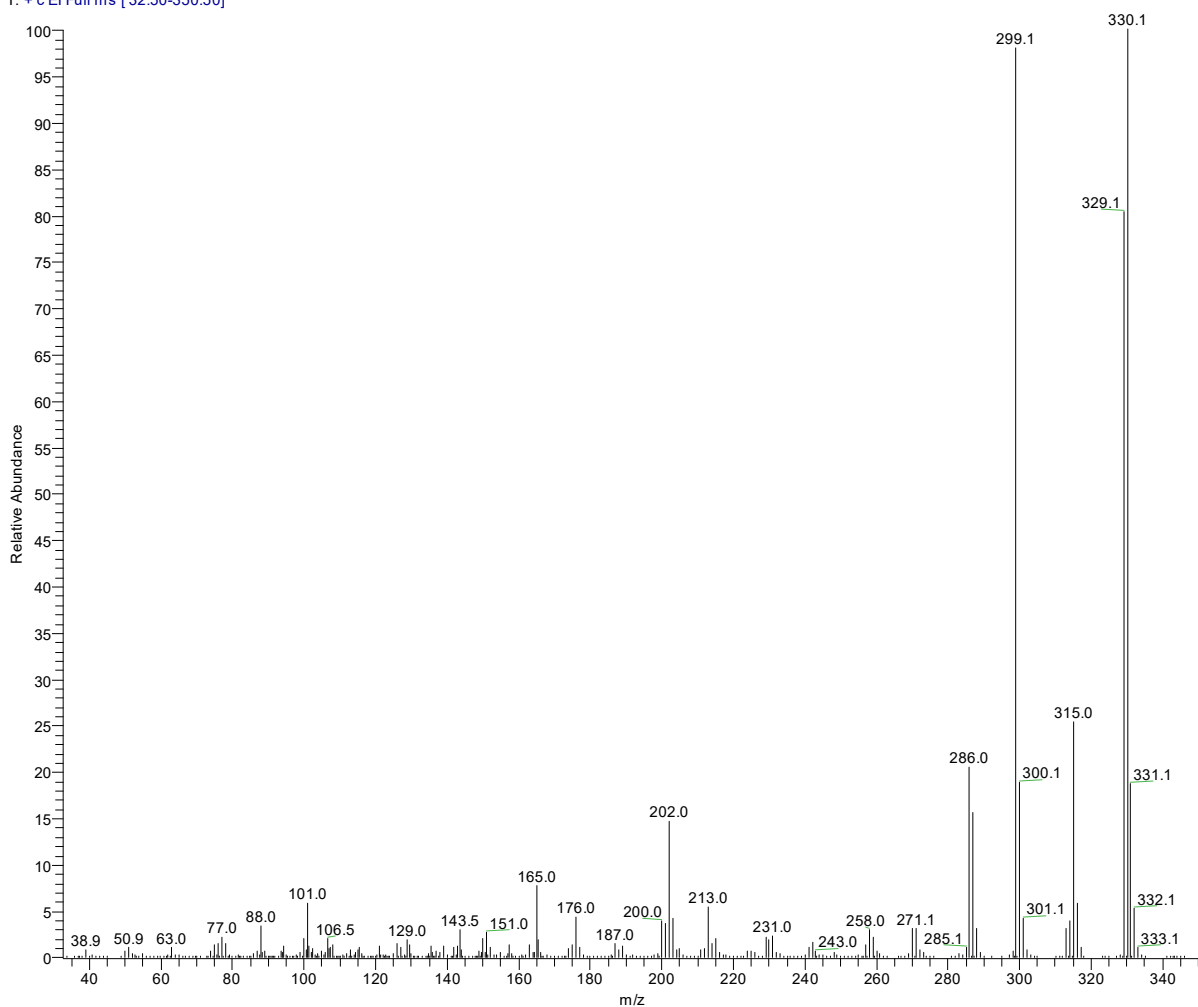
1-Hydroxy-4-(o-tolyl)anthracene-9,10-dione (14)

HC-57 #2 RT: 0.08 AV: 1 NL: 1.82E6
T: + c EI Full ms [14.50-340.50]



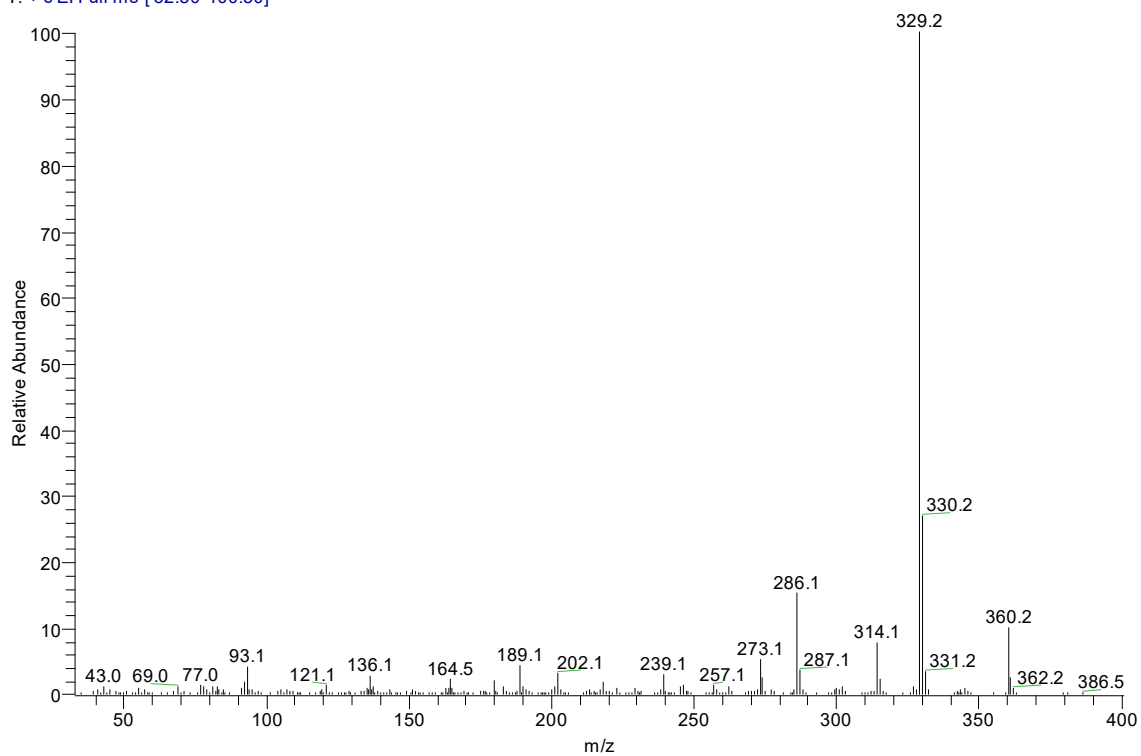
1-Hydroxy-4-(4-methoxyphenyl)anthracene-9,10-dione (15)

HC-84 #8 RT: 0.39 AV: 1 NL: 4.71E7
T: + c EI Full ms [32.50-350.50]



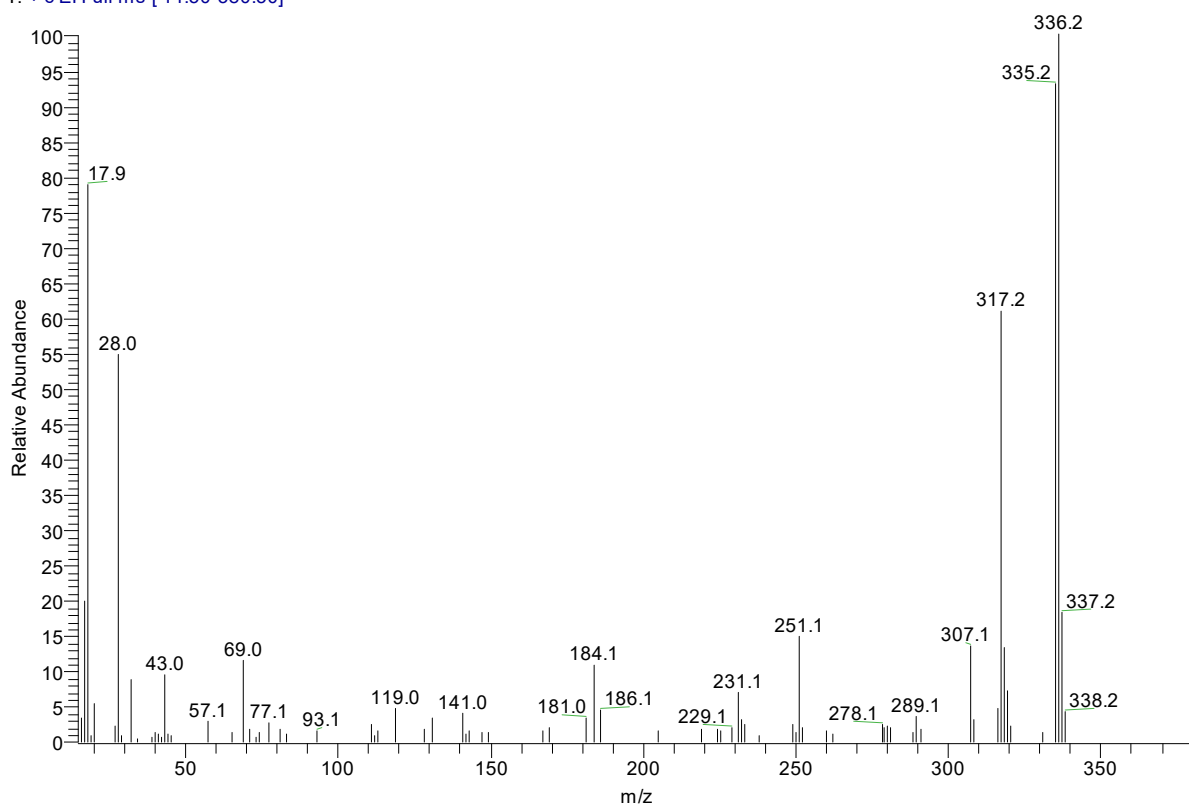
1-(2,3-Dimethoxyphenyl)-4-hydroxyanthracene-9,10-dione (16)

HC-53 _180504153944 #2 RT: 0.06 AV: 1 NL: 3.40E6
T: + c EI Full ms [32.50-400.50]



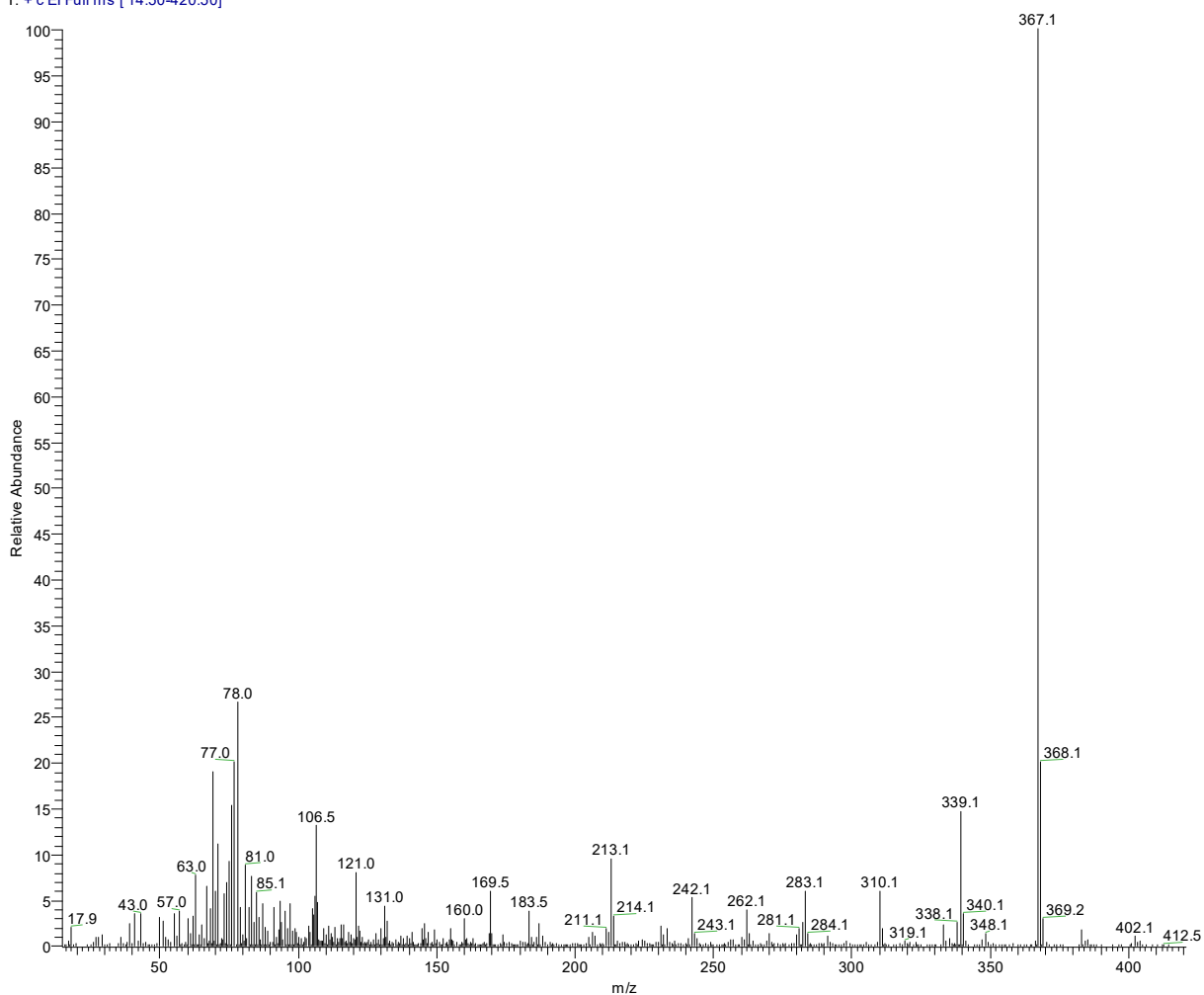
1-(3,5-Difluorophenyl)-4-hydroxyanthracene-9,10-dione (17)

HC-56_180604193113 #4 RT: 0.30 AV: 1 NL: 2.70E6
T: + c EI Full ms [14.50-380.50]



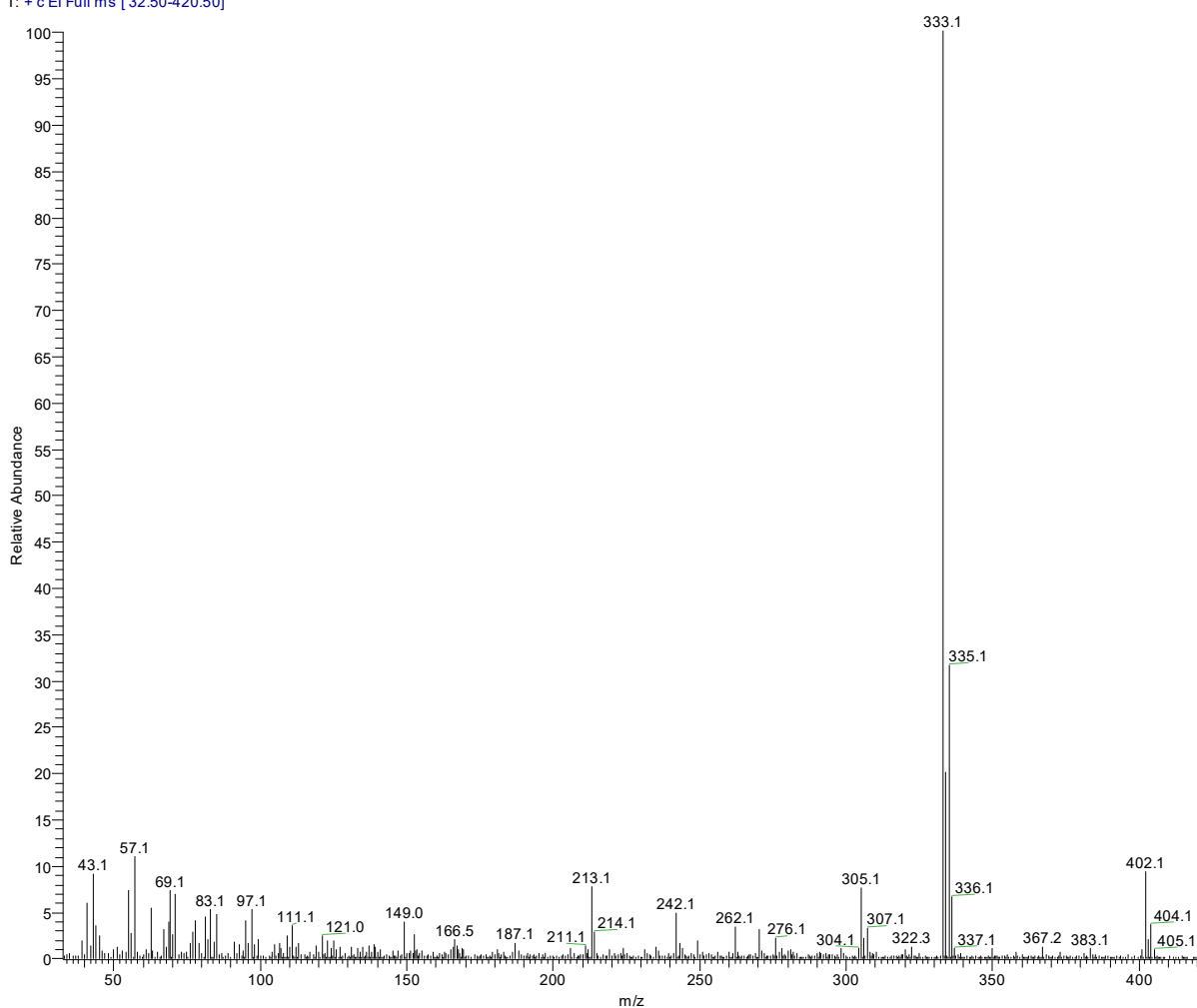
1-(2-Chloro-5-(trifluoromethyl)phenyl)-4-hydroxyanthracene-9,10-dione (18)

HC-79 #29 RT: 1.81 AV: 1 NL: 3.23E7
T: + c EI Full ms [14.50-420.50]



