Supporting Information

Synthesis and anti-tubercular activity of 1-and 3-substituted benzo[*g*]isoquinoline-5,10-diones

Robert J. Smets,[a] Eveline Torfs[b], Filip Lemière[c], Paul Cos[b], Davie Cappoen[b] and Kourosch Abbaspour Tehrani[a*]

[a] Organic Synthesis, Faculty of Sciences, University of Antwerp, Groenenborgerlaan 171, B-2020 Antwerp Belgium.

[b] Laboratory of Microbiology, Parasitology and Hygiene (LMPH), S7, Faculty of Pharmaceutical, Biomedical and Veterinary Sciences, University of Antwerp, Universiteitsplein 1, B-2610 Wilrijk, Belgium.

[c] Biomolecular & Analytical Mass Spectrometry and Center for Proteomics, Department of Chemistry, University of Antwerp, B-2020 Antwerp, Belgium.

E-mail: Kourosch.AbbaspourTehrani@uantwerpen.be

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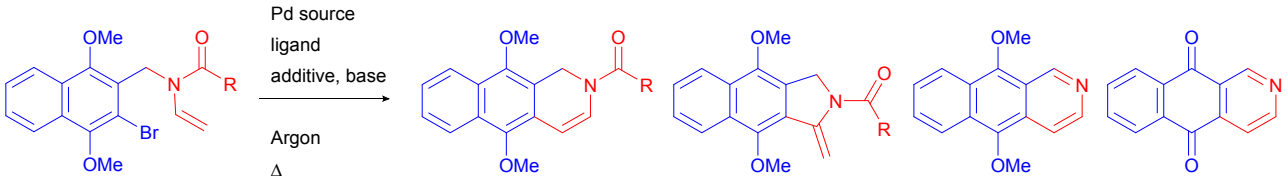
Table S1. Intramolecular Heck reaction of **19** to induce a 6-*endo-trig* ring closure[a]



19a R = H
19b R = CH_3

20a R = H
20b R = CH_3

24a R = H
24b R = CH_3

21

5

Entry	R	Pd source (eq.)	Ligand (eq.)	Base (eq.)	Additive (eq.)	Solvent	T, t (°C, h)	**20** (%)[b]	**24** (%)[b]	**21** (%)[b]	**5** (%)[b]	**Rec. 19** (%)[b]
1	H	$Pd(OAc)_2$ (0.05)	P(*o*-Tol)$_3$ (0.1)	*i*PrNEt$_2$ (1.5)	/	ACN	90, 24 then 105, 24	4[f]	0[f]	0[f]	0[f]	0[f]
2	H	$Pd(OAc)_2$ (0.2)	TPP (0.3)	K_2CO_3 (2.0)	TBAB (2.0)	DMF	100, 6	15[f]	6[f]	0[f]	0[f]	0[f]
3	H	$Pd(OAc)_2$ (0.00025)	/	NaOAc (1.2)	/	NMP	135, 19	0[f]	0[f]	0[f]	0[f]	0[f]
4	H	$Pd(OAc)_2$ (0.0005)	/	NaOAc (1.2)	/	NMP	135, 19	0[f]	0[f]	0[f]	0[f]	0[f]
5	H	$Pd(OAc)_2$ (0.001)	/	NaOAc (1.2)	/	NMP	135, 19	0[f]	0[f]	0[f]	0[f]	0[f]
6	H	$Pd(OAc)_2$ (0.2)	TPP (0.3)	K_2CO_3 (2.0)	TBAB (2.0)	DMA	100, 16	10[f]	8[f]	0[f]	0[f]	0[f]
7	H	$Pd(OAc)_2$ (0.2)	TPP (0.3)	K_2CO_3 (2.0)	TBAB (2.0)	EtOH	100, 16	5[f]	2[f]	0[f]	0[f]	0[f]
8	H	$Pd(OAc)_2$ (0.1)	/	KOAc (5.5)	TBAC (2.0)	DMF	100, 16	5[f]	4[f]	0[f]	0[f]	0[f]
9	H	$Pd(OAc)_2$ (0.1)	/	KOAc (5.5)	TBAC (2.0)	Toluene	100, 16	5[f]	6[f]	0[f]	0[f]	0[f]
10	H	$Pd(OAc)_2$ (0.2)	TPP (0.3)	K_2CO_3 (2.0)	TBAB (2.0)	DMF	100, 6	15	<6	0	0	0
11	H	$Pd(OAc)_2$ (0.2)	*rac*-BINAP (0.3)	K_2CO_3 (2.0)	TBAB (2.0)	DMF	100, 16	15	<20	0	0	0
12	H	$Pd(OAc)_2$ (0.1)	^{t}BuCy$_2$P.HBF$_4$ (0.2)	Cs_2CO_3 (5.0)	/	DMF	130, 22.5	10	0	4	11	0

13	CH_3	$Pd(OAc)_2$ (0.1)	$^tBuCy_2P.HBF_4$ (0.2)	Cs_2CO_3 (5.0)	/	DMF	130, 17.5	49 [c]	6 [c]	4 [c]	1 [c]	0 [c]
14	CH_3	$Pd(OAc)_2$ (0.1)	$^tBuCy_2P.HBF_4$ (0.2)	Cs_2CO_3 (4.0)	/	DMF	130, 17.5	58 [d]	1 [d]	0 [d]	2 [d]	0 [d]
15	CH_3	$Pd(OAc)_2$ (0.1)	$^tBuCy_2P.HBF_4$ (0.2)	Cs_2CO_3 (3.0)	/	DMF	130, 16.5	57 [d]	trace [d]	3 [d]	2 [d]	0 [d]
16	CH_3	$Pd(OAc)_2$ (0.1)	$^tBuCy_2P.HBF_4$ (0.2)	Cs_2CO_3 (2.0)	/	DMF	130, 16.5	63 [d]	4 [d]	2 [d]	1 [d]	0 [d]
17	CH_3	$Pd(OAc)_2$ (0.1)	$^tBuCy_2P.HBF_4$ (0.2)	Cs_2CO_3 (1.2)	/	DMF	130, 19	75 [d]	6 [d]	trace [d]	trace [d]	0 [d]
18	CH_3	$Pd(OAc)_2$ (0.1)	$^tBuCy_2P.HBF_4$ (0.2)	Cs_2CO_3 (1.2)	/	DMF	130, 16	71 [d]	11 [d]	trace [d]	trace [d]	0 [d]
19	CH_3	$Pd(OAc)_2$ (0.1)	$Cy_3P.HBF_4$ (0.2)	Cs_2CO_3 (1.2)	/	DMF	130, 16	74 [d]	8 [d]	trace [d]	trace [d]	0 [d]
20	CH_3	$Pd(OAc)_2$ (0.1)	$^tBu_3P.HBF_4$ (0.2)	Cs_2CO_3 (1.2)	/	DMF	130, 16	15 [d]	36 [d]	0 [d]	0 [d]	16 [d]
21	CH_3	$Pd(OAc)_2$ (0.1)	TPP (0.2)	Cs_2CO_3 (1.2)	/	DMF	130, 16	48 [d]	29 [d]	0 [d]	0 [d]	0 [d]
22	CH_3	$Pd(OAc)_2$ (0.1)	JohnPhos (0.2)	Cs_2CO_3 (1.2)	/	DMF	130, 16	29 [d]	38 [d]	0 [d]	0 [d]	0 [d]
23	CH_3	$Pd(OAc)_2$ (0.1)	DPPP (0.1)	Cs_2CO_3 (1.2)	/	DMF	130, 16	45 [d]	29 [d]	0 [d]	0 [d]	0 [d]
24	CH_3	$Pd(OAc)_2$ (0.1)	DPPF (0.1)	Cs_2CO_3 (1.2)	/	DMF	130, 16	49 [d]	31 [d]	0 [d]	0 [d]	0 [d]
25	CH_3	$Pd(OAc)_2$ (0.1)	DPPE (0.1)	Cs_2CO_3 (1.2)	/	DMF	130, 16	41 [d]	32 [d]	0 [d]	0 [d]	0 [d]
26	CH_3	$Pd(OAc)_2$ (0.1)	Xantphos (0.1)	Cs_2CO_3 (1.2)	/	DMF	130, 16	17 [d]	34 [d]	0 [d]	0 [d]	15 [d]
27	CH_3	$Pd(OAc)_2$ (0.1)	*rac*-BINAP (0.1)	Cs_2CO_3 (1.2)	/	DMF	130, 16	26 [d]	44 [d]	0 [d]	0 [d]	0 [d]
28	CH_3	Pd_2dba_3 (0.05)	*rac*-BINAP (0.1)	Cs_2CO_3 (1.2)	/	DMF	130, 16	36 [d]	44 [d]	0 [d]	0 [d]	0 [d]
29	CH_3	*rac*-BINAP-Pd-G3 Buchwald precat. (0.1)		Cs_2CO_3 (1.1)	/	DMF	DMF	31 [d]	49 [d]	0 [d]	0 [d]	0 [d]
30	CH_3	*rac*-BINAP-Pd-G3 Buchwald precat. (0.1)		Et_3N (2.0)	/	DMF	DMF	39 [d]	37 [d]	0 [d]	0 [d]	0 [d]
31 [e]	CH_3	*rac*-BINAP-Pd-G3 Buchwald precat. (0.1)		K_3PO_4 (1.1)	/	DMF	DMF	23 [d]	27 [d]	0 [d]	0 [d]	8 [d]
32	CH_3	*rac*-BINAP-Pd-G3 Buchwald precat. (0.1)		Na_2CO_3 (1.1)	/	DMF	DMF	31 [d]	42 [d]	0 [d]	0 [d]	0 [d]
33	**CH_3**	***rac*-BINAP-Pd-G3**		**K_2CO_3**	**/**	**DMF**	**130,**	**31 [d]**	**50 [d]**	**0 [d]**	**0 [d]**	**0 [d]**

		Buchwald precat. (0.1)		**(1.1)**			**16**					
34	CH_3	*rac*-BINAP-Pd-G3		K_2CO_3	TBAC	DMF	130,	25 [d]	45 [d]	0 [d]	0 [d]	0 [d]
		Buchwald precat. (0.1)		(1.1)	(1.0)		16					
35 [g]	**CH_3**	**$Pd(OAc)_2$**	**$^tBuCy_2P.HBF_4$**	**Cs_2CO_3**	**/**	DMF	**130,**	**92**	**0**	**0**	**0**	**0**
		(0.05)	**(0.1)**	**(1.1)**			**16.5**					
36 [h]	CH_3	$Pd(OAc)_2$	$Cy_3P.HBF_4$	Cs_2CO_3	/	DMF	130,	65	0	0	0	0
		(0.1)	(0.2)	(1.2)			16					
37	CH_3	$Pd(OAc)_2$	$^tBuCy_2P.HBF_4$	Et_3N	/	DMF	130,	67 [d]	12 [d]	0 [d]	0 [d]	0 [d]
		(0.1)	(0.2)	(2.0)			16					
38	CH_3	$Pd(OAc)_2$	$^tBuCy_2P.HBF_4$	K_3PO_4	/	DMF	130,	61 [d]	15 [d]	0 [d]	0 [d]	0 [d]
		(0.1)	(0.2)	(1.2)			16					
39 [i]	CH_3	$Pd(OAc)_2$	$^tBuCy_2P.HBF_4$	Ag_2CO_3	/	DMF	130,	trace [d]	0 [d]	0 [d]	0 [d]	0 [d]
		(0.1)	(0.2)	(1.2)			16					

[a]**19** (0.28 mmol), $Pd(OAc)_2$, ligand, base and additive were dissolved in the suitable solvent (2.8 mL), stirred and heated to the indicated temperature during the indicated time under Ar. [b]Isolated yield. [c]^{1}H NMR yield, calculated with 1,4-diacetylbenzene as internal standard. [d]^{1}H NMR yield, calculated with dimethyl sulfon as internal standard. [e]Among the other products, C-N bond cleavage of the vinyl functionality of the starting material by presumably hydrolysis was also observed in 4% (NMR yield) (structure not depicted). [f]^{1}H NMR yield, calculated with 1,3,5-trimethoxybenzene as internal standard. [g]Reaction performed on a 4.35 mmol scale. [h]Reaction performed on a 20.70 mmol scale. [i] C-N bond cleavage of the vinyl functionality of the starting material by presumably hydrolysis was observed in 60% (NMR yield) (structure not depicted).

^{1}H, ^{13}C & 2D NMR spectra of compounds

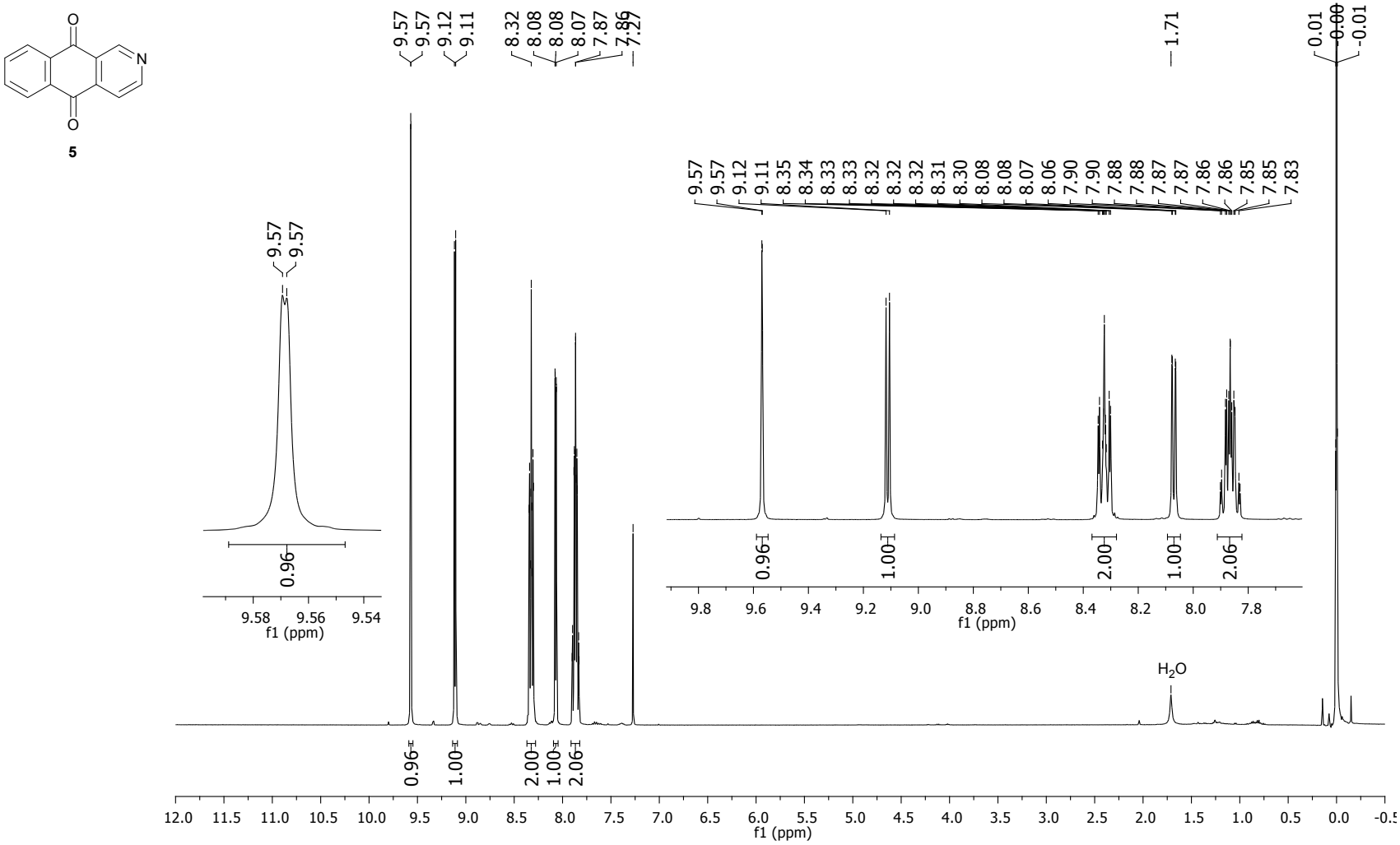


Figure 1 ^{1}H NMR spectrum of benzo[*g*]isoquinoline-5,10-dione (**5**) ($CDCl_3$, 400 MHz).

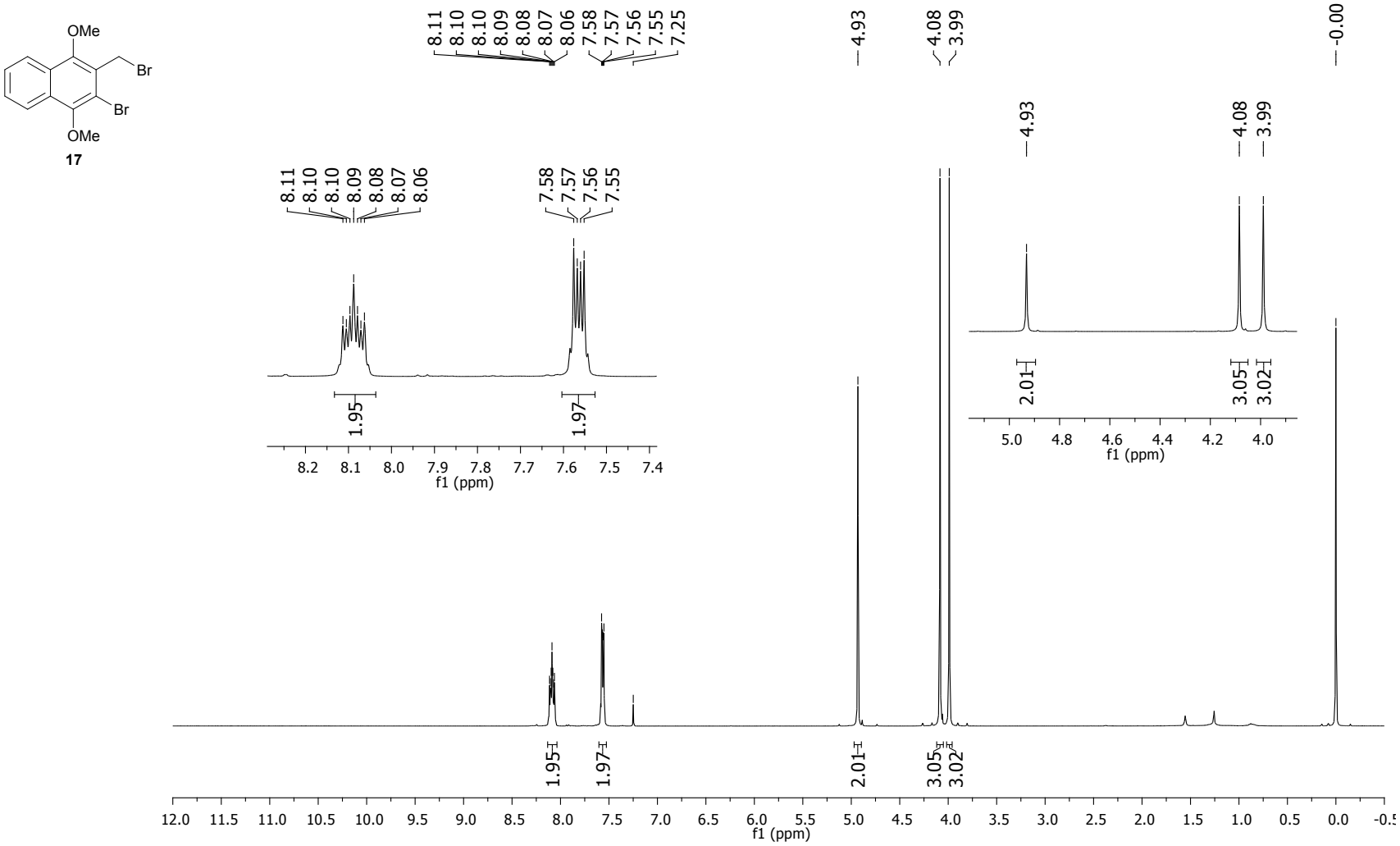


Figure 2 ^{1}H NMR spectrum of 2-bromo-3-(2-bromomethyl)-1,4-dimethoxynaphthalene (**17**) ($CDCl_3$, 400 MHz).

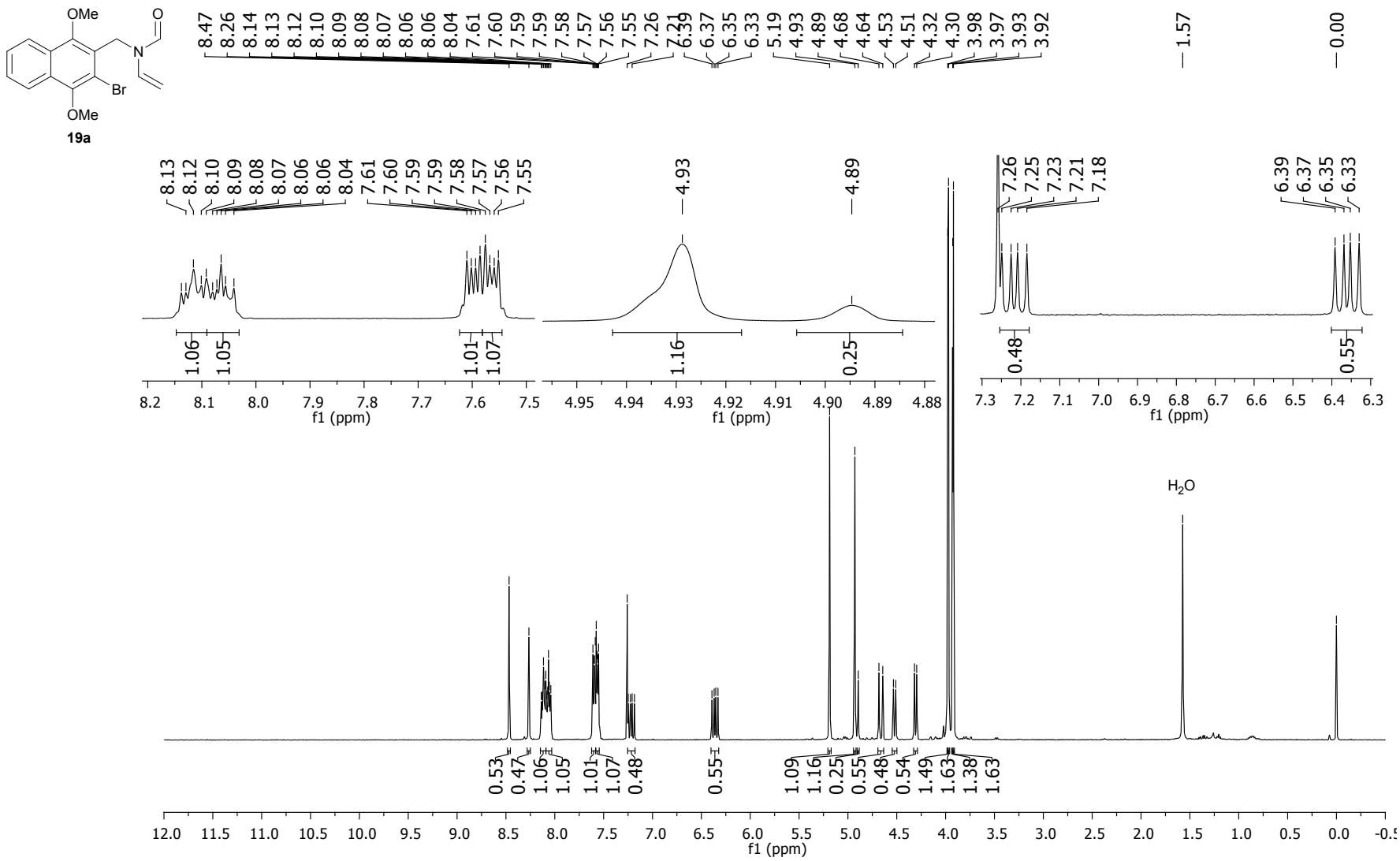


Figure 3 ^{1}H NMR spectrum of *N*-((3-bromo-1,4-dimethoxynaphthalen-2-yl)methyl)-*N*-vinylformamide (**19a**) ($CDCl_3$, 400 MHz).

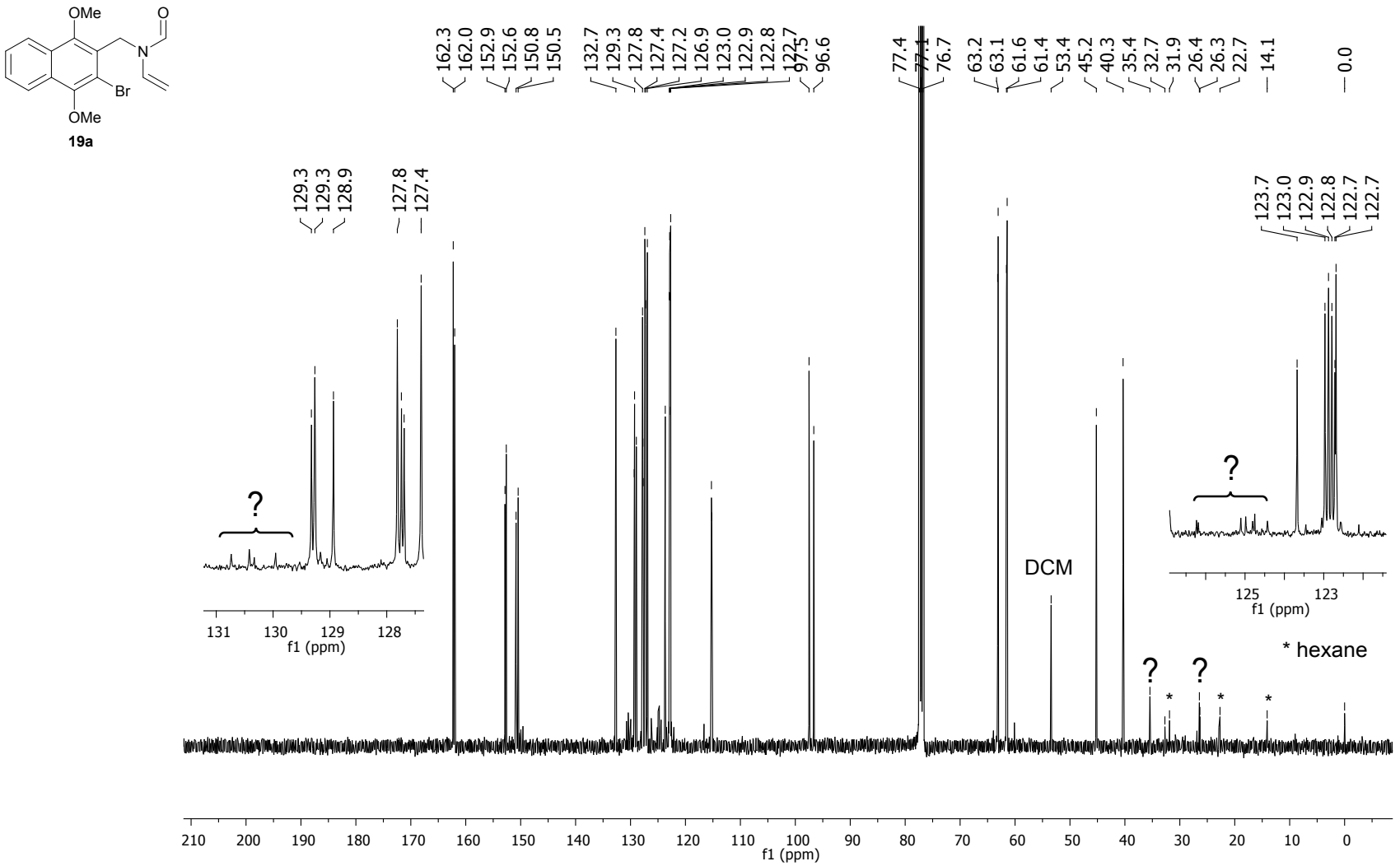


Figure 4 ^{13}C NMR spectrum of *N*-((3-bromo-1,4-dimethoxynaphthalen-2-yl)methyl)-*N*-vinylformamide (**19a**) ($CDCl_3$, 100 MHz).

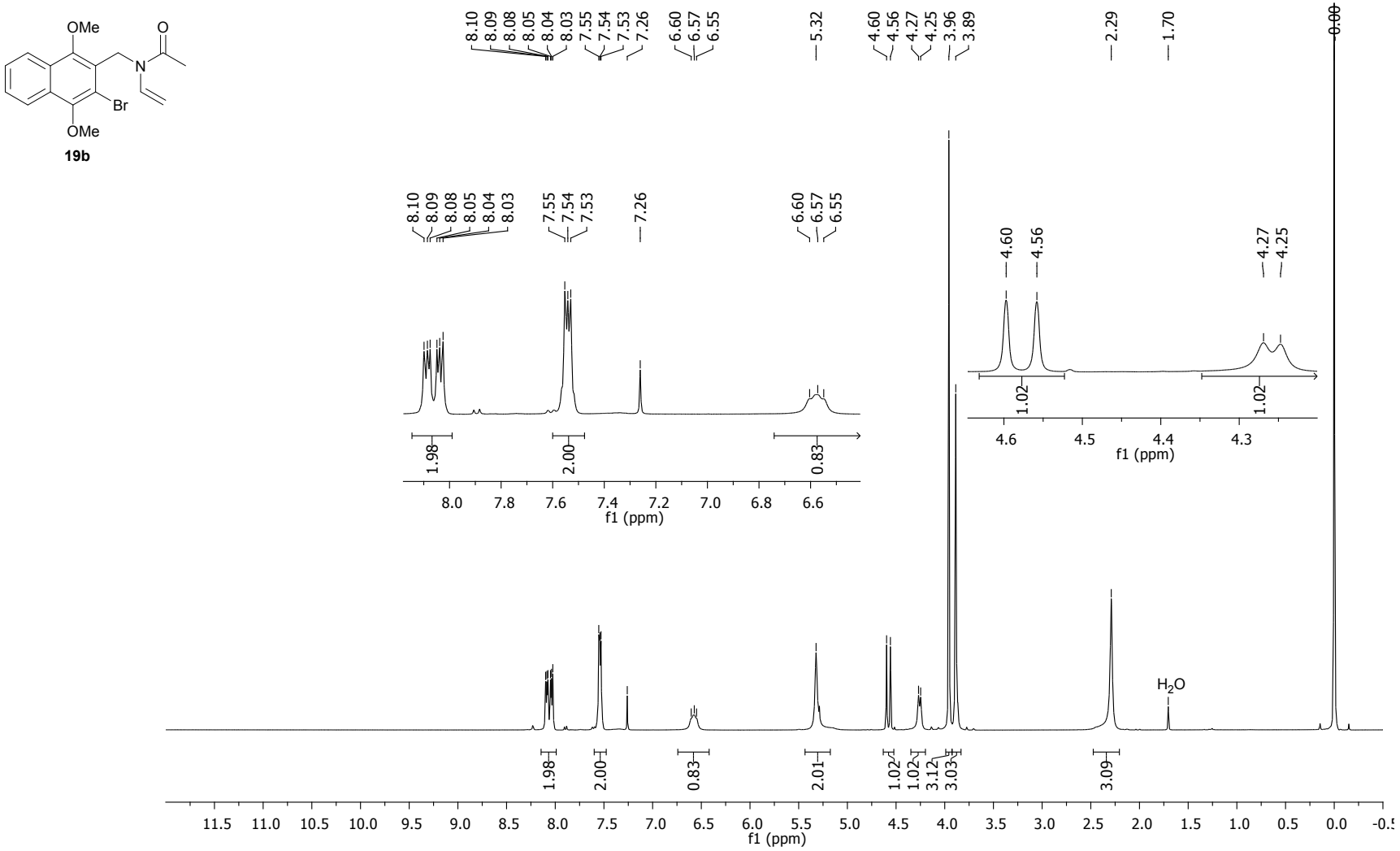


Figure 5 ^{1}H NMR spectrum of *N*-((3-bromo-1,4-dimethoxynaphthalen-2-yl)methyl)-*N*-vinylacetamide (**19b**) ($CDCl_3$, 400 MHz).

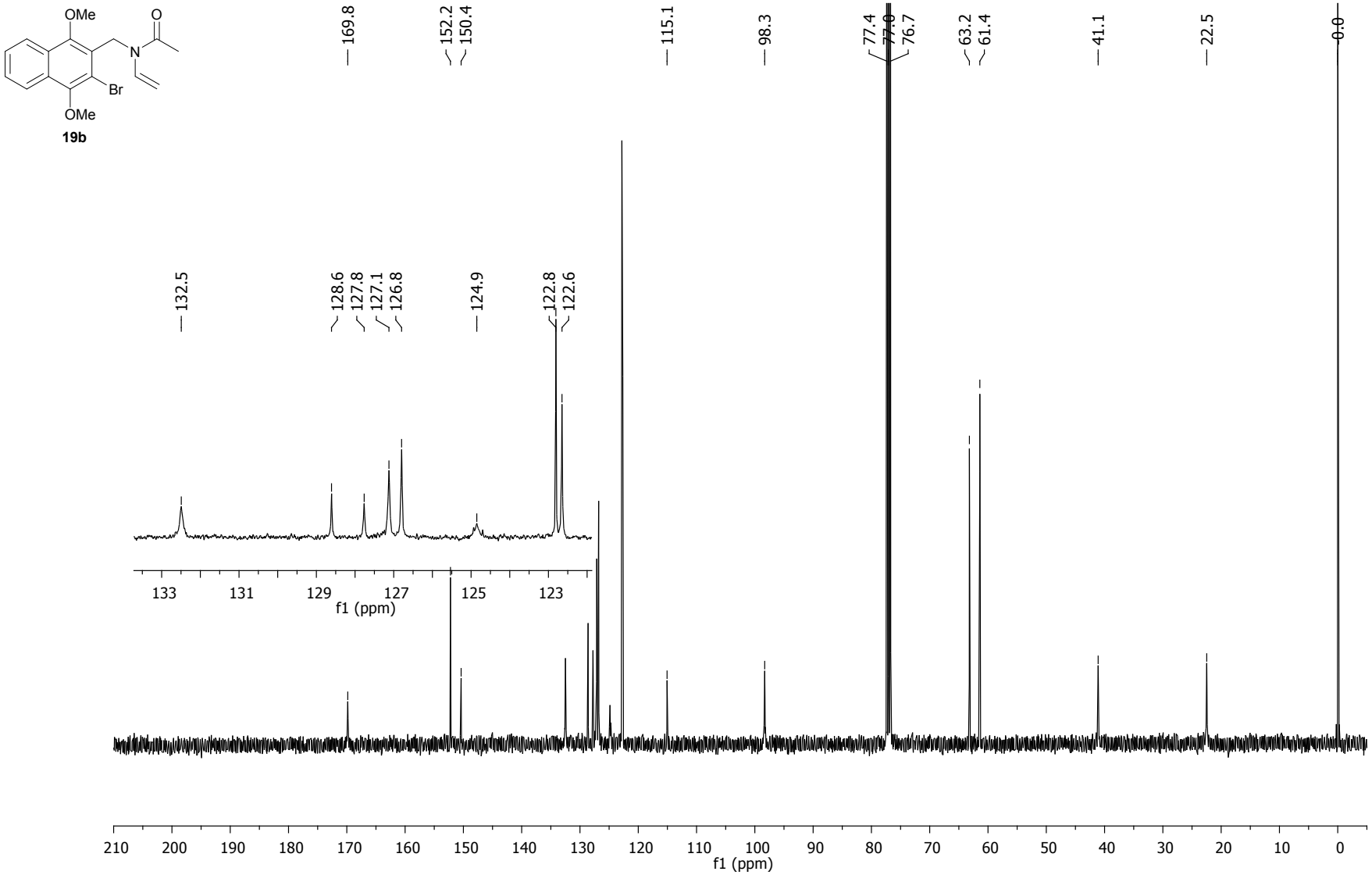


Figure 6 ^{13}C NMR spectrum of *N*-((3-bromo-1,4-dimethoxynaphthalen-2-yl)methyl)-*N*-vinylacetamide (**19b**) ($CDCl_3$, 400 MHz).

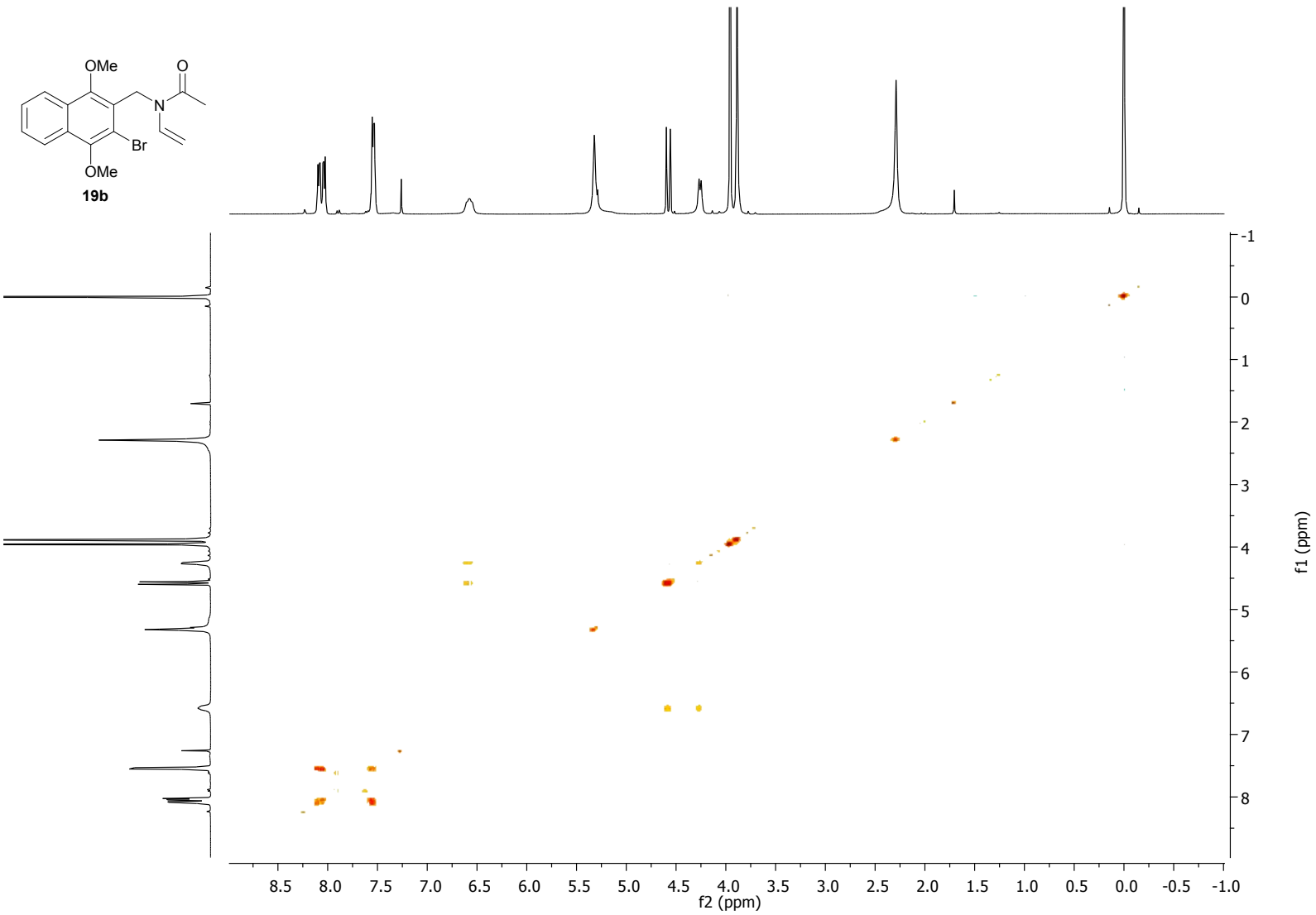


Figure 7 COSY spectrum of *N*-((3-bromo-1,4-dimethoxynaphthalen-2-yl)methyl)-*N*-vinylacetamide (**19b**) ($CDCl_3$, 400 MHz).

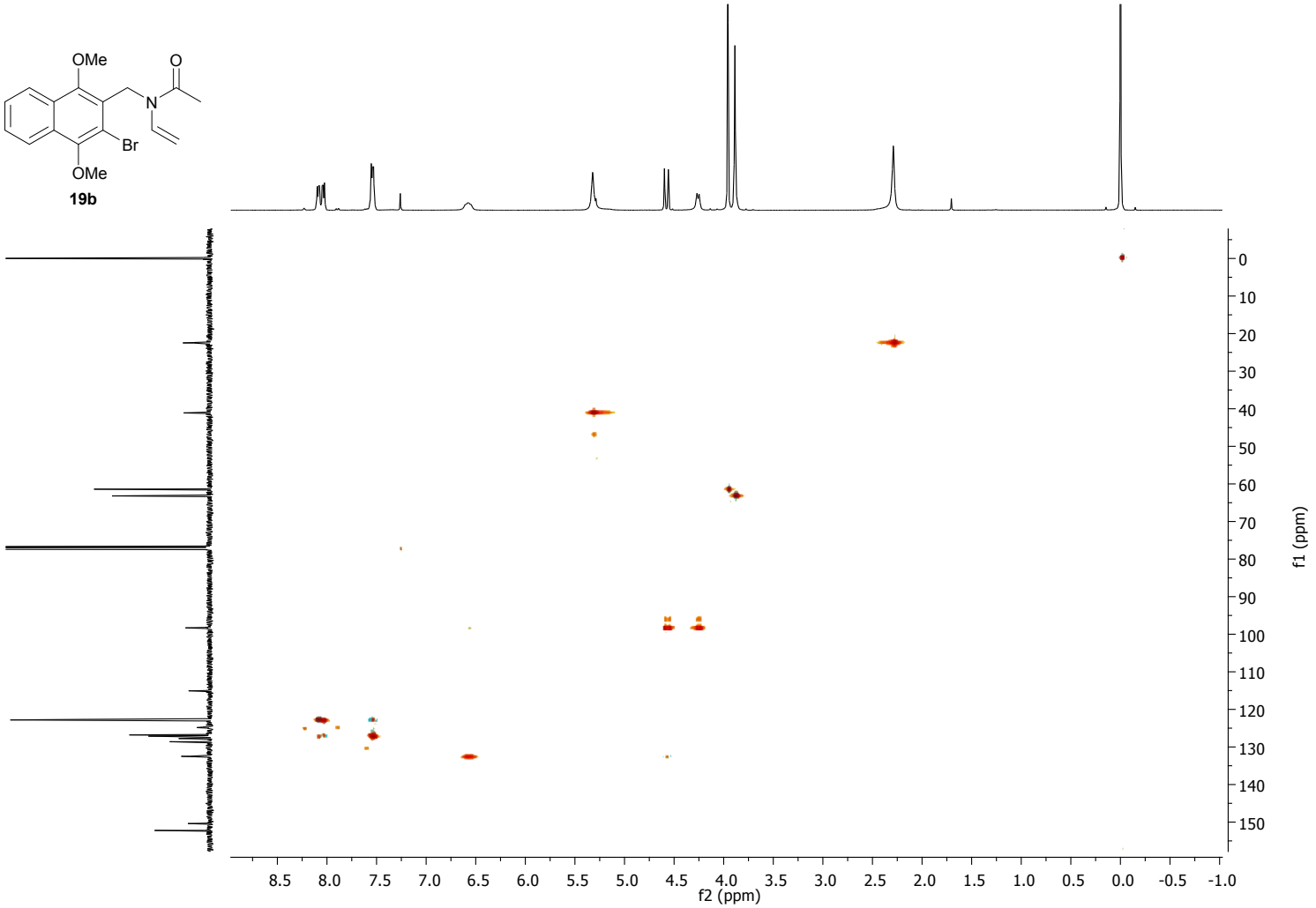


Figure 8 HSQC spectrum of *N*-((3-bromo-1,4-dimethoxynaphthalen-2-yl)methyl)-*N*-vinylacetamide (**19b**) ($CDCl_3$, 400 MHz).

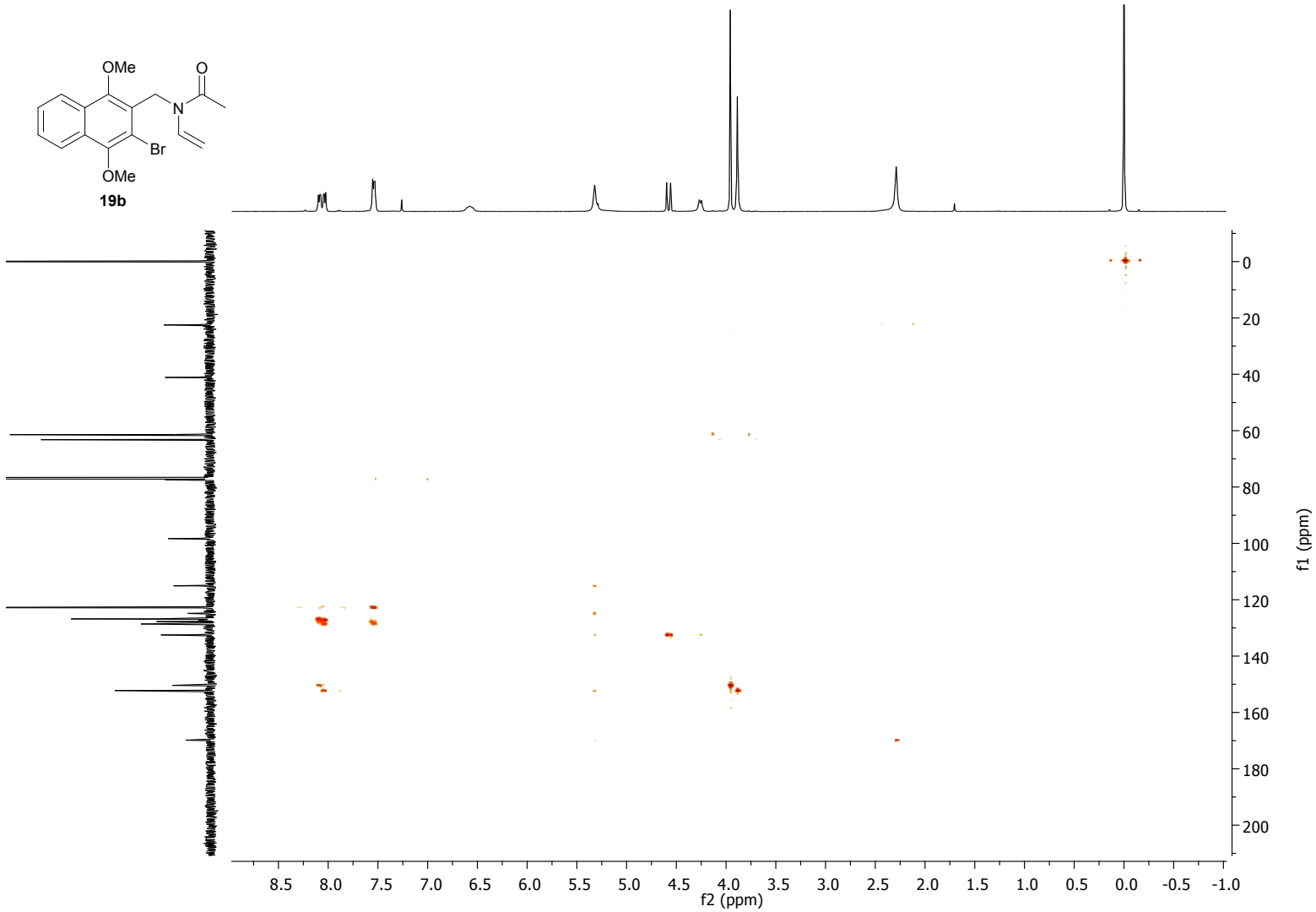


Figure 9 HMBC spectrum of *N*-((3-bromo-1,4-dimethoxynaphthalen-2-yl)methyl)-*N*-vinylacetamide (**19b**) ($CDCl_3$, 400 MHz).

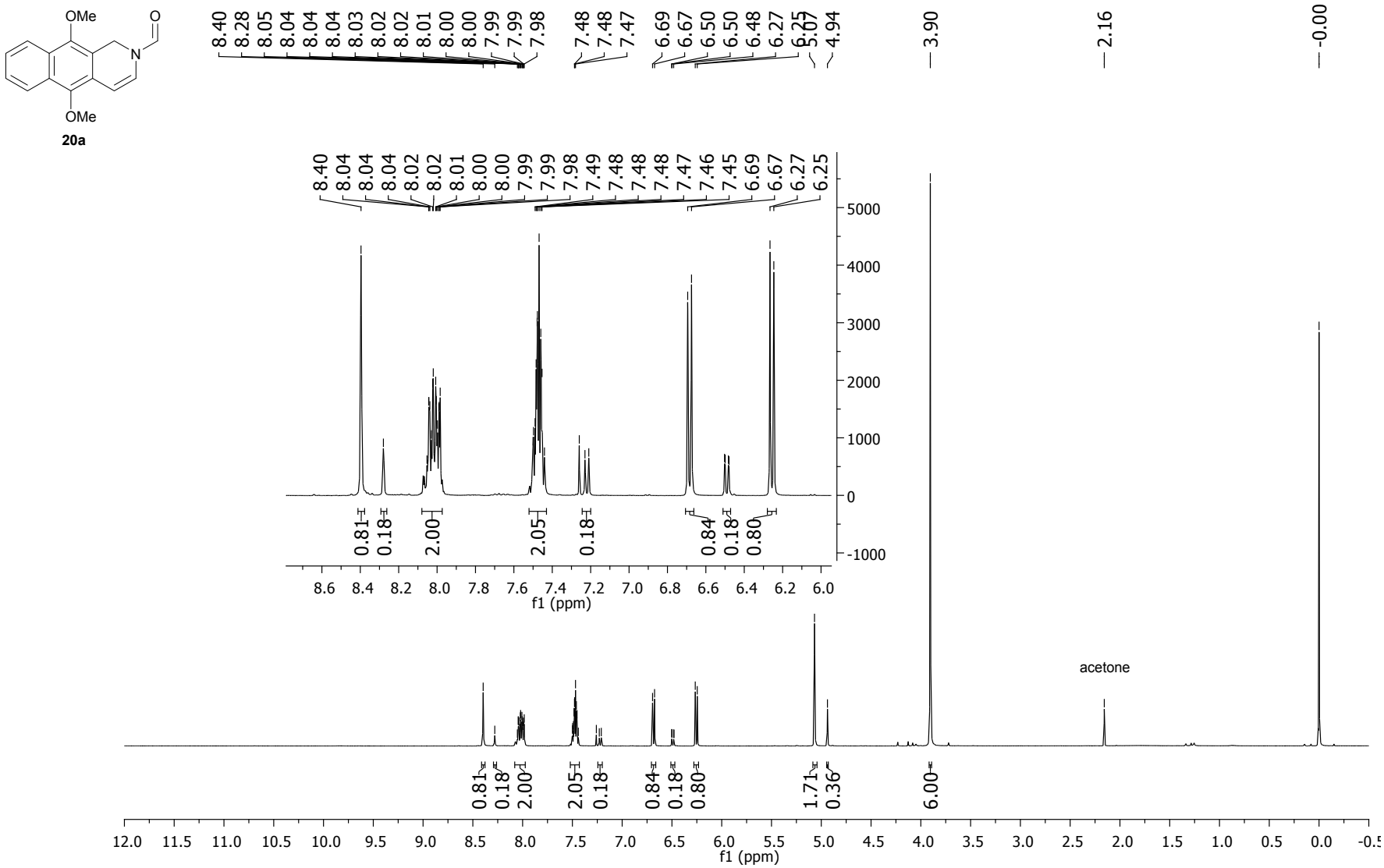


Figure 10 ^{1}H NMR spectrum of 5,10-dimethoxybenzo[*g*]isoquinoline-2(1*H*)-carbaldehyde (**20a**) ($CDCl_3$, 400 MHz).

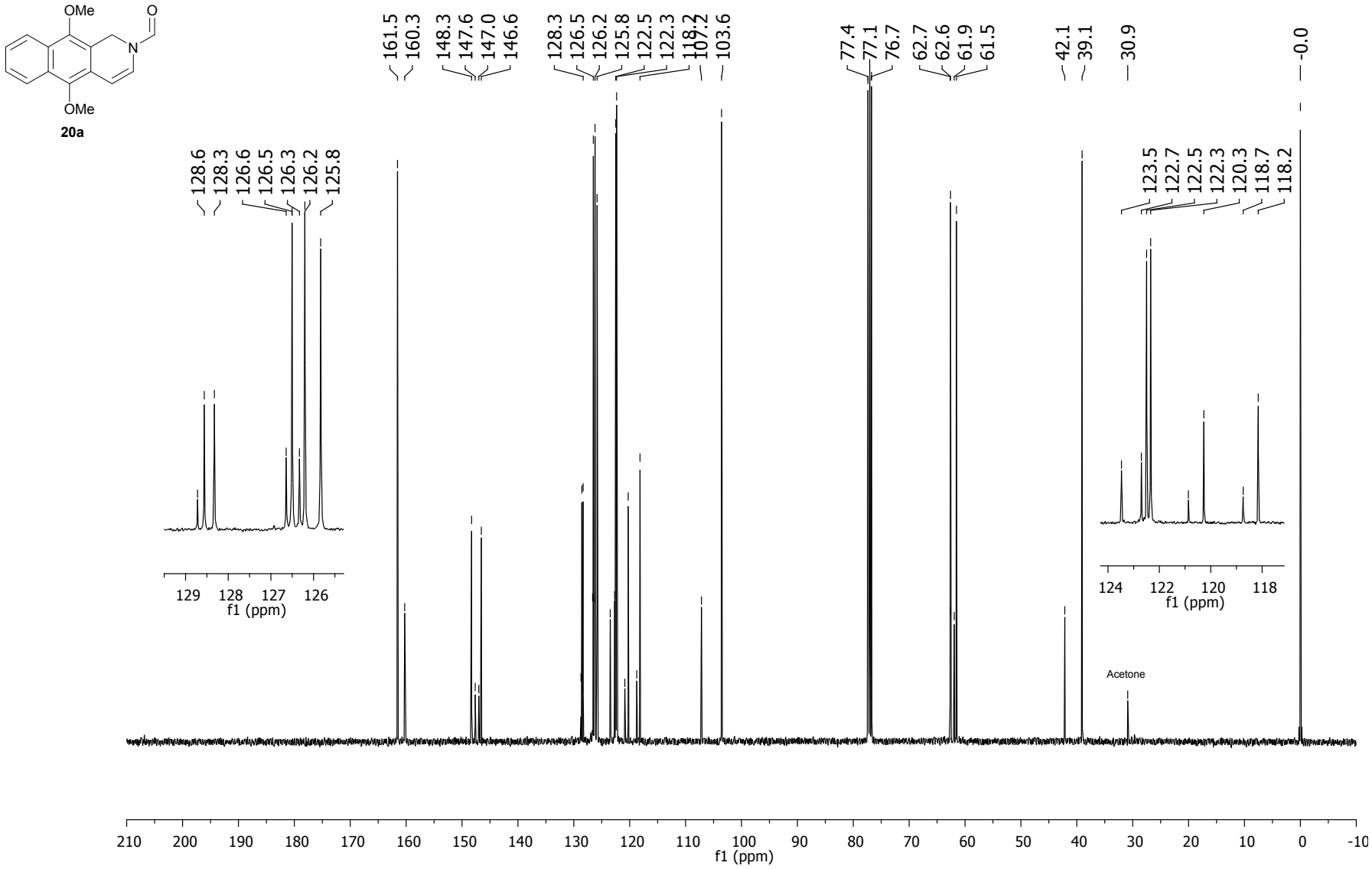


Figure 11 ^{13}C NMR spectrum of 5,10-dimethoxybenzo[*g*]isoquinoline-2(1*H*)-carbaldehyde (**20a**) ($CDCl_3$, 100 MHz).

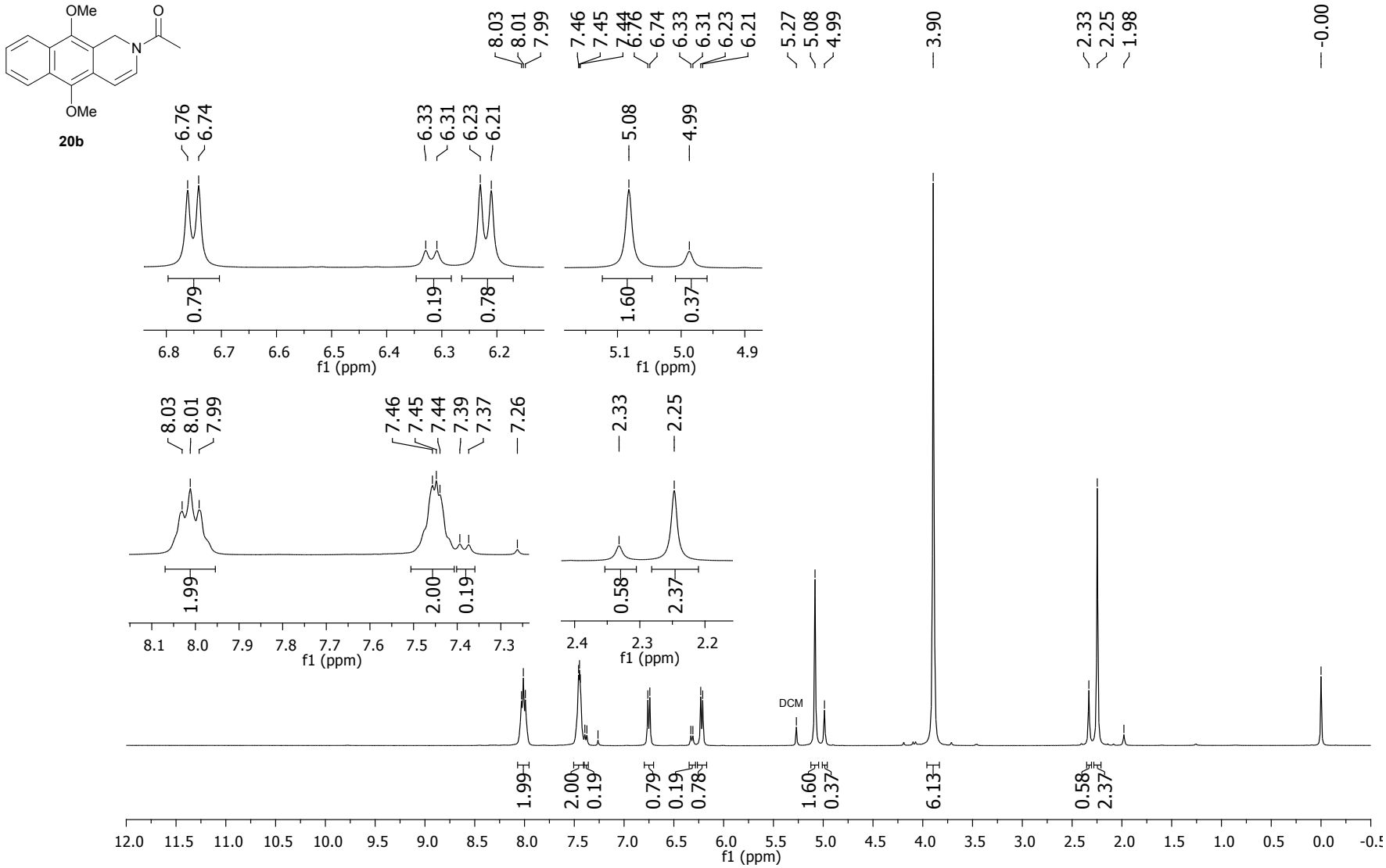


Figure 12 ^{1}H NMR spectrum of 1-(5,10-dimethoxybenzo[*g*]isoquinolin-2(1*H*)-yl)ethanone (**20b**) ($CDCl_3$, 400 MHz).

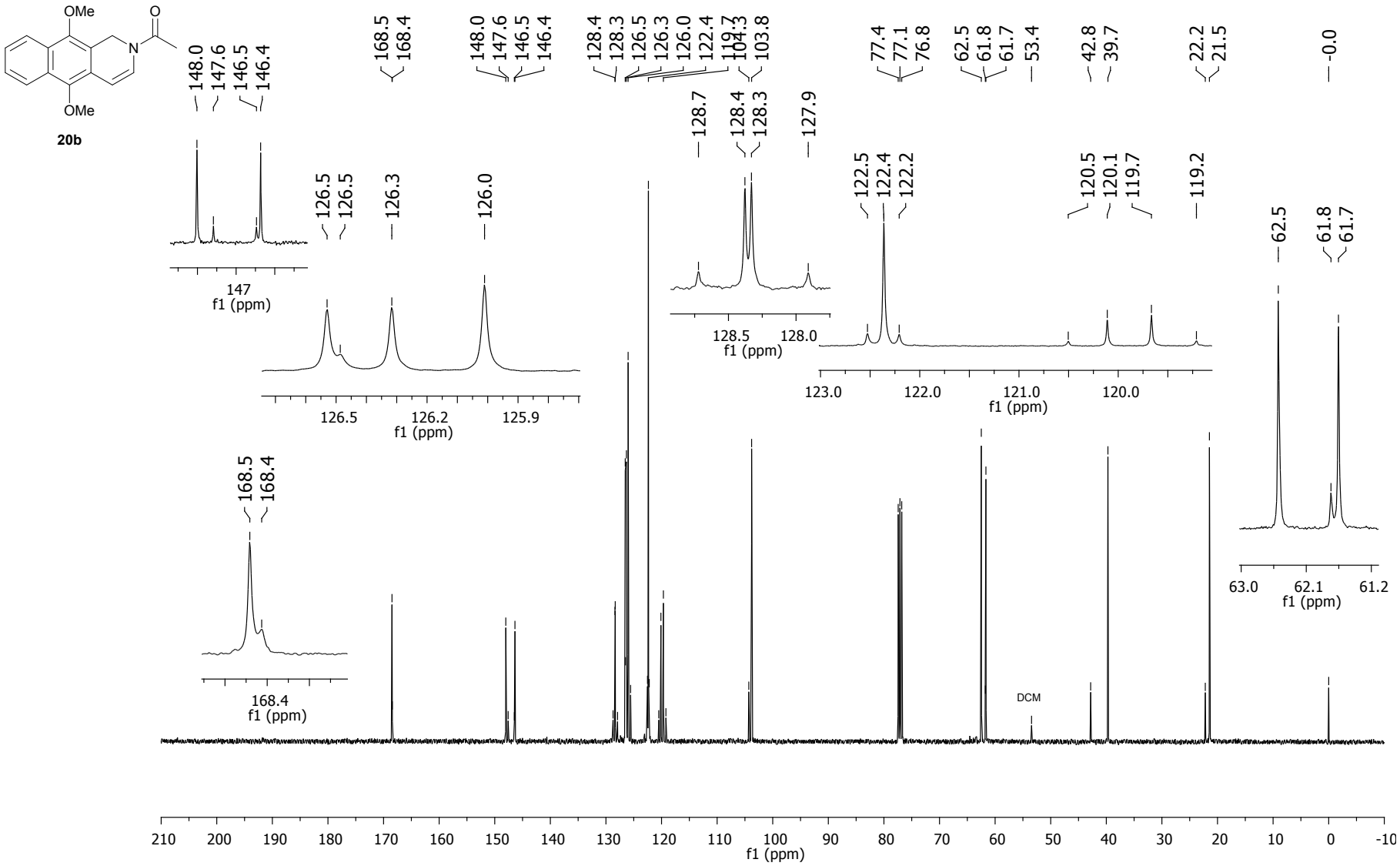


Figure 13 ^{13}C NMR spectrum of 1-(5,10-dimethoxybenzo[*g*]isoquinolin-2(1*H*)-yl)ethanone (**20b**) ($CDCl_3$, 100 MHz).

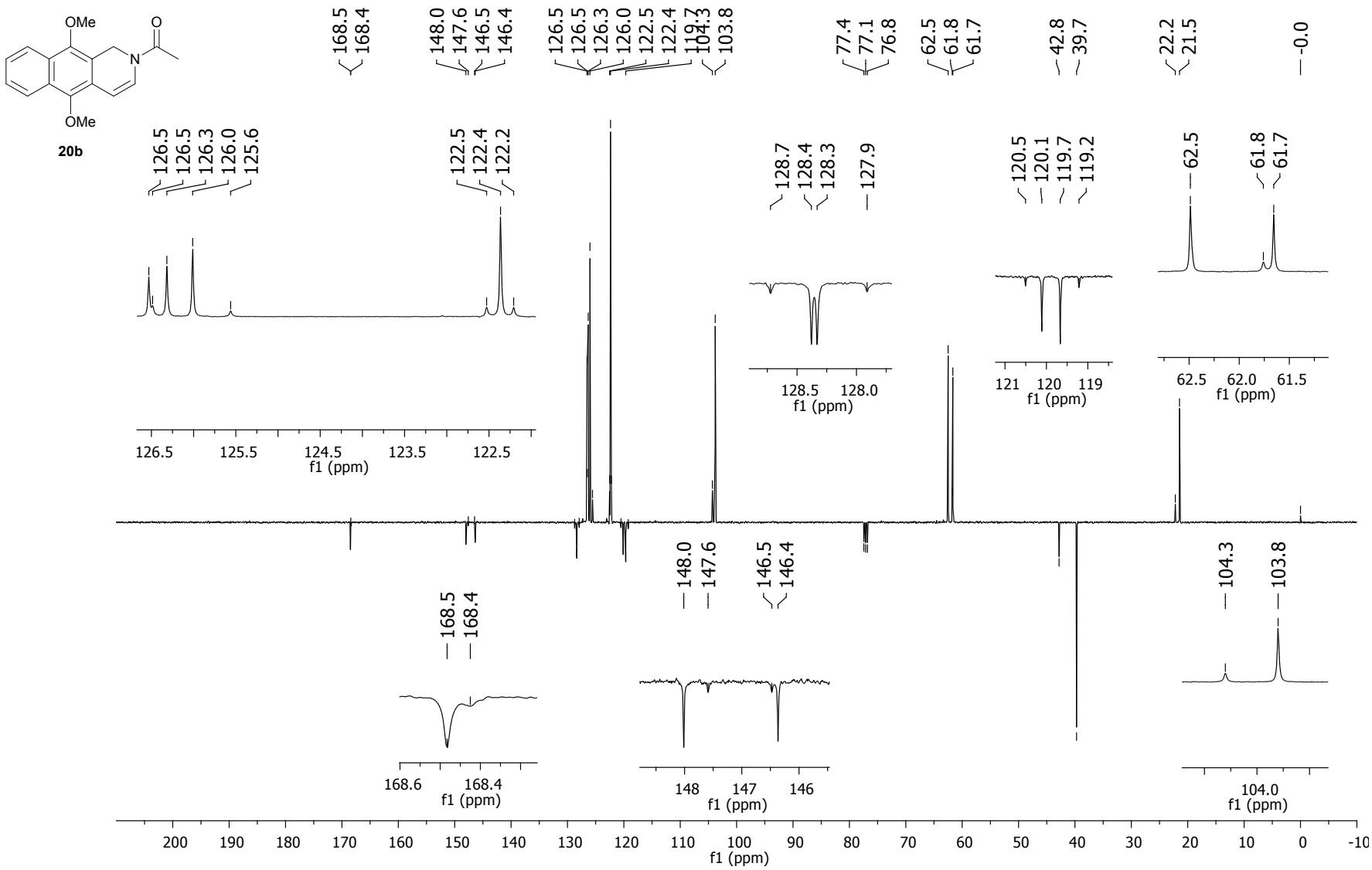


Figure 14 APT spectrum of 1-(5,10-dimethoxybenzo[*g*]isoquinolin-2(1*H*)-yl)ethanone (**20b**) ($CDCl_3$, 100 MHz).

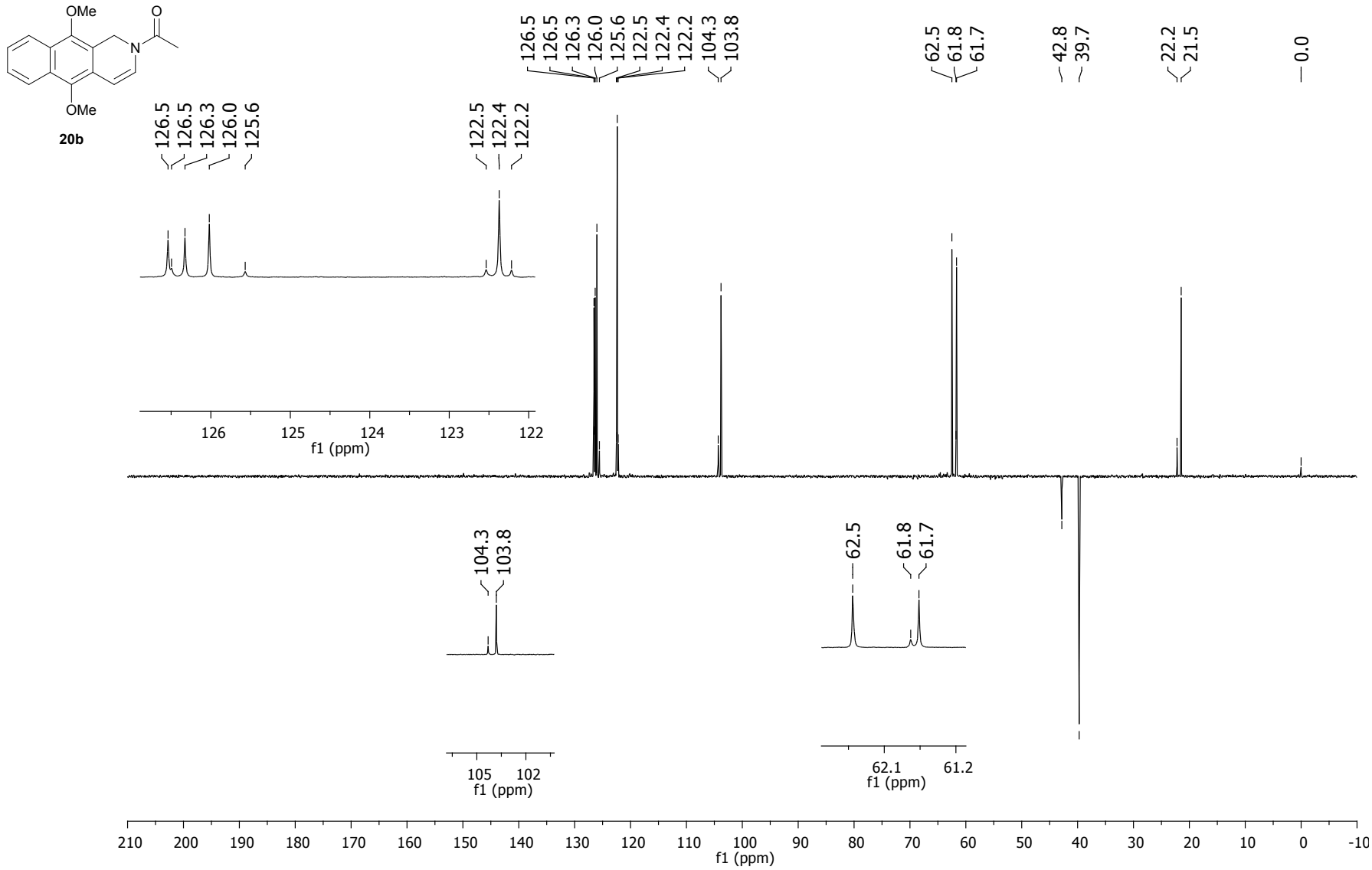


Figure 15 DEPT 135 spectrum of 1-(5,10-dimethoxybenzo[*g*]isoquinolin-2(1*H*)-yl)ethanone (**20b**) ($CDCl_3$, 100 MHz).

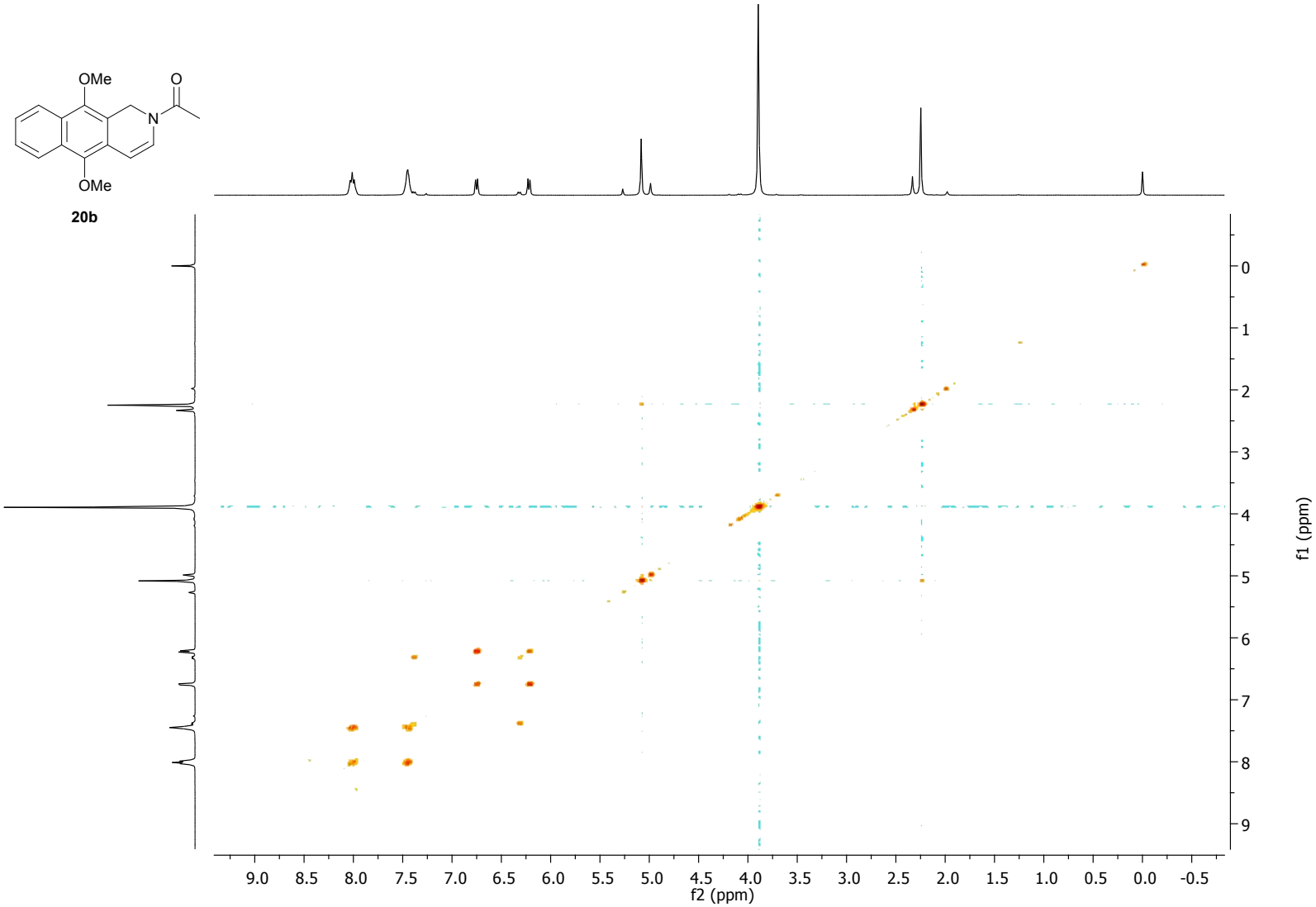


Figure 16 COSY spectrum of 1-(5,10-dimethoxybenzo[*g*]isoquinolin-2(1*H*)-yl)ethanone (**20b**) ($CDCl_3$, 400 MHz).

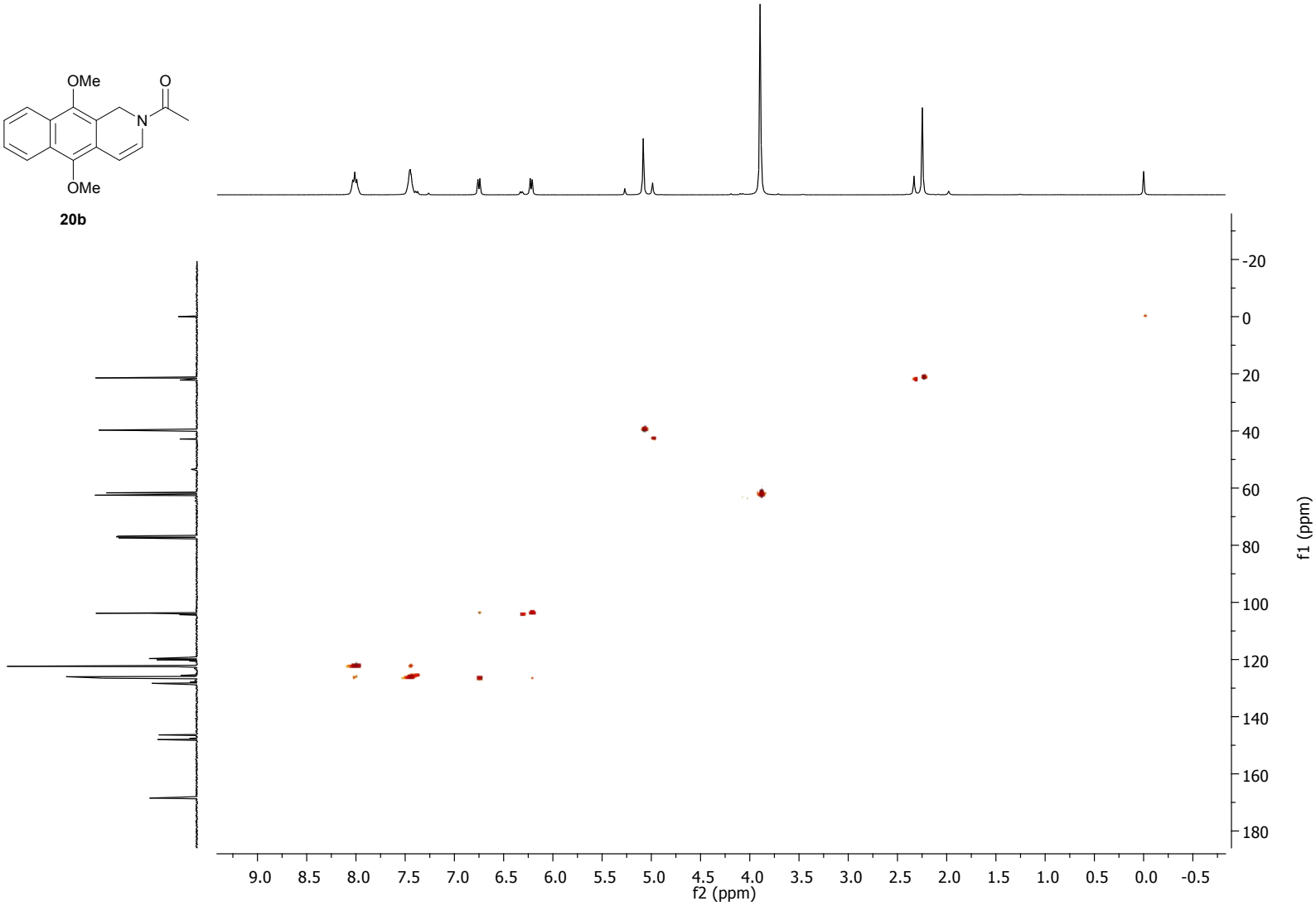


Figure 17 HSQC spectrum of 1-(5,10-dimethoxybenzo[*g*]isoquinolin-2(1*H*)-yl)ethanone (**20b**) ($CDCl_3$, 400 MHz).

