Supporting Information

Tribenzopentaphene Derivatives with Lateral Aromatic Groups: Effect of Substituents' Nature and Position on Emission Properties

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CONTENTS

Synthesis of **1,4-bis(4-(5'-hexyl-2,2'-bithiophen-5-yl)phenyl)triphenylene, 5a**: A Schlenck tube was charged with 1,4-bis(4-bromophenyl)triphenylene, **4a** (200 mg, 0.37 mmol), 5'-Hexyl-2,2'-bithiophene-5-boronicacid pinacolester (559 mg, 5.59 mmol.), Tris(dibenzylideneacetone)dipalladium (37 mg, 3.3 x 10^{-2} mmol), Sphos (30 mg, 7.4 x 10^{-2} mmol), and K_3PO_4 (315 mg, 1.48 mmol) in 15 mL of degassed 1:1 mixture of toluene and 1-butanol. The reaction was refluxed under argon for 4 days. The solvent was evaporated under vacuo and the resulting black mixture was extracted with dichloromethane (x3) from a saturated aqueous solution of $NaHCO_3$. The combined organic layer was washed with H_2O, concentrated, precipitated using hexane followed by Millipore filtration affording the desired product as a yellow solid (22 mg, 7 %).

5a: ^{1}H-NMR: (360 MHz, $CDCl_3$): δ_{TMS} 8.46 (*d*, 2H, ArH), 7.82 (*d*, 2H, ArH), 7.64 (*d*, 4H, ArH), 7.55 (*s*, 2H, ArH), 7.48 (*d*, 6H, ArH), 7.27 (*d*, 2H, ArH), 7.16 (*t*, 2H, ArH), 7.12 (*d*, 2H, ArH), 7.03 (*d*, 2H, ArH), 6.71 (*d*, 2H, ArH); EI-MS = m/z (% int): 876.300 ($M^{\bullet+}$, 100), (m/z calcd for $C_{58}H_{52}S_4^+$: 876.295).

