

Supporting Information

Sustainable access to acridin-9-(10*H*)-ones with an embedded mterphenyl moiety based on a three- component reaction

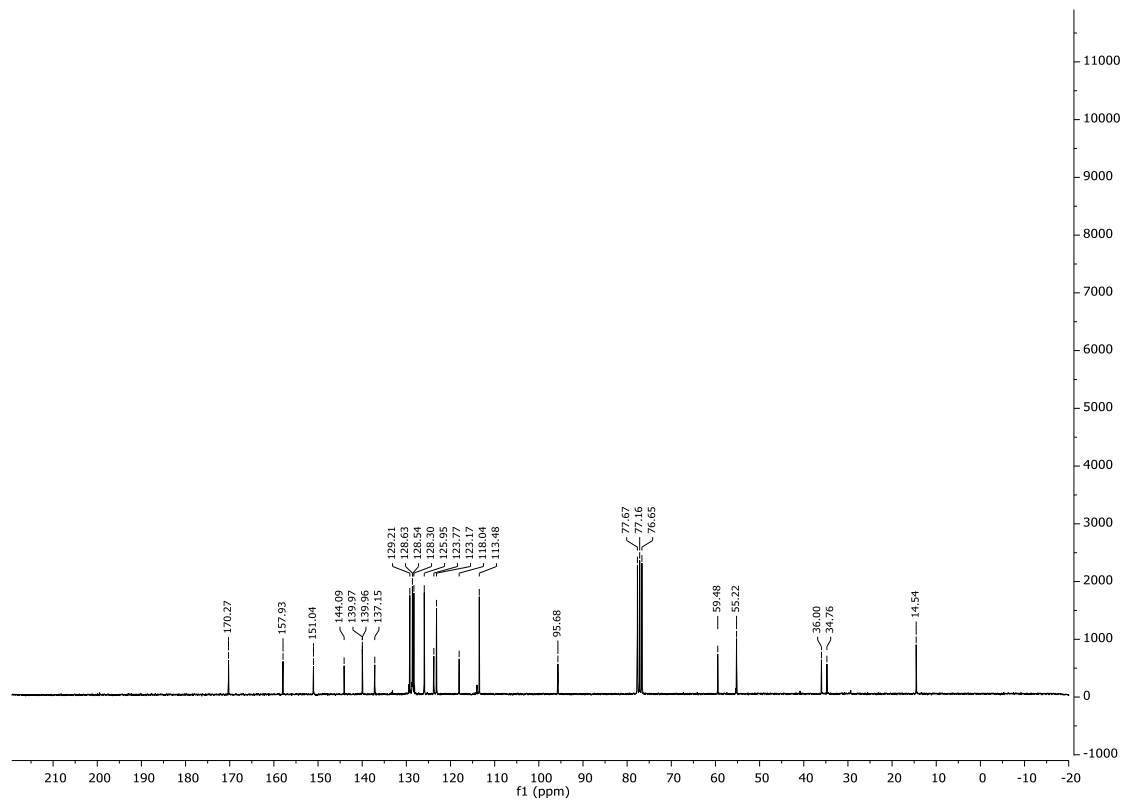
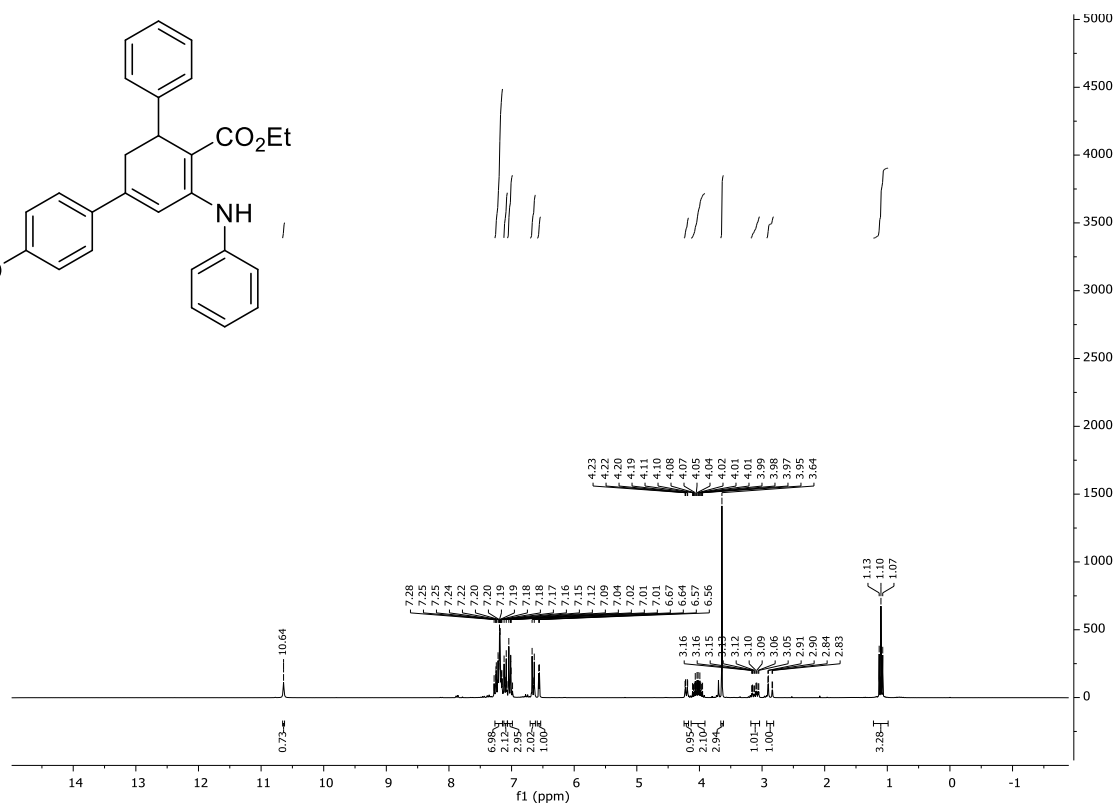
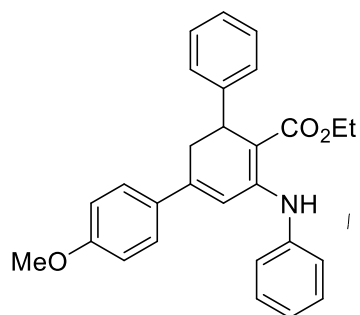
Damiano Rocchi, Jorge Gómez-Carpintero, Juan F. González* and J. Carlos Menéndez*

Unidad de Química Orgánica y Farmacéutica, Departamento de Química en Ciencias Farmacéuticas, Facultad de Farmacia, Universidad Complutense, 28040 Madrid, Spain

Content:

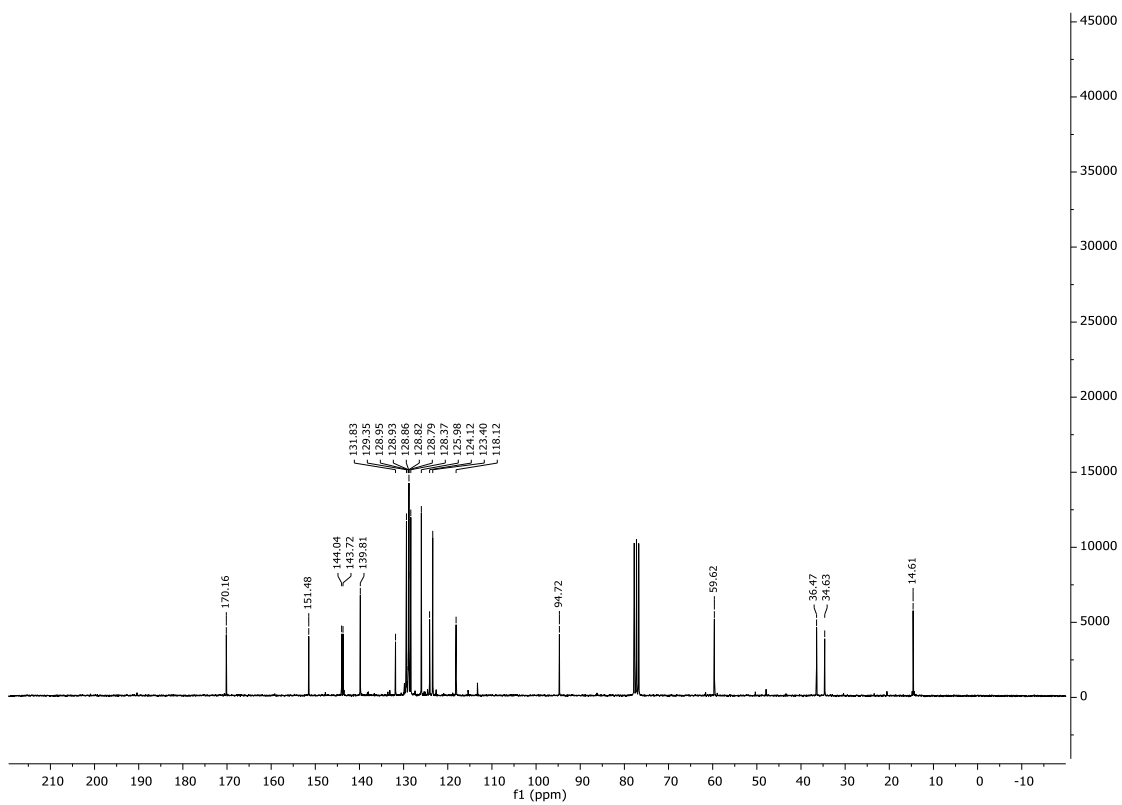
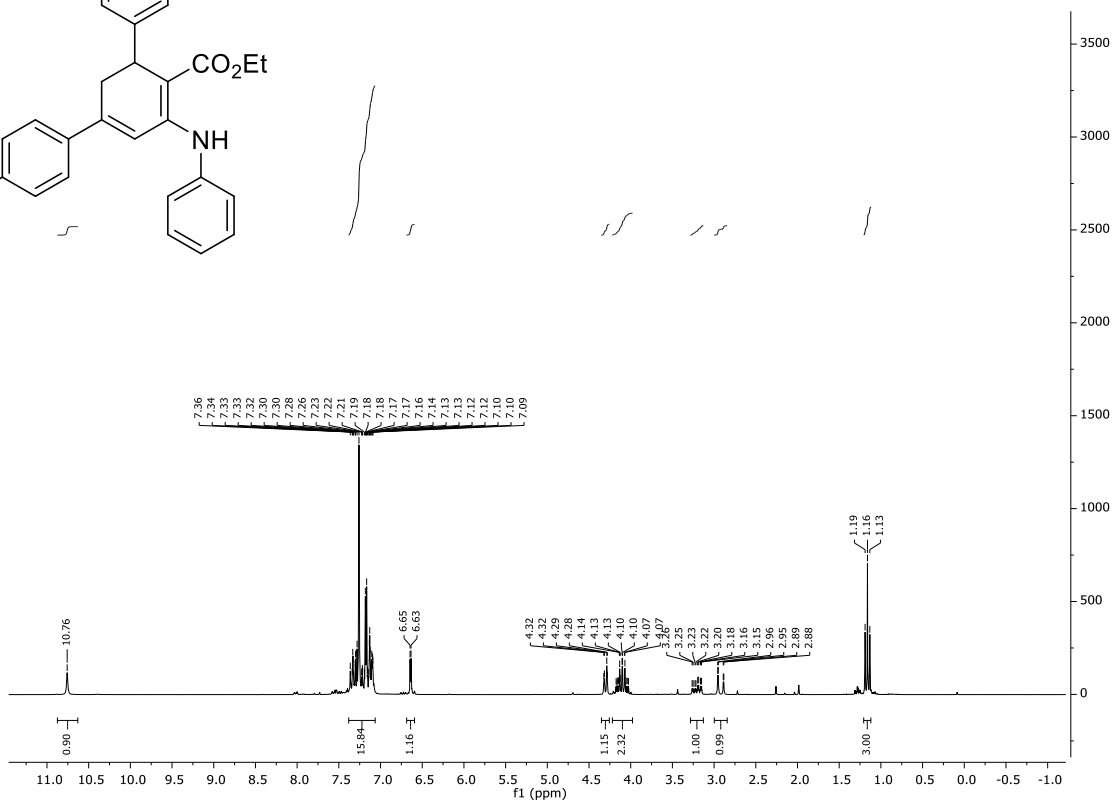
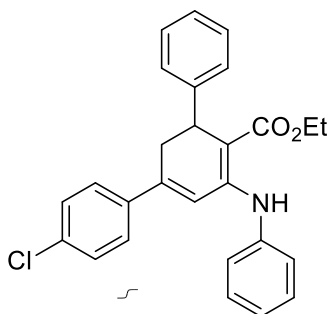
1. Copies of NMR spectra of new compounds
2. Structural study of compound 2a and 3a

Ethyl 4-methoxy-5'-(phenylamino)-2',3'-dihydro-[1,1':3',1''-terphenyl]-4'-carboxylate (II)

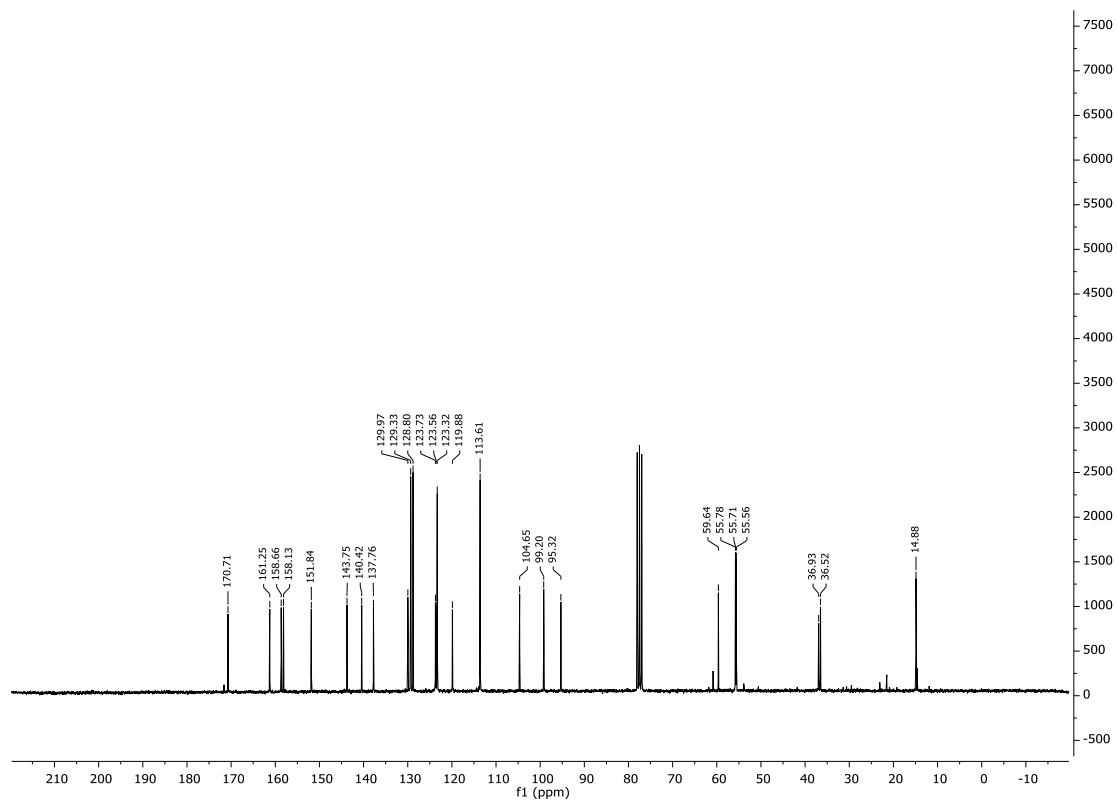
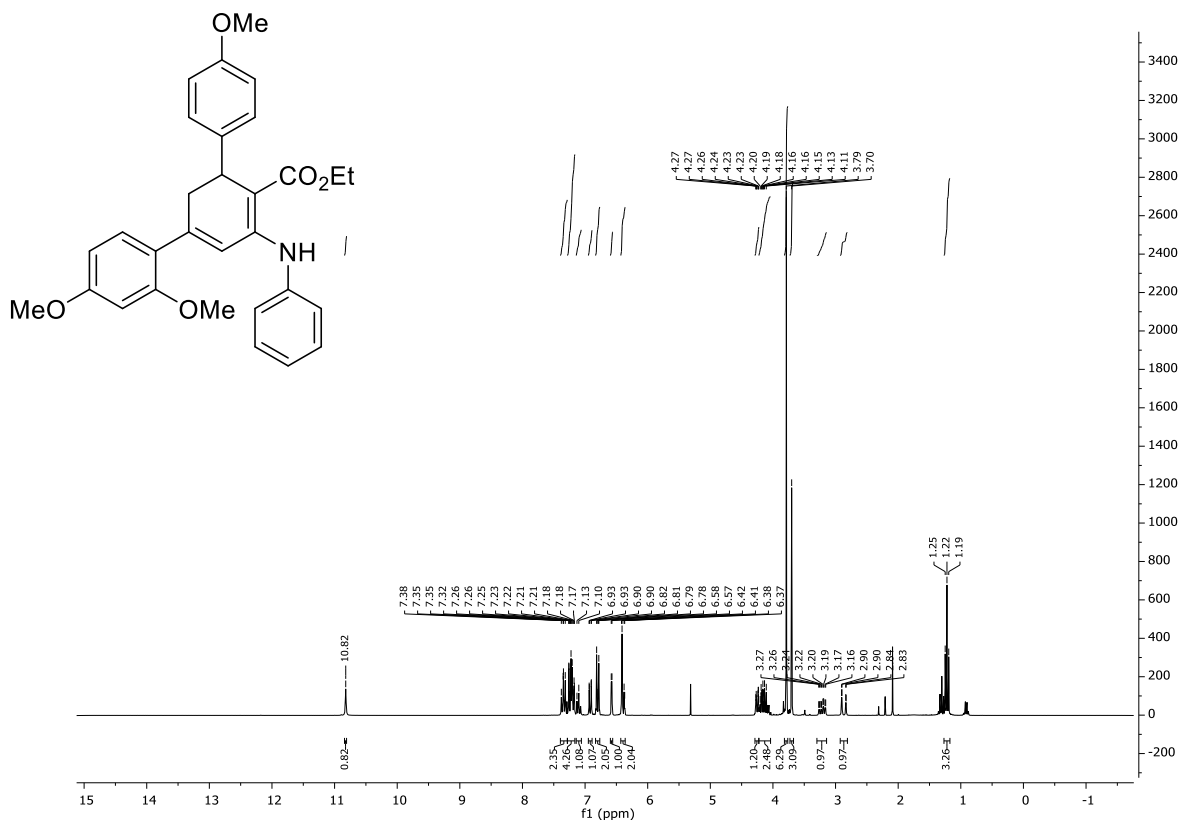


Ethyl
carboxylate (1m)

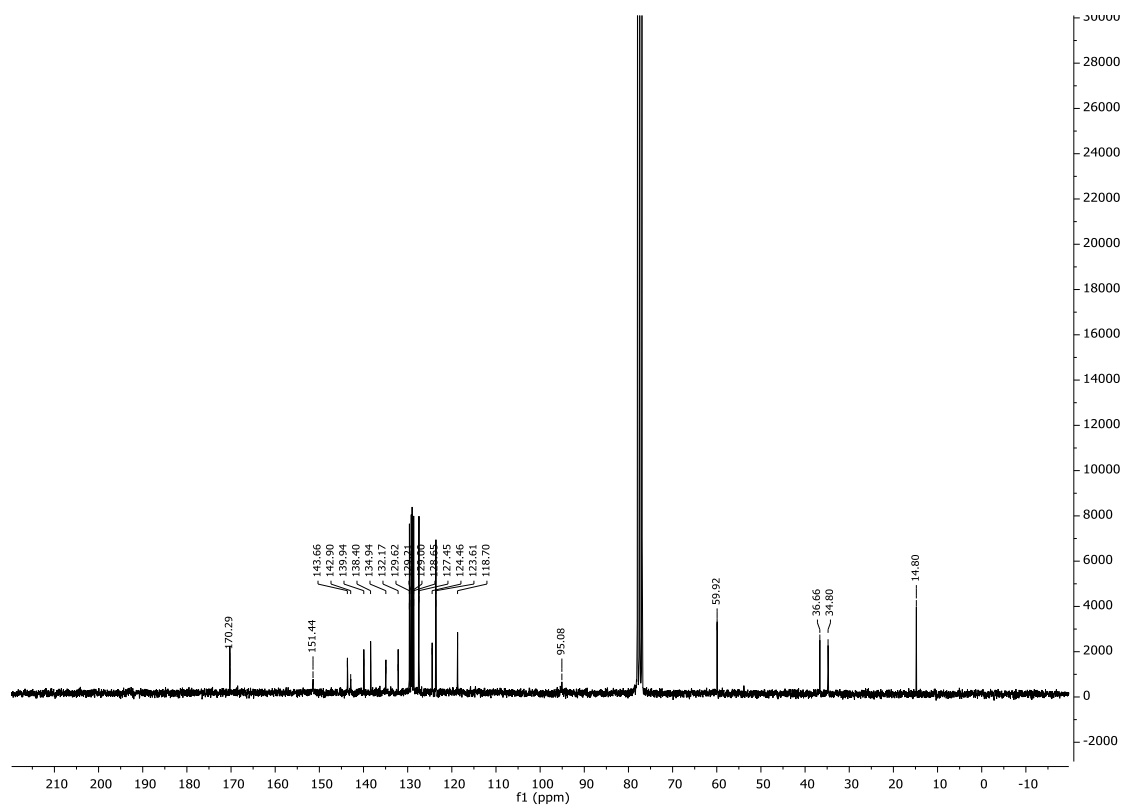
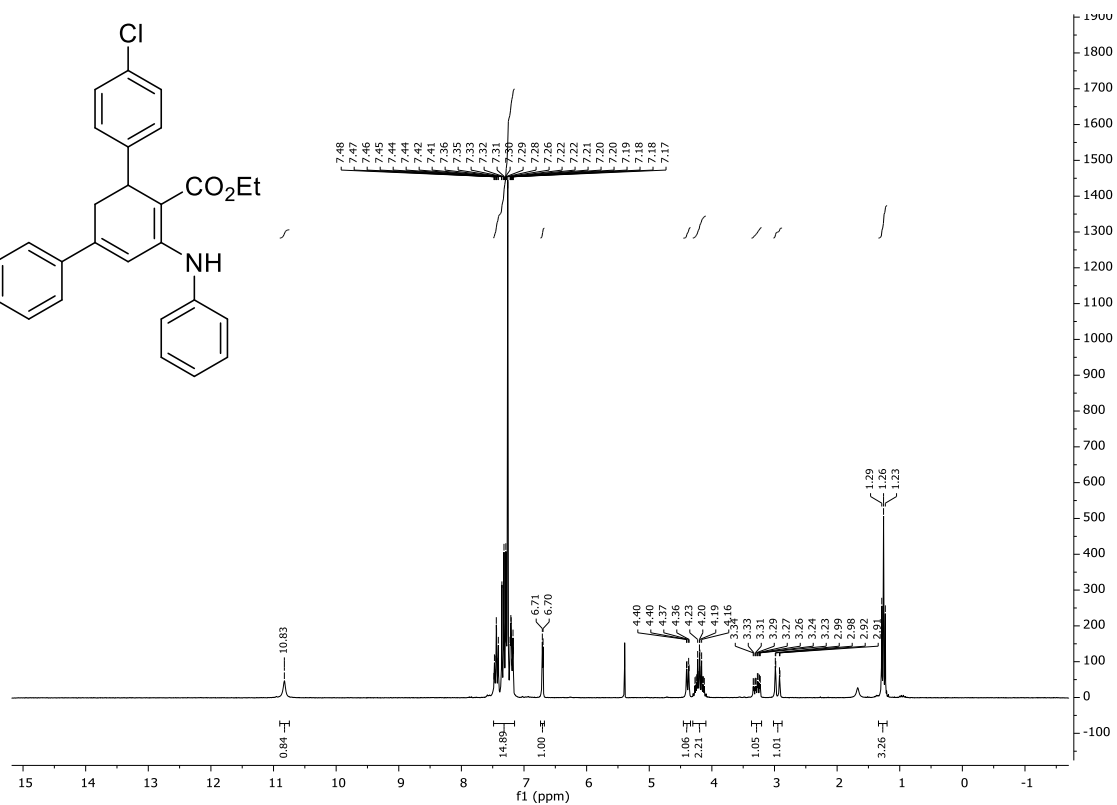
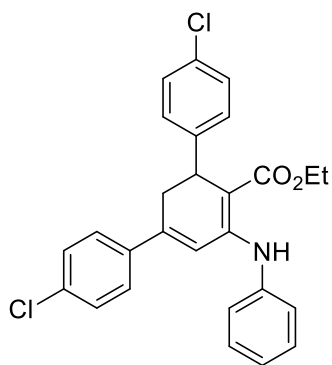
4-chloro-5'-(phenylamino)-2',3'-dihydro-[1,1':3',1''-terphenyl]-4'-