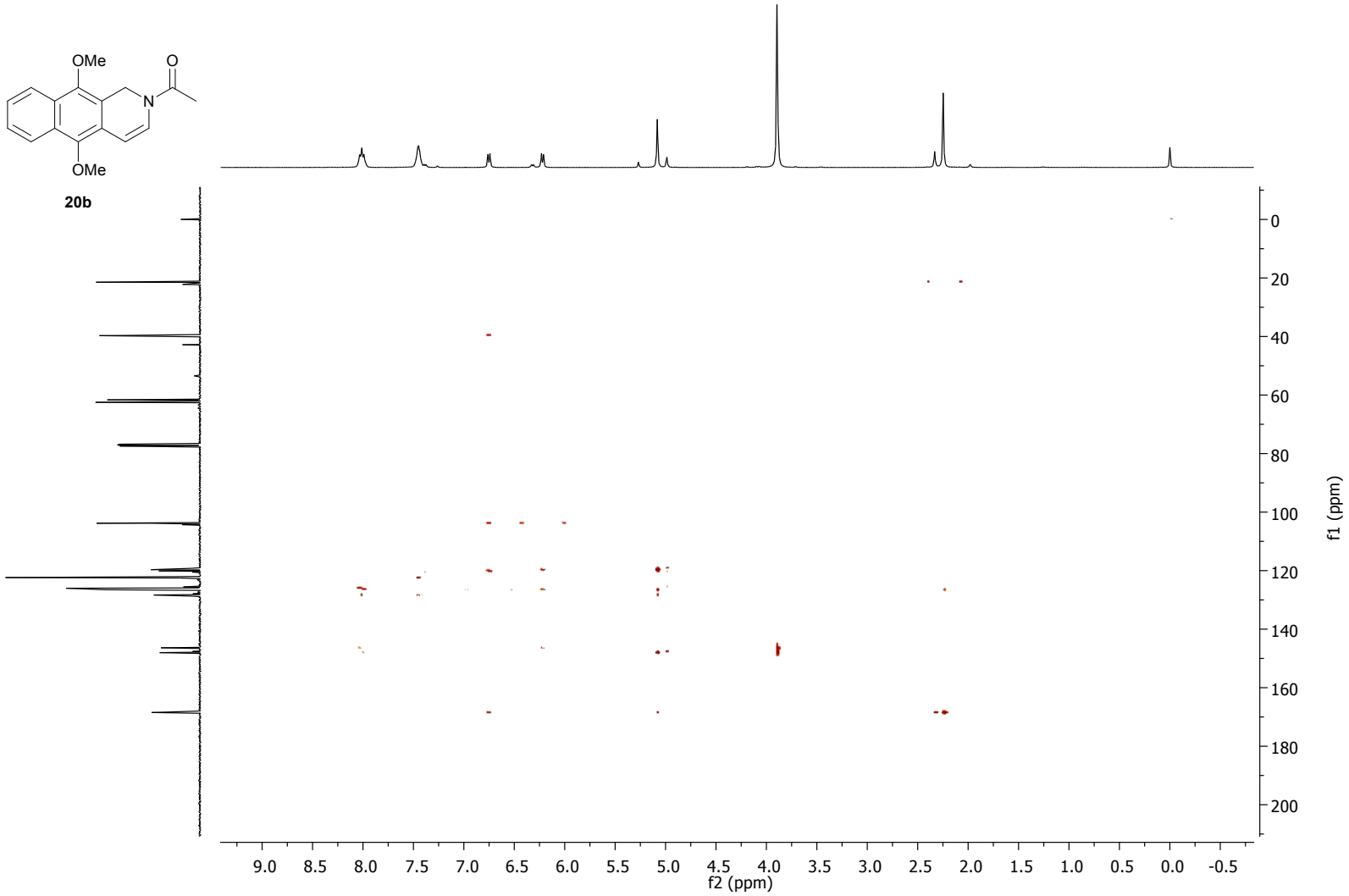


Figure 18 HMBC spectrum of 1-(5,10-dimethoxybenzo[*g*]isoquinolin-2(1*H*)-yl)ethanone (**20b**) ($CDCl_3$, 400 MHz).

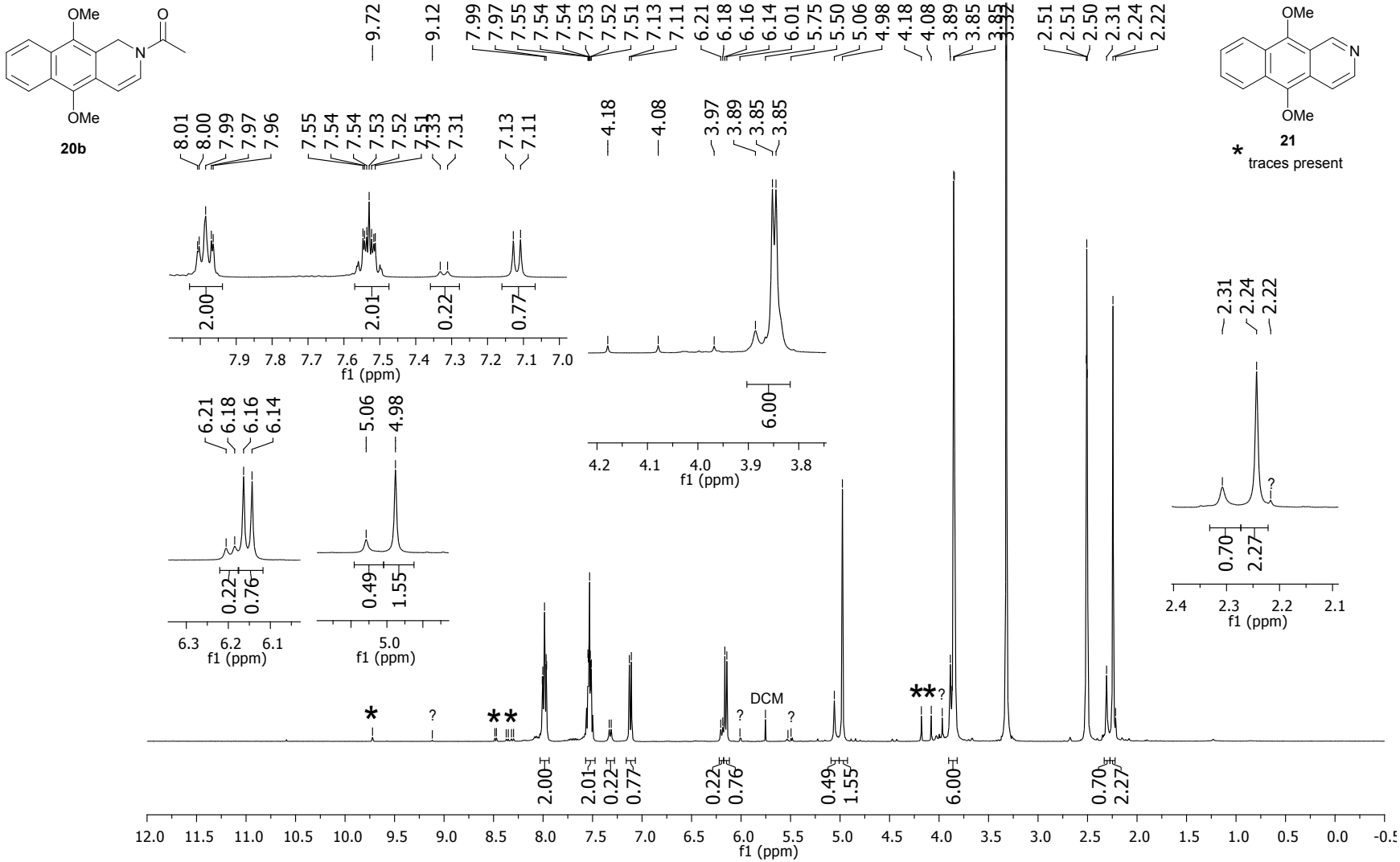


Figure 19 ^{1}H NMR spectrum of 1-(5,10-dimethoxybenzo[*g*]isoquinolin-2(1*H*)-yl)ethanone (**20b**) (DMSO-d_6, 400 MHz). Traces of **21** are present due to limited stability of **20b** in DMSO-d6.

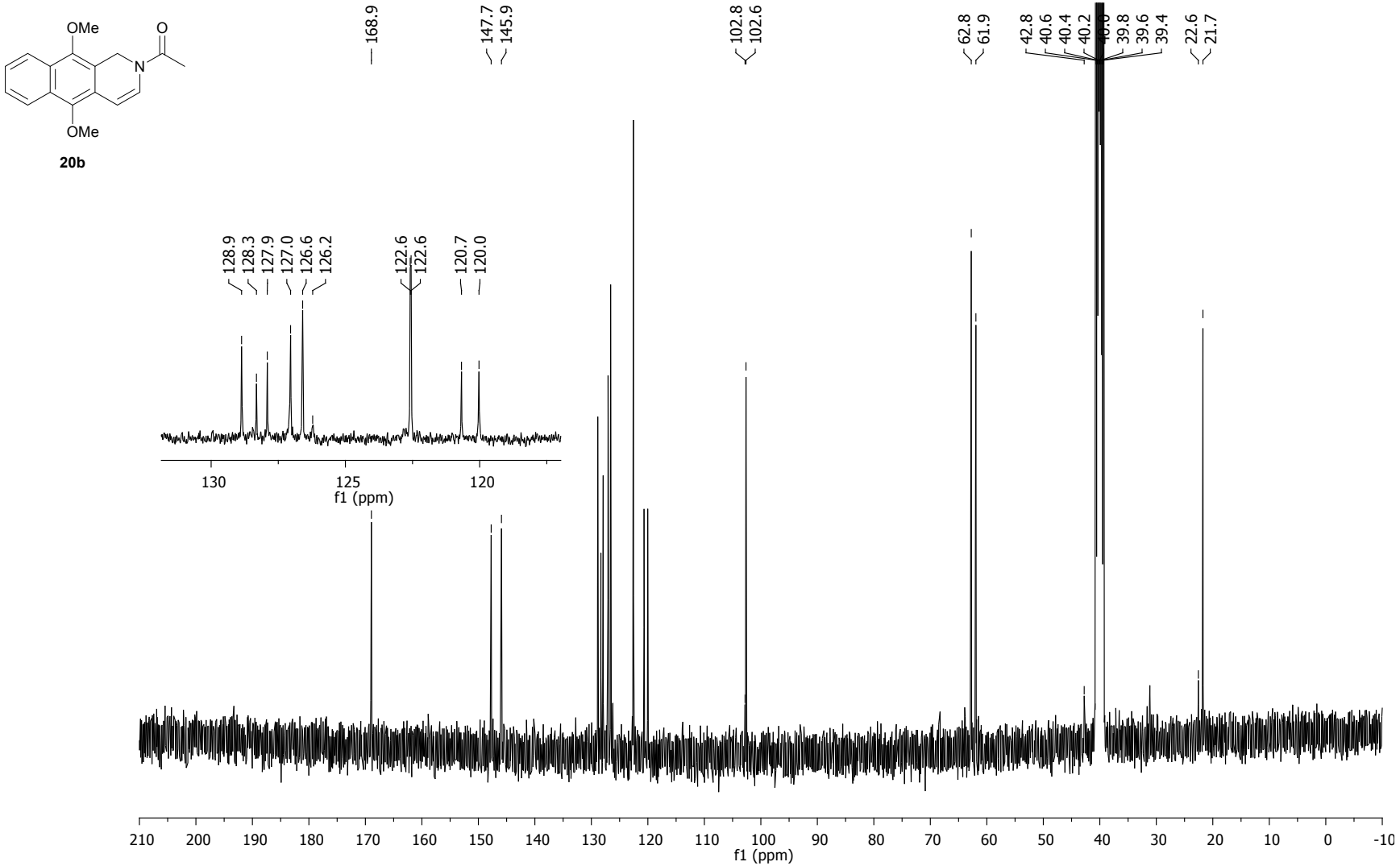


Figure 20 ^{13}C NMR spectrum of 1-(5,10-dimethoxybenzo[*g*]isoquinolin-2(1*H*)-yl)ethanone (**20b**) (DMSO-d_6, 100 MHz).

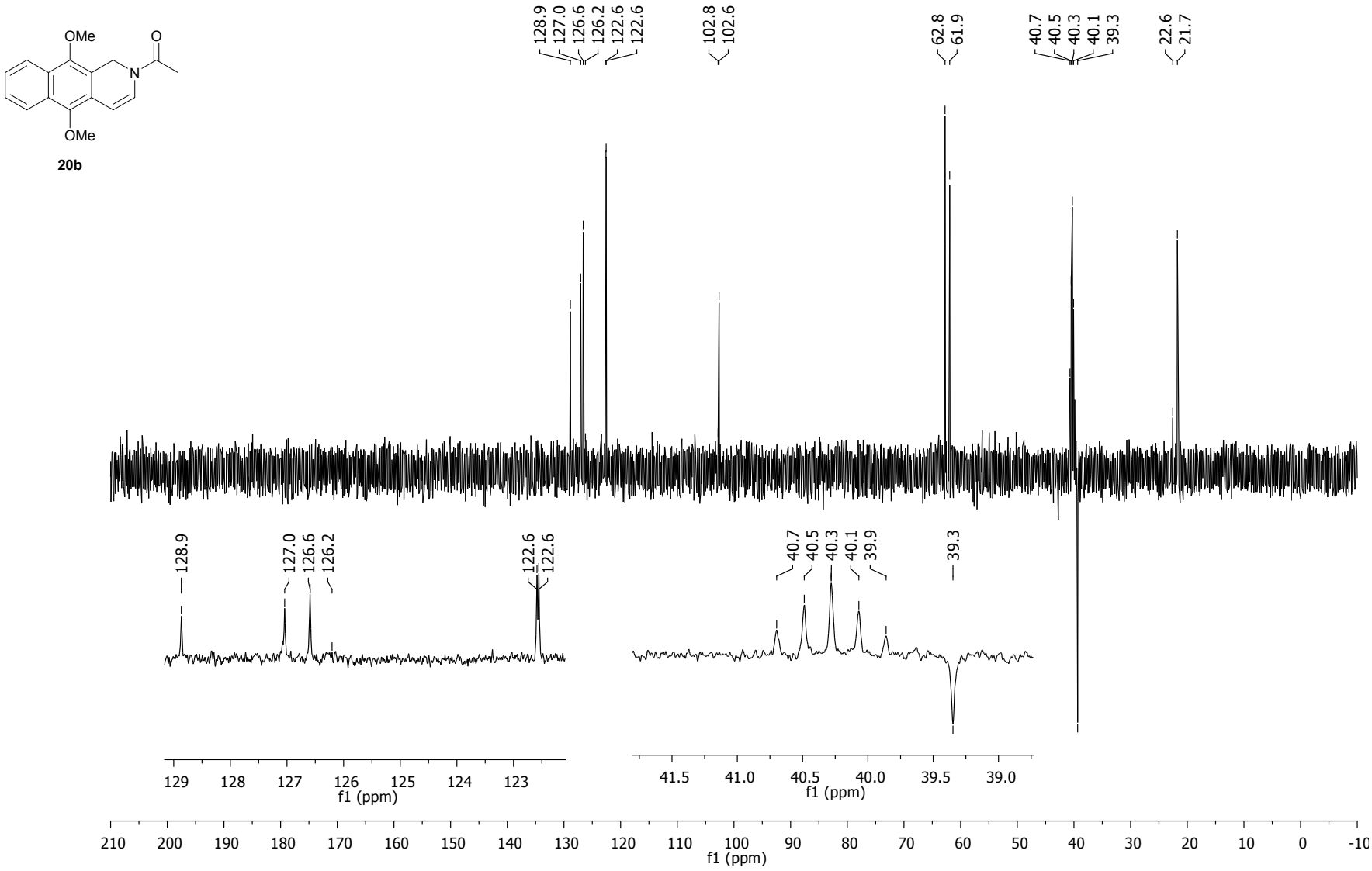


Figure 21 DEPT-135 spectrum of 1-(5,10-dimethoxybenzo[*g*]isoquinolin-2(1*H*)-yl)ethanone (DMSO-d_6, 100 MHz).

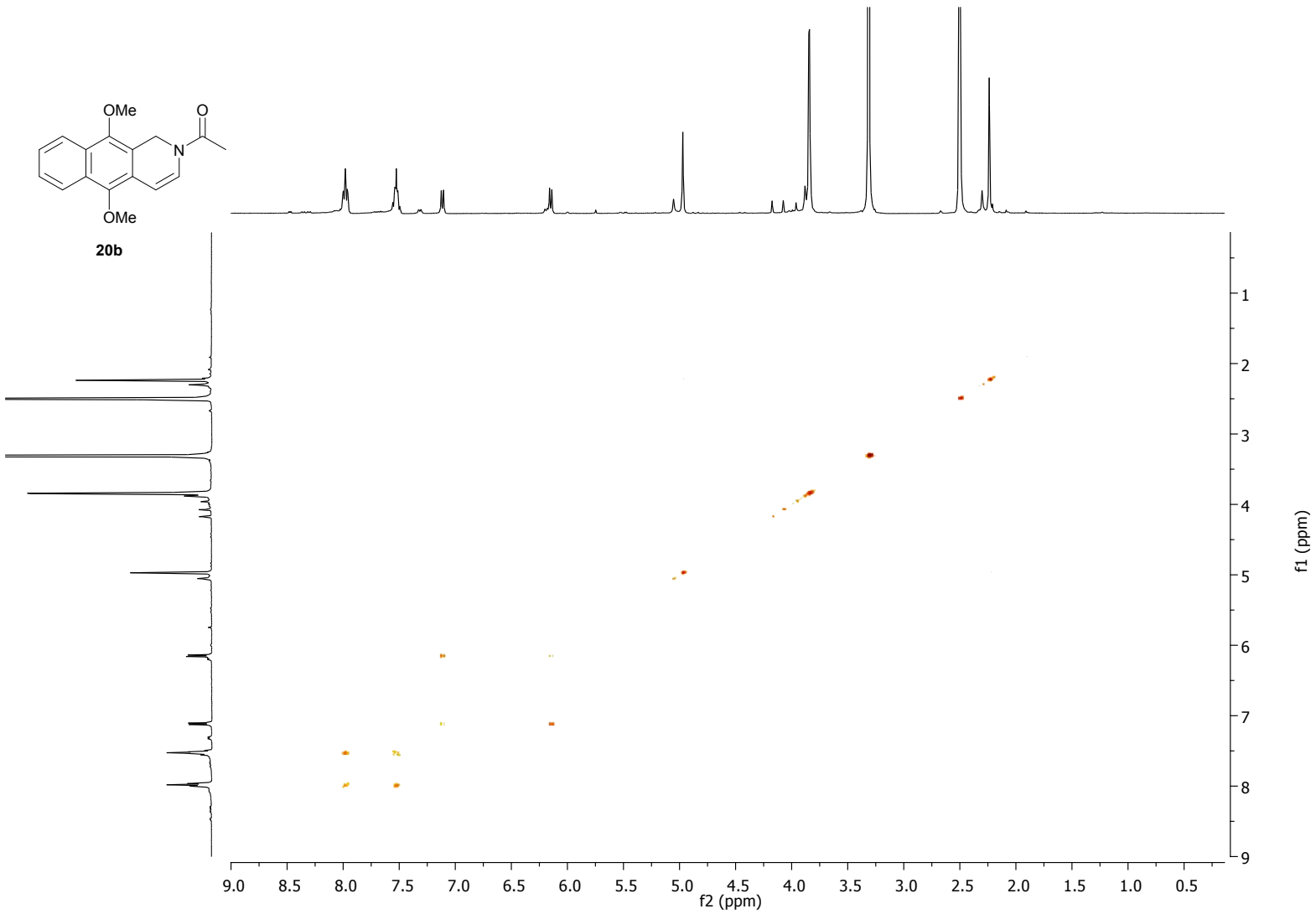


Figure 22 COSY spectrum of 1-(5,10-dimethoxybenzo[*g*]isoquinolin-2(1*H*)-yl)ethanone (DMSO-d_6, 400 MHz).

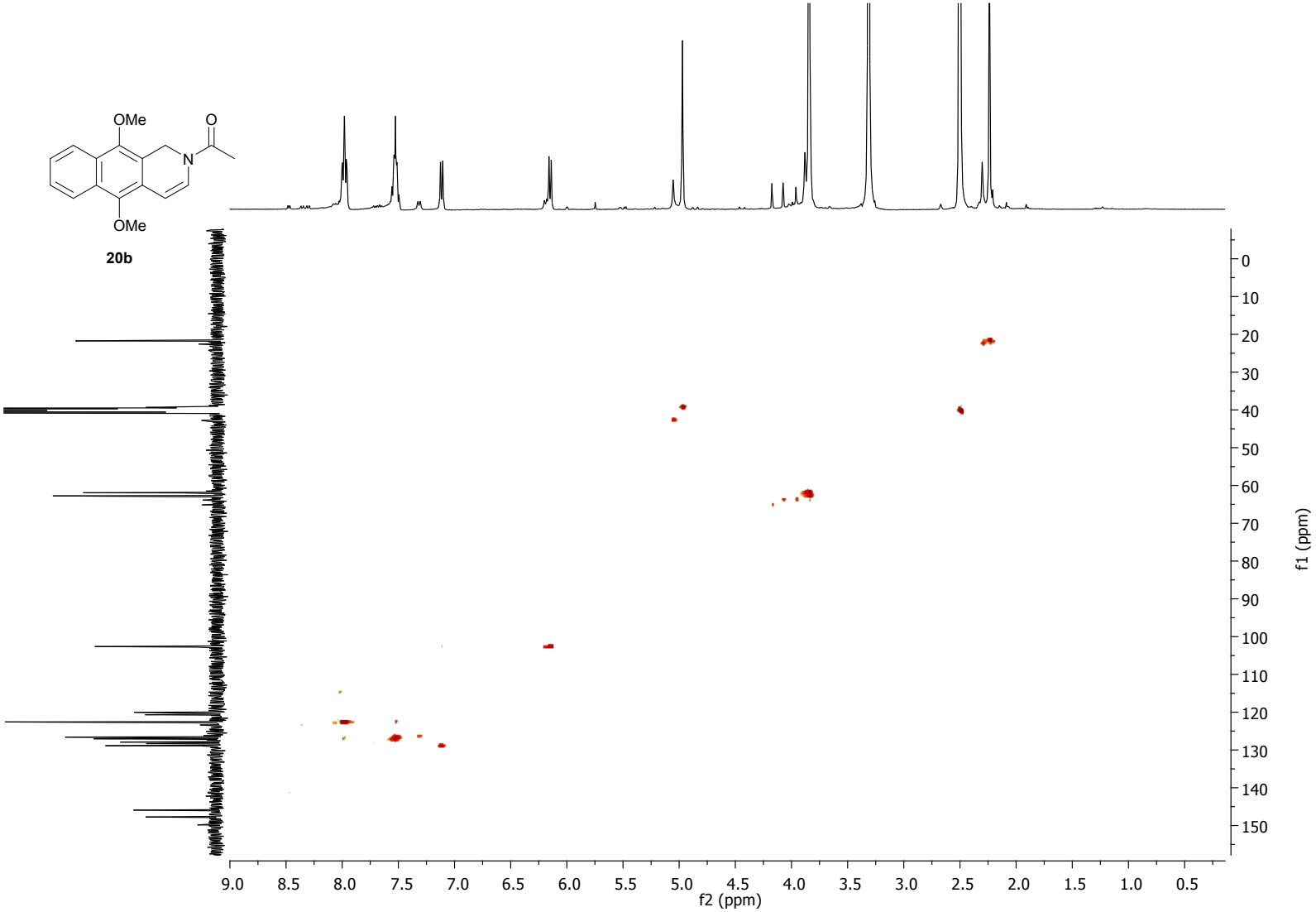


Figure 23 HSQC spectrum of 1-(5,10-dimethoxybenzo[*g*]isoquinolin-2(1*H*)-yl)ethanone (DMSO-d_6, 400 MHz).

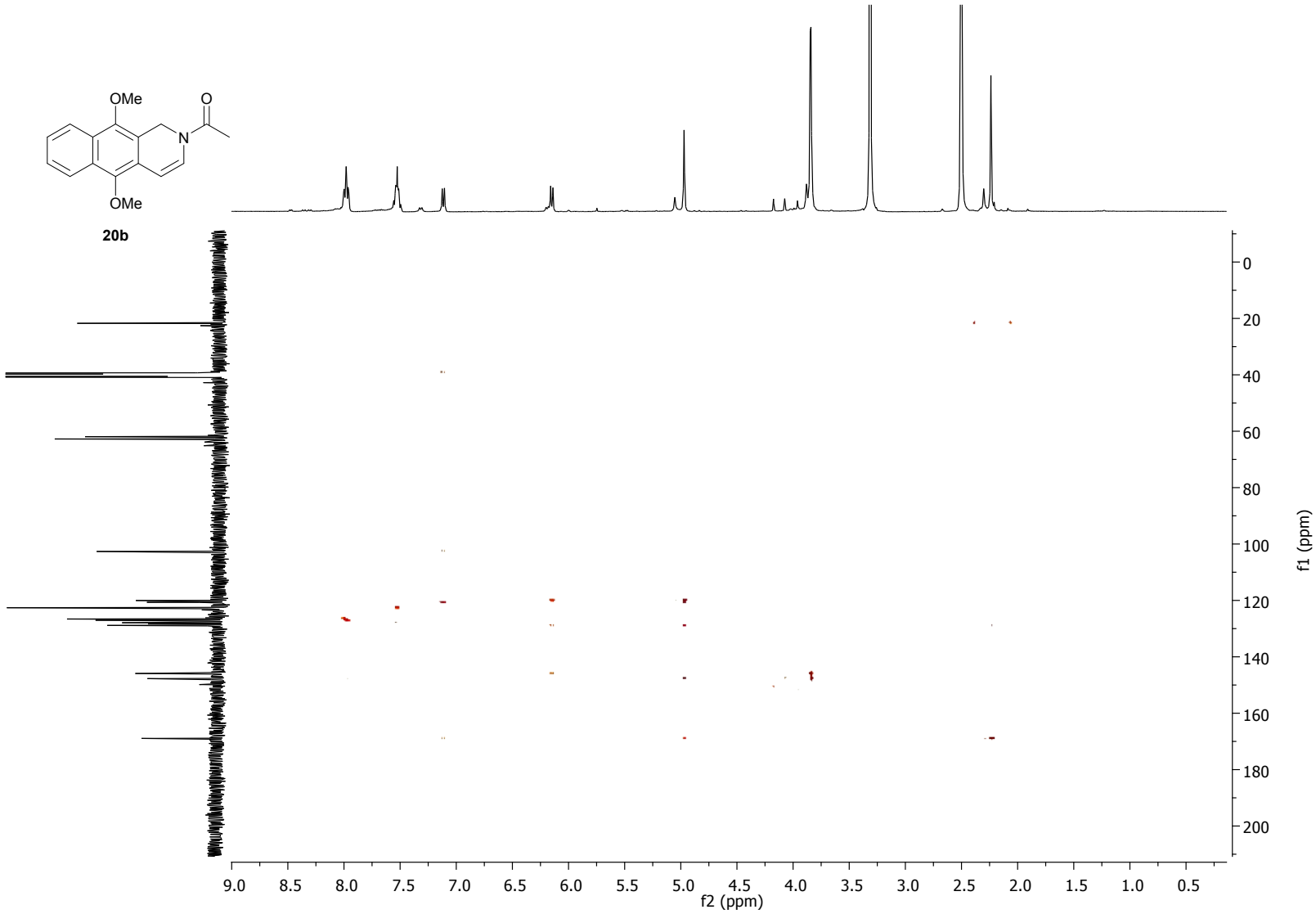


Figure 24 HMBC spectrum of 1-(5,10-dimethoxybenzo[*g*]isoquinolin-2(1*H*)-yl)ethanone (DMSO-d_6, 400 MHz).

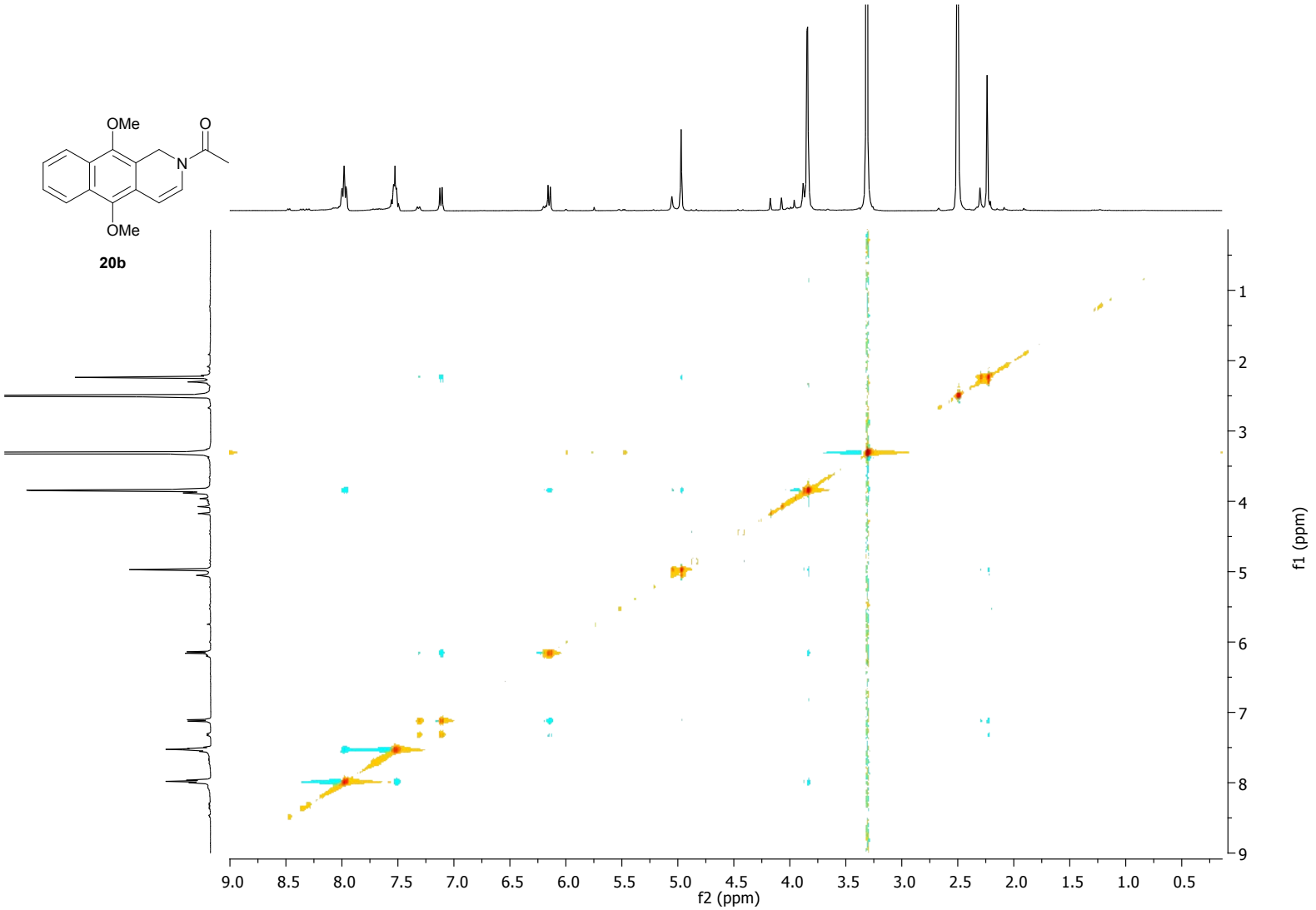


Figure 25 NOESY spectrum of 1-(5,10-dimethoxybenzo[*g*]isoquinolin-2(1*H*)-yl)ethanone (DMSO-d_6, 400 MHz).

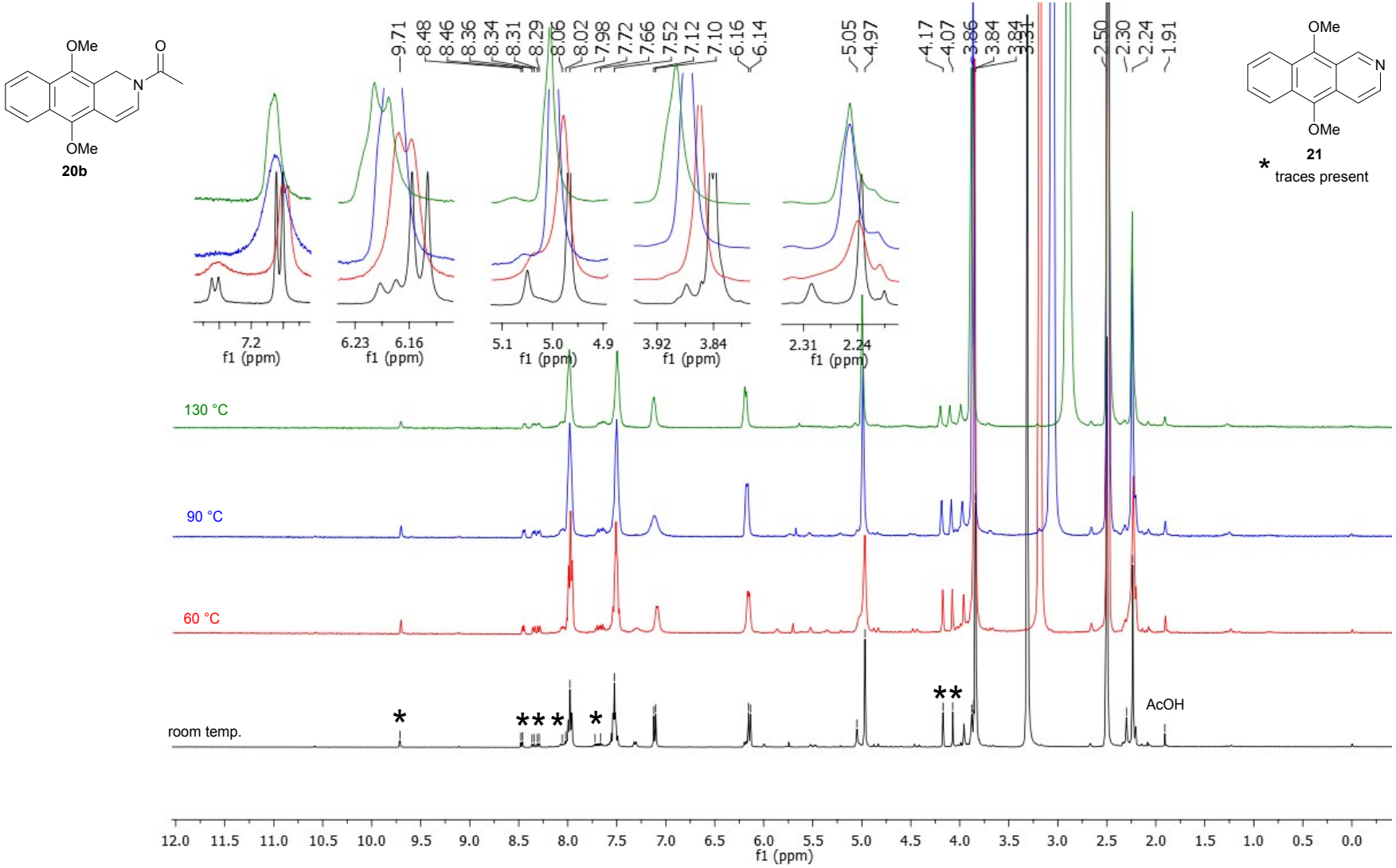


Figure 26 VT-^{1}H NMR spectrum of 1-(5,10-dimethoxybenzo[*g*]isoquinolin-2(1*H*)-yl)ethanone (**20b**) (DMSO-d_6, 400 MHz, rt-130 °C). Traces of **21** are present due to limited stability of **20b** in DMSO-d6.

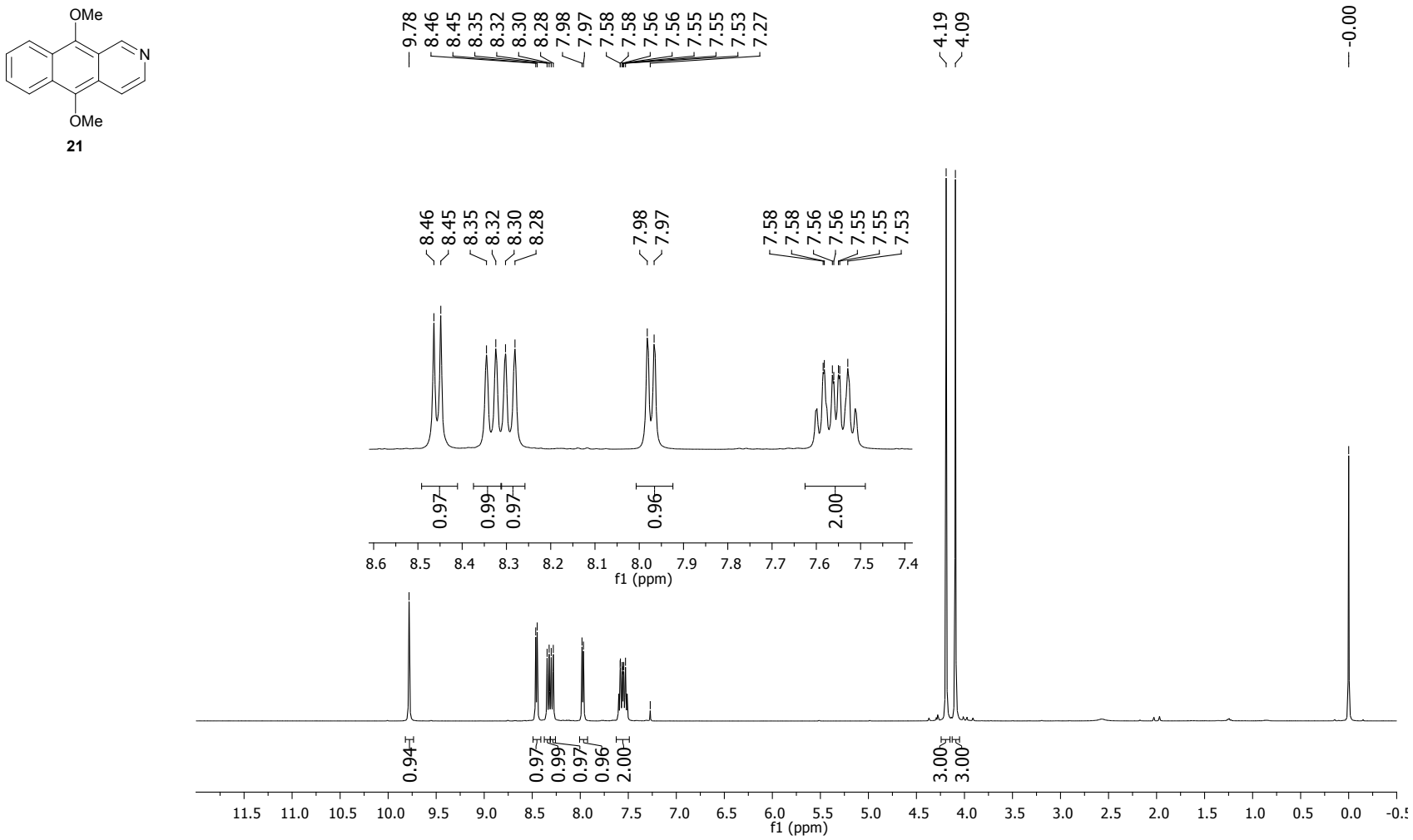


Figure 27 ^{1}H NMR spectrum of 5,10-dimethoxybenzo[*g*]isoquinoline (**21**) ($CDCl_3$, 400 MHz).

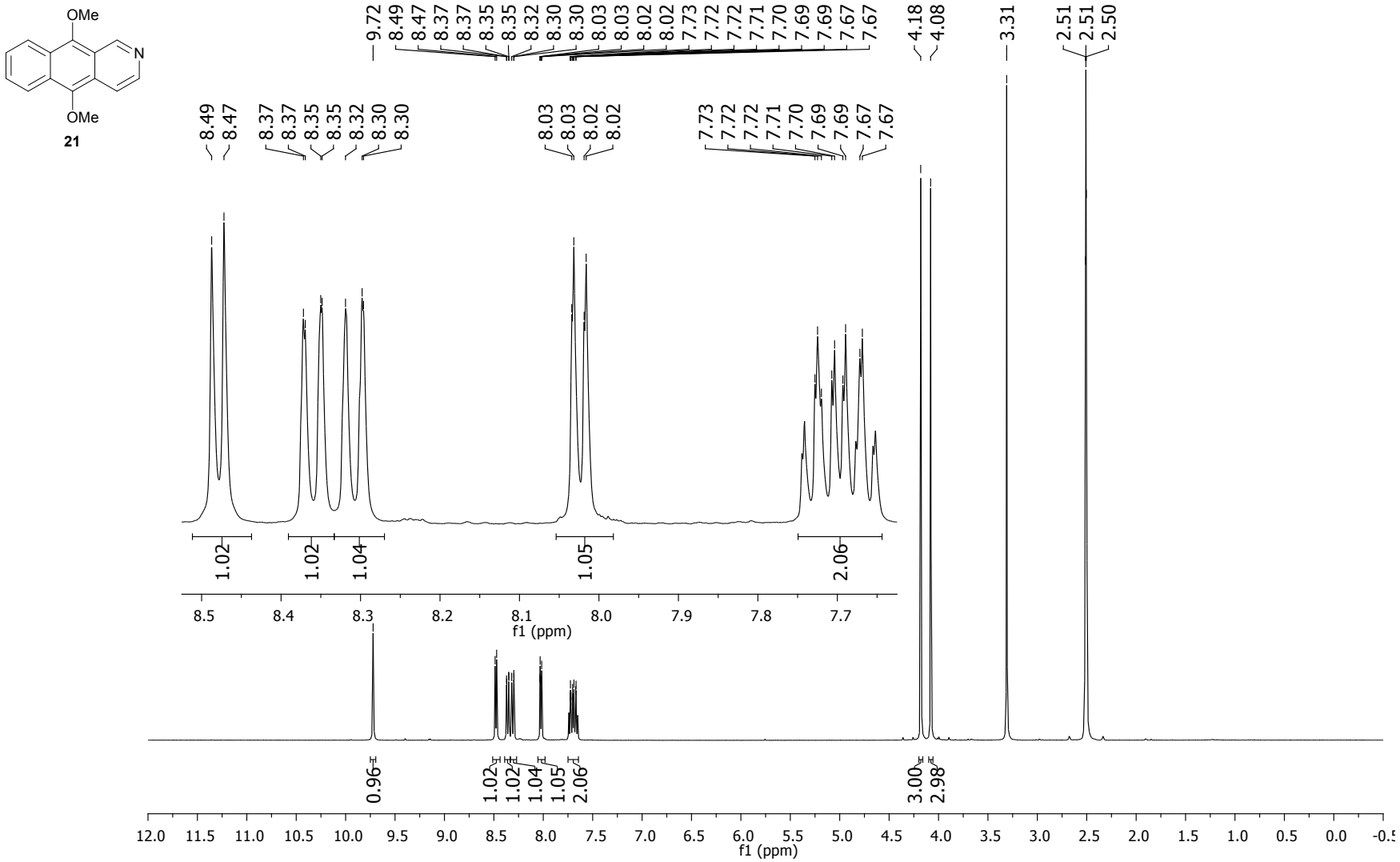


Figure 28 ^{1}H NMR spectrum of 5,10-dimethoxybenzo[*g*]isoquinoline (**21**) (DMSO-d6, 400 MHz).

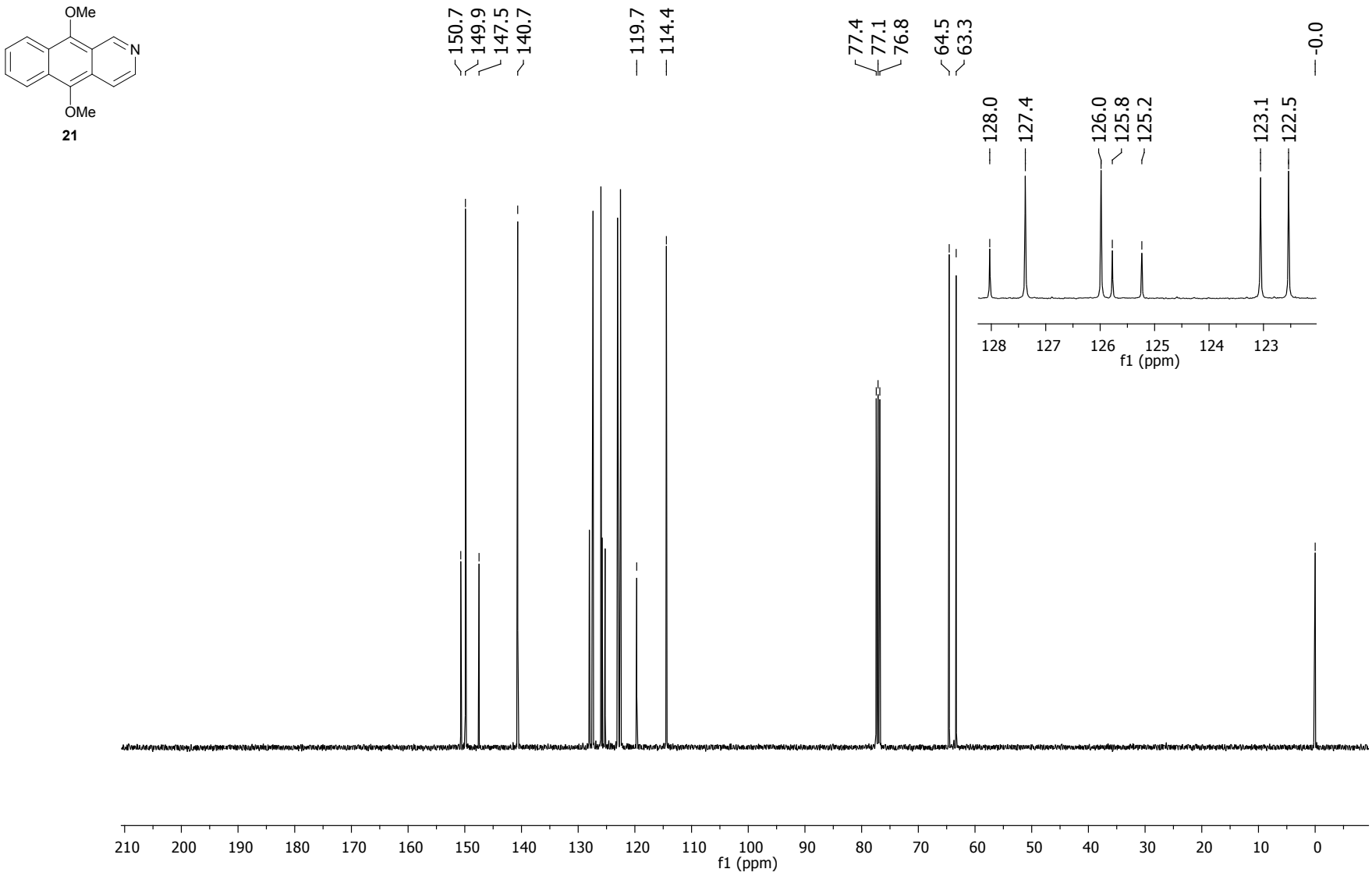


Figure 29 ^{13}C NMR spectrum of 5,10-dimethoxybenzo[*g*]isoquinoline (**21**) ($CDCl_3$, 100 MHz).

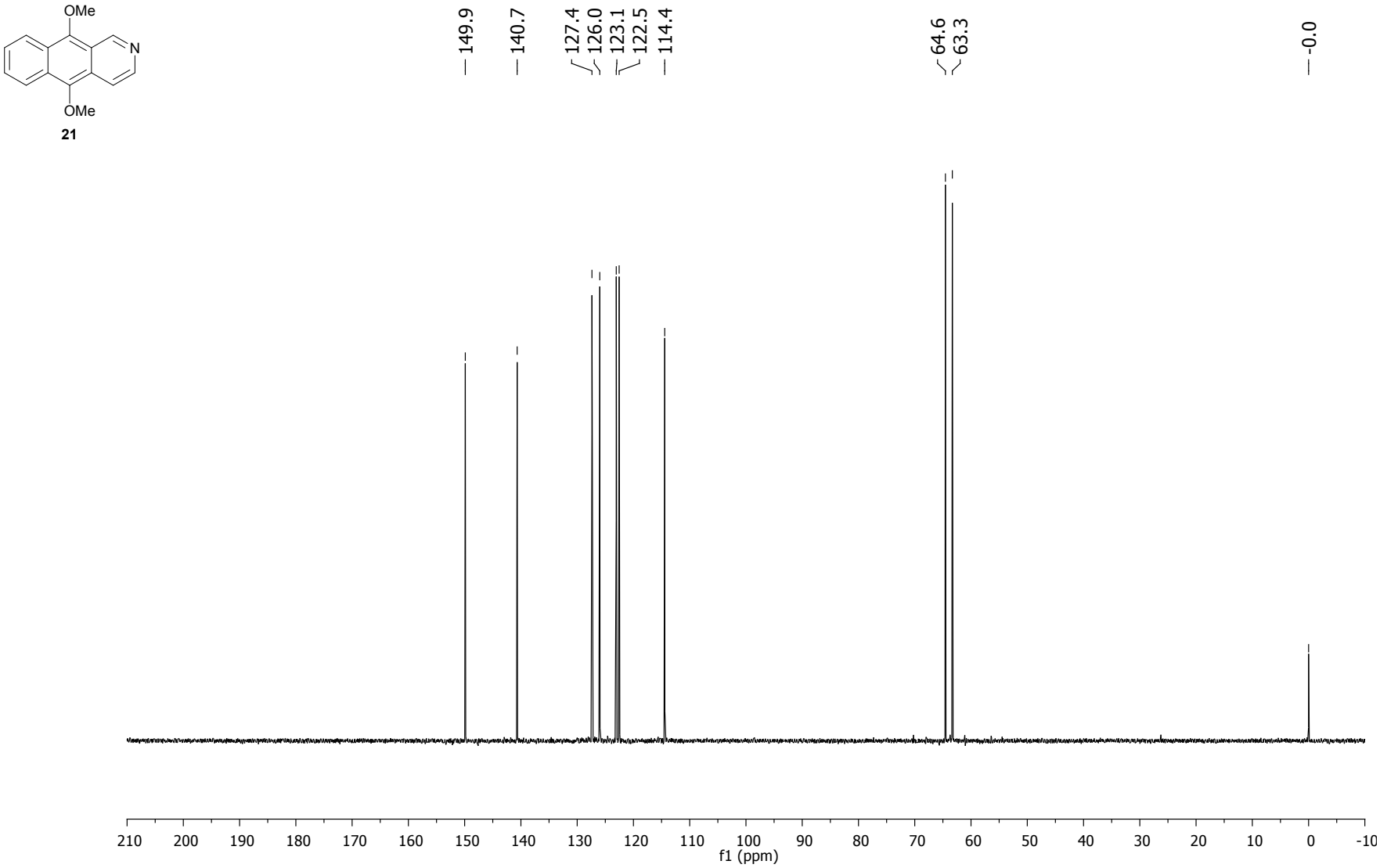


Figure 30 DEPT-135 spectrum of 5,10-dimethoxybenzo[*g*]isoquinoline (**21**) ($CDCl_3$, 100 MHz).

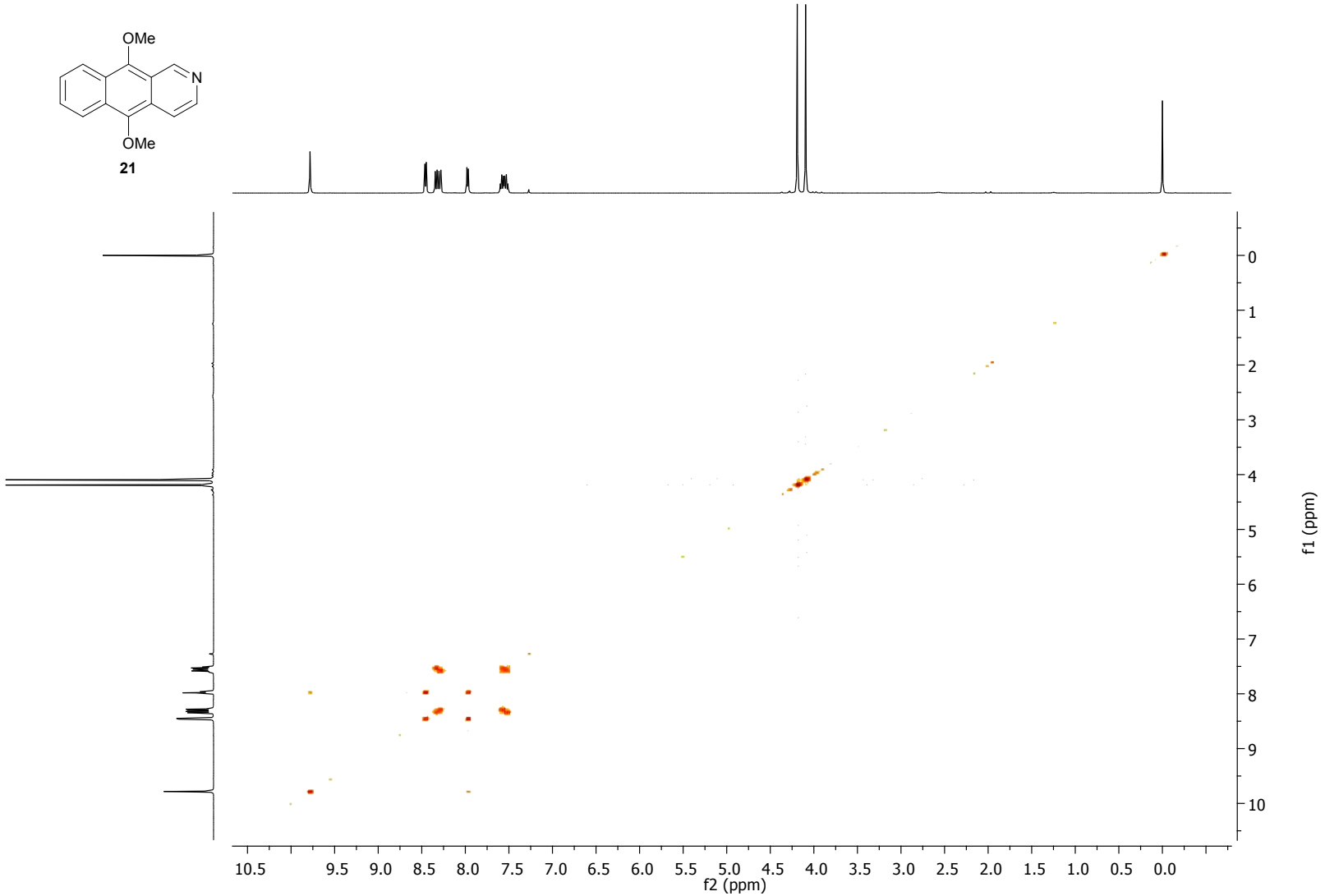


Figure 31 COSY spectrum of 5,10-dimethoxybenzo[*g*]isoquinoline (**21**) ($CDCl_3$, 400 MHz).

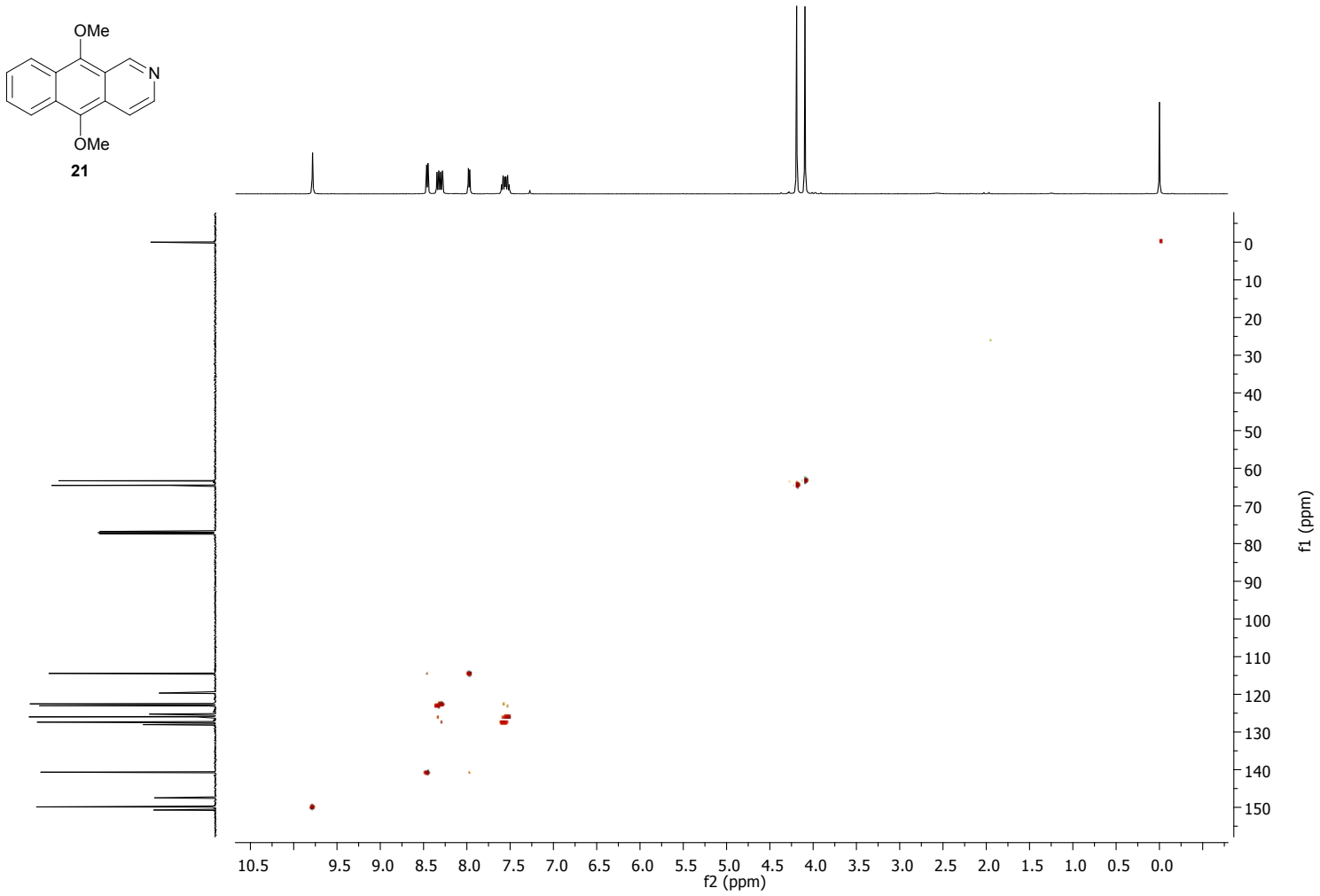


Figure 32 HSQC spectrum of 5,10-dimethoxybenzo[*g*]isoquinoline (**21**) ($CDCl_3$, 400 MHz).

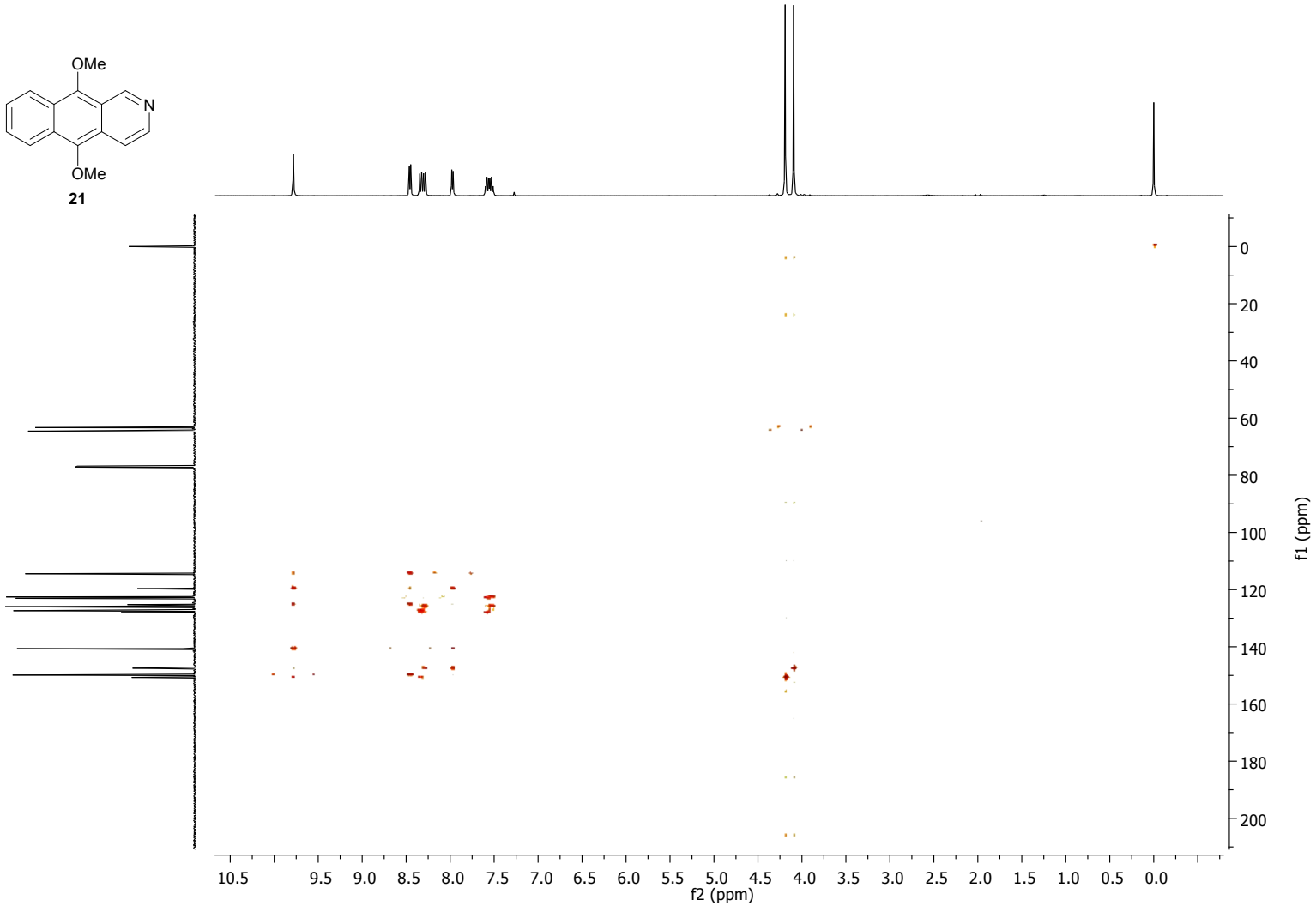


Figure 33 HMBC spectrum of 5,10-dimethoxybenzo[*g*]isoquinoline (**21**) ($CDCl_3$, 400 MHz).

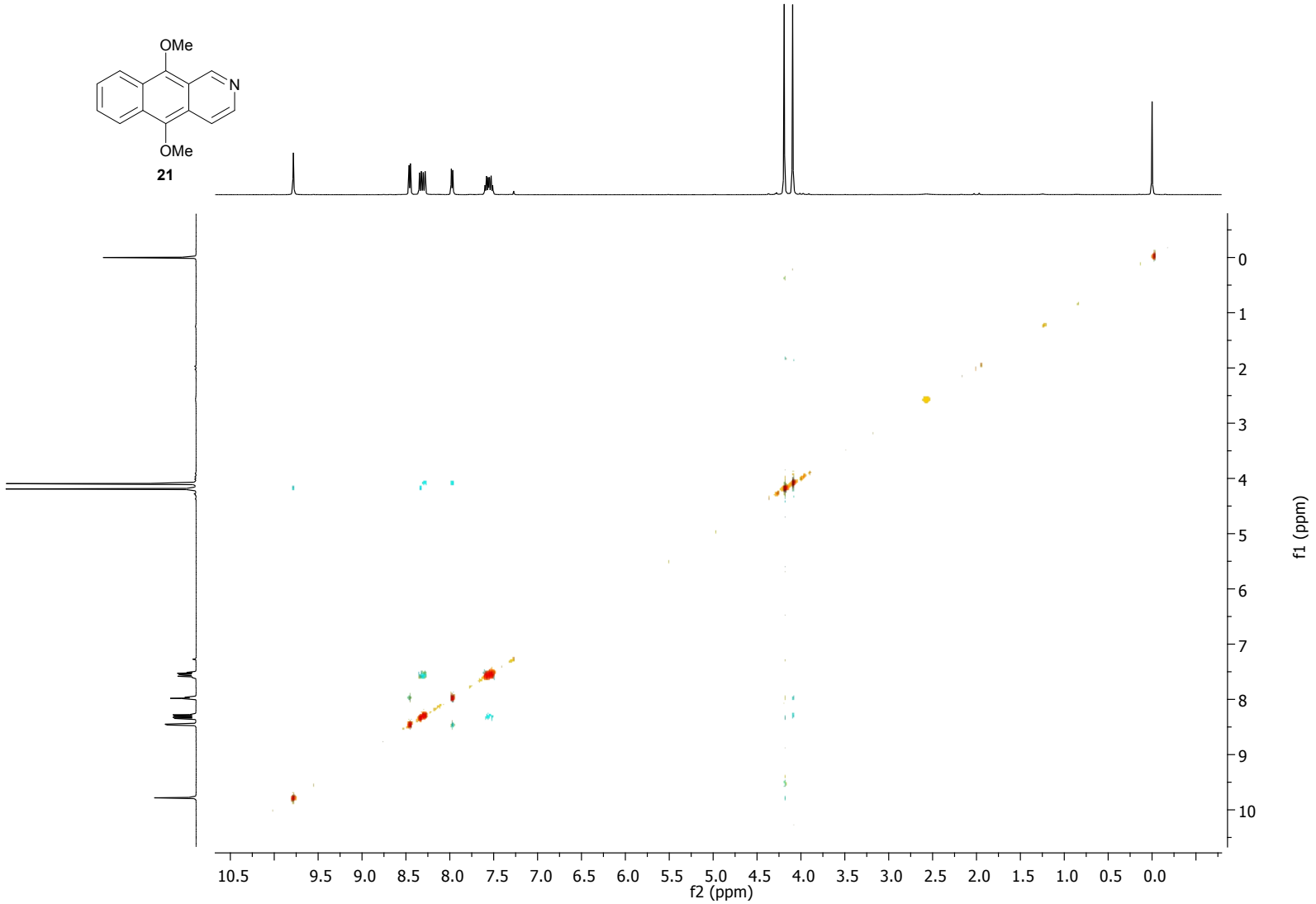


Figure 34 NOESY spectrum of 5,10-dimethoxybenzo[*g*]isoquinoline (**21**) ($CDCl_3$, 400 MHz).

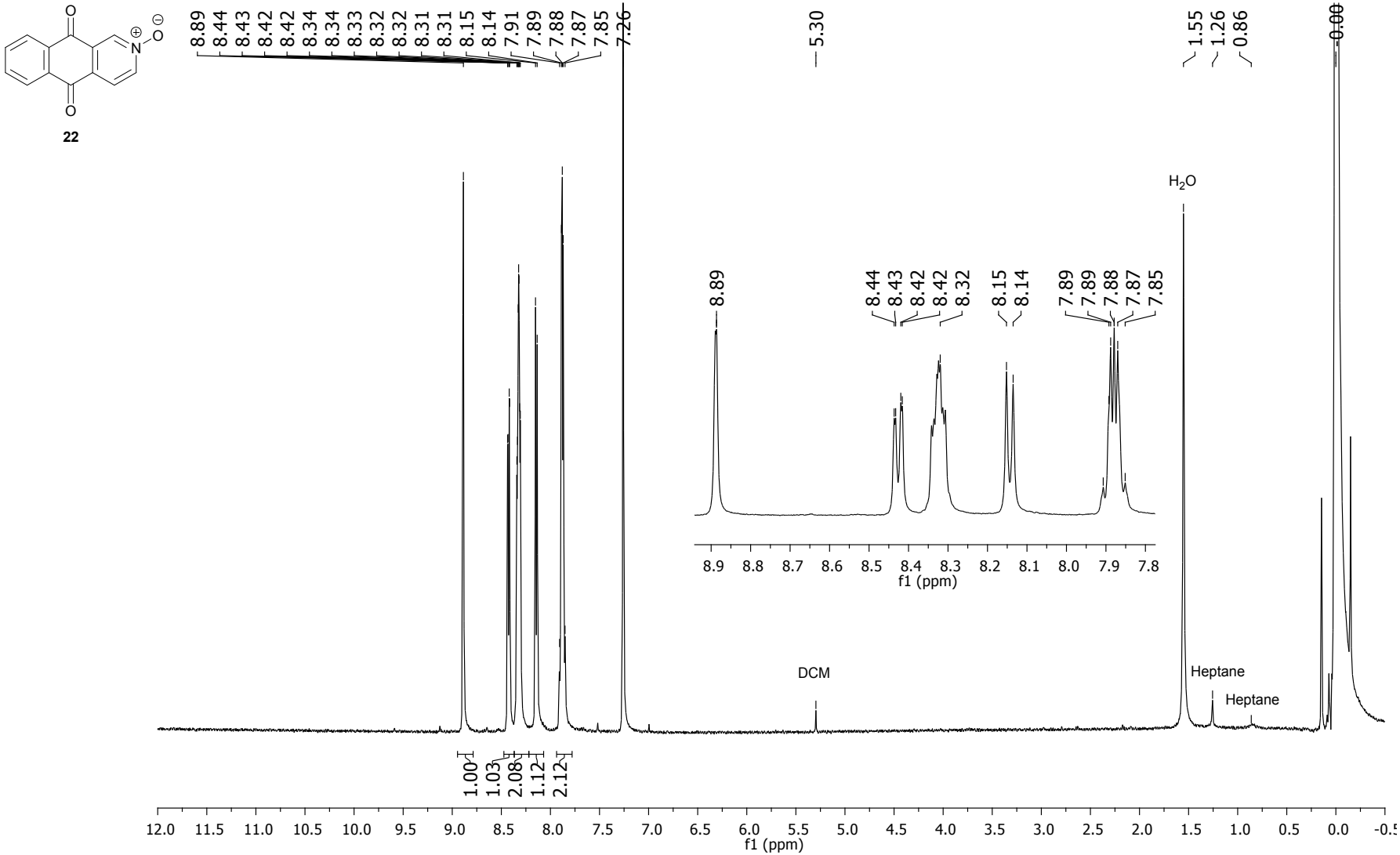


Figure 35 ^{1}H NMR spectrum of 5,10-dioxo-5,10-dihydrobenzo[*g*]isoquinoline 2-oxide (**22**) ($CDCl_3$, 400 MHz).

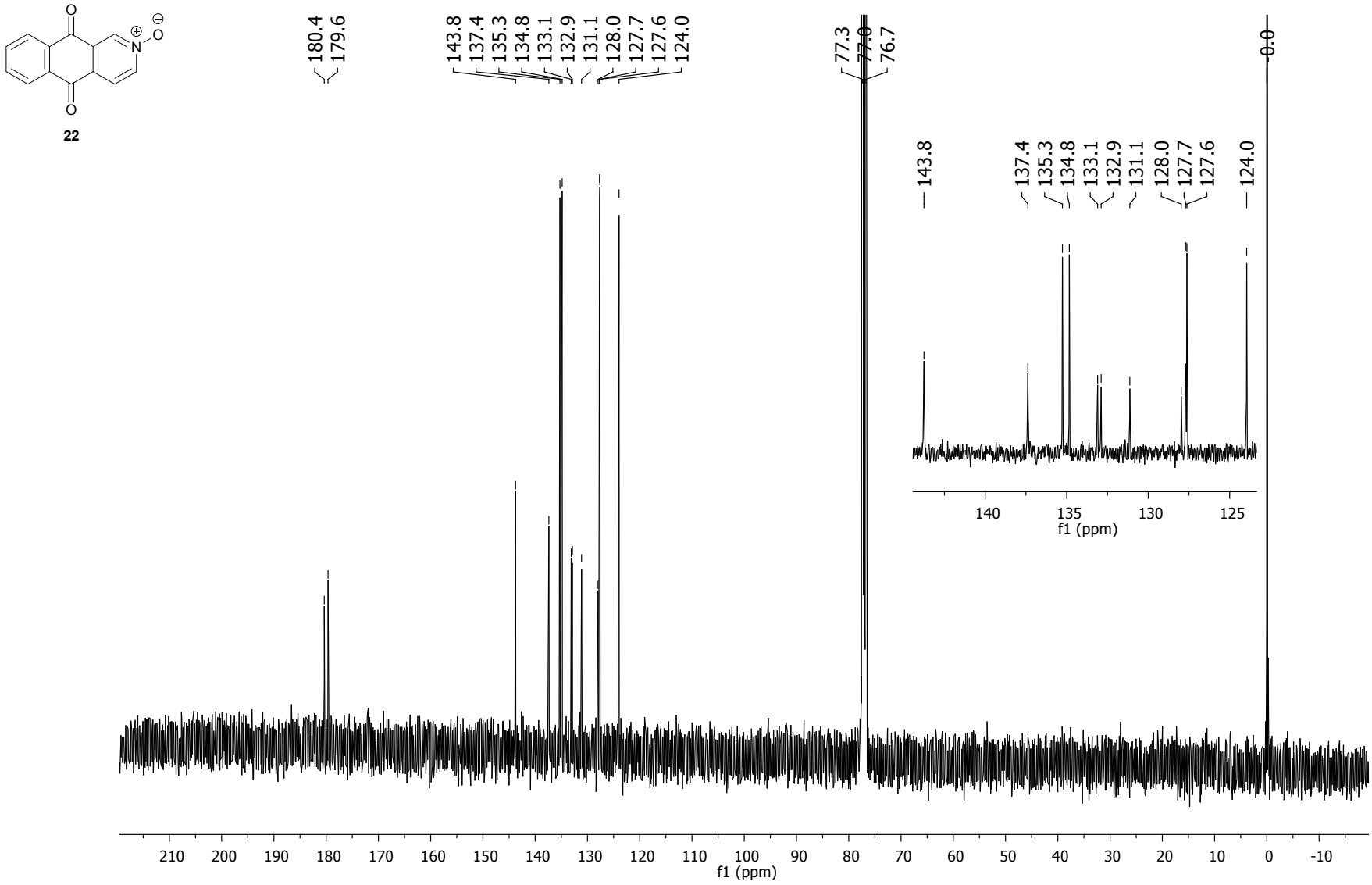


Figure 36 ^{13}C NMR spectrum of 5,10-dioxo-5,10-dihydrobenzo[*g*]isoquinoline 2-oxide (**22**) ($CDCl_3$, 400 MHz).

