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Supporting Information (SI)

Design, synthesis and amplified spontaneous emission (ASE) of 1,2,5-benzothiadiazole derivatives

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1. Supplementary Figures and Tables

1.1 *Computational study*

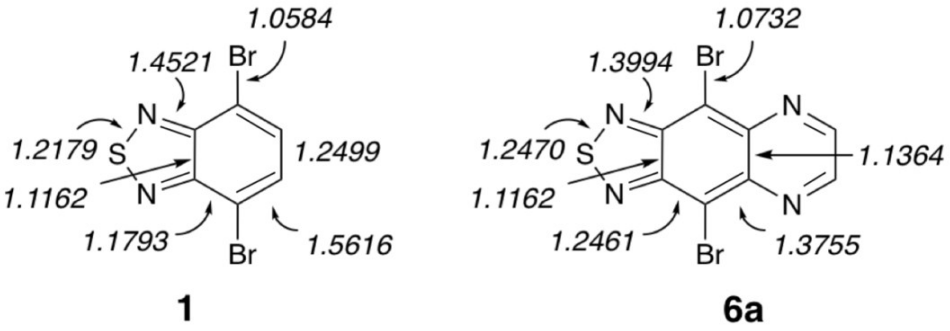


Figure S1. NBO Wiberg indexes of compounds 1 and 6a computed at B3LYP-D3/6-31G* level

Table S1. Total electronic energies, zero-point correction of the energy (ZPCE), thermal corrections to Gibbs free energies (TCGFE, in a.u.), and number of imaginary frequencies (NIMAG) of all stationary points discussed in the main text.

Structure	E (a.u.) [a]	ZPCE[b]	TCGFE [c]	NIMAG(ν)
1	-5880.933424	0.070811	0.033801	0
6a	-6066.638812	0.093342	0.053265	0
Br·[c]	-2571.656918	–	–	–
1(monoBr)· [c]	-3309.135007	–	–	–
6a(monoBr)· [c]	-3494.839086	–	–	–

[a]Computed at B3LYP-D3/6-31G* level of theory. [b]Computed at 298.15K. [c]Values computed for calculation of the heterolytitc bond energy dissociation.

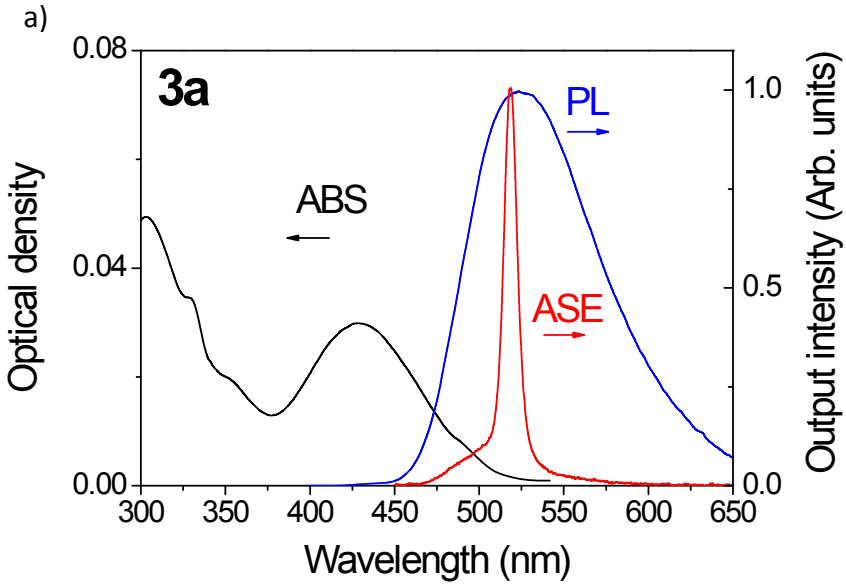
Table S2. Topology and energy values of HOMO-LUMO orbitals calculated at B3LYP/6-31G(d,p).

Compound	E_{HOMO} (eV)	E_{LUMO} (eV)	E_{GAP}(eV)
3a[a]	-5.16	-2.59	2.57
3b[a]	-4.78	-2.46	2.32
3c	-5.27	-2.79	2.48

3d	-4.71	-2.93	1.78
8a	-5.28	-3.25	2.03
8b	-5.18	-3.07	2.11
8c	-5.01	-2.96	2.05

[a]Values are according with the previously calculated in reference [1] and [2] for **3a** and **3b**, respectively

1.2 ASE properties of PS films doped with benzothiadiazole derivatives



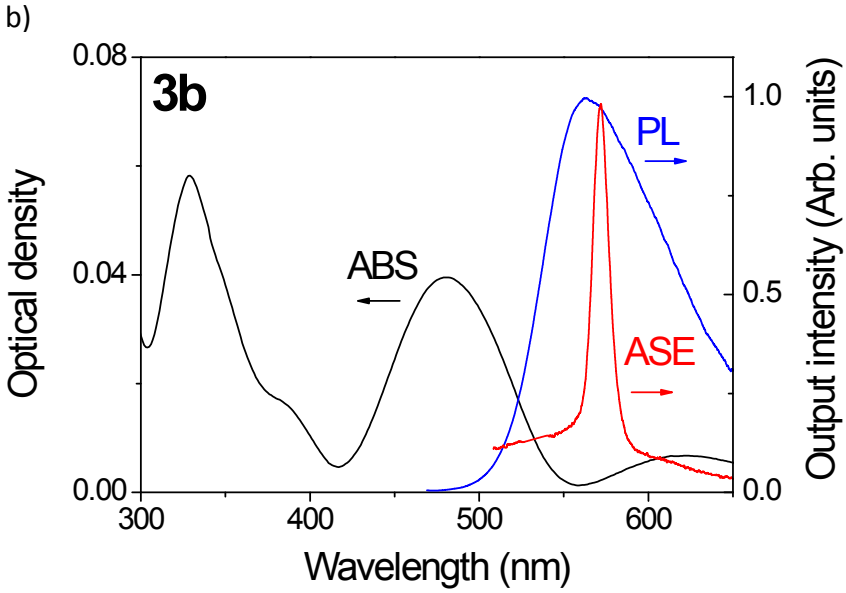


Figure S2. Optical density (ABS, black line, left axis), normalized photoluminiscence (PL,blue line, right axis) and amplified spontaneous emission (ASE, red line, right axis) for PS films doped with 19.44 and 19.67 µmol BTD/g PS of **3a** (a) and **3b** (b), respectively.

Table S3. ASE properties of compounds **3a-d** and **8a-c**

Compound	µmol BTD,TDQ/g PS	*h* (nm)	*α* (nm) 436 nm	$I_{th\text{-}ASE}$ (kW/cm2)	λ_{PLmax} (nm)	λ_{ASE} (nm)	$FWHM_{ASE}$ (nm)	$\tau_{1/2}$ (min) (*I*p, kW/cm2)
3a	9.55	550	631.0	229	521.4	516.1	14.5	9.5 (684)
	19.44	590	807.0	189	523.6	518.5	8.7	
	61.4	578	2475.0	229	531.0	520.1	7.5	
	125.0	590	4441.0	> 2000	540.3			
	238.0	591	8506.4	> 1500	545.2			
3b	9.55	589	158.3	270	558.2	567.2	13.2	37.4 (674)
	19.67	570	691.9	194	563.9	571.6	10.5	
	61.4	625	1804.4	260	574.3	576.7	12.3	
	125.7	587	4201.6	540	579.3	578.8		
	246.3	643	6960.4	> 1340	584.6			
3c	4.56	538	703.1	71	502.3	509.5	15.5	6.2 (681)
	9.54	548	889.3	57	506.3	514.2	15.8	
	20.65	529	1340.1	40	509.1	515.1	10.3	
	61.4	607	3247.0	43	515.5	518.6	11.0	
	124.5	601	6528.8	66	523.1	522.9	8.4	
8b	20.67	604		439.5	605.3	636.1	16.6	
	61.4	595		1039.0	616.5	639.4	13.6	

h, thickness of the films α, absorption coefficient; $I_{th\text{-}ASE}$, ASE threshold; λ_{ASE}, ASE wavelength; $FWHM_{ASE}$, ASE linewidth; $\tau_{1/2}$, ASE half-life; *I*p, pump intensity.

1.3 Optical properties in solution

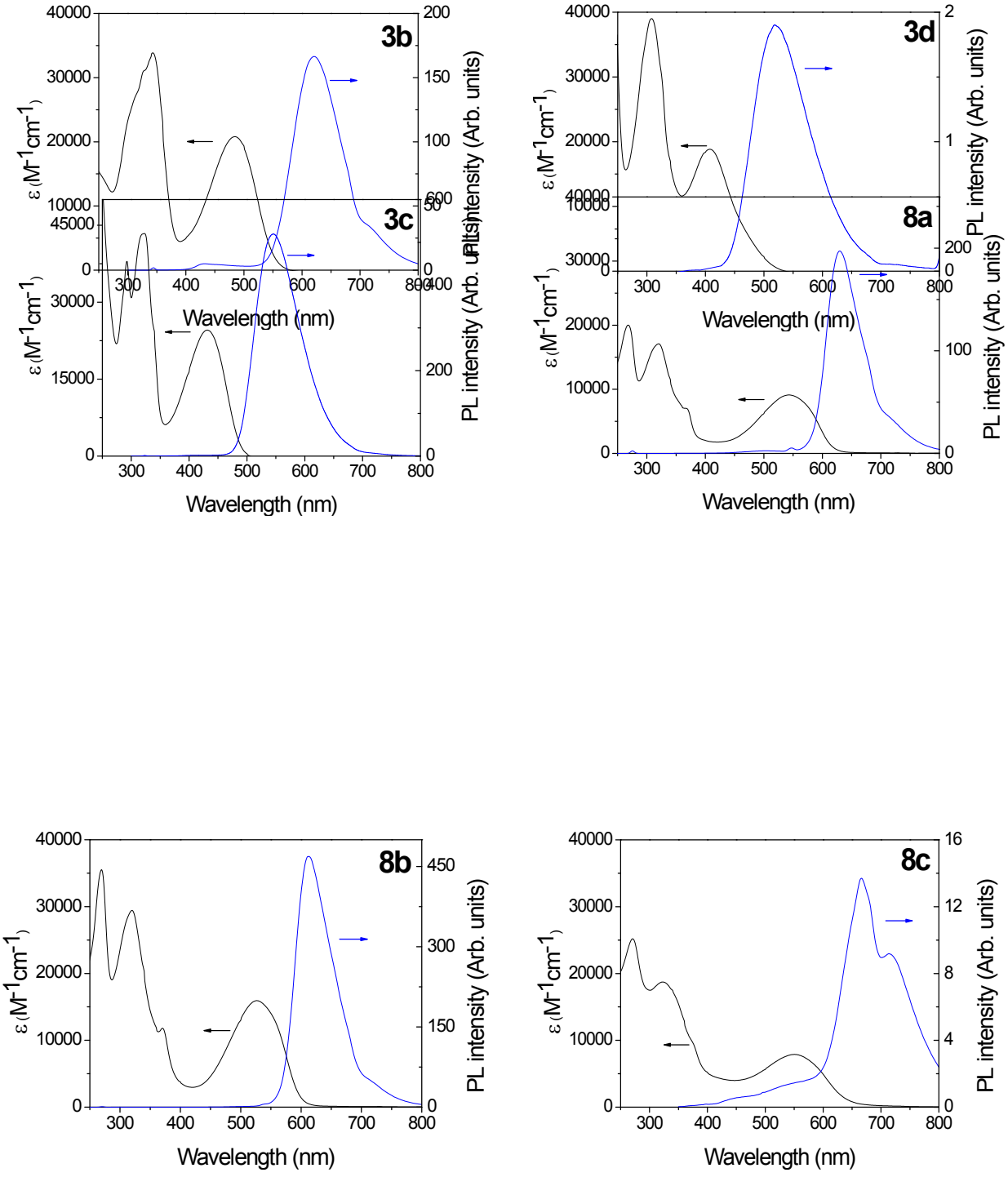


Figure S3. Absorption (**black**) and PL (**blue**) spectra for compounds **3b-c** and **8a-c** at room temperature in $CHCl_3$. The concentration of solutions were 2.0 x 10^{-5} M and 3.3 x 10^{-5} for **3** and **8**, respectively. The PL spectra were obtained by exciting all compounds at their absorption maxima wavelength

Table S4. Photophysical properties of **3a-d** and **8a-c** in solution

Compound	ε (M^{-1} cm^{-1})	λ_{abs} (nm)	λ_{em} (nm)	Stokes shift[e] (cm^{-1})	ϕ_F (%)
3a[a]	20000/15500	318/428	590	6415	49
3b	33900/20800	343/484	624	4636	26[b]
3c	43400/24600	323/431	546	4887	36[b]
3d	39000/18800	308/408	518	5205	-[d]
8a	17100/9100	321/543	628	2493	45[c]
8b	29400/15900	320/527	613	2662	67[c]
8c	18700/7900	323/551	666/713(sh)	3134	8[c]

[a] Values for **3a** were taken from reference[1]; [b]using Quinine Sulfate in H_2SO_4 1 M (ϕ_F = 0.54) as internal standard ; [c] using Rhodamine 101 in Ethanol+0.01% HCl (ϕ_F = 1.00) as internal standard; [d]The PLQY for compound **3d** could not be determined accurately due to its very low PL emission; [e]The Stokes shift is determined as the difference in cm^{-1} between the lowest energy absorption and the highest energy florescence band.

Low quantum yield for **8c** in a polar solvent ($CHCl_3$) shows it pronounced ICT characteristics. Generally, ICT transitions are characterized by high Stokes shifts and low fluorescence quantum yields in solvents with high polarity. One of the main reasons for the low fluorescence efficiency under these conditions is that the ICT state is so favoured that the excited and the ground states are energetically very close, and the excited state deactivates mainly *vía* non-radiative pathways, leading to lower quantum yields[3,4]. When we compare the fluorescence spectrum of this compound in a polar solvent ($CHCl_3$) vs. a non-polar solvent (toluene) we observe a difference of 54% of intensity (**Figure S4a**) asserting the above hypothesis. Besides, when we compare dilute solutions of this compound in solvents with different polarity under 365 nm light we can observe different emission intensity (**Figure S4b**).

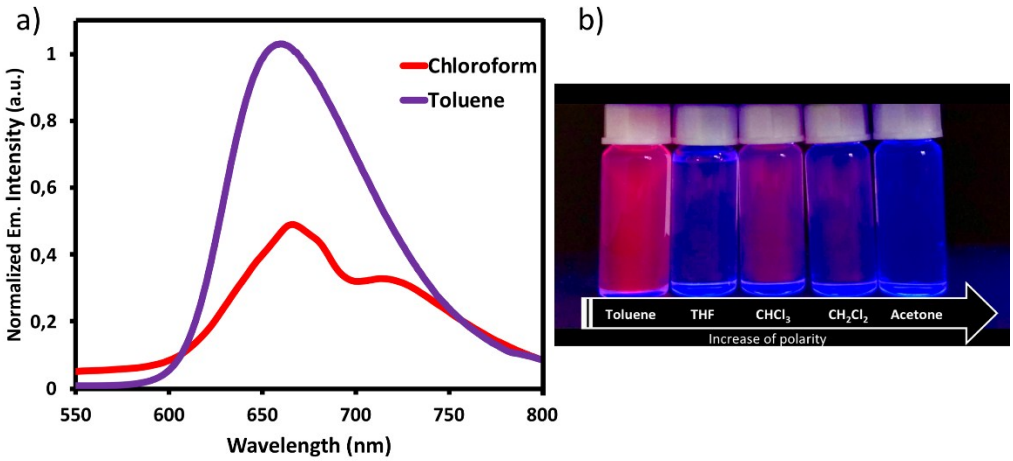


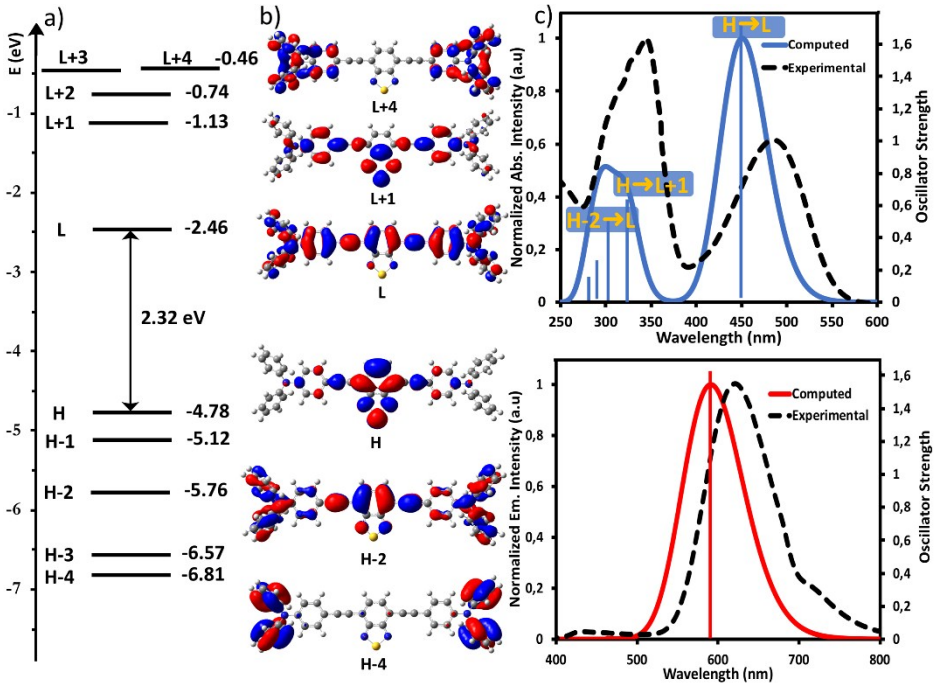
Figure S4. a) Emission spectra of **8c** in chloroform and toluene; b) Luminescence photographs of solutions of **8c** in solvents with different polarity upon excitation at 365 nm light.

1.4 TD-DFT calculations

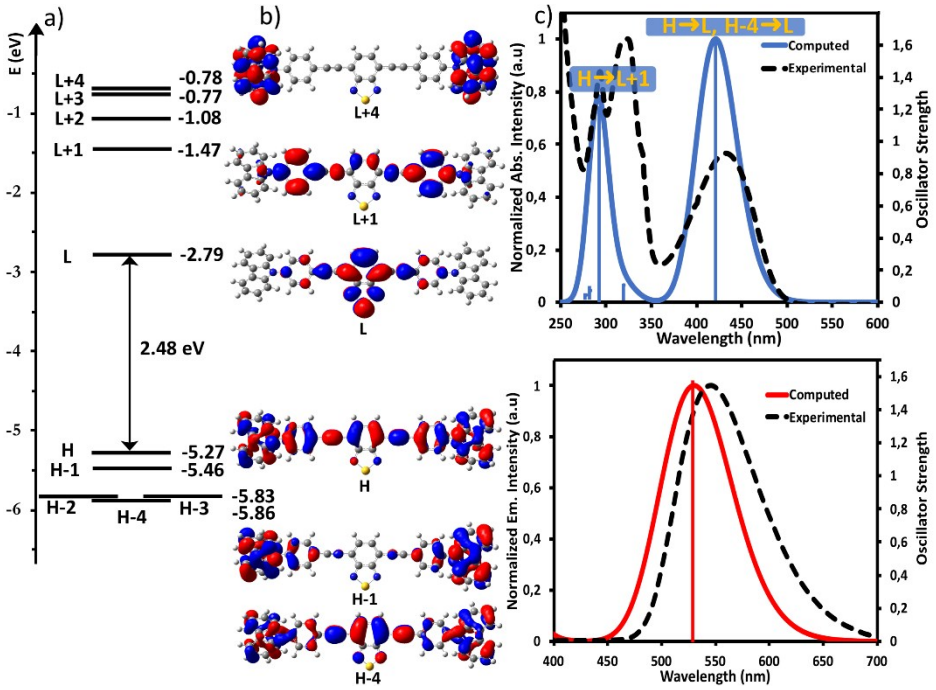
Density functional theory (DFT) calculations were performed with the Gaussian 09 suite of programs.[5] Geometry optimizations were performed using the B3LYP/6-31G(d,p)[6,7] level of theory. All the optimized compounds were characterized by harmonic vibrational analysis[8] in which the optimized compounds showed only positive definite Hessians.
Geometry optimizations were performed using the medium-sized 6-31G(d) basis set and frequency calculations were performed to confirm the nature of ground state stationary points. Solvent effects on molecular geometries and energies were estimated by means of polarization continuum models (CPCM)[9] using chloroform as solvent. For the calculation of emission spectra, TD-DFT calculations were performed at the optimized geometry of the first excited state using an identical model chemistry (M06-2x/6-311+G(2d,p)//M06-2x/6-31G*) and solvation model.
Molecular orbital contour plots were obtained using the Gaussview 5.0 software[10]. GaussSum 3.0[11] software was used for the electronic spectrum simulation. The equation employed by the program to calculate the theoretical spectrum and the extinction coefficients is based on Gaussian convolution and is reported in the open source code of the program (available at http://gausssum.sourceforge.net.). The full- width at half-maximum (FWHM) value used for the simulated spectrum was 3000 cm^{-1} for each peak.

All compound revels two absorption bands. The first, around 250-400 nm represent π-π transitions between the acceptor and donor arms, respectively. Thus, this band can be ascribed to a π-π* locally excited (LE) transition. The second band between 400-600 nm represent the transition from donor arms to acceptor core, which is attributed to an intramolecular charge transfer band (ICT). Comparison of the computed and experimental results are shown in **Figure S5**. As an example, we comment the results for **8b**. The first absorption band (250-400 nm) includes the transition H$\rightarrow$L+1 and H-2$\rightarrow$L. Both H and L+1 orbitals are mainly located on the donor arm, which means that it is a π-π* transition from the absorption of the donor arm. H-2 and L orbitals are located in the acceptor core which means that this transition represents a transition from the acceptor core. The sum of H$\rightarrow$L+1 and H-2$\rightarrow$L transitions make the LE band. The second absorption transition (400-600 nm) involves H$\rightarrow$L transition, which represent intramolecular charge transfer from donor arm (HOMO) to acceptor core (LUMO). Same analysis can be carried out for the rest of molecules.
It is interesting to mention the case of **3d.** In this compound LE band is formed by the contribution of several transitions (**Table S4**). This can be explained according to the molecular orbital diagram of the molecule, in which we can observe that a considerable number of molecular orbitals are degenerated. For that reason, transitions involve a greater number of orbitals. Besides, for this molecule ICT band involves H-2$\rightarrow$L transition, unlike the rest of molecules which implicate H$\rightarrow$L transition. This fact can be explain taking into account the perpendicularity of phenoxazine groups. The perpendicular disposition of phenoxazine groups with respect to the rest of the molecule lead a situation in which the conjugation between phenoxazine groups and the donor branch is blocked. For that reason, it can not be intramolecular charge transfer between HOMO an LUMO orbitals in **3d**. H-2$\rightarrow$L transition directs an ICT band in which phenoxazine groups are not involved.

