Electronic Supplementary Material (ESI) for Materials Advances.

Two types of two-step mechanochromic luminescence of phenanthroimidazolylbenzothiadiazoles

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1. Absorption and fluorescence spectra

Both absorption and fluorescence spectra of **1a**–**g** in toluene solutions were observed in the same regions irrespective to the substituent R on the *N*-phenyl group (Fig. S1).

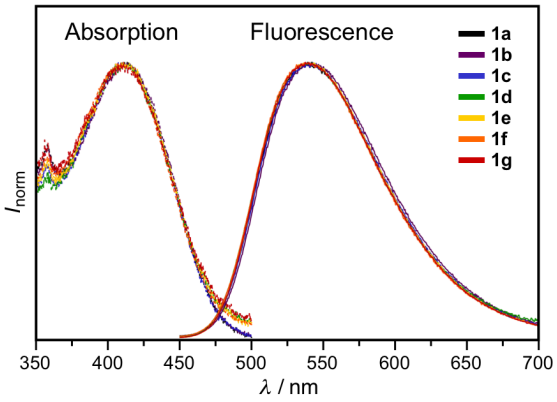

Fig. S1 Absorption and fluorescence spectra of **1a**–**g** in toluene (1.0×10^{-5} M).

The maximum emission wavelength of crystalline **1a**–**g** were observed over a wide range of 490 –563 nm (Fig. S2).

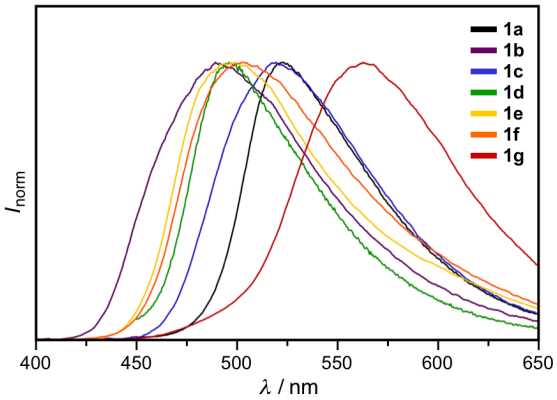

Fig. S2 Solid-state fluorescence spectra of crystalline **1a**–**g**.

2. Single-crystal X-ray diffraction analyses

*X-ray analysis of **1a***

A single crystal of **1a** was obtained from vapor diffusion of hexane into a chloroform solution of **1a** and was mounted on a glass fiber. All measurements were made on a Rigaku XtaLAB P200 diffractometer using multi-layer mirror monochromated Cu-Kα radiation (λ = 1.54184 Å). The data were collected at a temperature of –50 ± 1 °C to a maximum 2θ value of 148.8°. A total of 2306 oscillation images were collected. The crystal-to-detector distance was 40.00 mm. Readout was performed in the 0.172 mm pixel mode.

Of the 15141 reflections that were collected, 4685 were unique (R_{int} = 0.0326); equivalent reflections were merged. Data were collected and processed using CrysAlisPro (Rigaku Oxford Diffraction).[1] The linear absorption coefficient, μ, for Cu-Kα radiation is 13.683 cm^{-1}. An empirical absorption correction was applied which resulted in transmission factors ranging from 0.280 to 0.611. The data were corrected for Lorentz and polarization effects.

The structure was solved by direct methods (SIR2011)[2] and expanded using Fourier techniques. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were refined using the riding model. All calculations were performed using the CrystalStructure[3] crystallographic software package except for refinement, which was performed using SHELXL Version 2014/7.[4]

Crystal data for **1a** (CCDC 1995249): $C_{34}H_{23}N_4S$, M = 518.63, monoclinic, a = 13.13381(11) Å, b = 16.14963(13) Å, c = 24.1369(2) Å, β = 94.3385(7)°, V = 5104.92(7) Å^3, space group C_2/c (no. 15), Z = 8, D_c = 1.350 g cm^{-3}, F(000) = 2160.00, T = 223(1) K, μ(Cu-Kα) = 13.683 cm^{-1}, 15141 reflections measured, 4685 independent (R_{int} = 0.0326). The final refinement converged to R_1 = 0.0451 for $I > 2.0\sigma(I)$, wR_2 = 0.1217 for all data.

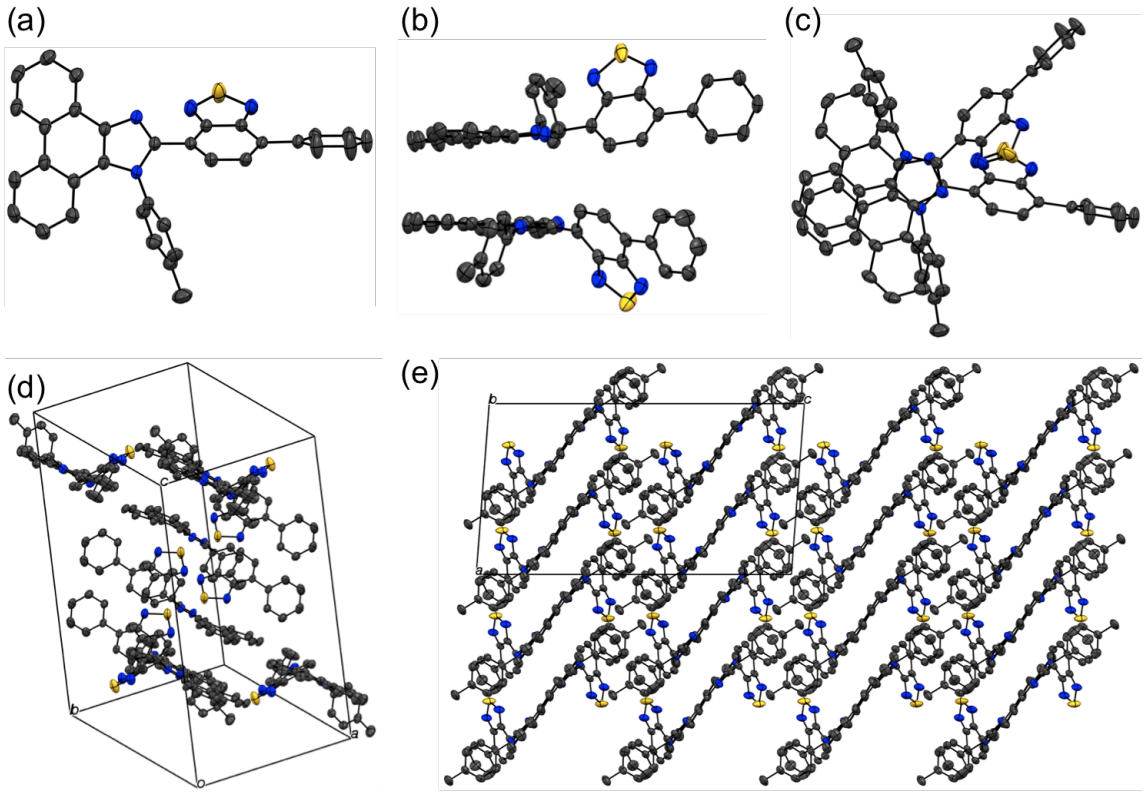

Fig. S3 The molecular structure of **1a** with atomic displacement parameters set at 50% probability (Color code: gray = C, blue = N, yellow = S). All hydrogen atoms are omitted for clarity. (a) Front view. (b) Side view of adjacent two molecules. (c) Top view of adjacent two molecules. (d) Unit cell structure. (e) Packing structure viewed along *b* axis.

*X-ray analysis of **1b***

A single crystal of **1b** was obtained from vapor diffusion of hexane into a chloroform solution of **1b** and was mounted on a glass fiber. All measurements were made on a Rigaku XtaLAB P200 diffractometer using graphite monochromated Cu-Kα radiation (λ = 1.54184 Å). The data were collected at a temperature of –50 ± 1 °C to a maximum 2θ value of 150.8°. A total of 2794 oscillation images were collected. The crystal-to-detector distance was 40.00 mm. Readout was performed in the 0.172 mm pixel mode.

Of the 14064 reflections that were collected, 4822 were unique (R_{int} = 0.0292); equivalent reflections were merged. Data were collected and processed using CrysAlisPro (Rigaku Oxford Diffraction).[1] The linear absorption coefficient, μ, for Cu-Kα radiation is 13.711 cm^{-1}. An empirical absorption correction was applied which resulted in transmission factors ranging from 0.714 to 0.916. The data were corrected for Lorentz and polarization effects.

The structure was solved by direct methods (SIR2011)[2] and expanded using Fourier techniques. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were refined using the riding model. All calculations were performed using the CrystalStructure[3] crystallographic software package except for refinement, which was performed using SHELXL Version 2014/7.[4]

Crystal data for **1b** (CCDC 1995250): $C_{34}H_{22}N_4OS$, M = 534.63, triclinic, a = 9.72015(13) Å, b = 10.26595(12) Å, c = 14.23572(16) Å, α = 100.4892(9)°, β = 96.5213(10)°, γ = 106.5436(11)°, V = 1318.19(3) Å^3, space group P-1 (no. 2), Z = 2, D_c = 1.347 g cm^{-3}, F(000) = 556.00, T = 223(1) K, μ(Cu-Kα) = 13.711 cm^{-1}, 14064 reflections measured, 4822 independent (R_{int} = 0.0292). The final refinement converged to R_1 = 0.0448 for $I > 2.0\sigma(I)$, wR_2 = 0.1214 for all data.

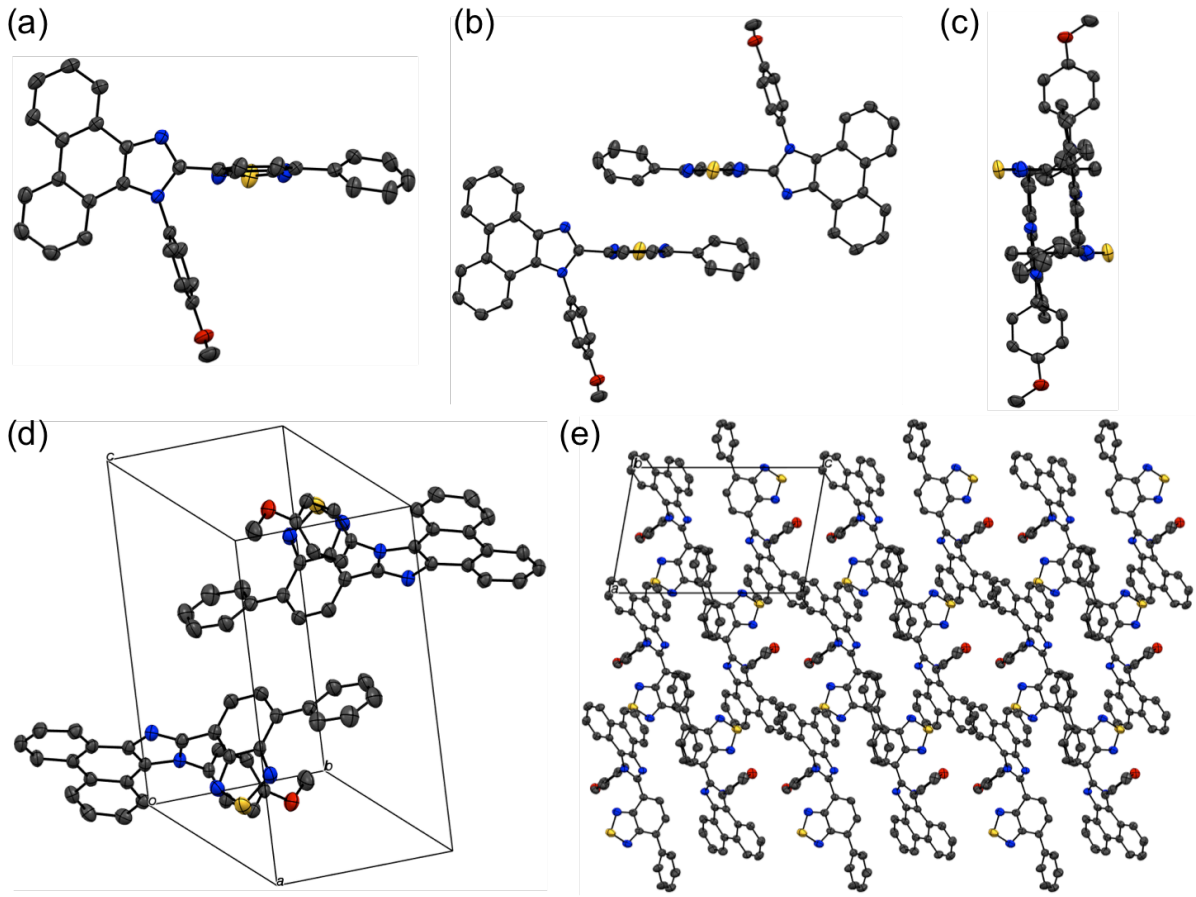

Fig. S4 The molecular structure of **1b** with atomic displacement parameters set at 50% probability (Color code: gray = C, blue = N, red = O, yellow = S). All hydrogen atoms are omitted for clarity. (a) Front view. (b) Front view of adjacent two molecules. (c) Side view of adjacent two molecules. (d) Unit cell structure. (e) Packing structure viewed along *b* axis.

*X-ray analysis of **1d***

A single crystal of **1d** was obtained from vapor diffusion of hexane into a chloroform solution of **1d** and was mounted on a glass fiber. All measurements were made on a Rigaku XtaLAB P200 diffractometer using graphite monochromated Cu-Kα radiation (λ = 1.54184 Å). The data were collected at a temperature of –50 ± 1 °C to a maximum 2θ value of 150.4°. A total of 2878 oscillation images were collected. The crystal-to-detector distance was 40.00 mm. Readout was performed in the 0.172 mm pixel mode.

Of the 12728 reflections that were collected, 4685 were unique (R_{int} = 0.1047); equivalent reflections were merged. Data were collected and processed using CrysAlisPro (Rigaku Oxford Diffraction).[1] The linear absorption coefficient, μ, for Cu-Kα radiation is 15.859 cm^{-1}. An empirical absorption correction was applied which resulted in transmission factors ranging from 0.576 to 0.863. The data were corrected for Lorentz and polarization effects.

The structure was solved by direct methods (SIR2011)[2] and expanded using Fourier techniques. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were refined using the riding model. All calculations were performed using the CrystalStructure[3] crystallographic software package except for refinement, which was performed using SHELXL Version 2014/7.[4]

Crystal data for **1d** (CCDC 1995251): $C_{34}H_{19}F_3N_4S$, M = 572.61, triclinic, a = 6.7391(3) Å, b = 13.8406(5) Å, c = 15.2075(5) Å, α = 113.486(3)°, β = 90.031(3)°, γ = 96.987(3)°, V = 1289.41(9) Å^3, space group P-1 (no. 2), Z = 2, D_c = 1.475 g cm^{-3}, F(000) = 588.00, T = 223(1) K, μ(Cu-Kα) = 15.859 cm^{-1}, 12728 reflections measured, 4685 independent (R_{int} = 0.1047). The final refinement converged to R_1 = 0.0695 for $I > 2.0\sigma(I)$, wR_2 = 0.2109 for all data.

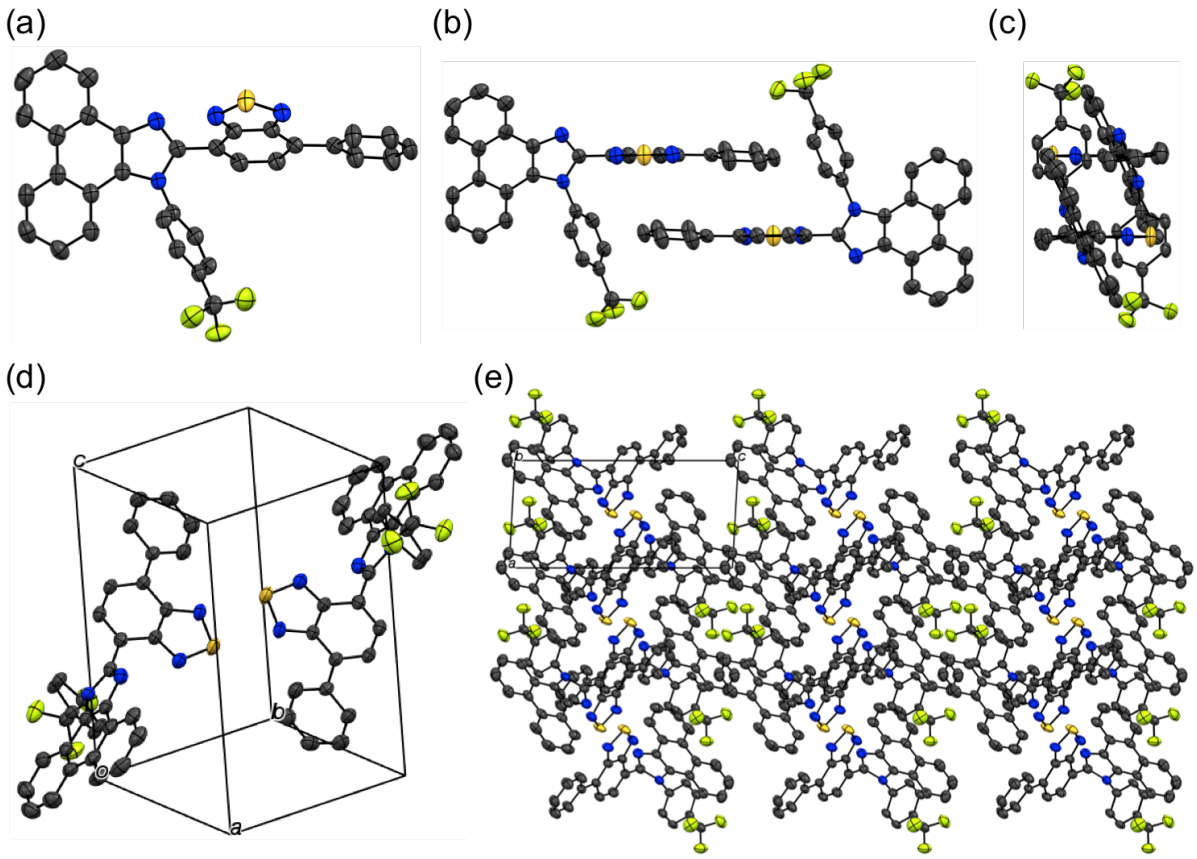

Fig. S5 The molecular structure of **1d** with atomic displacement parameters set at 50% probability (Color code: gray = C, blue = N, green = F, yellow = S). All hydrogen atoms are omitted for clarity. (a) Front view. (b) Front view of adjacent two molecules. (c) Side view of adjacent two molecules. (d) Unit cell structure. (e) Packing structure viewed along *b* axis.

*X-ray analysis of **1e***

A single crystal of **1e** was obtained from vapor diffusion of hexane into a chloroform solution of **1e** and was mounted on a glass fiber. All measurements were made on a Rigaku XtaLAB P200 diffractometer using graphite monochromated Cu-Kα radiation (λ = 1.54184 Å). The data were collected at a temperature of –50 ± 1 °C to a maximum 2θ value of 153.0°. A total of 2912 oscillation images were collected. The crystal-to-detector distance was 40.00 mm. Readout was performed in the 0.172 mm pixel mode.

Of the 14175 reflections that were collected, 5135 were unique (R_{int} = 0.0664); equivalent reflections were merged. Data were collected and processed using CrysAlisPro (Rigaku Oxford Diffraction).[1] The linear absorption coefficient, μ, for Cu-Kα radiation is 32.341 cm^{-1}. An empirical absorption correction was applied which resulted in transmission factors ranging from 0.375 to 0.674. The data were corrected for Lorentz and polarization effects.

The structure was solved by direct methods (SIR2011)[2] and expanded using Fourier techniques. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were refined using the riding model. All calculations were performed using the CrystalStructure[3] crystallographic software package except for refinement, which was performed using SHELXL Version 2014/7.[4]

Crystal data for **1e** (CCDC 1995252): $C_{33}H_{19}BrN_4S$, M = 583.50, triclinic, a = 6.63294(10) Å, b = 13.8905(2) Å, c = 15.0996(2) Å, α = 66.2986(14)°, β = 88.1740(12)°, γ = 83.1236(13)°, V = 1264.49(3) Å^3, space group P-1 (no. 2), Z = 2, D_c = 1.532 g cm^{-3}, F(000) = 592.00, T = 223(1) K, μ(Cu-Kα) = 32.341 cm^{-1}, 14175 reflections measured, 5135 independent (R_{int} = 0.0664). The final refinement converged to R_1 = 0.0506 for $I > 2.0\sigma(I)$, wR_2 = 0.1436 for all data.

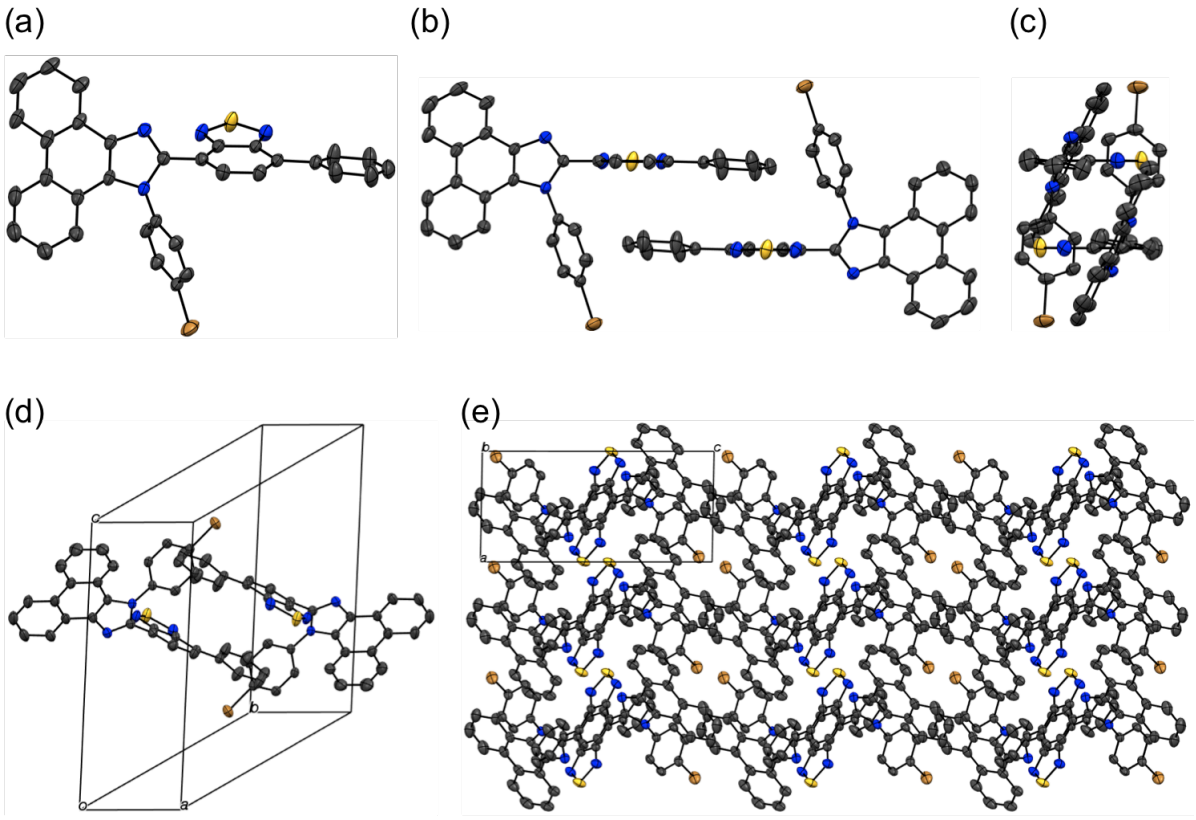

Fig. S6 The molecular structure of **1e** with atomic displacement parameters set at 50% probability (Color code: gray = C, blue = N, yellow = S, orange = Br). All hydrogen atoms are omitted for clarity. (a) Front view. (b) Front view of adjacent two molecules. (c) Side view of adjacent two molecules. (d) Unit cell structure. (e) Packing structure viewed along *b* axis.

*X-ray analysis of **1g***

A single crystal of **1g** was obtained from vapor diffusion of hexane into a chloroform solution of **1g** and was mounted on a glass fiber. All measurements were made on a Rigaku XtaLAB P200 diffractometer using graphite monochromated Cu-Kα radiation (λ = 1.54184 Å). The data were collected at a temperature of –50 ± 1 °C to a maximum 2θ value of 150.4°. A total of 1920 oscillation images were collected. The crystal-to-detector distance was 40.00 mm. Readout was performed in the 0.172 mm pixel mode.

Of the 17435 reflections that were collected, 4612 were unique (R_{int} = 0.0499); equivalent reflections were merged. Data were collected and processed using CrysAlisPro (Rigaku Oxford Diffraction).[1] The linear absorption coefficient, μ, for Cu-Kα radiation is 32.439 cm^{-1}. An empirical absorption correction was applied which resulted in transmission factors ranging from 0.375 to 0.674. The data were corrected for Lorentz and polarization effects.

The structure was solved by direct methods (SIR2011)[2] and expanded using Fourier techniques. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were refined using the riding model. All calculations were performed using the CrystalStructure[3] crystallographic software package except for refinement, which was performed using SHELXL Version 2014/7.[4]

Crystal data for **1g** (CCDC 1995253): $C_{33}H_{19}BrN_4S$, M = 583.50, monoclinic, a = 10.39805(19) Å, b = 18.2187(4) Å, c = 13.3287(2) Å, β = 93.0879(17)°, V = 2521.31(8) Å^3, space group $P2_1/n$ (no. 14), Z = 4, D_c = 1.537 g cm^{-3}, F(000) = 1184.00, T = 223(1) K, μ(Cu-Kα) = 32.439 cm^{-1}, 17435 reflections measured, 4612 independent (R_{int} = 0.0499). The final refinement converged to R_1 = 0.0540 for $I > 2.0\sigma(I)$, wR_2 = 0.1569 for all data.

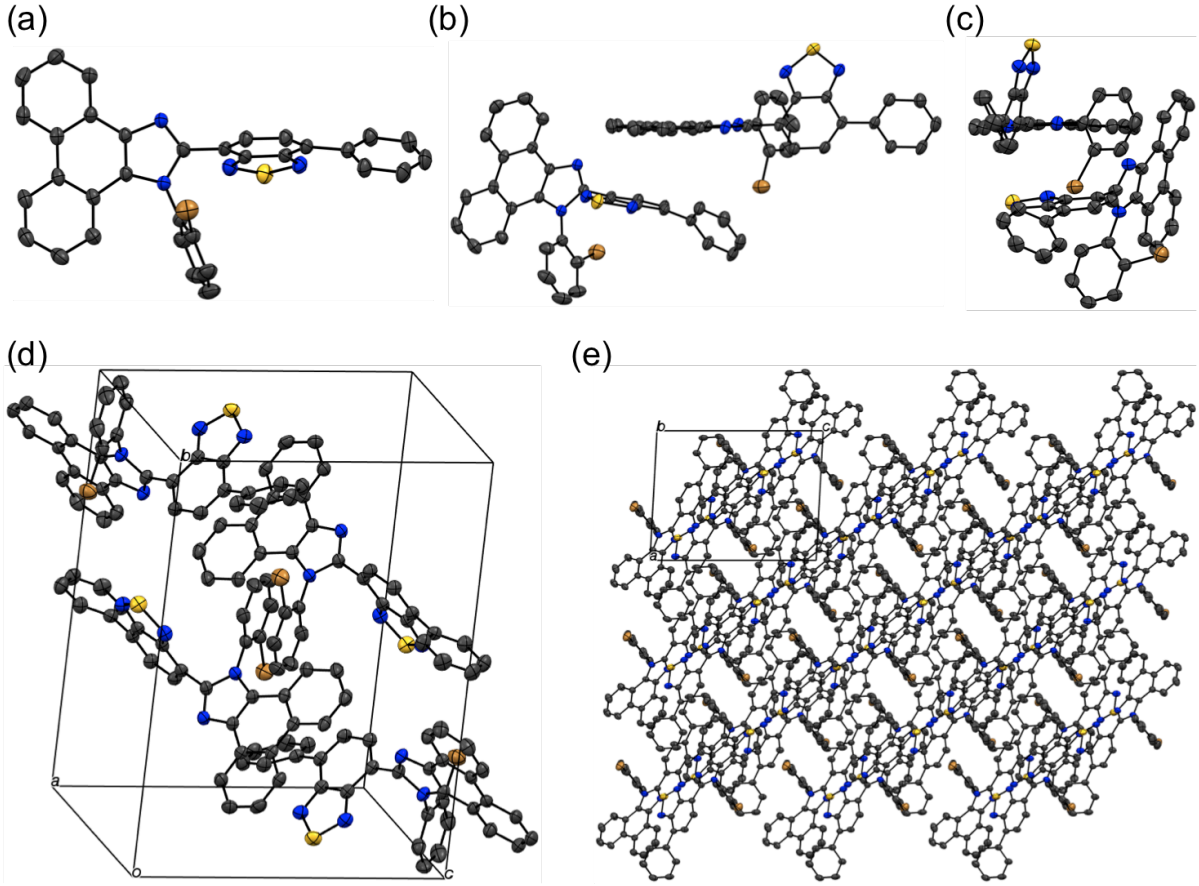

Fig. S7 The molecular structure of **1g** with atomic displacement parameters set at 50% probability (Color code: gray = C, blue = N, yellow = S, orange = Br). All hydrogen atoms are omitted for clarity. (a) Front view. (b) Front view of adjacent two molecules. (c) Side view of adjacent two molecules. (d) Unit cell structure. (e) Packing structure viewed along *b* axis.