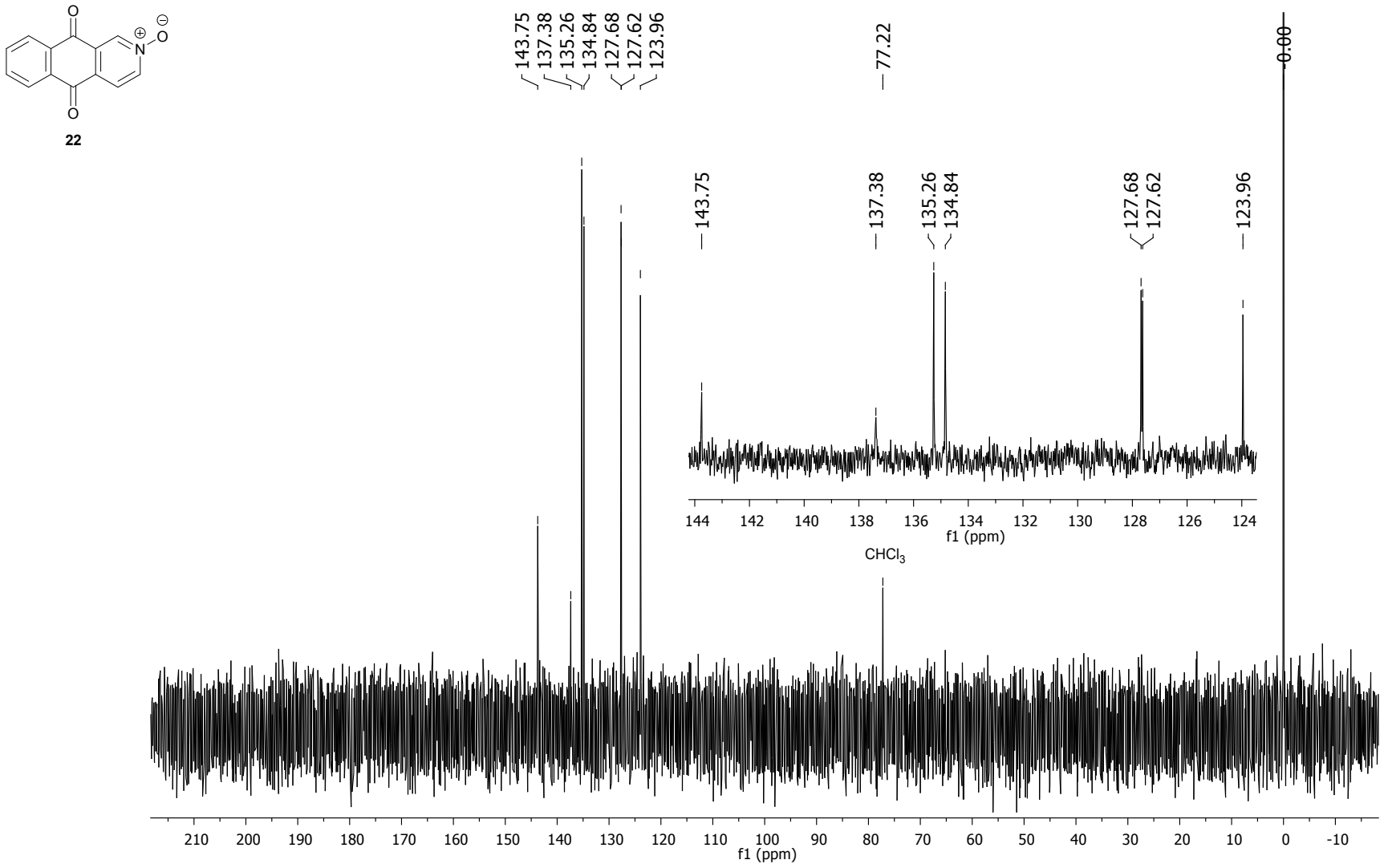


Figure 37 DEPT-135 spectrum of 5,10-dioxo-5,10-dihydrobenzo[*g*]isoquinoline 2-oxide (**22**) ($CDCl_3$, 100 MHz).

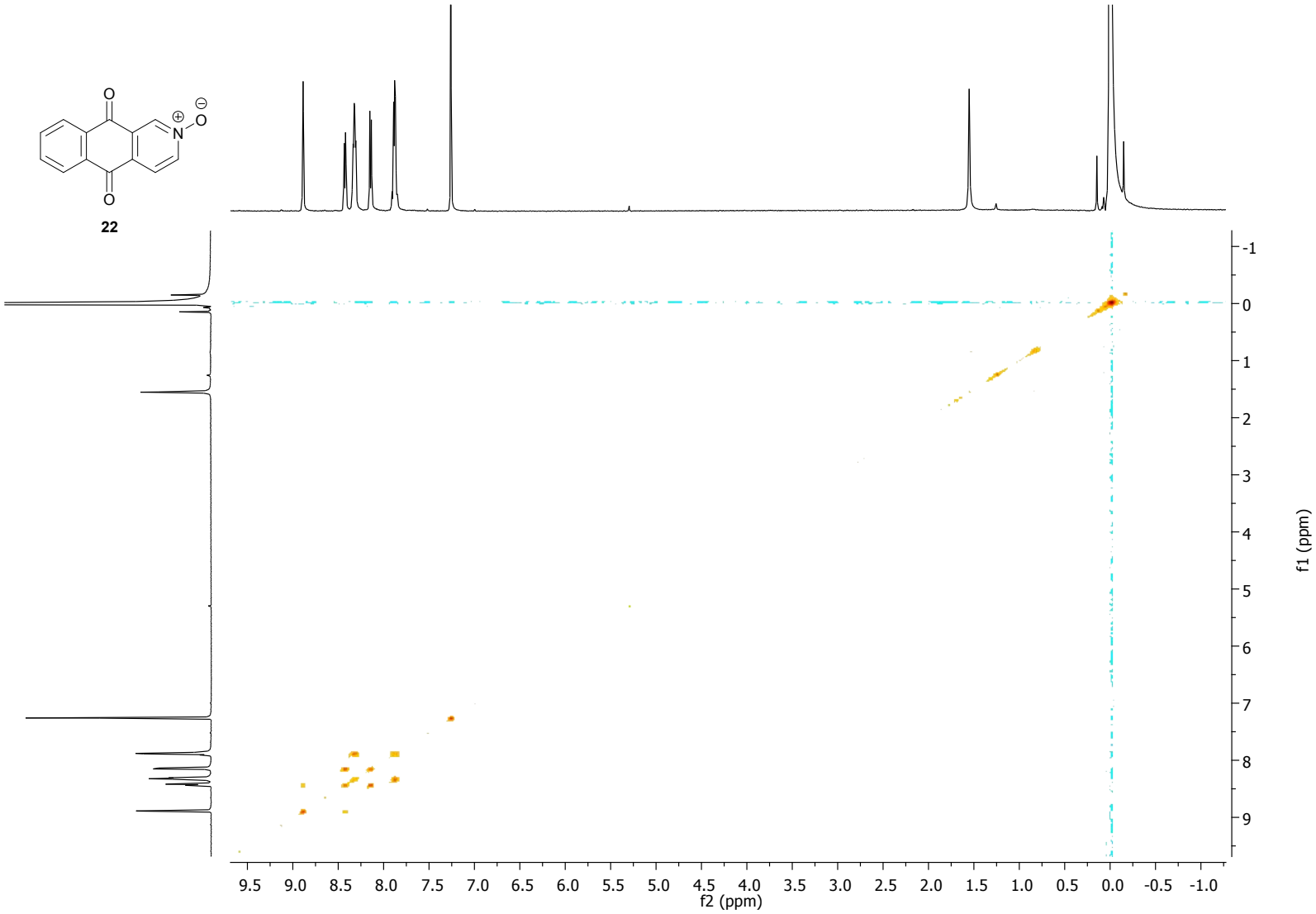


Figure 38 COSY spectrum of 5,10-dioxo-5,10-dihydrobenzo[*g*]isoquinoline 2-oxide (**22**) ($CDCl_3$, 400 MHz).

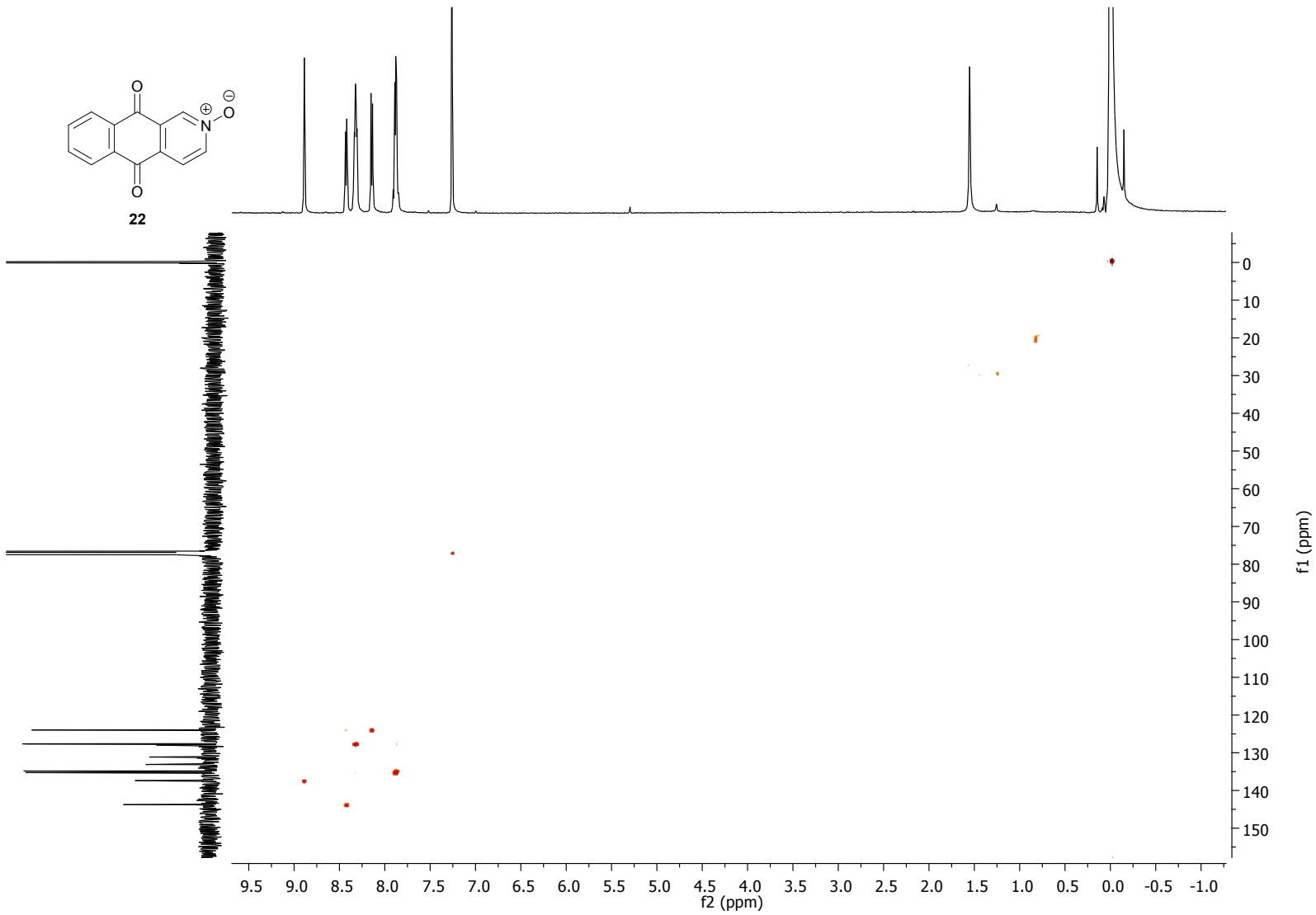


Figure 39 HSQC spectrum of 5,10-dioxo-5,10-dihydrobenzo[*g*]isoquinoline 2-oxide (**22**) ($CDCl_3$, 400 MHz).

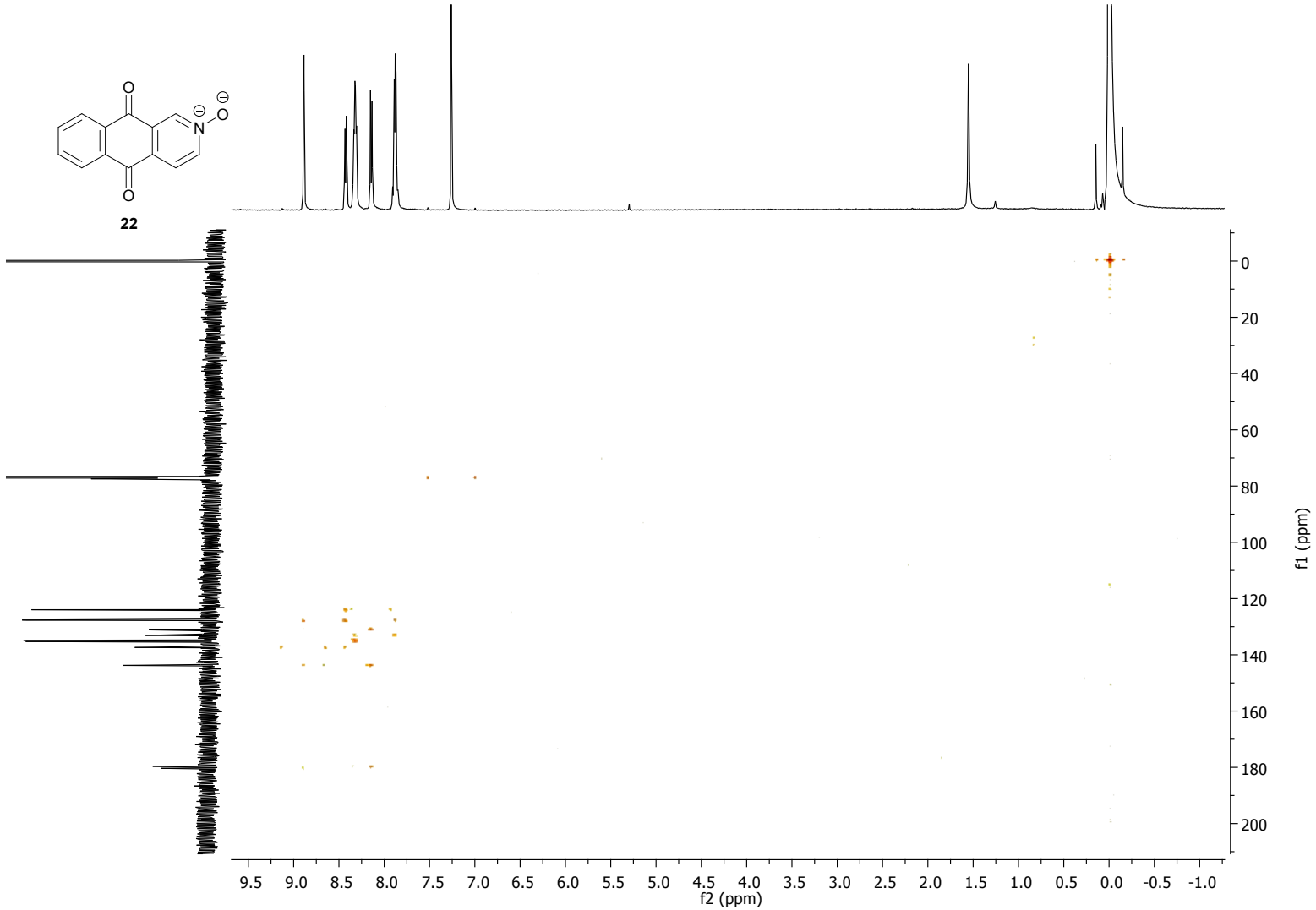


Figure 40 HMBC spectrum of 5,10-dioxo-5,10-dihydrobenzo[*g*]isoquinoline 2-oxide (**22**) ($CDCl_3$, 400 MHz).

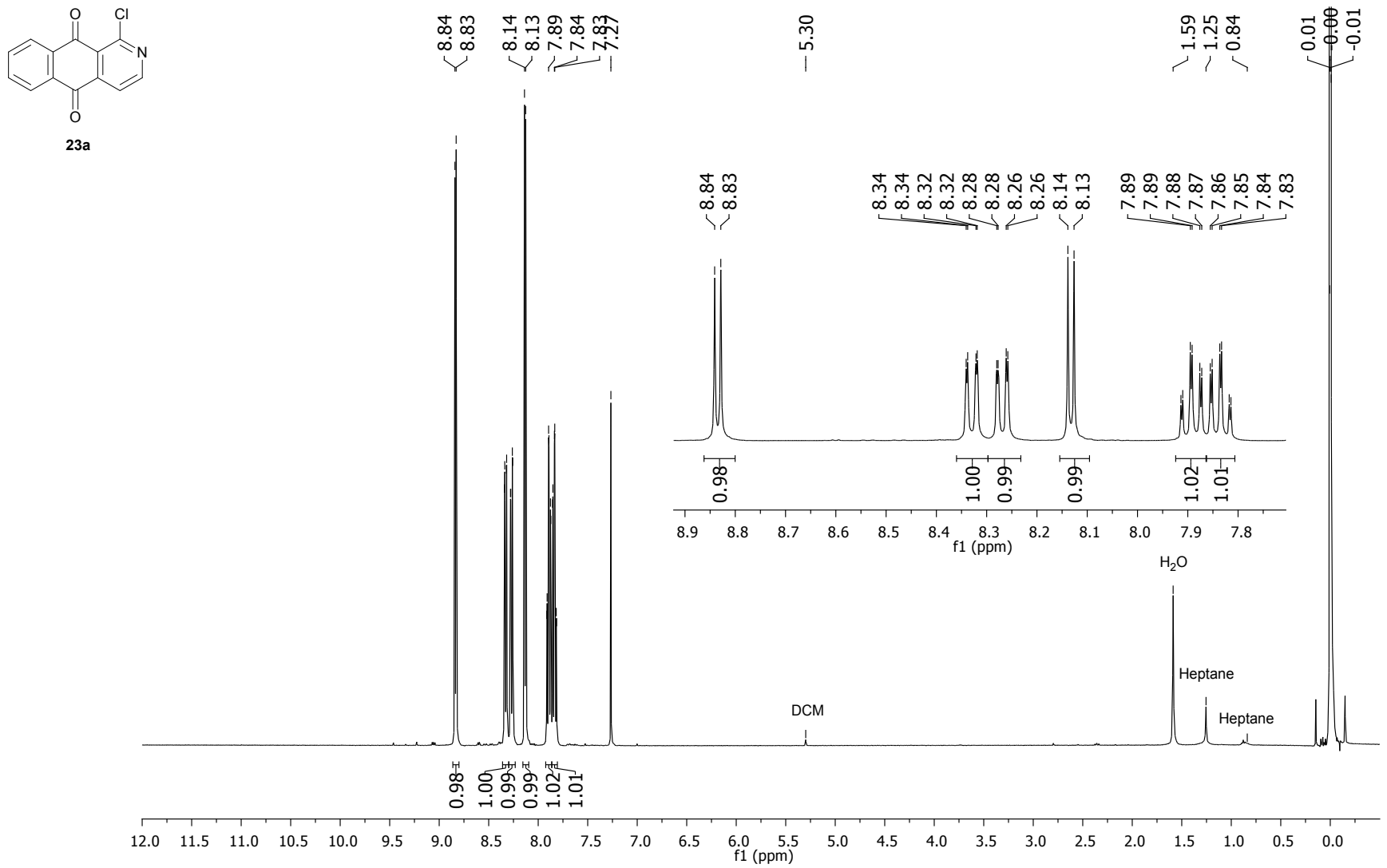


Figure 41 ^{1}H NMR spectrum of 1-chlorobenzo[*g*]isoquinoline-5,10-dione (**23a**) ($CDCl_3$, 400 MHz).

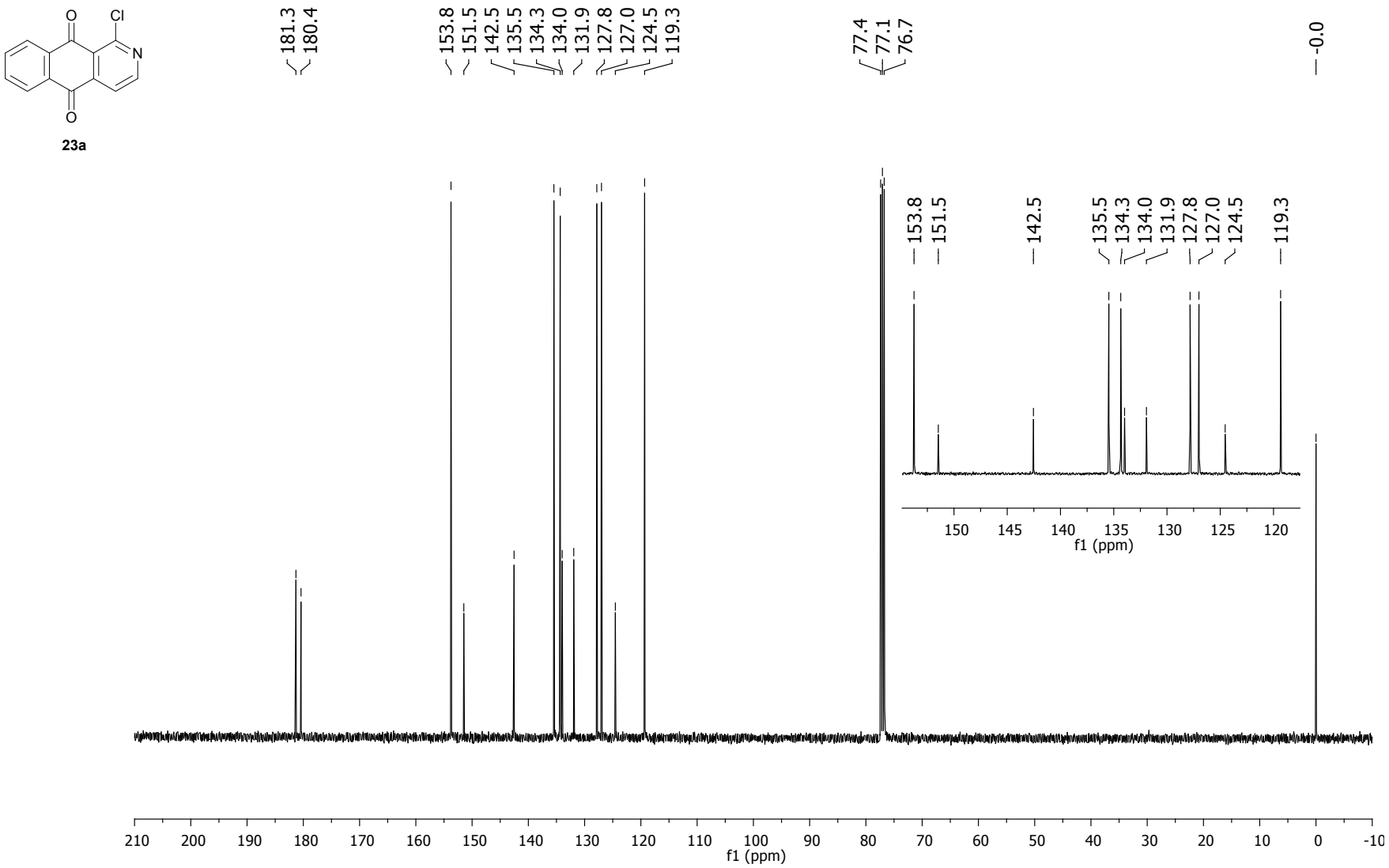


Figure 42^{13}C NMR spectrum of 1-chlorobenzo[*g*]isoquinoline-5,10-dione (**23a**) ($CDCl_3$, 100 MHz).

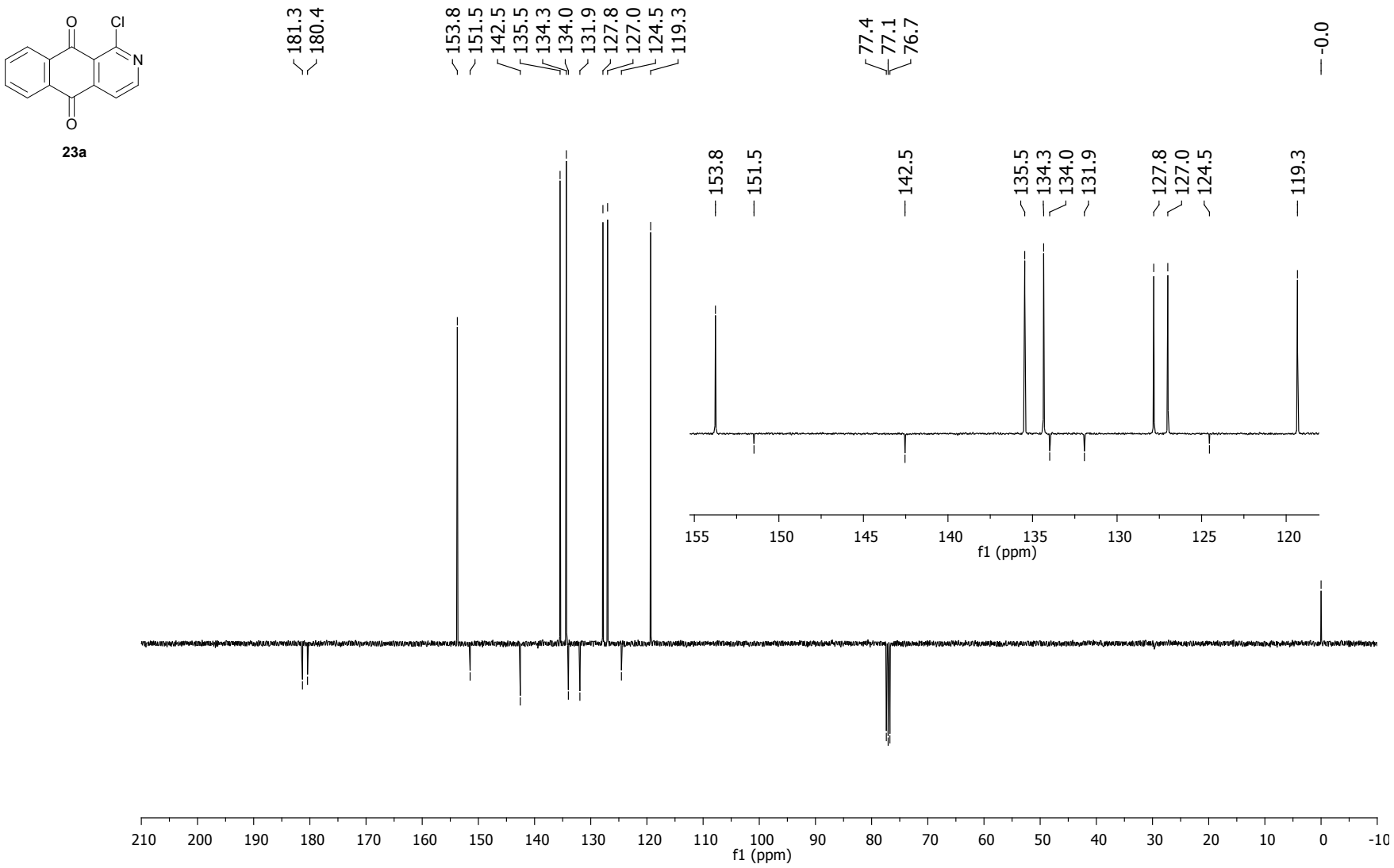


Figure 43 APT spectrum of 1-chlorobenzo[*g*]isoquinoline-5,10-dione (**23a**) ($CDCl_3$, 100 MHz).

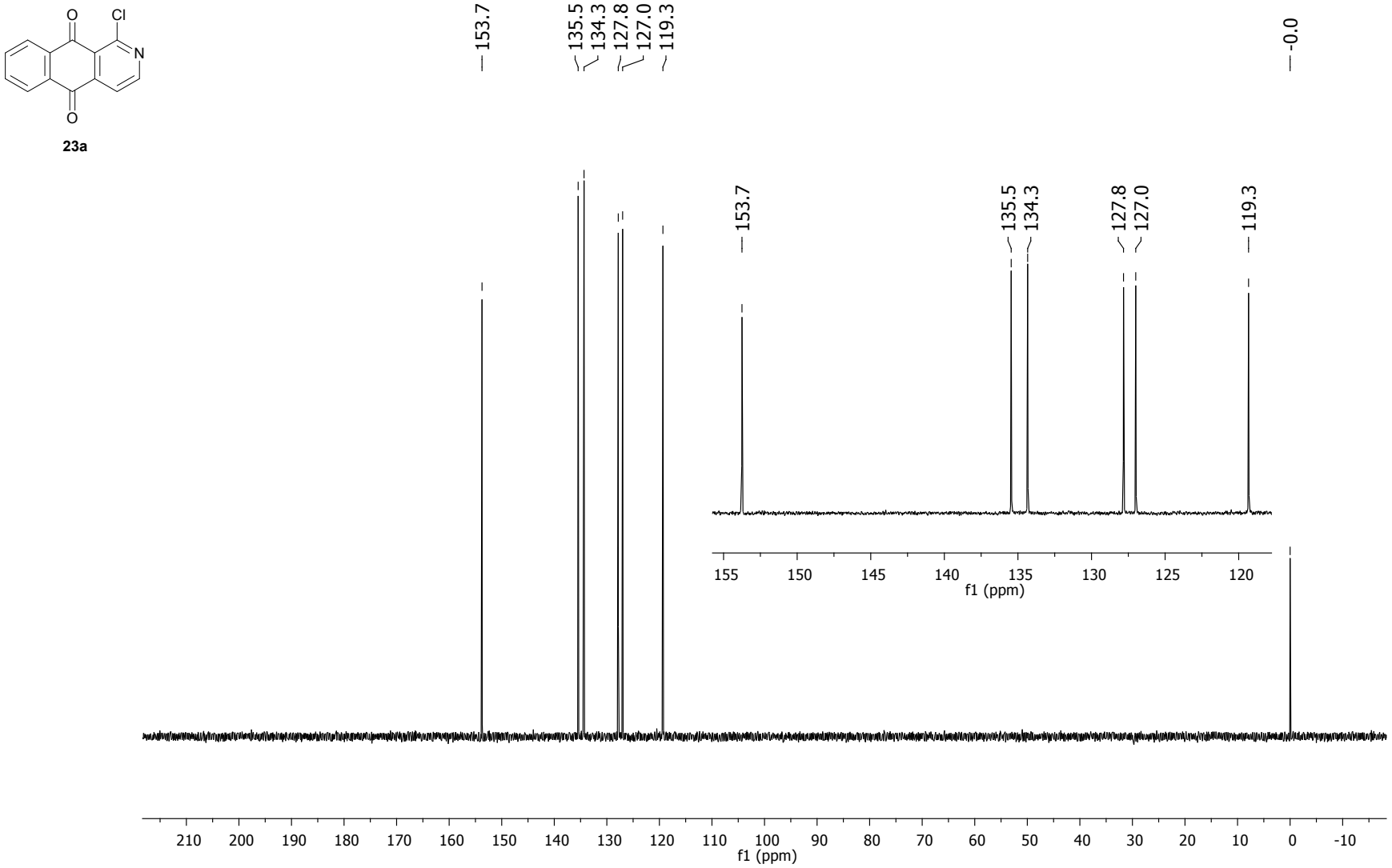


Figure 44 DEPT 135 spectrum of 1-chlorobenzo[*g*]isoquinoline-5,10-dione (**23a**) ($CDCl_3$, 100 MHz).

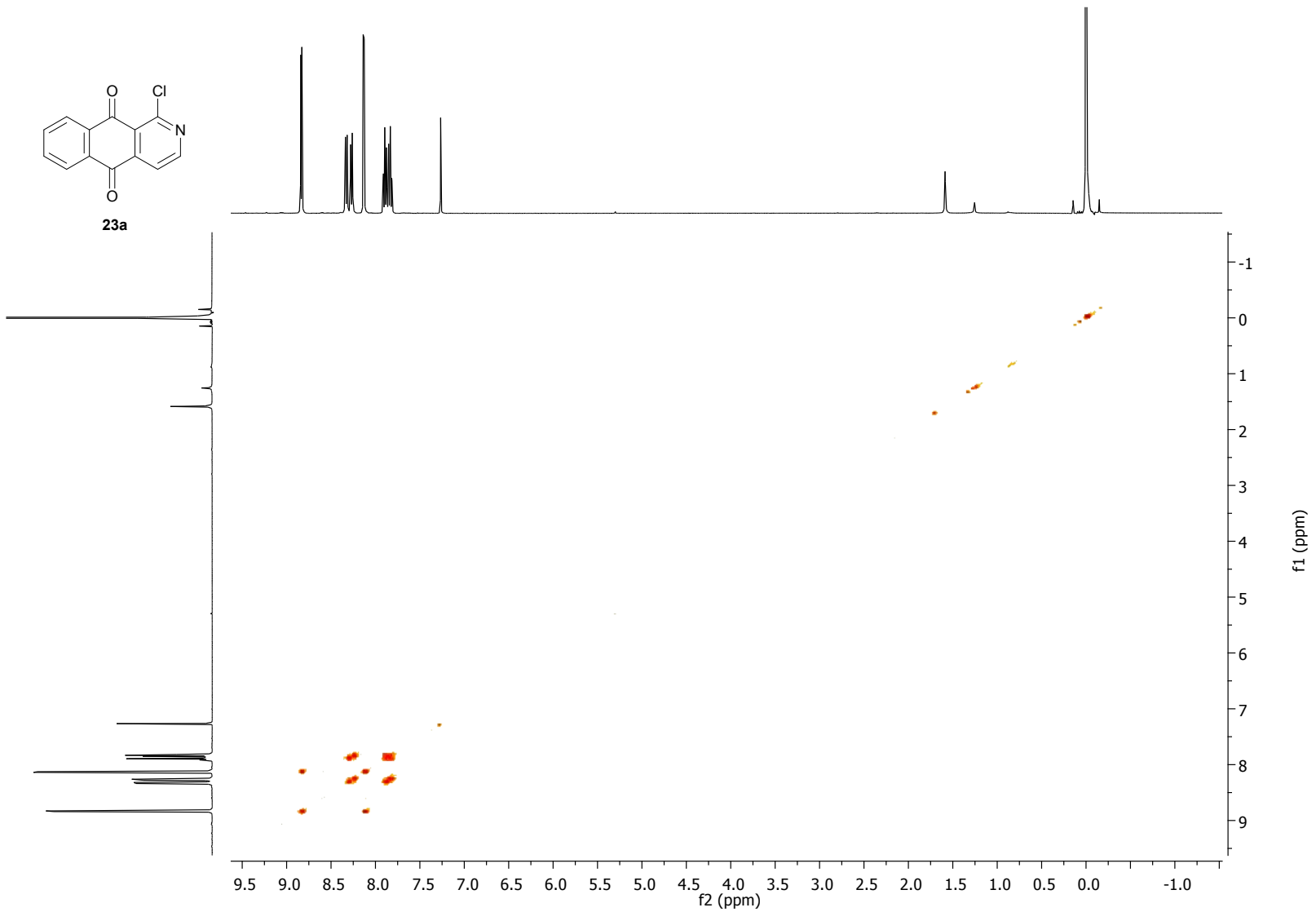


Figure 45 COSY spectrum of 1-chlorobenzo[*g*]isoquinoline-5,10-dione (**23a**) ($CDCl_3$, 400 MHz).

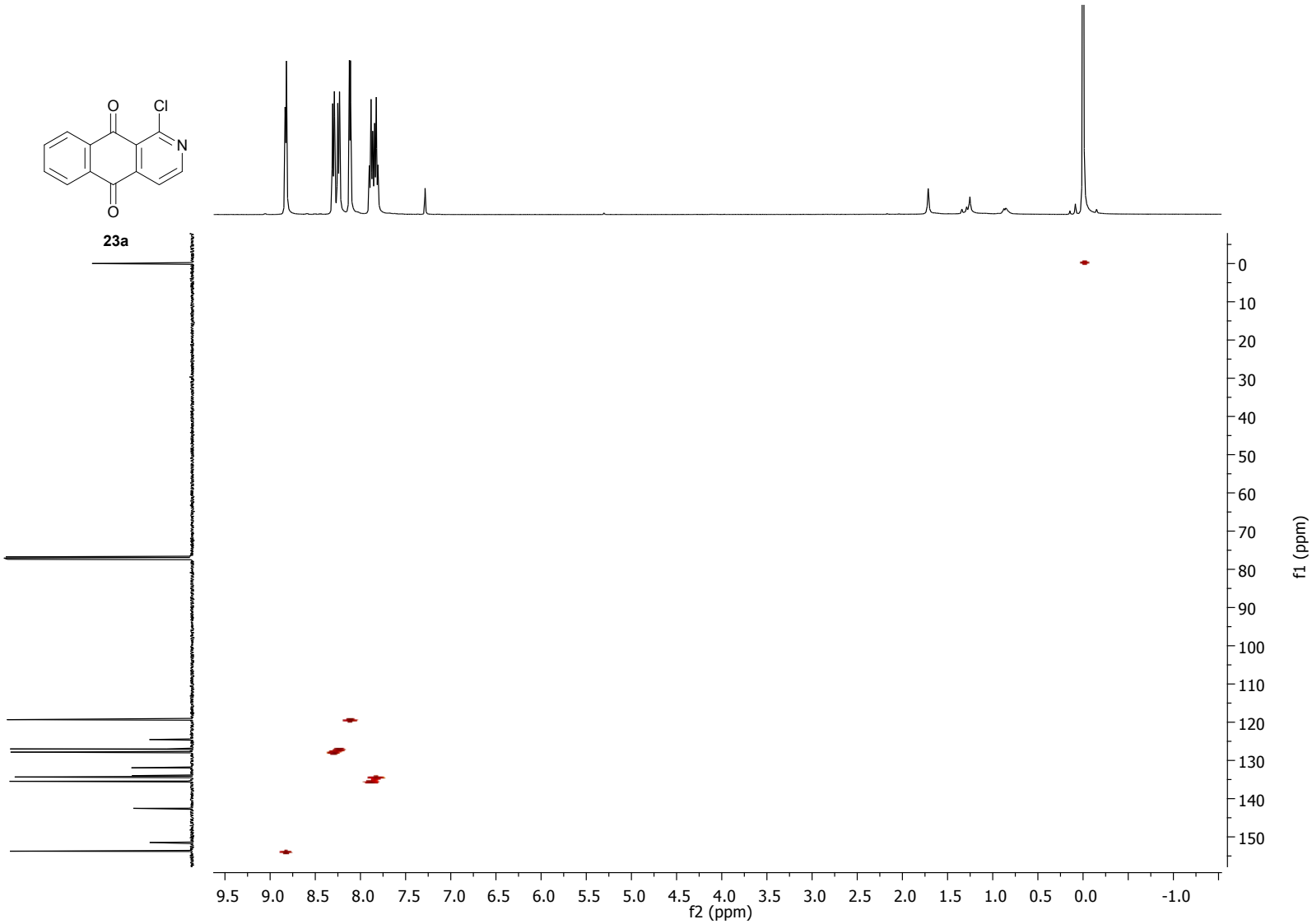


Figure 46 HSQC spectrum of 1-chlorobenzo[*g*]isoquinoline-5,10-dione (**23a**) ($CDCl_3$, 400 MHz).

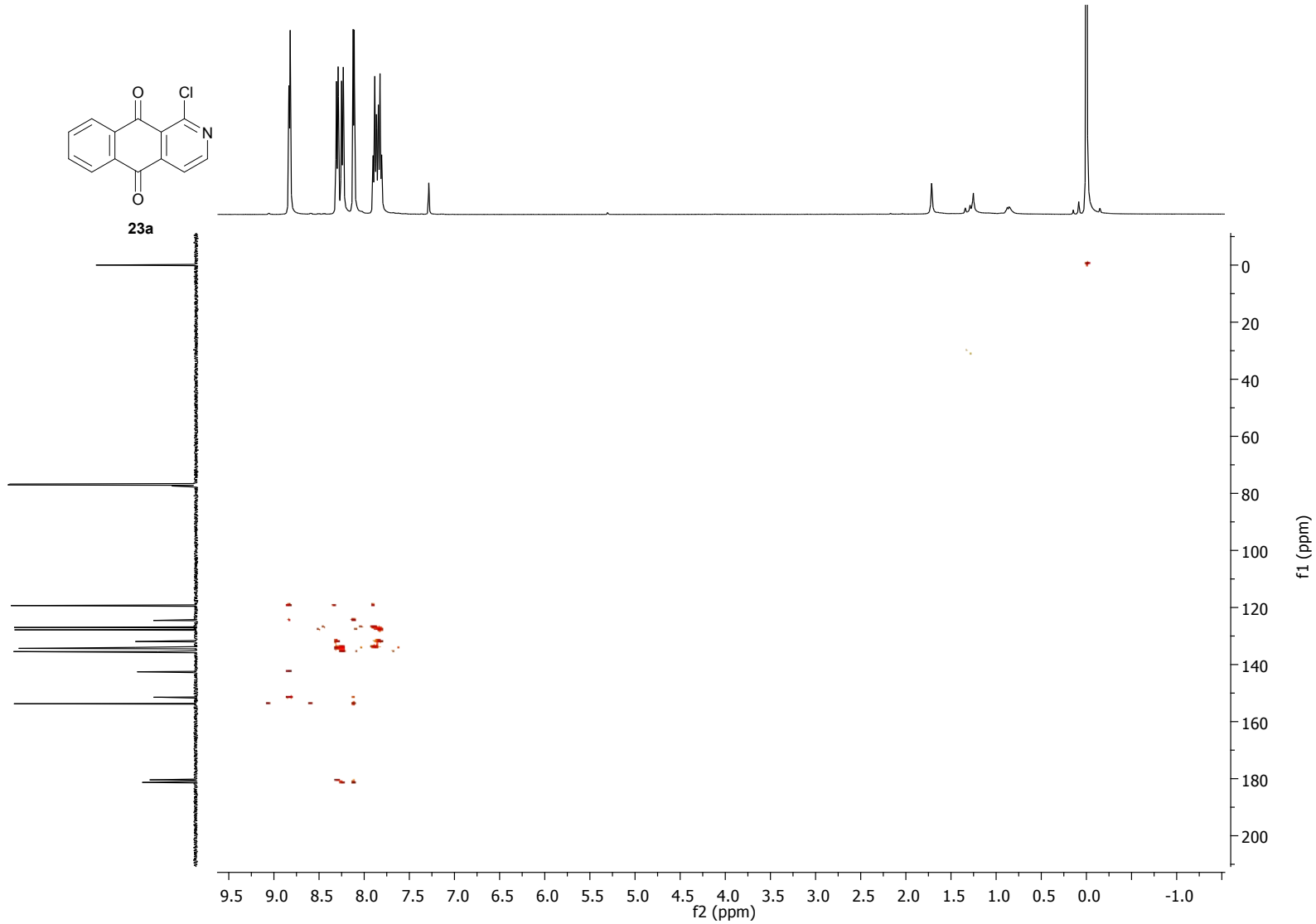


Figure 47 HMBC spectrum of 1-chlorobenzo[*g*]isoquinoline-5,10-dione (**23a**) ($CDCl_3$, 400 MHz).

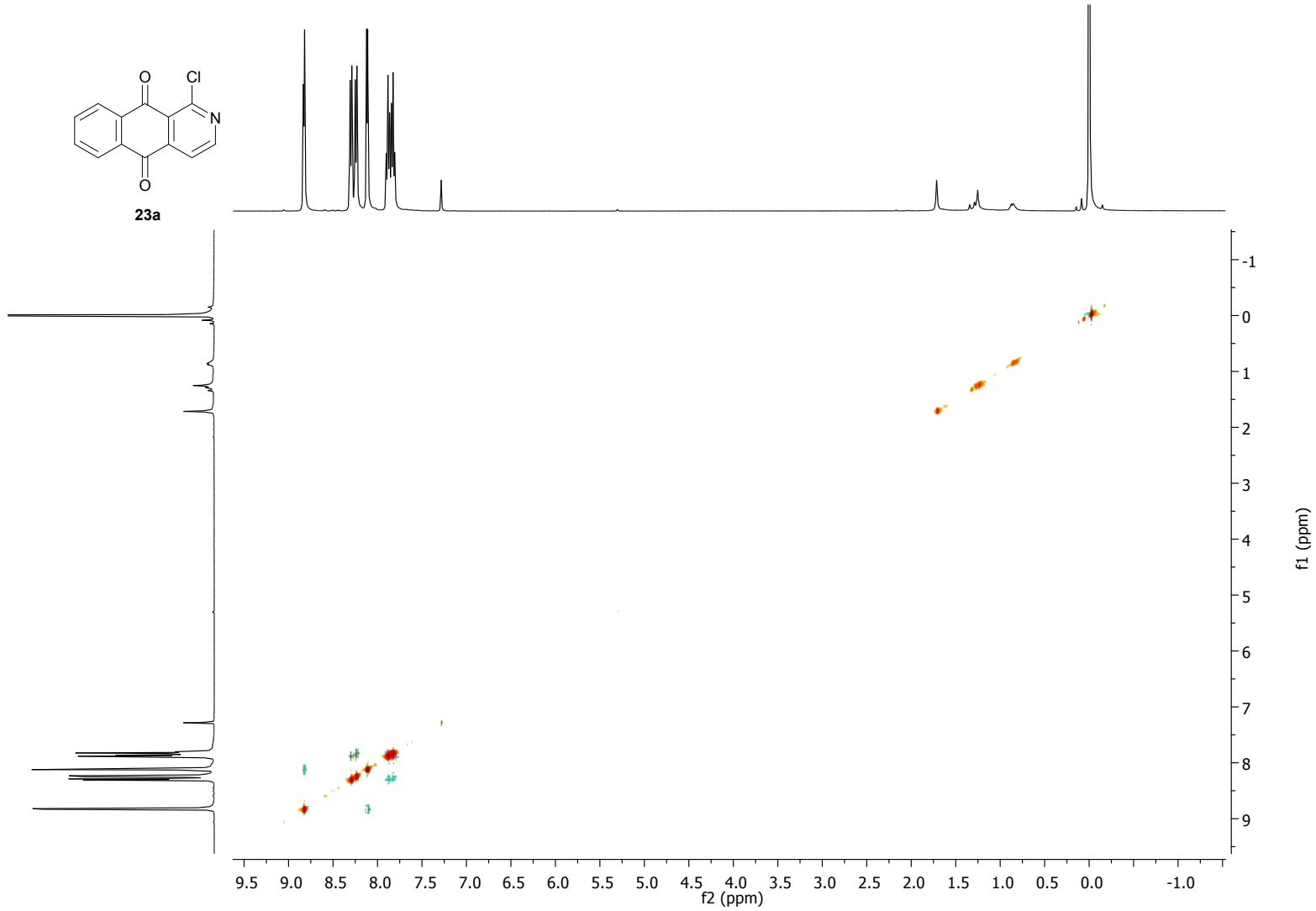


Figure 48 NOESY spectrum of 1-chlorobenzo[*g*]isoquinoline-5,10-dione (**23a**) ($CDCl_3$, 400 MHz).

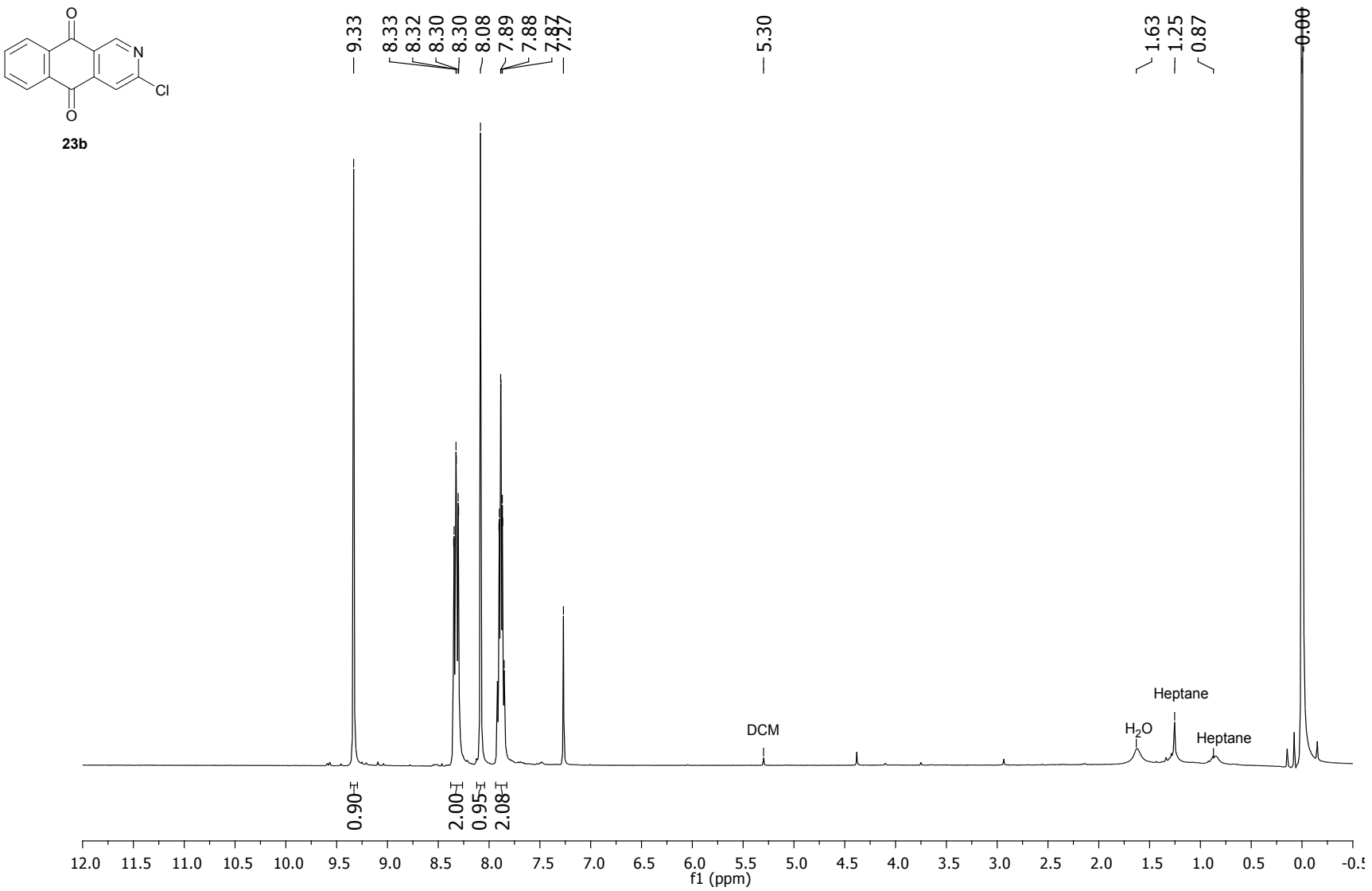


Figure 49^{1}H NMR spectrum of 3-chlorobenzo[*g*]isoquinoline-5,10-dione (**23b**) ($CDCl_3$, 400 MHz).

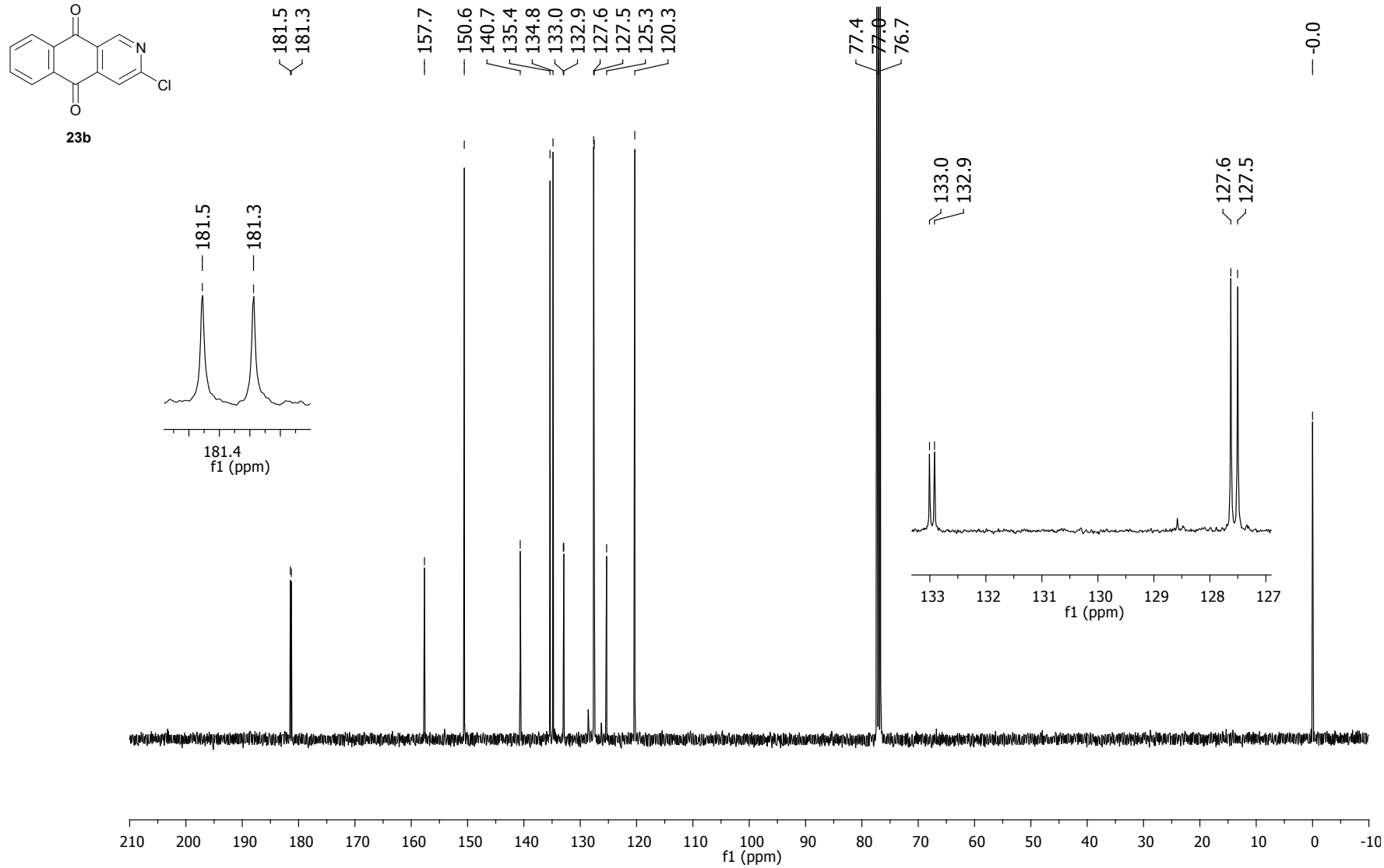


Figure 50 ^{13}C NMR spectrum of 3-chlorobenzo[*g*]isoquinoline-5,10-dione (**23b**) ($CDCl_3$, 100 MHz).

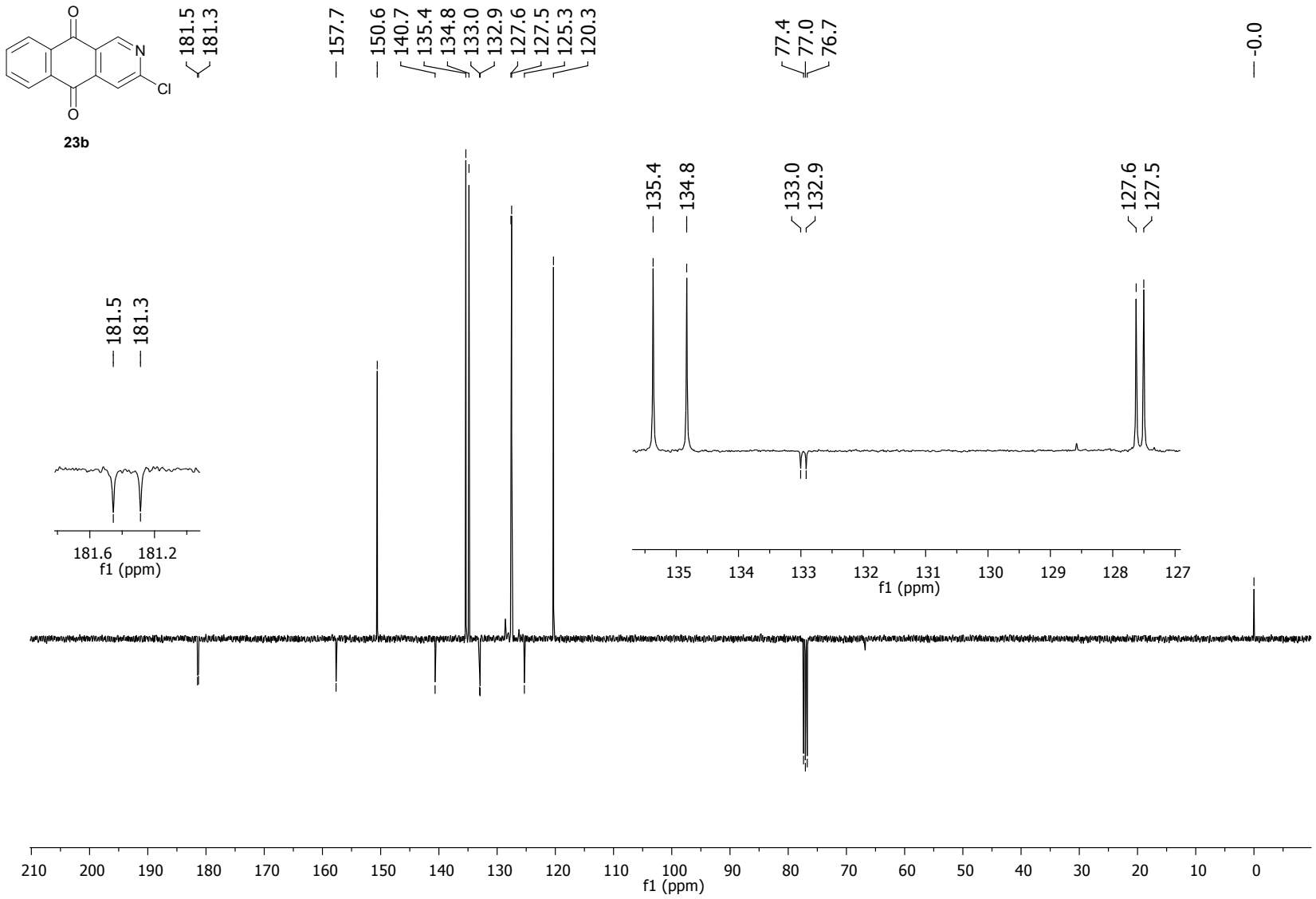


Figure 51 APT spectrum of 3-chlorobenzo[*g*]isoquinoline-5,10-dione (**23b**) ($CDCl_3$, 100 MHz).

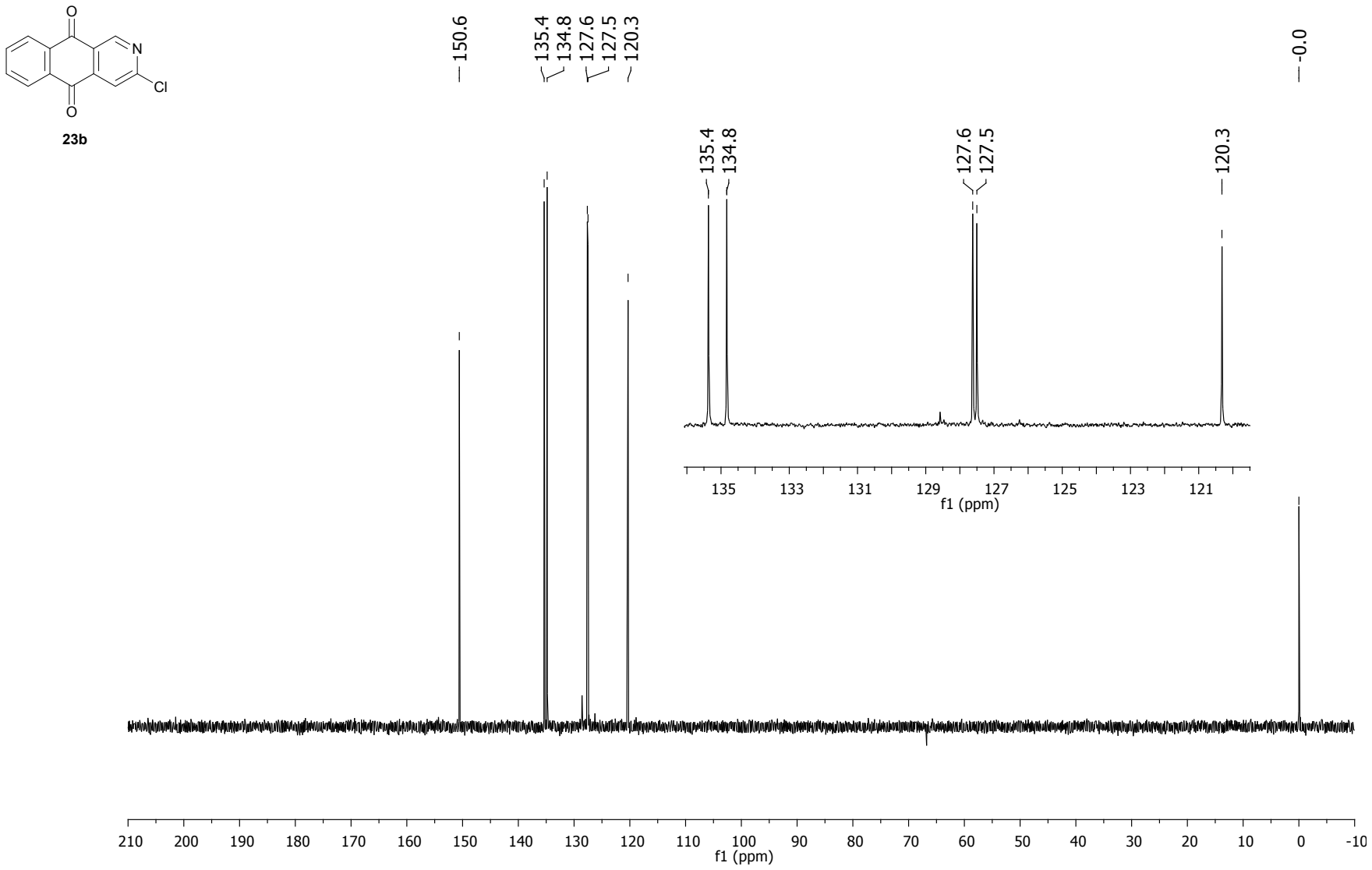


Figure 52 DEPT 135 spectrum of 3-chlorobenzo[*g*]isoquinoline-5,10-dione (**23b**) ($CDCl_3$, 100 MHz).

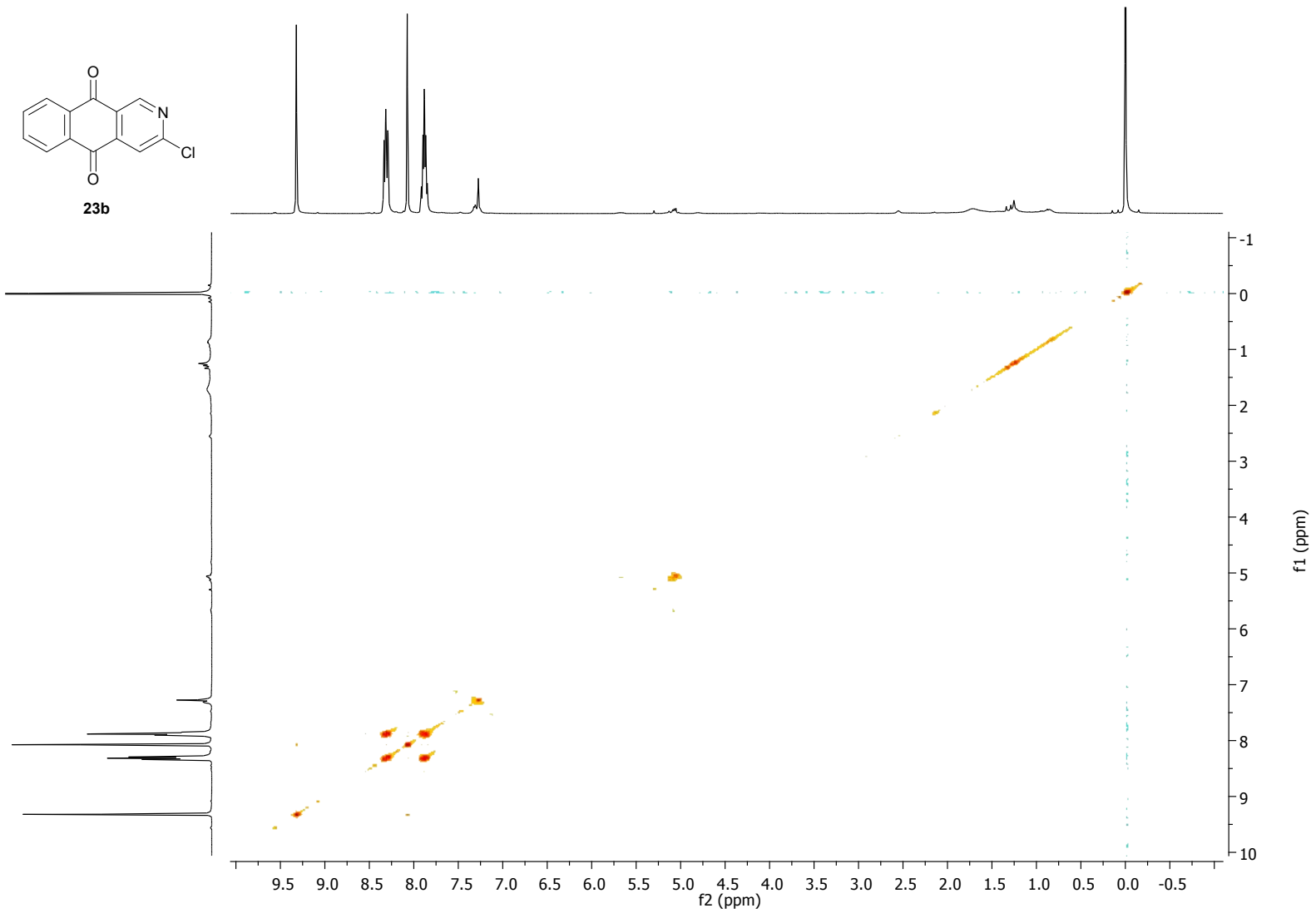


Figure 53 COSY spectrum of 3-chlorobenzo[*g*]isoquinoline-5,10-dione (**23b**) ($CDCl_3$, 400 MHz).

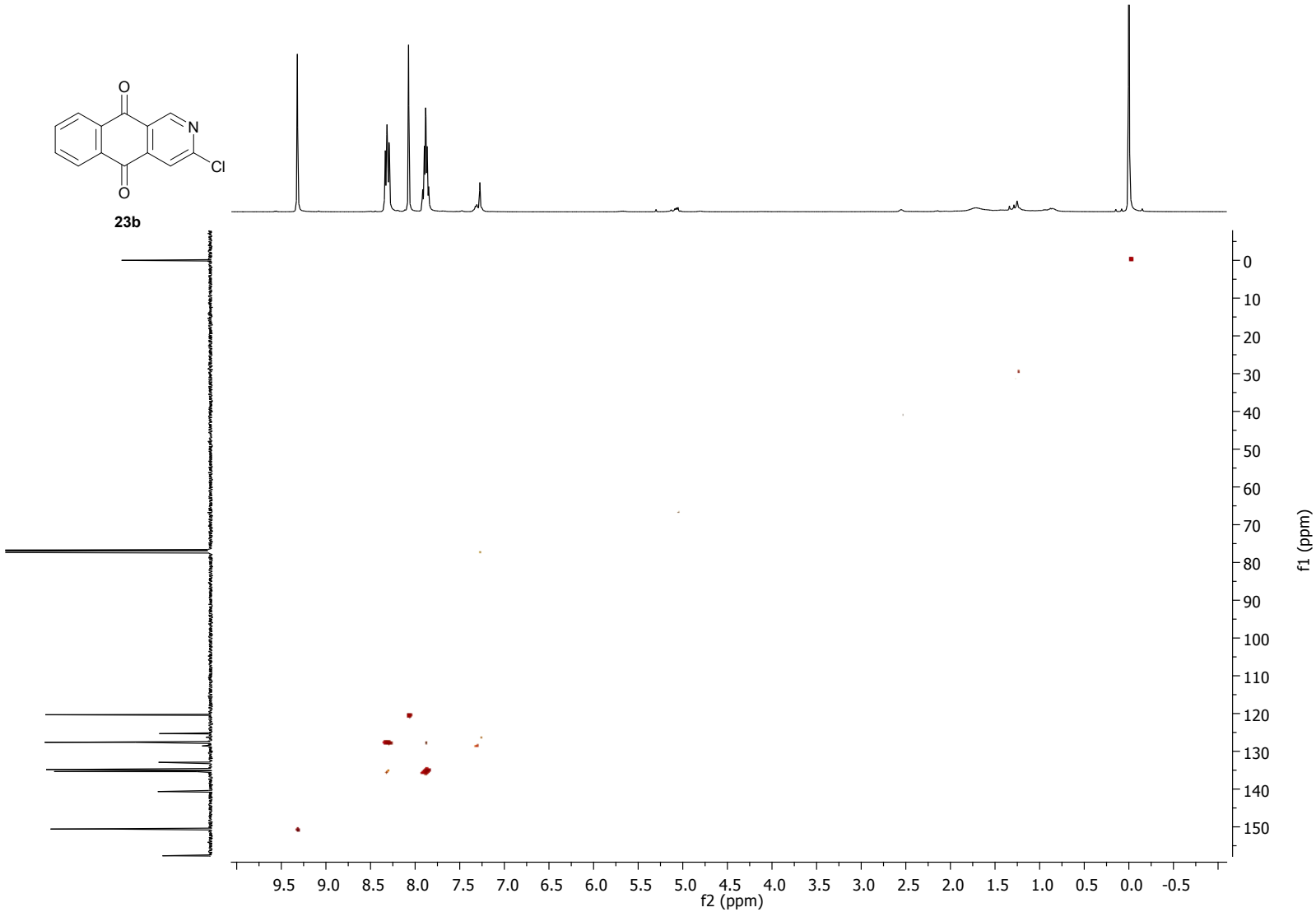


Figure 54 HSQC spectrum of 3-chlorobenzo[*g*]isoquinoline-5,10-dione (**23b**) ($CDCl_3$, 400 MHz).

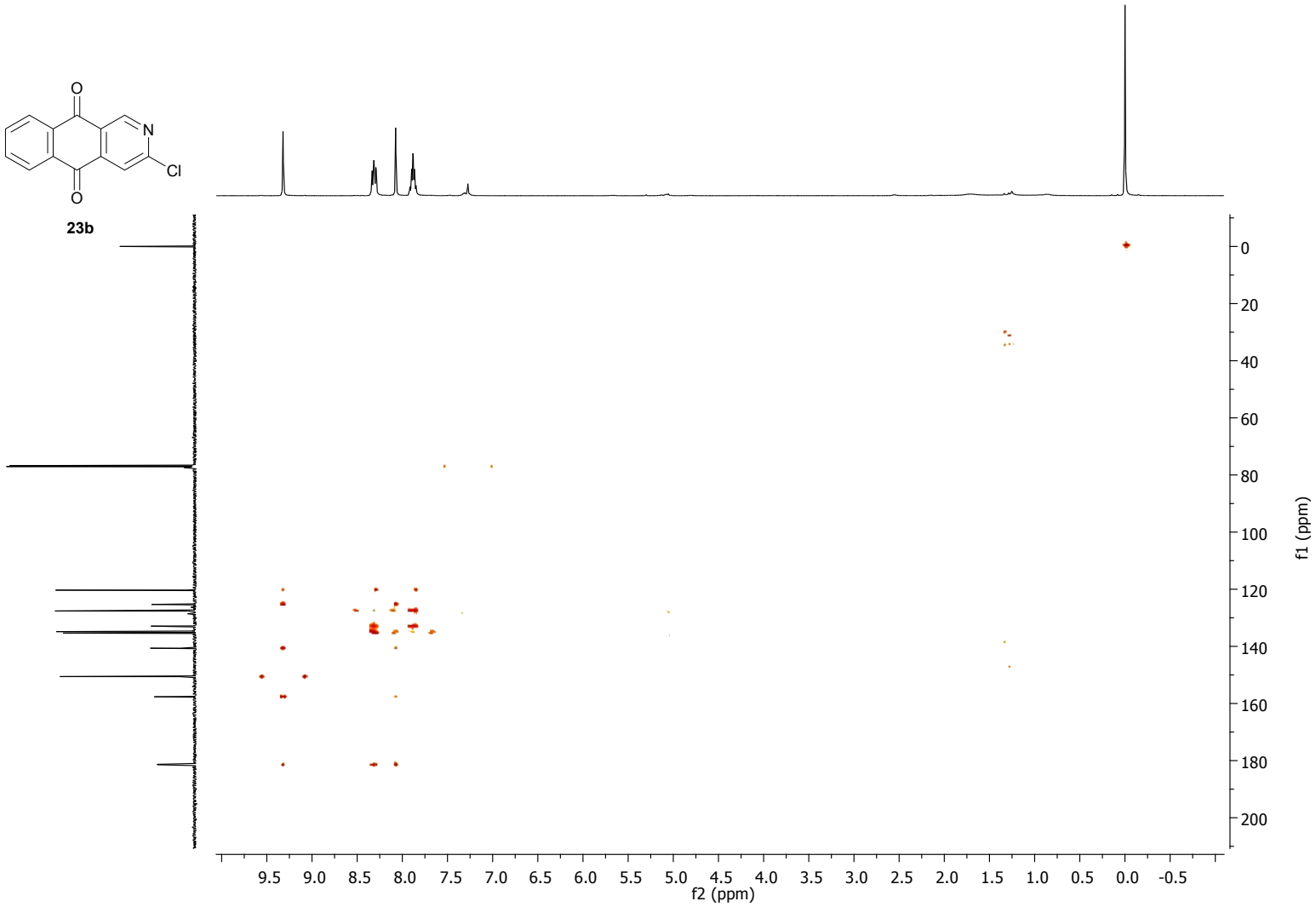


Figure 55 HMBC spectrum of 3-chlorobenzo[*g*]isoquinoline-5,10-dione (**23b**) ($CDCl_3$, 400 MHz).

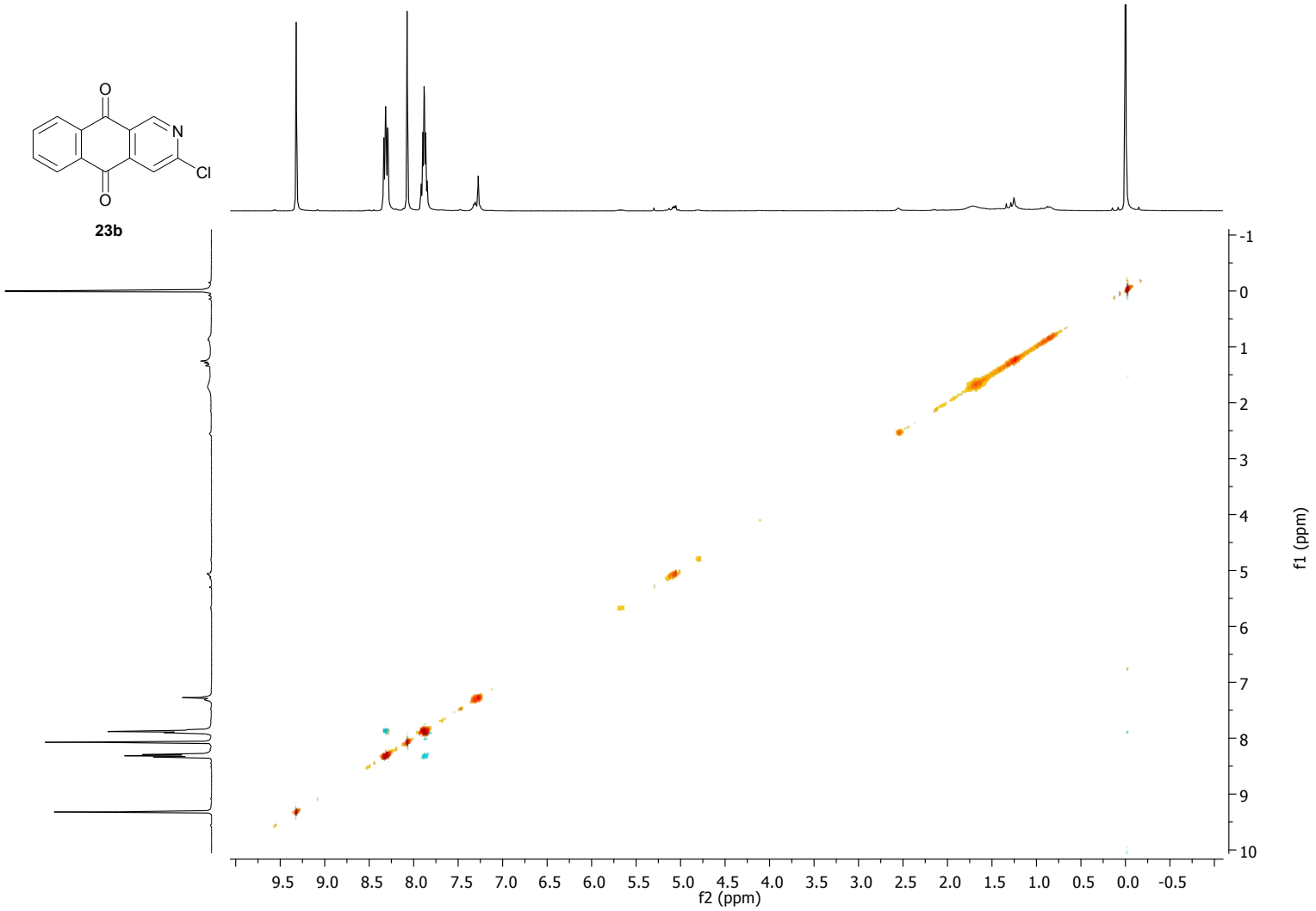


Figure 56 NOESY spectrum of 3-chlorobenzo[*g*]isoquinoline-5,10-dione (**23b**) ($CDCl_3$, 400 MHz).

