SUPPLEMENTARY DATA

New 1,4-anthracenedione derivatives with fused heterocyclic rings: synthesis and biological evaluation.

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Table S1. Antifungal evaluation (GM-MIC_{90}, μg/mL) against pathogenic yeasts (*Candida spp*.)

Compound	*Candida parapsilosis* ATCC 22019 (*Cp*)	*C. krusei* ATCC 6258 (*Ck*)	*C. lusitaniae* ATCC 200951 (*Cl*)	*C. tropicalis* CECT 11901 (*Ct*1)	*C. tropicalis* ATCC 200956 (*Ct*2, INM13)	*C. albicans* ATTC 10231 (*Ca*1)	*C. albicans* ATCC 90028 (*Ca*2)
1	4,75 ± 2	4 ± 0	5,04 ± 2,07	12,7 ± 4,13	5,04 ± 2,07	17,96 ± 9,8	22,63 ± 8,76
2	2 ± 0	1 ± 0	2 ± 0	> 32	5,04 ± 2,31	> 32	8 ± 0
3a	4 ± 0	2 ± 0	5,04 ± 2,07	12,7 ± 4,13	8 ± 0	20,16 ± 8,26	16 ± 10,93
4b	> 32	> 32	> 32	> 32	> 32	> 32	> 32
10a	> 32	> 32	> 32	> 32	> 32	> 32	> 32
12a	8 ± 0	2,82 ± 1,15	2.24 ± 0.82	6,35 ± 2,07	4 ± 0	4 ± 0	8 ± 5,47
14	6,72 ± 2	19,02 ±6,94	20,16 ± 8,26	> 32	32 ± 0	> 32	> 32
21	> 32	> 32	> 32	> 32	> 32	> 32	> 32
23	> 32	> 32	> 32	> 32	> 32	> 32	> 32
32	> 32	> 32	> 32	> 32	> 32	> 32	> 32
34	> 32	> 32	> 32	> 32	> 32	> 32	> 32
35	> 32	> 32	> 32	> 32	> 32	> 32	> 32
36	> 32	> 32	> 32	> 32	> 32	> 32	> 32
37	> 32	> 32	> 32	> 32	> 32	> 32	> 32
38	> 32	> 32	> 32	> 32	> 32	> 32	> 32
39	> 32	> 32	> 32	> 32	> 32	> 32	> 32
43	> 32	> 32	> 32	> 32	> 32	> 32	> 32
TRB	--	--	--	--	--	--	--
ITZ	0,25 ± 0	0,5 ± 0	--	--	--	--	--
AM B	2 ± 0	2 ± 0	--	--	--	--	--

Table S1 (cont.). Antifungal evaluation (GM-MIC_{90}, μg/mL) against filamentous fungi and dermatophytes.

Compound	*Aspergillus fumigatus* ATCC 204305 (*Afu*)	*A. flavus* ATCC 204304 (*Afl*)	*A. terreus* CDC 317 (*At*, INM7)	*A. niger* ATCC 16404 (*An*, INM9)	*Fusarium oxysporum* ATCC 48112 (*Fo*)	*Trichophyton mentagrophytes* ATCC 24198 (*Tm*)	*Trichophyton rubrum* ATCC 28188 (*Tr*)
1	> 32	> 32	> 32	> 32	> 32	1.26 ± 0.52	4 ± 0
2	8 ± 0	4,75 ± 2	> 32	> 32	> 32	6.06 ± 3.10	8 ± 7.23
3a	16 ± 0	> 32	> 32	> 32	16 ± 0	3.17 ± 3.10	5.03 ± 2.7
4b	> 32	> 32	> 32	> 32	> 32	5.04 ± 2.07	3.17 ± 1.03
10a	> 32	> 32	> 32	> 32	> 32	> 32	> 32
12a	22,6 ± 8,02	> 32	> 32	> 32	32 ± 0	3.17 ± 1.03	5.04 ± 3.10
14	16 ± 0	> 32	> 32	> 32	> 32	32 ± 0	8 ± 5.47
21	> 32	> 32	> 32	> 32	> 32	> 32	> 32
23	> 32	> 32	> 32	> 32	> 32	> 32	> 32
32	> 32	> 32	> 32	> 32	> 32	> 32	> 32
34	> 32	> 32	> 32	> 32	> 32	> 32	> 32
35	> 32	> 32	> 32	> 32	> 32	> 32	> 32
36	> 32	> 32	> 32	> 32	> 32	> 32	> 32
37	> 32	> 32	> 32	> 32	> 32	> 32	> 32
38	> 32	> 32	> 32	> 32	>32	25.4 ± 8.26	25.4 ± 8.26
39	> 32	> 32	> 32	> 32	> 32	> 32	> 32
43	> 32	> 32	> 32	> 32	> 32	> 32	> 32
TRB	--	--	--	--	--	0.03 ± 0	<0,08
ITZ	0,17 ± 0,09	0,13 ± 0	--	--	--	--	--
AM B	2 ± 0	4 ± 0	--	--	--	< 0,004	< 0,004

Table S2. Antiviral activity of selected AQ derivatives.

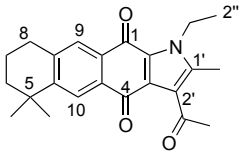
Compound	Vero ATCC CCL-81[a]						Vero cells
	1 $TCID_{50}$[b] HHV-1			10 $TCID_{50}$[c] HHV-2			
	(*Rf*)[d]	Antiviral activity [e] (μg/mL)	SI[f]	(R*f*)[d]	Antiviral activity [e] (μg/mL)	SI[f]	IC_{50} (μg/mL)
1	$10^{0.5}$	6.25	1.37	nd	>50	nd	8.6
2	$10^{0.5}$	50	0.85	10^{2}	25	1.7	42.2
3a	10^{2}	6.25	17.5	nd	>50	nd	109.3
4b	nd	na	nd	nd	na	nd	35.6
10a	nd	>50	nd	10^{1}	50	1,39	69.5
12a	nd	>50	nd	10^{1}	12.5	1.78	22.3
14	nd	>50	nd	10^{1}	25	0,18	4.6
21	nd	na	nd	nd	na	nd	14.4
23	nd	na	nd	nd	na	nd	≤25
32a/b	nd	na	nd	nd	na	nd	85.4
34a/b	nd	na	nd	nd	na	nd	67.4
35a/b	nd	na	nd	nd	na	nd	88.2
36a/b	nd	na	nd	nd	na	nd	95.6
37a/b	10^{1}	50	1.42	nd	>50	nd	71.0
38a/b	10^{1}	50	1.01	nd	>50	nd	50.5
39a/b	10^{1}	50	≤0.5	nd	>50	nd	≤25
43	nd	>50	nd	10^{1}	50	0.33	16.4
Dextran sulphate	10^{2}	0.5	nd	10^{2}	0.5	nd	
Acyclovir	10^{4}	1.5	nd	10^{4}	1.5	nd	

[a]**Vero** *Cercopithecus aethiops* African green monkey kidney cell line ATCC CCL 81; [b] **1$TCID_{50}$:**1 Cell Culture Infectious Dose Fifty percent. [c] **10$TCID_{50}$:**10 Cell Culture Infectious Dose Fifty percent; [d]***Rf***: Value obtained by dividing the viral titer in the absence of the compound on the titer obtained in presence of the compound; [e]Maximum non-toxic concentration of compound which had the highest factor of reduction of viral titer; [f]**SI:** Selectivity Index (IC_{50} Vero/$TCID_{50}$); **na**: Not active; **nd**: Not determined.

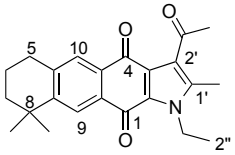
Table S3. IC_{50} (μg/mL) against mammalian Vero cells

Compound	IC_{50} ± DS	R2.adj
1	8.6 ± 1.1	0.9
2	42.2 ± 4.4	0.9
3a	109.3±6.1	0.9
4b	35.6 ± 6.2	0.7
10a	69.5 ± 15.9	0.7
12a	22.3 ± 1.3	0.7
14	4.6 ± 0.4	0.9
21	14.4 ± 1.5	0.9
23	≤ 25	NA
32	85.4 ± 25.7	0.6
34	67.4 ± 16.3	0.7
35	88.2 ± 28.2	0.5
36	95.6 ± 5.7	1.0
37	71.0 ± 12.9	0.7
38	50.5 ± 15.9	0.8
39	≤ 25	NA
43	16.4 ± 7.9	0.8
TRB	30.9±9.1	0.97
ITZ	>50	-
AMB	28.6±7.7	0.93

Table S4. ^{1}H and ^{13}C NMR data and assignments for the new synthesized compounds.

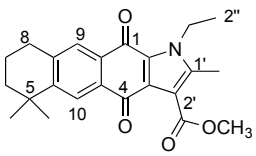


9a

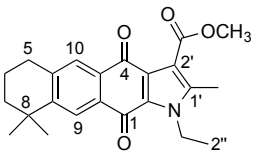


9b

	H	**C**	**H**	**C**
1		176.3		176.4
2		129.5		129.6
3		125.3		125.3
4		181.1		180.9
4a		131.4		130.6
5		34.6	2.88 t (6.3)	31.0
6	1.70-1.82 m	38.6	1.71-1.83 m	19.2
7	1.70-1.82 m	19.2	1.71-1.83 m	38.6
8	2.88 t (6.3)	31.0		34.5
8a		140.5		151.9
9	7.78 s	127.3	8.09 s	125.0
9a		130.3		131.1
10	8.09 s	125.4	7.79 s	127.3
10a		152.1		142.6
5-Me	1.34 s	31.3		
8-Me			1.35 s	31.4
1´		140.5		140.5
2´		122.8		122.7
1´´	4.52 m	40.8	4.52 m	40.8
2´´	1.39 t (7.1)	15.3	1.41 t (7.1)	15.3
1´-Me	2.42 s	10.4	2.43 s	10.4
2´-CO$\underline{CH_3}$	2.72 s	31.7	2.70 s	31.6
2´-$\underline{C}$OCH$_3$		199.6		199.7



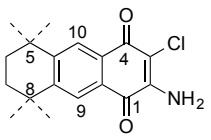
10a



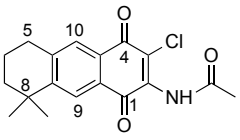
10b

	H	C	H	C
1		176.5		176.3
2		-		-[a]
3		-		130.1[a]
4		179.8		180.0
4a		131.1		130.4
5		34.6	2.87 t (6.0)	31.0
6	1.69-1.81 m	38.7	1.72-1.82 m	19.3
7	1.69-1.81 m	19.3	1.72-1.82 m	38.7
8	2.86 t (6.2)	31.0		34.6
8a		142.6		152.1
9	7.78 s	127.8	8.11 s	125.6
9a		130.0		131.7
10	8.07 s	124.9	7.77 s	127.3
10a		151.7		142.2
1´		141.2		141.1
2´		113.5		113.5
1´´	4.52 m	41.0	4.52 m	41.0
2´´	1.40 t (7.1)	15.4	1.39 t (7.1)	15.5
1´-Me	2.48 s	10.5	2.48 s	10.6
5-Me	1.32 s	31.4		
8-Me			1.33 s	31.4
2´-COO<u>C</u>H$_3$	3.95 s	52.1	3.97 s	52.1
2´-<u>C</u>OOCH$_3$		165.4		165.5

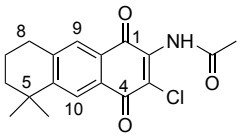
[a] Exchangeable assignments



11a/11b



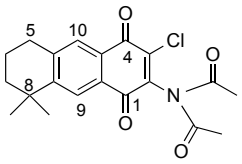
12a



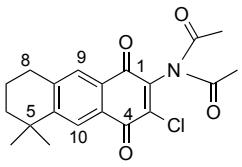
12b

	H	C	H	C	H	C
1		176.6		177.8		177.8
2		-		139.0		138.8
3		145.1/145.2		133.4		-
4		179.0		180.0		180.0
4a		130.3/-[a]		124.1[a]		127.3[a]
5	2.84 m	34.8/30.8	2.89 t (6.2)	31.2		34.9
6	1.71-1.82 m	38.4/19.0	1.70-1.83 m	19.1	1.70-1.83 m	38.4
7	1.71-1.82 m	19.0/38.4	1.70-1.83 m	38.4	1.70-1.83 m	19.1
8	2.84 m	30.8/34.4		34.8	2.88 t (6.2)	31.1
8a		145.2/154.1		153.4		143.8
9	7.70 s /7.99 s	127.9/125.6	8.05 s	125.9	7.76 s	128.1
9a		126.9/127.7[a]		128.6[a]		129.4[a]
10	8.07 s /7.78 s	125.4/127.7	7.82 s	128.6	8.11 s	126.4
10a		151.4/145.1		144.7		154.2
5-Me	1.32 s	31.2			1.33 s	31.4
8-Me	1.32 s	31.2	1.33 s	31.4		
2-CO$\underline{CH_3}$			2.29 s	24.2	2.28 s	24.2
2-$\underline{C}OCH_3$				166.7		166.6

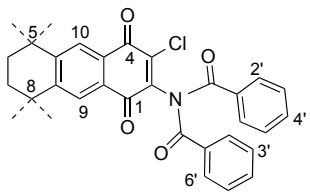
[a] Exchangeable assignments



13a



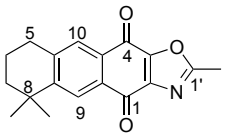
13b



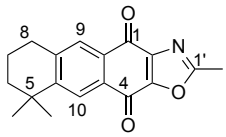
15a/15b

	H*	C*	H**	C**		H	C
1		177.7		177.2	**1**		178.7
2		138.9		143.1	**2**		-
3		133.2		-	**3**		-
4		179.8		178.6	**4**		177.4
4a		128.0[a]		128.8[a]	**4a**		-
5	2.90 t (6.2)	31.1		34.9	**5**	2.87 m	31.1/34.9
6	1.71-1.86 m	18.9	1.74-1.84 m	38.4	**6**	1.71-1.81 m	19.0/38.4
7	1.71-1.86 m	38.3	1.74-1.84 m	19.0	**7**	1.71-1.81 m	38.4/19.0
8		34.7	2.91 t	31.2	**8**	2.87m	34.9/31.1
8a		153.3		144.8	**8a**		154.1/144.6
9	8.04 s	125.8	7.82 s	128.8	**9**	8.07/7.77 s	126.6/132.9
9a		128.5		129.3	**9a**		-
10	7.83 s	128.5	8.17 s	126.6	**10**	7.84/8.12 s	132.9/126.6
10a		144.6		154.5	**10a**		144.6/154.1
5-Me			1.34 s	31.4	**5-Me**	1.30 s	31.4
8-Me	1.34 s	31.3			**8-Me**	1.33 s	31.4
2-CO$\underline{CH}_3$	2.28 s	24.1	2.36 s	25.6	**2-N-$\underline{C}$O**		
2-$\underline{C}$OCH_3		166.4		170.7	**1´**		
					2´, 6´	7.75 m	128.6
					3´, 5´	7.33 m	129.3
					4´	7.33 m	132.9

[a] Exchangeable assignments. * Spectra done at 400 MHz. ** Signals obtained after elimination of those from isomer a.



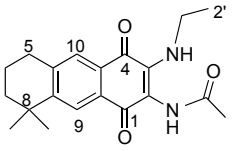
14a



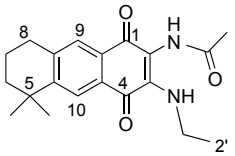
14b

	H*	C*	H	C
1		179.9		179.9
2		-[a]		140.3[a]
3		154.7[a]		-[a]
4		172.5		172.7
4a		123.3		127.4
5	2.82 t (6.2)	30.6		34.5
6	1.71-1.83 m	19.0	1.67-186 m	38.5
7	1.71-1.83 m	38.3	1.67-186 m	19.0
8		34.7	2.82 m	29.7
8a		154.7		145.3
9	7.81 s	121.4	7.32 s	130.3
9a		126.4		122.7
10	7.57 s	132.5	8.10 s	130.3
10a		140.2		149.9
5-Me			1.31 s	31.3
8-Me	1.35 s	31.2		
1´		162.9		163.1
1´-Me	2.63 s	14.0	2.61	14.1

[a] Exchangeable assignments
* Spectra done at 400 MHz



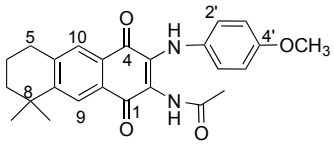
16a



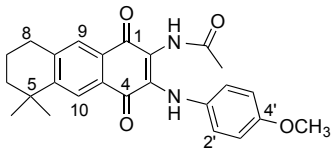
16b

	H	C	H	C
1		180.2[a]		179.8[a]
2		141.5[b]		142.1[b]
3		112.0[b]		112.2[b]
4		182.2[a]		182.2[a]
4a		127.7		129.3
5	2.83 t (6.1)	30.9		34.5
6	1.69-1.80 m	19.2	1.66-1.80 m	38.6
7	1.69-180 m	38.4	1.66-1.80 m	19.2
8		34.8	2.85 t (6.1)	31.2
8a		153.9		144.3
9	7.99 s	124.9	7.69 s	127.1
9a		130.1		128.4
10	7.68 s	127.7	7.97 s	125.4
10a		142.1		151.1
5-Me			1.31 s	31.4
8-Me	1.31 s	31.4		
1´	3.45 m	38.6	3.45 m	38.6
2´	1.24 t (7.2)	15.7	1.24 t (7.0)	15.7
2-CO$\underline{C}H_3$	2.23 s	23.5	2.22 s	23.5
2-$\underline{C}OCH_3$		170.6		170.4

[a,b] Exchangeable assignments



17a

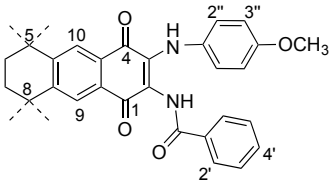


17b

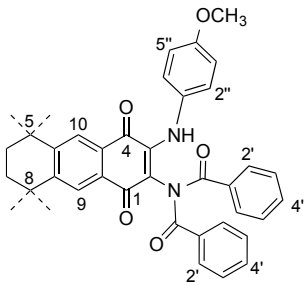
	H	C	H*	C*
1		180.3[a]		180.2[a]
2		142.1[a]		-[a]
3		114.1[a]		114.2[a]
4		182.1[a]		182.2[a]
4a		129.9		129.0
5	2.87 t (6.4)	30.9		34.6
6	1.67-1.85 m	19.2	1.67-1.85 m	38.6
7	1.67-1.85 m	38.7	1.67-1.85 m	19.2
8		34.8	2.88 t (6.36)	31.2
8a		153.7		144.2
9	8.02 s	125.1	7.76 s	127.3
9a		130.4		128.6
10	7.75 s	127.8	8.04 s	125.6
10a		142.1		151.7
5-Me			1.34 s	31.4
8-Me	1.33 s	31.3		
1´		135.3		135.5
2´-6´	6.89 d (9.1)	124.5	6.90 d (8.8)	124.5
3´-5´	6.81 d (9.1)	113.2	6.80 d (9.1)	113.2
4´		156.8		156.8
4´-OCH_3	3.80 s	55.6	3.80 s	55.6
2-$CO\underline{CH_3}$	1.62 s	22.8	1.61 s	22.8
2-$\underline{C}OCH_3$		166.7		166.7

[a] Exchangeable assignments

* Spectra done at 400 MHz



18a/18b

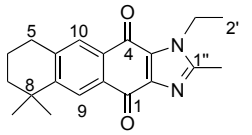


19a/19b

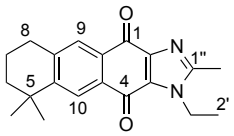
	H	C	H	C
1		182.2		182.1
2		C_{cuat}		C_{cuat}
3		C_{cuat}		C_{cuat}
4		180.3		180.1
4a		C_{cuat}		C_{cuat}
5	2.88 t (6.2)	31.0/34.6	2.86 m	31.2/34.9
6	1.68-1.83 m	19.2/38.6	1.67-1.82 m	19.1/38.5
7	1.68-1.83 m	38.6/19.2	1.67-1.82 m	38.5/19.1
8	2.88 t (6.2)	34.9/31.0	2.86 m	34.9/31.2
8a		151.8/142.2		152.8/143.2
9	8.05/7.75 s	CH_{arom}	8.04 s	CH_{arom}
9a		C_{cuat}		C_{cuat}
10	7.77/8.07 s	CH_{arom}	7.76 s	CH_{arom}
10a		144.3/153.8		144.7/154.2
5. 8-Me	1.30/1.33 s	31.4	1.30/1.33 s	31.4
2-N-CO		164.2		170.3/164.3
1´		C_{cuat}		C_{cuat}
2´. 6´	7.30-8.06 m	CH_{arom}	7.21-7.76 m	CH_{arom}
3´. 5´	7.30-8.06 m	CH_{arom}	7.21-7.76 m	CH_{arom}
4´	7.30-8.06 m	C_{cuat}	7.21-7.76 m	C_{cuat}
1´´		C_{cuat}		C_{cuat}
2´´. 6´´	6.91 d (8.7)	CH_{arom}	6.89 d (8.8)	CH_{arom}
3´´. 5´´	6.64 d (8.7)	113.4	6.56 d (8.8)	114.5
4´´		156.8		157.8
4´´-OCH_3	3.59 s	55.5	3.66 s	55.4

18: ***CH_{arom}***.: 131.6, 128.2, 127.9, 127.4, 125.7, 125.1, 124.4 ; ***C_{cuat}***: 135.1, 133.8, 130.3, 129.8, 129.0, 128.5, 114.4.

19*:* ***CH_{arom}***.: 133.6, 130.4, 129.5, 128.7, 127.9, 126.3, 125.3 ; ***C_{cuat}***: 135.9, 135.6, 135.2, 134.1, 132.5.

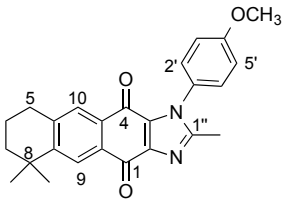


20a

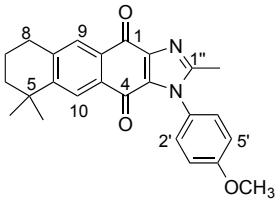


20b

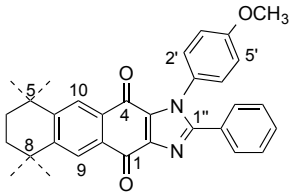
	H	**C**	**H**	**C**
1		179.2		179.3
2		143.3		143.2
3		131.8		132.0
4		176.5		176.6
4a		130.2		131.0
5	2.88 t (6.3)	31.0		34.5
6	1.70-1.82 m	19.1	1.70-1.82 m	38.5
7	1.70-1.82 m	38.6	1.70-1.82 m	19.1
8		34.6	2.87 t (6.3)	31.0
8a		152.5		143.1
9	8.17 s	125.8	7.89 s	128.1
9a		130.7		129.8
10	7.77 s	127.5	8.08 s	125.2
10a		142.6		152.1
5-Me			1.34 s	31.3
8-Me	1.34 s	31.3		
1´	4.43 m	40.7	4.43 m	40.8
2´	1.43 t (7.2)	15.4	1.45 t (7.1)	15.4
1´´		152.2		152.3
1´´-Me	2.57 s	13.0	2.56 s	13.0



21a



21b

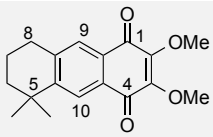
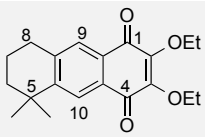


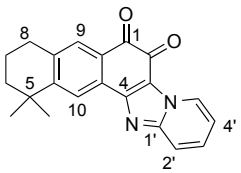
22a/22b

	H	C	H*	C*	H	C
1		179.4		179.5		179.7
2		142.7		143.2		C_{cuat}
3		-		132.0		C_{cuat}
4		174.3		175.7		176.0
4a		130.4		130.9		C_{cuat}
5	2.82 t (6.2)	31.0		34.5	2.86 m	31.1/34.7
6	1.65-1.79 m	19.2	1.61-1.84 m	38.4	1.67-1.84 m	19.2/38.7
7	1.65-1.79 m	38.7	1.61-1.84 m	19.1	1.67-1.84 m	38.7/19.2
8		34.7	2.87 t (6.3)	30.9	2.86 m	34.6/31.1
8a		153.6		143.1		152.4/142.9
9	8.18 s	125.8	7.91 s	128.0	8.23/7.95 s	CH_{arom}
9a		130.9		129.8		C_{cuat}
10	7.65 s	127.6	7.99 s	125.3	7.69/8.03 s	CH_{arom}
10a		142.7		153.6		143.2/152.7
5-Me			1.27 s	31.2	1.36 s	31.4
8-Me	1.34 s	31.3			1.28 s	31.4
1´		-		-		C_{cuat}
2´-6´	7.24 d (8.4)	127.9	7.25 d (6.8)	127.8	6.96-7.59 m	CH_{arom}
3´-5´	7.06 d (9.1)	114.5	7.07 d (6.8)	114.7	6.96-7.59 m	114.7
4´		160.4		160.4		160.3
4´-OCH_3	3.89 s	55.6	3.90 s	55.6	3.88 s	55.6
1´´		152.6		152.2		153.7
1´´-Me	2.38 s	13.6	2.39 s	13.6		
1´´-Ph					6.96-7.59 m	$C_{cuat.}/CH_{arom}$

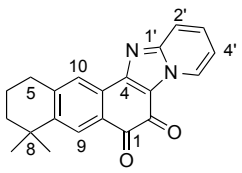
22: ***$CH_{arom:}$*** 130.1, 129.5, 128.6, 128.3, 127.7, 125.9, 125.3; ***$C_{cuat:}$*** 134.0, 133.8, 131.3, 130.8, 130.6, 127.0.