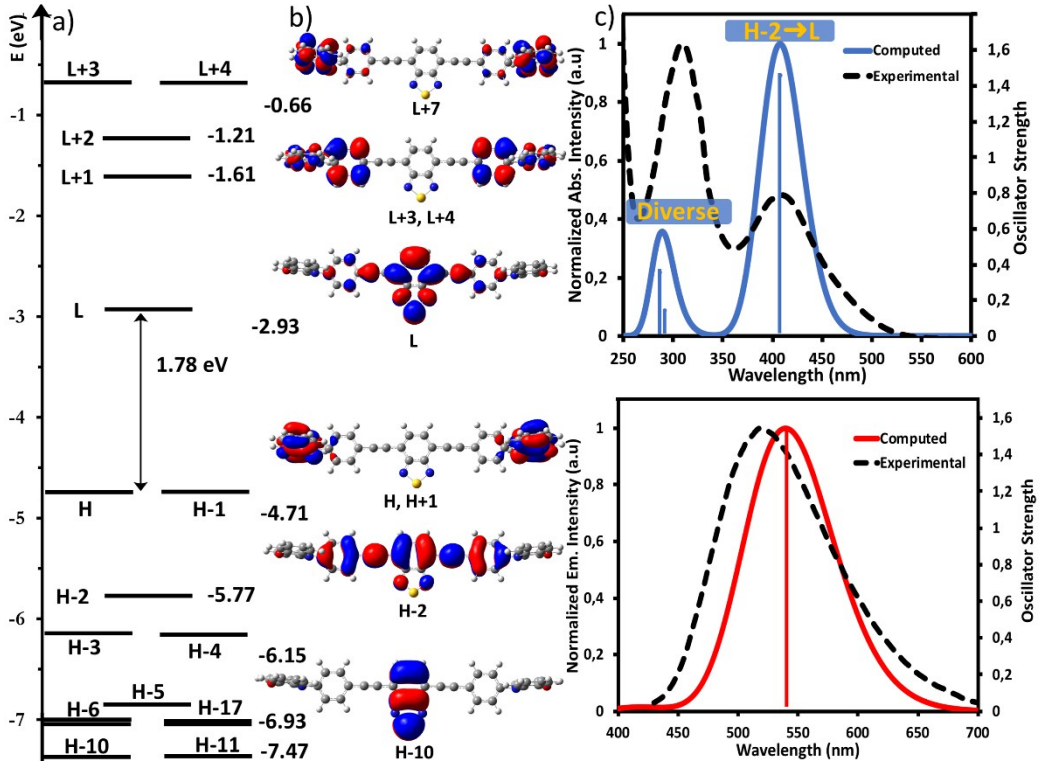
Compound 3b



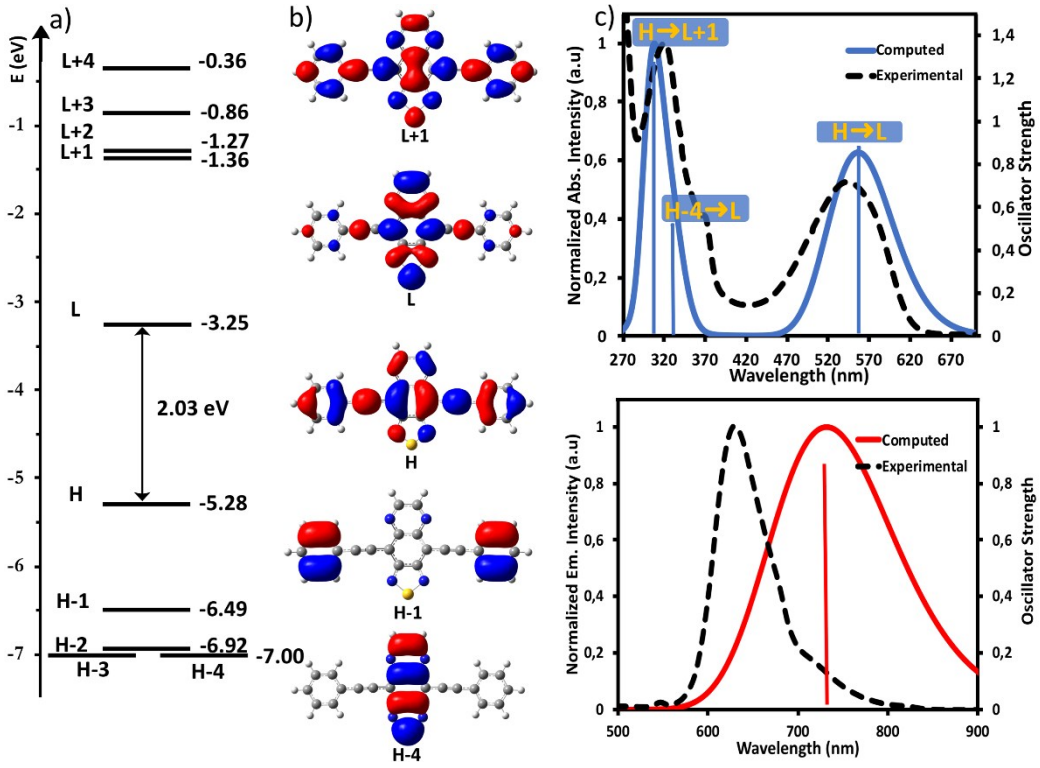
Compound 3c



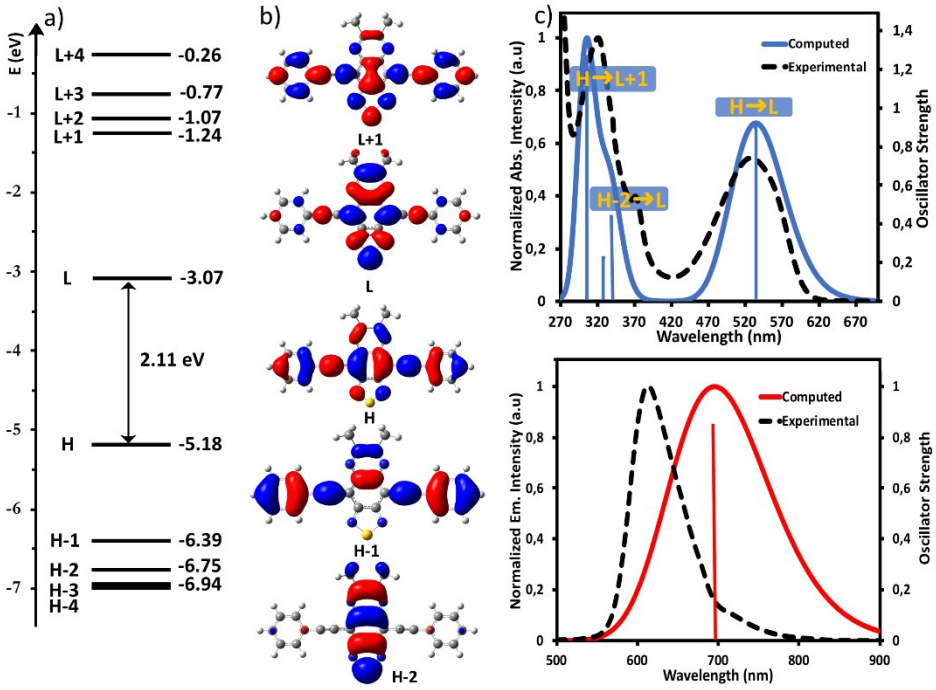
Compound 3d



Compound 8a



Compound 8b



Compound 8c

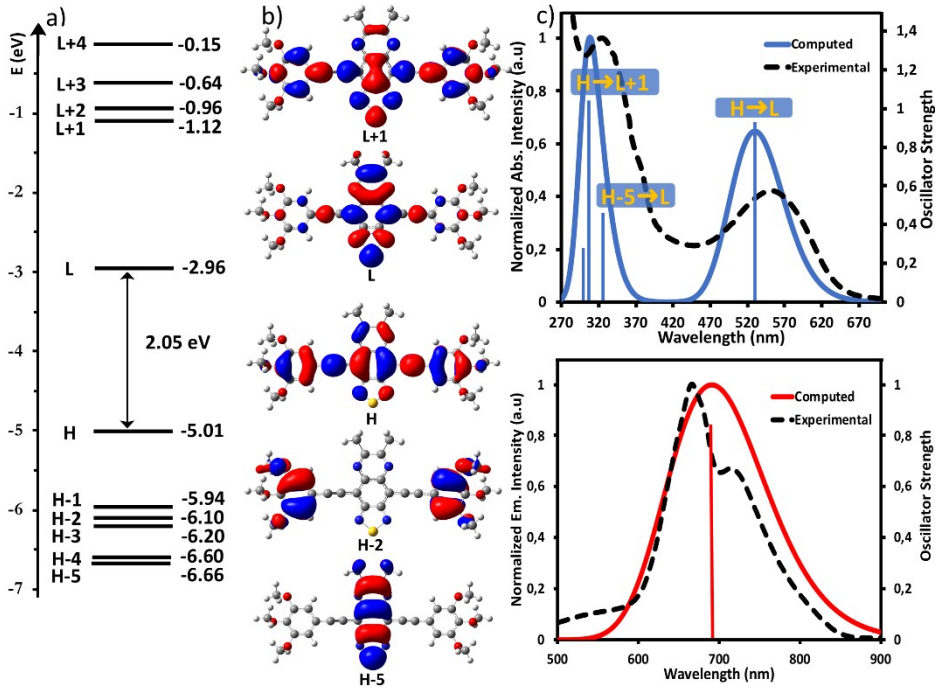


Figure S5. a) Partial Molecular Orbital energy level diagram of **3b-d** and **8a-c** calculated at B3LYP/6-31g(d,p); b) Electronic density distribution of some molecular orbitals for the studied compounds calculated at CPCM-M06-2X/6-311+G(2d,p) in chloroform; c) Absorption and emission experimental spectra (**black dash line**) and calculated at CPCM-M06-2X/6-311+G(2d,p) in chloroform (**solid blue: absorption**, **solid red: emission**). Oscillator strength values are also plotted.

Table S5. Calculated electronic transitions and oscillator strength (*f*) for **3a-d** and **8a-c** by TD-DFT at M06-2X/6-311+G(2d,p). H: HOMO. L: LUMO. Only transitions with $f \geq 0.2$ and contribution greater than 10% are shown.

	Spectrum	Elec.Trans.	λ (nm)	*f*	MO (coeficient %)
3a[a]	**Absorption**	$S_0 \rightarrow S_1$	421	1.27	H→L (94%)
		$S_0 \rightarrow S_5$	288	1.01	H→L+1 (78%)
		$S_0 \rightarrow S_6$	284	0.25	H-5→L (83%)
	Emission	$S_1 \rightarrow S_0$	543	1.33	L→H (97%)
3b	**Absorption**	$S_0 \rightarrow S_1$	450	1.72	H→L (86%)
		$S_0 \rightarrow S_3$	323	0.63	H→L+1 (45%), H-2→L (32%), H-1→L+2 (15%)
		$S_0 \rightarrow S_6$	301	0.51	H-2→L (52%), H→L+1 (27%), H→L (11%),
		$S_0 \rightarrow S_9$	288	0.26	H-1→L+6 (42%), H→L+5 (44%)
	Emission	$S_1 \rightarrow S_0$	591	1.61	L→H (92%)
3c	**Absorption**	$S_0 \rightarrow S_1$	421	1.64	H→L (75%), H-4→L (21%)
		$S_0 \rightarrow S_{10}$	292	1.20	H-4→L (10%), H-4→L+1 (10%), H→L+1 (51%)
	Emission	$S_1 \rightarrow S_0$	530	1.56	L→H (90%)
3d	**Absorption**	$S_0 \rightarrow S_1$	408	1.47	H-2→L (93%)
		$S_0 \rightarrow S_8$	292	0.15	H-10→L (39%), H-5→L (43%)
		$S_0 \rightarrow S_{10}$	287	0.36	H-1→L+3 (13%), H-1→L+7 (28%), H→L+4 (13%), H→L+8 (29%)
	Emission	$S_1 \rightarrow S_0$	539	1.61	H-2→L (28%), H→L (68%)
8a	**Absorption**	$S_0 \rightarrow S_2$	557	0.88	H→L (98%)
		$S_0 \rightarrow S_6$	329	0.52	H-4→L (89%)
		$S_1 \rightarrow S_0$	306	1.27	H→L+1 (78%), H-5→L (13%)
	Emission	$S_1 \rightarrow S_0$	731	0.79	L→H (99%)
8b	**Absorption**	$S_0 \rightarrow S_1$	534	0.90	H→L (98%)
		$S_0 \rightarrow S_3$	339	0.43	H-2→L (34%), H-1→L (61%)
		$S_1 \rightarrow S_4$	328	0.23	H-2→L (56%), H-1→L (33%)
		$S_1 \rightarrow S_5$	305	1.27	H→L+1 (83%)
	Emission	$S_1 \rightarrow S_0$	695	0.81	L→H (99%)
8c	**Absorption**	$S_0 \rightarrow S_1$	530	0.92	H→L (98%)
		$S_0 \rightarrow S_4$	327	0.43	H-5→L (83%)
		$S_0 \rightarrow S_5$	308	1.03	H-4→L (17%), H-2→L 21%), H→L+1 (52%)
		$S_0 \rightarrow S_7$	301	0.26	H-2→L (70%), H→L+1 (19%)
	Emission	$S_1 \rightarrow S_0$	690	0.83	L→H (99%)

[a] Values for **3a** were taken from reference[1]

1.5 Solvathocromism study

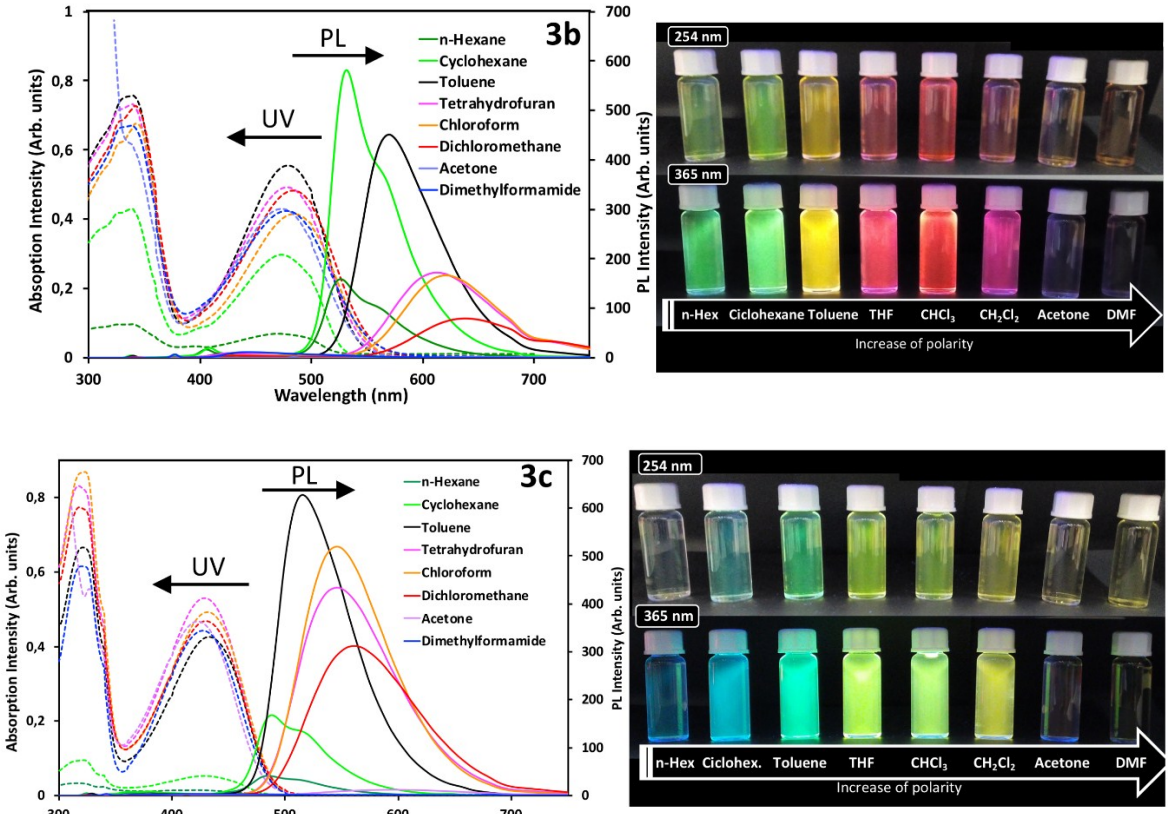


Figure S6. UV/Vis absorption and fluorescence spectra of **3b** (2 x 10^{-5} M, excited at 340 nm) and **3c** (2 x 10^{-5} M, excited at 323 nm) in toluene, chloroform, tetrahydrofuran, dichloromethane, acetone and dimethylformamide. Right of spectra, luminescence photographs of **3b** and **3c** by varying solvent polarities upon excitation at 254 nm and 365 nm.

Table S6. Maximum absorption and emission wavelengths for compounds **3b** and **3c** in different solvents. Measurements were taking with 2·10^{-5}M solutions, excited at 340 nm for **3b** and 323 nm for **3c.**

	Compound 3b		Compound 3c	
Solvent	λ_{abs}	λ_{em}	λ_{abs}	λ_{em}
n-Hexane	331/470	527	318/420	485
Cyclohexane	339/473	532	322/428	489
Toluene	340/479	570	321/433	516
Tetrahydrofuran	340/479	612	317/429	548
Chloroform	342/484	621	322/431	546
Dichloromethane	342/484	638	318/431	562
Acetone	347/474	-	327/423	-
Dimethylformamide	340/478	-	320/427	-

1.6 PL spectra of doped PS film

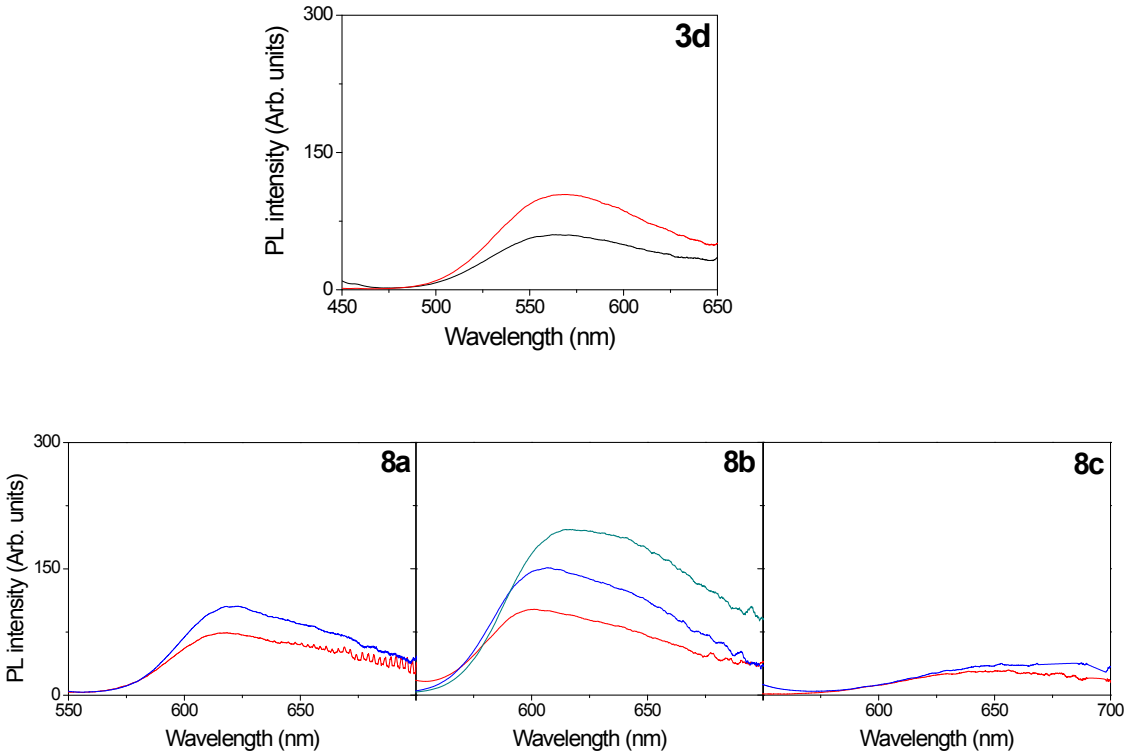


Figure S7. PL spectra of PS film doped with **9.55**, **20.67** and **61.4** µmol BTD,TDQ/g PS (**red**, **blue** and **green** lines, respectivelly) of compounds **3d** and **8a-c**

2. X-ray data and figures

Data collection for compounds **3b** and **3c** was performed at X8 APEX II diffractometer, using MoKα radiation at room temperature. The data reduction was performed with the APEX3[12] software and corrected for absorption using SADABS.[13] Crystal structure was solved by direct methods using the SIR97 program[14] and refined by full-matrix least-squares on F2 including all reflections using anisotropic displacement parameters by means of the WINGX crystallographic package.[15,16] All non-hydrogen atoms were refined anisotropically and all hydrogen atoms were geometrically placed and refined using a riding model. The molecule **3b** is disordered over an inversion center. CCDC code 1912850 for **3b** and 1912851 for **3c** contain the supplementary crystallographic data for this paper.

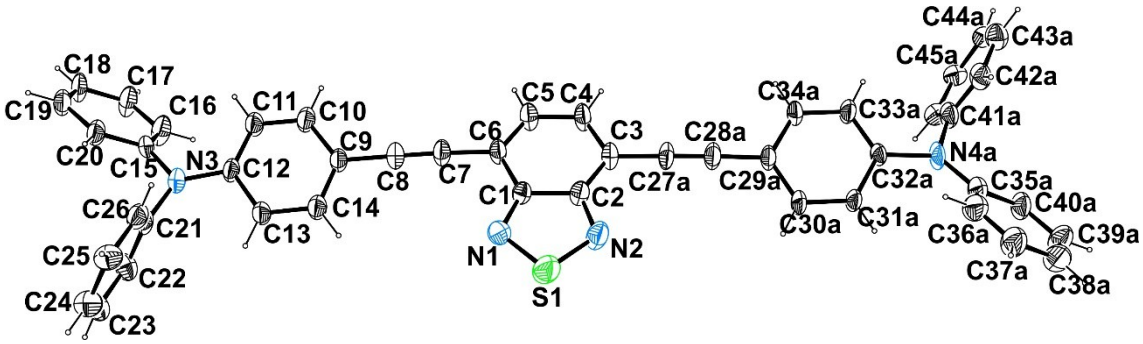


Table S7. Crystal data and structure refinement for compound **3b**.

Empirical formula	C46 H30 N4 S	
Formula weight	670.80	
Temperature	290(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P ī	
Unit cell dimensions	a = 8.2931(15) Å	α= 76.505(5)°.
	b = 9.7165(18) Å	β= 83.078(5)°.
	c = 11.6820(16) Å	γ = 75.073(5)°.
Volume	882.6(3) Å3	
Z	1	
Density (calculated)	1.262 Mg/m3	
Absorption coefficient	0.131 mm-1	
F(000)	350	
Crystal size	0.170 x 0.090 x 0.040 mm3	
Theta range for data collection	2.219 to 24.985°.	
Index ranges	-9≤h≤9, -11≤k≤11, -13≤l≤9	

Reflections collected	10421
Independent reflections	3071 [R(int) = 0.0615]
Completeness to theta = 25.242°	96.3 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.746 and 0.597
Refinement method	Full-matrix least-squares on F2
Data / restraints / parameters	3071 / 399 / 425
Goodness-of-fit on F2	0.972
Final R indices [I>2sigma(I)]	R1 = 0.0650, wR2 = 0.1557
R indices (all data)	R1 = 0.1522, wR2 = 0.2048
Extinction coefficient	0.038(8)
Largest diff. peak and hole	0.199 and -0.231 e.Å-3

Table S8. Atomic coordinates (x 104) and equivalent isotropic displacement parameters (Å2x 103) for 3b. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
S(1)	8744(3)	12300(3)	11447(2)	107(1)
N(1)	7794(8)	11919(7)	10486(6)	69(2)
N(2)	10498(13)	11178(12)	11370(10)	77(3)
N(3)	-800(30)	13760(30)	6780(20)	55(3)
C(1)	8807(12)	10844(10)	10072(9)	49(2)
C(2)	10440(12)	10399(11)	10574(7)	57(2)
C(3)	11709(11)	9358(11)	10251(11)	55(3)
C(4)	11361(11)	8734(11)	9376(9)	66(3)
C(5)	9818(14)	9151(13)	8894(13)	62(3)
C(6)	8546(11)	10146(10)	9199(7)	55(2)
C(7)	6924(10)	10632(10)	8721(8)	61(3)
C(8)	5570(12)	11126(12)	8351(9)	57(3)
C(9)	3911(15)	11745(14)	7912(11)	51(3)
C(10)	3458(18)	11564(17)	6858(11)	64(3)
C(11)	1930(20)	12130(20)	6472(14)	61(4)
C(12)	770(20)	12940(20)	7112(16)	54(4)
C(13)	1150(20)	13170(20)	8176(18)	61(4)
C(14)	2783(10)	12564(8)	8574(7)	64(4)
C(15)	-1496(10)	13206(8)	5939(7)	53(4)
C(16)	-1375(10)	11753(8)	5937(7)	81(8)
C(17)	-2167(10)	11395(8)	5102(7)	84(5)
C(18)	-3078(10)	12491(8)	4269(7)	72(4)
C(19)	-3199(10)	13944(8)	4270(7)	67(4)

C(20)	-2407(10)	14302(8)	5105(7)	62(4)
C(21)	-1947(10)	14921(8)	7197(7)	51(4)
C(22)	-3335(10)	14854(8)	7985(7)	64(6)
C(23)	-4267(10)	16103(8)	8350(7)	65(5)
C(24)	-3811(10)	17420(8)	7927(7)	69(4)
C(25)	-2423(10)	17487(8)	7139(7)	67(4)
C(26)	-1491(10)	16237(8)	6774(7)	61(3)
C(27)	6682(10)	11077(10)	9268(7)	60(2)
C(28)	5374(12)	11462(14)	8858(9)	67(3)
C(29)	3823(16)	11992(16)	8317(10)	56(3)
C(30)	3558(15)	11682(16)	7259(12)	65(4)
C(31)	1990(20)	12290(20)	6786(13)	62(4)
C(32)	680(20)	13170(20)	7354(16)	47(4)
N(4)	-970(30)	13620(30)	6820(30)	70(5)
C(33)	950(20)	13480(30)	8391(18)	62(4)
C(34)	2479(11)	12902(12)	8854(9)	59(3)
C(35)	-1623(16)	13162(13)	5985(10)	67(5)
C(36)	-1272(15)	11707(13)	6039(11)	75(6)
C(37)	-1839(17)	11126(16)	5291(11)	86(4)
C(38)	-2823(17)	11998(14)	4436(11)	81(4)
C(39)	-3239(16)	13454(15)	4348(11)	81(4)
C(40)	-2634(15)	14057(13)	5109(11)	70(4)
C(41)	-1898(14)	14958(13)	7257(11)	64(5)
C(42)	-3297(13)	14686(14)	7934(10)	66(5)
C(43)	-4366(16)	15780(15)	8403(11)	69(4)
C(44)	-4071(13)	17124(14)	8187(10)	56(3)
C(45)	-2740(15)	17400(12)	7482(11)	61(3)
C(46)	-1574(15)	16300(15)	7029(11)	69(3)

Table S9. Bond lengths [Å] and angles [°] for **3b.**

S(1)-C(4)#1	1.567(11)	C(4)#1-N(1)-C(1)	37.1(8)	C(6)#1-C(3)-C(2)	41.7(8)
S(1)-N(2)	1.584(10)	C(4)#1-N(1)-S(1)	72.5(10)	C(1)#1-C(3)-C(4)	25.1(13)
S(1)-N(1)	1.606(7)	C(1)-N(1)-S(1)	107.9(7)	C(6)#1-C(3)-C(4)	154.9(13)
S(1)-C(5)#1	1.689(12)	C(4)#1-N(1)-C(3)#1	59.9(9)	C(2)-C(3)-C(4)	114.7(9)
N(1)-C(4)#1	0.819(8)	C(1)-N(1)-C(3)#1	24.8(5)	C(1)#1-C(3)-N(1)#1	52.4(13)
N(1)-C(1)	1.310(11)	S(1)-N(1)-C(3)#1	132.2(6)	C(6)#1-C(3)-N(1)#1	165.0(12)
N(1)-C(3)#1	1.613(13)	C(5)#1-N(2)-C(2)	23.7(18)	C(2)-C(3)-N(1)#1	144.0(9)
N(2)-C(5)#1	0.613(12)	C(5)#1-N(2)-S(1)	89.0(19)	C(4)-C(3)-N(1)#1	30.5(4)