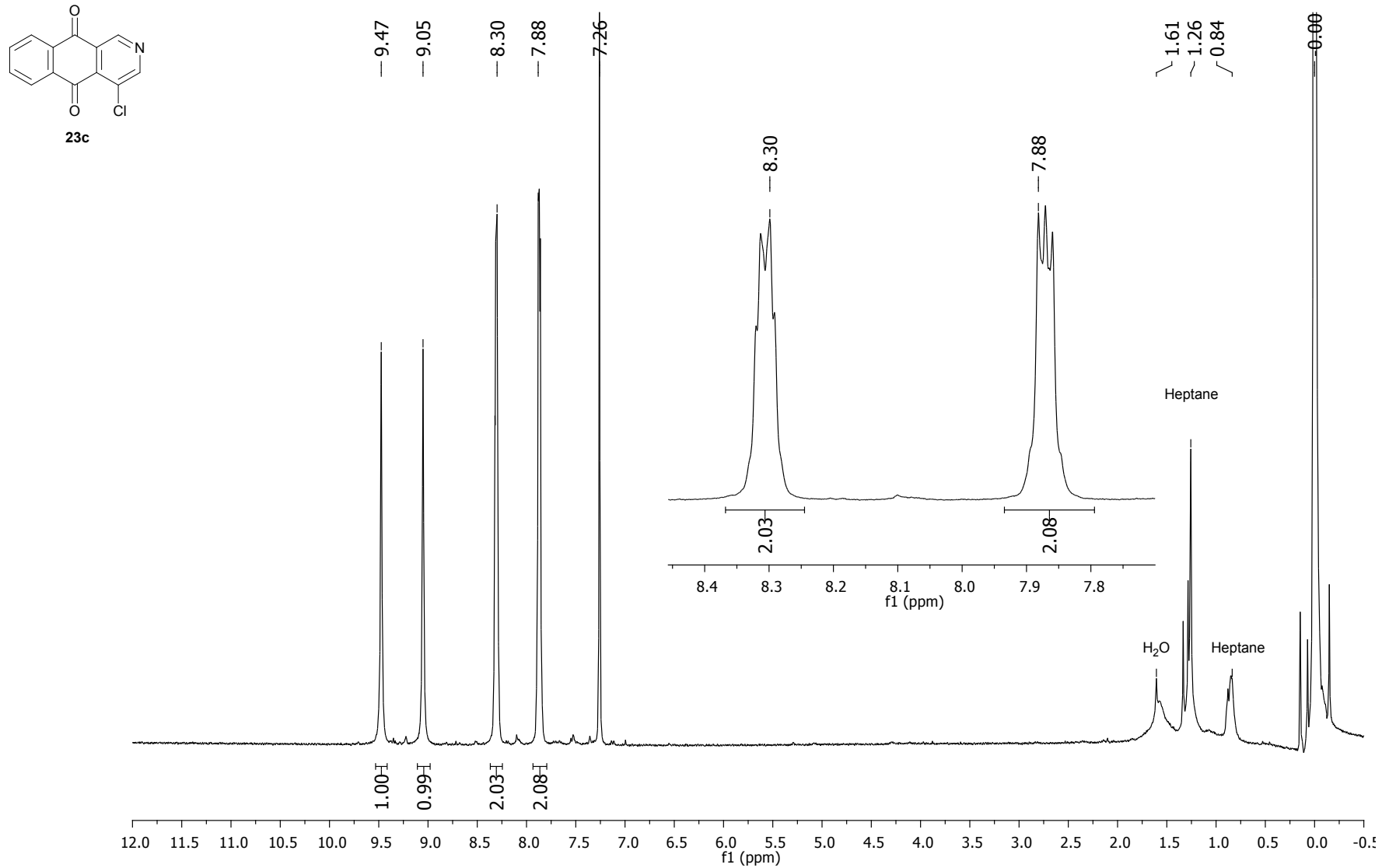


Figure 57 ^{1}H NMR spectrum of 4-chlorobenzo[*g*]isoquinoline-5,10-dione (**23c**) ($CDCl_3$, 400 MHz).

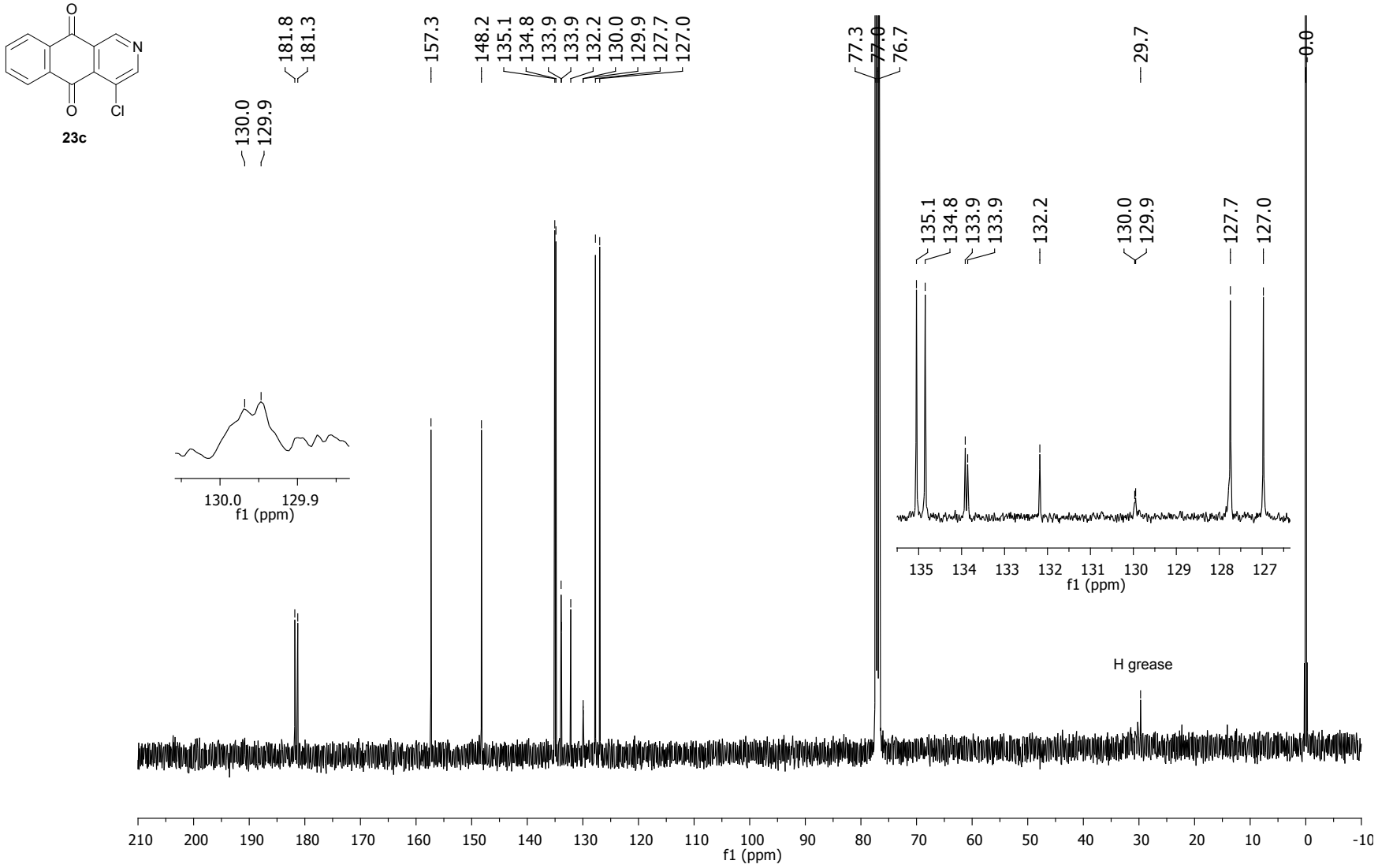


Figure 58 ^{13}C NMR spectrum of 4-chlorobenzo[*g*]isoquinoline-5,10-dione (**23c**) ($CDCl_3$, 100 MHz).

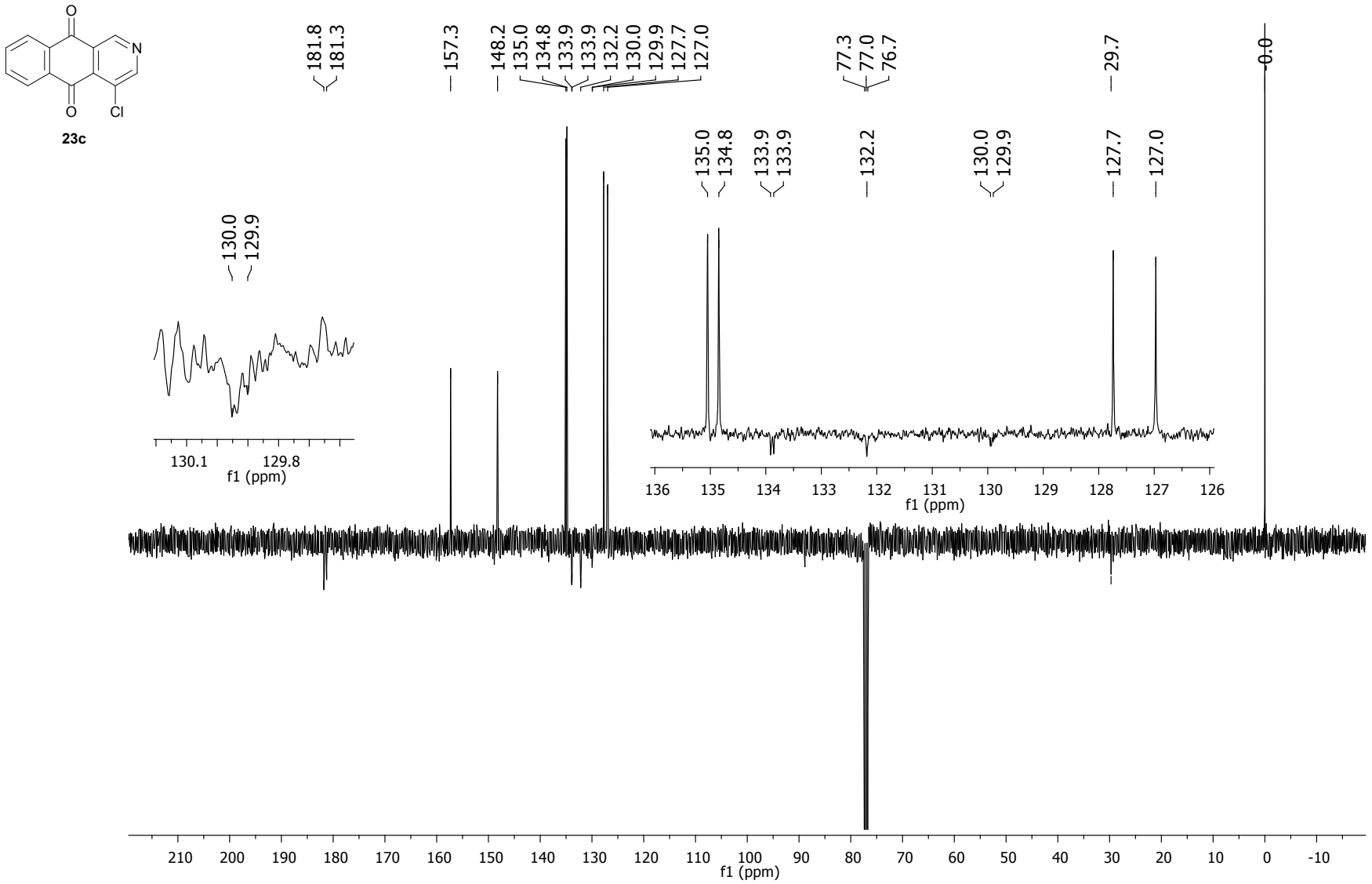


Figure 59 APT spectrum of 4-chlorobenzo[*g*]isoquinoline-5,10-dione (**23c**) ($CDCl_3$, 100 MHz).

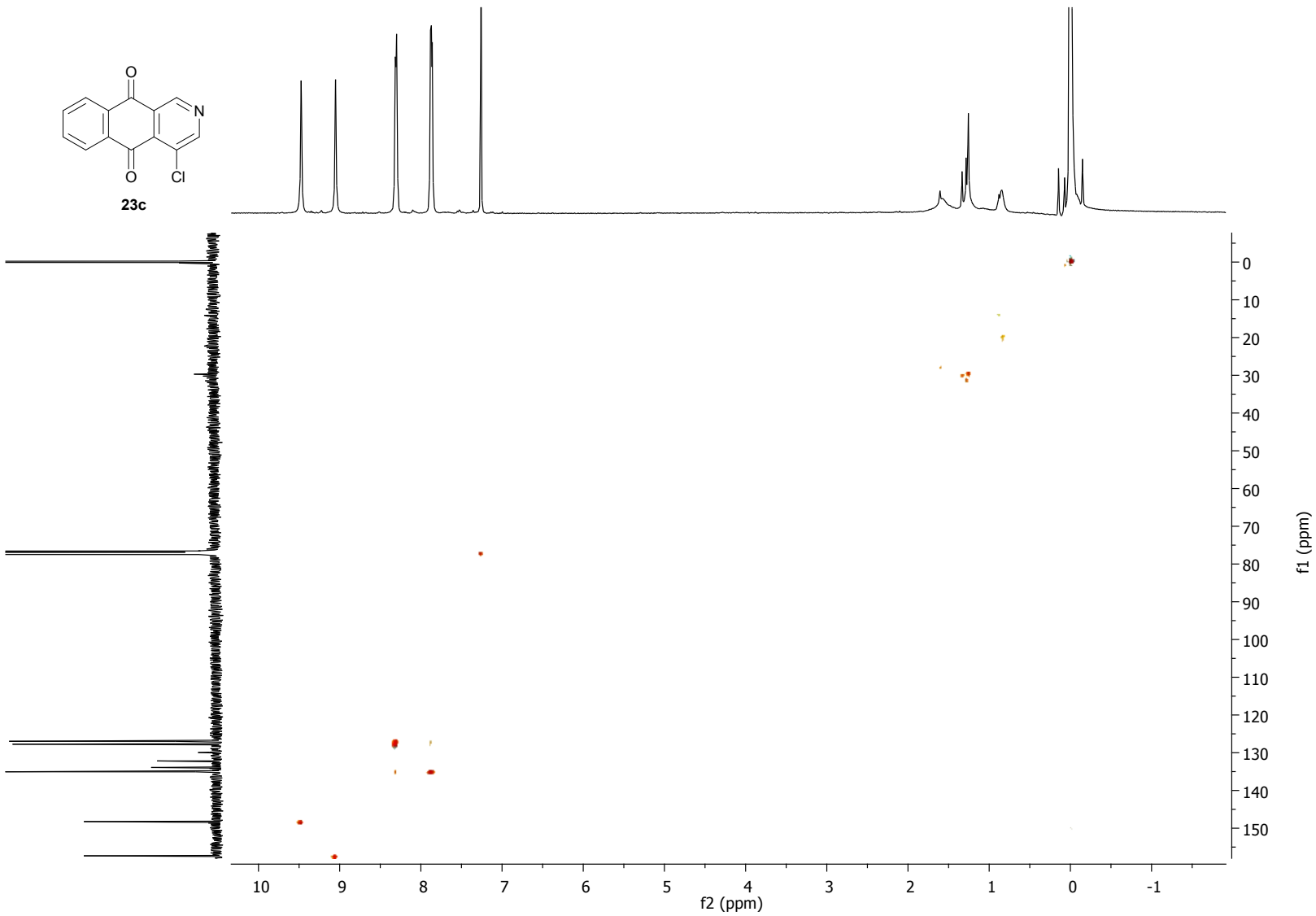


Figure 60 HSQC spectrum of 4-chlorobenzo[*g*]isoquinoline-5,10-dione (**23c**) ($CDCl_3$, 400 MHz).

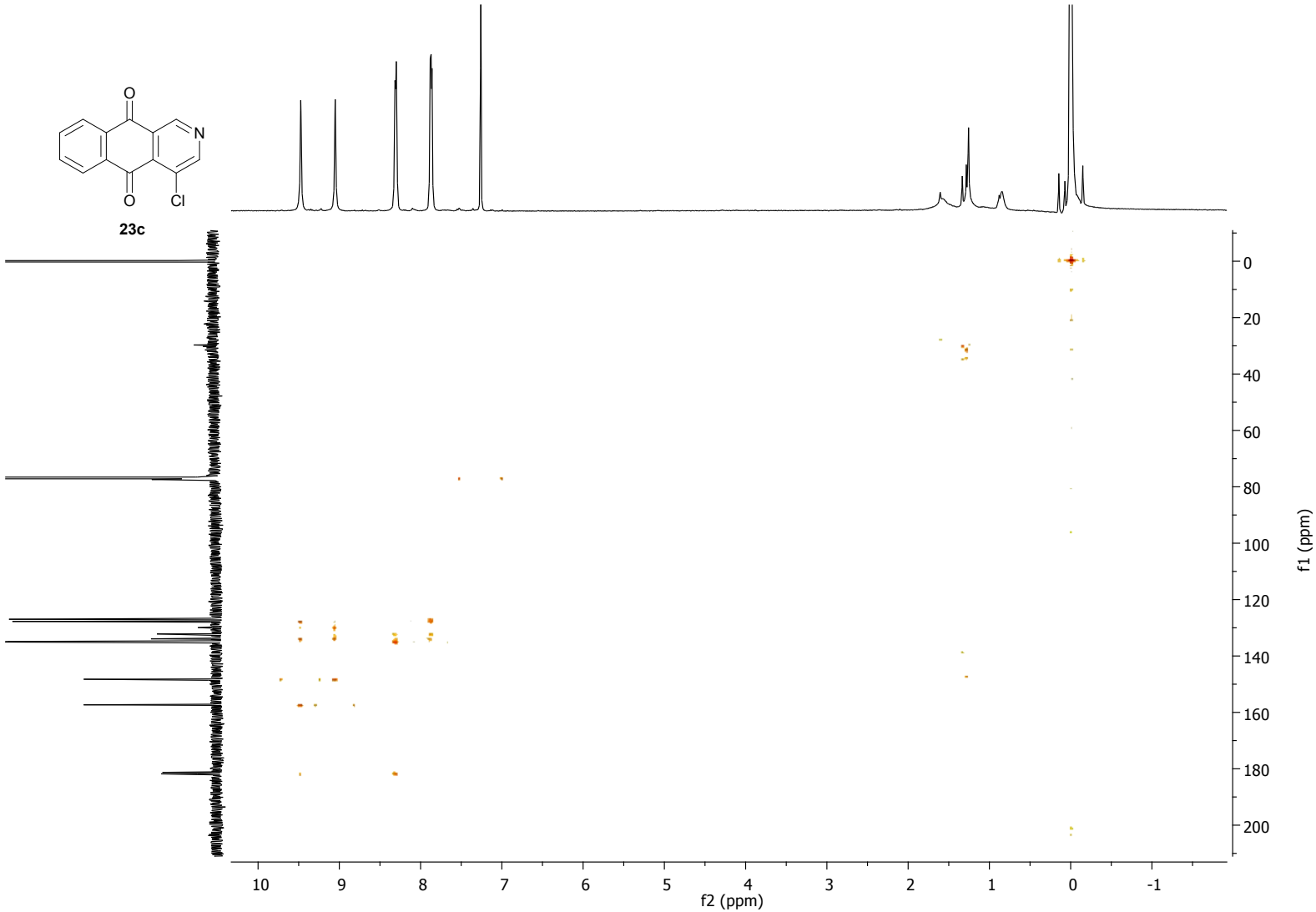


Figure 61 HMBC spectrum of 4-chlorobenzo[*g*]isoquinoline-5,10-dione (**23c**) ($CDCl_3$, 400 MHz).

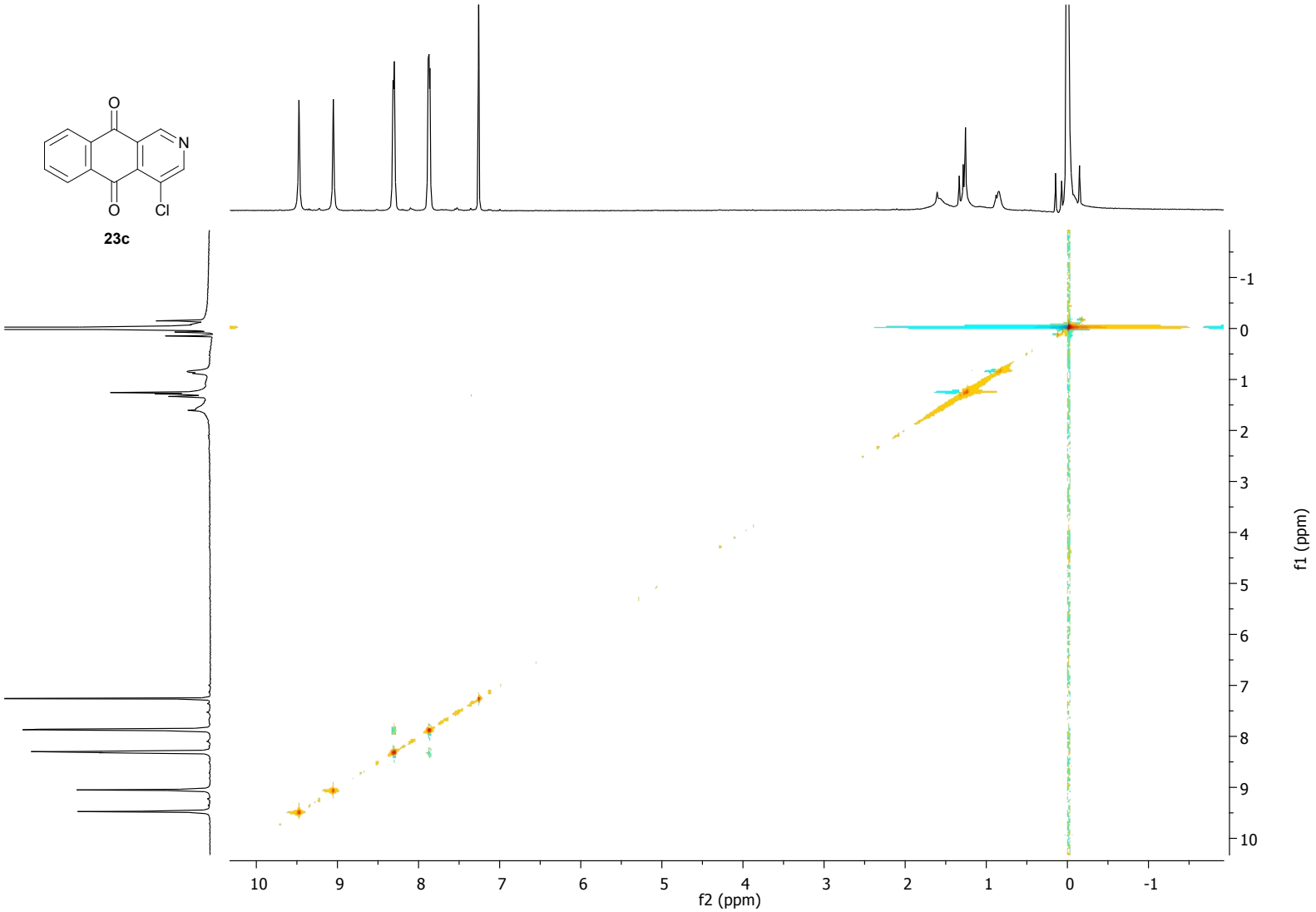


Figure 62 NOESY spectrum of 4-chlorobenzo[*g*]isoquinoline-5,10-dione (**23c**) ($CDCl_3$, 400 MHz).

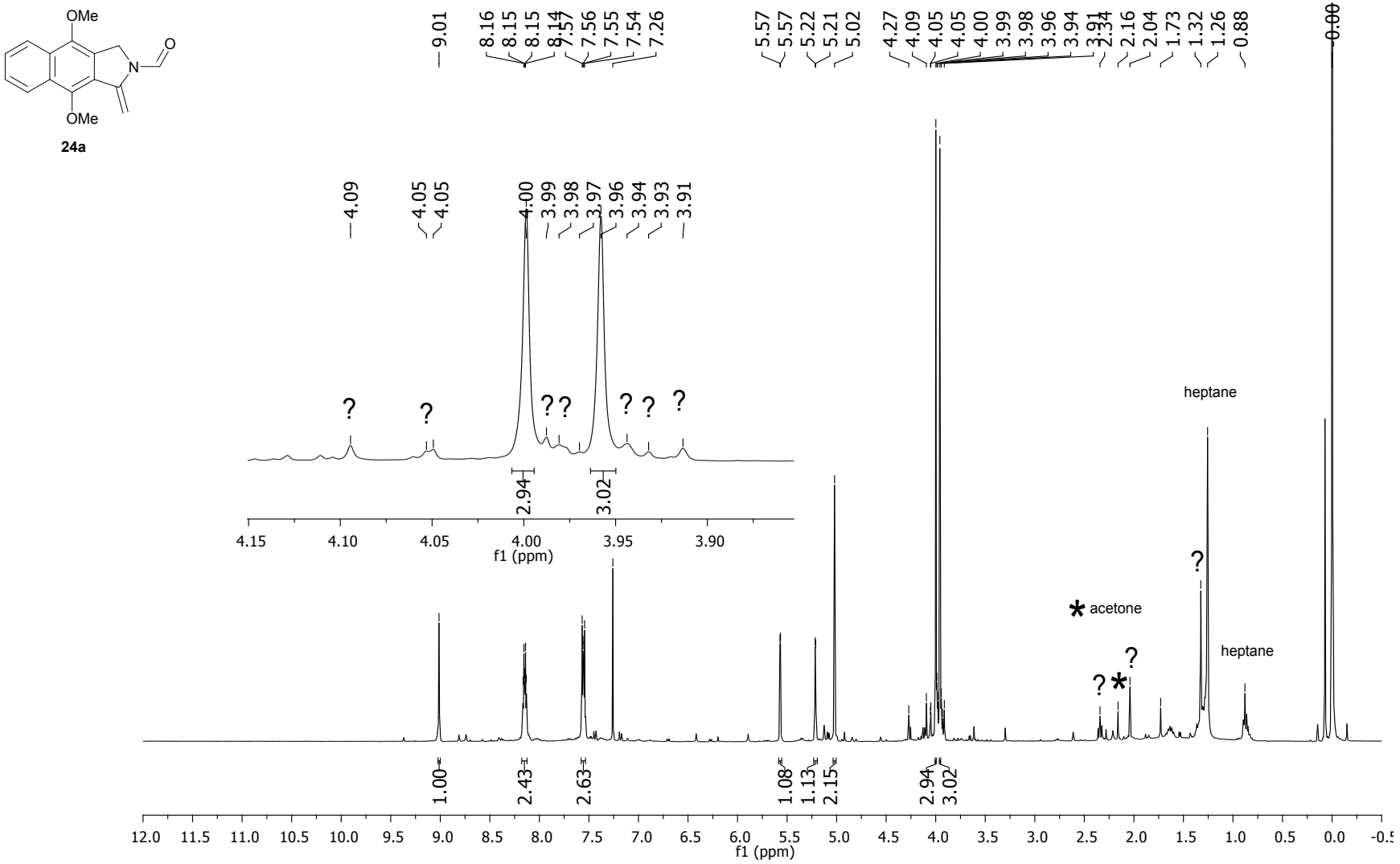


Figure 63 ^{1}H NMR spectrum of 4,9-dimethoxy-1-methylene-1,3-dihydro-2*H*-benzo[*f*]isoindole-2-carbaldehyde (**24a**) ($CDCl_3$, 400 MHz). Due to limited stability of **24a** no clearer spectrum could be measured.

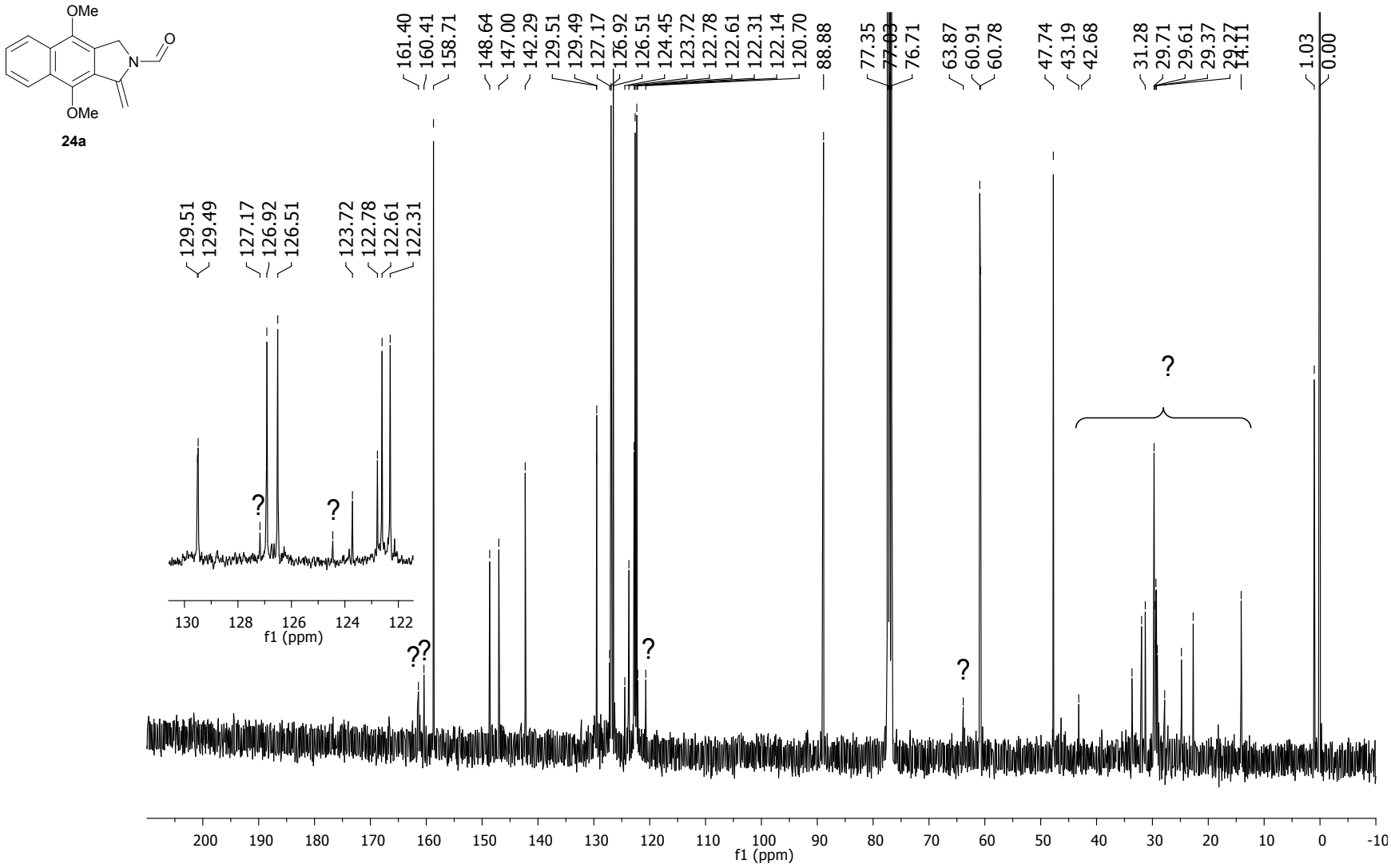


Figure 64 ^{13}C NMR spectrum of 4,9-dimethoxy-1-methylene-1,3-dihydro-2*H*-benzo[*f*]isoindole-2-carbaldehyde (**24a**) ($CDCl_3$, 100 MHz). Due to limited stability of **24a** no clearer spectrum could be measured.

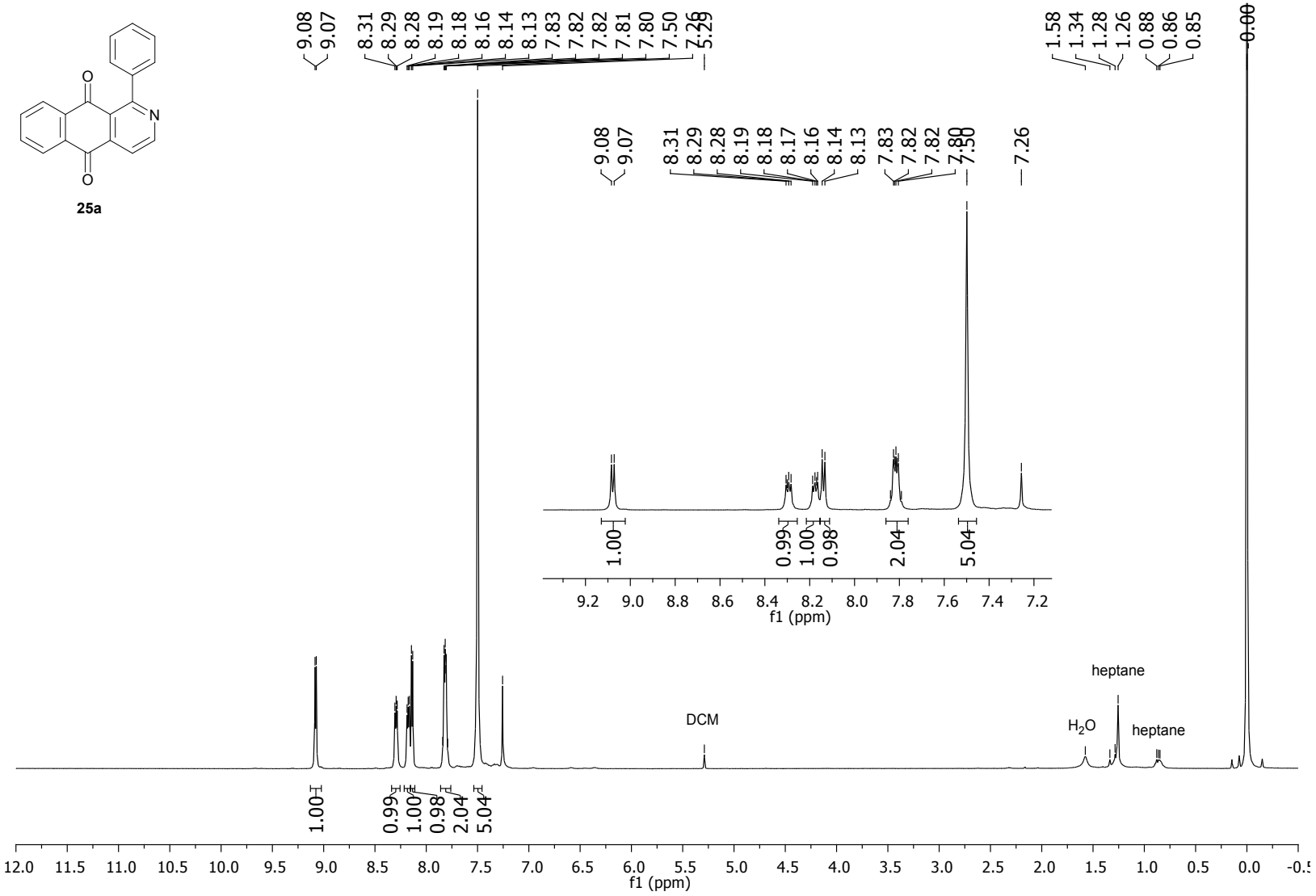


Figure 65 ^{1}H NMR spectrum of 1-phenylbenzo[*g*]isoquinoline-5,10-dione (**25a**) ($CDCl_3$, 400 MHz).

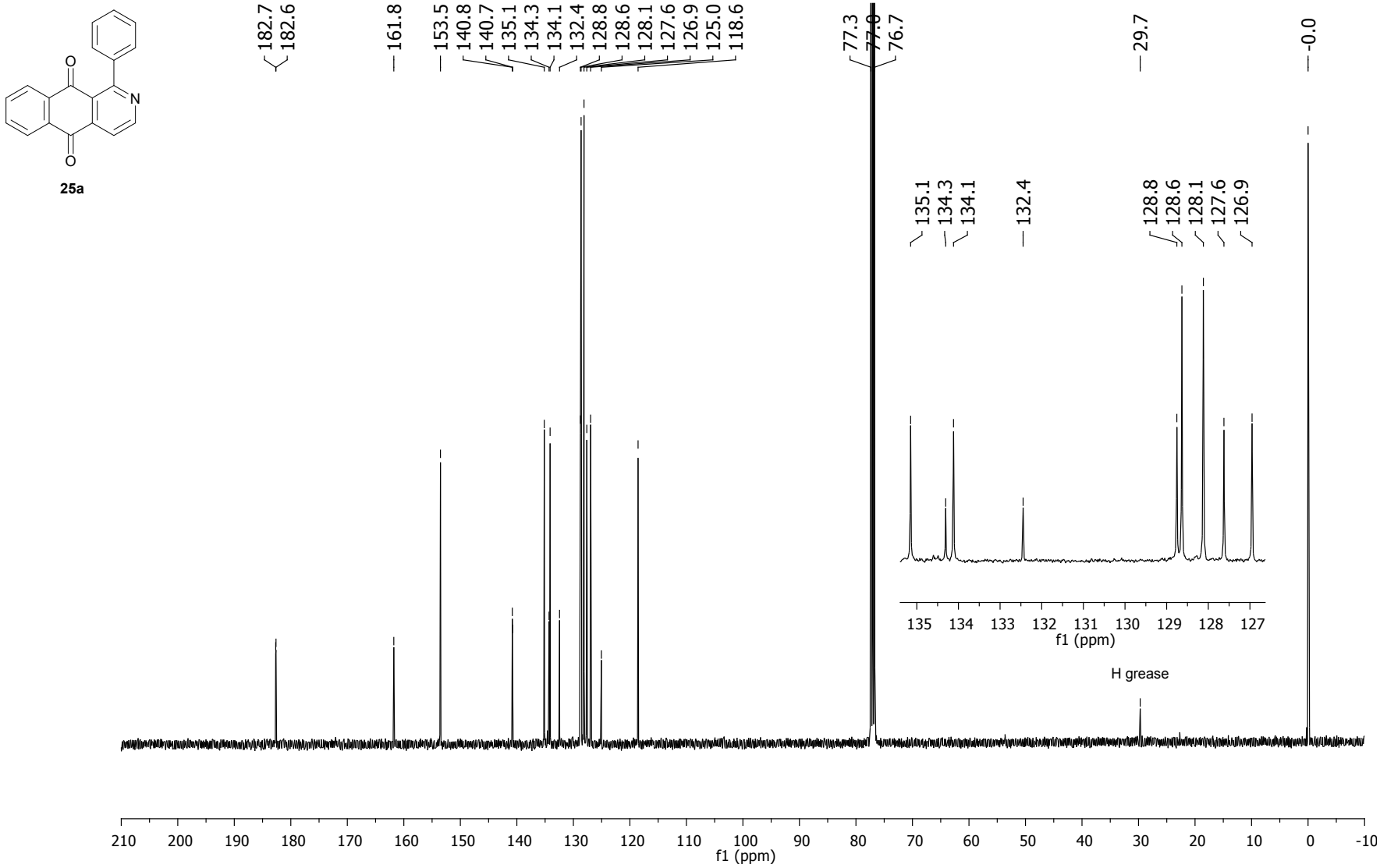


Figure 66 ^{13}C NMR spectrum of 1-phenylbenzo[*g*]isoquinoline-5,10-dione (**25a**) ($CDCl_3$, 100 MHz).

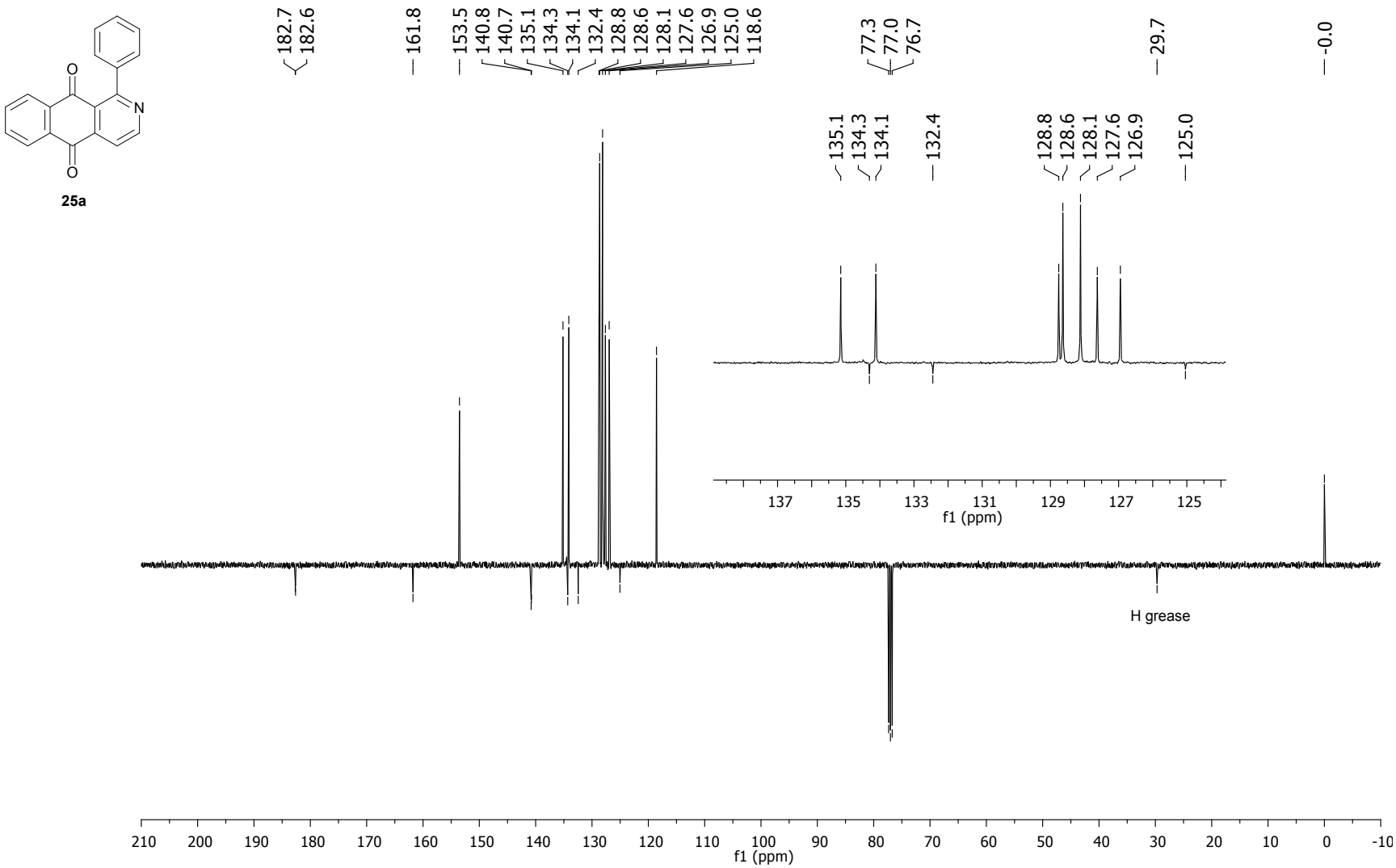


Figure 67 APT spectrum of 1-phenylbenzo[*g*]isoquinoline-5,10-dione (**25a**) ($CDCl_3$, 100 MHz).

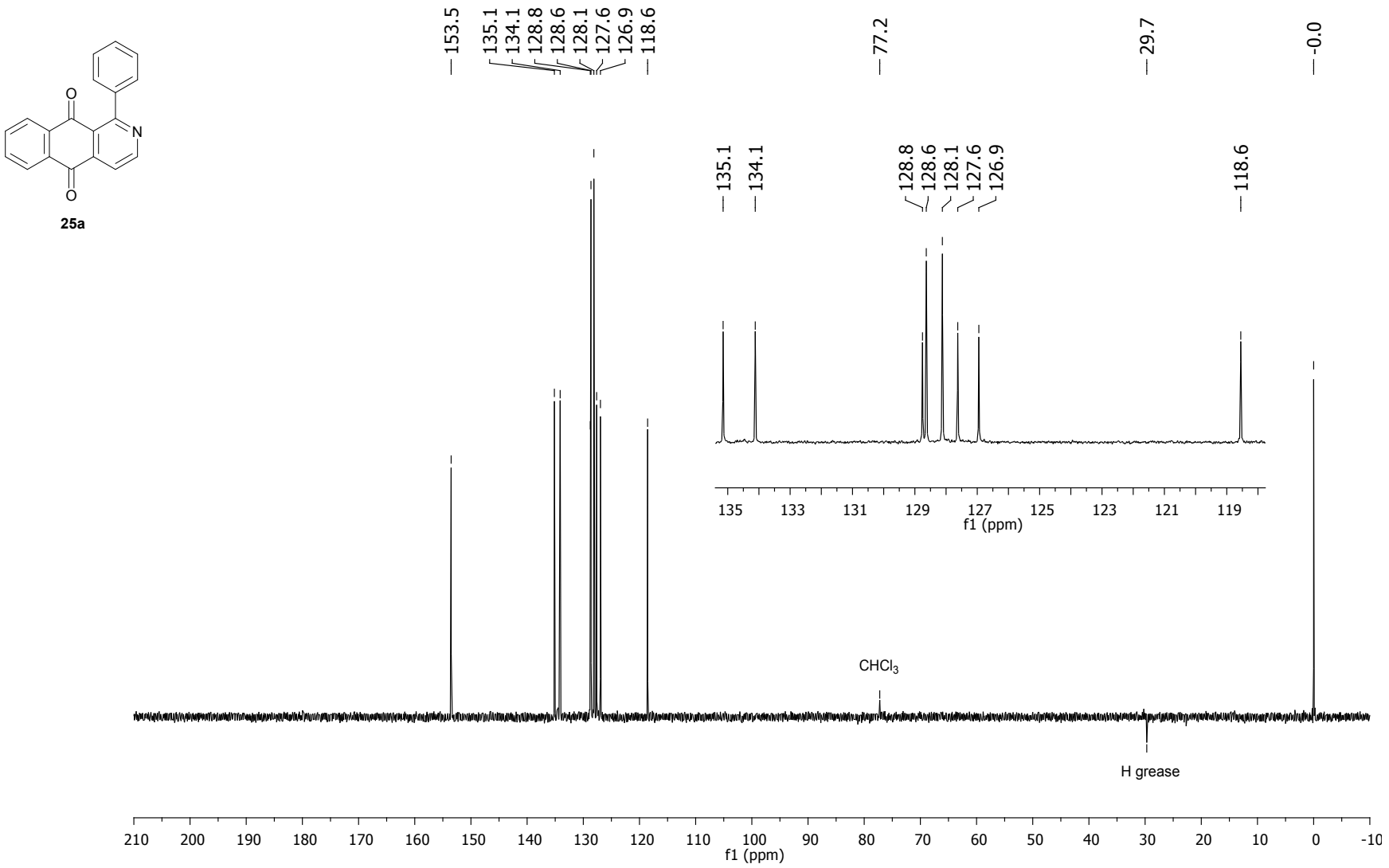


Figure 68 DEPT 135 spectrum of 1-phenylbenzo[*g*]isoquinoline-5,10-dione (**25a**) ($CDCl_3$, 100 MHz).

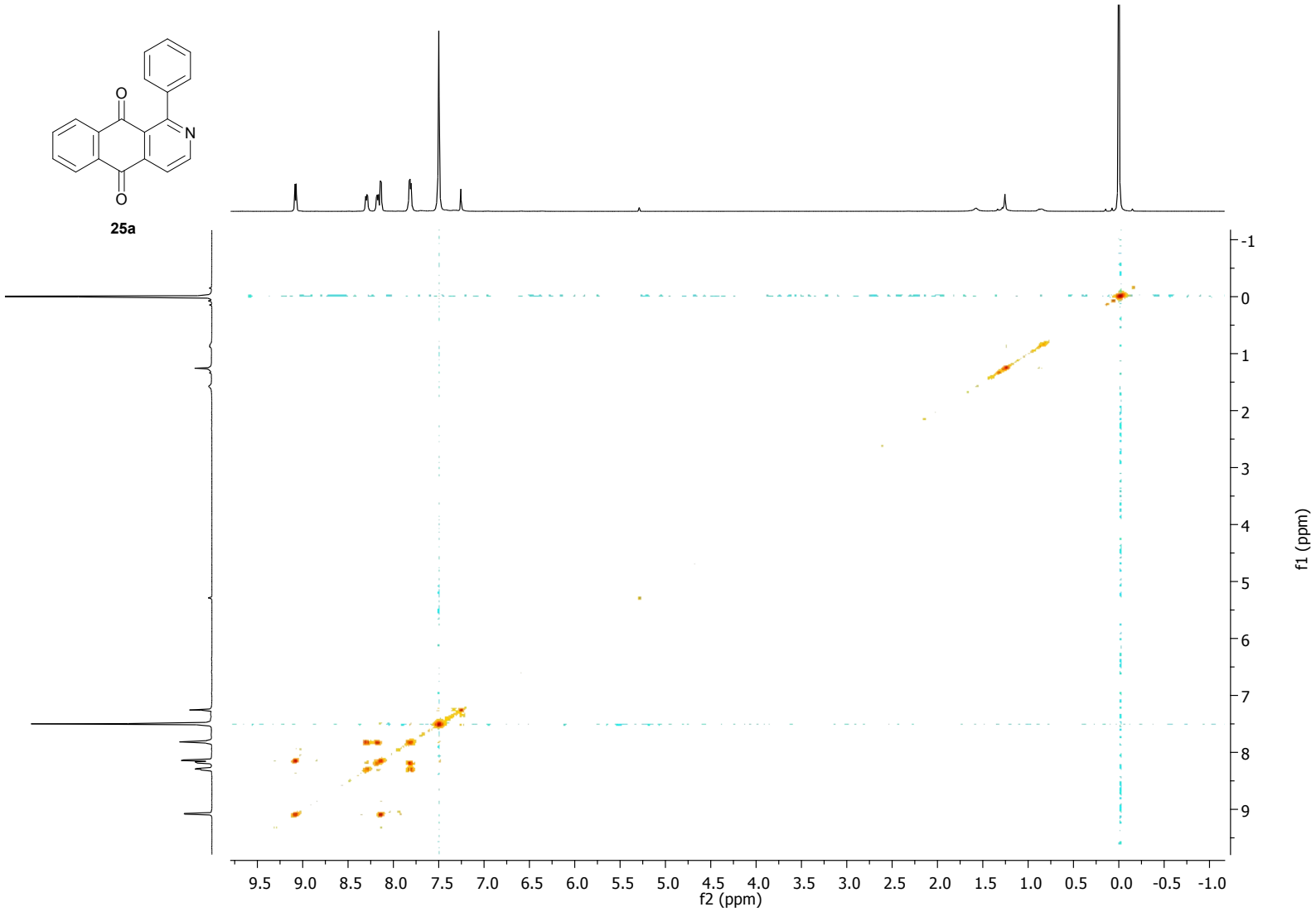


Figure 69 COSY spectrum of 1-phenylbenzo[*g*]isoquinoline-5,10-dione (**25a**) ($CDCl_3$, 400 MHz).

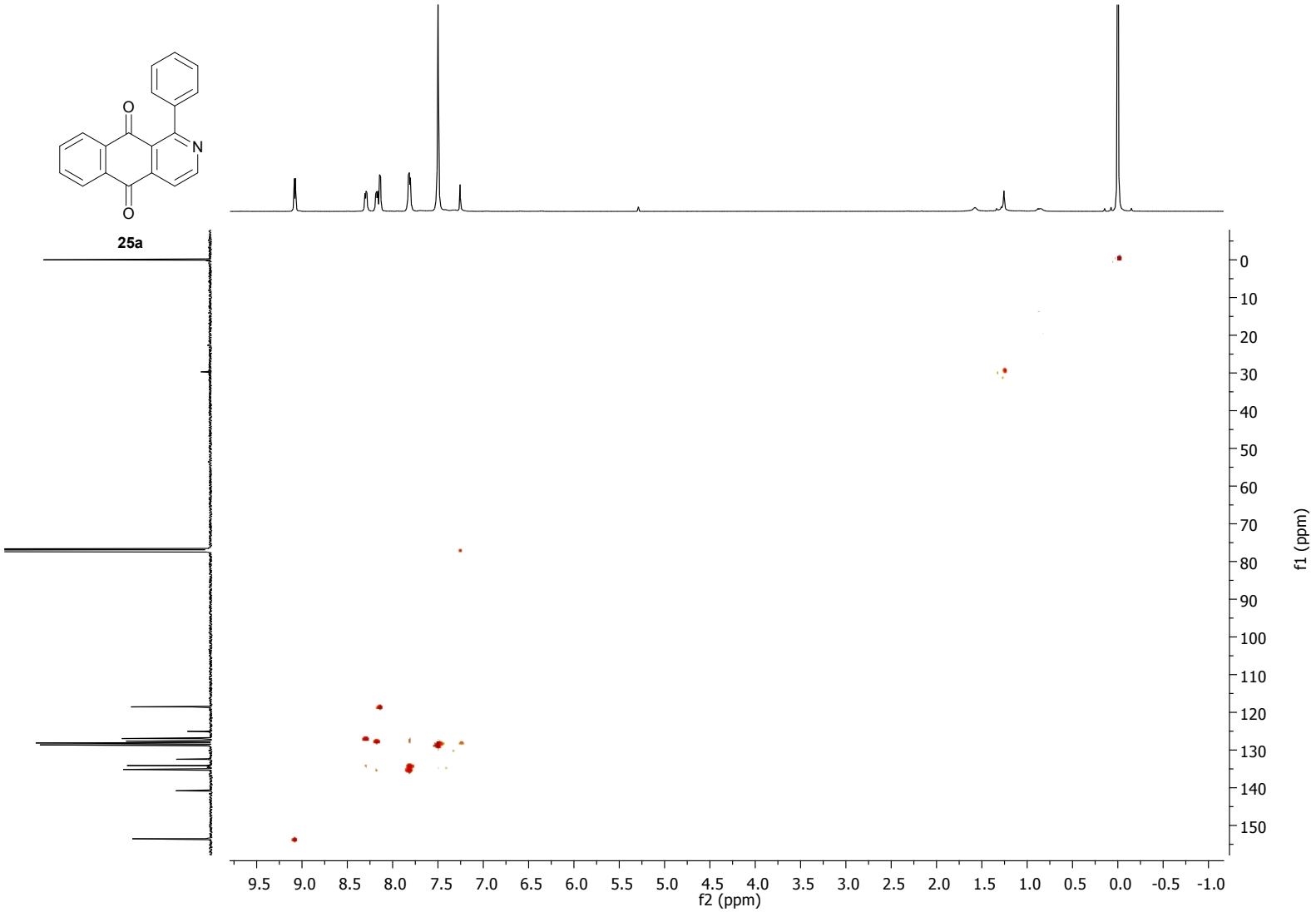


Figure 70 HSQC spectrum of 1-phenylbenzo[*g*]isoquinoline-5,10-dione (**25a**) ($CDCl_3$, 400 MHz).

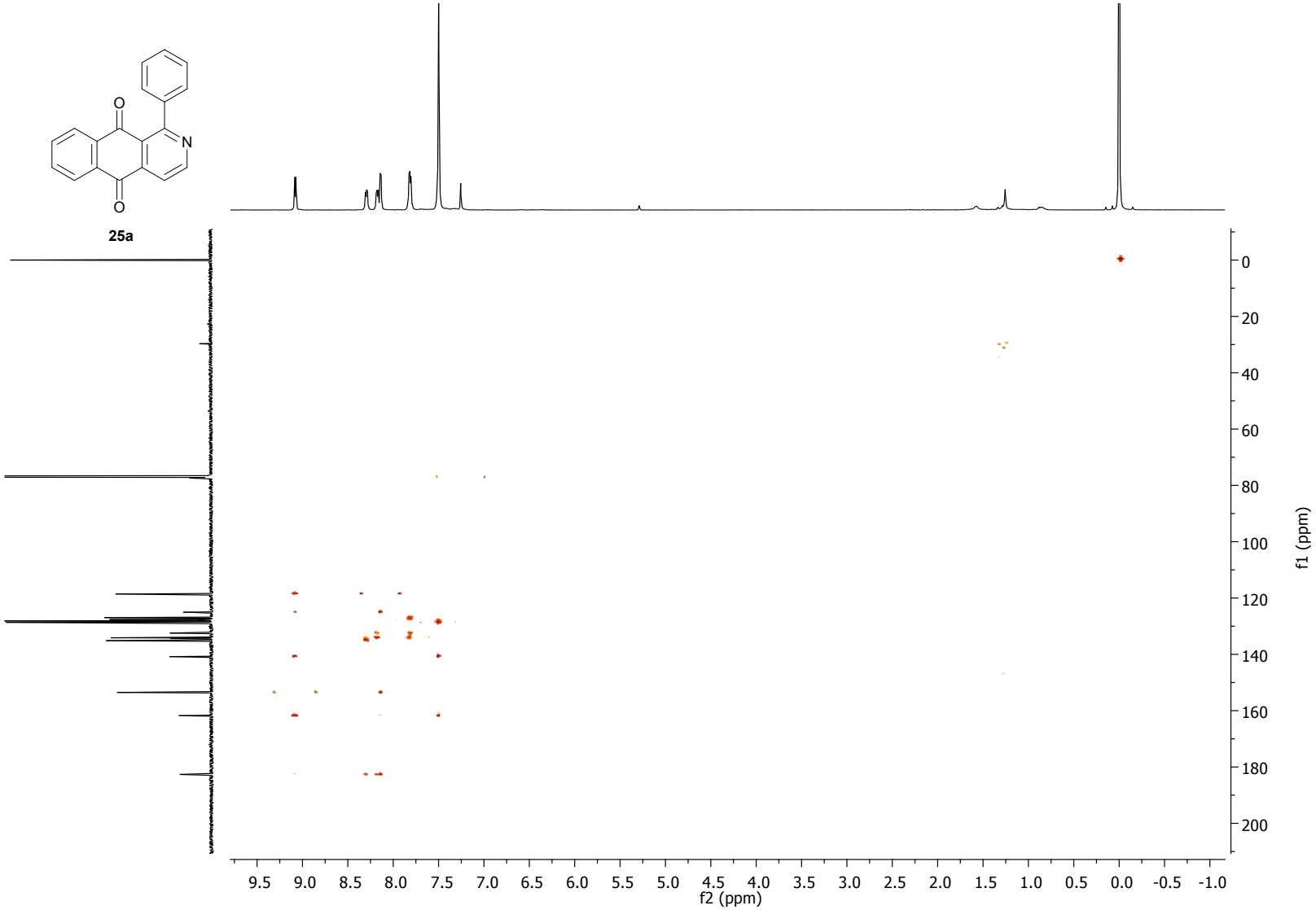


Figure 71 HMBC spectrum of 1-phenylbenzo[*g*]isoquinoline-5,10-dione (**25a**) ($CDCl_3$, 400 MHz).

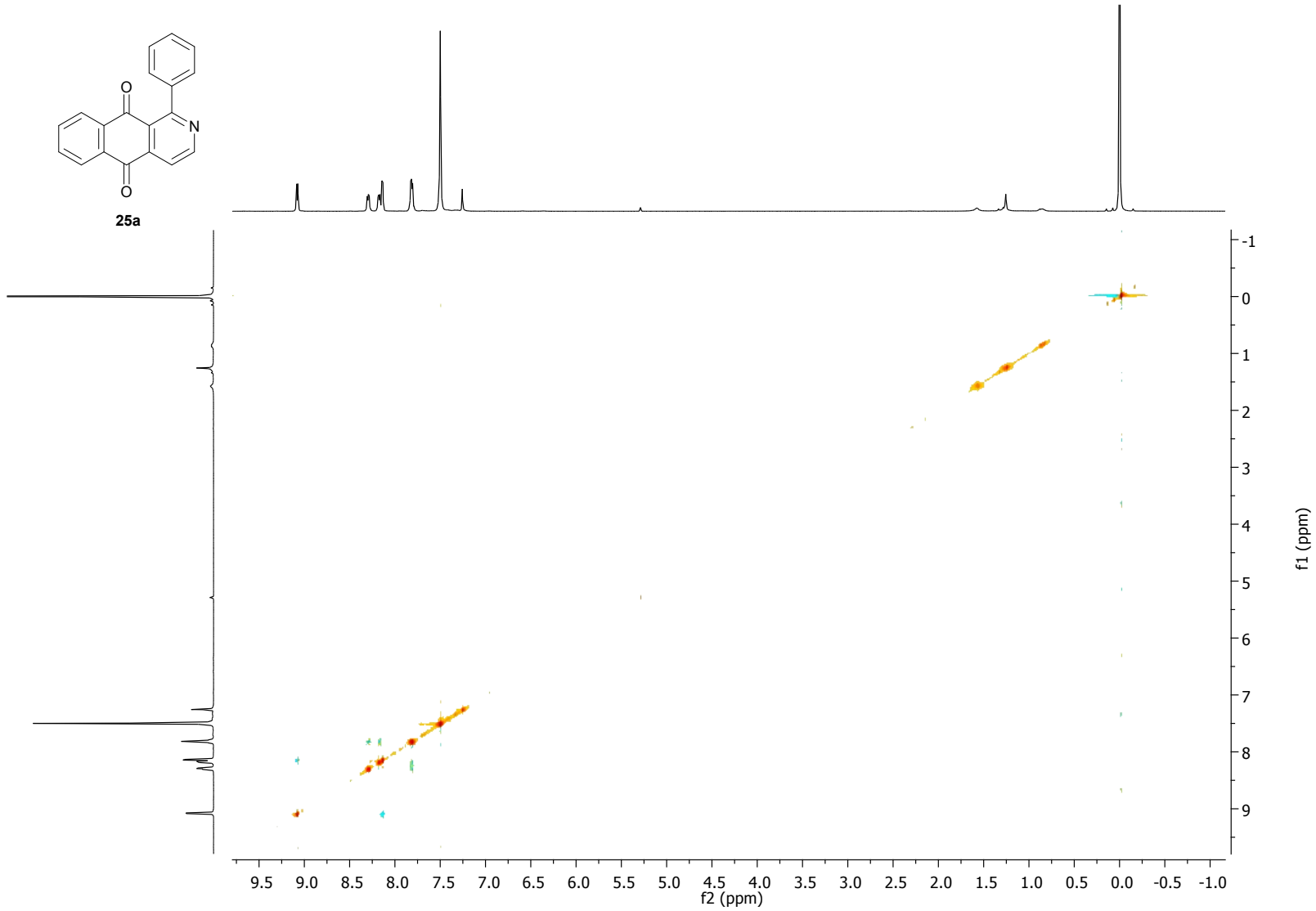


Figure 72 NOESY spectrum of 1-phenylbenzo[*g*]isoquinoline-5,10-dione (**25a**) ($CDCl_3$, 400 MHz).

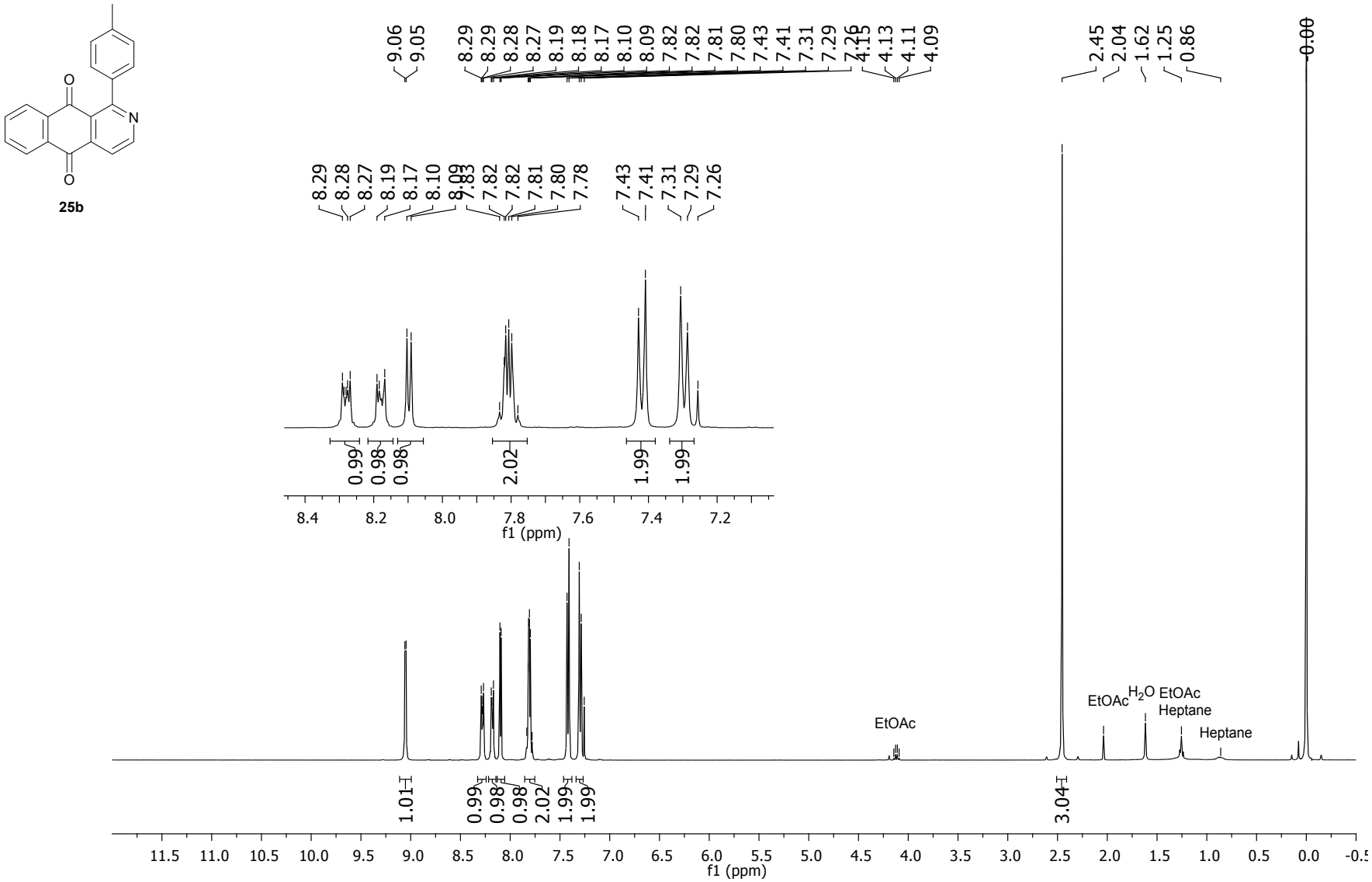


Figure 73 ^{1}H NMR spectrum of 1-*p*-tolylbenzo[*g*]isoquinoline-5,10-dione (**25b**) ($CDCl_3$, 400 MHz).

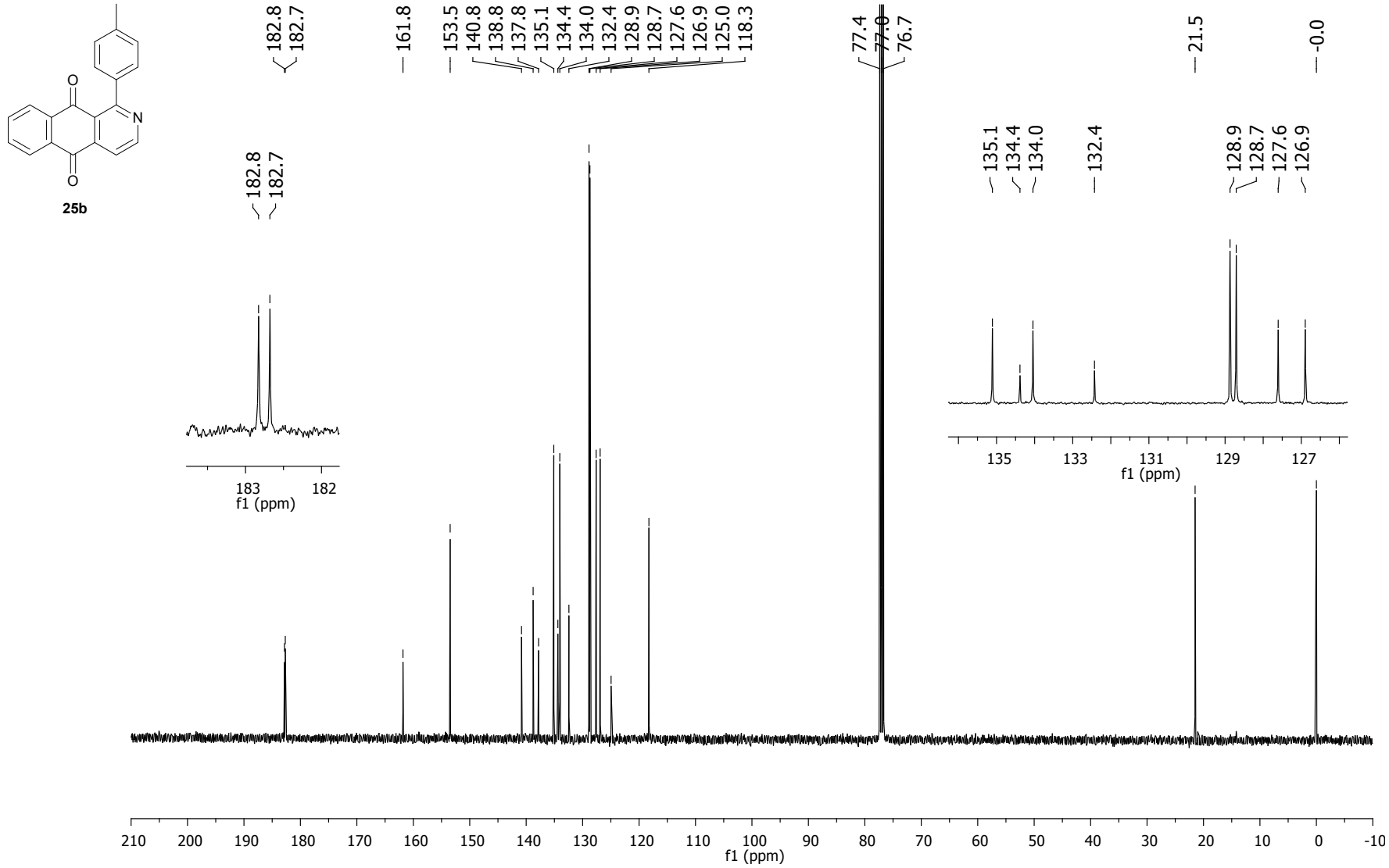


Figure 74 ^{13}C NMR spectrum of 1-*p*-tolylbenzo[*g*]isoquinoline-5,10-dione (**25b**) ($CDCl_3$, 100 MHz).

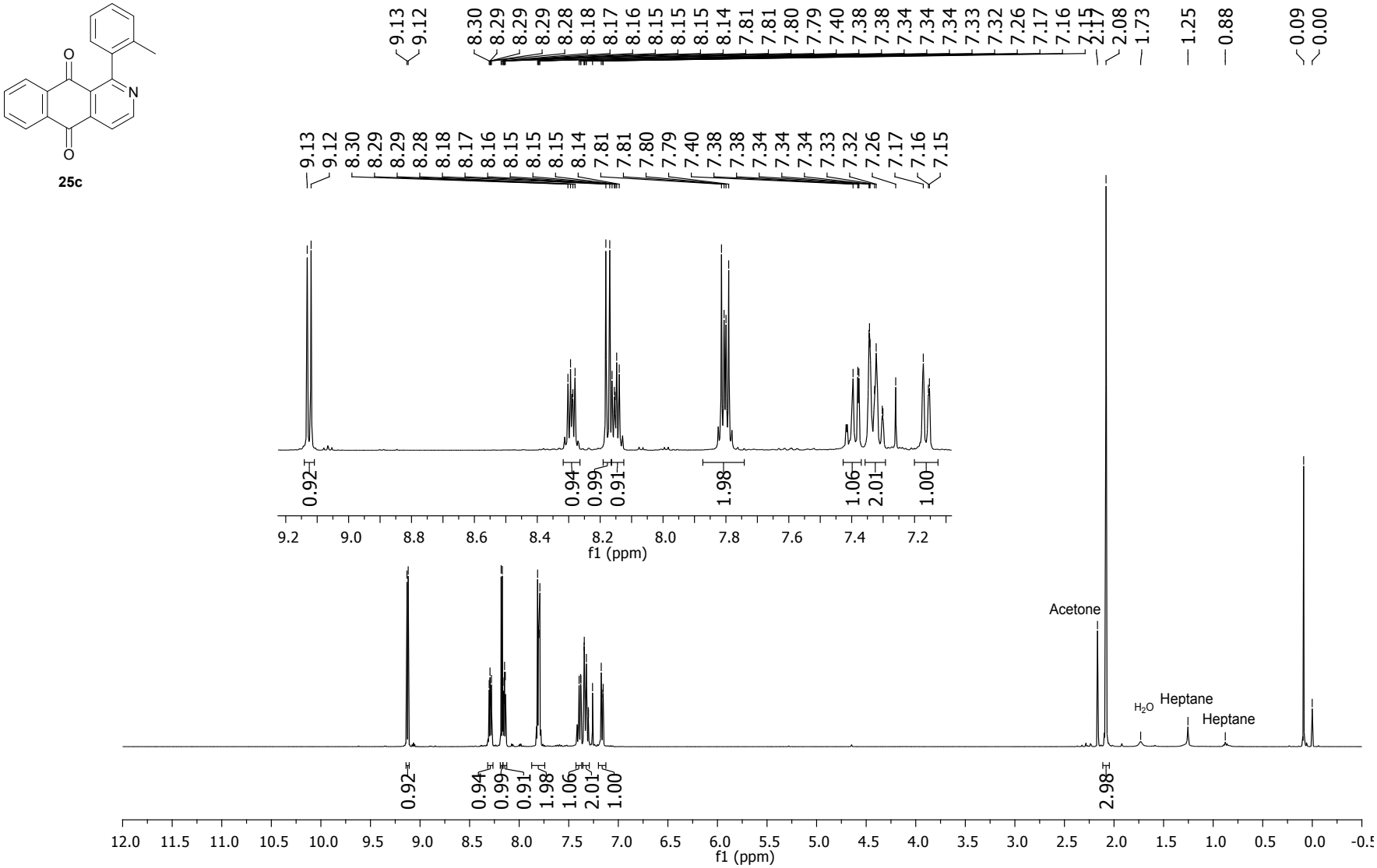


Figure 75 ^{1}H NMR spectrum of 1-*o*-tolylbenzo[*g*]isoquinoline-5,10-dione (**25c**) ($CDCl_3$, 400 MHz).

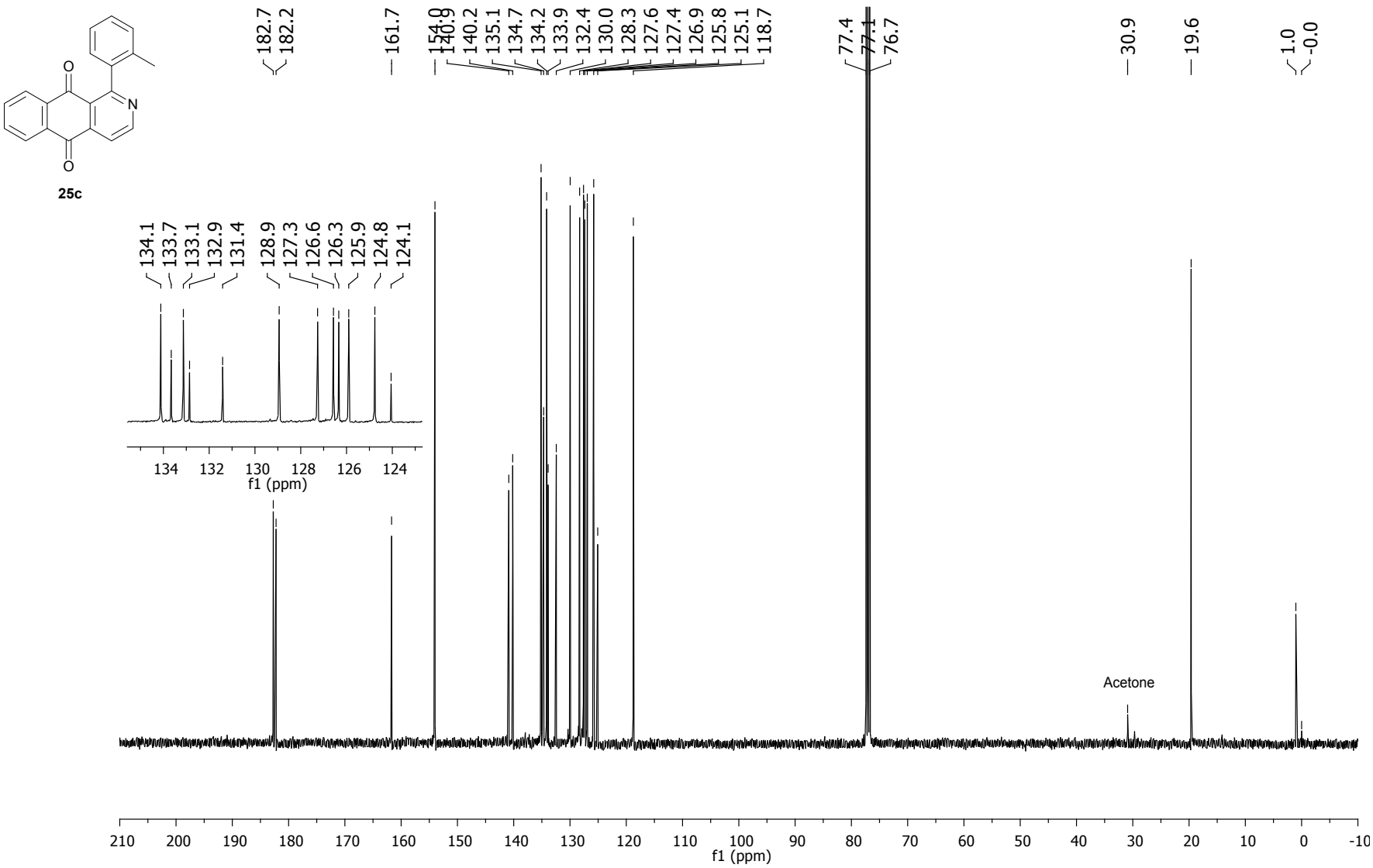


Figure 76 ^{13}C NMR spectrum of 1-*o*-tolylbenzo[*g*]isoquinoline-5,10-dione (**25c**) ($CDCl_3$, 100 MHz).