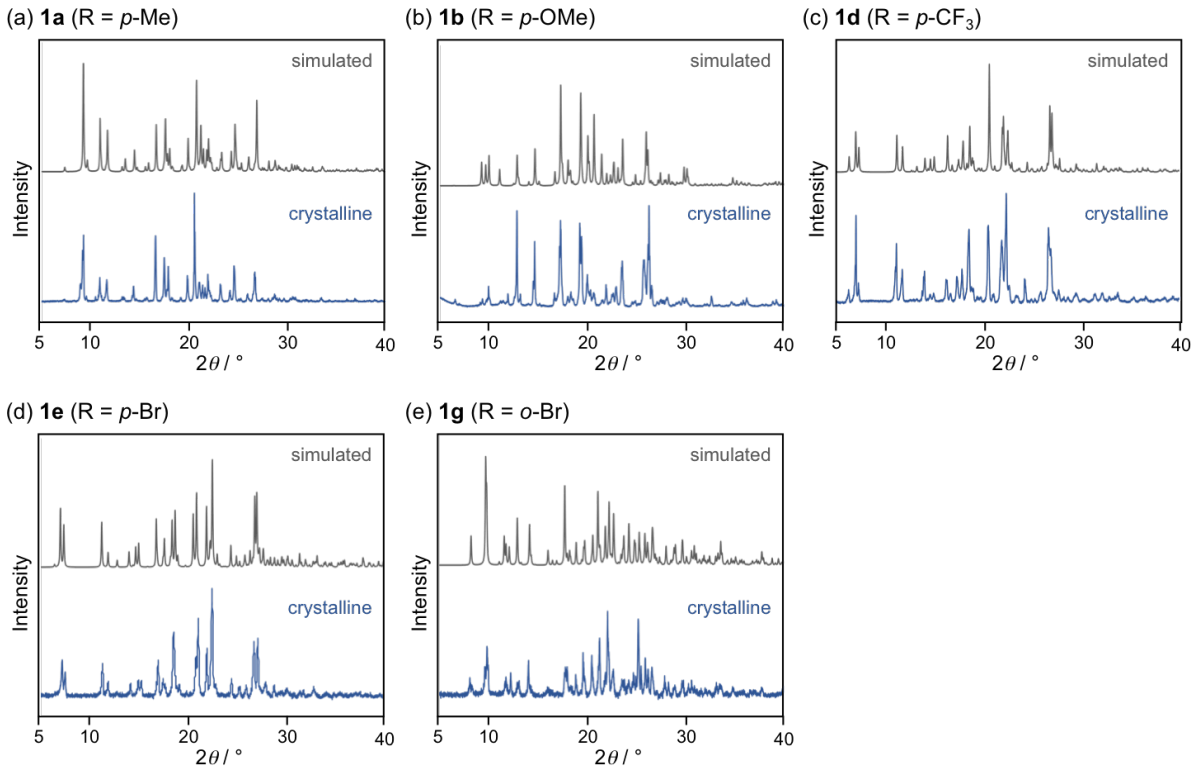

Fig. S8 PXRD patterns for **1a** (a), **1b** (b), **1d** (c), **1e** (d), and **1g** (e). Simulated patterns of the single crystals obtained from vapor diffusion of hexane into chloroform solutions (black). Experimental patterns of the crystalline samples obtained from toluene solutions (blue).

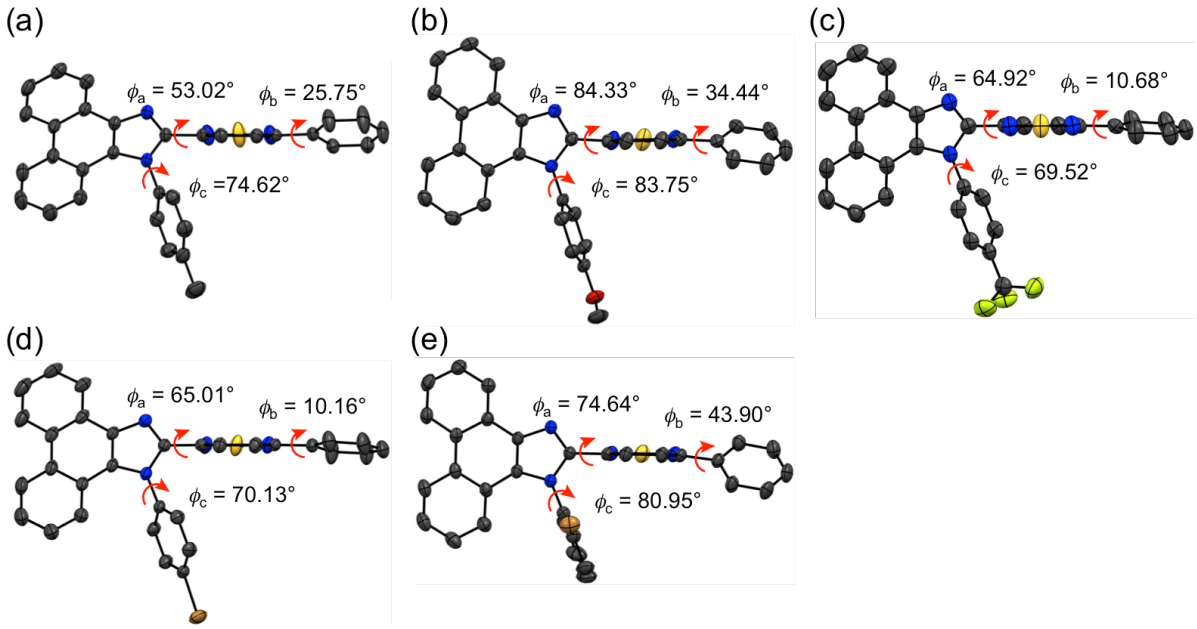

Fig. S9 Molecular structures for **1a** (a), **1b** (b), **1d** (c), **1e** (d), and **1g** (e) determined by X-ray diffraction analysis. Atomic displacement parameters set at 50% probability (Color code: gray = C, blue = N, red = O, green = F, yellow = S, orange = Br). All hydrogen atoms are omitted for clarity.

3. Theoretical calculations

Theoretical absorption wavelengths of **1a, 1b, 1d**, **1e**, and **1g** were calculated by time-dependent density functional theory (TD-DFT) at the CAM-B3LYP/6-31G(d) and B3LYP/6-31G(d) level of theories (Table S1 and S2). The CAM-B3LYP approach gave better results than the B3LYP approach.

Table S1 Calculated absorption properties of **1a, 1b, 1d**, **1e**, and **1g** at the CAM-B3LYP/6-31G(d) level of theory.

Compd	Calcd absorption λ_{abs} (nm)	Transition from HOMO to LUMO	Oscillator strength	HOMO (eV)	LUMO (eV)	Dipole moment (D)
1a	363.28	0.63387	0.3977	–6.46	–1.18	5.30
	310.34	0.61354[a]	0.0766	–7.36[b]	–1.18	
1b	352.42	0.68023	0.0368	–6.46	–1.22	5.78
	330.53	0.67871[a]	0.3171	–7.36[b]	–1.22	
1d	359.78	0.58804	0.3767	–6.69	–1.40	1.84
	322.07	0.56595[a]	0.0848	–7.42[b]	–1.40	
1e	354.81	0.60550	0.3153	–6.66	–1.35	2.64
	320.15	0.59458[a]	0.1191	–7.45[b]	–1.35	
1g	349.67	0.63855	0.1881	–6.56	–1.25	4.40
	315.03	0.63223[a]	0.1438	–7.53[b]	–1.25	

[a]Transition from HOMO–2 to LUMO. [b]Energy level of HOMO–2.

Table S2 Calculated absorption properties of **1a, 1b, 1d**, **1e**, and **1g** at the B3LYP/6-31G(d) level of theory.

Compd	Calcd absorption λ_{abs} (nm)	Transition from HOMO to LUMO	Oscillator strength	HOMO (eV)	LUMO (eV)	Dipole moment (D)
1a	499.33	0.70549	0.1339	–5.22	–2.28	5.25
	372.97	0.69663[a]	0.1681	–6.04[b]	–2.28	
1b	529.29	0.70522	0.0054	–5.19	–2.34	5.84
	384.05	0.69633[a]	0.1962	–6.05[b]	–2.34	
1d	502.01	0.70537	0.0814	–5.44	–2.50	1.84
	386.76	0.69552[a]	0.1962	–6.12[b]	–2.50	
1e	501.38	0.70534	0.0651	–5.41	–2.45	2.64
	380.70	0.69779[a]	0.2087	–6.14[b]	–2.45	
1g	506.40	0.70547	0.0400	–5.30	–2.37	4.34
	370.81	0.69718[a]	0.1686	–6.20[b]	–2.37	

[a]Transition from HOMO–2 to LUMO. [b]Energy level of HOMO–2.

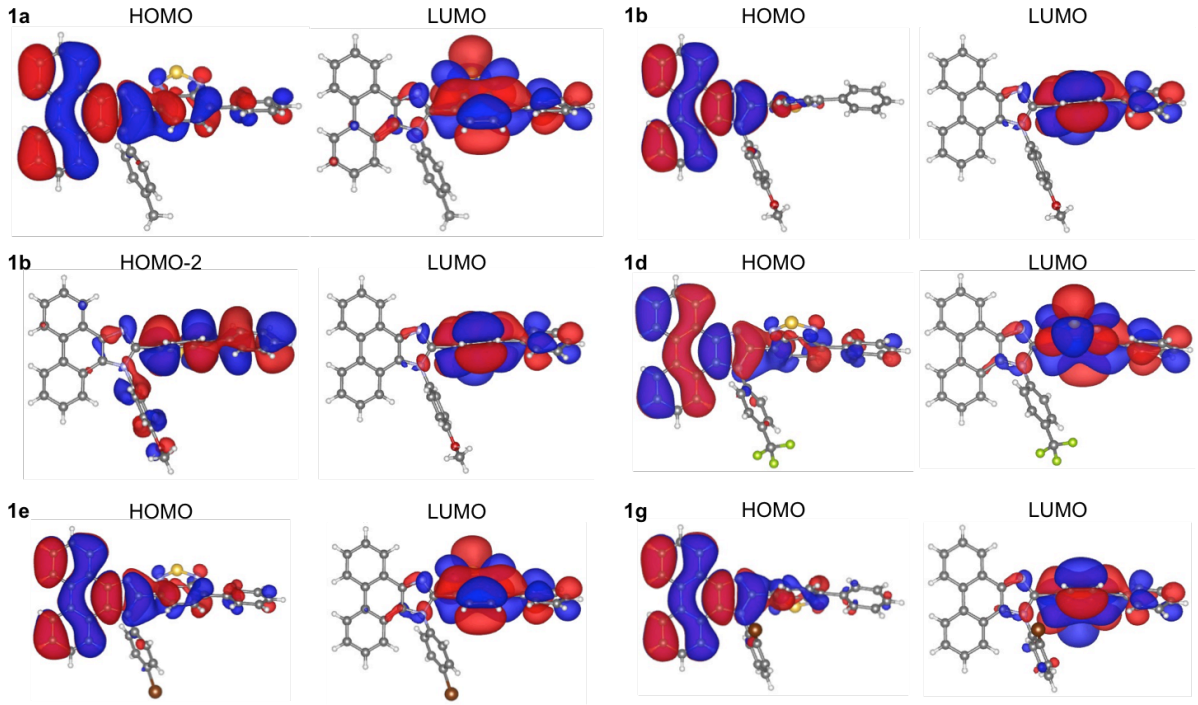

Fig. S10 HOMO, HOMO–2 (**1b**), and LUMO of **1a**, **1b**, **1d**, **1e**, and **1g** calculated at the CAM-B3LYP/6-31G(d) level. The structures are drawn by VESTA.[5]

Table S3 Calculated absorption properties of the optimized structures of **1a, 1b, 1d**, **1e**, and **1g** at the CAM-B3LYP/6-31G(d) level of theory.

Compd	Calcd absorption λ_{abs} (nm)	Transition from HOMO to LUMO	Oscillator strength	HOMO (eV)	LUMO (eV)	Dipole moment (D)
1a	367.38	0.64470	0.4318	–6.46	–1.19	5.52
	302.34	0.61348[a]	0.0469	–7.47[b]	–1.19	
1b	373.74	0.64460	0.3819	–6.46	–1.27	4.77
	308.71	0.62011[a]	0.0568	–7.49[b]	–1.27	
1d	371.40	0.63601	0.4079	–6.64	–1.41	1.40
	307.52	0.61447[a]	0.0410	–7.61[b]	–1.41	
1e	372.05	0.63757	0.3989	–6.60	–1.38	1.99
	308.05	0.61695[a]	0.0453	–7.58[b]	–1.38	
1g	366.85	0.63356	0.3320	–6.54	–1.32	3.96
	313.21	0.61864[a]	0.0747	–7.52[b]	–1.32	

[a]Transition from HOMO–2 to LUMO. [b]Energy level of HOMO–2.

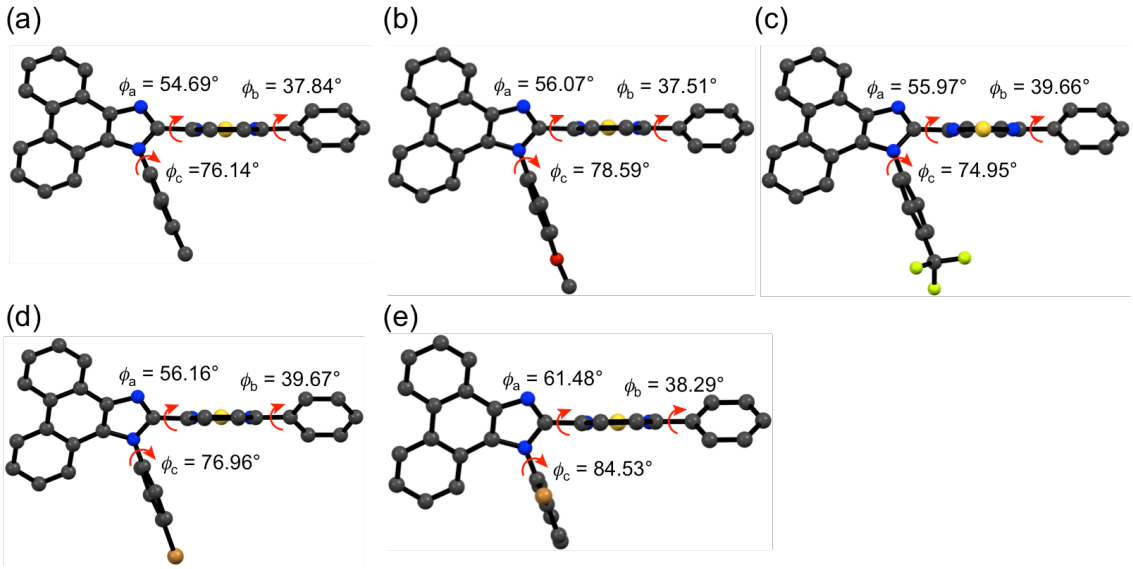

Fig. S11 Optimized molecular structures for **1a** (a), **1b** (b), **1d** (c), **1e** (d), and **1g** (e) calculated at the CAM-B3LYP/6-31G(d) level of theory (Color code: gray = C, blue = N, red = O, green = F, yellow = S, orange = Br). All hydrogen atoms are omitted for clarity.

Table S4 Calculated absorption properties of the stacked dimers of **1a, 1b, 1d**, **1e**, and **1g** at the CAM-B3LYP/6-31G(d) level of theory.

Compd	Calcd absorption λ_{abs} (nm)	Transition	Oscillator strength	Energy level (eV)		Dipole moment (D)
1a	366.25	HOMO to LUMO 0.51762	0.4318	HOMO –6.21	LUMO –1.040	2.292000
	362.30	HOMO to LUMO+1 0.52217	0.5644	HOMO –6.21	LUMO+1 –1.039	
1b	339.00	HOMO–1 to LUMO 0.40708	0.3636	HOMO–1 –6.49	LUMO –1.11	0.000748
1d	355.86	HOMO to LUMO 0.43691	0.8623	HOMO –6.70	LUMO –1.38	0.001556
1e	350.15	HOMO to LUMO 0.44350	0.7380	HOMO –6.68	LUMO –1.33	0.000510
1g	356.66	HOMO to LUMO+1 0.57774	0.0073	HOMO –6.40	LUMO+1 –1.00	5.245622
	355.63	HOMO to LUMO 0.55624	0.2179	HOMO –6.40	LUMO –1.19	
	331.72	HOMO–1 to LUMO+1 0.54743	0.1924	HOMO–1 –6.57	LUMO –1.00	

[a]Transition from HOMO–2 to LUMO. [b]Energy level of HOMO–2.

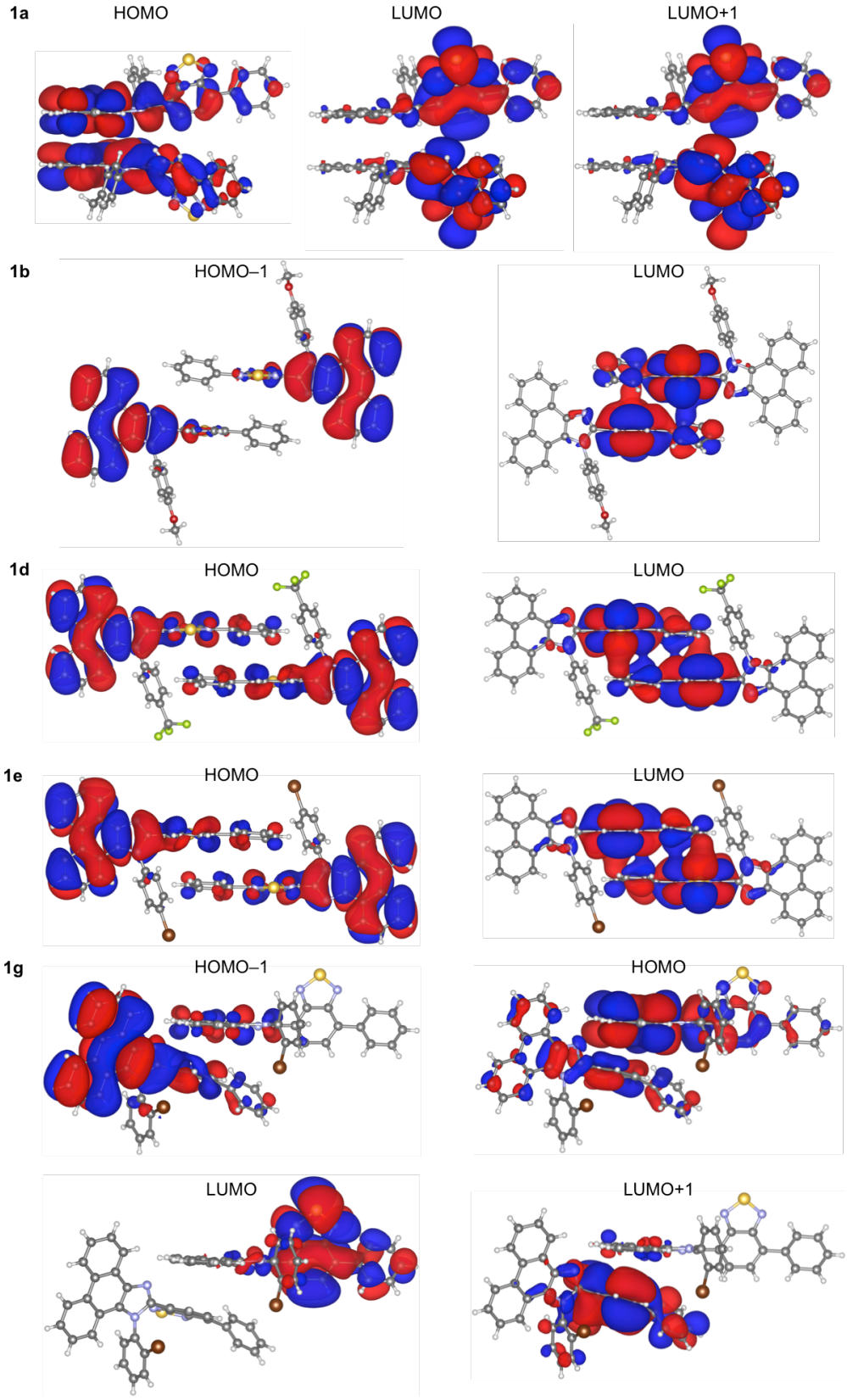

Fig. S12 Molecular orbitals for the stacked dimers of **1a**, **1b**, **1d**, **1e**, and **1g** calculated at the CAM-B3LYP/6-31G(d) level. The structures are drawn by VESTA.[5]

4. Solid-state absorption spectra

The solid-state absorption band of **1a** was observed at the longest-wavelength region, followed in order by **1e** ≈ **1g**, **1d**, and **1b** (Fig. S13).

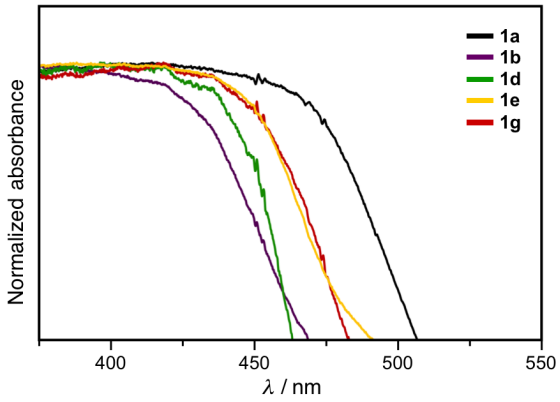

Fig. S13 Solid-state absorption spectra of crystalline **1a, 1b, 1d**, **1e**, and **1g**.

5. Supplementary data for bicolor MCL

Fluorescence spectra of crystalline **1b**–**d** and **1f** shifted in bathochromic direction after grinding (Fig. S14).

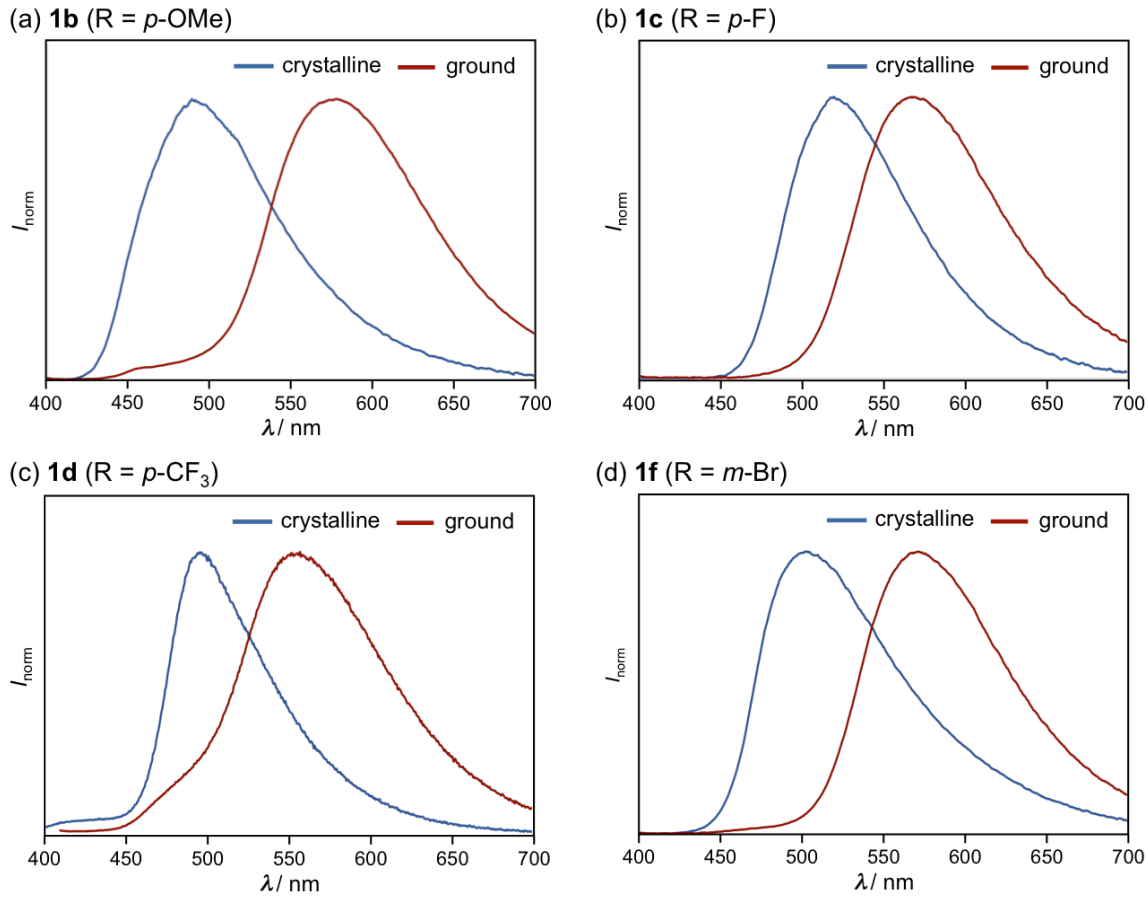

Fig. S14 Fluorescence spectra of crystalline and ground **1b** (a), **1c** (b), **1d** (c), and **1f** (d).

The intense peaks of the diffraction for crystalline samples of **1b**–**d** and **1f** almost disappeared after grinding and significantly recovered after heating (Fig. S15).