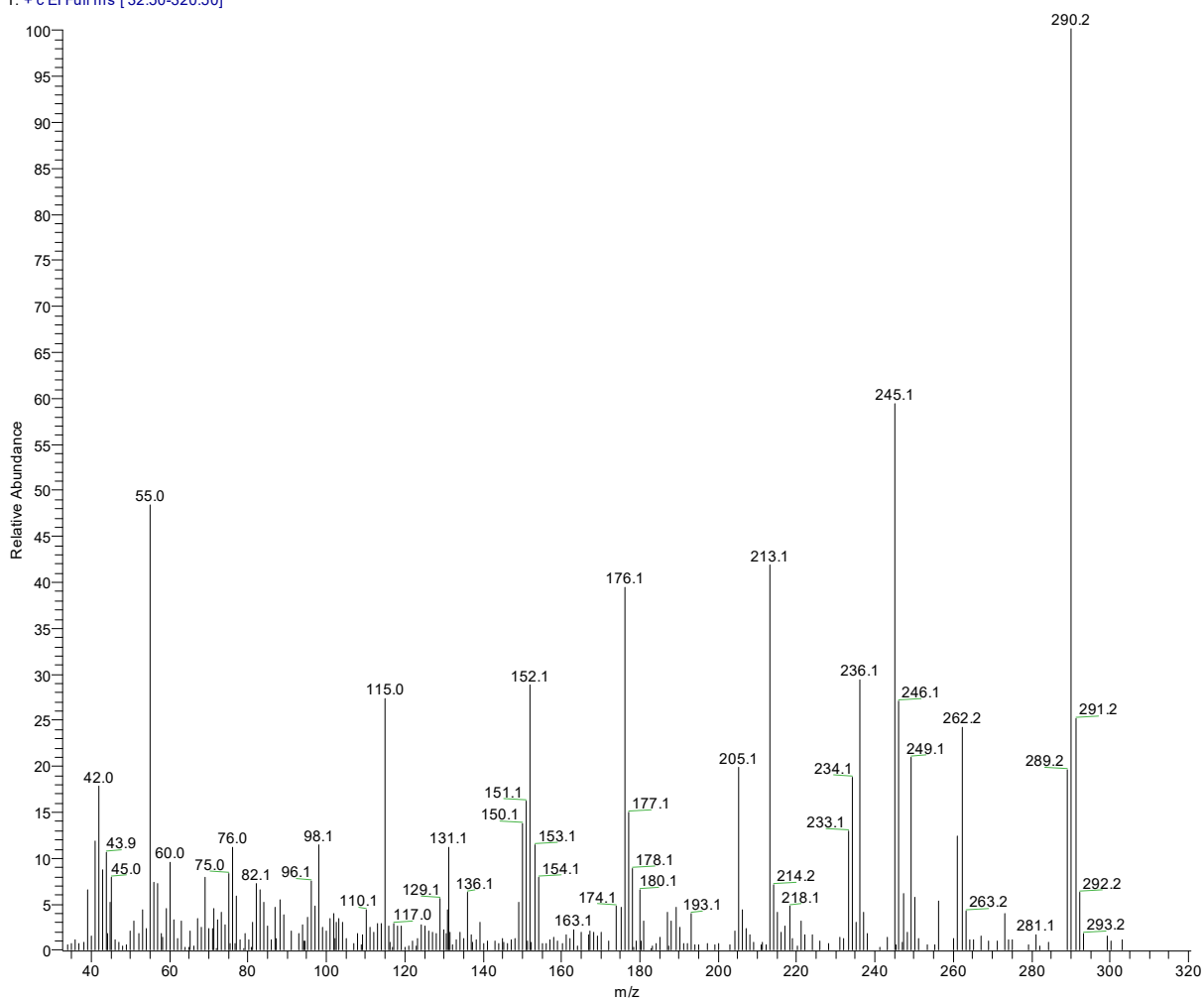
1-(4-Chloro-2-(trifluoromethyl)phenyl)-4-hydroxyanthracene-9,10-dione (19)

HC-80 #18 RT: 1.02 AV: 1 NL: 2.66E7
T: + c EI Full ms [32.50-420.50]



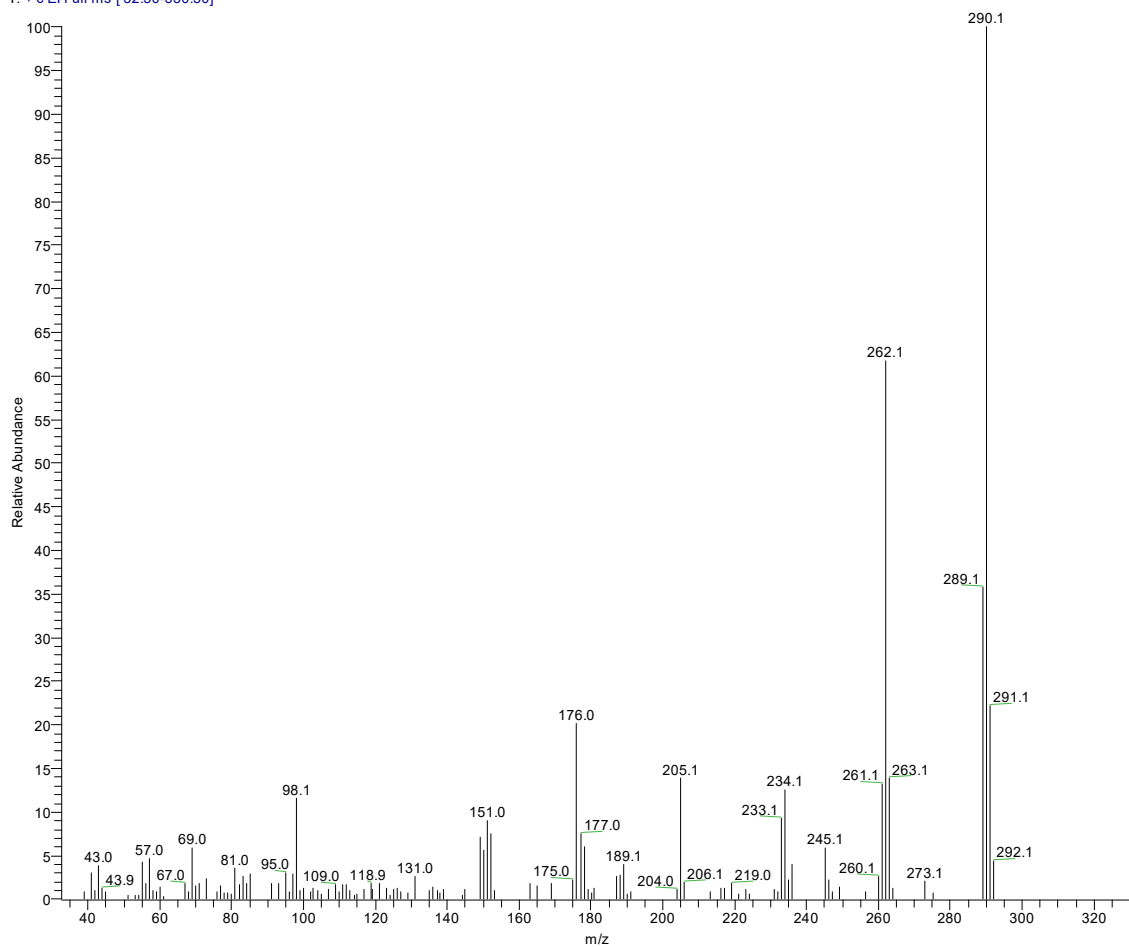
1-(Furan-2-yl)-4-hydroxyanthracene-9,10-dione (22)

HC-59 #23 RT: 1.19 AV: 1 NL: 5.75E6
T: + c EI Full ms [32.50-320.50]



1-(Furan-3-yl)-4-hydroxyanthracene-9,10-dione (23)

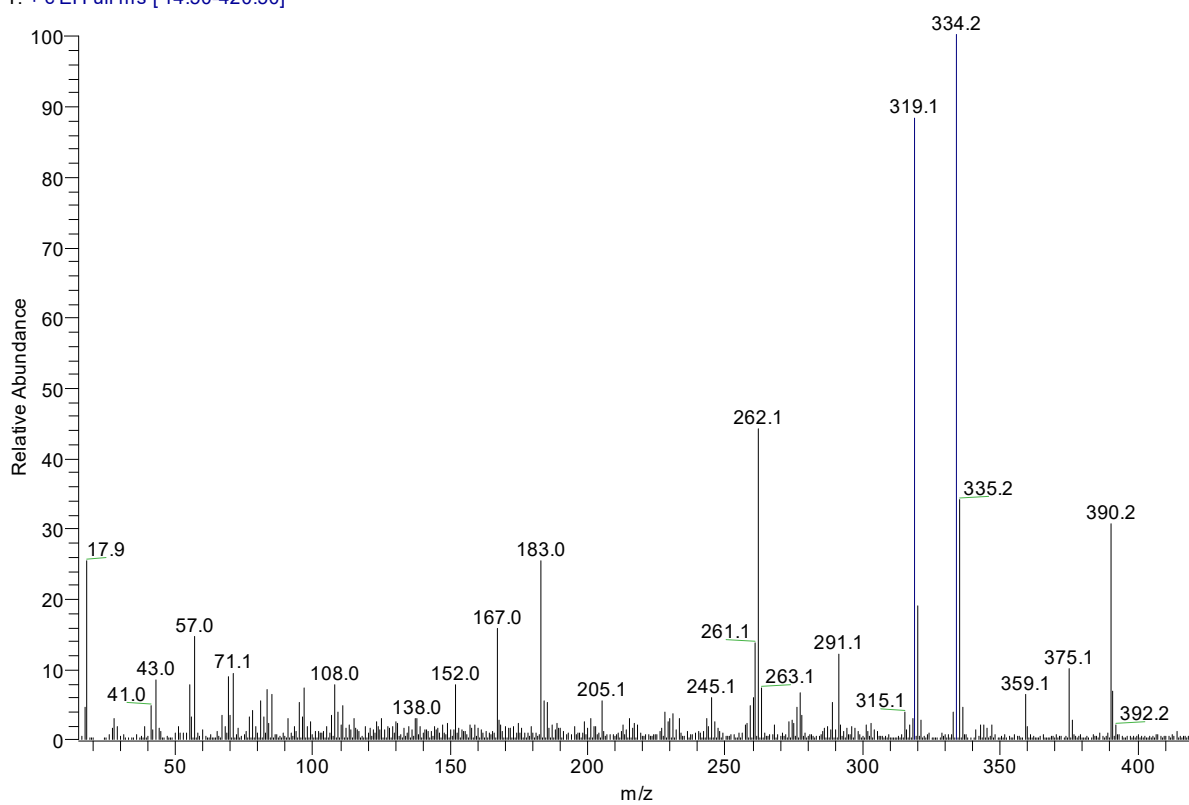
C-18-10kp #18 RT: 0.93 AV: 1 NL: 1.79E6
T: + c EI Full ms [32.50-330.50]



1-Hydroxy-2-(3,4,5-trimethoxyphenyl)anthracene-9,10-dione (24)

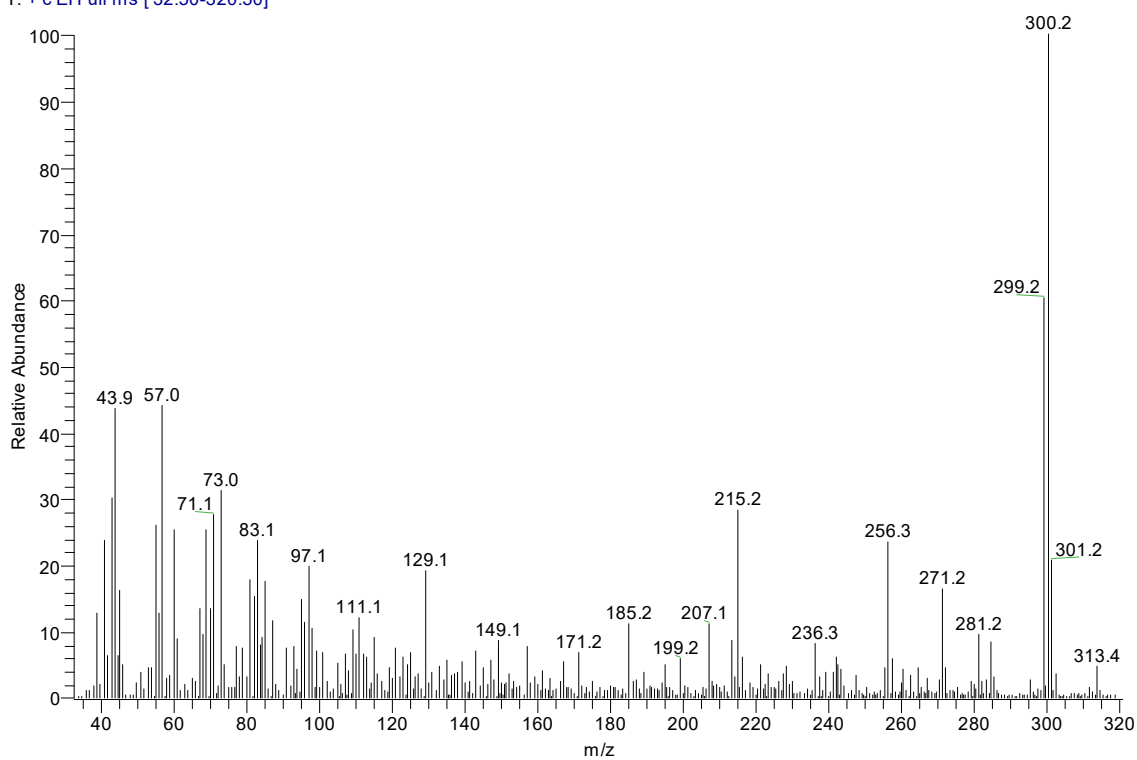
HC-87 #5 RT: 0.31 AV: 1 NL: 1.43E8

T: + c EI Full ms [14.50-420.50]



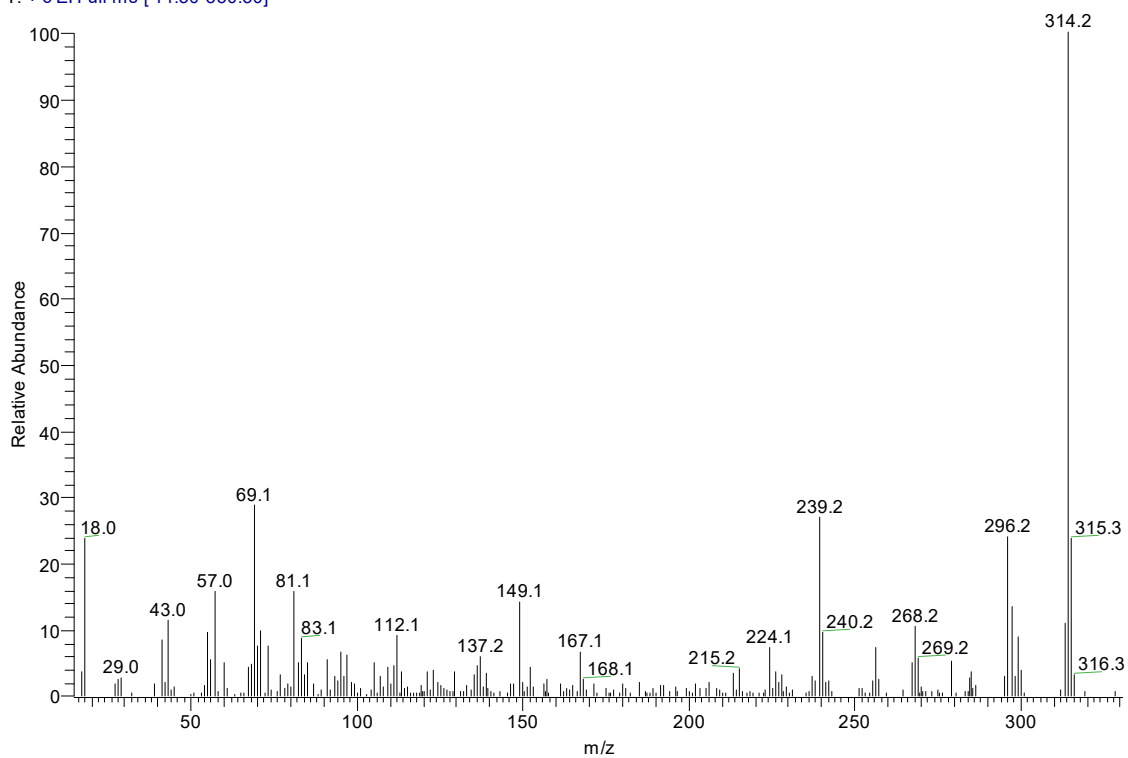
1-Hydroxy-2-phenylanthracene-9,10-dione (25)

HC-38-1_180523155353 #16 RT: 1.07 AV: 1 NL: 1.62E7
T: + c EI Full ms [32.50-320.50]



1-Hydroxy-2-(o-tolyl)anthracene-9,10-dione (26)

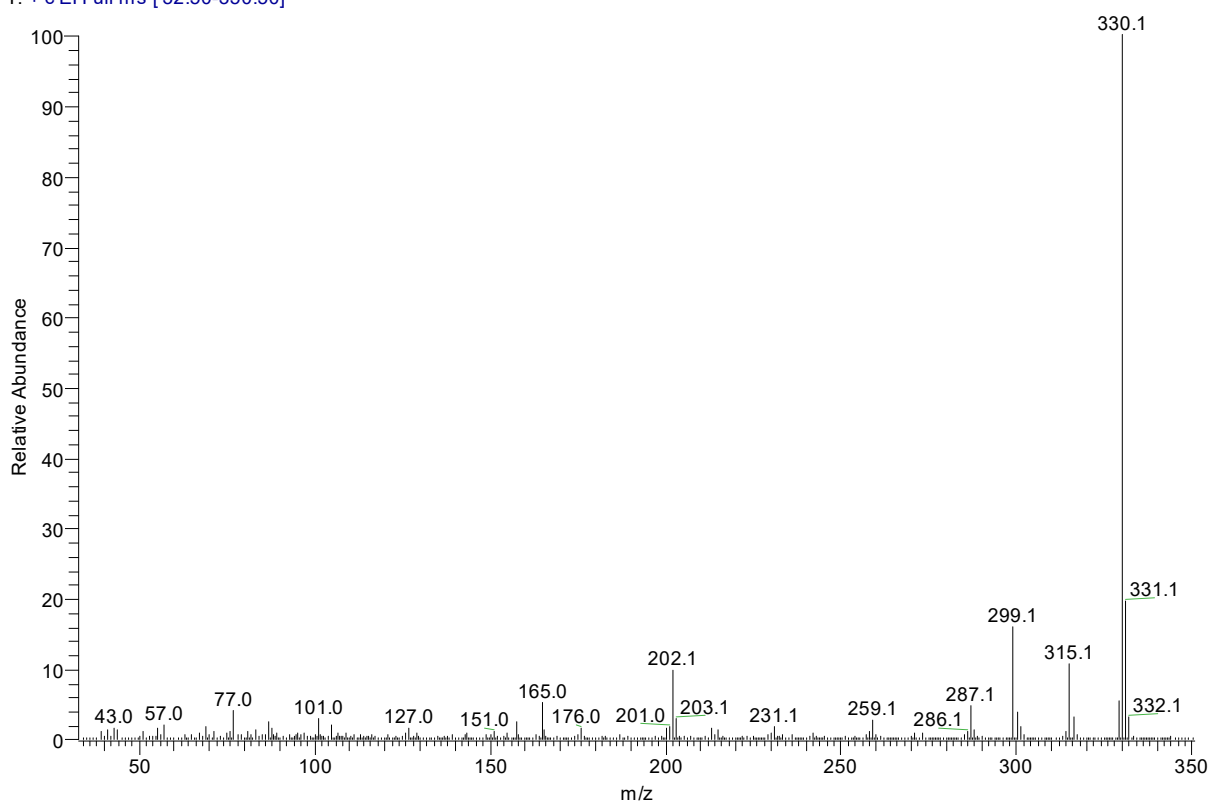
HC-45 #15 RT: 1.08 AV: 1 NL: 8.63E5
T: + c EI Full ms [14.50-330.50]