I. Experimental details MALDI of 9-11

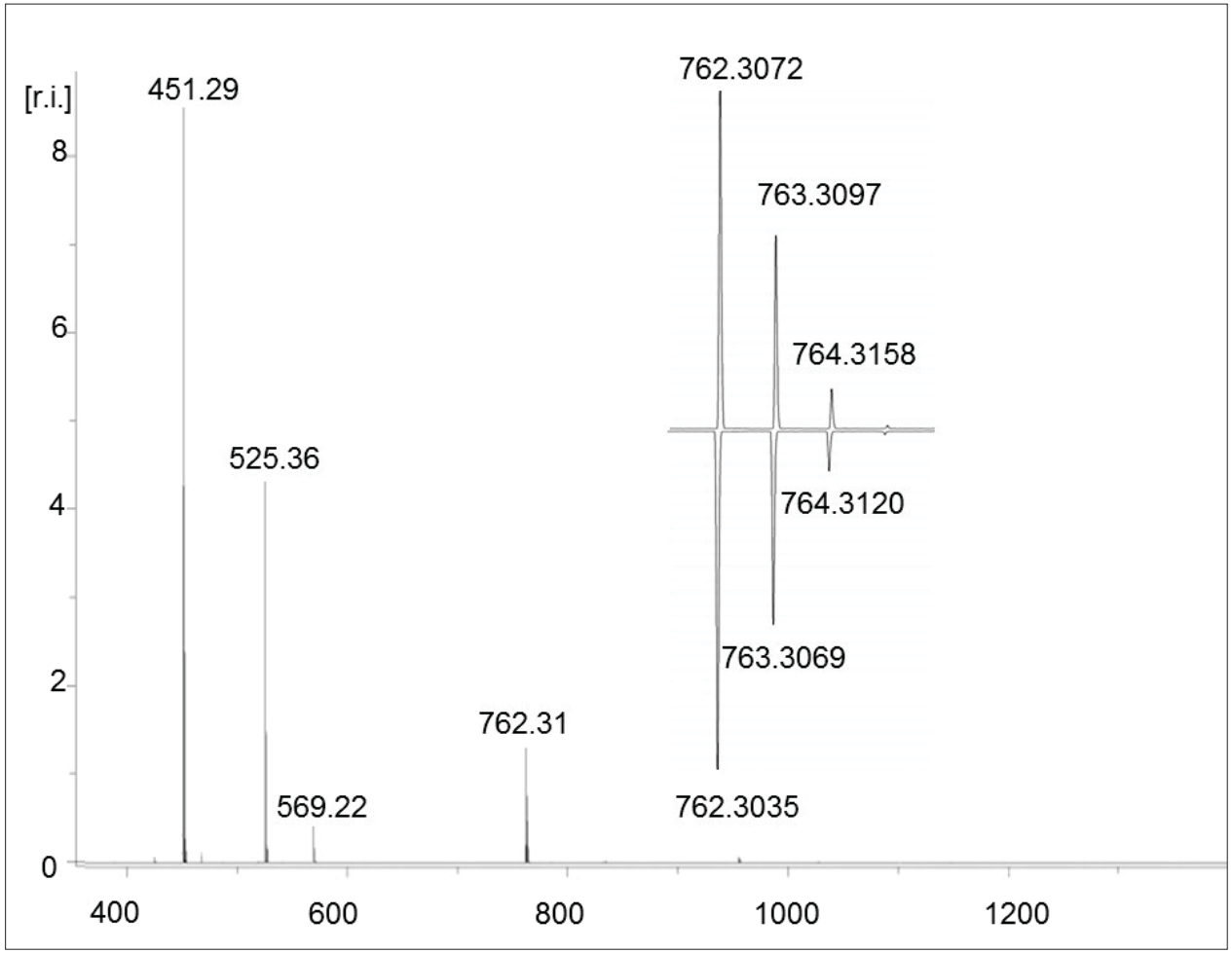


Figure S1. HR-MALDI spectrum of **9a**

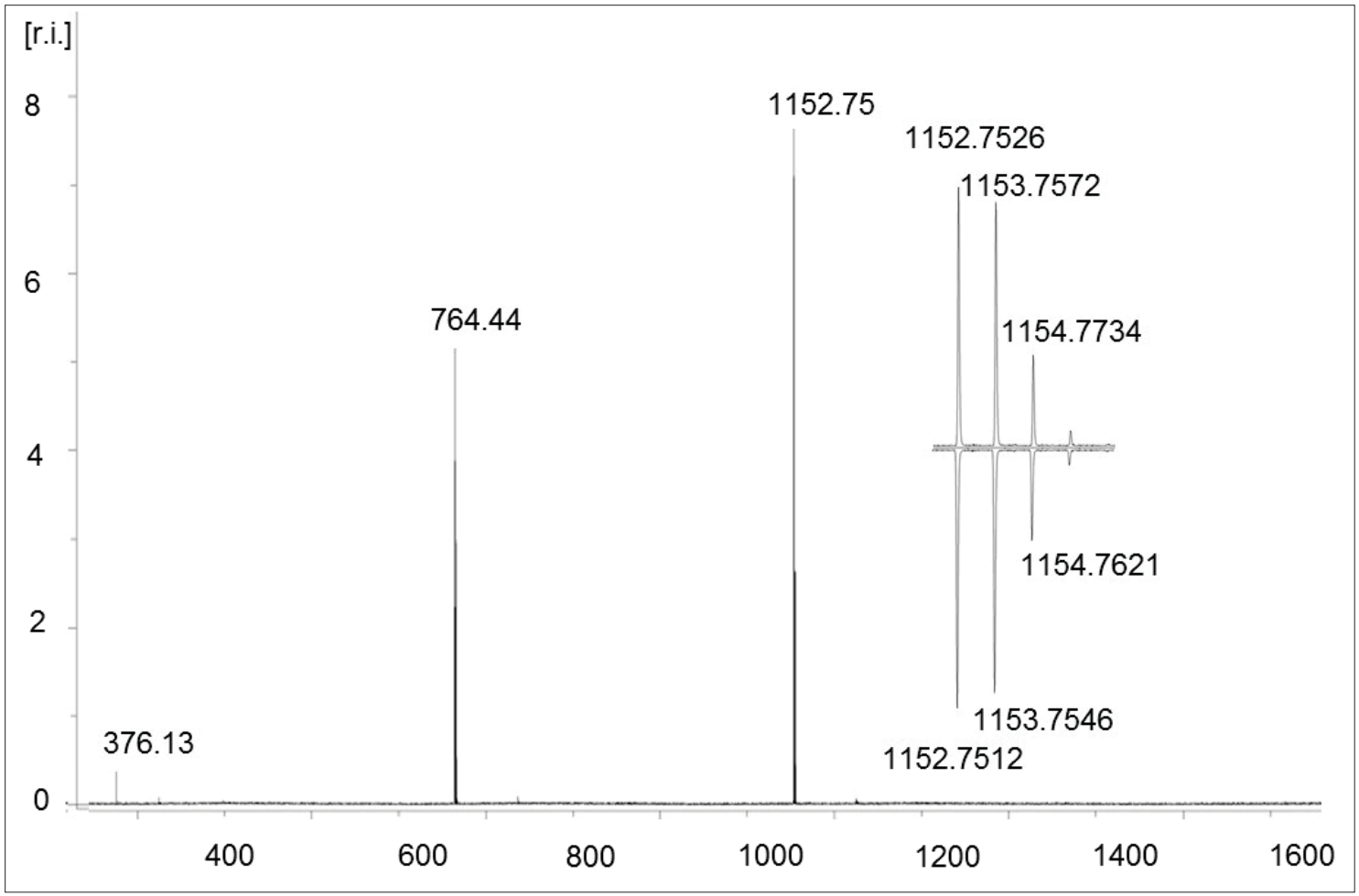


Figure S2. HR-MALDI spectrum of **9b**

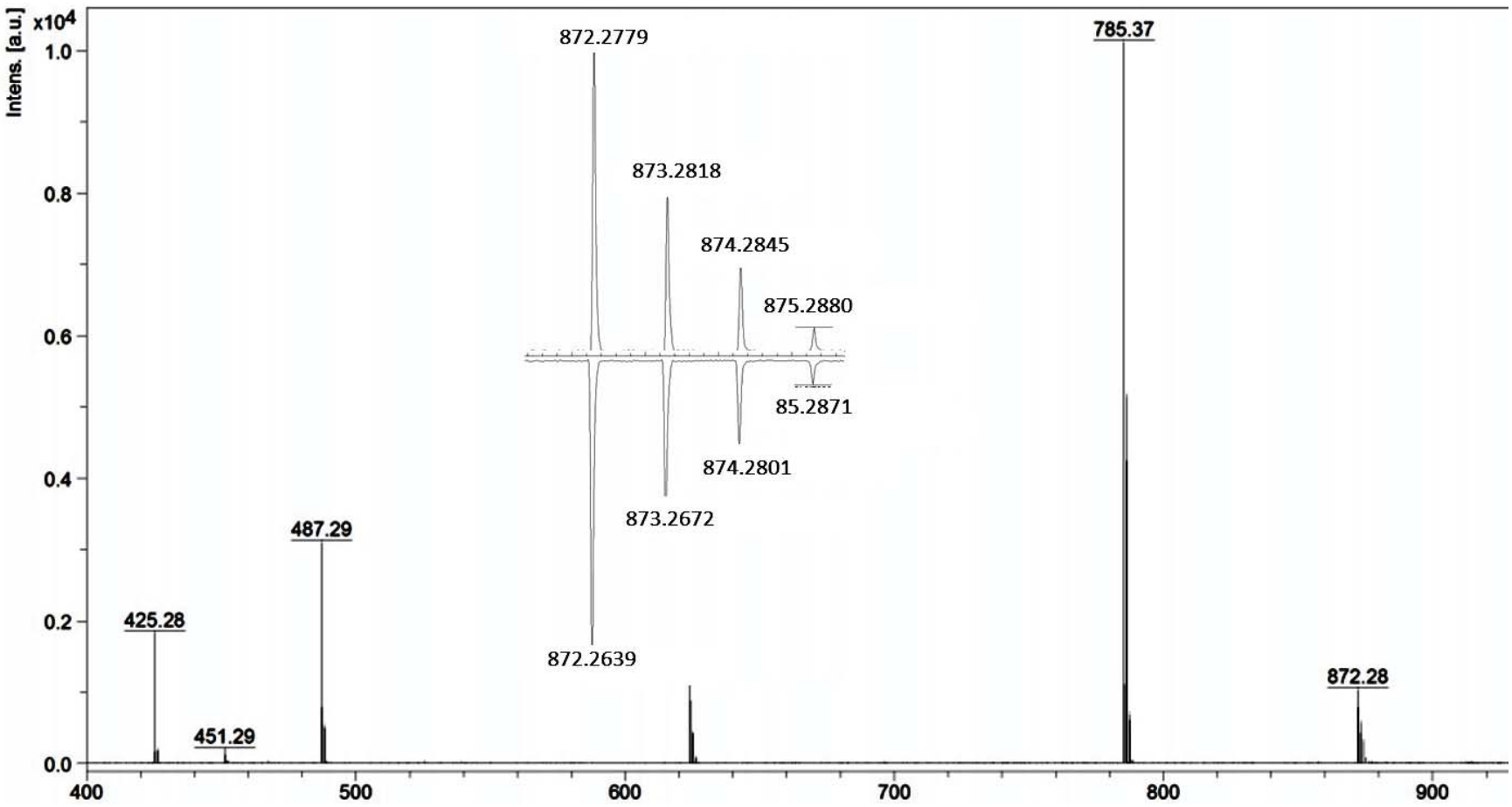


Figure S3. HR-MALDI spectrum of **9c**

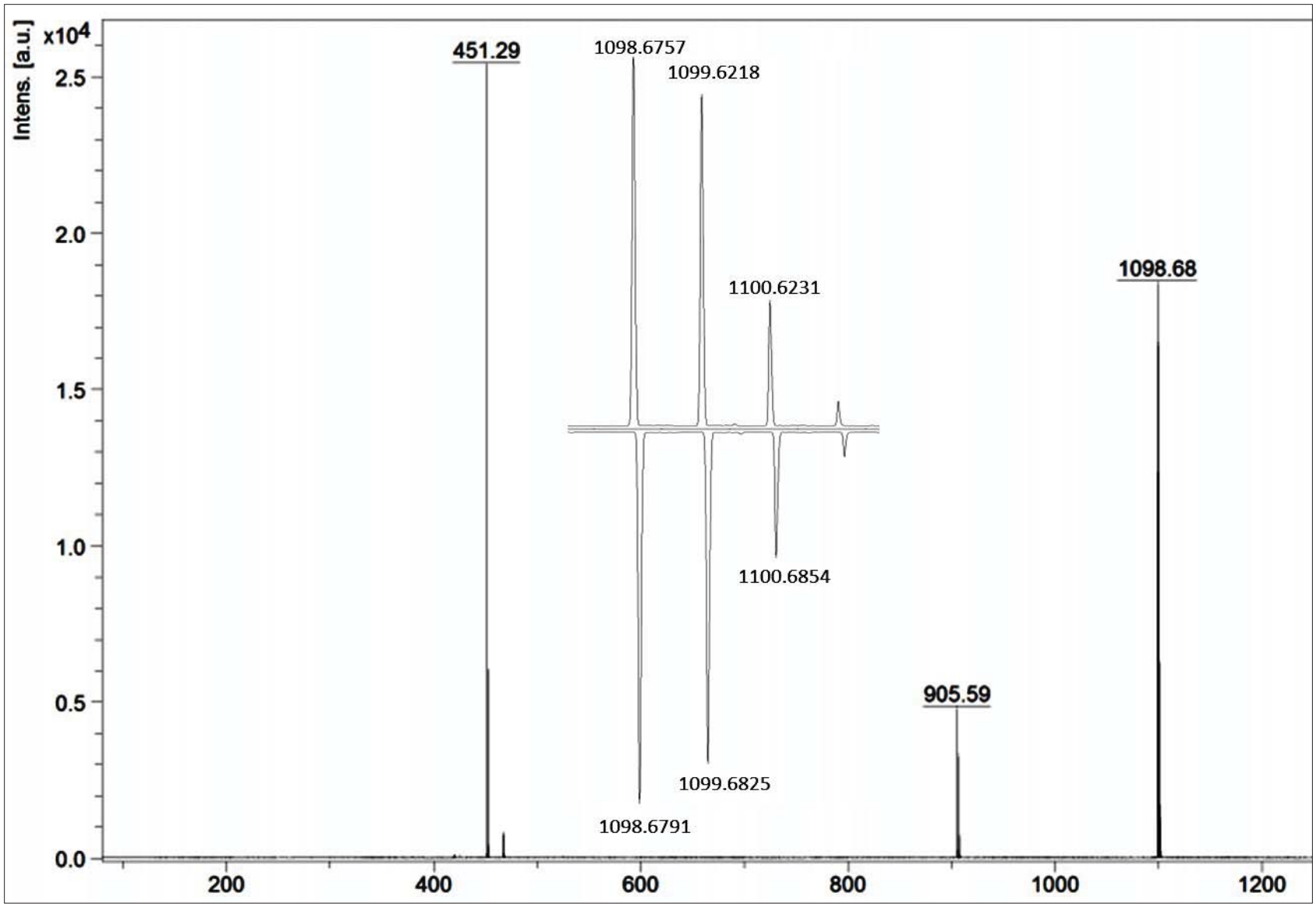