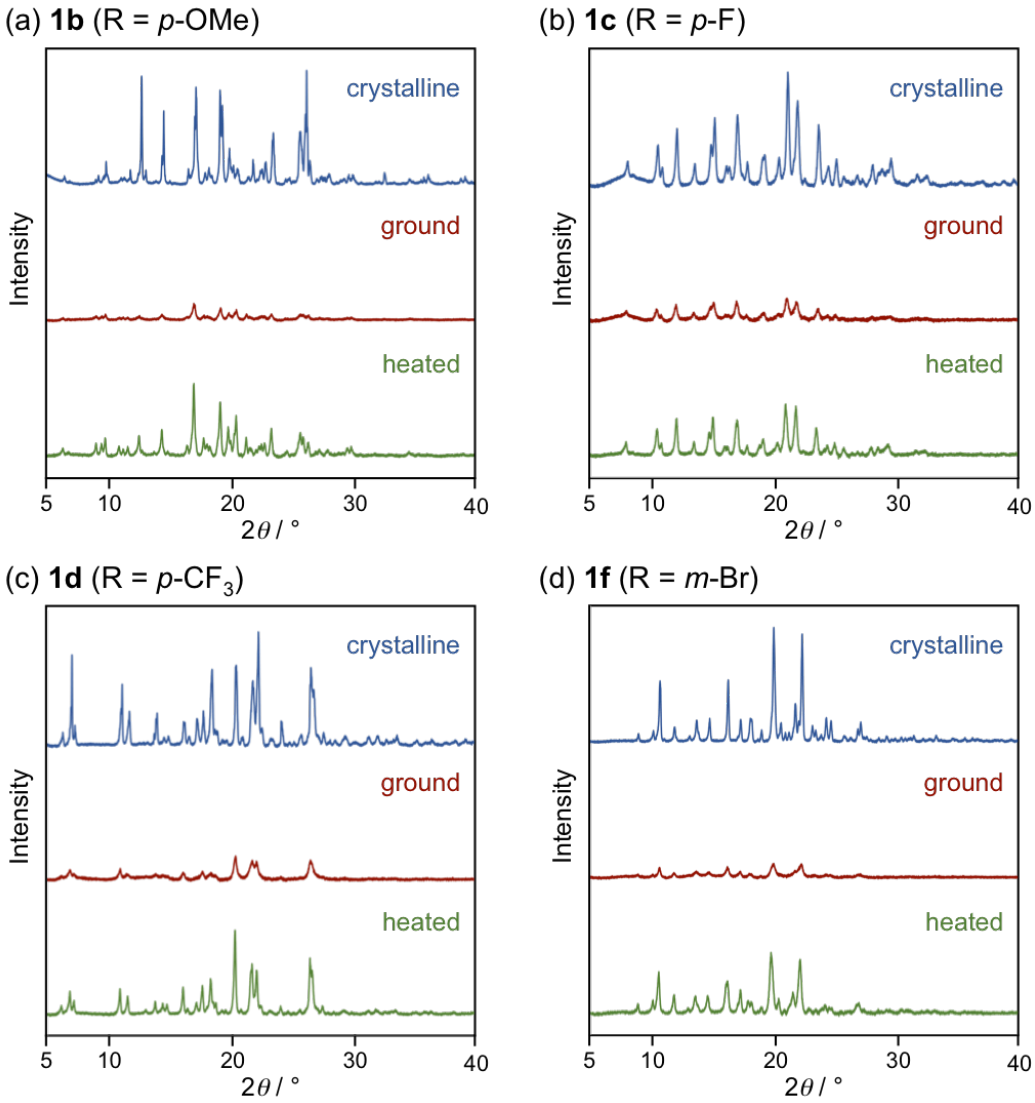

Fig. S15 PXRD patterns for the crystalline (blue), ground (red), and heated (green) samples of **1b** (a), **1c** (b), **1d** (c), and **1f** (d).

In the DSC thermograms of **1b–d** and **1f**, endothermic peaks that correspond to their melting points (T_m) were observed for crystalline samples. Glass transition steps (T_g) were observed in the 2nd heating of molten samples. Cold crystallization transition peaks (T_c) followed by T_m were observed for ground samples (Fig. S16).

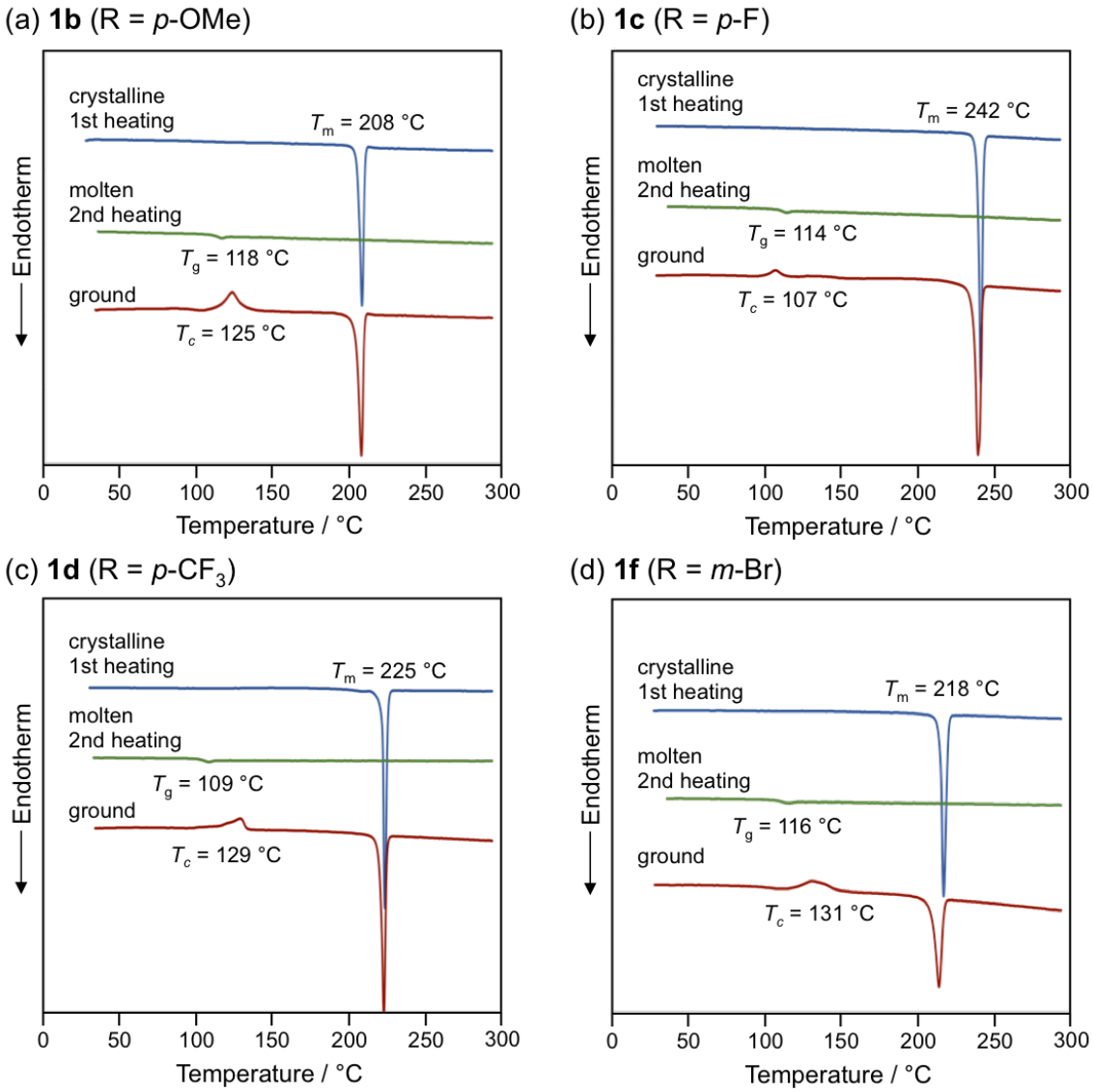

Fig. S16 DSC scans for the crystalline (1st heating: blue), molten (2nd heating: green), and ground (red) samples of **1b** (a), **1c** (b), **1d** (c), and **1f** (d). T_m, T_g, and T_c values are noted near the corresponding peaks and steps.

6. Supplementary data for two-step MCL

Upon gently crushing a crystalline sample of a phenanthroimidazolylbenzothiadiazole derivative into a fine powder, the particle size changed from several hundreds of μm to several tens of μm (Fig. S17a and S17b). No significant reduction in particle size was observed in the samples obtained after grinding the crushed sample (Fig. S17c).

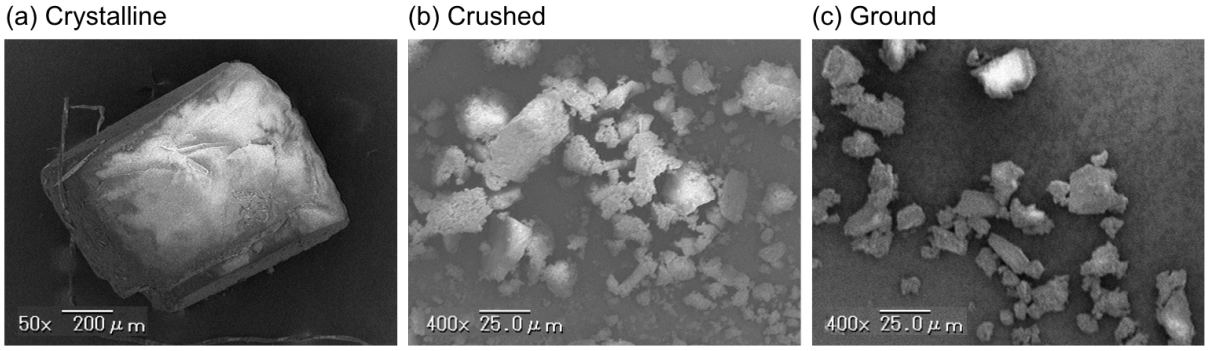

Fig. S17 Typical SEM images for the crystalline (a), crushed (b), and ground (c) samples of a phenanthroimidazolylbenzothiadiazole derivative (R = H).

Fluorescence band of crystalline **1e** shifted in one direction upon gentle crushing followed by strong grinding (Fig. S18a). The maximum emission wavelength of crystalline **1g** shifted in hypsochromic direction after gentle crushing. Upon strong grinding, the emission band of crushed **1g** shifted in bathochromic direction (Fig. S18b).

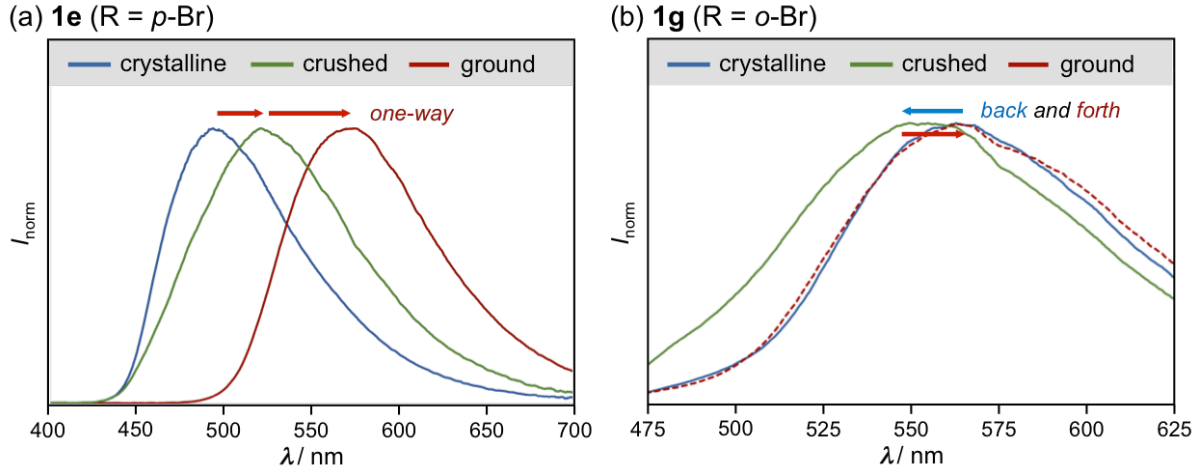

Fig. S18 (a) Fluorescence spectra for the one-way type two-step MCL of **1e**. (b) Fluorescence spectra for the back-and-forth type two-step MCL of **1g**.

Excitation spectrum of crushed samples shifted in hypsochromic direction compared to those of crystalline and ground samples (Fig. S19).

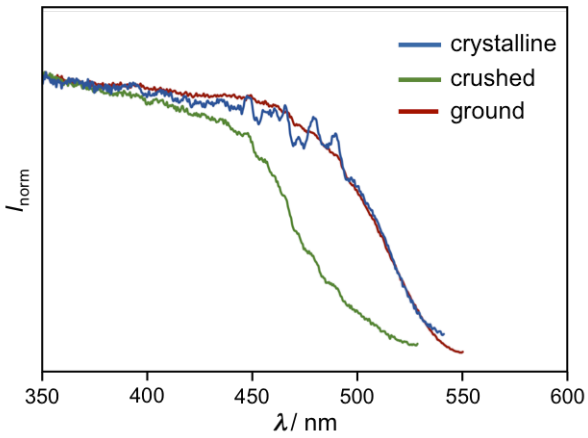

Fig. S19 Excitation spectra for the crystalline (blue), crushed (green), and ground (red) samples of **1g**.

7. References

1) CrysAlisPro: Data Collection and Processing Software, Rigaku Corporation (2015). Tokyo 196-8666, Japan.
2) SIR2011: M. C. Burla, R. Caliandro, M. Camalli, B. Carrozzini, G. L. Cascarano, C. Giacovazzo, M. Mallamo, A. Mazzone, G. Polidori and R. Spagna, *J. Appl. Cryst.*, 2012, **45**, 357.
3) CrystalStructure 4.2.5: Crystal Structure Analysis Package, Rigaku Corporation (2000-2017). Tokyo 196-8666, Japan.
4) SHELXL Version 2014/7: G. M. Sheldrick, *Acta Cryst.*, 2008, **A64**, 112.
5) K. Momma and F. Izumi, *J. Appl. Crystallogr.*, 2011, **44**, 1272.

^{1}H NMR (500 MHz, in $CDCl_3$)

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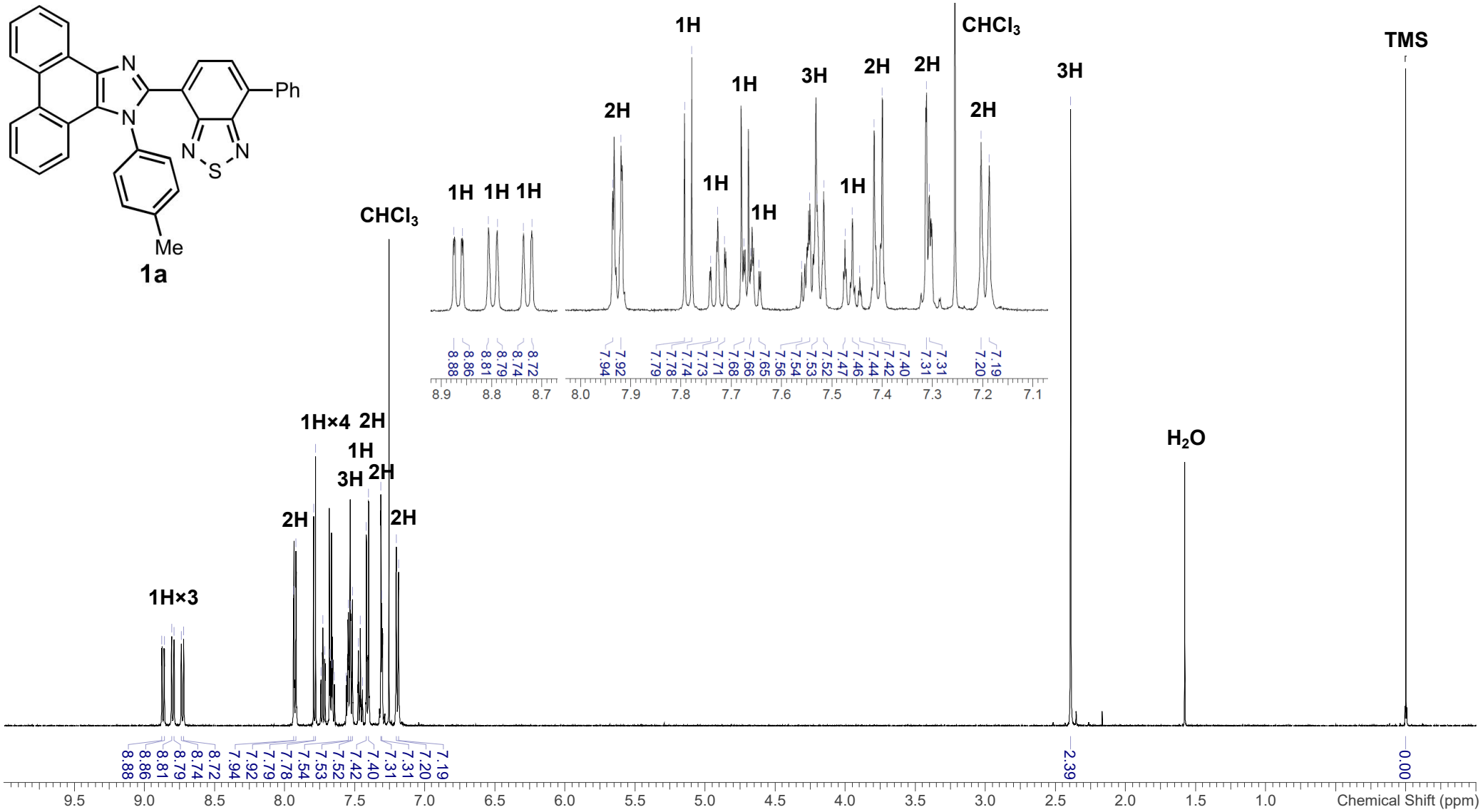
SWH	10330.5785123967			**Solvent**	CHLOROFORM-d			**Spectrum Offset (Hz)**	3072.7070
Spectrum Type	standard	**Sweep Width (Hz)**	10330.26	**TD**	65536	**TD0**	1	**TE**	298.5
Temperature (degree C)	25.500	**WDW**	1						



^{13}C NMR (126 MHz, in $CDCl_3$)

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File Name	E:¥NMR¥ 1a_STA_Ph_PhMe_13C¥10¥PDATA¥1¥1r			**Frequency (MHz)**	125.7578	**GB**	0	**INSTRUM**	<spect>
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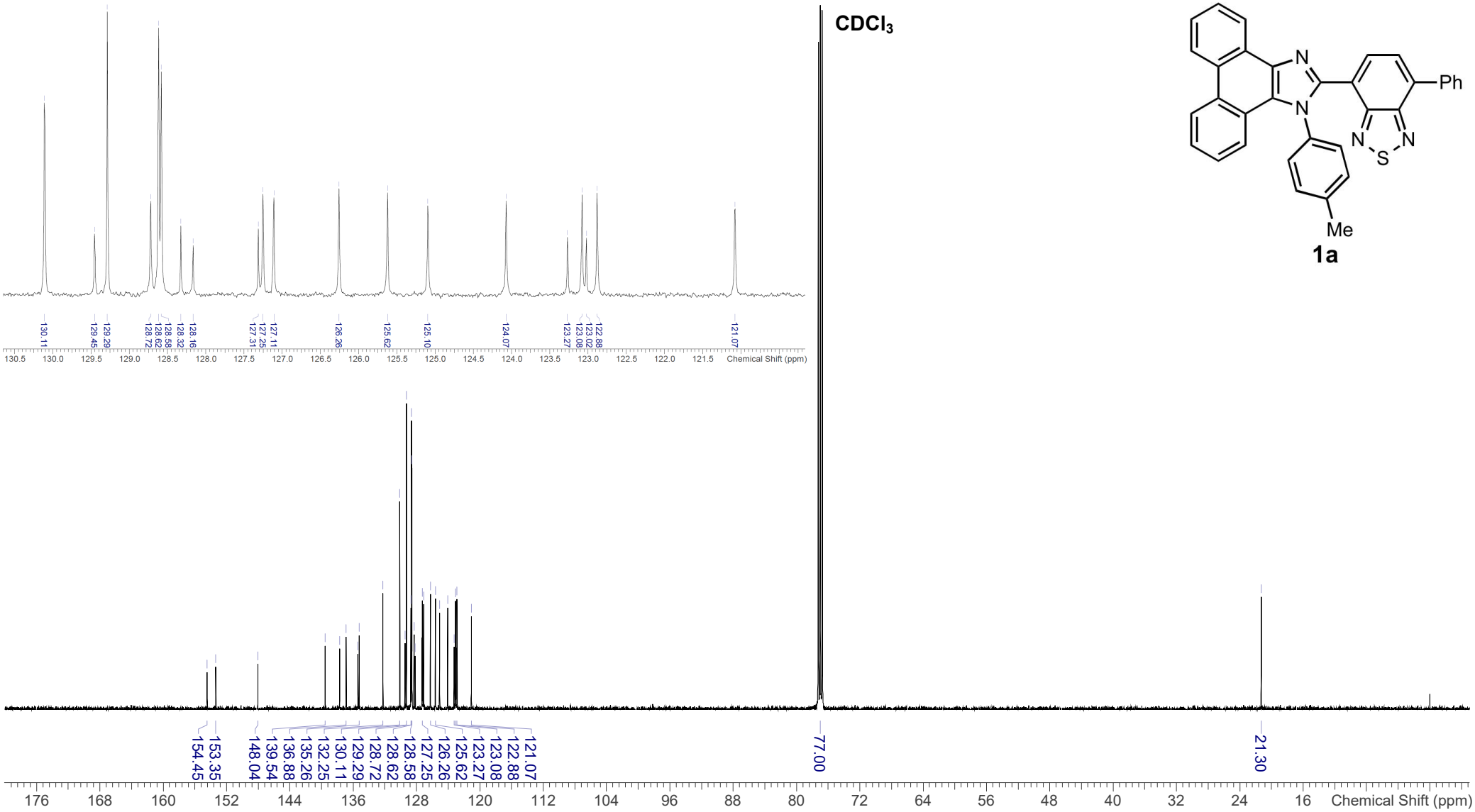
Original Points Count	32768	**Owner**	root	**PC**	1.4	**PROBHD**	<5 mm BBO BB-1H Z-GRD Z859001/0006 >		
PULPROG	<zgpg30>	**Points Count**	32768	**Pulse Sequence**	zgpg30	**Receiver Gain**	4096.00	**SF**	125.757789
SFO1	125.770364304853			**SI**	32768	**SSB**	0	**SW(cyclical) (Hz)**	30030.03
SWH	30030.03003003			**Solvent**	CHLOROFORM-d			**Spectrum Offset (Hz)**	12569.6934
Spectrum Type	standard	**Sweep Width (Hz)**	30029.11	**TD**	65536	**TD0**	1	**TE**	299.7
Temperature (degree C)	26.700	**WDW**	1						



^{1}H NMR (500 MHz, in $CDCl_3$)

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File Name	E:¥2DNMR¥1b_Ph_PhOMe¥ 1b_STA_Ph_PhOMe_1H¥1¥PDATA¥1¥1r				**Frequency (MHz)**	500.1300	**GB**	0
INSTRUM	<spect>	**LB**	0.1	**NS**	8	**Nucleus**	1H	**Number of Transients**	8
Origin	spect	**Original Points Count**	32768	**Owner**	root	**PC**	1		
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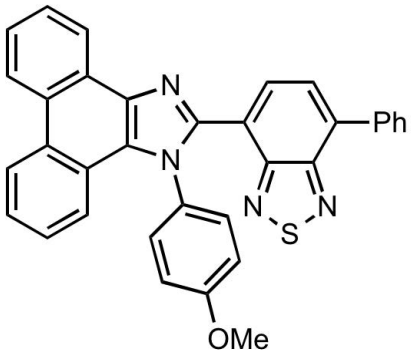
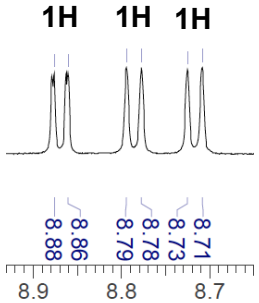
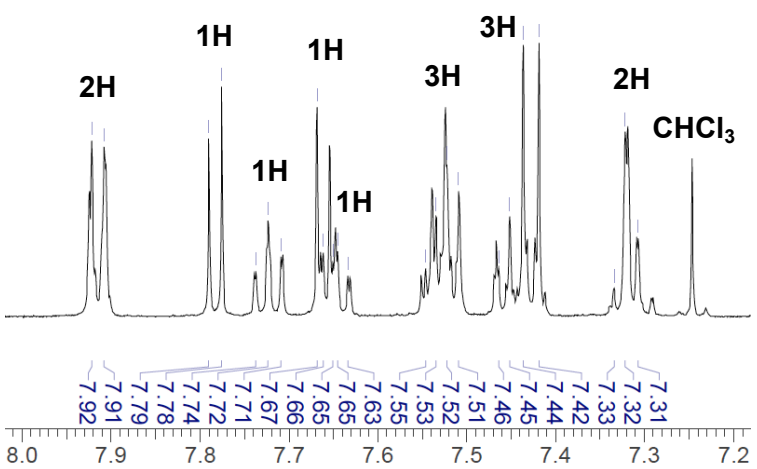
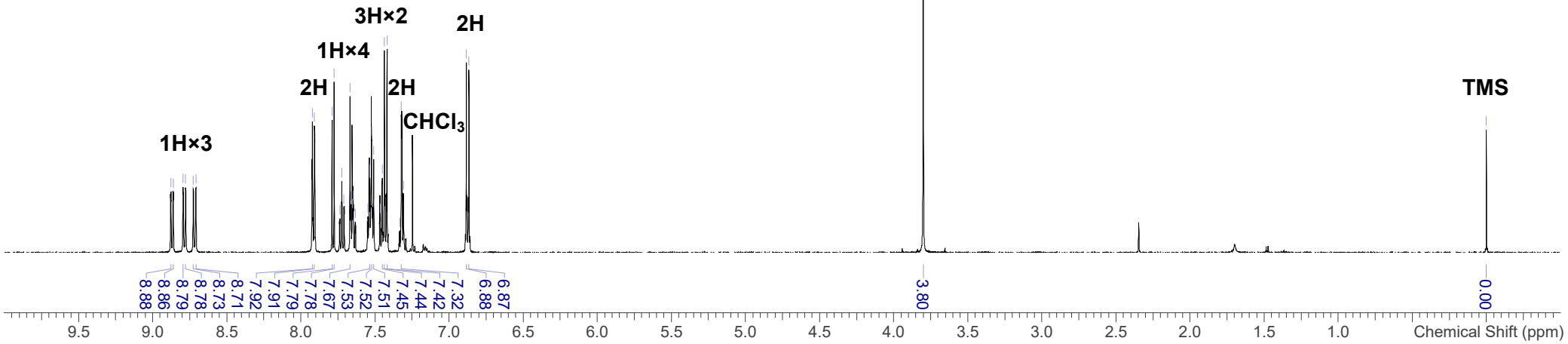
Receiver Gain	362.00	**SF**	500.130006648269			**SFO1**	500.133088507478		
SI	32768	**SSB**	0	**SW(cyclical) (Hz)**	10330.58	**SWH**	10330.5785123967		
Solvent	CHLOROFORM-d			**Spectrum Offset (Hz)**	3068.3059	**Spectrum Type**	standard	**Sweep Width (Hz)**	10330.26
TD	65536	**TD0**	1	**TE**	297.5	**Temperature (degree C)**	24.500	**WDW**	1



1b







^{13}C NMR (126 MHz, in $CDCl_3$)

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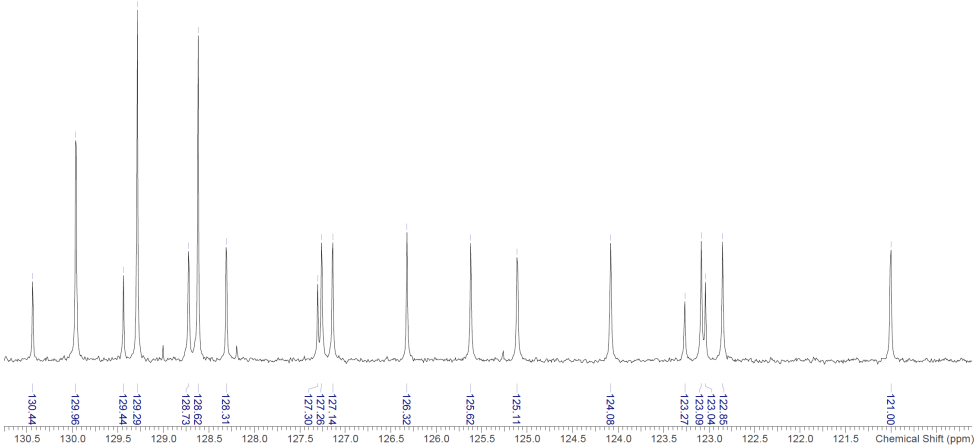
PROBHD	<5 mm BBO BB-1H Z-GRD Z859001/0006 >			**PULPROG**	<zgpg30>	**Points Count**	32768	**Pulse Sequence**	zgpg30
Receiver Gain	16384.00	**SF**	125.757789	**SFO1**	125.770364304853			**SI**	32768
SSB	0	**SW(cyclical) (Hz)**	30030.03	**SWH**	30030.03003003			**Solvent**	CHLOROFORM-d
Spectrum Offset (Hz)	12568.7744	**Spectrum Type**	standard	**Sweep Width (Hz)**	30029.11	**TD**	65536	**TD0**	1
TE	299	**Temperature (degree C)**	26.000	**WDW**	1				



1b

^{1}H NMR (500 MHz, in $CDCl_3$)