***** Spectra done at 400 MHZ

	 **23**		 **24**	
	H	**C**	**H**	**C**
1		182.2		182.4
2		143.2		143.1
3		143.2		143.1
4		182.2		187.6
4a		128.8		128.9
5		34.7		34.7
6	1.71-1.80 m	38.6	1.68-1.78 m	38.6
7	1.71-1.80 m	19.2	1.68-1.78 m	19.2
8	2.86 t (6.2)	31.0	2.85 t (6.2)	31.0
8a		147.6		147.5
9	7.71 s	127.3	7.69 s	127.2
9a		128.0		128.1
10	8.00 s	125.1	7.98 s	125.0
10a		152.8		152.6
5-Me	1.32 s	31.4	1.31 s	31.4
2,3-OCH_3	4.08 s	61.4		
2,3-$O\underline{CH_2}CH_3$			4.34 m	69.6
2,3-$OCH_2\underline{CH_3}$			1.37 t (6.8)	15.7

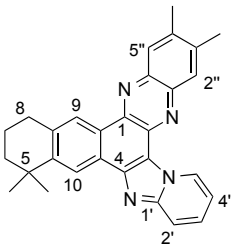


25a

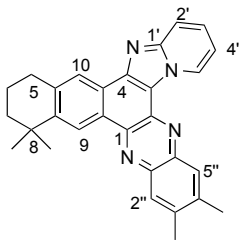


25b

	H	**C**	**H**	**C**
1		181.9		181.9
2		167.8		168.0
3		120.4		120.4
4		154.8		154.5
4a		128.7		128.0
5		34.8	2.89 t (6.4)	31.1
6	1.70-1.85 m	38.6	1.70-1.87 m	19.1
7	1.70-1.85 m	19.1	1.70-1.87 m	38.6
8	2.82 t (6.4)	30.6		34.3
8a		139.7		149.3
9	7.79 s	131.4	8.10 s	129.2
9a		128.1		128.9
10	8.10 s	123.1	7.84 s	125.4
10a		154.6		145.1
5-Me	1.39 s	31.2		
8-Me			1.34 s	31.3
1´		150.3		150.3
2´	7.80 d (8.9)	117.9	7.78 d (8.7)	117.9
3´	7.60 dd (7.6;8.8)	131.9	7.61 dd (7.4;8.7)	131.9
4´	7.16 dd (6.2;7.6)	116.3	7.17 dd (6.3;7.4)	116.3
5´	9.29 d (6.2)	129.0	9.29 d (6.3)	129.0



26a



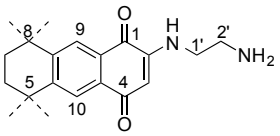
26b

	H*	C*	H	C
1		141.3		141.6
2		C_{cuat}		C_{cuat}
3		C_{cuat}		C_{cuat}
4		C_{cuat}		C_{cuat}
4a		C_{cuat}		C_{cuat}
5		34.7	3.11 t (6.2)	31.1
6	1.84-1.97 m	39.4	1.75-1.95 m	19.8
7	1.84-1.97 m	19.8	1.75-1.95 m	39.5
8	3.14 t (6.2)	31.3		34.7
8a		136.7		148.3
9	8.94 s	126.1	8.39 s	123.3
9a		C_{cuat}		C_{cuat}
10	8.70s	121.2	9.31 s	124.1
10a		149.1		
5-Me	1.48 s	32.1		
8-Me			1.57 s	32.4
1´		148.1		146.4
2´	7.94 d (8.2)	117.0	7.88 d (8.4)	117.2
3´	7.51 dd (7.0;8.2)	127.6	7.48 m	127.3[a]
4´	7.10 dd (6.7;7.0)	112.7	7.08 dd (6.7;7.0)	112.8
5´	10.12 d (6.7)	129.0	10.13 d (6.7)	129.0
1´´		C_{cuat}		C_{cuat}
2´´	7.80 s[a]	127.2[a]	7.98 s[a]	127.6[a]
3´´		140.3[b]		C_{cuat}
4´´		138.8[b]		C_{cuat}
5´´	7.90 s[a]	128.4[a]	7.85 s[a]	128.6[a]
6´´		C_{cuat}		
3´´-Me	2.46 s[b]	20.2[c]	2.49 s[b]	20.4
4´´-Me	2.49 s[b]	20.3[c]	2.52 s[b]	20.4

26a: ***C*****$_{cuat}$**: 144.5, 139.9, 137.1, 127.8, 126.7

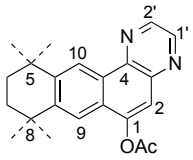
26b: C_{cuat}: 144.5, 140.3, 139.9, 139.4, 138.9, 126.4

* Spectra done at 400 MHz



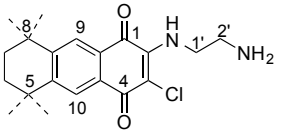
27a/27b

	H	C
1		184.2
2		-
3	5.63 s	101.7
4		184.3
4a		130.3
5		34.4
6	1.72-1.80 m	37.4
7	1.72-1.80 m	19.5
8	2.81 t (6.1)	31.0
8a		140.6/149.4
9	7.73 s	124.2
9a		130.0
10	7.99 s	123.9
10a		154.4/144.8
5-Me	1.30 s	31.6
1´	4.02 t (6.2)	48.5
2´	3.28 t (6.2)	39.0
3´		

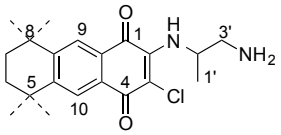


29a/29b

	H	C
1		148.8
2	7.64/7.63s	116.9/116.5
3		140.3[a]
4		140.4[a]
4a		130.2/129.2
5	3.12 t (6.3)	31.1/34.7
6	1.78-1.95 m	19.5/39.2
7	1.78-1.95 m	39.0/19.5
8	3.05 t (6.3)	34.7/31.4
8a		148.6/139.0
9	7.90/7.62 s	119.1/121.3
9a		126.3/125.5
10	8.89/9.22 s	124.6/122.7
10a		138.0/147.7
5-Me	1.44 s	32.3
8-Me	1.42 s	32.3
1-OCOCH$_3$	2.54/2.53 s	21.1
2-OCOCH$_3$		168.8
1´		
2´	8.84[a]	142.5[b]
3´	8.86[a]	144.2[b]
4´		
5´		
6´		
3´-Me		
4´-Me		

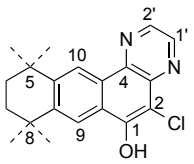


30a/30b

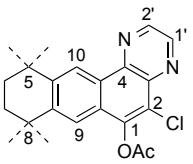


31a/31b

	H	**C**	**H**	**C**
1		174.5		176.7
2		152.4		151.0
3		139.5/139.7		139.0/139.1
4		176.6		176.7
4a		129.7/128.4		129.7/129.2
5		34.4	2.85 t (6.0)	34.4/31.0
6	1.60-1.82 m	37.4	1.65-1.93 m	38.9
7	1.60-1.82 m	19.4	1.65-1.93m	19.4
8	2.85 m	31.0/30.8	2.85 t (6.0)	30.8
8a		140.3/149.9		140.3/149.9
9	7.80/8.10	127.0/122.4	7.80/8.10	127.0/124.5
9a		-/129.2		128.5/129.5
10	8.12/7.81	124.5/124.9	8.14/7.83	122.5/124.8
10a		150.7/141.1		150.6/141.9
5-Me	1.33/1.34 s	31.6	1.32/1.34 s	31.7
1´	4.14 m	48.3	1.66/1.69 d (3.3)	19.4
2´	3.45 m	38.9	3.51 m	52.9
3´			3.13 m	43.2



32a/32b

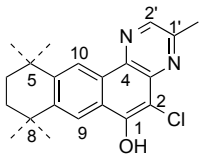


34a/34b

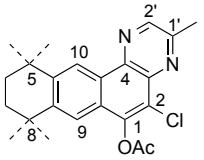
	H	C	H*	C*
1		150.2/150.4		146.1/145.8
2		108.5/108.3		120.7/121.0
3		138.8[a]		141.0/140.8[a]
4		139.9[a]		139.2/139.4[a]
4a		124.5/128.2		127.5/128.3
5	3.06 m	31.3/34.8	3.08 t (6.3)	31.1/34.7
6	1.75-1.93 m	19.6/39.2	1.76-1.92 m	19.4/39.0
7	1.75-1.93 m	39.2/19.6	1.76-1.92 m	38.9/19.4
8	3.06 m	34.8/31.3	3.03 t (6.3)	34.6/31.4
8a		149.1/139.3		149.5/139.8
9	8.28/7.99 s	120.4/122.3	7.83/7.55 s	119.1/121.2
9a		127.4/123.7		126.4/125.7
10	8.77/9.11 s	124.5/122.5	8.83/9.17 s	124.8/122.9
10a		139.3/148.1		138.4/148.1
5-Me	1.46 s	32.3	1.46 s	32.2
8-Me	1.44 s	32.3	1.40 s	32.2
1-OCOCH$_3$			2.59/2.57 s	20.6/20.5
2-OCOCH$_3$				167.7/167.5
1´	8.84 d (2.2)[a]	143.6[b]	8.91/8.88 d (2.1)[a]	143.1[b]
2´	8.74 d (2.2)[a]	140.8[b]	8.95 d (2.1)[a]	143.9/144.0[b]

[a] Exchangeable assignments

* NMR data at 400 MHz



33a/33b

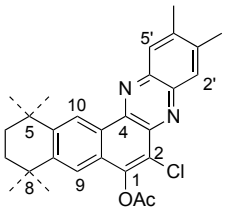


35a/35b

	H	C	H*	C*
1		150.1		144.9
2		*C*$_{cuat}$		129.1[a]
3		*C*$_{cuat}$		140.0/139.4[a]
4		*C*$_{cuat}$		136.9/137.0
4a		128.1/124.7		127.4/128.2
5	3.08 m	31.3/34.8	3.10 t (6.3)	31.4/34.7
6	1.76-1.94 m	19.7/39.3	1.77-1.94 m	19.5/39.1
7	1.76-1.94 m	39.3/19.7	1.77-1.94 m	38.9/19.5
8	3.08 m	34.8/31.3	3.04 t (6.3)	34.6/31.6
8a		148.7/138.9		149.1/139.5
9	8.28/7.99 s	120.2/122.2	7.81/7.54 s	118.9/121.0
9a		124.7/128.1		126.5/125.4
10	8.82/9.14 s	124.4/122.4	8.88/9.20 s	124.7/122.8
10a		138.0/147.7		137.9/147.6
5-Me	1.49 s	32.4	1.48 s	32.3
8-Me	1.45 s	32.4	1.41 s	32.3
1-OCOC$\underline{\mathbf{H}}$**$_3$**			2.59/2.58 s	20.6
2-O$\underline{\mathbf{C}}$**OCH$_3$**				167.7/167.9
1´		*C*$_{cuat}$		152.6
1´-Me	2.80/2.82 s	22.1	2.85/2.87 s	22.3
2´	8.73 s	144.0/144.1	8.83/8.82 s	144.6/144.5

[a] Exchangeable assignments

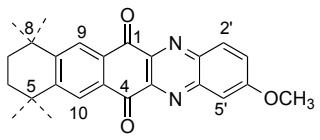
33: ***C*$_{cuat}$**: 149.2, 148.9, 148.7.



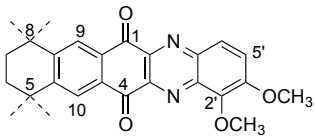
36a/36b

	H	C
1		146.2/146.1
2		C_{cuat}
3		C_{cuat}
4		C_{cuat}
4a		126.4/128.6
5	3.13 t (6.2)	31.4/34.6
6	1.78-1.94 m	19.6/39.0
7	1.78-1.94 m	39.2/19.6
8	3.04 t (6.2)	34.8/31.2
8a		139.5/149.2
9	7.52/7.81 s	121.8/119.7
9a		128.6/126.4
10	9.34/9.01 s	123.7/125.6
10a		147.9/138.2
5-Me	1.52 s	32.3
8-Me	1.42 s	32.3
1-OCO$\underline{CH_3}$	2.56/2.58 s	20.6
2-O$\underline{C}$OCH$_3$		167.6/167.8
1´		C_{cuat}
2´	8.07 s[a]	128.2
3´		C_{cuat}
4´		C_{cuat}
5´	8.13 s[a]	128.2
6´		C_{cuat}
3´-Me	2.59 s[b]	20.6
4´-Me	2.59 s[b]	20.6

36: ***C*$_{cuat}$:** 141.5, 140.9, 140.7.



40a/40b



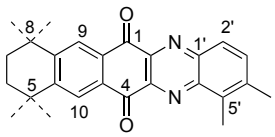
41a/41b

	H	C	H*	C*
1		181.5		181.4
2		C_{cuat}		C_{cuat}
3		C_{cuat}		C_{cuat}
4		181.2		180.8
4a		C_{cuat}		132.0/131.2
5	2.97 t (6.5)	35.0/31.2	2.99 t (6.2)	35.0/31.3
6	1.76-1.87 m	38.5/19.1	1.41-1.80 m	38.5/19.1
7	1.76-1.87 m	19.1/38.5	1.41-1.80 m	19.1/38.5
8	2.97 t (6.5)	31.2/35.0	2.99 t (6.2)	31.3/35.0
8a		145.0/154.6		145.2/154.3
9	8.13/8.41 s	128.1/126.9	8.13/8.42 s	126.9
9a		C_{cuat}		131.1/132.0
10	8.41/8.13 s	126.9/128.1	8.42/8.15 s	126.9
10a		154.8/146.1		154.7/145.2
5. 8-Me	1.41 s	31.5	1.41/1.42 s	31.5
1´		C_{cuat}		C_{cuat}
2´	8.33/8.31 d (9.1;9.5)	129.0[a]		C_{cuat}
3´	7.62/7.60 d (9.4;9.1)	107.3		C_{cuat}
4´		163.7		C_{cuat}
5´	7.69 s /7.71 s	132.0[a]	7.83 d (9.3)	129.1
6´		C_{cuat}	8.25/8.26 d (9.3)	122.3
3´-OCH_3			4.32/4.33 s[a]	57.2[a]
4´-OCH_3	4.03 s	56.4	4.14 s[a]	62.9[a]

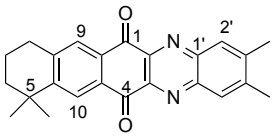
[a] Exchangeable assignments

40: C_{cuat}: 145.3, 144.6, 144.5, 142.5, 142.4, 140.7, 131.7, 130.9, 130.8.

41: C_{cuat}: 143.8, 143.4, 142.5, 139.5, 139.3



42a/42b



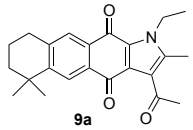
43

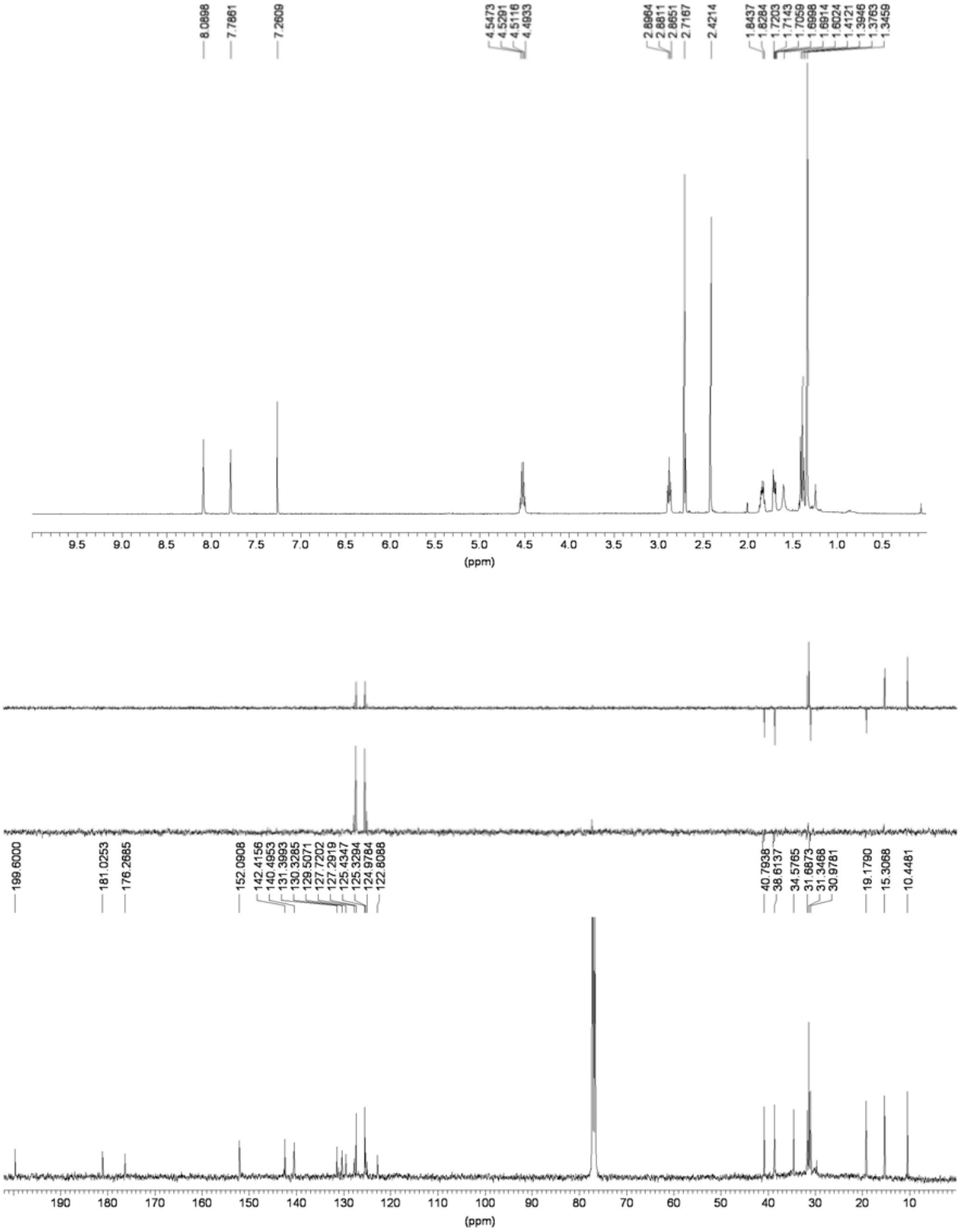
	H*	**C***	**H***	**C***
1		181.5/181.4		181.3
2		*C*$_{cuat}$		143.8
3		*C*$_{cuat}$		144.0
4		181.3		181.3
4a		131.1/131.2		131.8
5	2.99 m	34.9/31.0		34.9
6	1.64-1.77 m	38.5/19.0	1.73-1.90 m	38.4
7	1.64-1.77 m	19.0/38.5	1.73-1.90 m	19.0
8	2.99 m	31.0/34.9	2.98 t (6.3)	31.1
8a		145.1/154.5		145.0
9	8.12/8.41 s	127.8/126.7	8.13 s	129.0
9a		131.0/131.2		131.0
10	8.42/8.14 s	126.7/127.8	8.41 s	126.8
10a		154.6/145.1		154.6
5.8-Me	1.42 s	31.4	1.41 s	31.4
1´		137.0		143.1
2´		*C*$_{cuat}$	8.18[a]	129.7
3´		*C*$_{cuat}$		145.3
4´		*C*$_{cuat}$		145.3
5´	7.79 d (8.6)	136.9	8.20[a]	129.7
6´	8.20/8.21 d(8.6)	126.8		143.1
3´-Me	2.91s[a]	13.4[a]	2.56 s	20.8
4´-Me	2.60s[a]	20.8[a]	2.56 s	20.8

42a/42b: ***C*$_{cua.}$**: 145.0, 143.4, 143.3, 143.2, 143.0, 142.8, 142.7.

* Spectra done at 400 MHz

Figure S1: ^{1}H and ^{13}C NMR spectra for compound **9a**





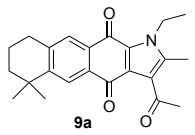
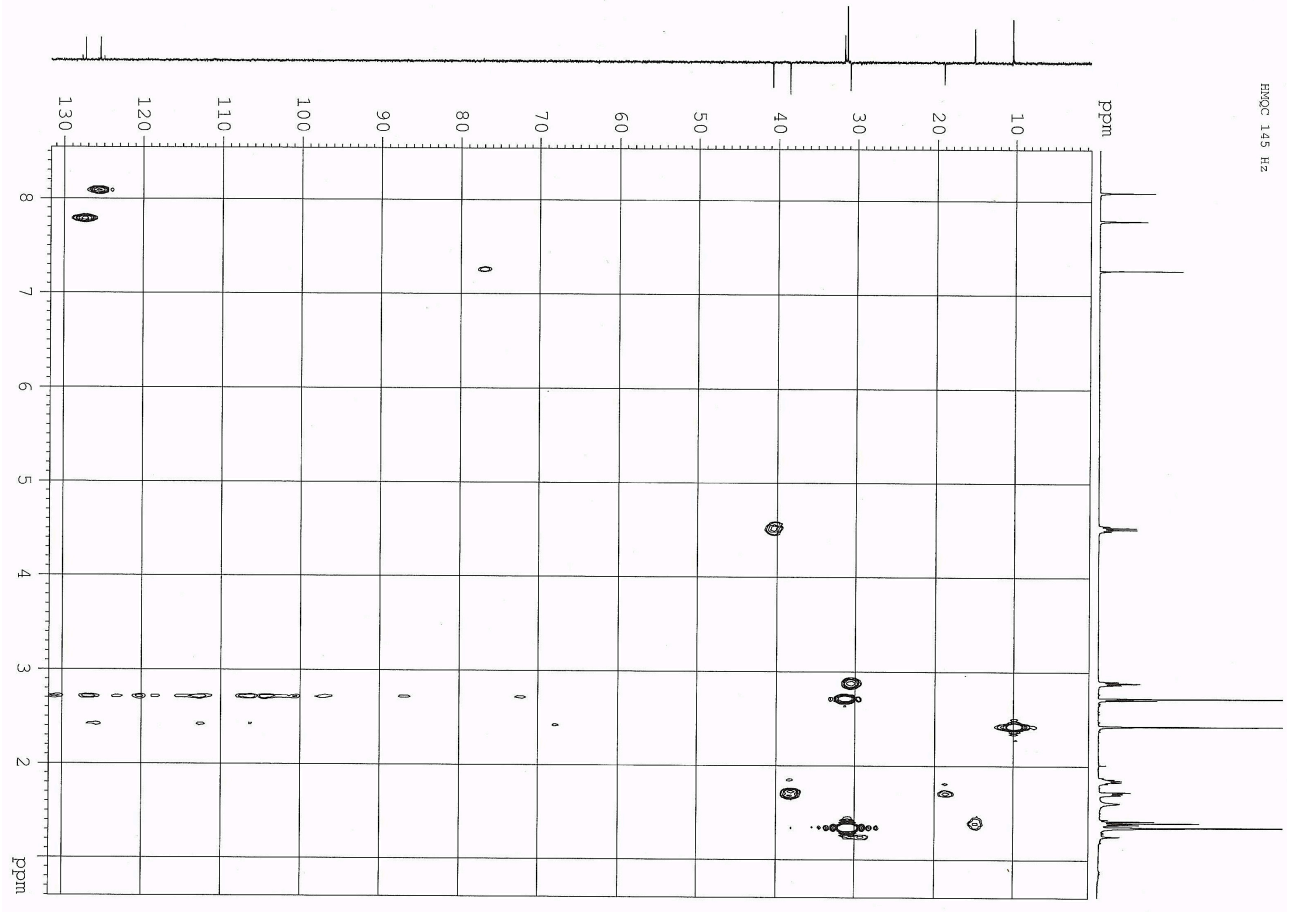