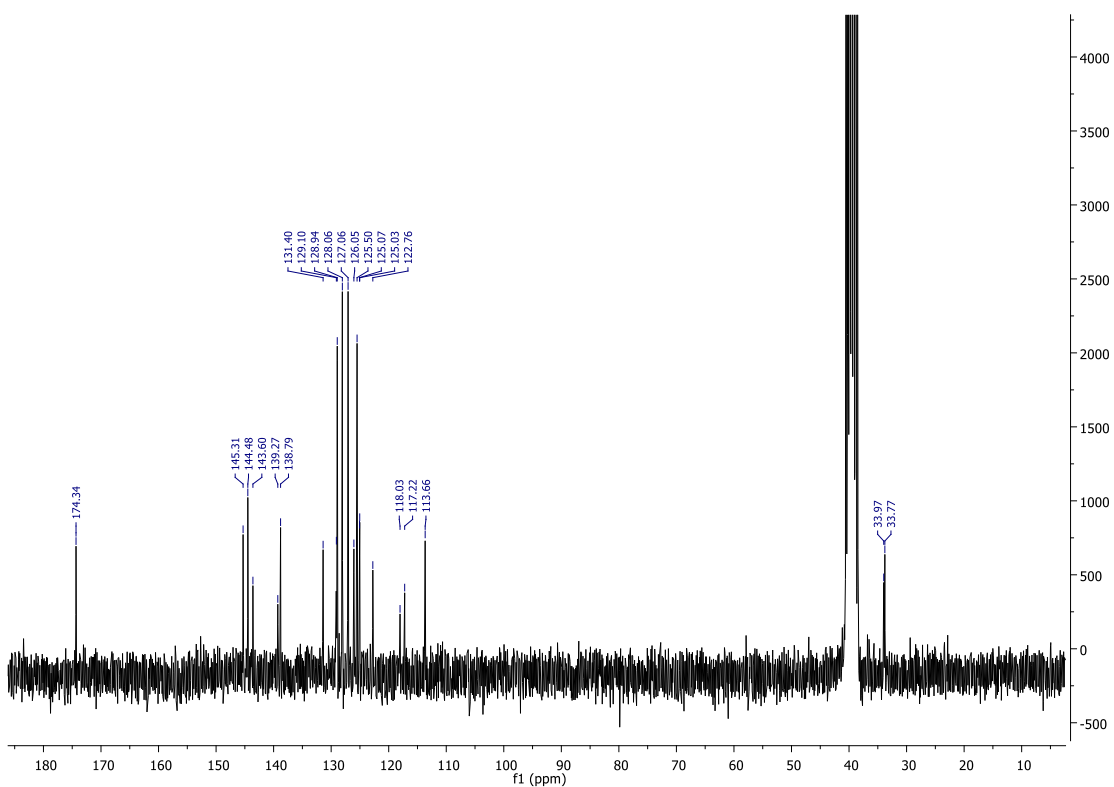
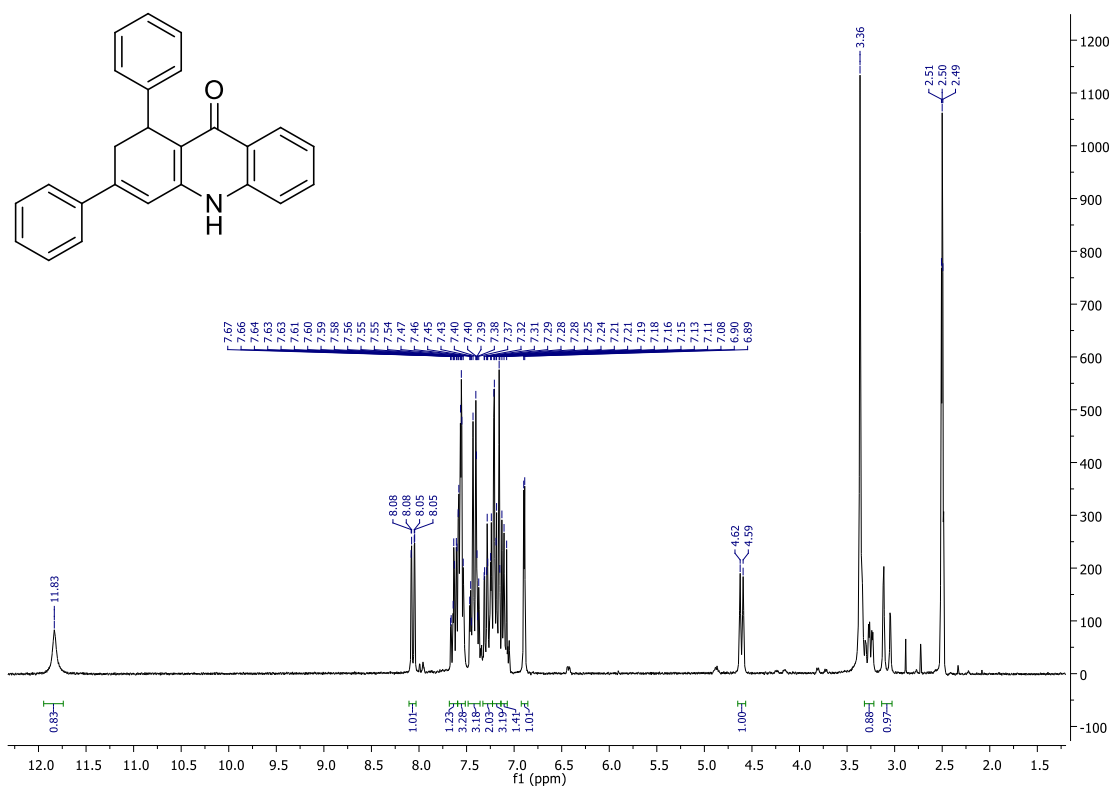
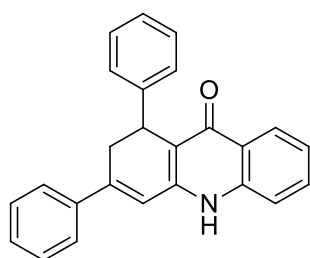
Ethyl 2,4,4''-trimethoxy-5'-(phenylamino)-2',3'-dihydro-[1,1':3',1''-terphenyl]-4'-carboxylate (1n)



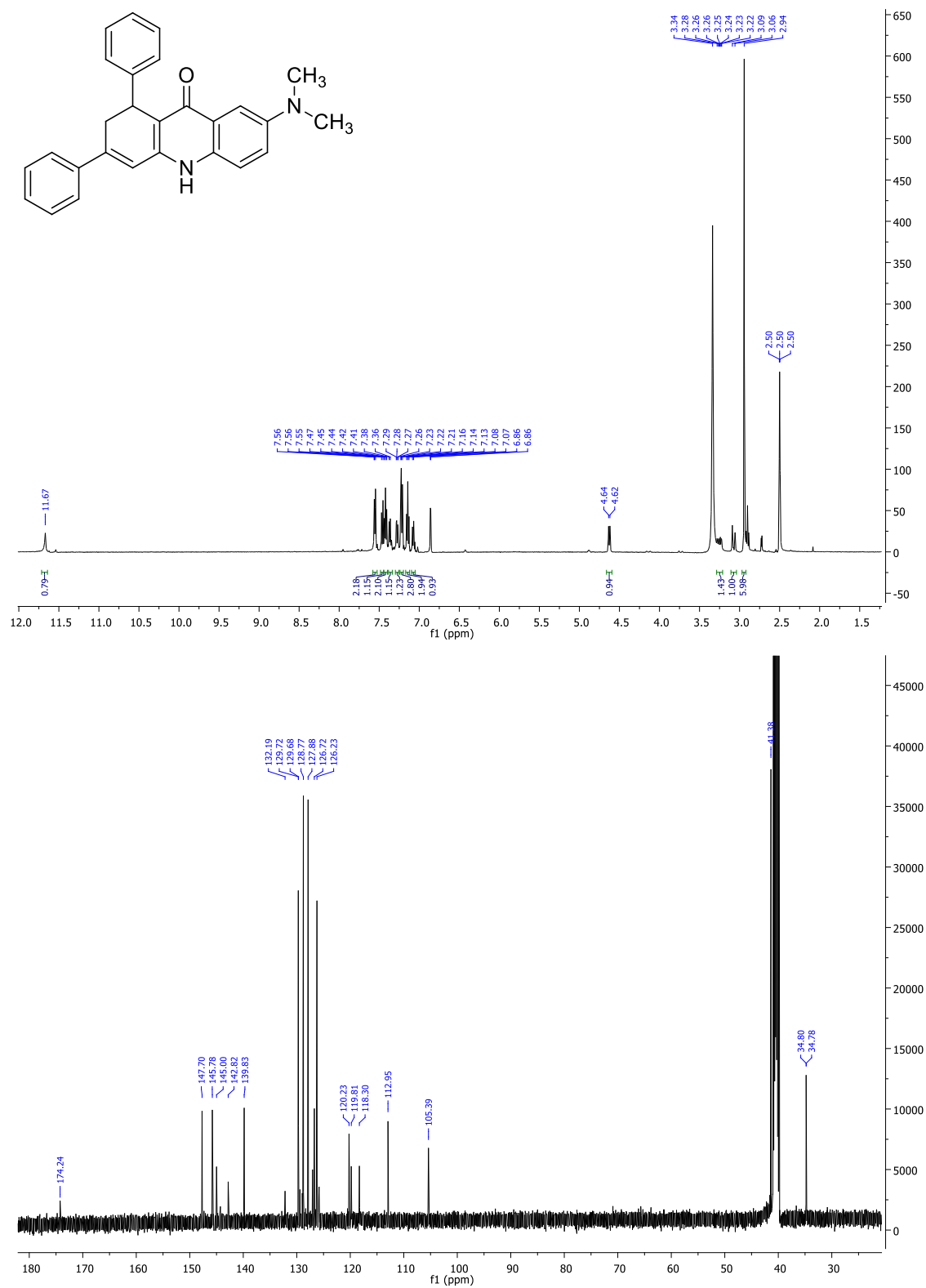
Ethyl 4,4'-dichloro-5'-(phenylamino)-2',3'-dihydro-[1,1':3',1''-terphenyl]-4'-carboxylate (10)



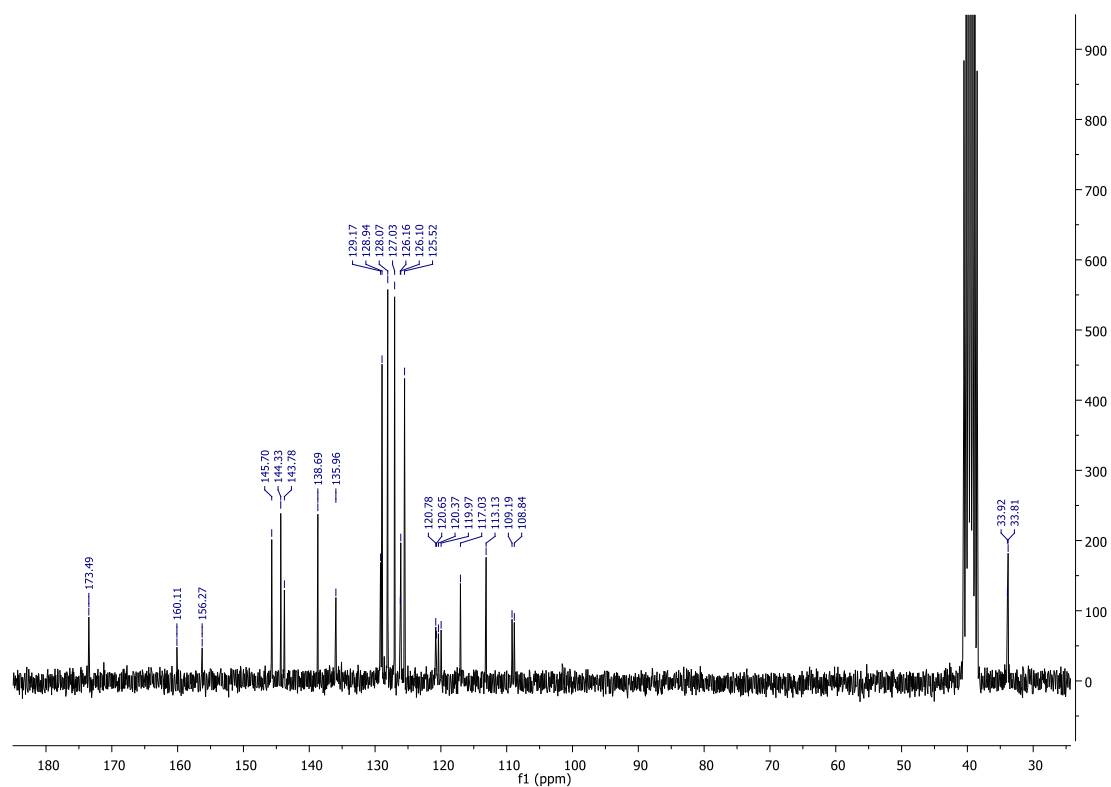
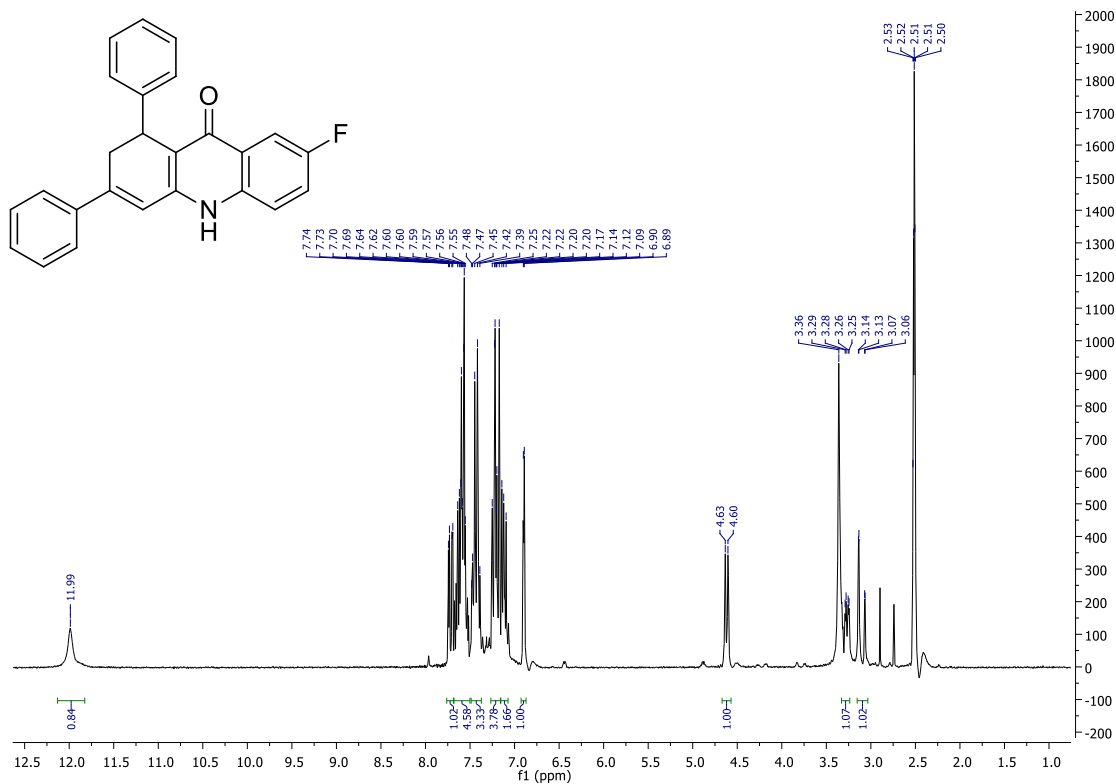
1,3-diphenyl-1,2-dihydroacridin-9(10H)-one (2a)



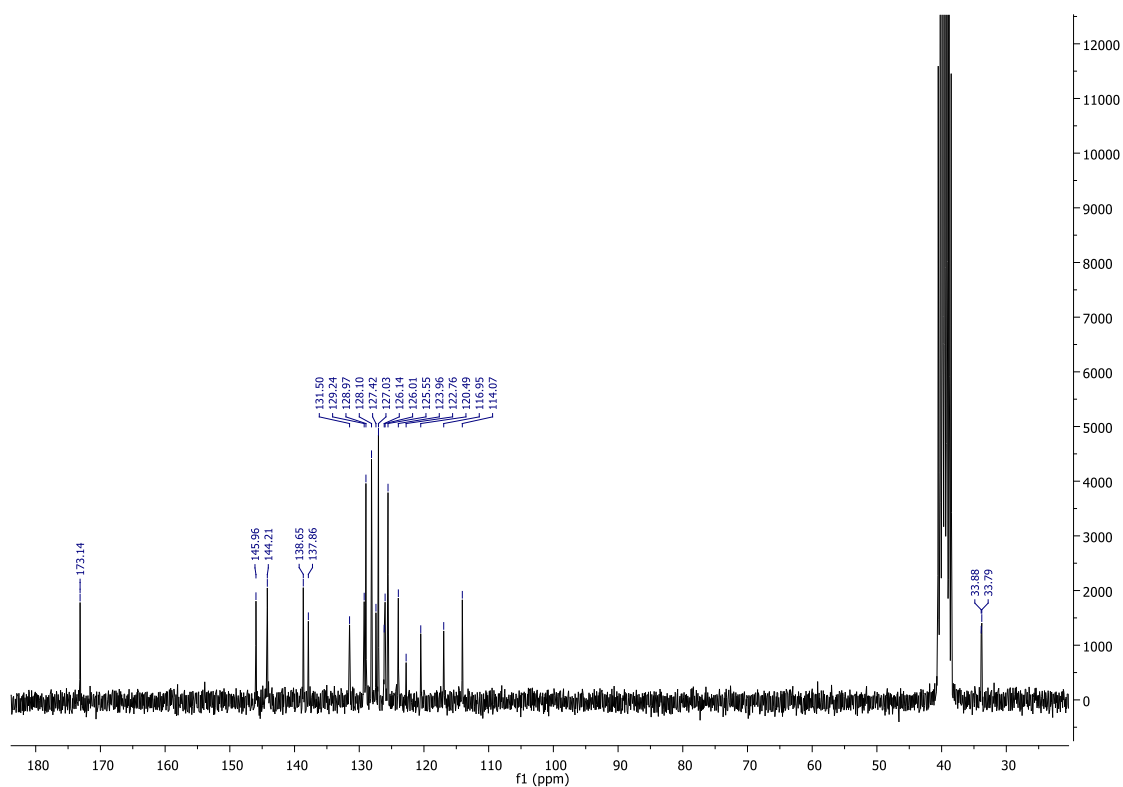
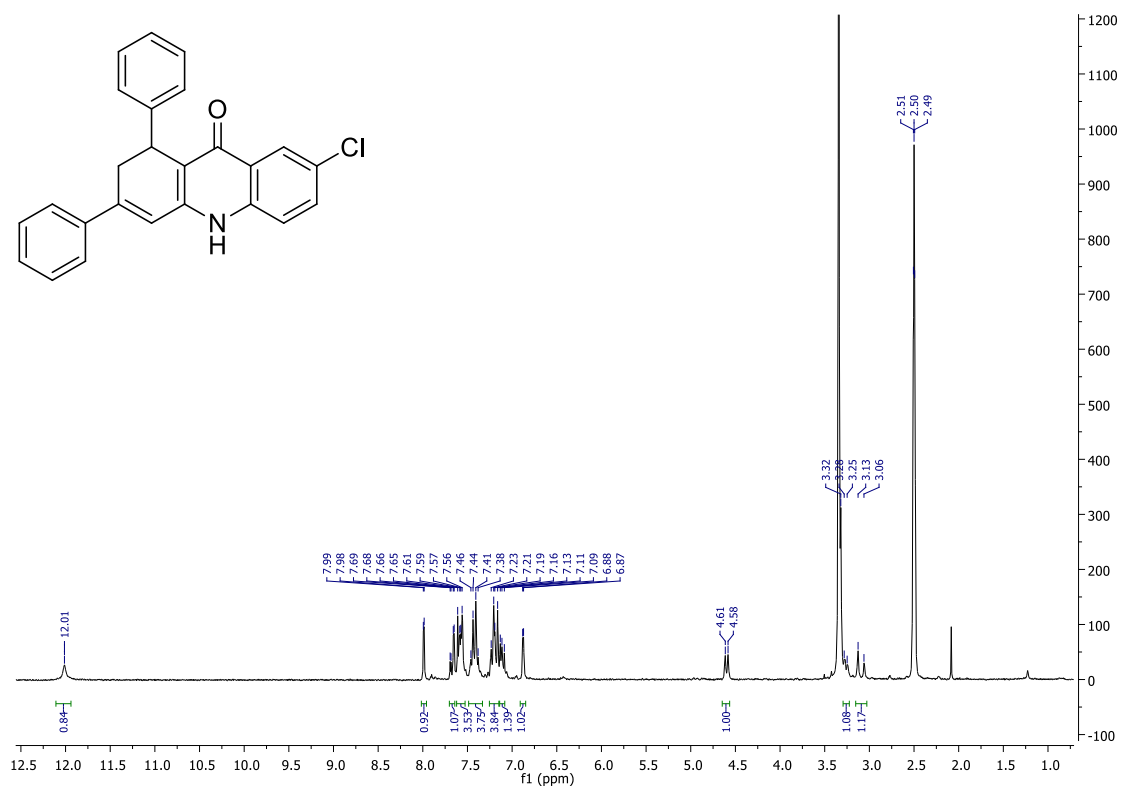
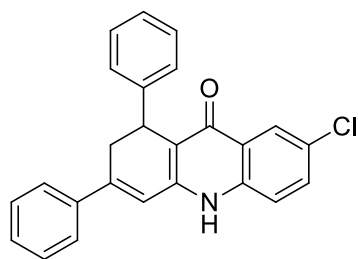
7-(dimethylamino)-1,3-diphenyl-1,2-dihydroacridin-9(10H)-one (2b)