N(2)-C(2)	1.341(12)	C(2)-N(2)-S(1)	108.1(8)	C(1)#1-C(3)-C(7)#1	164.1(16)
N(2)-C(6)#1	1.572(13)	C(5)#1-N(2)-C(6)#1	54.1(17)	C(6)#1-C(3)-C(7)#1	55.0(9)
N(2)-C(4)#1	1.834(11)	C(2)-N(2)-C(6)#1	35.0(5)	C(2)-C(3)-C(7)#1	96.2(9)
N(3)-C(12)	1.39(3)	S(1)-N(2)-C(6)#1	142.7(6)	C(4)-C(3)-C(7)#1	148.9(8)
N(3)-C(21)	1.42(3)	C(5)#1-N(2)-C(4)#1	35.9(16)	N(1)#1-C(3)-C(7)#1	118.5(6)
N(3)-C(15)	1.45(2)	C(2)-N(2)-C(4)#1	54.4(7)	C(3)-C(4)-C(5)	122.1(10)
C(1)-C(3)#1	0.693(9)	S(1)-N(2)-C(4)#1	54.0(4)	C(6)-C(5)-C(4)	124.8(11)
C(1)-C(4)#1	0.823(9)	C(6)#1-N(2)-C(4)#1	88.8(6)	C(3)#1-C(6)-C(2)#1	98.8(13)
C(1)-C(6)	1.414(12)	C(12)-N(3)-C(21)	132.2(19)	C(3)#1-C(6)-C(5)	136.8(13)
C(1)-C(2)	1.462(11)	C(12)-N(3)-C(15)	113.8(19)	C(2)#1-C(6)-C(5)	38.1(7)
C(1)-C(2)#1	1.530(13)	C(21)-N(3)-C(15)	113.5(16)	C(3)#1-C(6)-C(1)	22.1(9)
C(1)-C(5)#1	1.760(16)	C(3)#1-C(1)-C(4)#1	134(2)	C(2)#1-C(6)-C(1)	79.3(9)
C(2)-C(5)#1	0.818(10)	C(3)#1-C(1)-N(1)	102.8(16)	C(5)-C(6)-C(1)	116.5(9)
C(2)-C(6)#1	0.904(10)	C(4)#1-C(1)-N(1)	36.9(8)	C(3)#1-C(6)-C(7)	95.6(11)
C(2)-C(3)	1.344(13)	C(3)#1-C(1)-C(6)	28.0(13)	C(2)#1-C(6)-C(7)	163.1(12)
C(2)-C(4)#1	1.516(15)	C(4)#1-C(1)-C(6)	161.7(16)	C(5)-C(6)-C(7)	127.2(9)
C(2)-C(1)#1	1.530(13)	N(1)-C(1)-C(6)	129.0(10)	C(1)-C(6)-C(7)	116.3(9)
C(2)-C(2)#1	1.986(17)	C(3)#1-C(1)-C(2)	143.7(17)	C(3)#1-C(6)-N(2)#1	155.2(12)
C(2)-C(3)#1	2.062(12)	C(4)#1-C(1)-C(2)	77.6(13)	C(2)#1-C(6)-N(2)#1	58.4(8)
C(2)-C(3)#2	19.983(16)	N(1)-C(1)-C(2)	112.5(11)	C(5)-C(6)-N(2)#1	22.3(5)
C(3)-C(1)#1	0.693(9)	C(6)-C(1)-C(2)	118.4(8)	C(1)-C(6)-N(2)#1	137.7(8)
C(3)-C(6)#1	0.866(10)	C(3)#1-C(1)-C(2)#1	61.4(13)	C(7)-C(6)-N(2)#1	105.7(7)
C(3)-C(4)	1.396(14)	C(4)#1-C(1)-C(2)#1	156.3(13)	C(8)-C(7)-C(6)	175.3(10)
C(3)-N(1)#1	1.613(13)	N(1)-C(1)-C(2)#1	164.2(11)	C(8)-C(7)-C(3)#1	146.4(9)
C(3)-C(7)#1	1.751(13)	C(6)-C(1)-C(2)#1	35.5(4)	C(6)-C(7)-C(3)#1	29.5(4)
C(4)-C(5)	1.385(13)	C(2)-C(1)-C(2)#1	83.2(7)	C(7)-C(8)-C(9)	179.1(10)
C(5)-C(6)	1.310(14)	C(3)#1-C(1)-C(5)#1	163.9(16)	C(14)-C(9)-C(10)	119.6(10)
C(6)-C(3)#1	0.866(10)	C(4)#1-C(1)-C(5)#1	50.2(11)	C(14)-C(9)-C(8)	116.6(10)
C(6)-C(2)#1	0.904(10)	N(1)-C(1)-C(5)#1	85.6(9)	C(10)-C(9)-C(8)	123.7(10)
C(6)-C(7)	1.441(11)	C(6)-C(1)-C(5)#1	145.3(8)	C(11)-C(10)-C(9)	123.0(12)
C(6)-N(2)#1	1.572(13)	C(2)-C(1)-C(5)#1	27.5(5)	C(10)-C(11)-C(12)	119.1(11)
C(7)-C(8)	1.192(10)	C(2)#1-C(1)-C(5)#1	109.8(8)	C(11)-C(12)-C(13)	120.7(14)
C(7)-C(3)#1	1.751(13)	C(5)#1-C(2)-C(6)#1	99.0(14)	C(11)-C(12)-N(3)	126.8(16)
C(8)-C(9) 1.455(14)		C(5)#1-C(2)-C(3)	138.5(15)	C(13)-C(12)-N(3)	112.1(16)
C(9)-C(14)	1.355(11)	C(6)#1-C(2)-C(3)	39.5(7)	C(12)-C(13)-C(14)	119.5(11)
C(9)-C(10)	1.390(12)	C(5)#1-C(2)-N(2)	17.5(13)	C(9)-C(14)-C(13)	118.1(9)
C(10)-C(11)	1.330(17)	C(6)#1-C(2)-N(2)	86.6(10)	C(16)-C(15)-C(20)	120.0
C(11)-C(12)	1.349(18)	C(3)-C(2)-N(2)	125.4(10)	C(16)-C(15)-N(3)	126.8(11)

C(12)-C(13)	1.398(16)	C(5)#1-C(2)-C(1)	97.0(14)	C(20)-C(15)-N(3)	113.2(11)
C(13)-C(14)	1.416(18)	C(6)#1-C(2)-C(1)	160.9(13)	C(15)-C(16)-C(17)	120.0
C(15)-C(16)	1.3900	C(3)-C(2)-C(1)	123.5(8)	C(18)-C(17)-C(16)	120.0
C(15)-C(20)	1.3901	N(2)-C(2)-C(1)	111.2(10)	C(17)-C(18)-C(19)	120.0
C(16)-C(17)	1.3901	C(5)#1-C(2)-C(4)#1	65.0(12)	C(20)-C(19)-C(18)	120.0
C(17)-C(18)	1.3900	C(6)#1-C(2)-C(4)#1	161.2(12)	C(19)-C(20)-C(15)	120.0
C(18)-C(19)	1.3900	C(3)-C(2)-C(4)#1	154.7(9)	C(26)-C(21)-C(22)	120.0
C(19)-C(20)	1.3900	N(2)-C(2)-C(4)#1	79.6(9)	C(26)-C(21)-N(3)	111.9(11)
C(21)-C(26)	1.3900	C(1)-C(2)-C(4)#1	32.0(4)	C(22)-C(21)-N(3)	128.0(11)
C(21)-C(22)	1.3901	C(5)#1-C(2)-C(1)#1	160.4(14)	C(23)-C(22)-C(21)	120.0
C(22)-C(23)	1.3899	C(6)#1-C(2)-C(1)#1	65.2(9)	C(22)-C(23)-C(24)	120.0
C(23)-C(24)	1.3900	C(3)-C(2)-C(1)#1	26.9(4)	C(23)-C(24)-C(25)	120.0
C(24)-C(25)	1.3900	N(2)-C(2)-C(1)#1	151.8(10)	C(26)-C(25)-C(24)	120.0
C(25)-C(26)	1.3900	C(1)-C(2)-C(1)#1	96.8(7)	C(21)-C(26)-C(25)	120.0
C(27)-C(28)	1.174(10)	C(4)#1-C(2)-C(1)#1	127.7(8)	C(27)-C(28)-C(29)	176.9(14)
C(28)-C(29)	1.422(13)	C(5)#1-C(2)-C(2)#1	144.6(16)	C(30)-C(29)-C(34)	117.5(9)
C(29)-C(30)	1.393(12)	C(6)#1-C(2)-C(2)#1	111.9(12)	C(30)-C(29)-C(28)	123.2(10)
C(29)-C(34)	1.415(14)	C(3)-C(2)-C(2)#1	73.7(7)	C(34)-C(29)-C(28)	119.3(9)
C(30)-C(31)	1.401(16)	N(2)-C(2)-C(2)#1	160.9(11)	C(29)-C(30)-C(31)	118.6(10)
C(31)-C(32)	1.406(16)	C(1)-C(2)-C(2)#1	49.9(6)	C(30)-C(31)-C(32)	122.4(10)
C(32)-C(33)	1.371(17)	C(4)#1-C(2)-C(2)#1	81.2(7)	C(33)-C(32)-C(31)	118.5(13)
C(32)-N(4)	1.49(3)	C(1)#1-C(2)-C(2)#1	46.9(5)	C(33)-C(32)-N(4)	124.3(15)
N(4)-C(35)	1.38(3)	C(5)#1-C(2)-C(3)#1	107.3(14)	C(31)-C(32)-N(4)	117.0(16)
N(4)-C(41)	1.49(3)	C(6)#1-C(2)-C(3)#1	149.5(11)	C(35)-N(4)-C(32)	133(2)
C(33)-C(34)	1.366(17)	C(3)-C(2)-C(3)#1	112.4(6)	C(35)-N(4)-C(41)	120.3(17)
C(35)-C(36)	1.356(11)	N(2)-C(2)-C(3)#1	122.2(9)	C(32)-N(4)-C(41)	105.7(18)
C(35)-C(40)	1.386(10)	C(1)-C(2)-C(3)#1	11.5(5)	C(34)-C(33)-C(32)	119.5(12)
C(36)-C(37)	1.329(12)	C(4)#1-C(2)-C(3)#1	42.6(6)	C(33)-C(34)-C(29)	123.4(10)
C(37)-C(38)	1.351(14)	C(1)#1-C(2)-C(3)#1	85.6(5)	C(36)-C(35)-N(4)	117.1(14)
C(38)-C(39)	1.349(14)	C(2)#1-C(2)-C(3)#1	38.7(4)	C(36)-C(35)-C(40)	117.2(8)
C(39)-C(40)	1.375(12)	C(5)#1-C(2)-C(3)#2	131.1(12)	N(4)-C(35)-C(40)	125.7(14)
C(41)-C(46)	1.359(11)	C(6)#1-C(2)-C(3)#2	79.6(9)	C(37)-C(36)-C(35)	123.0(10)
C(41)-C(42)	1.371(11)	C(3)-C(2)-C(3)#2	55.9(6)	C(36)-C(37)-C(38)	119.9(11)
C(42)-C(43)	1.373(11)	N(2)-C(2)-C(3)#2	140.4(7)	C(39)-C(38)-C(37)	120.0(10)
C(43)-C(44)	1.351(14)	C(1)-C(2)-C(3)#2	82.1(6)	C(38)-C(39)-C(40)	120.2(9)
C(44)-C(45)	1.341(13)	C(4)#1-C(2)-C(3)#2	103.1(5)	C(39)-C(40)-C(35)	119.8(9)
C(45)-C(46)	1.402(11)	C(1)#1-C(2)-C(3)#2	38.3(5)	C(46)-C(41)-C(42)	120.8(9)
C(4)#1-S(1)-N(2)	71.2(4)	C(2)#1-C(2)-C(3)#2	45.1(5)	C(46)-C(41)-N(4)	129.7(15)

C(4)#1-S(1)-N(1)	29.9(3)	C(3)#1-C(2)-C(3)#2	71.7(4)	C(42)-C(41)-N(4)	109.4(14)
N(2)-S(1)-N(1)	100.3(4)	C(1)#1-C(3)-C(6)#1	130(2)	C(41)-C(42)-C(43)	119.5(10)
C(4)#1-S(1)-C(5)#1	50.2(5)	C(1)#1-C(3)-C(2)	91.7(14)	C(44)-C(43)-C(42)	120.8(10)
N(2)-S(1)-C(5)#1	21.3(4)	C(44)-C(45)-C(46)	121.6(10)	C(45)-C(44)-C(43)	119.5(9)
N(1)-S(1)-C(5)#1	79.7(4)	C(41)-C(46)-C(45)	117.7(9)		

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,-y+2,-z+2 #2 -x+2,-y,-z+2

Table S10. Anisotropic displacement parameters (Å2x 103) for 3b. The anisotropic displacement factor exponent takes the form: -2π2[h2a*2U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
S(1)	108(2)	114(2)	96(2)	-52(2)	-33(1)	20(2)
N(1)	66(4)	68(4)	65(4)	-18(3)	-11(3)	7(3)
N(2)	80(5)	70(6)	77(5)	-19(4)	-36(4)	4(4)
N(3)	41(5)	61(6)	61(6)	-7(4)	-19(4)	-7(4)
C(1)	48(4)	46(5)	50(5)	-4(4)	-12(4)	-6(3)
C(2)	53(4)	58(5)	58(5)	-9(4)	-18(4)	-8(3)
C(3)	41(4)	48(5)	75(6)	-7(4)	-24(4)	-7(3)
C(4)	42(4)	62(6)	91(6)	-21(5)	-28(4)	6(4)
C(5)	46(4)	53(6)	93(9)	-25(5)	-25(4)	-2(4)
C(6)	41(4)	53(5)	69(5)	-14(4)	-21(3)	3(3)
C(7)	45(4)	62(6)	78(6)	-20(5)	-26(4)	-3(3)
C(8)	44(4)	53(6)	72(7)	-4(5)	-20(4)	-8(3)
C(9)	40(4)	55(6)	59(7)	-14(5)	-17(4)	-3(3)
C(10)	54(5)	70(7)	67(7)	-20(5)	-26(4)	1(4)
C(11)	49(4)	70(7)	69(7)	-30(6)	-23(5)	3(4)
C(12)	44(5)	60(8)	59(7)	-18(5)	-25(4)	-1(4)
C(13)	45(5)	74(9)	67(7)	-31(5)	-19(5)	4(5)
C(14)	51(5)	72(7)	70(6)	-28(5)	-23(4)	1(5)
C(15)	31(7)	68(7)	55(7)	-14(5)	-13(6)	3(5)
C(16)	83(15)	72(7)	91(11)	-13(6)	-48(11)	-3(6)
C(17)	86(9)	67(7)	98(8)	-22(5)	-57(7)	8(5)
C(18)	60(7)	64(7)	89(7)	-20(5)	-47(6)	11(5)
C(19)	59(6)	65(6)	72(6)	-20(4)	-32(5)	13(4)
C(20)	49(7)	71(6)	63(6)	-10(5)	-25(5)	-6(5)
C(21)	39(6)	60(6)	55(7)	-12(5)	-28(5)	-4(4)
C(22)	55(8)	51(6)	80(10)	-5(6)	-7(7)	-6(5)
C(23)	56(7)	53(6)	80(9)	-9(5)	-4(6)	-6(5)

C(24)	86(8)	52(6)	67(8)	-7(5)	0(6)	-18(5)
C(25)	80(7)	61(6)	61(7)	-9(5)	2(5)	-24(5)
C(26)	58(6)	69(6)	58(6)	-14(4)	-21(4)	-13(4)
C(27)	41(4)	68(7)	64(6)	9(4)	-26(4)	-10(4)
C(28)	44(4)	84(8)	68(7)	-4(5)	-24(4)	-10(4)
C(29)	35(4)	68(7)	62(6)	-9(5)	-21(4)	-6(4)
C(30)	37(4)	84(7)	67(8)	-23(6)	-25(5)	13(4)
C(31)	40(5)	79(8)	66(7)	-39(6)	-26(4)	20(5)
C(32)	31(4)	47(7)	59(7)	-15(5)	-15(4)	8(4)
N(4)	35(6)	76(8)	95(9)	-32(7)	-33(5)	19(5)
C(33)	42(5)	75(9)	67(7)	-29(5)	-26(5)	11(5)
C(34)	35(4)	76(6)	62(5)	-7(5)	-19(3)	-2(4)
C(35)	45(9)	80(8)	71(8)	-20(6)	-18(7)	6(5)
C(36)	71(12)	78(8)	69(8)	-16(5)	-16(9)	0(6)
C(37)	76(7)	85(7)	90(7)	-22(5)	-28(7)	5(5)
C(38)	80(7)	72(7)	88(7)	-35(5)	-21(6)	12(5)
C(39)	83(9)	80(7)	78(7)	-23(5)	-38(6)	8(6)
C(40)	51(6)	74(7)	83(8)	-20(5)	-28(5)	6(5)
C(41)	43(7)	64(7)	79(9)	-20(6)	-22(6)	8(5)
C(42)	52(7)	59(6)	78(10)	-11(6)	-21(7)	8(5)
C(43)	59(7)	64(5)	82(8)	-15(5)	-12(5)	-6(5)
C(44)	53(5)	65(6)	49(5)	-12(5)	-7(4)	-9(4)
C(45)	68(5)	62(6)	56(6)	-16(4)	0(5)	-18(4)
C(46)	66(6)	84(7)	62(6)	-27(5)	-7(4)	-15(5)

Table S11. Hydrogen coordinates (x 104) and isotropic displacement parameters (Å2 103) for **3b.**

	x	y	z	U(eq)
H(4)	12193	8014	9107	79
H(5)	9673	8692	8312	75
H(10)	4257	11022	6403	77
H(11)	1671	11966	5771	74
H(13)	341	13722	8618	74
H(14)	3071	12722	9270	76
H(16)	-765	11020	6495	98
H(17)	-2086	10423	5102	100
H(18)	-3608	12252	3710	86
H(19)	-3809	14677	3713	81
H(20)	-2488	15274	5106	74
H(22)	-3640	13973	8268	77
H(23)	-5195	16059	8878	78
H(24)	-4434	18256	8172	83
H(25)	-2118	18367	6856	80
H(26)	-562	16282	6247	73
H(30)	4401	11084	6875	78
H(31)	1821	12106	6070	74
H(33)	108	14074	8775	75
H(34)	2642	13120	9559	71
H(36)	-606	11087	6625	90
H(37)	-1558	10122	5356	103
H(38)	-3214	11594	3909	97
H(39)	-3936	14050	3770	98
H(40)	-2901	15063	5037	84
H(42)	-3520	13768	8075	79
H(43)	-5305	15593	8875	83
H(44)	-4785	17852	8525	68
H(45)	-2586	18344	7290	74
H(46)	-613	16483	6587	83

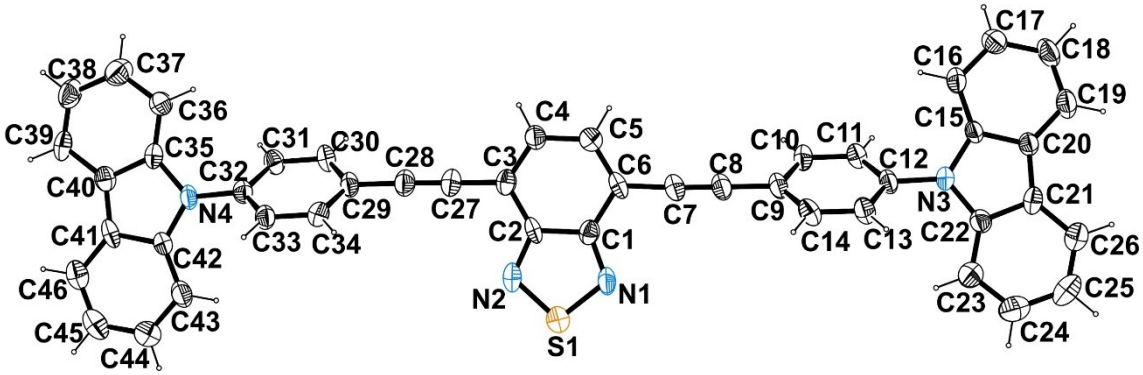


Table S12. Crystal data and structure refinement for **3c**.

Empirical formula	C48 H28 Cl6 N4 S	
Formula weight	905.50	
Temperature	290(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 2_1/c	
Unit cell dimensions	a = 11.8955(16) Å	α= 90°.
	b = 17.813(2) Å	β= 95.537(3)°.
	c = 20.278(3) Å	γ = 90°.
Volume	4276.9(10) Å^3	
Z	4	
Density (calculated)	1.406 Mg/m^3	
Absorption coefficient	0.491 mm^{-1}	
F(000)	1848	
Crystal size	0.120 x 0.080 x 0.040 mm^3	
Theta range for data collection	2.225 to 24.999°.	
Index ranges	-14≤h≤14, -19≤k≤21, -18≤l≤24	
Reflections collected	23480	
Independent reflections	7454 [R(int) = 0.1165]	
Completeness to theta = 25.242°	96.2 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.746 and 0.679	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7454 / 0 / 532	
Goodness-of-fit on F^2	0.945	
Final R indices [I>2sigma(I)]	R1 = 0.0898, wR2 = 0.2264	
R indices (all data)	R1 = 0.2317, wR2 = 0.2921	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.791 and -0.448 e.Å^{-3}	

Table S13. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3)

for **3c.**U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	7604(2)	3299(1)	2371(1)	85(1)
Cl(1)	14425(3)	2937(2)	3011(1)	145(1)
Cl(2)	14520(2)	2842(2)	4432(1)	117(1)
Cl(5)	9547(3)	2406(2)	9242(2)	189(2)
Cl(4)	10130(3)	2703(2)	7953(2)	166(1)
Cl(6)	11556(3)	1813(2)	8844(2)	220(2)
N(3)	15305(4)	5966(3)	3859(3)	57(1)
N(4)	-606(4)	4404(3)	1028(2)	58(1)
N(1)	8538(4)	3931(3)	2607(3)	70(2)
C(15)	15806(4)	6675(4)	3922(3)	50(2)
C(7)	9677(5)	5377(4)	2949(3)	64(2)
C(1)	8016(5)	4594(4)	2562(3)	57(2)
C(11)	13601(5)	6164(4)	3108(3)	60(2)
C(12)	14131(4)	5825(4)	3663(3)	56(2)
C(29)	2810(5)	4864(4)	1628(3)	58(2)
C(10)	12459(5)	6048(4)	2938(3)	62(2)
N(2)	6508(4)	3815(3)	2201(3)	72(2)
C(32)	544(5)	4577(4)	1248(3)	56(2)
C(30)	2268(5)	5219(4)	1076(3)	61(2)
C(42)	-1040(5)	3689(4)	927(3)	59(2)
C(5)	7781(5)	5917(4)	2635(3)	65(2)
C(3)	6130(5)	5168(4)	2236(3)	58(2)
C(16)	15328(5)	7382(4)	3796(3)	61(2)
C(9)	11836(5)	5578(4)	3301(3)	61(2)
C(2)	6839(5)	4526(4)	2325(3)	53(2)
C(22)	16127(5)	5422(4)	4047(3)	58(2)
C(21)	17151(5)	5799(4)	4225(3)	61(2)
C(8)	10650(5)	5466(4)	3120(3)	66(2)
C(13)	13515(5)	5354(4)	4045(3)	66(2)
C(43)	-493(6)	2997(4)	1028(4)	74(2)
C(40)	-2457(5)	4522(4)	654(3)	58(2)
C(33)	1070(5)	4245(4)	1809(3)	59(2)
C(4)	6623(5)	5854(4)	2404(3)	60(2)

C(34)	2188(5)	4381(4)	1998(3)	64(2)
C(20)	16940(5)	6588(4)	4161(3)	53(2)
C(41)	-2189(5)	3744(4)	692(3)	62(2)
C(28)	3986(5)	4984(4)	1834(3)	70(2)
C(27)	4961(5)	5065(4)	2006(3)	66(2)
C(14)	12390(5)	5238(4)	3861(3)	67(2)
C(31)	1156(5)	5075(4)	887(3)	60(2)
C(6)	8484(5)	5315(4)	2717(3)	58(2)
C(17)	16032(6)	7996(4)	3903(4)	71(2)
C(35)	-1475(4)	4938(4)	859(3)	54(2)
C(26)	18117(5)	5365(5)	4417(3)	73(2)
C(38)	-3455(6)	5694(5)	480(4)	86(2)
C(36)	-1467(5)	5704(4)	888(3)	68(2)
C(19)	17625(6)	7224(5)	4268(4)	77(2)
C(37)	-2459(7)	6085(5)	695(4)	88(2)
C(39)	-3471(5)	4931(5)	472(3)	76(2)
C(23)	16060(6)	4651(5)	4022(4)	79(2)
C(18)	17164(6)	7922(5)	4133(4)	81(2)
C(46)	-2799(6)	3086(5)	547(4)	76(2)
C(25)	18041(7)	4599(6)	4408(4)	92(3)
C(48)	10186(7)	2035(5)	8590(4)	105(3)
C(24)	17021(7)	4246(5)	4207(4)	88(2)
C(45)	-2268(7)	2407(5)	631(4)	90(2)
C(47)	14762(9)	2414(6)	3714(5)	136(4)
C(44)	-1122(7)	2361(4)	874(4)	84(2)
Cl(3)	16089(3)	2050(2)	3717(2)	175(1)

Table S14. Bond lengths [Å] and angles [°] for **3c**.