Figure S4. HR-MALDI spectrum of **10a**

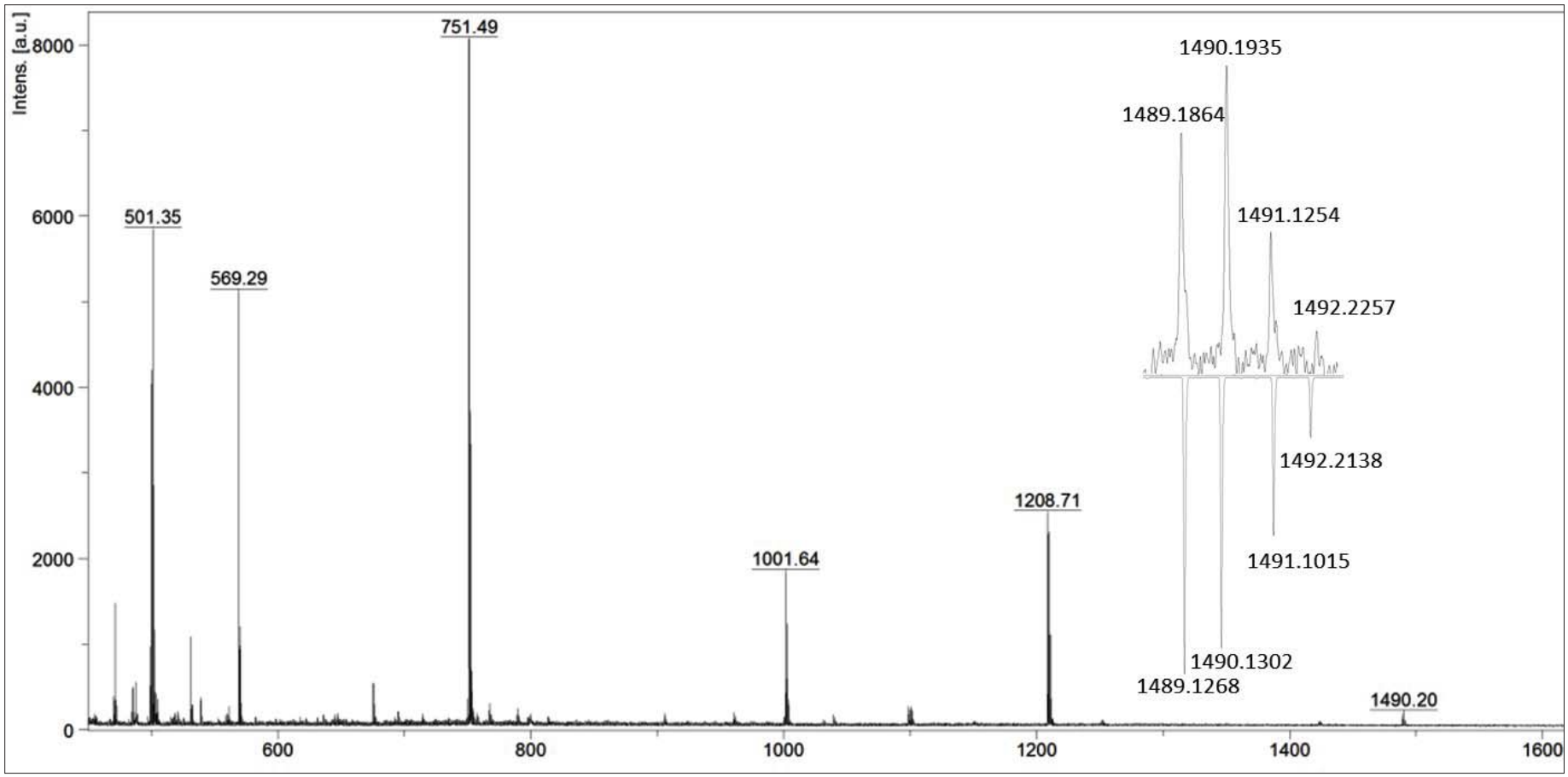


Figure S5. HR-MALDI spectrum of **10b**

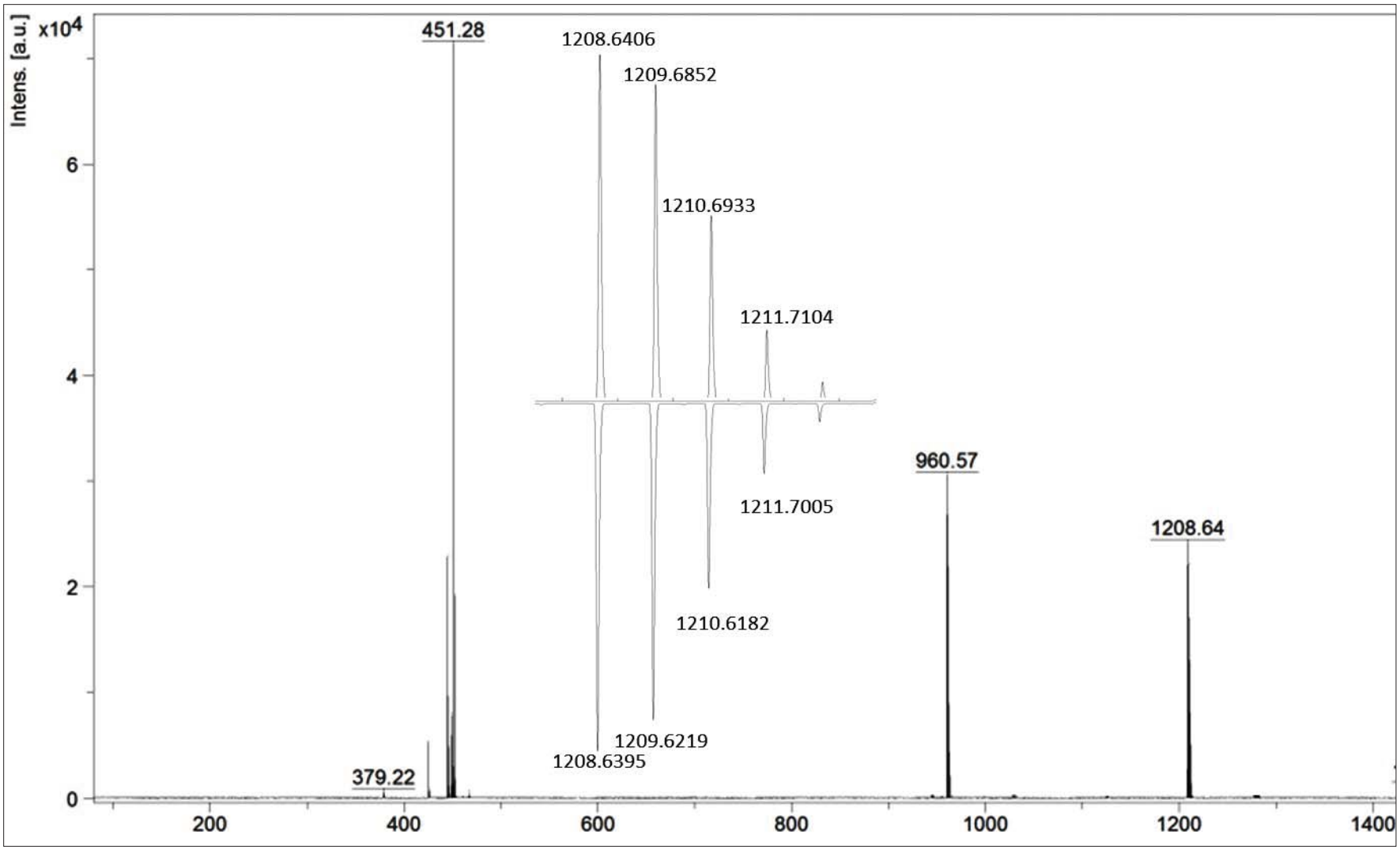


Figure S6. HR-MALDI spectrum of **10c**

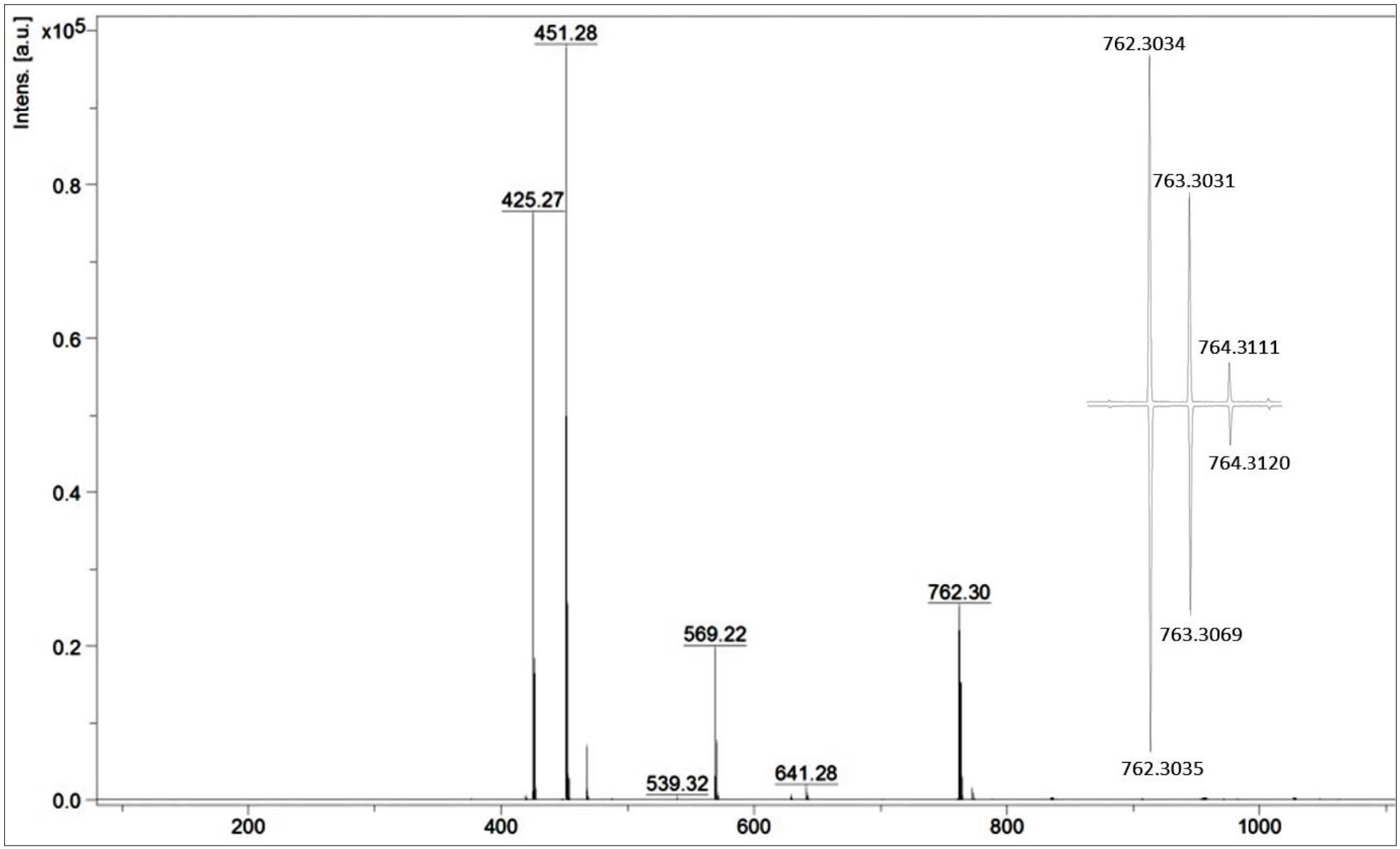


Figure S7. HR-MALDI spectrum of **11a**

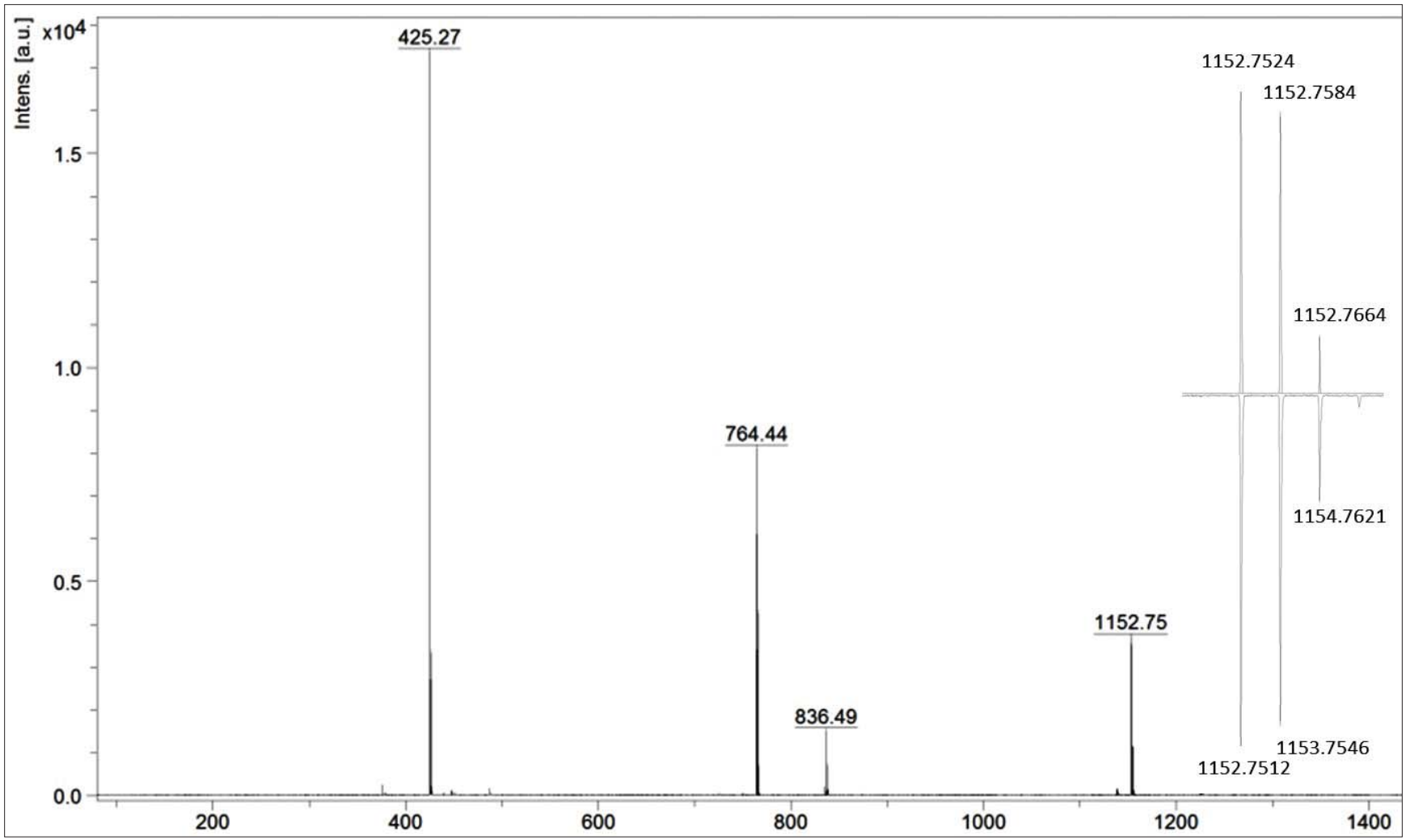


Figure S8. HR-MALDI spectrum of **11b**