Acquisition Time (sec)	3.1719	**Comment**	5 mm BBO BB-1H Z-GRD Z859001/0006		**D**	3.827959	**D1**	3.827959
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GB	0	**INSTRUM**	<spect>	**LB**	0.1	**NS**	8	**Nucleus**	1H
Number of Transients	8	**Origin**	spect	**Original Points Count**	32768	**Owner**	root	**PC**	1
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Receiver Gain	645.10	**SF**	500.130006648269			**SFO1**	500.133088507478		
SI	32768	**SSB**	0	**SW(cyclical) (Hz)**	10330.58	**SWH**	10330.5785123967		
Solvent	CHLOROFORM-d			**Spectrum Offset (Hz)**	3071.7568	**Spectrum Type**	standard	**Sweep Width (Hz)**	10330.26
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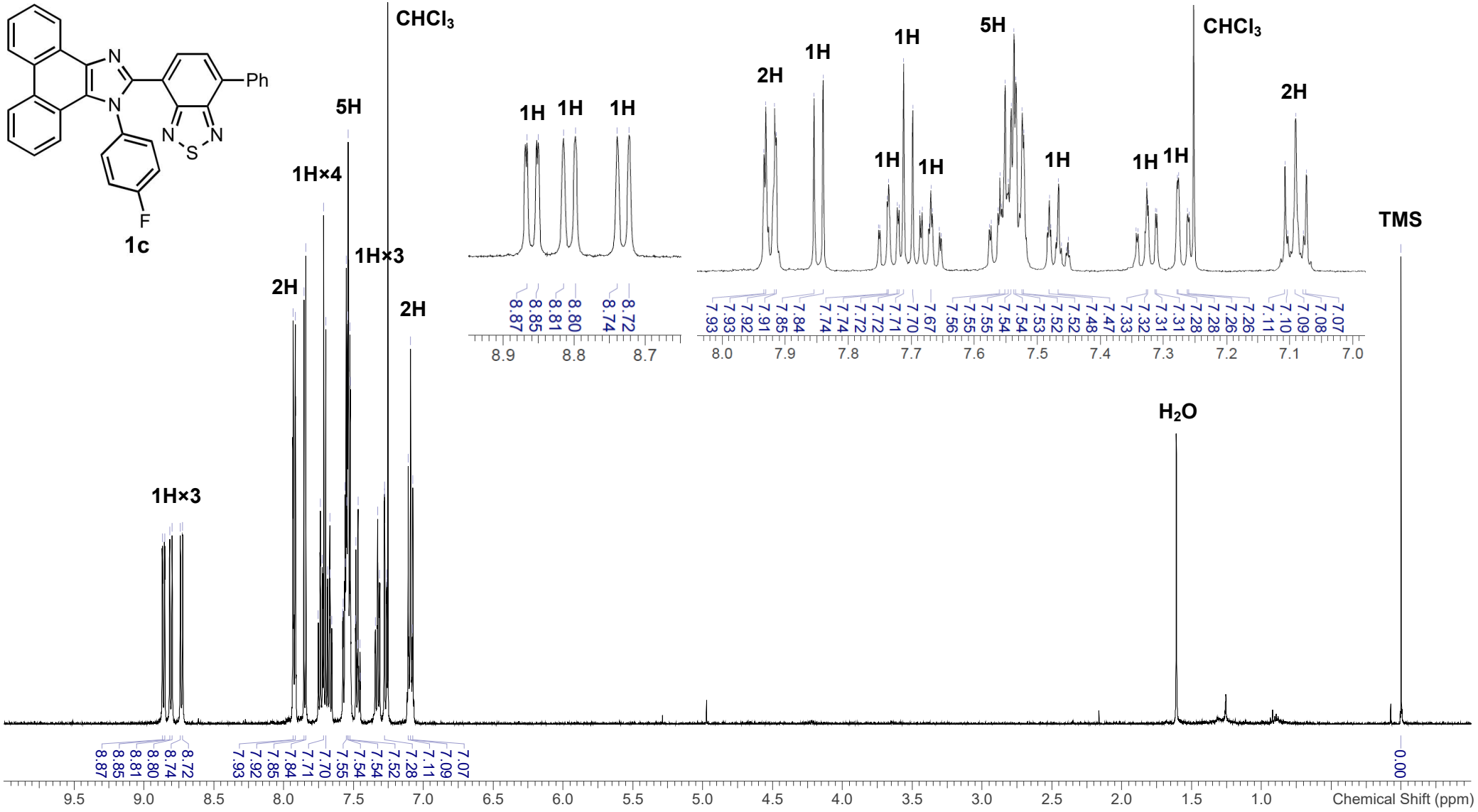

^{13}C NMR (126 MHz, in $CDCl_3$)

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Origin	spect	**Original Points Count**	32768	**Owner**	root	**PC**	1.4		
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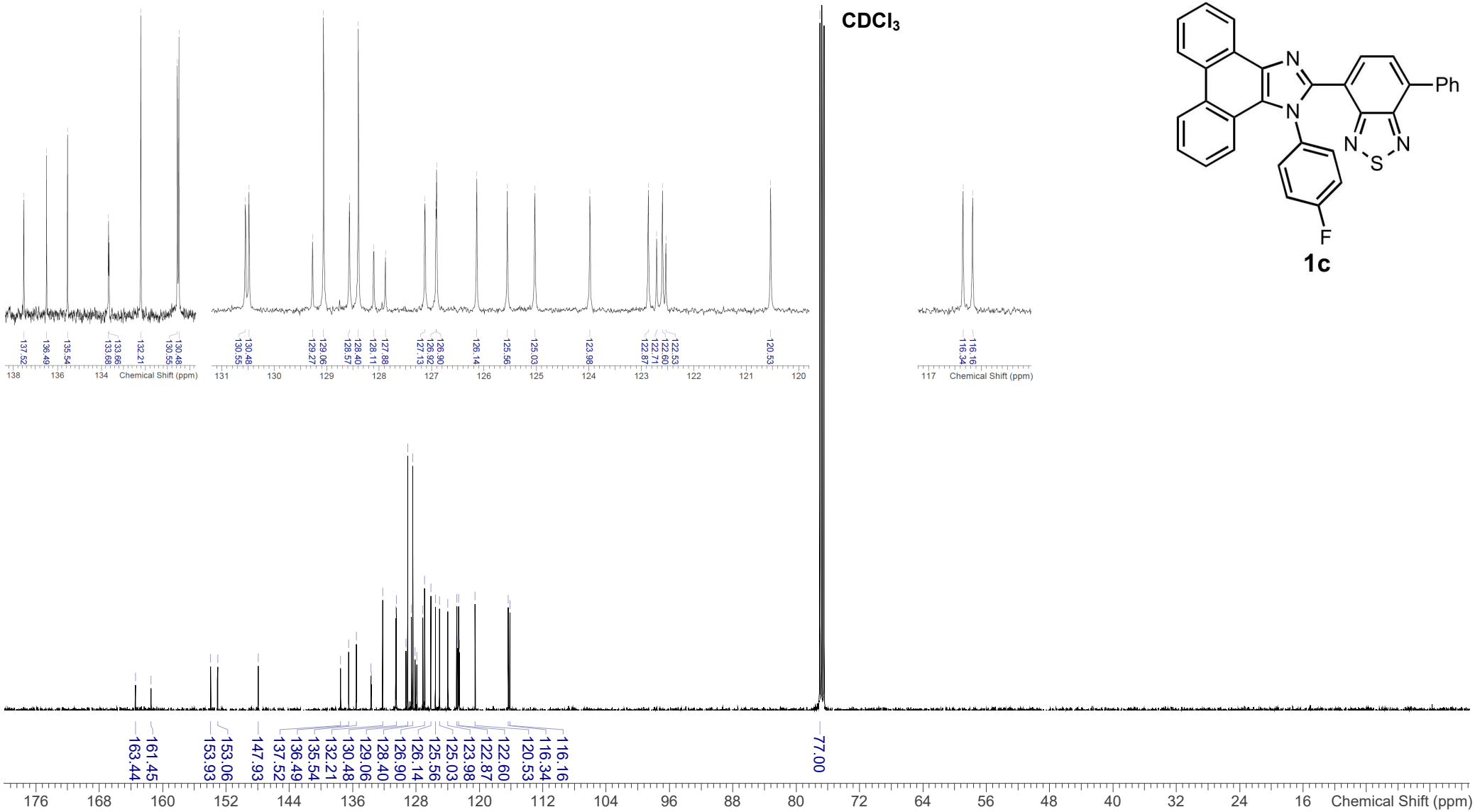
Receiver Gain	3251.00	**SF**	125.757789	**SFO1**	125.770364304853			**SI**	32768
SSB	0	**SW(cyclical) (Hz)**	30030.03	**SWH**	30030.03003003			**Solvent**	CHLOROFORM-d
Spectrum Offset (Hz)	12537.6123	**Spectrum Type**	standard	**Sweep Width (Hz)**	30029.11	**TD**	65536	**TD0**	1
TE	298.3	**Temperature (degree C)**	25.300	**WDW**	1				



^{1}H NMR (500 MHz, in $CDCl_3$)

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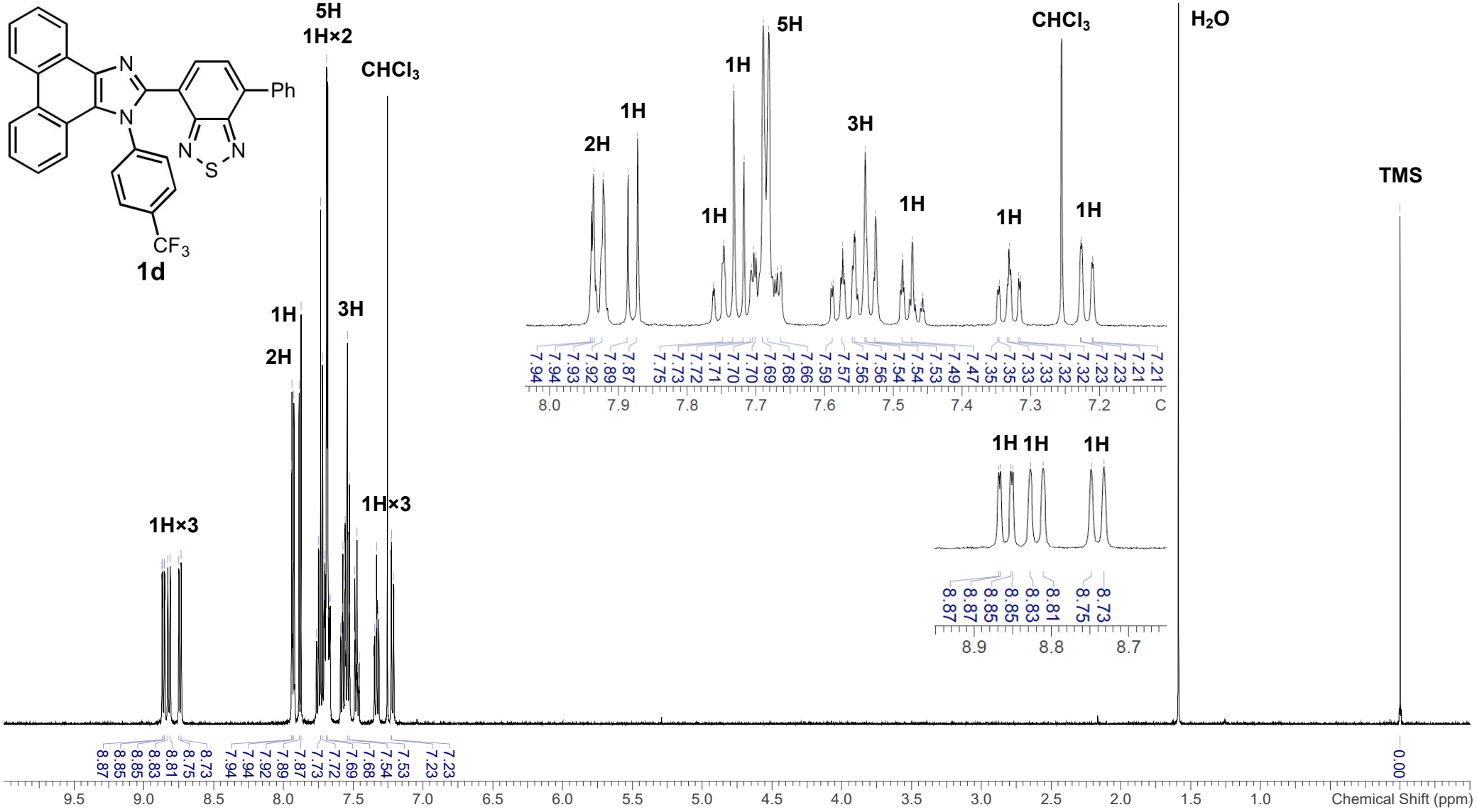
Original Points Count	32768	**Owner**	root	**PC**	1	**PROBHD**	<5 mm BBO BB-1H Z-GRD Z859001/0006 >		
PULPROG	<zg30>	**Points Count**	32768	**Pulse Sequence**	zg30	**Receiver Gain**	645.10	**SF**	500.130006648269
SFO1	500.133088507478			**SI**	32768	**SSB**	0	**SW(cyclical) (Hz)**	10330.58
SWH	10330.5785123967			**Solvent**	CHLOROFORM-d			**Spectrum Offset (Hz)**	3072.7070
Spectrum Type	standard	**Sweep Width (Hz)**	10330.26	**TD**	65536	**TD0**	1	**TE**	297.6
Temperature (degree C)	24.600	**WDW**	1						



^{13}C NMR (126 MHz, in $CDCl_3$)

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INSTRUM	<spect>	**LB**	1	**NS**	1024	**Nucleus**	13C	**Number of Transients**	1024
Origin	spect	**Original Points Count**	32768	**Owner**	root	**PC**	1.4		
PROBHD	<5 mm BBO BB-1H Z-GRD Z859001/0006 >			**PULPROG**	<zgpg30>	**Points Count**	32768	**Pulse Sequence**	zgpg30
Receiver Gain	4096.00	**SF**	125.757789	**SFO1**	125.770364304853			**SI**	32768
SSB	0	**SW(cyclical) (Hz)**	30030.03	**SWH**	30030.03003003			**Solvent**	CHLOROFORM-d
Spectrum Offset (Hz)	12568.7764	**Spectrum Type**	standard	**Sweep Width (Hz)**	30029.11	**TD**	65536	**TD0**	1
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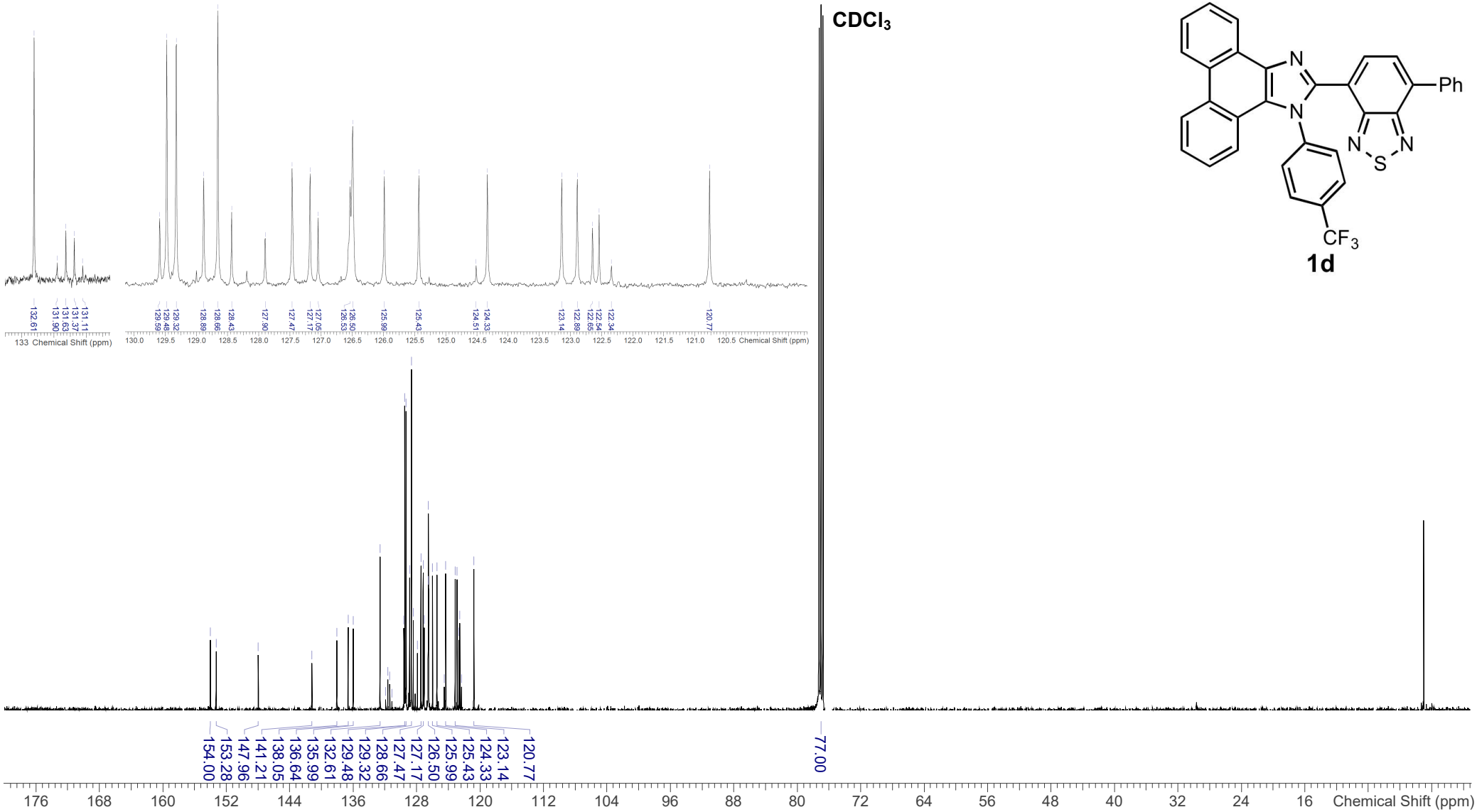

^{1}H NMR (500 MHz, in $CDCl_3$)

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Original Points Count	32768	**Owner**	root	**PC**	1	**PROBHD**	<5 mm BBO BB-1H Z-GRD Z859001/0006 >		
PULPROG	<zg30>	**Points Count**	32768	**Pulse Sequence**	zg30	**Receiver Gain**	456.10	**SF**	500.130006648269
SFO1	500.133088507478			**SI**	32768	**SSB**	0	**SW(cyclical) (Hz)**	10330.58
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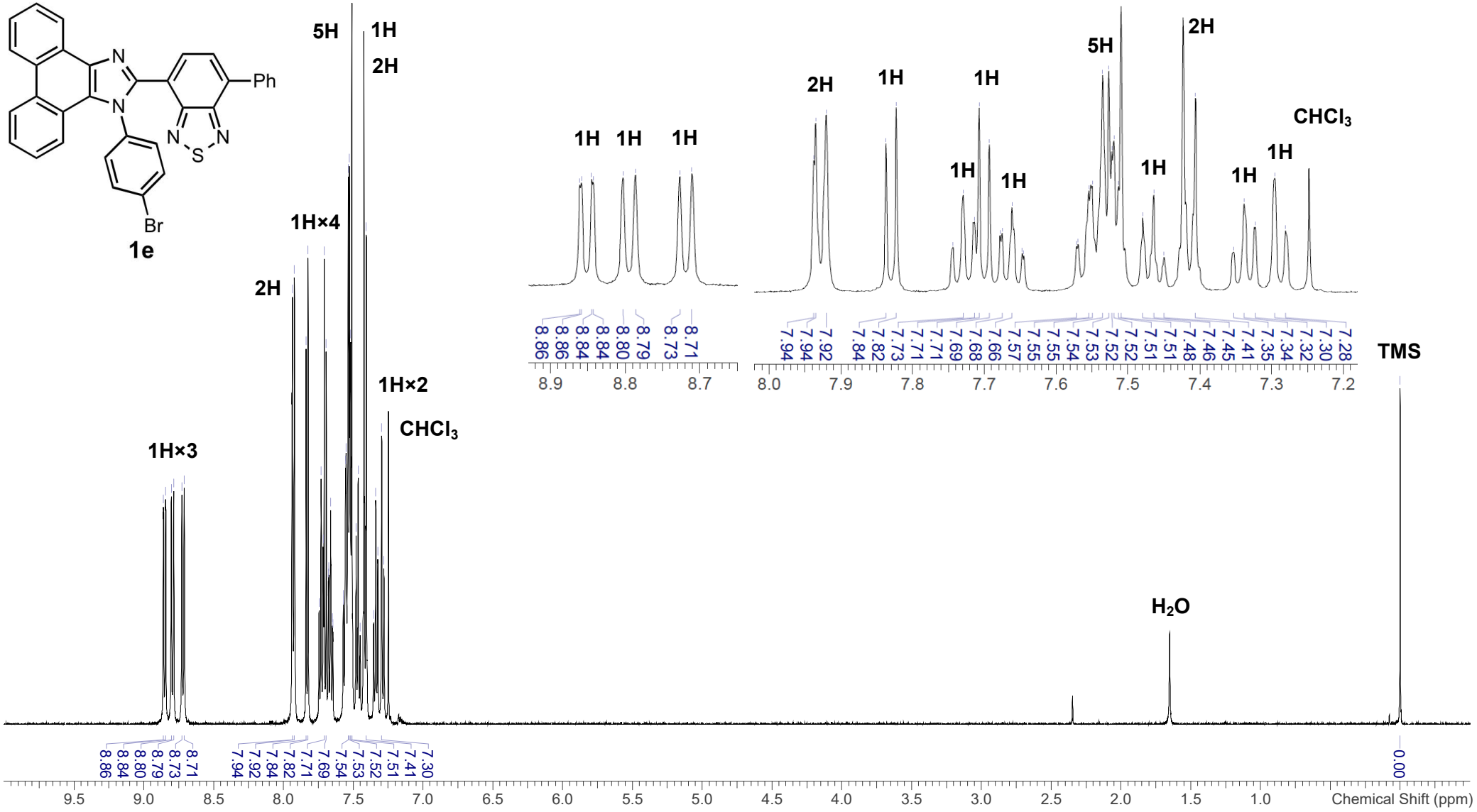
Temperature (degree C)	25.300	**WDW**	1						



^{13}C NMR (126 MHz, in $CDCl_3$)

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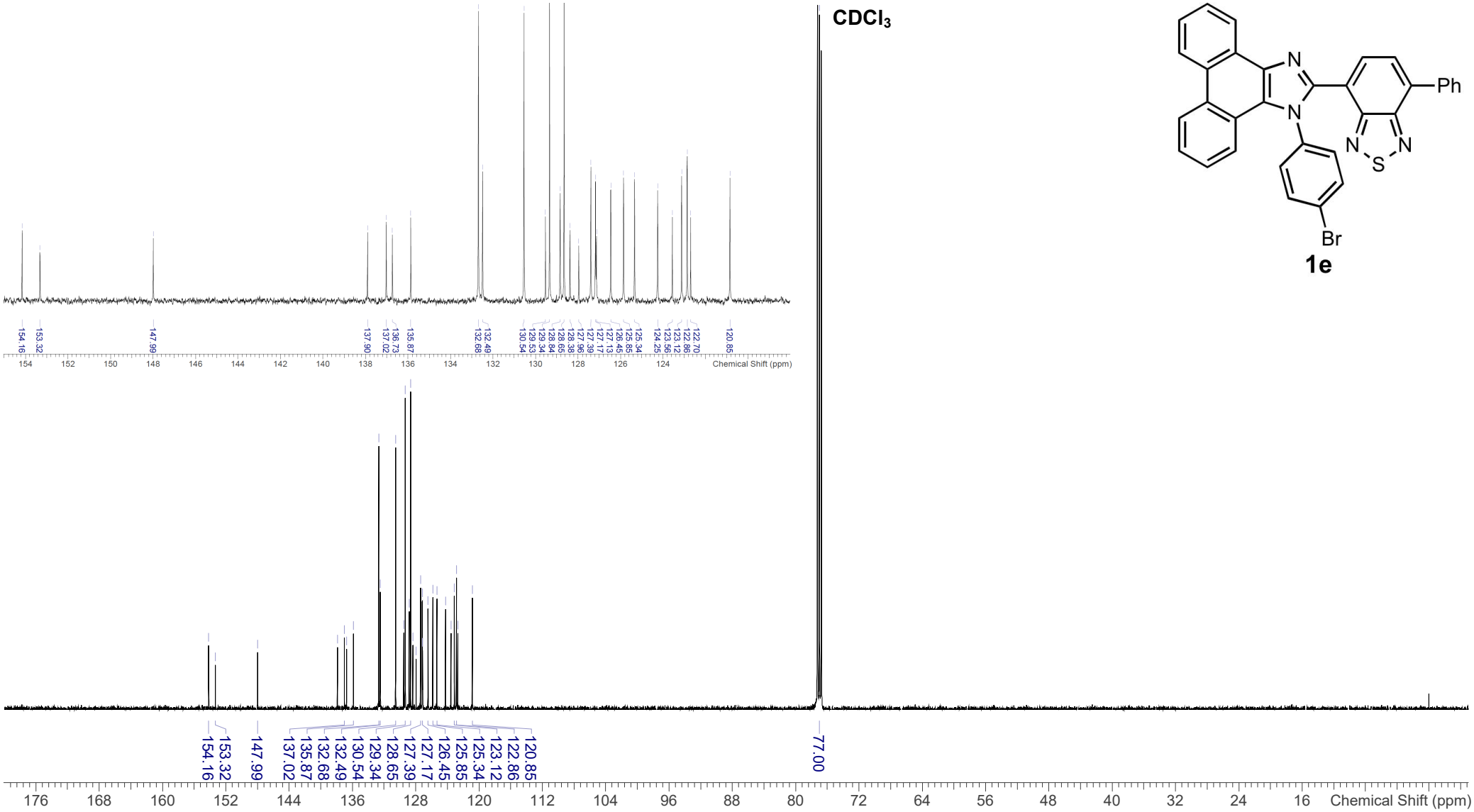
Original Points Count	32768	**Owner**	root	**PC**	1.4	**PROBHD**	<5 mm BBO BB-1H Z-GRD Z859001/0006 >		
PULPROG	<zgpg30>	**Points Count**	32768	**Pulse Sequence**	zgpg30	**Receiver Gain**	4096.00	**SF**	125.757789
SFO1	125.770364304853			**SI**	32768	**SSB**	0	**SW(cyclical) (Hz)**	30030.03
SWH	30030.03003003			**Solvent**	CHLOROFORM-d			**Spectrum Offset (Hz)**	12569.6924
Spectrum Type	standard	**Sweep Width (Hz)**	30029.11	**TD**	65536	**TD0**	1	**TE**	298.9
Temperature (degree C)	25.900	**WDW**	1						



^{1}H NMR (500 MHz, in $CDCl_3$)