Figure S2: HMQC and HMBC experiments for compound **9a**



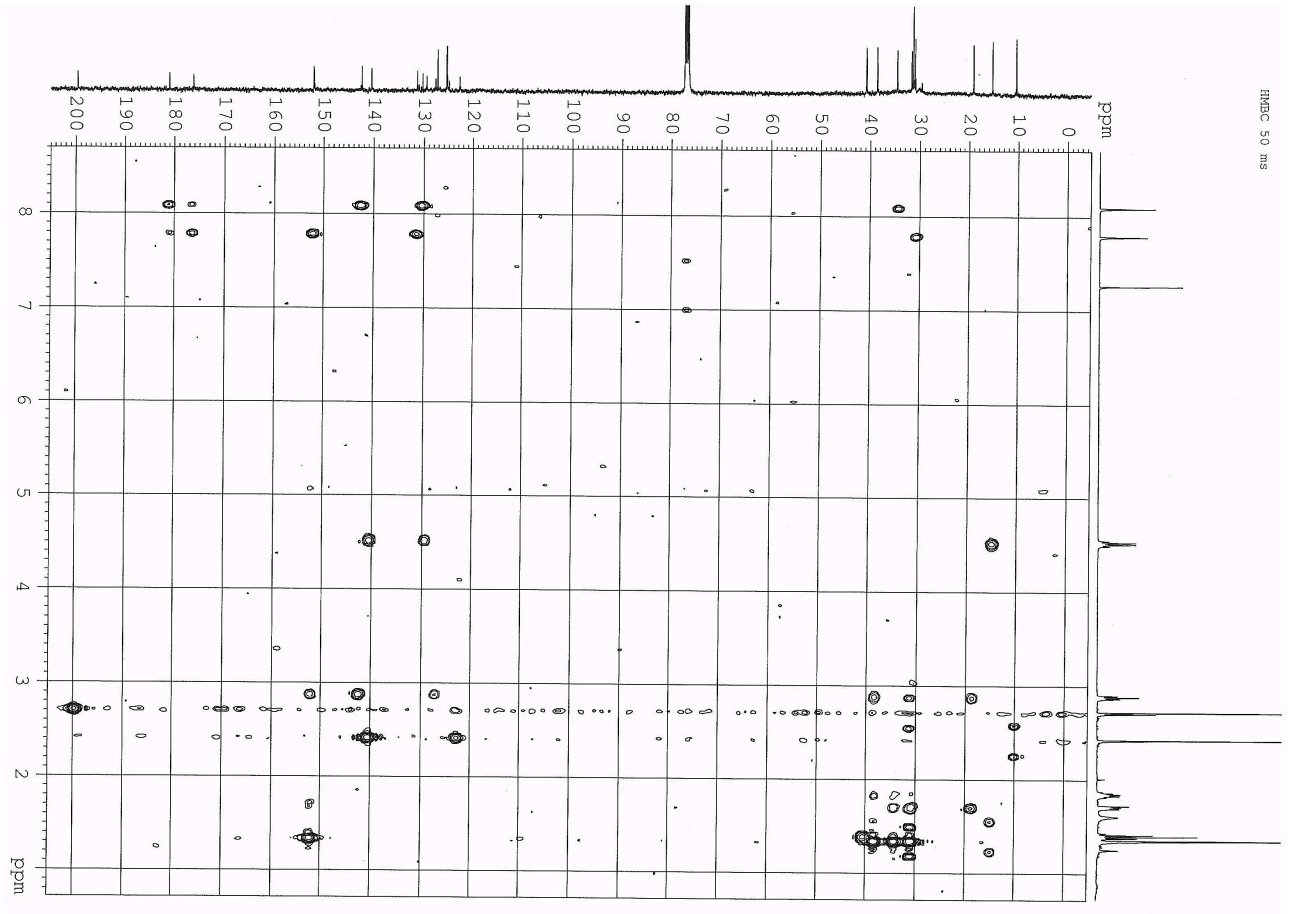
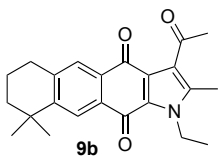


Figure S3: ^{1}H and ^{13}C NMR spectra for compound **9b**



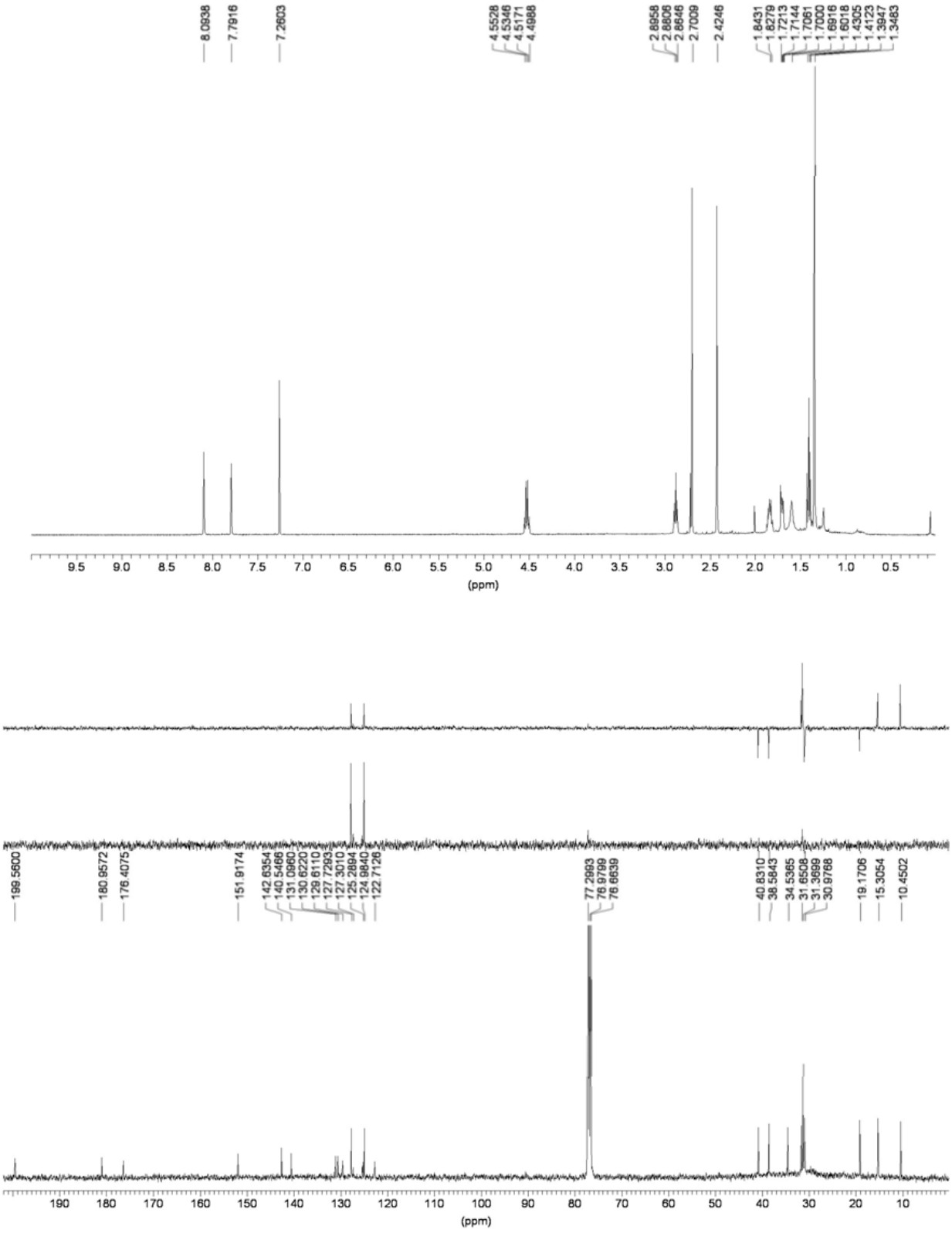
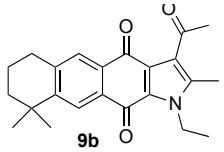
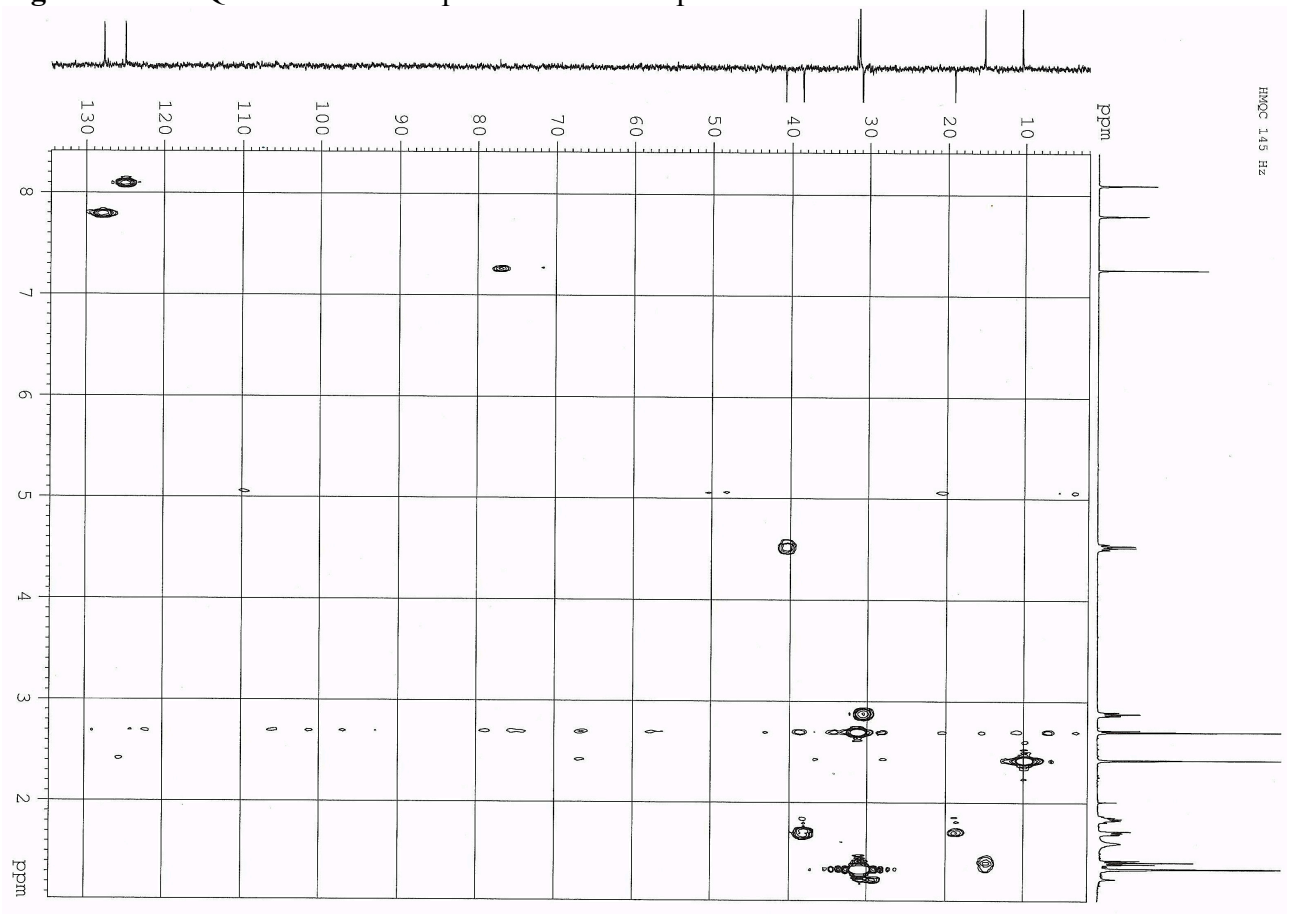


Figure S4: HMQC and HMBC experiments for compound **9b**





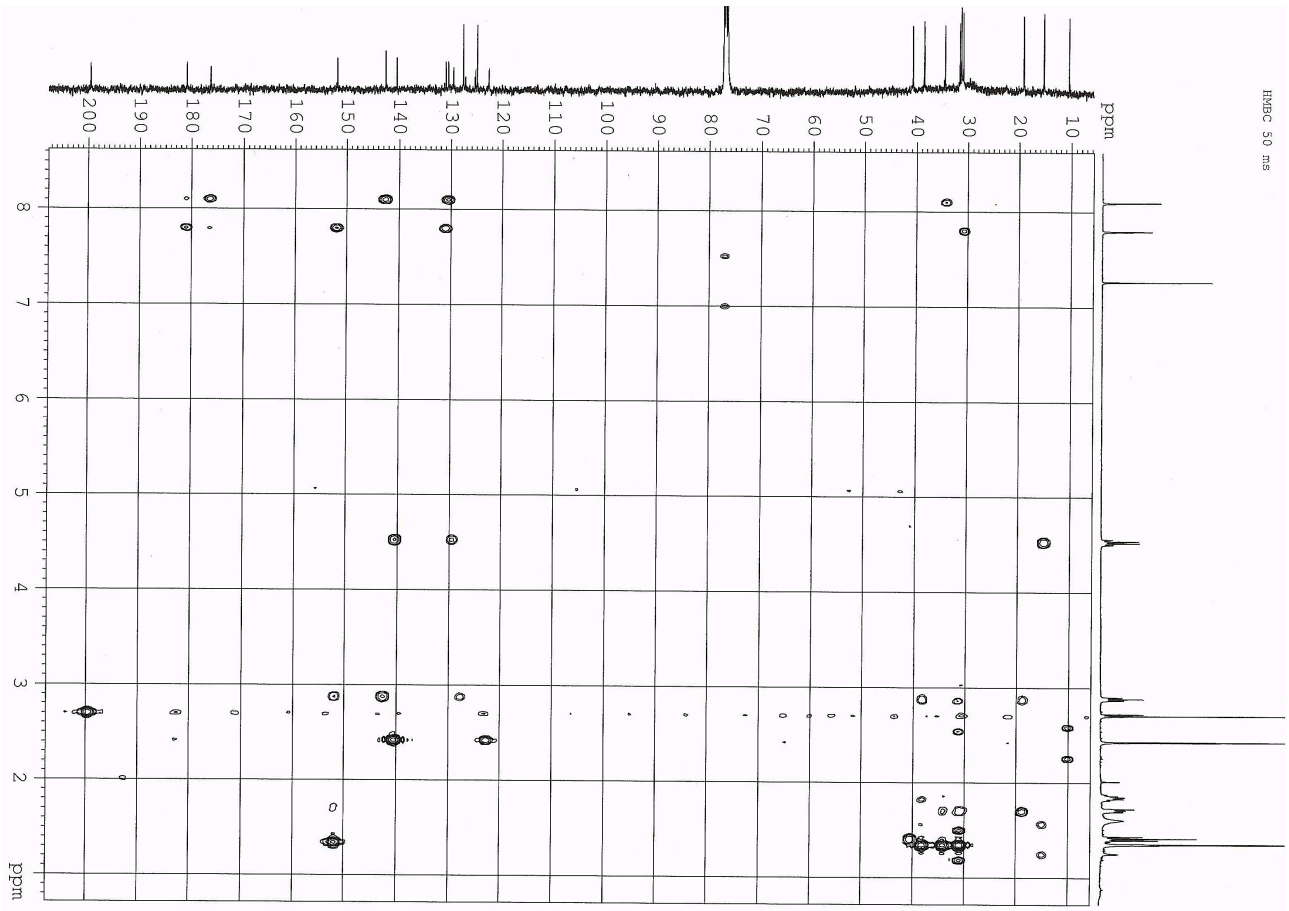
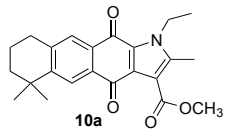


Figure S5: ^{1}H and ^{13}C NMR spectra for compound **10a**



10a

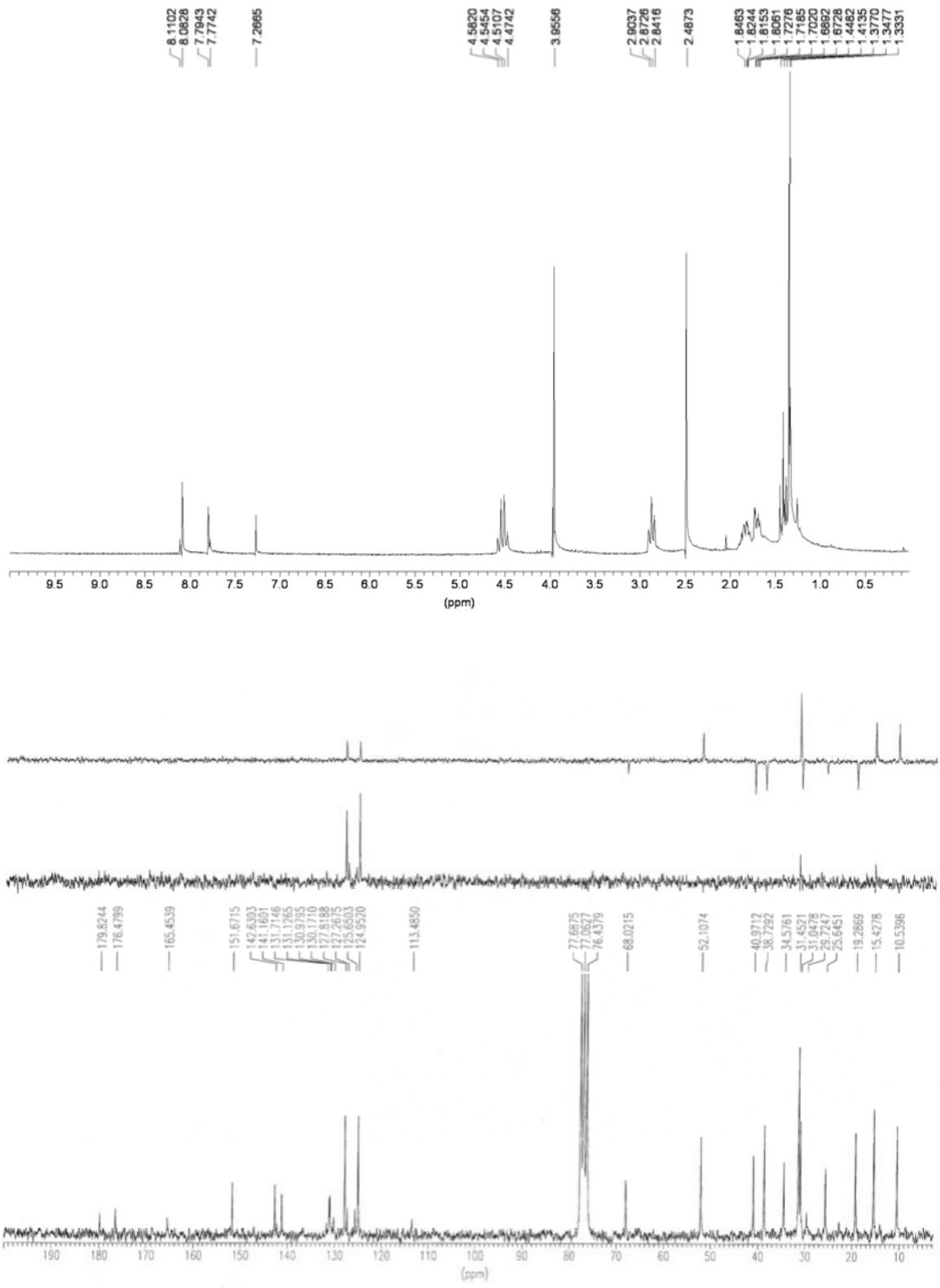
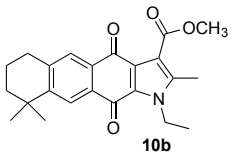
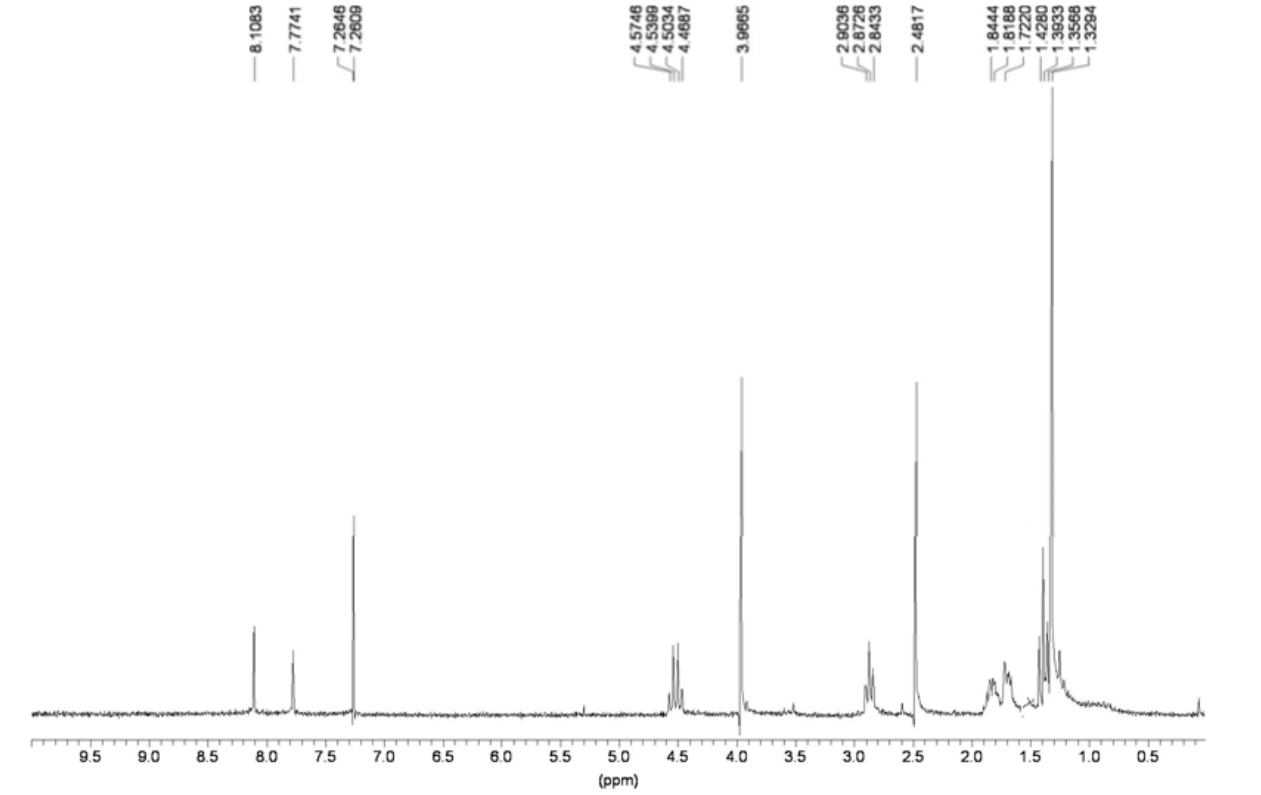


Figure S6: ^{1}H and ^{13}C NMR spectra for compound **10b**



10b



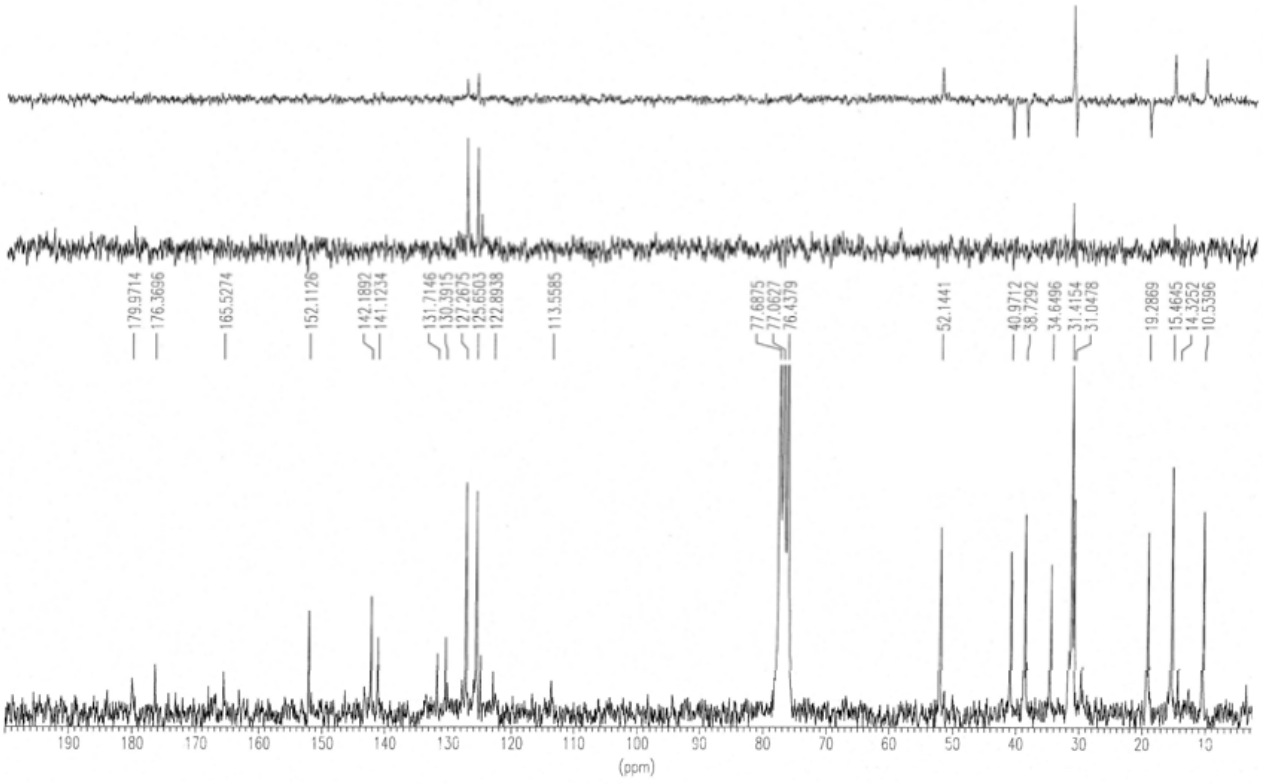
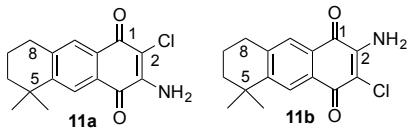