1-Hydroxy-2-(4-methoxyphenyl)anthracene-9,10-dione (27)

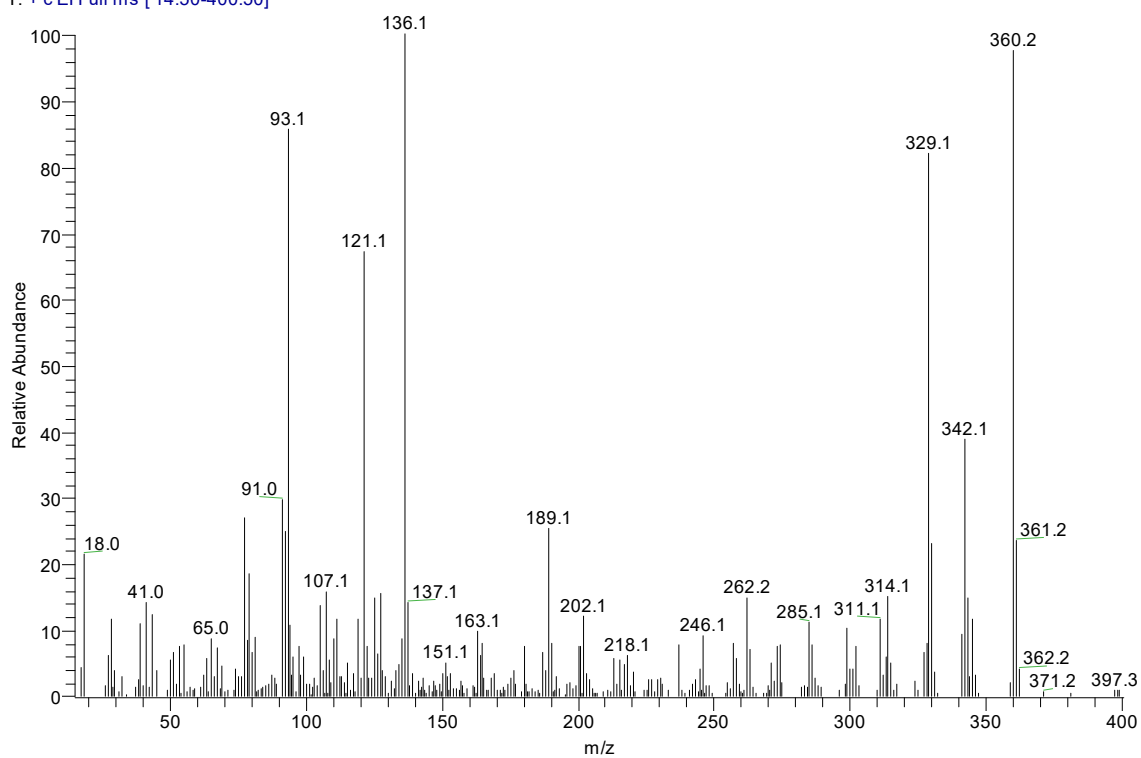
HC-85 #13 RT: 0.78 AV: 1 NL: 6.24E7

T: + c EI Full ms [32.50-350.50]



2-(2,3-Dimethoxyphenyl)-1-hydroxyanthracene-9,10-dione (28)

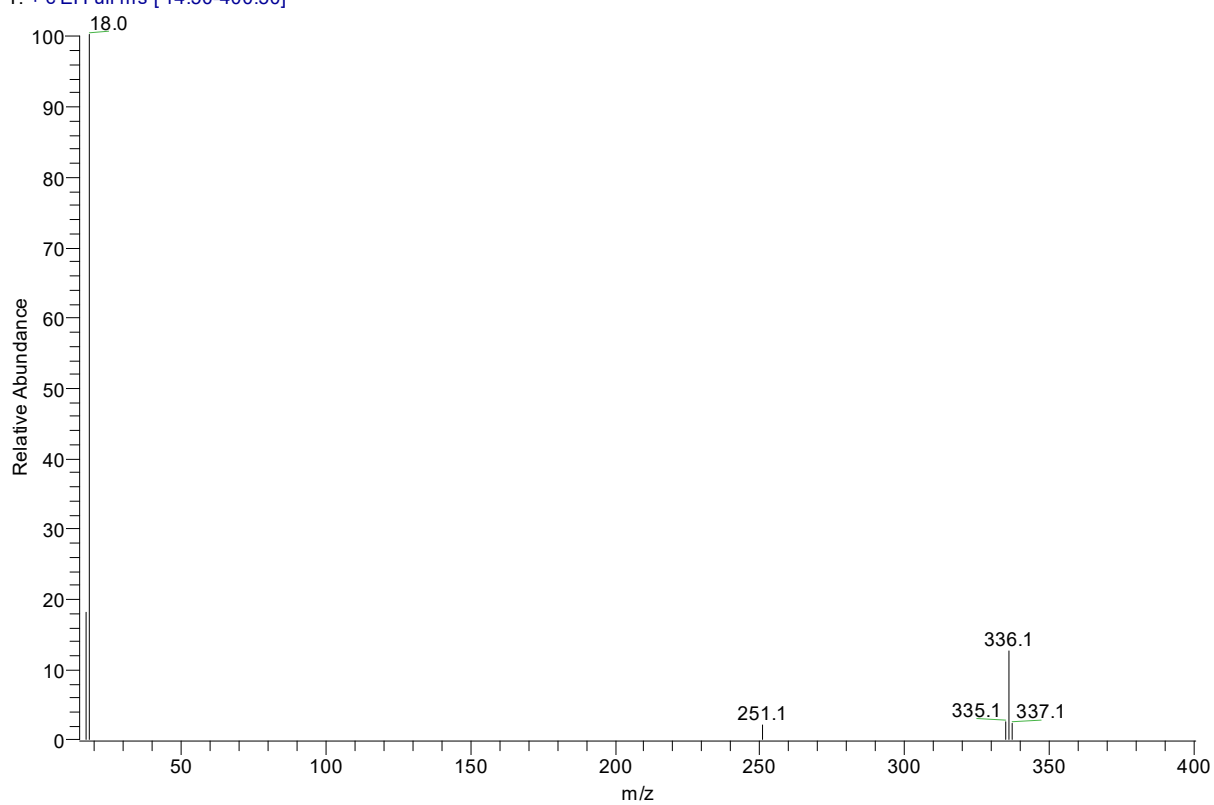
HC-51_180427165923 #1 RT: 0.00 AV: 1 NL: 6.85E5
T: + c EI Full ms [14.50-400.50]



2-(3,5-Difluorophenyl)-1-hydroxyanthracene-9,10-dione (29)

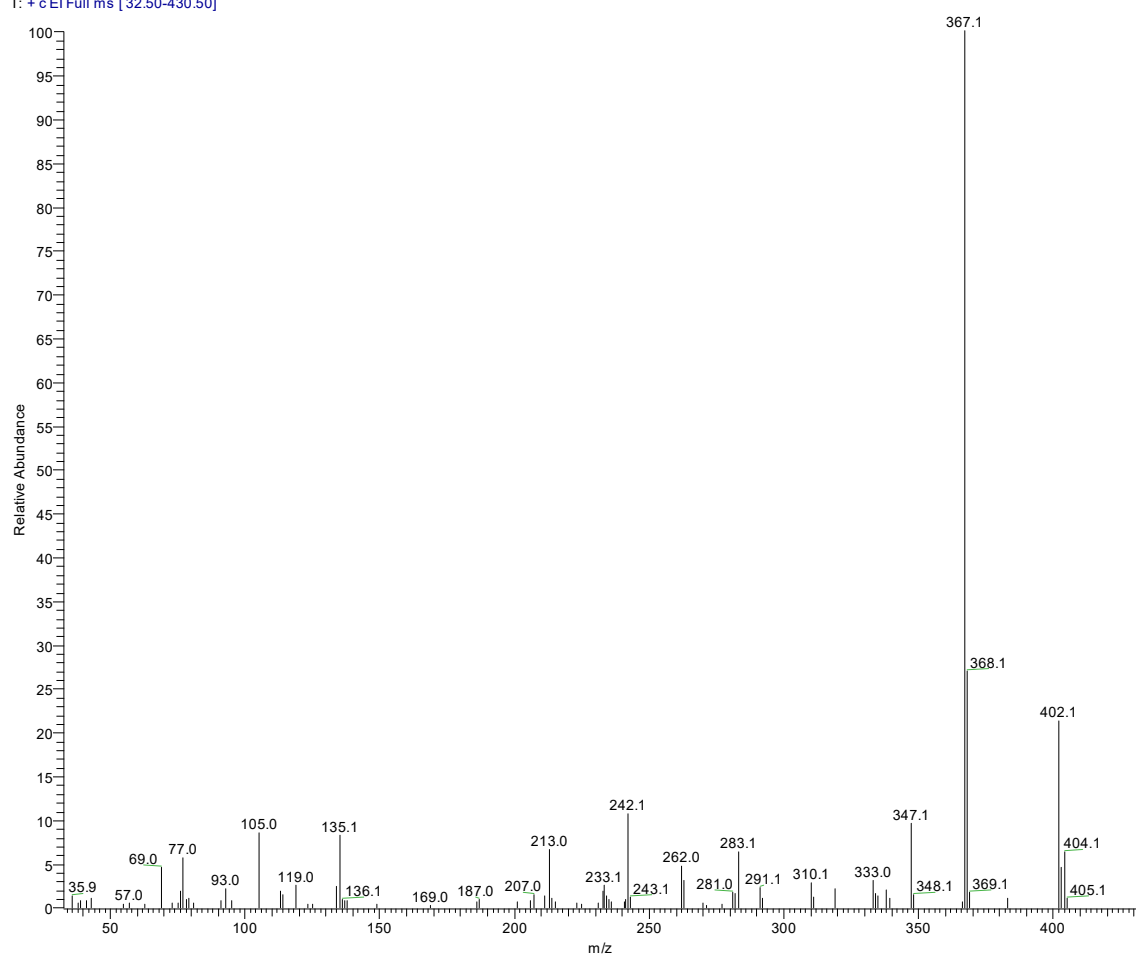
HC-54 #5 RT: 0.40 AV: 1 NL: 5.92E4

T: + c EI Full ms [14.50-400.50]



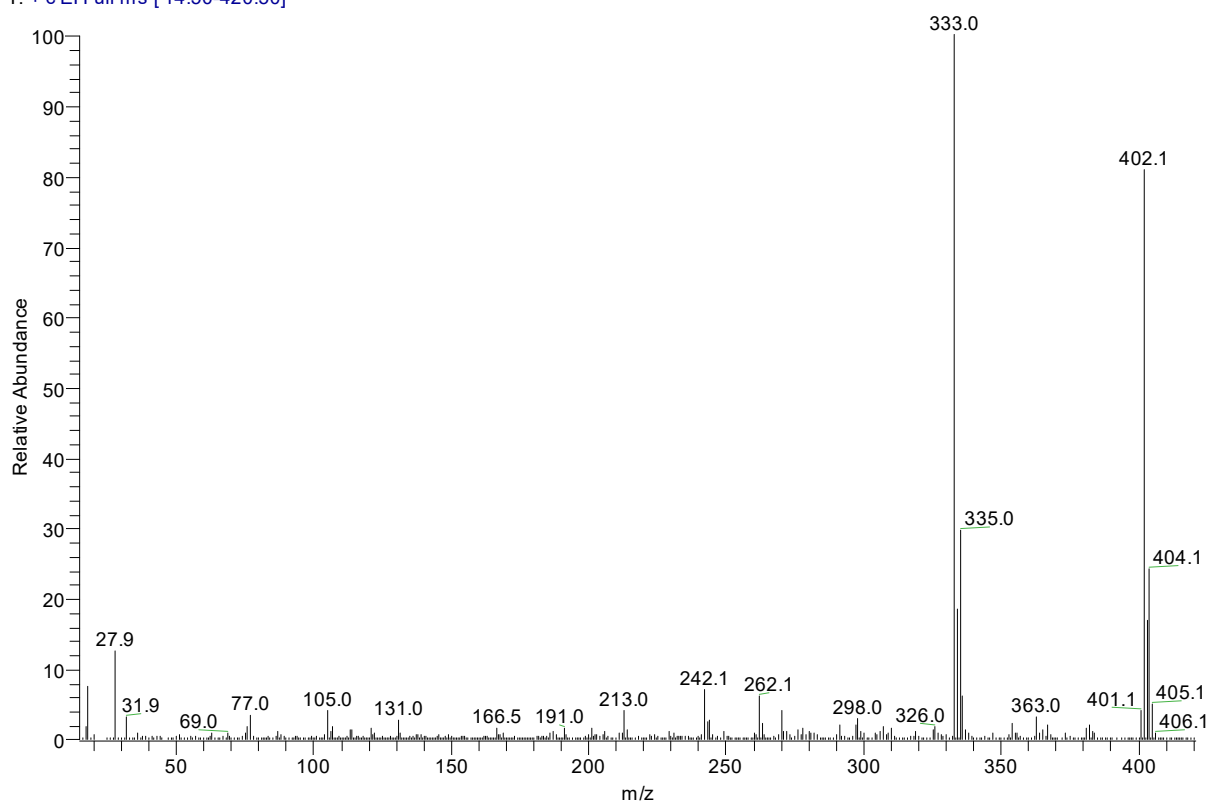
2-(2-Chloro-5-(trifluoromethyl)phenyl)-1-hydroxyanthracene-9,10-dione (30)

HC-48-2kp #4 RT: 0.18 AV: 1 NL: 1.79E6
T: + c EI Full ms [32.50-430.50]



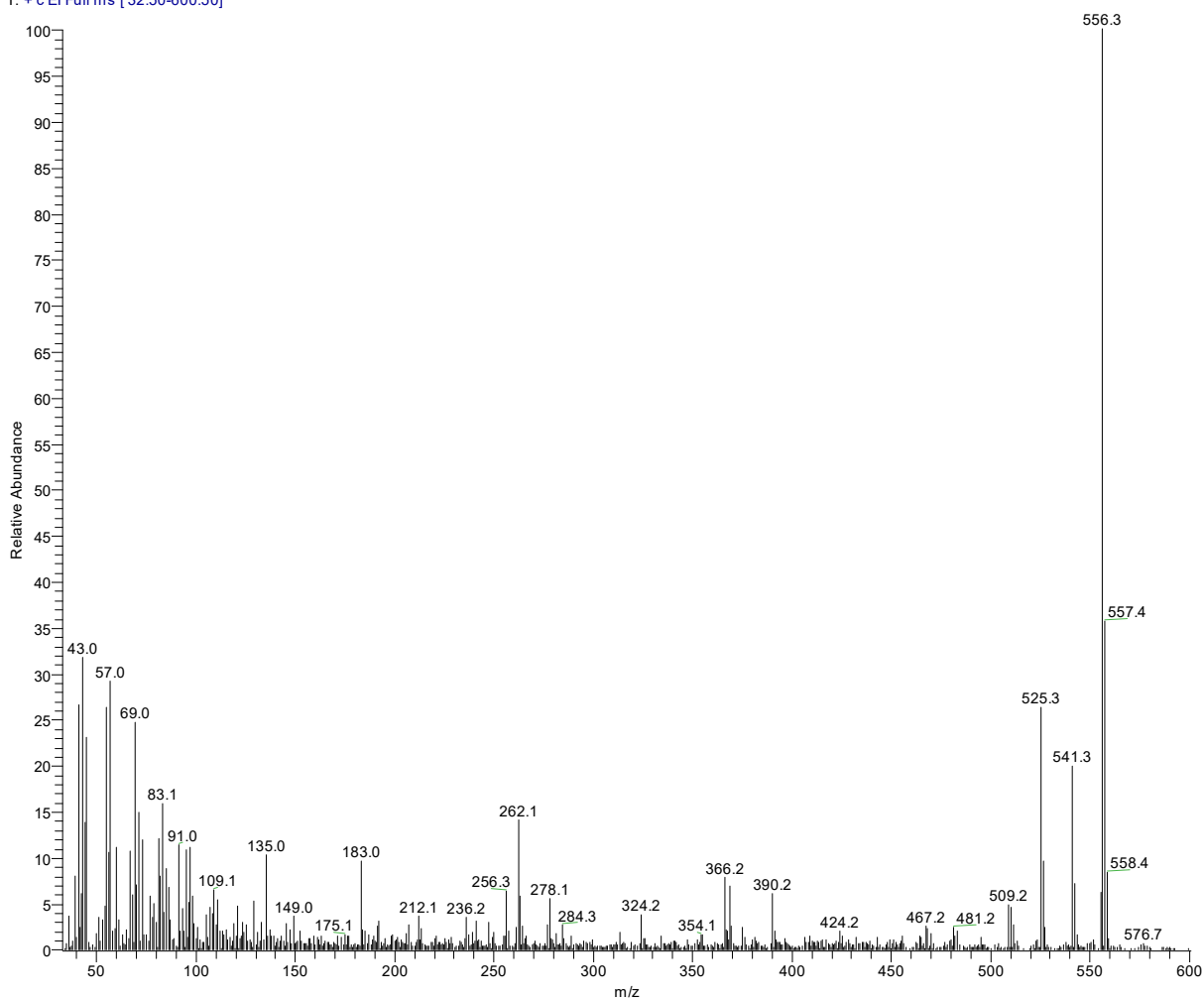
2-(4-Chloro-2-(trifluoromethyl)phenyl)-1-hydroxyanthracene-9,10-dione (31)

HC-81_181023142054 #16 RT: 1.15 AV: 1 NL: 6.86E7
T: + c EI Full ms [14.50-420.50]