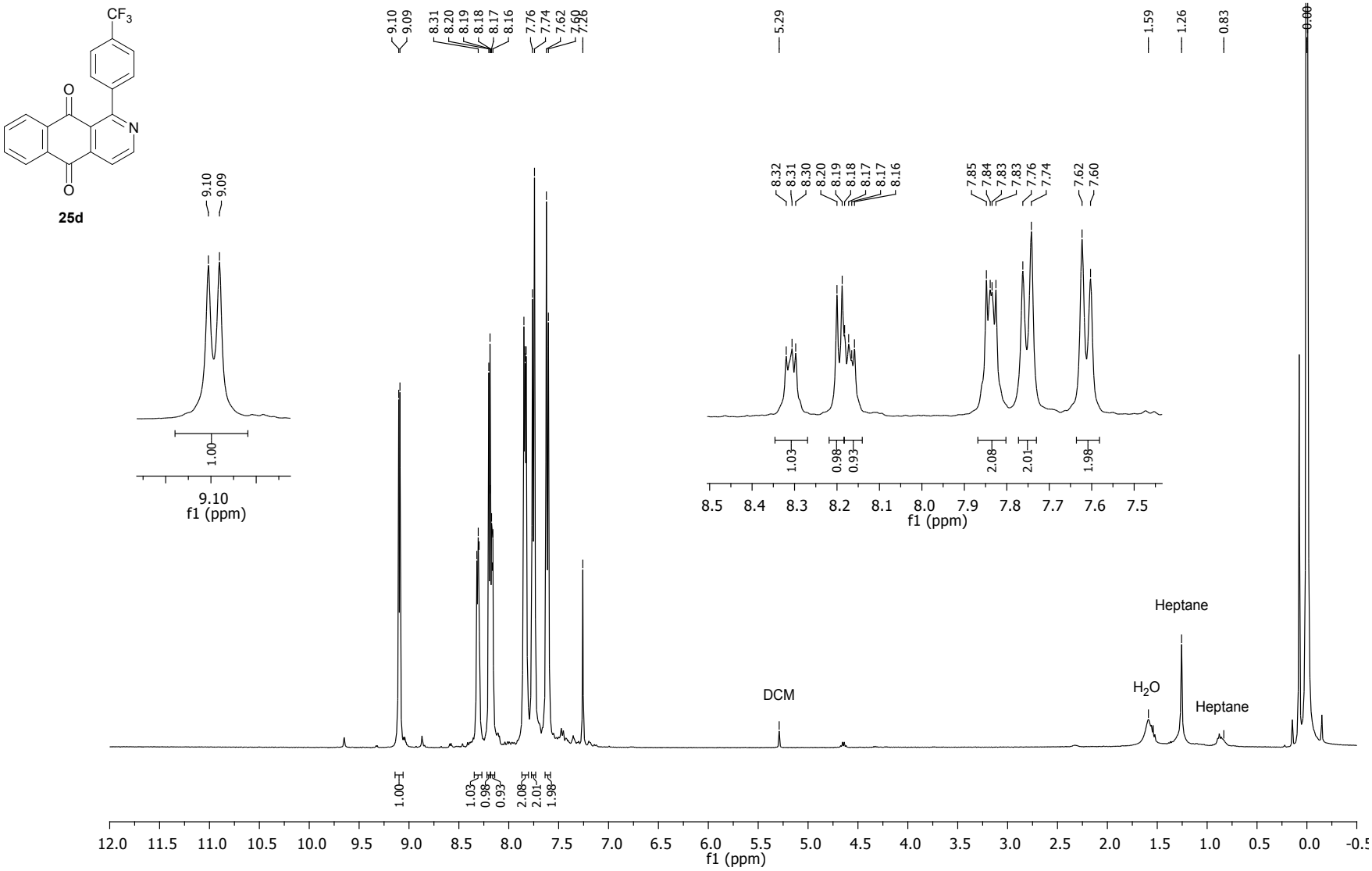


Figure 77 ^{1}H NMR spectrum of 1-(*p*-(trifluoromethyl)phenyl)benzo[*g*]isoquinoline-5,10-dione (**25d**) ($CDCl_3$, 400 MHz).

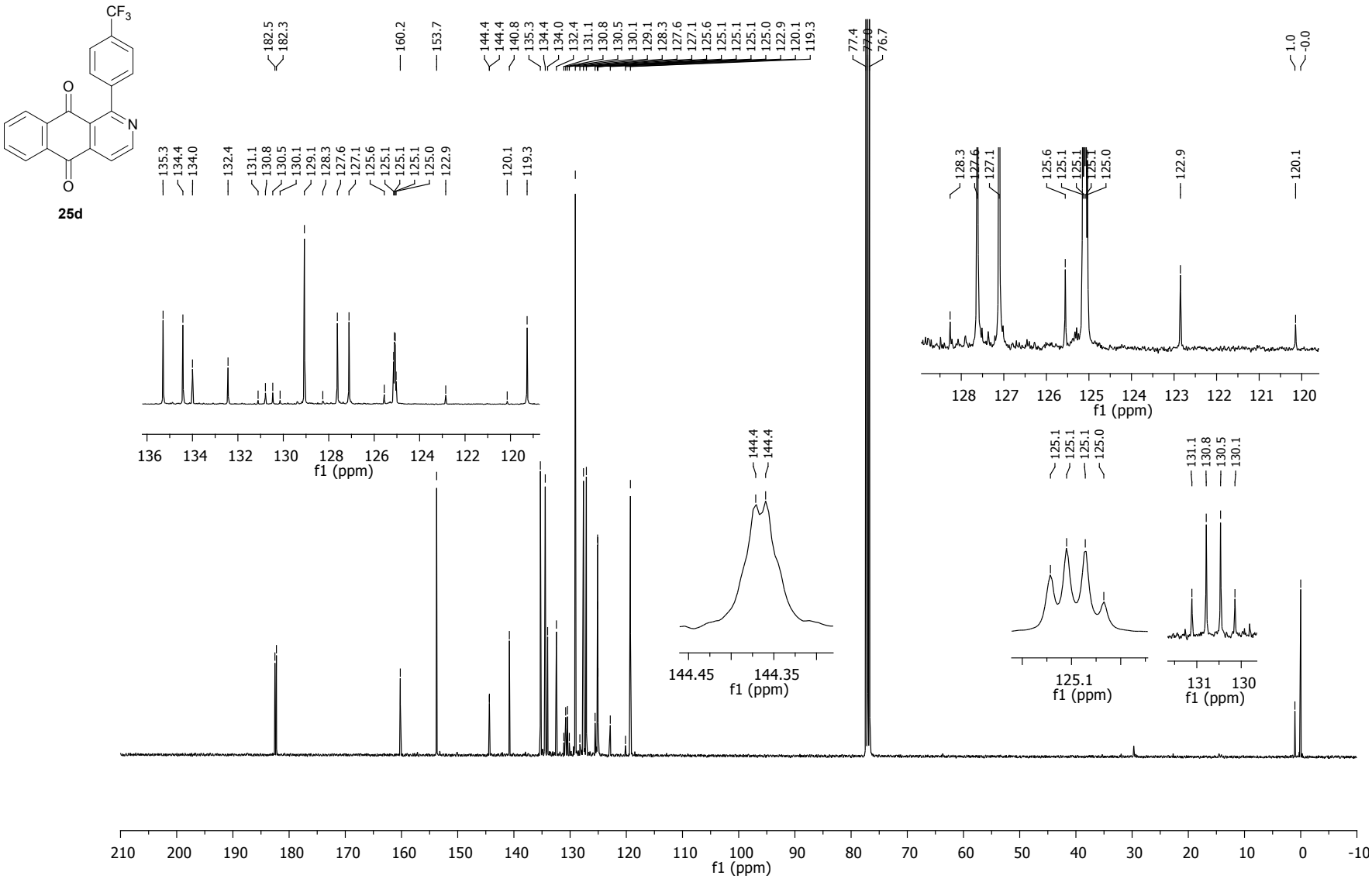


Figure 78 ^{13}C NMR spectrum of 1-(*p*-(trifluoromethyl)phenyl)benzo[*g*]isoquinoline-5,10-dione (**25d**) ($CDCl_3$, 100 MHz).

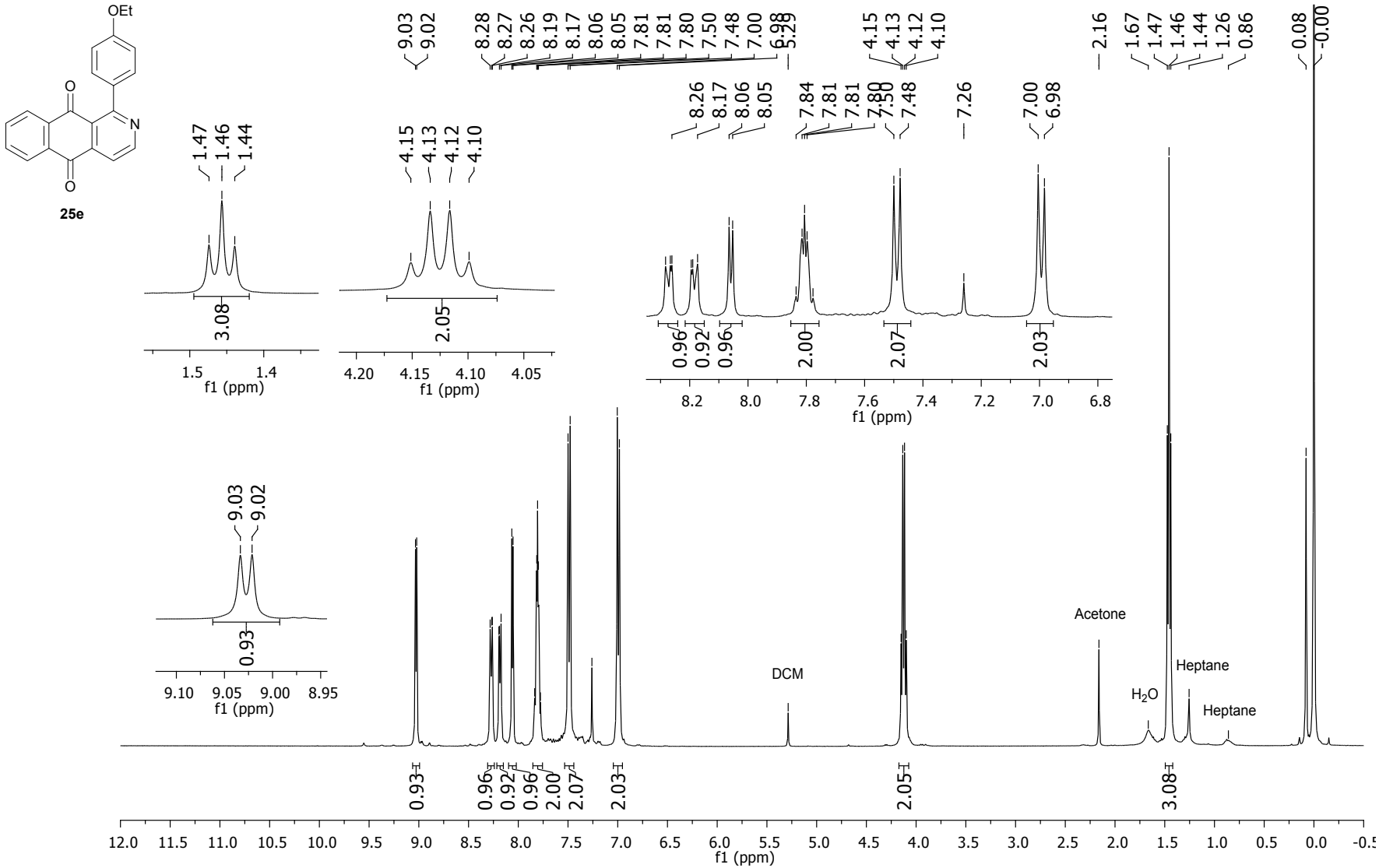


Figure 79 ^{1}H NMR spectrum of 1-(*p*-ethoxyphenyl)benzo[*g*]isoquinoline-5,10-dione (**25e**) ($CDCl_3$, 400 MHz).

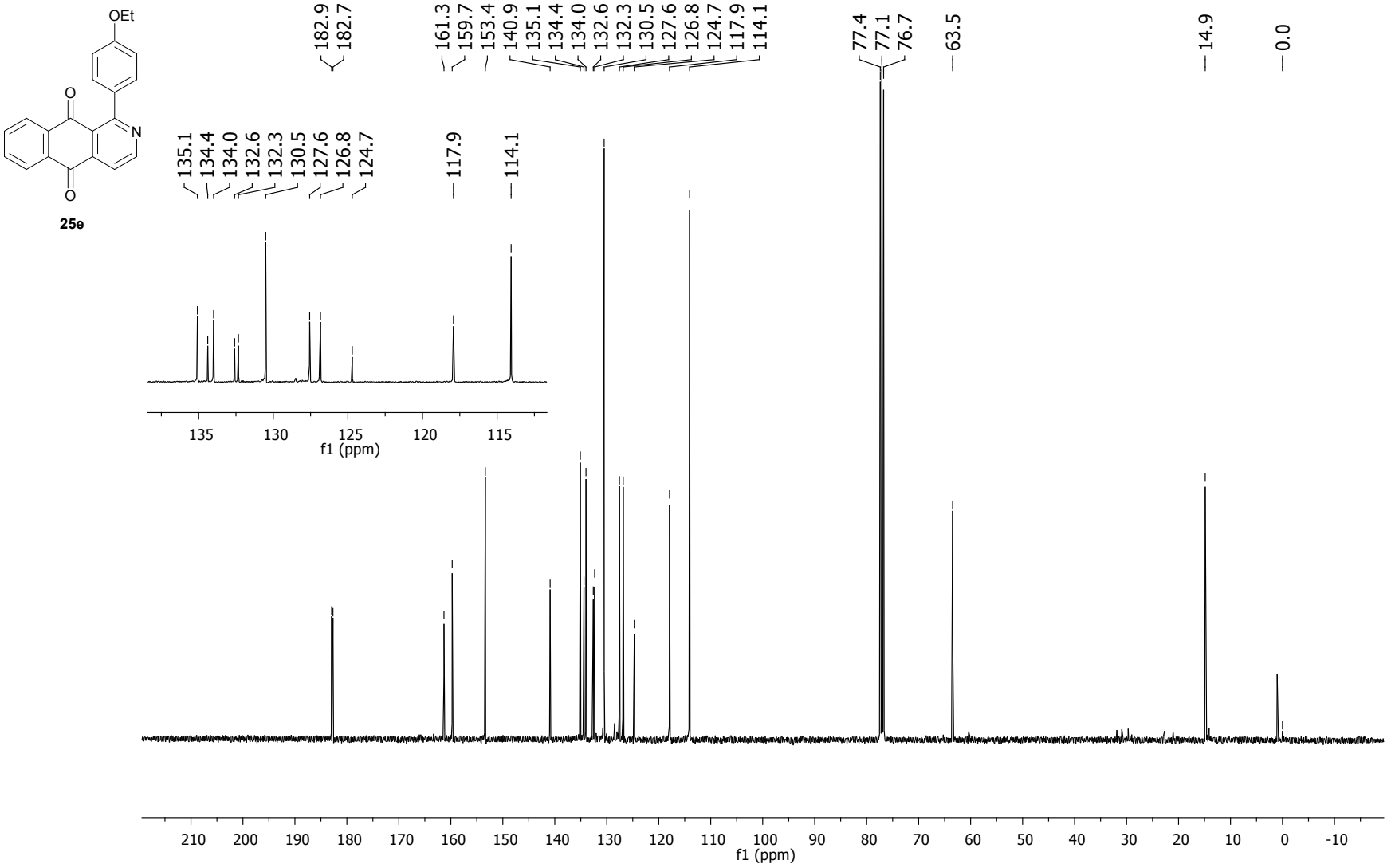


Figure 80 ^{13}C NMR spectrum of 1-(*p*-ethoxyphenyl)benzo[*g*]isoquinoline-5,10-dione (**25e**) ($CDCl_3$, 100 MHz).

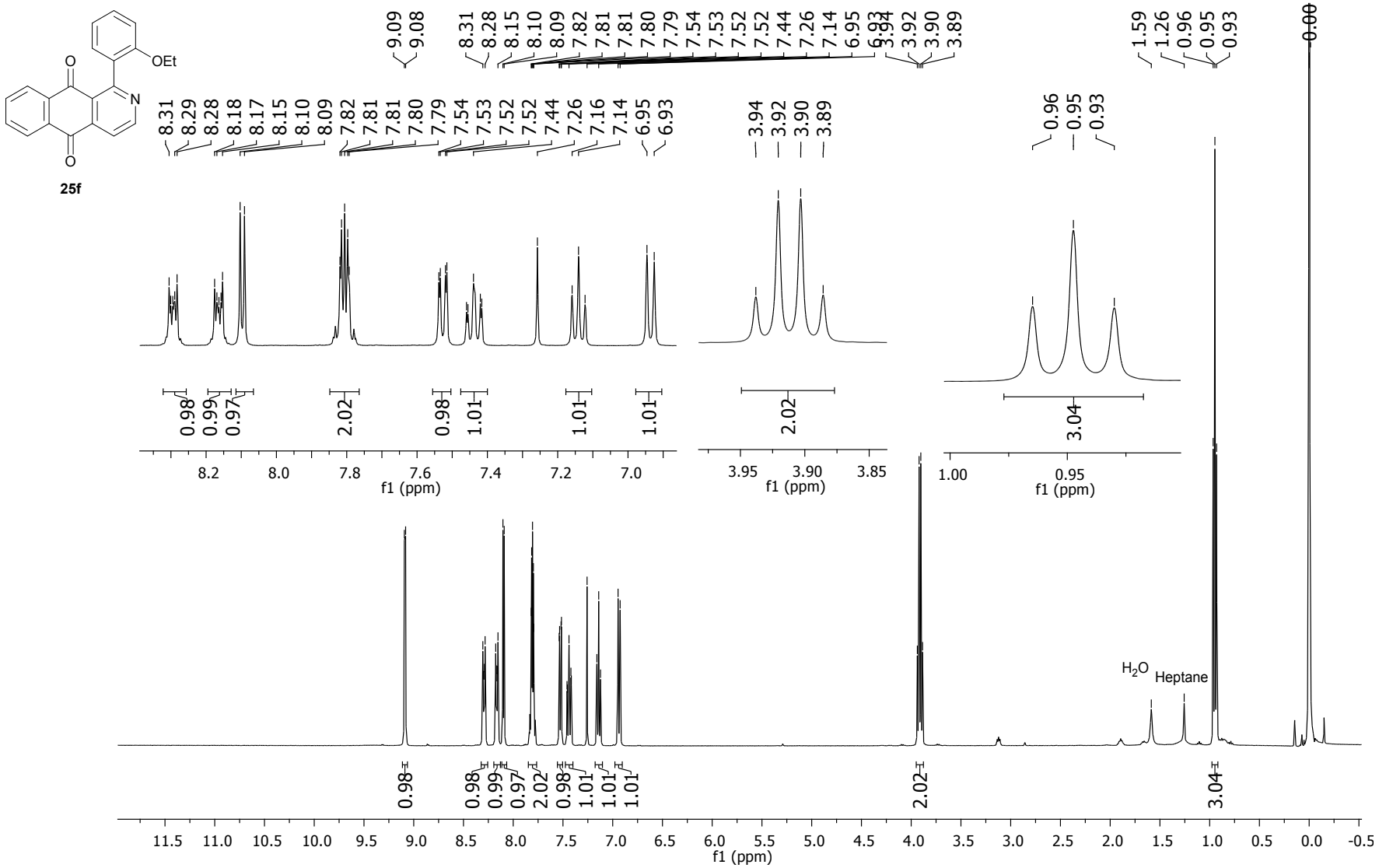


Figure 81 ^{1}H NMR spectrum of 1-(*o*-ethoxyphenyl)benzo[*g*]isoquinoline-5,10-dione (**25f**) ($CDCl_3$, 400 MHz).

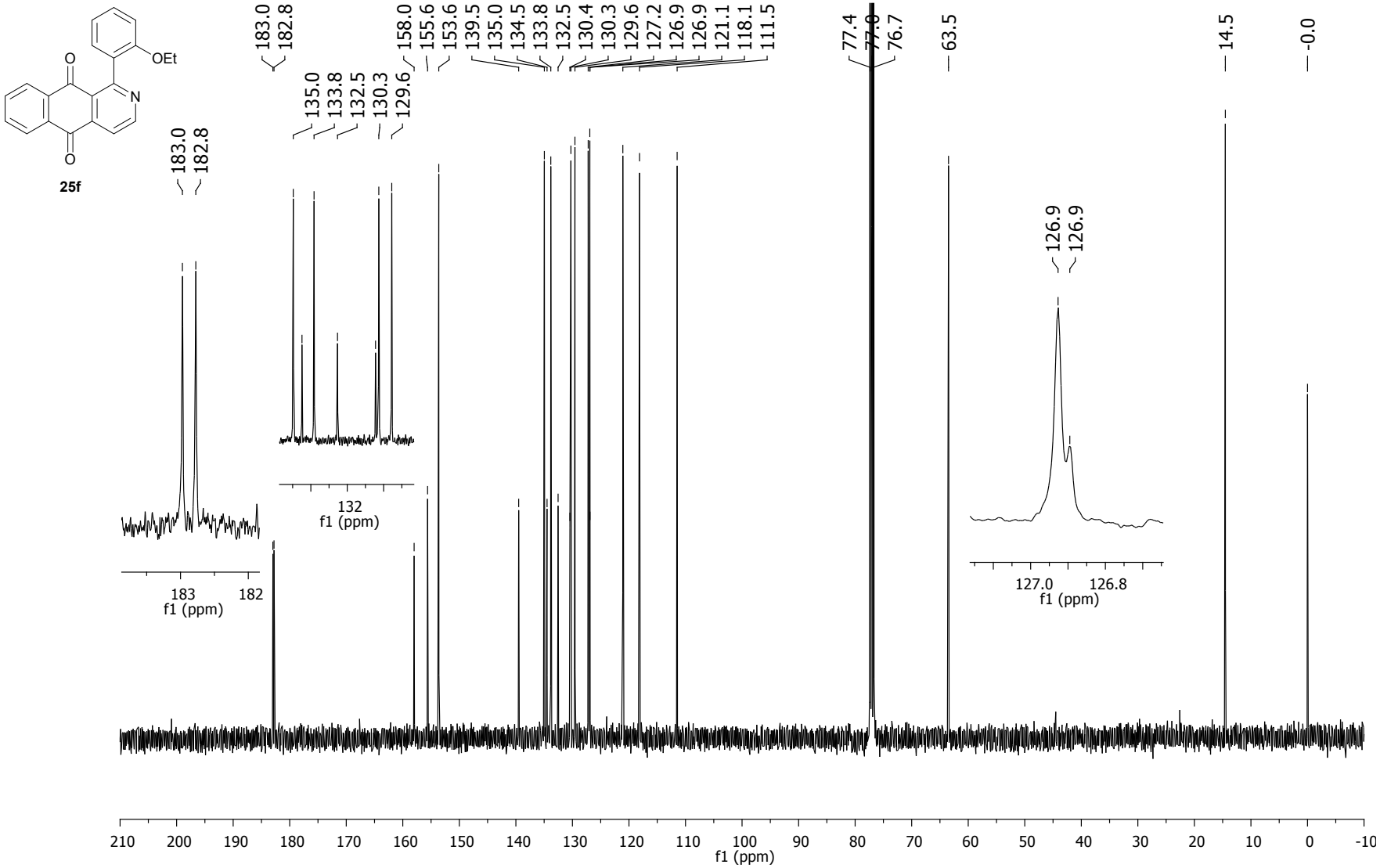


Figure 82 ^{13}C NMR spectrum of 1-(*o*-ethoxyphenyl)benzo[*g*]isoquinoline-5,10-dione (**25f**) ($CDCl_3$, 100 MHz).

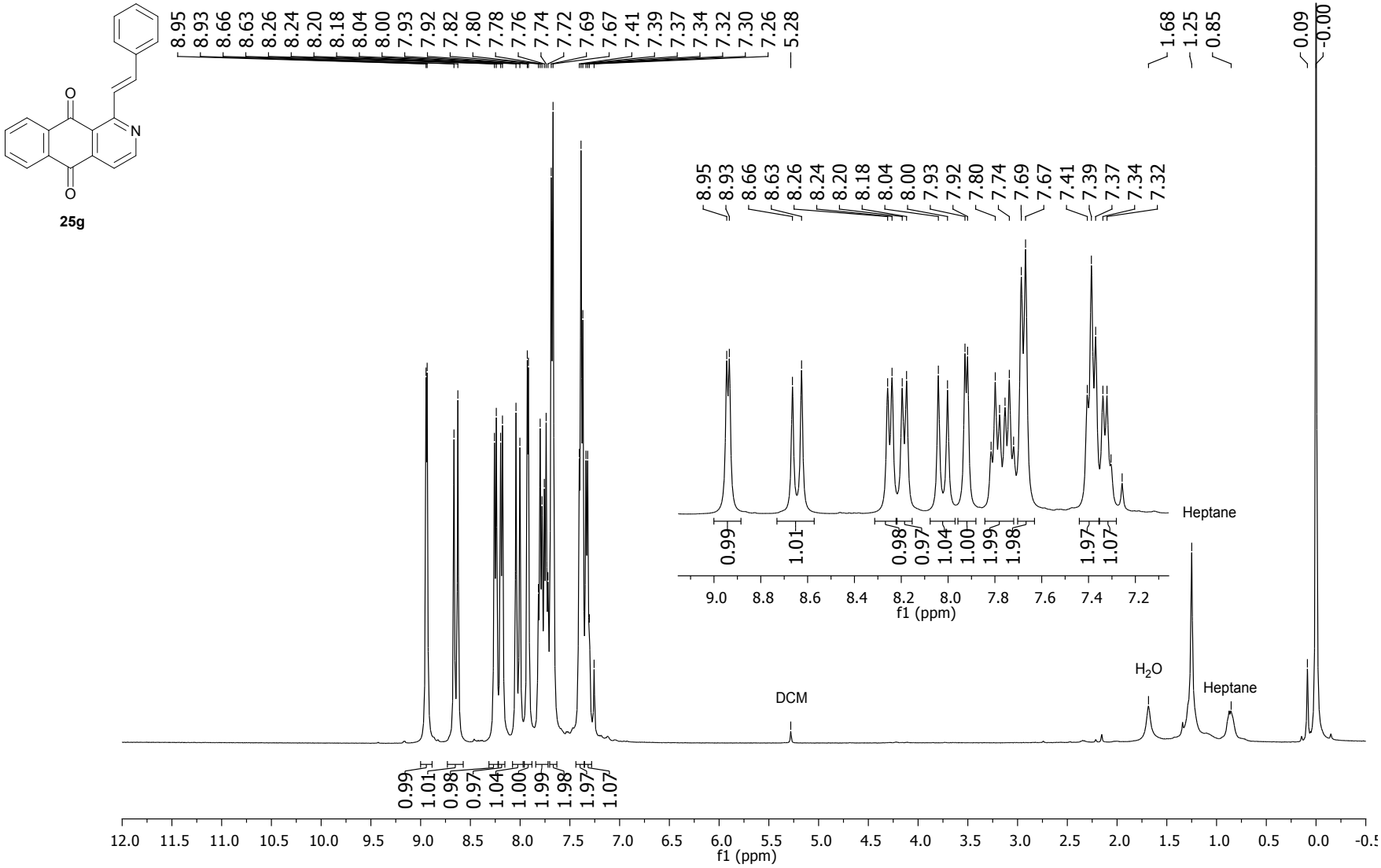


Figure 83 ^{1}H NMR spectrum of (*E*)-1-styrylbenzo[*g*]isoquinoline-5,10-dione (**25g**) ($CDCl_3$, 400 MHz).

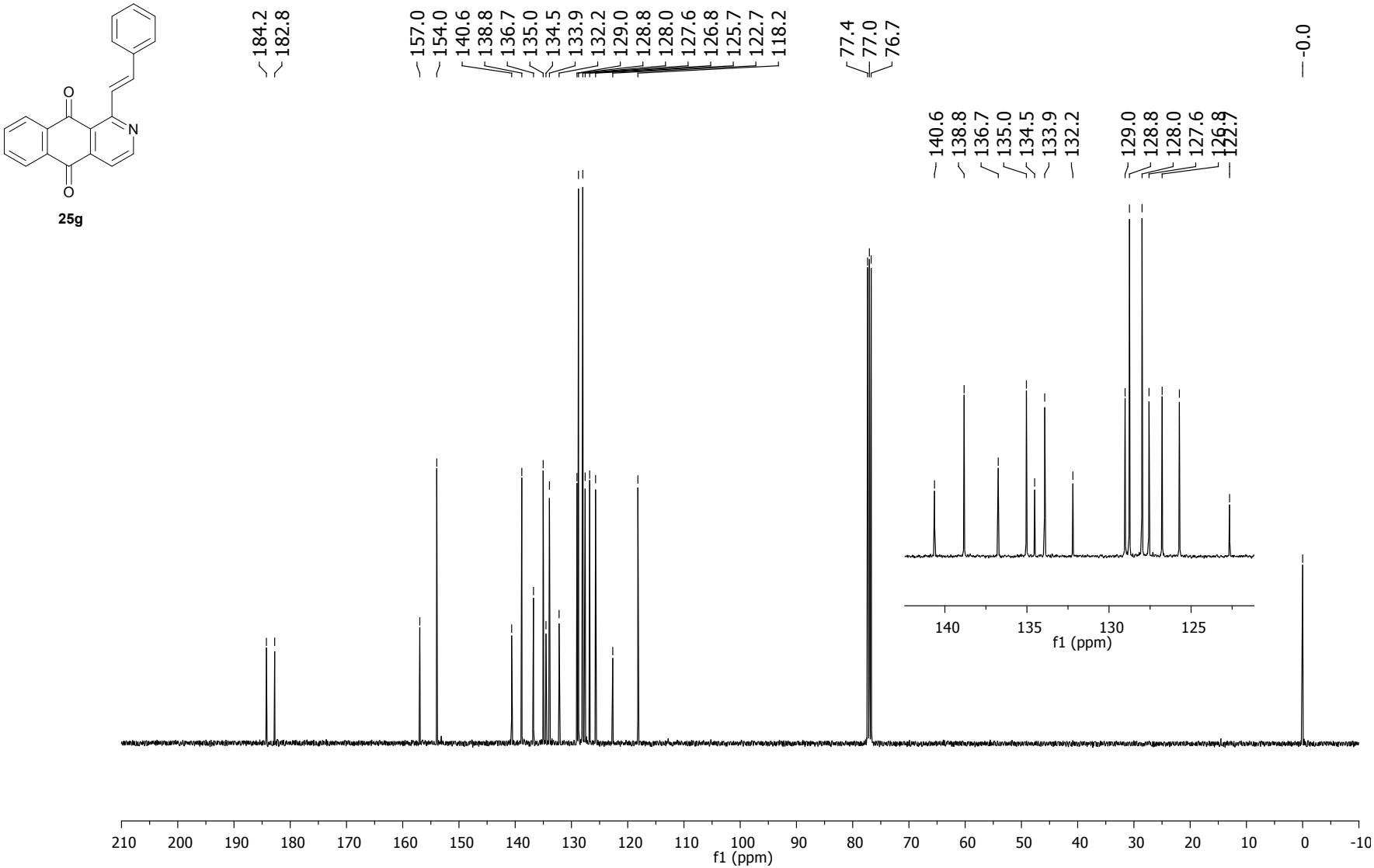


Figure 84[13]C NMR spectrum of (*E*)-1-styrylbenzo[*g*]isoquinoline-5,10-dione (**25g**) ($CDCl_3$, 100 MHz).

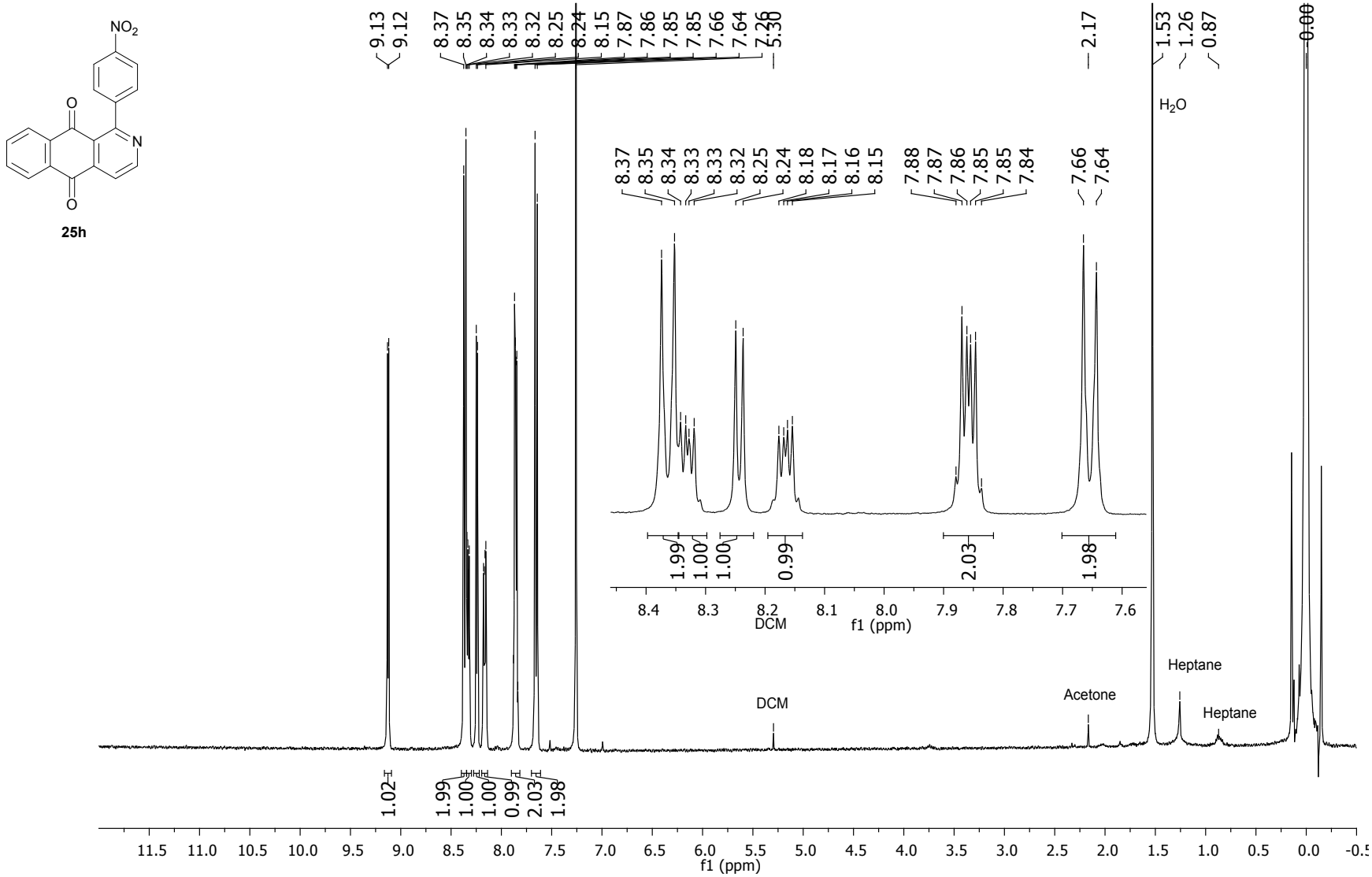


Figure 85 ^{1}H NMR spectrum of 1-(*p*-nitrophenyl)benzo[*g*]isoquinoline-5,10-dione (**25h**) ($CDCl_3$, 400 MHz).

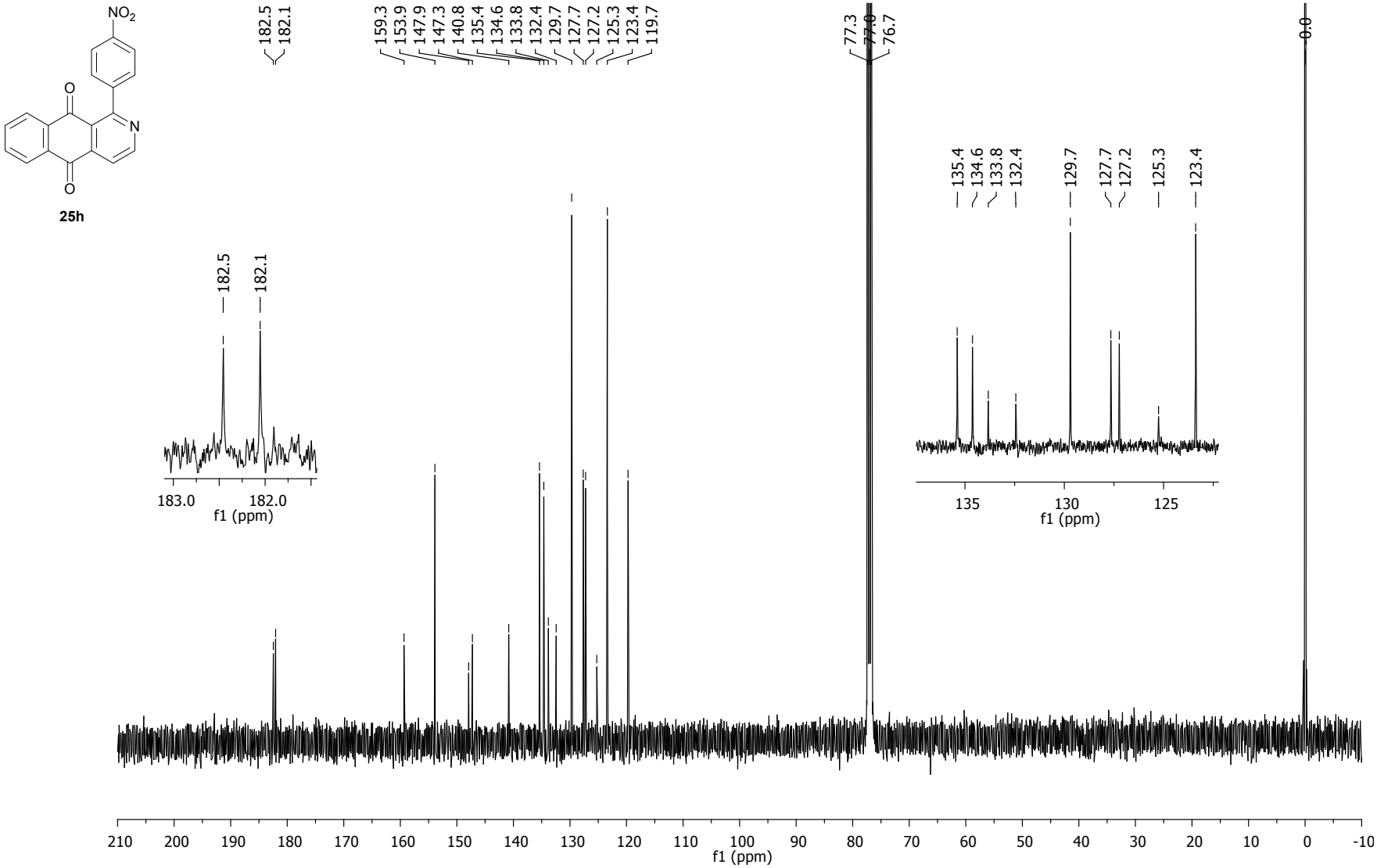


Figure 86 ^{13}C NMR spectrum of 1-(*p*-nitrophenyl)benzo[*g*]isoquinoline-5,10-dione (**25h**) ($CDCl_3$, 100 MHz).

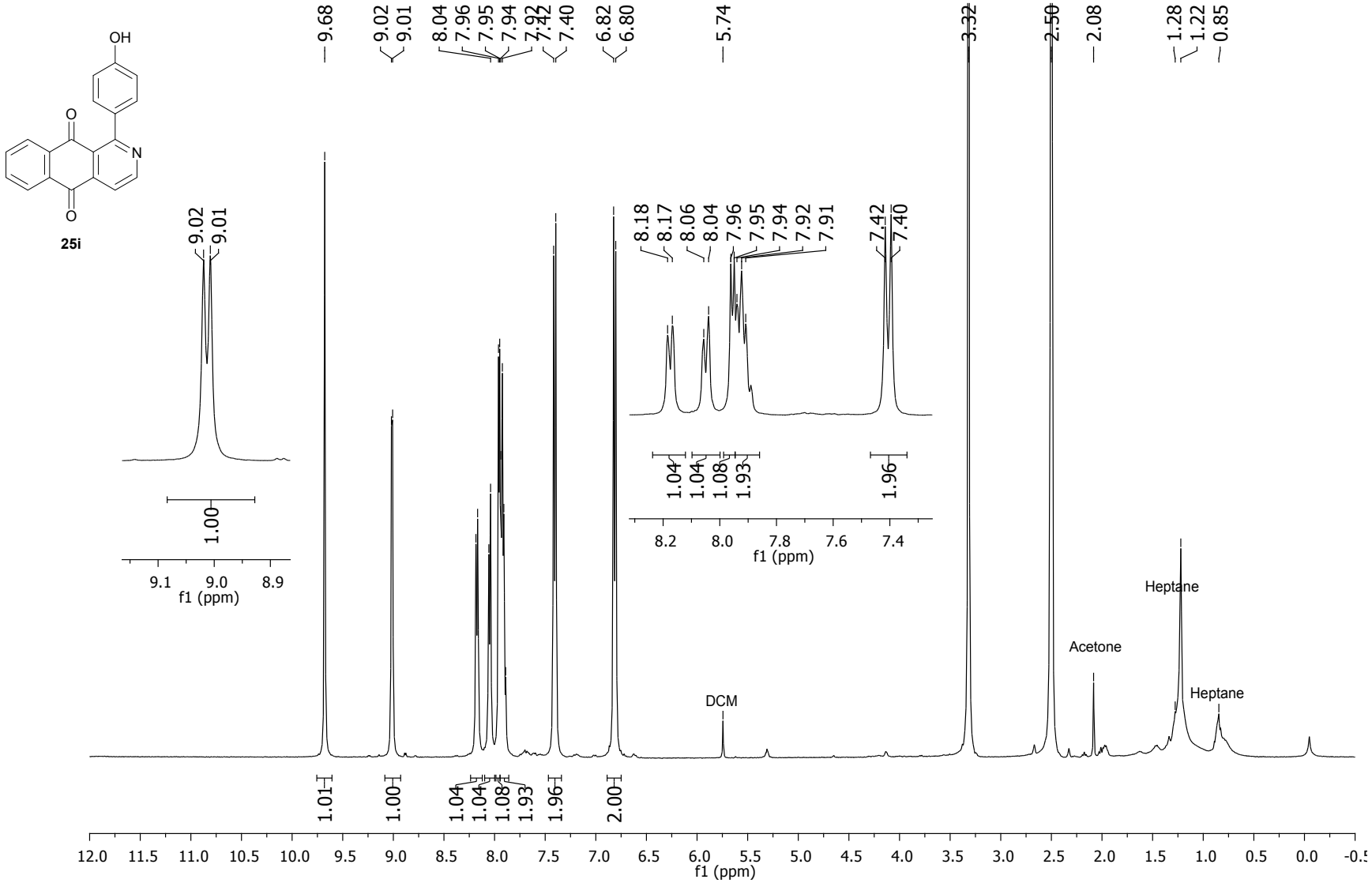


Figure 87 ^{1}H NMR spectrum of 1-(*p*-hydroxyphenyl)benzo[*g*]isoquinoline-5,10-dione (**25i**) (DMSO-d6, 400 MHz).

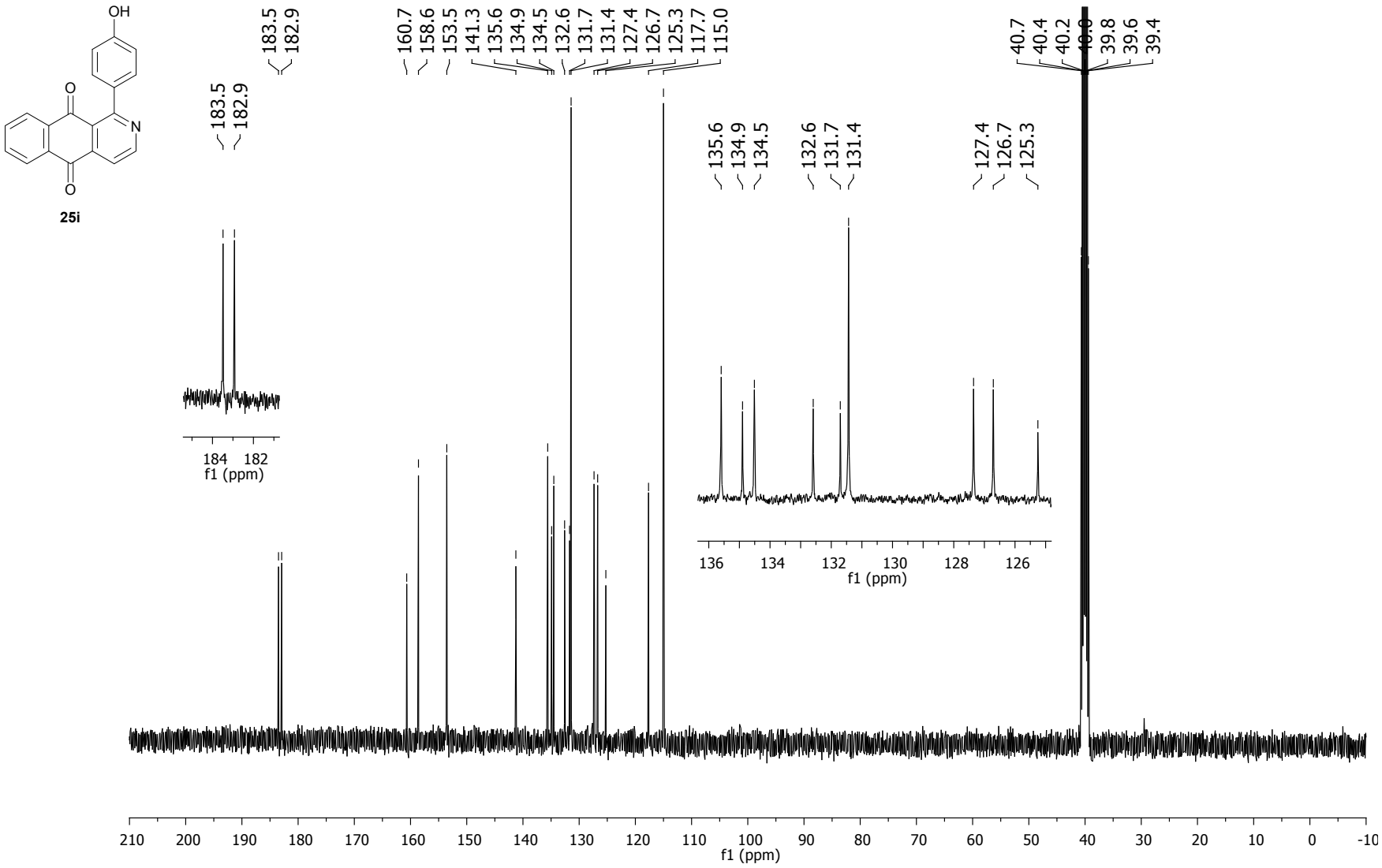


Figure 88 ^{13}C NMR spectrum of 1-(*p*-hydroxyphenyl)benzo[*g*]isoquinoline-5,10-dione (**25i**) (DMSO-d6, 100 MHz).

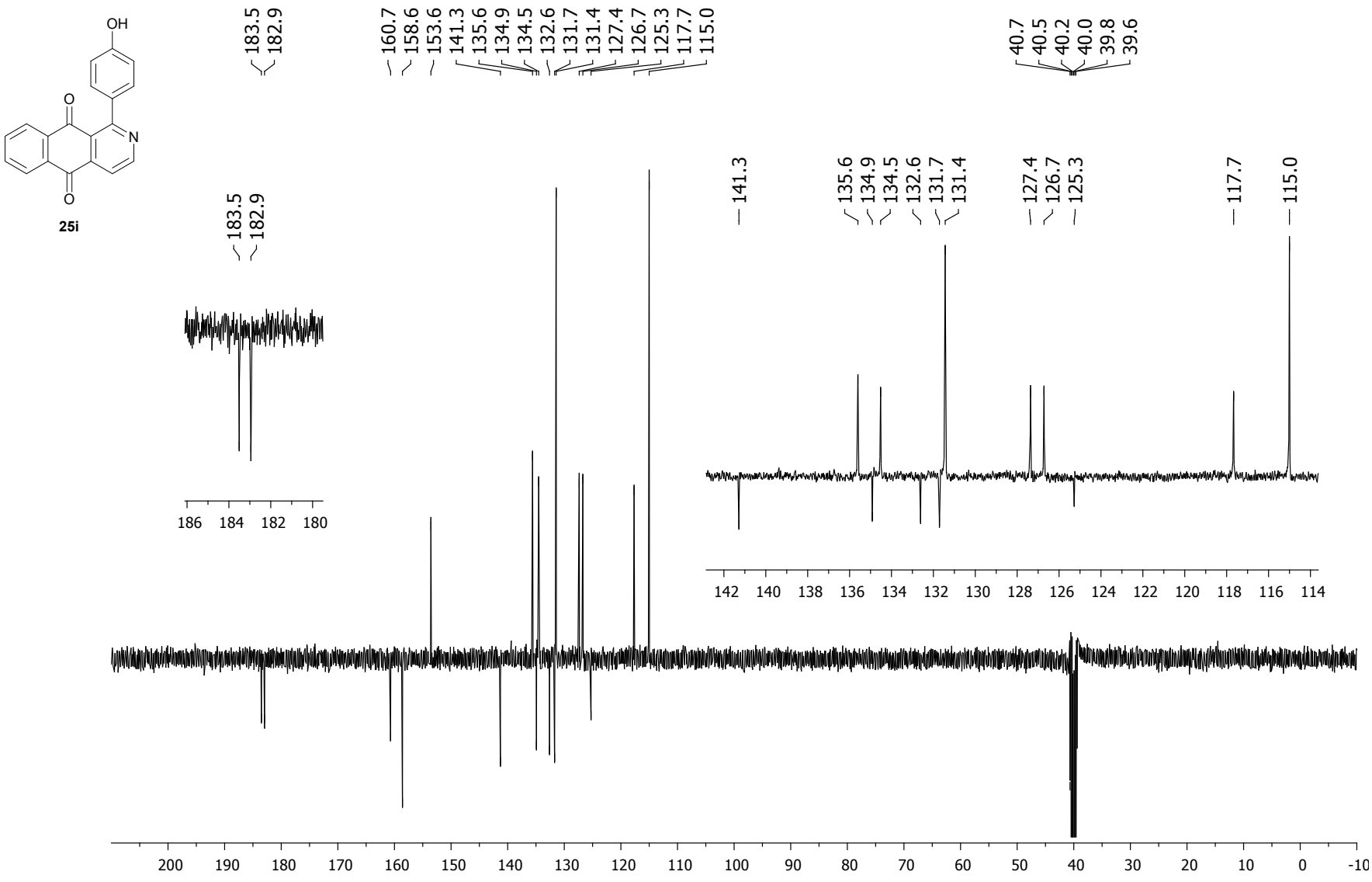


Figure 89 APT spectrum of 1-(*p*-hydroxyphenyl)benzo[*g*]isoquinoline-5,10-dione (**25i**) (DMSO-d6, 100 MHz).

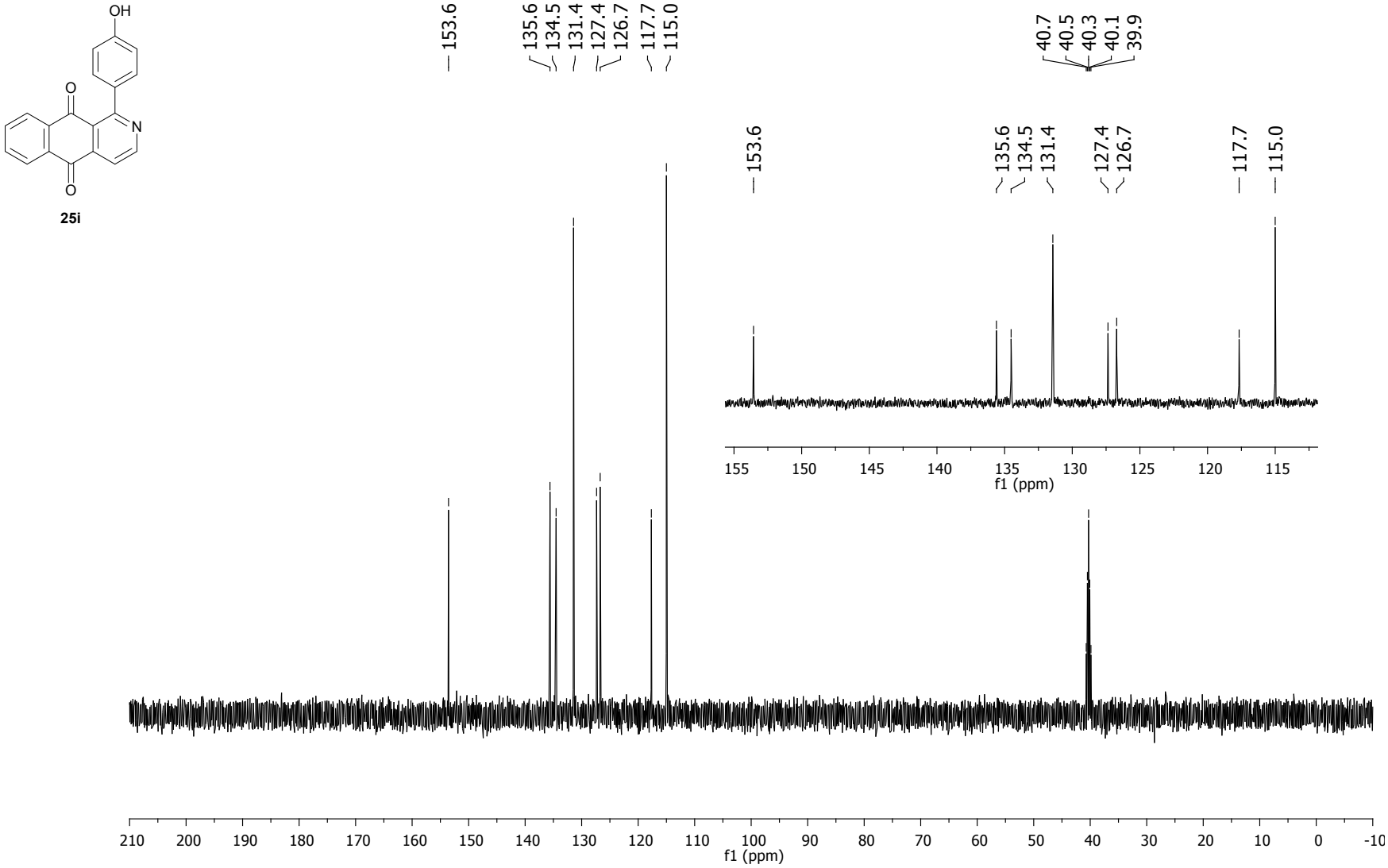


Figure 90 DEPT 135 spectrum of 1-(*p*-hydroxyphenyl)benzo[*g*]isoquinoline-5,10-dione (**25i**) (DMSO-d6, 100 MHz).

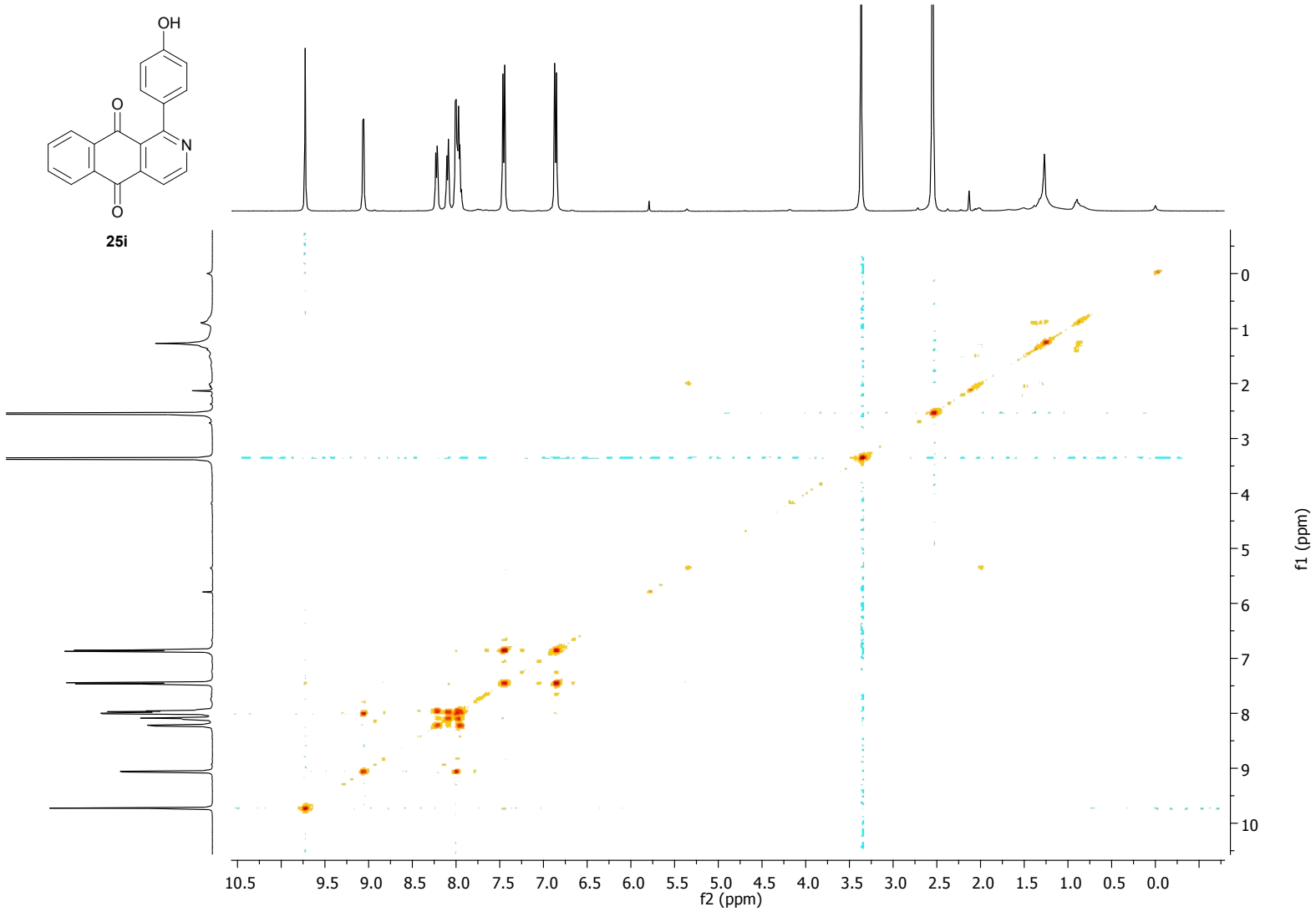


Figure 91 COSY spectrum of 1-(*p*-hydroxyphenyl)benzo[*g*]isoquinoline-5,10-dione (**25i**) (DMSO-d6, 400 MHz).

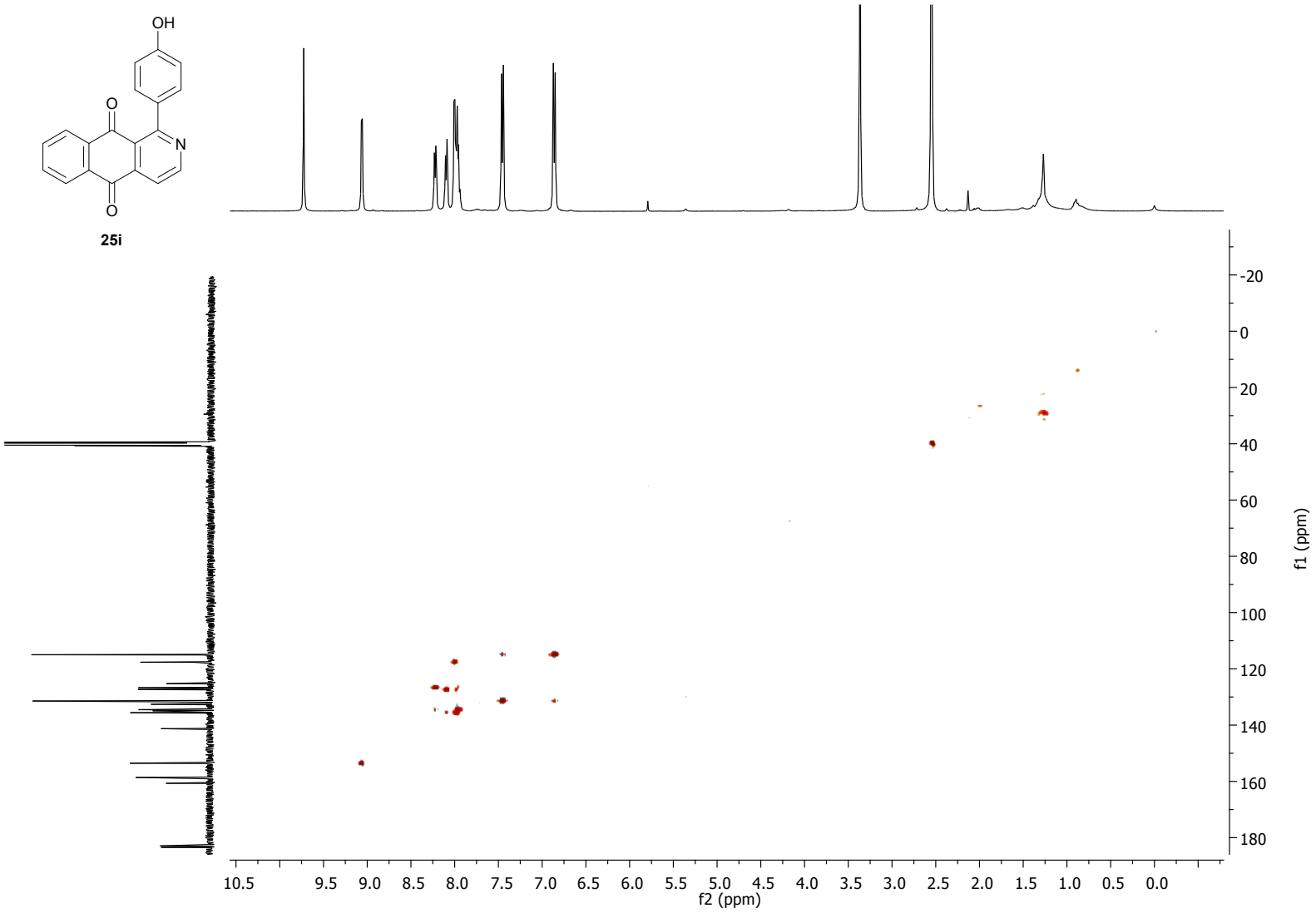


Figure 92 HSQC spectrum of 1-(*p*-hydroxyphenyl)benzo[*g*]isoquinoline-5,10-dione (**25i**) (DMSO-d6, 400 MHz).

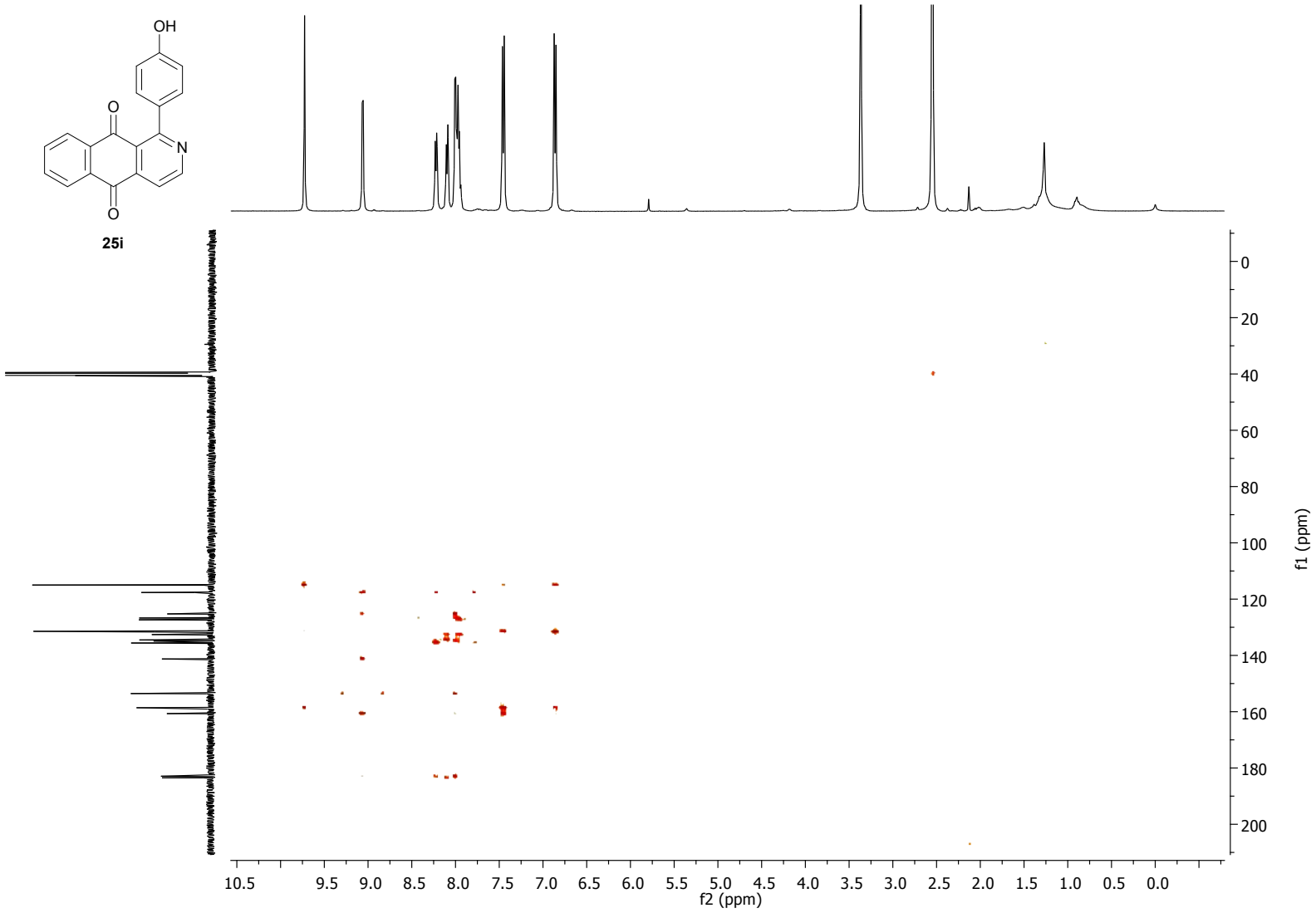


Figure 93 HMBC spectrum of 1-(*p*-hydroxyphenyl)benzo[*g*]isoquinoline-5,10-dione (**25i**) (DMSO-d6, 400 MHz).

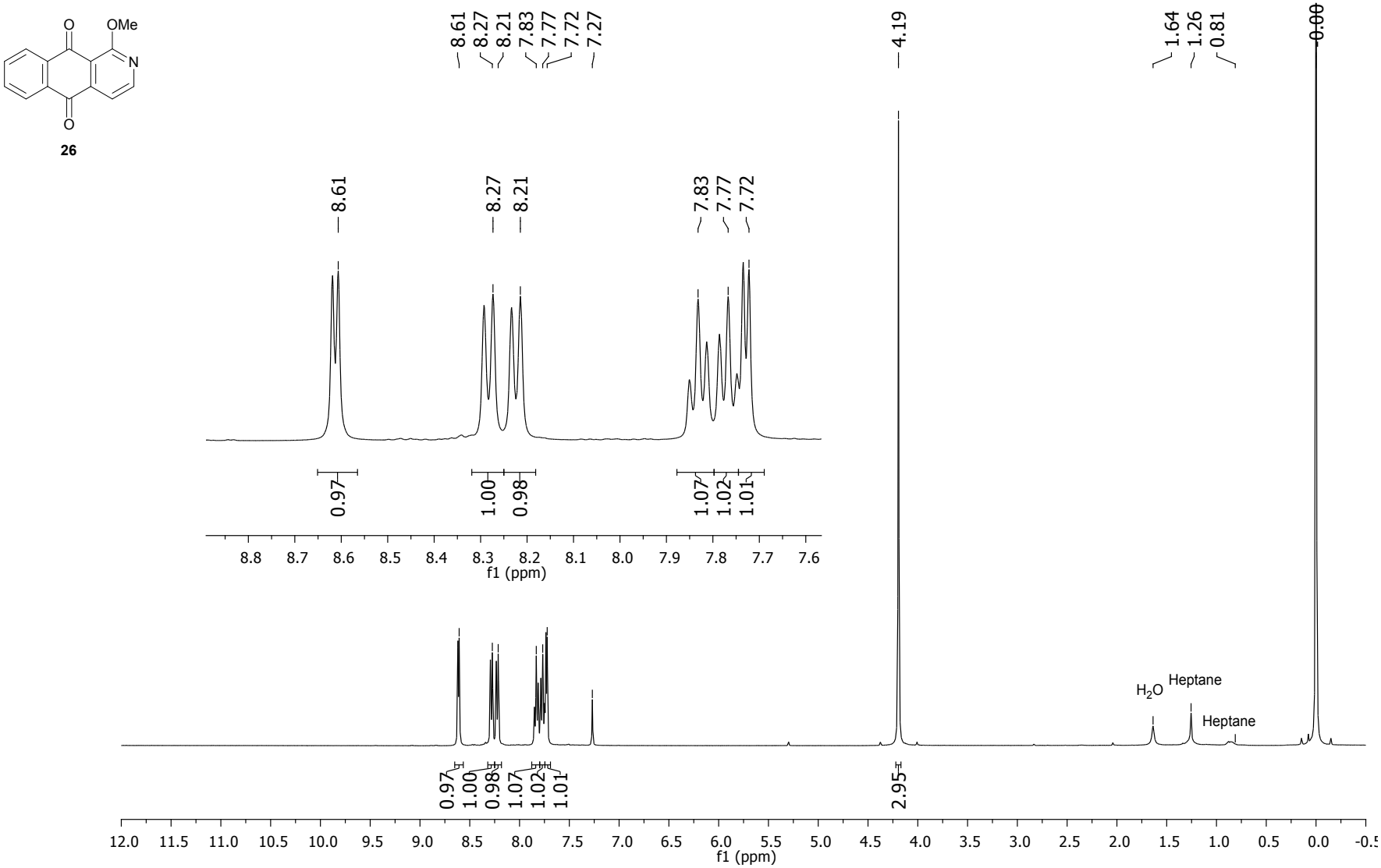


Figure 94 ^{1}H NMR spectrum of 1-methoxybenzo[*g*]isoquinoline-5,10-dione (**26**) ($CDCl_3$, 400 MHz).

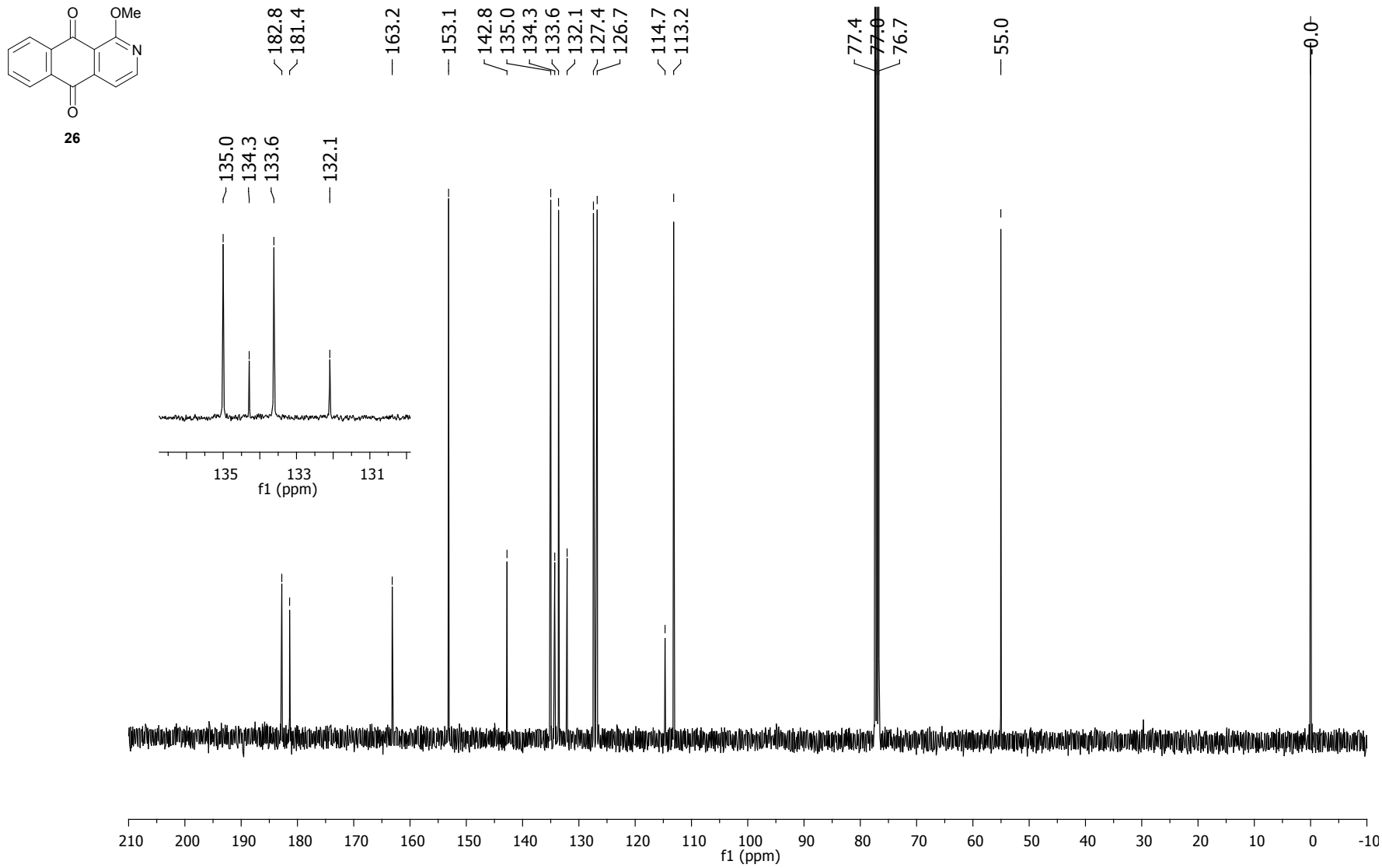


Figure 95 ^{13}C NMR spectrum of 1-methoxybenzo[*g*]isoquinoline-5,10-dione (**26**) ($CDCl_3$, 100 MHz).

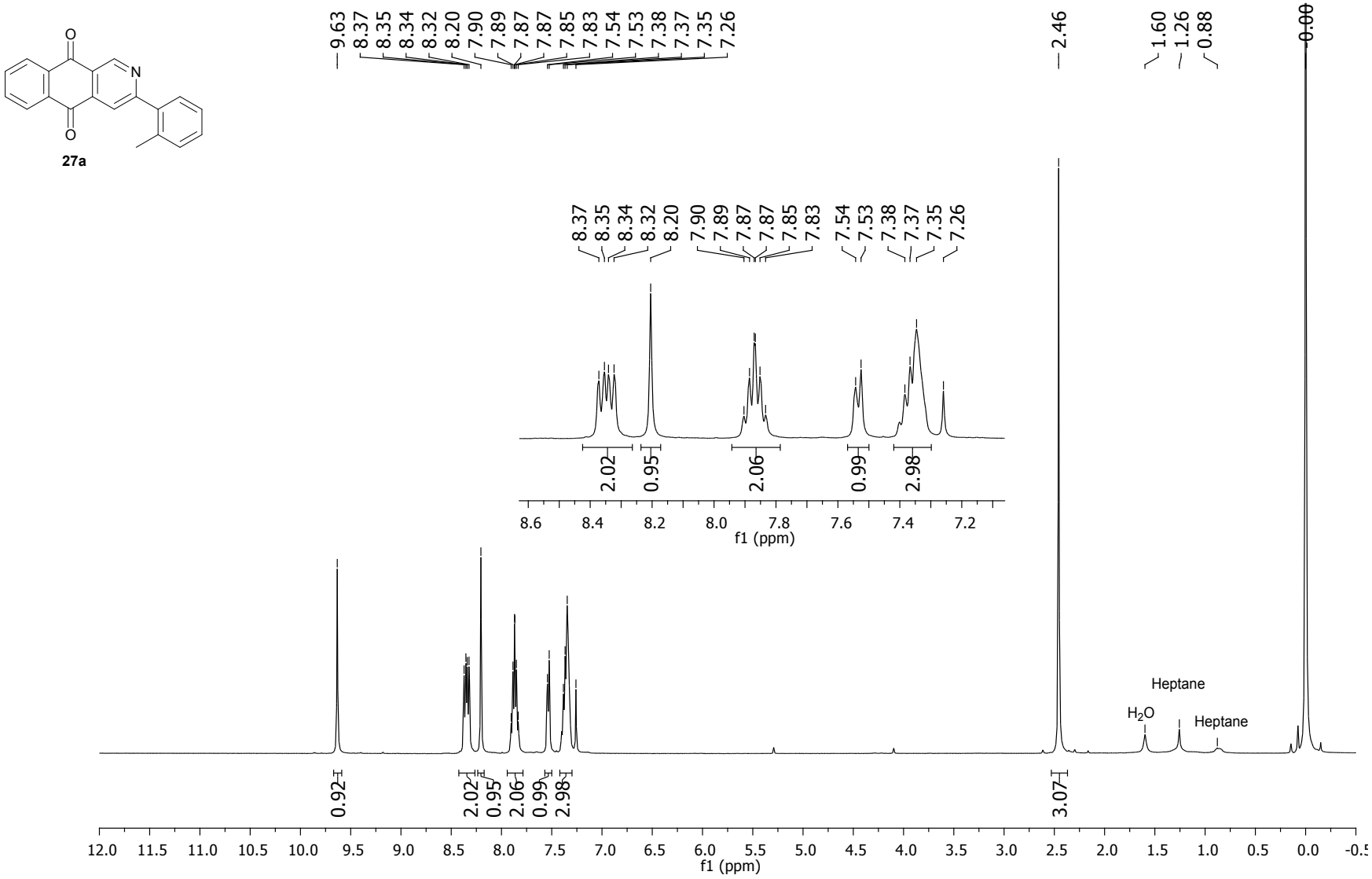


Figure 96^{1}H NMR spectrum of 3-(*o*-tolyl)benzo[*g*]isoquinoline-5,10-dione (**27a**) ($CDCl_3$, 400 MHz).