Figure S7: ^{1}H and ^{13}C NMR spectra for compound **11a/11b**



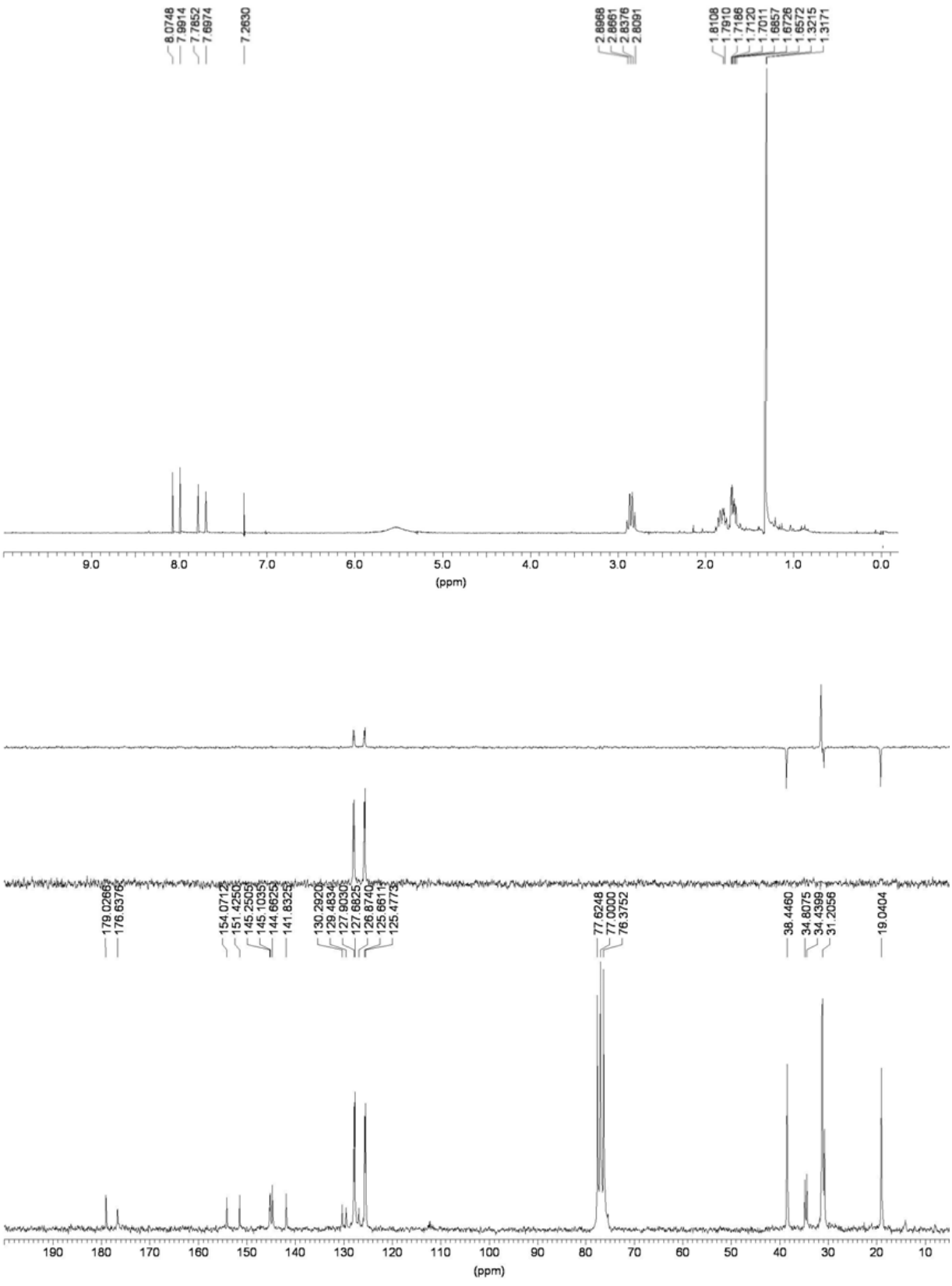
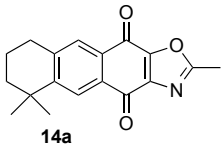


Figure S8: ^{1}H and ^{13}C NMR spectra for compound **14a**



14a

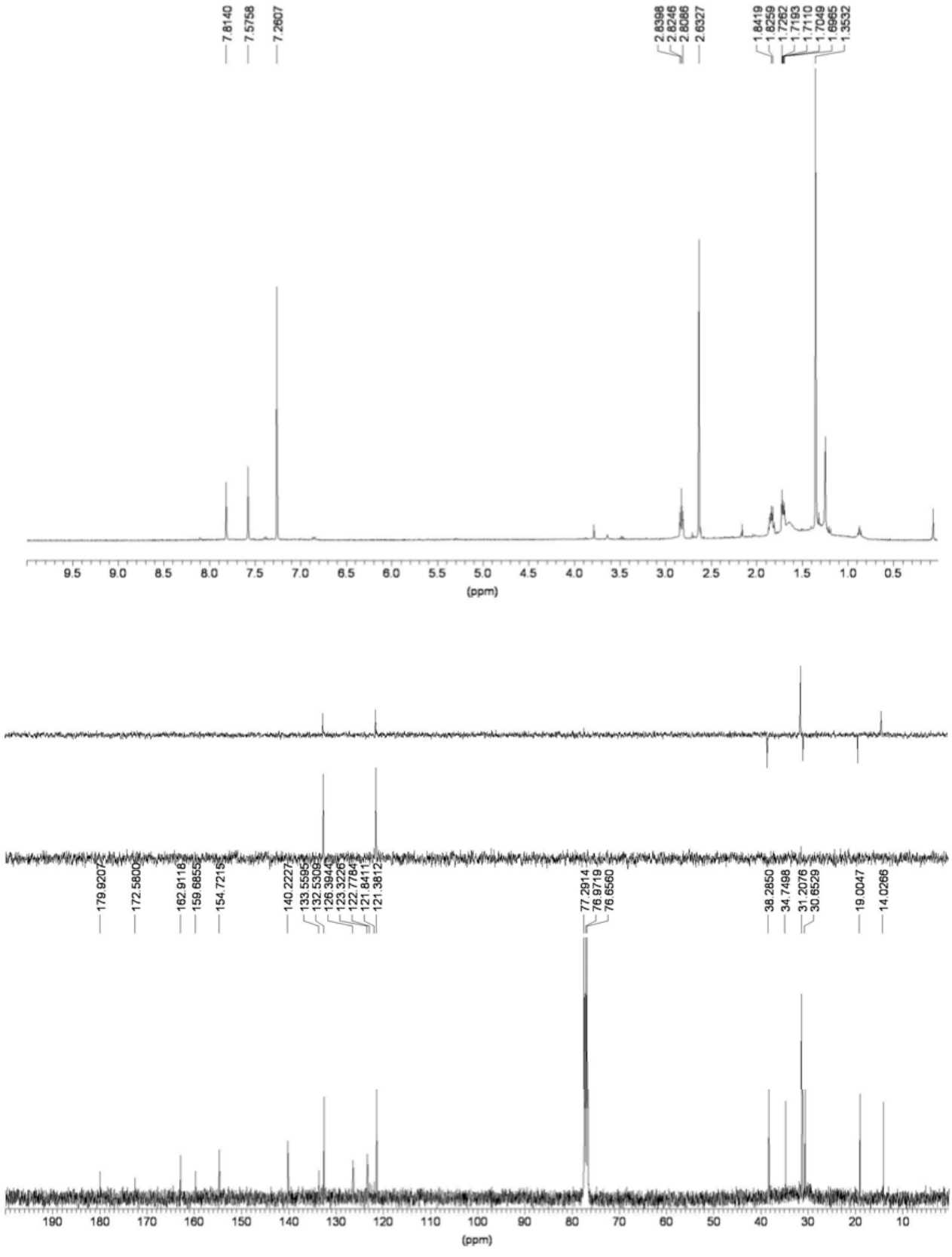
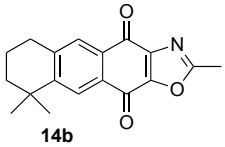


Figure S9: ^{1}H and ^{13}C NMR spectra for compound **14b**



14b

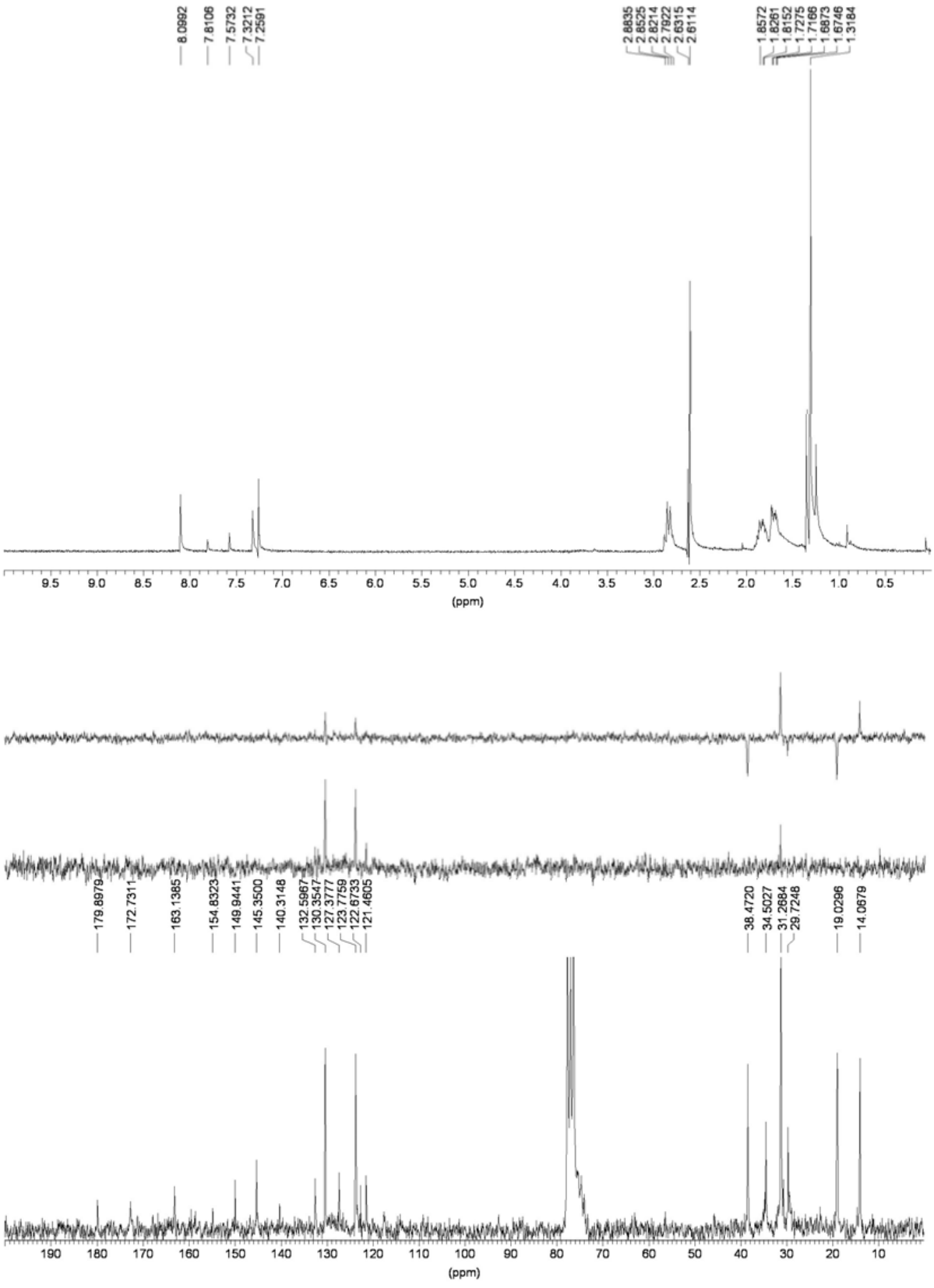
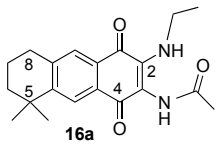


Figure S10: ^{1}H and ^{13}C NMR spectra for compound **16a**



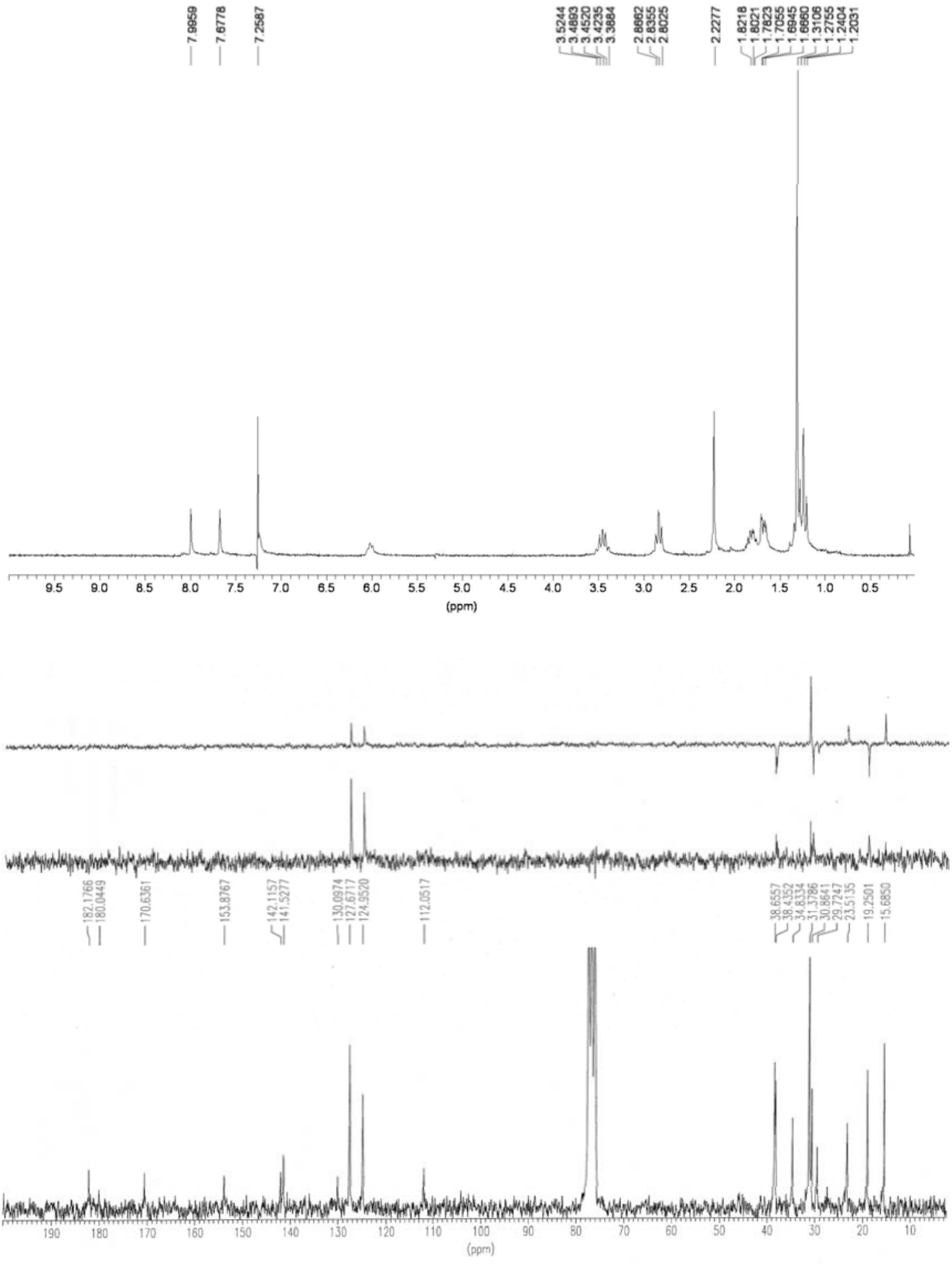
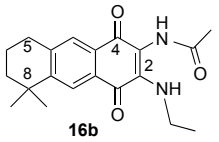


Figure S11: ^{1}H and ^{13}C NMR spectra for compound **16b**



16b

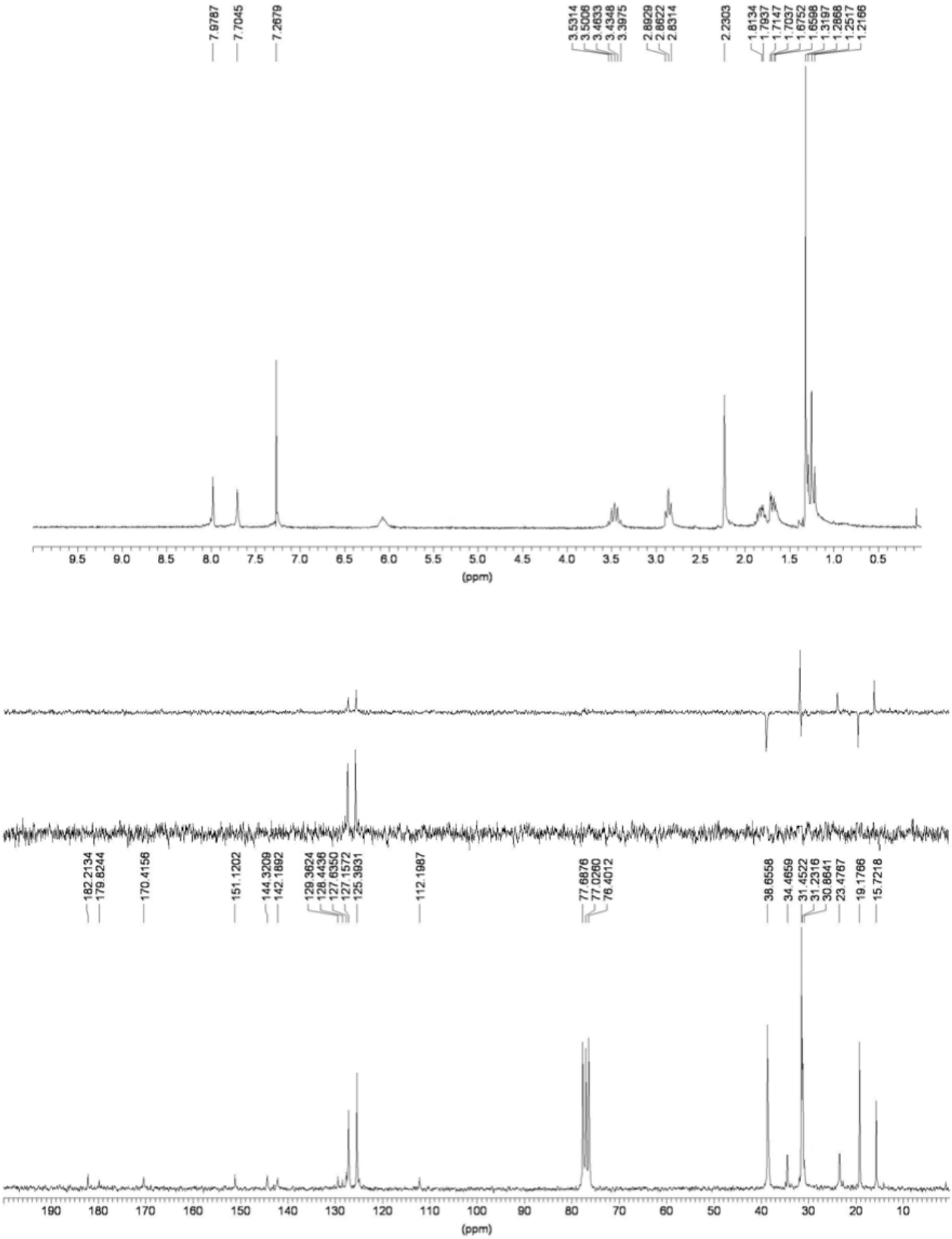
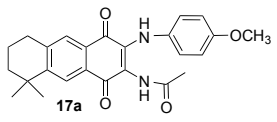


Figure S12: ^{1}H and ^{13}C NMR spectra for compound **17a**



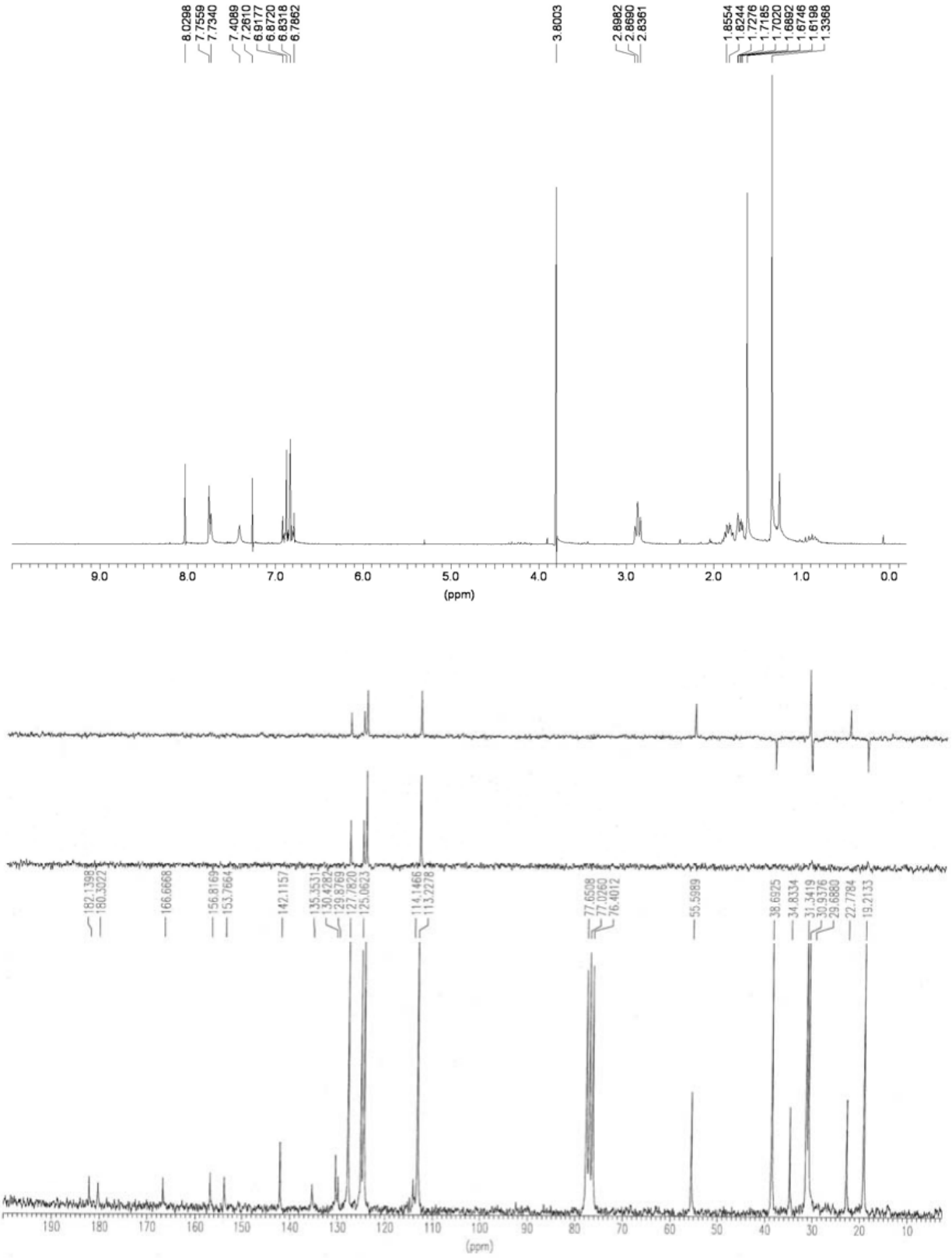
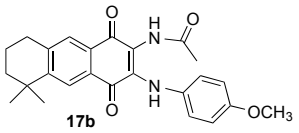
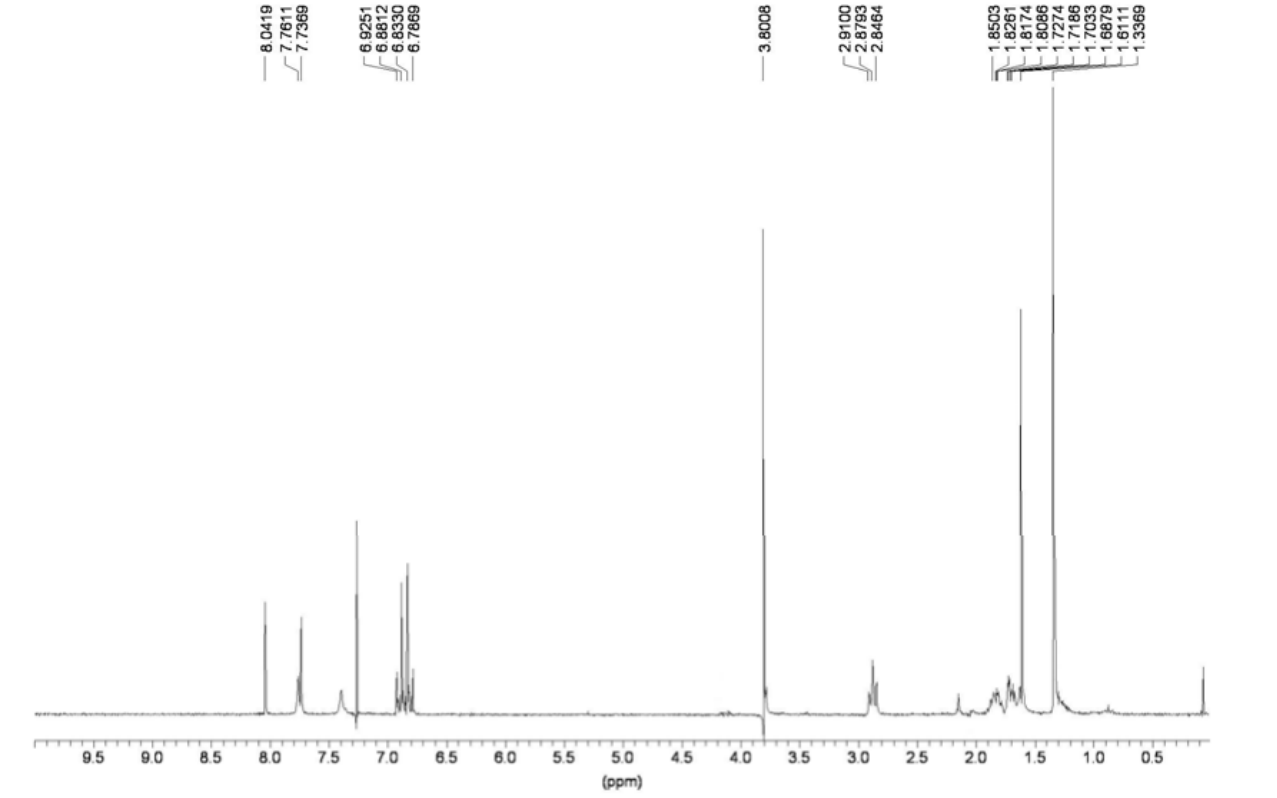