S(1)-N(2)	1	C(45)-H(45)		C(42)-C(43)-H(43)	12
S(1)-N(1)	1	C(47)-Cl(3)		C(35)-C(40)-C(39)	11
Cl(1)-C(47)	1	C(47)-H(47)		C(35)-C(40)-C(41)	10
Cl(2)-C(47)	1	C(44)-H(44)		C(39)-C(40)-C(41)	13
Cl(5)-C(48)	1	N(2)-S(1)-N(1)	10	C(34)-C(33)-C(32)	12
Cl(4)-C(48)	1	C(15)-N(3)-C(22)	10	C(34)-C(33)-H(33)	11
Cl(6)-C(48)	1	C(36)-C(37)		C(32)-C(33)-H(33)	11
N(3)-C(15)	1	C(36)-H(36)		C(3)-C(4)-C(5)	12
N(3)-C(22)	1	C(19)-C(18)		C(3)-C(4)-H(4)	11

N(3)-C(12)	1	C(19)-H(19)		C(5)-C(4)-H(4)	11
N(4)-C(42)	1	C(37)-H(37)			
N(4)-C(35)	1	C(39)-H(39)		C(33)-C(34)-C(29)	12
N(4)-C(32)	1	C(23)-C(24)		C(33)-C(34)-H(34)	11
N(1)-C(1)	1	C(23)-H(23)		C(29)-C(34)-H(34)	11
C(15)-C(16)	1	C(15)-N(3)-C(12)	12	C(19)-C(20)-C(15)	11
C(15)-C(20)	1	C(22)-N(3)-C(12)	12	C(19)-C(20)-C(21)	13
C(7)-C(8)	1	C(42)-N(4)-C(35)	10	C(15)-C(20)-C(21)	10
C(7)-C(6)	1	C(42)-N(4)-C(32)	12	C(46)-C(41)-C(42)	11
C(1)-C(6)	1	C(35)-N(4)-C(32)	12	C(46)-C(41)-C(40)	13
C(1)-C(2)	1	C(1)-N(1)-S(1)	10	C(42)-C(41)-C(40)	10
C(11)-C(12)	1	C(16)-C(15)-N(3)	12	C(27)-C(28)-C(29)	17
C(11)-C(10)	1	C(16)-C(15)-C(20)	12	C(28)-C(27)-C(3)	17
C(11)-H(11)	0	N(3)-C(15)-C(20)	10	C(13)-C(14)-C(9)	12
C(12)-C(13)	1	C(8)-C(7)-C(6)	17	C(13)-C(14)-H(14)	11
C(29)-C(30)	1	N(1)-C(1)-C(6)	12	C(9)-C(14)-H(14)	11
C(29)-C(34)	1	N(1)-C(1)-C(2)	11	C(30)-C(31)-C(32)	12
C(29)-C(28)	1	C(6)-C(1)-C(2)	11	C(30)-C(31)-H(31)	11
C(10)-C(9)	1	C(12)-C(11)-C(10)	11	C(32)-C(31)-H(31)	11
C(10)-H(10)	0	C(12)-C(11)-H(11)	12	C(5)-C(6)-C(1)	11
N(2)-C(2)	1	C(10)-C(11)-H(11)	12	C(5)-C(6)-C(7)	12
C(32)-C(33)	1	C(11)-C(12)-C(13)	11	C(1)-C(6)-C(7)	11
C(32)-C(31)	1	C(11)-C(12)-N(3)	12	C(16)-C(17)-C(18)	12
C(30)-C(31)	1	C(13)-C(12)-N(3)	12	C(16)-C(17)-H(17)	11
C(30)-H(30)	0	C(30)-C(29)-C(34)	11	C(18)-C(17)-H(17)	11
C(42)-C(43)	1	C(30)-C(29)-C(28)	12	C(36)-C(35)-C(40)	12
C(42)-C(41)	1	C(34)-C(29)-C(28)	11	C(36)-C(35)-N(4)	13
C(5)-C(6)	1	C(9)-C(10)-C(11)	12	C(40)-C(35)-N(4)	10
C(5)-C(4)	1	C(9)-C(10)-H(10)	11	C(25)-C(26)-C(21)	11
C(5)-H(5)	0	C(11)-C(10)-H(10)	11	C(25)-C(26)-H(26)	12
C(3)-C(4)	1	C(2)-N(2)-S(1)	10	C(21)-C(26)-H(26)	12
C(3)-C(2)	1	C(33)-C(32)-C(31)	11	C(39)-C(38)-C(37)	12
C(3)-C(27)	1	C(33)-C(32)-N(4)	12	C(39)-C(38)-H(38)	11
C(16)-C(17)	1	C(31)-C(32)-N(4)	12	C(37)-C(38)-H(38)	11
C(16)-H(16)	0	C(31)-C(30)-C(29)	12	C(35)-C(36)-C(37)	11
C(9)-C(14)	1	C(31)-C(30)-H(30)	11	C(35)-C(36)-H(36)	12
C(9)-C(8)	1	C(29)-C(30)-H(30)	11	C(37)-C(36)-H(36)	12
C(22)-C(23)	1	N(4)-C(42)-C(43)	12	C(18)-C(19)-C(20)	11

C(22)-C(21)	1	N(4)-C(42)-C(41)	10	C(18)-C(19)-H(19)	12
C(21)-C(26)	1	C(43)-C(42)-C(41)	12	C(20)-C(19)-H(19)	12
C(21)-C(20)	1	C(6)-C(5)-C(4)	12	C(36)-C(37)-C(38)	12
C(13)-C(14)	1	C(6)-C(5)-H(5)	11	C(36)-C(37)-H(37)	11
C(13)-H(13)	0	C(4)-C(5)-H(5)	11	C(38)-C(37)-H(37)	11
C(43)-C(44)	1	C(4)-C(3)-C(2)	11	C(38)-C(39)-C(40)	11
C(43)-H(43)	0	C(4)-C(3)-C(27)	12	C(38)-C(39)-H(39)	12
C(40)-C(35)	1	C(2)-C(3)-C(27)	11	C(40)-C(39)-H(39)	12
C(40)-C(39)	1	C(17)-C(16)-C(15)	11	C(22)-C(23)-C(24)	11
C(40)-C(41)	1	C(17)-C(16)-H(16)	12	C(26)-C(25)-C(24)	12
C(33)-C(34)	1	C(15)-C(16)-H(16)	12	C(26)-C(25)-H(25)	11
C(33)-H(33)	0	C(10)-C(9)-C(14)	11	C(24)-C(25)-H(25)	11
C(4)-H(4)	0	C(10)-C(9)-C(8)	12	Cl(6)-C(48)-Cl(5)	10
C(34)-H(34)	0	C(14)-C(9)-C(8)	12	Cl(6)-C(48)-Cl(4)	11
C(20)-C(19)	1	N(2)-C(2)-C(3)	12	Cl(5)-C(48)-Cl(4)	10
C(41)-C(46)	1	N(2)-C(2)-C(1)	11	Cl(6)-C(48)-H(48)	10
C(28)-C(27)	1	C(3)-C(2)-C(1)	12	Cl(5)-C(48)-H(48)	10
C(14)-H(14)	0	C(23)-C(22)-N(3)	12	Cl(4)-C(48)-H(48)	10
C(31)-H(31)	0	C(23)-C(22)-C(21)	12	C(23)-C(24)-C(25)	12
C(17)-C(18)	1	N(3)-C(22)-C(21)	10	C(23)-C(24)-H(24)	11
C(17)-H(17)	0	C(22)-C(21)-C(26)	11	C(25)-C(24)-H(24)	11
C(35)-C(36)	1	C(22)-C(21)-C(20)	10	C(46)-C(45)-C(44)	12
C(26)-C(25)	1	C(22)-C(23)-H(23)	12	C(46)-C(45)-H(45)	11
C(26)-H(26)	0	C(24)-C(23)-H(23)	12	C(44)-C(45)-H(45)	11
C(38)-C(39)	1	C(19)-C(18)-C(17)	12	Cl(2)-C(47)-Cl(3)	11
C(38)-C(37)	1	C(19)-C(18)-H(18)	11	Cl(2)-C(47)-Cl(1)	11
C(38)-H(38)	0	C(17)-C(18)-H(18)	11	Cl(3)-C(47)-Cl(1)	11
C(18)-H(18)	0	C(45)-C(46)-C(41)	11	Cl(2)-C(47)-H(47)	10
C(46)-C(45)	1	C(45)-C(46)-H(46)	12	Cl(3)-C(47)-H(47)	10
C(46)-H(46)	0	C(41)-C(46)-H(46)	12	Cl(1)-C(47)-H(47)	10
C(25)-C(24)	1	C(26)-C(21)-C(20)	13	C(43)-C(44)-C(45)	12
C(25)-H(25)	0	C(7)-C(8)-C(9)	17	C(43)-C(44)-H(44)	11
C(48)-H(48)	0	C(14)-C(13)-C(12)	11	C(45)-C(44)-H(44)	11
C(24)-H(24)	0	C(14)-C(13)-H(13)	12	C(44)-C(43)-H(43)	12
C(45)-C(44)	1	C(12)-C(13)-H(13)	12	C(44)-C(43)-C(42)	11

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,-y+2,-z+2 #2 -x+2,-y,-z+2

Table S15. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **3c** The anisotropic 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}
S(1)	64(1)	76(2)	113(2)	-1(1)	0(1)	-6(1)
Cl(1)	188(3)	154(3)	91(2)	35(2)	5(2)	-12(2)
Cl(2)	121(2)	148(2)	84(2)	-7(2)	19(1)	-31(1)
Cl(5)	210(3)	192(4)	177(3)	-32(3)	77(3)	-66(3)
Cl(4)	218(3)	155(3)	119(2)	26(2)	-14(2)	-81(2)
Cl(6)	169(3)	159(3)	310(6)	-58(3)	-90(3)	24(2)
N(3)	39(3)	61(4)	69(4)	0(3)	-4(2)	-3(3)
N(4)	35(3)	69(4)	69(4)	-3(3)	1(2)	-10(3)
N(1)	47(3)	76(5)	84(4)	3(3)	-4(3)	-10(3)
C(15)	39(4)	52(5)	60(4)	-4(3)	2(3)	-10(3)
C(7)	53(4)	76(5)	63(5)	-11(4)	6(3)	-14(3)
C(1)	47(4)	73(5)	51(4)	11(4)	1(3)	-3(4)
C(11)	49(4)	70(5)	59(5)	0(4)	1(3)	-14(3)
C(12)	37(4)	63(5)	67(5)	-10(4)	2(3)	-13(3)
C(29)	42(4)	70(5)	62(5)	-19(4)	4(3)	-7(3)
C(10)	46(4)	77(5)	61(5)	-6(4)	-7(3)	-5(3)
N(2)	47(3)	87(5)	80(4)	1(3)	3(3)	-3(3)
C(32)	44(4)	64(5)	60(4)	-3(4)	8(3)	-4(3)
C(30)	46(4)	83(5)	52(4)	0(4)	2(3)	-17(3)
C(42)	43(4)	58(5)	75(5)	2(4)	5(3)	-11(3)
C(5)	58(4)	63(5)	73(5)	-2(4)	4(3)	-3(3)
C(3)	49(4)	78(6)	46(4)	2(3)	4(3)	0(4)
C(16)	42(4)	74(5)	66(5)	-6(4)	2(3)	-8(3)
C(9)	44(4)	71(5)	67(5)	-13(4)	3(3)	-14(3)
C(2)	40(4)	71(5)	49(4)	-4(3)	5(3)	-21(3)
C(22)	56(4)	57(5)	57(4)	-2(3)	-1(3)	-6(3)
C(21)	41(4)	84(6)	55(4)	7(4)	-5(3)	0(3)
C(8)	44(4)	77(5)	77(5)	-14(4)	2(3)	-14(3)
C(13)	53(4)	77(5)	65(5)	2(4)	-5(3)	-16(3)
C(43)	55(4)	79(6)	90(6)	-11(4)	12(4)	-17(4)
C(40)	52(4)	72(5)	49(4)	3(3)	2(3)	-5(3)
C(33)	42(4)	67(5)	68(5)	6(4)	7(3)	-3(3)
C(4)	50(4)	63(5)	65(5)	9(4)	-1(3)	-4(3)
C(34)	53(4)	68(5)	70(5)	3(4)	-1(3)	5(3)
C(20)	43(4)	58(5)	57(4)	6(3)	-1(3)	-8(3)

C(41)	44(4)	90(6)	53(4)	-5(4)	2(3)	-29(4)
C(28)	46(4)	83(5)	80(5)	-15(4)	-3(3)	-1(3)
C(27)	45(4)	88(6)	65(5)	-5(4)	0(3)	1(3)
C(14)	62(5)	74(5)	66(5)	-1(4)	8(4)	-26(3)
C(31)	52(4)	73(5)	52(4)	2(3)	-6(3)	-13(3)
C(6)	45(4)	75(5)	53(4)	-11(3)	6(3)	-26(4)
C(17)	72(5)	65(5)	78(5)	-6(4)	10(4)	-7(4)
C(35)	36(4)	75(6)	49(4)	-1(3)	1(3)	-2(3)
C(26)	58(5)	89(6)	72(5)	9(4)	5(3)	4(4)
C(38)	61(5)	102(7)	90(6)	-6(5)	-15(4)	15(4)
C(36)	59(5)	64(6)	79(5)	-12(4)	-7(3)	-2(4)
C(19)	49(4)	93(7)	88(6)	5(5)	-6(4)	-17(4)
C(37)	83(6)	88(6)	91(6)	-11(5)	-6(4)	14(5)
C(39)	37(4)	110(7)	79(5)	2(5)	-5(3)	3(4)
C(23)	70(5)	75(6)	92(6)	9(5)	1(4)	1(4)
C(18)	63(5)	80(6)	99(6)	5(5)	-1(4)	-33(4)
C(46)	61(5)	96(7)	71(5)	6(5)	1(4)	-19(5)
C(25)	77(6)	120(8)	79(6)	20(5)	8(4)	37(5)
C(48)	108(7)	96(7)	105(7)	-9(5)	-29(5)	-38(5)
C(24)	104(7)	76(6)	83(6)	2(5)	5(5)	18(5)
C(45)	86(6)	98(8)	87(6)	-10(5)	7(5)	-37(5)
C(47)	155(9)	139(10)	111(9)	3(7)	-9(7)	-17(7)
C(44)	85(6)	73(6)	95(6)	-2(4)	11(5)	-7(4)
Cl(3)	239(4)	145(3)	141(3)	-13(2)	22(2)	60(2)

Table S16. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **3c.**

	x	y	z	U(eq)
–				
H(11)	14009	6471	2846	72
H(10)	12104	6293	2571	75
H(30)	2663	5555	835	73
H(5)	8074	6392	2736	78
H(16)	14569	7437	3647	73
H(13)	13865	5120	4420	79
H(43)	263	2968	1191	89
H(33)	663	3926	2061	71
H(4)	6181	6285	2364	72
H(34)	2536	4151	2376	77
H(14)	11983	4924	4116	80
H(31)	802	5310	513	72
H(17)	15739	8474	3818	86
H(26)	18801	5597	4550	88
H(38)	-4108	5960	341	103
H(36)	-812	5963	1035	82
H(19)	18381	7175	4428	93
H(37)	-2467	6607	708	106
H(39)	-4141	4676	349	91
H(23)	15384	4412	3883	95
H(18)	17614	8347	4196	98
H(46)	-3561	3109	393	92
H(25)	18676	4311	4537	110
H(48)	9782	1581	8429	127
H(24)	16990	3725	4197	106
H(45)	-2671	1969	526	108
H(47)	14252	1981	3675	163
H(44)	-783	1892	933	101

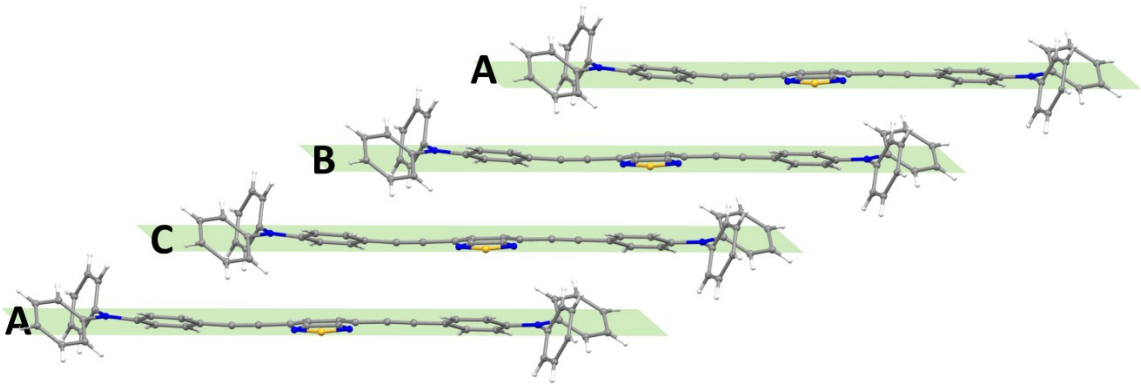


Figure S8. Front view of 1D lamellae arrangement for molecules of **3b**. Green panels show molecules in the same plane.

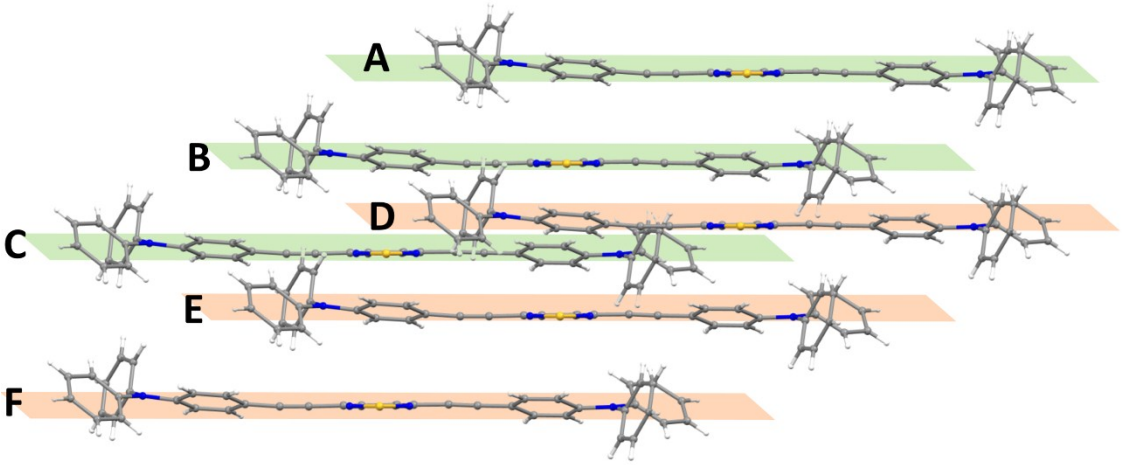


Figure S9. Front view of 2D lamellae arrangement for molecules of **3b.** Green and orange panels show molecules in the same plane, respectively.

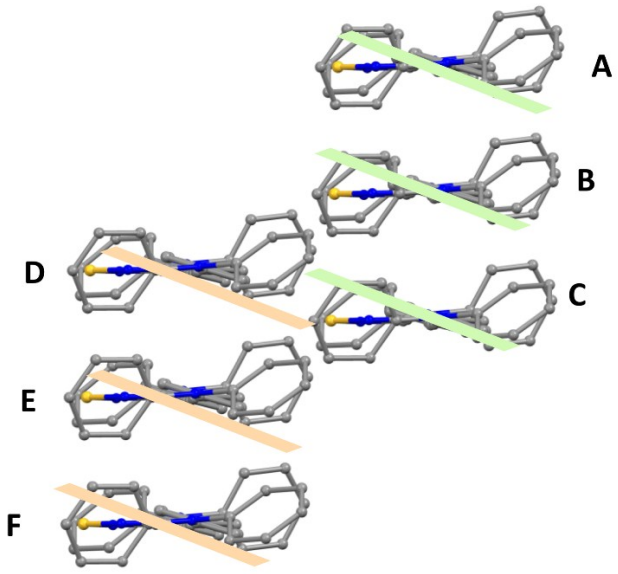


Figure S10. Side view of 2D lamellae arrangement for molecules of **3b.** Green and orange panels show molecules in the same plane, respectively. Hydrogen atoms has been removed to clarify

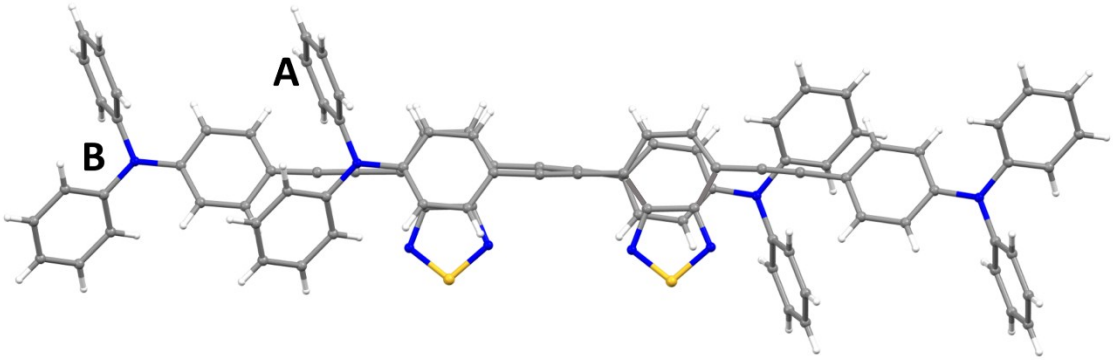


Figure S11. Top view of **3b** molecules in the same lamellae (A and B)

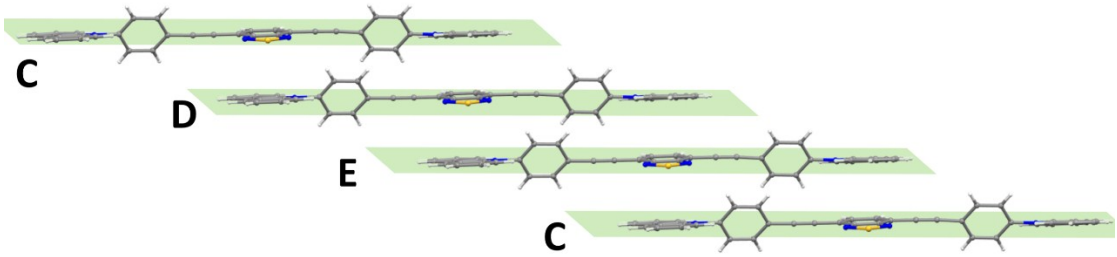


Figure S12. Front view of 1D lamellae arrangement for molecules of **3c.** Green panels show molecules in the same plane, respectively.

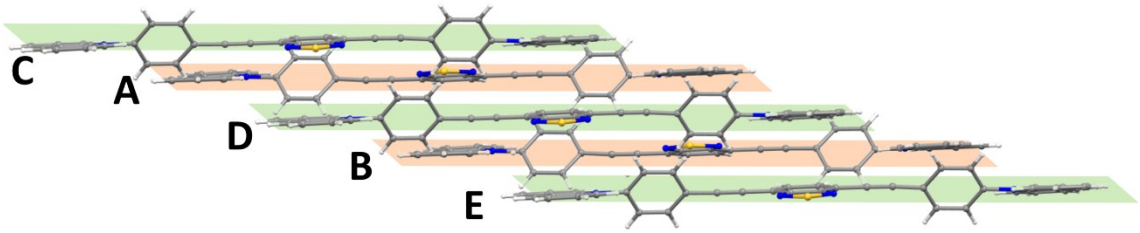


Figure S13. Front view of 2D lamellae arrangement for molecules of **3c.** Green and orange panels show molecules in the same plane, respectively.

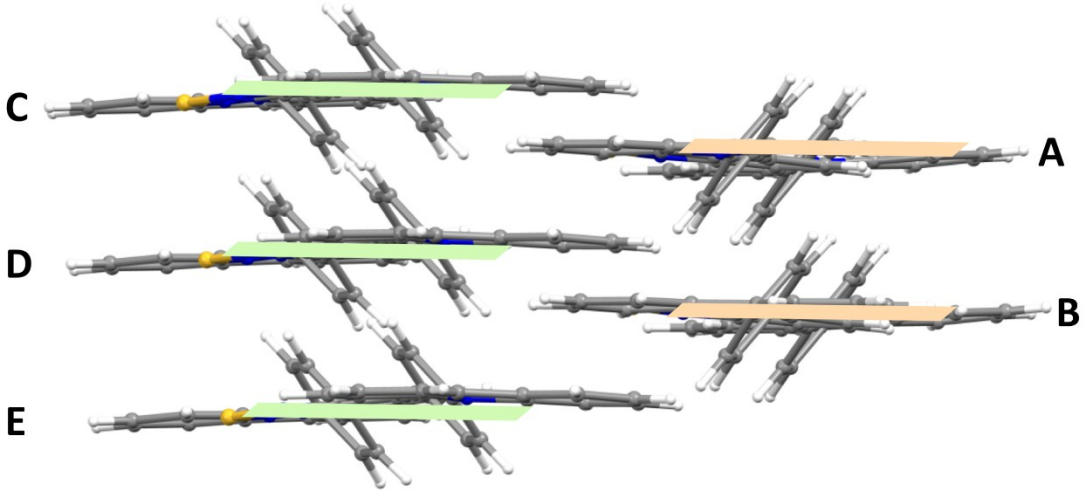


Figure S14. Side view of 2D lamellae arrangement for molecules of **3c.** Green and orange panels show molecules in the same plane, respectively.

