SUPPLEMENTARY MATERIAL

Experimental Validation of Quantum Circuit Rules in Molecular Junctions

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Table S1. *Crystal and refinement details*

Structure	1	2	3	5	7	8
Chemical formula	$C_{22}H_{22}S_2$	$2(C_8H_7S)$	$2(C_7H_6N)$	$C_{19}H_{18}S_2$	$C_{15}H_{13}NS$	$C_{17}H_{14}OS_2$
M_r	350.51	270.39	208.26	310.45	239.32	298.40
Crystal system, space group	Monoclinic, $P2_1/n$	Triclinic, $P\bar{1}$	Monoclinic, $P2_1/n$	Orthorhombic, $Pbca$	Monoclinic, $P2_1/n$	Orthorhombic, $P2_12_12_1$
Temperature (K)	100	100	100	100	100	100
a, b, c (Å)	6.8023 (1), 8.6989 (1), 15.8992 (3)	8.7859 (5), 8.9288 (5), 10.2064 (4)	13.3461 (4), 5.7693 (2), 14.1264 (4)	11.8352 (3), 11.3040 (2), 24.1403 (5)	5.6632 (1), 19.1076 (4), 11.1134 (2)	5.6138 (1), 7.6625 (1), 34.9847 (4)
α, β, γ (°)	90, 101.747 (2), 90	75.109 (4), 84.568 (4), 64.069 (6)	90, 93.841 (3), 90	90, 90, 90	90, 95.806 (2), 90	90, 90, 90
V (Å^3)	921.09 (3)	695.73 (7)	1085.26 (6)	3229.61 (12)	1196.41 (4)	1504.89 (4)
Z	2	2	4	8	4	4
μ (mm^{-1})	2.59	3.27	0.59	2.89	2.17	3.13
Crystal size (mm)	0.24 × 0.21 × 0.17	0.38 × 0.17 × 0.08	0.13 × 0.09 × 0.06	0.22 × 0.14 × 0.11	0.14 × 0.05 × 0.05	0.28 × 0.19 × 0.1
Absorption correction	Multi-scan *CrysAlis PRO*	Gaussian *CrysAlis PRO*	Multi-scan *CrysAlis PRO*	Multi-scan *CrysAlis PRO*	Gaussian *CrysAlis PRO*	Multi-scan *CrysAlis PRO*

	1.171.40.53 (Rigaku Oxford Diffraction, 2019) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.	1.171.40.53 (Rigaku Oxford Diffraction, 2019) Numerical absorption correction based on gaussian integration over a multifaceted crystal model using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.	1.171.40.53 (Rigaku Oxford Diffraction, 2019) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.	1.171.40.53 (Rigaku Oxford Diffraction, 2019) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.	1.171.40.53 (Rigaku Oxford Diffraction, 2019) Numerical absorption correction based on gaussian integration over a multifaceted crystal model using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.	1.171.41.103a (Rigaku Oxford Diffraction, 2021) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.
T_{min}, T_{max}	0.698, 1.000	0.392, 1.000	0.821, 1.000	0.747, 1.000	0.736, 1.000	0.757, 1.000
No. of measured, independent and observed [$I > 2s(I)$] reflections	31951, 1864, 1792	24911, 2755, 2494	18035, 2186, 1911	45677, 3339, 3024	22134, 2427, 2126	14332, 3019, 2968
R_{int}	0.108	0.116	0.104	0.160	0.086	0.051
$(\sin q/l)_{max}$ (Å^{-1})	0.628	0.627	0.630	0.629	0.628	0.627
$R[F^2 > 2s(F^2)]$,	0.037, 0.099, 1.13	0.054, 0.172, 1.13	0.059, 0.172, 1.13	0.048, 0.140, 1.11	0.039, 0.108, 1.06	0.057, 0.153, 1.18

$wR(F^2), S$						
No. of reflections	1864	2755	2186	3339	2427	3019
No. of parameters	111	165	145	193	155	184
$D\rho_{max}, D\rho_{min}$ (e Å^{-3})	0.28, -0.40	0.45, -0.71	0.25, -0.28	0.42, -0.45	0.28, -0.22	1.63, -0.39
Absolute structure	–	–	–	–	–	Refined as an inversion twin.