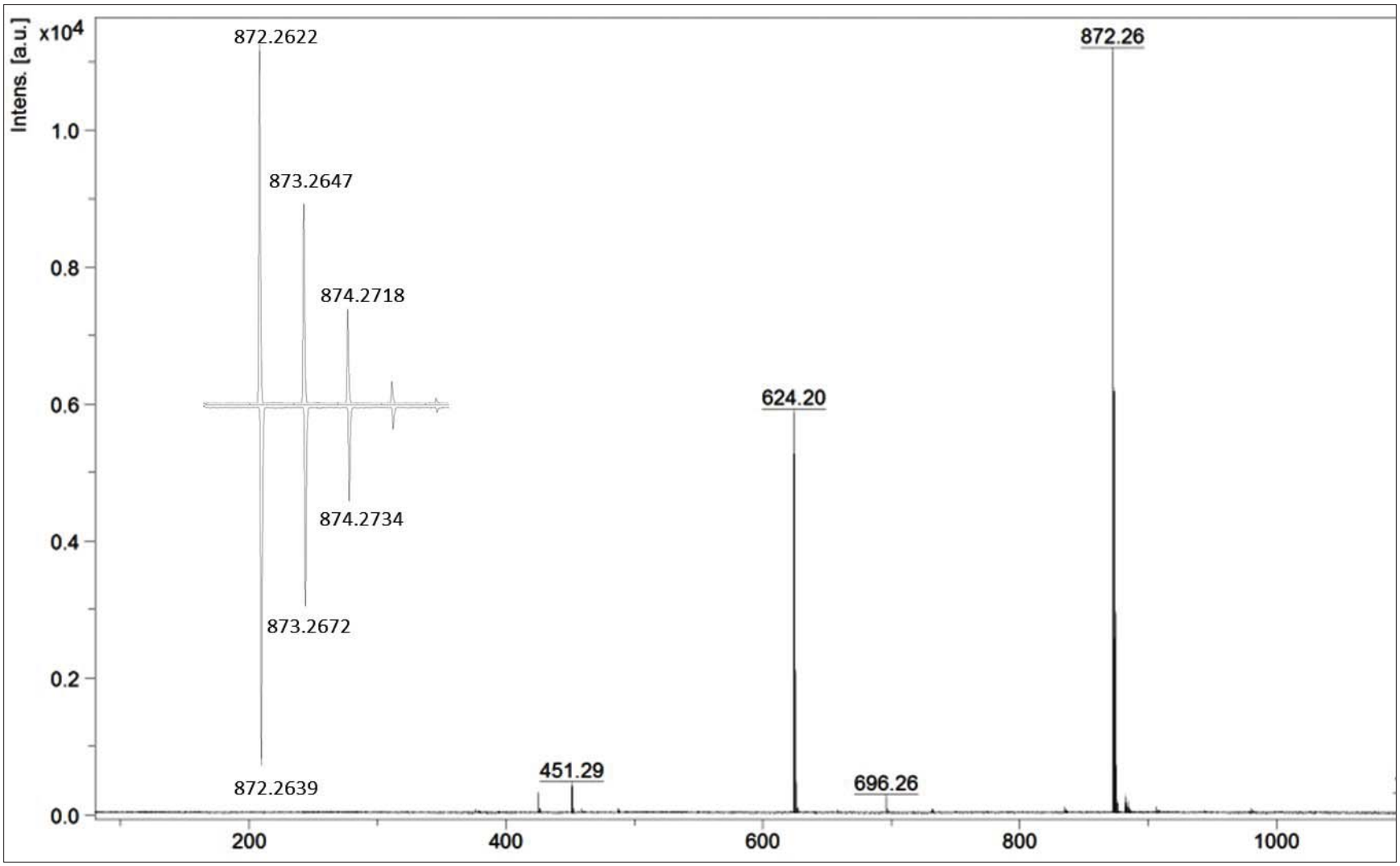


Figure S9. HR-MALDI spectrum of **11c**

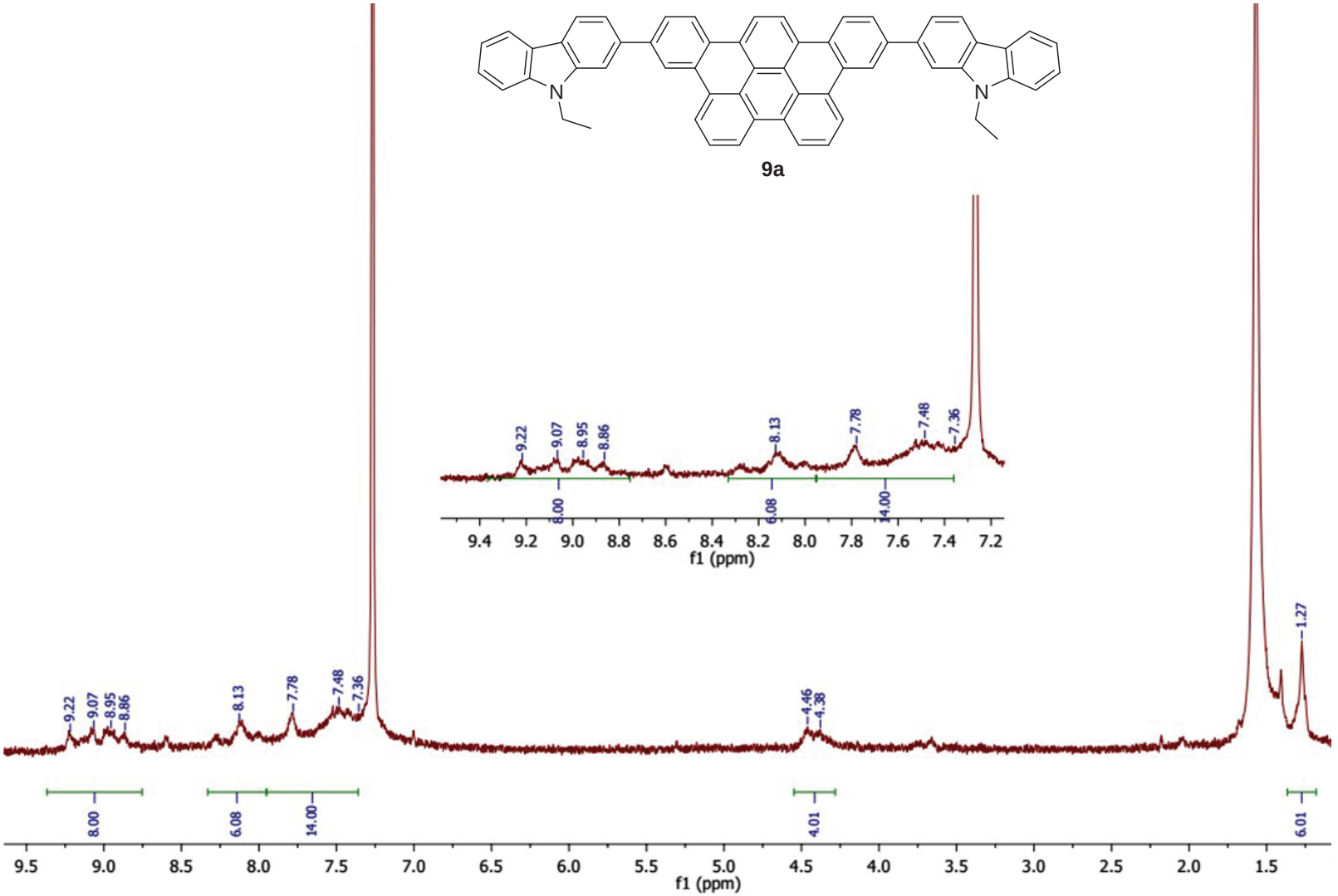


Figure S10. ^{1}H-NMR spectrum of **9a**

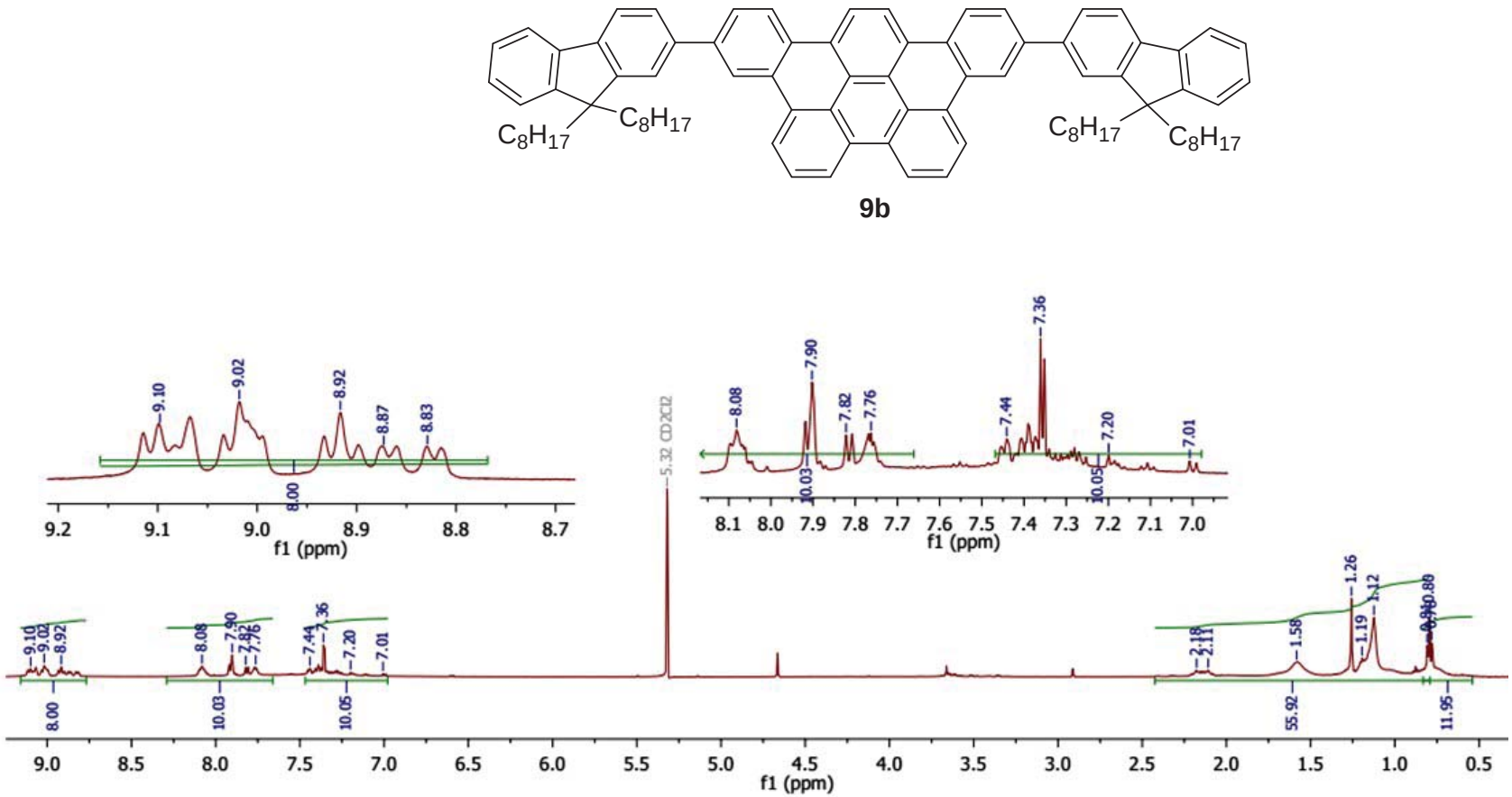


Figure S11. ^{1}H-NMR spectrum of **9b**

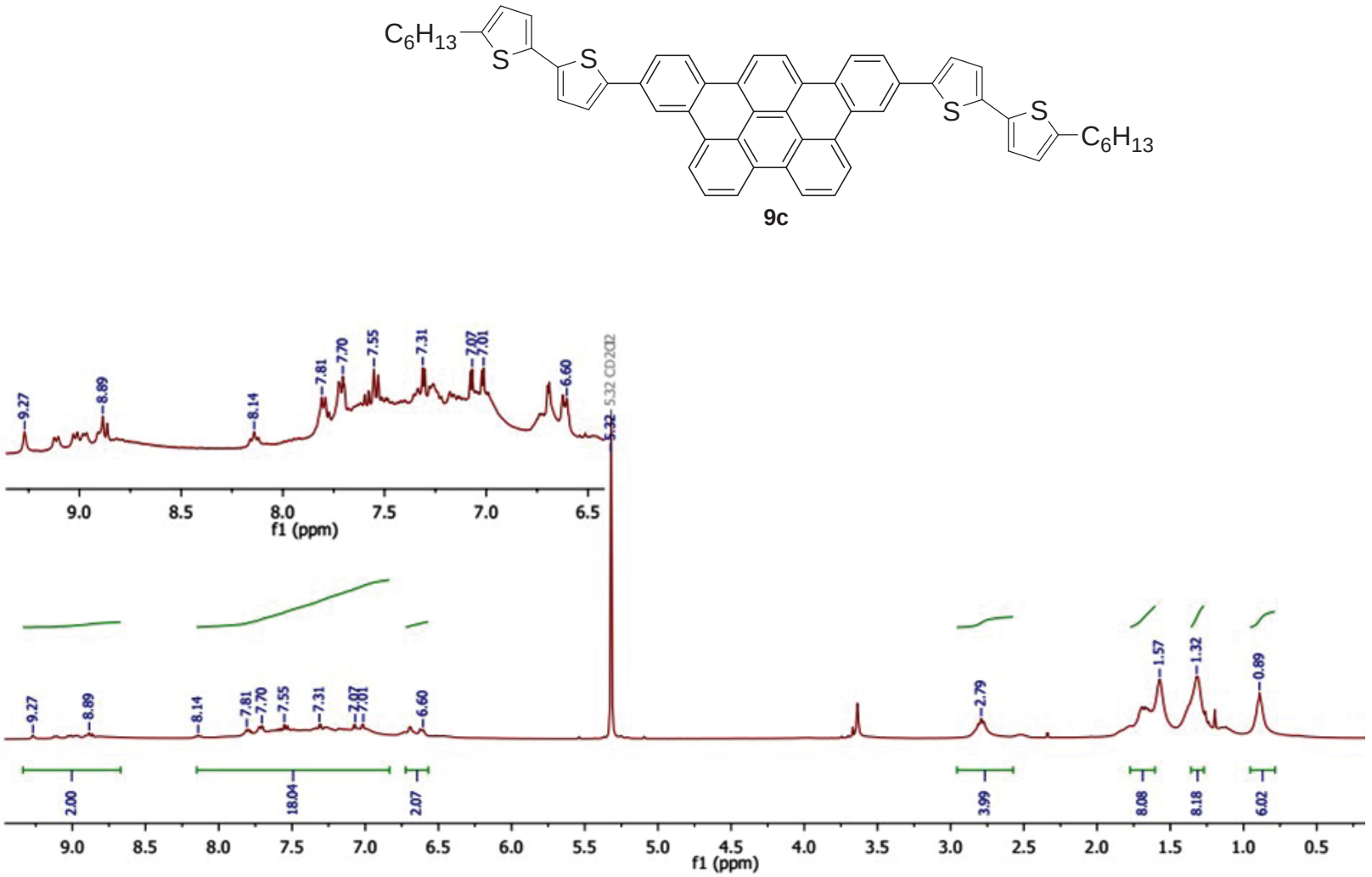
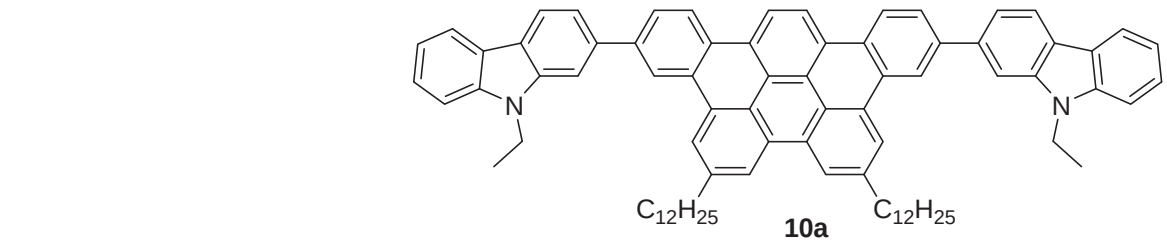