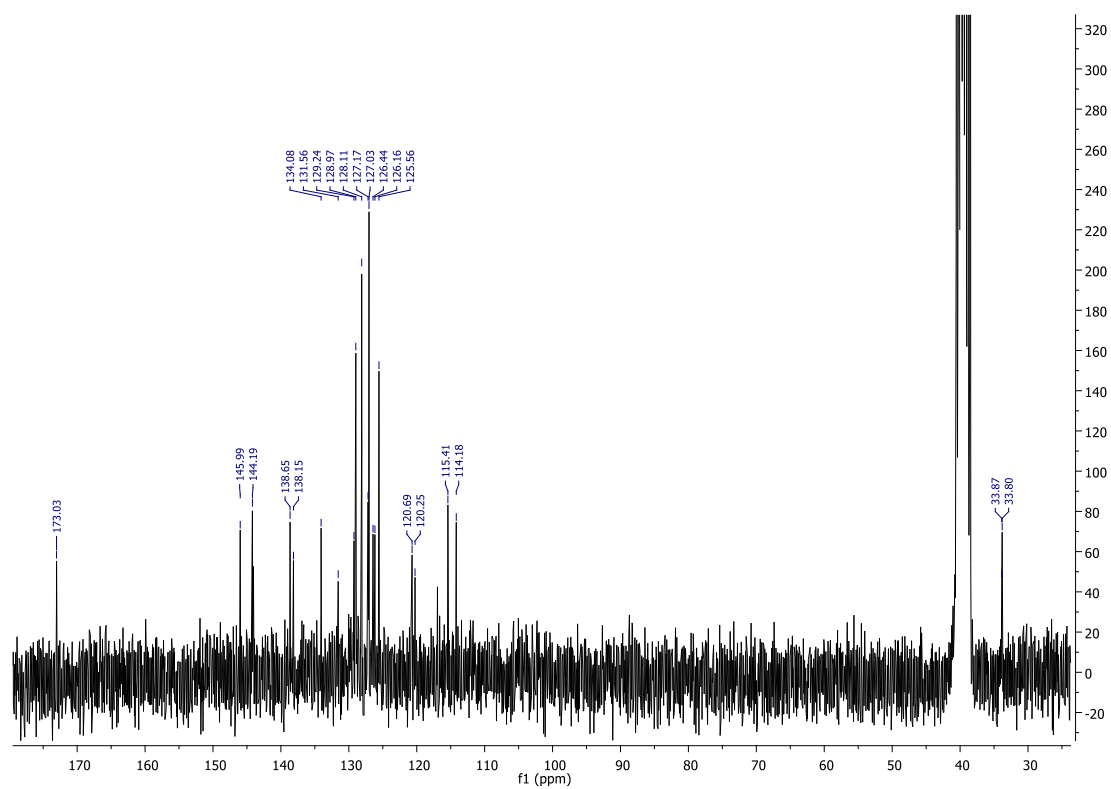
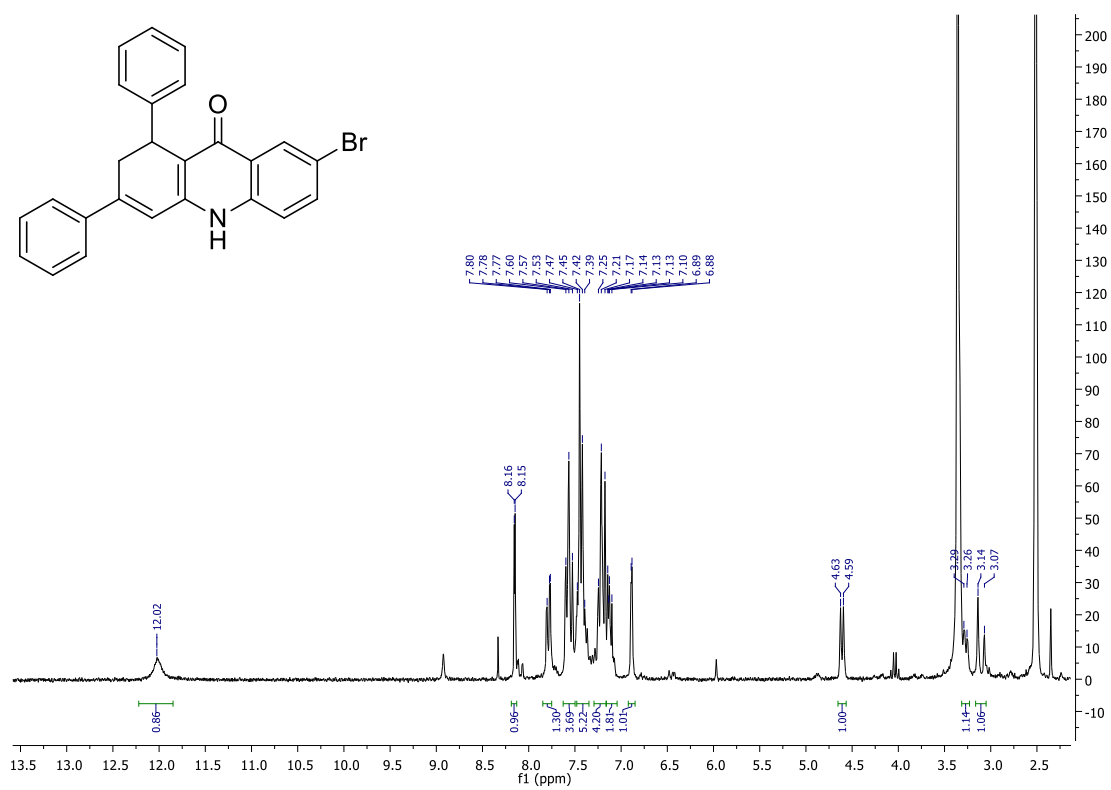
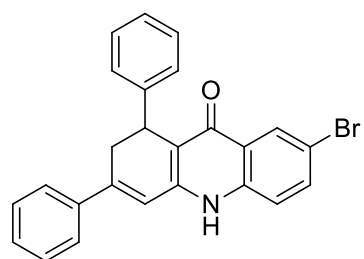
7-fluoro-1,3-diphenyl-1,2-dihydroacridin-9(10H)-one (2c)



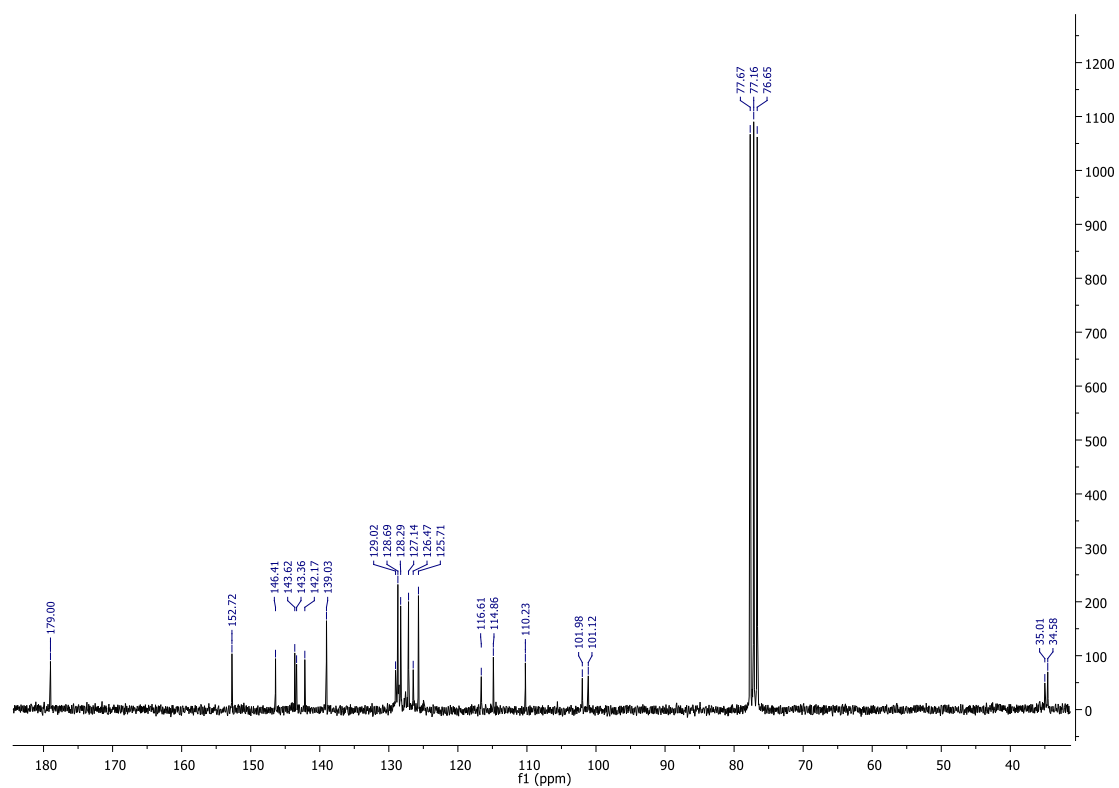
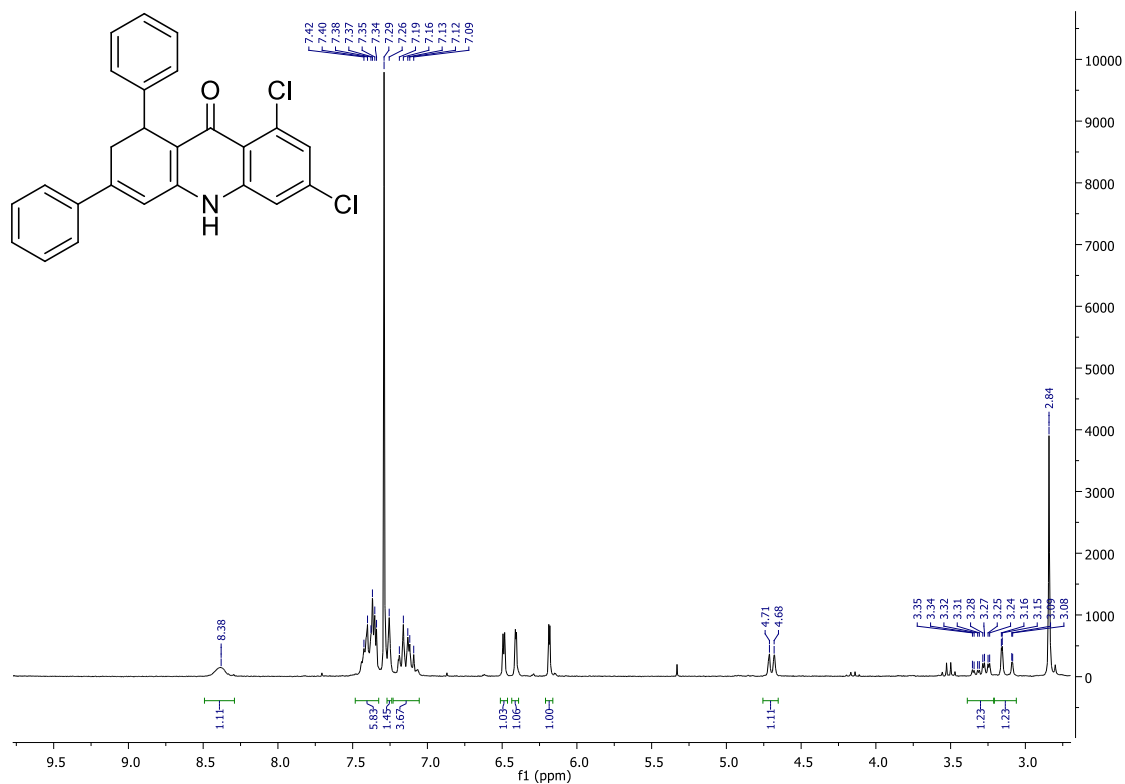
7-chloro-1,3-diphenyl-1,2-dihydroacridin-9(10H)-one (2d)



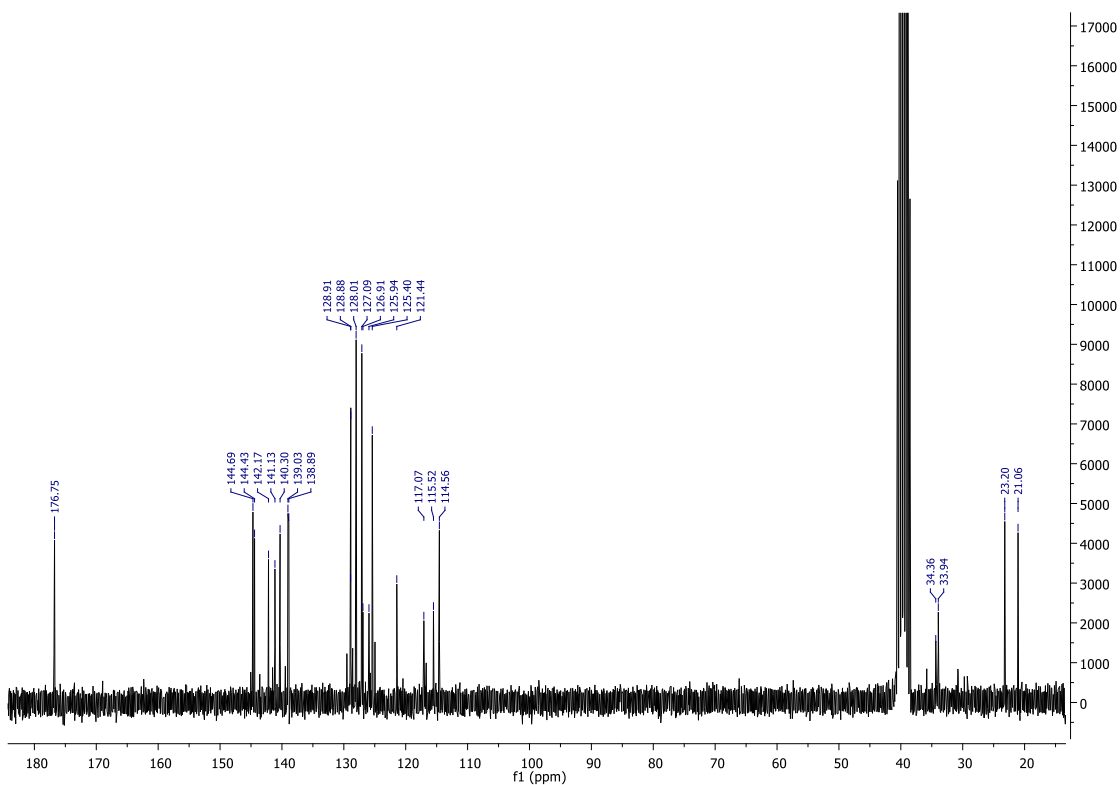
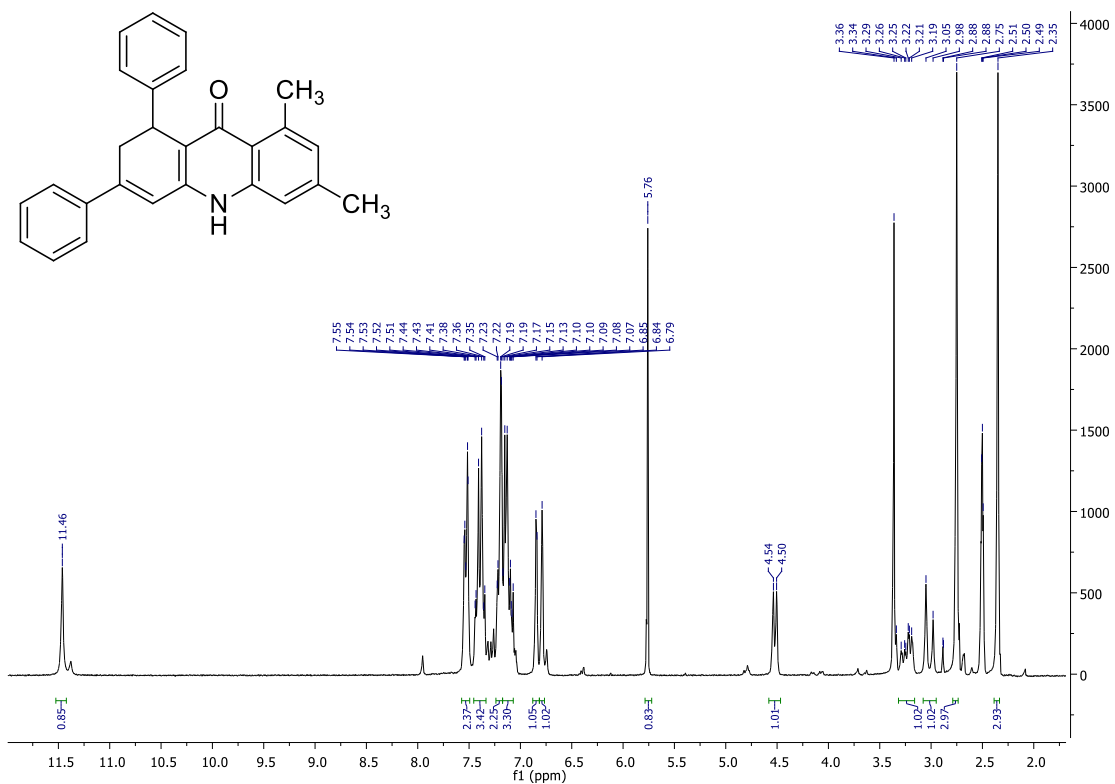
7-bromo-1,3-diphenyl-1,2-dihydroacridin-9(10H)-one (2e)



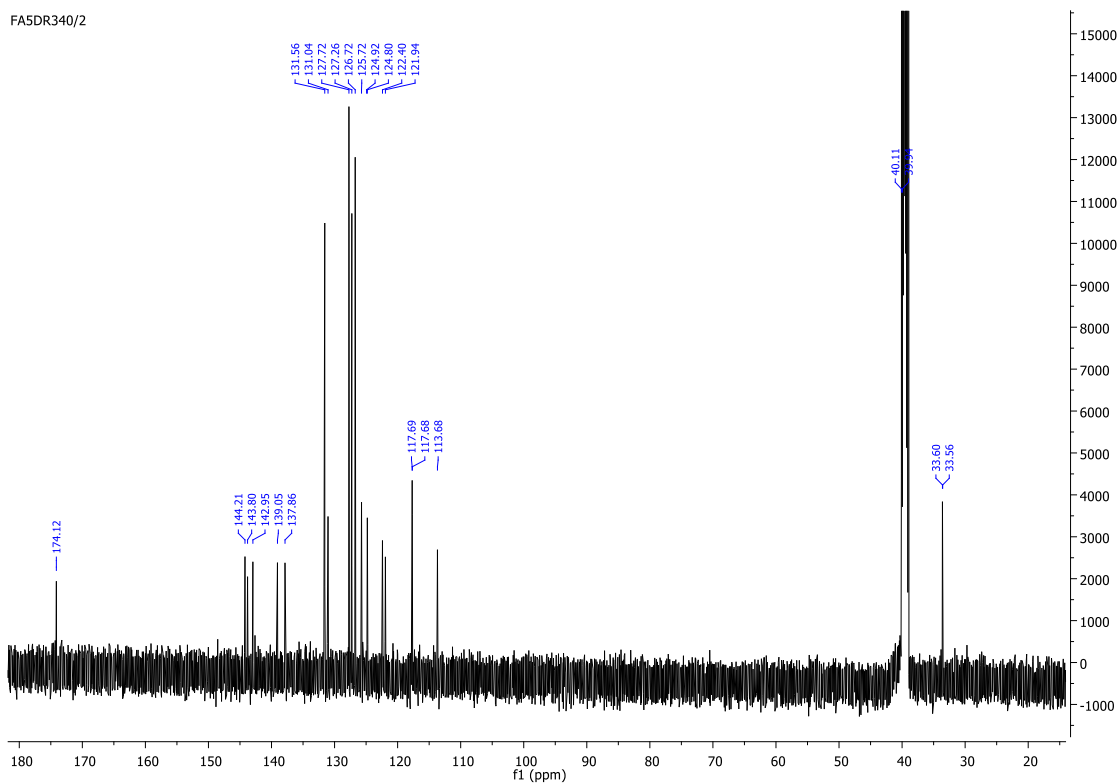
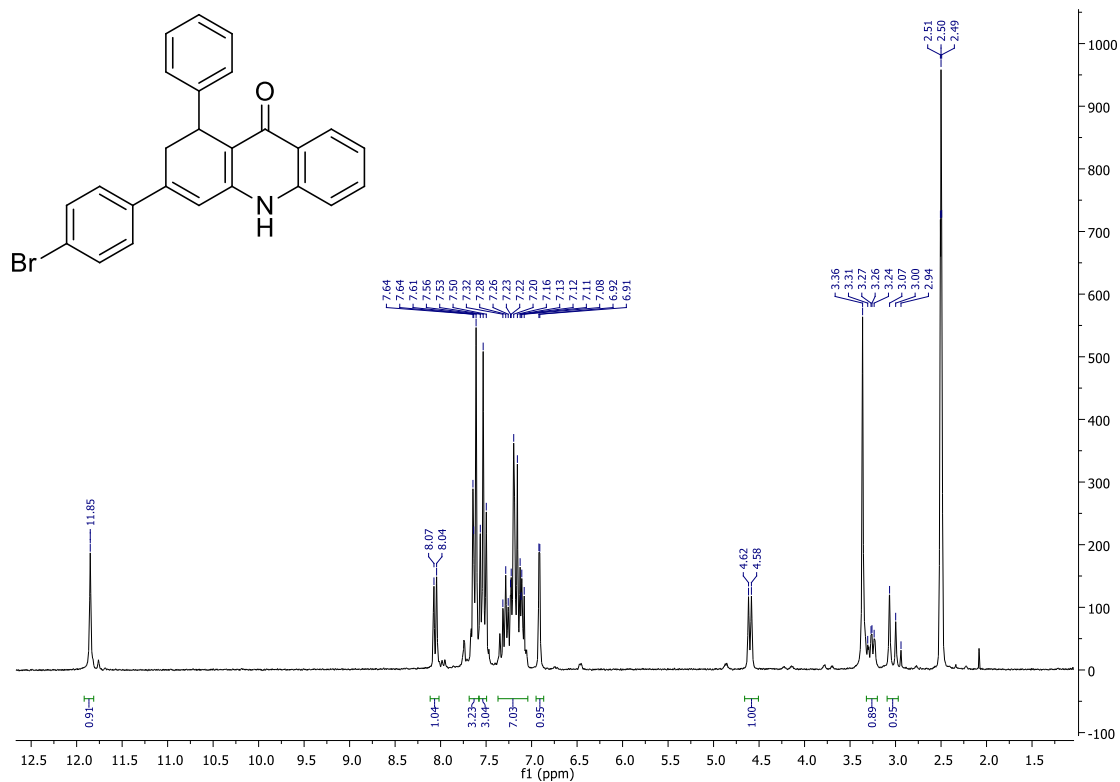
6,8-dichloro-1,3-diphenyl-1,2-dihydroacridin-9(10H)-one (2f)