Absolute structure parameter	–	–	–	–	–	0.39 (4)

500 MHz, CDCl3
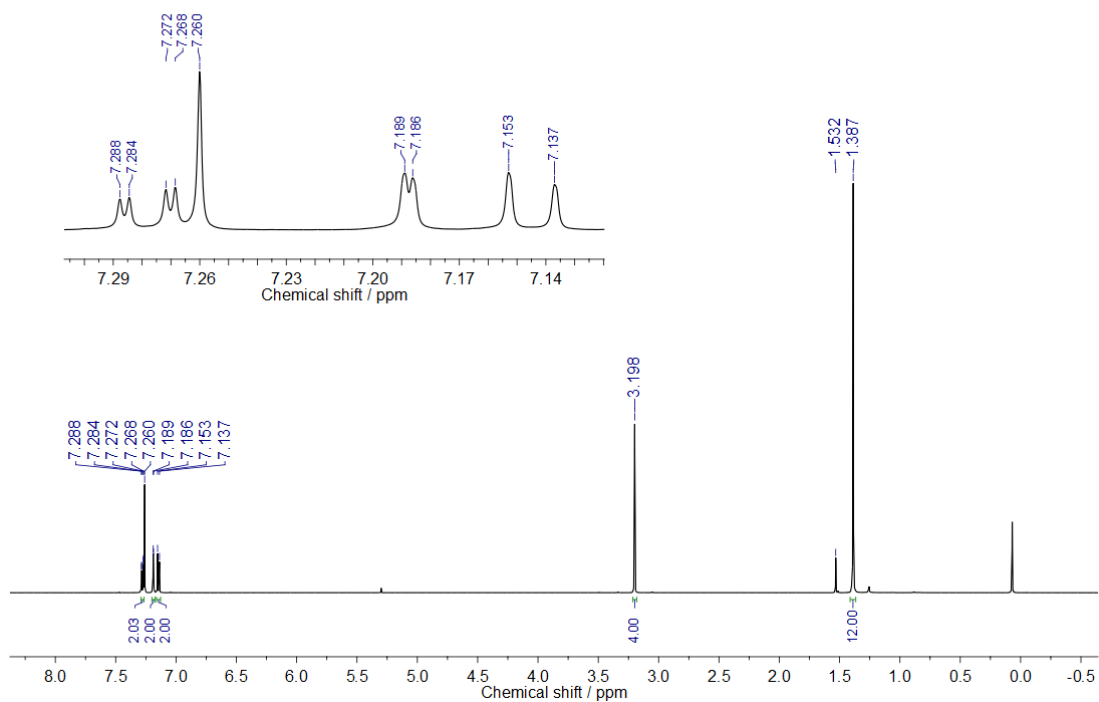
Figure S1. ^{1}H NMR spectrum of **1** recorded in CDCl$_3$.