Figure S13: ^{1}H and ^{13}C NMR spectra for compound **17b**



17b



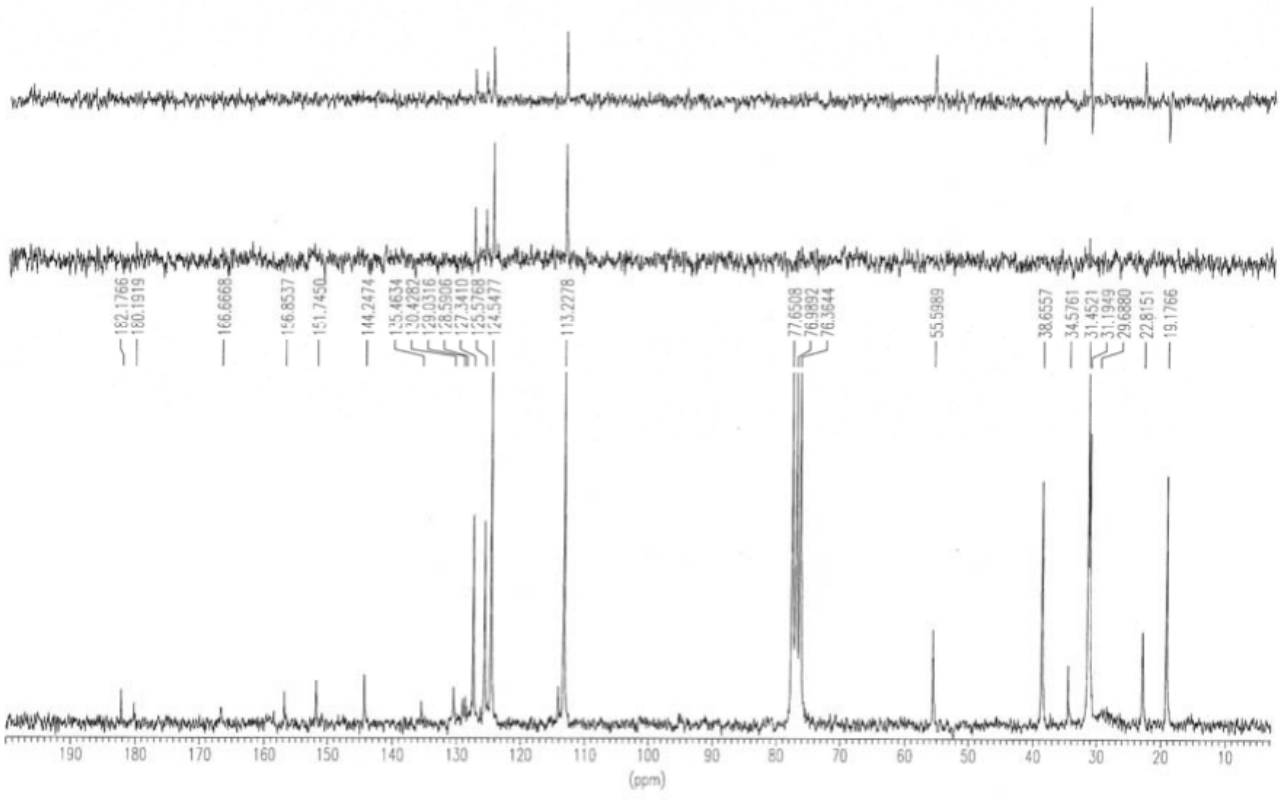
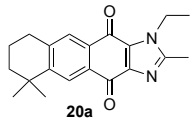
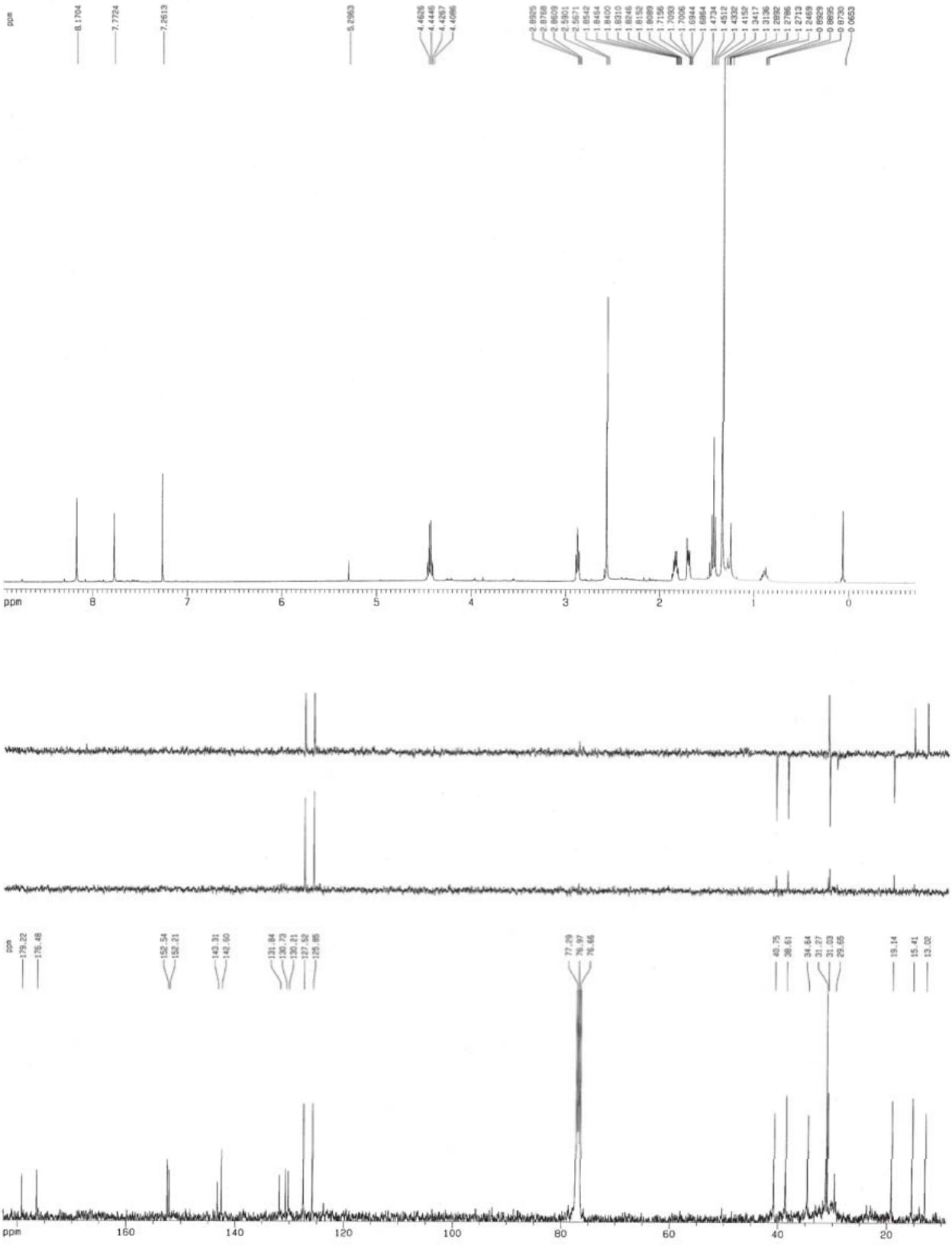


Figure S14: ^{1}H and ^{13}C NMR spectra for compound **20a**





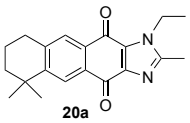
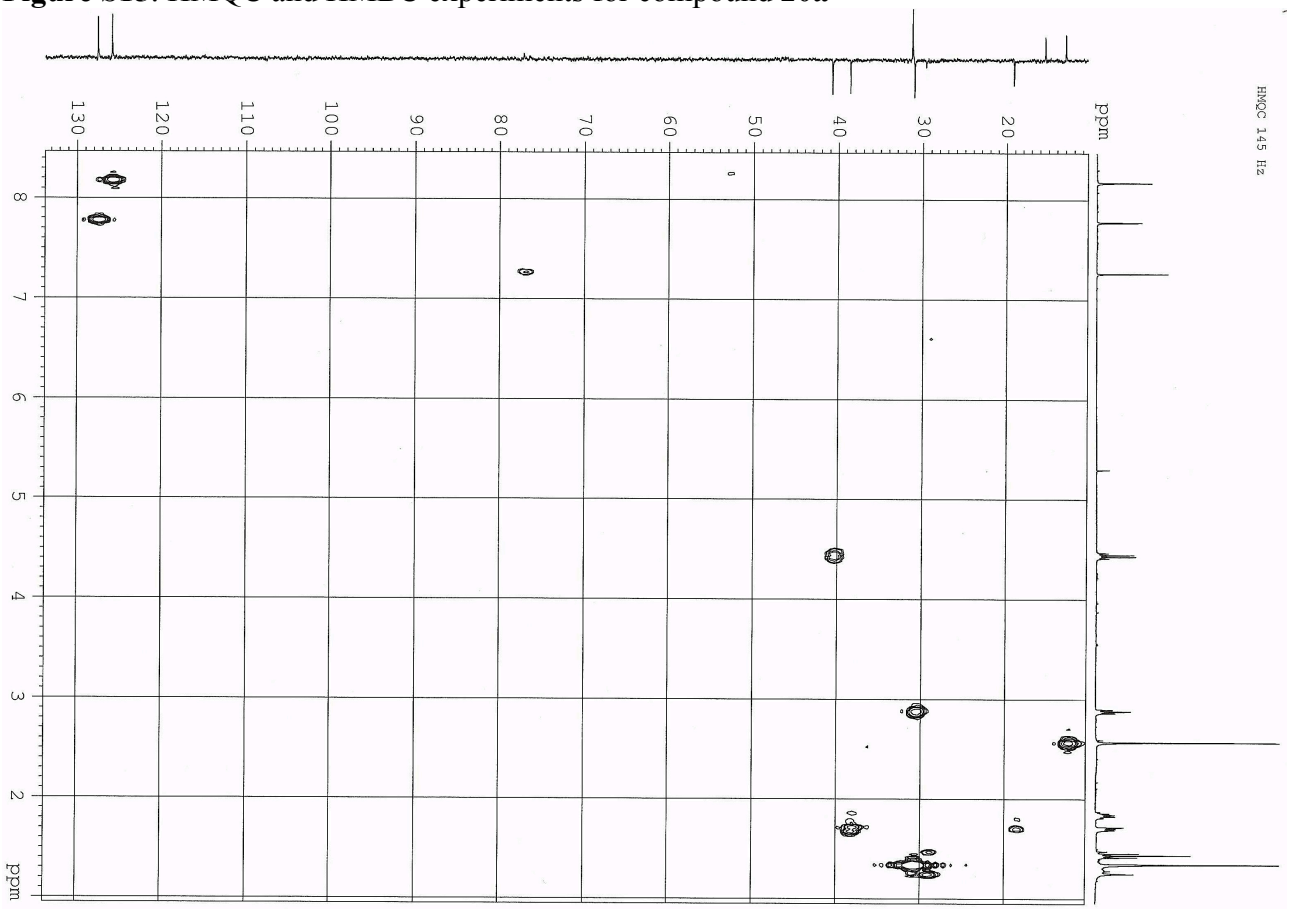


Figure S15: HMQC and HMBC experiments for compound **20a**



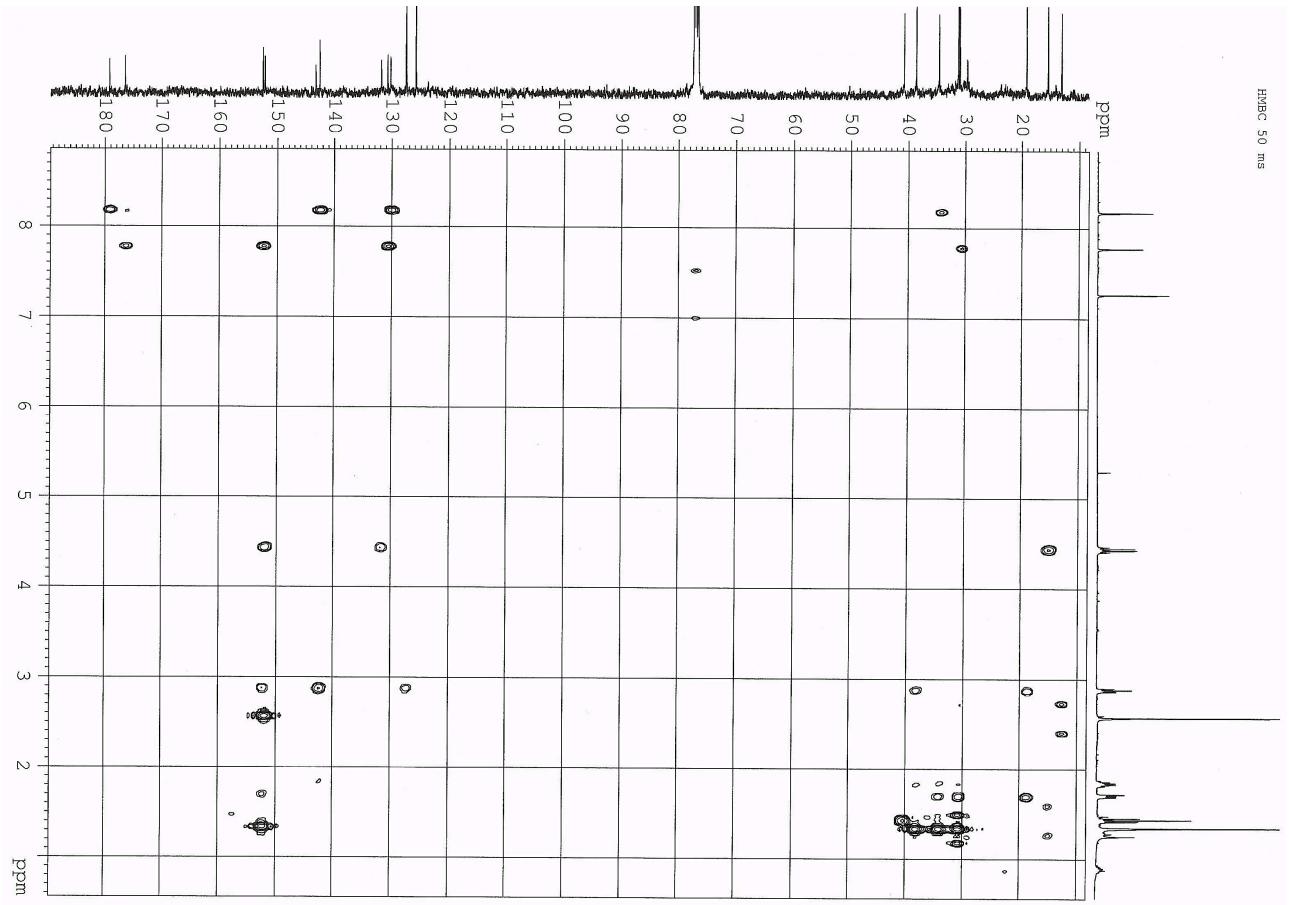
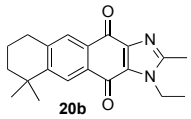
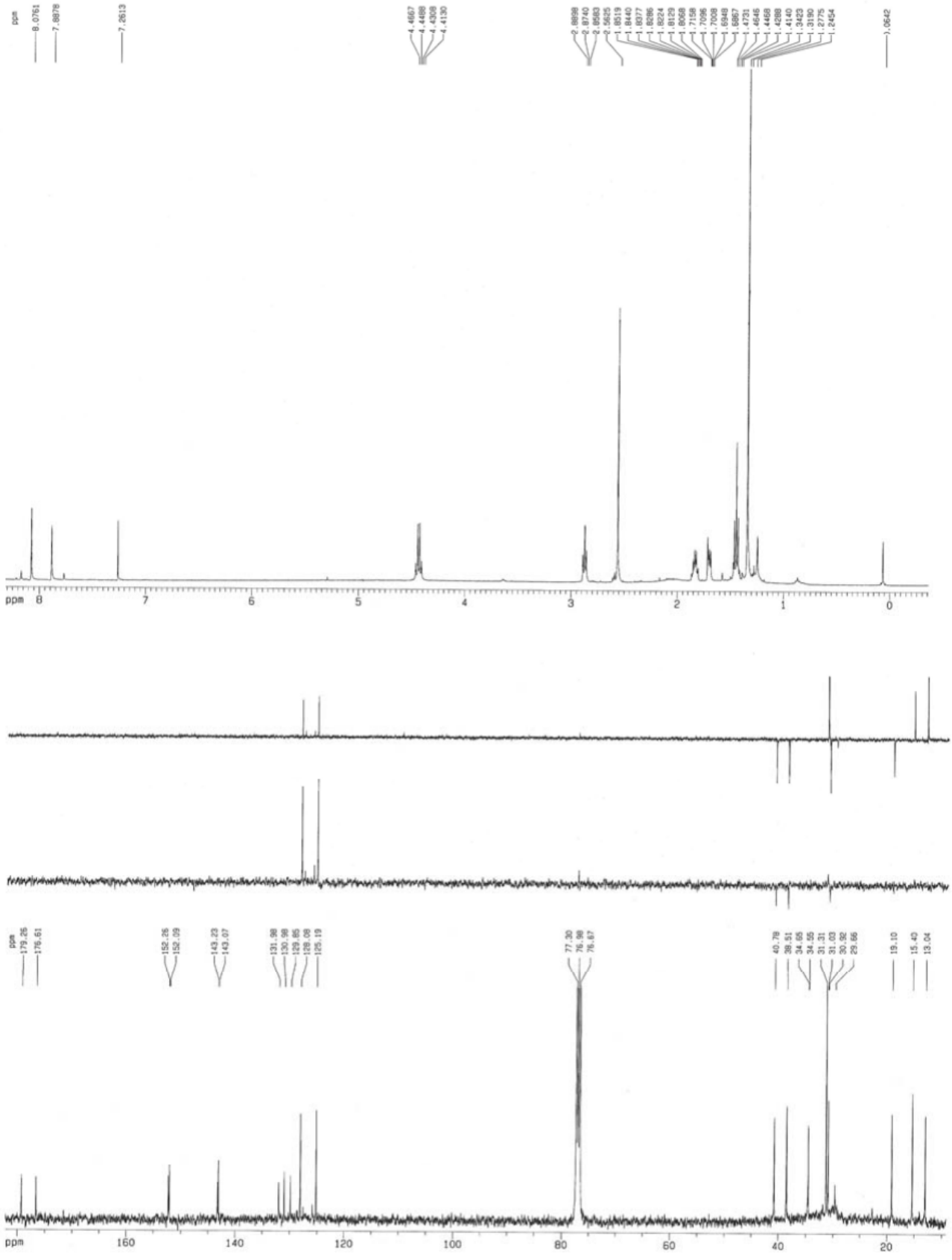


Figure S16: ^{1}H and ^{13}C NMR spectra for compound **20b**





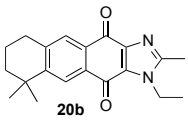
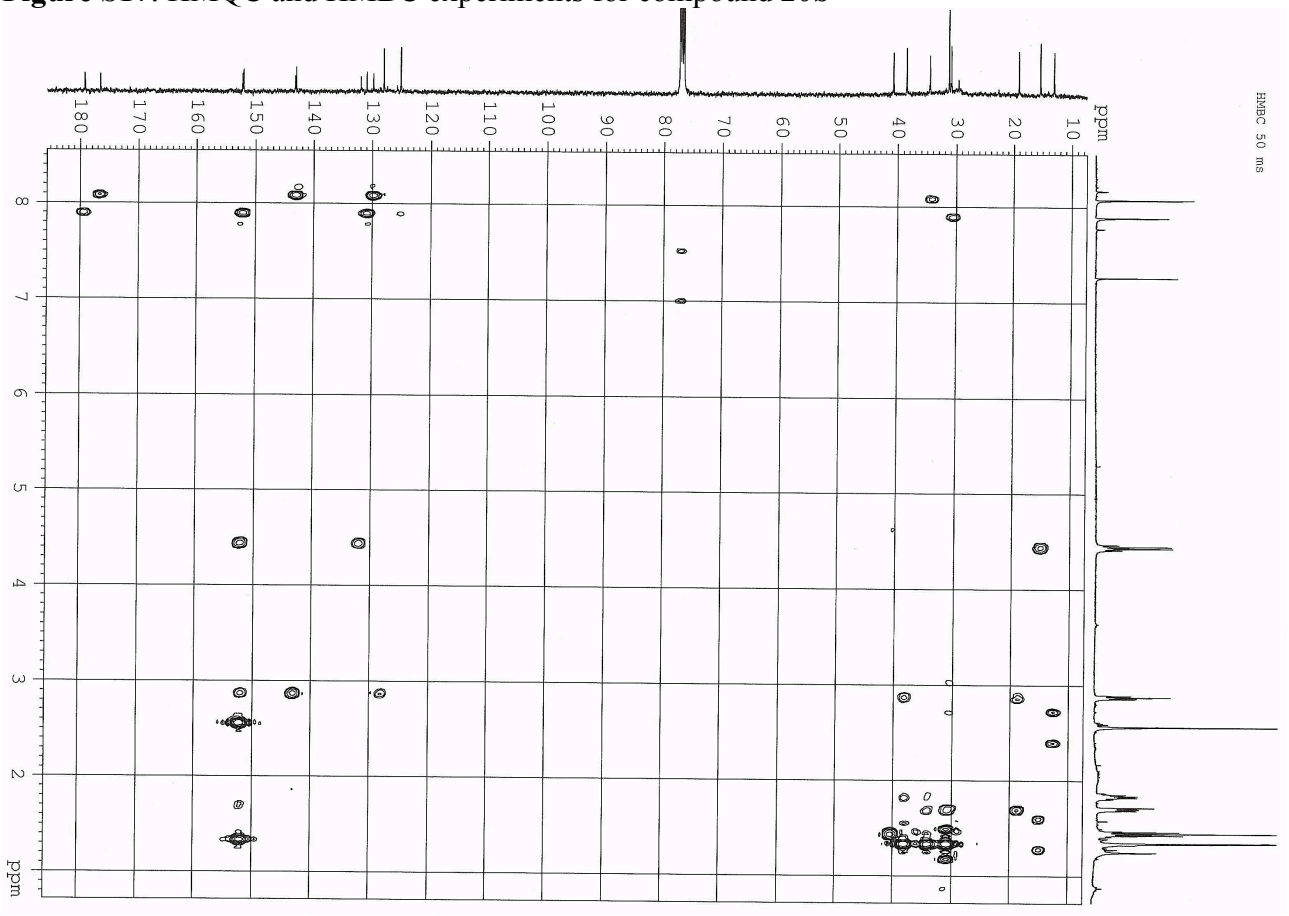