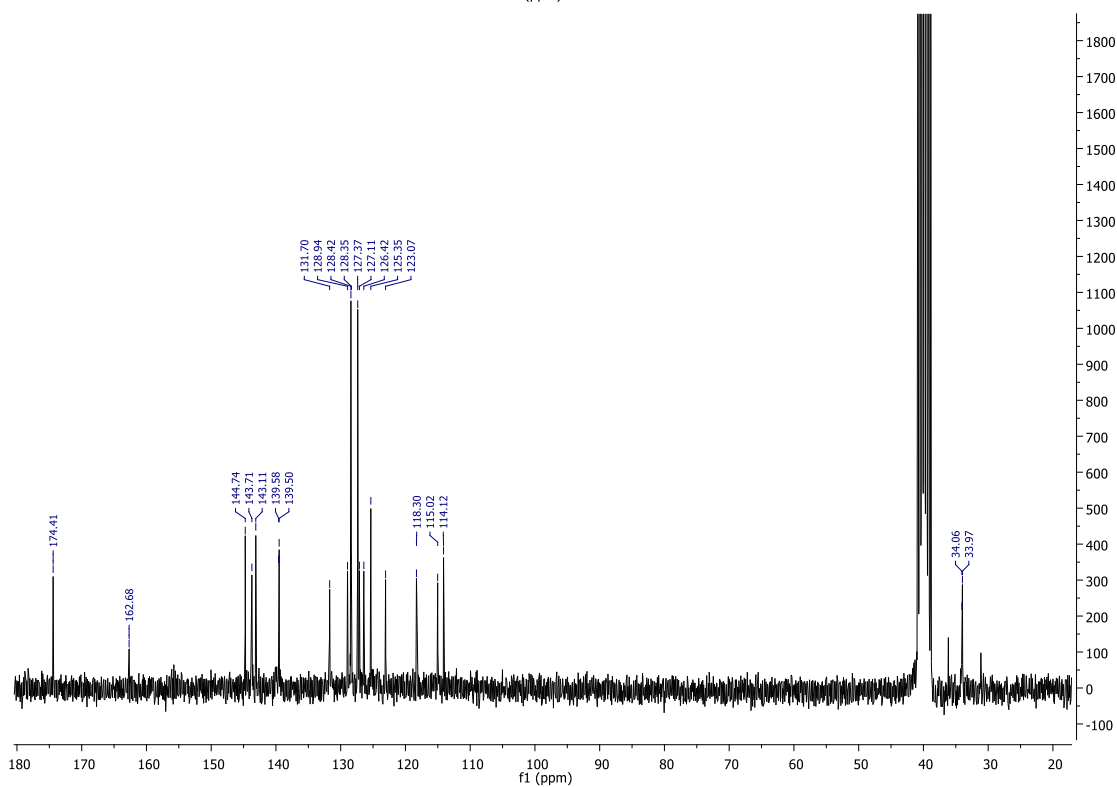
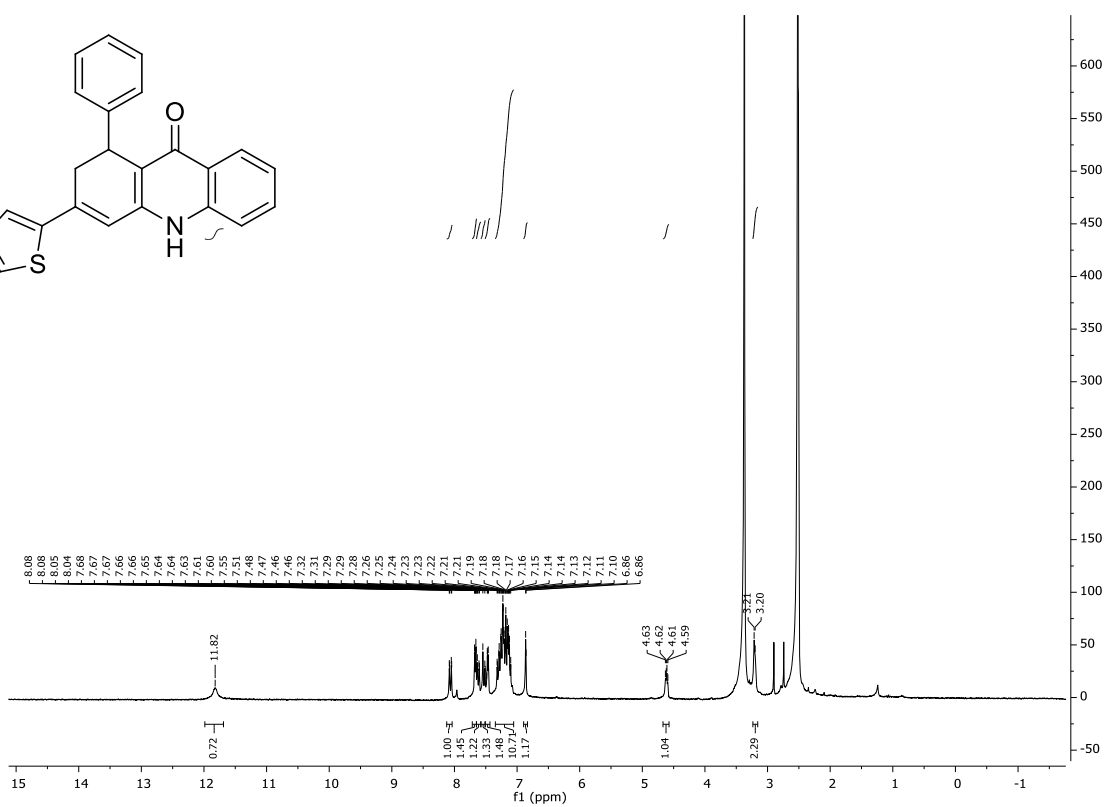
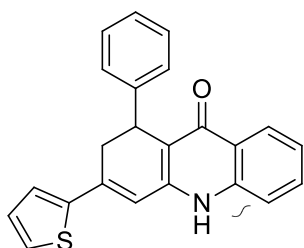
6,8-dimethyl-1,3-diphenyl-1,2-dihydroacridin-9(10H)-one (2g)



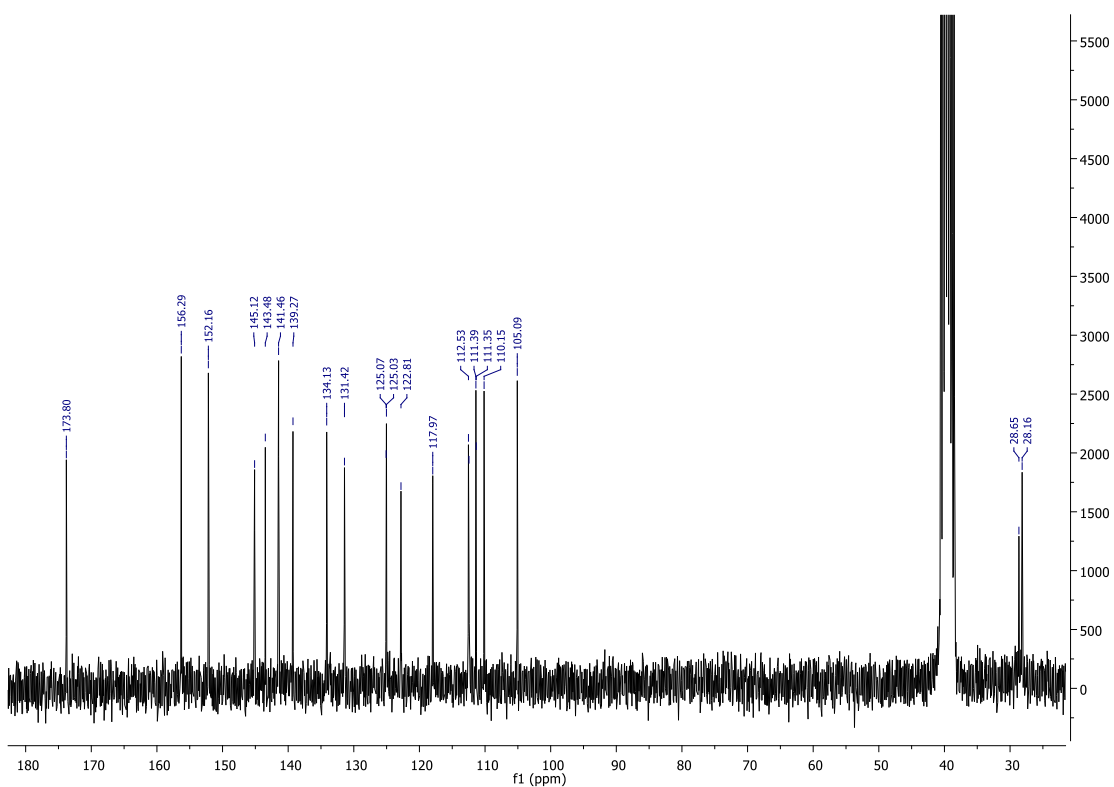
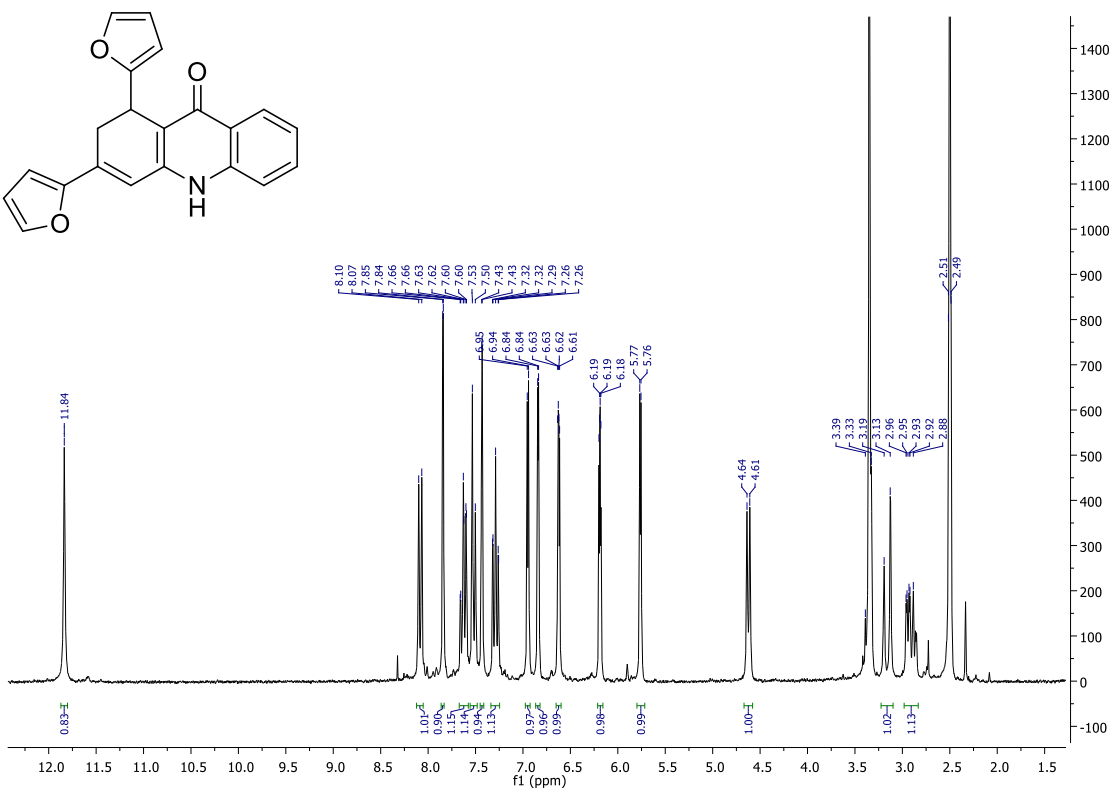
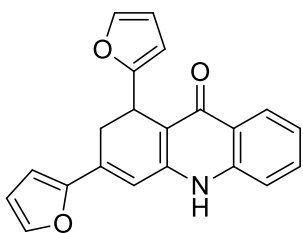
3-(4-bromophenyl)-1-phenyl-1,2-dihydroacridin-9(10H)-one (2i)



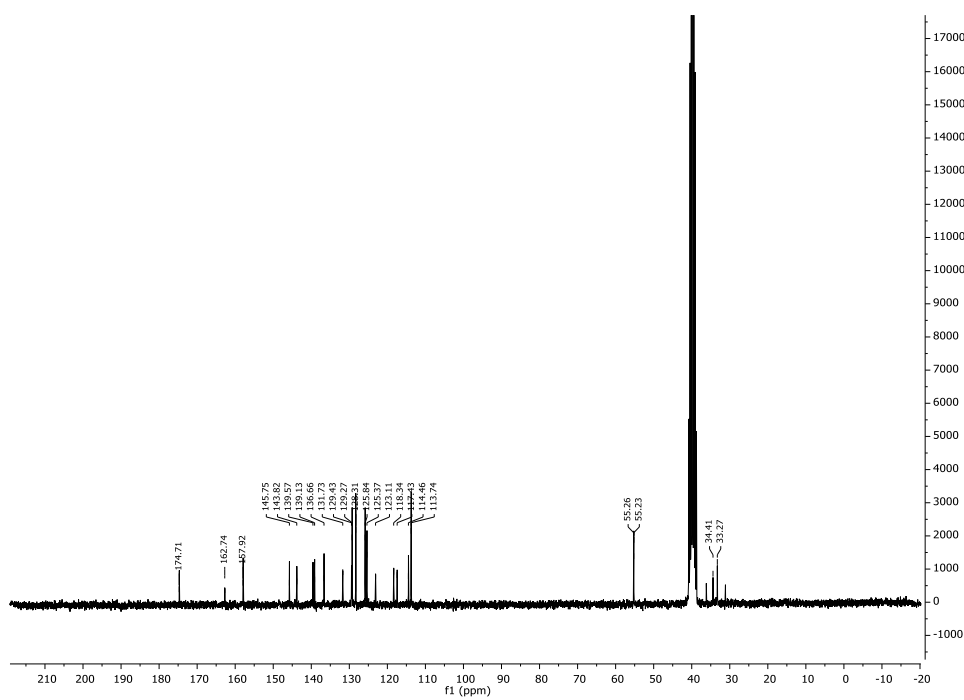
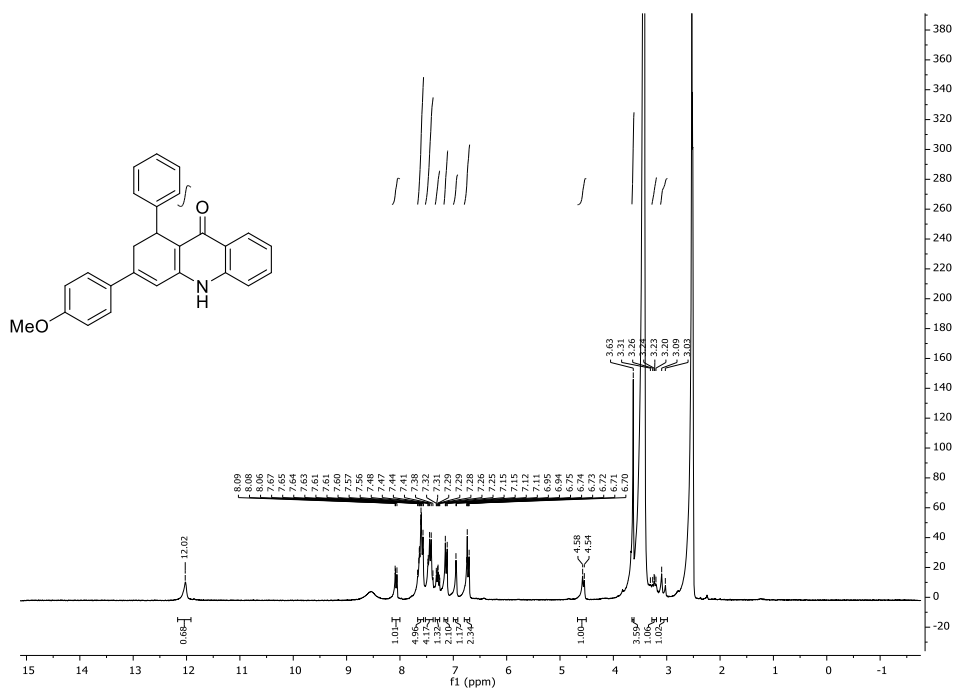
1-phenyl-3-(thiophen-2-yl)-1,2-dihydroacridin-9(10H)-one (2j)



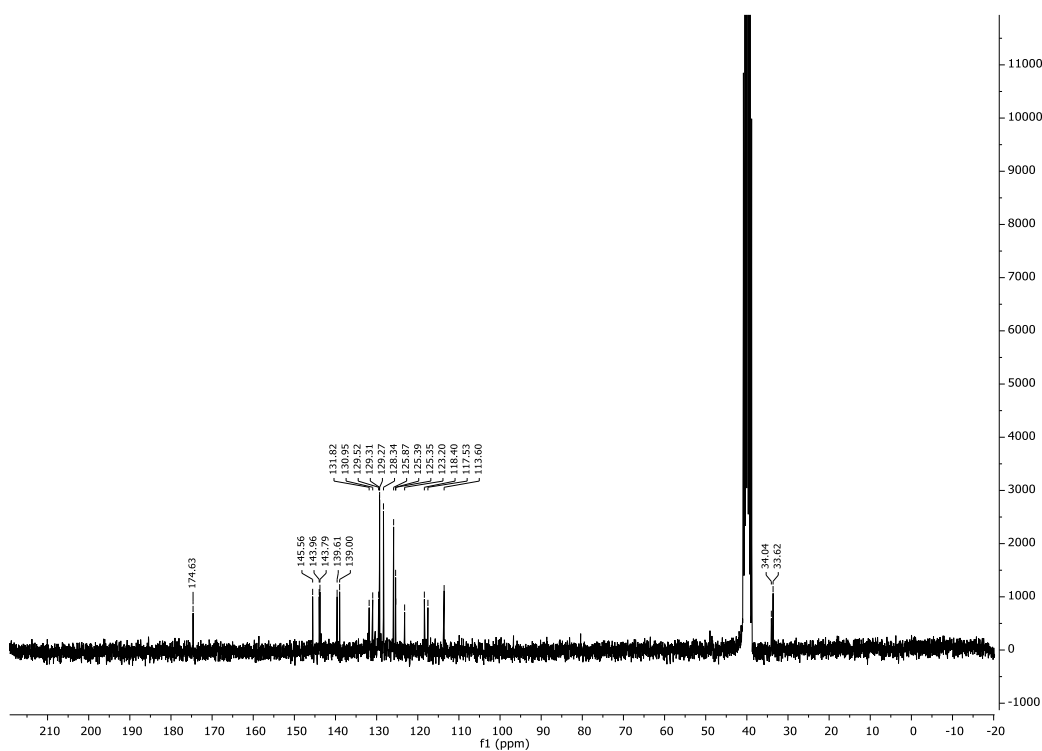
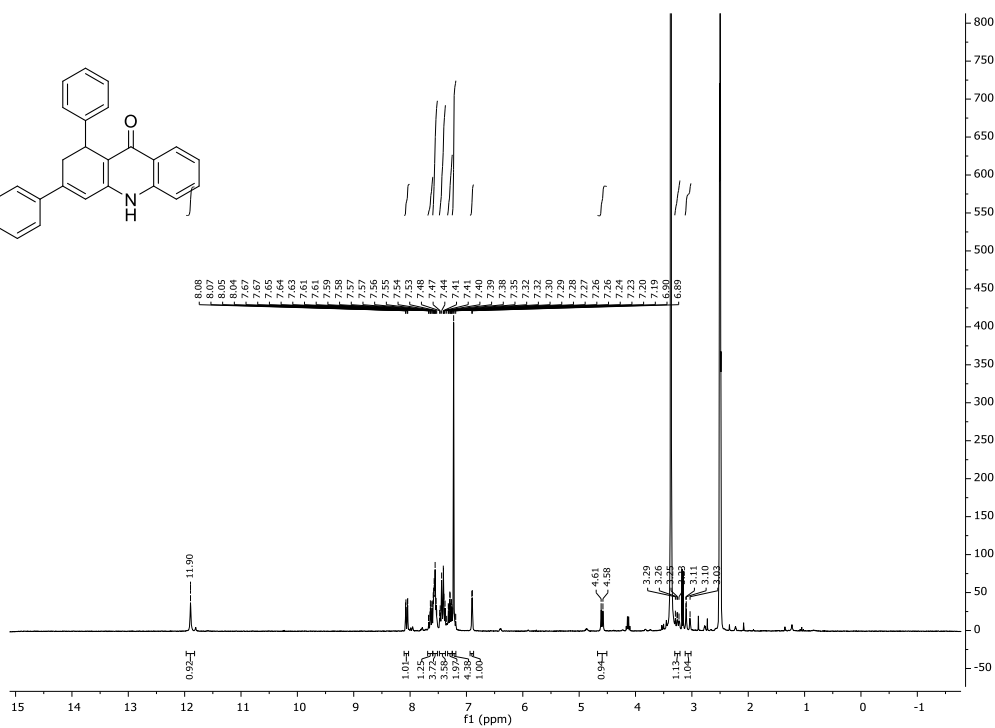
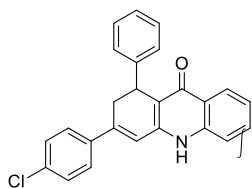
1,3-di(furan-2-yl)-1,2-dihydroacridin-9(10H)-one (2k)