Acquisition Time (sec)	3.1719	**Comment**	5 mm BBO BB-1H Z-GRD Z859001/0006			**D**	3.827959	**D1**	3.827959
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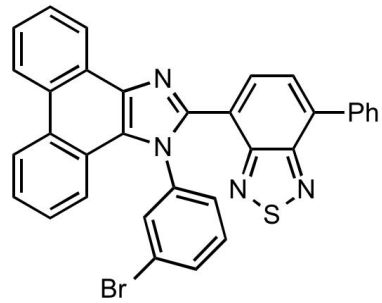
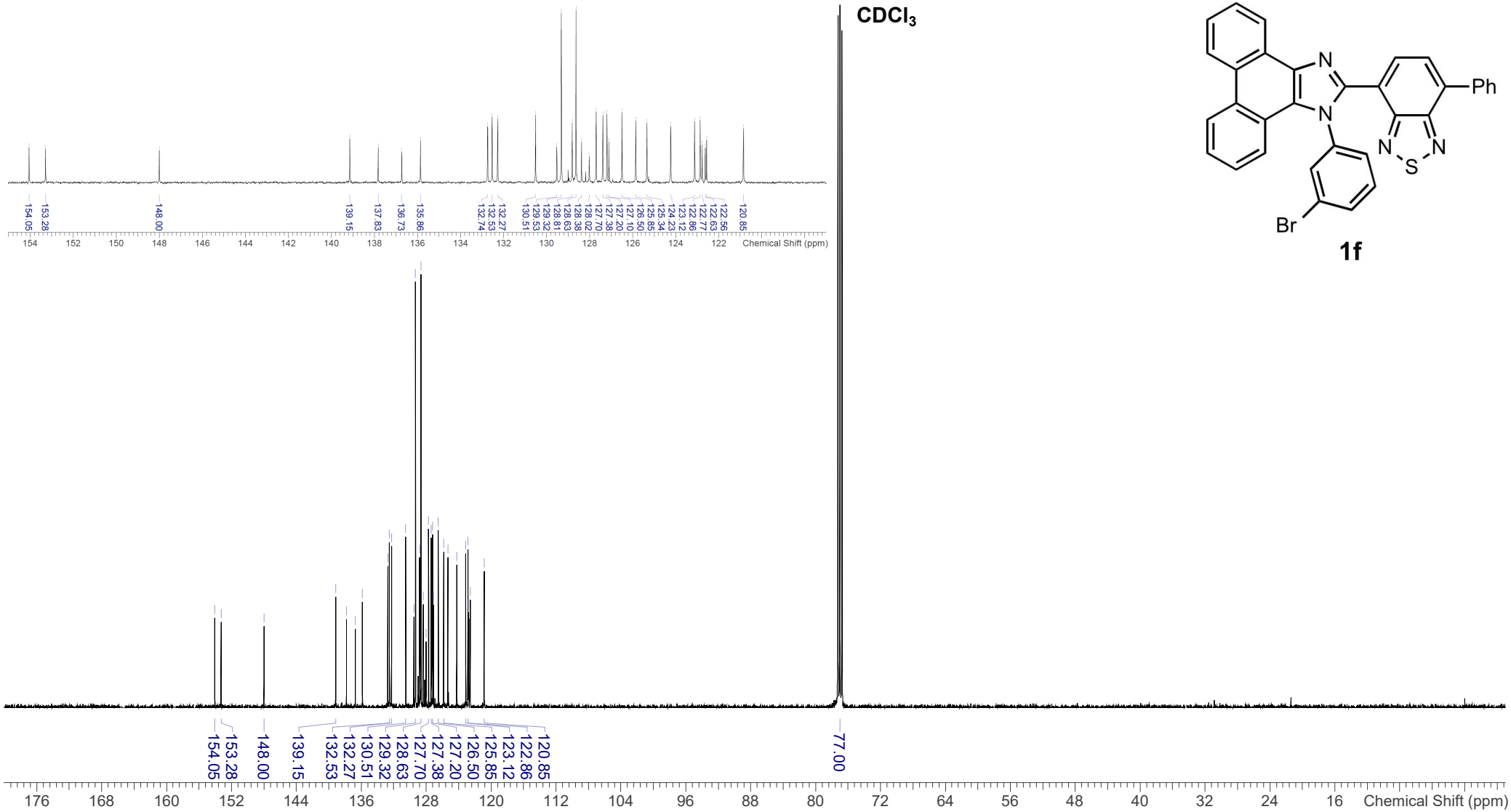
File Name	E:¥STA_1f_1H¥1¥PDATA¥1¥1r			**Frequency (MHz)**	500.1300	**GB**	0	**INSTRUM**	<spect>
LB	0.1	**NS**	8	**Nucleus**	1H	**Number of Transients**	8	**Origin**	spect
Original Points Count	32768	**Owner**	root	**PC**	1	**PROBHD**	<5 mm BBO BB-1H Z-GRD Z859001/0006 >		
PULPROG	<zg30>	**Points Count**	32768	**Pulse Sequence**	zg30	**Receiver Gain**	645.10	**SF**	500.130006648269
SFO1	500.133088507478			**SI**	32768	**SSB**	0	**SW(cyclical) (Hz)**	10330.58
SWH	10330.5785123967			**Solvent**	CHLOROFORM-d			**Spectrum Offset (Hz)**	3073.3533
Spectrum Type	standard	**Sweep Width (Hz)**	10330.26	**TD**	65536	**TD0**	1	**TE**	296.5
Temperature (degree C)	23.500	**WDW**	1						



1f

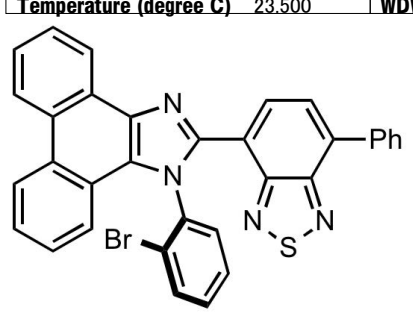
^{13}C NMR (126 MHz, in $CDCl_3$)

Acquisition Time (sec)	1.0912	**D**	0.00345	**D1**	2	**DE**	6	**DS**	4
Date	26 Dec 2019 17:11:44			**Date Stamp**	26 Dec 2019 17:11:44				
File Name	E:¥NMR¥ 1f_STA_Ph_PhBr(m)_13C¥1¥PDATA¥1¥1r					**Frequency (MHz)**	125.7578	**GB**	0
INSTRUM	<spect>	**LB**	1	**NS**	1024	**Nucleus**	13C	**Number of Transients**	1024
Origin	spect	**Original Points Count**	32768	**Owner**	root	**PC**	1.4		
PROBHD	<5 mm BBO BB-1H Z-GRD Z859001/0006 >			**PULPROG**	<zgpg30>	**Points Count**	32768	**Pulse Sequence**	zgpg30
Receiver Gain	3649.10	**SF**	125.757789			**SFO1**	125.770364304853		
SI	32768	**SSB**	0	**SW(cyclical) (Hz)**	30030.03	**SWH**	30030.03003003		
Solvent	CHLOROFORM-d			**Spectrum Offset (Hz)**	12566.9395			**Spectrum Type**	standard
Sweep Width (Hz)	30029.11	**TD**	65536	**TD0**	1	**TE**	298.7	**Temperature (degree C)**	25.700
WDW	1								



^{1}H NMR (500 MHz, in $CDCl_3$)

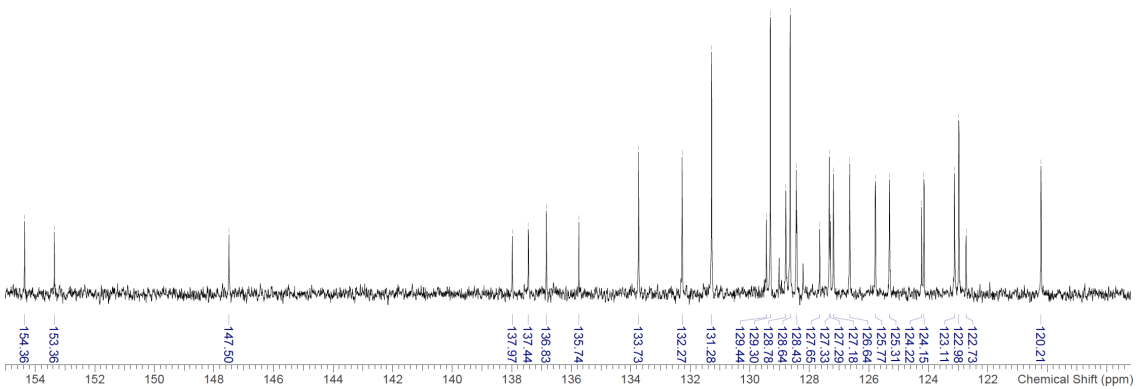
Acquisition Time (sec)	3.1719	**Comment**	5 mm BBO BB-1H Z-GRD Z859001/0006	**D**	3.827959	**D1**	3.827959
DE	6	**DS**	2	**Date**	28 Mar 2020 05:39:20	**Date Stamp**	28 Mar 2020 05:39:20
File Name	E:¥STA_1g_1H¥1¥PDATA¥1¥1r			**Frequency (MHz)**	500.1300	**GB**	0	**INSTRUM**	<spect>
LB	0.1	**NS**	8	**Nucleus**	1H	**Number of Transients**	8	**Origin**	spect
Original Points Count	32768	**Owner**	root	**PC**	1	**PROBHD**	<5 mm BBO BB-1H Z-GRD Z859001/0006 >		
PULPROG	<zg30>	**Points Count**	32768	**Pulse Sequence**	zg30	**Receiver Gain**	645.10	**SF**	500.130006648269
SFO1	500.133088507478			**SI**	32768	**SSB**	0	**SW(cyclical) (Hz)**	10330.58
SWH	10330.5785123967			**Solvent**	CHLOROFORM-d			**Spectrum Offset (Hz)**	3073.3572
Spectrum Type	standard	**Sweep Width (Hz)**	10330.26	**TD**	65536	**TD0**	1	**TE**	296.5
Temperature (degree C)	23.500	**WDW**	1						

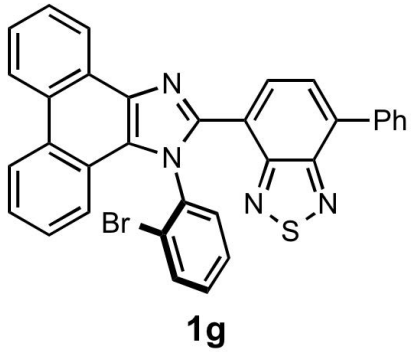


1g

^{13}C NMR (126 MHz, in $CDCl_3$)

Acquisition Time (sec)	1.0912	**D**	0.00345	**D1**	2	**DE**	6	**DS**	4
Date	16 Jan 2020 16:58:20			**Date Stamp**	16 Jan 2020 16:58:20				
File Name	E:¥2DNMR¥1g_Ph_PhBr(o)¥ 1e_STA_Ph_PhBr(o)_13C¥10¥PDATA¥1¥1r					**Frequency (MHz)**	125.7578	**GB**	0
INSTRUM	<spect>	**LB**	1	**NS**	1024	**Nucleus**	13C	**Number of Transients**	1024
Origin	spect	**Original Points Count**	32768	**Owner**	root	**PC**	1.4		
PROBHD	<5 mm BBO BB-1H Z-GRD Z859001/0006 >			**PULPROG**	<zgpg30>	**Points Count**	32768	**Pulse Sequence**	zgpg30
Receiver Gain	5160.60	**SF**	125.757789	**SFO1**	125.770364304853			**SI**	32768
SSB	0	**SW(cyclical) (Hz)**	30030.03	**SWH**	30030.03003003			**Solvent**	CHLOROFORM-d
Spectrum Offset (Hz)	12571.5166	**Spectrum Type**	standard	**Sweep Width (Hz)**	30029.11	**TD**	65536	**TD0**	1
TE	299.2	**Temperature (degree C)**	26.200	**WDW**	1				



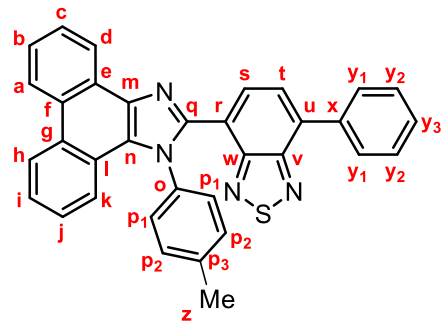


1g

Partial ^{1}H NMR spectrum of **1a** (500 MHz, in $CDCl_3$, rt)

Acquisition Time (sec)	3.1719	*Comment*	5 mm BBO BB-1H Z-GRD Z859001/0006			*D*	3.827959	*D1*	3.827959
DE	6	*DS*	2	*Date*	04 Dec 2019 14:20:40			*Date Stamp*	04 Dec 2019 14:20:40
File Name	E:¥NMR¥ 1a_STA_Ph_PhMe_1H¥1¥PDATA¥1¥1r			*Frequency (MHz)*	500.1300	*GB*	0	*INSTRUM*	<spect>
LB	0.1	*NS*	8	*Nucleus*	1H	*Number of Transients*	8	*Origin*	spect
Original Points Count	32768	*Owner*	root	*PC*	1	*PROBHD*	<5 mm BBO BB-1H Z-GRD Z859001/0006 >		
PULPROG	<zg30>	*Points Count*	32768	*Pulse Sequence*	zg30	*Receiver Gain*	812.70	*SF*	500.130006648269
SFO1	500.133088507478			*SI*	32768	*SSB*	0	*SW(cyclical) (Hz)*	10330.58
SWH	10330.5785123967			*Solvent*	CHLOROFORM-d			*Spectrum Offset (Hz)*	3072.7070
Spectrum Type	standard	*Sweep Width (Hz)*	10330.26	*TD*	65536	*TD0*	1	*TE*	298.5
Temperature (degree C)	25.500	*WDW*	1						

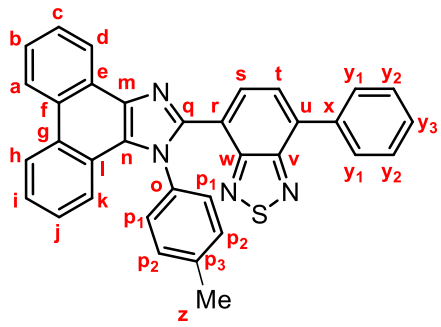
1a_STA_Ph_PhMe_1H.001.001.1r.esp



Partial ^{13}C NMR spectrum of **1a** (500 MHz, in $CDCl_3$, rt)

Acquisition Time (sec)	1.0912	*D*	0.00345	*D1*	2	*DE*	6	*DS*	4
Date	03 Dec 2019 15:36:34			*Date Stamp*	03 Dec 2019 15:36:34				
File Name	E:¥NMR¥	1a_STA_Ph_PhMe_13C¥10¥PDATA¥1¥1r		*Frequency (MHz)*	125.7578	*GB*	0	*INSTRUM*	<spect>
LB	1	*NS*	1024	*Nucleus*	13C	*Number of Transients*	1024	*Origin*	spect
Original Points Count	32768	*Owner*	root	*PC*	1.4	*PROBHD*	<5 mm BBO BB-1H Z-GRD Z859001/0006 >		
PULPROG	<zgpg30>	*Points Count*	32768	*Pulse Sequence*	zgpg30	*Receiver Gain*	4096.00	*SF*	125.757789
SFO1	125.770364304853			*SI*	32768	*SSB*	0	*SW(cyclical) (Hz)*	30030.03
SWH	30030.03003003			*Solvent*	CHLOROFORM-d			*Spectrum Offset (Hz)*	12569.6934
Spectrum Type	standard	*Sweep Width (Hz)*	30029.11	*TD*	65536	*TD0*	1	*TE*	299.7
Temperature (degree C)	26.700	*WDW*	1						

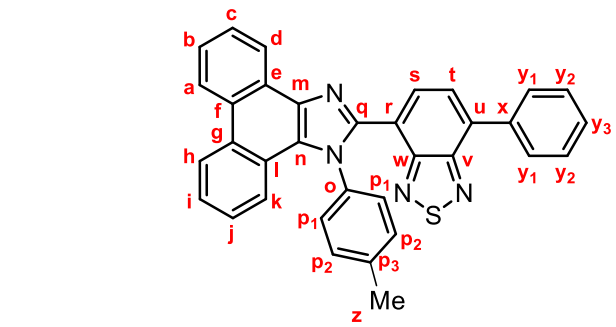
1a_STA_Ph_PhMe_13C.010.001.1r.esp



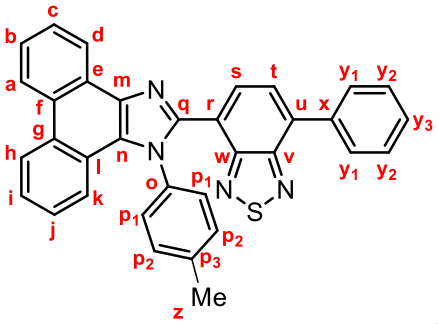
Partial ^{13}C NMR spectrum of **1a** (500 MHz, in $CDCl_3$, rt)

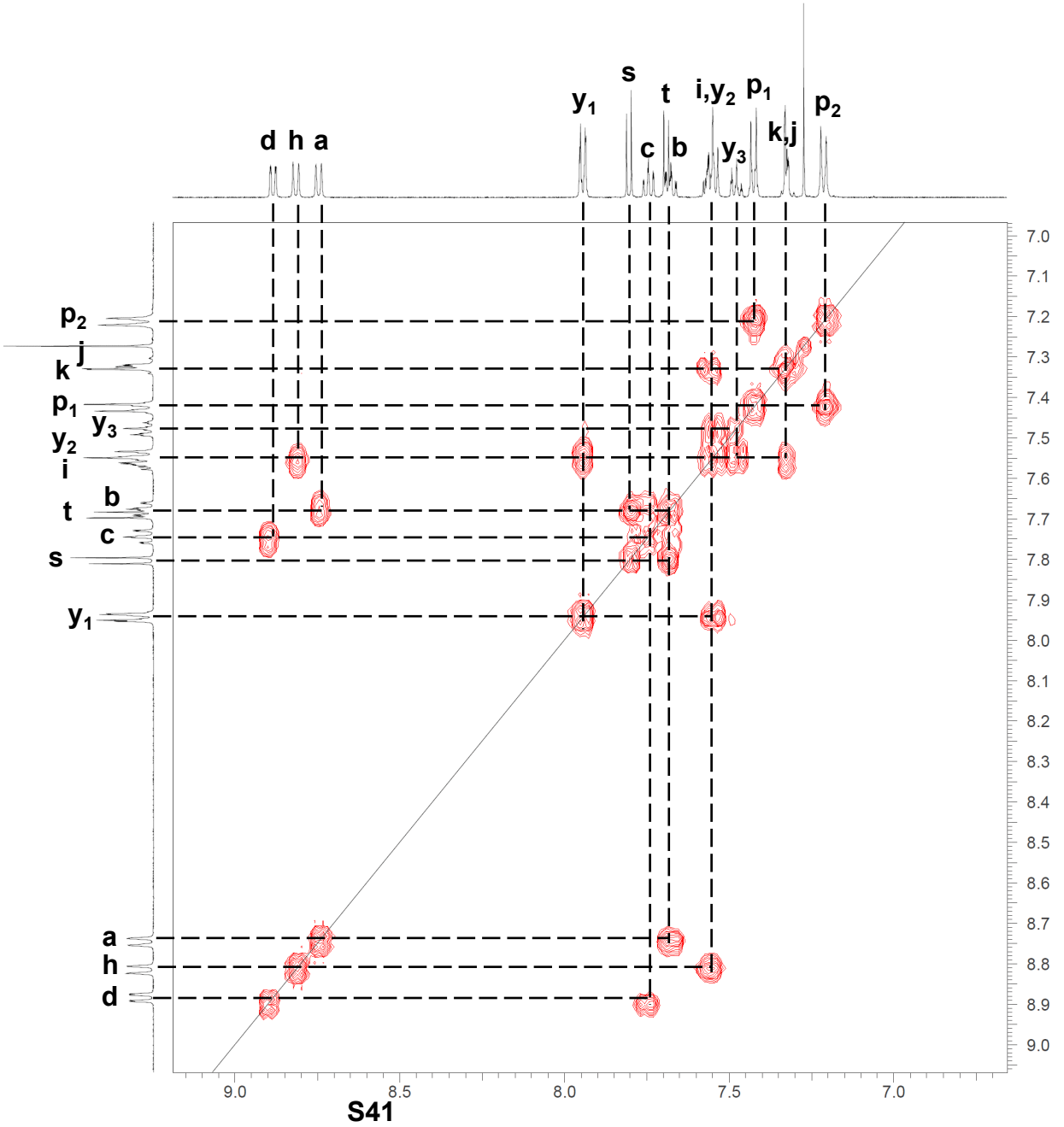
Acquisition Time (sec)	1.0912	*D*	0.00345	*D1*	2	*DE*	6	*DS*	4
Date	03 Dec 2019 15:36:34			*Date Stamp*	03 Dec 2019 15:36:34				
File Name	E:¥NMR¥ 1a_STA_Ph_PhMe_13C¥10¥PDATA¥1¥1r			*Frequency (MHz)*	125.7578	*GB*	0	*INSTRUM*	<spect>
LB	1	*NS*	1024	*Nucleus*	13C	*Number of Transients*	1024	*Origin*	spect
Original Points Count	32768	*Owner*	root	*PC*	1.4	*PROBHD*	<5 mm BBO BB-1H Z-GRD Z859001/0006 >		
PULPROG	<zgpg30>	*Points Count*	32768	*Pulse Sequence*	zgpg30	*Receiver Gain*	4096.00	*SF*	125.757789
SFO1	125.770364304853			*SI*	32768	*SSB*	0	*SW(cyclical) (Hz)*	30030.03
SWH	30030.03003003			*Solvent*	CHLOROFORM-d			*Spectrum Offset (Hz)*	12569.6934
Spectrum Type	standard	*Sweep Width (Hz)*	30029.11	*TD*	65536	*TD0*	1	*TE*	299.7
Temperature (degree C)	26.700	*WDW*	1						

1a_STA_Ph_PhMe_13C.010.001.1r.esp

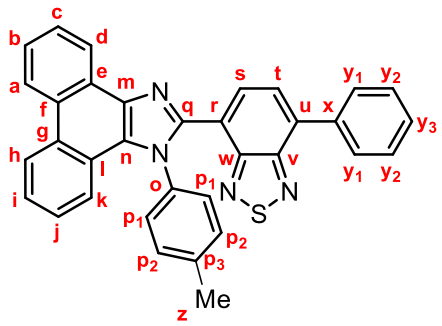


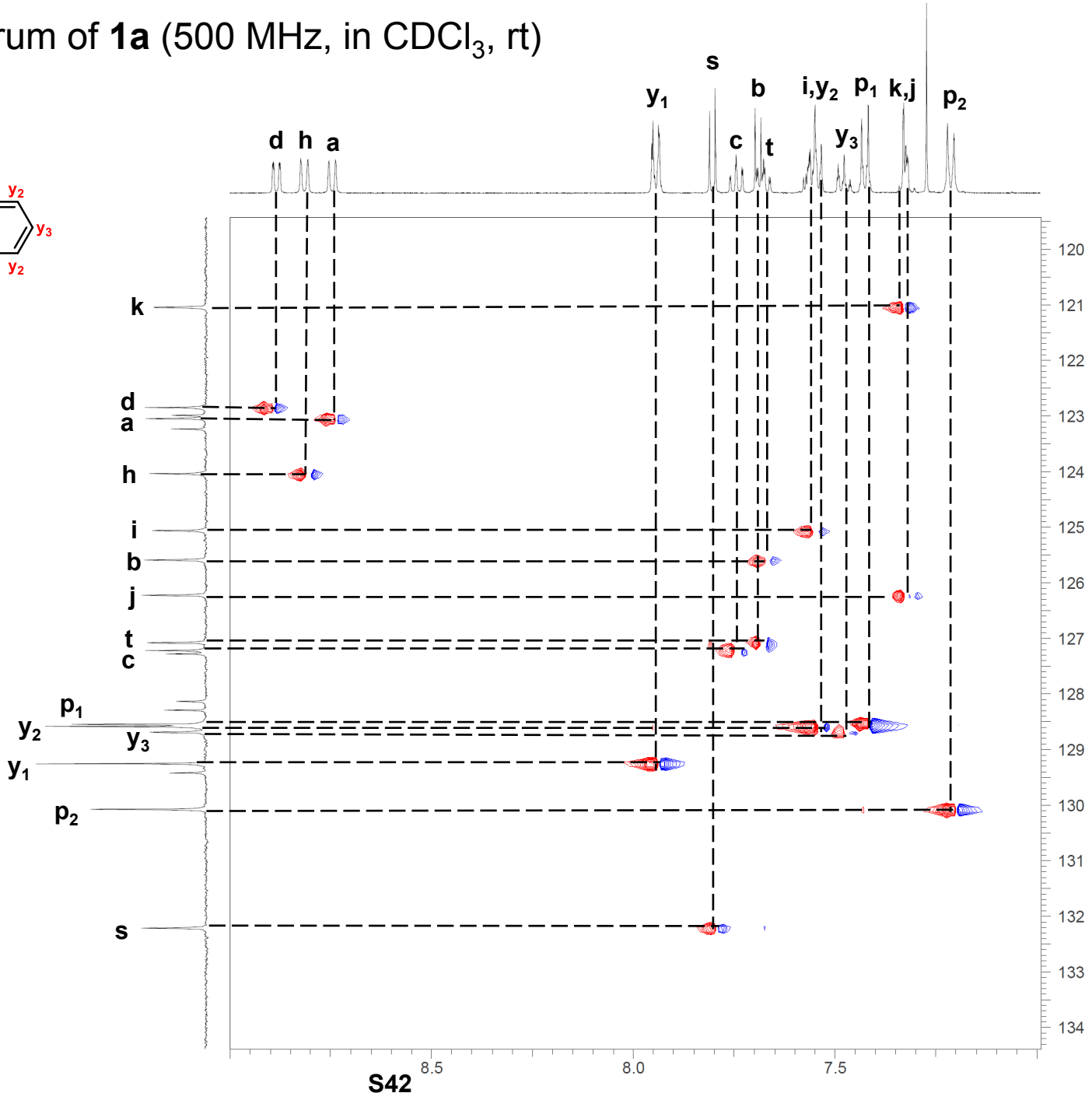
Partial COSY spectrum of **1a** (500 MHz, in $CDCl_3$, rt)



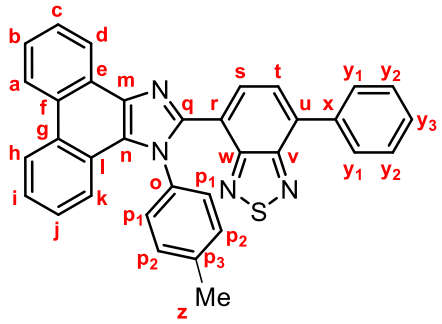


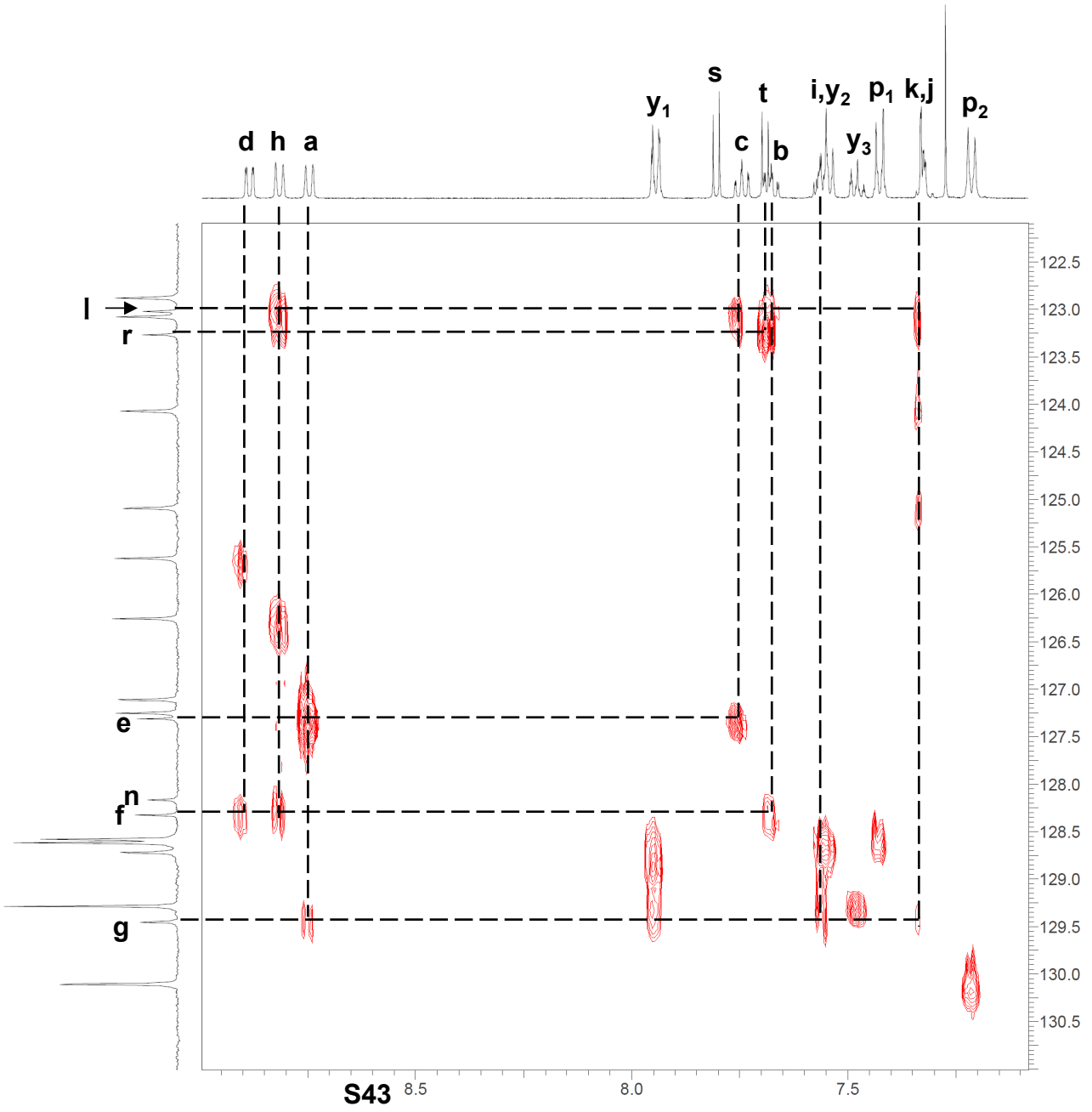
Partial HSQC spectrum of **1a** (500 MHz, in $CDCl_3$, rt)