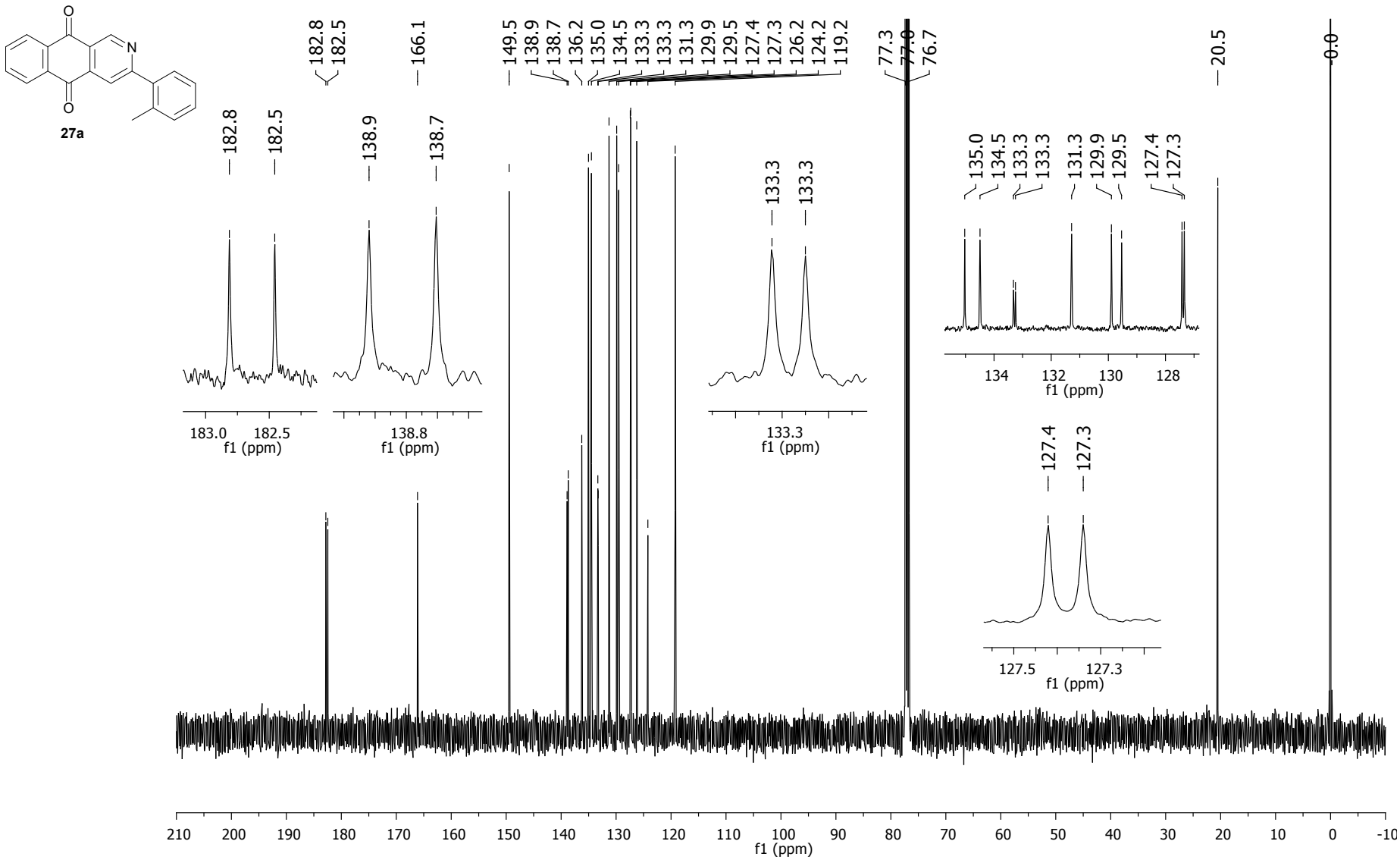


Figure 97 ^{13}C NMR spectrum of 3-(*o*-tolyl)benzo[*g*]isoquinoline-5,10-dione (**27a**) ($CDCl_3$, 100 MHz).

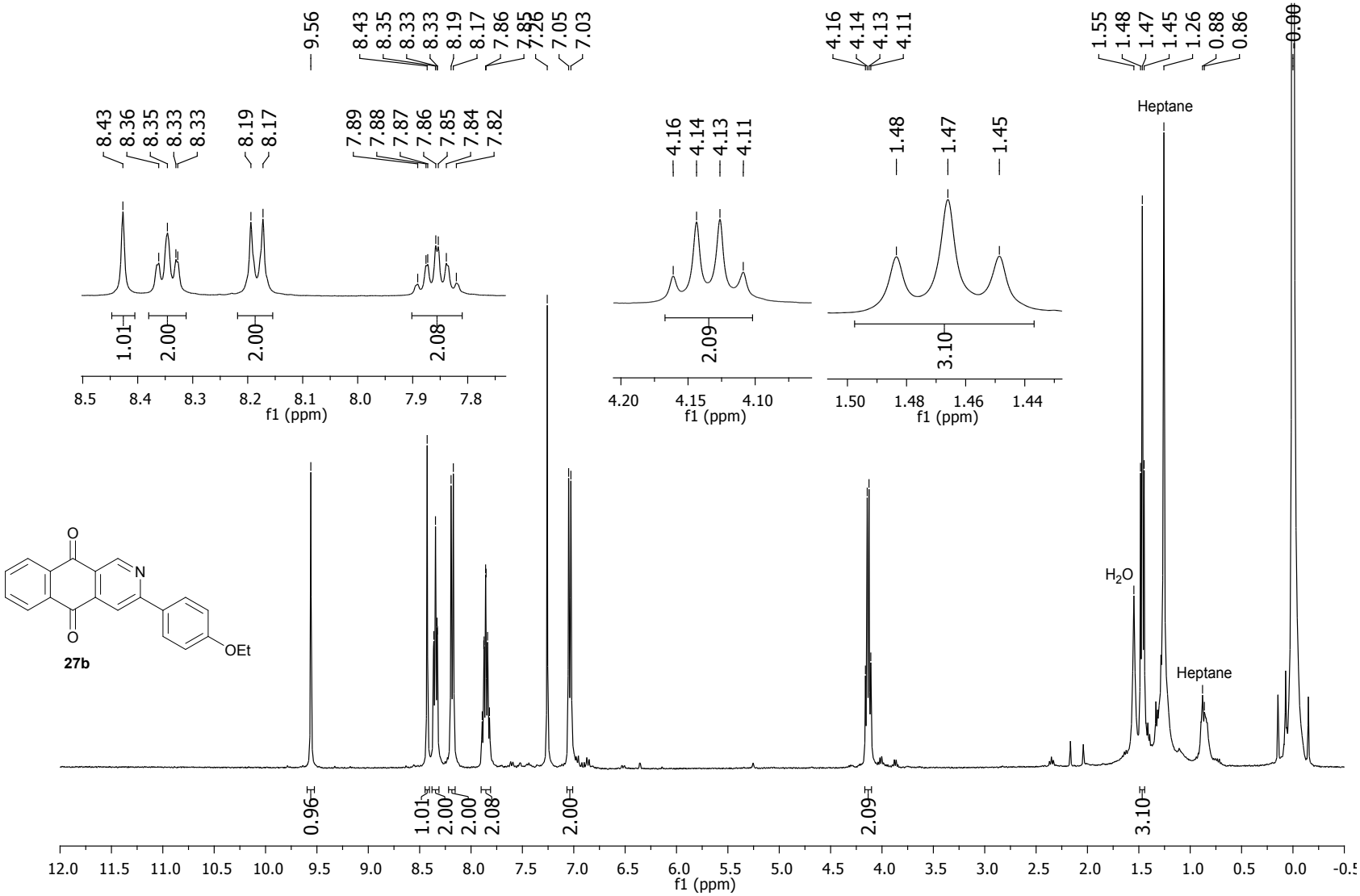


Figure 98 ^{1}H NMR spectrum of 3-(*p*-ethoxyphenyl)benzo[*g*]isoquinoline-5,10-dione (**27b**) ($CDCl_3$, 400 MHz).

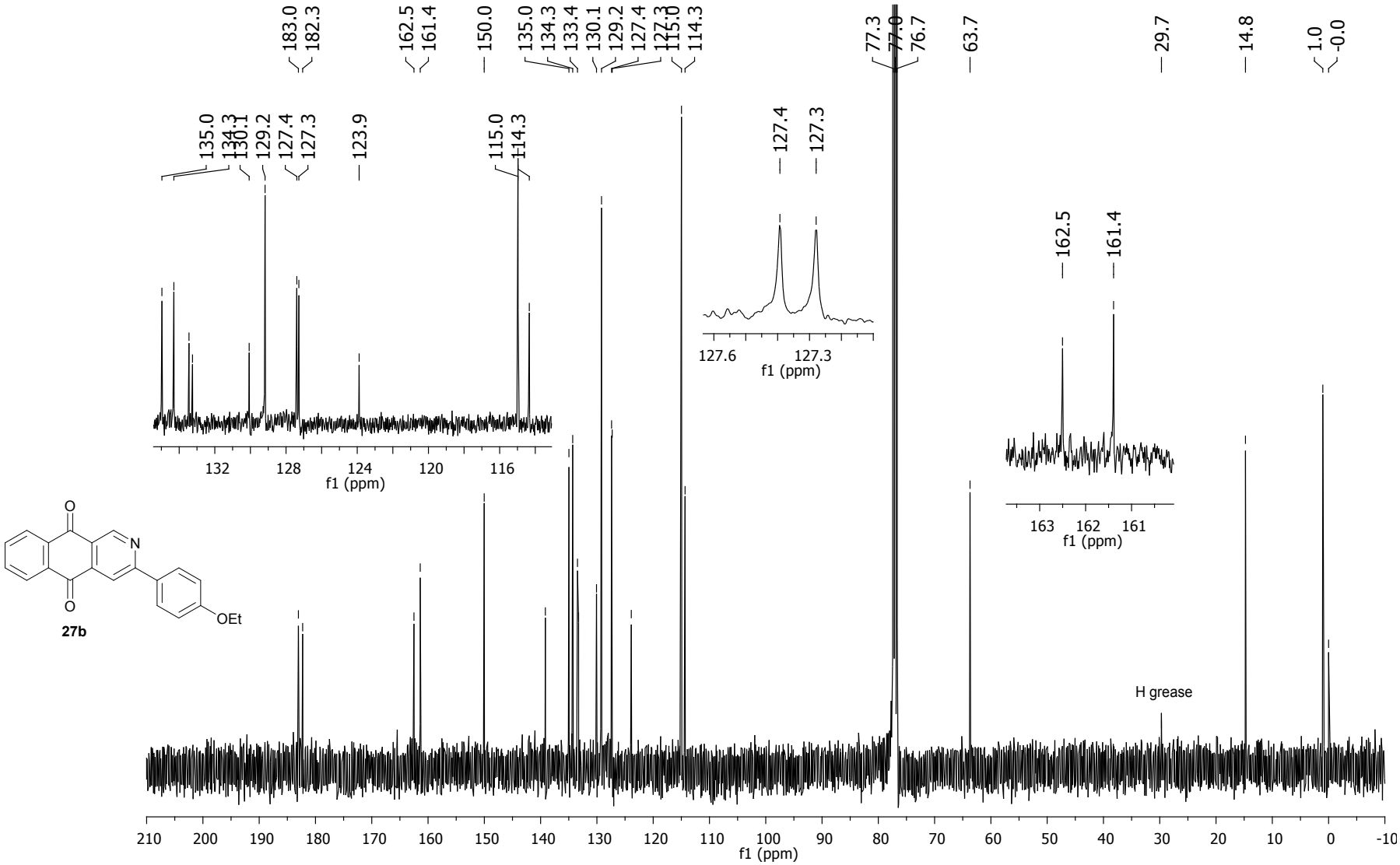


Figure 99 ^{13}C NMR spectrum of 3-(*p*-ethoxyphenyl)benzo[*g*]isoquinoline-5,10-dione (**27b**) ($CDCl_3$, 100 MHz).

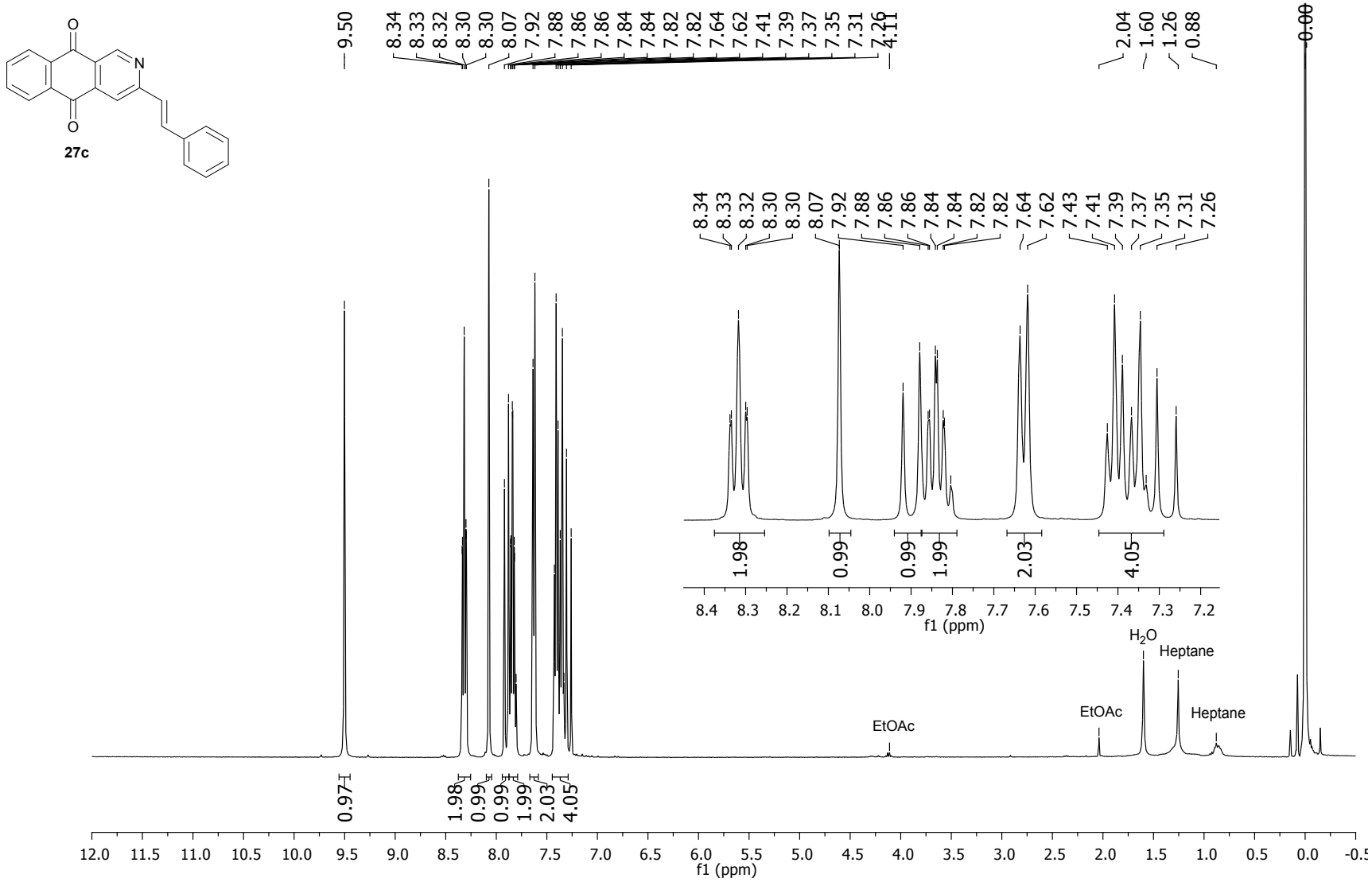


Figure 100 ^{1}H NMR spectrum of (*E*)-3-styrylbenzo[*g*]isoquinoline-5,10-dione (**27c**) ($CDCl_3$, 400 MHz).

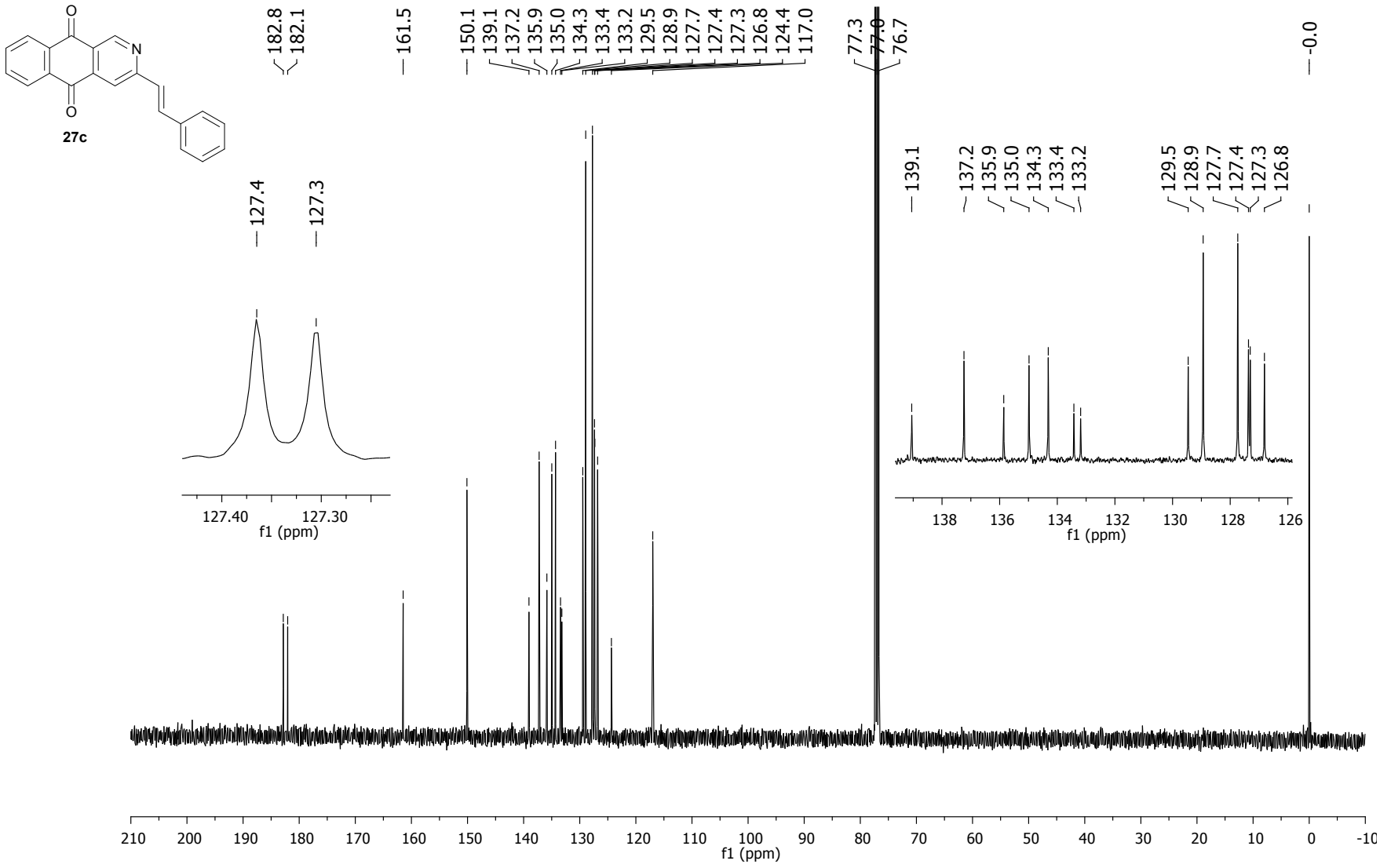


Figure 101 ^{13}C NMR spectrum of (*E*)-3-styrylbenzo[*g*]isoquinoline-5,10-dione (**27c**) ($CDCl_3$, 100 MHz).

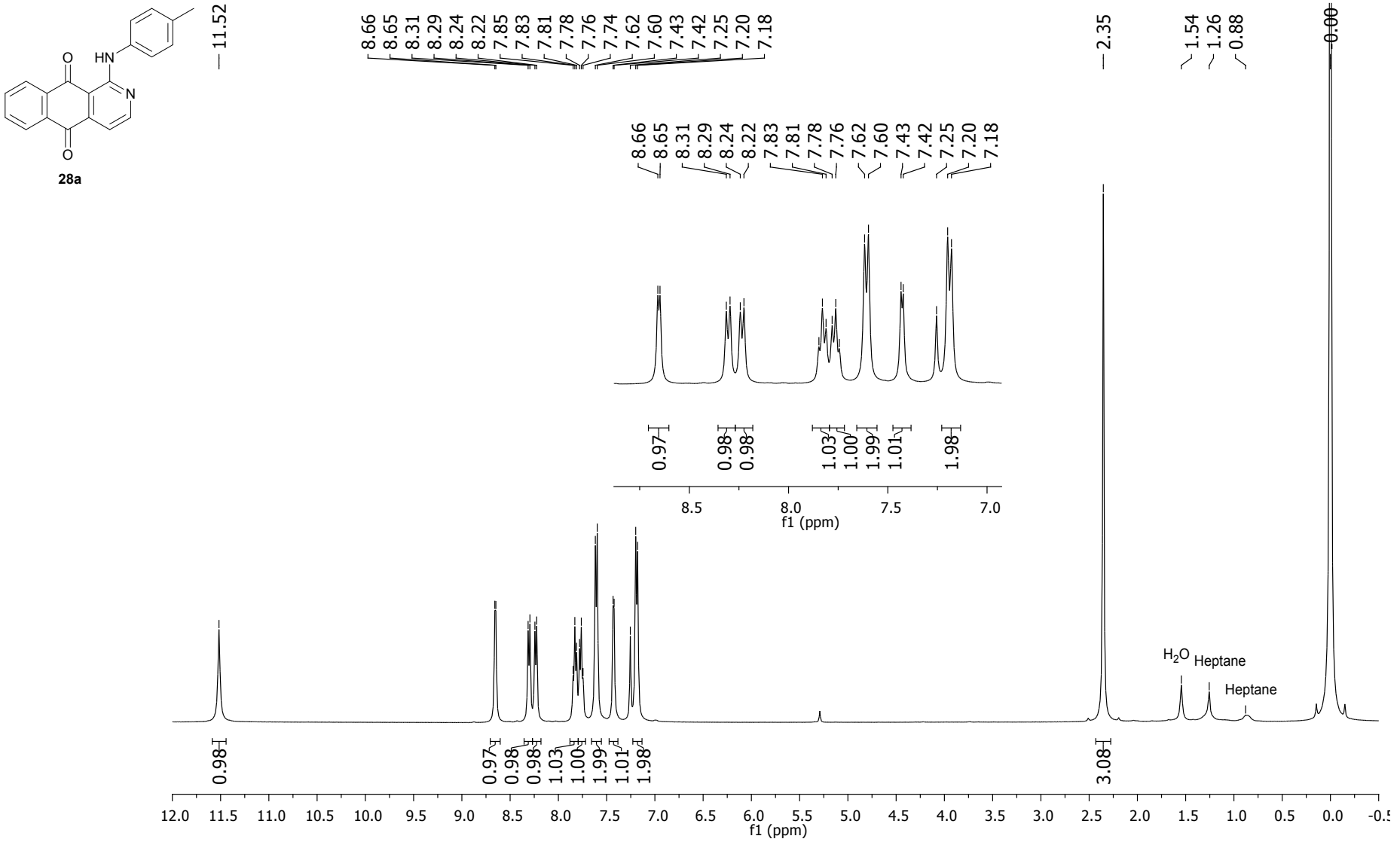


Figure 102 ^{1}H NMR spectrum of 1-(*p*-tolylamino)benzo[*g*]isoquinoline-5,10-dione (**28a**) ($CDCl_3$, 400 MHz).

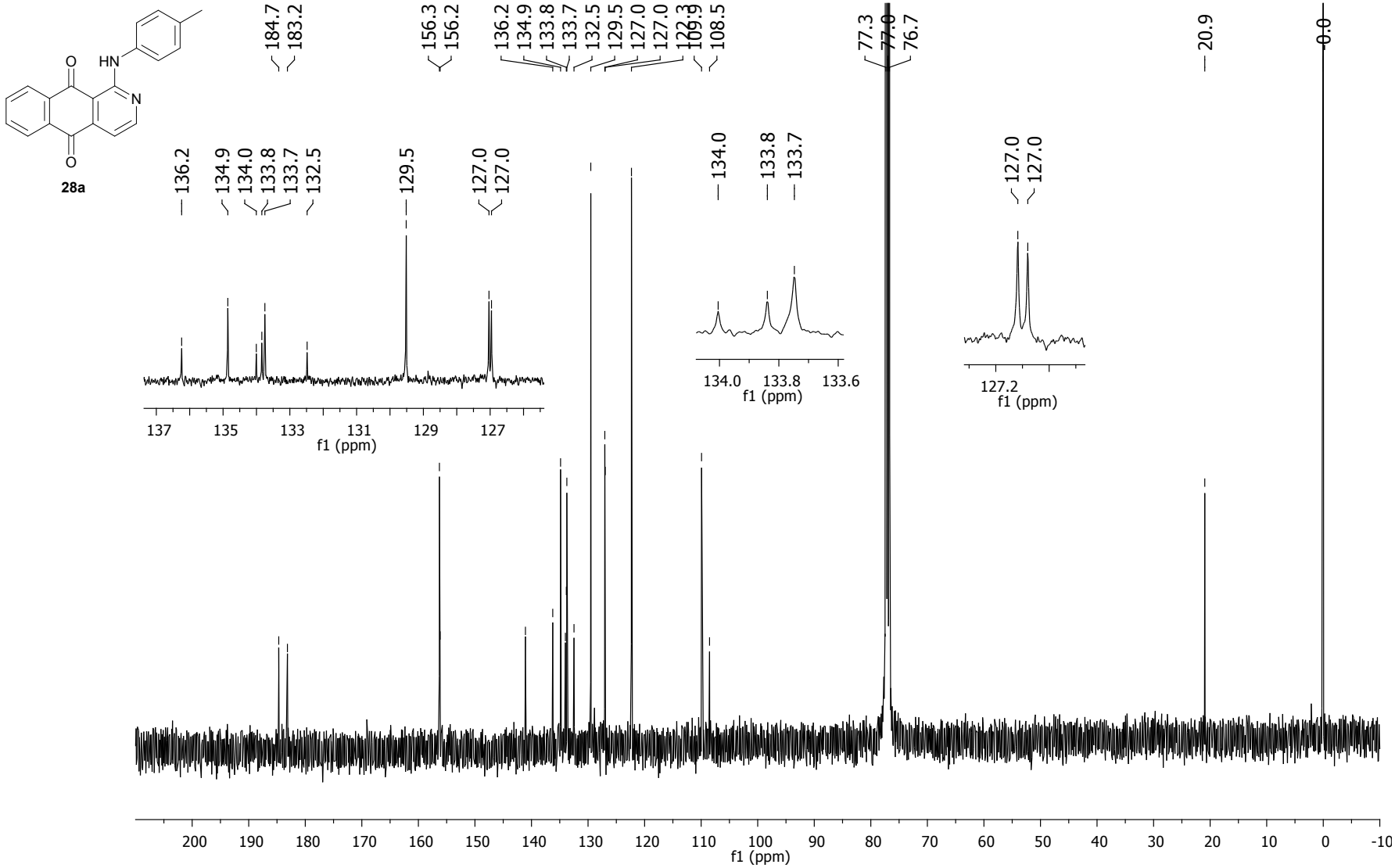


Figure 103 ^{13}C NMR spectrum of 1-(*p*-tolylamino)benzo[*g*]isoquinoline-5,10-dione (**28a**) ($CDCl_3$, 100 MHz).

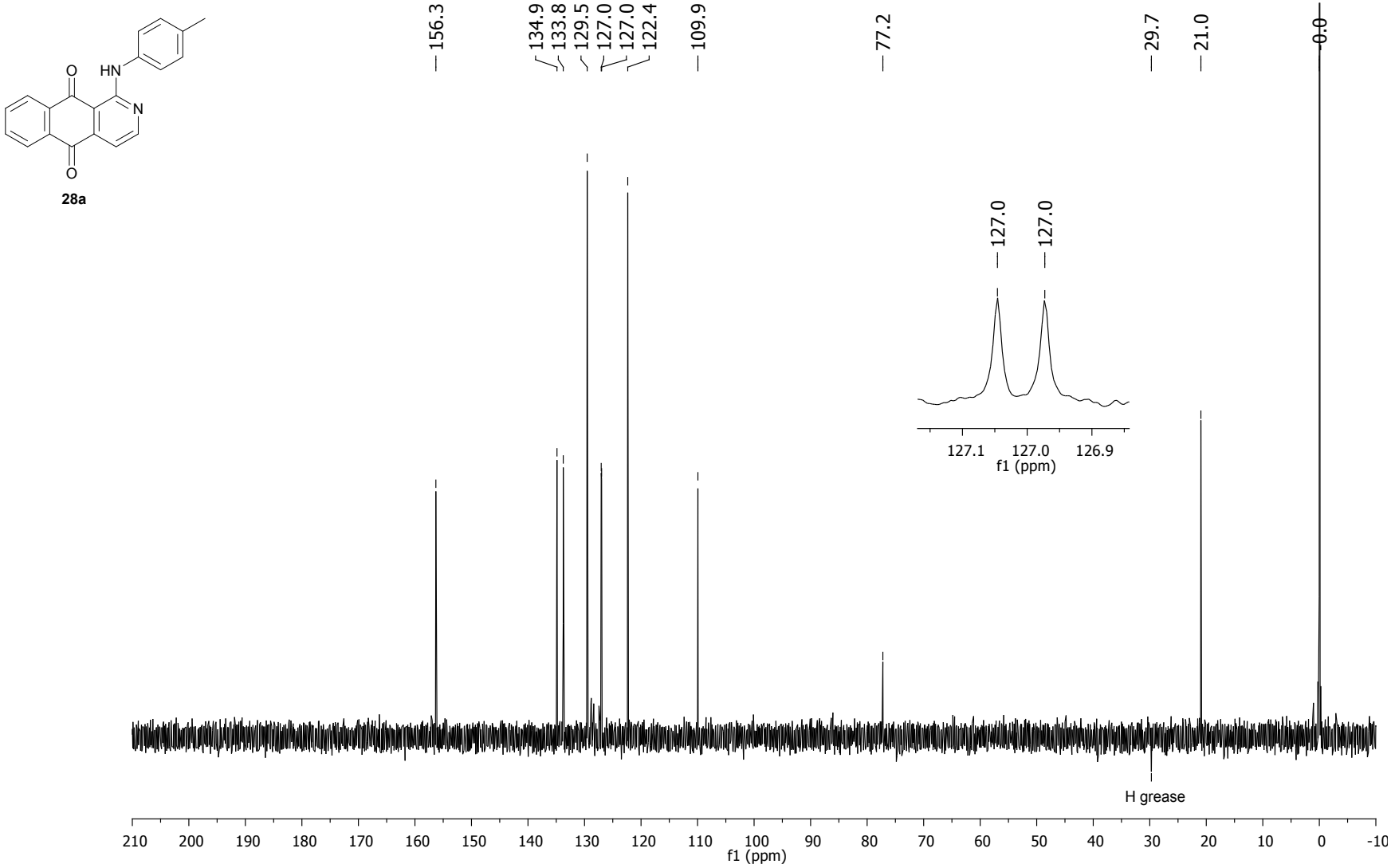


Figure 104 DEPT 135 spectrum of 1-(*p*-tolylamino)benzo[*g*]isoquinoline-5,10-dione (**28a**) ($CDCl_3$, 100 MHz).

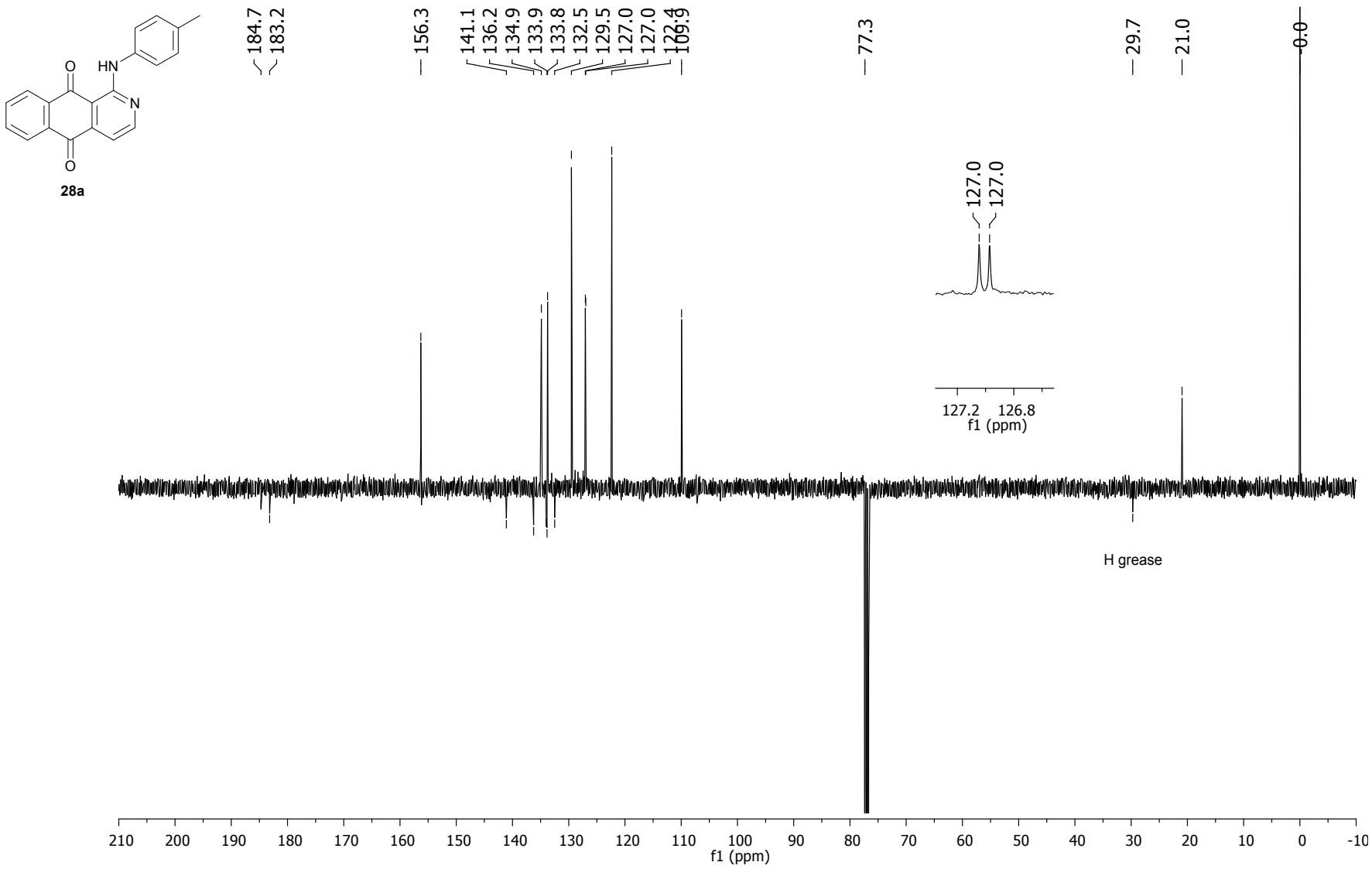


Figure 105 APT spectrum of 1-(*p*-tolylamino)benzo[*g*]isoquinoline-5,10-dione (**28a**) ($CDCl_3$, 100 MHz).

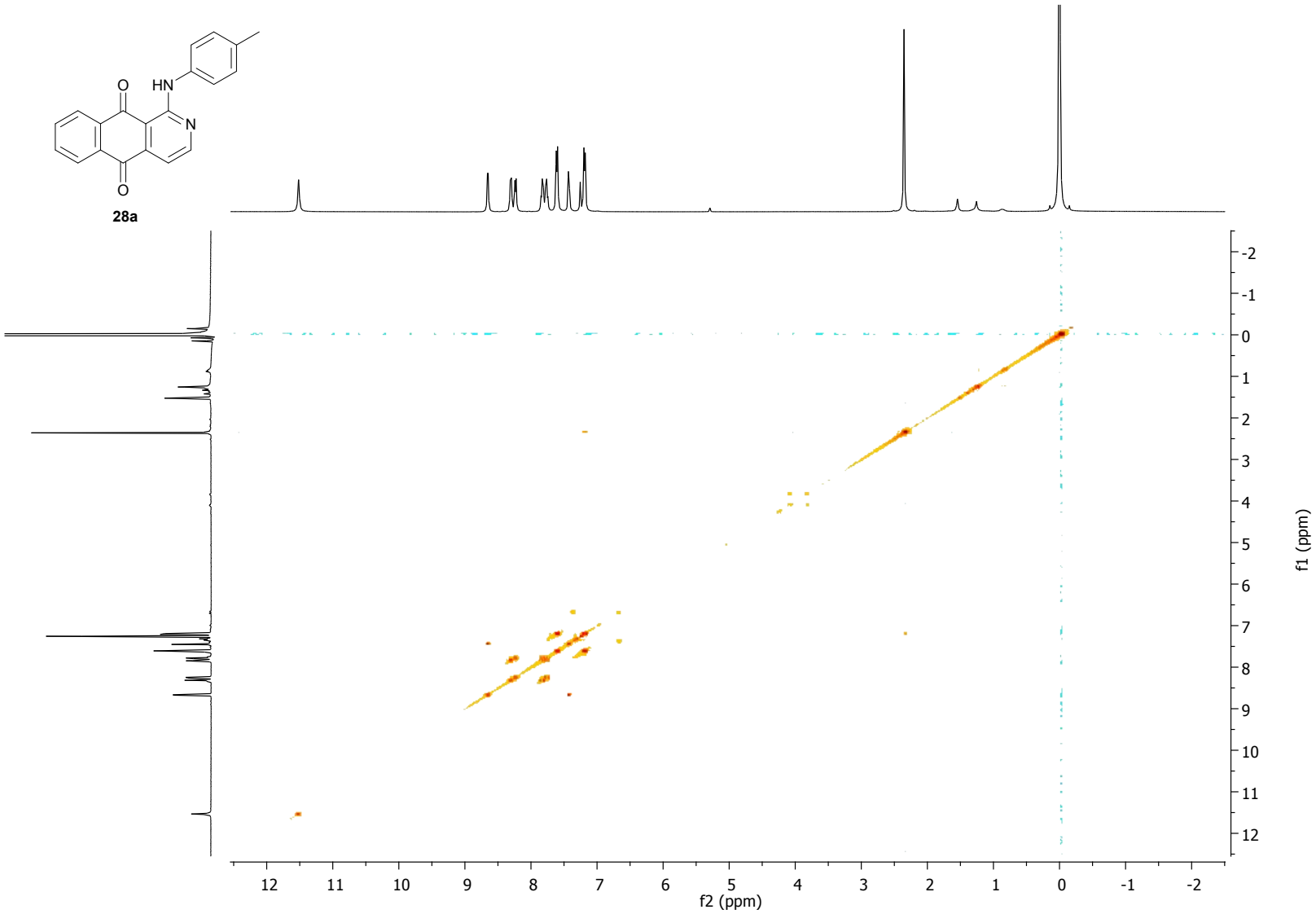


Figure 106 COSY spectrum of 1-(*p*-tolylamino)benzo[*g*]isoquinoline-5,10-dione (**28a**) ($CDCl_3$, 400 MHz).

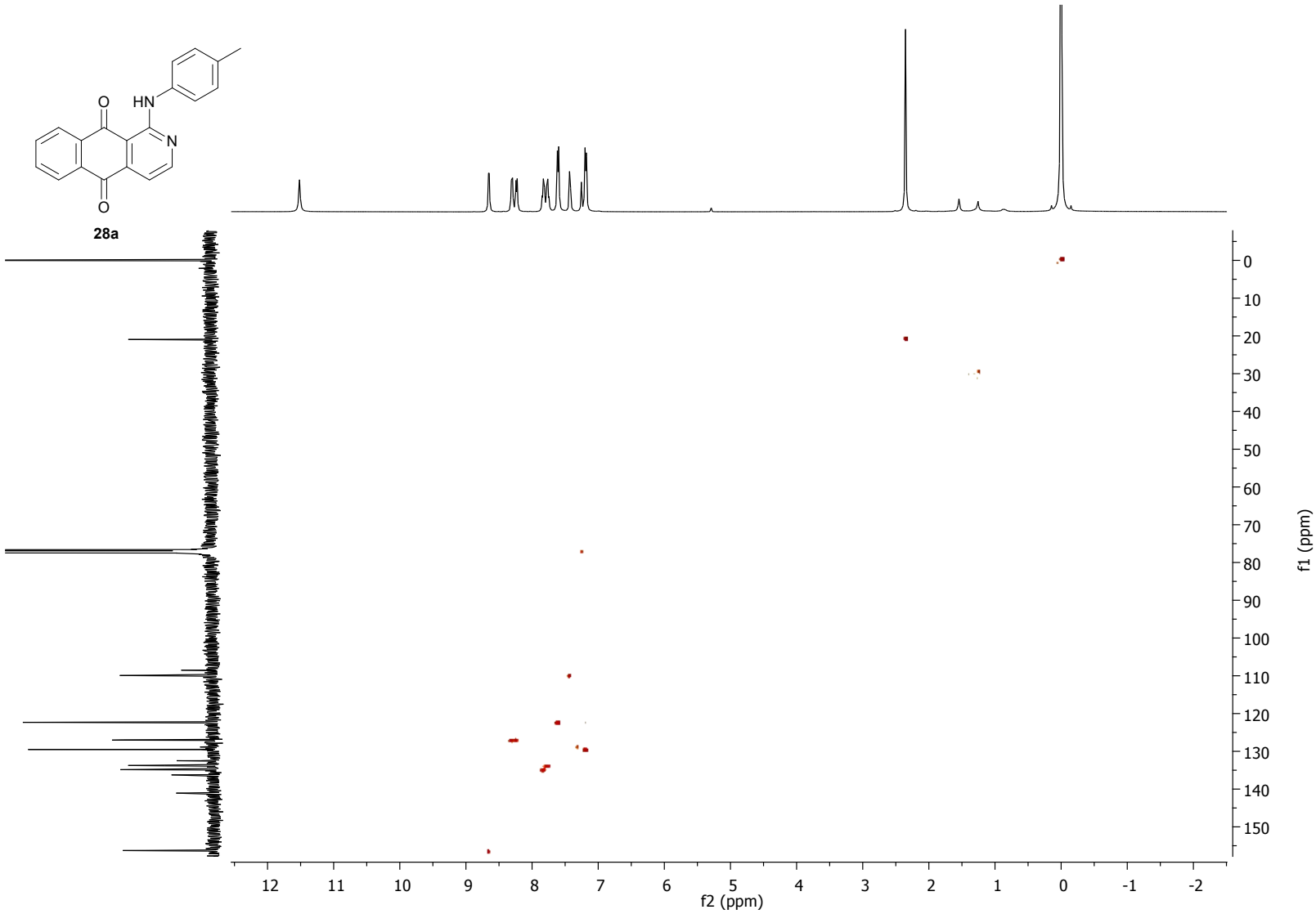


Figure 107 HSQC spectrum of 1-(*p*-tolylamino)benzo[*g*]isoquinoline-5,10-dione (**28a**) ($CDCl_3$, 400 MHz).

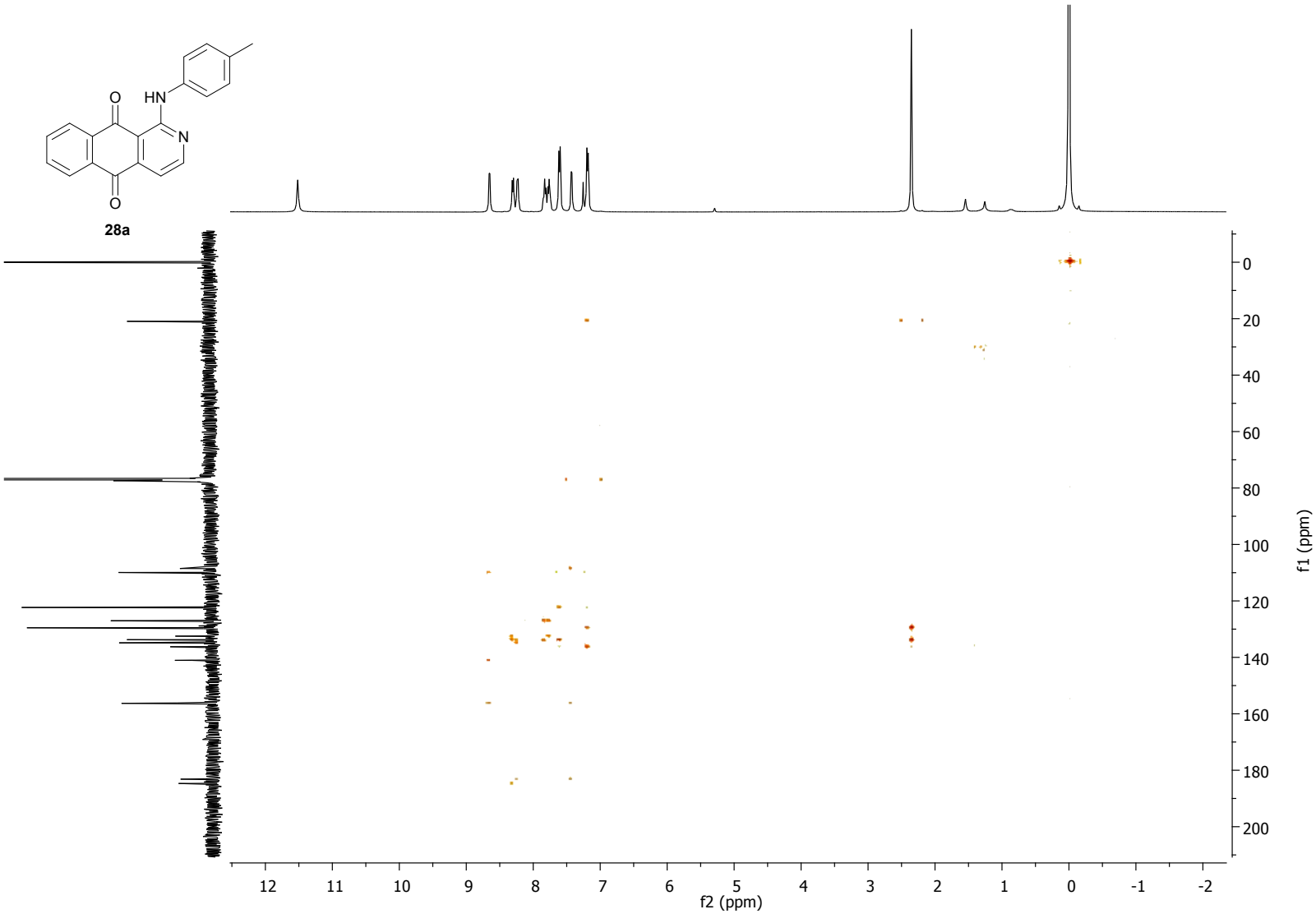


Figure 108 HMBC spectrum of 1-(*p*-tolylamino)benzo[*g*]isoquinoline-5,10-dione (**28a**) ($CDCl_3$, 400 MHz).

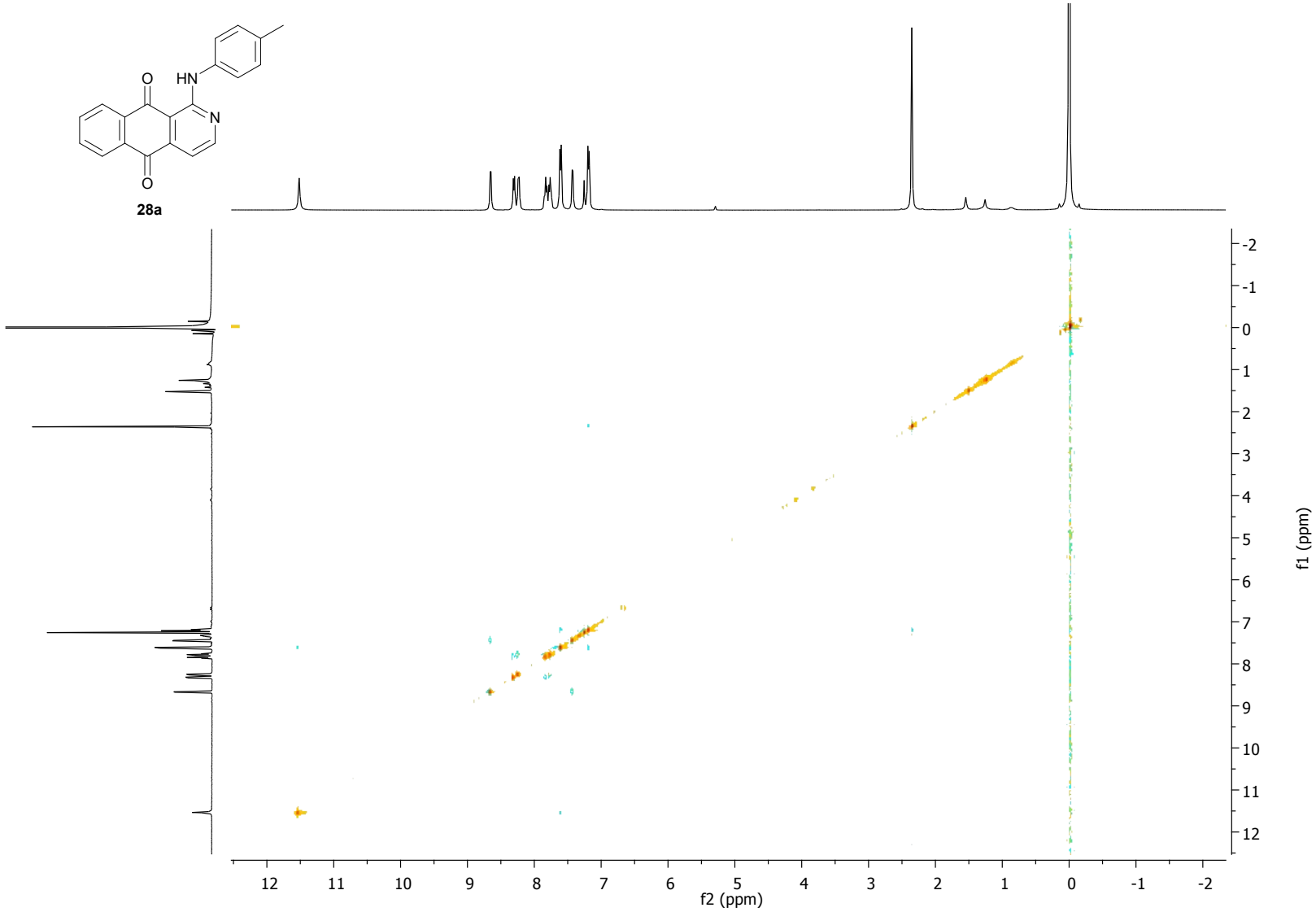


Figure 109 NOESY spectrum of 1-(*p*-tolylamino)benzo[*g*]isoquinoline-5,10-dione (**28a**) ($CDCl_3$, 400 MHz).

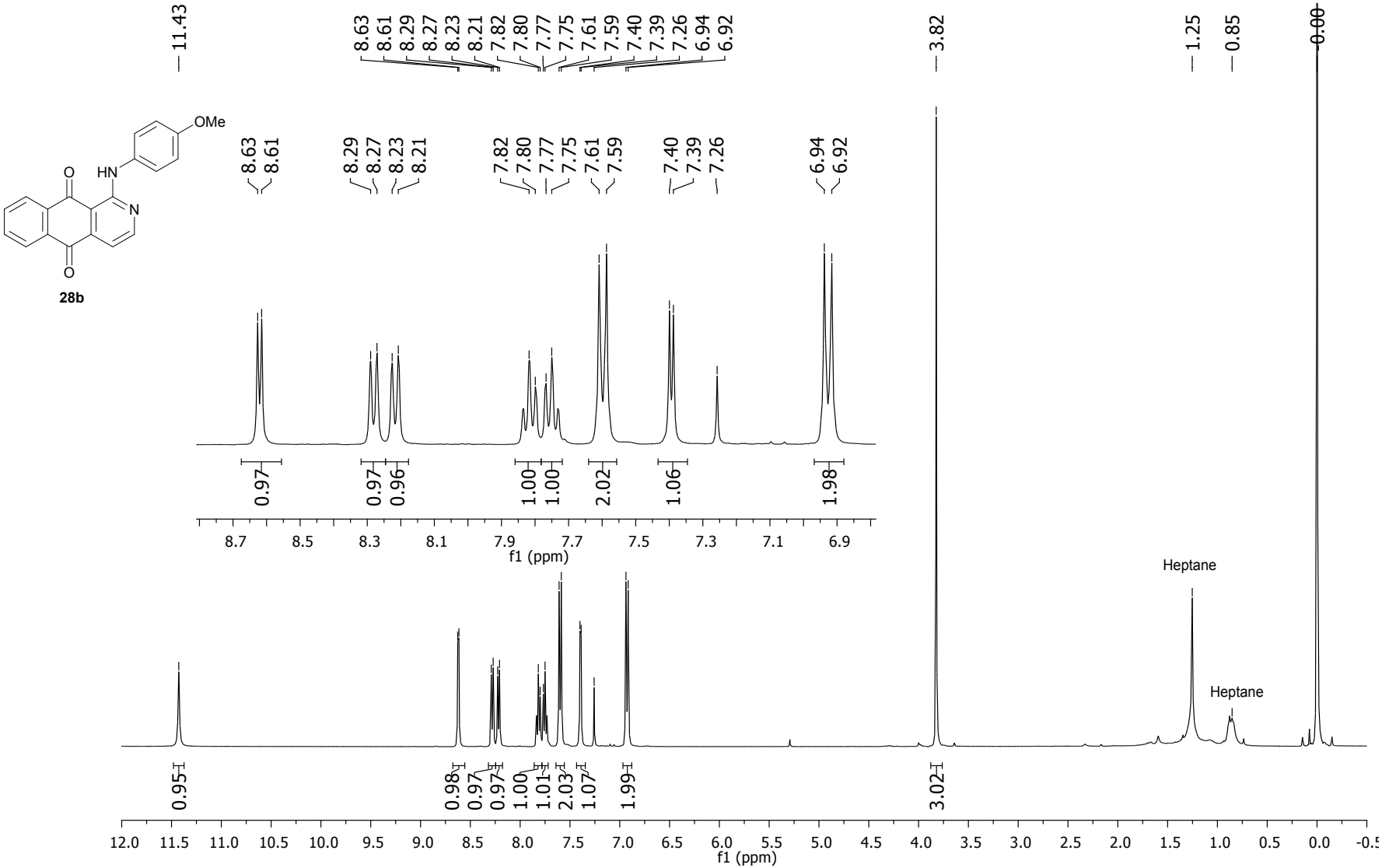


Figure 110 ^{1}H NMR spectrum of 1-((*p*-methoxyphenyl)amino)benzo[*g*]isoquinoline-5,10-dione (**28b**) ($CDCl_3$, 400 MHz).

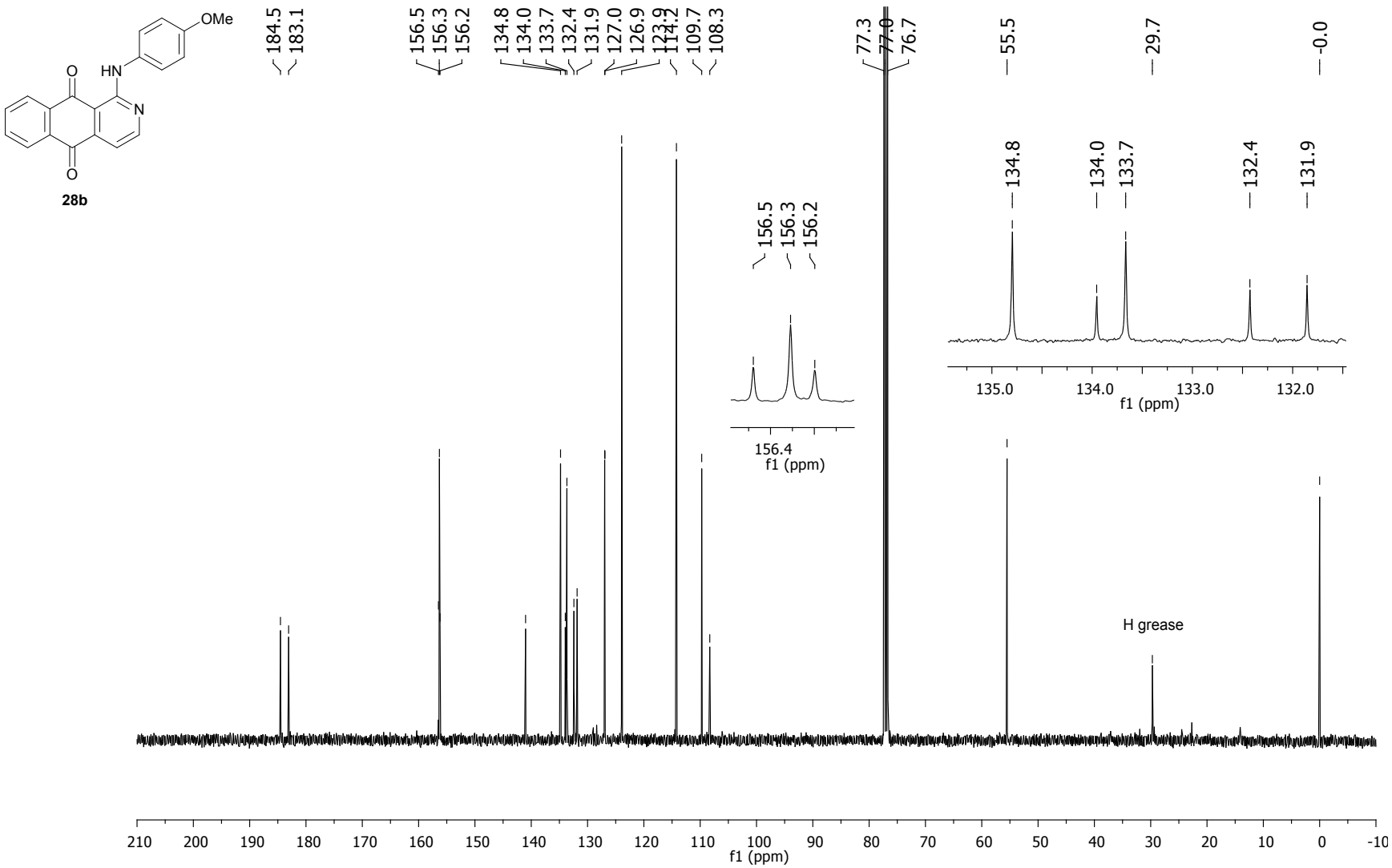


Figure 111 ^{13}C NMR spectrum of 1-((*p*-methoxyphenyl)amino)benzo[*g*]isoquinoline-5,10-dione (**28b**) ($CDCl_3$, 100 MHz).

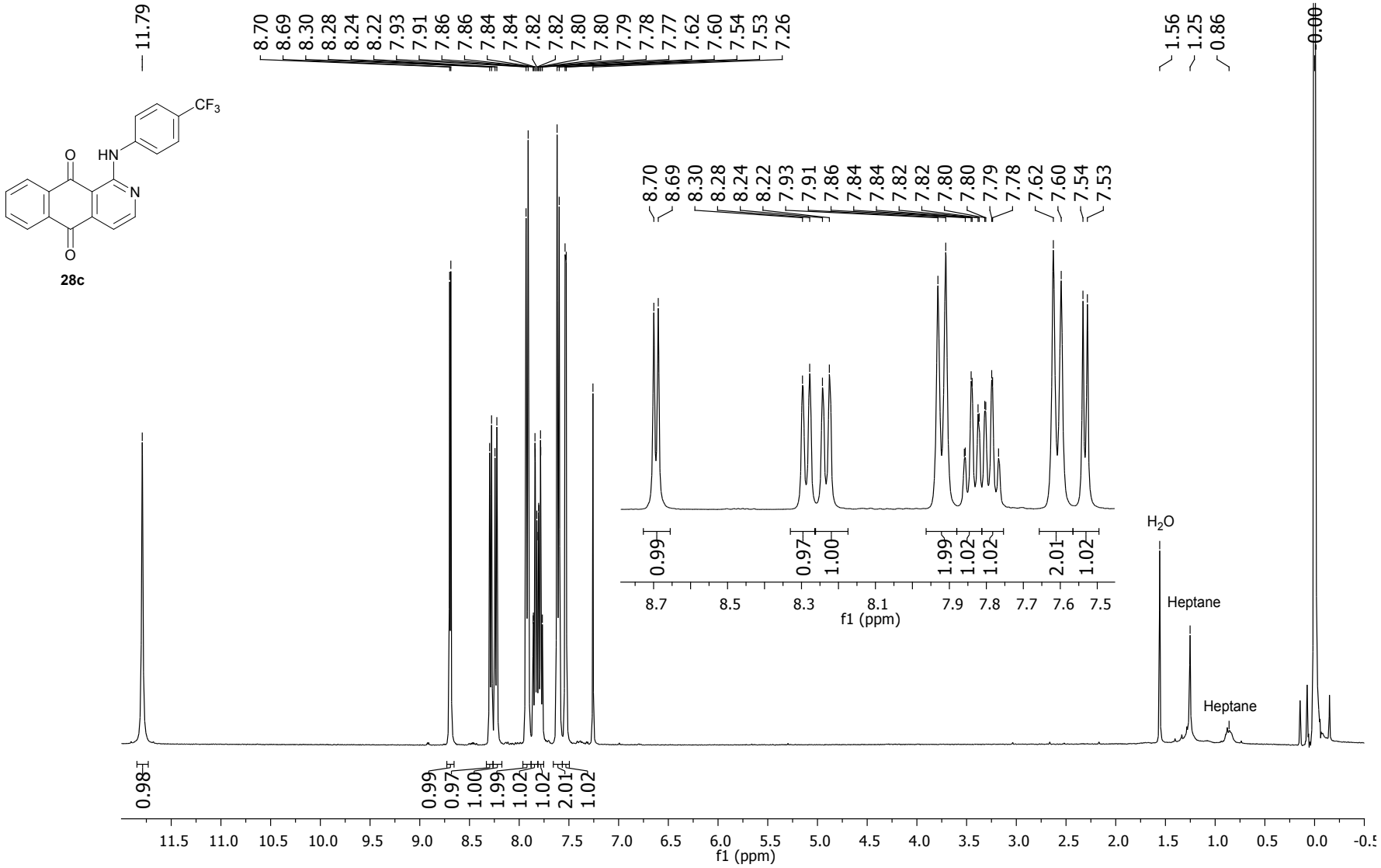


Figure 112 ^{1}H NMR spectrum of 1-((*p*-(trifluoromethyl)phenyl)amino)benzo[*g*]isoquinoline-5,10-dione (**28c**) ($CDCl_3$, 400 MHz).

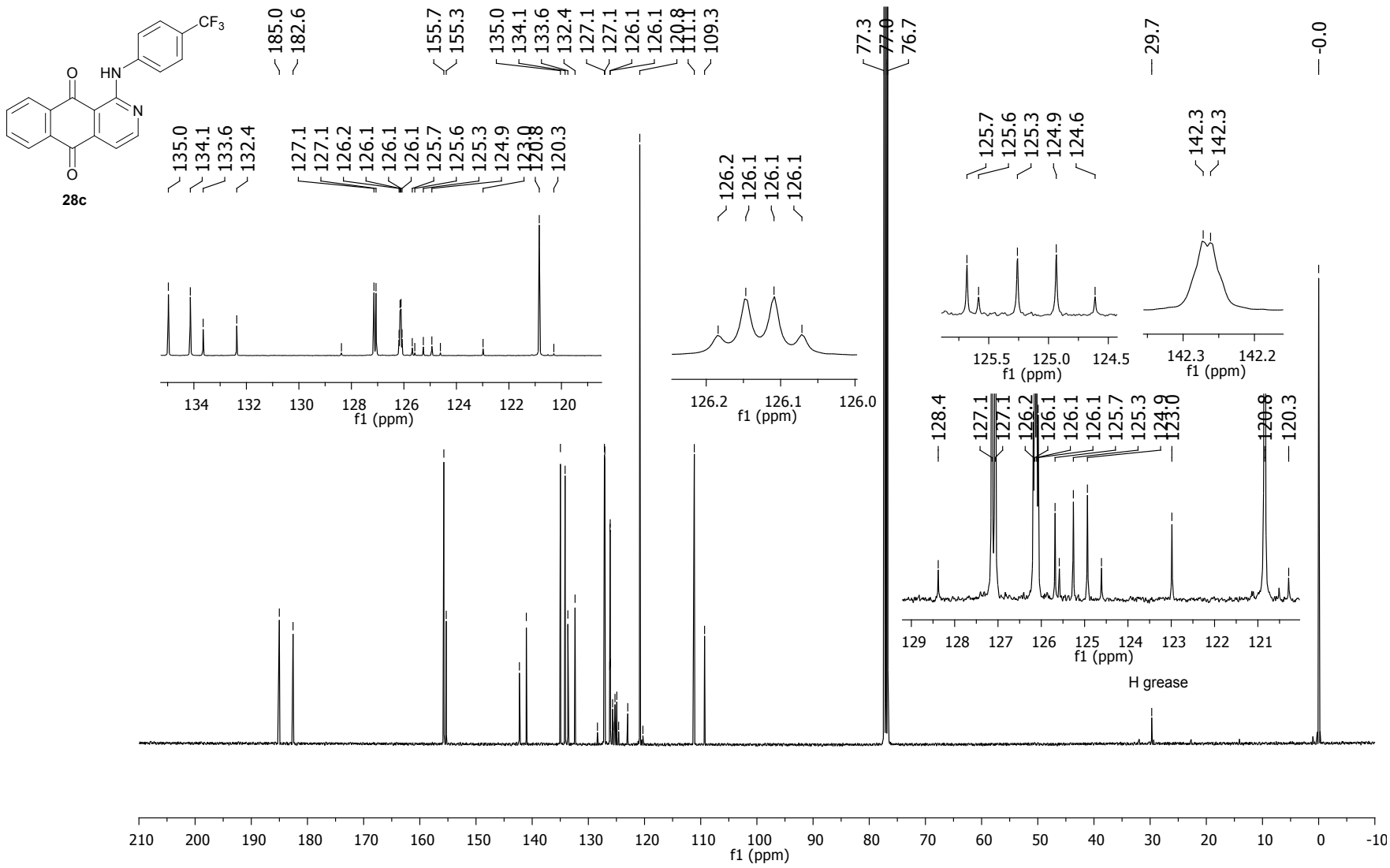


Figure 113 ^{13}C NMR spectrum of 1-((*p*-(trifluoromethyl)phenyl)amino)benzo[*g*]isoquinoline-5,10-dione (**28c**) ($CDCl_3$, 100 MHz).

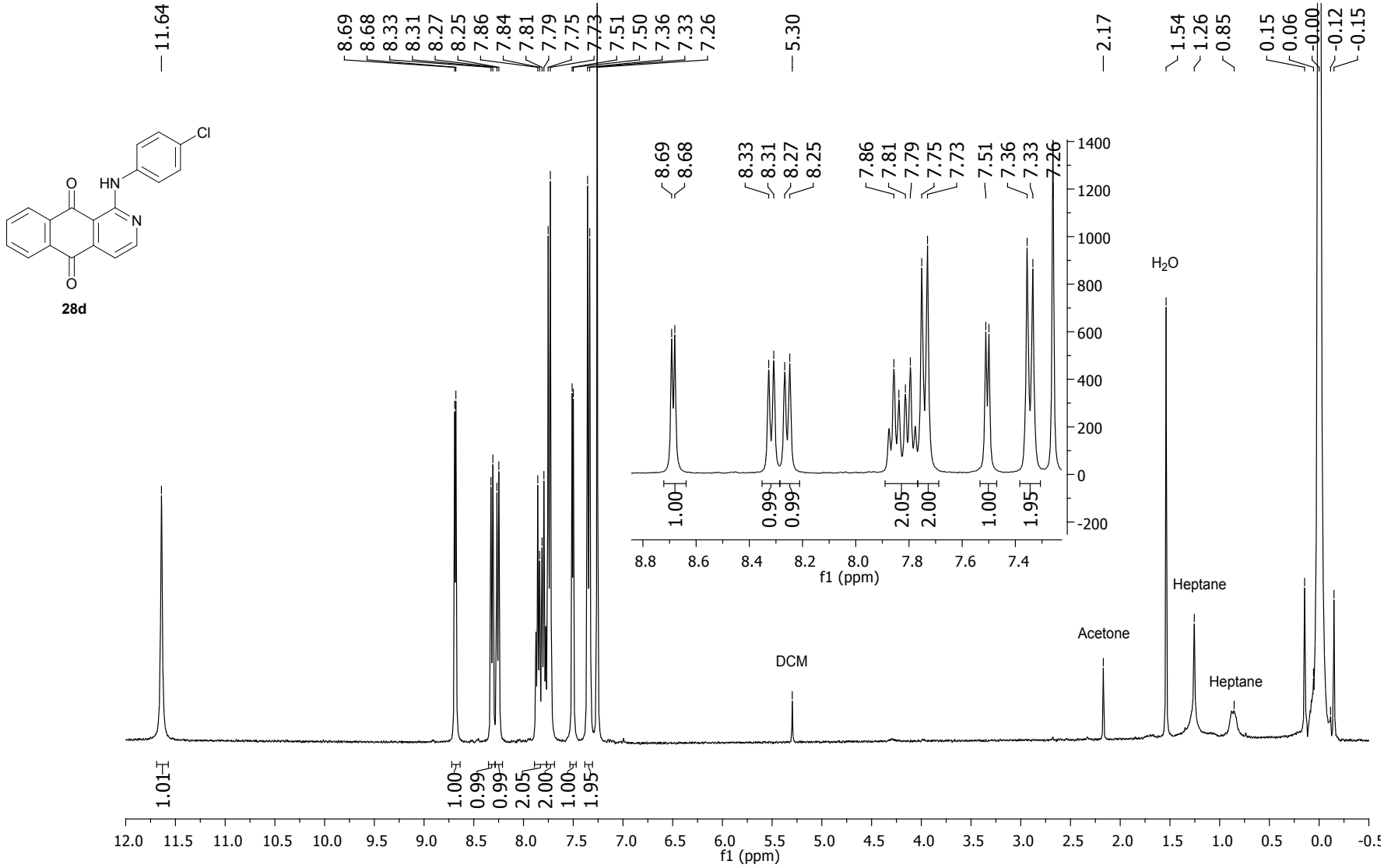


Figure 114 ^{1}H NMR spectrum of 1-((*p*-chlorophenyl)amino)benzo[*g*]isoquinoline-5,10-dione (**28d**) ($CDCl_3$, 400 MHz).

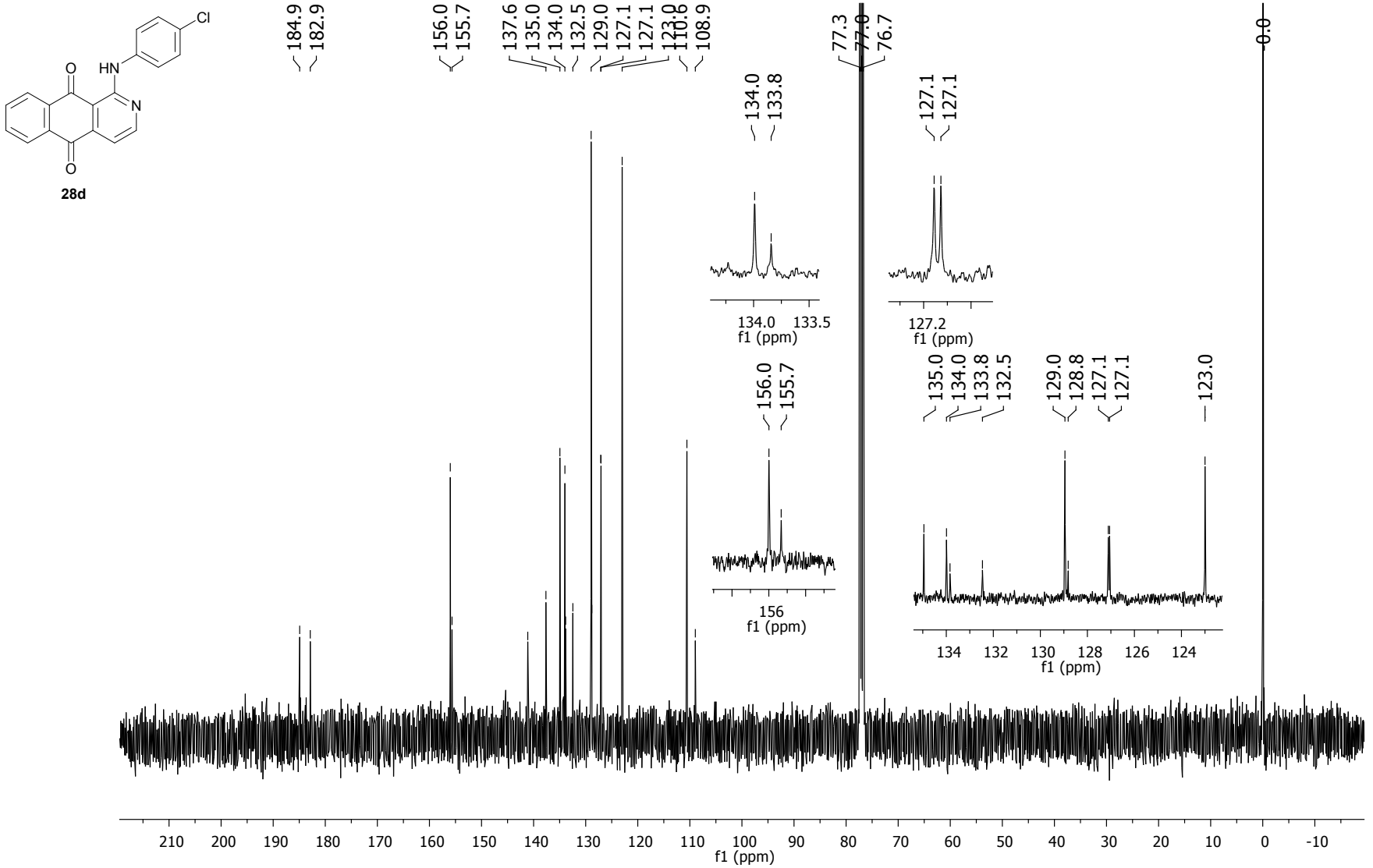


Figure 115 ^{13}C NMR spectrum of 1-((*p*-chlorophenyl)amino)benzo[*g*]isoquinoline-5,10-dione (**28d**) ($CDCl_3$, 100 MHz).

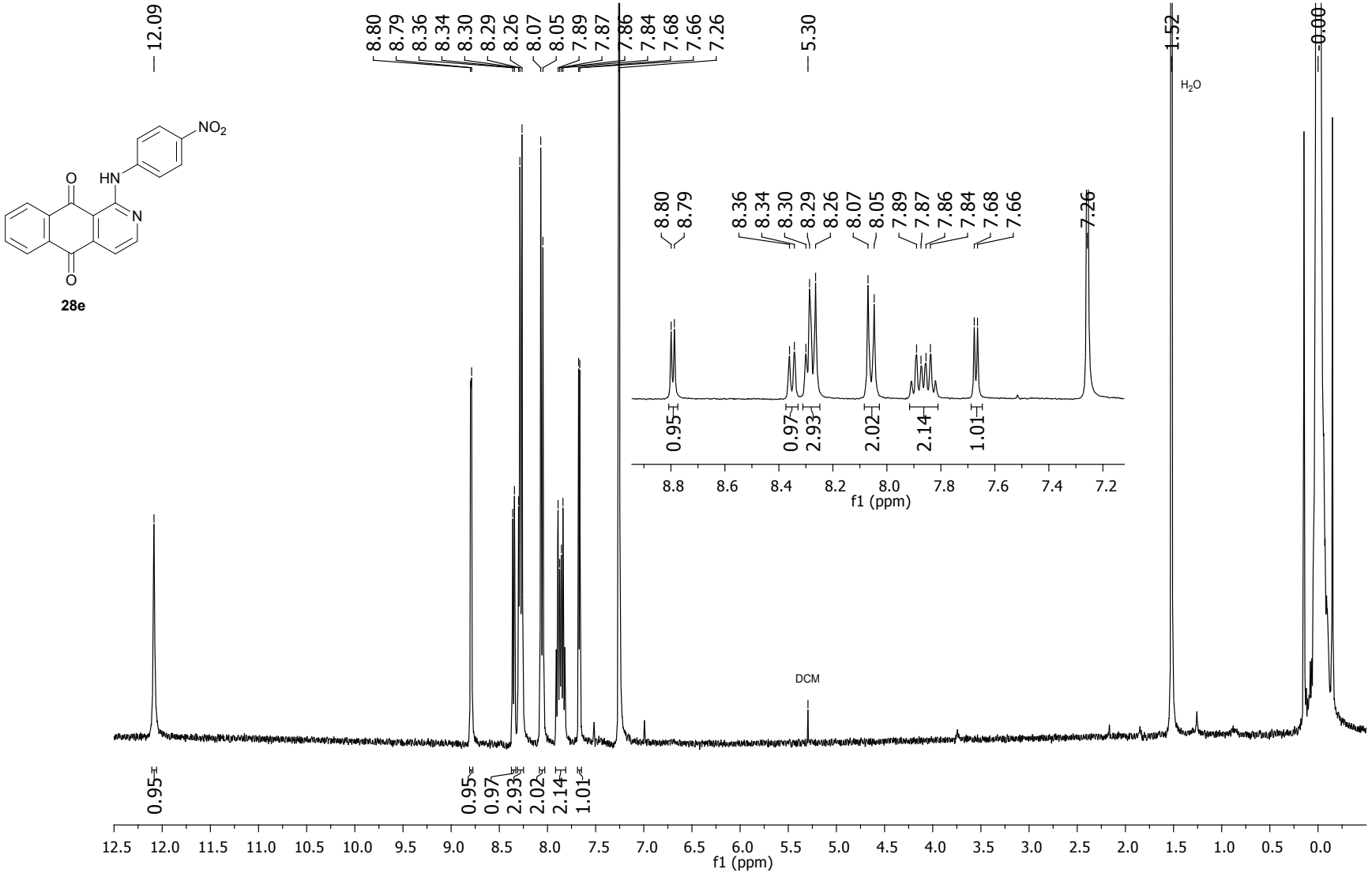


Figure 116 ^{1}H NMR spectrum of 1-((*p*-nitrophenyl)amino)benzo[*g*]isoquinoline-5,10-dione (**28e**) ($CDCl_3$, 400 MHz).