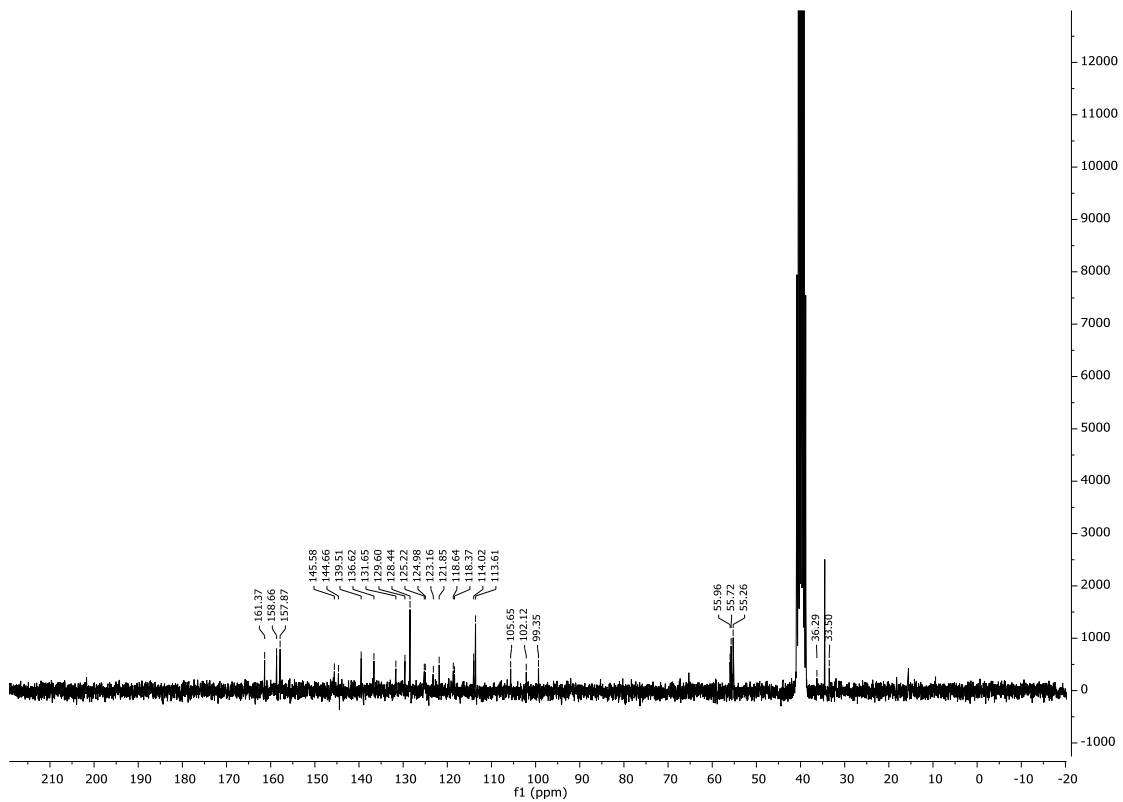
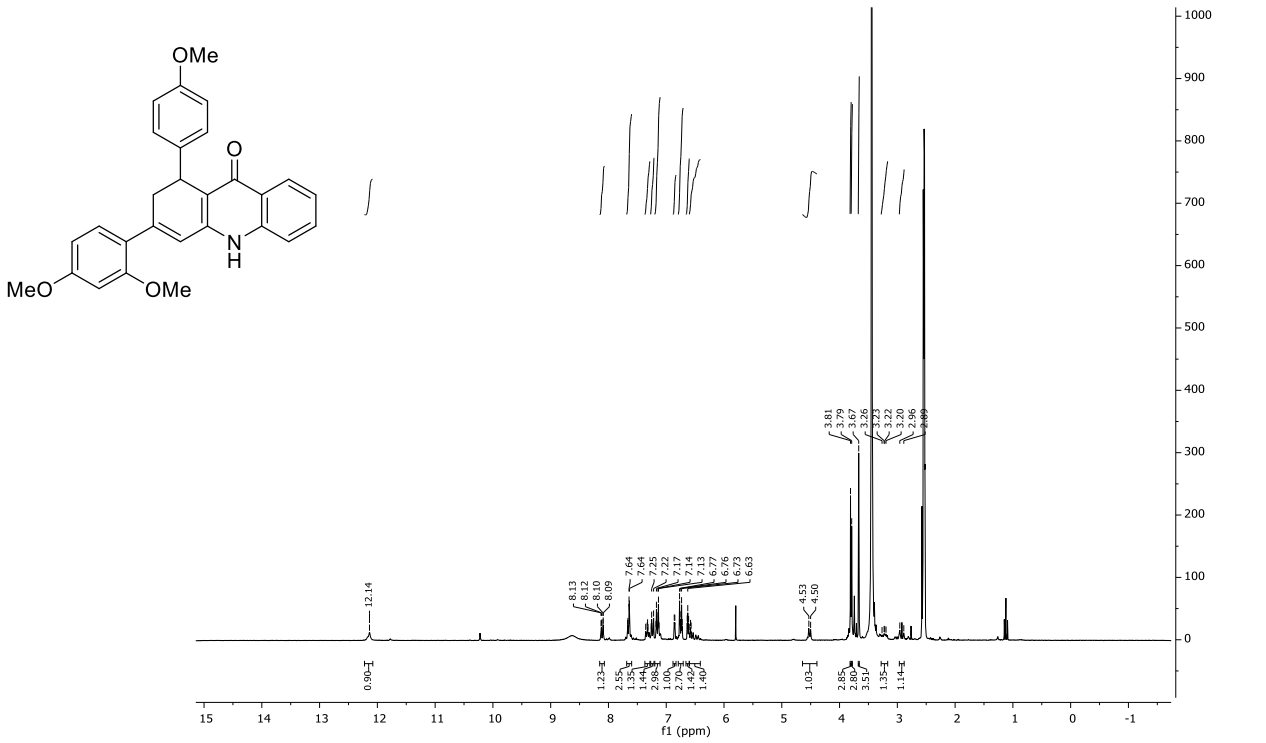
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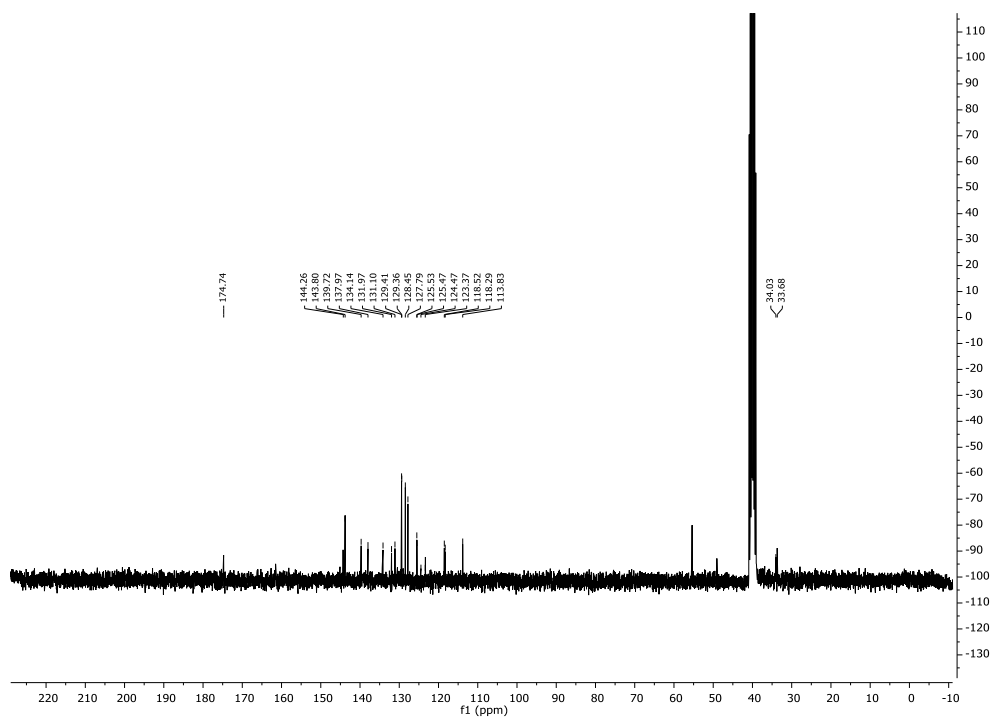
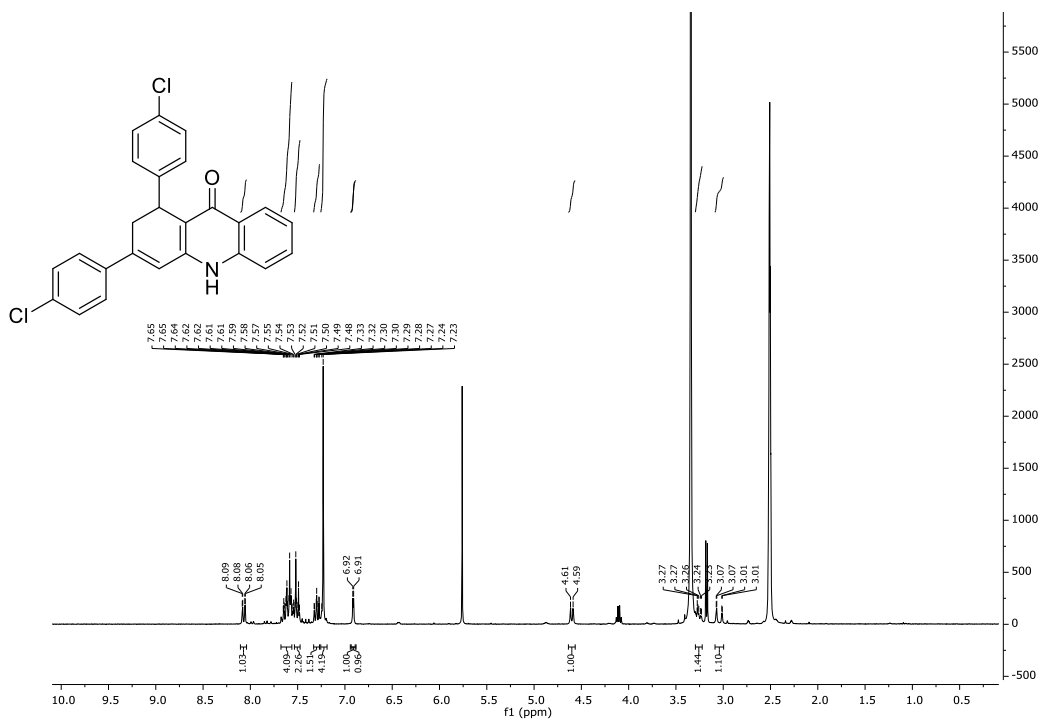
1-(4-chlorophenyl)-3-phenyl-1,10-dihydroacridin-9(2H)-one (2m)



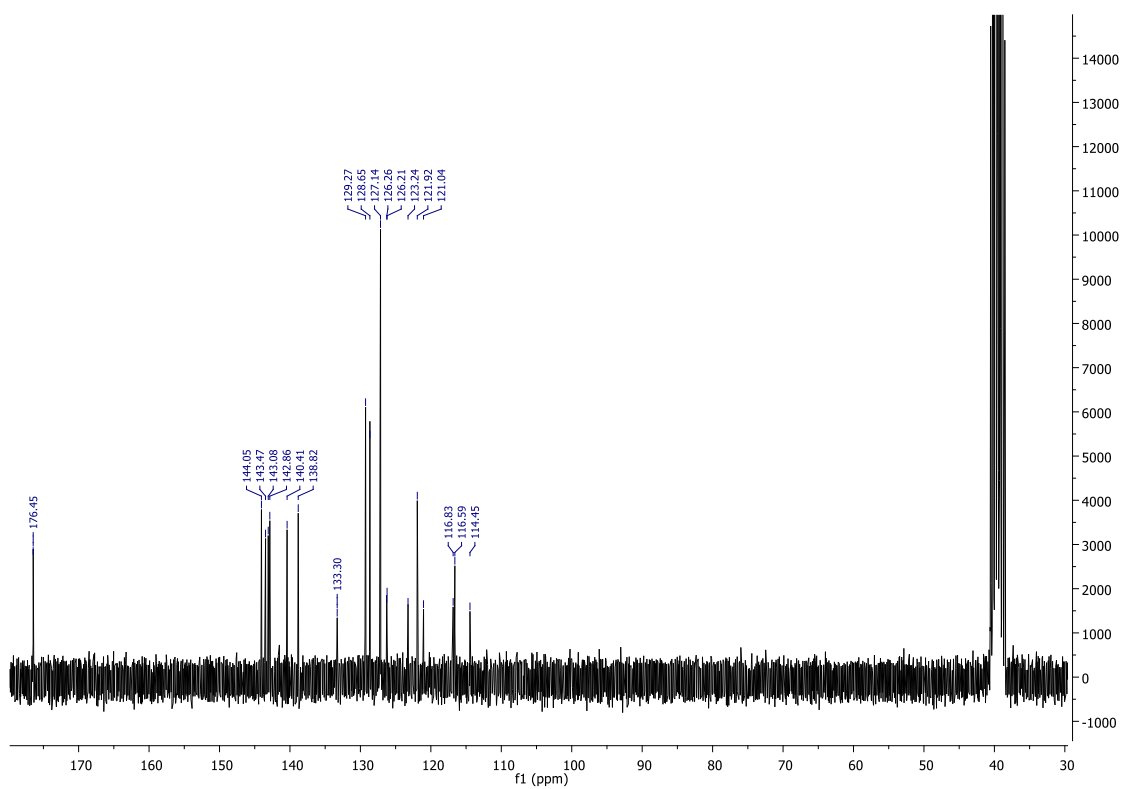
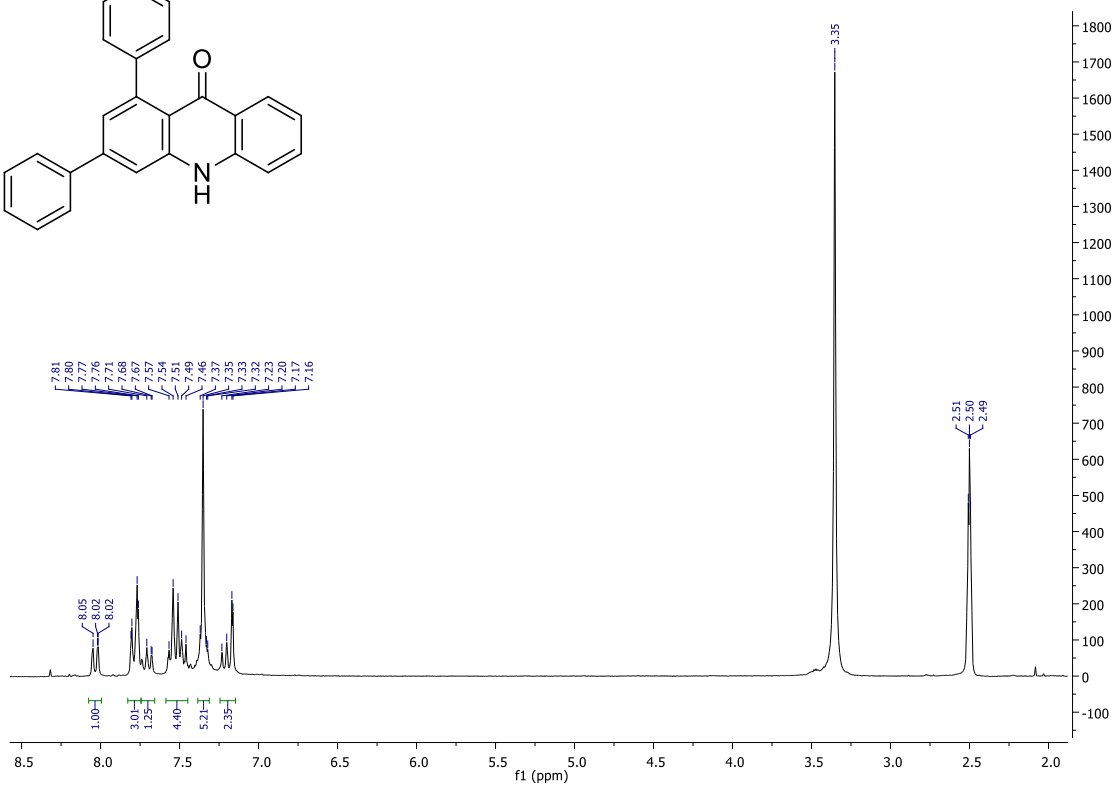
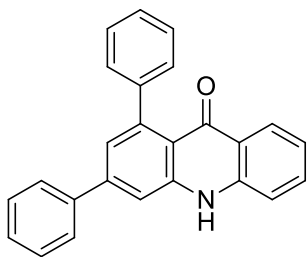
1-(2,4-dimethoxyphenyl)-3-(4-methoxyphenyl)-1,10-dihydroacridin-9(2H)-one (2n)



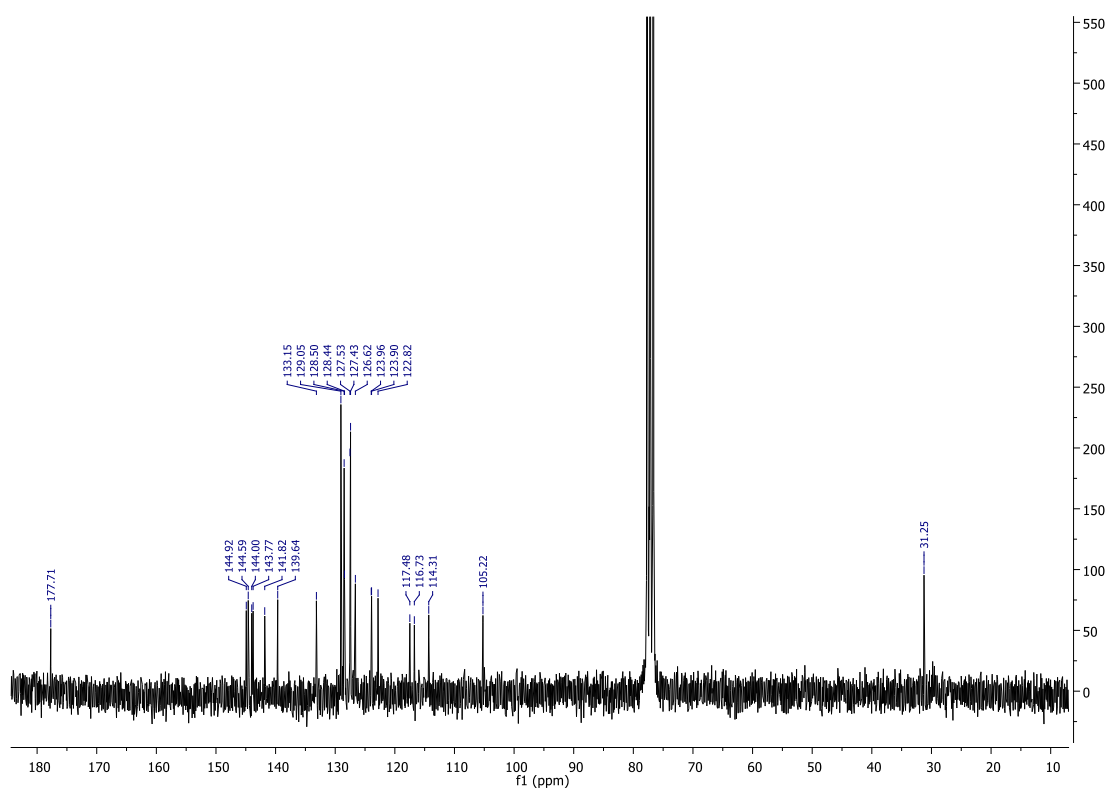
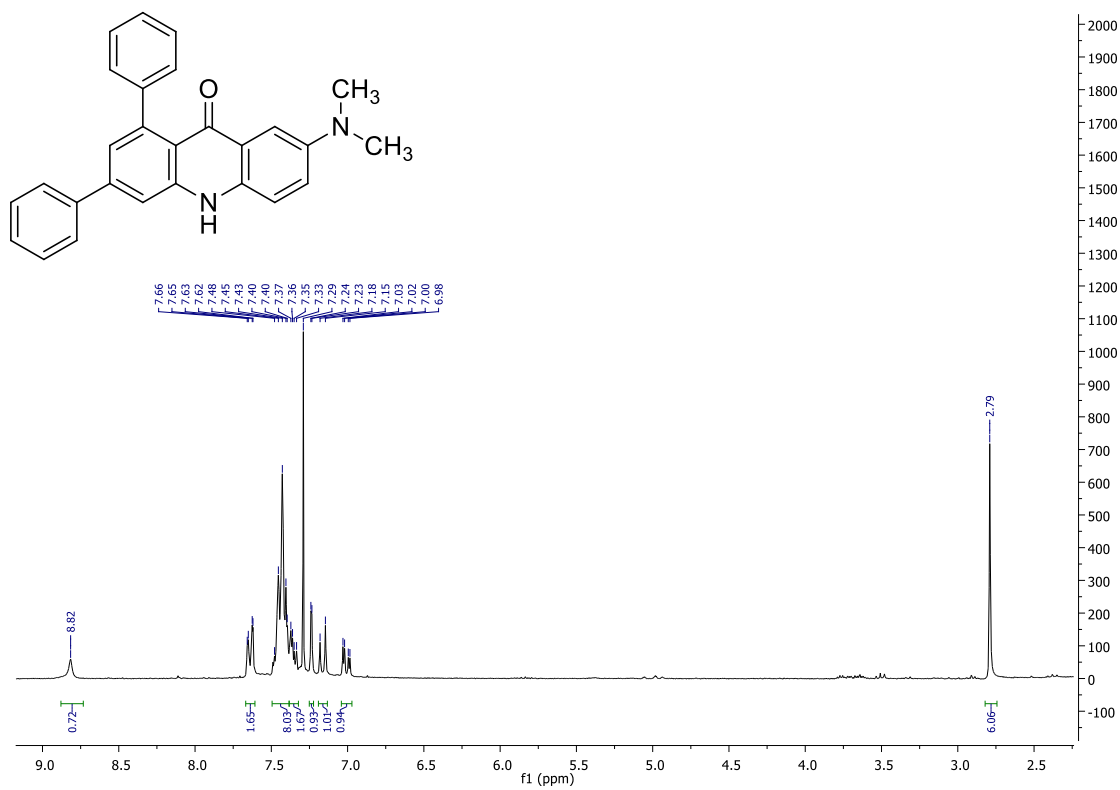
1,3-bis(4-chlorophenyl)-1,10-dihydroacridin-9(2H)-one (2o)



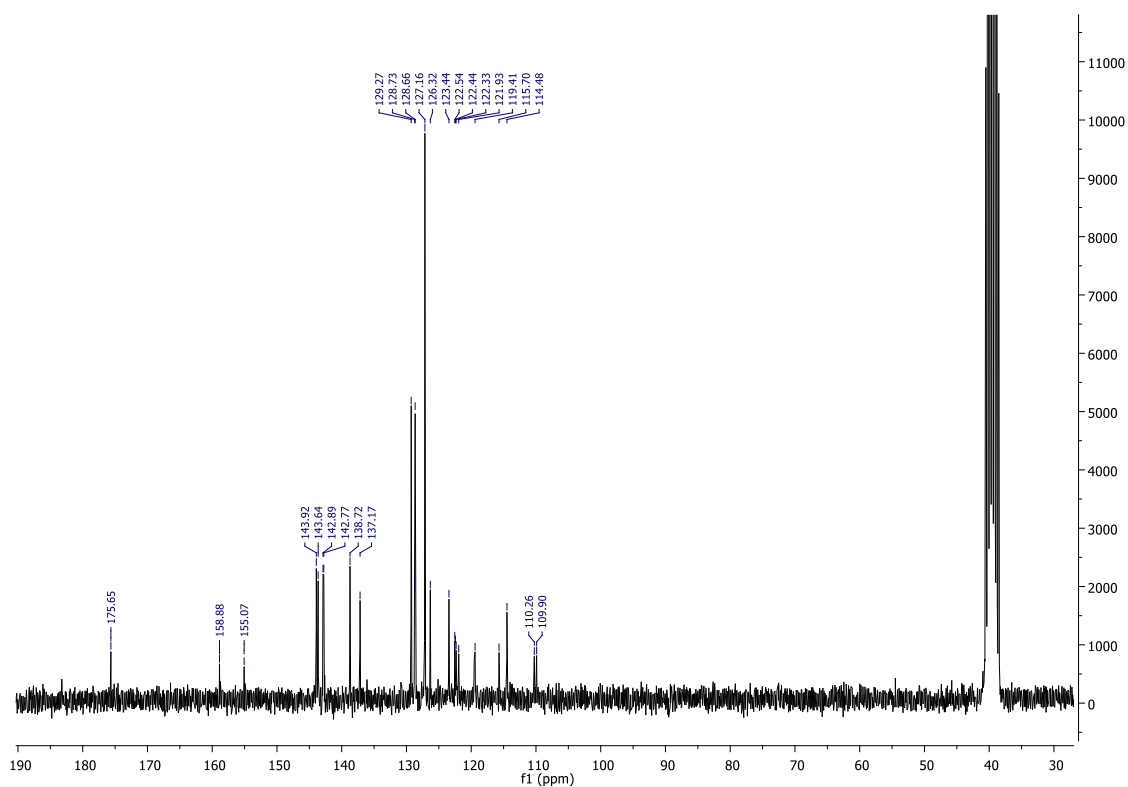
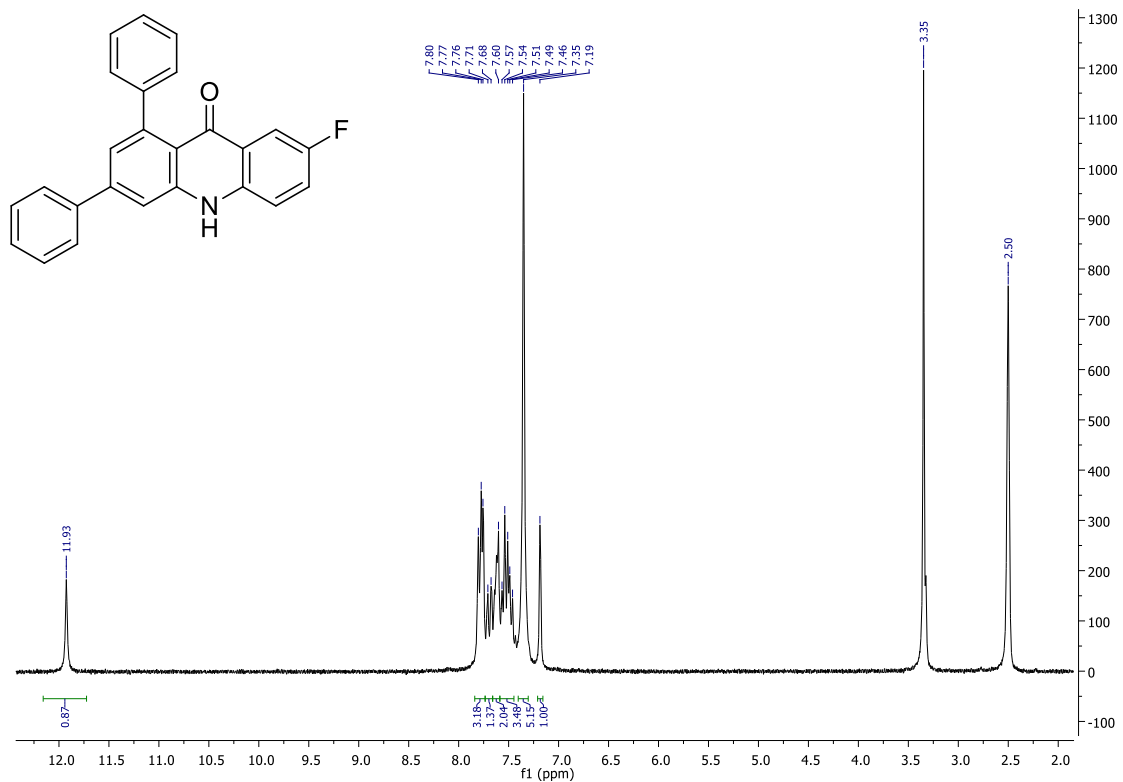
1,3-diphenylacridin-9(10H)-one (3a)