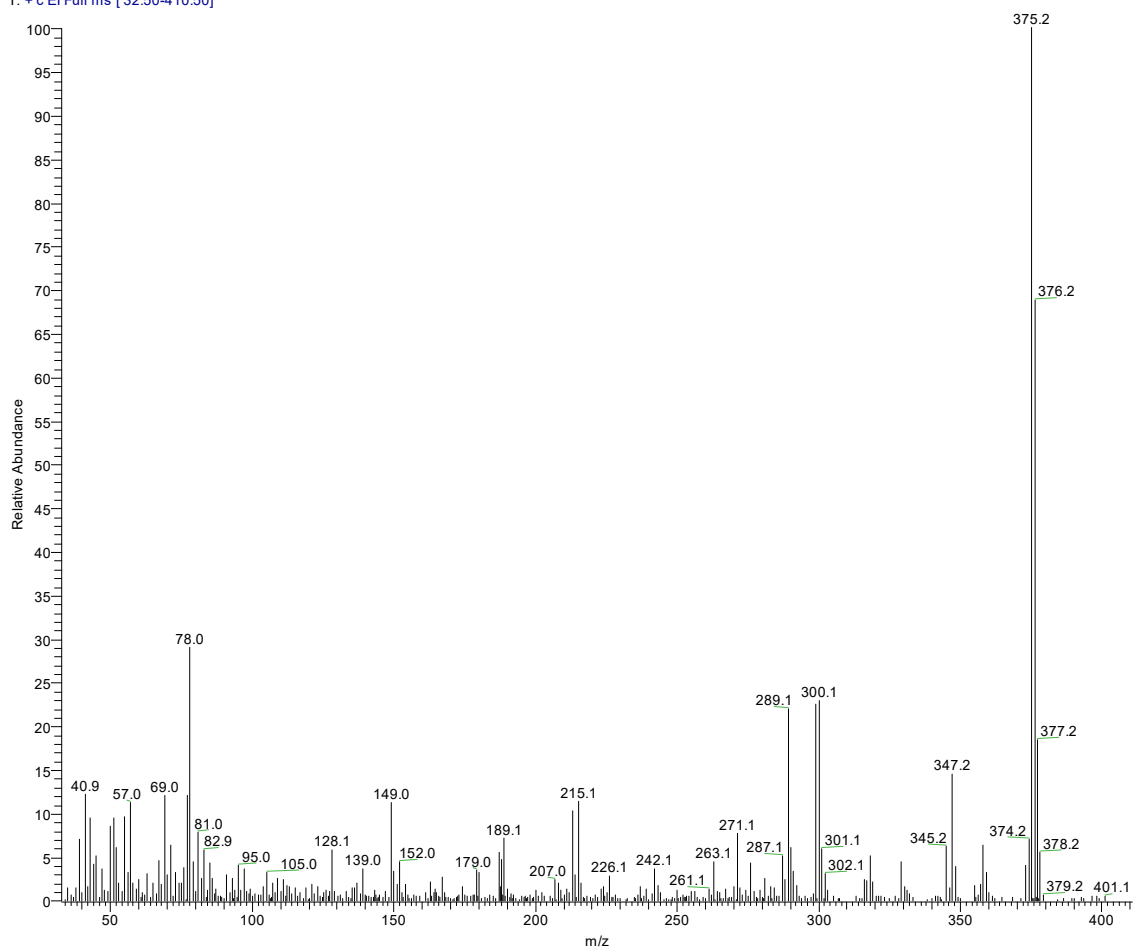
1-Hydroxy-2,4-di-(3,4,5-trimethoxyphenyl)anthracene-9,10-dione (32)

HC-88 #17 RT: 1.08 AV: 1 NL: 6.71E6
T: + c EI Full ms [32.50-600.50]



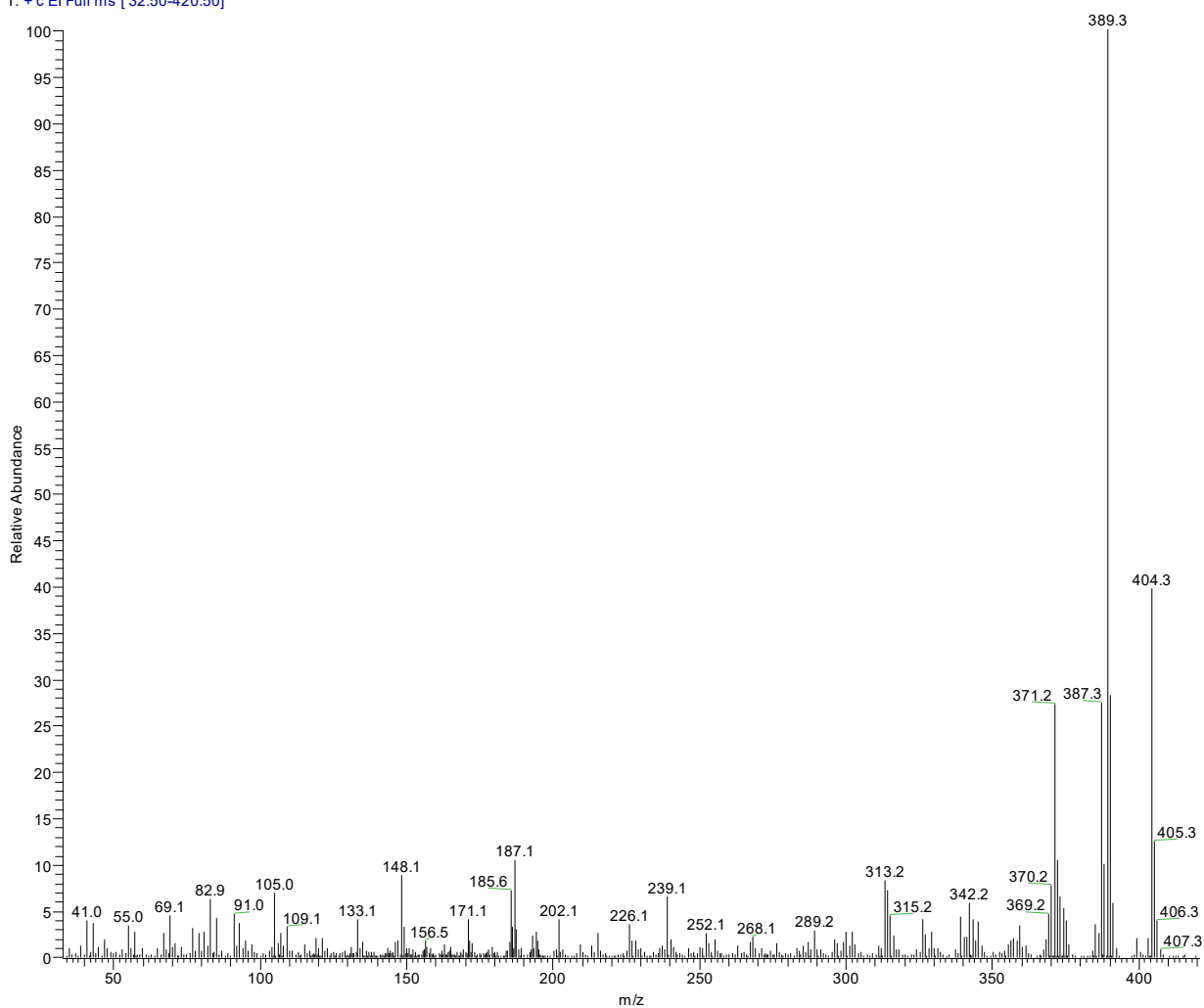
1-Hydroxy-2,4-diphenylanthracene-9,10-dione (33)

HC-34_3#37 RT: 2.14 AV: 1 NL: 7.82E6
T: + c EI Full ms [32.50-410.50]



1-Hydroxy-2,4-di-(*o*-tolyl)anthracene-9,10-dione (34)

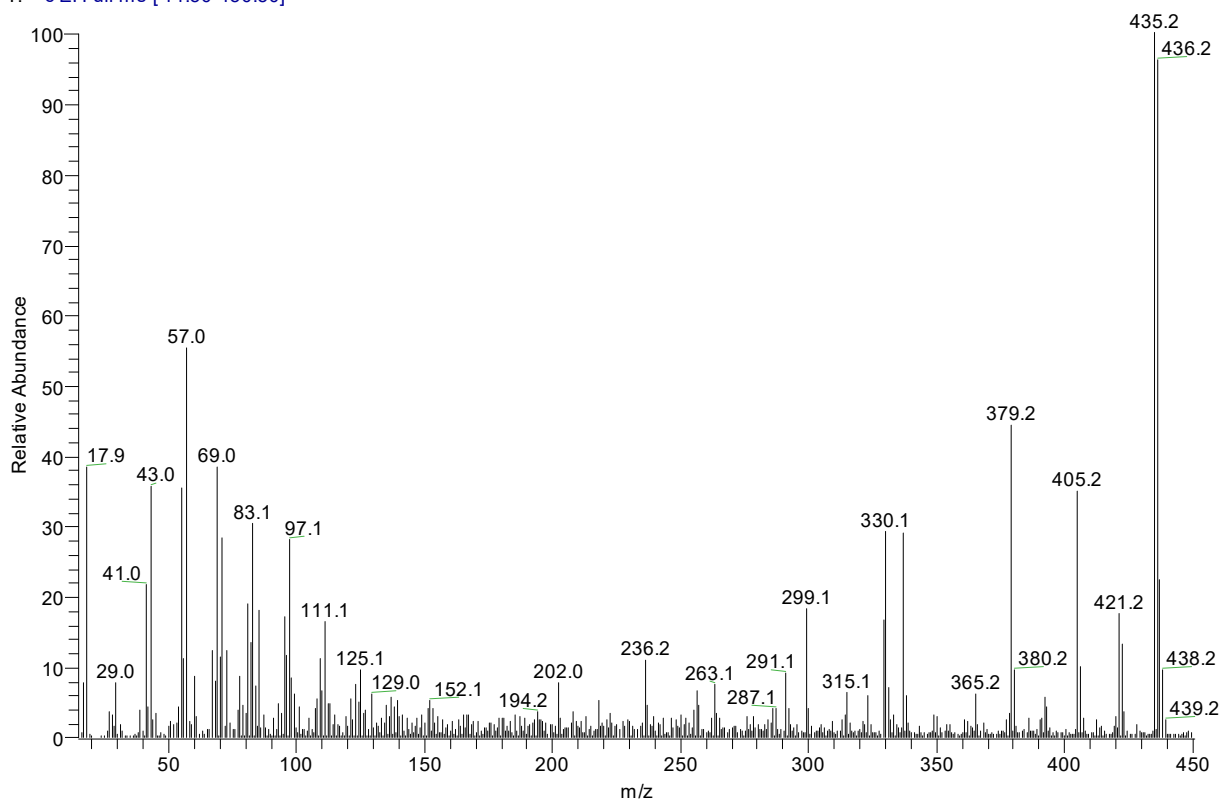
HC-42 #24 RT: 1.38 AV: 1 NL: 2.27E7
T: + c EI Full ms [32.50-420.50]



1-Hydroxy-2,4-di-(4-methoxyphenyl)anthracene-9,10-dione (35)

HC-86 #27 RT: 1.84 AV: 1 NL: 5.12E7

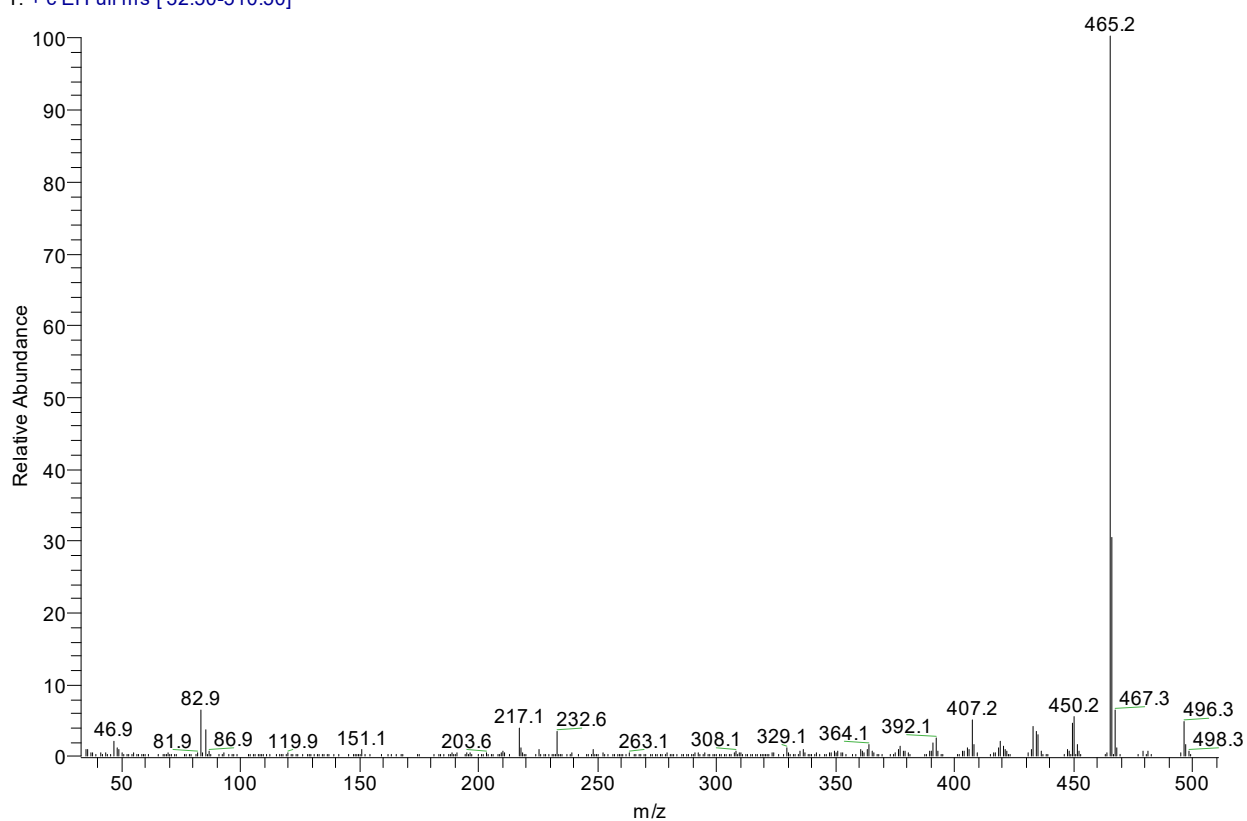
T: + c EI Full ms [14.50-450.50]



2,4-Di-(2,3-dimethoxyphenyl)-1-hydroxyanthracene-9,10-dione (36)

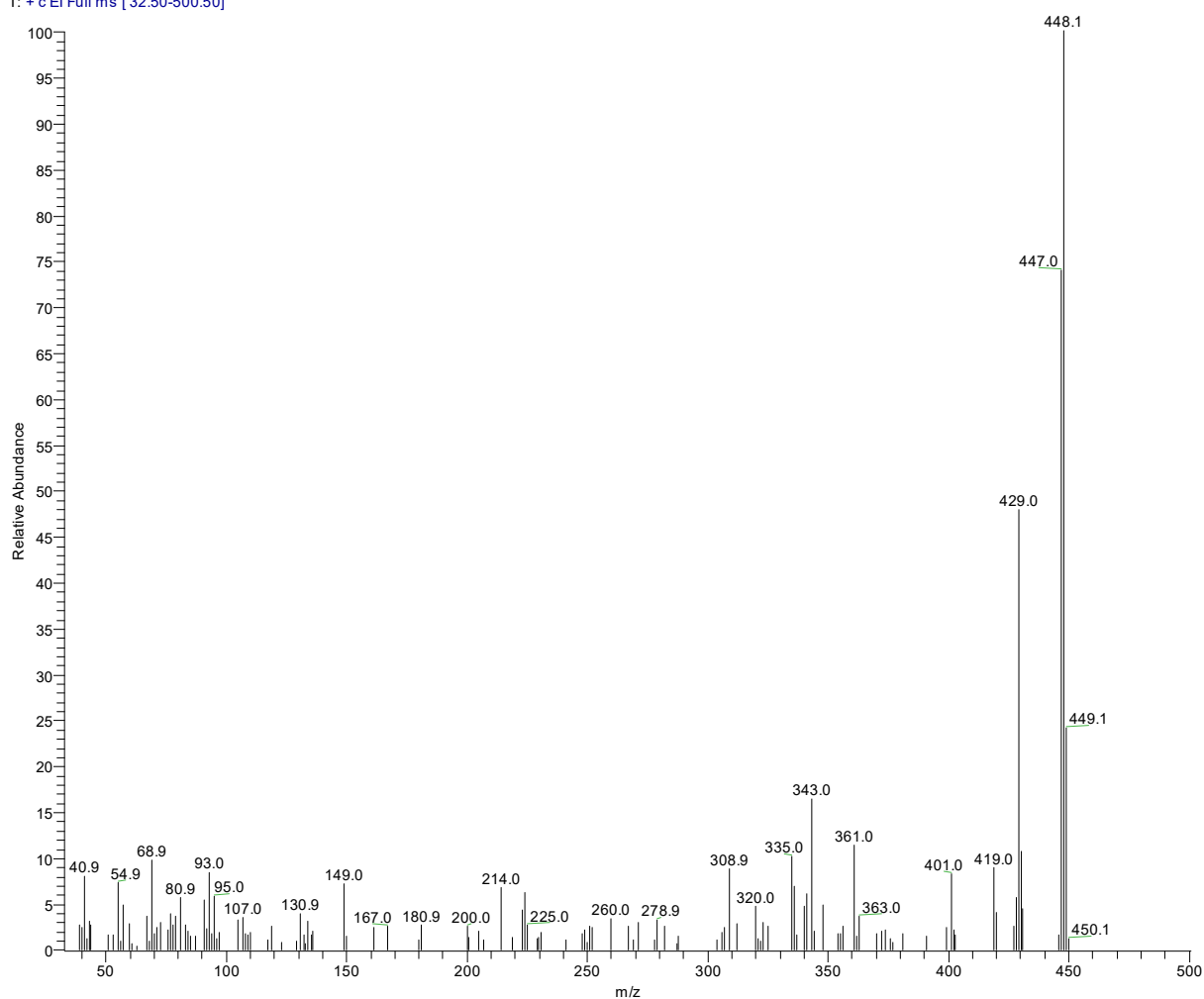
HC-52-2 #22 RT: 1.35 AV: 1 NL: 1.97E7

T: + c EI Full ms [32.50-510.50]



2,4-Di-(3,5-difluorophenyl)-1-hydroxyanthracene-9,10-dione (37)