Figure S12. ^{1}H-NMR spectrum of **9c**



10a

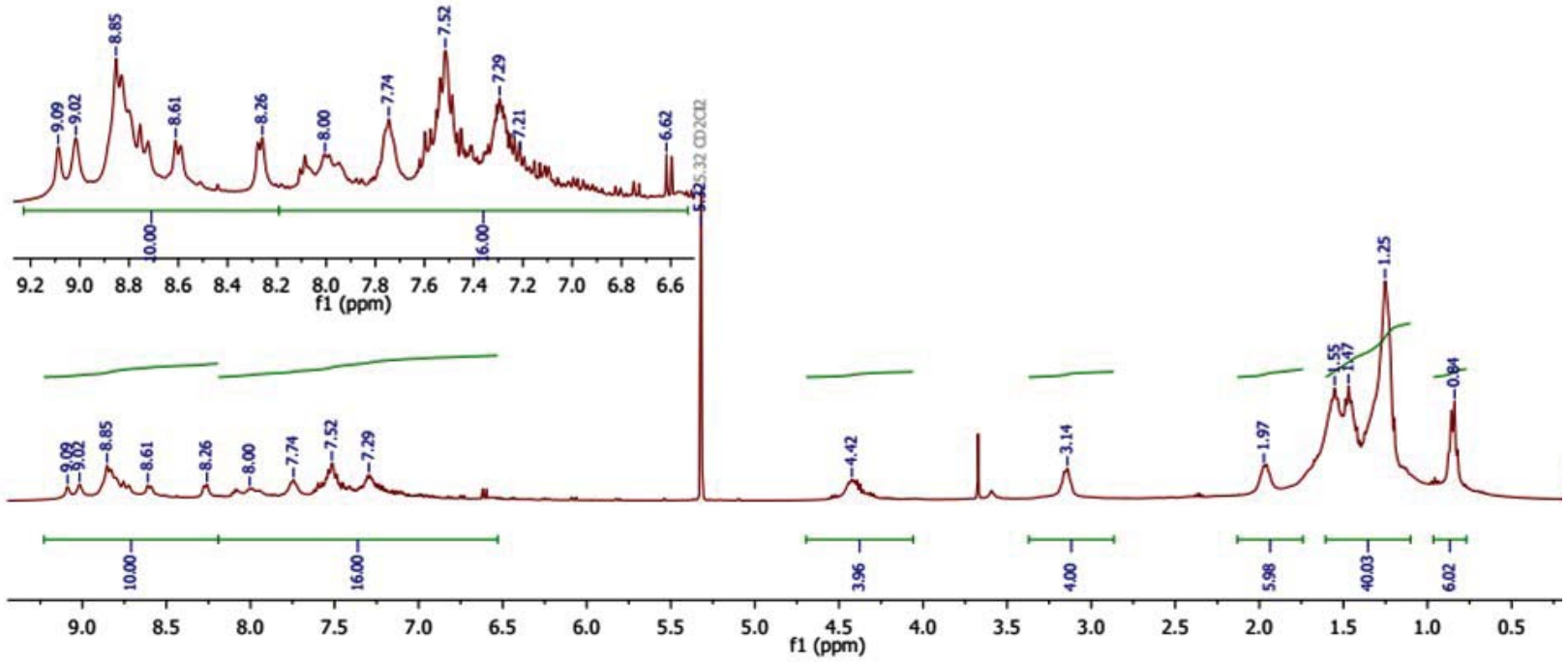


Figure S13. ^{1}H-NMR spectrum of **10a**

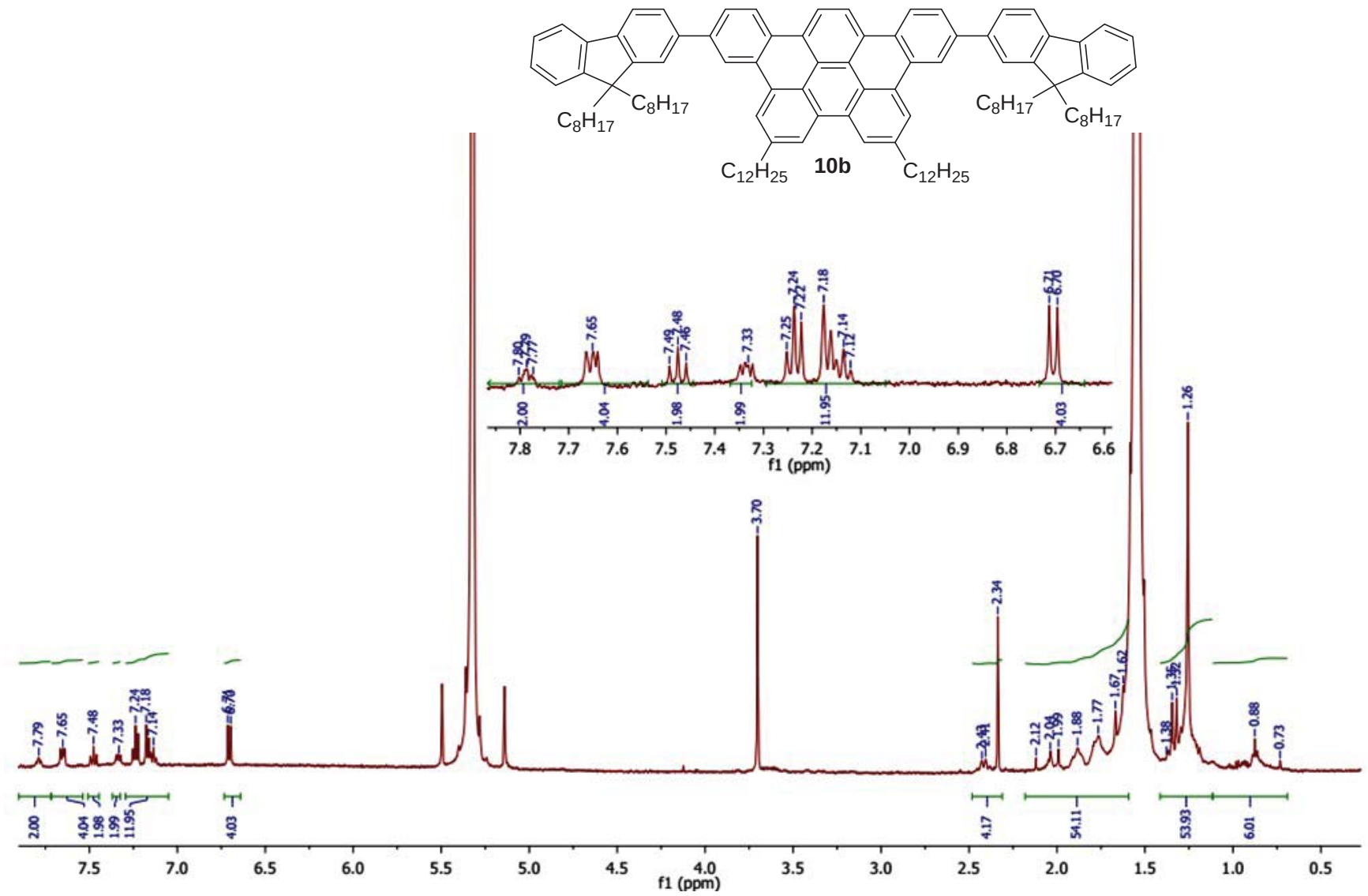


Figure S14. ^{1}H-NMR spectrum of **10b**

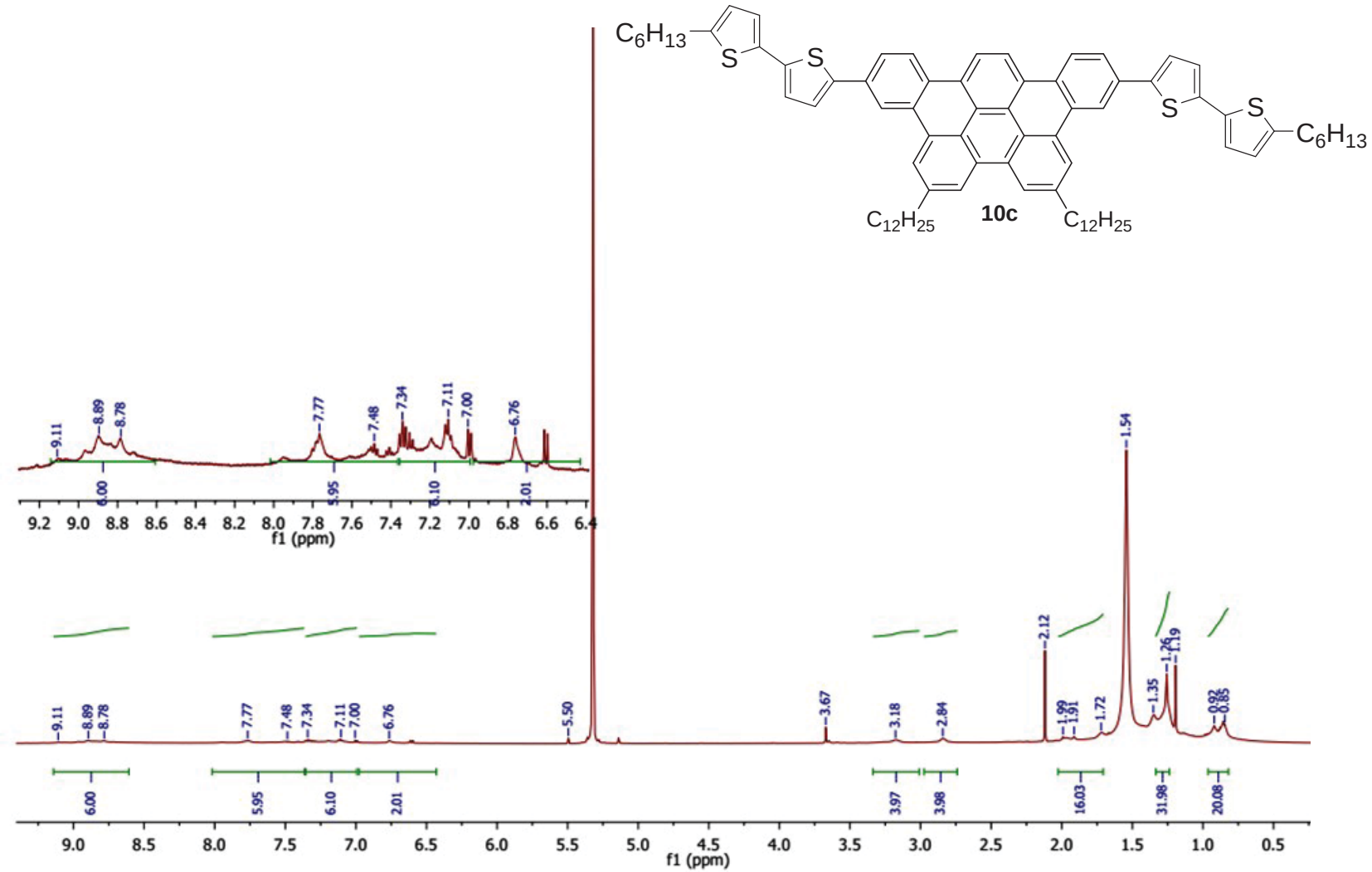


Figure S15. [1]H-NMR spectrum of **10c**

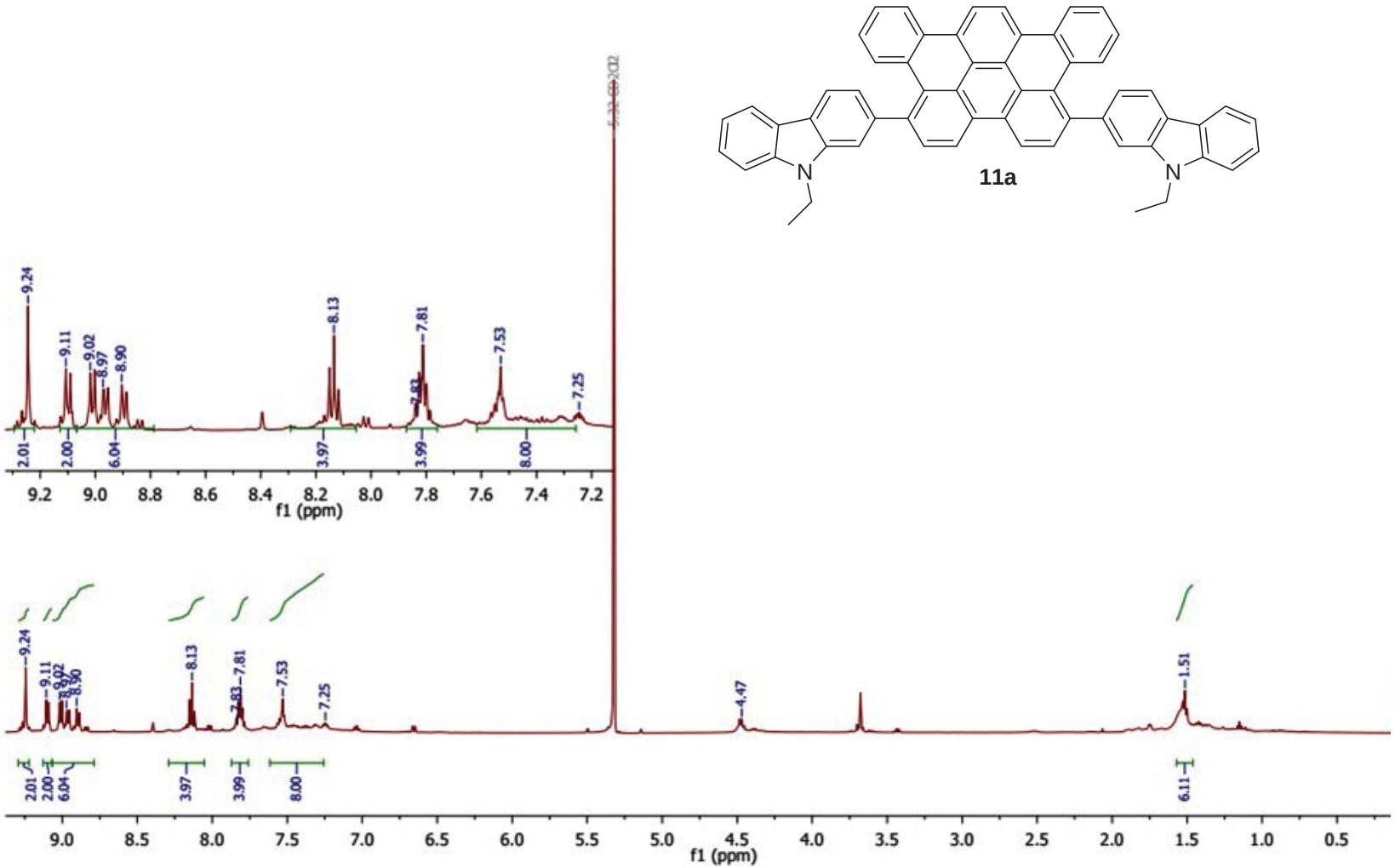


Figure S16. ^{1}H-NMR spectrum of **11**

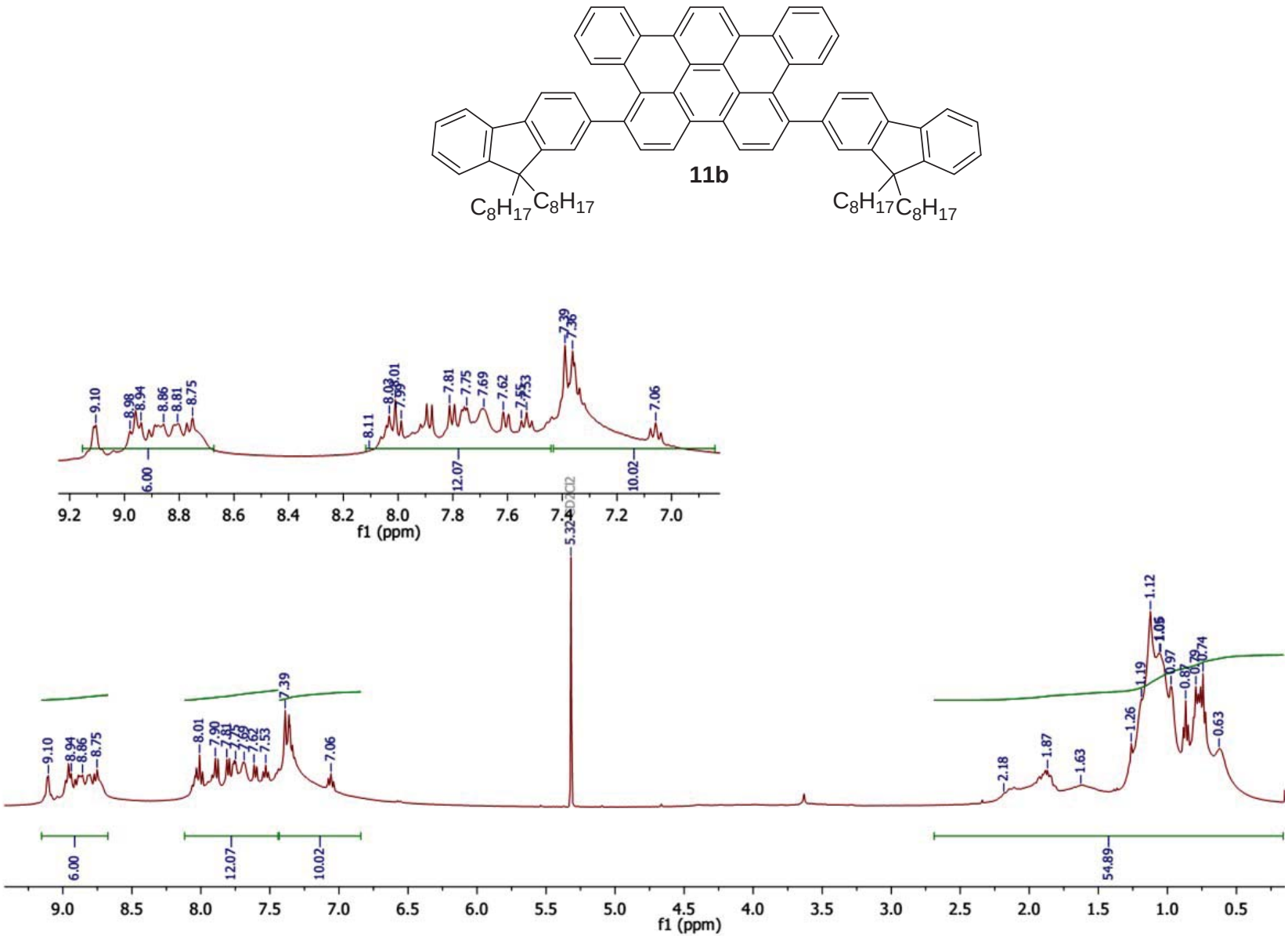


Figure S17. ^{1}H-NMR spectrum of **11b**

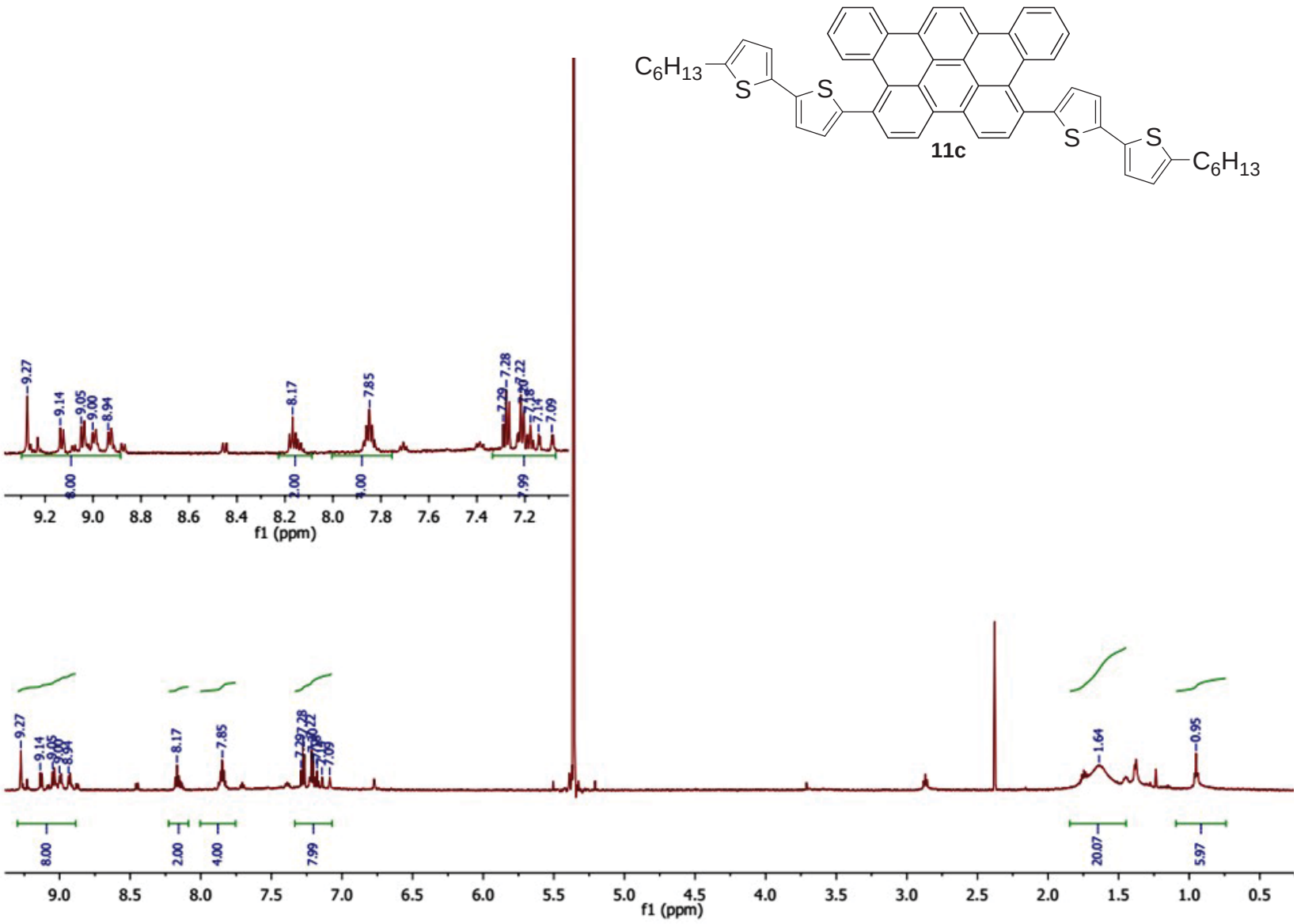


Figure S18. ^{1}H-NMR spectrum of **11c**

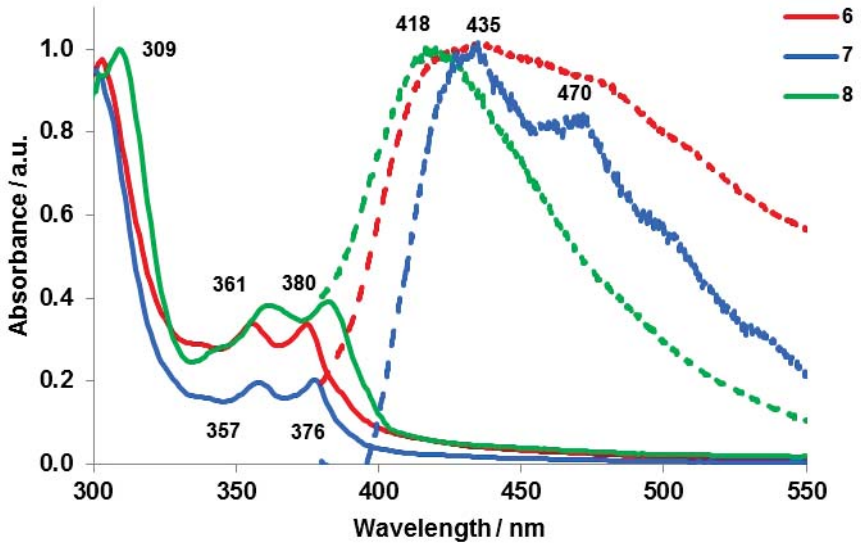
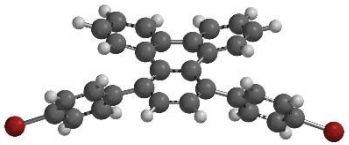
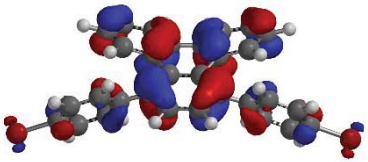
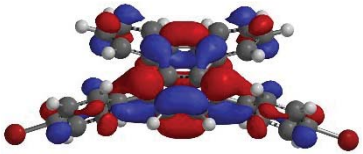
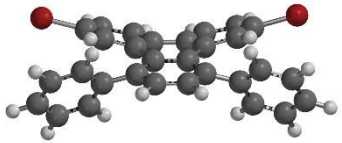
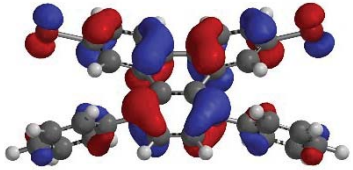