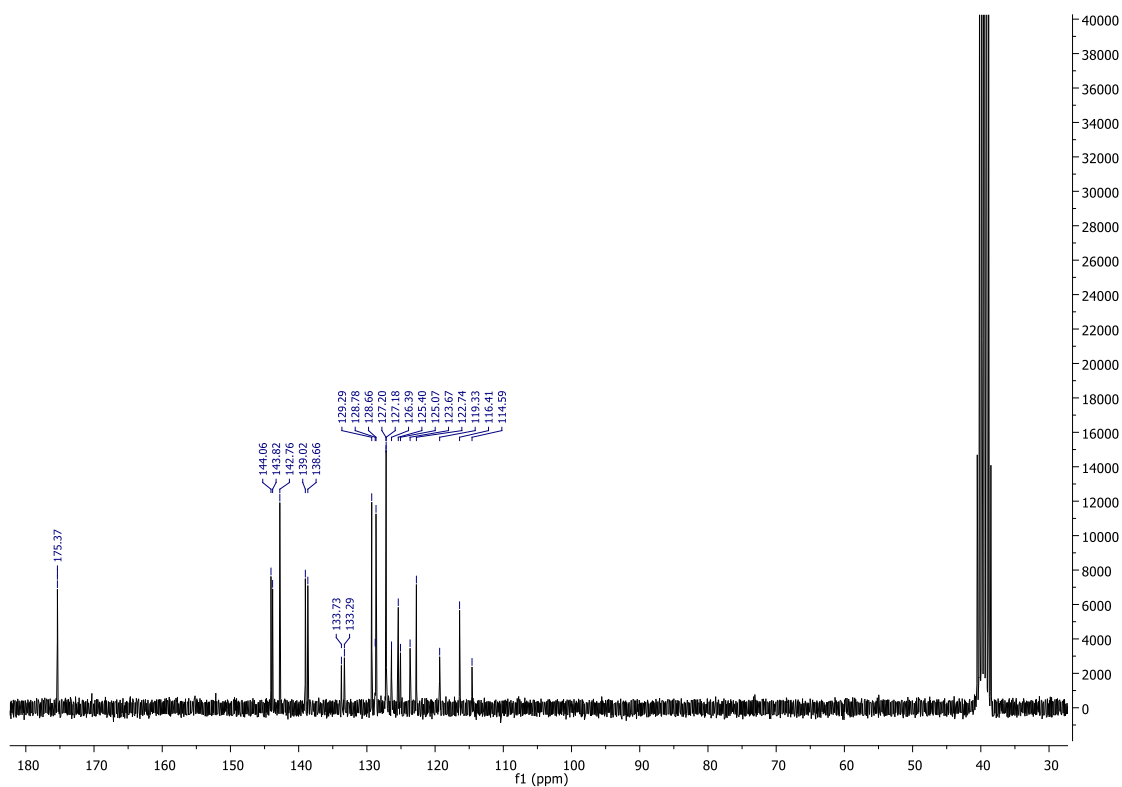
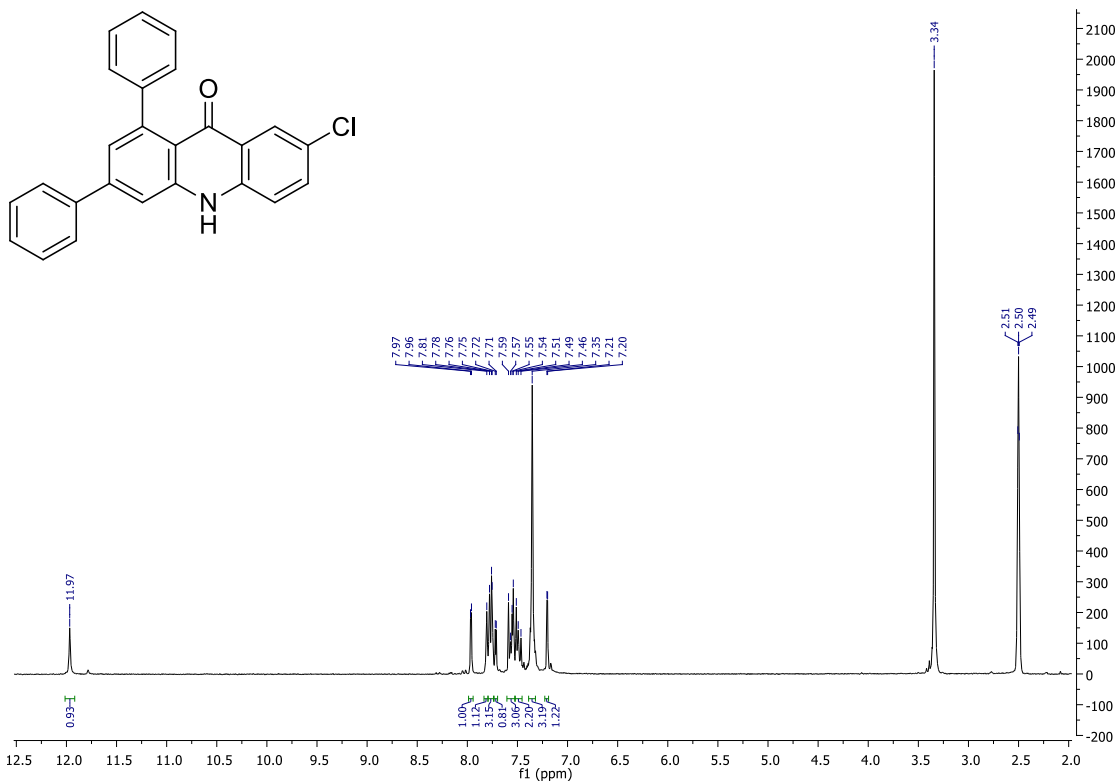
7-(dimethylamino)-1,3-diphenylacridin-9(10H)-one (3b)



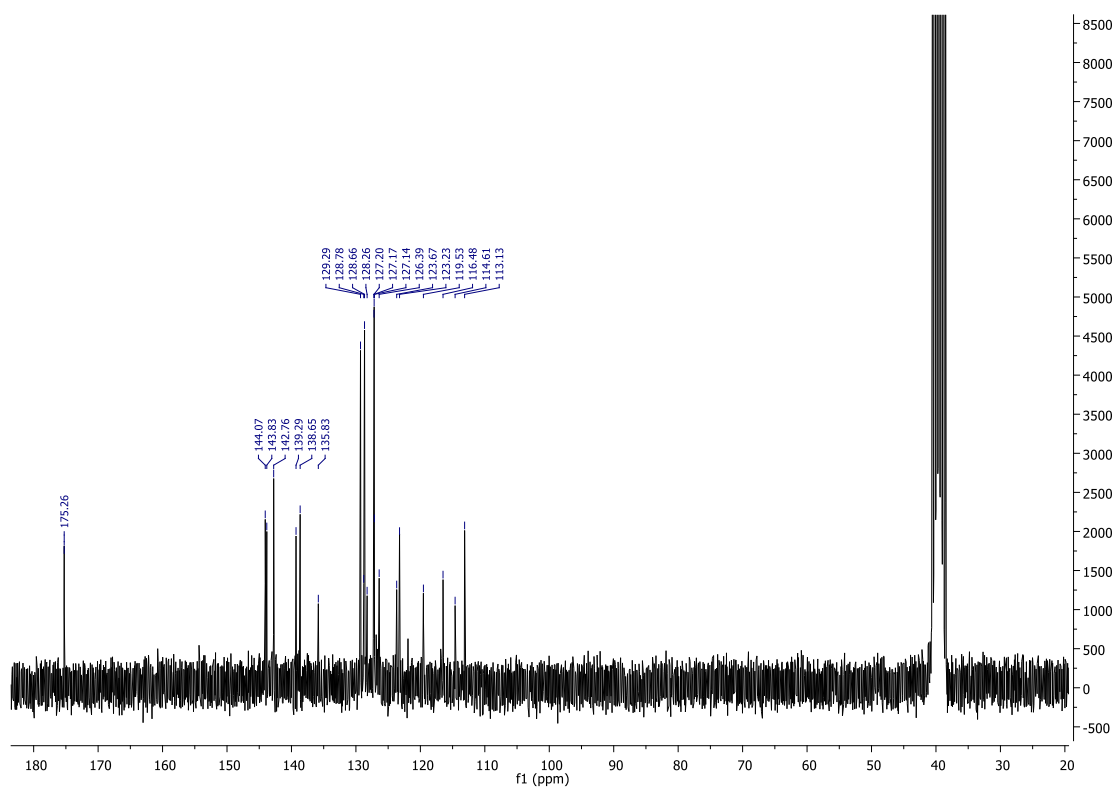
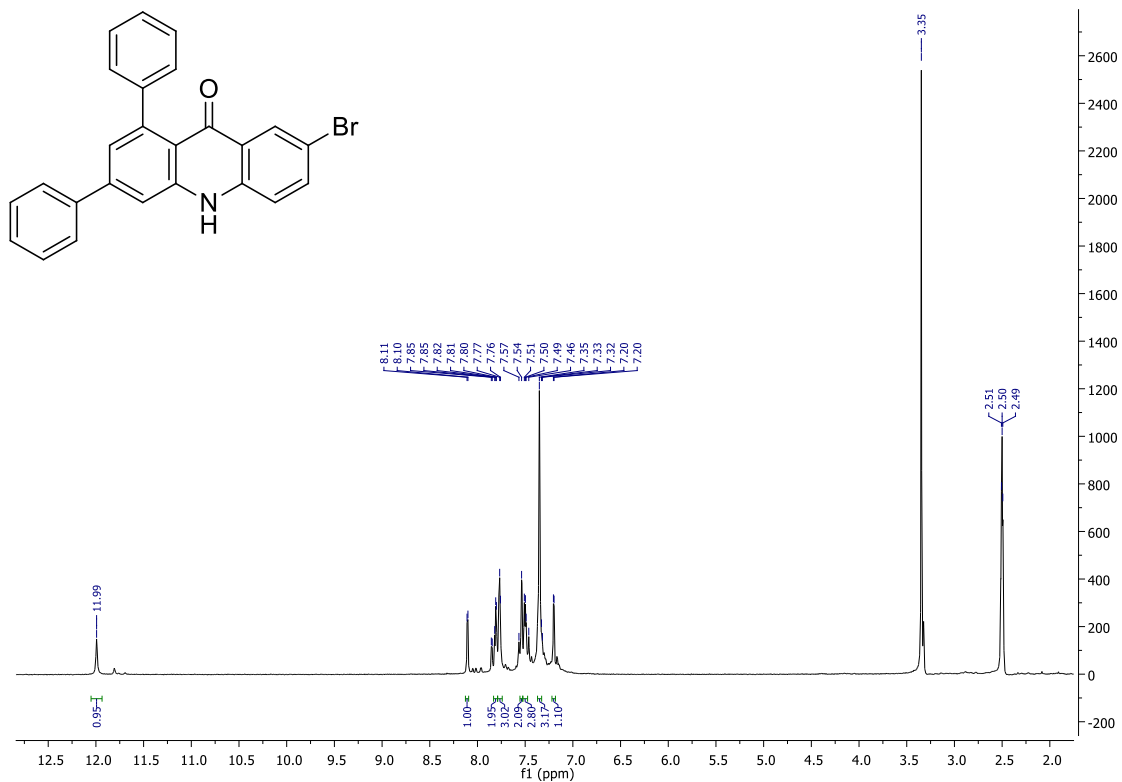
7-fluoro-1,3-diphenylacridin-9(10H)-one (3c)



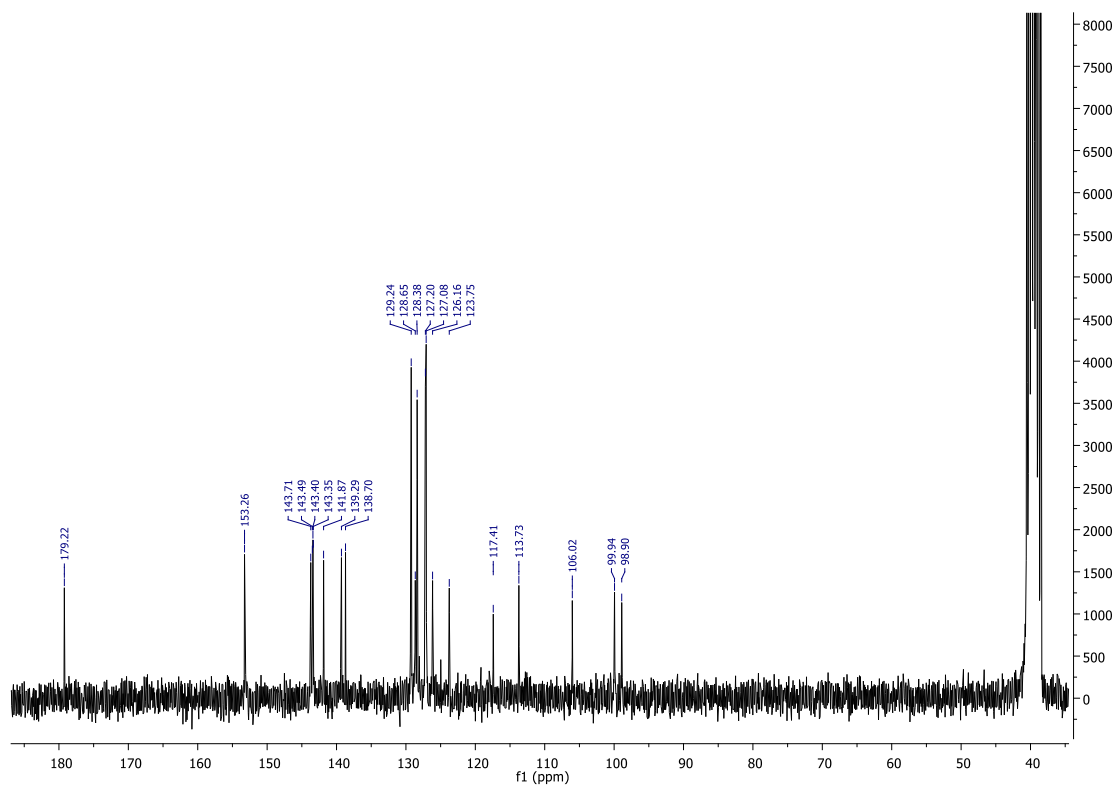
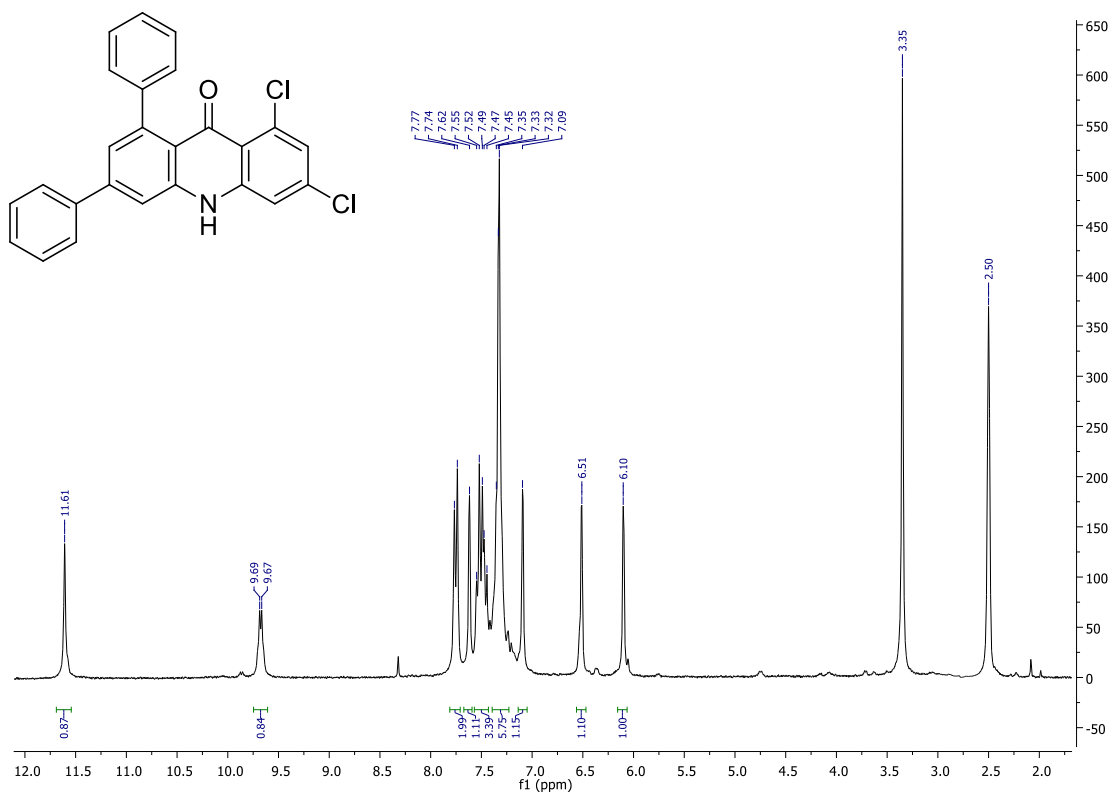
7-chloro-1,3-diphenylacridin-9(10H)-one (3d)



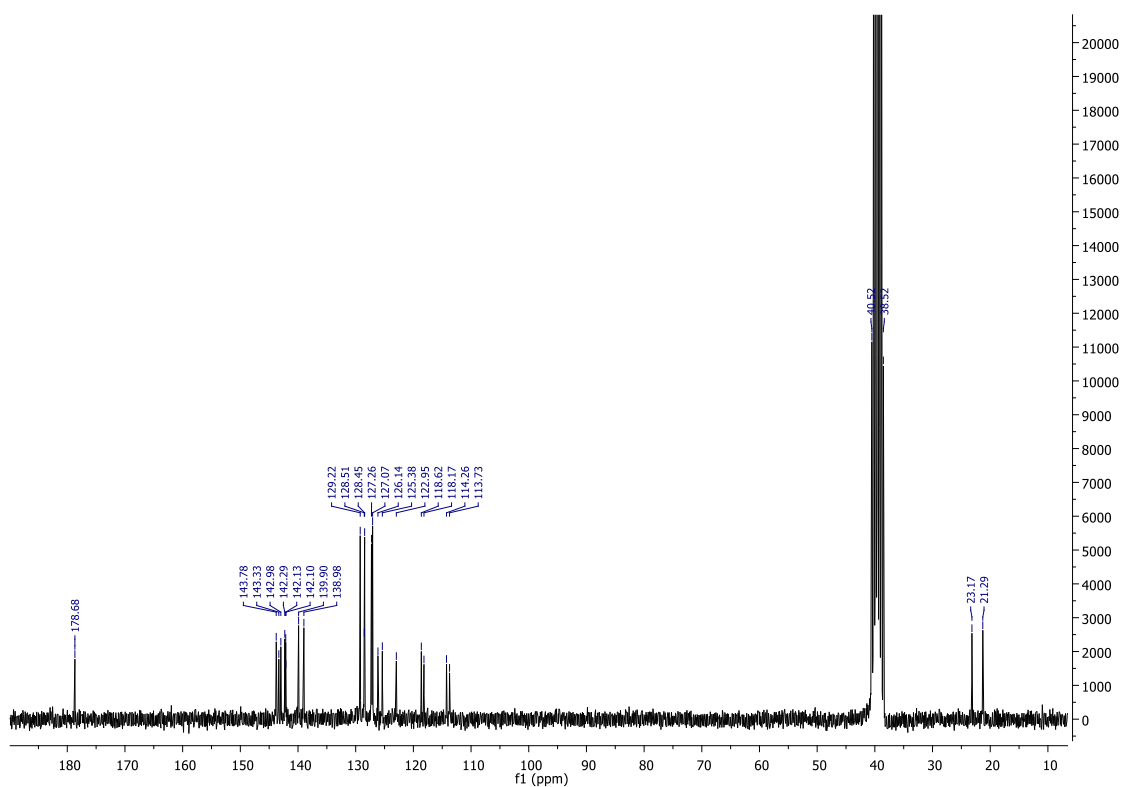
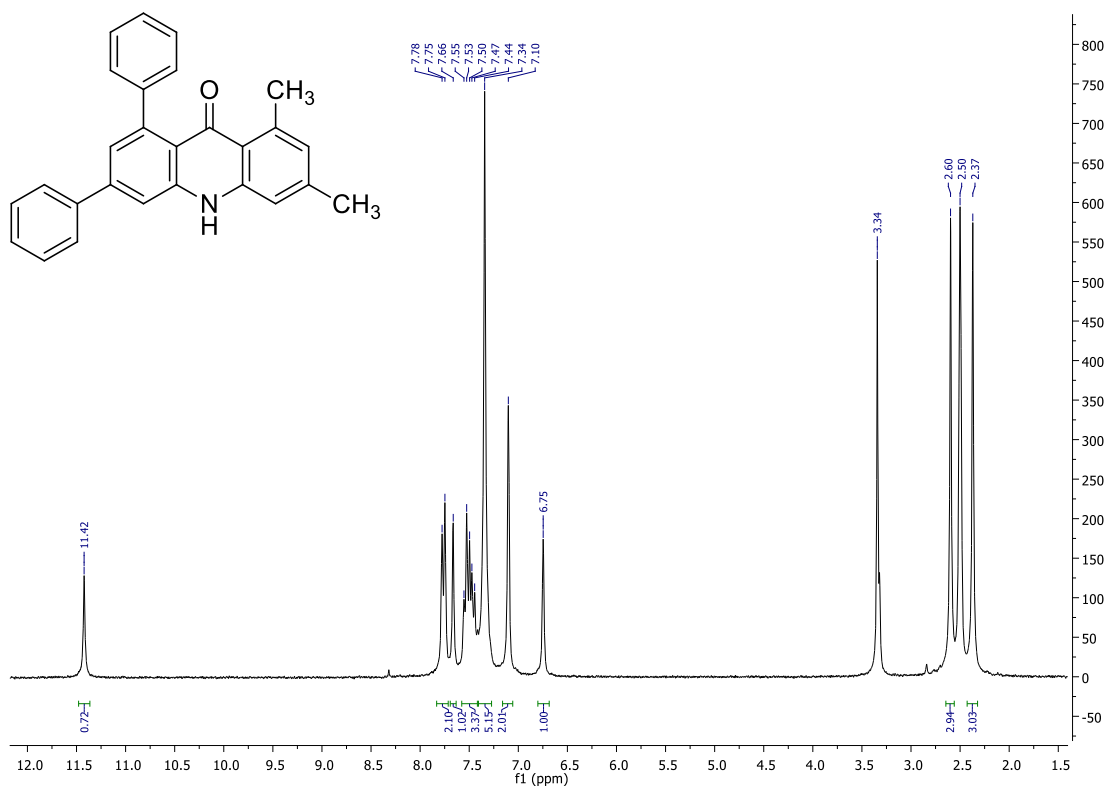
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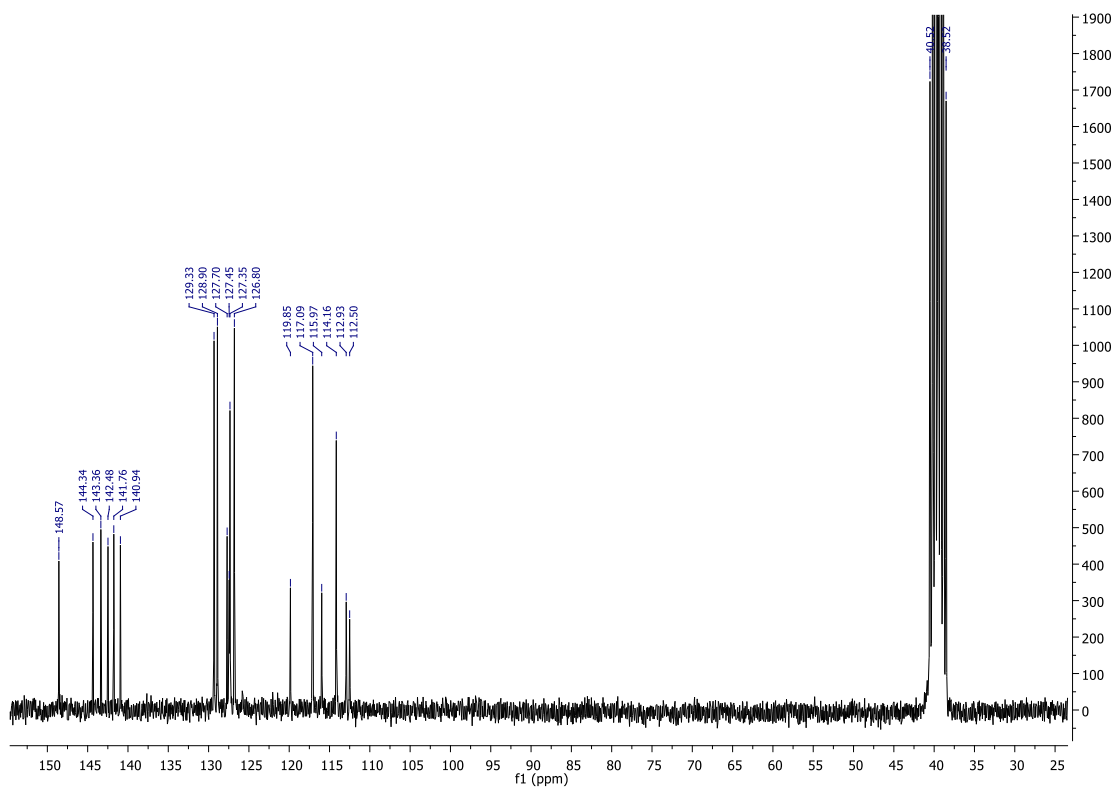
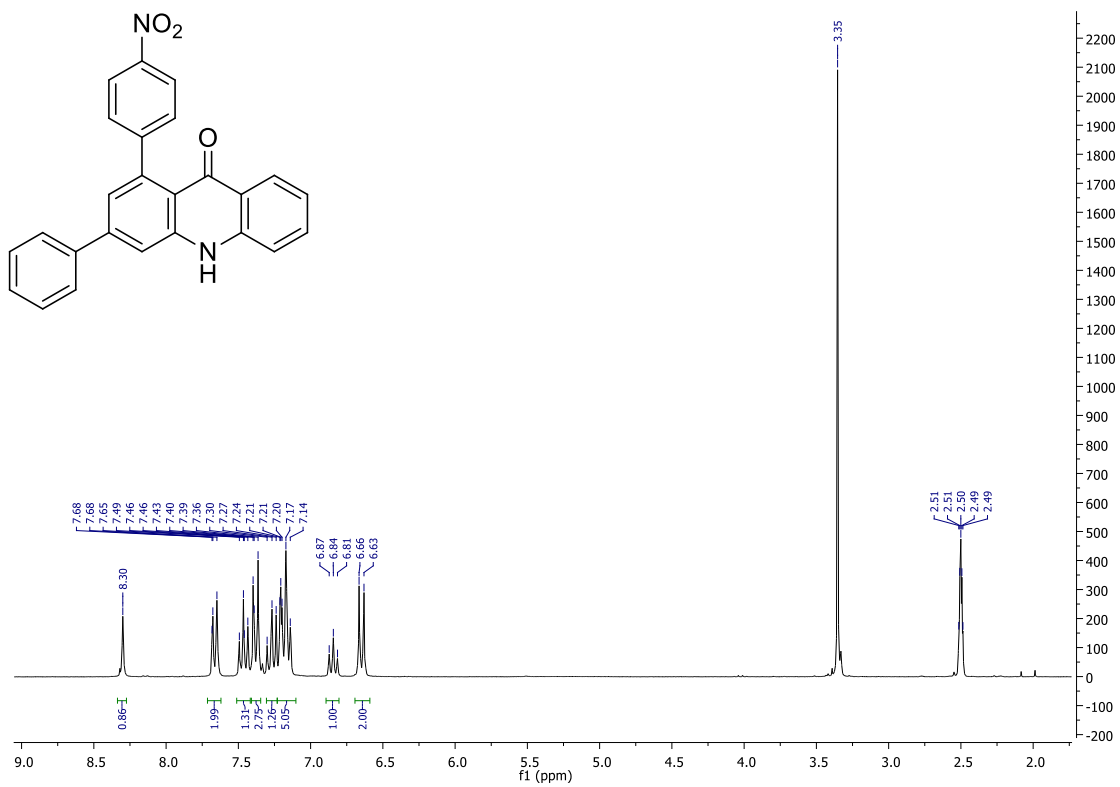
6,8-dichloro-1,3-diphenylacridin-9(10H)-one (3f)