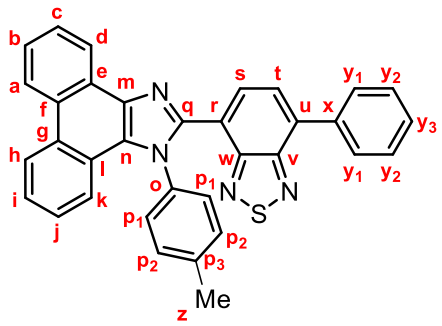


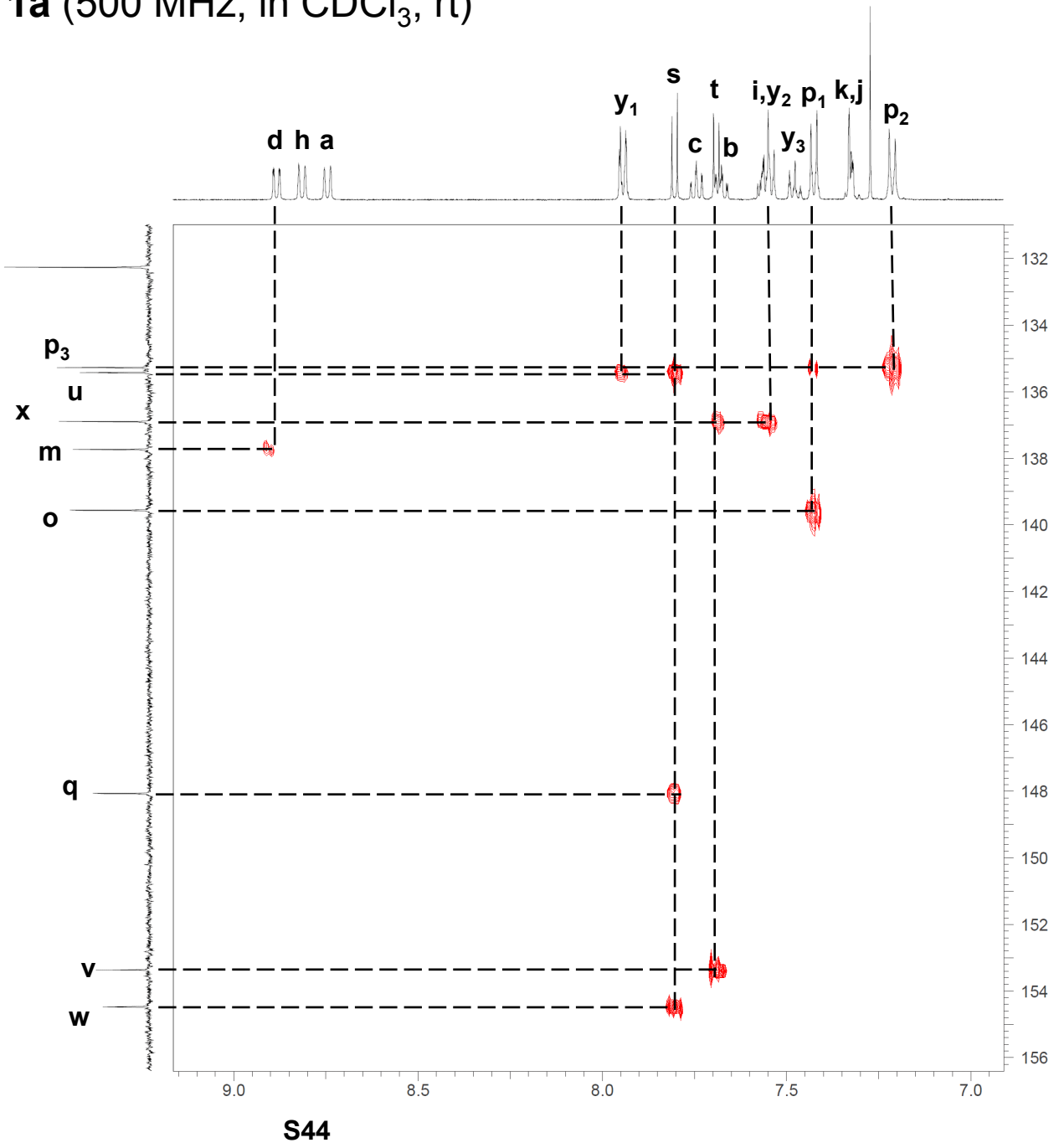
Partial HMBC spectrum of **1a** (500 MHz, in $CDCl_3$, rt)





Partial HMBC spectrum of **1a** (500 MHz, in $CDCl_3$, rt)

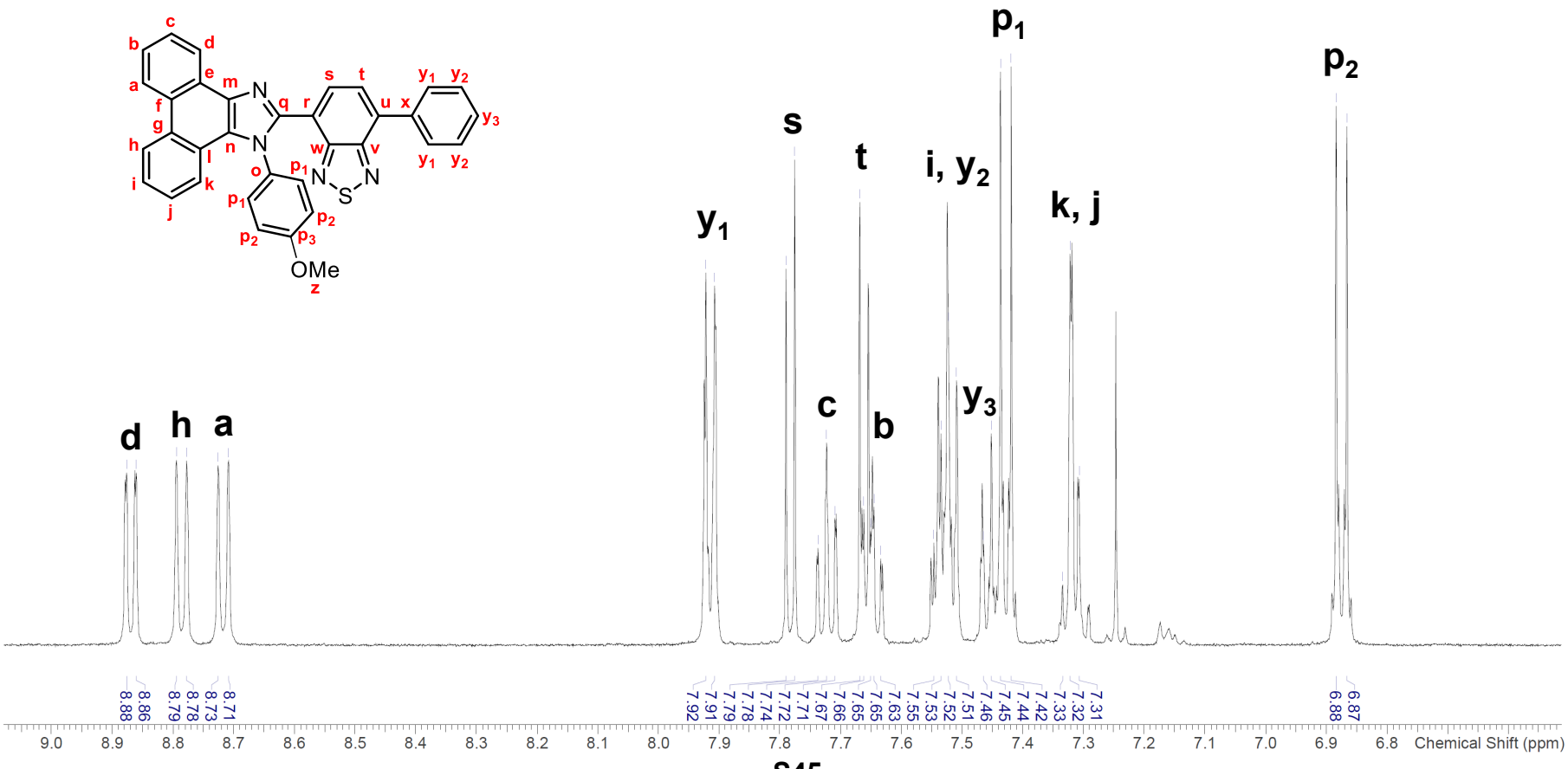




Partial ^{1}H NMR spectrum of **1b** (500 MHz, in $CDCl_3$, rt)

Acquisition Time (sec)	3.1719	*Comment*	5 mm BBO BB-1H Z-GRD Z859001/0006		*D*	3.827959	*D1*	3.827959
DE	6	*DS*	2	*Date*	04 Dec 2019 10:47:11		*Date Stamp*	04 Dec 2019 10:47:11
File Name	E:¥2DNMR¥1b_Ph_PhOMe¥ 1b_STA_Ph_PhOMe_1H¥1¥PDATA¥1¥1r				*Frequency (MHz)*	500.1300	*GB*	0
INSTRUM	<spect>	*LB*	0.1	*NS*	8	*Nucleus*	1H	*Number of Transients*	8
Origin	spect	*Original Points Count*	32768	*Owner*	root	*PC*	1		
PROBHD	<5 mm BBO BB-1H Z-GRD Z859001/0006 >			*PULPROG*	<zg30>	*Points Count*	32768	*Pulse Sequence*	zg30
Receiver Gain	362.00	*SF*	500.130006648269			*SFO1*	500.133088507478		
SI	32768	*SSB*	0	*SW(cyclical) (Hz)*	10330.58	*SWH*	10330.5785123967		
Solvent	CHLOROFORM-d			*Spectrum Offset (Hz)*	3068.3059	*Spectrum Type*	standard	*Sweep Width (Hz)*	10330.26
TD	65536	*TD0*	1	*TE*	297.5	*Temperature (degree C)*	24.500	*WDW*	1

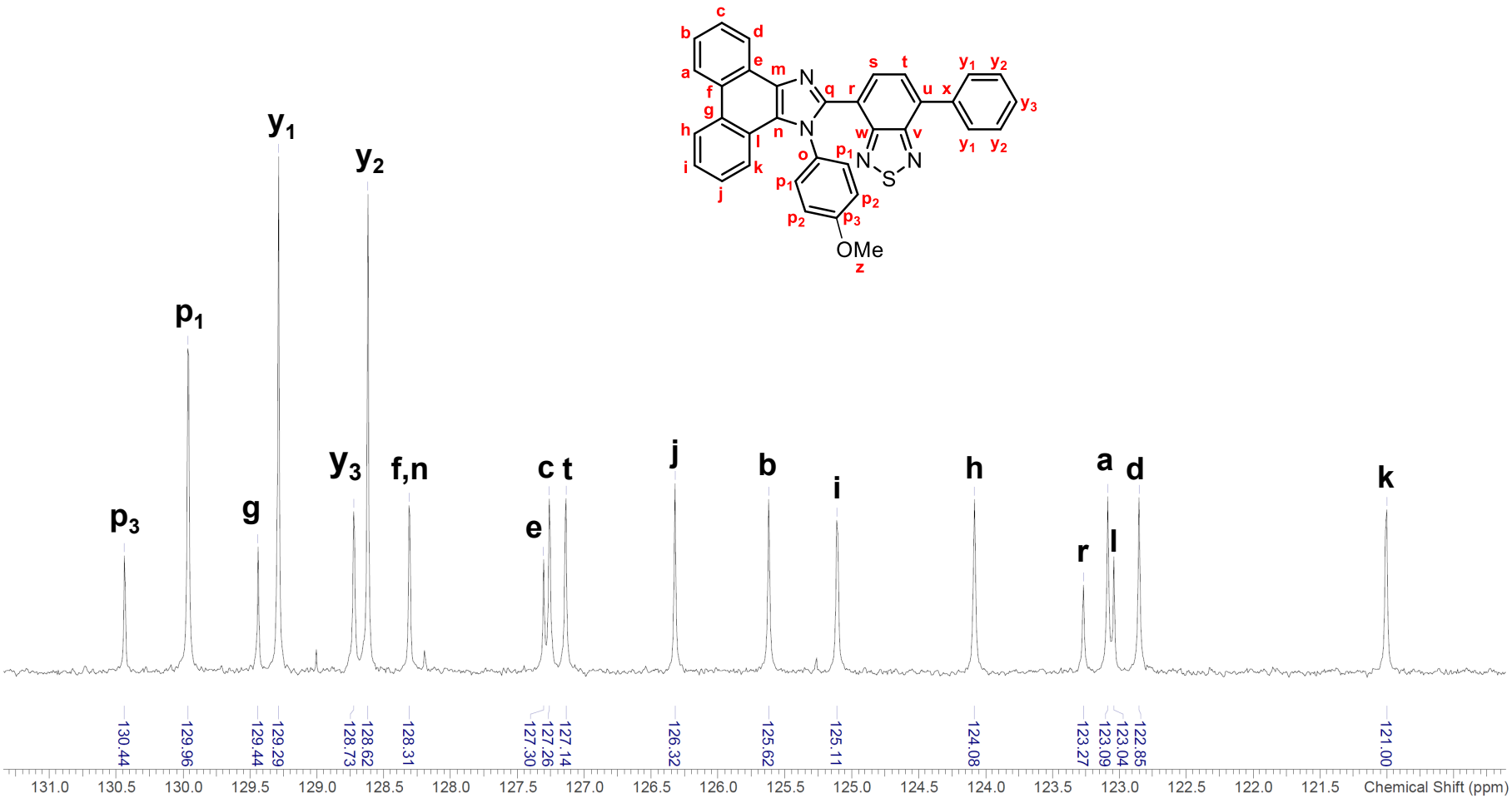
1b_STA_Ph_PhOMe_1H.001.001.1r.esp



Partial ^{13}C NMR spectrum of **1b** (500 MHz, in $CDCl_3$, rt)

Acquisition Time (sec)	1.0912	*D*	0.00345	*D1*	2	*DE*	6	*DS*	4
Date	04 Dec 2019 11:45:43			*Date Stamp*	04 Dec 2019 11:45:43				
File Name	E:¥2DNMR¥1b_Ph_PhOMe¥ 1b_STA_Ph_PhOMe_13C¥10¥PDATA¥1¥1r					*Frequency (MHz)*	125.7578	*GB*	0
INSTRUM	<spect>	*LB*	1	*NS*	1024	*Nucleus*	13C	*Number of Transients*	1024
Origin	spect	*Original Points Count*	32768	*Owner*	root	*PC*	1.4		
PROBHD	<5 mm BBO BB-1H Z-GRD Z859001/0006 >			*PULPROG*	<zgpg30>	*Points Count*	32768	*Pulse Sequence*	zgpg30
Receiver Gain	16384.00	*SF*	125.757789	*SFO1*	125.770364304853			*SI*	32768
SSB	0	*SW(cyclical) (Hz)*	30030.03	*SWH*	30030.03003003			*Solvent*	CHLOROFORM-d
Spectrum Offset (Hz)	12568.7744	*Spectrum Type*	standard	*Sweep Width (Hz)*	30029.11	*TD*	65536	*TD0*	1
TE	299	*Temperature (degree C)*	26.000	*WDW*	1				

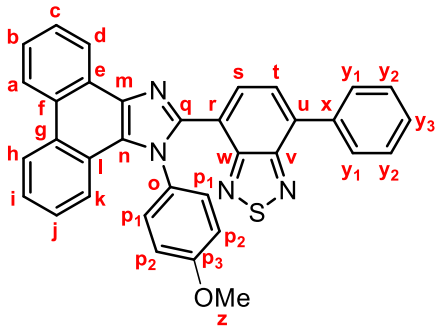
1b_STA_Ph_PhOMe_13C.010.001.1r.esp



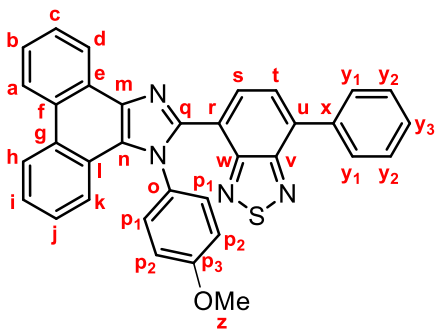
Partial ^{13}C NMR spectrum of **1b** (500 MHz, in $CDCl_3$, rt)

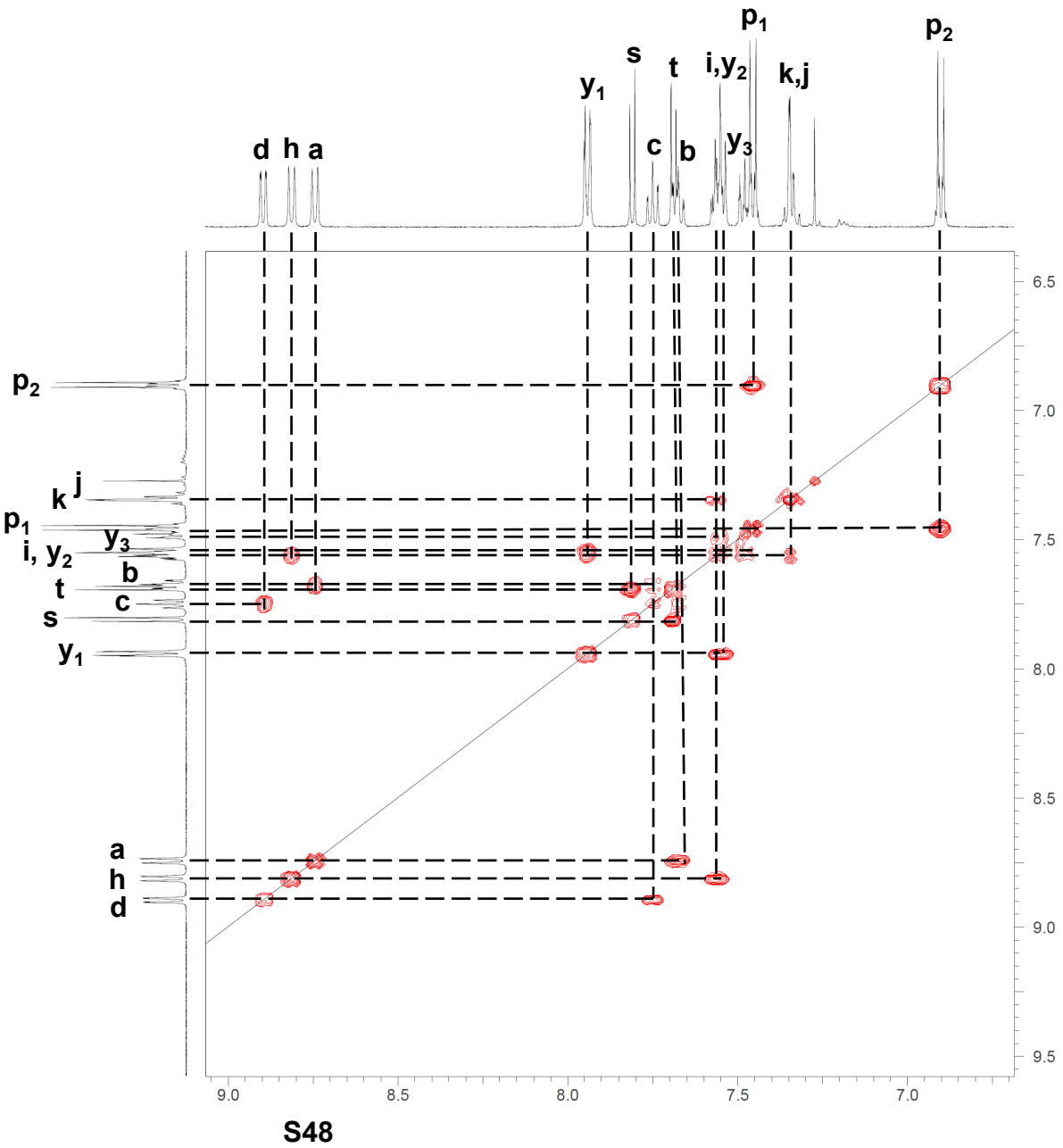
Acquisition Time (sec)	1.0912	*D*	0.00345	*D1*	2	*DE*	6	*DS*	4
Date	04 Dec 2019 11:45:43			*Date Stamp*	04 Dec 2019 11:45:43				
File Name	E:¥2DNMR¥1b_Ph_PhOMe¥ 1b_STA_Ph_PhOMe_13C¥10¥PDATA¥1¥1r					*Frequency (MHz)*	125.7578	*GB*	0
INSTRUM	<spect>	*LB*	1	*NS*	1024	*Nucleus*	13C	*Number of Transients*	1024
Origin	spect	*Original Points Count*	32768	*Owner*	root	*PC*	1.4		
PROBHD	<5 mm BBO BB-1H Z-GRD Z859001/0006 >			*PULPROG*	<zgpg30>	*Points Count*	32768	*Pulse Sequence*	zgpg30
Receiver Gain	16384.00	*SF*	125.757789	*SFO1*	125.770364304853			*SI*	32768
SSB	0	*SW(cyclical) (Hz)*	30030.03	*SWH*	30030.03003003			*Solvent*	CHLOROFORM-d
Spectrum Offset (Hz)	12568.7744	*Spectrum Type*	standard	*Sweep Width (Hz)*	30029.11	*TD*	65536	*TD0*	1
TE	299	*Temperature (degree C)*	26.000	*WDW*	1				

1b_STA_Ph_PhOMe_13C.010.001.1r.esp

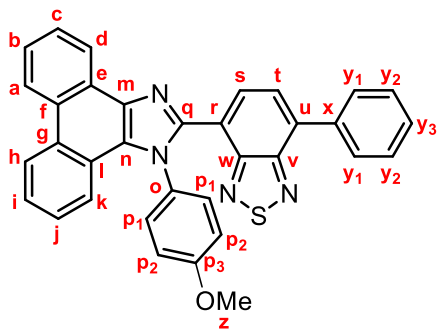


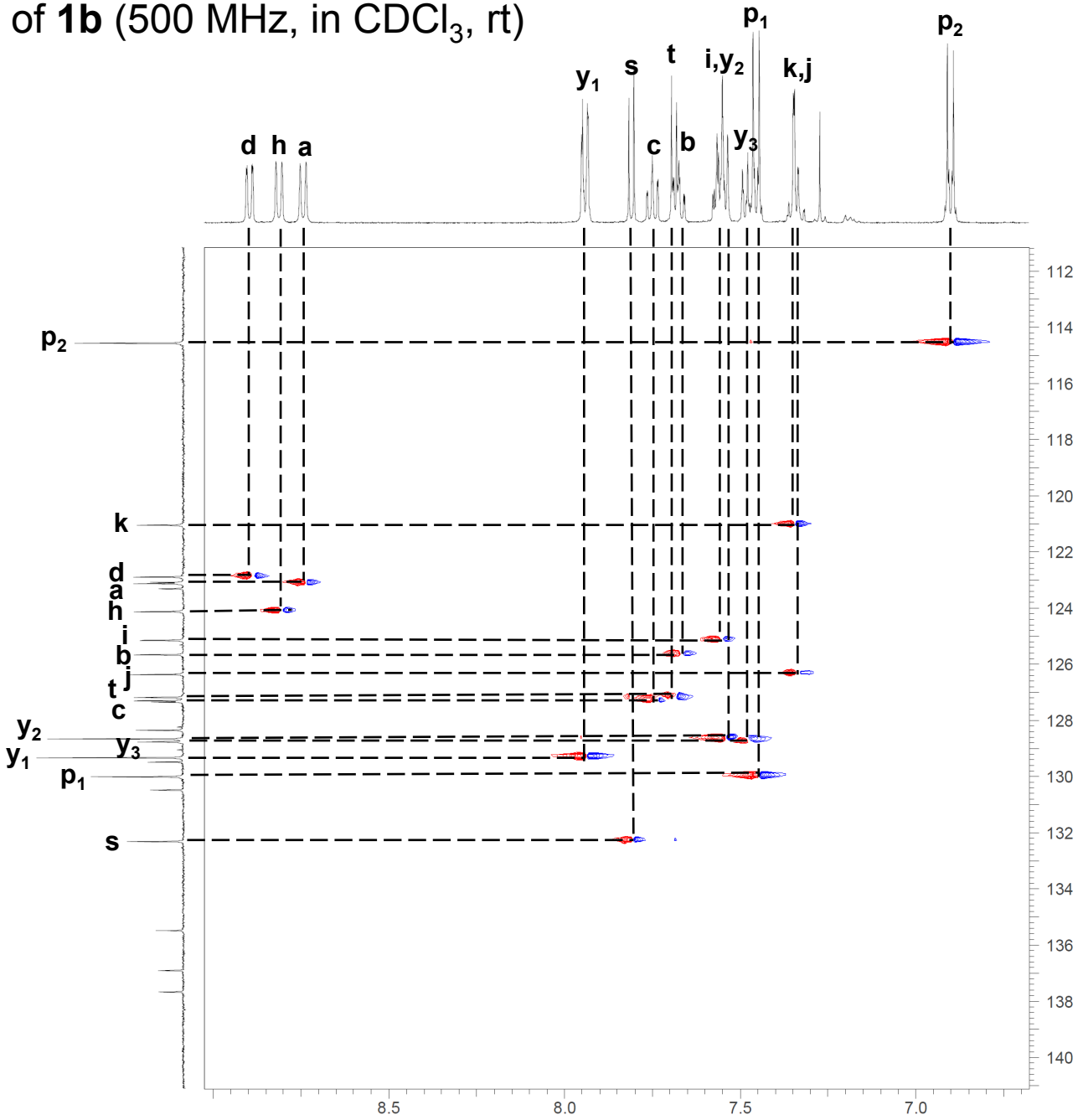
Partial COSY spectrum of **1b** (500 MHz, in $CDCl_3$, rt)