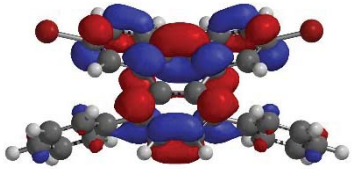
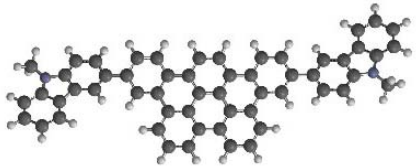
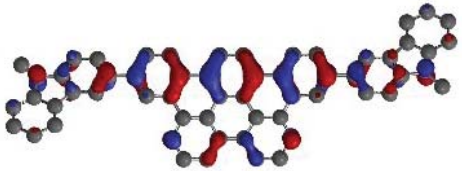
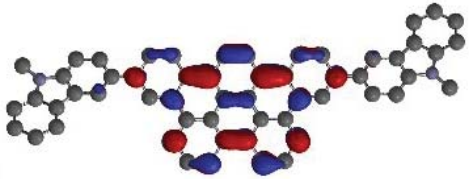
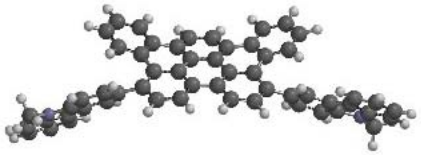
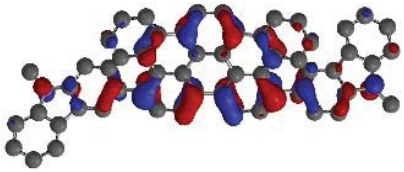
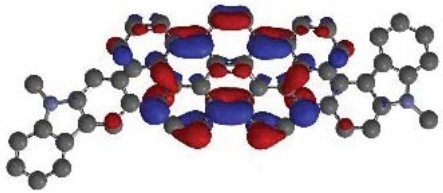
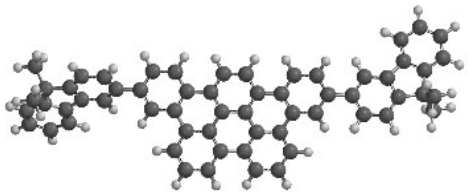
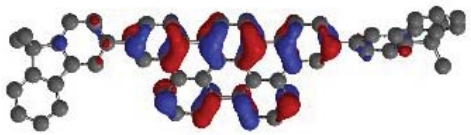
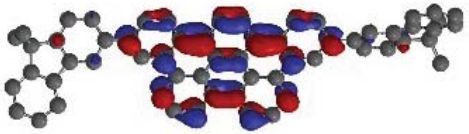
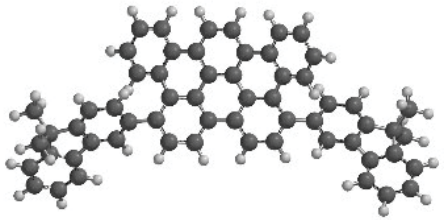
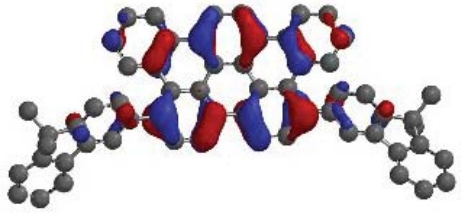
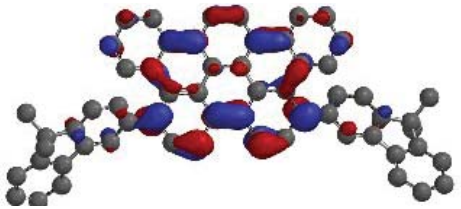
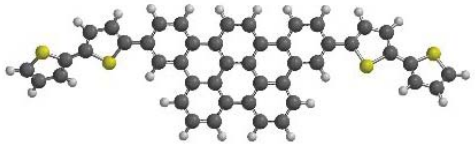
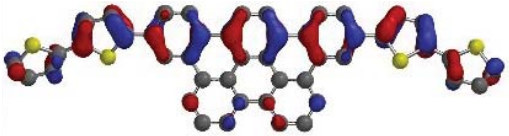
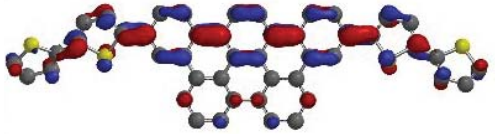
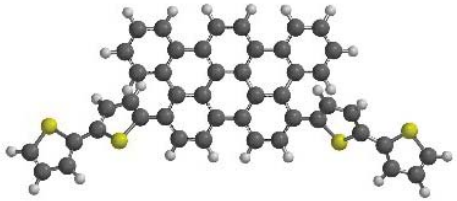
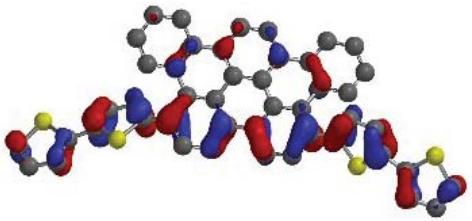
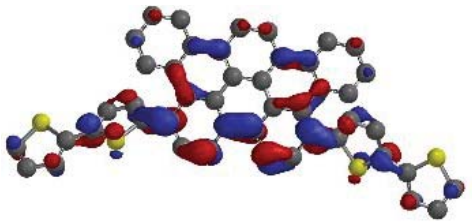