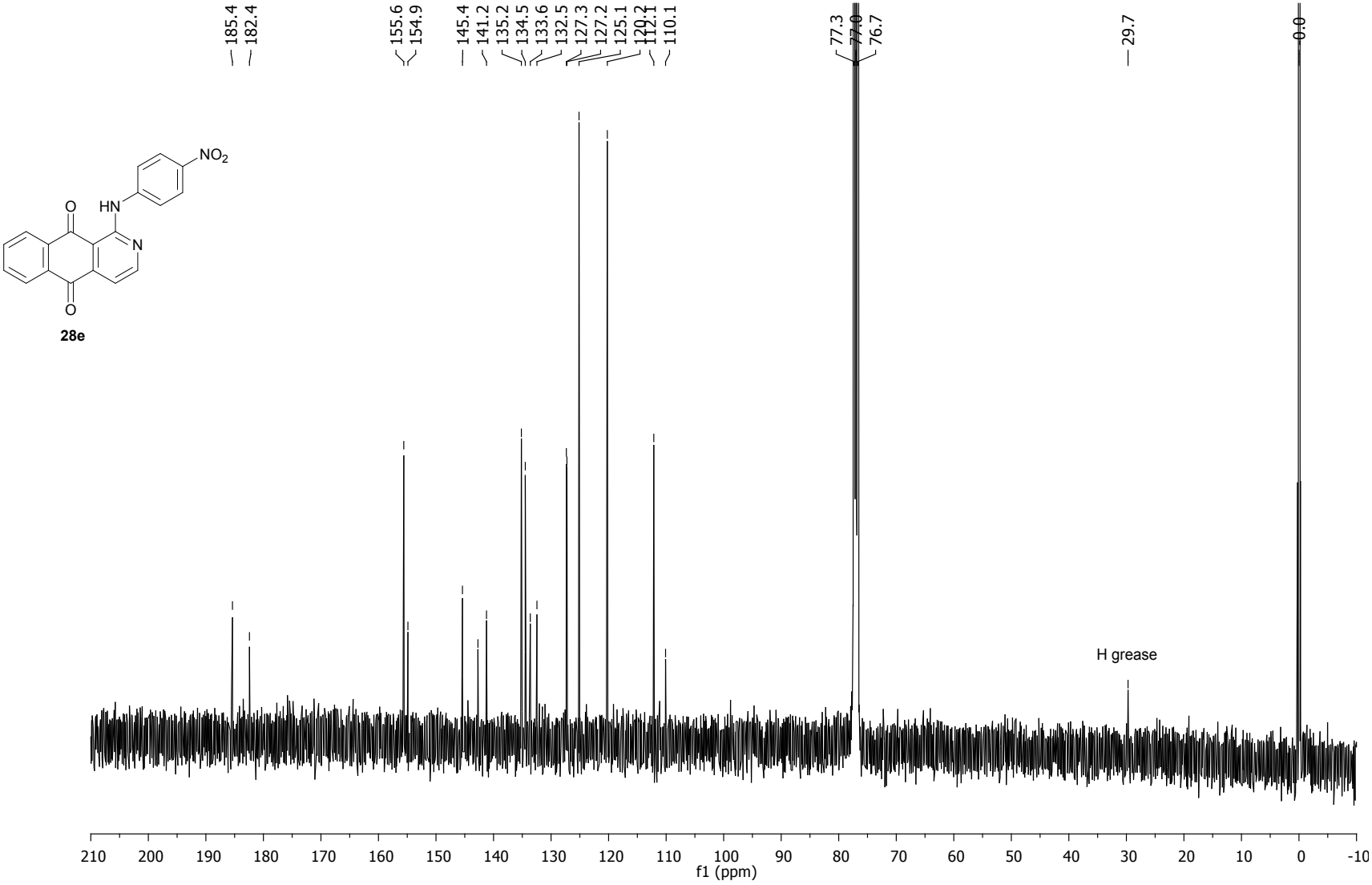


Figure 117 ^{13}C NMR spectrum of 1-((*p*-nitrophenyl)amino)benzo[*g*]isoquinoline-5,10-dione (**28e**) ($CDCl_3$, 100 MHz).

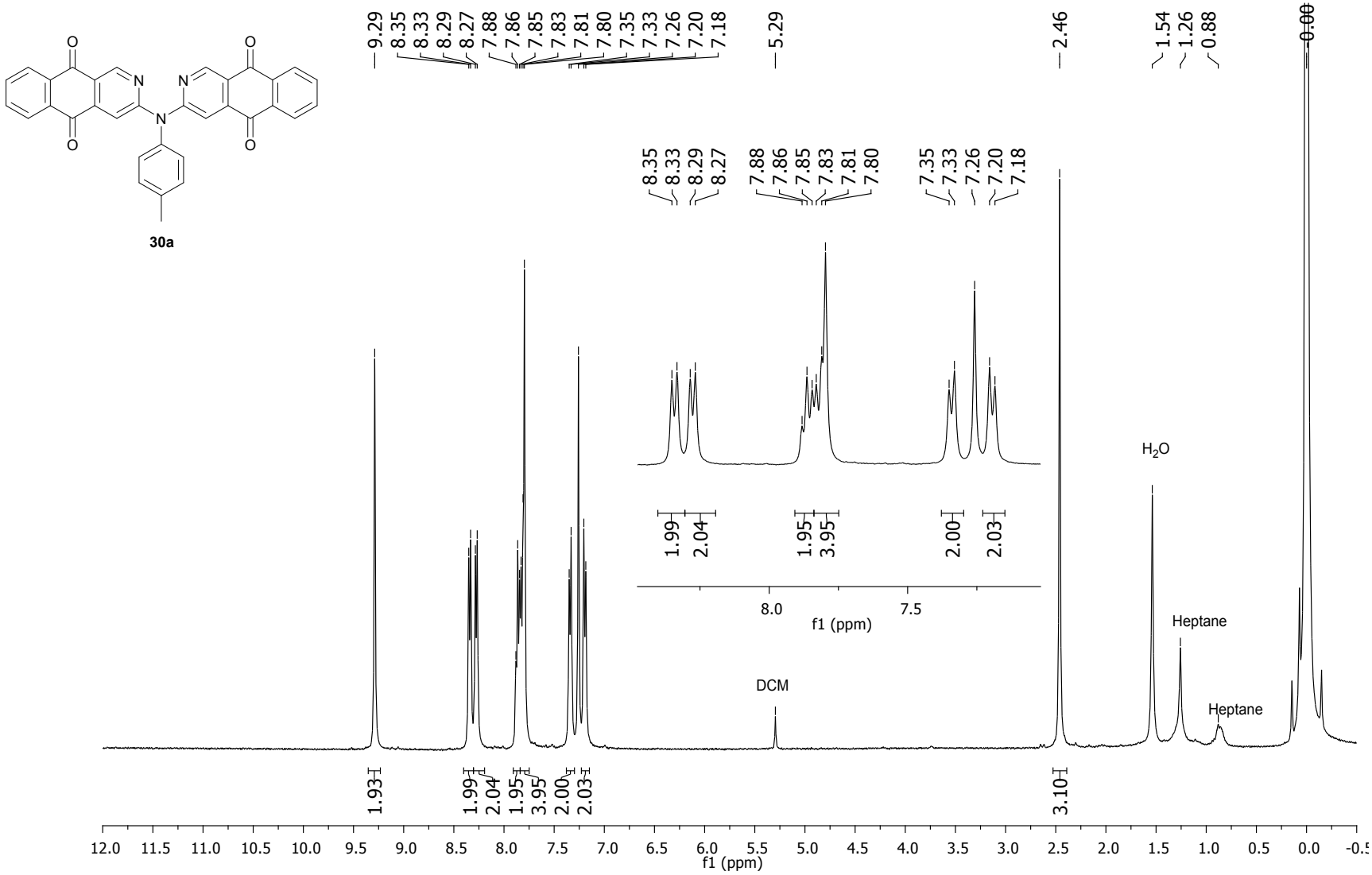


Figure 118 ^{1}H NMR spectrum of 3,3'-(*p*-tolylazanediyl)bis(benzo[*g*]isoquinoline-5,10-dione) (**30a**) ($CDCl_3$, 400 MHz).

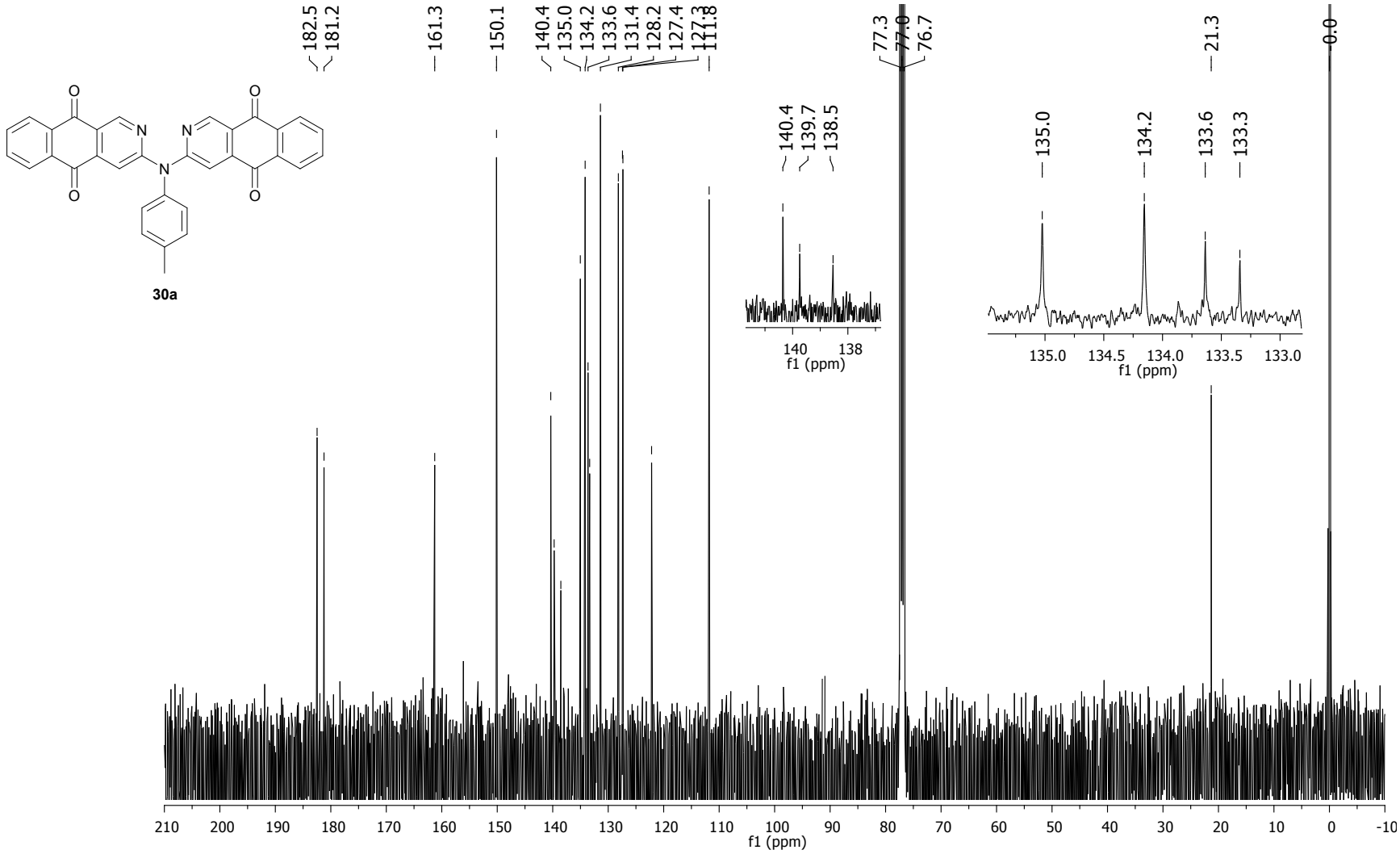


Figure 119 ^{13}C NMR spectrum of 3,3'-(*p*-tolylazanediyl)bis(benzo[*g*]isoquinoline-5,10-dione) (**30a**) ($CDCl_3$, 100 MHz).

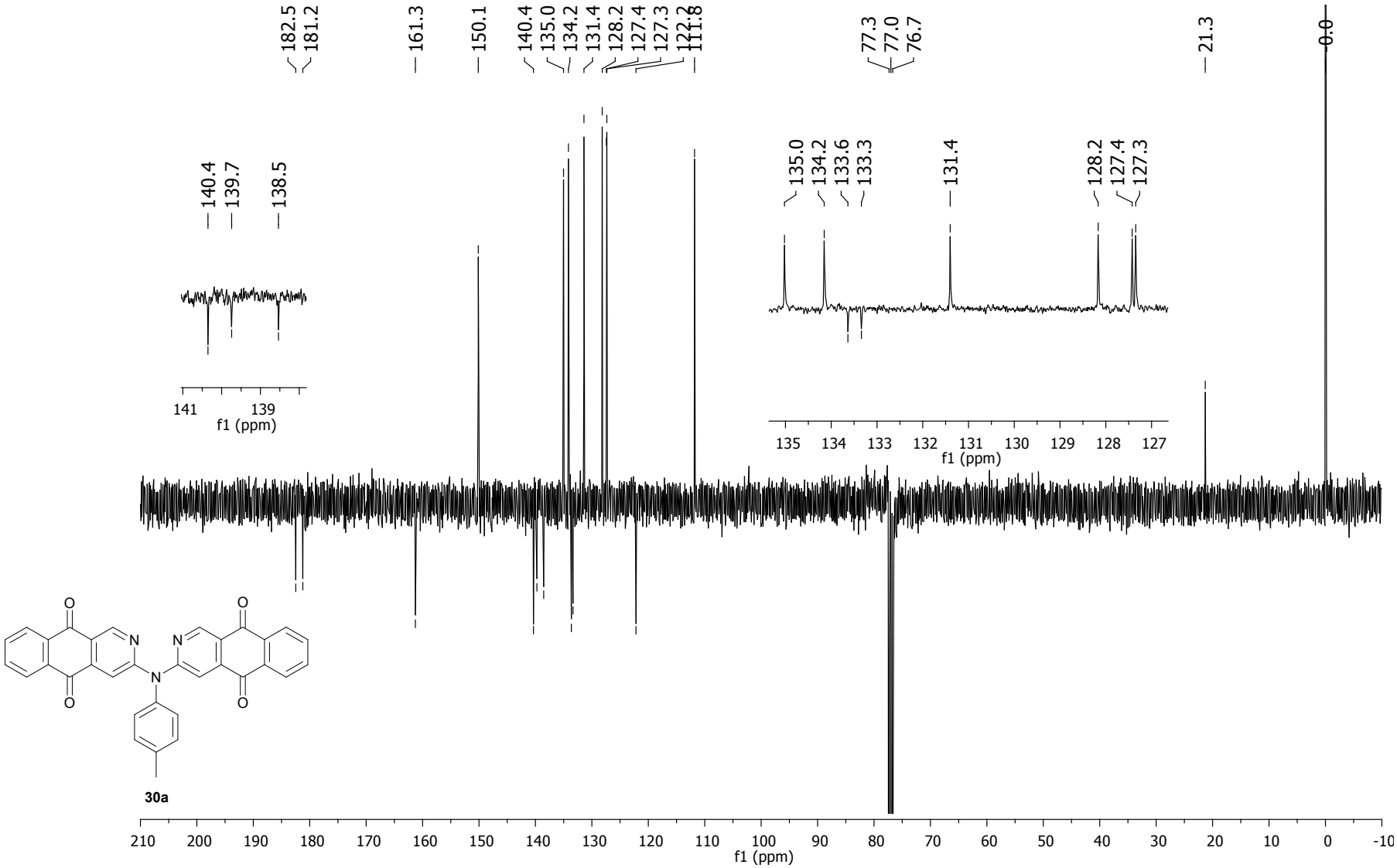


Figure 120 APT spectrum of 3,3'-(*p*-tolylazanediyl)bis(benzo[*g*]isoquinoline-5,10-dione) (**30a**) ($CDCl_3$, 100 MHz).

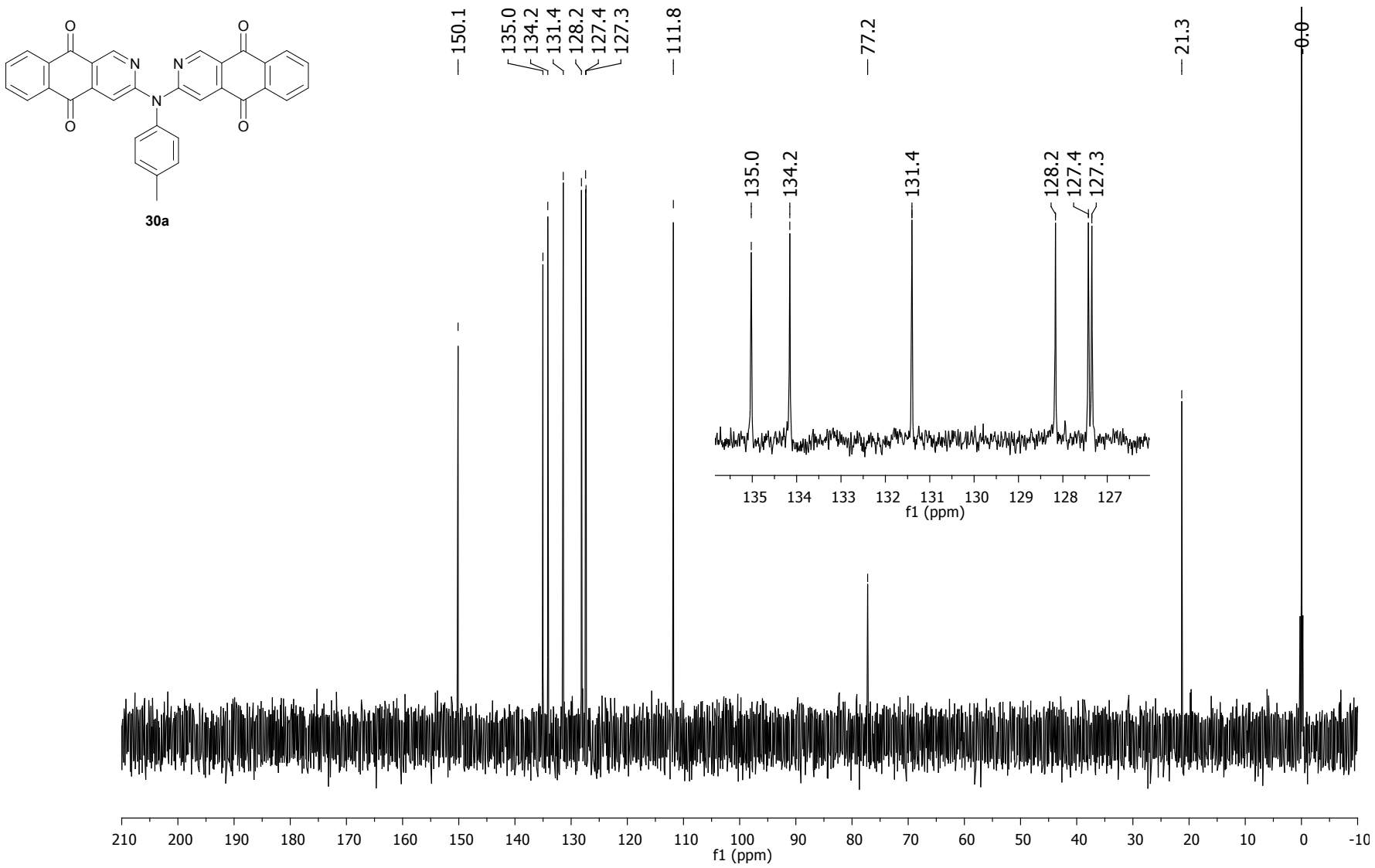


Figure 121 DEPT 135 spectrum of 3,3'-(*p*-tolylazanediyl)bis(benzo[*g*]isoquinoline-5,10-dione) (**30a**) ($CDCl_3$, 100 MHz).

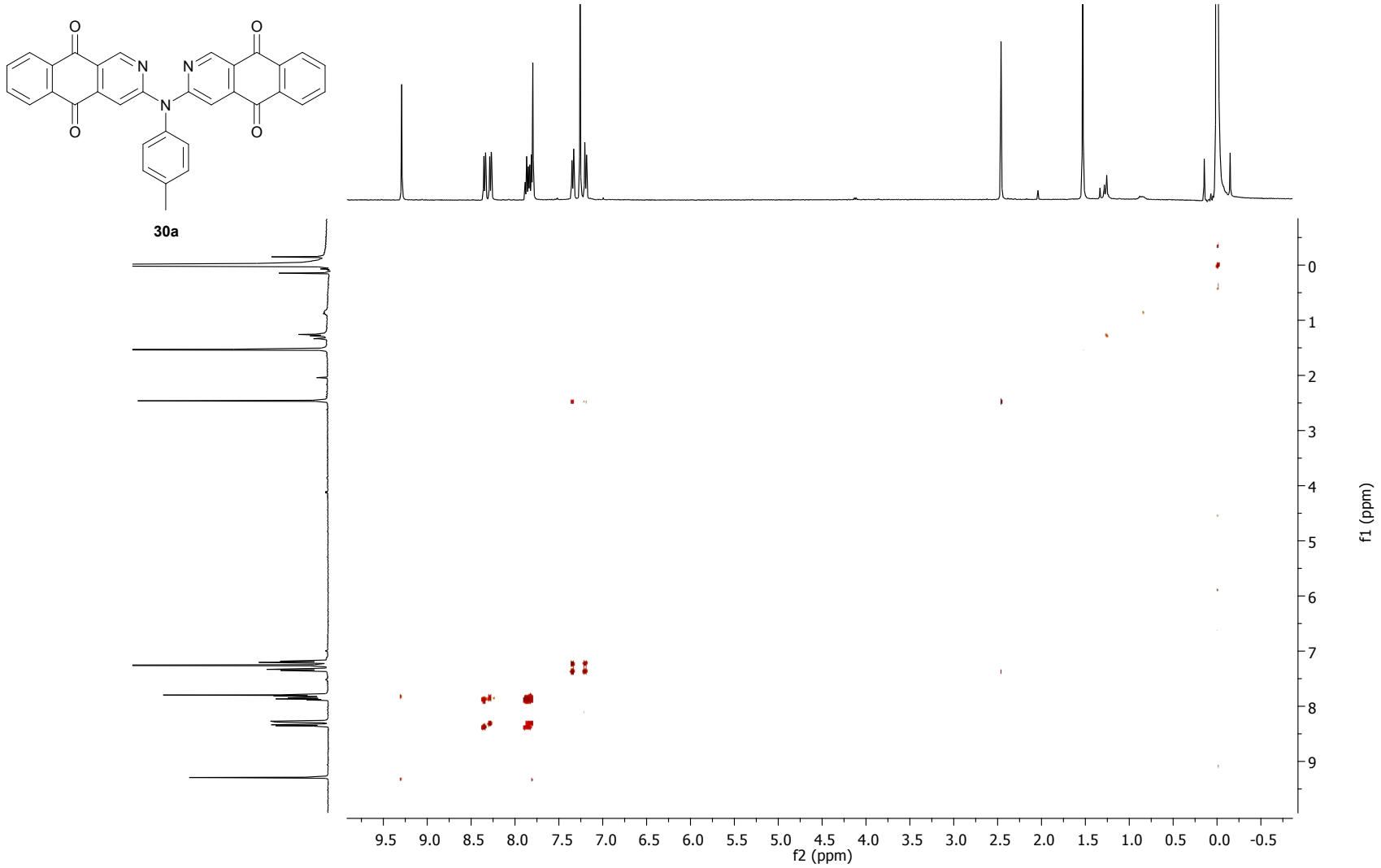


Figure 122 COSY spectrum of 3,3'-(*p*-tolylazanediyl)bis(benzo[*g*]isoquinoline-5,10-dione) (**30a**) ($CDCl_3$, 400 MHz).

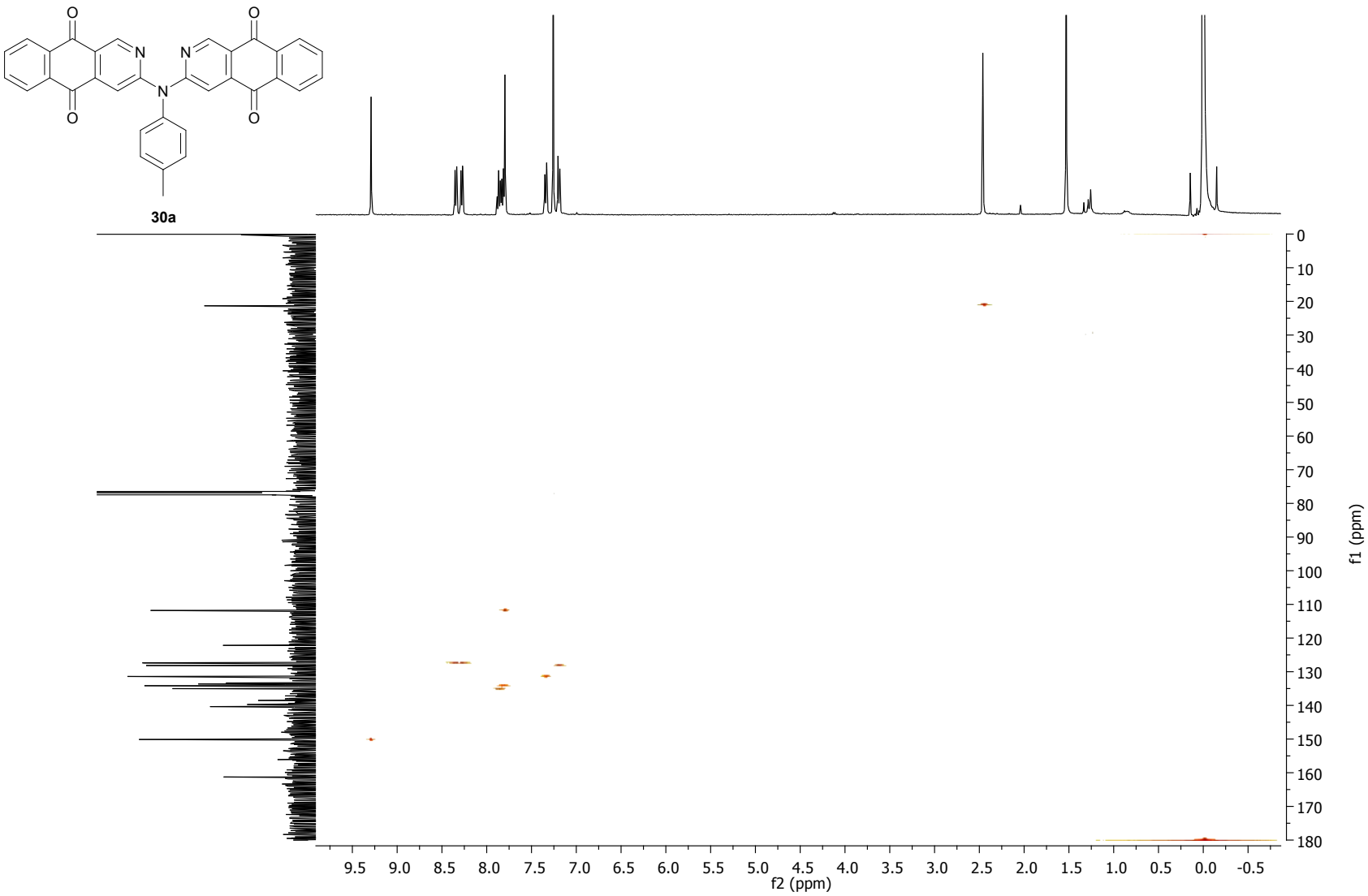


Figure 123 HSQC spectrum of 3,3'-(*p*-tolylazanediyl)bis(benzo[*g*]isoquinoline-5,10-dione) (**30a**) ($CDCl_3$, 400 MHz).

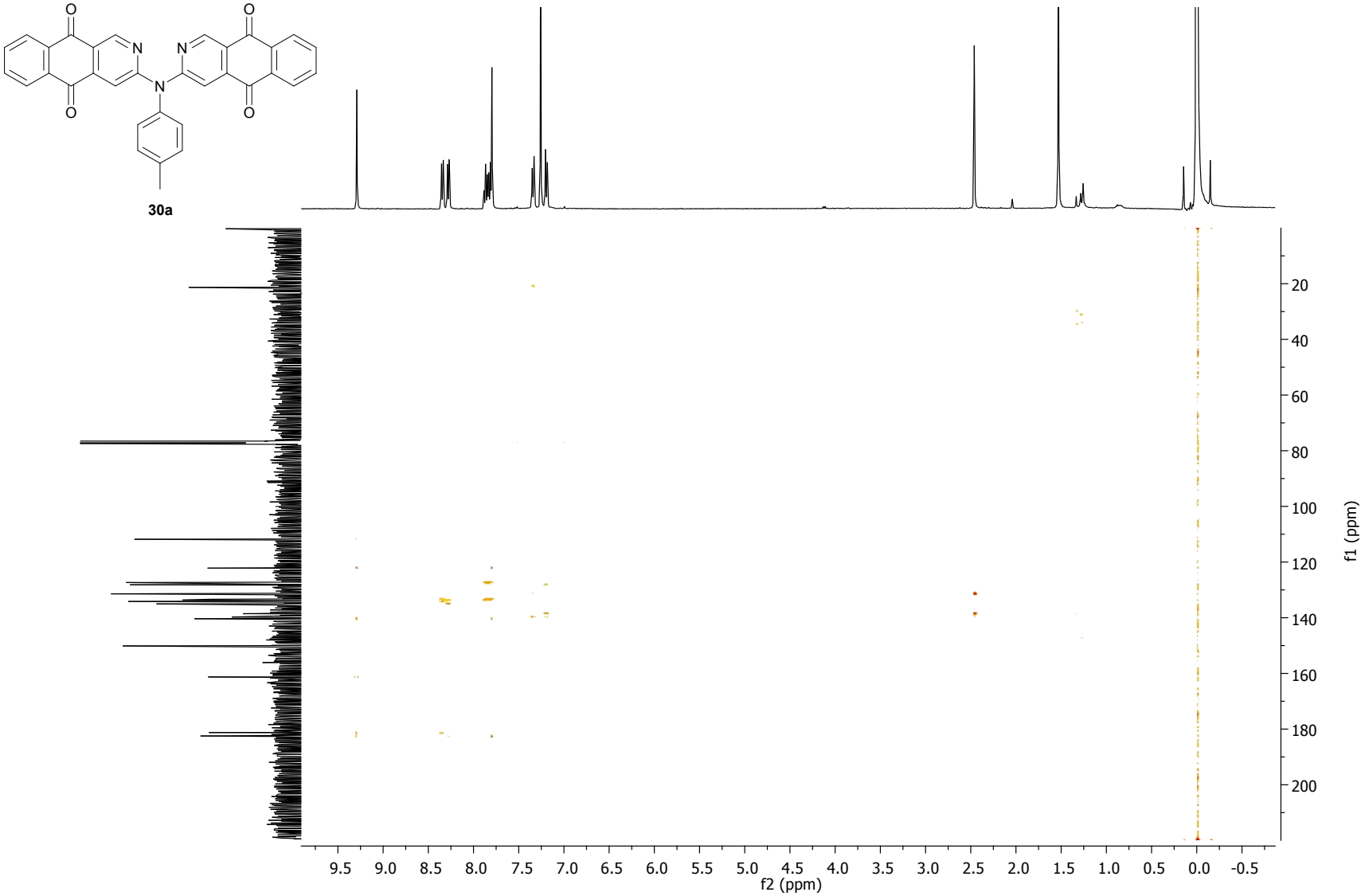


Figure 124 HMBC spectrum of 3,3'-(*p*-tolylazanediyl)bis(benzo[*g*]isoquinoline-5,10-dione) (**30a**) ($CDCl_3$, 400 MHz).

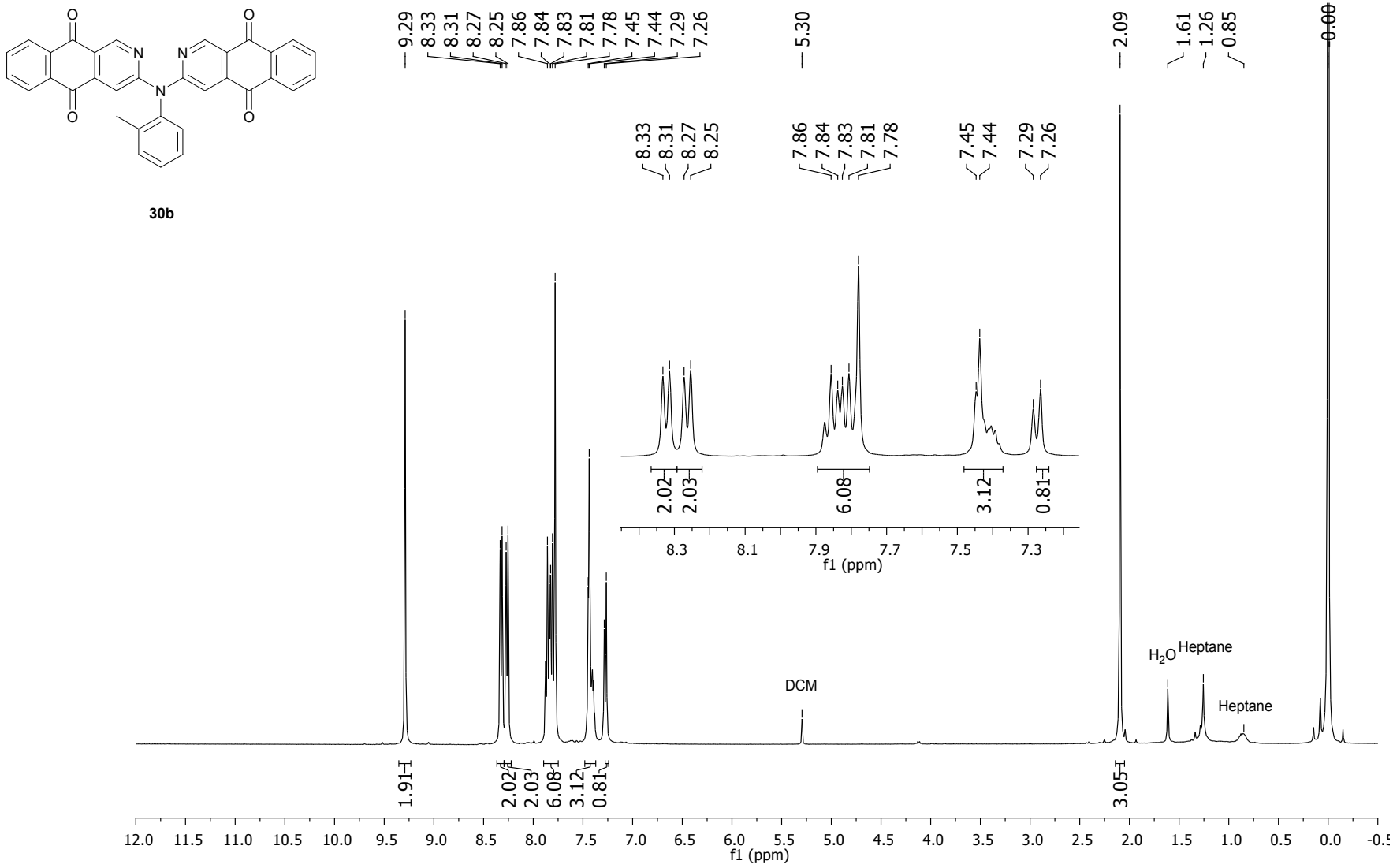


Figure 125 ^{1}H NMR spectrum of 3,3'-(*o*-tolylazanediyl)bis(benzo[*g*]isoquinoline-5,10-dione) (**30b**) ($CDCl_3$, 400 MHz).

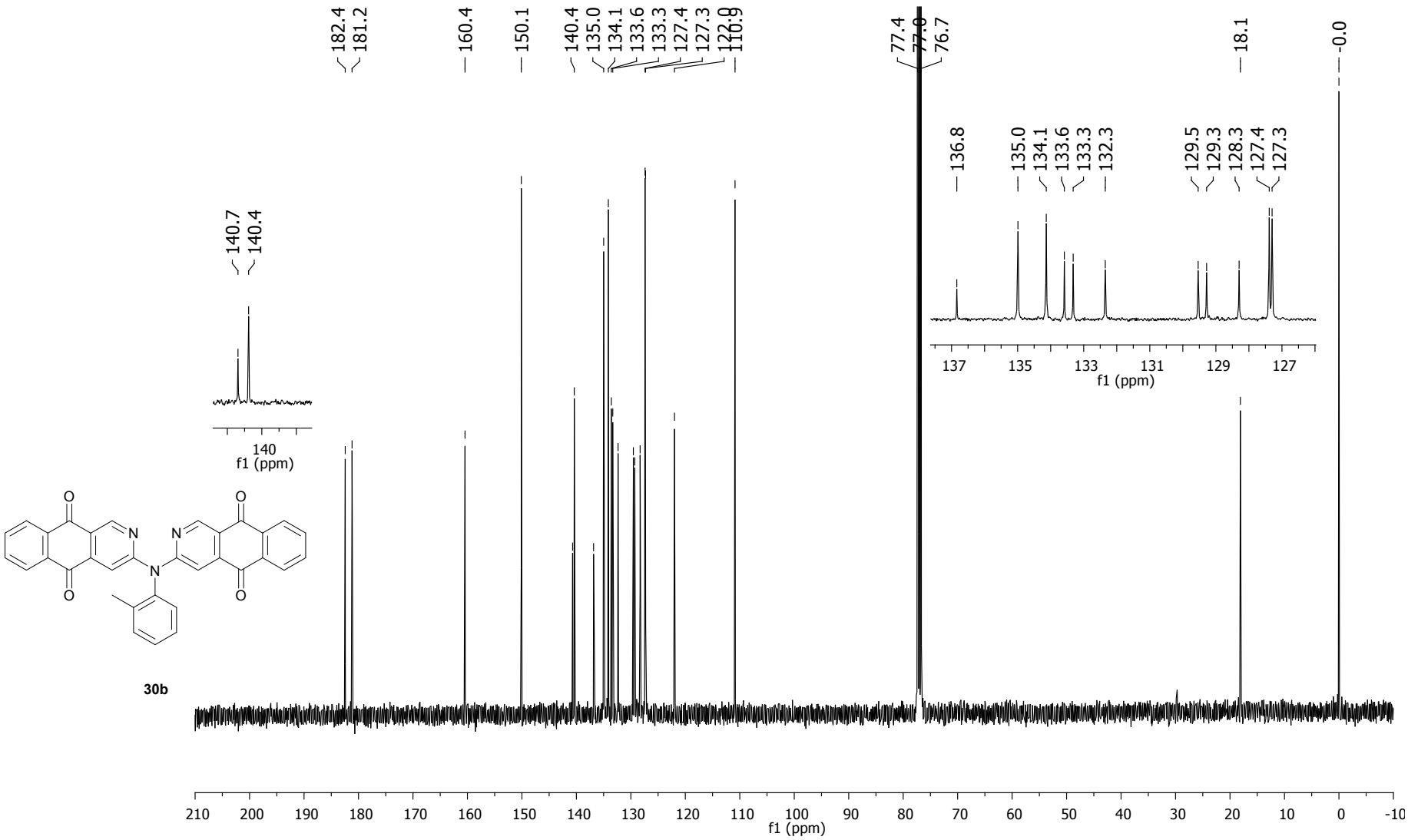
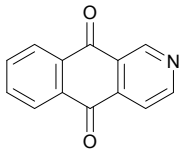


Figure 126 ^{13}C NMR spectrum of 3,3'-(*o*-tolylazanediyl)bis(benzo[*g*]isoquinoline-5,10-dione) (**30b**) ($CDCl_3$, 100 MHz).

UPLC spectra of compounds



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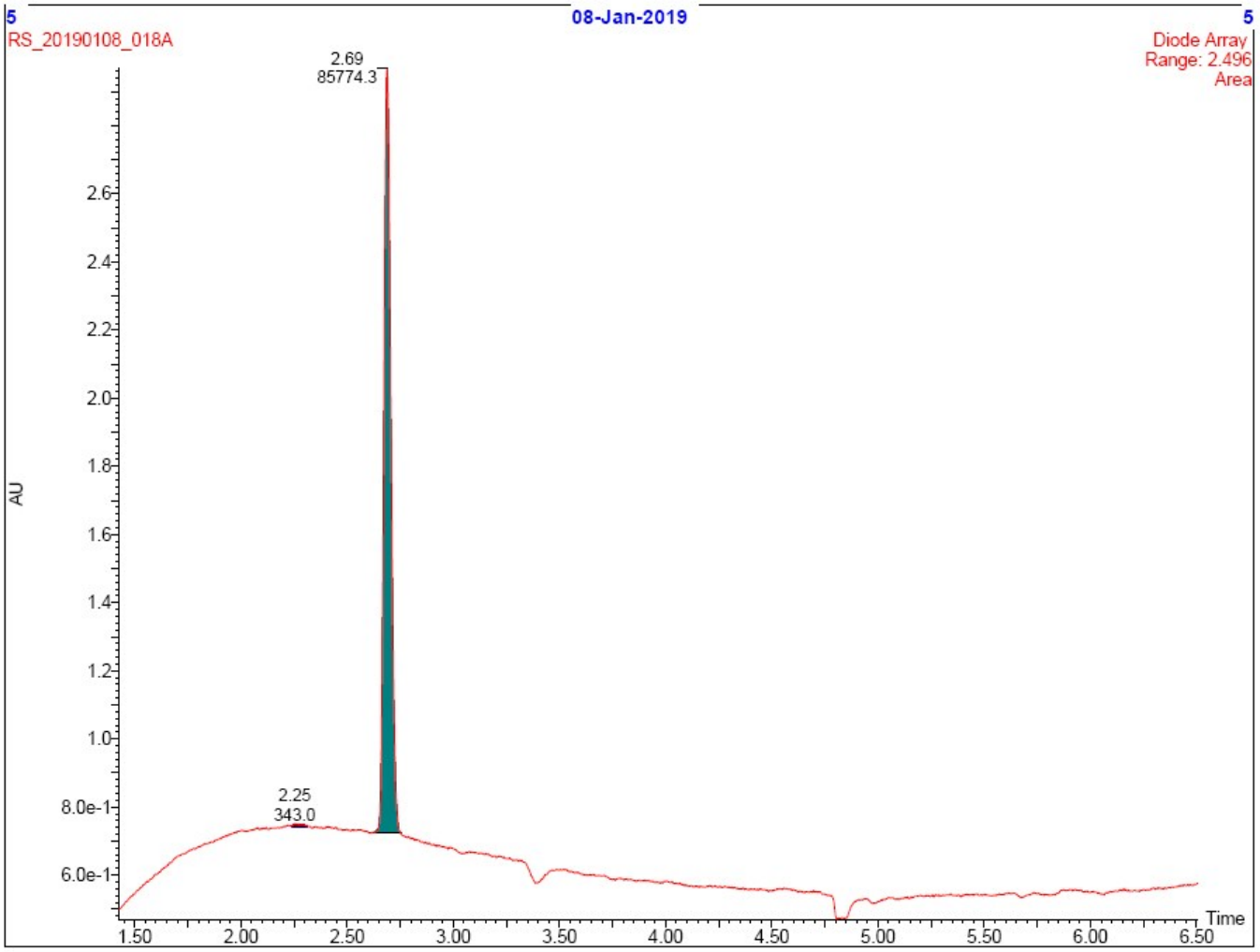
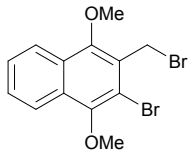


Figure 127 UPLC spectrum of benzo[*g*]isoquinoline-5,10-dione (**5**).



17

unpurified

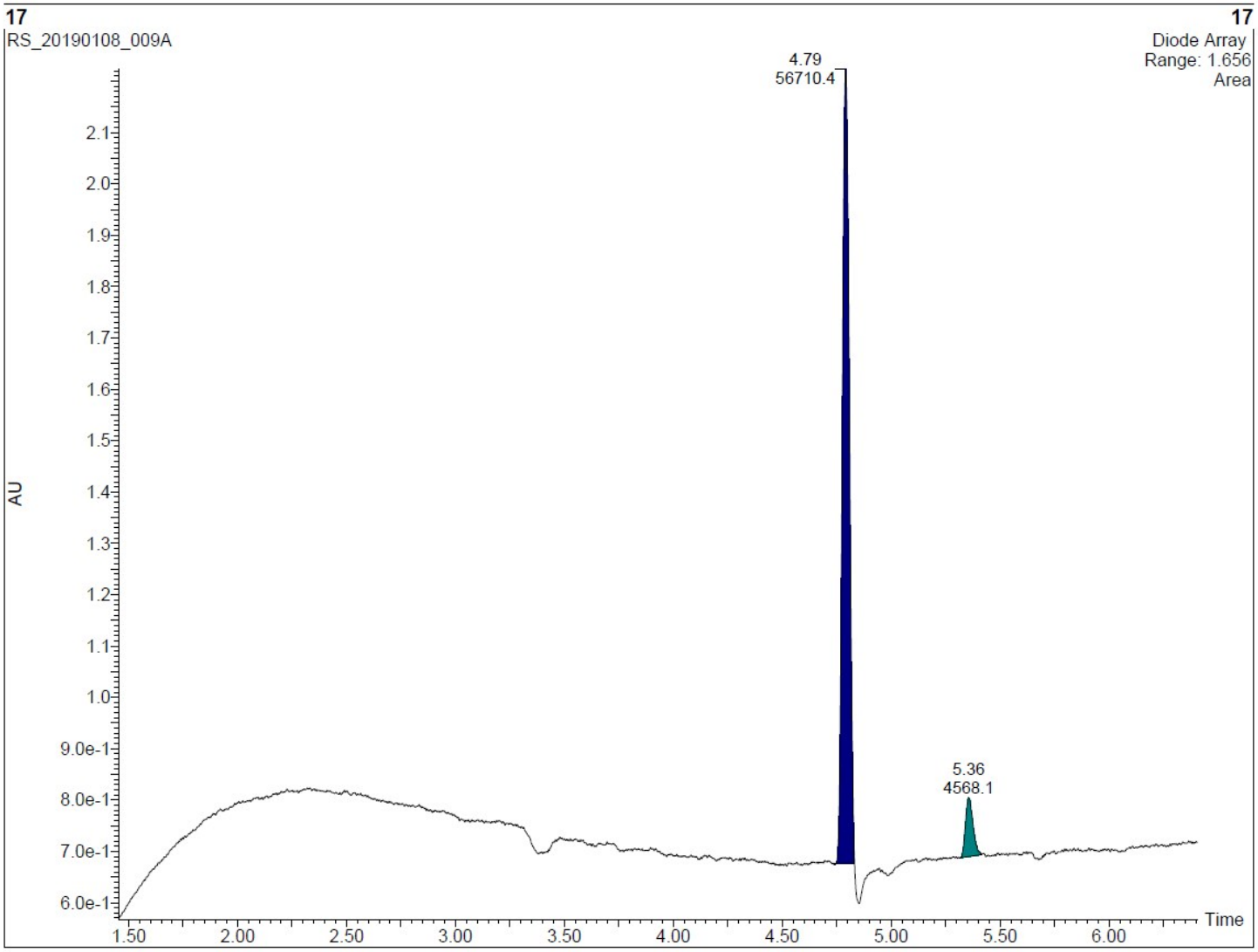
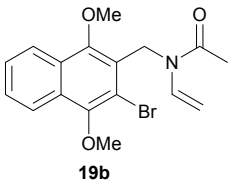


Figure 128 UPLC spectrum of 2-bromo-3-(2-bromomethyl)-1,4-dimethoxynaphthalene (**17**).



19b

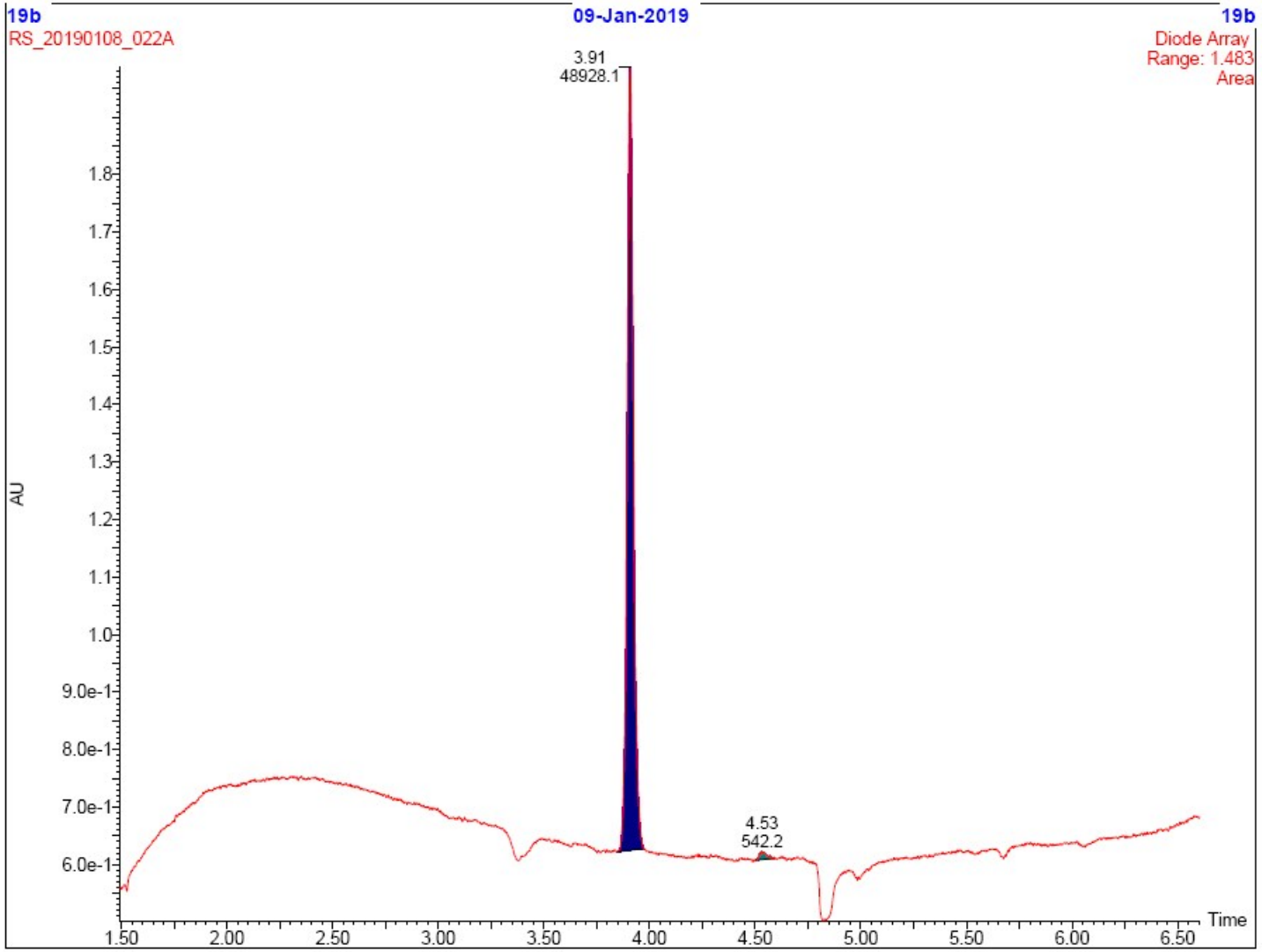
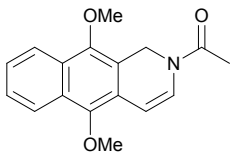


Figure 129 UPLC spectrum of *N*-((3-bromo-1,4-dimethoxynaphthalen-2-yl)methyl)-*N*-vinylacetamide (**19b**).



20b

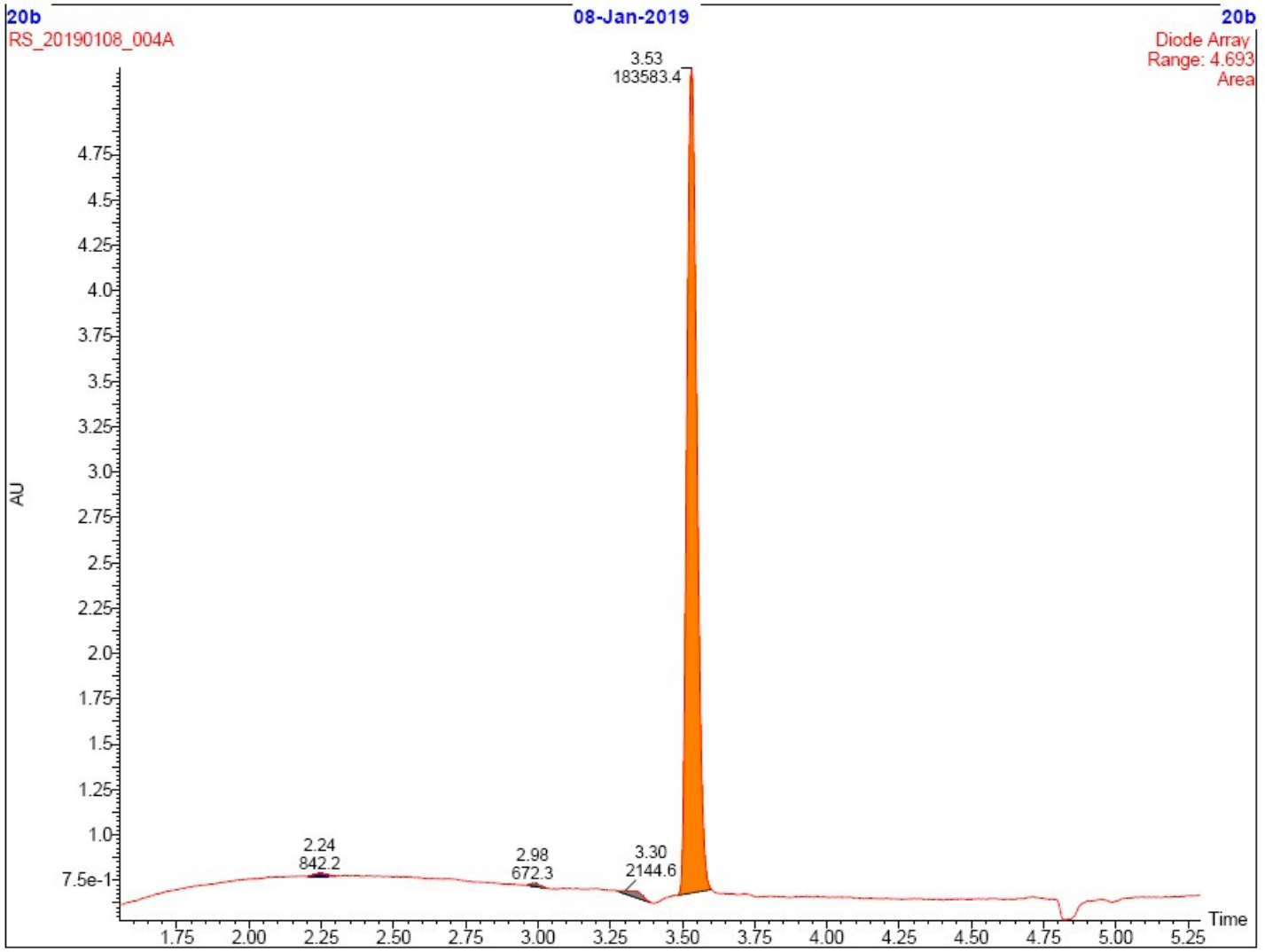
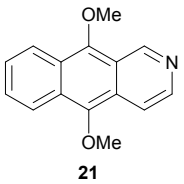


Figure 130 UPLC spectrum of 1-(5,10-dimethoxybenzo[*g*]isoquinolin-2(1*H*)-yl)ethanone (**20b**).



21

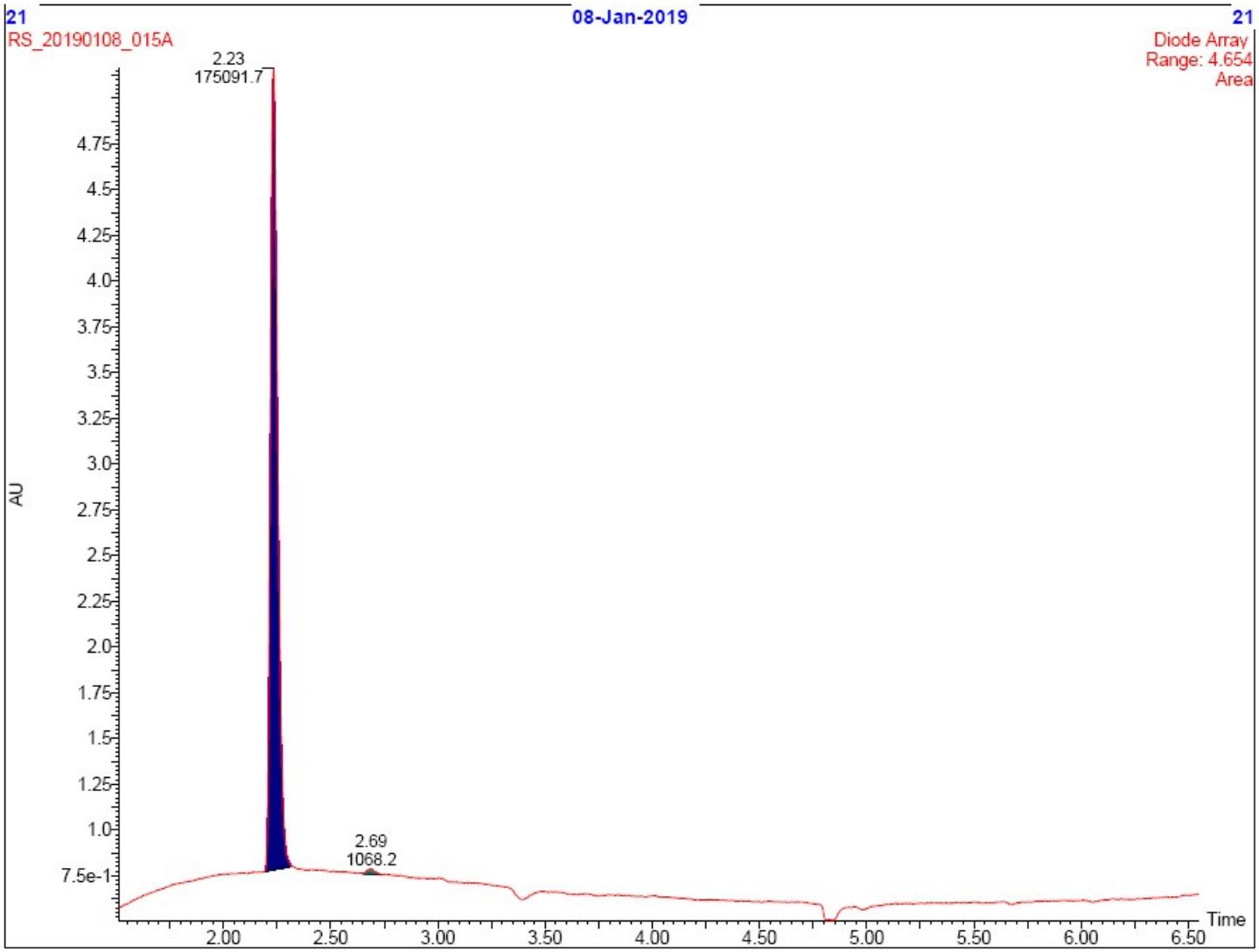
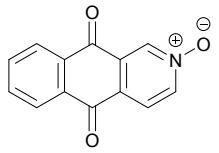


Figure 131 UPLC spectrum of 5,10-dimethoxybenzo[*g*]isoquinoline (**21**).



22

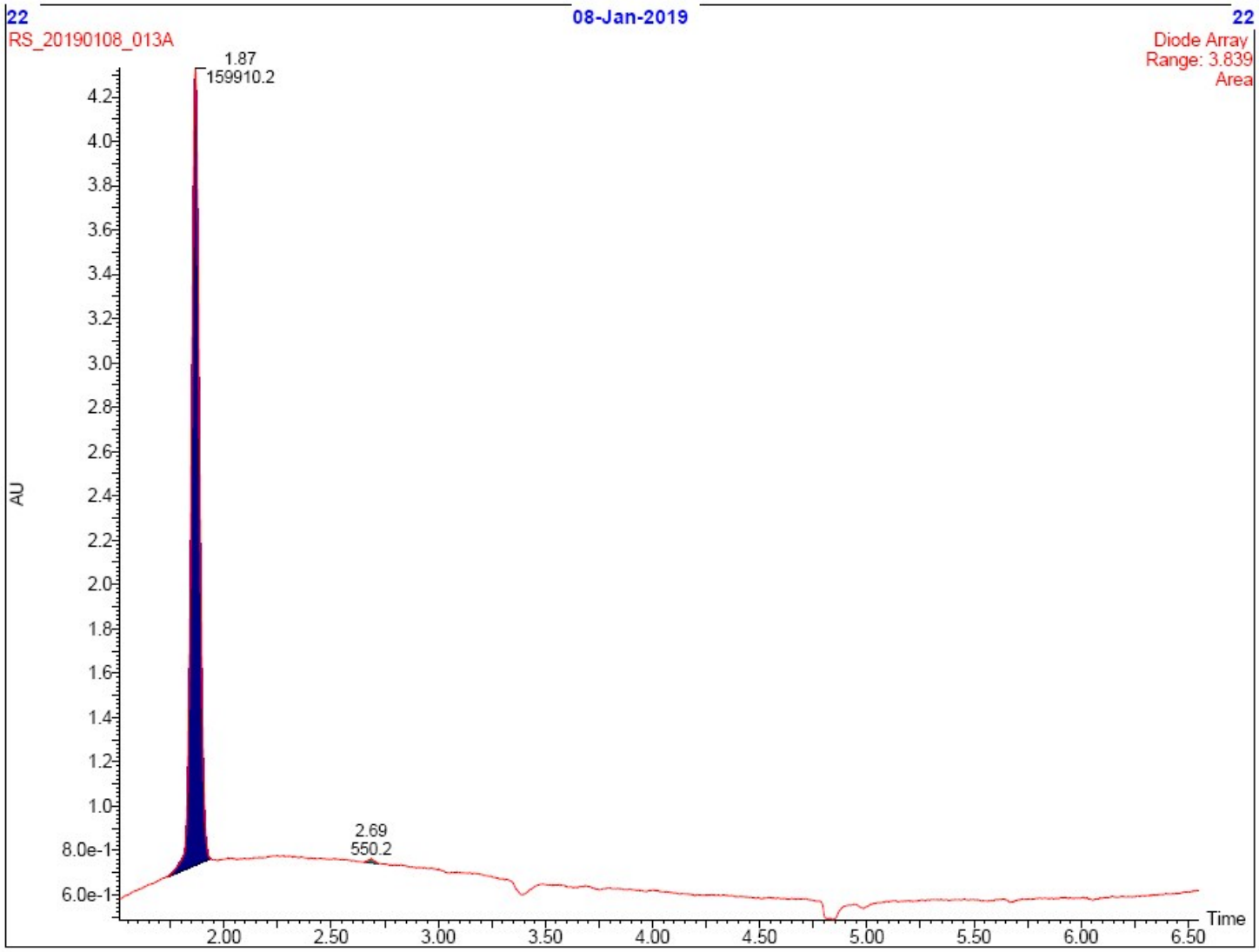


Figure 132 UPLC spectrum of 5,10-dioxo-5,10-dihydrobenzo[*g*]isoquinoline 2-oxide (**22**).

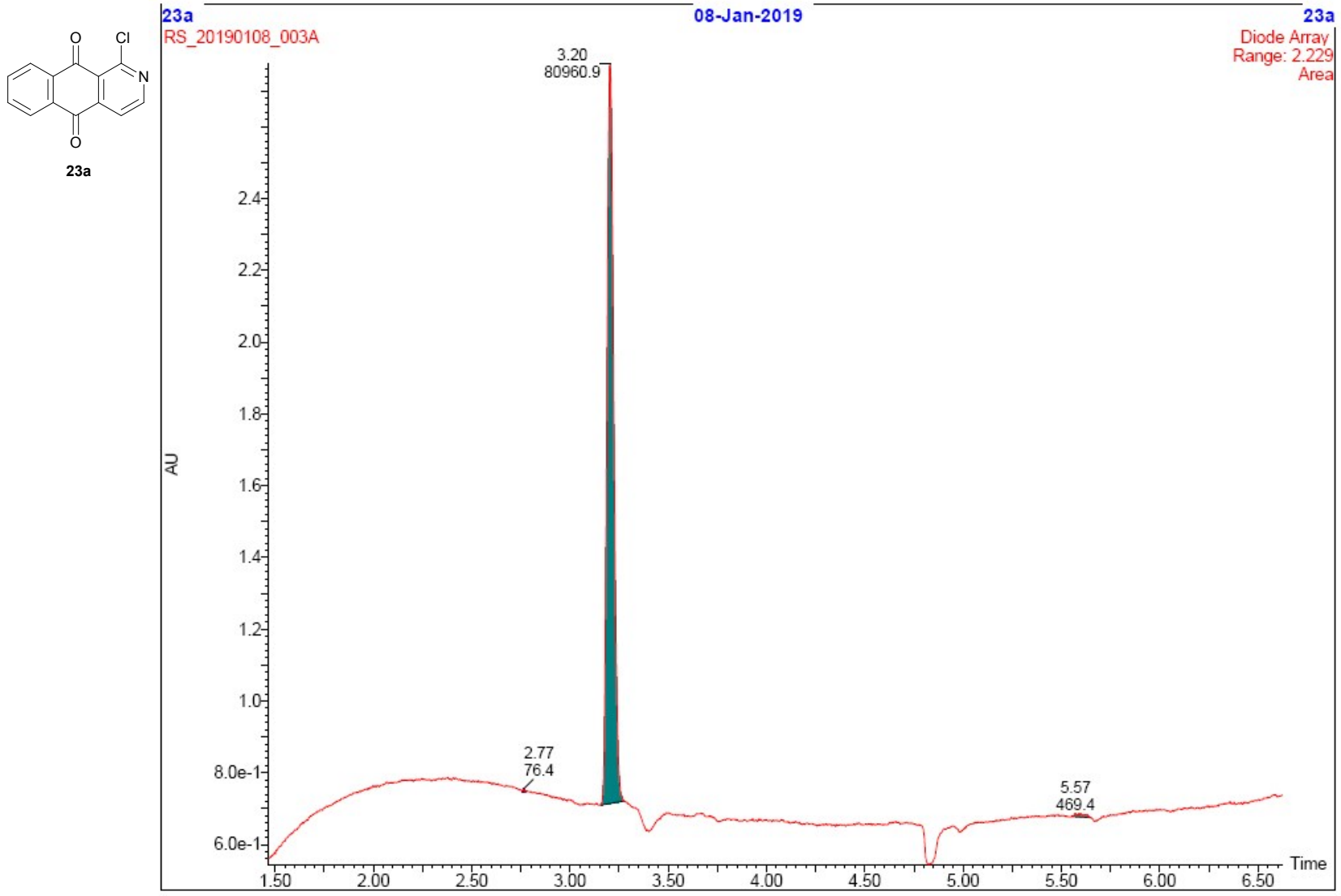
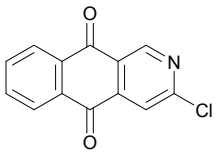


Figure 133 UPLC spectrum of 1-chlorobenzo[*g*]isoquinoline-5,10-dione (**23a**).



23b

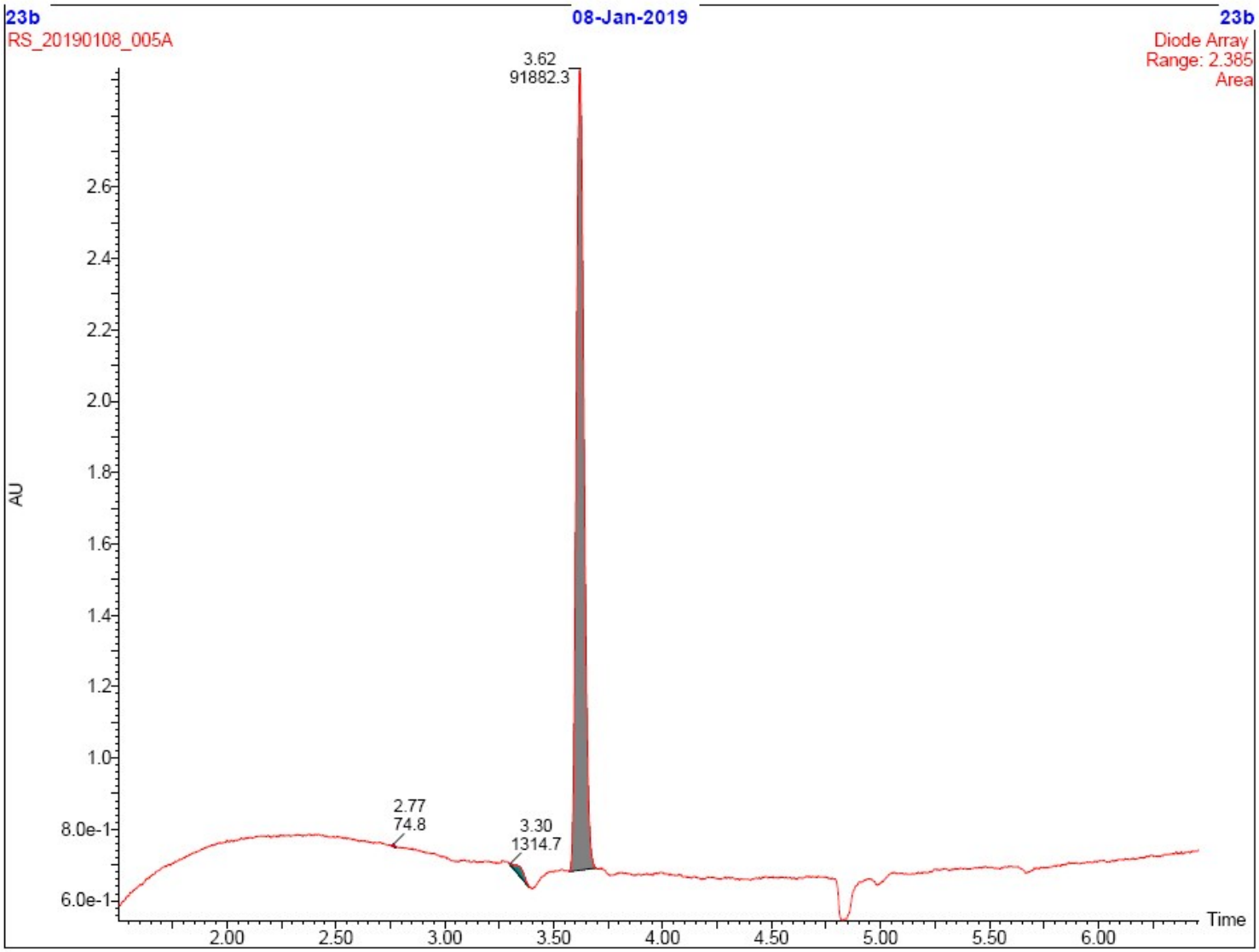


Figure 134 UPLC spectrum of 3-chlorobenzo[*g*]isoquinoline-5,10-dione (**23b**).

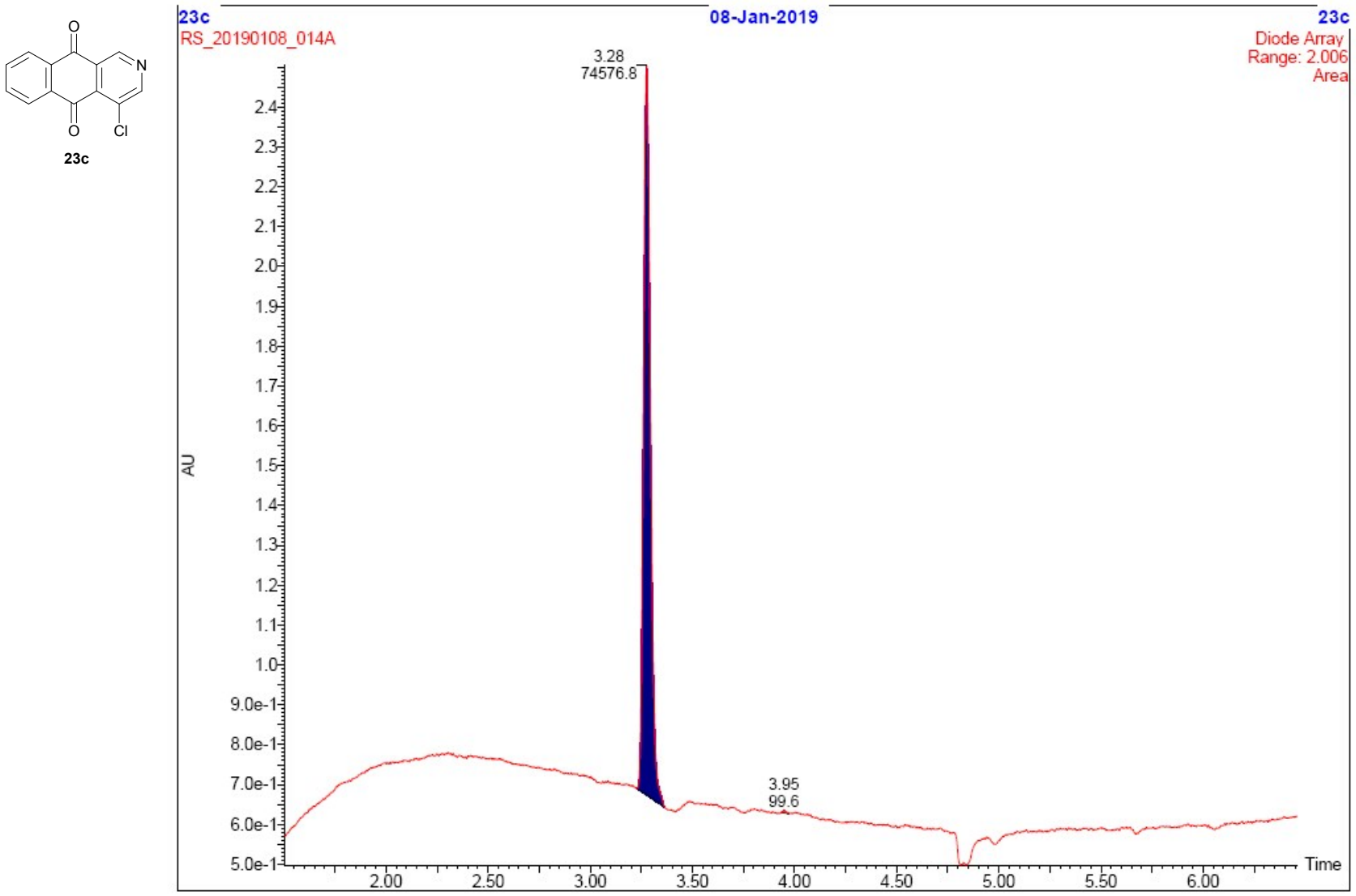
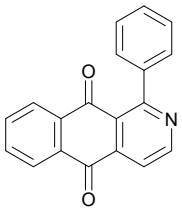


Figure 135 UPLC spectrum of 4-chlorobenzo[*g*]isoquinoline-5,10-dione (**23c**).