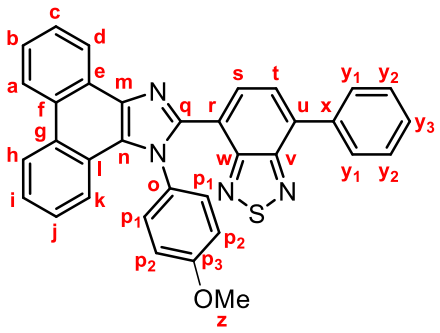


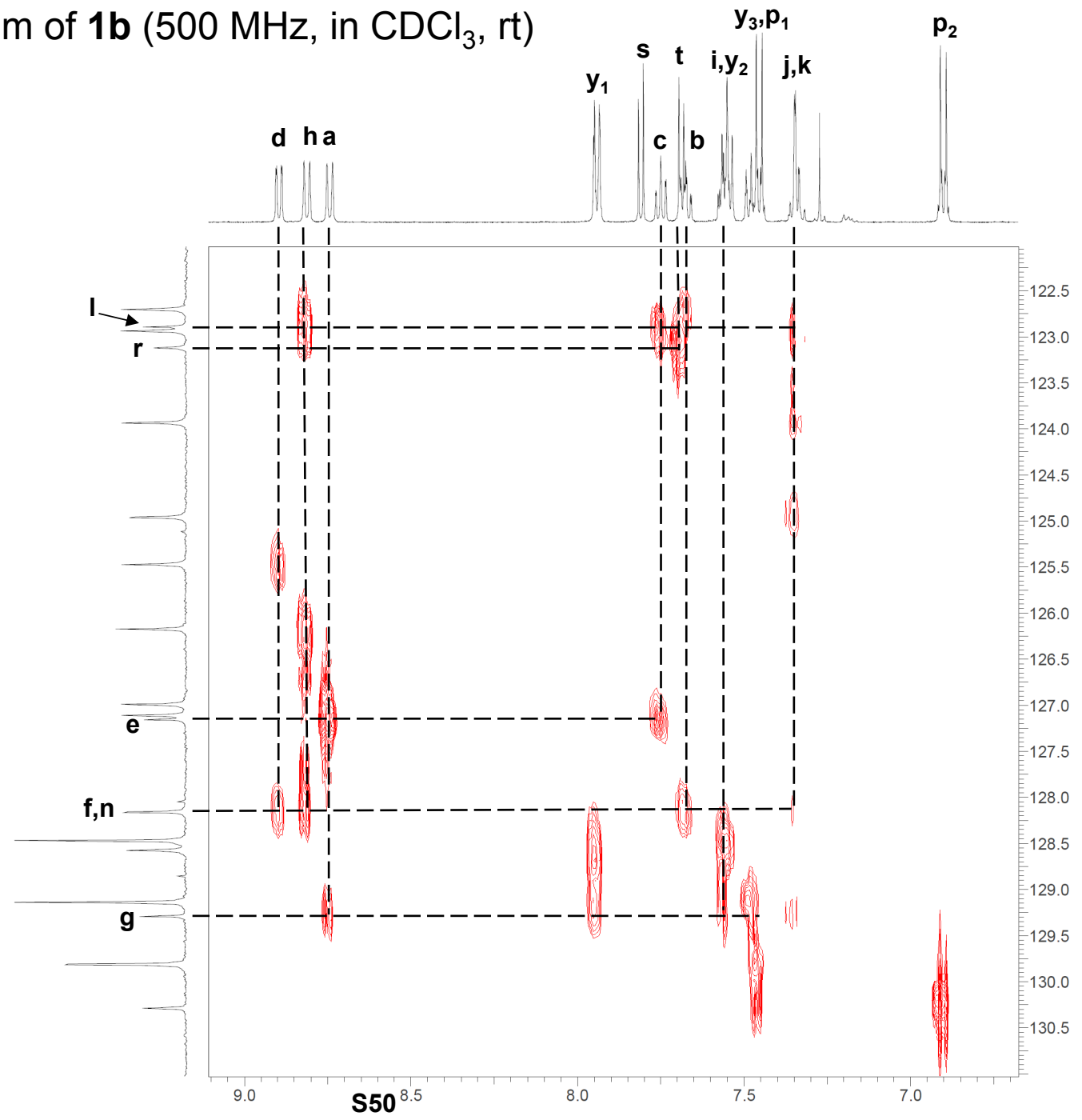
Partial HSQC spectrum of **1b** (500 MHz, in $CDCl_3$, rt)



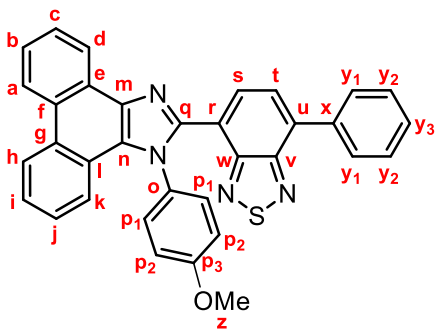


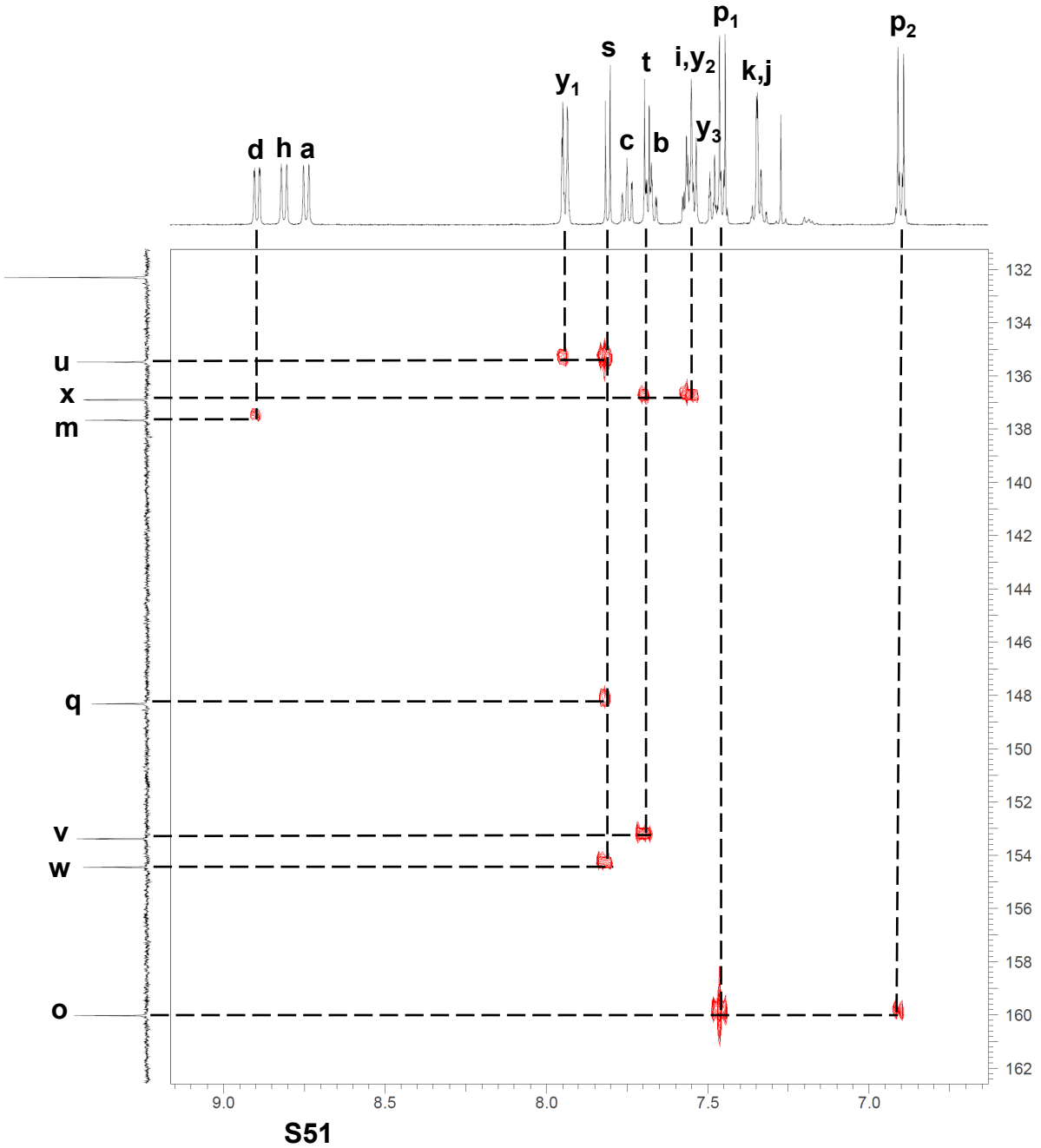
Partial HMBC spectrum of **1b** (500 MHz, in $CDCl_3$, rt)





Partial HMBC spectrum of **1b** (500 MHz, in $CDCl_3$, rt)

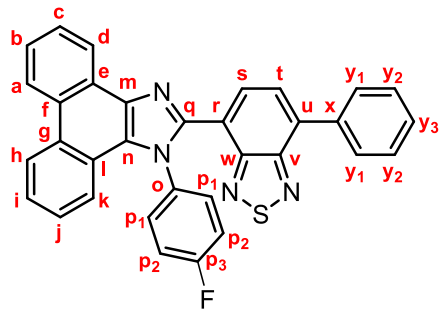




Partial ^{1}H NMR spectrum of **1c** (500 MHz, in $CDCl_3$, rt)

Acquisition Time (sec)	3.1719	*Comment*	5 mm BBO BB-1H Z-GRD Z859001/0006			*D*	3.827959	*D1*	3.827959
DE	6	*DS*	2	*Date*	11 Dec 2019 16:07:10			*Date Stamp*	11 Dec 2019 16:07:10
File Name	E:¥NMR¥ 1c_STA_Ph_PhF_1H¥1¥PDATA¥1¥1r			*Frequency (MHz)*	500.1300	*GB*	0	*INSTRUM*	<spect>
LB	0.1	*NS*	8	*Nucleus*	1H	*Number of Transients*	8	*Origin*	spect
Original Points Count	32768	*Owner*	root	*PC*	1	*PROBHD*	<5 mm BBO BB-1H Z-GRD Z859001/0006 >		
PULPROG	<zg30>	*Points Count*	32768	*Pulse Sequence*	zg30	*Receiver Gain*	724.10	*SF*	500.130006648269
SFO1	500.133088507478			*SI*	32768	*SSB*	0	*SW(cyclical) (Hz)*	10330.58
SWH	10330.5785123967			*Solvent*	CHLOROFORM-d			*Spectrum Offset (Hz)*	3072.7070
Spectrum Type	standard	*Sweep Width (Hz)*	10330.26	*TD*	65536	*TD0*	1	*TE*	297.6
Temperature (degree C)	24.600	*WDW*	1						

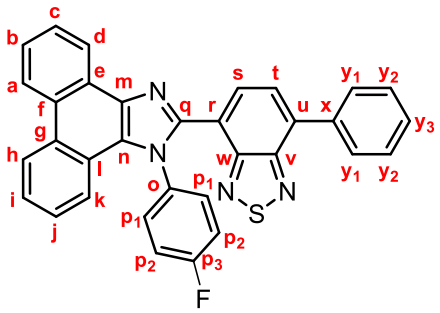
1c_STA_Ph_PhF_1H.001.001.1r.esp



Partial ^{13}C NMR spectrum of **1c** (500 MHz, in $CDCl_3$, rt)

Acquisition Time (sec)	1.0912	*D*	0.00345	*D1*	2	*DE*	6	*DS*	4
Date	12 Dec 2019 17:04:43			*Date Stamp*	12 Dec 2019 17:04:43				
File Name	E:¥2DNMR¥1c_Ph_PhF¥ 1c_STA_Ph_PhF_13C¥10¥PDATA¥1¥1r					*Frequency (MHz)*	125.7578	*GB*	0
INSTRUM	<spect>	*LB*	1	*NS*	1024	*Nucleus*	13C	*Number of Transients*	1024
Origin	spect	*Original Points Count*	32768	*Owner*	root	*PC*	1.4		
PROBHD	<5 mm BBO BB-1H Z-GRD Z859001/0006 >			*PULPROG*	<zgpg30>	*Points Count*	32768	*Pulse Sequence*	zgpg30
Receiver Gain	3251.00	*SF*	125.757789	*SFO1*	125.770364304853			*SI*	32768
SSB	0	*SW(cyclical) (Hz)*	30030.03	*SWH*	30030.03003003			*Solvent*	CHLOROFORM-d
Spectrum Offset (Hz)	12537.6123	*Spectrum Type*	standard	*Sweep Width (Hz)*	30029.11	*TD*	65536	*TD0*	1
TE	298.3	*Temperature (degree C)*	25.300	*WDW*	1				

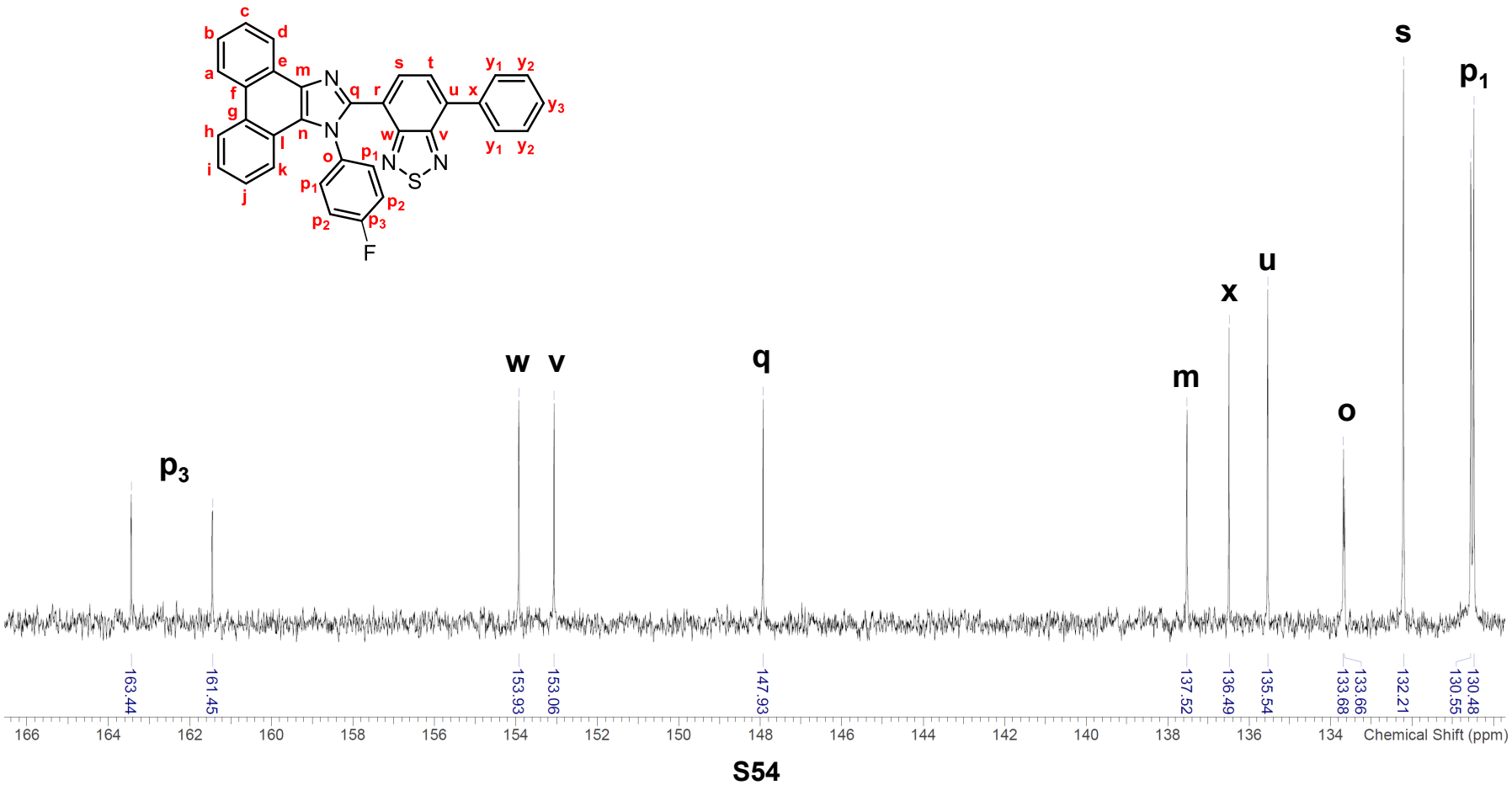
1c_STA_Ph_PhF_13C.010.001.1r.esp



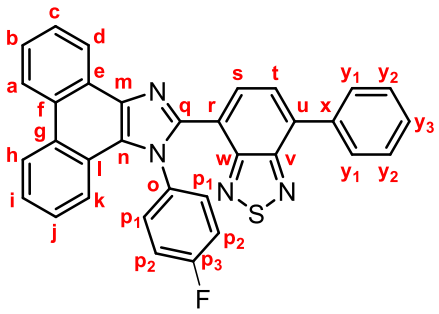
Partial ^{13}C NMR spectrum of **1c** (500 MHz, in $CDCl_3$, rt)

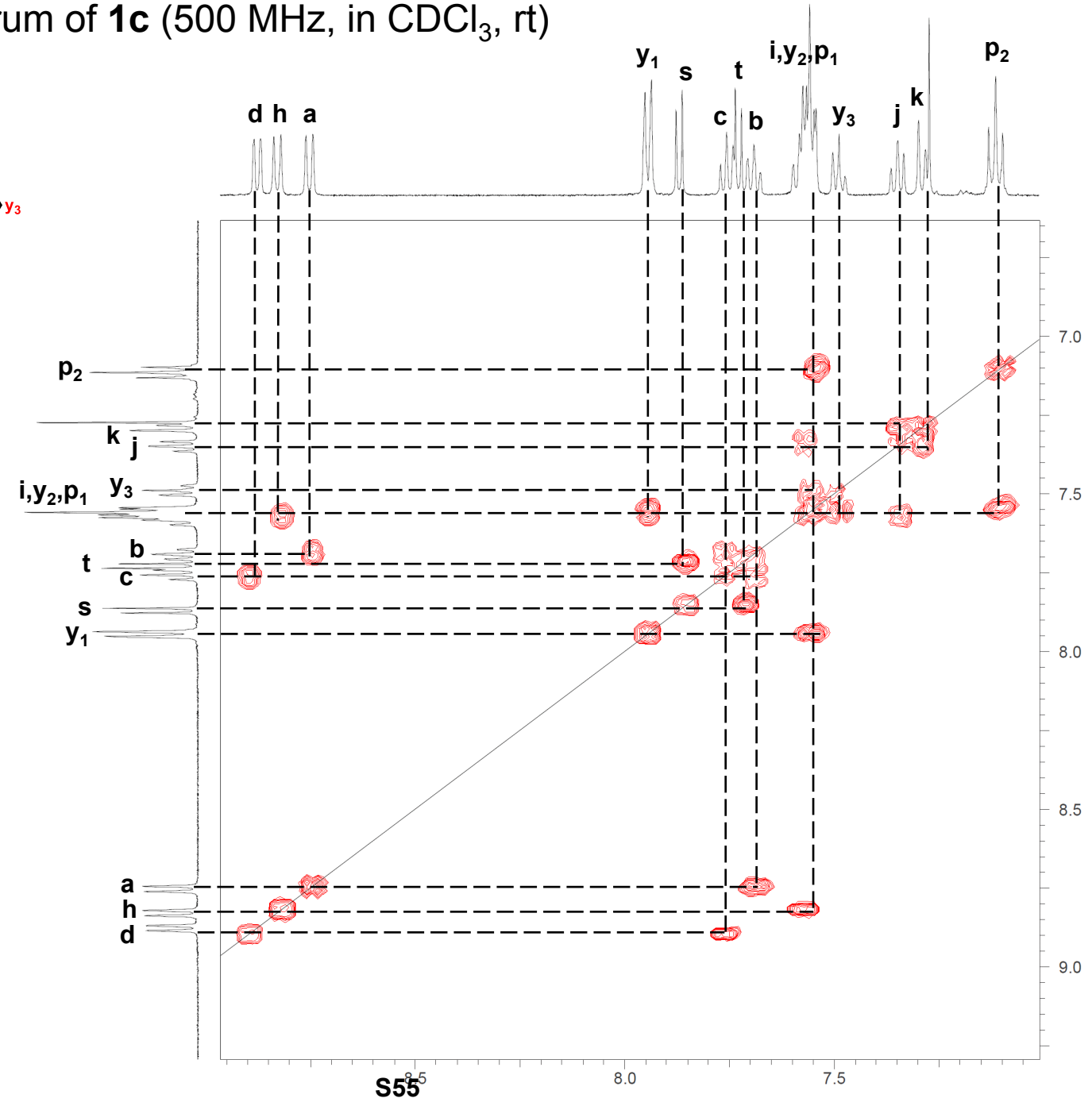
Acquisition Time (sec)	1.0912	*D*	0.00345	*D1*	2	*DE*	6	*DS*	4
Date	12 Dec 2019 17:04:43			*Date Stamp*	12 Dec 2019 17:04:43				
File Name	E:¥2DNMR¥1c_Ph_PhF¥ 1c_STA_Ph_PhF_13C¥10¥PDATA¥1¥1r					*Frequency (MHz)*	125.7578	*GB*	0
INSTRUM	<spect>	*LB*	1	*NS*	1024	*Nucleus*	13C	*Number of Transients*	1024
Origin	spect	*Original Points Count*	32768	*Owner*	root	*PC*	1.4		
PROBHD	<5 mm BBO BB-1H Z-GRD Z859001/0006 >			*PULPROG*	<zgpg30>	*Points Count*	32768	*Pulse Sequence*	zgpg30
Receiver Gain	3251.00	*SF*	125.757789	*SFO1*	125.770364304853			*SI*	32768
SSB	0	*SW(cyclical) (Hz)*	30030.03	*SWH*	30030.03003003			*Solvent*	CHLOROFORM-d
Spectrum Offset (Hz)	12537.6123	*Spectrum Type*	standard	*Sweep Width (Hz)*	30029.11	*TD*	65536	*TD0*	1
TE	298.3	*Temperature (degree C)*	25.300	*WDW*	1				

1c_STA_Ph_PhF_13C.010.001.1r.esp

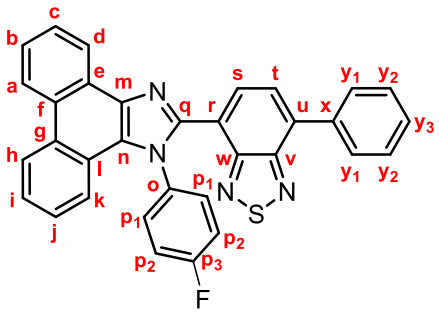


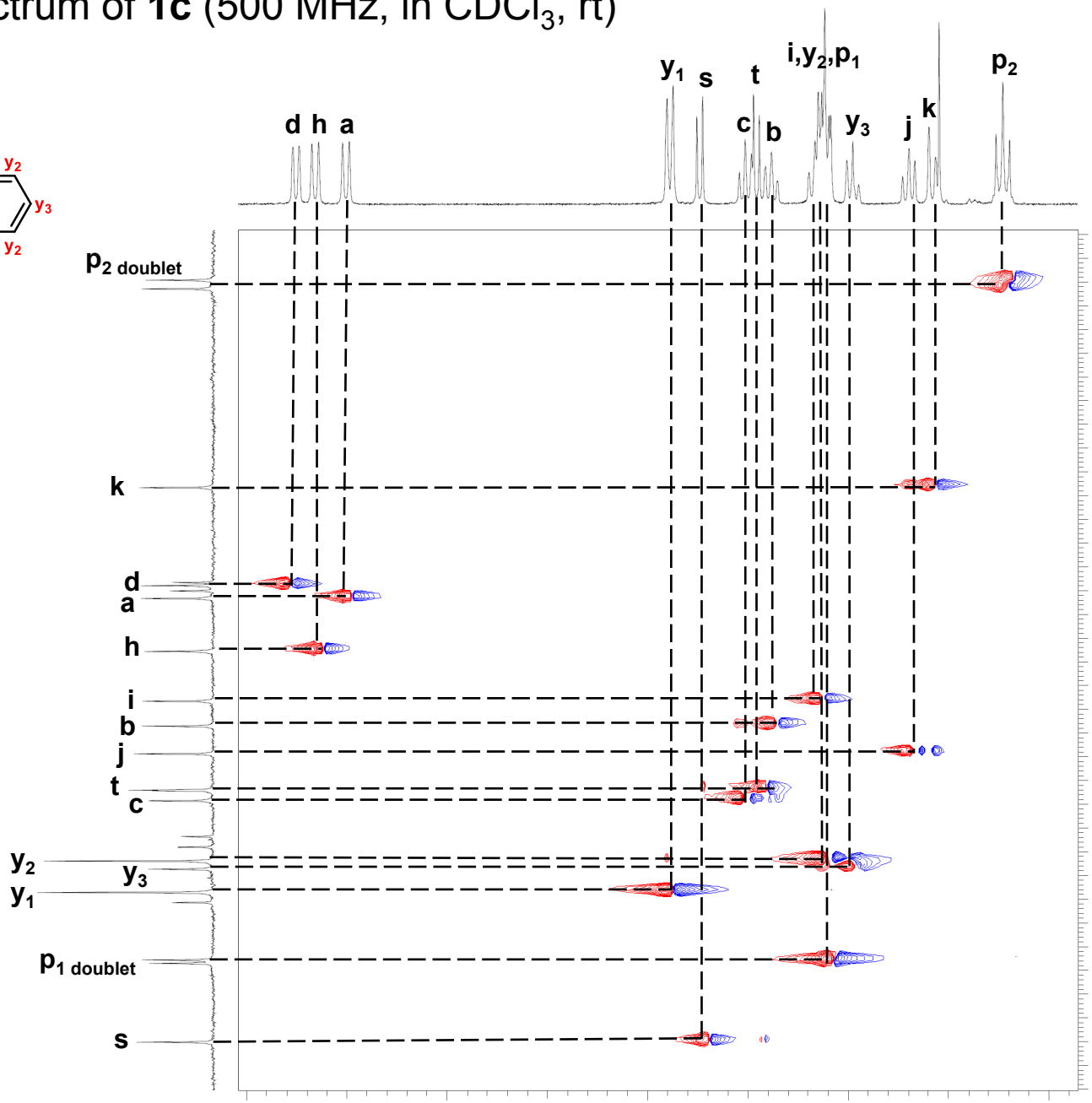
Partial COSY spectrum of **1c** (500 MHz, in $CDCl_3$, rt)



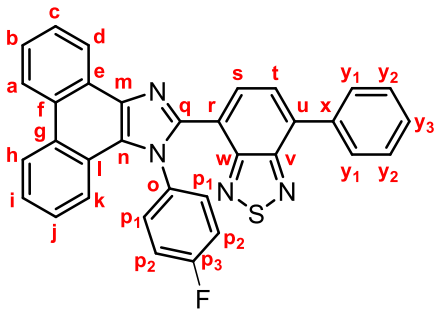


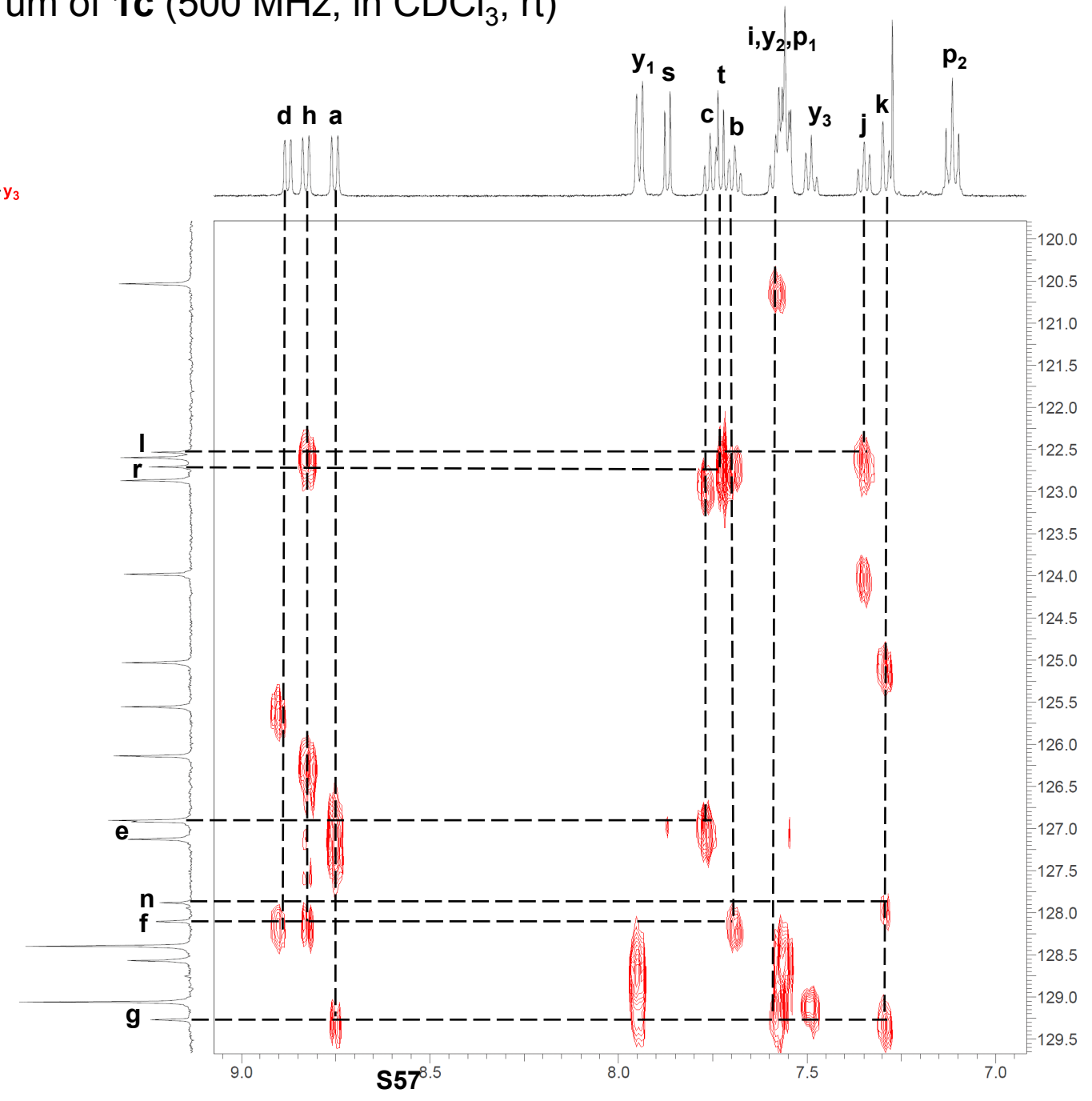
Partial HSQC spectrum of **1c** (500 MHz, in $CDCl_3$, rt)