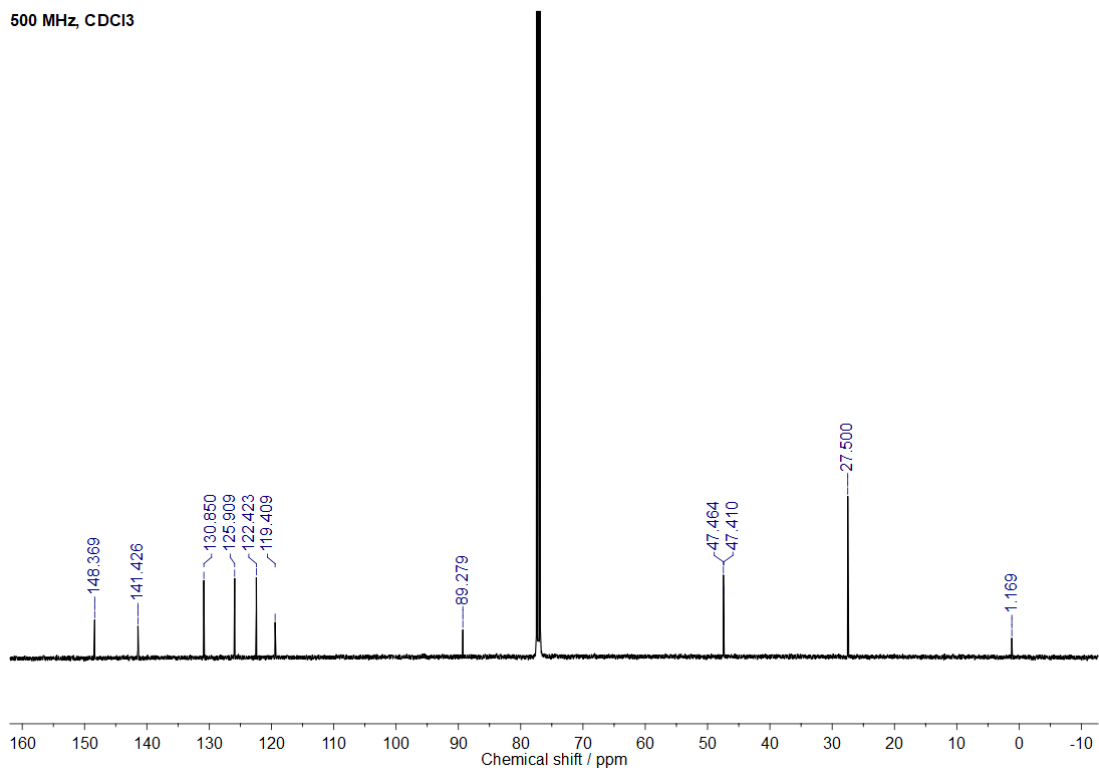
500 MHz, CDCl3

Figure S2. $^{13}C\{^{1}H\}$ NMR spectrum of **1** recorded in CDCl$_3$.
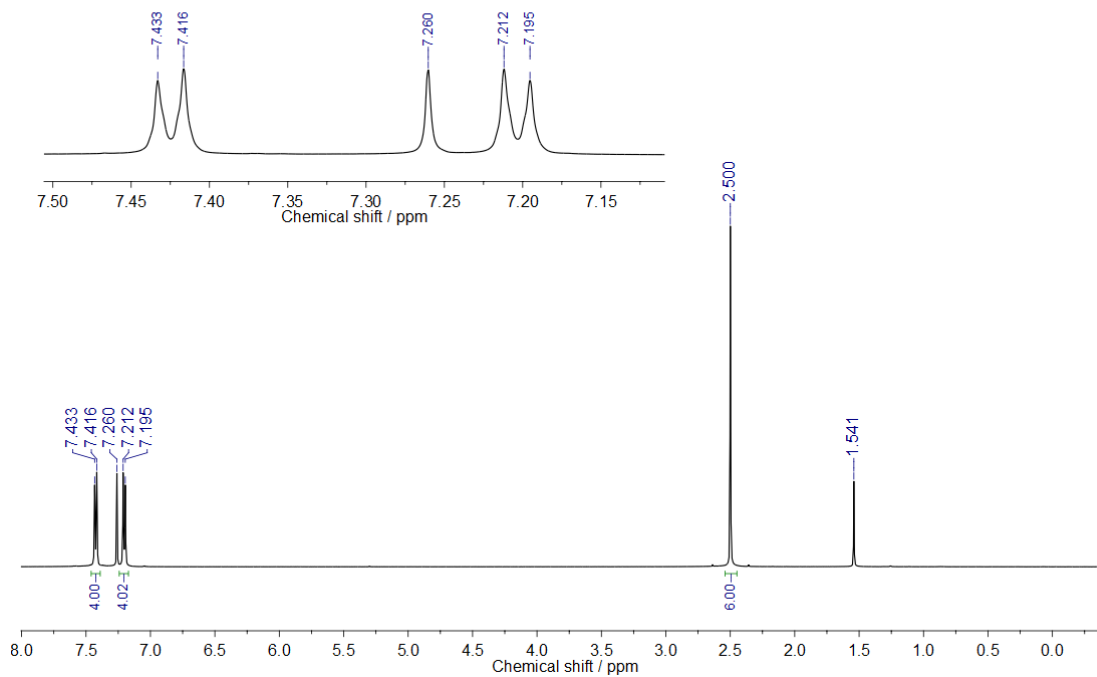
Figure S3. ¹H NMR spectrum of **2** recorded in CDCl₃.