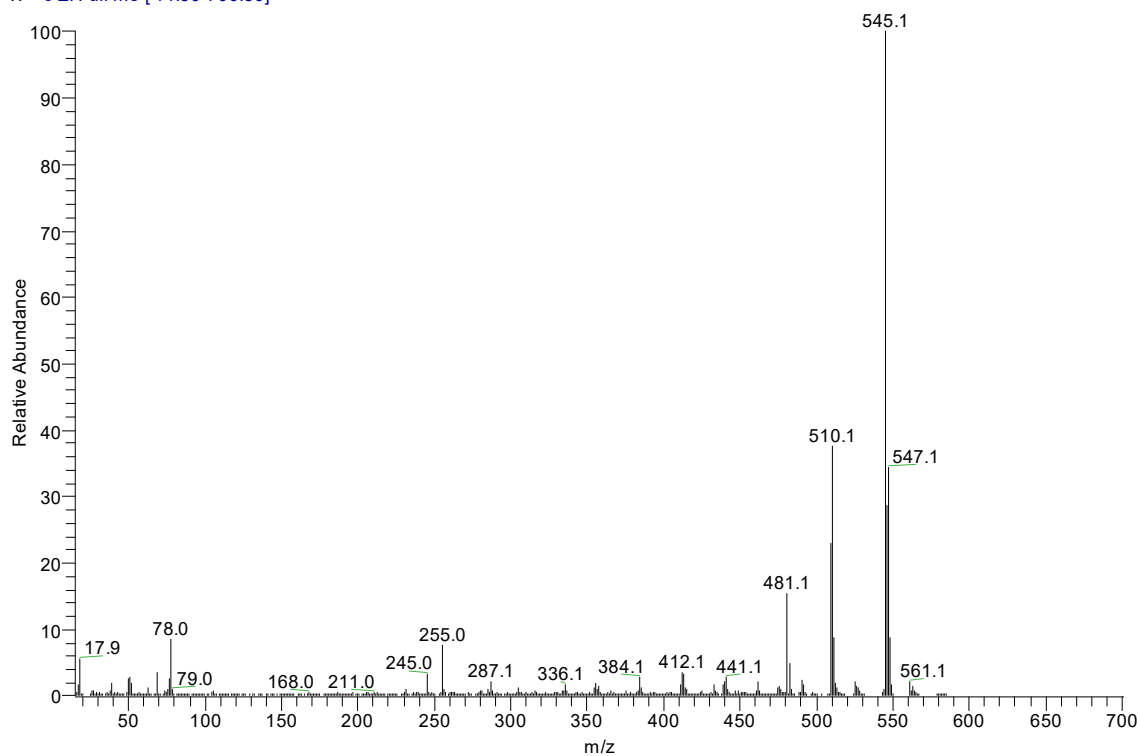
HC-55 #4 RT: 0.19 AV: 1 NL: 7.23E5
T: + c EI Full ms [32.50-500.50]



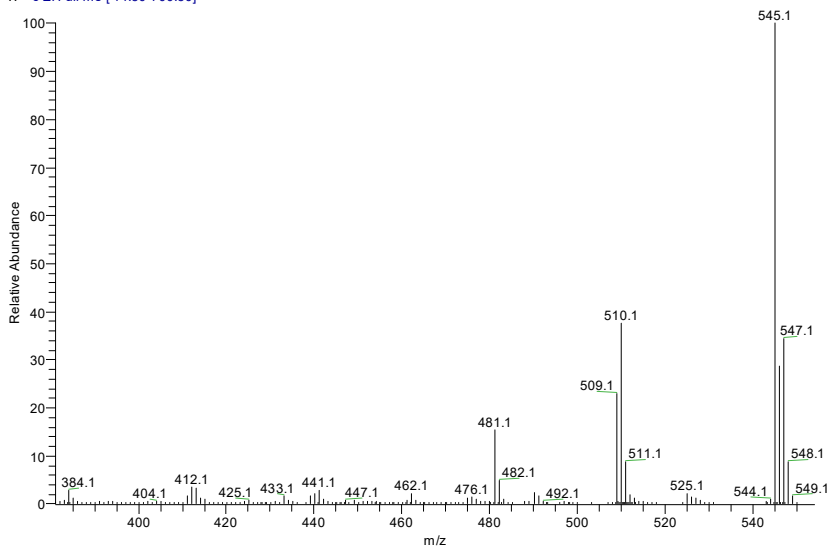
2,4-Di-(2-chloro-5-(trifluoromethyl)phenyl)-1-hydroxyanthracene-9,10-dione

(38)

HC-46-1kp_ #18 RT: 1.51 AV: 1 NL: 8.12E7
T: + c EI Full ms [14.50-700.50]

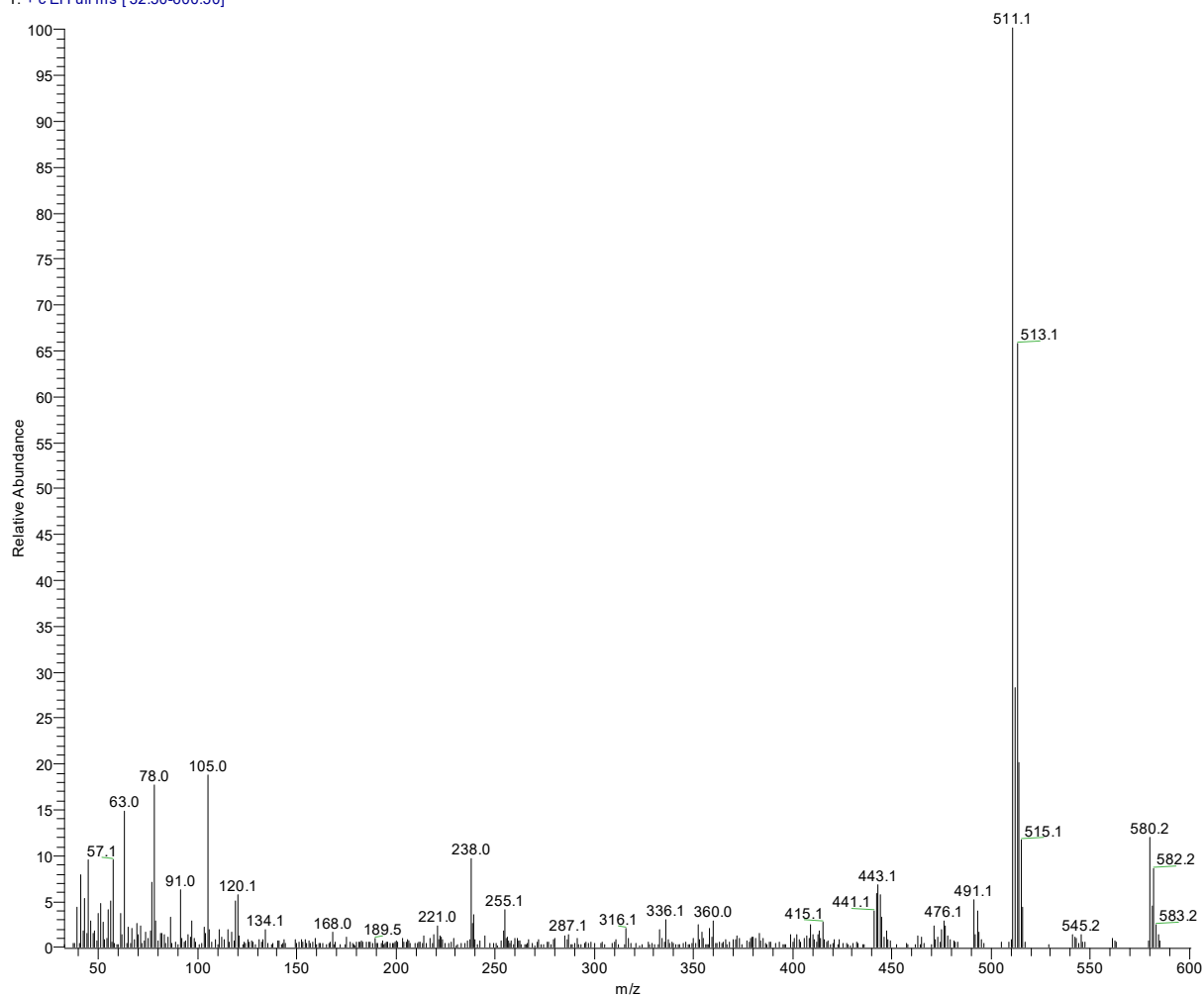


HC-46-1kp_ #18 RT: 1.51 AV: 1 NL: 8.12E7
T: + c EI Full ms [14.50-700.50]



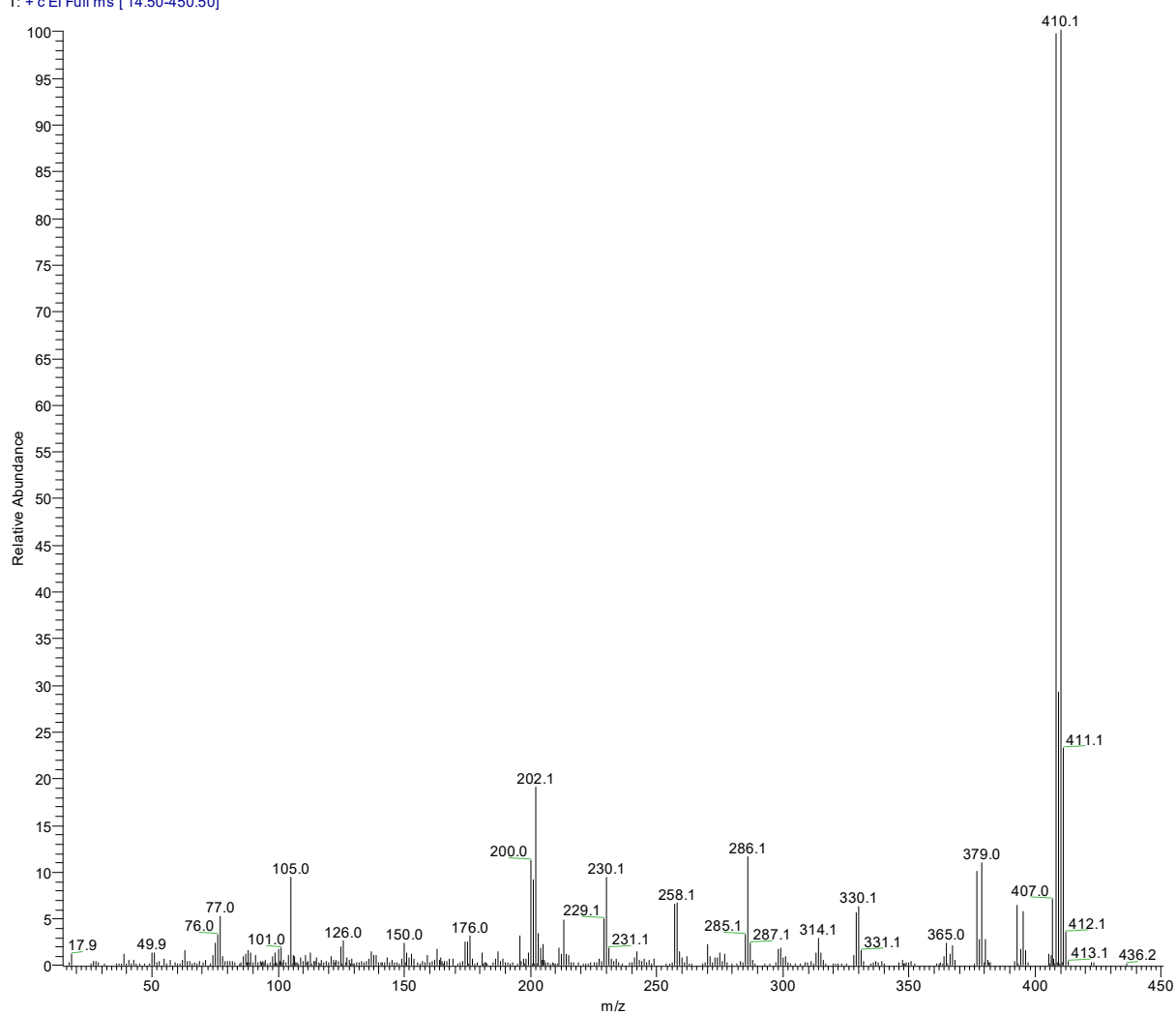
2,4-Di-(4-chloro-2-(trifluoromethyl)phenyl)-1-hydroxyanthracene-9,10-dione (39)

HC-82 #25 RT: 1.81 AV: 1 NL: 5.44E6
T: + c EI Full ms [32.50-600.50]



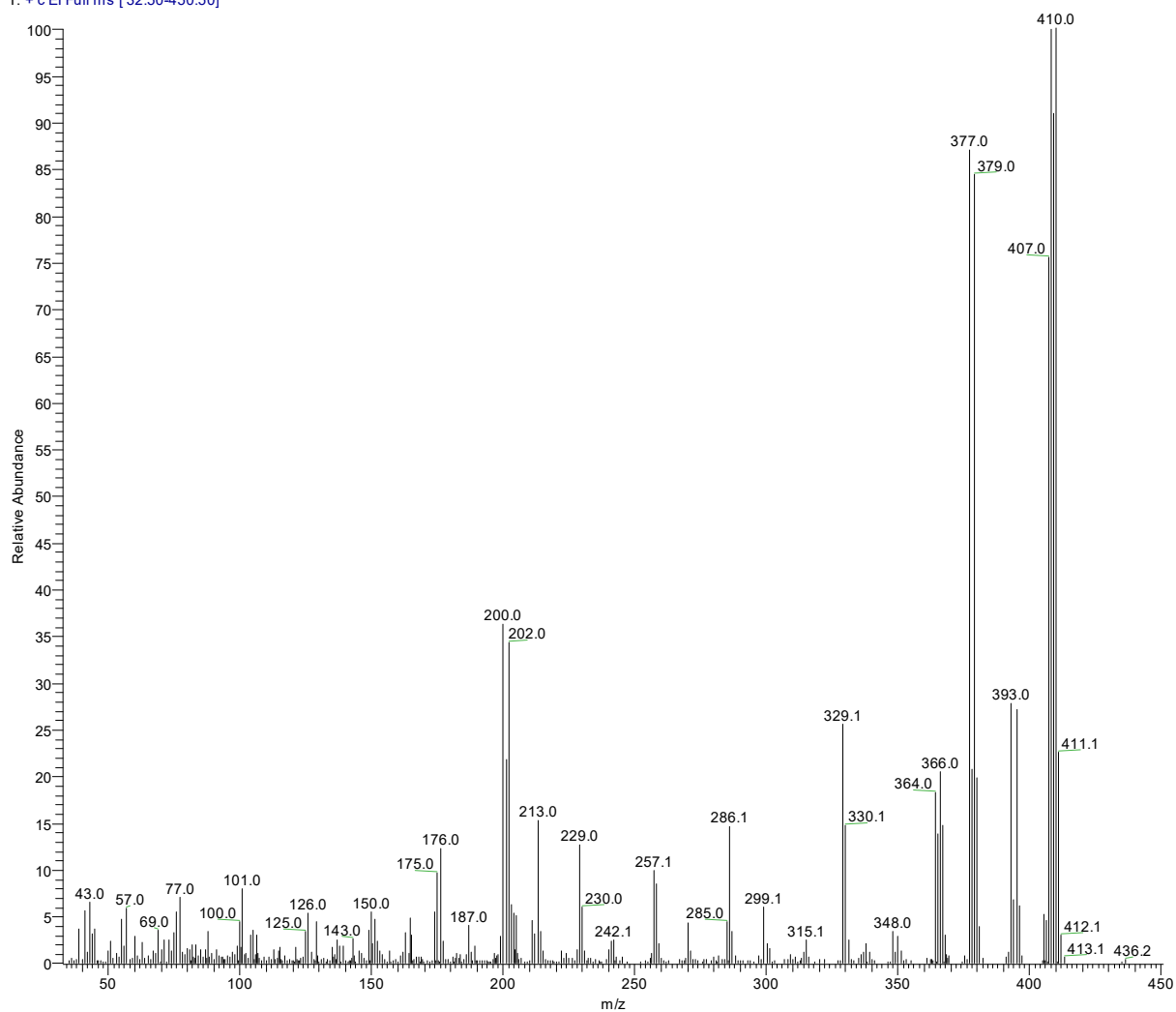
4-bromo-1-hydroxy-2-(4-methoxyphenyl)anthracene-9,10-dione (40)

HC-158-1-2 #6 RT: 0.40 AV: 1 NL: 9.44E6
T: + c EI Full ms [14.50-450.50]



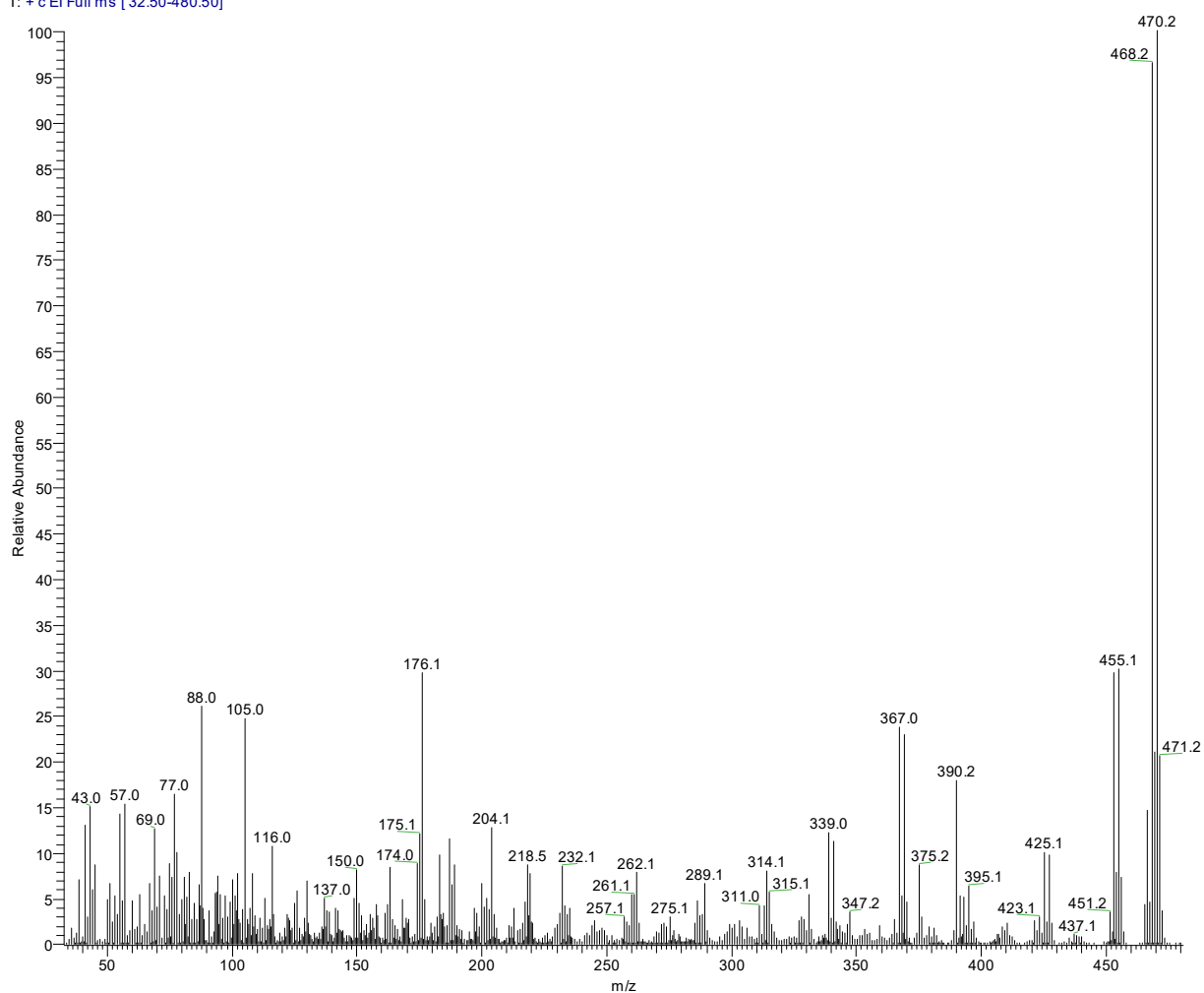
2-bromo-1-hydroxy-4-(4-methoxyphenyl)anthracene-9,10-dione (41)