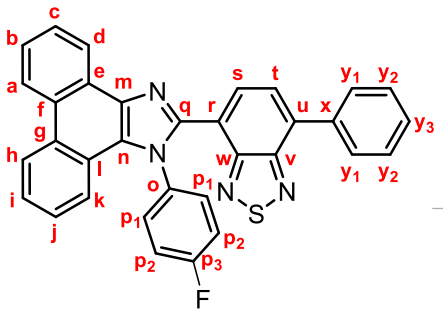


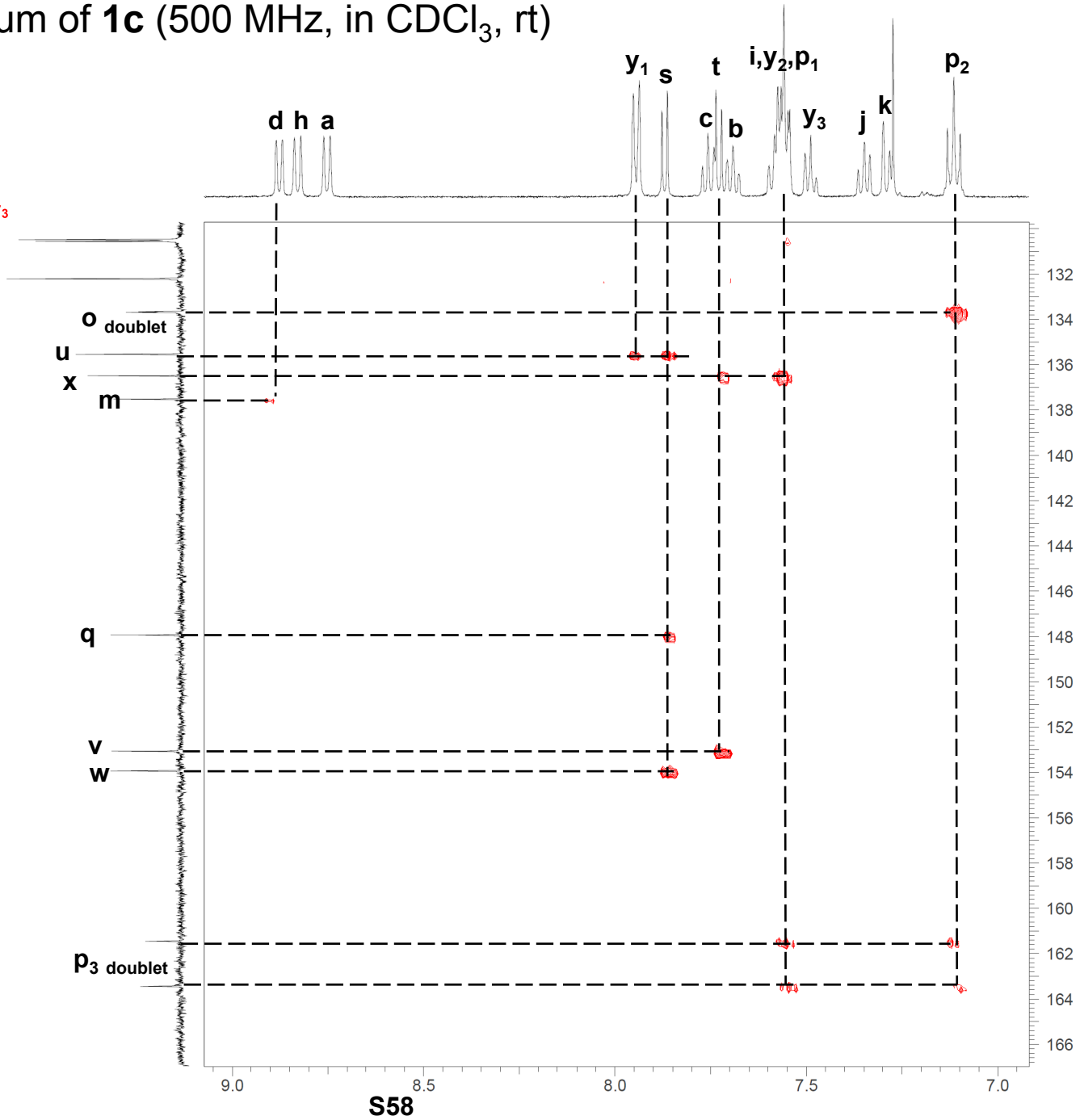
Partial HMBC spectrum of **1c** (500 MHz, in $CDCl_3$, rt)





Partial HMBC spectrum of **1c** (500 MHz, in $CDCl_3$, rt)

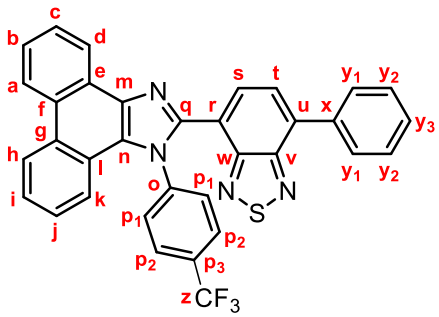




Partial ^{1}H NMR spectrum of **1d** (500 MHz, in $CDCl_3$, rt)

Acquisition Time (sec)	3.1719	*Comment*	5 mm BBO BB-1H Z-GRD Z859001/0006			*D*	3.827959	*D1*	3.827959
DE	6	*DS*	2	*Date*	05 Dec 2019 17:01:33			*Date Stamp*	05 Dec 2019 17:01:33
File Name	E:¥NMR¥ 1d_STA_Ph_PhCF3_1H¥1¥PDATA¥1¥1r			*Frequency (MHz)*	500.1300	*GB*	0	*INSTRUM*	<spect>
LB	0.1	*NS*	8	*Nucleus*	1H	*Number of Transients*	8	*Origin*	spect
Original Points Count	32768	*Owner*	root	*PC*	1	*PROBHD*	<5 mm BBO BB-1H Z-GRD Z859001/0006 >		
PULPROG	<zg30>	*Points Count*	32768	*Pulse Sequence*	zg30	*Receiver Gain*	322.50	*SF*	500.130006648269
SFO1	500.133088507478			*SI*	32768	*SSB*	0	*SW(cyclical) (Hz)*	10330.58
SWH	10330.5785123967			*Solvent*	CHLOROFORM-d			*Spectrum Offset (Hz)*	3067.3557
Spectrum Type	standard	*Sweep Width (Hz)*	10330.26	*TD*	65536	*TD0*	1	*TE*	298.5
Temperature (degree C)	25.500	*WDW*	1						

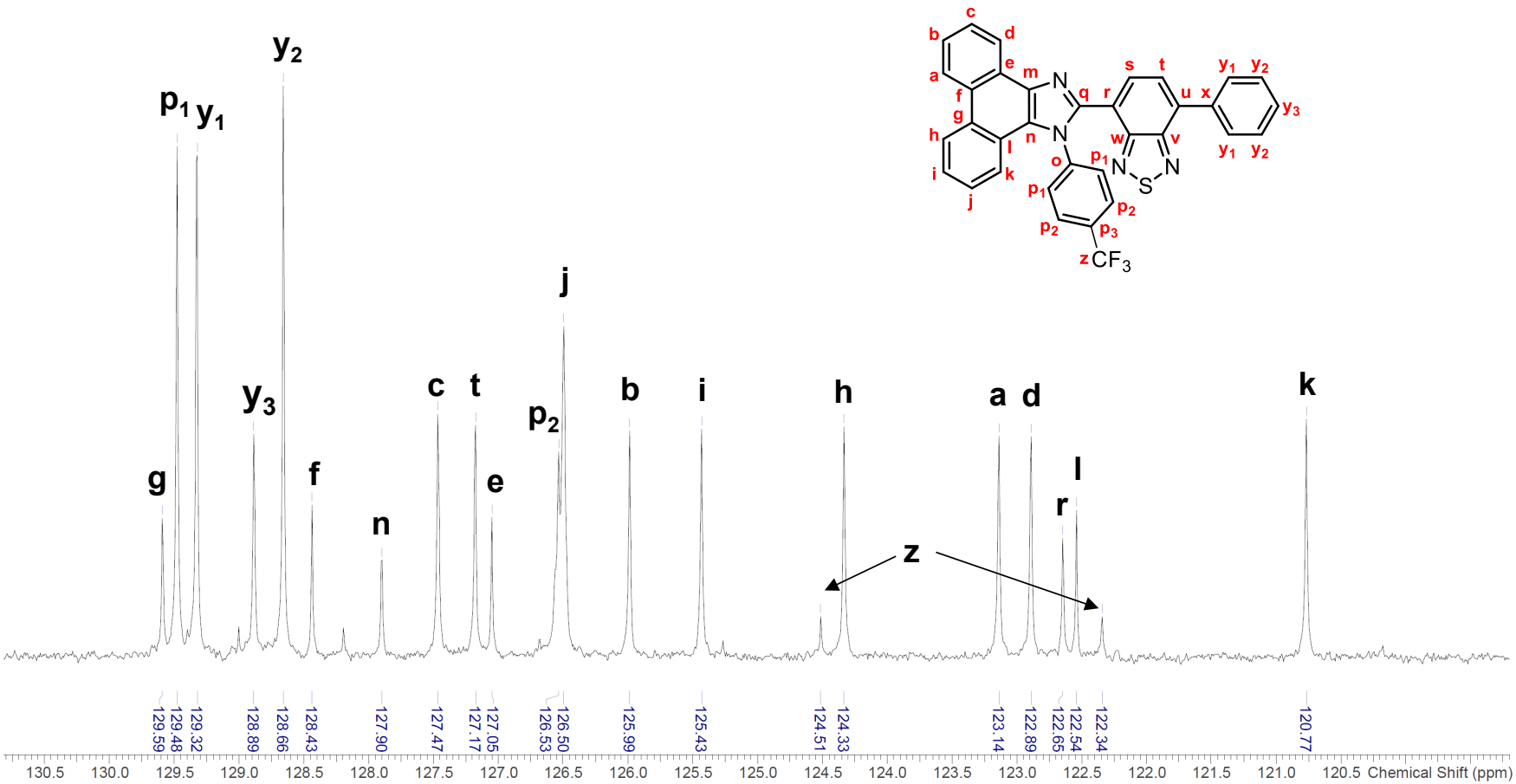
1d_STA_Ph_PhCF3_1H.001.001.1r.esp



Partial ^{13}C NMR spectrum of **1d** (500 MHz, in $CDCl_3$, rt)

Acquisition Time (sec)	1.0912	*D*	0.00345	*D1*	2	*DE*	6	*DS*	4
Date	05 Dec 2019 18:01:16			*Date Stamp*	05 Dec 2019 18:01:16				
File Name	E:¥2DNMR¥1d_Ph_PhCF3¥ 1d_STA_Ph_PhCF3_13C¥10¥pdata¥1¥1r					*Frequency (MHz)*	125.7578	*GB*	0
INSTRUM	<spect>	*LB*	1	*NS*	1024	*Nucleus*	13C	*Number of Transients*	1024
Origin	spect	*Original Points Count*	32768	*Owner*	root	*PC*	1.4		
PROBHD	<5 mm BBO BB-1H Z-GRD Z859001/0006 >			*PULPROG*	<zgpg30>	*Points Count*	32768	*Pulse Sequence*	zgpg30
Receiver Gain	4096.00	*SF*	125.757789	*SFO1*	125.770364304853			*SI*	32768
SSB	0	*SW(cyclical) (Hz)*	30030.03	*SWH*	30030.03003003			*Solvent*	CHLOROFORM-d
Spectrum Offset (Hz)	12568.7764	*Spectrum Type*	standard	*Sweep Width (Hz)*	30029.11	*TD*	65536	*TD0*	1
TE	299.5	*Temperature (degree C)*	26.500	*WDW*	1				

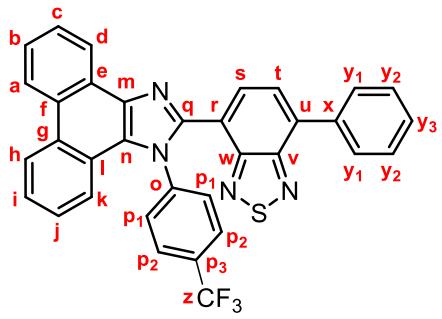
1d_STA_Ph_PhCF3_13C.010.001.1r.esp



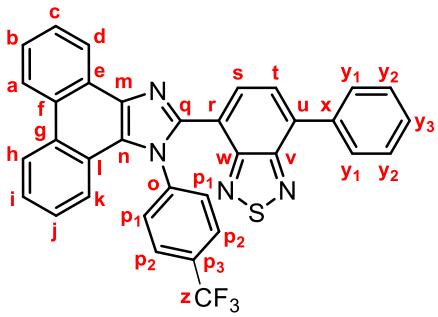
Partial ^{13}C NMR spectrum of **1d** (500 MHz, in $CDCl_3$, rt)

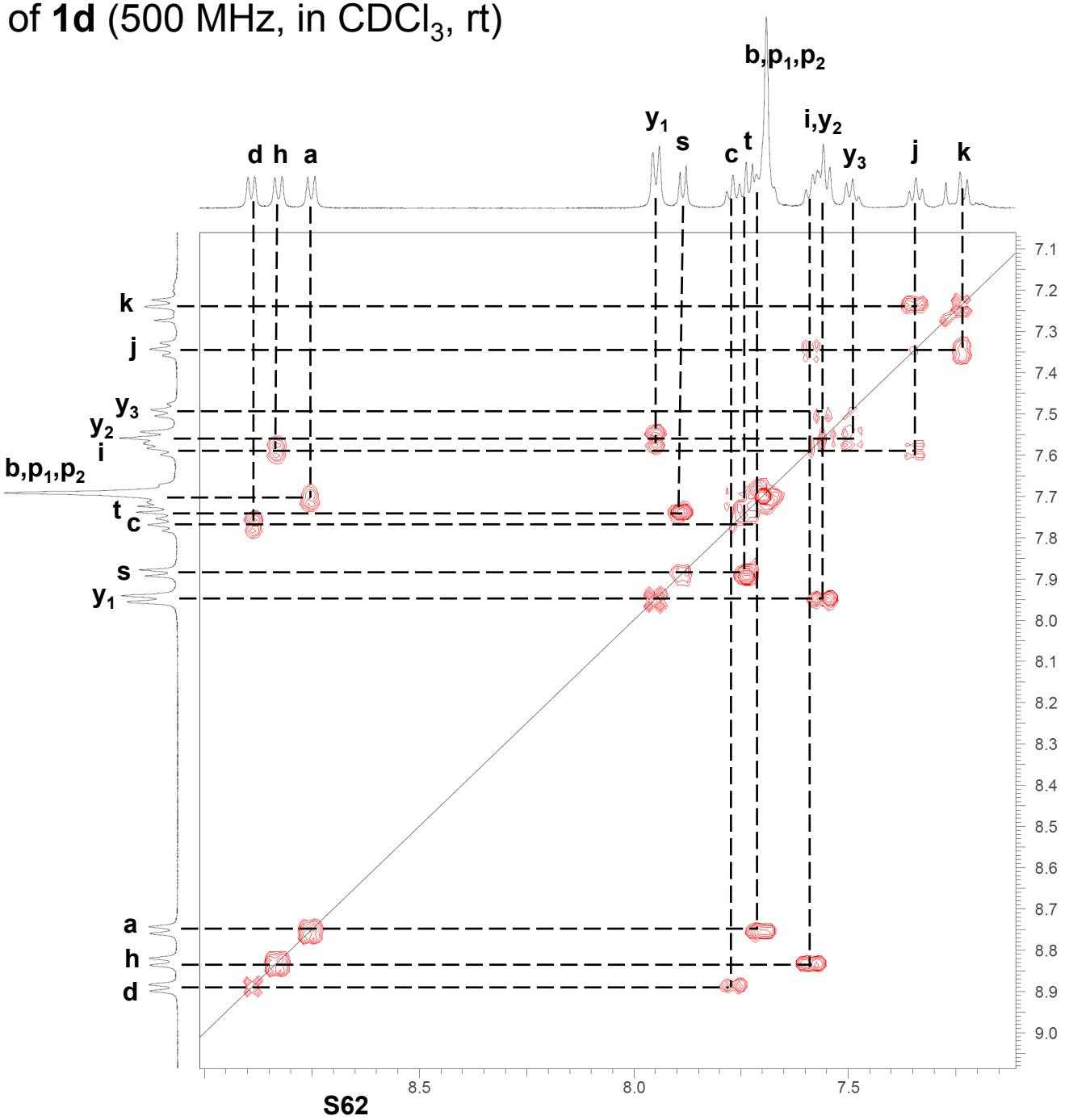
Acquisition Time (sec)	1.0912	*D*	0.00345	*D1*	2	*DE*	6	*DS*	4
Date	05 Dec 2019 18:01:16			*Date Stamp*	05 Dec 2019 18:01:16				
File Name	E:¥2DNMR¥1d_Ph_PhCF3¥ 1d_STA_Ph_PhCF3_13C¥10¥pdata¥1¥1r					*Frequency (MHz)*	125.7578	*GB*	0
INSTRUM	<spect>	*LB*	1	*NS*	1024	*Nucleus*	13C	*Number of Transients*	1024
Origin	spect	*Original Points Count*	32768	*Owner*	root	*PC*	1.4		
PROBHD	<5 mm BBO BB-1H Z-GRD Z859001/0006 >			*PULPROG*	<zgpg30>	*Points Count*	32768	*Pulse Sequence*	zgpg30
Receiver Gain	4096.00	*SF*	125.757789	*SFO1*	125.770364304853			*SI*	32768
SSB	0	*SW(cyclical) (Hz)*	30030.03	*SWH*	30030.03003003			*Solvent*	CHLOROFORM-d
Spectrum Offset (Hz)	12568.7764	*Spectrum Type*	standard	*Sweep Width (Hz)*	30029.11	*TD*	65536	*TD0*	1
TE	299.5	*Temperature (degree C)*	26.500	*WDW*	1				

1d_STA_Ph_PhCF3_13C.010.001.1r.esp

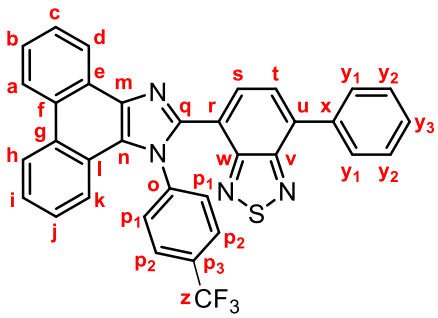


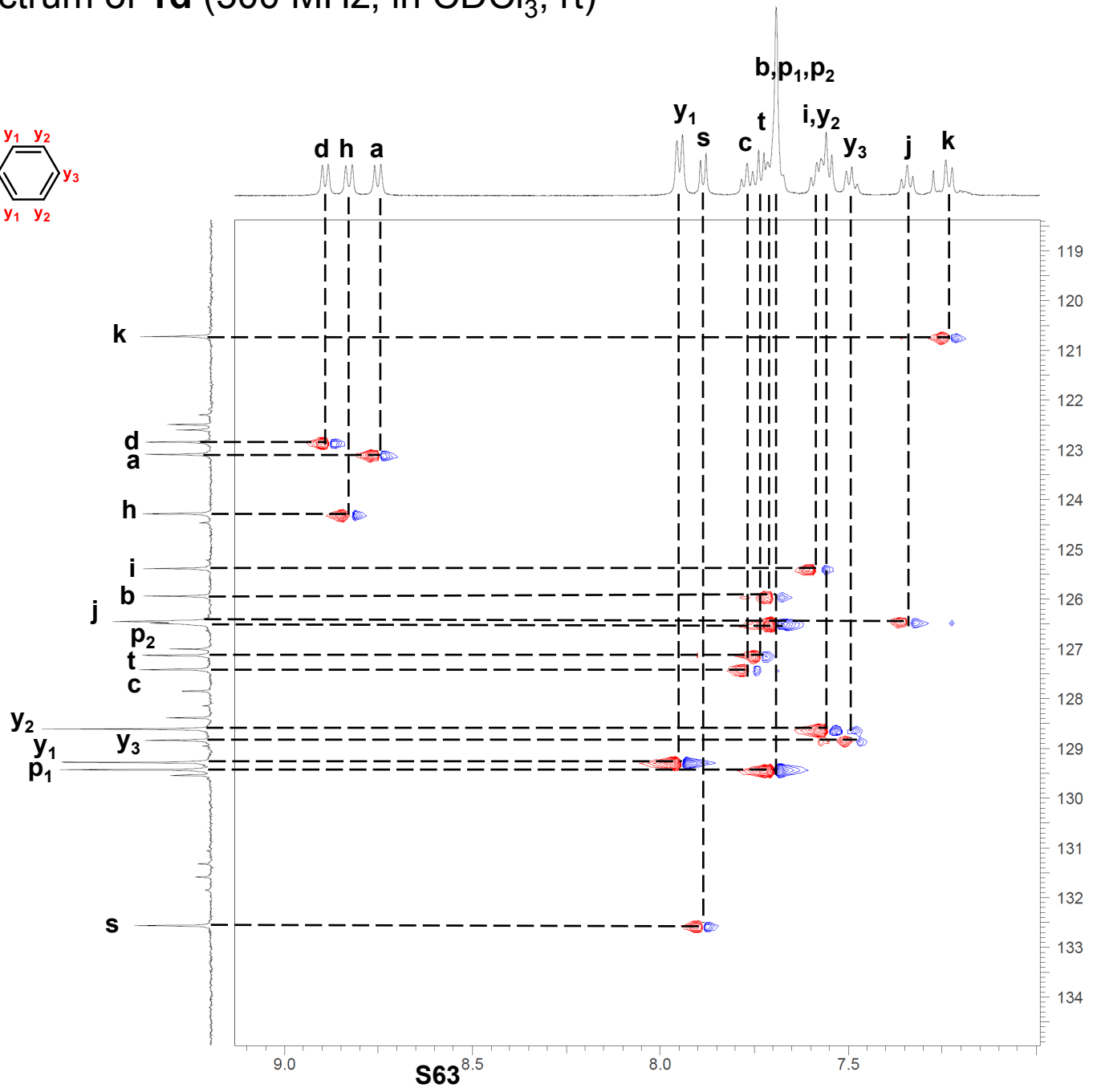
Partial COSY spectrum of **1d** (500 MHz, in $CDCl_3$, rt)



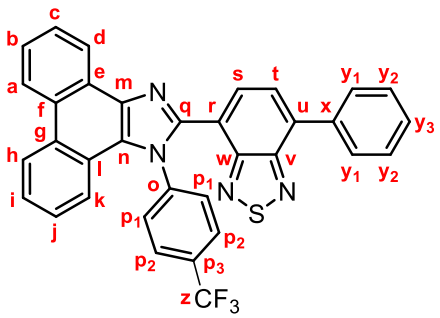


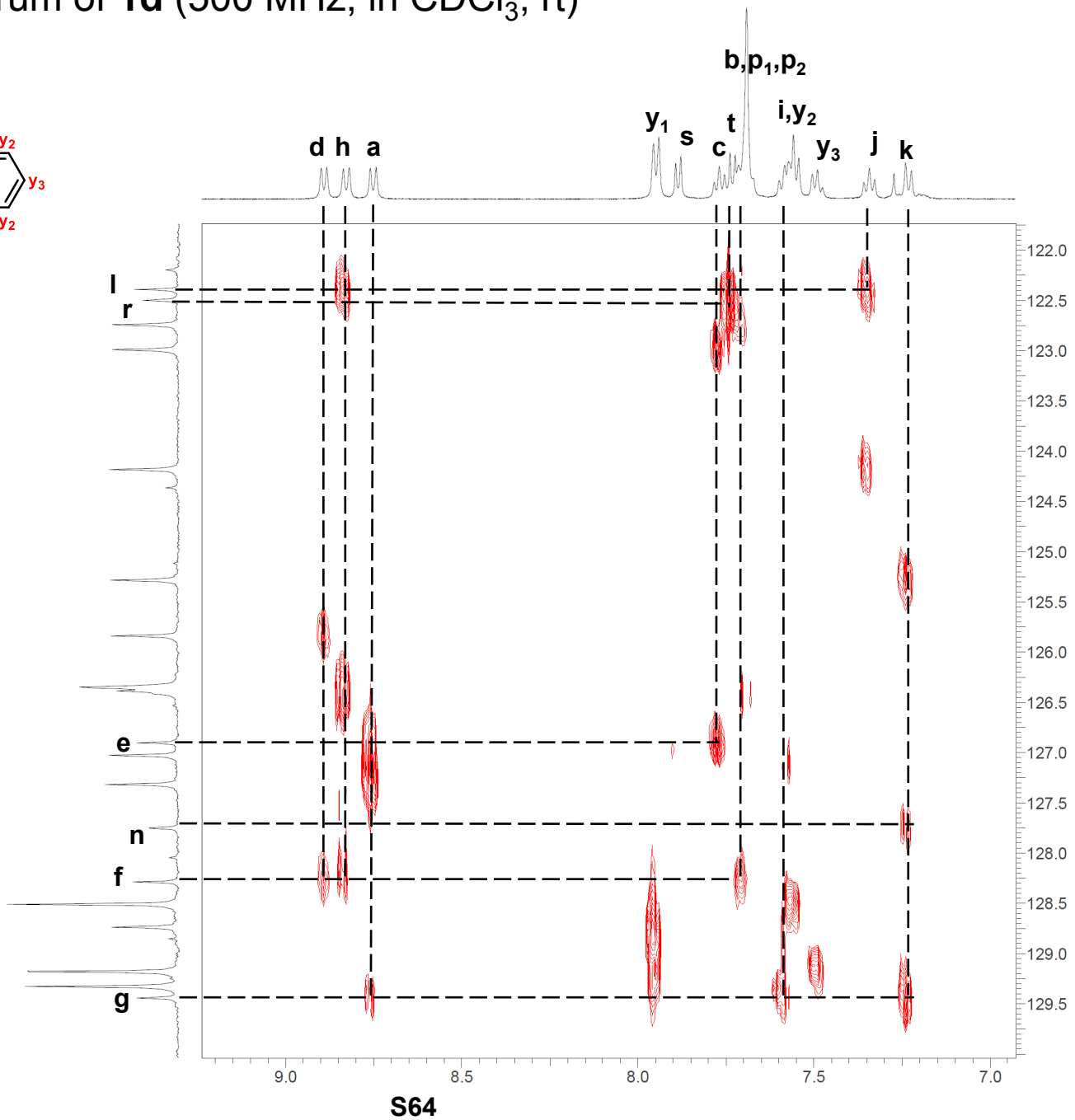
Partial HSQC spectrum of **1d** (500 MHz, in $CDCl_3$, rt)





Partial HMBC spectrum of **1d** (500 MHz, in $CDCl_3$, rt)





Partial HMBC spectrum of **1d** (500 MHz, in $CDCl_3$, rt)