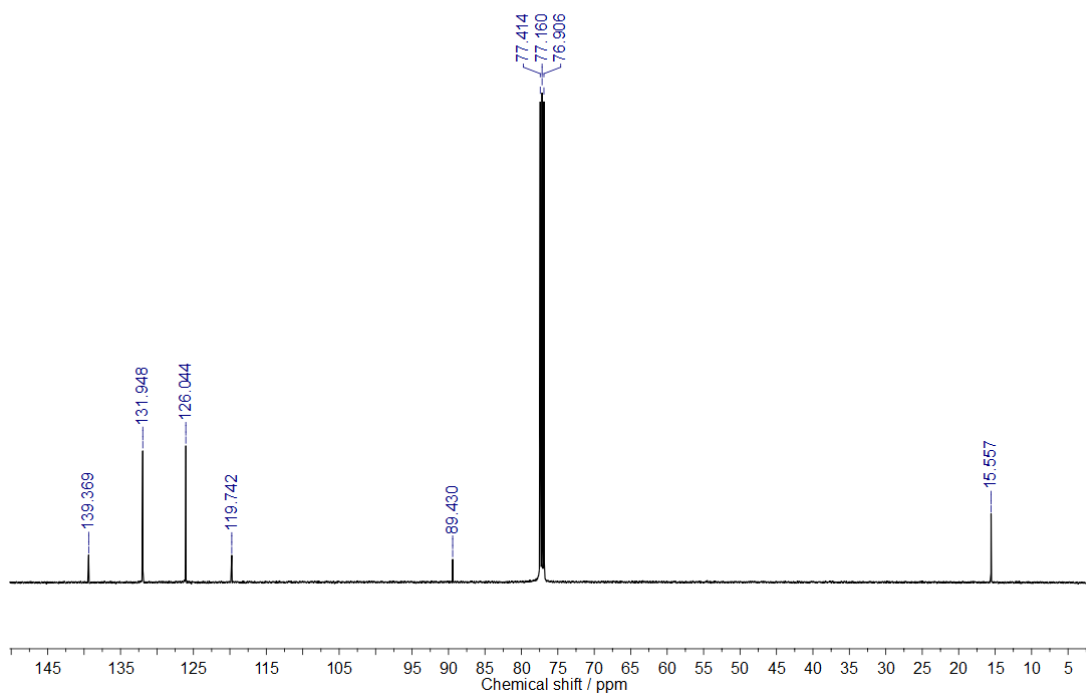
Figure S4. ¹³C{¹H} NMR spectrum of **2** recorded in CDCl₃.