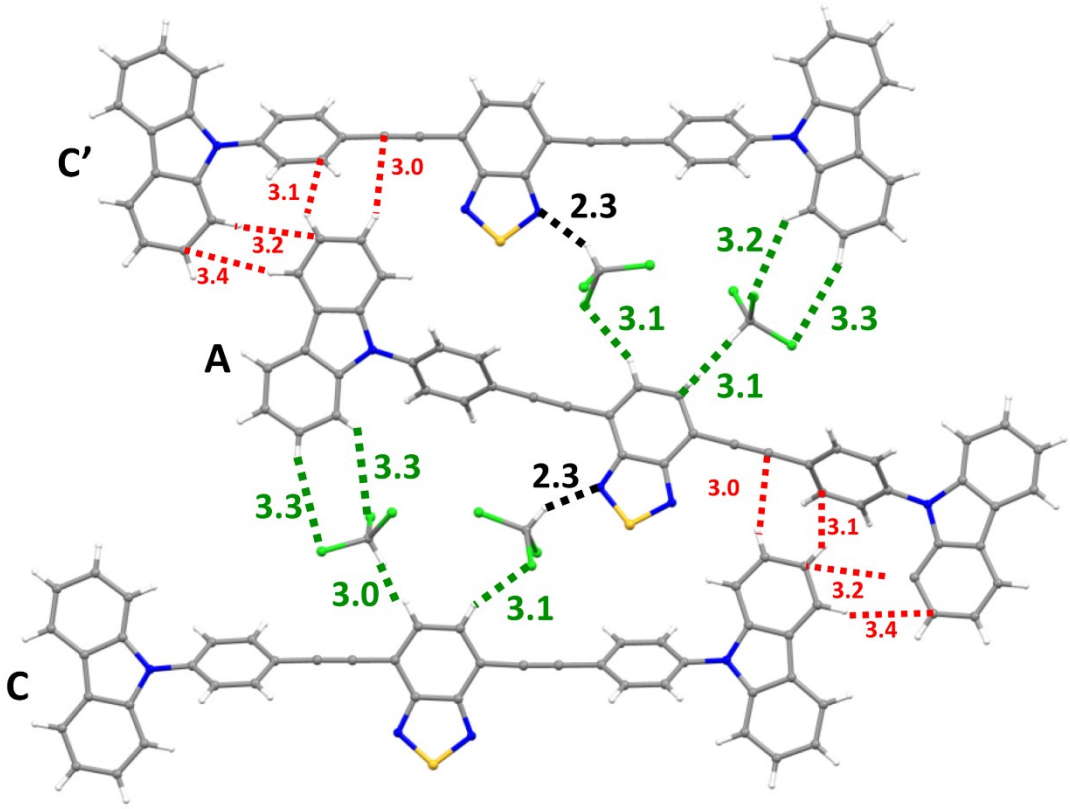


Figure S15. Top view of **3c** molecules of different lamellae (A and C) showing the important role of CH_3Cl solvent molecules in the formation of the crystal packing along b-axis. C and C' are located in the same plane

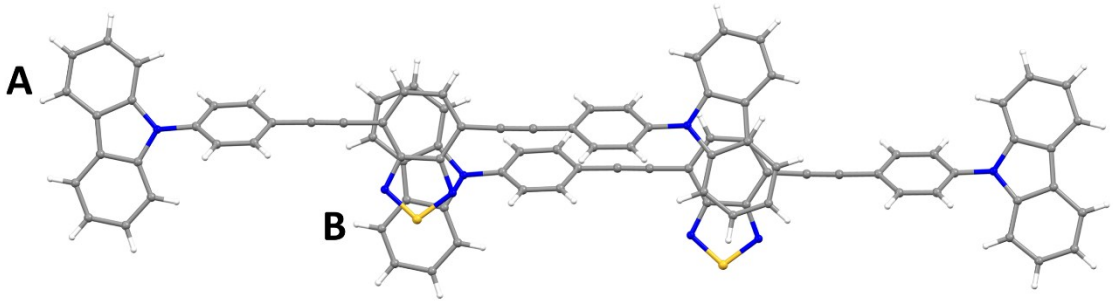
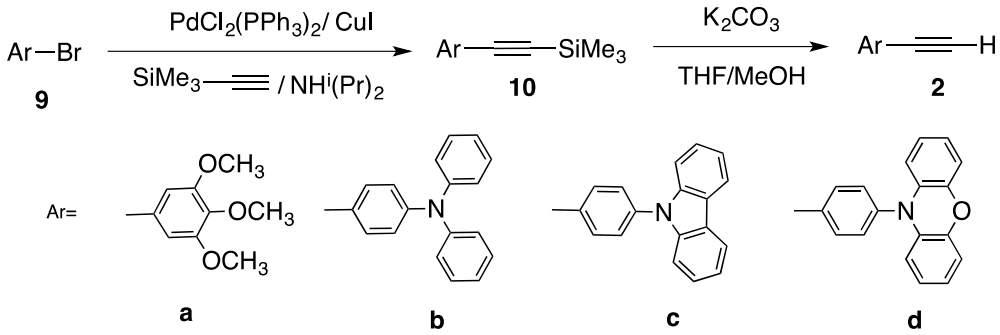


Figure S16. Top view of **3c** molecules in the same lamellae (A and B)

3. Synthesis of aryl alkynyl derivatives



Scheme S1. Synthesis of aryl alkynyl derivatives **2**

3.1 Preparation of arylethynyl silane derivatives (10)

***General procedure**:* To a solution of the corresponding bromide derivative (**9**) (11.87 mmol) in $HN^i(Pr)_2$ (60 mL), $PdCl_2(PPh_3)_2$, (1.645 g, 1.42 mmol) and CuI (0.027 g, 0.14 mmol) were added. Argon was bubbled through the solution for 30 minutes. Then, trimethylsilylacetylene (1.750 g, 17.80 mmol.) were added and the reaction mixture was stirring one hour at 80 ºC. After this time, trimethylsilylacetylene (1.750 g, 17.80 mmol) was added and the mixture was heated five hours. After cooling, the reaction was quenched with 40 mL of saturated ammonium chloride aqueous solution. The aqueous phase was extracted with ethyl eter (3 x 60 mL) and the combined organic layers were dried over $MgSO_4$ and concentrated in vacuo. Flash chromatography in Hex/AcOEt yielded the desired compounds.

3.1.1 Preparation of trimethyl((3,4,5 trimethoxyphenyl)ethynyl)silane (10a)

From derivative **9a** (2.935 g, 11.87 mmol), derivative **10a** (2.790 g, 89%) was obtained as solid by chromatography eluting with Hex/AcOEt (9/1).
The spectral properties and analytical data are in agreement with those reported previously.[17]

3.1.2 Preparation of N,N-diphenyl-4-((trimethylsilyl)ethynyl)aniline(10b)

From derivative **9b** (3.850 g, 11.87 mmol), derivative **10b** (3.324 g, 82%) was obtained as solid by chromatography eluting with Hex/AcOEt (9/1).
The spectral properties and analytical data are in agreement with those reported previously.[18]

3.1.3 Preparation of 9-(4-((trimethylsilyl)ethynyl)phenyl)-9H-carbazole (10c)

From derivative **9c** (3.830 g, 11.87 mmol), derivative **10c** (2.821 g, 70%) was obtained as a solid by chromatography eluting with Hex/AcOEt (9/1).
The spectral properties and analytical data are in agreement with those reported previously.[19]

3.1.4 Preparation of 10-(4-((trimethylsilyl)ethynyl)phenyl)-10H-phenoxazine (10d)

From derivative **9d** (4.000 g, 11.87 mmol), derivative **10d** (2.742 g, 65%) was obtained as a solid by chromatography eluting with Hex
^{1}H-NMR ($CDCl_3$, ppm) δ: 7.68 (d, *J* = 8.8 Hz, 2H, *m*-N-Ph), 7.28 (d, *J* = 8.8 Hz, 2H, *o*-N-Ph), 6.68 (d, *J* = 7.8 Hz, 4H, H1-phenoxacine), 6.64 (t, *J* = 7.8 Hz, 4H, H2- phenoxacine), 6.58 (t, *J* = 7.8 Hz, 4H, H3- phenoxacine), 5.90 (d, *J* = 7.8 Hz, 4H, H4- phenoxacine).

3.2 Preparation of arylethynyl derivatives (2)

General procedure: A mixture of the corresponding arylethynyl silane derivative (**10**) (5.90 mmol) and potassium carbonate (1.630 g, 11.80 mmol) was dissolved in 100 mL of a mixture of THF:MeOH (1:1). The mixture was stirred for 30 minutes at room temperature. Solvent was removed under reduce pressure. Solid residue was dissolved in 100 mL de $CHCl_3$ and washed with water (3 x 30 mL). The combined organic layers were dried over $MgSO_4$ and concentrated in vacuo. Flash chromatography in Hex/AcOEt yielded the desired compounds.

3.2.1 Preparation of 5-ethynyl-1,2,3-trimethoxybenzene (2a)

From derivative **10a** (1.560 g, 5.90 mmol), derivative **2a** (1.840 g, 81%) was obtained as a pale-yellow solid by chromatography eluting with Hex/AcOEt (9/1).
The spectral properties and analytical data are in agreement with those reported previously.[17]

3.2.2 Preparation of 4-ethynyl-N,N-diphenylaniline (2b)

From derivative **10b** (2.020 g, 5.90 mmol), derivative **2b** (1.122 g, 70%) was obtained as a pale yellow solid by chromatography eluting with Hex/AcOEt (9/1).
The spectral properties and analytical data are in agreement with those reported previously.[18]

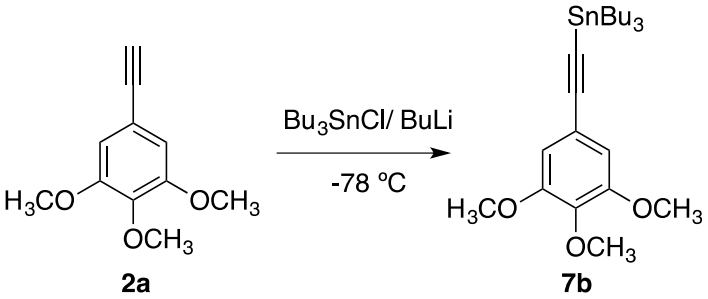
3.2.3 Preparation of 9-(4-ethynylphenyl)-9H-carbazole (2c)

From derivative **10c** (2.000 g, 5.90 mmol), derivative **2c** (1.457 g, 92%) was obtained as a pale yellow solid by chromatography eluting with hexane.
Reproduced by permission of Wiley Periodicals, Inc. Journal of Polymer Science: Part A: Polymer Chemistry , Vol. 48, 3744–3757 (2010)
The spectral properties and analytical data are in agreement with those reported previously.[19]

3.2.4 Preparation of 10-(4-ethynylphenyl)-10H-phenoxazine (2d)

From derivative **10d** (2.100 g, 5.90 mmol), derivative **2d** (1.200 g, 77%) was obtained as a red solid by chromatography eluting with hexane.
^{1}H-NMR ($CDCl_3$, ppm) δ: 7.70 (d, *J* = 8.3 Hz, 2H, *m*-N-Ph), 7.31 (d, *J* = 8.3 Hz, 2H, *o*-N-Ph), 6.68 (d, *J* = 7.8 Hz, 4H, H1-phenoxacine), 6.65 (t, *J* = 7.8 Hz, 4H, H2-phenoxacine), 6.59 (t, *J* = 7.8 Hz, 4H, H3- phenoxacine), 5.91 (d, *J* = 7.8 Hz, 4H, H4-phenoxacine), 3.17 (s, 1H, CCH). ^{13}C-NMR ($CDCl_3$, ppm) δ: 143.9, 139.4, 134.8, 133.9, 130.9, 123.2, 122.4, 121.5, 115.5, 82.7, 78.5

4. Synthesis of tributyl((3,4,5-trimethoxyphenyl)ethynyl)tin (7b)



2a **7b**

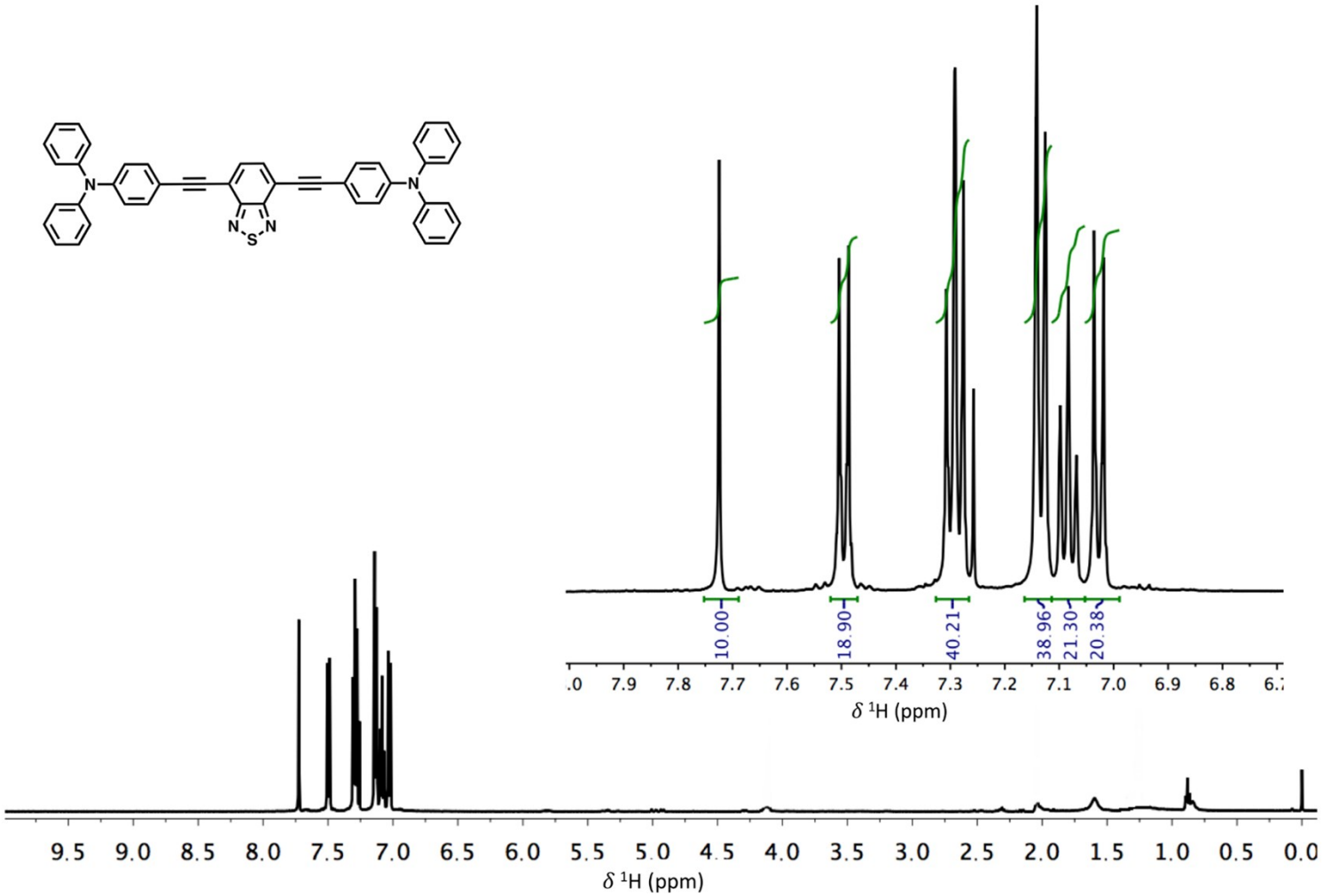
Scheme S2. *Synthesis of tributyl((3,4,5-trimethoxyphenyl)ethynyl)tin (**7b**)*

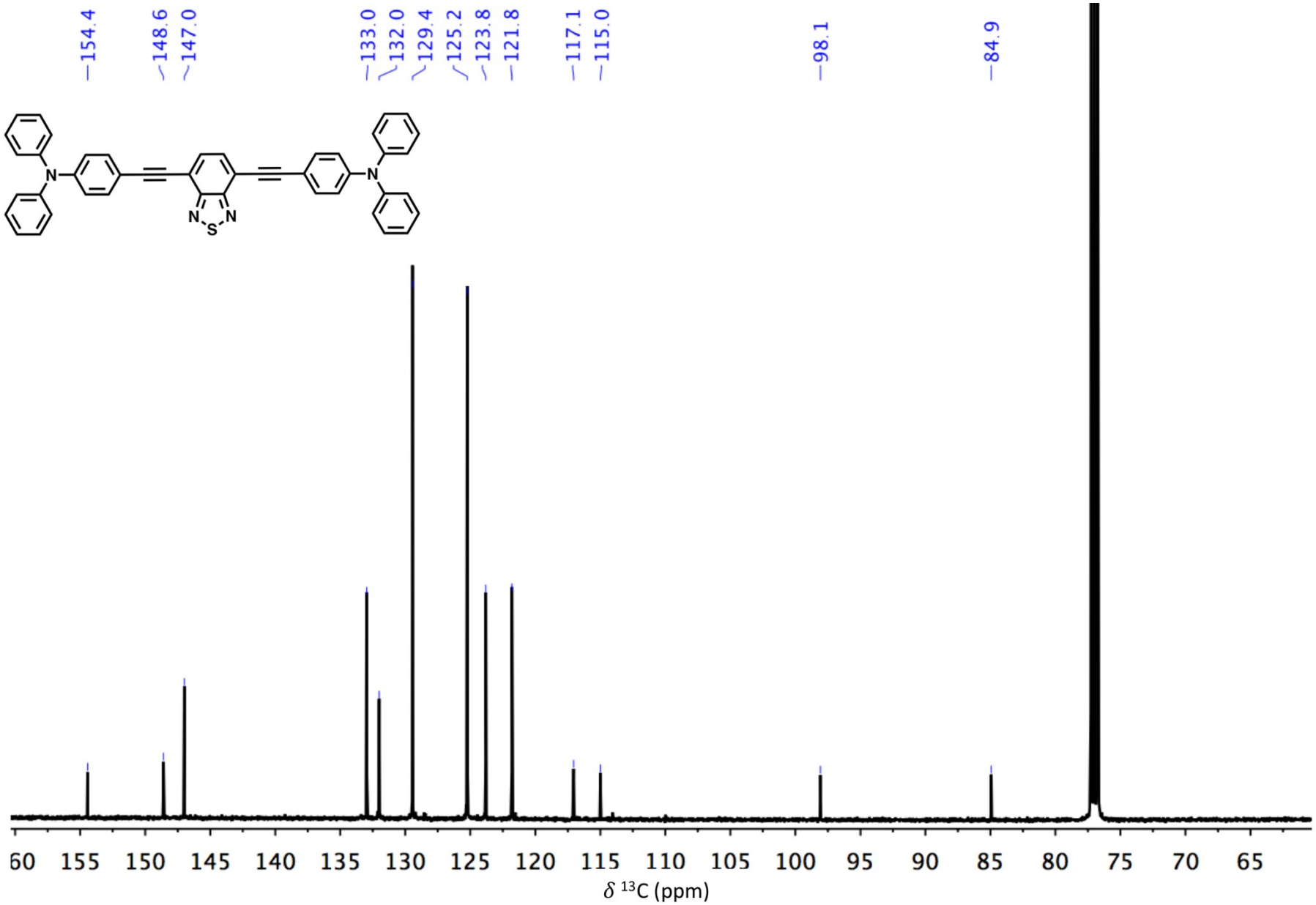
Preparation of tributyl((3,4,5-trimethoxyphenyl)ethynyl)tin (7b)

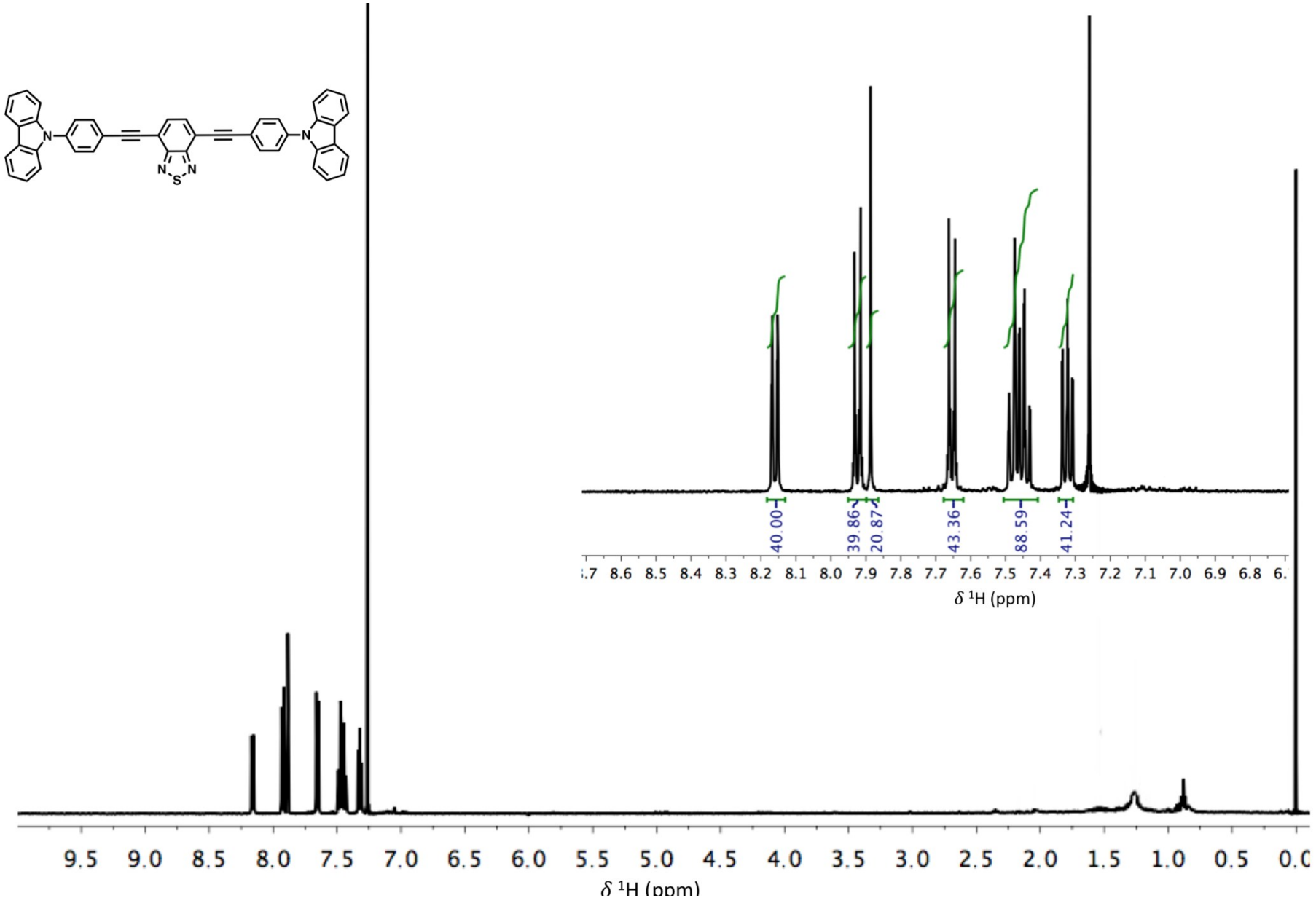
Butyllithium (0.63 ml of a 2.5 M solution in hexane, 1.15 mmol) was added dropwise over a period of 10 min to a vigorously stirred solution of 5-ethynyl-1,2,3-trimethoxybenzene (**2a**) (0.200 g, 1.042 mmol) in dry THF (10 ml) at −78 °C. The mixture was stirred for a further 10 min., then *n*Bu_3SnCl (0.34 ml, 1.25 mmol) was added dropwise over a period of *ca*. 10 min. The reaction mixture was then allowed to warm up to room temperature and it is stirring for two hours. After this time, 25 mL of water was added to the reaction mixture and it was neutralized with HCl 1M. The aqueous phase was extracted with CH_2Cl_2 (2 x15 mL) and the combined organic layers were dried over $MgSO_4$ and concentrated in vacuo to afford the product as a clear light-yellow liquid (0.488 g, 97%).

^{1}H-RMN ($CDCl_3$, ppm) δ: 6.67 (s, 2H, *o*-Ph); 3.84 (s, 6H, *m*-OCH_3); 3.83 (s, 3H, *p*-OCH_3); 1.61 (t, 6H, *J* = 7.8 Hz, Sn-CH_2); 1.42-1.35 (m, 6H, -C$\underline{H}_2$-CH_2); 1.04-1.09 (m, 6H, -C$\underline{H}_2$-CH_3); 0.92 (t, 9H, *J* = 7.3 Hz, -CH_3).