HC-158-1-2-2_191126122027 #7 RT: 0.38 AV: 1 NL: 7.78E6
T: + c EI Full ms [32.50-450.50]



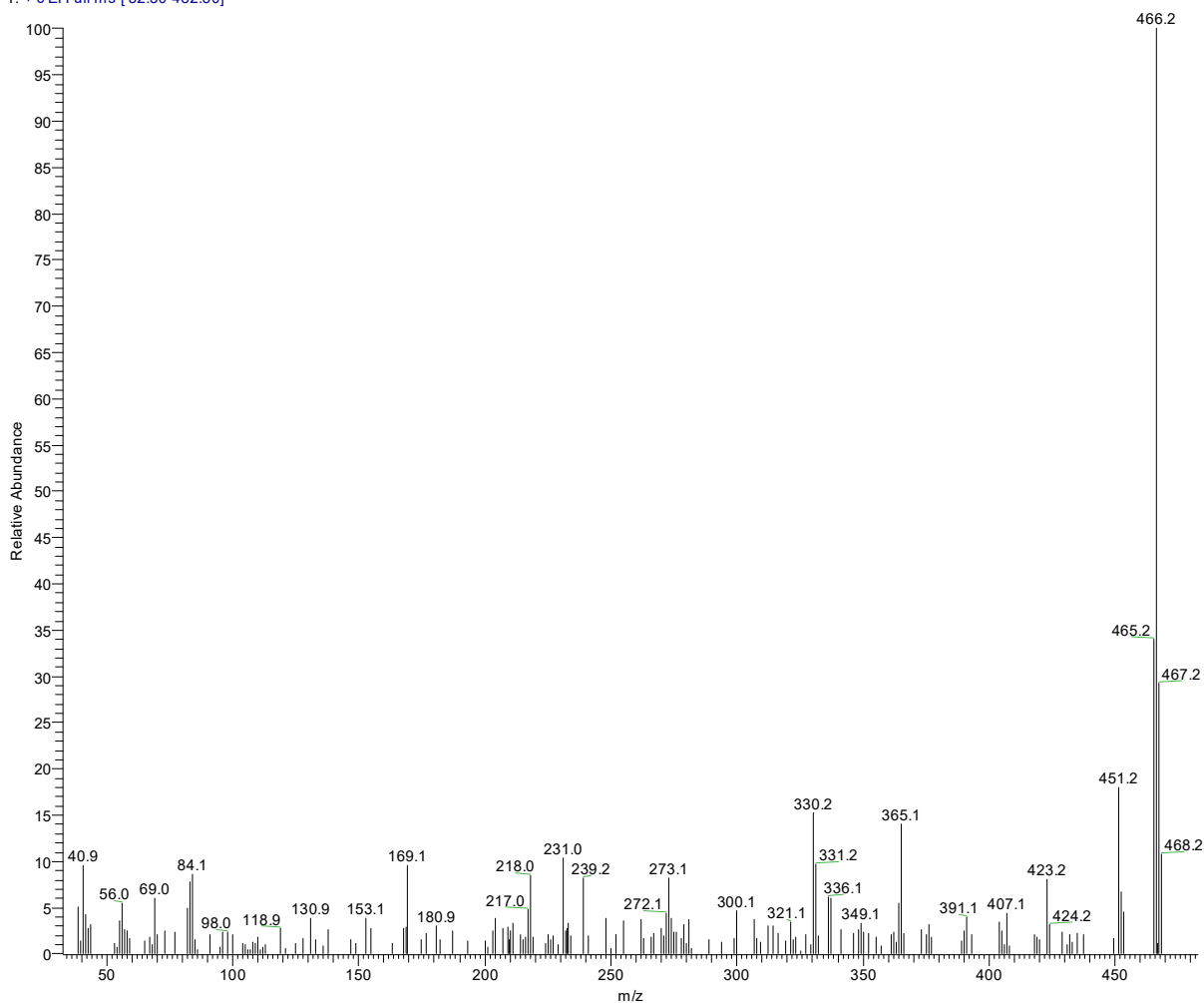
4-Bromo-1-hydroxy-2-(3,4,5-trimethoxyphenyl)anthracene-9,10-dione (42)

HC-90 #9 RT: 0.57 AV: 1 NL: 4.24E7
T: + c EI Full ms [32.50-480.50]



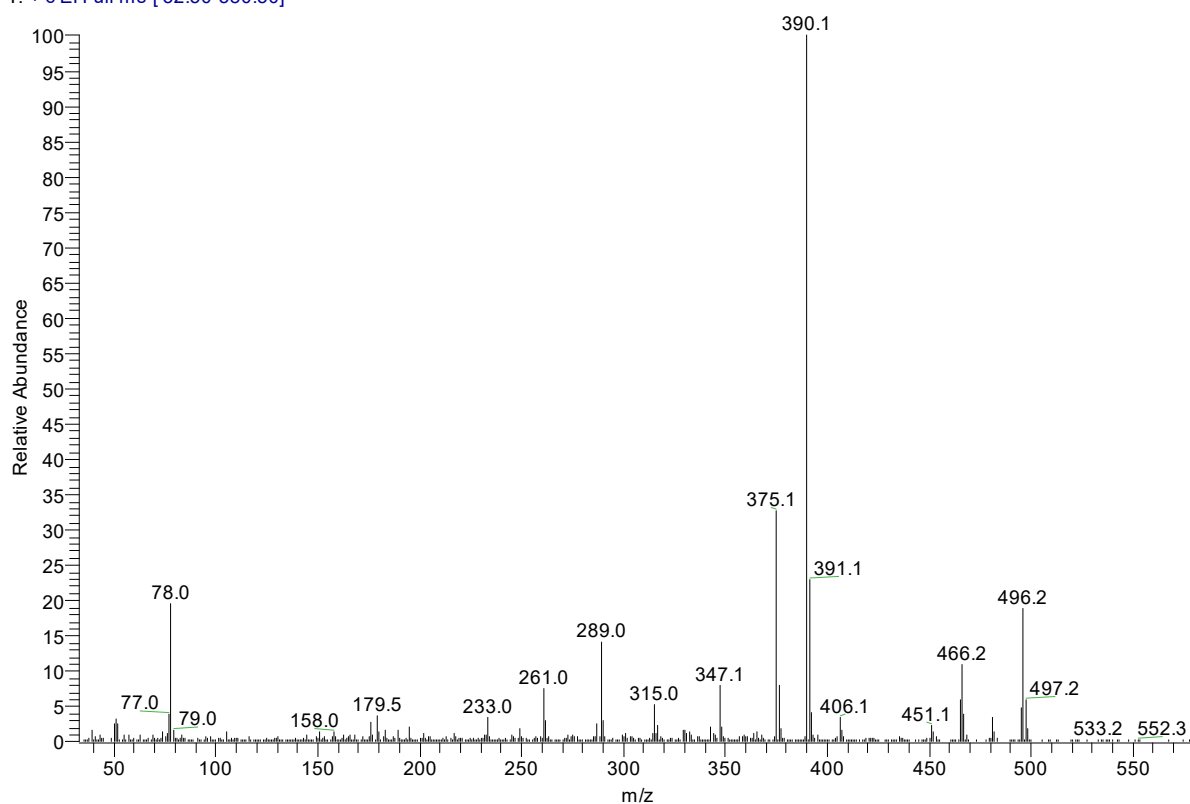
1-Hydroxy-4-phenyl-2-(3,4,5-trimethoxyphenyl)anthracene-9,10-dione (43)

HC_93 #7 RT: 0.38 AV: 1 NL: 1.46E6
T: + c EI Full ms [32.50-482.50]



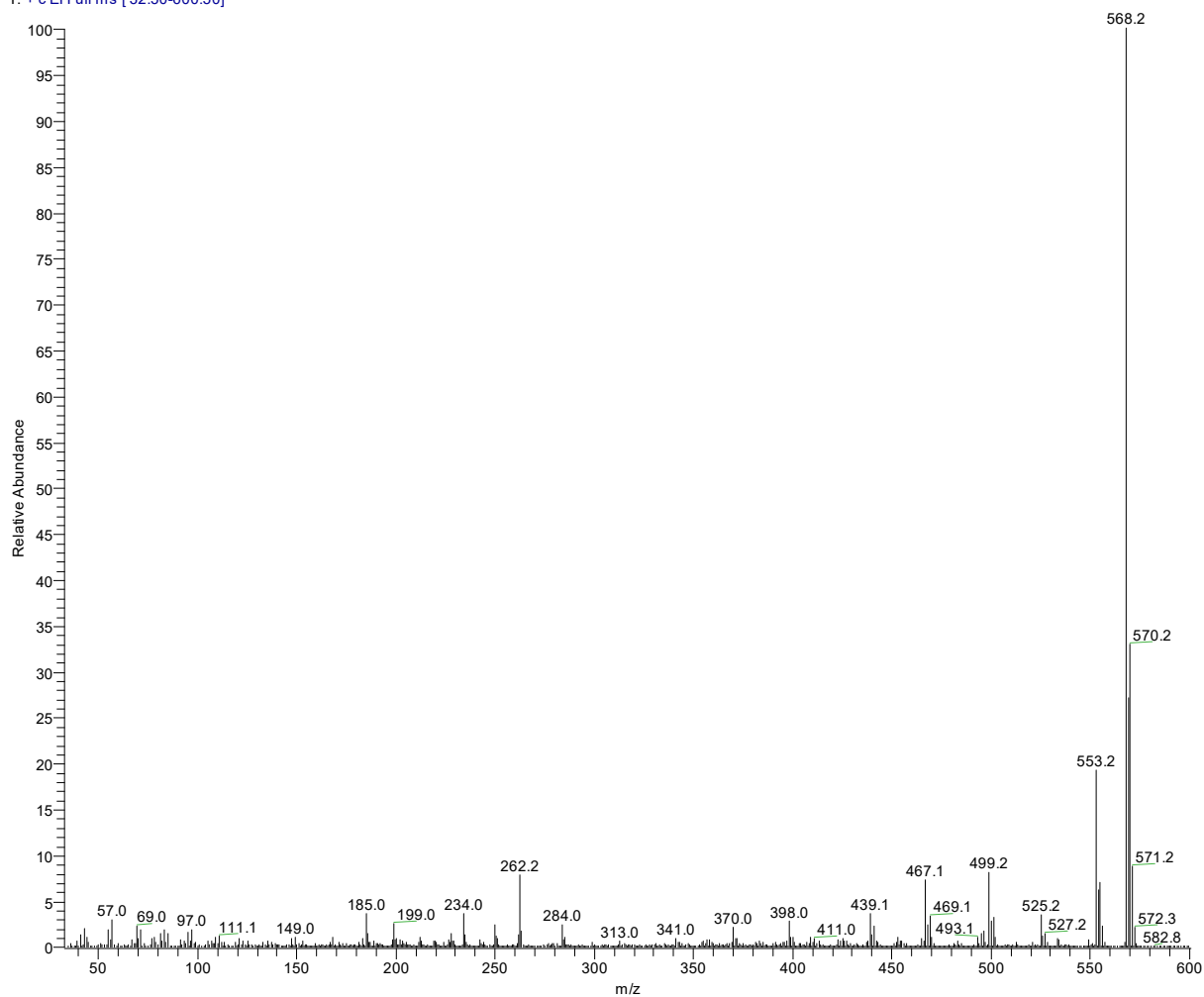
1-Hydroxy-4-(4-methoxyphenyl)-2-(3,4,5-trimethoxyphenyl)anthracene-9,10-dione (44)

HC-92 #26 RT: 1.65 AV: 1 NL: 5.64E7
T: + c EI Full ms [32.50-580.50]



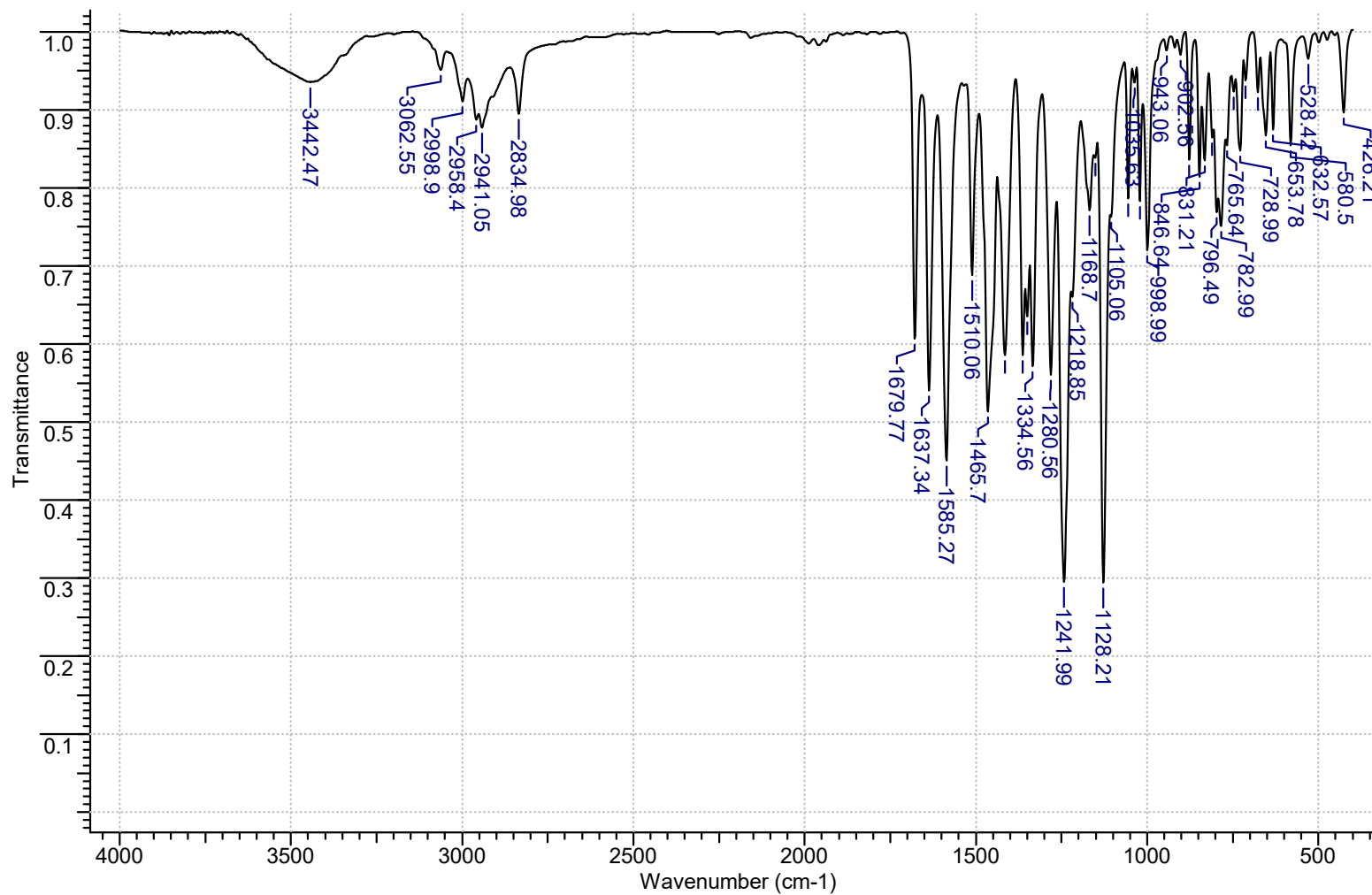
4-(4-Chloro-2-(trifluoromethyl)phenyl)-1-hydroxy-2-(3,4,5-trimethoxyphenyl)anthracene-9,10-dione (45)

HC-94 #23 RT: 1.76 AV: 1 NL: 6.22E7
T: + c EI Full ms [32.50-600.50]