Figure S17: HMQC and HMBC experiments for compound **20b**



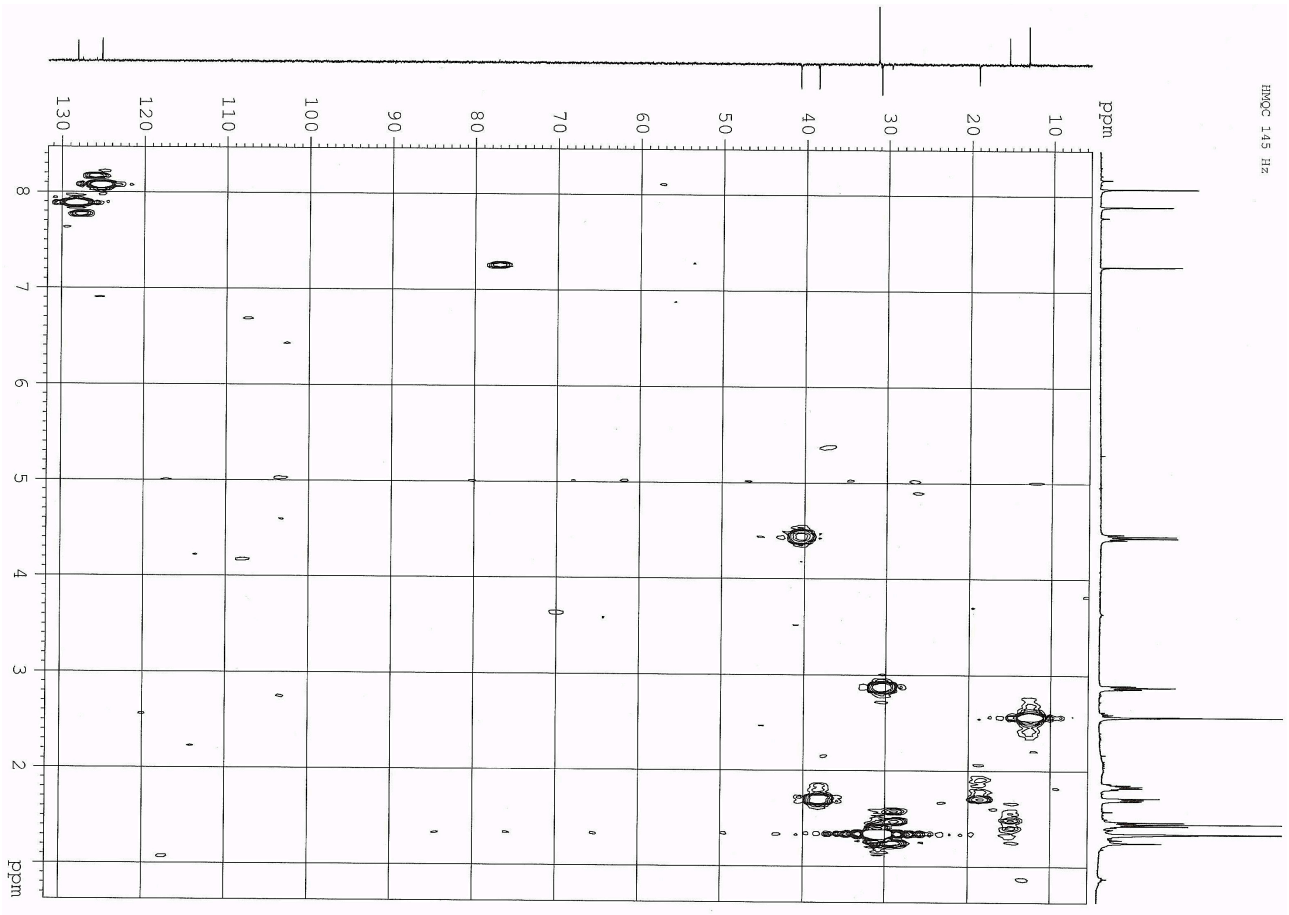
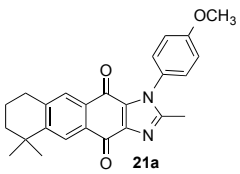


Figure S18: ^{1}H and ^{13}C NMR spectra for compound **21a**



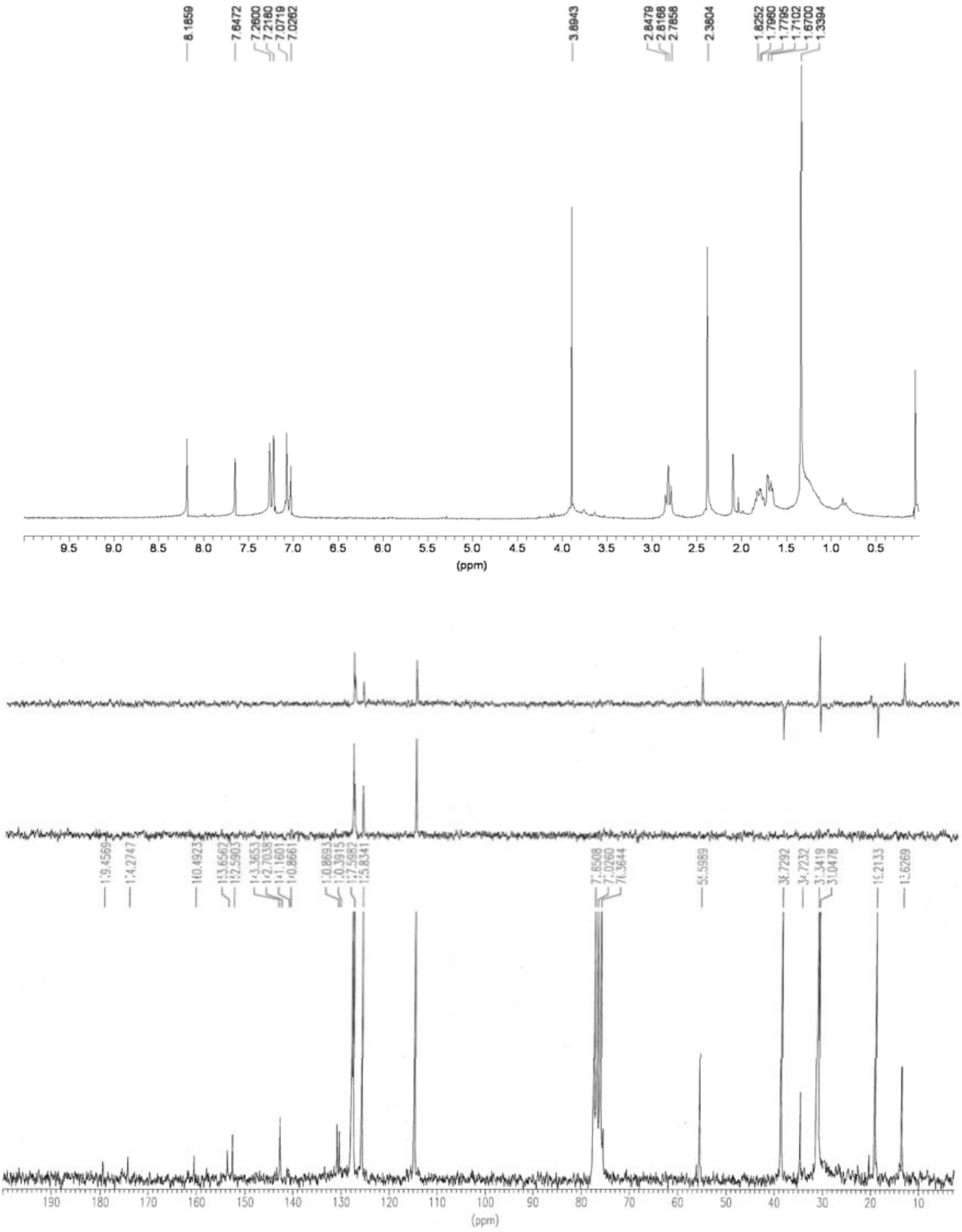
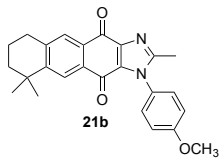


Figure S19: ^{1}H and ^{13}C NMR spectra for compound **21b**



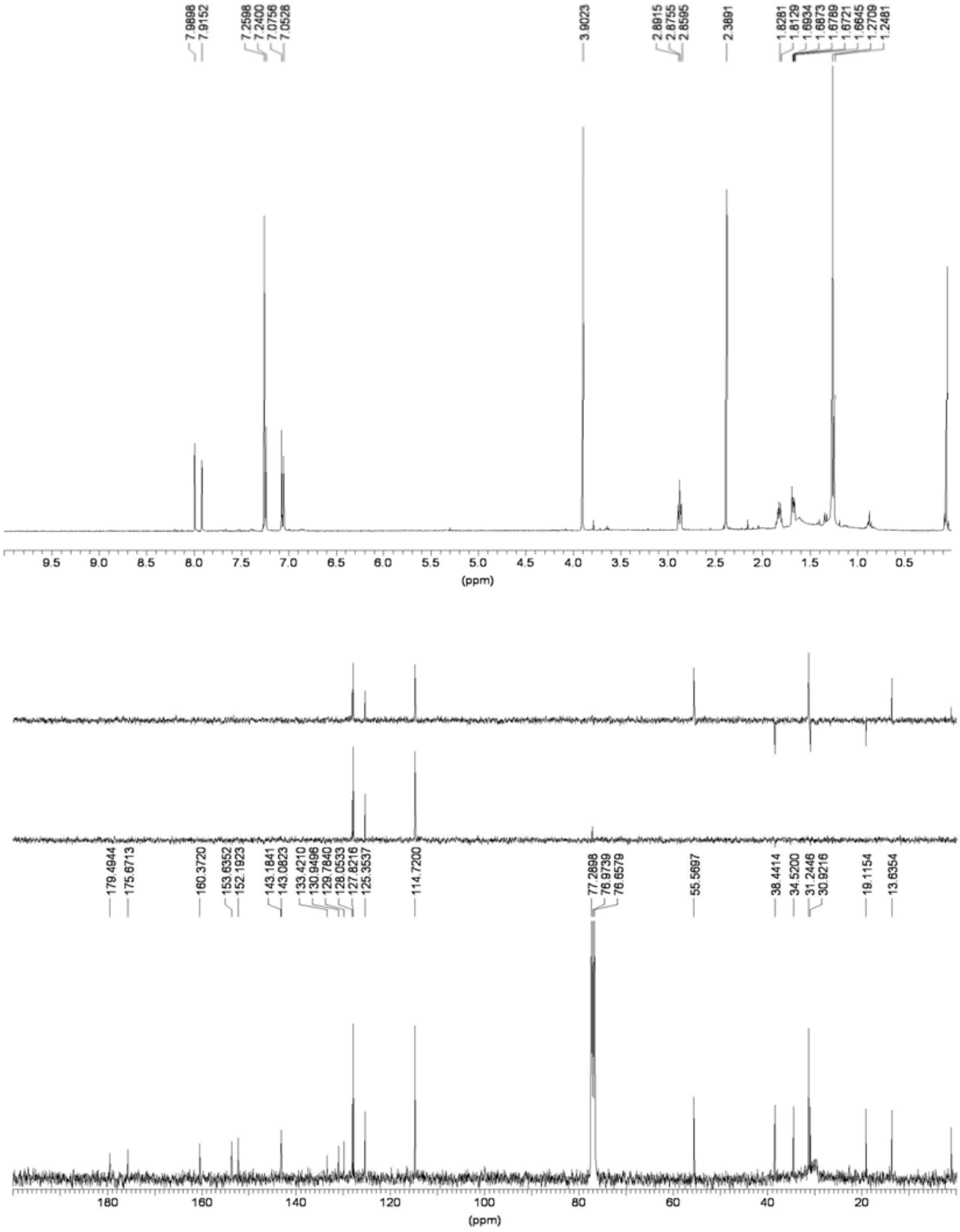
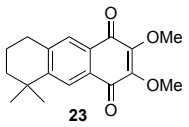
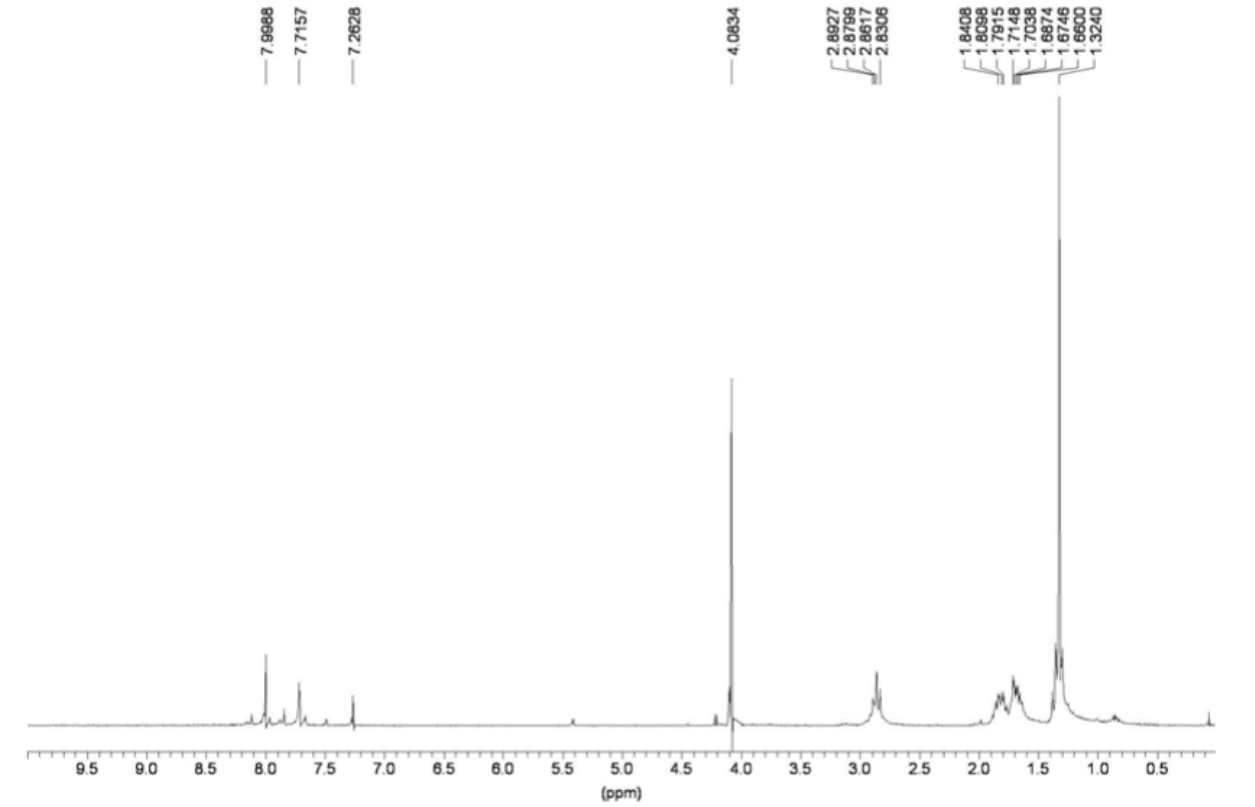


Figure S20: ^{1}H and ^{13}C NMR spectra for compound **23**





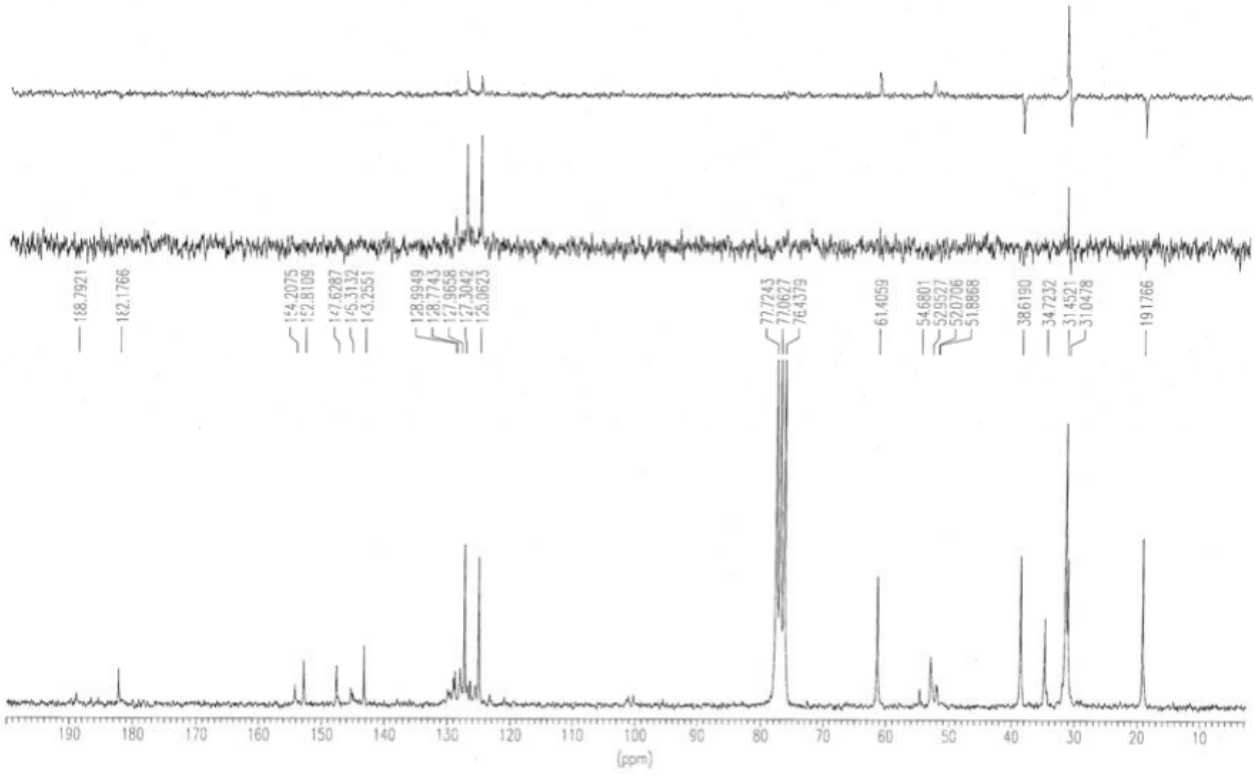
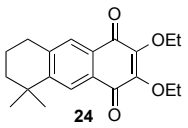


Figure S21: ^{1}H and ^{13}C NMR spectra for compound **24**



24

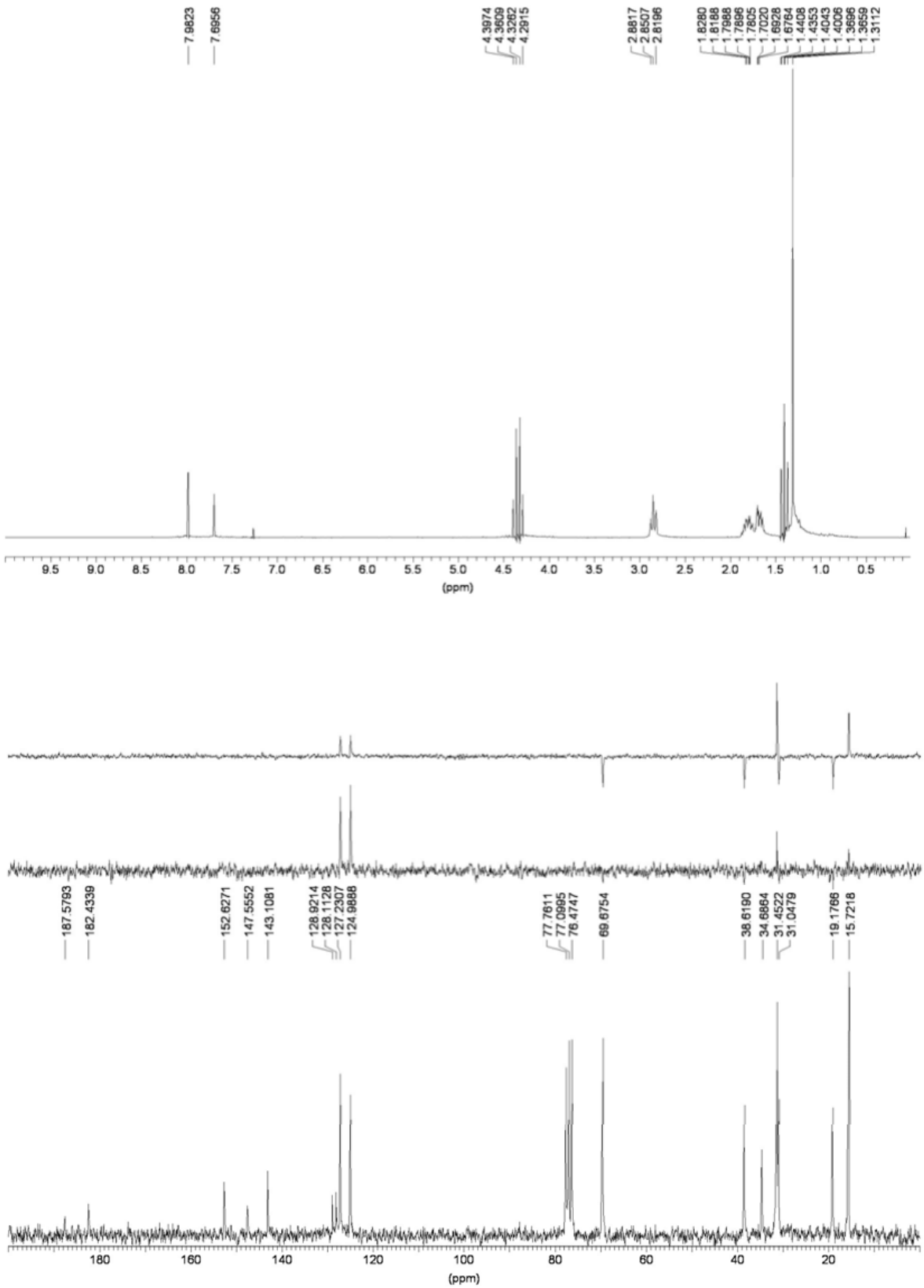
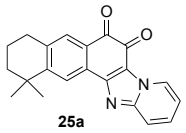
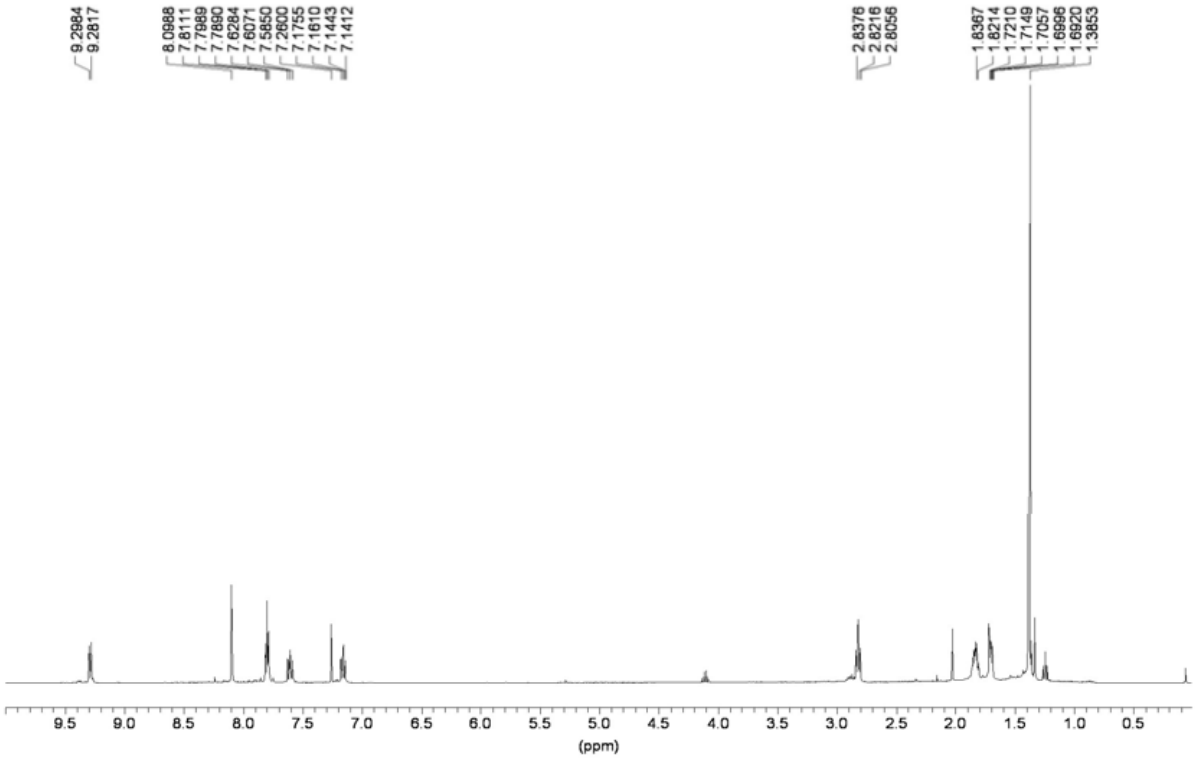