5. Collection of RMN spectra




154.4
148.6
147.0
133.0
132.0
129.4
125.2
123.8
121.8
117.1
115.0
98.1
84.9
N
N
N
S
60 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65
δ 13C (ppm)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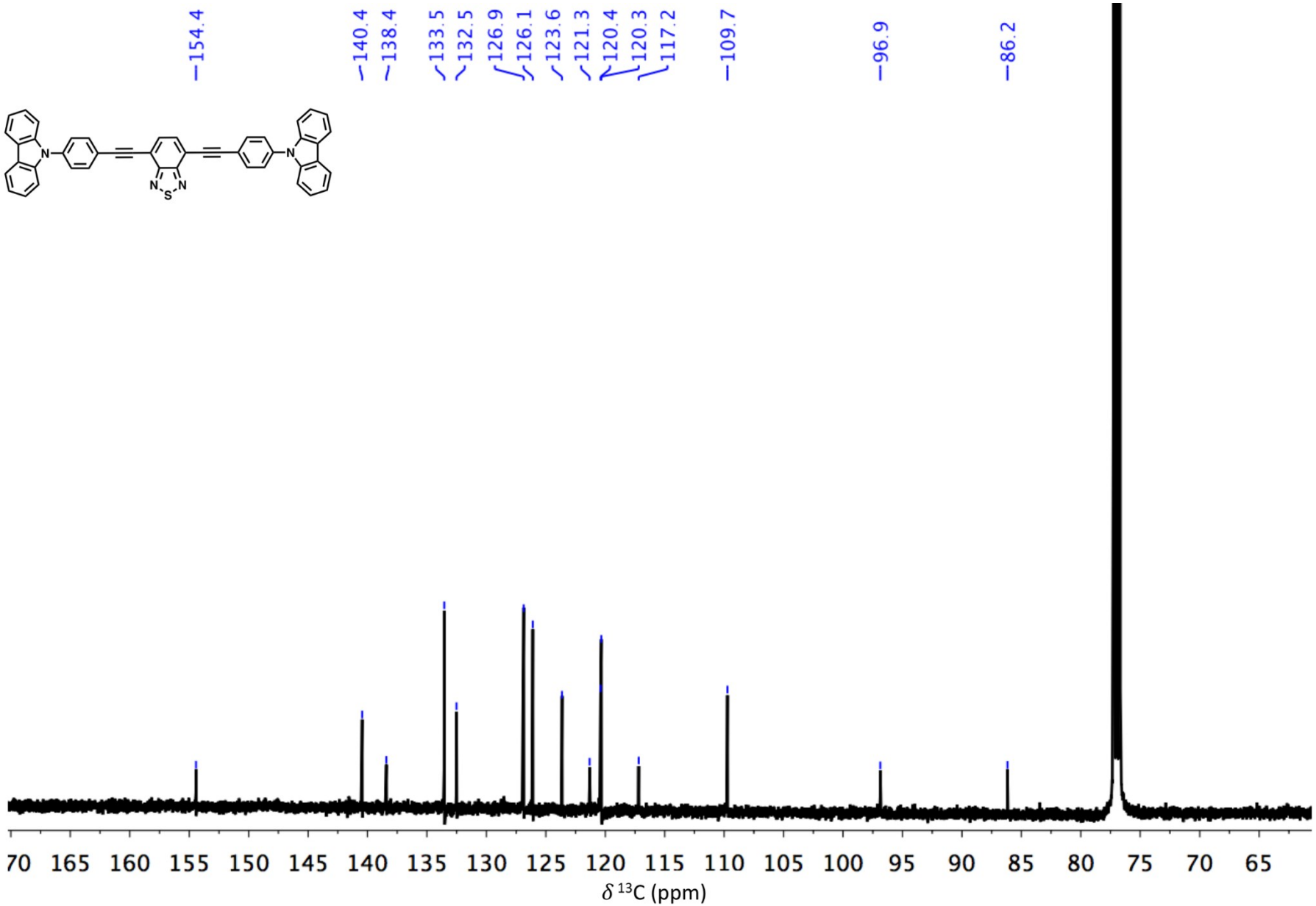
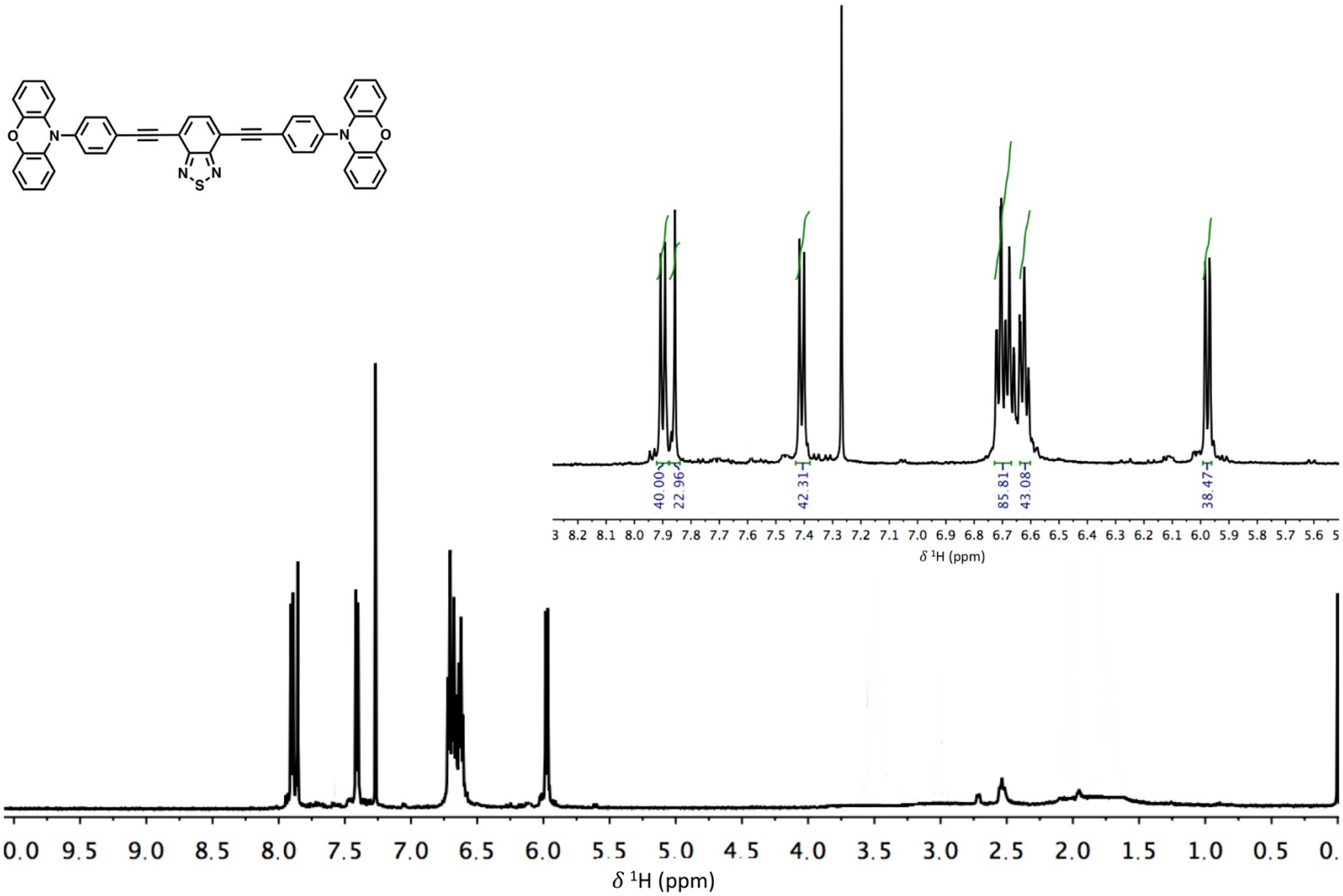
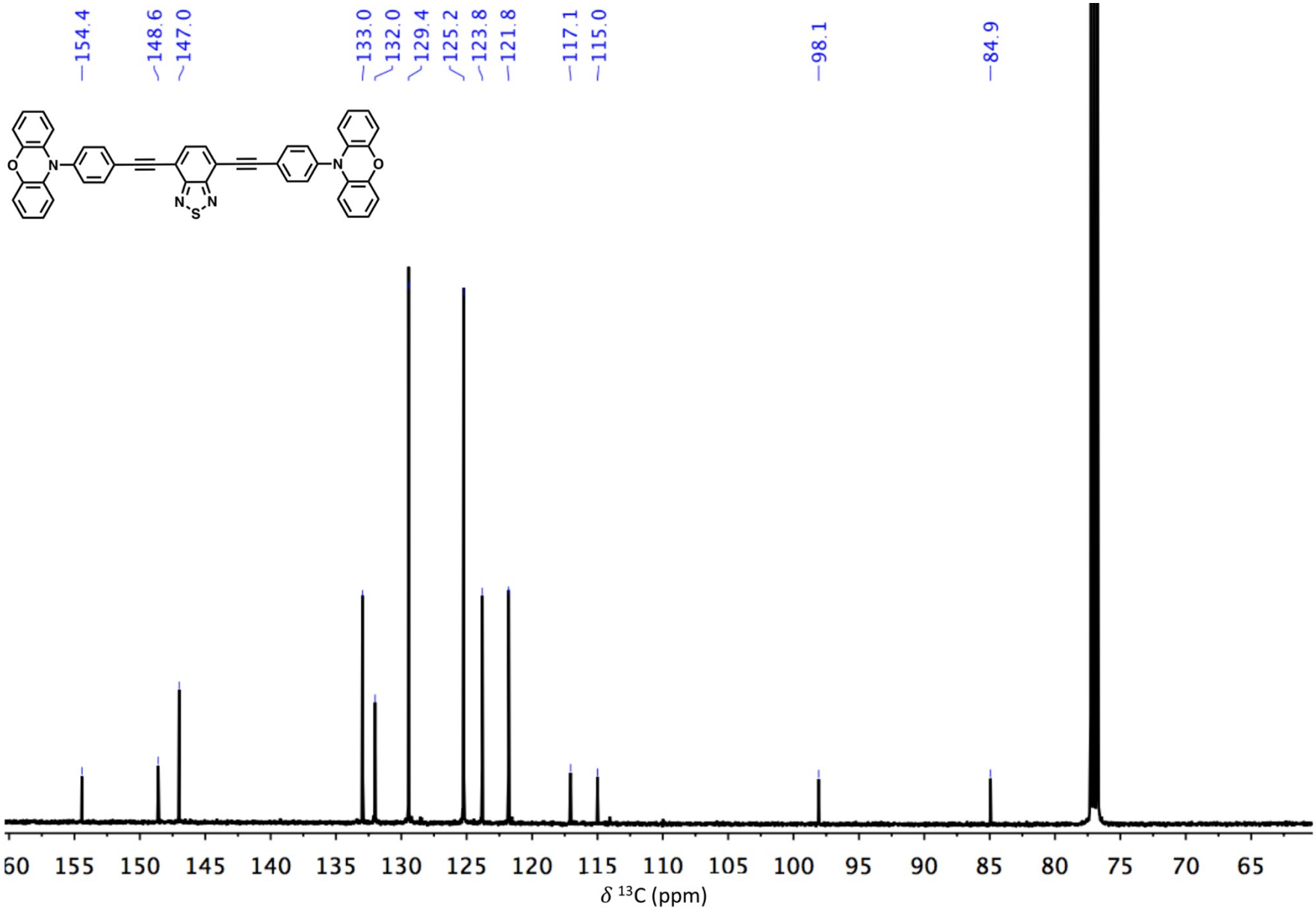
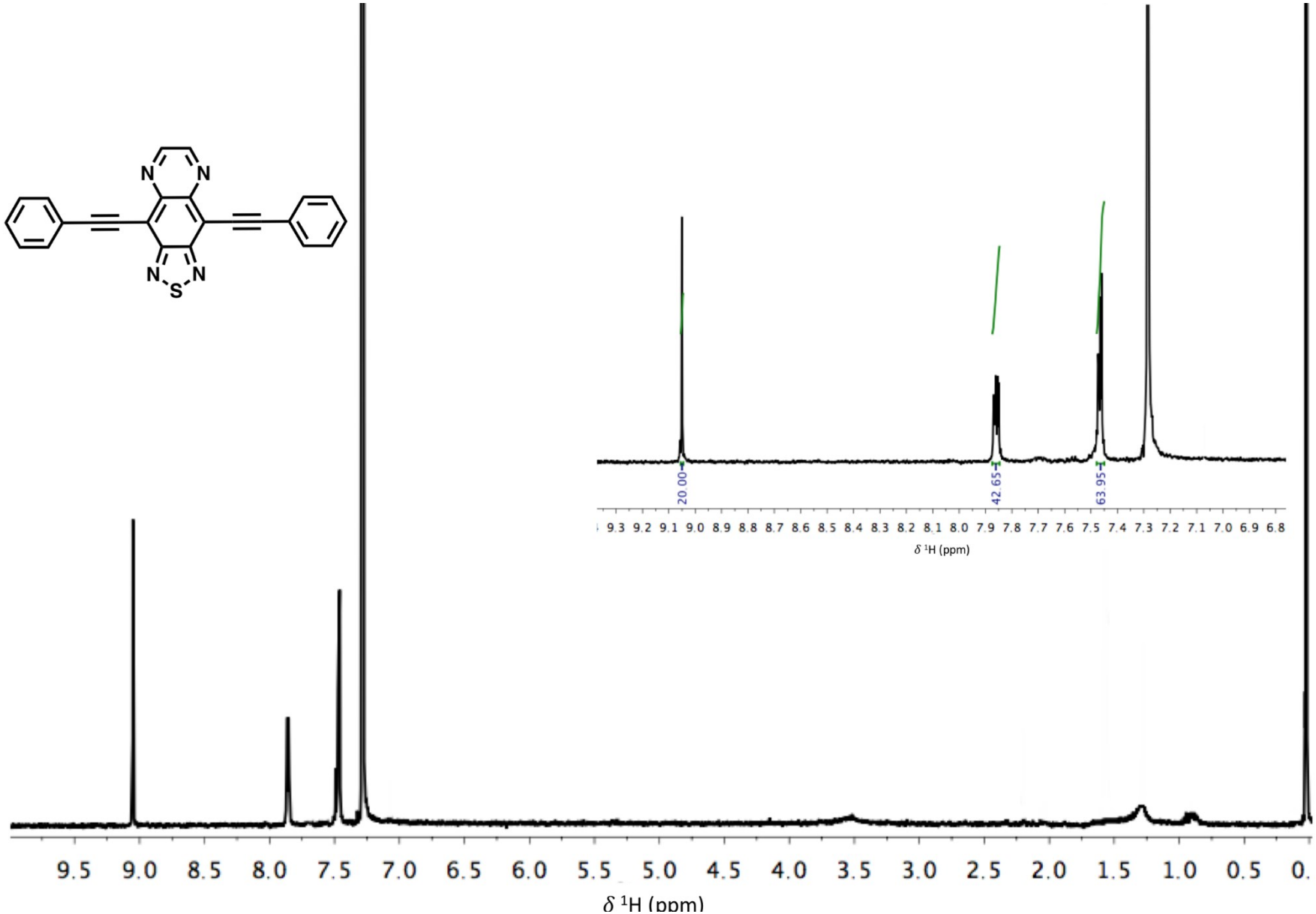
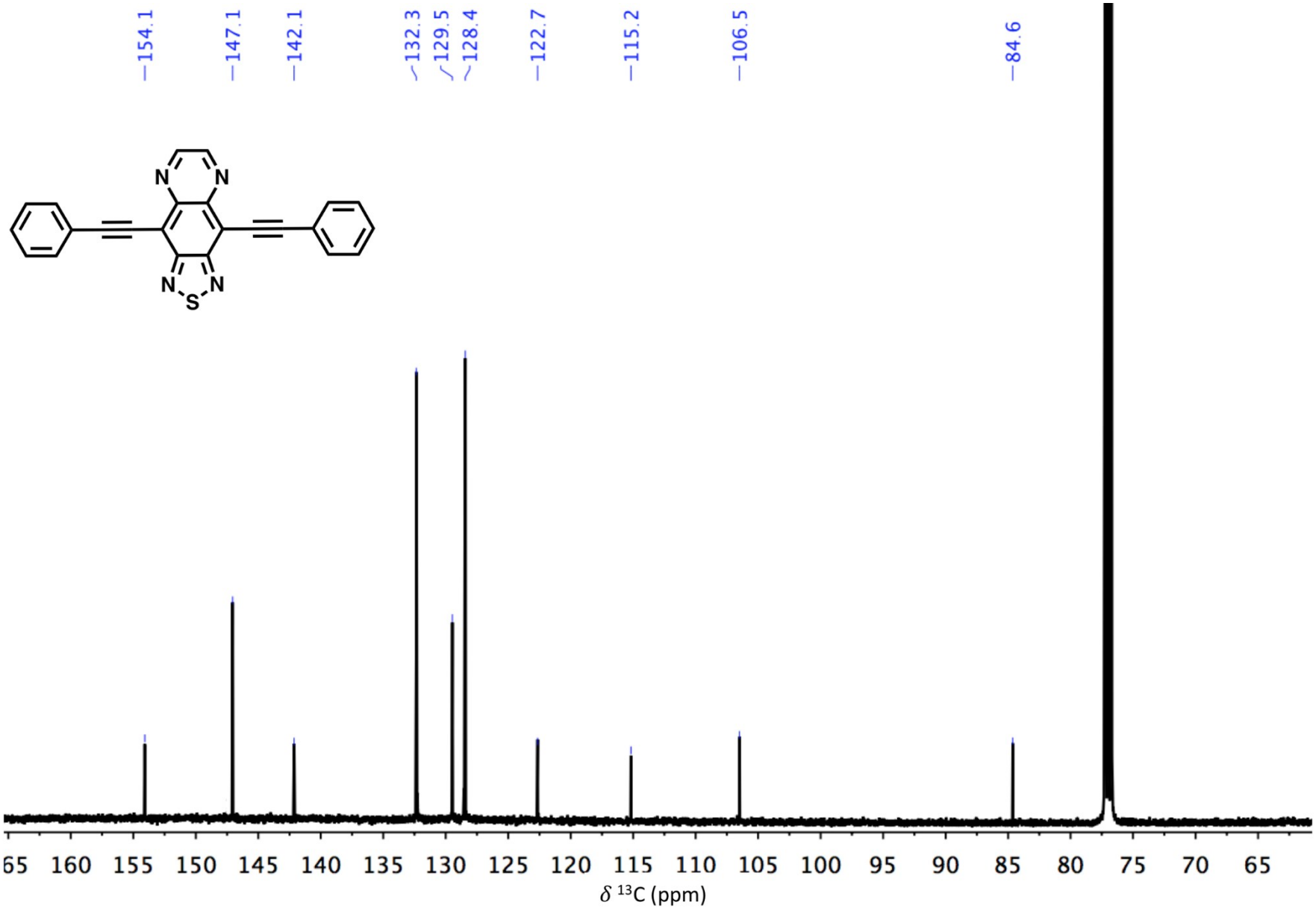
39.86
20.87
43.36
88.59
41.24
δ ¹H (ppm)
δ ¹H (ppm)

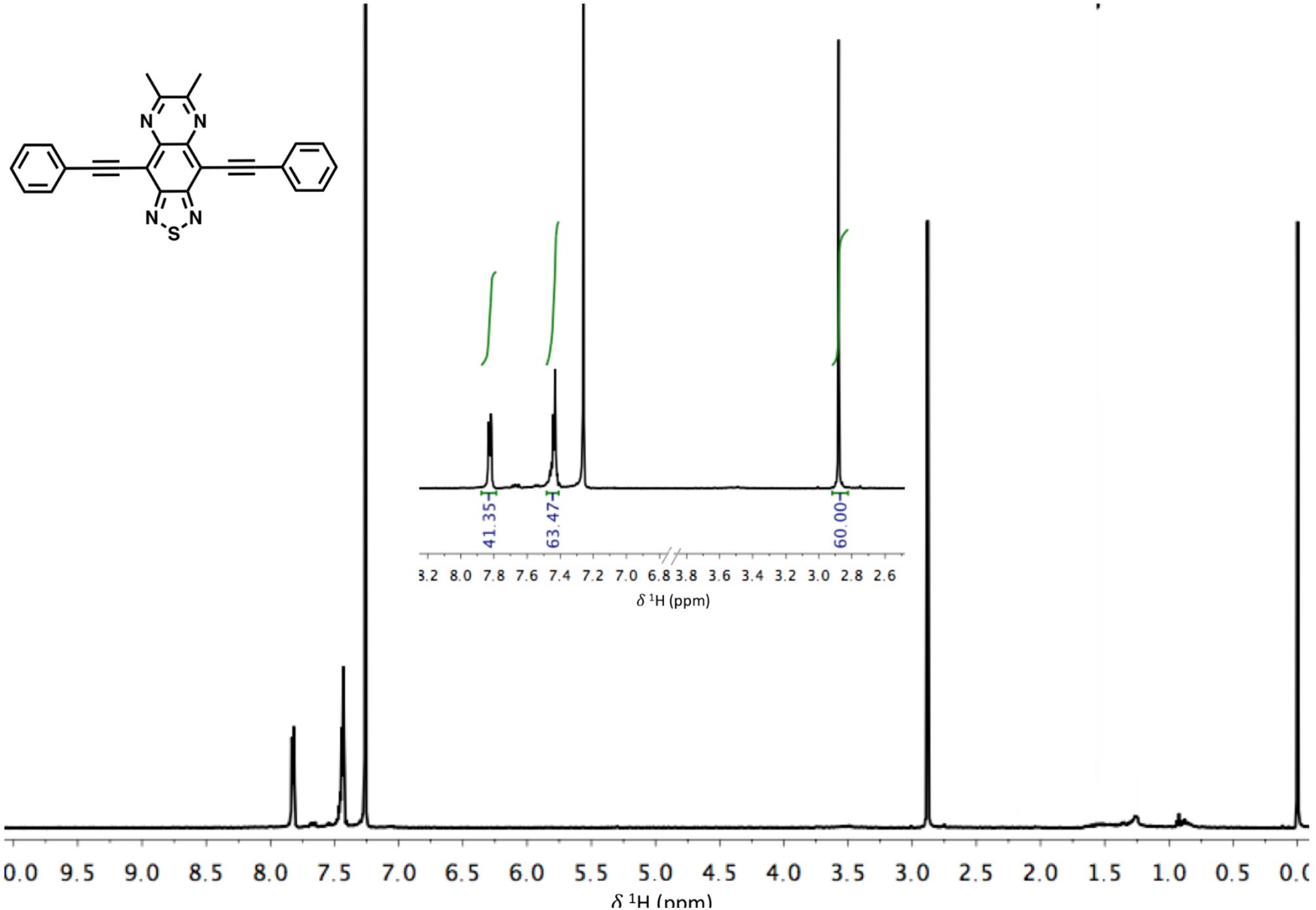

154.4
140.4
138.4
133.5
132.5
126.9
126.1
123.6
121.3
120.4
120.3
117.2
109.7
96.9
86.2
70 165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65
δ 13C (ppm)

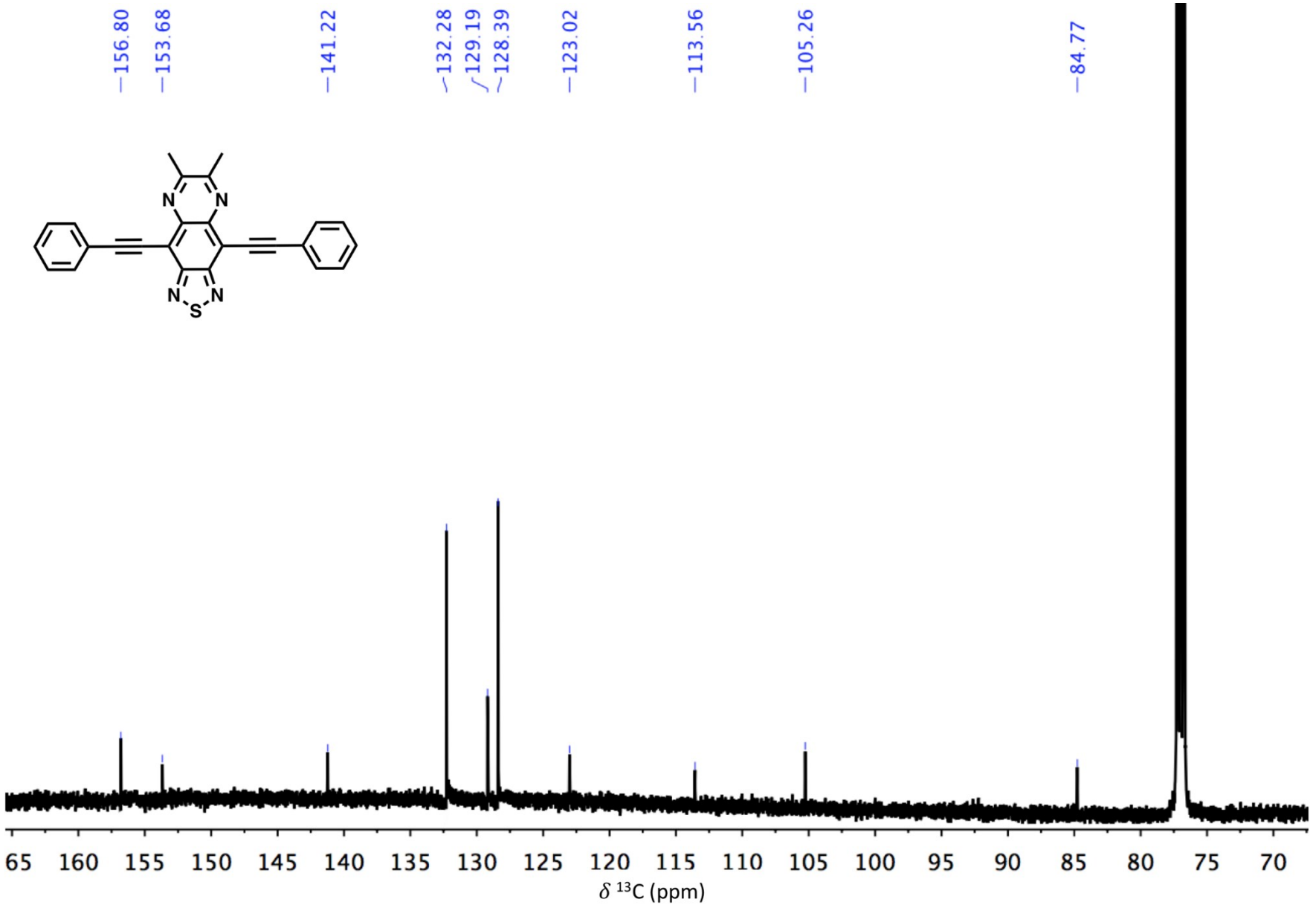

40.00
22.96
42.31
85.81
43.08
38.47
δ ¹H (ppm)
δ ¹H (ppm)