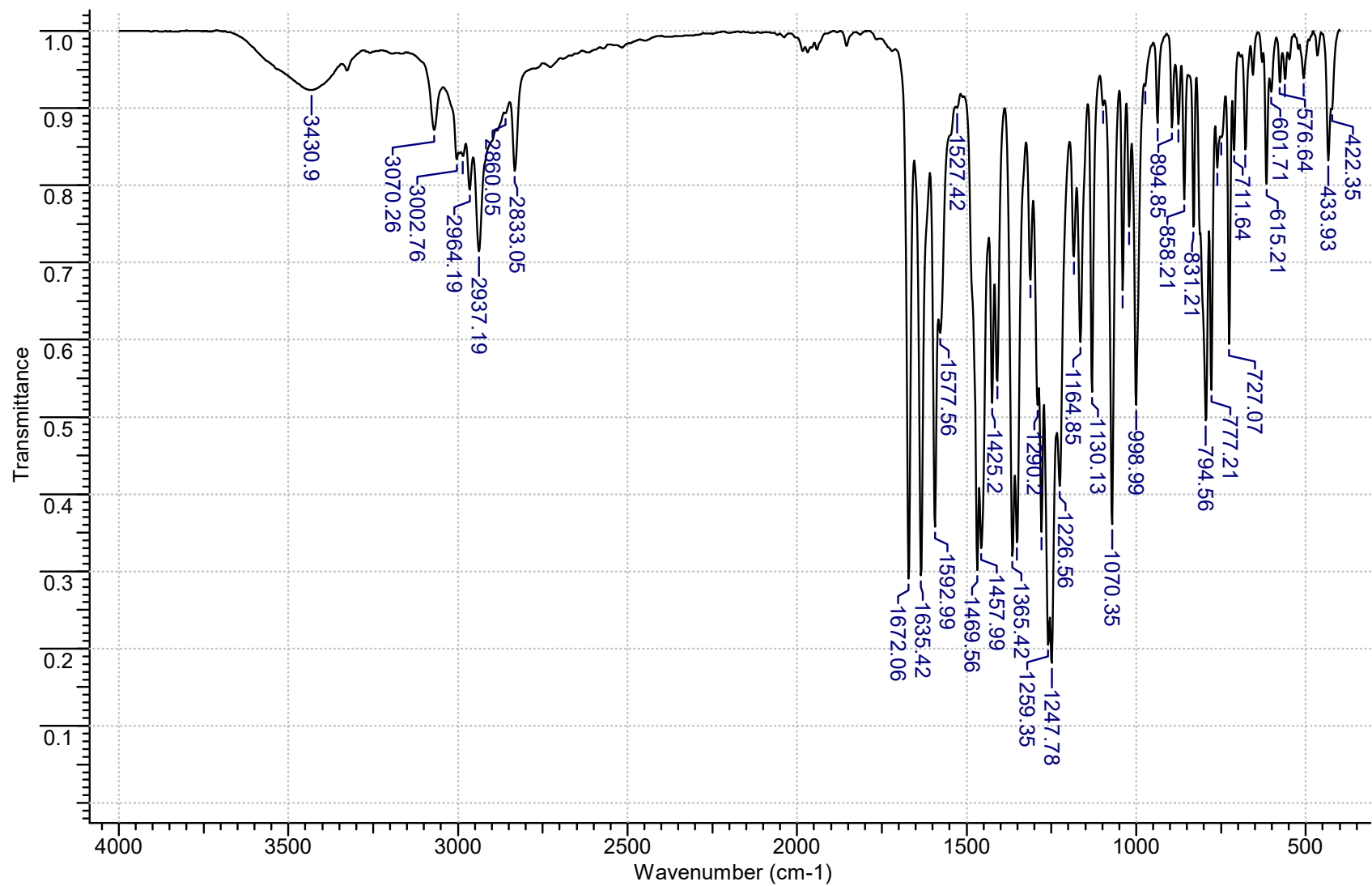


IR spectra of selected compounds

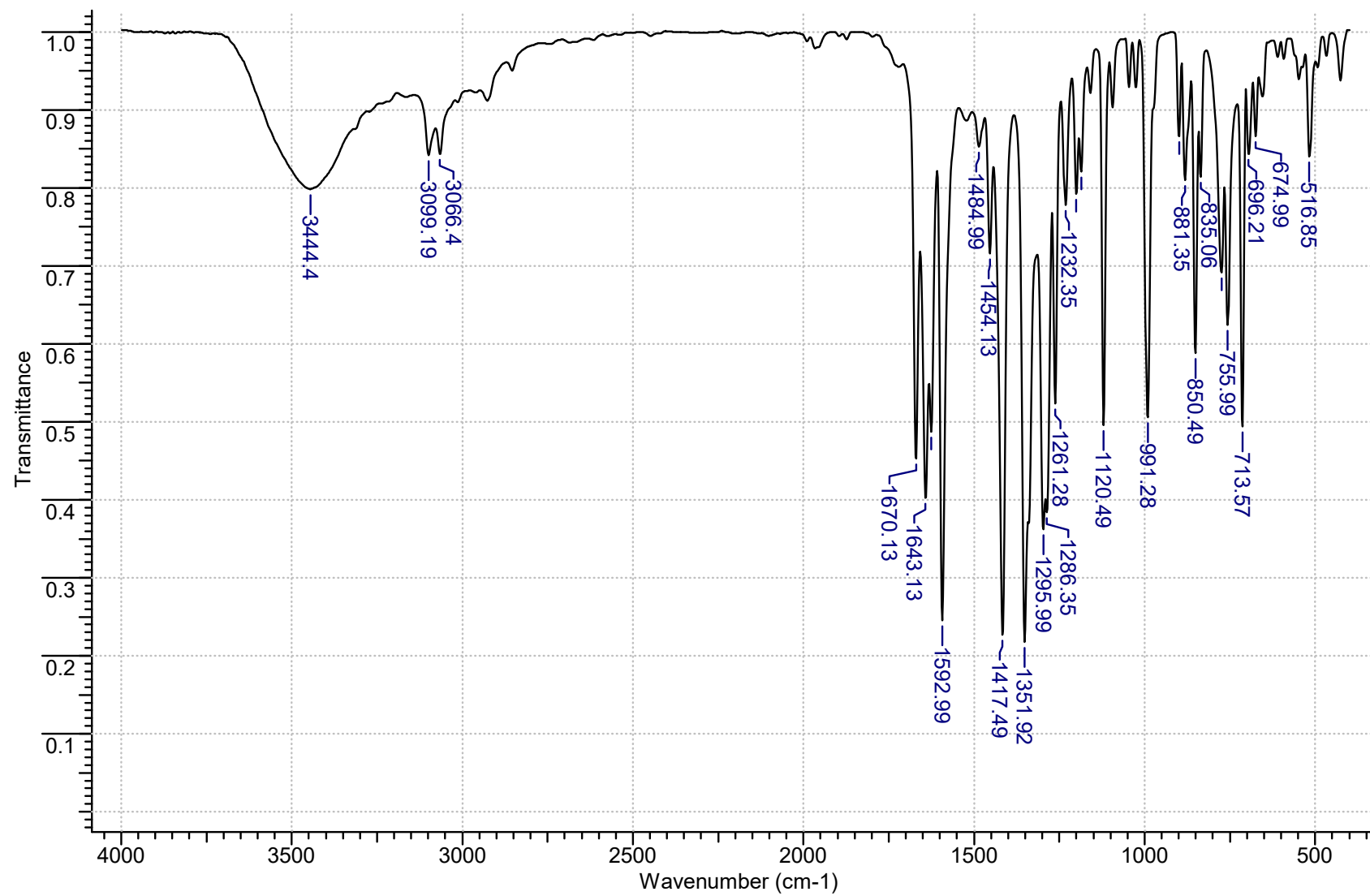
1-Hydroxy-4-(3,4,5-trimethoxyphenyl)anthracene-9,10-dione (5)



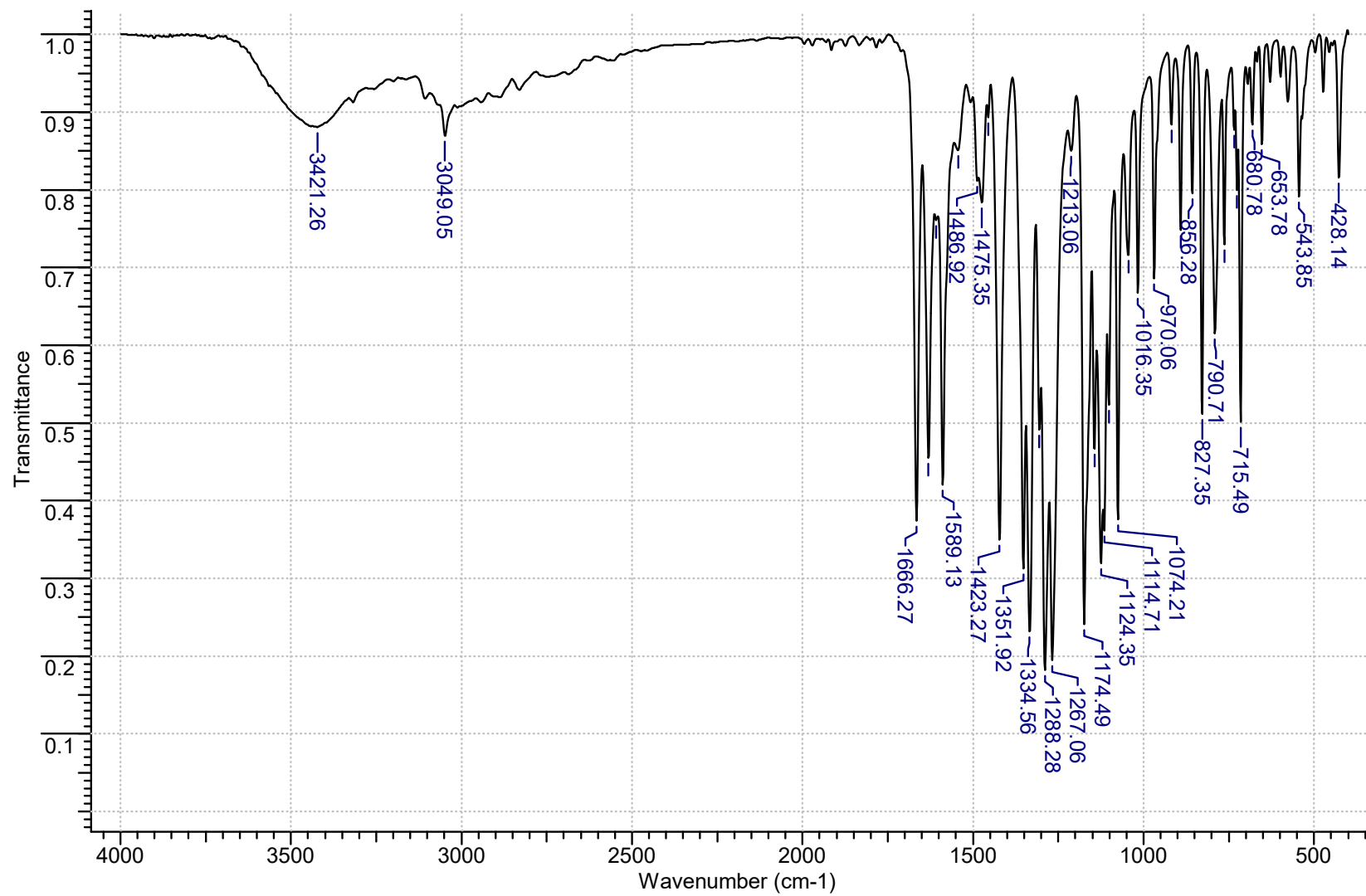
1-(2,3-Dimethoxyphenyl)-4-hydroxyanthracene-9,10-dione (16)



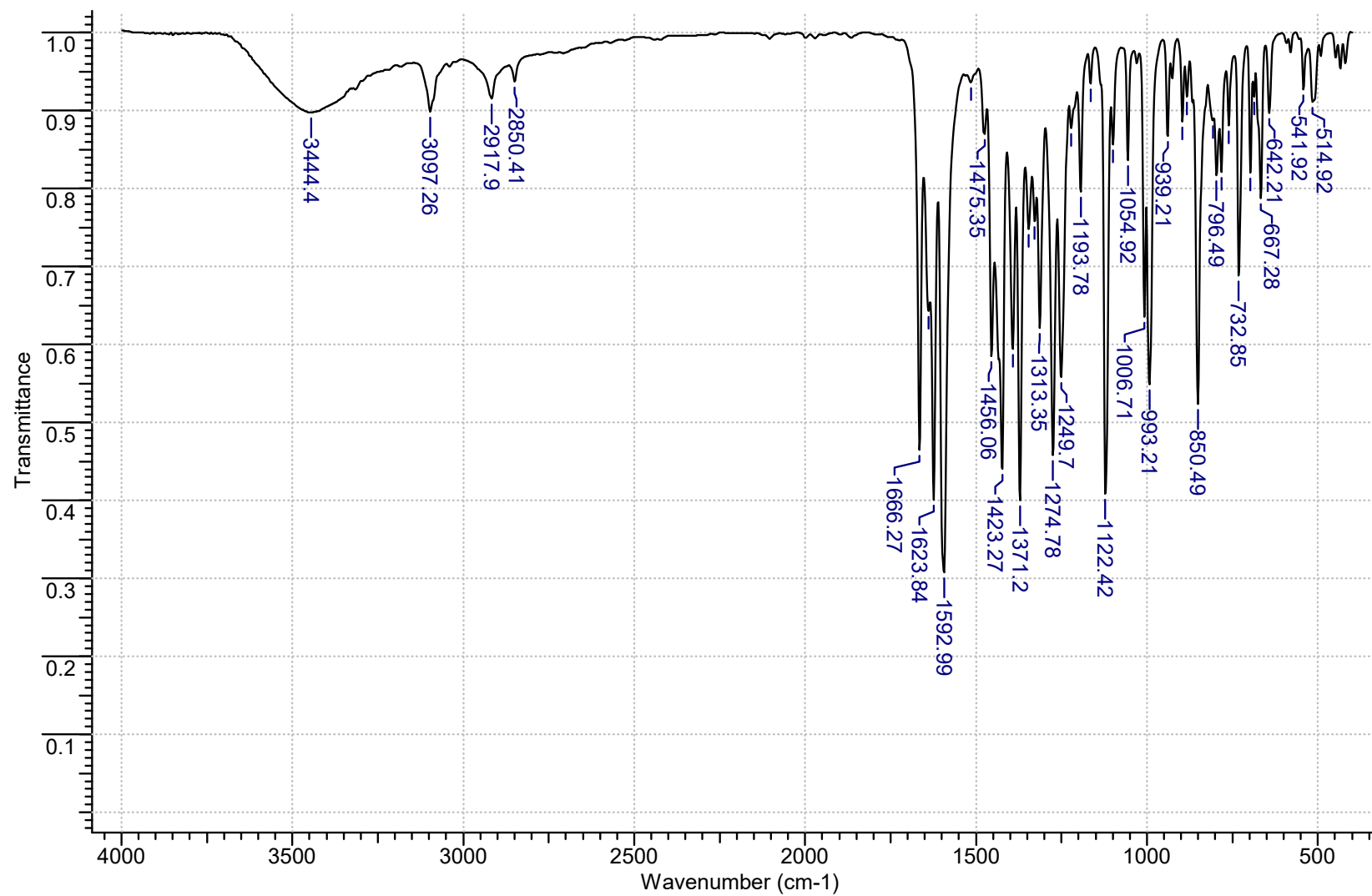
2-(3,5-Difluorophenyl)-1-hydroxyanthracene-9,10-dione (29)



2-(2-Chloro-5-(trifluoromethyl)phenyl)-1-hydroxyanthracene-9,10-dione (30)

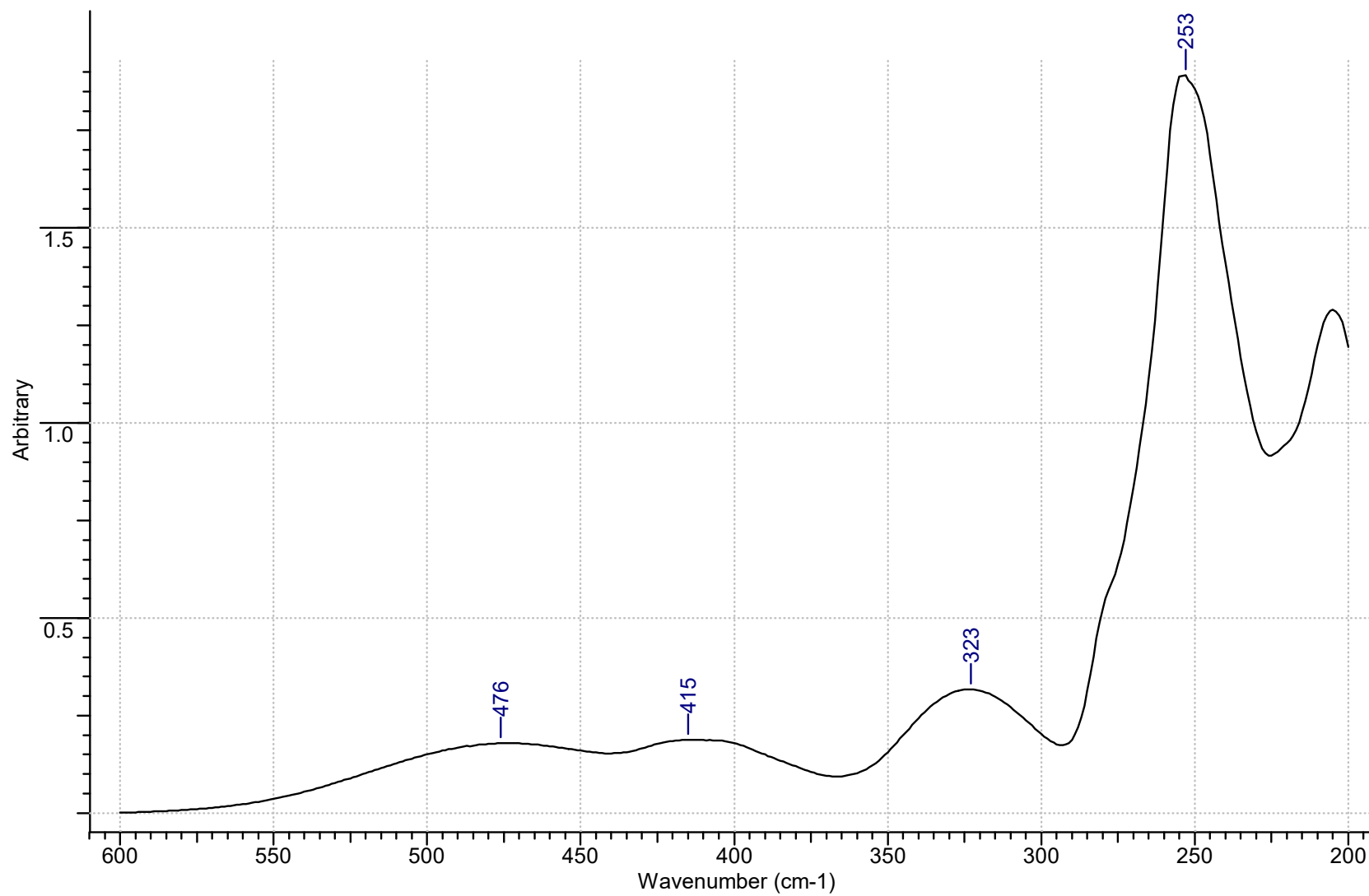


2,4-Di-(3,5-difluorophenyl)-1-hydroxyanthracene-9,10-dione (37)