Figure S22: ^{1}H and ^{13}C NMR spectra for compound **25a**



25a



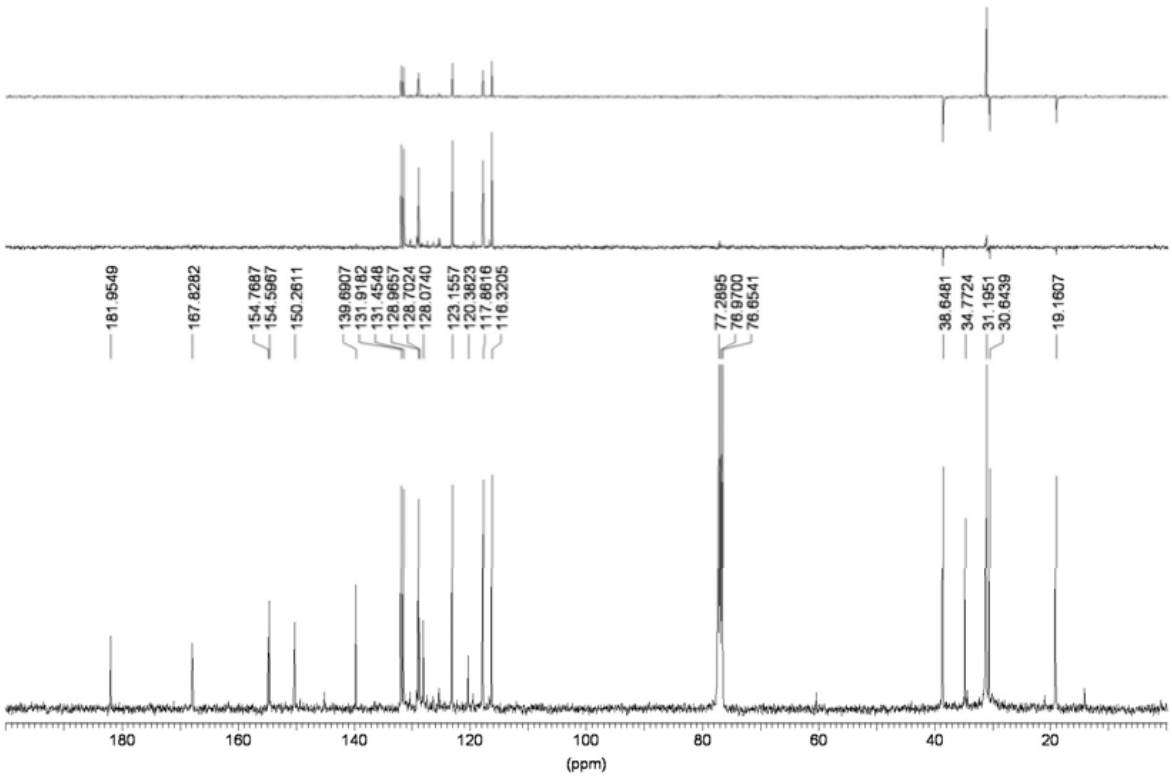
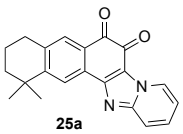
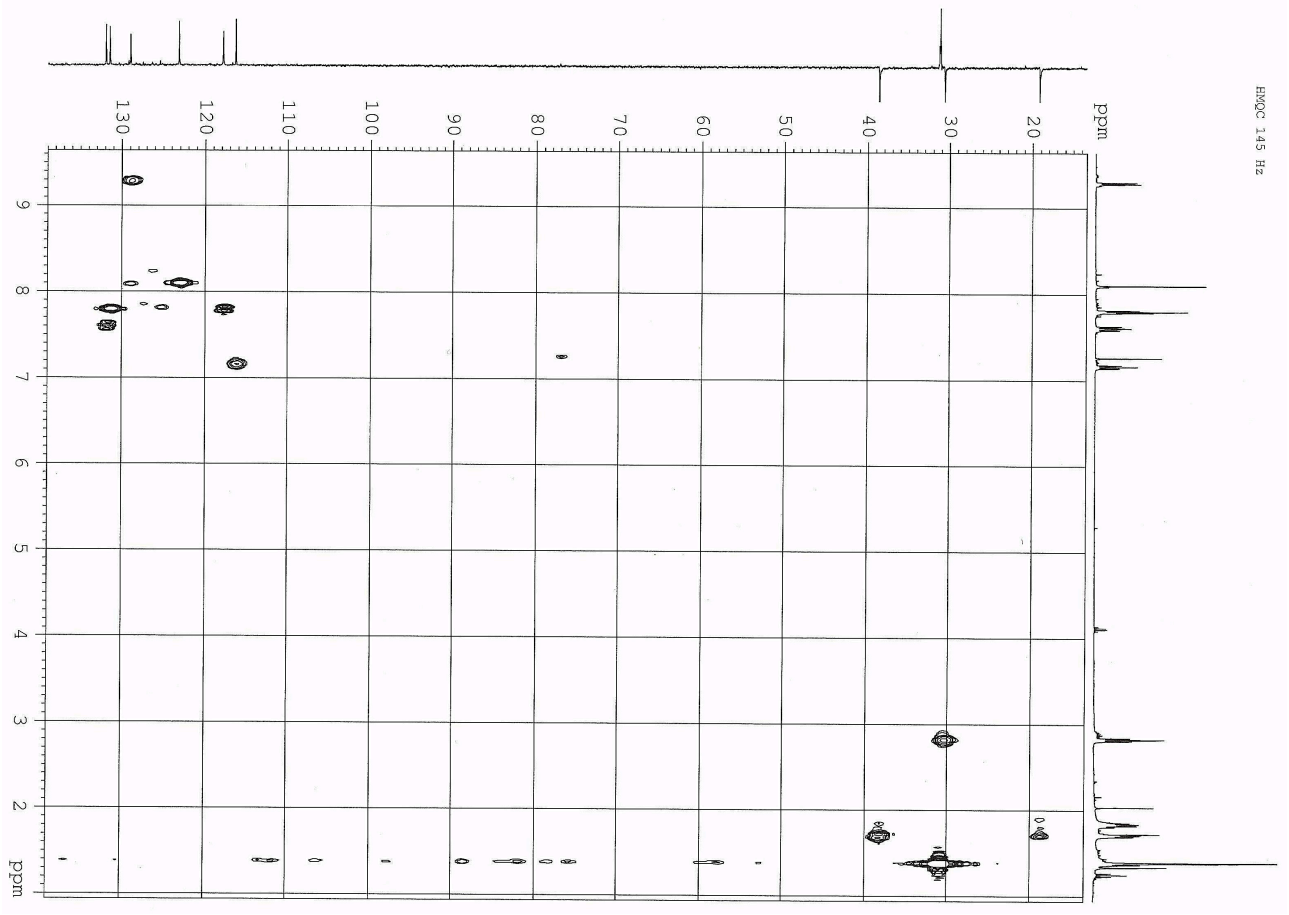


Figure S23: HMQC and HMBC experiments for compound **25a**



25a



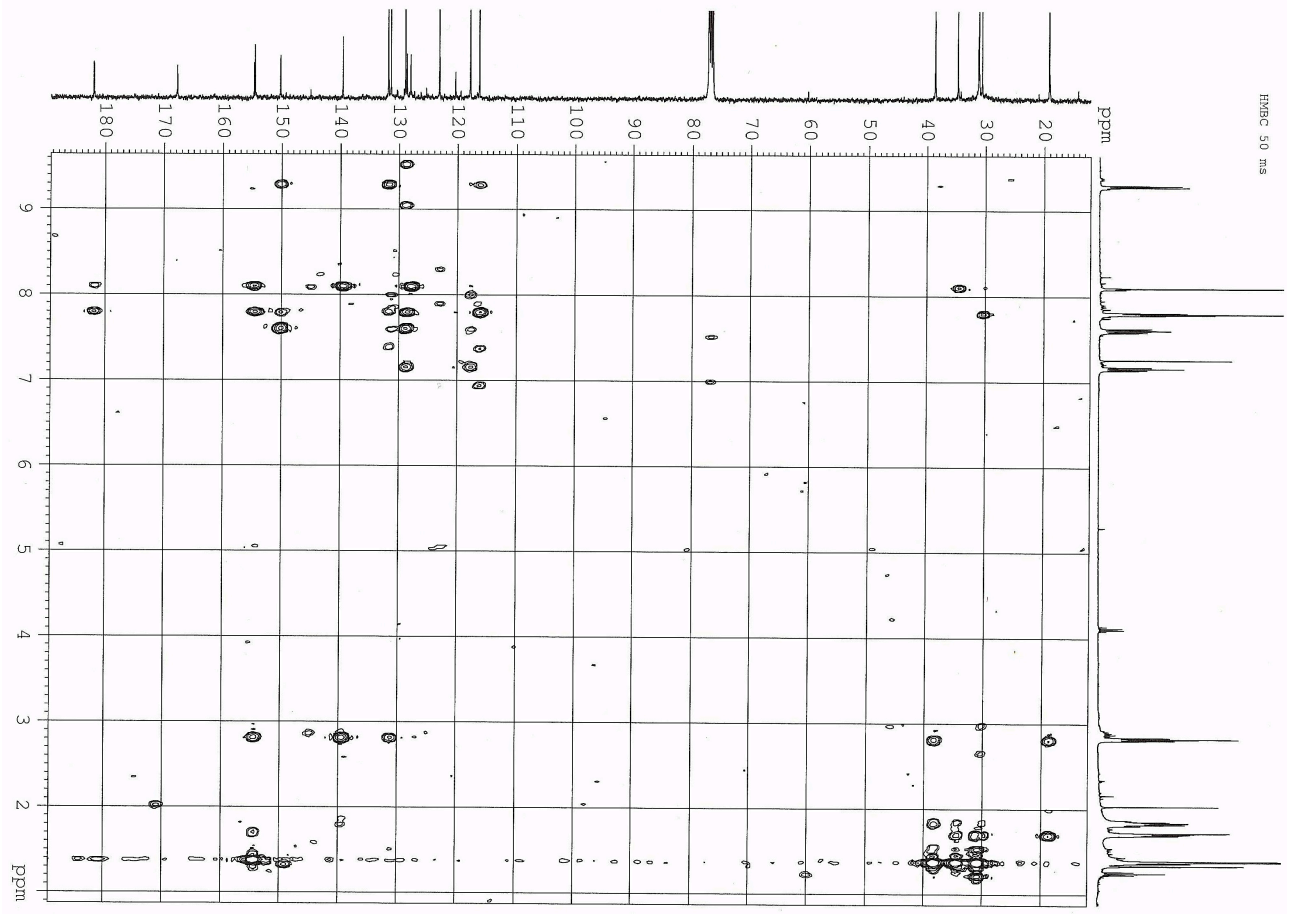
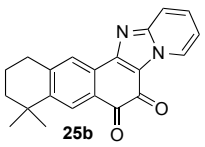
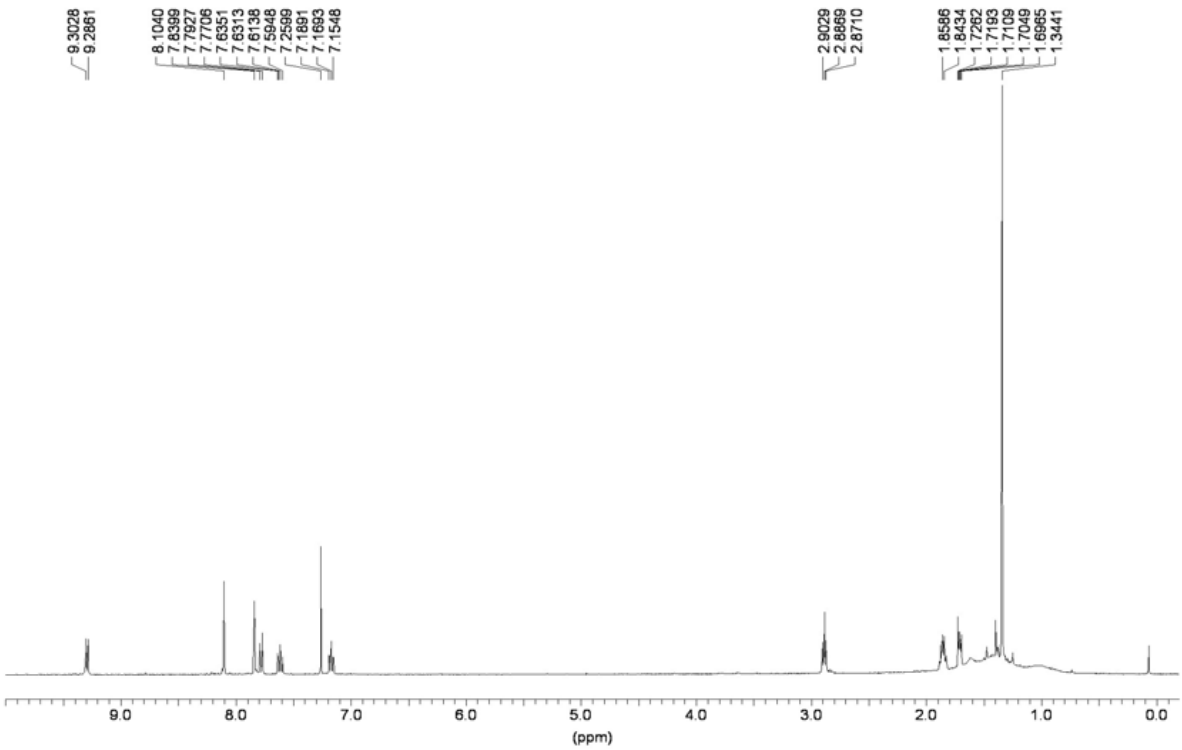


Figure S24: ^{1}H and ^{13}C NMR spectra for compound **25b**





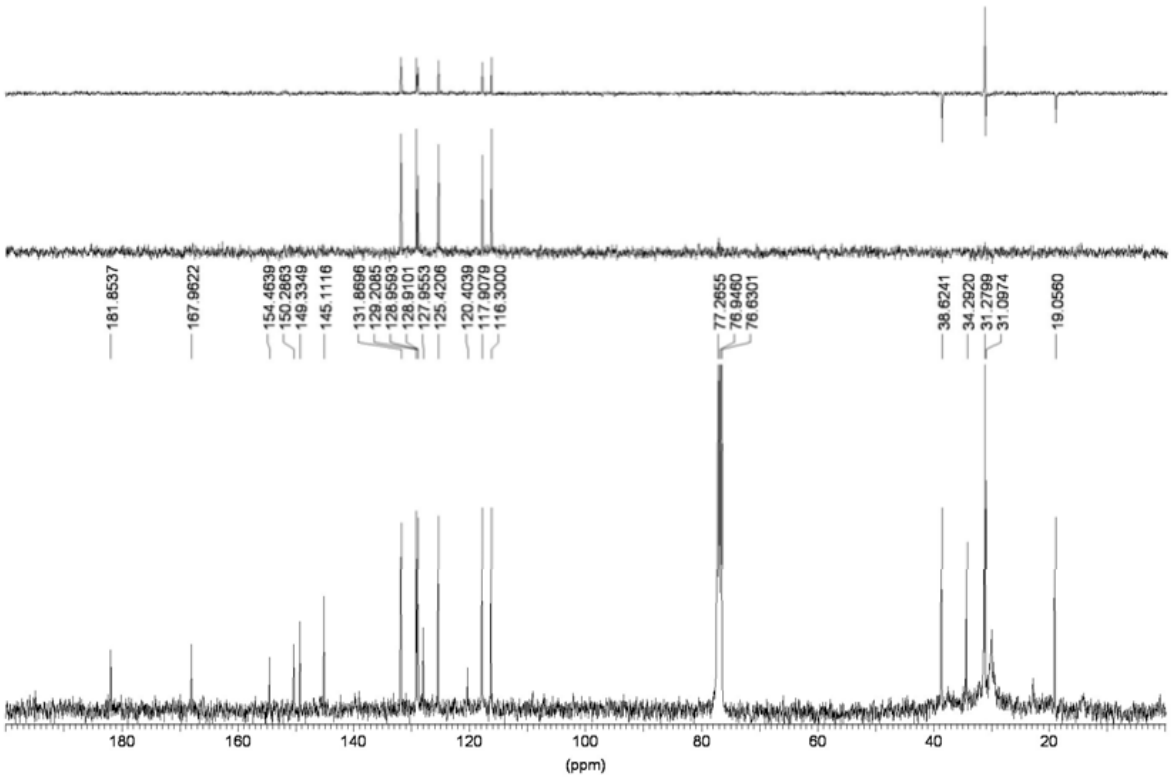
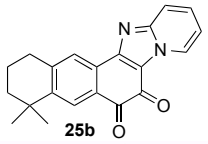
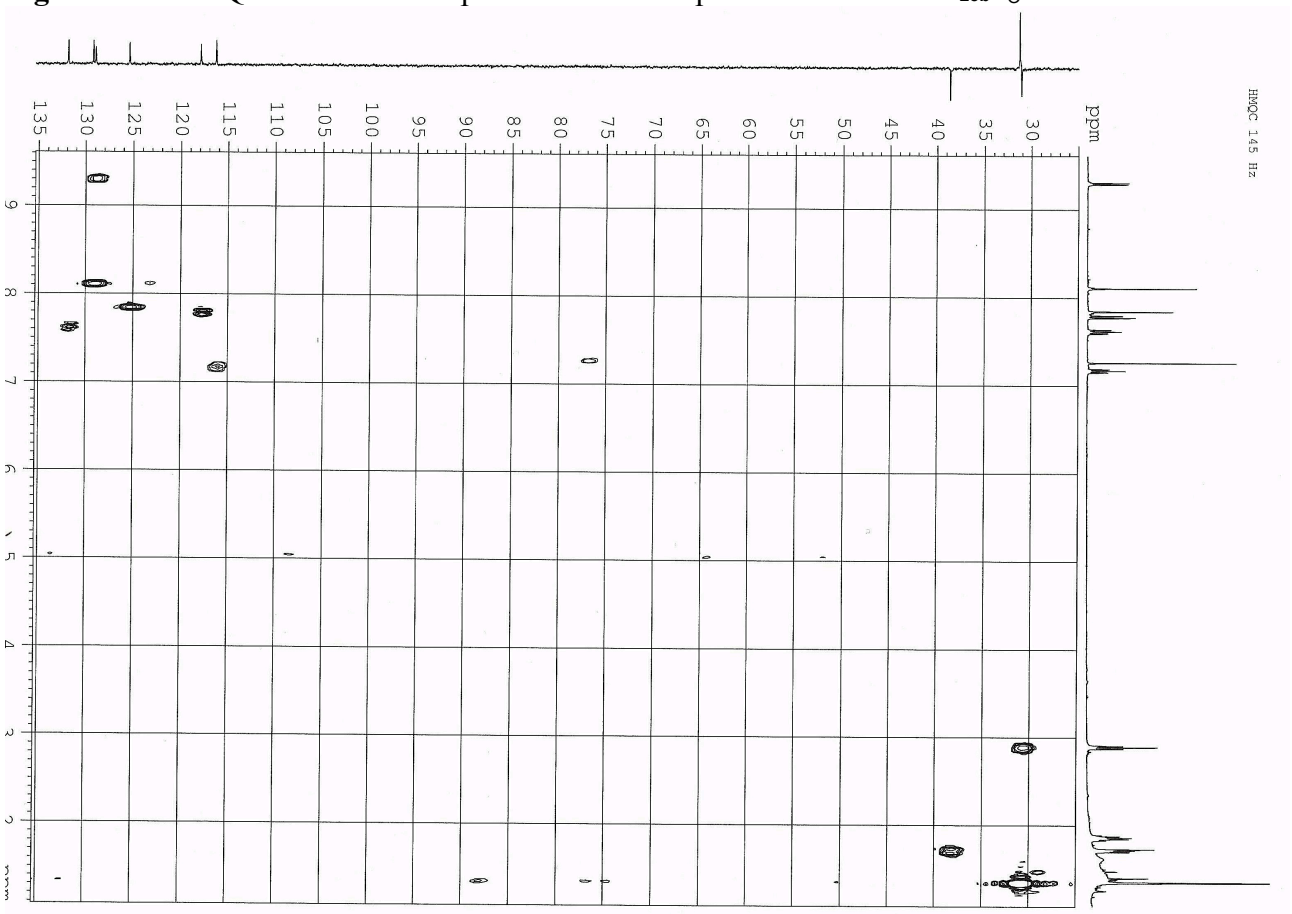


Figure S25: HMQC and HMBC experiments for compound **25b**



25b



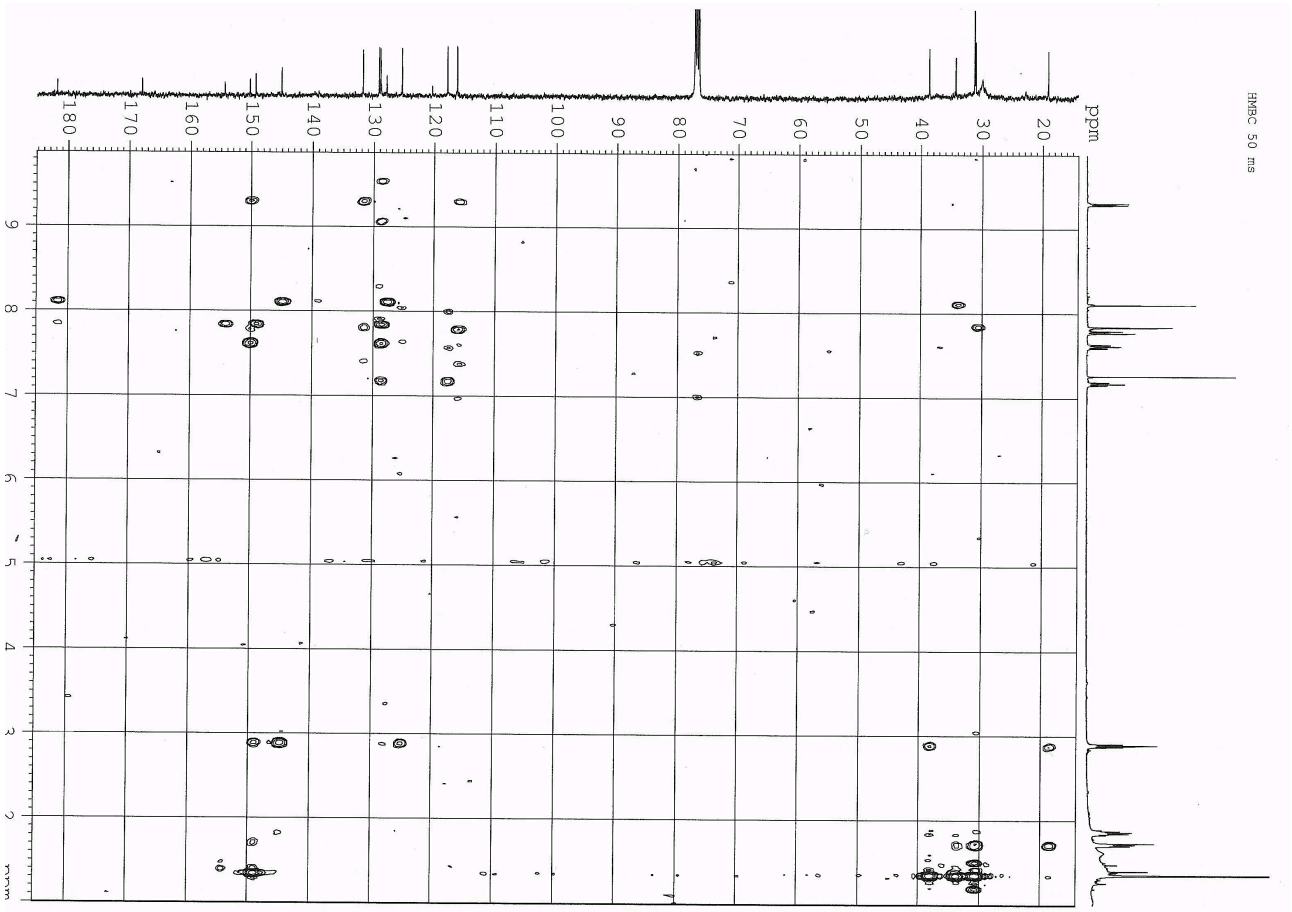
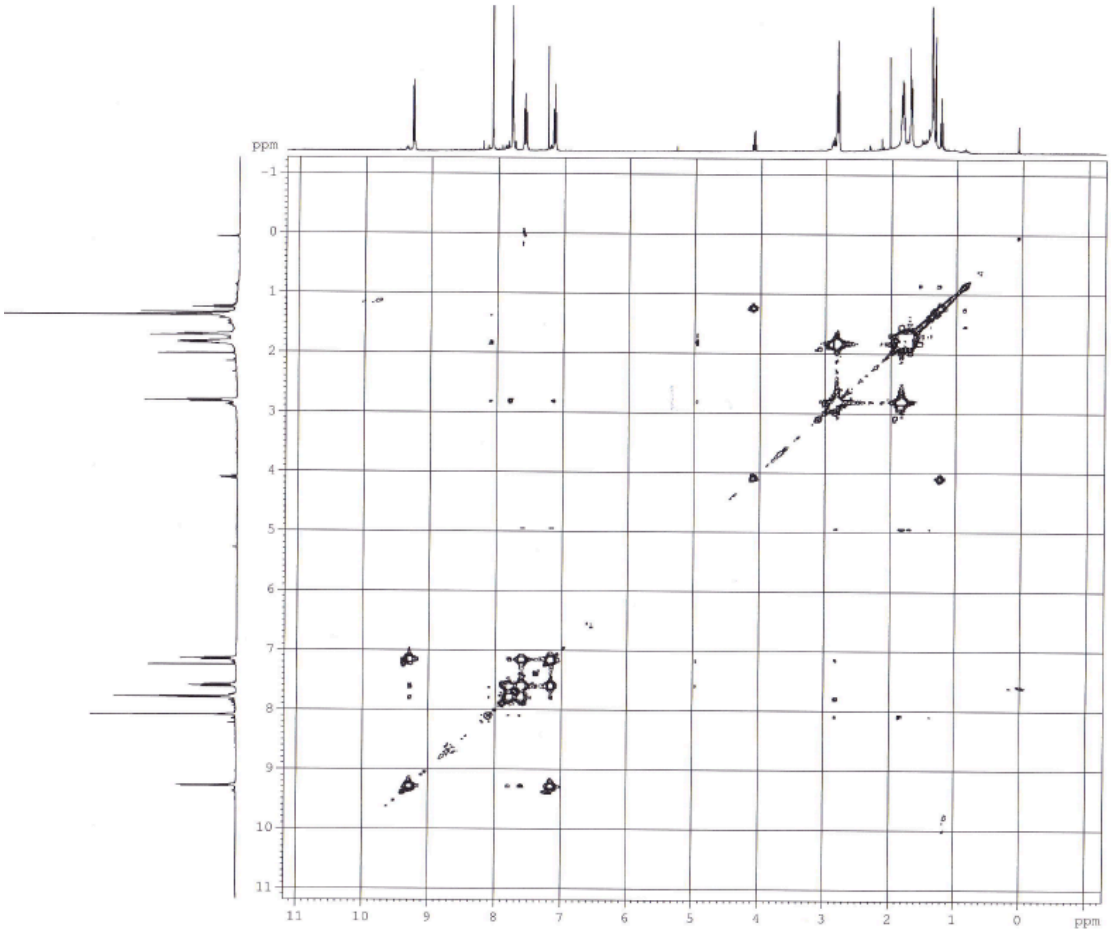
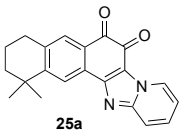
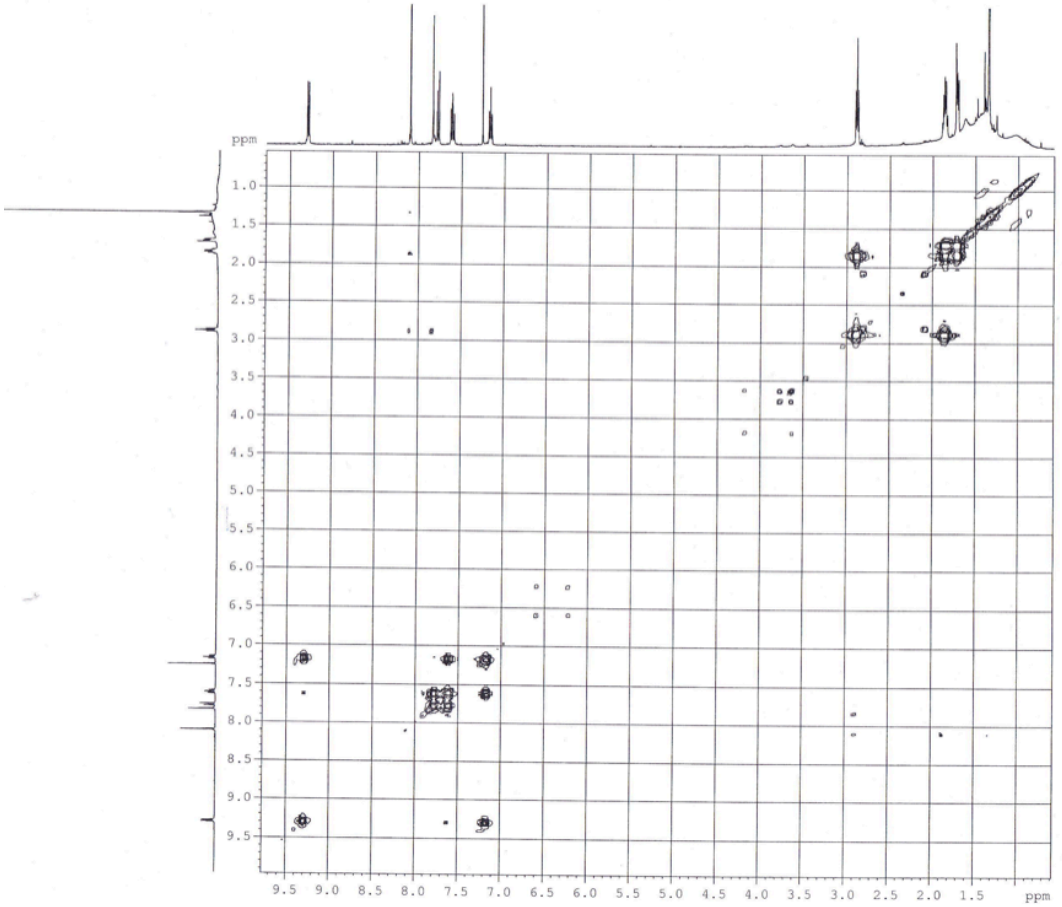