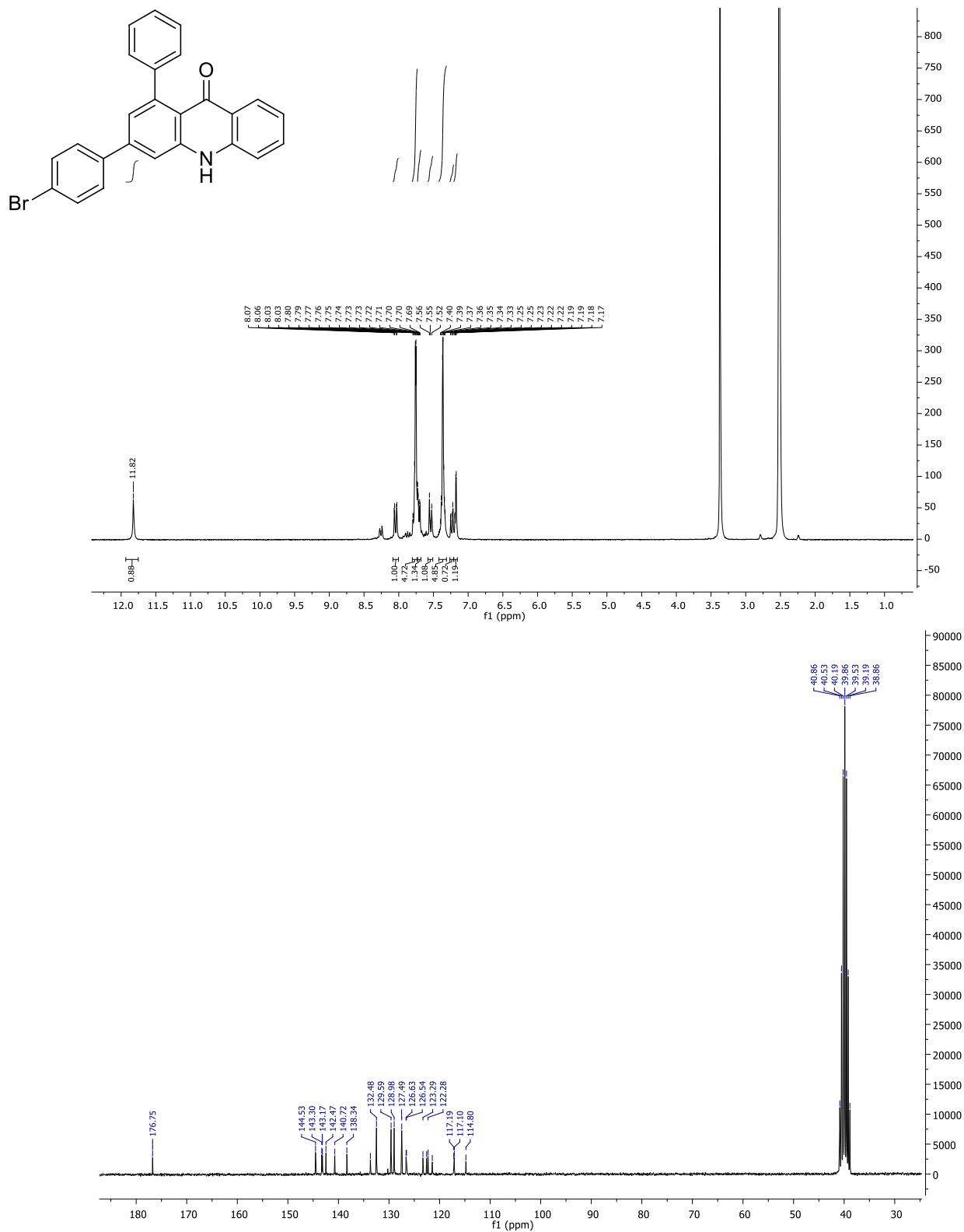
6,8-dimethyl-1,3-diphenylacridin-9(10H)-one (3g)



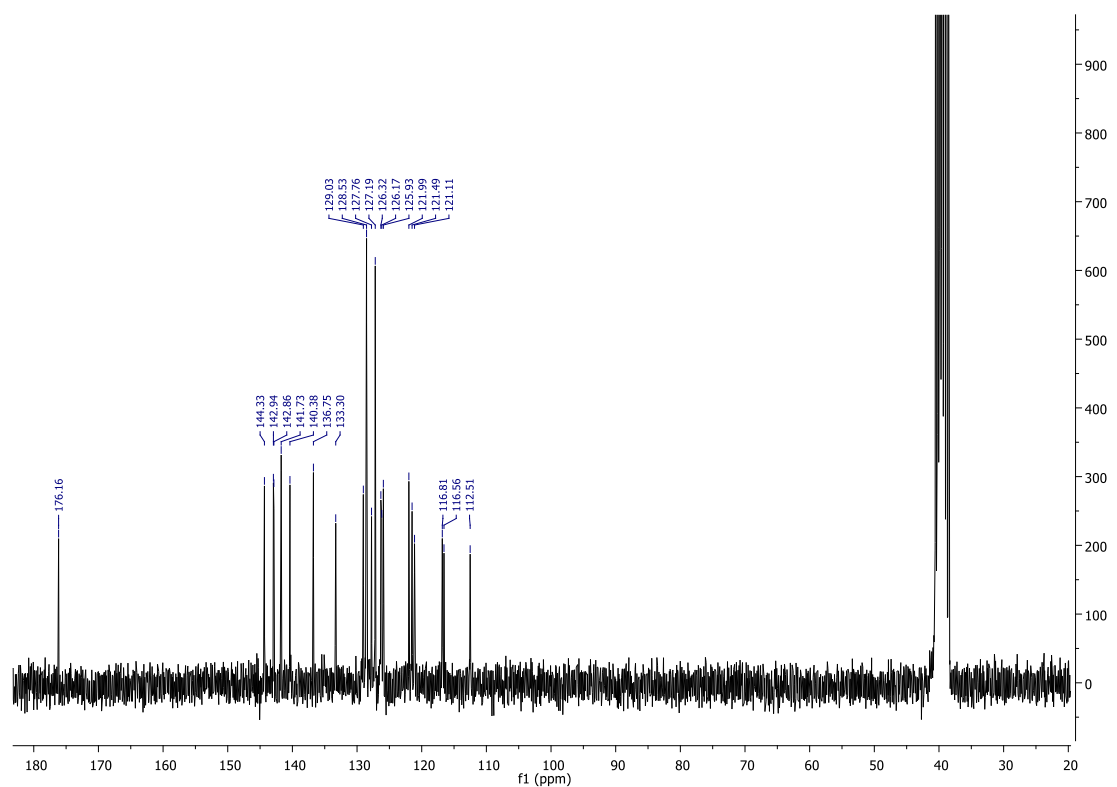
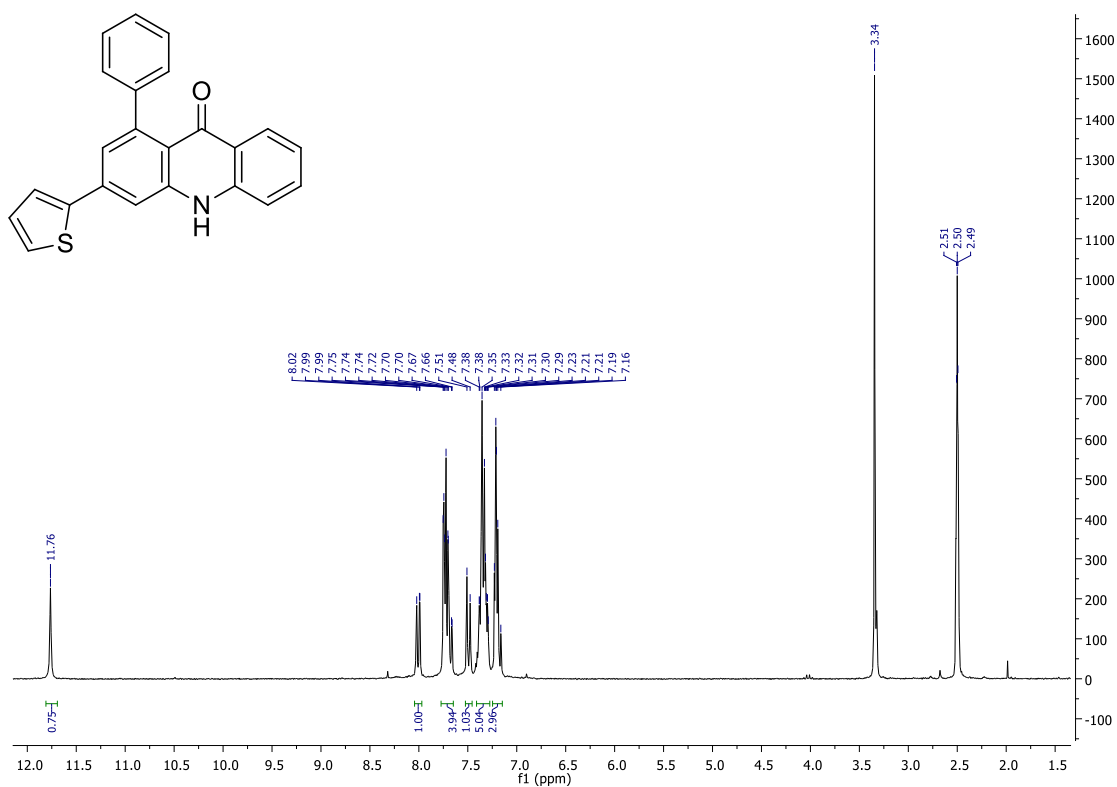
1-(4-nitrophenyl)-3-phenylacridin-9(10H)-one (3h)



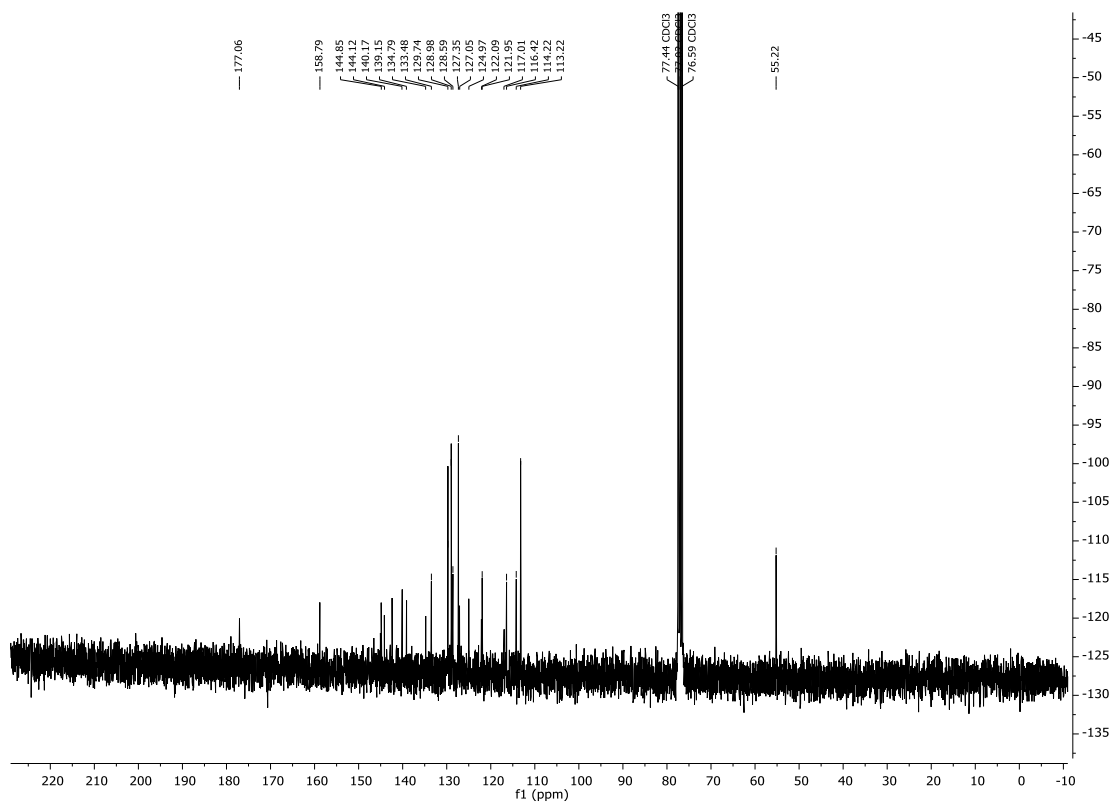
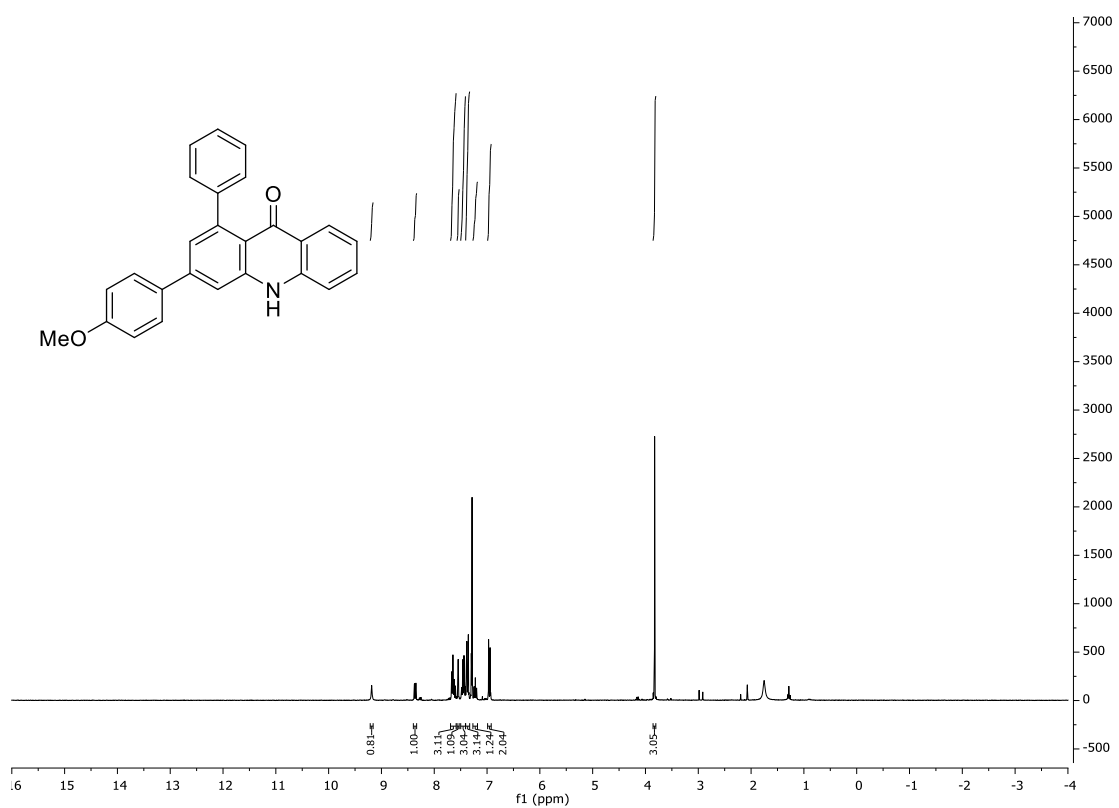
3-(4-bromophenyl)-1-phenylacridin-9(10H)-one (3i)



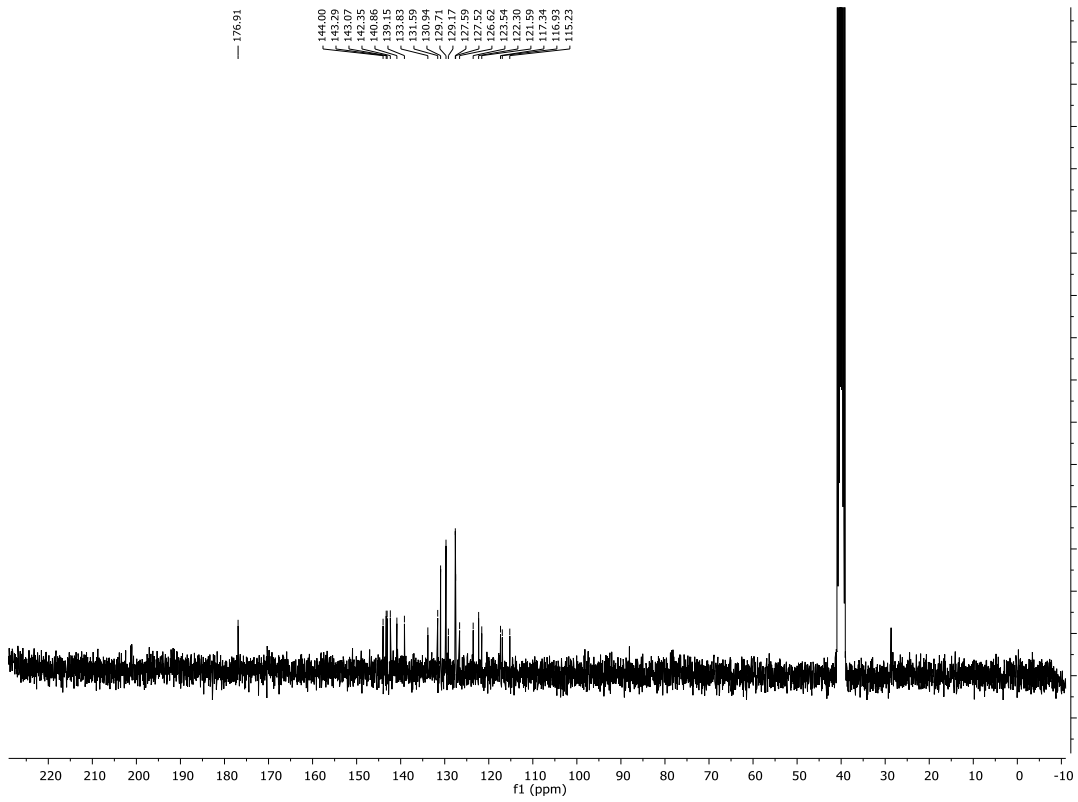
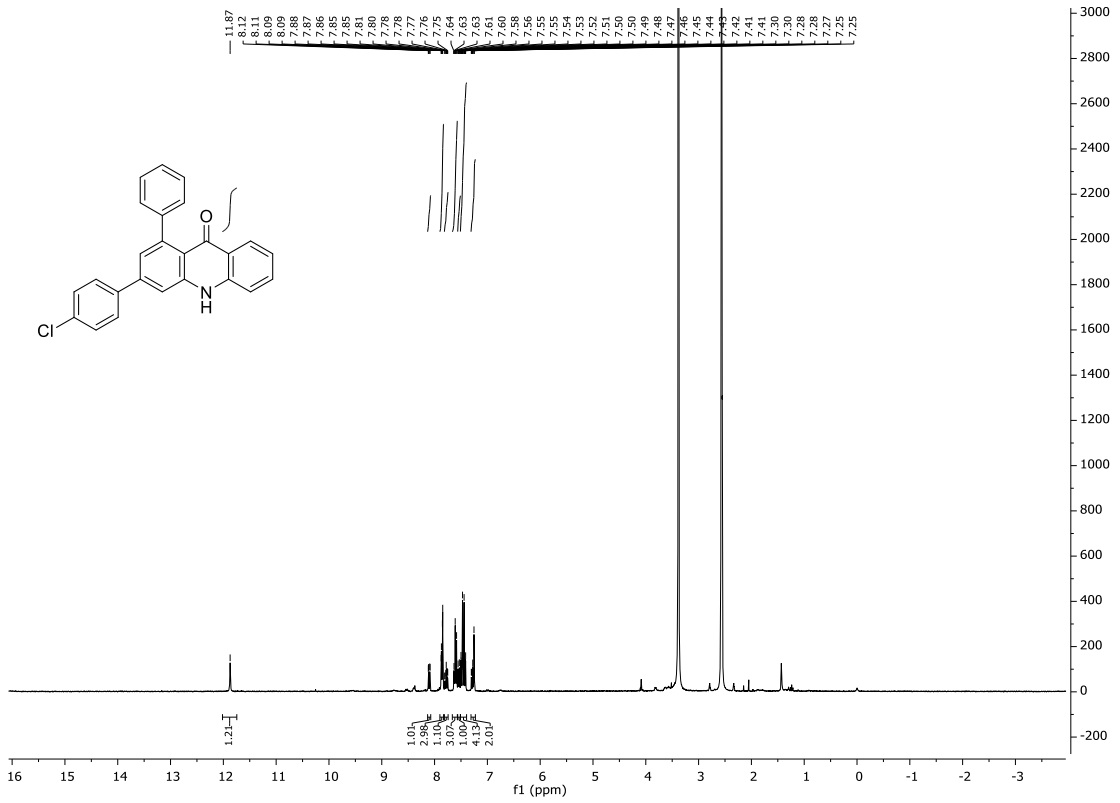
1-phenyl-3-(thiophen-2-yl)acridin-9(10H)-one (3j)