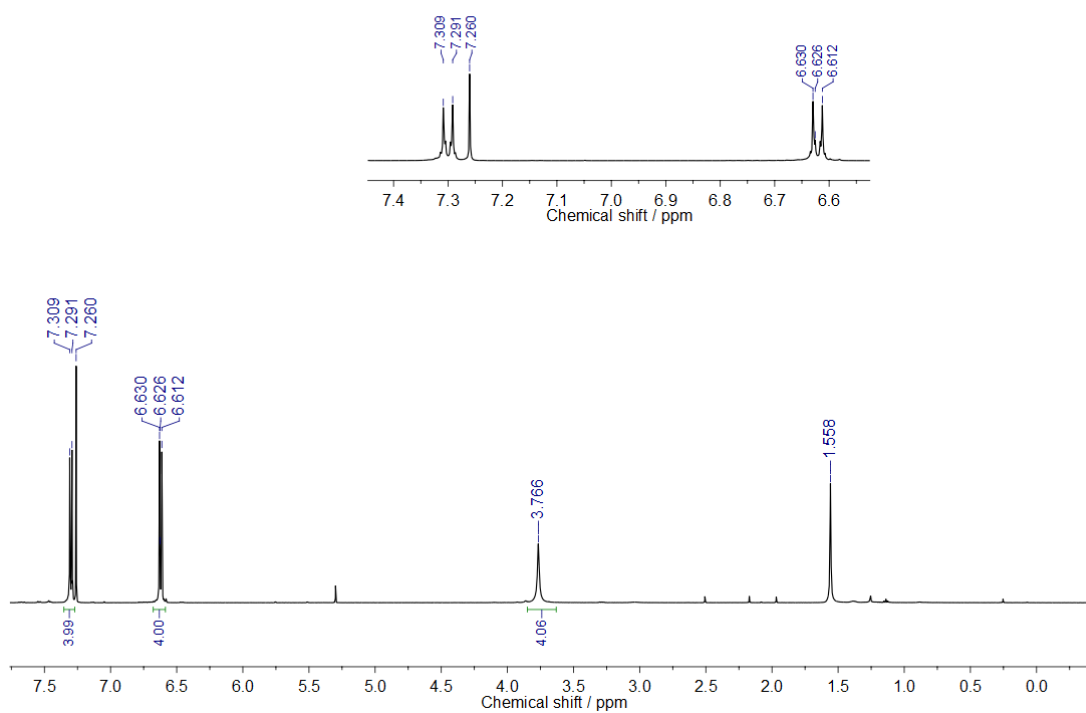
500 MHz, CDCl3

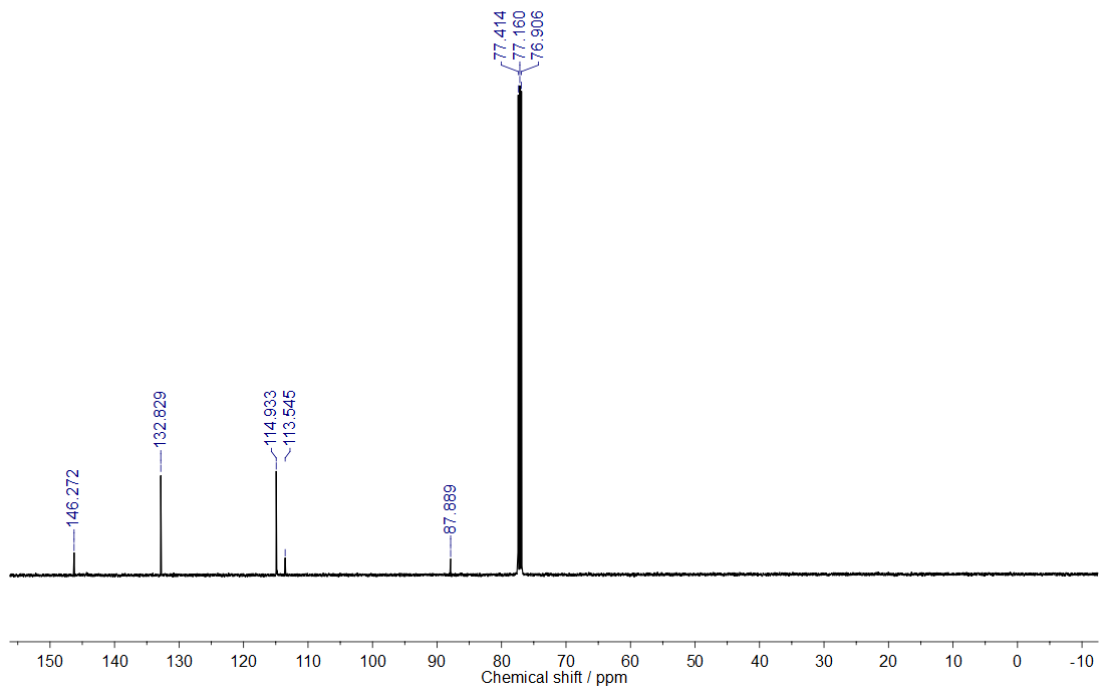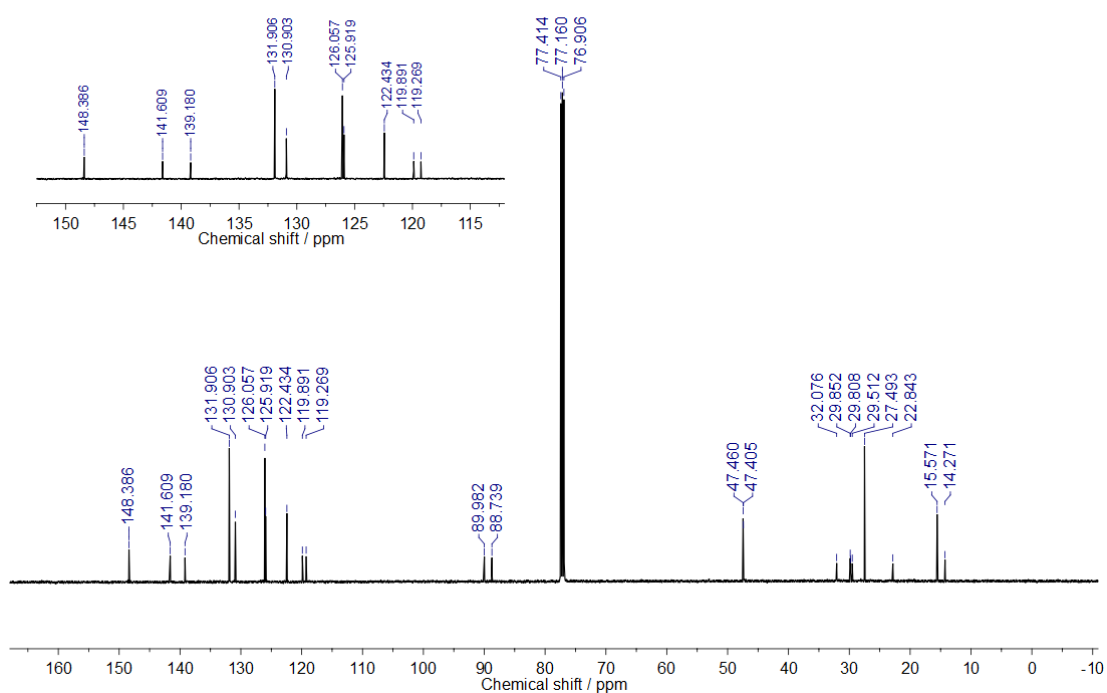