25a

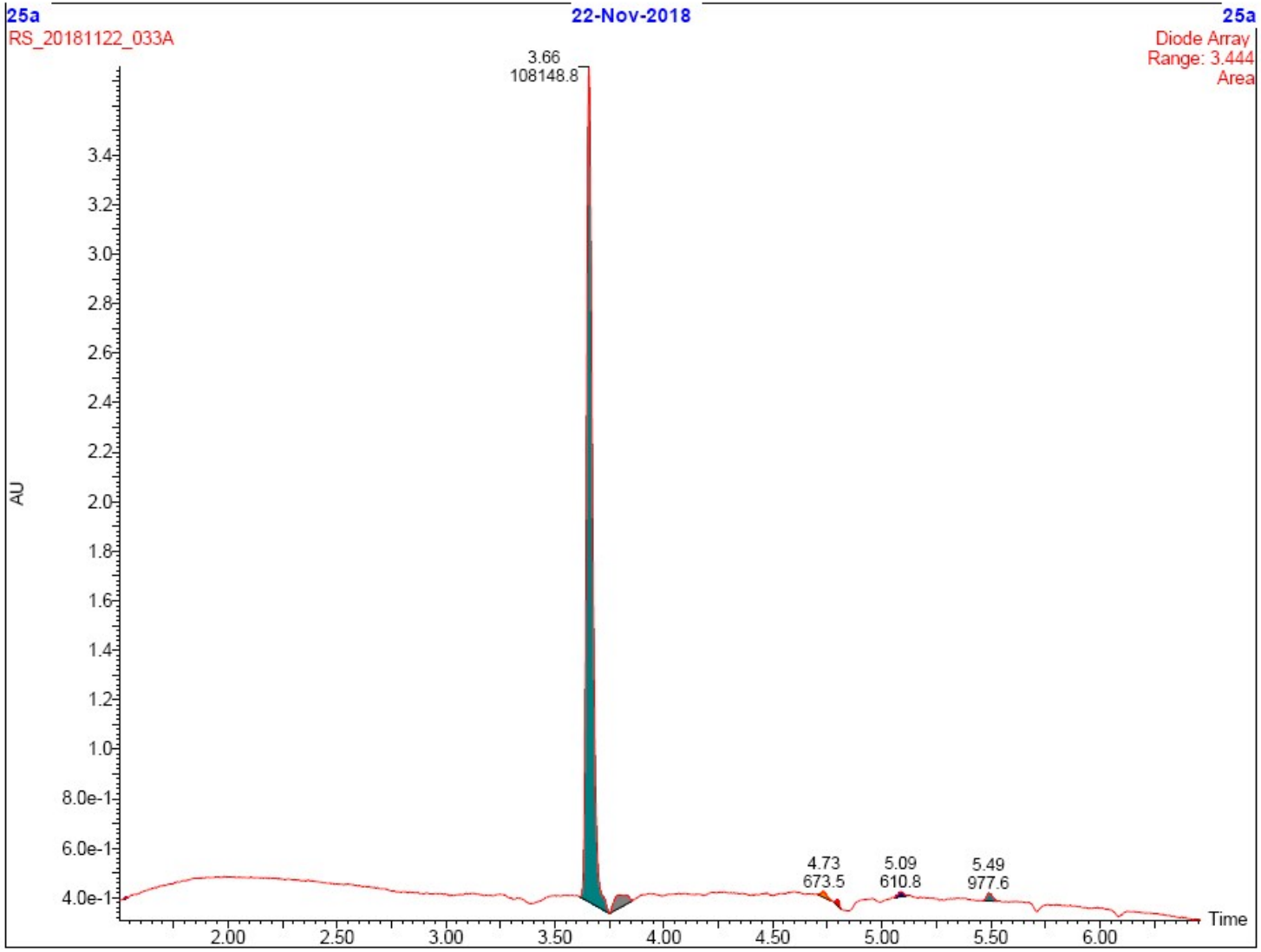
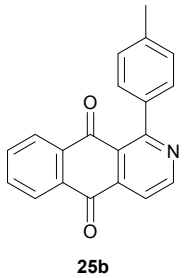


Figure 136 UPLC spectrum of 1-phenylbenzo[*g*]isoquinoline-5,10-dione (**25a**).



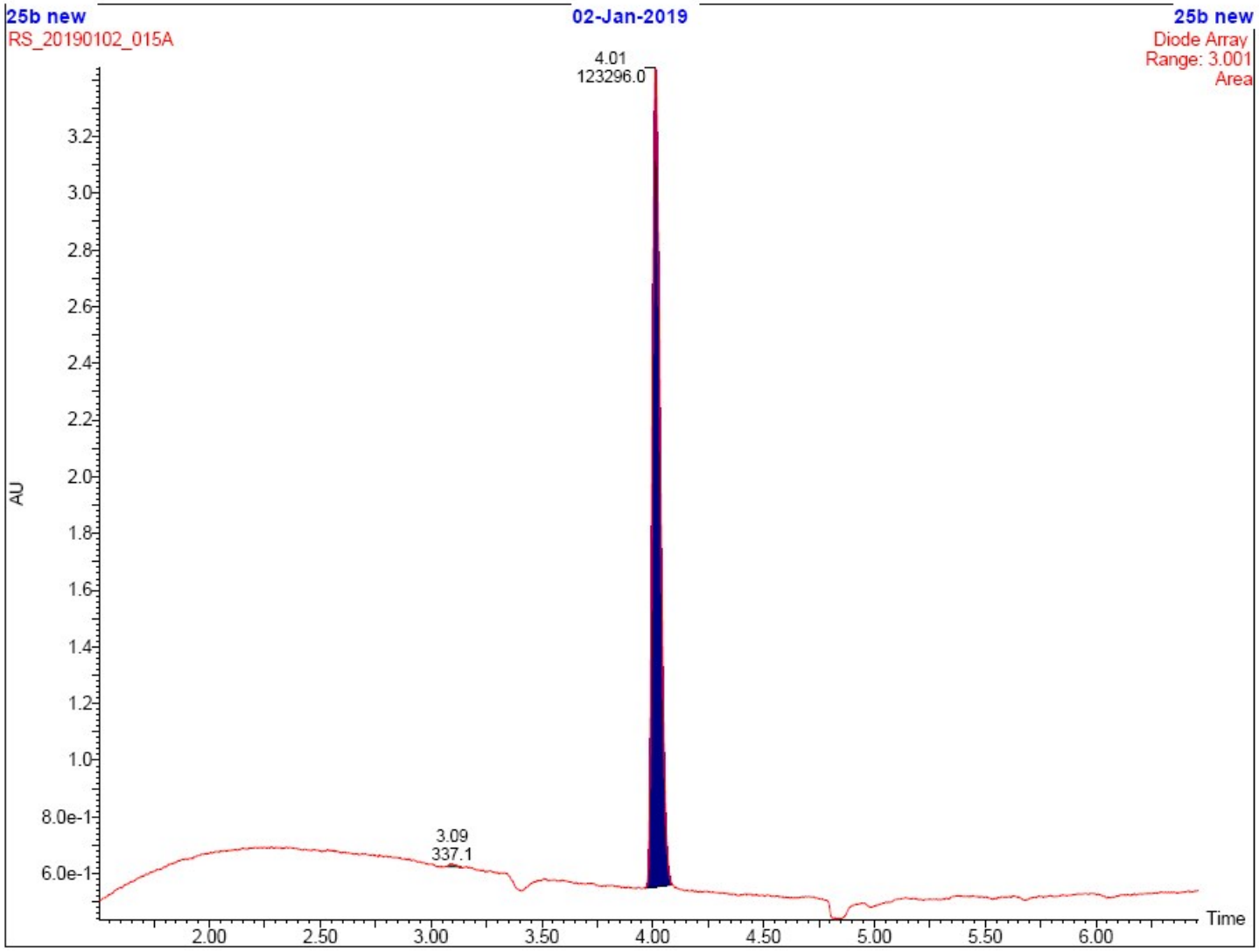
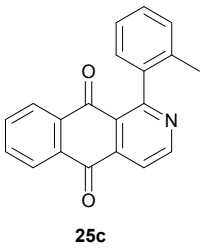


Figure 137 UPLC spectrum of 1-*p*-tolylbenzo[*g*]isoquinoline-5,10-dione (**25b**).



25c

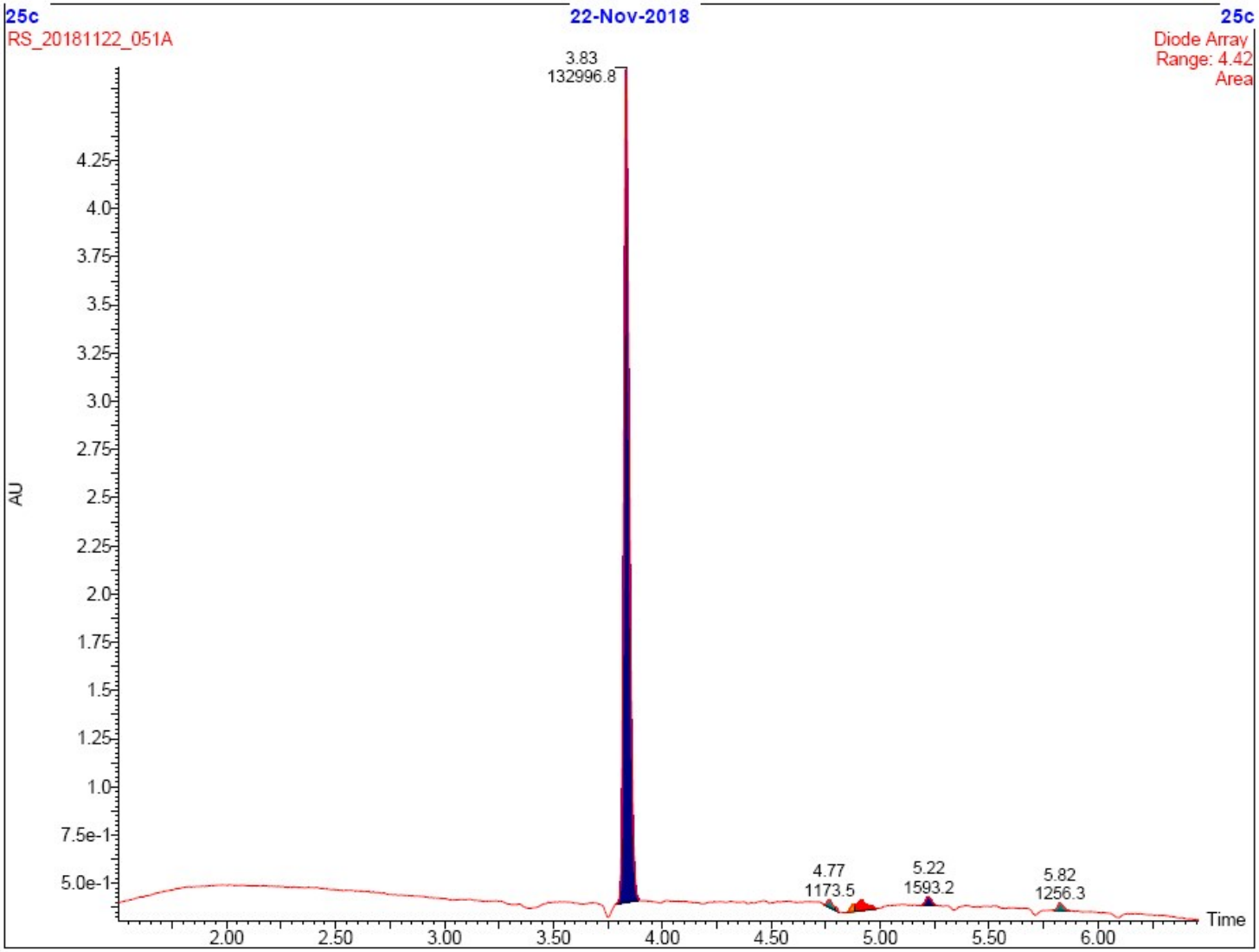
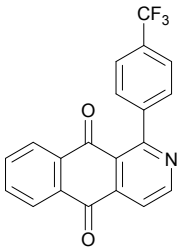


Figure 138 UPLC spectrum of 1-*o*-tolylbenzo[*g*]isoquinoline-5,10-dione (**25c**).



25d

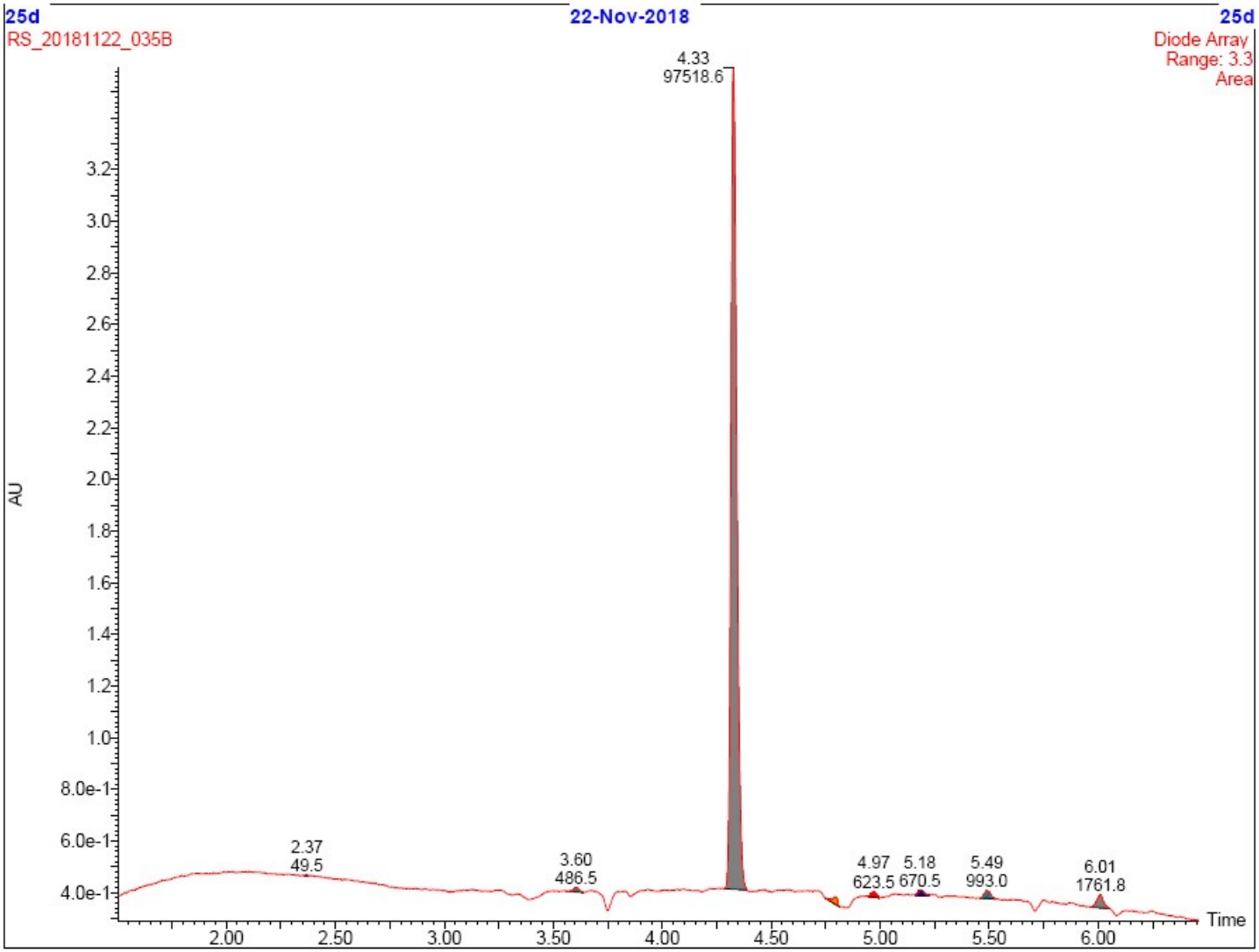
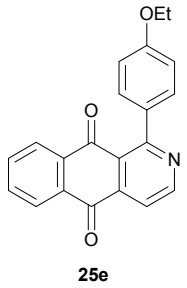


Figure 139 UPLC spectrum of 1-(*p*-(trifluoromethyl)phenyl)benzo[*g*]isoquinoline-5,10-dione (**25d**).



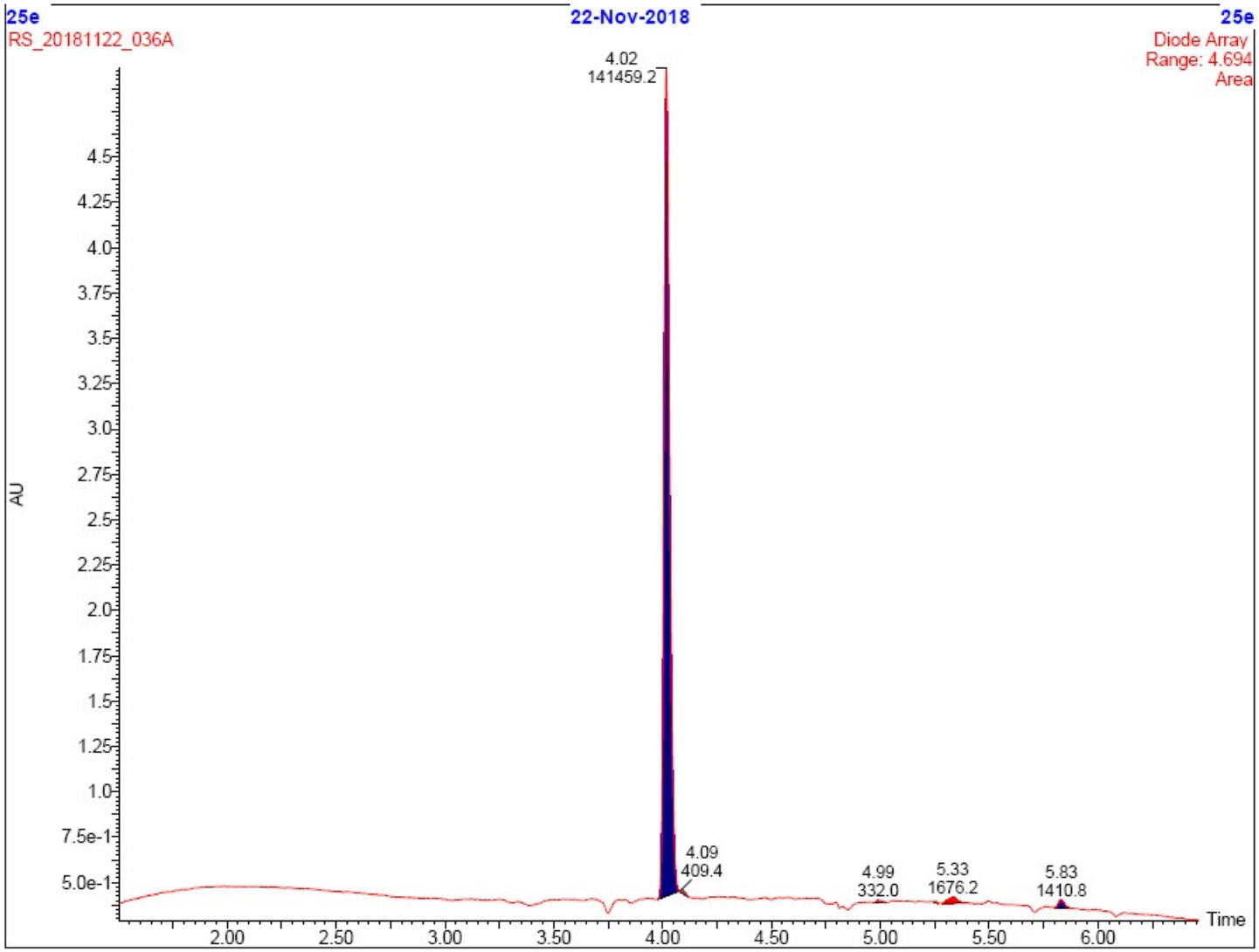
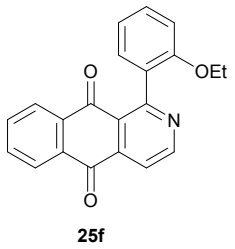


Figure 140 UPLC spectrum of 1-(*p*-ethoxyphenyl)benzo[*g*]isoquinoline-5,10-dione (**25e**).



25f

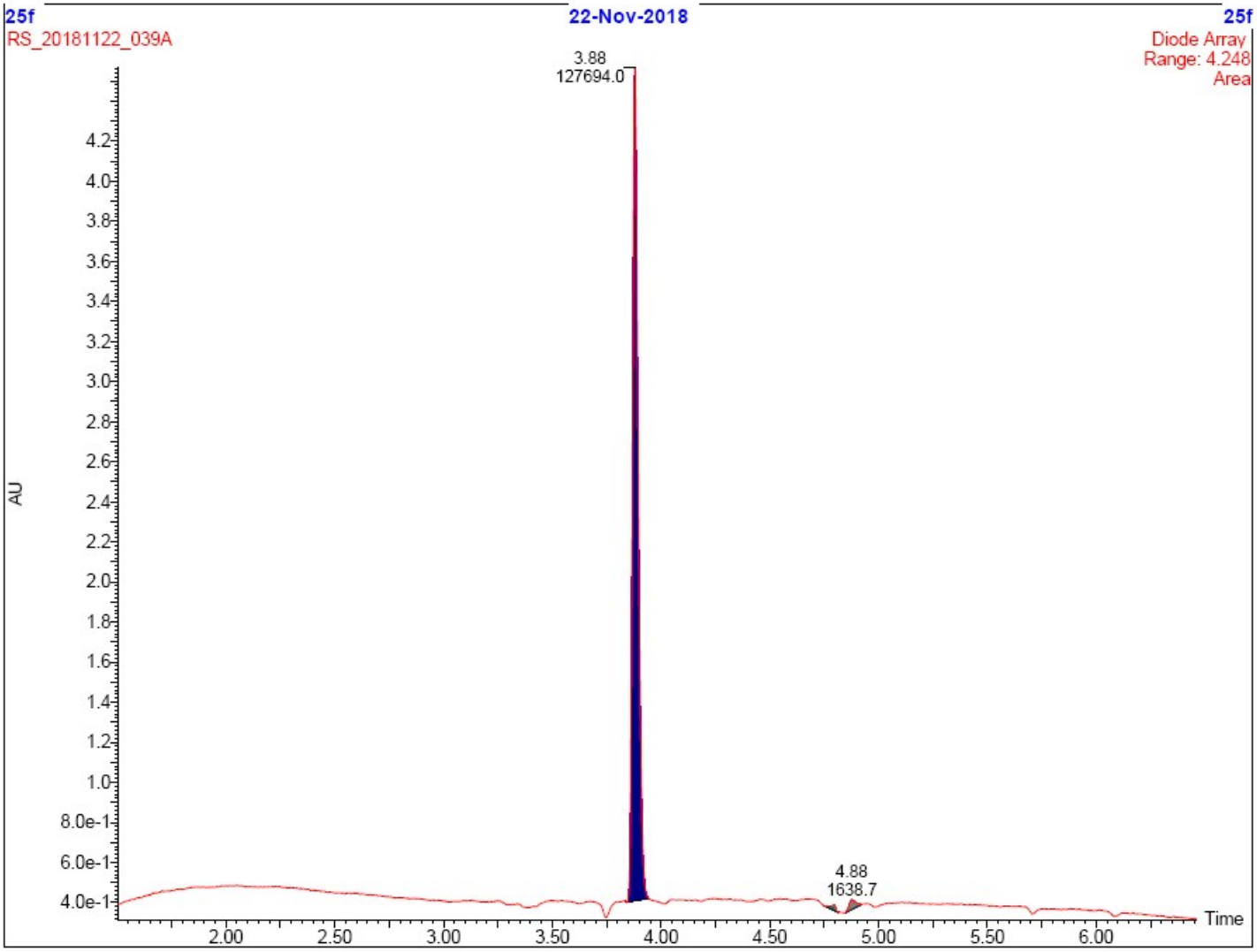


Figure 141 UPLC spectrum of 1-(*o*-ethoxyphenyl)benzo[*g*]isoquinoline-5,10-dione (**25f**).

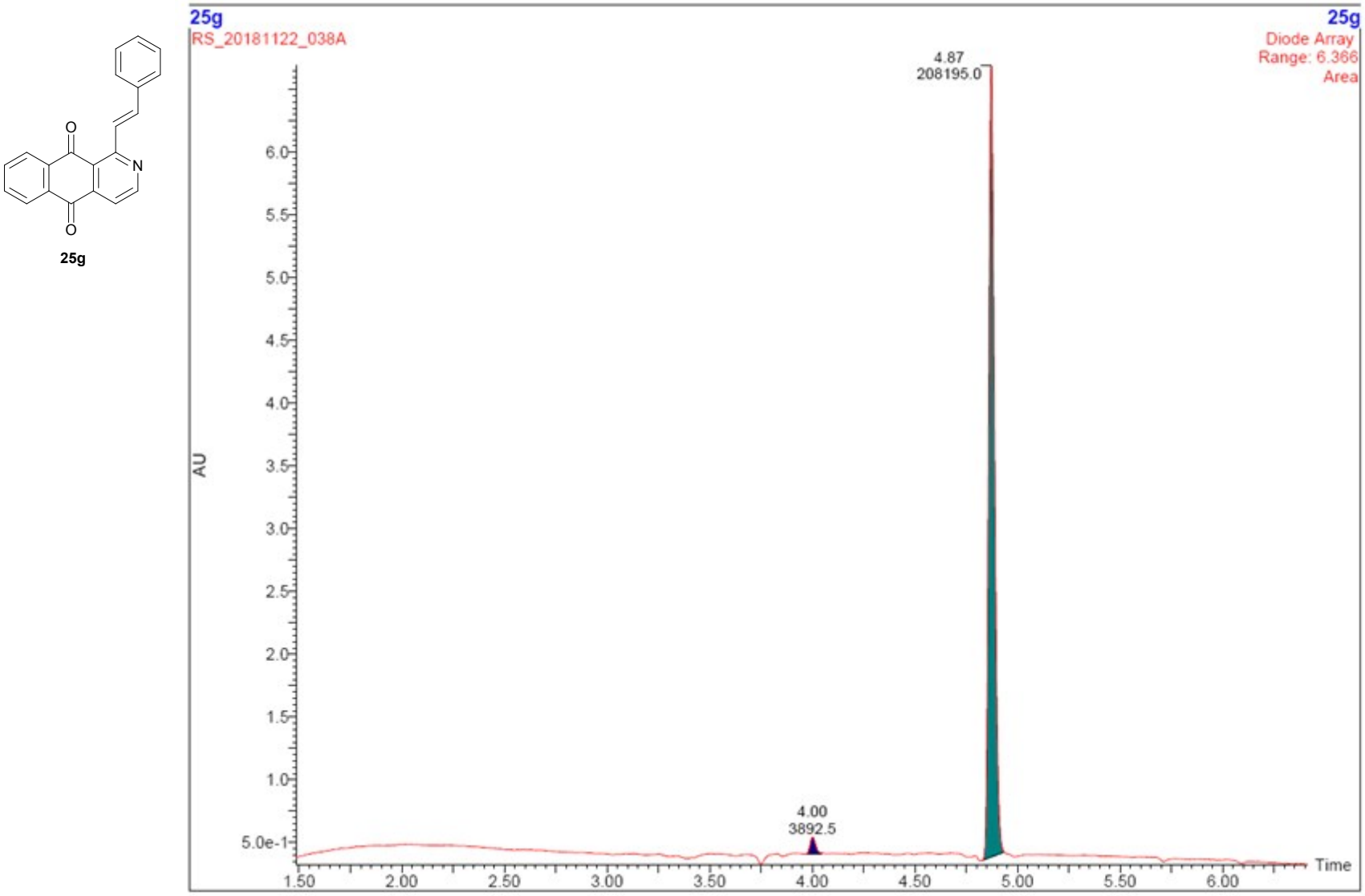
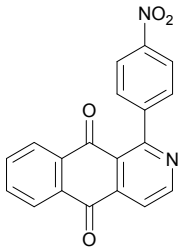


Figure 142 UPLC spectrum of (*E*)-1-styrylbenzo[*g*]isoquinoline-5,10-dione (**25g**).



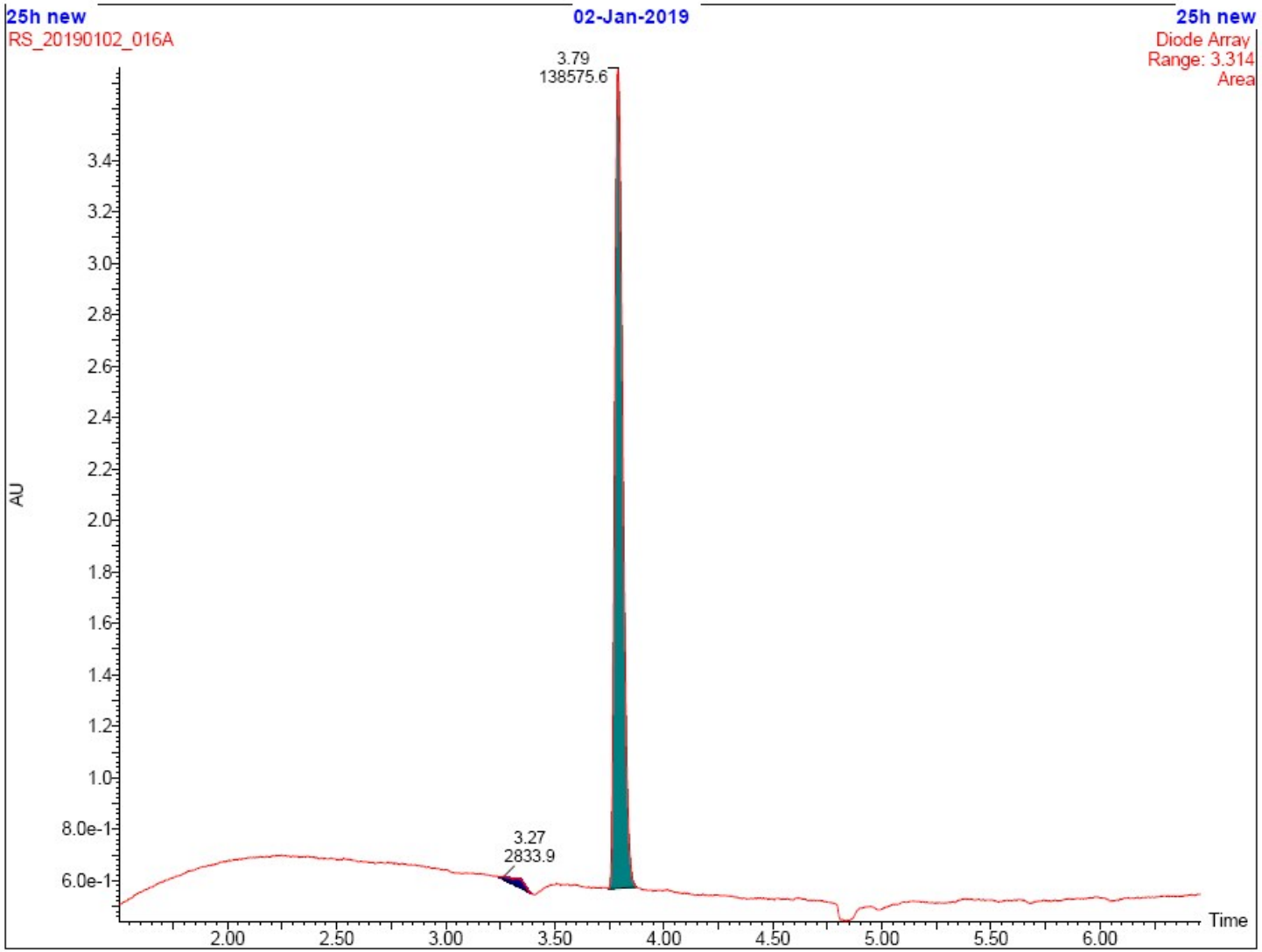


Figure 143 UPLC spectrum of 1-(*p*-nitrophenyl)benzo[*g*]isoquinoline-5,10-dione (**25h**).

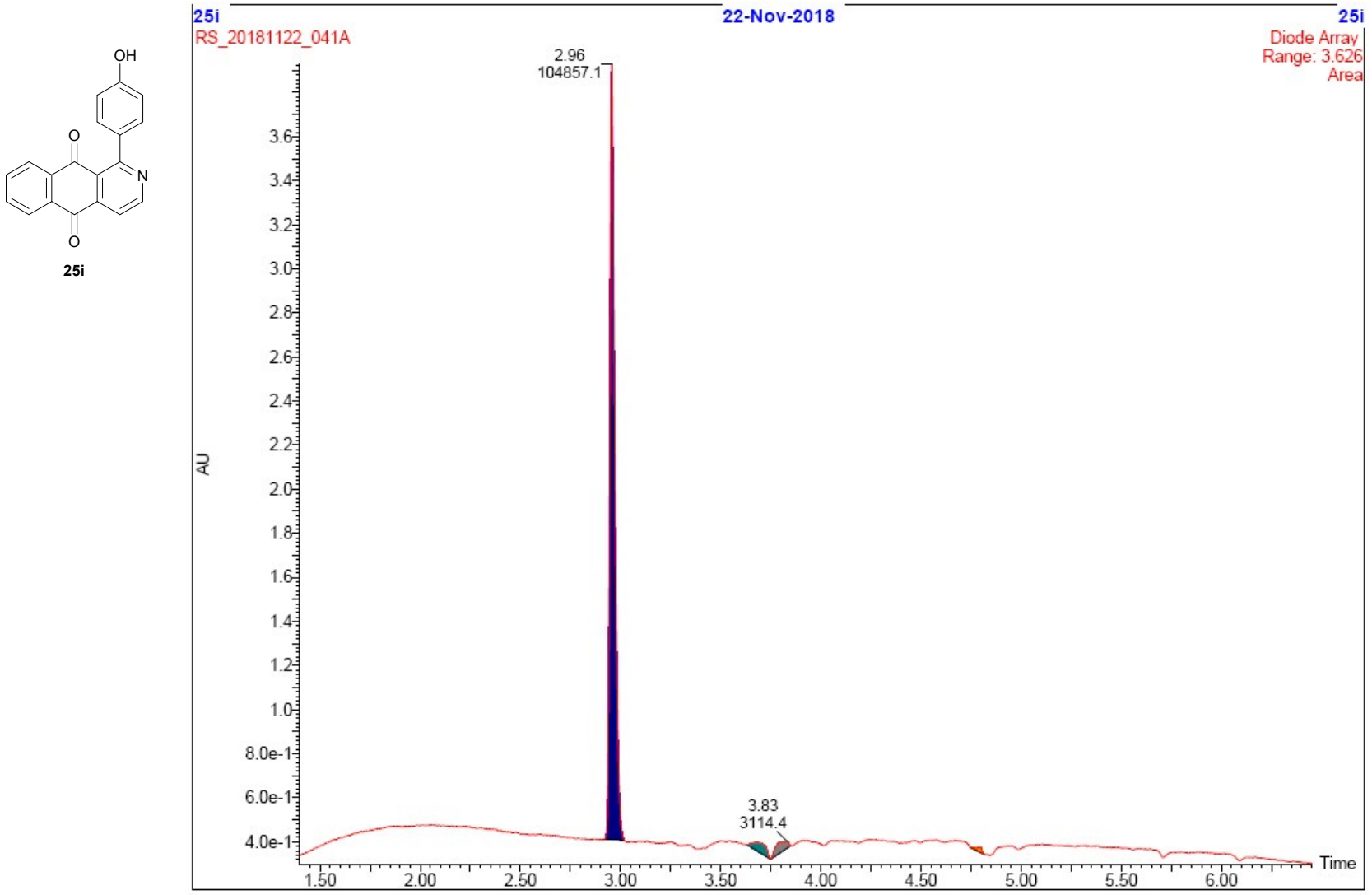


Figure 144 UPLC spectrum of 1-(*p*-hydroxyphenyl)benzo[*g*]isoquinoline-5,10-dione (**25i**).

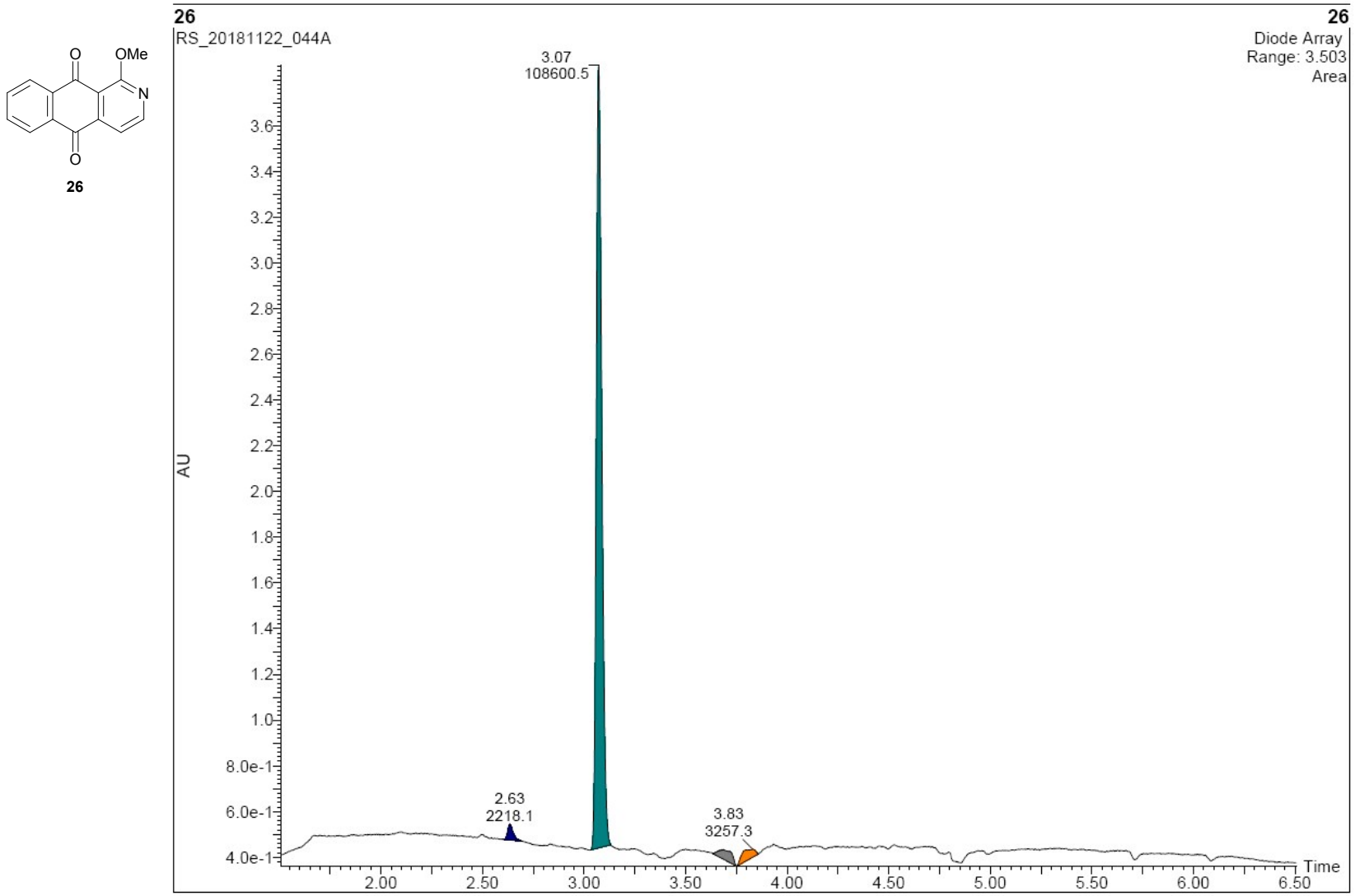
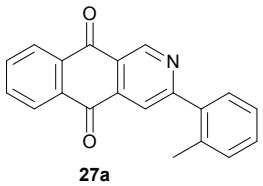


Figure 145 UPLC spectrum of 1-methoxybenzo[*g*]isoquinoline-5,10-dione (**26**).



27a

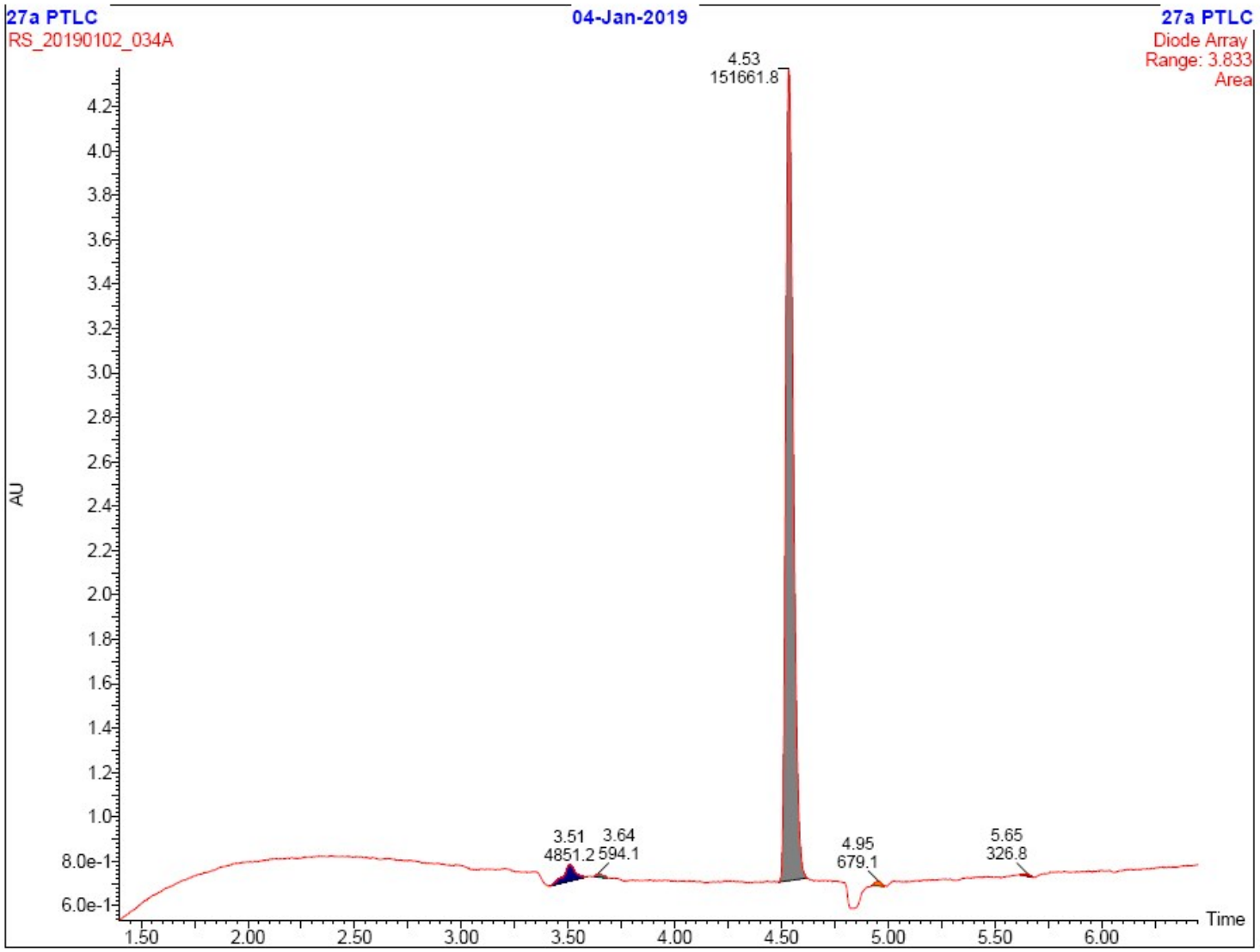
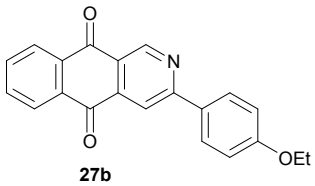


Figure 146 UPLC spectrum of 3-(*o*-tolyl)benzo[*g*]isoquinoline-5,10-dione (**27a**).



27b

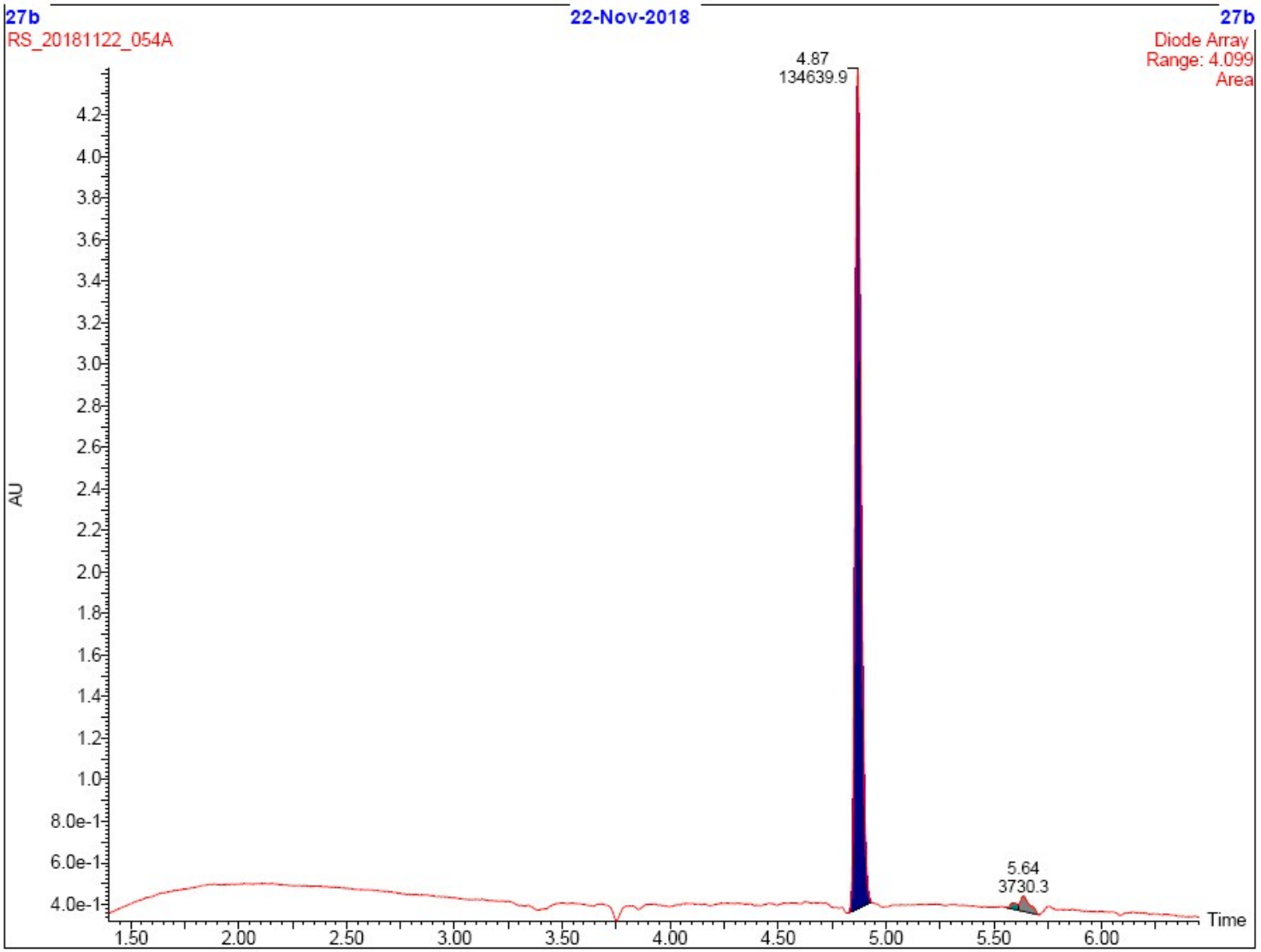
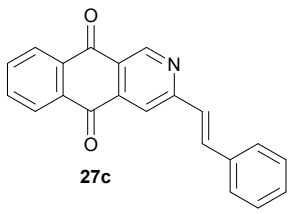


Figure 147 UPLC spectrum of 3-(*p*-ethoxyphenyl)benzo[*g*]isoquinoline-5,10-dione (**27b**).



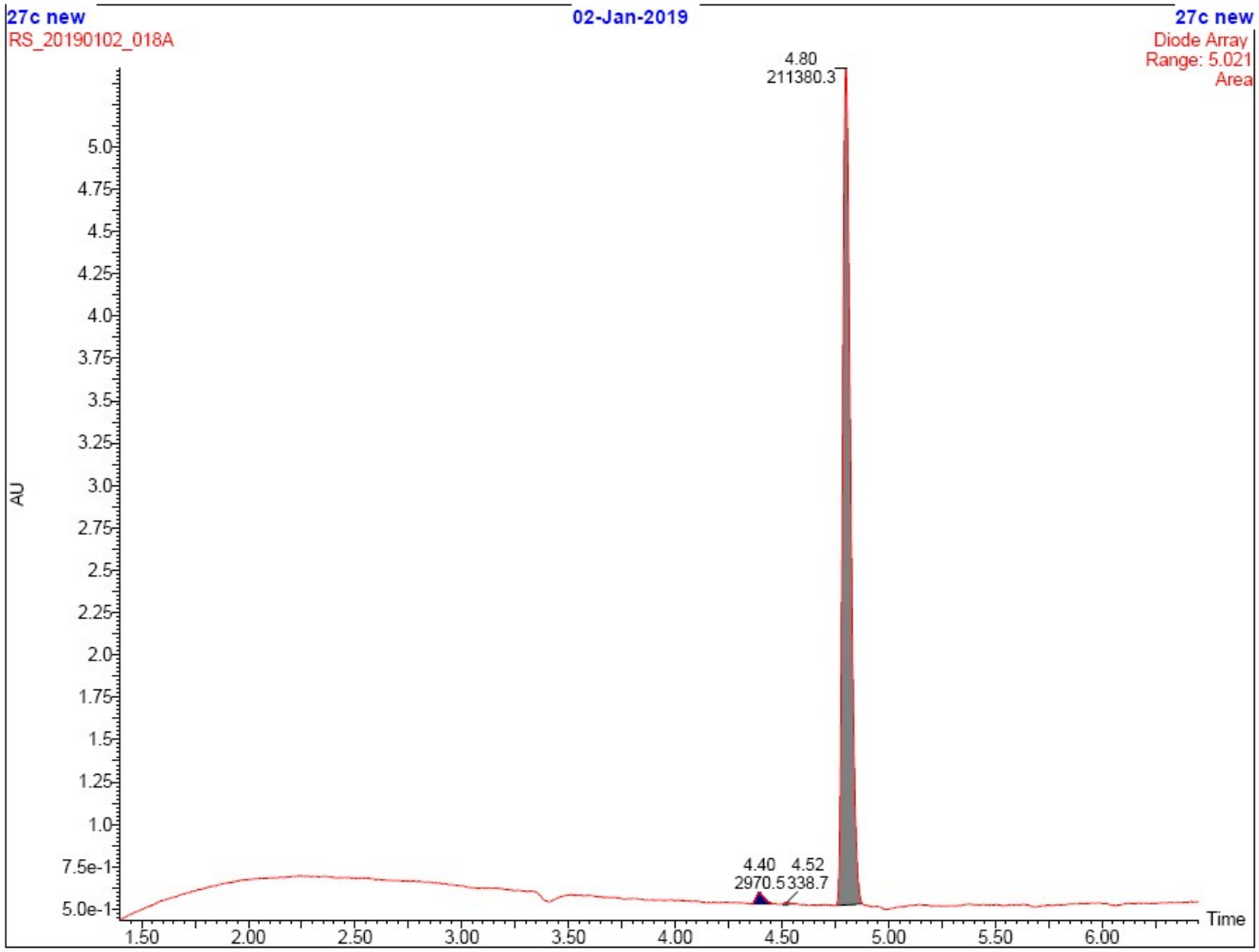
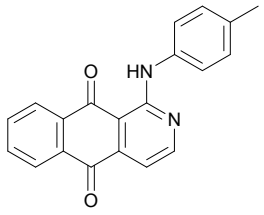


Figure 148 UPLC spectrum of (*E*)-3-styrylbenzo[*g*]isoquinoline-5,10-dione (**27c**).



28a

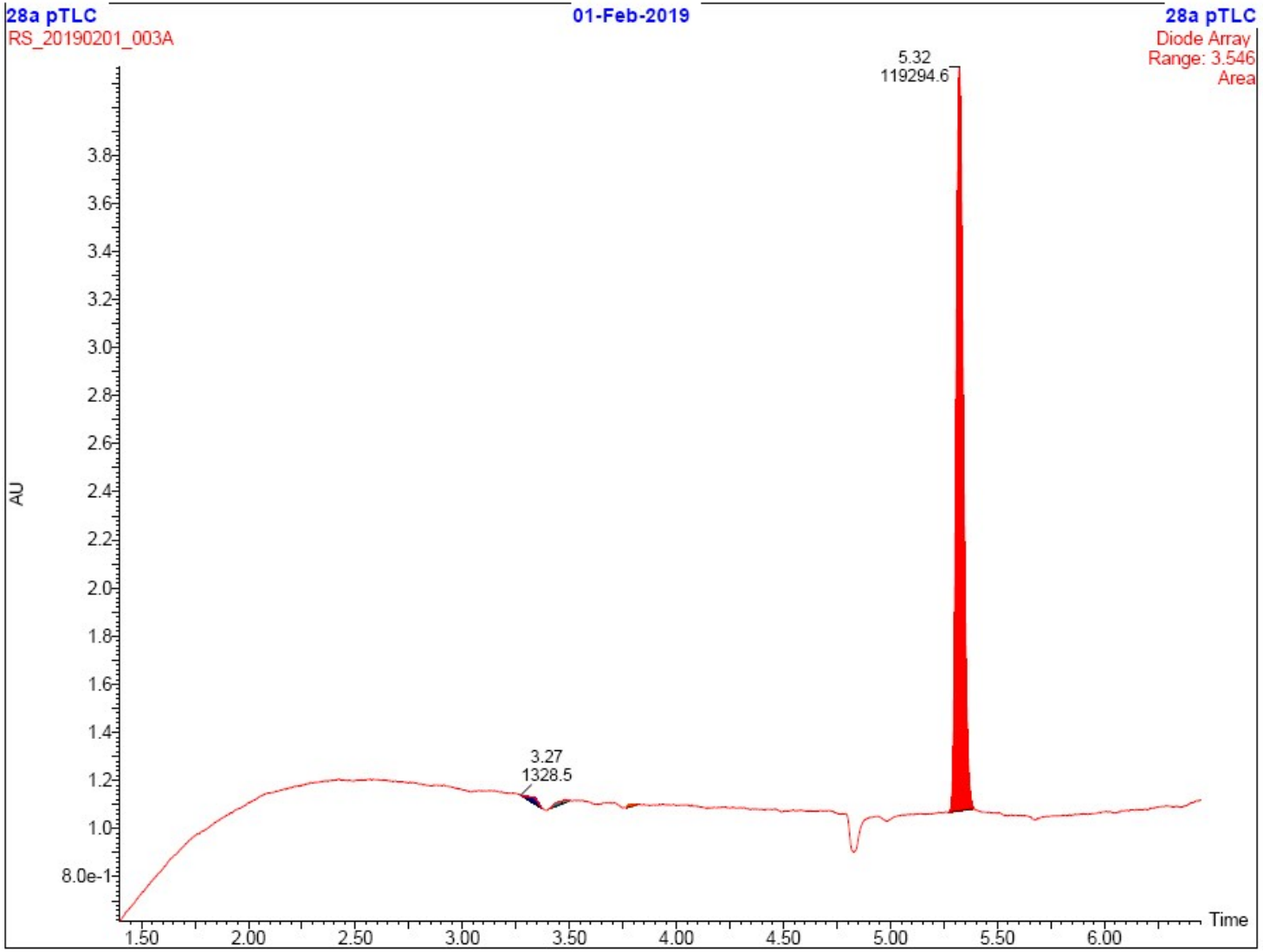
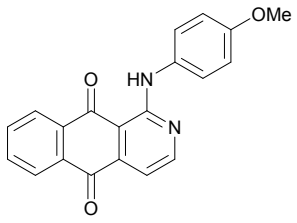


Figure 149 UPLC spectrum of 1-(*p*-tolylamino)benzo[*g*]isoquinoline-5,10-dione (**28a**).



28b

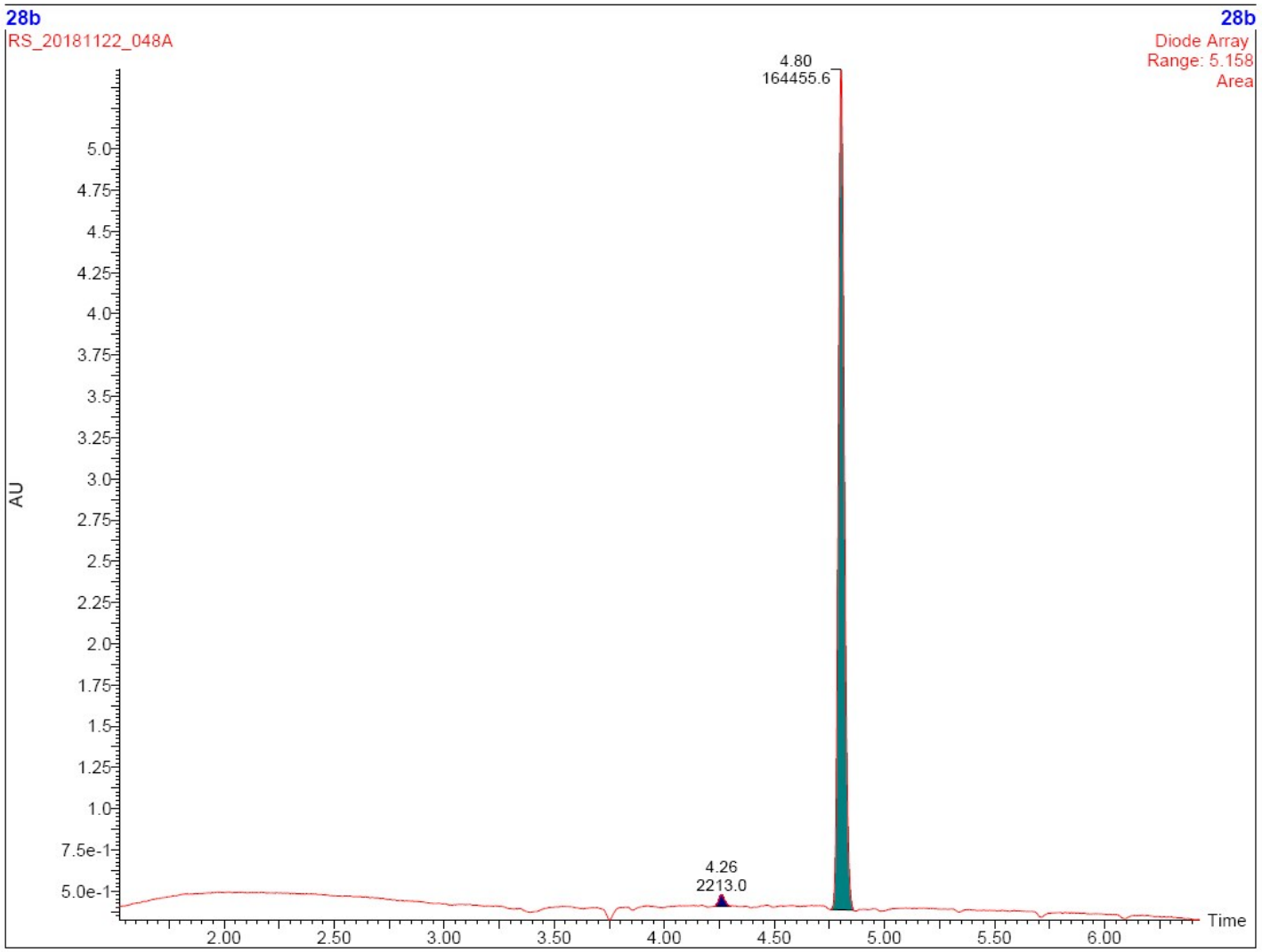
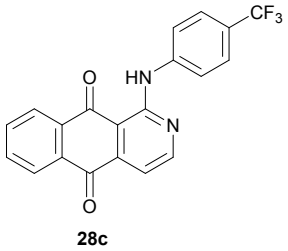


Figure 150 UPLC spectrum of 1-((*p*-methoxyphenyl)amino)benzo[*g*]isoquinoline-5,10-dione (**28b**).



28c

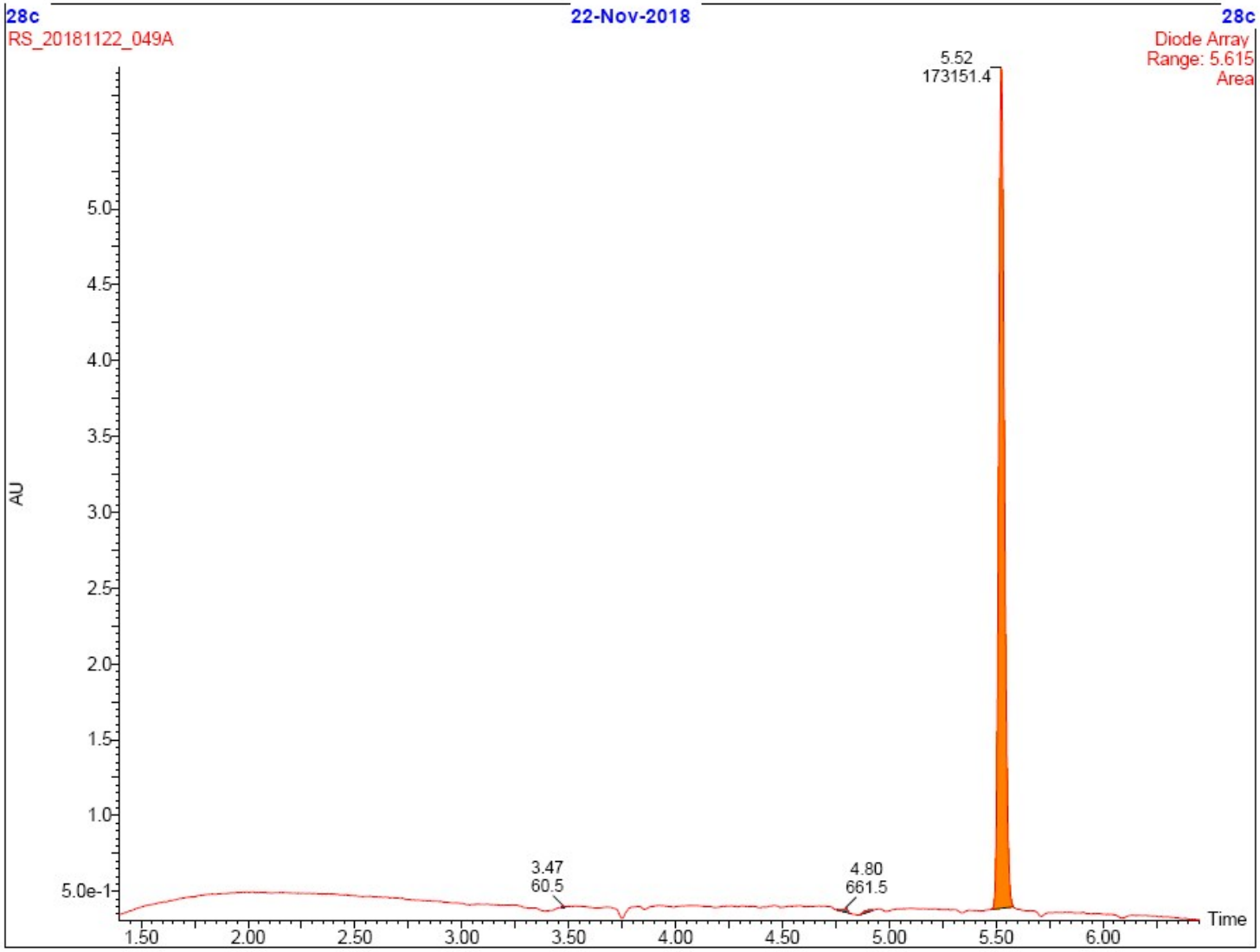


Figure 151 UPLC spectrum of 1-((*p*-(trifluoromethyl)phenyl)amino)benzo[*g*]isoquinoline-5,10-dione (**28c**).

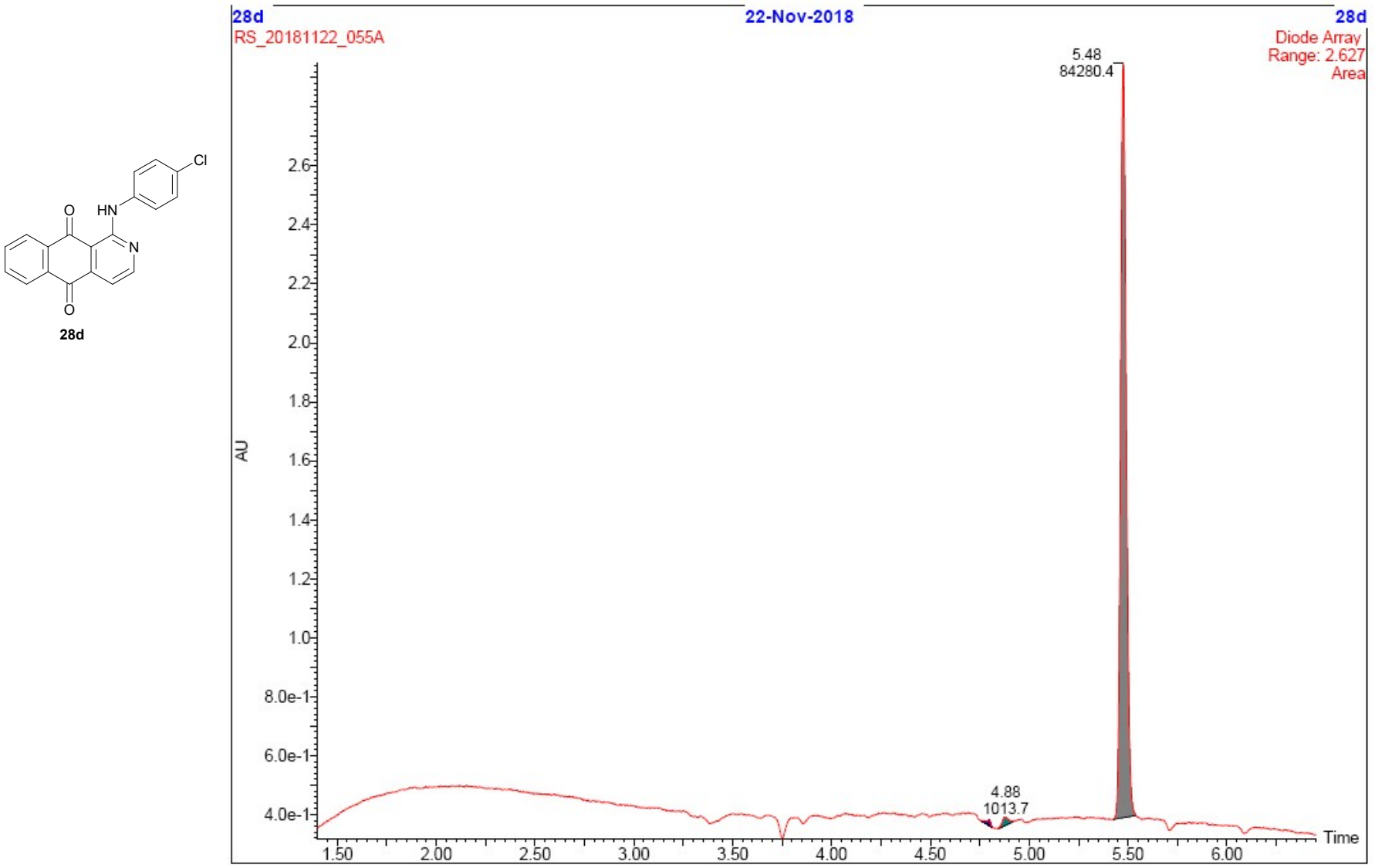


Figure 152 UPLC spectrum of 1-((*p*-chlorophenyl)amino)benzo[*g*]isoquinoline-5,10-dione (**28d**).

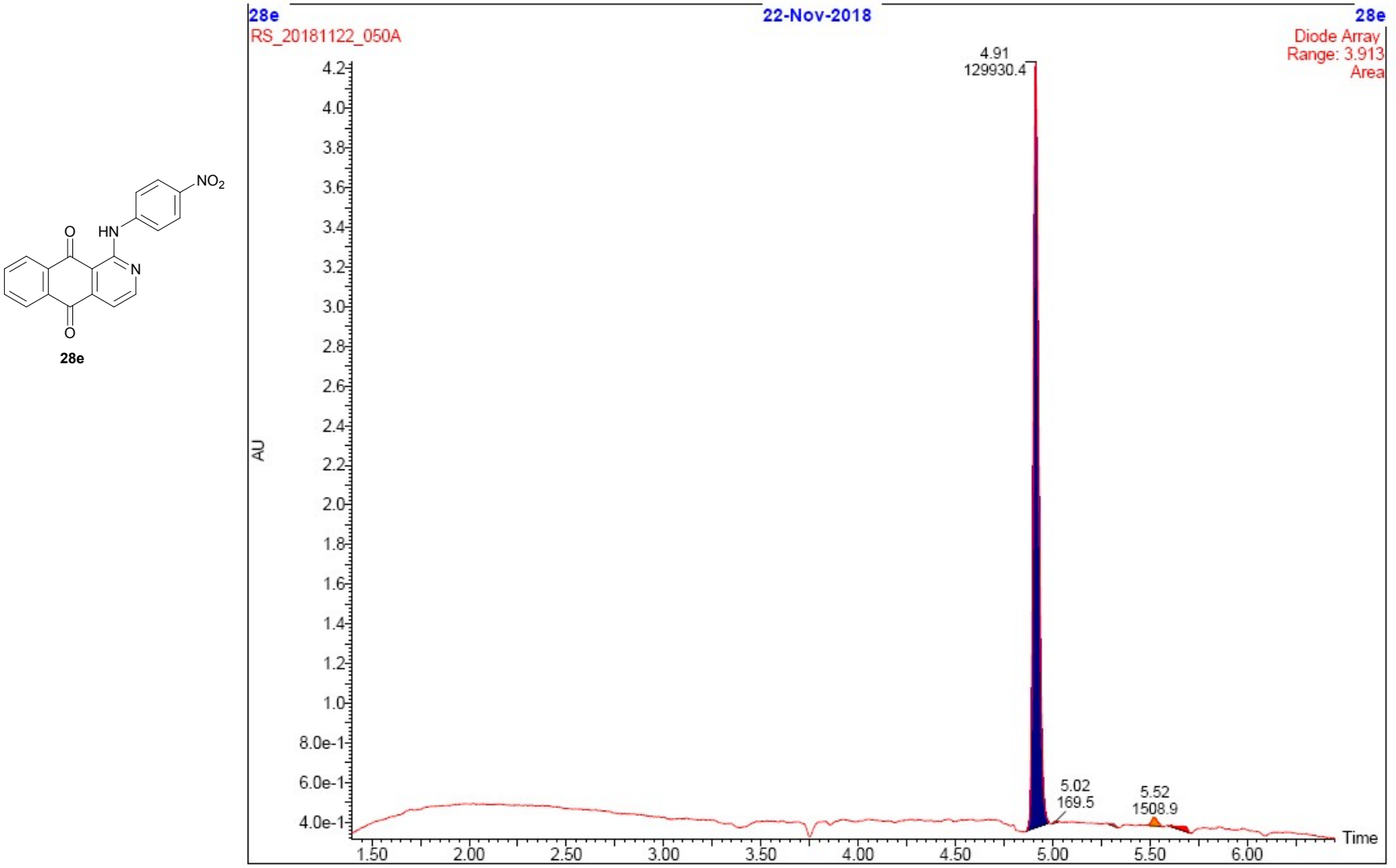


Figure 153 UPLC spectrum of 1-((*p*-nitrophenyl)amino)benzo[*g*]isoquinoline-5,10-dione (**28e**).

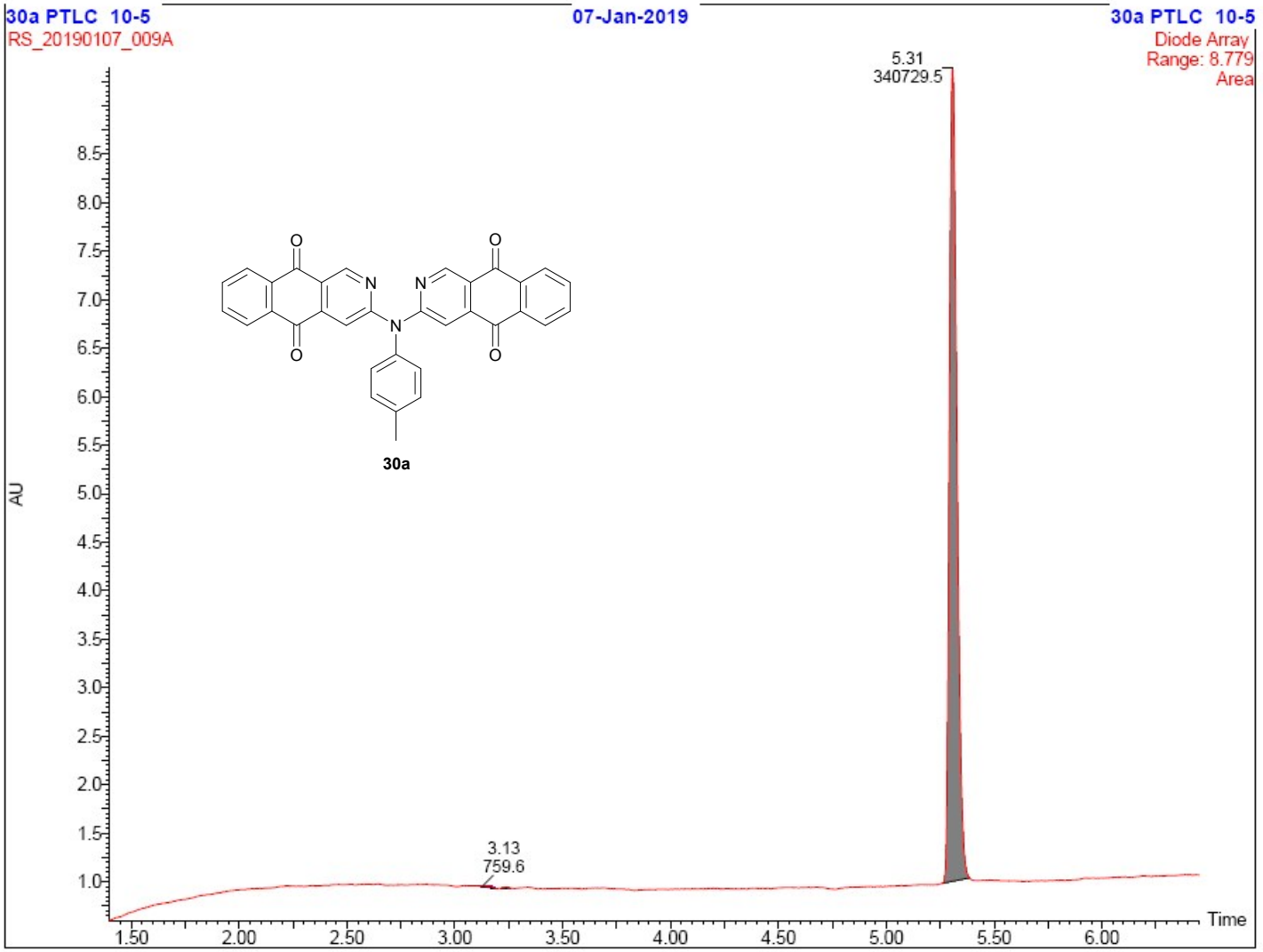


Figure 154 UPLC spectrum of 3,3'-(*p*-tolylazanediyl)bis(benzo[*g*]isoquinoline-5,10-dione) (**30a**).

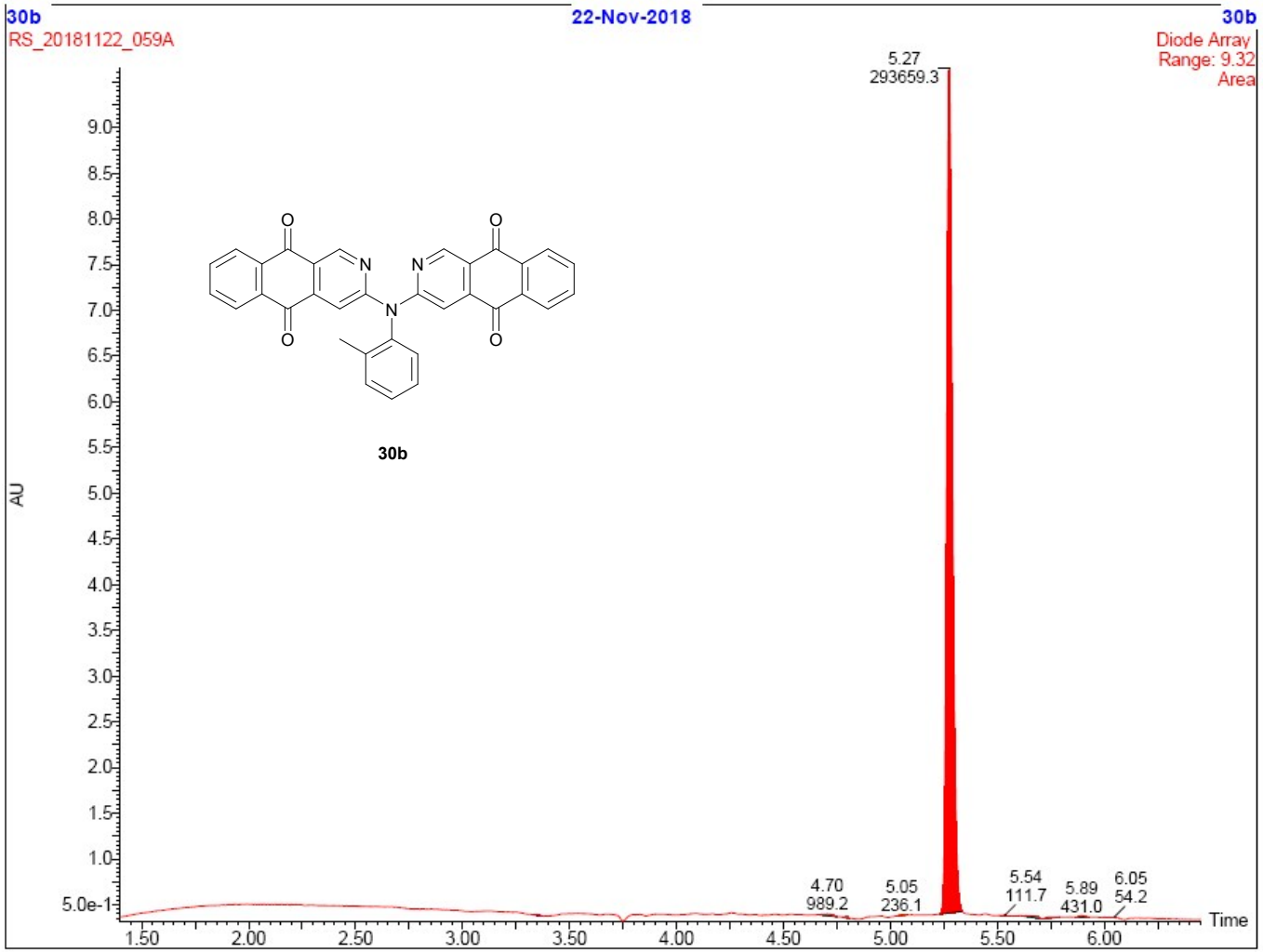


Figure 155 UPLC spectrum of 3,3'-(*o*-tolylazanediyl)bis(benzo[*g*]isoquinoline-5,10-dione) (**30b**).