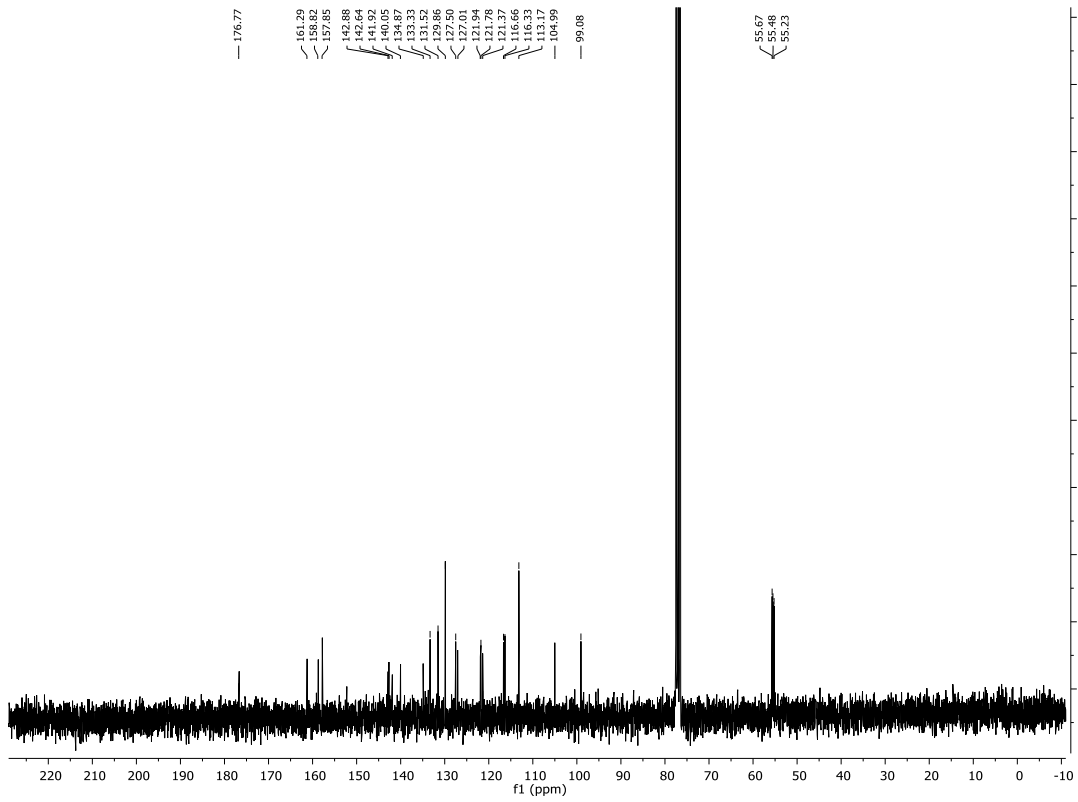
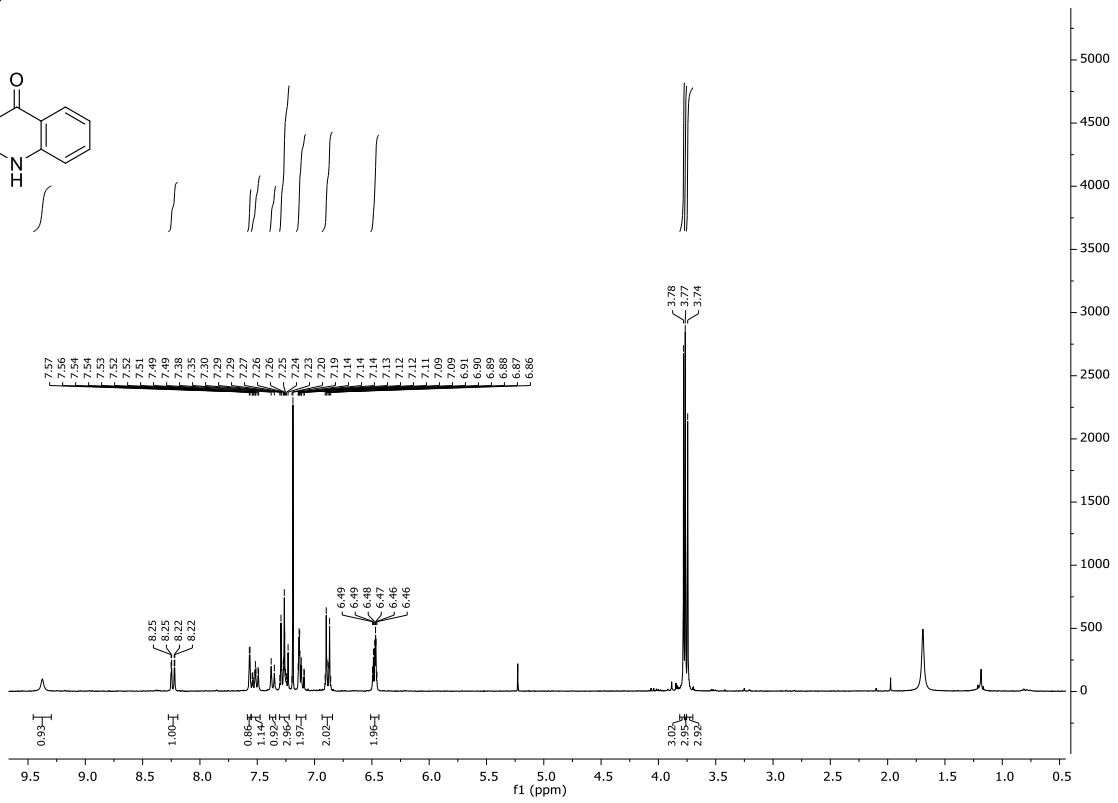
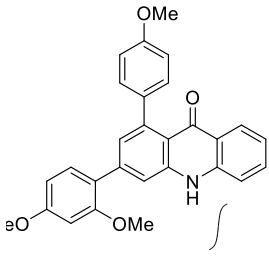
1-(4-methoxyphenyl)-3-phenylacridin-9(10H)-one (3l)



1-(4-chlorophenyl)-3-phenylacridin-9(10H)-one (3m)

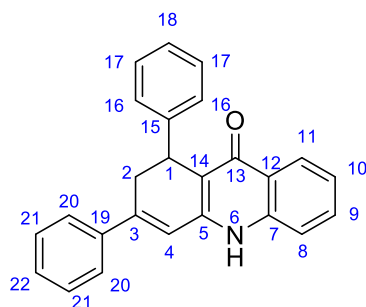


1-(2,4-dimethoxyphenyl)-3-(4-methoxyphenyl)-acridin-9(10H)-one (3n)

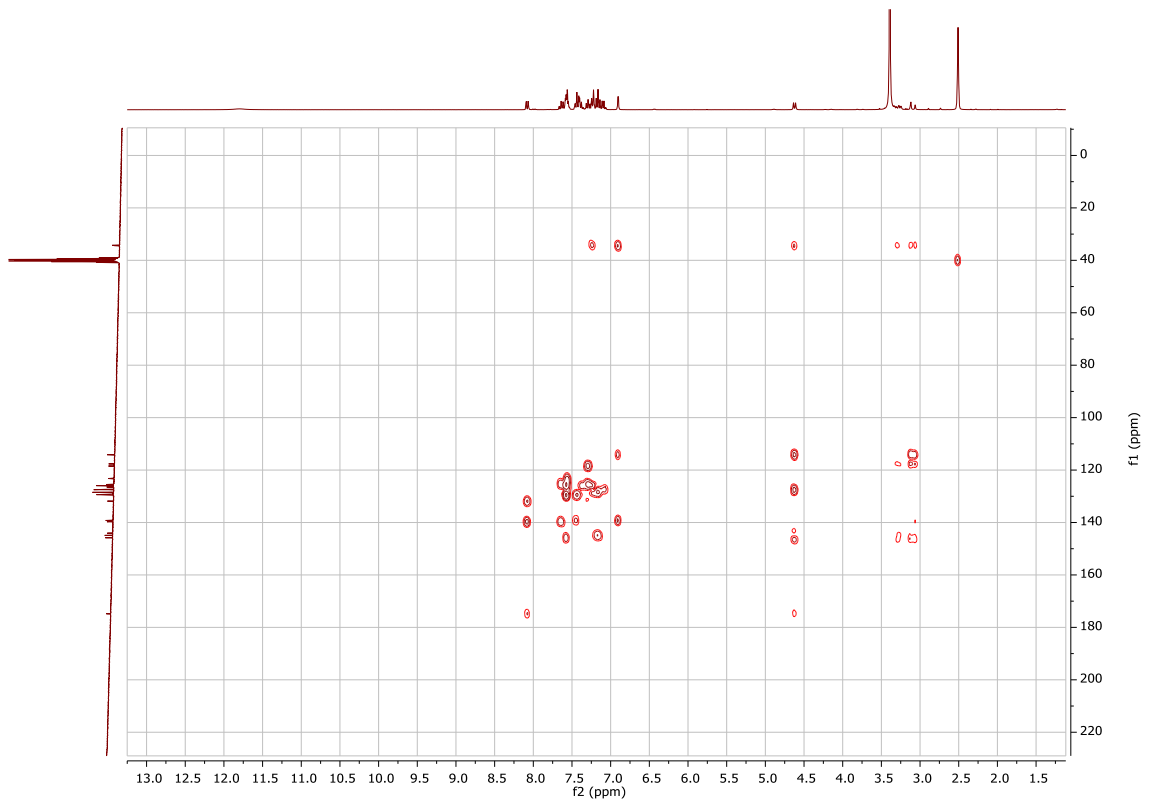
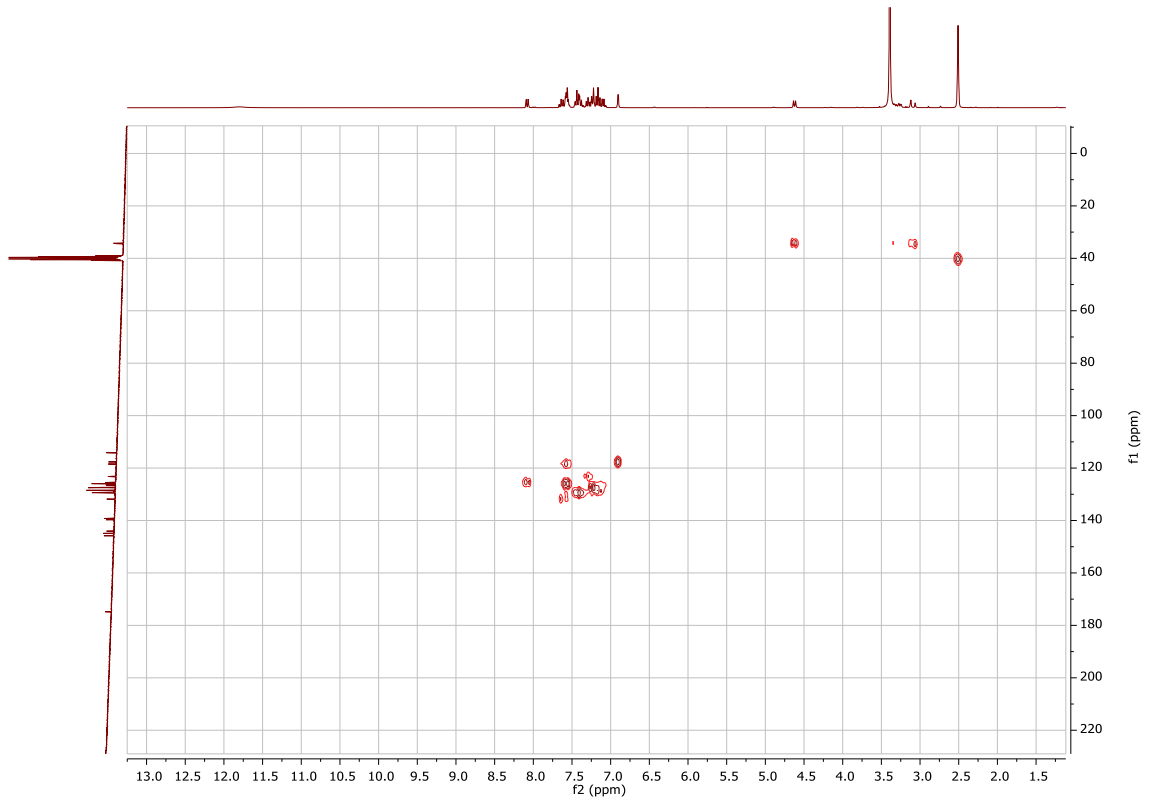


2. Structural study of compounds 2a y 3a.

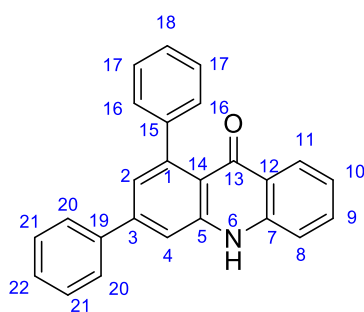
2D-NMR study of compound 2a



¹³ C chemical shift	HMQC	HMBC	Assignment
33.8	H-2	H-16	2
34.0	H-1	H-16	1
113.7		H-2	14
117.2	H-4		4
118.0	H-8	H-10	8
122.8	H-10	H-8	10
125.1	H-11	H-9	11
125.5	H-20		20
126.1	H-18	H-16	18
127.1	H-16	H-18	16
128.6	H-17		17
129.0	H-21		21
129.1	H-22		22
131.4	H-9	H-11	9
138.8		H-4, H20 and H-21	19
139.3		H-10, H-11	7 and 12
143.6			3
144.5			19
145.4		H-2	15
174.4		H-1	13

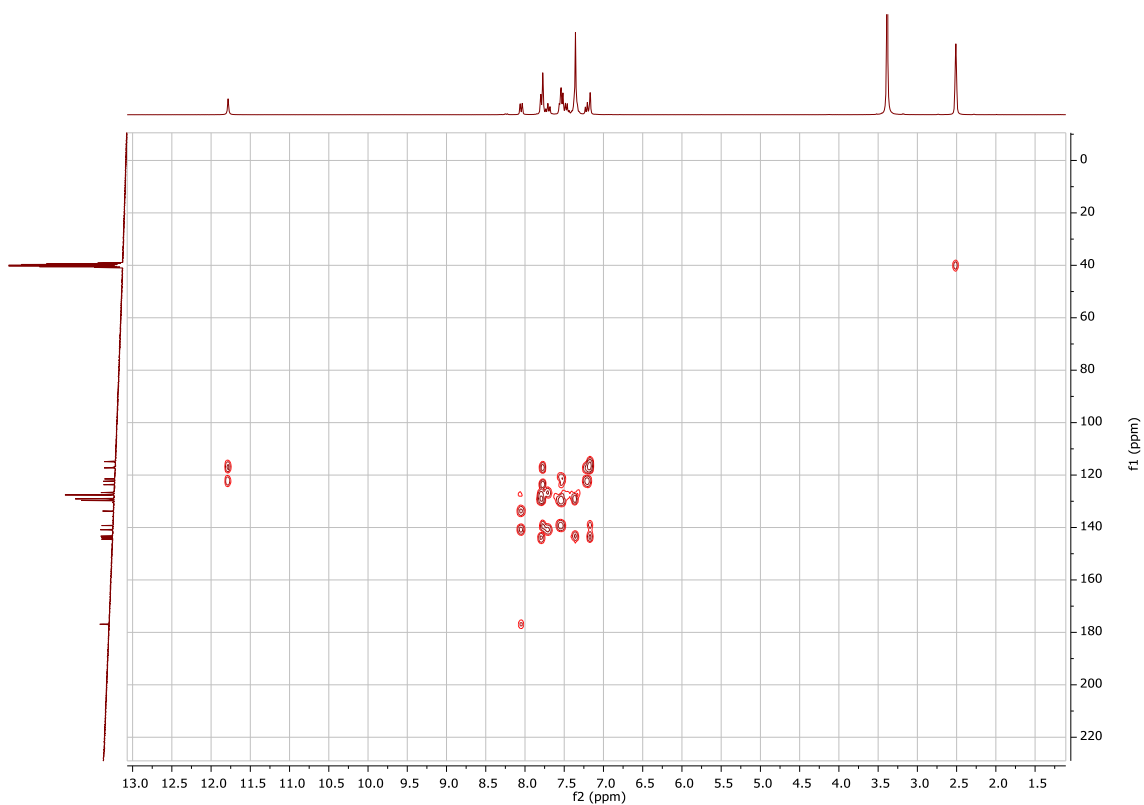
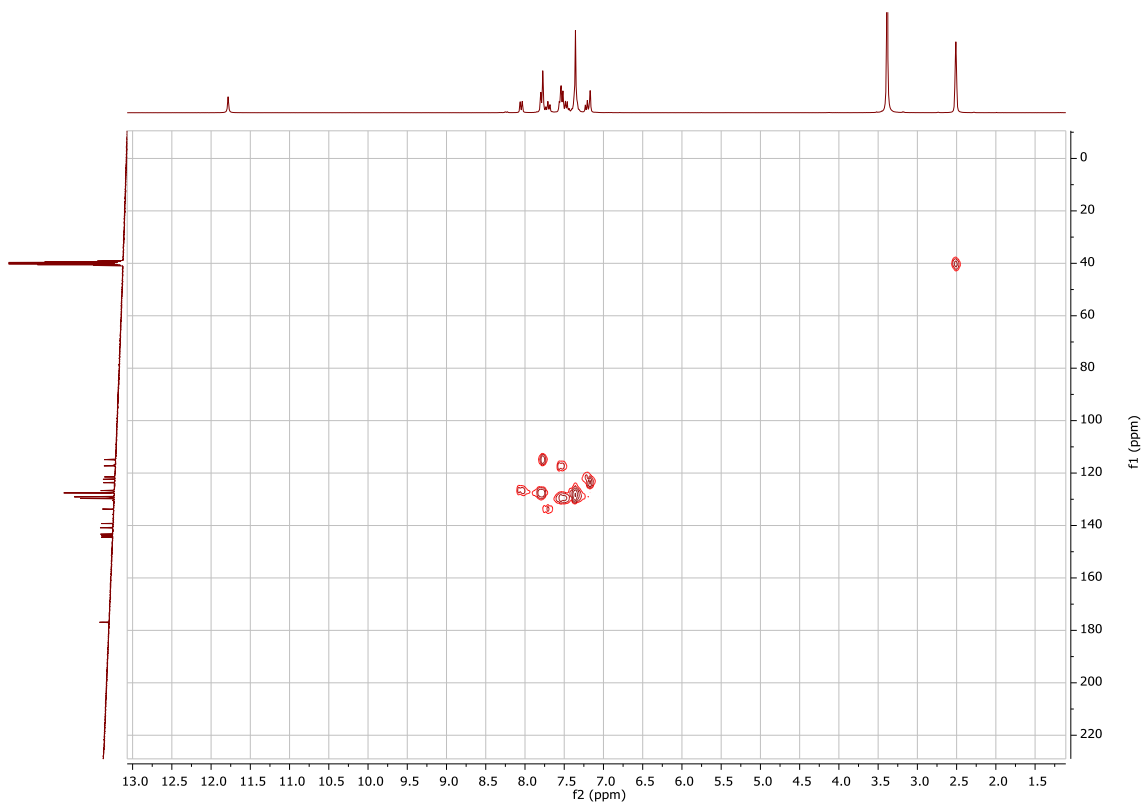


2D-NMR study of compound 3a



¹³ C chemical shift	HMQC	HMBC	Assignment
114.4 (CH)	H-4	H-2	4
116.6 (C)		H-6, H-10	12
116.8 (CH)	H-2	H-4	2
121.0 (CH)	H-10		10
121.9 (C)		H-6, H-2	14
123.2 (CH)	(H-16, 17, 20, 21 or 22)	H-4, H-14, H-13	*
126.2 (CH)	H-11	H-9	11
126.2 (CH)	H-18		*
127.1 (CH)	H-8, H-21	H-3, H-5, H-7	*
128.6 (CH)	(H-16, 17, 20, 21 or 22)		*
129.2 (CH)	(H-16, 17, 20, 21 or 22)		*
133.3 (CH)	H-9	H-11	9
138.1 (C)			*
140.4 (C)		H-11, H-9	7
142.9 (C)			*
143.1 (C)			*
143.5 (C)			*
144.0 (C)			*
176.5 (C=O)			13

* The signal was not able to be uniquely assigned



^1H NMR (250 MHz, Chloroform-*d*) δ 8.94 (s, 1H), 8.32 (d, $J = 8.1$ Hz, 1H), 7.65 (d, $J = 1.7$ Hz, 1H), 7.61 – 7.53 (m, 2H), 7.52 – 7.49 (m, 1H), 7.48 (d, $J = 1.6$ Hz, 1H), 7.34 (d, $J = 8.3$ Hz, 1H), 7.17 (m, 1H), 6.86 – 6.78 (d, $J = 3.8$ Hz, 1H), 6.59 (dd, $J = 3.2, 0.9$ Hz, 1H), 6.55 (dd, $J = 3.3, 1.8$ Hz, 1H), 6.51 (dd, $J = 3.4, 1.8$ Hz, 1H).