Figure S19. Normalized absorption and emission spectra for the pentaphene derivatives **6-8** in toluene. The solid lines represent absorption spectra and the dotted lines correspond to emission spectra.

II. Computational details

Table S1. Optimized structures and HOMO-LUMO frontier orbitals of **9-11** at the level of the B3LYP/6-31 G* basis set TBP derivatives (with R = H or Me instead of the alkyl groups for simplicity). The dihedral angle was measured between the TBP core and the lateral groups.

No	Optimized structure	HOMO	LUMO	Dihedral Angle
4a				-
4c				-
9a				38.65°
11a				34.98°

9b				38.7°
11b				36.9°
9c				24.43°
11c				34.77°

III. X-ray Crystallographic Data

Crystal data for **6**: CCDC: 1486177, $C_{30}H_{18}Br_2$, triclinic space group *P-1*, a = 6.9338(4) Å, b = 13.1529(7) Å, c = 13.7120(10) Å, α = 64.451(5)°, β = 83.600(6)°, γ = 79.575(6)°, V = 1108.84(12) Å^3, Z = 2, ρ_{calcd} = 1.612 mg·m^{-3}, μ = 3.672 mm^{-1}, F(000) = 536, R_1 = 0.0345, wR_2 = 0.102, 4158 independent reflections [2θ≤53°] and 290 parameters, goodness-of-fit 0.946.

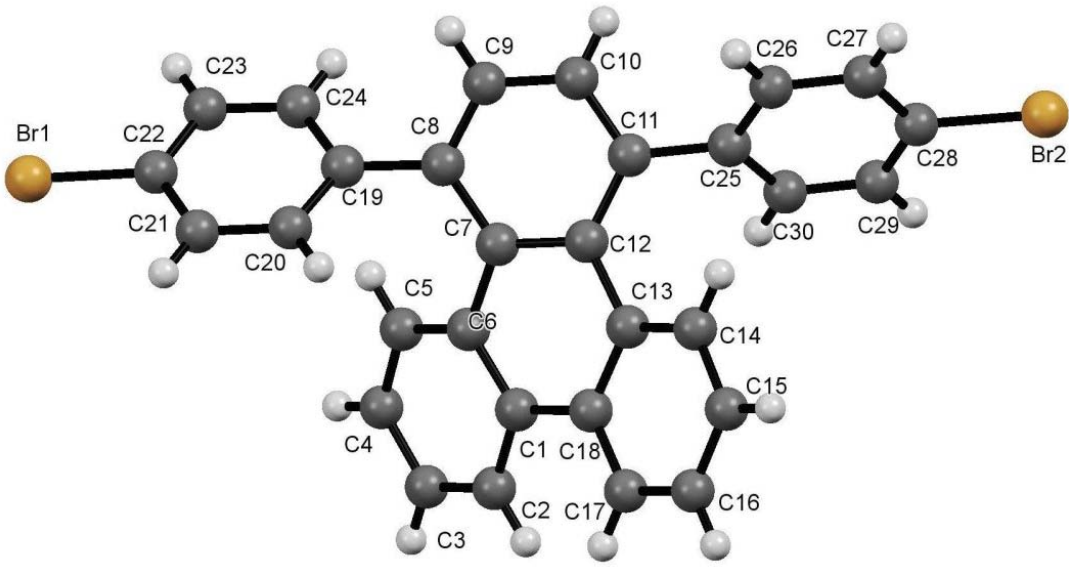


Figure S20. Crystallographically derived X-ray structure representations of **6**. Selected bond lengths (Å) and bond angles (º): Br2-C28 1.902(2), Br1-C22 1.900(3), C21-C22 1.375(4); C27-C28-Br2 119.95(18), C29-C28-Br2 118.95(19), C23-C22-Br1 119.5(2).

Table 1. Sample and crystal data for 6.

Identification code	Fakhriea_AA132_130915_RK
Chemical formula	$C_{30}H_{18}Br_2$
Formula weight	538.26
Temperature	298(2) K
Wavelength	0.71073 Å
Crystal size	0.150 x 0.200 x 0.200 mm
Crystal habit	yellow Block
Crystal system	triclinic

Space group	P -1	
Unit cell dimensions	a = 6.9338(4) Å	α = 64.451(5)°
	b = 13.1529(7) Å	β = 83.600(6)°
	c = 13.7120(10) Å	γ = 79.575(6)°
Volume	1108.84(12) $Å^3$	
Z	2	
Density (calculated)	1.612 g/cm^3	
Absorption coefficient	3.672 mm^{-1}	
F(000)	536	

Table 2. Data collection and structure refinement for 6.

Theta range for data collection	3.01 to 26.36°
Index ranges	-8<=h<=8, -16<=k<=16, -16<=l<=17
Reflections collected	9899
Independent reflections	4518 [R(int) = 0.0359]
Max. and min. transmission	0.6089 and 0.5271
Structure solution technique	direct methods
Structure solution program	SHELXS-97 (Sheldrick, 2008)
Refinement method	Full-matrix least-squares on F^2
Refinement program	SHELXL-97 (Sheldrick, 2008)
Function minimized	$\Sigma w(F_o^2 - F_c^2)^2$
Data / restraints / parameters	4518 / 0 / 290
Goodness-of-fit on F^2	0.946

Δ/σ_{max}	0.002
Final R indices	3519 data; I>2σ(I) R1 = 0.0345, wR2 = 0.0933
	all data R1 = 0.0475, wR2 = 0.1024
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0611P)^2+0.1344P]$ where $P=(F_o^2+2F_c^2)/3$
Extinction coefficient	0.0066(12)
Largest diff. peak and hole	0.421 and -0.456 eÅ^{-3}
R.M.S. deviation from mean	0.068 eÅ^{-3}

Table 3. Atomic coordinates and equivalent isotropic atomic displacement parameters (Å^2) for 6.

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)
Br2	0.22689(4)	0.94589(2)	0.59906(2)	0.05692(13)
Br1	0.37923(5)	0.35747(3)	0.10166(3)	0.07202(15)
C27	0.8426(4)	0.92450(19)	0.6961(2)	0.0462(6)
C26	0.6634(4)	0.96311(19)	0.7344(2)	0.0449(6)
C21	0.6039(4)	0.3266(2)	0.9275(2)	0.0537(7)
C29	0.9503(4)	0.1031(2)	0.6535(2)	0.0493(6)
C28	0.9834(4)	0.9950(2)	0.6557(2)	0.0421(6)
C25	0.6240(3)	0.07183(19)	0.7315(2)	0.0410(6)

	x/a	y/b	z/c	U(eq)
C12	0.3345(3)	0.22623(19)	0.7203(2)	0.0400(5)
C13	0.3510(3)	0.29274(19)	0.6025(2)	0.0389(5)
C18	0.2794(3)	0.41081(19)	0.5563(2)	0.0448(6)
C11	0.4367(3)	0.11392(19)	0.7753(2)	0.0423(6)
C10	0.3700(4)	0.0467(2)	0.8777(2)	0.0544(7)
C9	0.2085(4)	0.0865(2)	0.9270(2)	0.0569(7)
C8	0.1210(4)	0.1988(2)	0.8817(2)	0.0470(6)
C19	0.9412(4)	0.2353(2)	0.9357(2)	0.0474(6)
C20	0.7717(4)	0.2913(2)	0.8791(2)	0.0502(6)
C22	0.6051(4)	0.3045(2)	0.0350(2)	0.0485(6)
C30	0.7726(4)	0.1400(2)	0.6901(2)	0.0483(6)
C14	0.4108(4)	0.2395(2)	0.5319(2)	0.0449(6)
C15	0.4051(4)	0.2997(2)	0.4212(2)	0.0530(7)
C16	0.3422(4)	0.4160(3)	0.3763(2)	0.0607(8)
C17	0.2793(4)	0.4697(2)	0.4431(2)	0.0577(8)
C1	0.2039(3)	0.4657(2)	0.6277(2)	0.0470(6)
C2	0.1817(4)	0.5851(2)	0.5897(3)	0.0663(9)
C5	0.0982(4)	0.4544(3)	0.8056(3)	0.0575(7)
C6	0.1575(3)	0.3993(2)	0.7369(2)	0.0461(6)
C7	0.1985(3)	0.2733(2)	0.7798(2)	0.0418(6)
C23	0.7690(4)	0.2466(3)	0.0946(2)	0.0602(8)
C24	0.9354(4)	0.2121(3)	0.0444(2)	0.0604(8)
C4	0.0793(4)	0.5719(3)	0.7659(4)	0.0748(11)

	x/a	y/b	z/c	U(eq)
C3	0.1173(5)	0.6367(3)	0.6580(4)	0.0796(12)

Table 4. Bond lengths (Å) for 6.

Br2-C28	1.902(2)	Br1-C22	1.900(3)
C27-C28	1.373(4)	C27-C26	1.391(3)
C27-H27	0.93	C26-C25	1.390(3)
C26-H26	0.93	C21-C22	1.375(4)
C21-C20	1.381(4)	C21-H21	0.93
C29-C30	1.364(4)	C29-C28	1.386(3)
C29-H29	0.93	C25-C30	1.397(4)
C25-C11	1.485(3)	C12-C7	1.411(3)
C12-C11	1.426(3)	C12-C13	1.472(3)
C13-C14	1.409(4)	C13-C18	1.415(3)
C18-C17	1.405(4)	C18-C1	1.453(4)
C11-C10	1.378(4)	C10-C9	1.382(4)
C10-H10	0.93	C9-C8	1.380(4)
C9-H9	0.93	C8-C7	1.429(4)
C8-C19	1.490(4)	C19-C20	1.387(4)
C19-C24	1.383(4)	C20-H20	0.93
C22-C23	1.377(4)	C30-H30	0.93
C14-C15	1.378(4)	C14-H14	0.93

C15-C16	1.384(4)	C15-H15	0.93
C16-C17	1.374(5)	C16-H16	0.93
C17-H17	0.93	C1-C6	1.405(4)
C1-C2	1.409(3)	C2-C3	1.372(5)
C2-H2	0.93	C5-C4	1.386(4)
C5-C6	1.406(4)	C5-H5	0.93
C6-C7	1.482(3)	C23-C24	1.383(4)
C23-H23	0.93	C24-H24	0.93
C4-C3	1.376(5)	C4-H4	0.93
C3-H3	0.93		

Table 5. Bond angles (°) for 6.