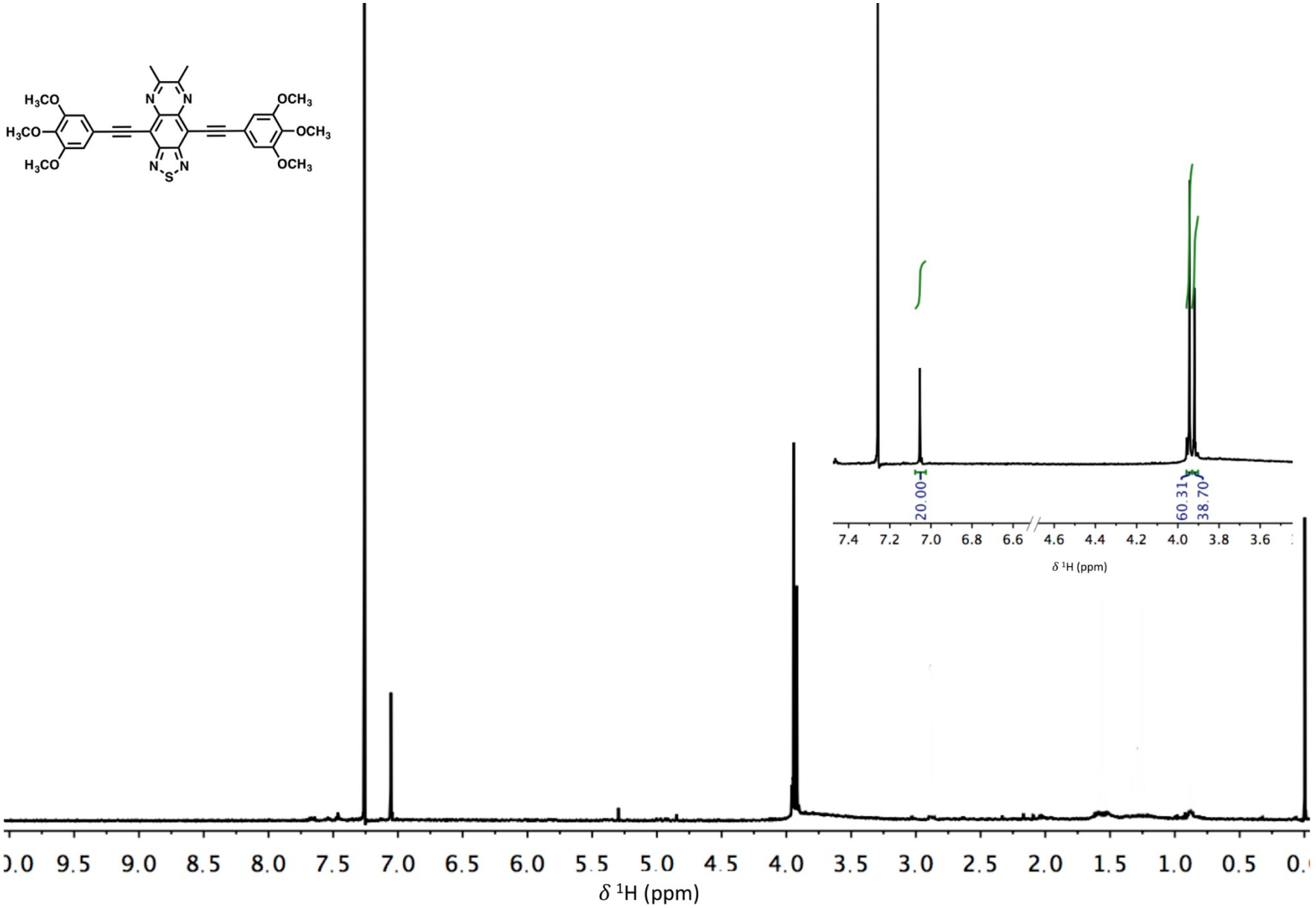

154.4
148.6
147.0
133.0
132.0
129.4
125.2
123.8
121.8
117.1
115.0
98.1
84.9
O
N
N
S
N
N
O
60 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65
δ 13C (ppm)

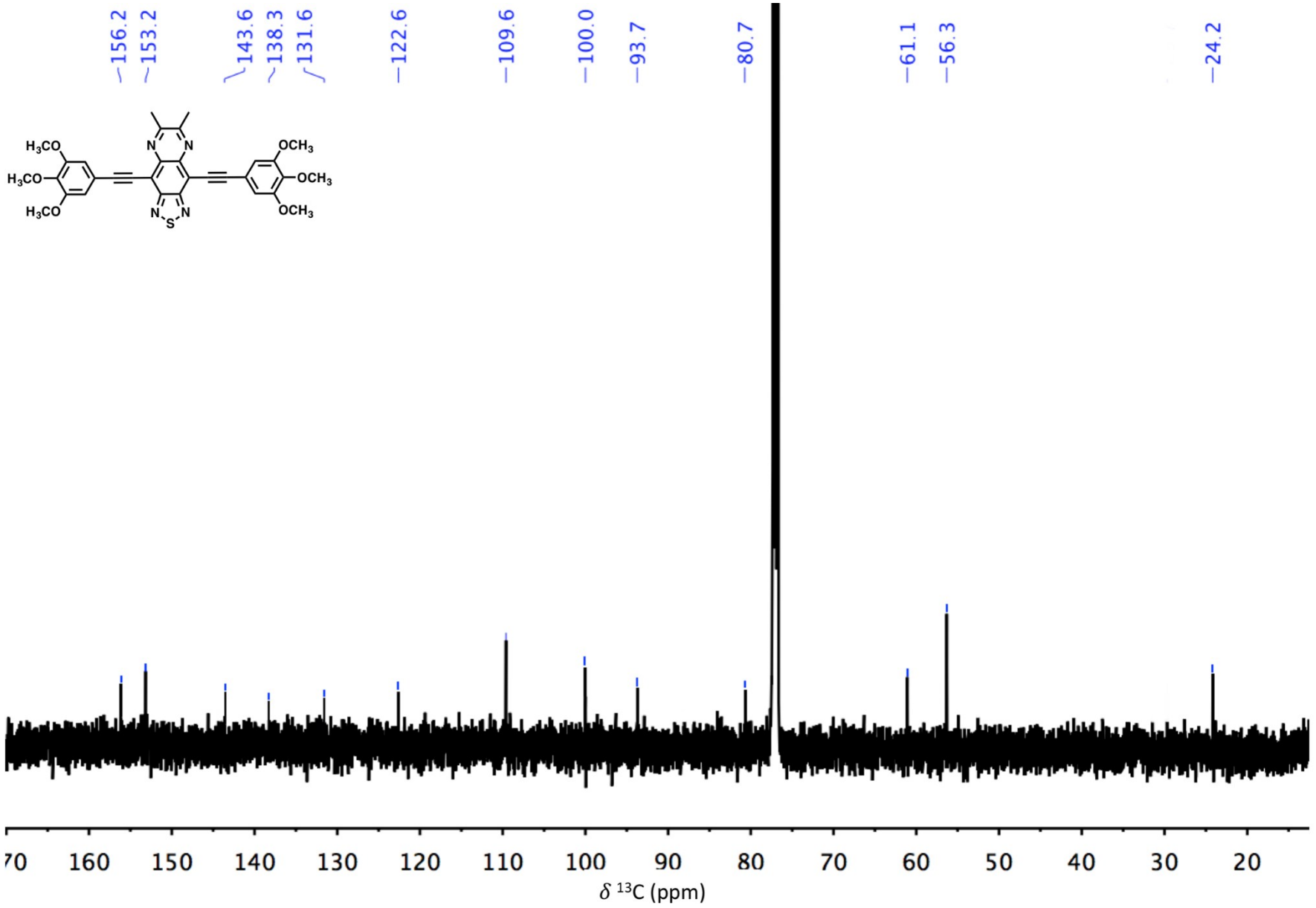

N
N
N
S
N
20.00
42.65
63.95
9.3 9.2 9.1 9.0 8.9 8.8 8.7 8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8
δ ¹H (ppm)
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.
δ ¹H (ppm)

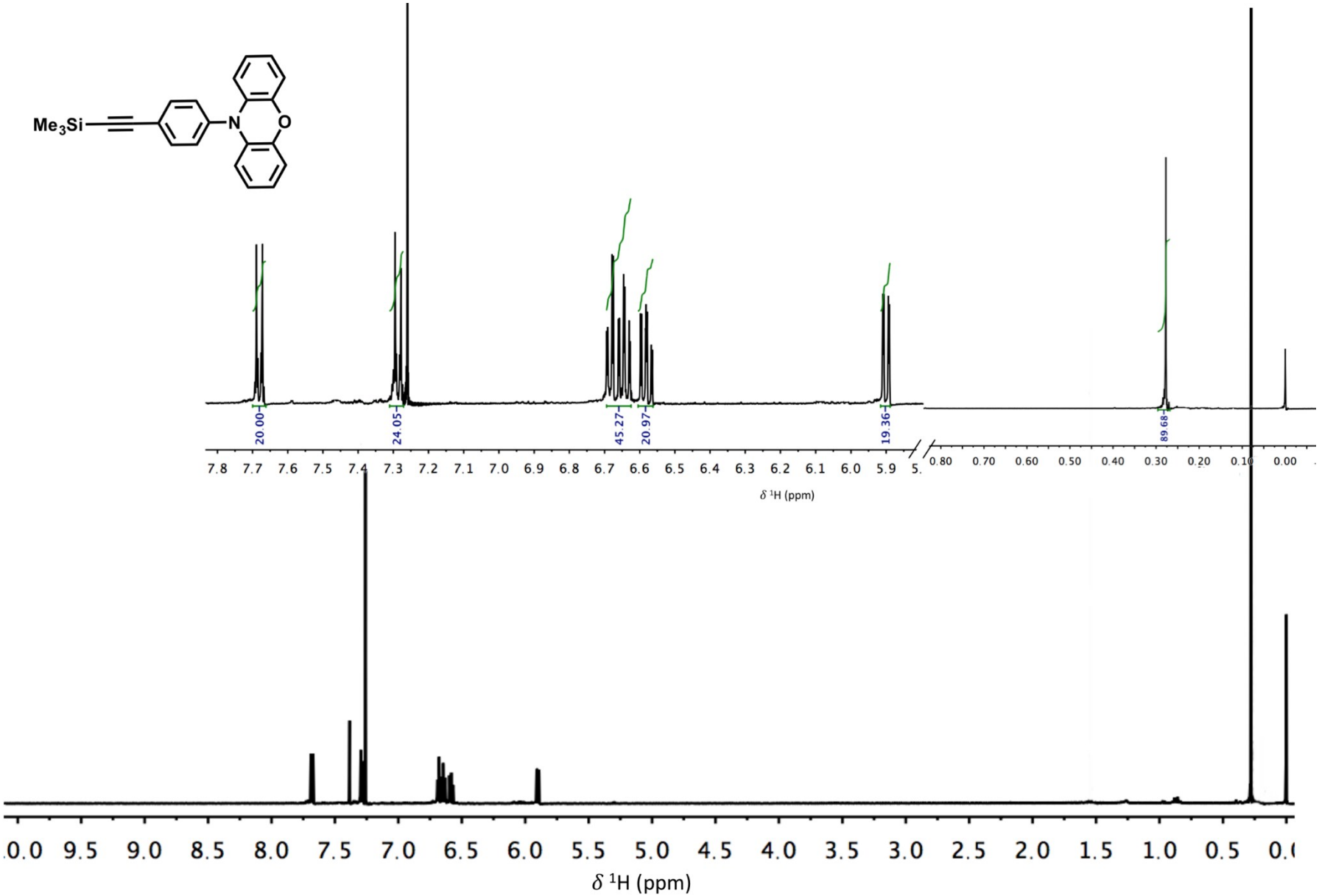

154.1
147.1
142.1
132.3
129.5
128.4
122.7
115.2
106.5
84.6
N
N
N
S
N
65 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65
δ 13C (ppm)

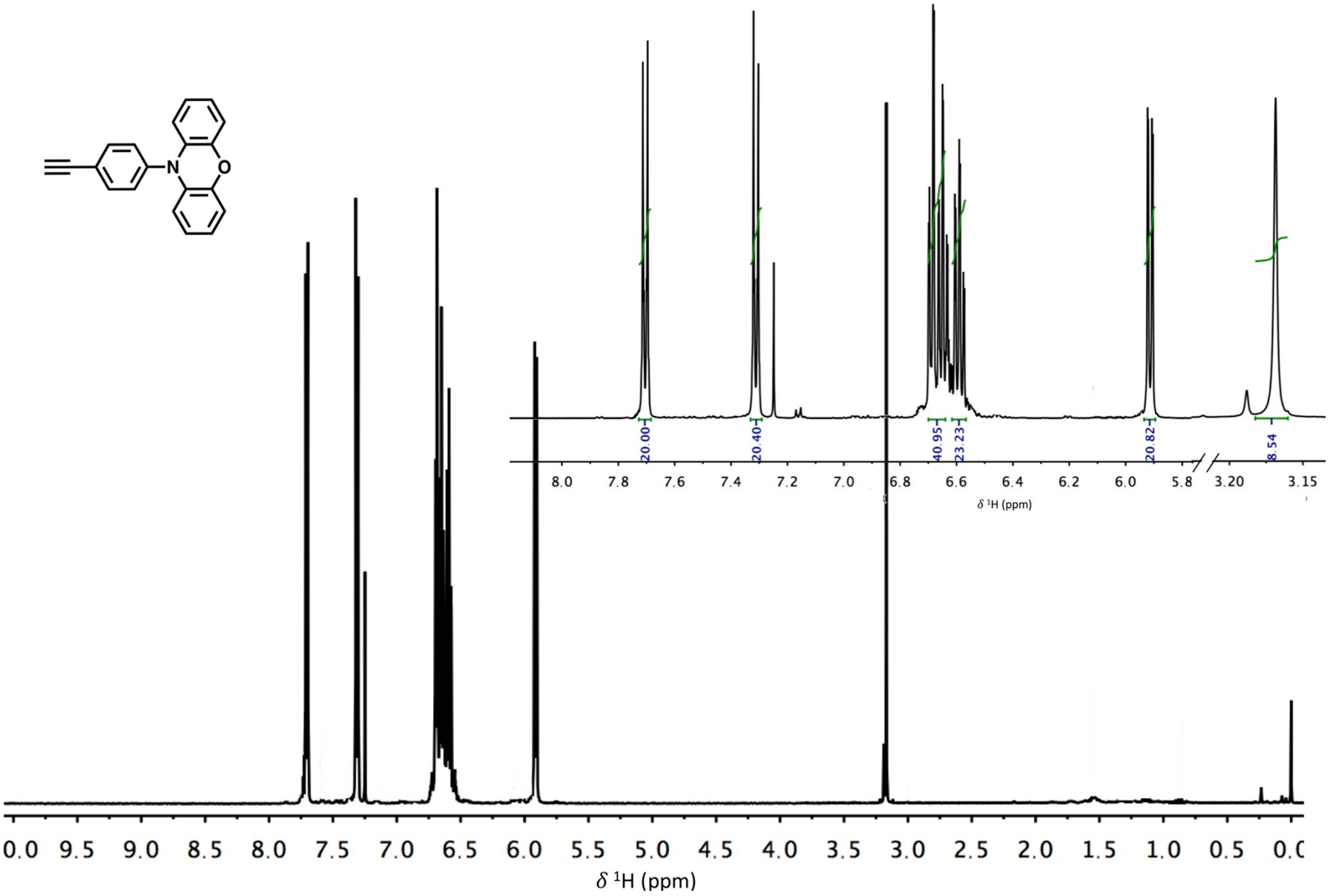

N
N
N
S
N
41.35
63.47
60.00
3.2 8.0 7.8 7.6 7.4 7.2 7.0 6.8 3.8 3.6 3.4 3.2 3.0 2.8 2.6
δ ¹H (ppm)
0.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
δ ¹H (ppm)

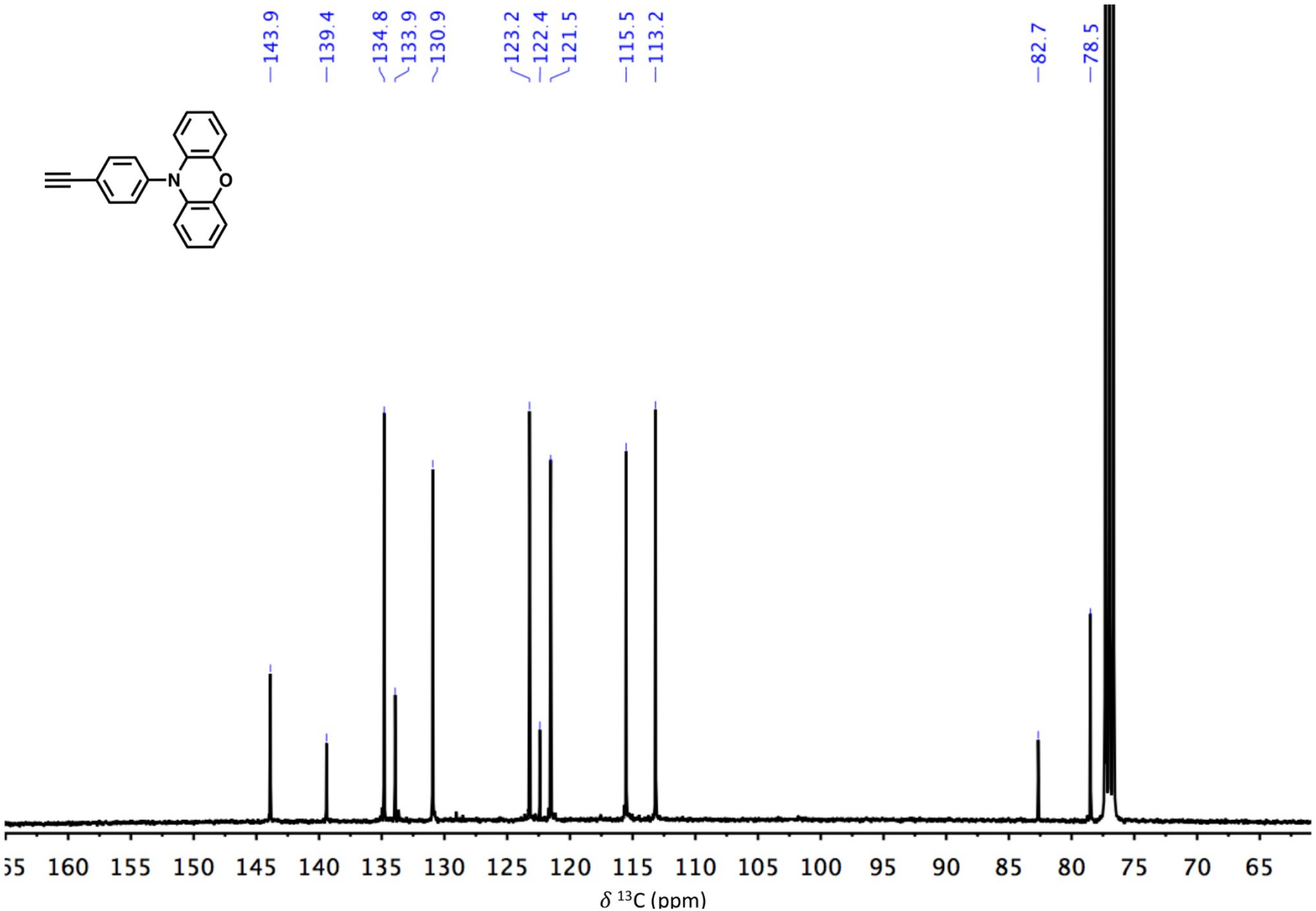

156.80
153.68
141.22
132.28
129.19
128.39
123.02
113.56
105.26
84.77
N
N
N
S
N
65 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70
δ 13C (ppm)

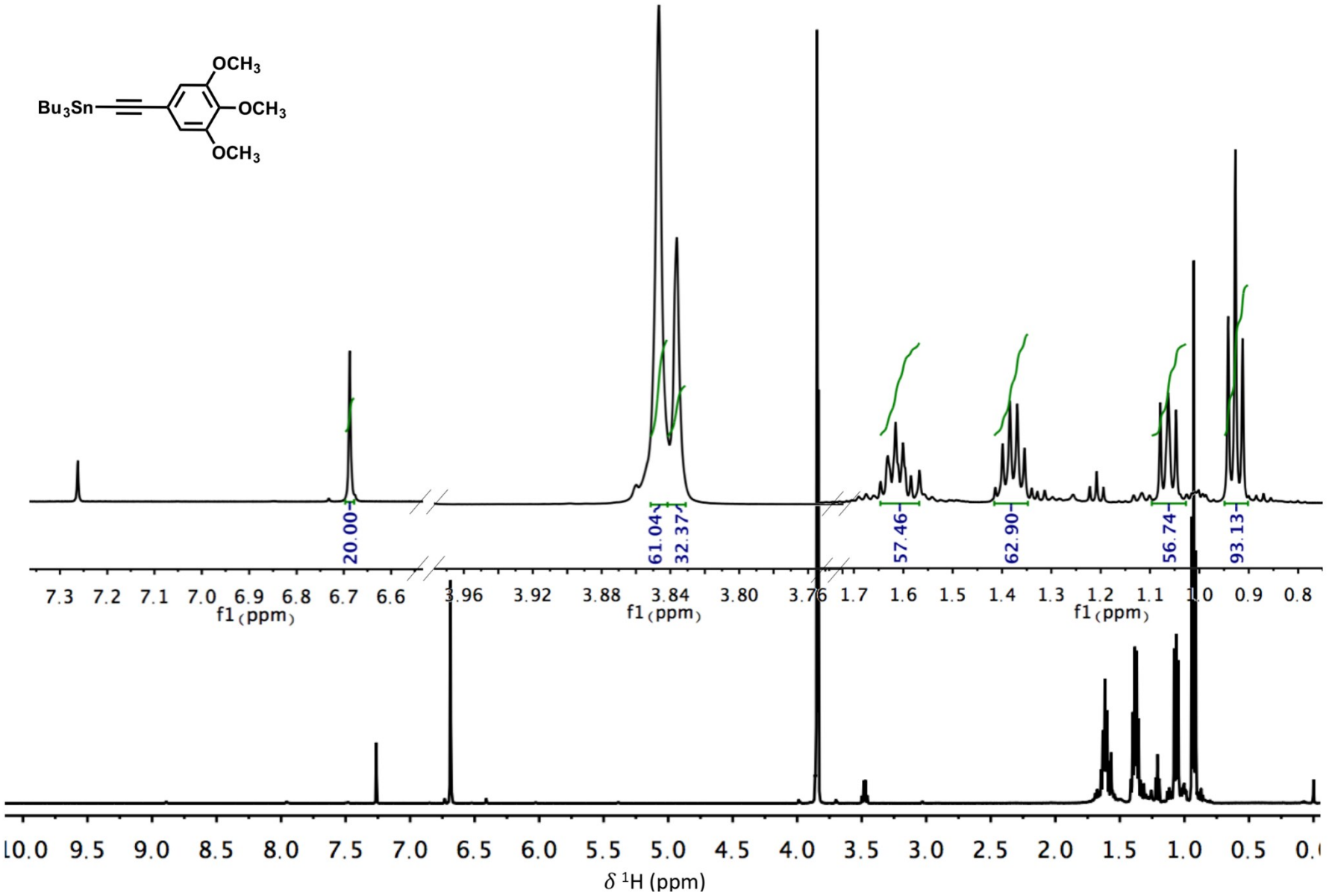

H3CO
H3CO
H3CO
OCH3
OCH3
OCH3
N
N
N
S
N
20.00
60.31
38.70
7.4 7.2 7.0 6.8 6.6 4.6 4.4 4.2 4.0 3.8 3.6
δ 1H (ppm)
0.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.
δ 1H (ppm)


156.2
153.2
143.6
138.3
131.6
122.6
109.6
100.0
93.7
80.7
61.1
56.3
24.2
H3CO
H3CO
H3CO
OCH3
OCH3
OCH3
N
N
N
N
S
70
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
δ 13C (ppm)


Me3Si
N
O
20.00
24.05
45.27
20.97
19.36
89.68
δ 1H (ppm)
δ 1H (ppm)


N
O
20.00
20.40
40.95
23.23
20.82
8.54
8.0 7.8 7.6 7.4 7.2 7.0 6.8 6.6 6.4 6.2 6.0 5.8 3.20 3.15
δ ¹H (ppm)
0.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
δ ¹H (ppm)


143.9
139.4
134.8
133.9
130.9
123.2
122.4
121.5
115.5
113.2
82.7
78.5
N
O
55 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65
δ 13C (ppm)


OCH3
Bu3Sn
OCH3
OCH3
20.00
61.04
32.37
57.46
62.90
56.74
93.13
f1 (ppm)
δ 1H (ppm)

6. Z-matrix coordinates

Standard orientation for optimised structures at B3LYP/6-31G(d,p)