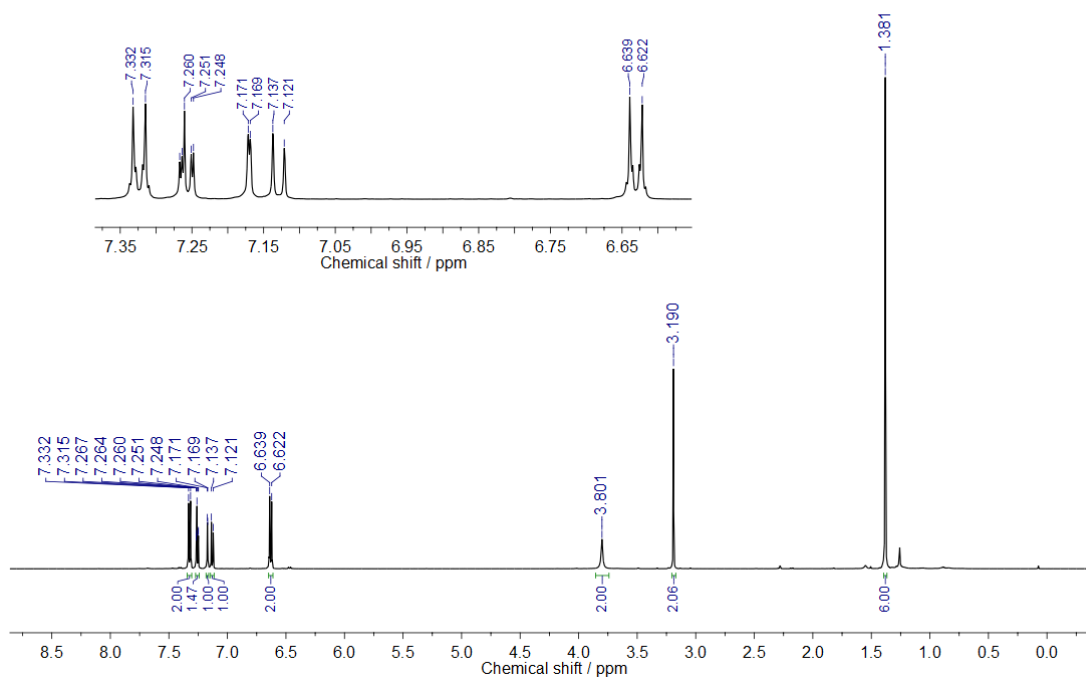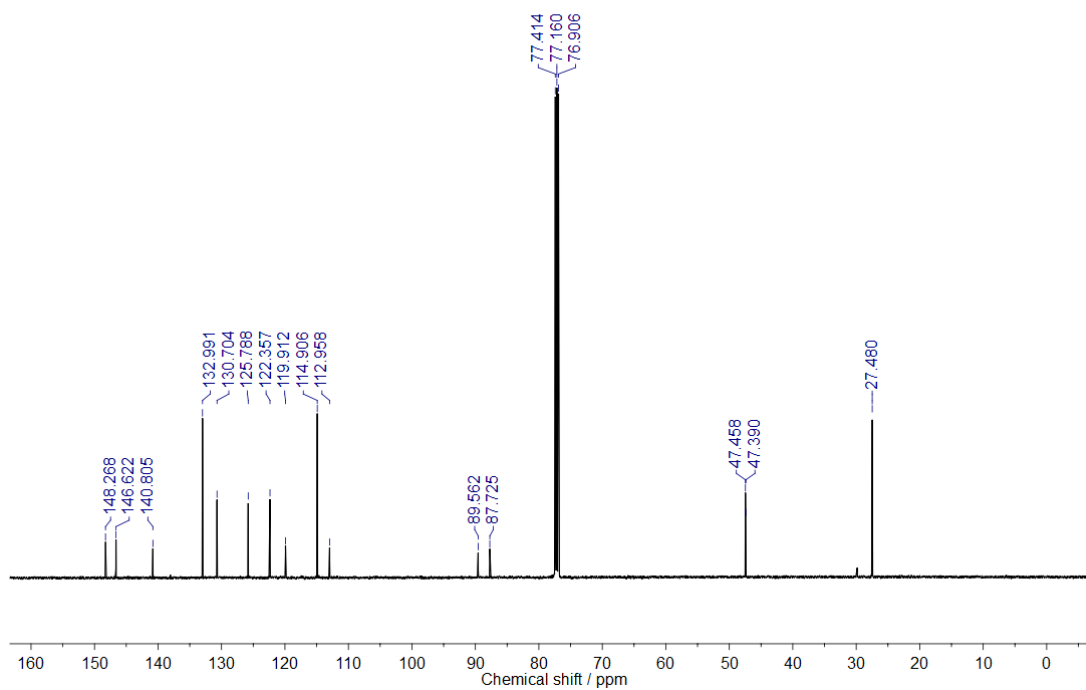