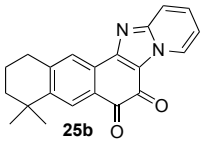
Figure S26: ^{1}H-^{1}H COSY experiments for compound **25a** and **25b.**





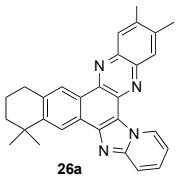
25a





25b

Figure S27: ^{1}H and ^{13}C NMR spectra for compound **26a**



26a

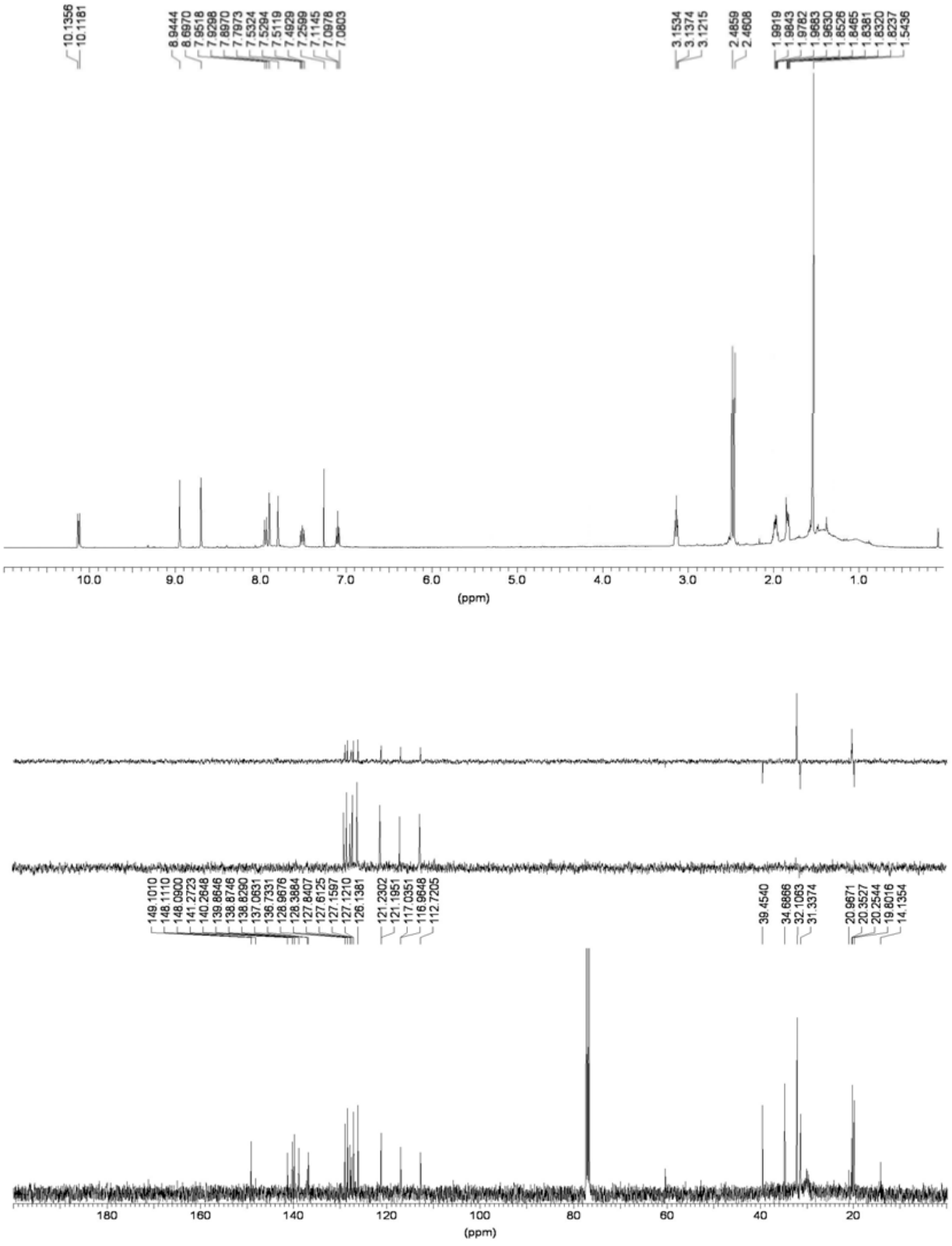
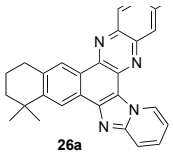
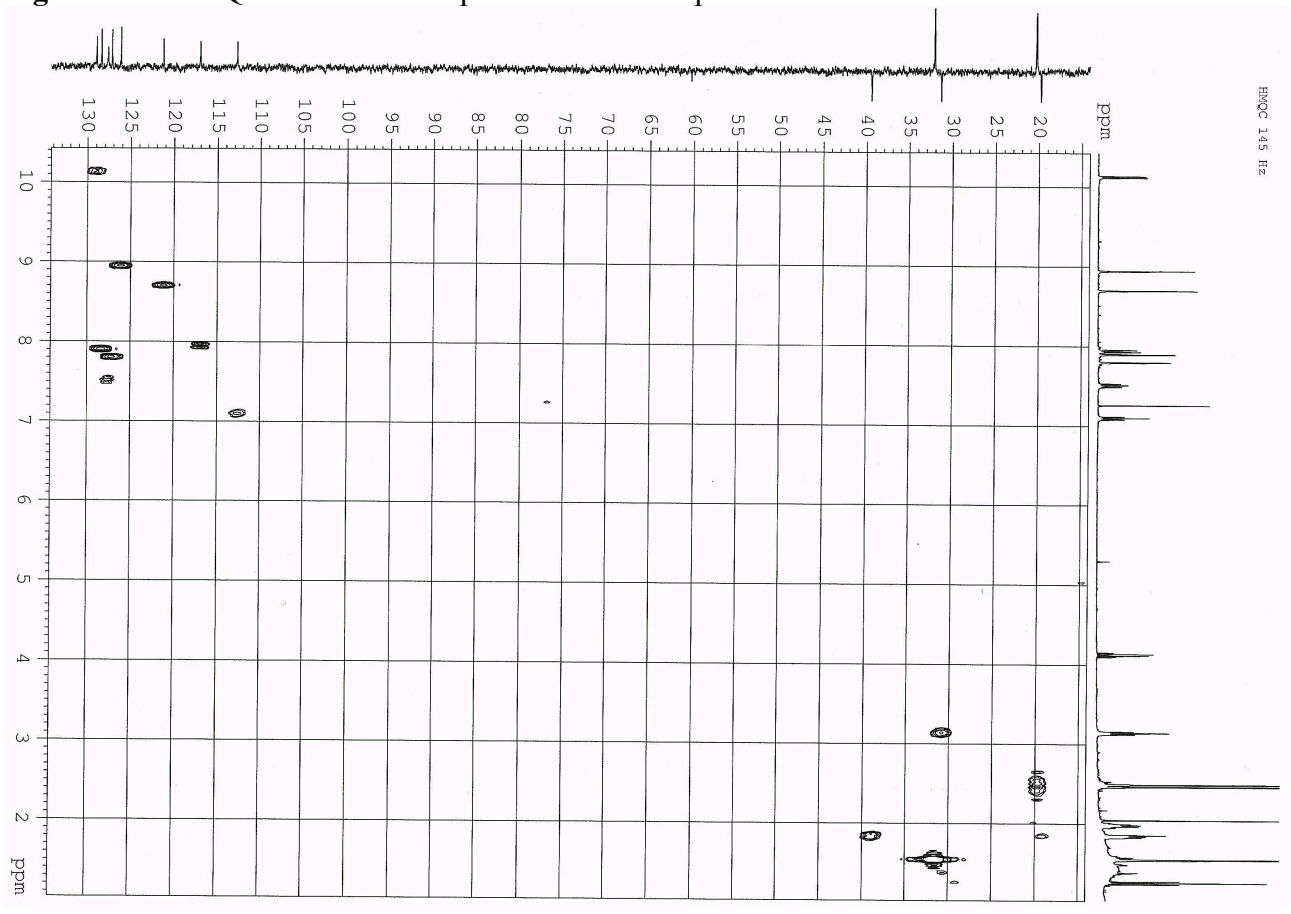


Figure S28: HMQC and HMBC experiments for compound **26a**



26a



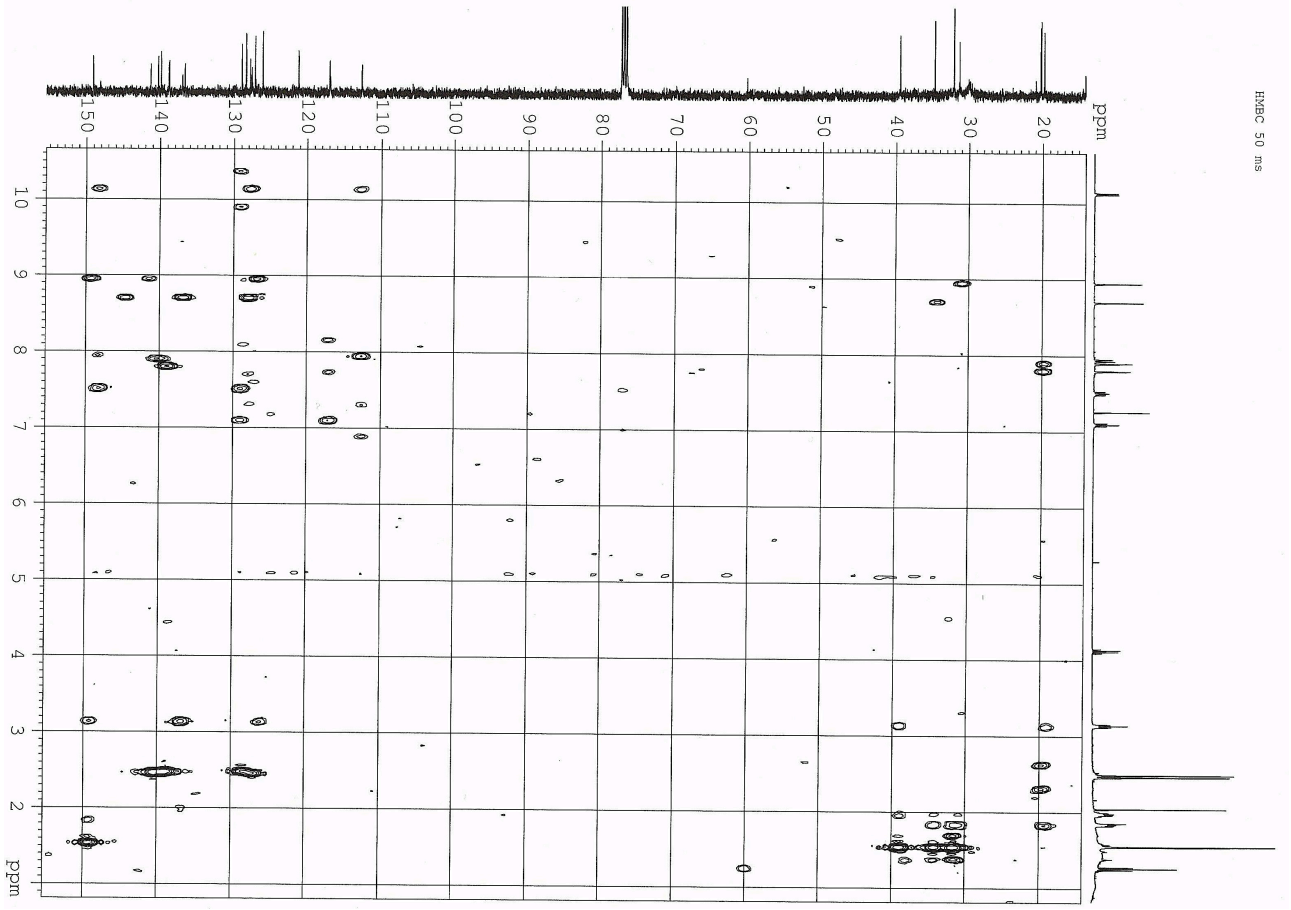
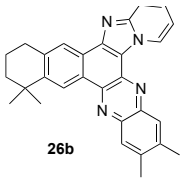


Figure S29: ^{1}H and ^{13}C NMR spectra for compound **26b**



26b

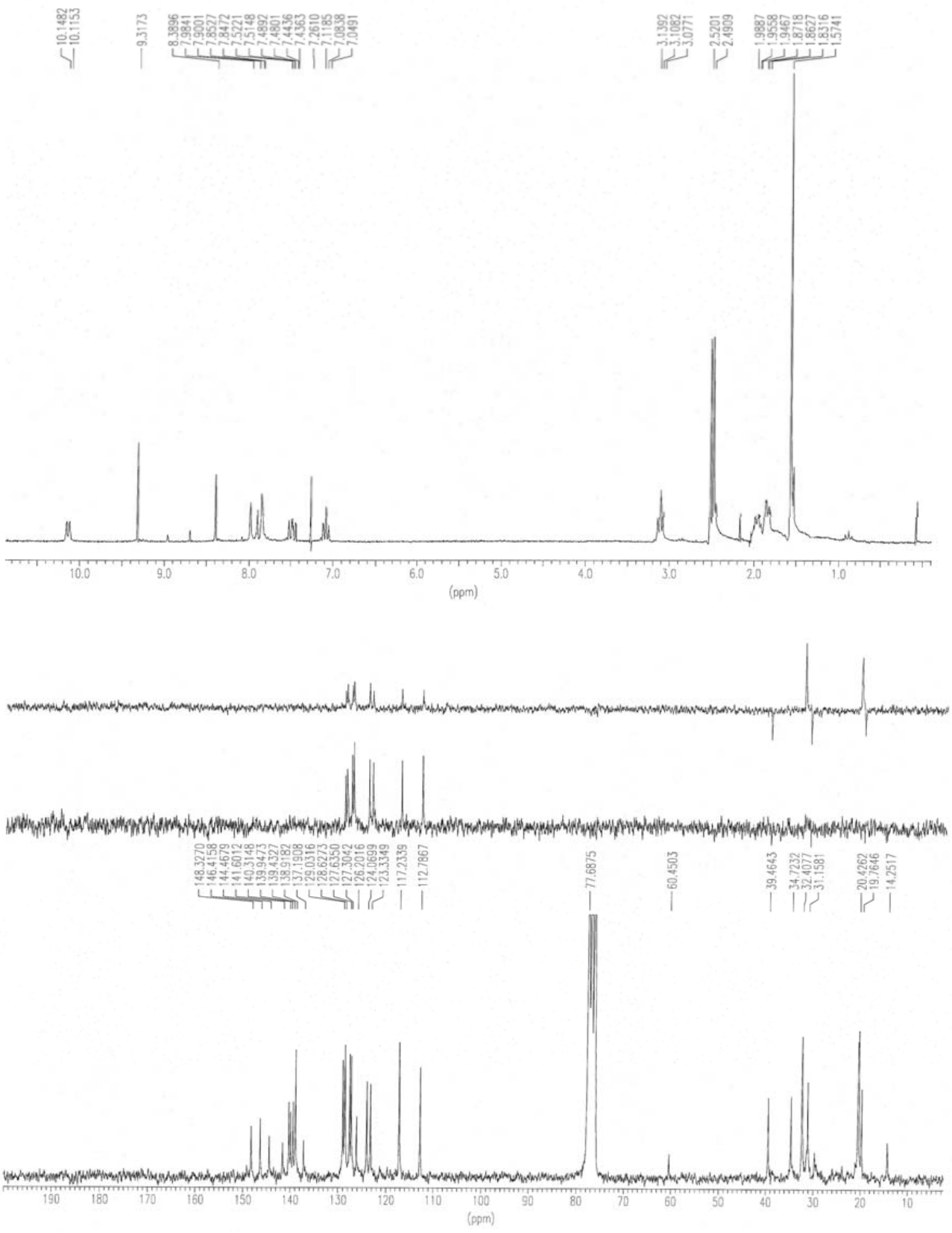
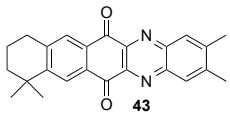
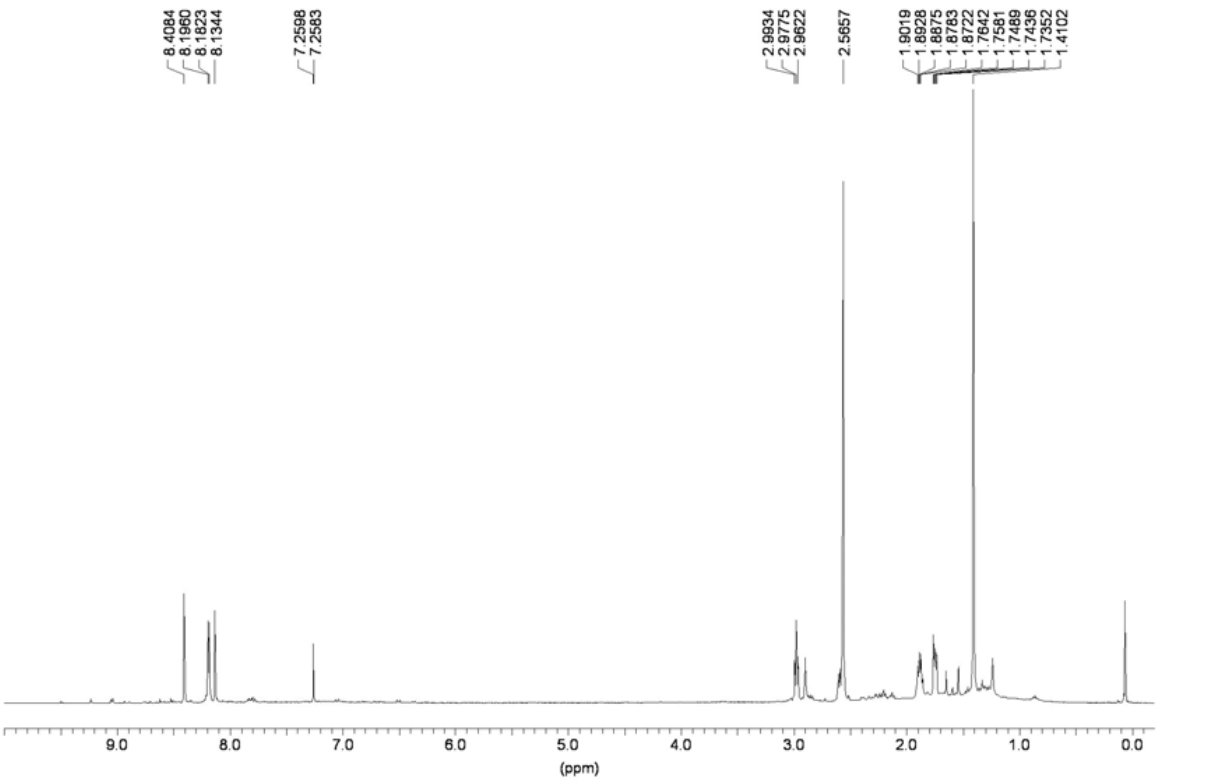
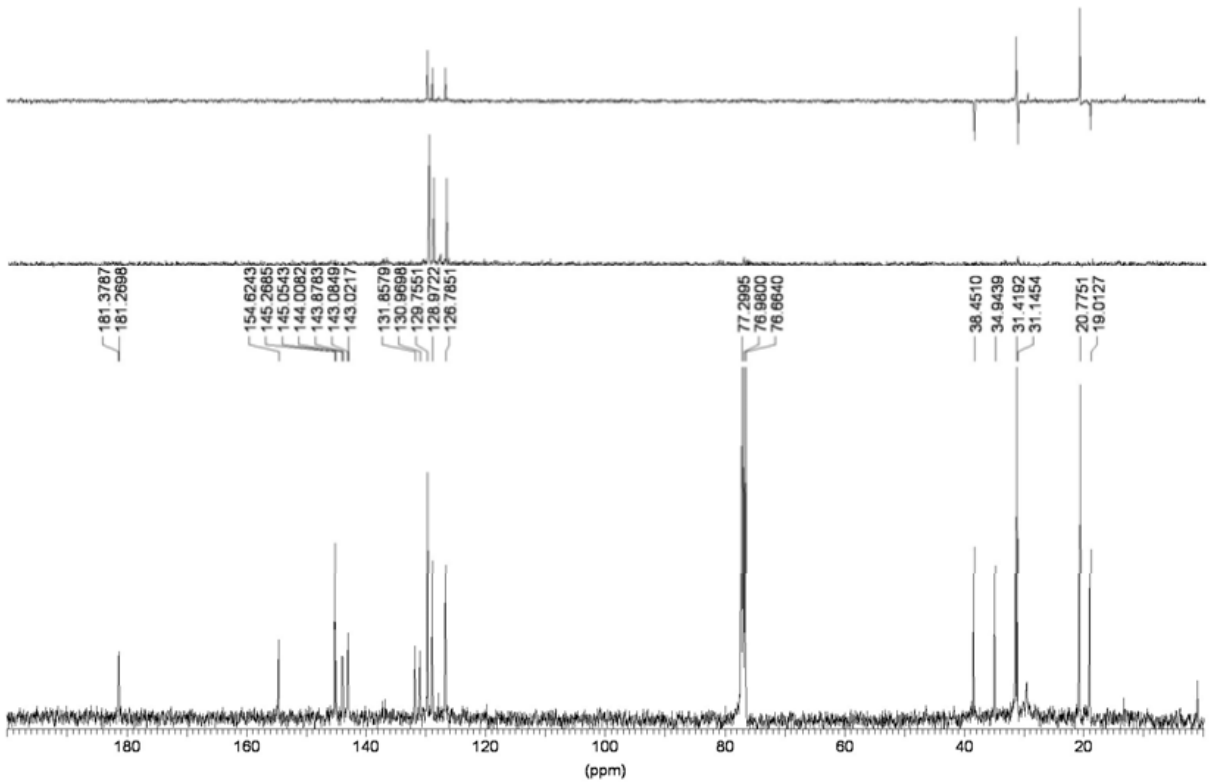


Figure S30: ^{1}H and ^{13}C NMR spectra for compound **43**







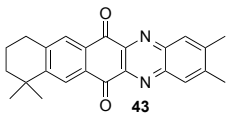


Figure S40: HMQC and HMBC experiments for compound **43**