Compound 3b

Center number	Atomic number	Atomic type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.723834	0.883932	0.002808
2	6	0	0.72381	0.883947	-0.00296
3	6	0	1.438931	-0.36119	-0.003638
4	6	0	0.688287	-1.571389	-0.000864
5	6	0	-0.688259	-1.571403	0.000676
6	6	0	-1.438928	-0.361222	0.003468
7	7	0	1.263202	2.093203	-0.005254
8	7	0	-1.263253	2.093176	0.00512
9	6	0	-2.832244	-0.375409	0.006703
10	6	0	-4.057549	-0.382873	0.00895
11	6	0	2.832247	-0.375347	-0.00687
12	6	0	4.057552	-0.382792	-0.009107
13	6	0	-5.461135	-0.347879	0.011001
14	6	0	-6.147907	0.88831	0.039437
15	6	0	-6.227524	-1.535229	-0.016131
16	6	0	-7.525509	0.93413	0.039073
17	1	0	-5.568429	1.805503	0.046525
18	6	0	-7.605289	-1.491159	-0.014196
19	1	0	-5.714506	-2.491223	-0.024497
20	6	0	-8.282539	-0.254952	0.012361
21	1	0	-8.037701	1.890404	0.045821
22	1	0	-8.179687	-2.411439	-0.020728
23	6	0	5.461138	-0.34782	-0.011108
24	6	0	6.14793	0.888359	-0.0395
25	6	0	6.227509	-1.535182	0.016032
26	6	0	7.525533	0.934158	-0.039086
27	1	0	5.568466	1.805561	-0.046594
28	6	0	7.605274	-1.491133	0.014147
29	1	0	5.714476	-2.491168	0.024364
30	6	0	8.282544	-0.254936	-0.012366
31	1	0	8.037739	1.890425	-0.0458
32	1	0	8.179658	-2.411422	0.020686
33	7	0	-9.680205	-0.210333	0.011626
34	7	0	9.680211	-0.210339	-0.011577
35	6	0	10.432947	-1.208845	0.660695
36	6	0	11.578478	-1.744934	0.063614
37	6	0	10.041627	-1.651965	1.928755
38	6	0	12.32121	-2.711401	0.731752
39	1	0	11.87682	-1.397796	-0.920739
40	6	0	10.782809	-2.629861	2.581378
41	1	0	9.158583	-1.223516	2.392842
42	6	0	11.926375	-3.162301	1.989572
43	1	0	13.208058	-3.122252	0.259444
44	1	0	10.47096	-2.966309	3.565183
45	1	0	12.505939	-3.920971	2.505145
46	6	0	10.370378	0.837032	-0.676759
47	6	0	11.480044	1.438824	-0.074476

48	6	0	9.953276	1.26408	-1.942074
49	6	0	12.161849	2.454268	-0.734764
50	1	0	11.798242	1.104813	0.908174
51	6	0	10.632679	2.291003	-2.586579
52	1	0	9.098127	0.786151	-2.410041
53	6	0	11.740644	2.889017	-1.989663
54	1	0	13.020827	2.91623	-0.258195
55	1	0	10.300449	2.615427	-3.567716
56	1	0	12.271861	3.686422	-2.498762
57	6	0	-10.432984	-1.208817	-0.660632
58	6	0	-11.578499	-1.744898	-0.063515
59	6	0	-10.04172	-1.651922	-1.928715
60	6	0	-12.321273	-2.711342	-0.73164
61	1	0	-11.876797	-1.397772	0.920855
62	6	0	-10.782943	-2.629796	-2.581325
63	1	0	-9.158688	-1.223478	-2.39283
64	6	0	-11.926494	-3.162228	-1.989482
65	1	0	-13.208108	-3.122188	-0.259304
66	1	0	-10.471138	-2.966232	-3.565148
67	1	0	-12.50609	-3.92088	-2.505045
68	6	0	-10.37033	0.837036	0.676854
69	6	0	-11.48001	1.438858	0.074627
70	6	0	-9.953169	1.264056	1.942161
71	6	0	-12.16177	2.454303	0.73496
72	1	0	-11.798253	1.10487	-0.908016
73	6	0	-10.632528	2.29098	2.58671
74	1	0	-9.098009	0.786104	2.410084
75	6	0	-11.740507	2.889023	1.989849
76	1	0	-13.020759	2.916287	0.258433
77	1	0	-10.300253	2.61538	3.567839
78	1	0	-12.27169	3.686428	2.498984
79	1	0	-1.233017	-2.509192	0.001313
80	1	0	1.233066	-2.509165	-0.001514
81	16	0	-0.000037	3.16853	-0.00006

Compound 3c

Center number	Atomic number	Atomic type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.72349	0.883668	-0.001037
2	6	0	-0.723471	0.883681	0.000975
3	6	0	-1.43832	-0.361832	0.002349
4	6	0	-0.687488	-1.575163	0.001296
5	6	0	0.687464	-1.575175	-0.001393
6	6	0	1.438317	-0.361857	-0.002428
7	7	0	-1.262295	2.092087	0.001726
8	7	0	1.262335	2.092065	-0.001772
9	6	0	2.830078	-0.376255	-0.004084
10	6	0	4.055443	-0.383131	-0.005246
11	6	0	-2.830081	-0.376205	0.004007
12	6	0	-4.055446	-0.383065	0.005174
13	1	0	1.233286	-2.512169	-0.002478
14	1	0	-1.233326	-2.512147	0.002368
15	6	0	-5.460671	-0.34888	0.005457
16	6	0	-6.142204	0.889548	-0.005635
17	6	0	-6.219738	-1.540292	0.016203
18	6	0	-7.522397	0.931855	-0.010314

19	1	0	-5.560986	1.805159	-0.02973
20	6	0	-7.599835	-1.495323	0.019776
21	1	0	-5.702924	-2.493716	0.040852
22	6	0	-8.265499	-0.259287	0.004308
23	1	0	-8.044117	1.882286	-0.055782
24	1	0	-8.181422	-2.41038	0.064542
25	6	0	5.460668	-0.348931	-0.005508
26	6	0	6.219747	-1.540336	-0.016264
27	6	0	6.142188	0.889503	0.005616
28	6	0	7.599843	-1.495353	-0.019814
29	1	0	5.702942	-2.493764	-0.040936
30	6	0	7.522381	0.931824	0.010317
31	1	0	5.560961	1.805108	0.029719
32	6	0	8.265495	-0.25931	-0.004315
33	1	0	8.18144	-2.410403	-0.064587
34	1	0	8.04409	1.882259	0.05581
35	6	0	-10.461488	0.600844	0.816106
36	6	0	-10.50904	-0.984504	-0.807096
37	6	0	-10.079968	1.489856	1.822199
38	6	0	-11.819034	0.352622	0.5251
39	6	0	-10.181739	-1.8932	-1.814729
40	6	0	-11.849435	-0.658788	-0.512938
41	6	0	-11.088818	2.156141	2.506053
42	1	0	-9.037307	1.646967	2.075022
43	6	0	-12.813884	1.033586	1.226814
44	6	0	-11.22868	-2.500132	-2.49654
45	1	0	-9.150282	-2.108708	-2.070568
46	6	0	-12.883304	-1.281266	-1.212464
47	6	0	-12.442317	1.939973	2.210447
48	1	0	-10.81916	2.855383	3.291115
49	1	0	-13.861987	0.849507	1.009703
50	6	0	-12.566825	-2.207042	-2.197345
51	1	0	-11.001561	-3.212483	-3.283304
52	1	0	-13.918608	-1.03734	-0.992933
53	1	0	-13.203838	2.479379	2.763797
54	1	0	-13.359376	-2.701344	-2.749228
55	6	0	10.50903	-0.98452	0.807113
56	6	0	10.461489	0.600856	-0.816061
57	6	0	10.18172	-1.893238	1.814725
58	6	0	11.849426	-0.658785	0.512985
59	6	0	10.079977	1.489883	-1.822144
60	6	0	11.819032	0.352644	-0.525036
61	6	0	11.228655	-2.500171	2.496543
62	1	0	9.150261	-2.108761	2.070542
63	6	0	12.883289	-1.281264	1.212518
64	6	0	11.088832	2.15619	-2.505968
65	1	0	9.037318	1.646987	-2.074982
66	6	0	12.813887	1.033631	-1.226719
67	6	0	12.566803	-2.207061	2.197377
68	1	0	11.001531	-3.212538	3.28329
69	1	0	13.918595	-1.037323	0.993009
70	6	0	12.442328	1.940031	-2.210343
71	1	0	10.81918	2.855444	-3.291023
72	1	0	13.861988	0.849559	-1.009594
73	1	0	13.35935	-2.701365	2.749265
74	1	0	13.203853	2.479456	-2.76367
75	7	0	9.667403	-0.215671	-0.003668

76	7	0	-9.667407	-0.215661	0.003686
77	16	0	0.000029	3.168086	-0.000015

Compound 3d

Center number	Atomic number	Atomic type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.725078	0.623789	0.73453
2	6	0	-0.725082	0.623756	0.734552
3	6	0	-1.44754	-0.168054	-0.225378
4	6	0	-0.687321	-0.936085	-1.158205
5	6	0	0.687329	-0.936056	-1.158225
6	6	0	1.447543	-0.167992	-0.22542
7	7	0	-1.256874	1.394152	1.668862
8	7	0	1.256864	1.39421	1.668821
9	6	0	2.836817	-0.176218	-0.2325
10	6	0	4.064039	-0.18075	-0.234784
11	6	0	-2.836817	-0.176342	-0.232416
12	6	0	-4.064038	-0.180915	-0.234671
13	1	0	1.227149	-1.534101	-1.884243
14	1	0	-1.227137	-1.534153	-1.884207
15	6	0	5.468377	-0.174849	-0.223003
16	6	0	6.205398	-0.946522	-1.152212
17	6	0	6.173478	0.606414	0.72326
18	6	0	7.58595	-0.934606	-1.133992
19	1	0	5.673042	-1.536671	-1.890317
20	6	0	7.554092	0.61277	0.737388
21	1	0	5.6146	1.188515	1.448053
22	6	0	8.274613	-0.156187	-0.190191
23	1	0	8.150931	-1.515785	-1.856333
24	1	0	8.094041	1.200945	1.473068
25	6	0	-5.468377	-0.174968	-0.222912
26	6	0	-6.173465	0.606319	0.72334
27	6	0	-6.205408	-0.946623	-1.152127
28	6	0	-7.55408	0.612716	0.73745
29	1	0	-5.614579	1.188404	1.448139
30	6	0	-7.585961	-0.934663	-1.133925
31	1	0	-5.67306	-1.536793	-1.89022
32	6	0	-8.274611	-0.156217	-0.190138
33	1	0	-8.094021	1.200907	1.473124
34	1	0	-8.150951	-1.515832	-1.856267
35	6	0	-10.409663	-1.340319	0.029562
36	6	0	-10.400598	1.053641	-0.359538
37	6	0	-9.792047	-2.565868	0.297721
38	6	0	-11.813651	-1.300992	0.024073
39	6	0	-11.804631	1.02862	-0.329079
40	6	0	-9.775375	2.273998	-0.633576
41	6	0	-10.548491	-3.71813	0.496036
42	1	0	-8.712163	-2.61908	0.359854
43	6	0	-12.567194	-2.446899	0.220781
44	6	0	-12.54978	2.182991	-0.507355
45	1	0	-8.696308	2.316837	-0.714664
46	6	0	-10.523425	3.434702	-0.813702
47	6	0	-11.937131	-3.667523	0.4491
48	1	0	-10.039137	-4.654513	0.696331

49	1	0	-13.64791	-2.354966	0.199836
50	6	0	-11.911441	3.398078	-0.742041
51	1	0	-13.630824	2.101985	-0.467368
52	1	0	-10.008075	4.366694	-1.019041
53	1	0	-12.530602	-4.562216	0.601001
54	1	0	-12.498291	4.299455	-0.87946
55	7	0	-9.687774	-0.14758	-0.174085
56	8	0	-12.511123	-0.133062	-0.149439
57	6	0	10.409635	-1.340347	0.029524
58	6	0	10.400628	1.053621	-0.359525
59	6	0	9.79199	-2.565901	0.297594
60	6	0	11.813625	-1.301035	0.024125
61	6	0	11.804658	1.028584	-0.328973
62	6	0	9.775436	2.273985	-0.633612
63	6	0	10.548409	-3.71818	0.495906
64	1	0	8.712103	-2.619106	0.359663
65	6	0	12.567143	-2.44696	0.220827
66	6	0	12.549832	2.182945	-0.507204
67	1	0	8.696376	2.316834	-0.714774
68	6	0	10.523511	3.434679	-0.813689
69	6	0	11.937053	-3.667586	0.449055
70	1	0	10.039033	-4.654565	0.696131
71	1	0	13.647861	-2.355036	0.199954
72	6	0	11.911523	3.398039	-0.741933
73	1	0	13.630873	2.101928	-0.467143
74	1	0	10.008187	4.366677	-1.019066
75	1	0	12.530505	-4.562293	0.600953
76	1	0	12.498392	4.29941	-0.879314
77	7	0	9.687774	-0.147589	-0.174117
78	8	0	12.511122	-0.133105	-0.149276
79	16	0	-0.000008	2.079146	2.500167

Compound 8a

Center number	Atomic number	Atomic type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.721326	-1.12032	-0.000299
2	6	0	-0.721491	-1.120221	-0.000103
3	6	0	-1.460195	0.094575	0.000148
4	6	0	-0.721077	1.2863	0.000191
5	6	0	0.721244	1.2862	-0.000005
6	6	0	1.460197	0.094374	-0.000245
7	6	0	0.720902	3.567728	0.000272
8	6	0	-0.72042	3.567827	0.00047
9	1	0	1.257228	4.513831	0.000311
10	1	0	-1.256616	4.514005	0.00066
11	16	0	-0.000238	-3.381893	-0.000494
12	7	0	1.417287	2.474767	0.000044
13	7	0	-1.416956	2.474963	0.000431
14	7	0	1.244205	-2.353225	-0.00052
15	7	0	-1.24454	-2.353054	-0.000181
16	6	0	-2.876021	0.079414	0.00034
17	6	0	2.876021	0.079014	-0.000419
18	6	0	4.088134	0.030342	-0.000565

19	6	0	-4.088138	0.030861	0.000511
20	6	0	-5.516398	-0.009288	0.000774
21	6	0	-6.190291	-1.240749	0.000664
22	6	0	-6.25376	1.185388	0.00114
23	6	0	-7.579425	-1.271582	0.000917
24	1	0	-5.614805	-2.160648	0.000379
25	6	0	-7.64249	1.14401	0.001392
26	1	0	-5.726678	2.133851	0.001223
27	6	0	-8.307342	-0.081997	0.001281
28	1	0	-8.096031	-2.225937	0.000829
29	1	0	-8.208264	2.070065	0.001676
30	1	0	-9.392327	-0.110291	0.001478
31	6	0	5.5164	-0.009568	-0.000719
32	6	0	6.190492	-1.240919	-0.000985
33	6	0	6.253569	1.185228	-0.000604
34	6	0	7.579632	-1.271525	-0.001133
35	1	0	5.615156	-2.160911	-0.001074
36	6	0	7.642305	1.144076	-0.000752
37	1	0	5.726333	2.133606	-0.000396
38	6	0	8.307356	-0.081822	-0.001017
39	1	0	8.096392	-2.225797	-0.00134
40	1	0	8.20793	2.070223	-0.000661
41	1	0	9.392346	-0.109941	-0.001132

Compound 8b

Center number	Atomic number	Atomic type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.721379	-1.51162	-0.000033
2	6	0	-0.721377	-1.511621	-0.000034
3	6	0	-1.458668	-0.293945	-0.000019
4	6	0	-0.719627	0.895205	-0.000005
5	6	0	0.719626	0.895206	-0.000001
6	6	0	1.458668	-0.293943	-0.000015
7	6	0	0.732268	3.191973	0.000036
8	6	0	-0.732272	3.191972	0.000025
9	16	0	0.000003	-3.774417	-0.000081
10	7	0	1.410286	2.086424	0.000022
11	7	0	-1.410289	2.086422	0.000008
12	7	0	1.244685	-2.742853	-0.000041
13	7	0	-1.244681	-2.742855	-0.000043
14	6	0	-2.875307	-0.306945	-0.000015
15	6	0	2.875308	-0.306941	-0.000008
16	6	0	4.087632	-0.348053	-0.000004
17	6	0	-4.087632	-0.348059	-0.000008
18	6	0	-5.516438	-0.375963	0.000006
19	6	0	-6.202315	-1.600687	0.000002
20	6	0	-6.242923	0.825393	0.000027
21	6	0	-7.591775	-1.618421	0.000017
22	1	0	-5.635759	-2.526124	-0.000014
23	6	0	-7.632029	0.797336	0.000042
24	1	0	-5.70661	1.768785	0.00003
25	6	0	-8.308657	-0.422204	0.000037
26	1	0	-8.117262	-2.567948	0.000014
27	1	0	-8.188894	1.728819	0.000058
28	1	0	-9.393866	-0.440279	0.000049
29	6	0	5.516439	-0.375959	0.000002

30	6	0	6.202314	-1.600685	-0.000042
31	6	0	6.242925	0.825395	0.000051
32	6	0	7.591773	-1.618421	-0.000036
33	1	0	5.635755	-2.526121	-0.00008
34	6	0	7.632032	0.797336	0.000056
35	1	0	5.706614	1.768789	0.000084
36	6	0	8.308657	-0.422205	0.000013
37	1	0	8.117259	-2.567948	-0.000071
38	1	0	8.188898	1.728818	0.000095
39	1	0	9.393867	-0.440282	0.000017
40	6	0	1.478459	4.493053	0.000067
41	1	0	1.222196	5.090394	0.881524
42	1	0	2.550542	4.295518	0.000057
43	1	0	1.222188	5.090445	-0.881354
44	6	0	-1.478466	4.493051	0.000033
45	1	0	-1.222198	5.090414	0.881474
46	1	0	-1.222201	5.090421	-0.881404
47	1	0	-2.550549	4.295514	0.000033

Compound 8c

Center number	Atomic number	Atomic type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.72441	1.501982	-0.007581
2	6	0	0.724517	1.501916	0.007735
3	6	0	1.452532	0.26787	0.015281
4	6	0	0.71373	-0.969311	0.008068
5	6	0	-0.713844	-0.969248	-0.00792
6	6	0	-1.452539	0.268002	-0.015131
7	7	0	1.256766	2.711892	0.013233
8	7	0	-1.256551	2.712005	-0.01308
9	6	0	-2.840688	0.269164	-0.028765
10	6	0	-4.065059	0.287461	-0.040088
11	6	0	2.840687	0.268919	0.028933
12	6	0	4.065055	0.287102	0.040254
13	6	0	-5.47432	0.290185	-0.053935
14	6	0	-6.182847	1.50635	-0.049815
15	6	0	-6.180369	-0.929472	-0.066858
16	6	0	-7.5699	1.511868	-0.052562
17	1	0	-5.655358	2.453058	-0.025807
18	6	0	-7.563155	-0.921167	-0.082214
19	1	0	-5.653601	-1.877082	-0.079847
20	6	0	-8.277238	0.292651	-0.07526
21	6	0	5.474322	0.289895	0.054017
22	6	0	6.182754	1.506108	0.049817
23	6	0	6.180452	-0.929709	0.066981
24	6	0	7.569812	1.511707	0.05253
25	1	0	5.655198	2.452776	0.025772
26	6	0	7.563243	-0.92132	0.082271
27	1	0	5.653745	-1.877353	0.079972
28	6	0	8.277246	0.292562	0.075318
29	8	0	-8.245883	-2.10751	-0.114227
30	8	0	-9.629884	0.336306	-0.143602
31	8	0	-8.197955	2.716114	-0.071553
32	8	0	8.245997	-2.107645	0.11413
33	8	0	9.629941	0.336347	0.143686

34	8	0	8.197774	2.716006	0.071438
35	6	0	-8.819736	-2.38951	-1.391667
36	1	0	-9.532881	-1.610416	-1.681158
37	1	0	-8.034299	-2.467725	-2.150469
38	1	0	-9.335028	-3.345105	-1.29345
39	6	0	-10.365958	-0.42921	0.817491
40	1	0	-9.807502	-0.505958	1.754376
41	1	0	-11.296531	0.114837	0.985058
42	1	0	-10.582513	-1.430053	0.438932
43	6	0	-9.273592	2.919301	0.846132
44	1	0	-10.229012	2.642184	0.398335
45	1	0	-9.116717	2.341345	1.762941
46	1	0	-9.26878	3.983667	1.085456
47	6	0	8.820292	-2.389605	1.39138
48	1	0	9.533521	-1.610488	1.680588
49	1	0	8.035115	-2.467817	2.150452
50	1	0	9.335566	-3.345193	1.293012
51	6	0	10.365961	-0.428414	-0.818048
52	1	0	9.808603	-0.502063	-1.755856
53	1	0	11.297679	0.114403	-0.983167
54	1	0	10.580271	-1.430475	-0.441467
55	6	0	9.273392	2.919199	-0.846271
56	1	0	10.228849	2.642341	-0.398395
57	1	0	9.116632	2.341021	-1.762959
58	1	0	9.2684	3.983513	-1.085823
59	16	0	0.000157	3.789404	0.000083
60	7	0	1.39796	-2.126895	0.016847
61	7	0	-1.398175	-2.126771	-0.016733
62	6	0	0.709399	-3.262311	0.009068
63	6	0	-0.709713	-3.262248	-0.008991
64	6	0	-1.480938	-4.54968	-0.020512
65	1	0	-2.549744	-4.333222	-0.032103
66	1	0	-1.230082	-5.152497	-0.90043
67	1	0	-1.250001	-5.15693	0.861739
68	6	0	1.480508	-4.549813	0.020553
69	1	0	1.22961	-5.152626	0.900462
70	1	0	1.249503	-5.157023	-0.861708
71	1	0	2.549334	-4.333453	0.032132

Compound 1

Center number	Atomic number	Atomic type	Coordinates (Angstroms)		
			X	Y	Z
1	16	0	-0.000028	2.883347	-0.000033
2	7	0	-1.261474	1.832689	0.000086
3	6	0	-0.727269	0.608967	-0.000012
4	6	0	0.727246	0.608938	0.000022
5	7	0	1.261709	1.83256	-0.000006
6	6	0	-1.43249	-0.631599	-0.000027
7	6	0	-0.714123	-1.798107	-0.000029
8	6	0	0.714099	-1.798141	-0.000016
9	6	0	1.4325	-0.631664	-0.000004
10	1	0	-1.233946	-2.749937	-0.000025
11	1	0	1.233825	-2.750022	-0.000019
12	35	0	3.32543	-0.63487	0.000008

13	35	0	-3.325455	-0.634864	0.000004
1	16	0	-0.000028	2.883347	-0.000033
2	7	0	-1.261474	1.832689	0.000086
3	6	0	-0.727269	0.608967	-0.000012
4	6	0	0.727246	0.608938	0.000022
5	7	0	1.261709	1.83256	-0.000006
6	6	0	-1.43249	-0.631599	-0.000027
7	6	0	-0.714123	-1.798107	-0.000029
8	6	0	0.714099	-1.798141	-0.000016
9	6	0	1.4325	-0.631664	-0.000004
10	1	0	-1.233946	-2.749937	-0.000025
11	1	0	1.233825	-2.750022	-0.000019
12	35	0	3.32543	-0.63487	0.000008
13	35	0	-3.325455	-0.634864	0.000004
1	16	0	-0.000028	2.883347	-0.000033
2	7	0	-1.261474	1.832689	0.000086
3	6	0	-0.727269	0.608967	-0.000012
4	6	0	0.727246	0.608938	0.000022
5	7	0	1.261709	1.83256	-0.000006
6	6	0	-1.43249	-0.631599	-0.000027
7	6	0	-0.714123	-1.798107	-0.000029
8	6	0	0.714099	-1.798141	-0.000016
9	6	0	1.4325	-0.631664	-0.000004

Compound 6a

Center number	Atomic number	Atomic type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	1.417127	2.440987	0.000022
2	6	0	0.729853	1.24984	0.000012
3	6	0	-0.729872	1.249825	0.000001
4	7	0	-1.417165	2.440967	0.000008
5	6	0	-0.718868	3.539839	0.000026
6	6	0	0.718814	3.53985	0.000039
7	6	0	-1.447163	0.050394	-0.000005
8	6	0	-0.729822	-1.164376	-0.000031
9	6	0	0.729831	-1.164352	0.000006
10	6	0	1.44716	0.050416	0.000024
11	7	0	-1.260025	-2.400673	-0.000014
12	16	0	0.000049	-3.436229	0.000076
13	7	0	1.260037	-2.400655	-0.000101
14	35	0	-3.330584	0.01913	-0.000016
15	35	0	3.33058	0.019168	-0.000015
16	1	0	1.263494	4.483146	0.000013
17	1	0	-1.263562	4.483128	0.000002
1	7	0	1.417127	2.440987	0.000022
2	6	0	0.729853	1.24984	0.000012
3	6	0	-0.729872	1.249825	0.000001
4	7	0	-1.417165	2.440967	0.000008
5	6	0	-0.718868	3.539839	0.000026
6	6	0	0.718814	3.53985	0.000039

7	6	0	-1.447163	0.050394	-0.000005
8	6	0	-0.729822	-1.164376	-0.000031
9	6	0	0.729831	-1.164352	0.000006
10	6	0	1.44716	0.050416	0.000024
11	7	0	-1.260025	-2.400673	-0.000014
12	16	0	0.000049	-3.436229	0.000076
13	7	0	1.260037	-2.400655	-0.000101
14	35	0	-3.330584	0.01913	-0.000016
15	35	0	3.33058	0.019168	-0.000015
16	1	0	1.263494	4.483146	0.000013
17	1	0	-1.263562	4.483128	0.000002

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