C28-C27-C26	119.1(2)	C28-C27-H27	120.4
C26-C27-H27	120.4	C25-C26-C27	121.2(2)
C25-C26-H26	119.4	C27-C26-H26	119.4
C22-C21-C20	118.9(3)	C22-C21-H21	120.6
C20-C21-H21	120.6	C30-C29-C28	118.9(2)
C30-C29-H29	120.6	C28-C29-H29	120.6
C27-C28-C29	121.1(2)	C27-C28-Br2	119.95(18)
C29-C28-Br2	118.95(19)	C26-C25-C30	117.4(2)
C26-C25-C11	122.4(2)	C30-C25-C11	120.1(2)
C7-C12-C11	118.8(2)	C7-C12-C13	117.7(2)
C11-C12-C13	123.3(2)	C14-C13-C18	117.9(2)

C14-C13-C12	121.6(2)	C18-C13-C12	119.9(2)
C17-C18-C13	118.6(3)	C17-C18-C1	122.6(2)
C13-C18-C1	118.8(2)	C10-C11-C12	118.5(2)
C10-C11-C25	118.9(2)	C12-C11-C25	122.3(2)
C9-C10-C11	121.3(2)	C9-C10-H10	119.4
C11-C10-H10	119.4	C8-C9-C10	121.5(3)
C8-C9-H9	119.2	C10-C9-H9	119.2
C9-C8-C7	118.2(2)	C9-C8-C19	119.1(2)
C7-C8-C19	122.6(2)	C20-C19-C24	117.6(2)
C20-C19-C8	120.9(2)	C24-C19-C8	121.4(2)
C21-C20-C19	121.9(3)	C21-C20-H20	119.1
C19-C20-H20	119.1	C21-C22-C23	121.0(2)
C21-C22-Br1	119.6(2)	C23-C22-Br1	119.5(2)
C29-C30-C25	122.3(2)	C29-C30-H30	118.9
C25-C30-H30	118.9	C15-C14-C13	121.8(2)
C15-C14-H14	119.1	C13-C14-H14	119.1
C14-C15-C16	120.1(3)	C14-C15-H15	120.0
C16-C15-H15	120.0	C17-C16-C15	119.4(3)
C17-C16-H16	120.3	C15-C16-H16	120.3
C16-C17-C18	122.2(3)	C16-C17-H17	118.9
C18-C17-H17	118.9	C6-C1-C2	119.2(3)
C6-C1-C18	119.9(2)	C2-C1-C18	120.9(3)
C3-C2-C1	120.9(3)	C3-C2-H2	119.5
C1-C2-H2	119.5	C4-C5-C6	120.8(3)

C4-C5-H5	119.6	C6-C5-H5	119.6
C5-C6-C1	118.5(2)	C5-C6-C7	121.5(3)
C1-C6-C7	119.4(2)	C12-C7-C8	119.0(2)
C12-C7-C6	117.4(2)	C8-C7-C6	123.4(2)
C24-C23-C22	119.1(3)	C24-C23-H23	120.4
C22-C23-H23	120.4	C23-C24-C19	121.5(3)
C23-C24-H24	119.2	C19-C24-H24	119.2
C3-C4-C5	120.2(3)	C3-C4-H4	119.9
C5-C4-H4	119.9	C4-C3-C2	120.2(3)
C4-C3-H3	119.9	C2-C3-H3	119.9

Table 6. Torsion angles (°) for 6.

C28-C27-C26-C25	0.7(4)	C26-C27-C28-C29	0.6(4)
C26-C27-C28-Br2	-178.2(2)	C30-C29-C28-C27	-1.4(4)
C30-C29-C28-Br2	177.4(2)	C27-C26-C25-C30	-1.0(4)
C27-C26-C25-C11	-177.8(2)	C7-C12-C13-C14	-152.3(2)
C11-C12-C13-C14	22.5(4)	C7-C12-C13-C18	18.4(3)
C11-C12-C13-C18	-166.7(2)	C14-C13-C18-C17	-2.6(3)
C12-C13-C18-C17	-173.7(2)	C14-C13-C18-C1	175.6(2)
C12-C13-C18-C1	4.6(3)	C7-C12-C11-C10	13.8(4)
C13-C12-C11-C10	-161.0(3)	C7-C12-C11-C25	-159.3(2)
C13-C12-C11-C25	25.9(4)	C26-C25-C11-C10	49.1(4)
C30-C25-C11-C10	-127.6(3)	C26-C25-C11-C12	-137.8(3)

C30-C25-C11-C12	45.5(4)	C12-C11-C10-C9	-0.3(4)
C25-C11-C10-C9	173.0(3)	C11-C10-C9-C8	-7.6(5)
C10-C9-C8-C7	1.8(5)	C10-C9-C8-C19	176.9(3)
C9-C8-C19-C20	-126.5(3)	C7-C8-C19-C20	48.4(4)
C9-C8-C19-C24	51.9(4)	C7-C8-C19-C24	-133.3(3)
C22-C21-C20-C19	-0.5(4)	C24-C19-C20-C21	2.1(4)
C8-C19-C20-C21	-179.6(3)	C20-C21-C22-C23	-1.1(4)
C20-C21-C22-Br1	177.5(2)	C28-C29-C30-C25	1.1(4)
C26-C25-C30-C29	0.1(4)	C11-C25-C30-C29	177.0(3)
C18-C13-C14-C15	1.5(4)	C12-C13-C14-C15	172.4(2)
C13-C14-C15-C16	1.0(4)	C14-C15-C16-C17	-2.3(4)
C15-C16-C17-C18	1.0(5)	C13-C18-C17-C16	1.5(4)
C1-C18-C17-C16	-176.8(3)	C17-C18-C1-C6	162.5(2)
C13-C18-C1-C6	-15.7(4)	C17-C18-C1-C2	-19.3(4)
C13-C18-C1-C2	162.4(2)	C6-C1-C2-C3	0.6(5)
C18-C1-C2-C3	-177.6(3)	C4-C5-C6-C1	2.2(4)
C4-C5-C6-C7	173.5(3)	C2-C1-C6-C5	-2.7(4)
C18-C1-C6-C5	175.5(2)	C2-C1-C6-C7	-174.2(2)
C18-C1-C6-C7	4.0(4)	C11-C12-C7-C8	-19.5(4)
C13-C12-C7-C8	155.6(2)	C11-C12-C7-C6	155.2(2)
C13-C12-C7-C6	-29.8(3)	C9-C8-C7-C12	11.7(4)
C19-C8-C7-C12	-163.2(3)	C9-C8-C7-C6	-162.6(3)
C19-C8-C7-C6	22.5(4)	C5-C6-C7-C12	-152.2(2)
C1-C6-C7-C12	19.0(3)	C5-C6-C7-C8	22.2(4)

C1-C6-C7-C8	-166.6(3)	C21-C22-C23-C24	1.1(5)
Br1-C22-C23-C24	-177.5(2)	C22-C23-C24-C19	0.5(5)
C20-C19-C24-C23	-2.1(5)	C8-C19-C24-C23	179.6(3)
C6-C5-C4-C3	0.5(5)	C5-C4-C3-C2	-2.6(5)
C1-C2-C3-C4	2.1(5)		

Table 7. Anisotropic atomic displacement parameters (Å^2) for 6.

The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Br2	0.04451(18)	0.0611(2)	0.0655(2)	-0.03237(15)	0.00333(14)	0.00306(13)
Br1	0.0665(2)	0.0684(2)	0.0758(3)	-0.03421(18)	0.02905(18)	-0.00611(16)
C27	0.0466(14)	0.0320(11)	0.0568(16)	-0.0174(11)	-0.0061(12)	0.0009(10)
C26	0.0412(13)	0.0341(11)	0.0543(15)	-0.0143(11)	-0.0024(11)	-0.0042(10)
C21	0.0430(14)	0.0617(16)	0.0532(17)	-0.0242(13)	-0.0006(12)	-0.0006(12)
C29	0.0419(13)	0.0457(13)	0.0641(18)	-0.0258(12)	-0.0017(13)	-0.0089(11)
C28	0.0381(12)	0.0423(12)	0.0430(14)	-0.0183(10)	-0.0071(11)	0.0055(10)
C25	0.0362(12)	0.0381(12	0.0465(14	-0.0171(10)	-0.0068(11)	0.0010(10)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
		)	)			
C12	0.0330(11)	0.0383(12)	0.0501(15)	-0.0203(10)	-0.0010(10)	-0.0043(10)
C13	0.0280(11)	0.0398(12)	0.0482(14)	-0.0182(10)	0.0016(10)	-0.0056(9)
C18	0.0322(11)	0.0379(12)	0.0579(16)	-0.0155(11)	0.0041(11)	-0.0052(10)
C11	0.0370(12)	0.0394(12)	0.0499(15)	-0.0198(11)	-0.0024(11)	-0.0013(10)
C10	0.0503(15)	0.0431(13)	0.0547(17)	-0.0111(12)	-0.0035(13)	0.0059(12)
C9	0.0528(15)	0.0555(15)	0.0467(16)	-0.0115(12)	0.0033(13)	0.0006(13)
C8	0.0405(13)	0.0553(15)	0.0455(15)	-0.0237(12)	-0.0032(11)	-0.0002(11)
C19	0.0431(13)	0.0548(14)	0.0449(15)	-0.0232(12)	0.0018(11)	-0.0052(11)
C20	0.0441(14)	0.0651(16)	0.0432(14)	-0.0265(12)	-0.0015(12)	-0.0027(12)
C22	0.0465(14)	0.0460(13)	0.0520(16)	-0.0229(12)	0.0135(12)	-0.0080(11)
C30	0.0419(13)	0.0405(12)	0.0696(18)	-0.0310(12)	-0.0028(13)	-0.0025(11)
C14	0.0376(12)	0.0421(12)	0.0514(15)	-0.0185(11)	0.0011(11)	-0.0019(10)
C15	0.0453(14)	0.0616(16)	0.0469(15)	-0.0217(13)	0.0009(12)	0.0002(12)
C16	0.0513(16)	0.0658(18)	0.0463(16)	-0.0098(14)	0.0023(13)	-0.0016(14)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C17	0.0488(15)	0.0419(13)	0.0609(18)	-0.0049(13)	0.0024(14)	-0.0009(12)
C1	0.0309(11)	0.0388(12)	0.0701(18)	-0.0239(12)	0.0058(12)	-0.0044(10)
C2	0.0508(16)	0.0406(13)	0.101(3)	-0.0282(15)	0.0196(16)	-0.0090(12)
C5	0.0432(14)	0.0648(17)	0.081(2)	-0.0472(16)	0.0076(14)	-0.0098(13)
C6	0.0298(11)	0.0475(13)	0.0681(18)	-0.0322(13)	-0.0002(11)	-0.0030(10)
C7	0.0339(11)	0.0433(12)	0.0491(15)	-0.0219(11)	-0.0036(11)	-0.0006(10)
C23	0.0618(17)	0.0739(18)	0.0421(15)	-0.0249(14)	0.0061(13)	-0.0071(15)
C24	0.0502(15)	0.080(2)	0.0441(16)	-0.0244(14)	-0.0051(13)	0.0031(14)
C4	0.0504(17)	0.0698(19)	0.132(3)	-0.072(2)	0.021(2)	-0.0135(15)
C3	0.0585(19)	0.0492(15)	0.137(4)	-0.051(2)	0.034(2)	-0.0161(14)

Table 8. Hydrogen atomic coordinates and isotropic atomic displacement parameters ($Å^2$) for 6.

	x/a	y/b	z/c	U(eq)
H27	0.8667	-0.1481	0.6978	0.055

	x/a	y/b	z/c	U(eq)
H26	0.5682	-0.0847	0.7626	0.054
H21	-0.5080	0.3646	0.8880	0.064
H29	1.0475	0.1497	0.6275	0.059
H10	0.4349	-0.0269	0.9143	0.065
H9	0.1575	0.0364	0.9922	0.068
H20	-0.2289	0.3056	0.8065	0.06
H30	0.7495	0.2130	0.6874	0.058
H14	0.4555	0.1616	0.5609	0.054
H15	0.4435	0.2621	0.3767	0.064
H16	0.3425	0.4573	0.3015	0.073
H17	0.2352	0.5477	0.4123	0.069
H2	0.2110	0.6295	0.5174	0.08
H5	0.0712	0.4114	0.8786	0.069
H23	-0.2322	0.2308	1.1676	0.072
H24	0.0459	0.1724	1.0846	0.072
H4	0.0408	0.6072	0.8124	0.09
H3	0.0993	0.7157	0.6312	0.096