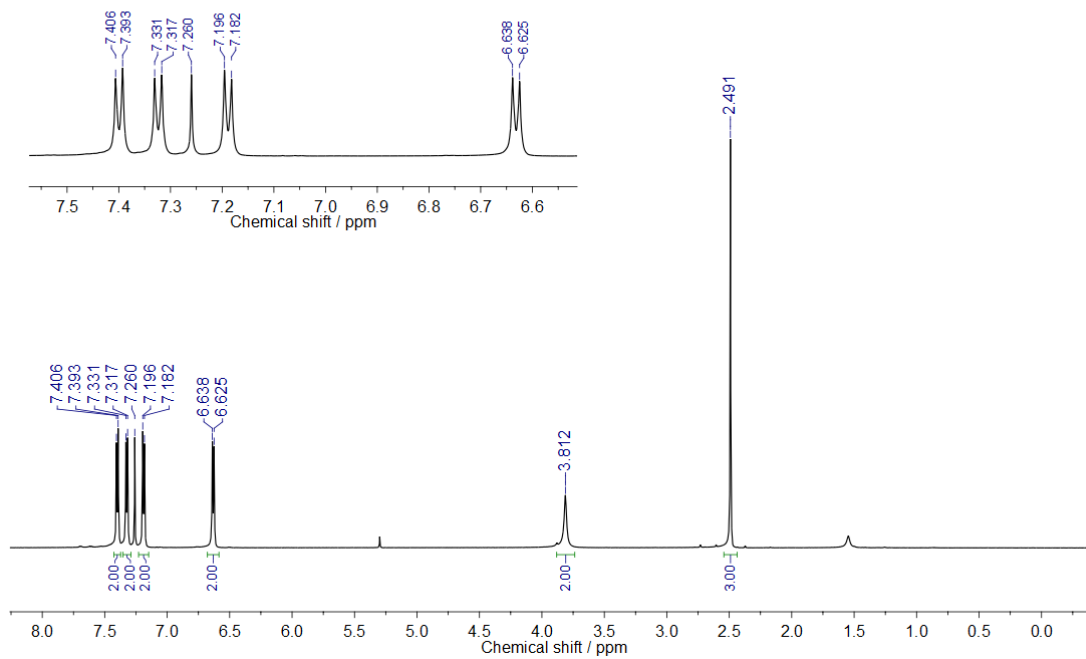**Figure S5**. ^{1}H NMR spectrum of **3** recorded in CDCl$_3$.