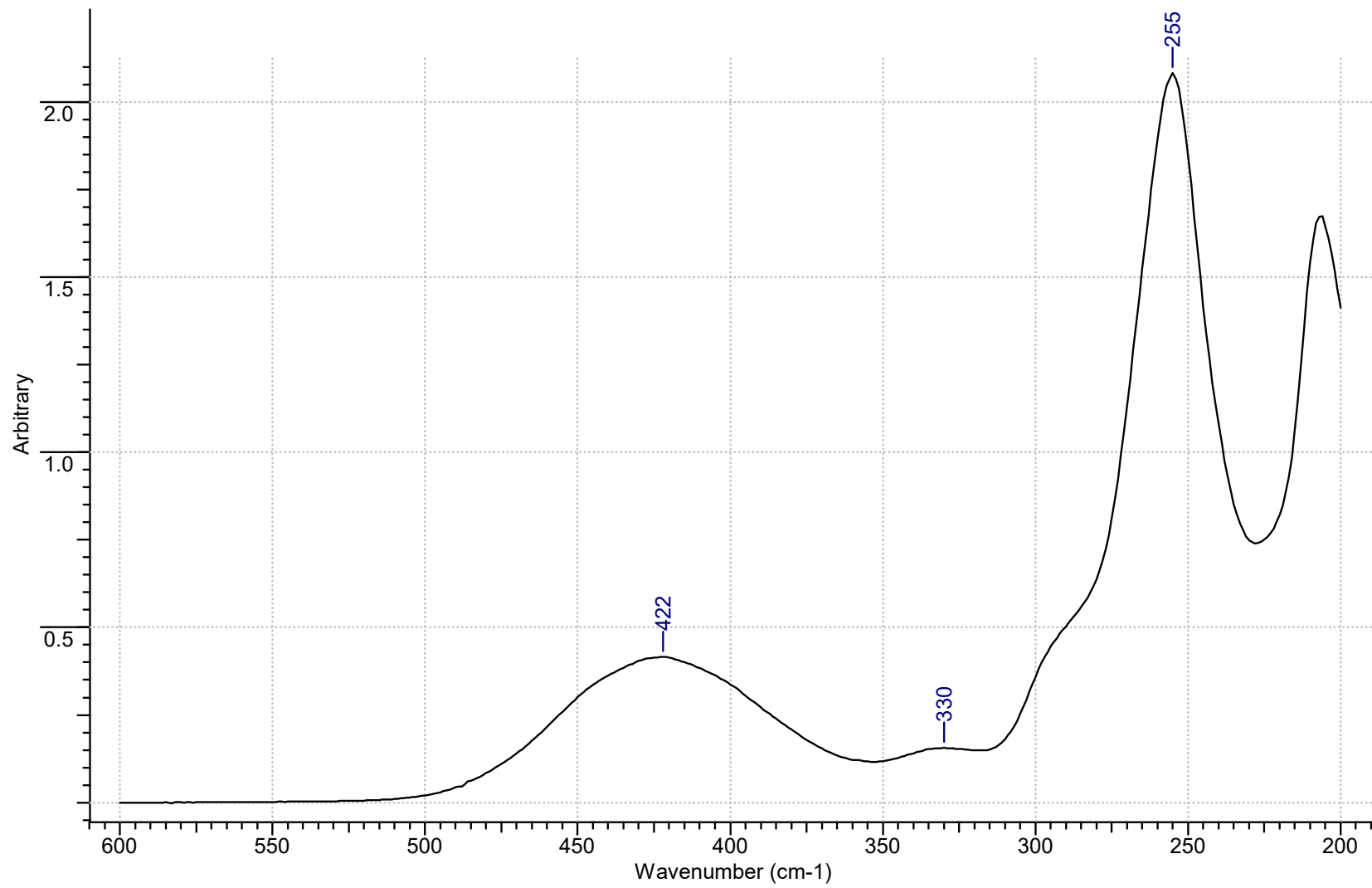


UV spectra of selected compounds

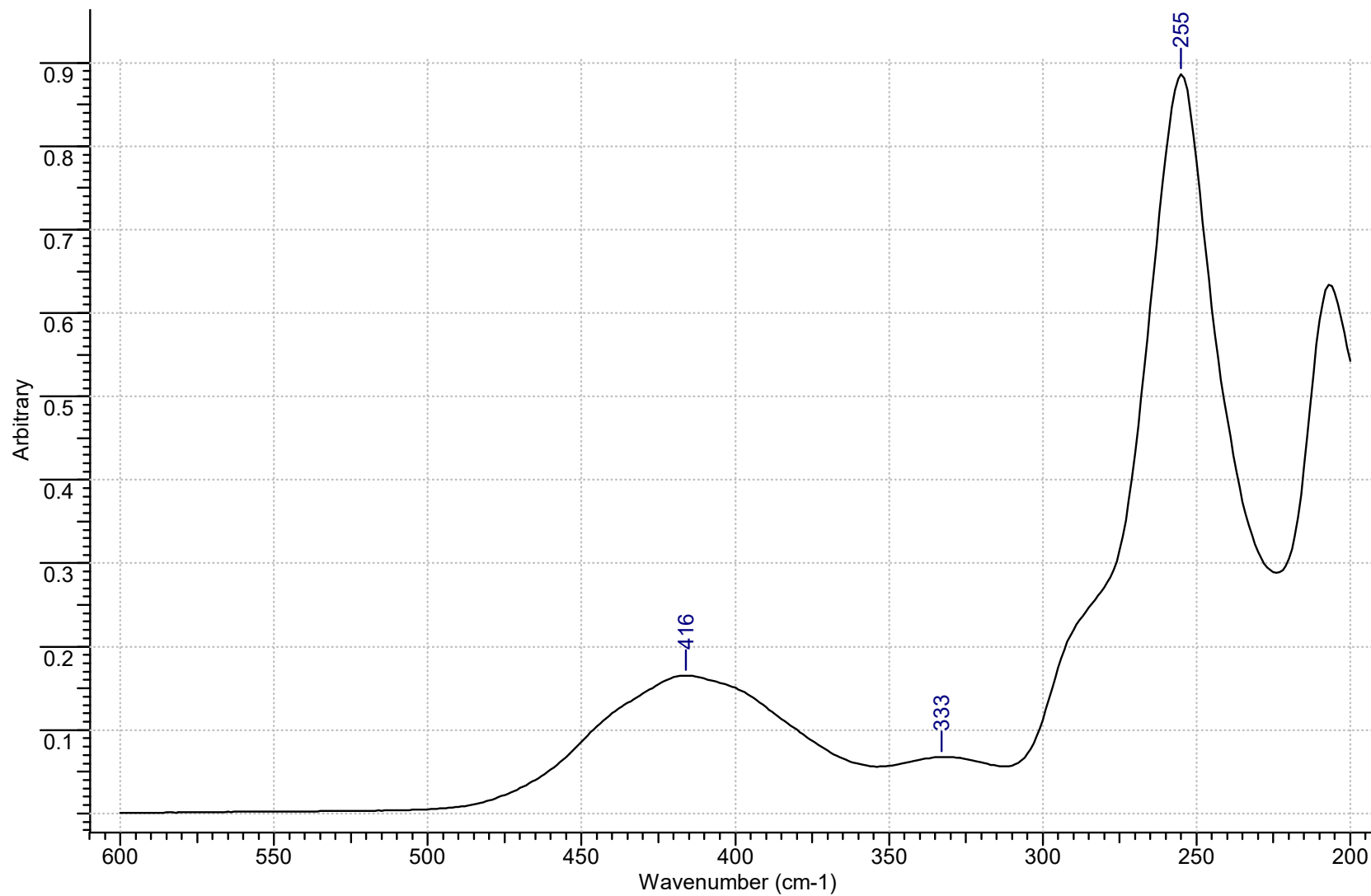
1-(Furan-2-yl)-4-hydroxyanthracene-9,10-dione (22)



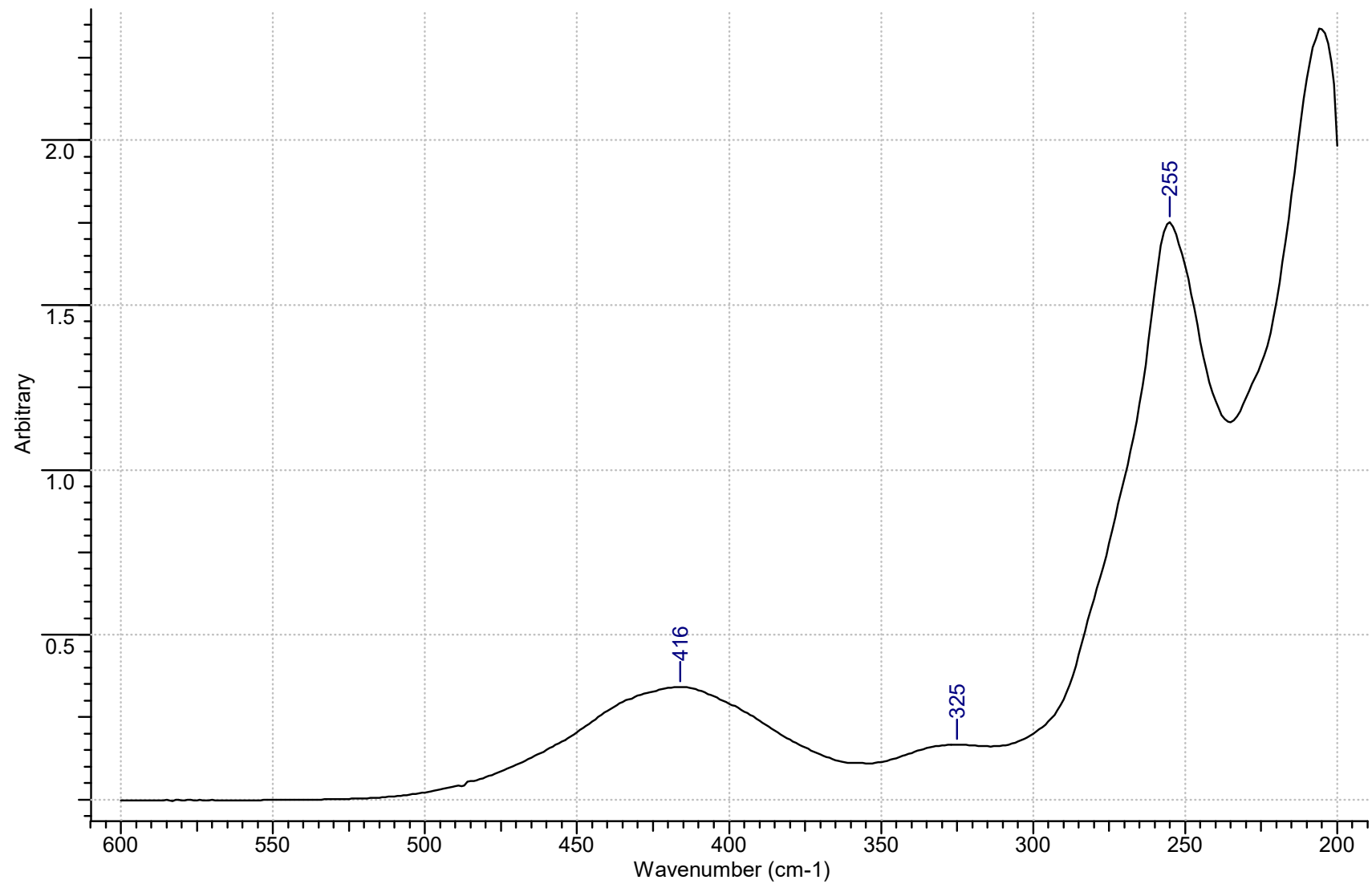
1-Hydroxy-2-phenylanthracene-9,10-dione (25)



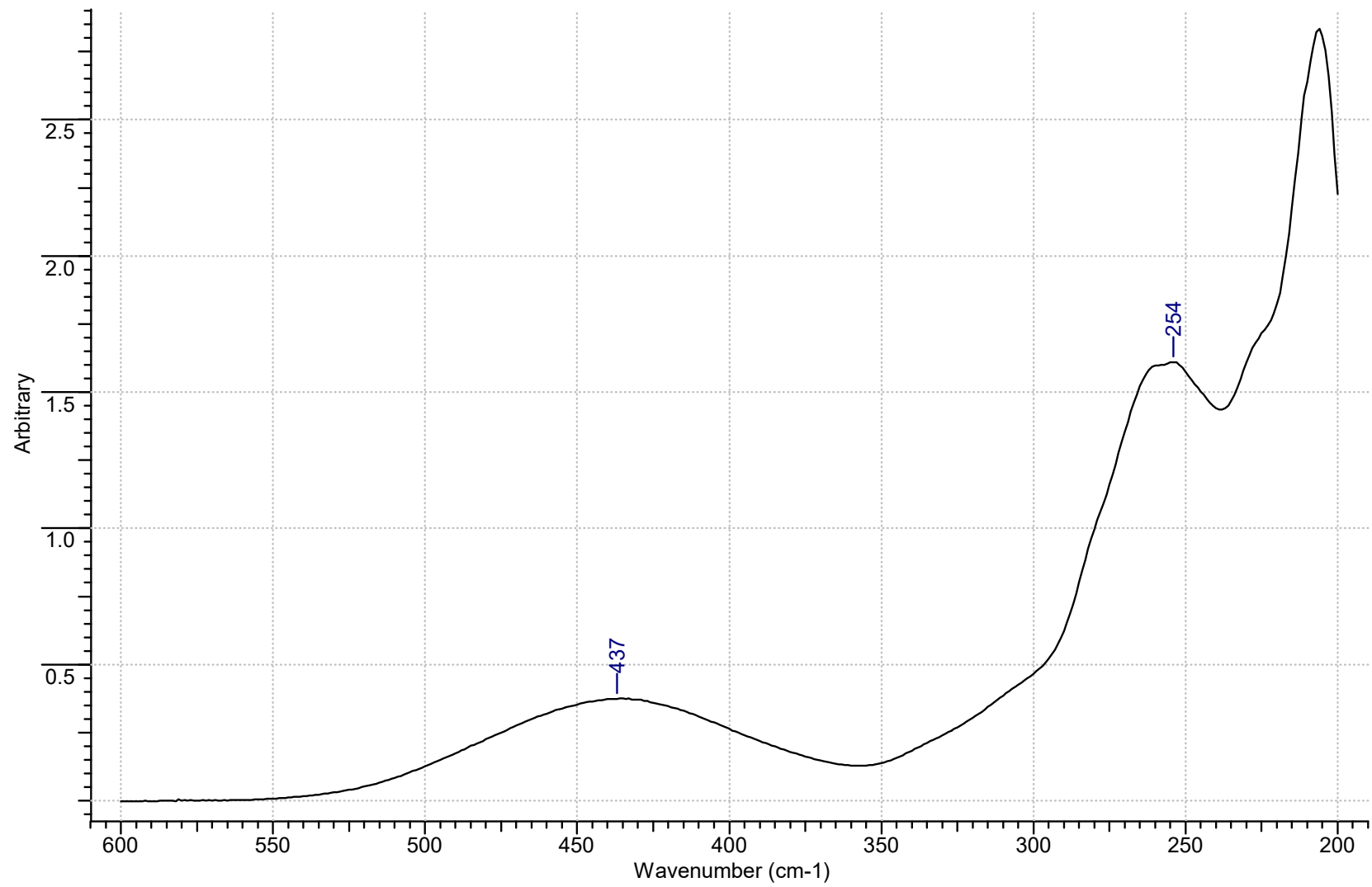
2-(3,5-Difluorophenyl)-1-hydroxyanthracene-9,10-dione (29)



1-Hydroxy-2,4-di-(*o*-tolyl)anthracene-9,10-dione (34)



1-Hydroxy-4-phenyl-2-(3,4,5-trimethoxyphenyl)anthracene-9,10-dione (43)



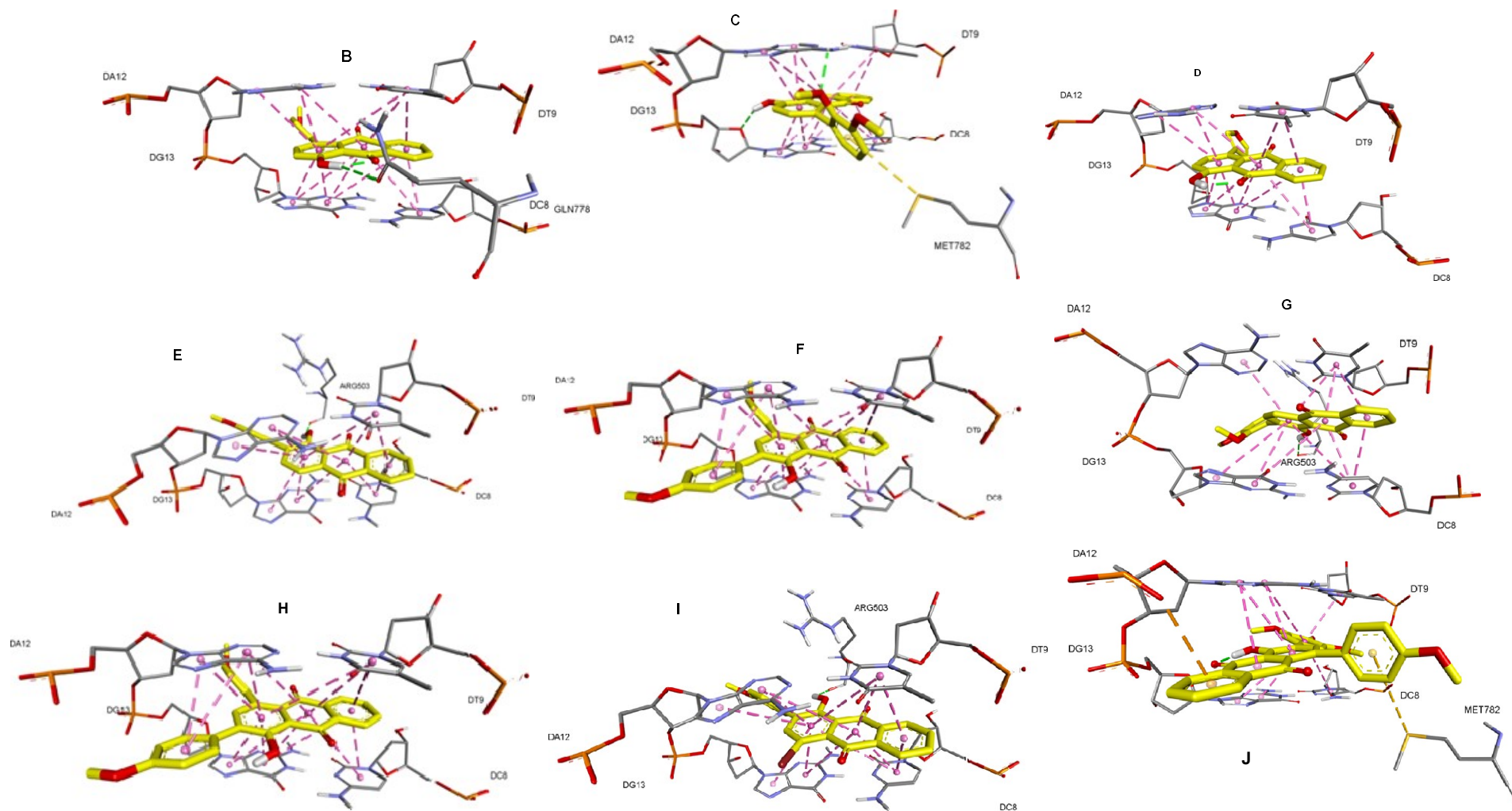


Figure 2S. Docking of new derivatives **15**, **16**, **23**, **25**, **27**, **28**, **35**, **40** and **44** in topoisomerase II β -DNA complex binding site. B – **15**, C – **16**, D **23**, E **25**, F **27**, G **28**, H – **35**, I – **40**, and J **44**. Non-covalent interactions of molecules are shown by dotted lines: green - hydrogen bonds, orange – electrostatic interactions, yellow – sulphur interactions, purple – stacking interactions.