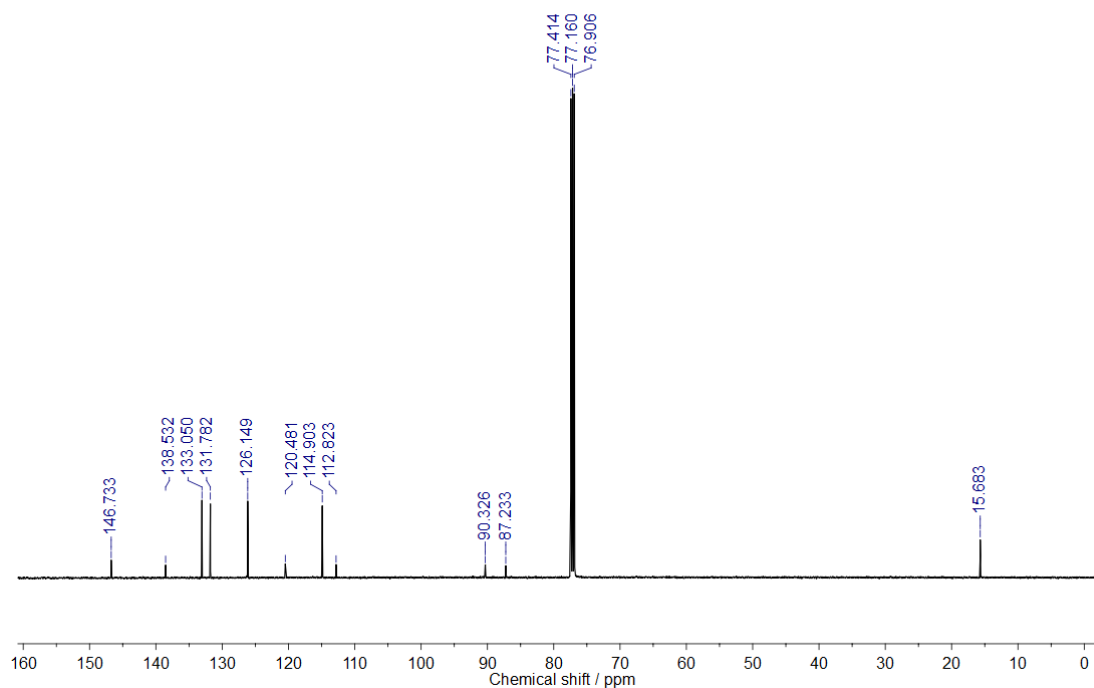
500 MHz, CDCl3

Figure S6. ^{13}C{^{1}H} NMR spectrum of **3** recorded in CDCl$_3$.
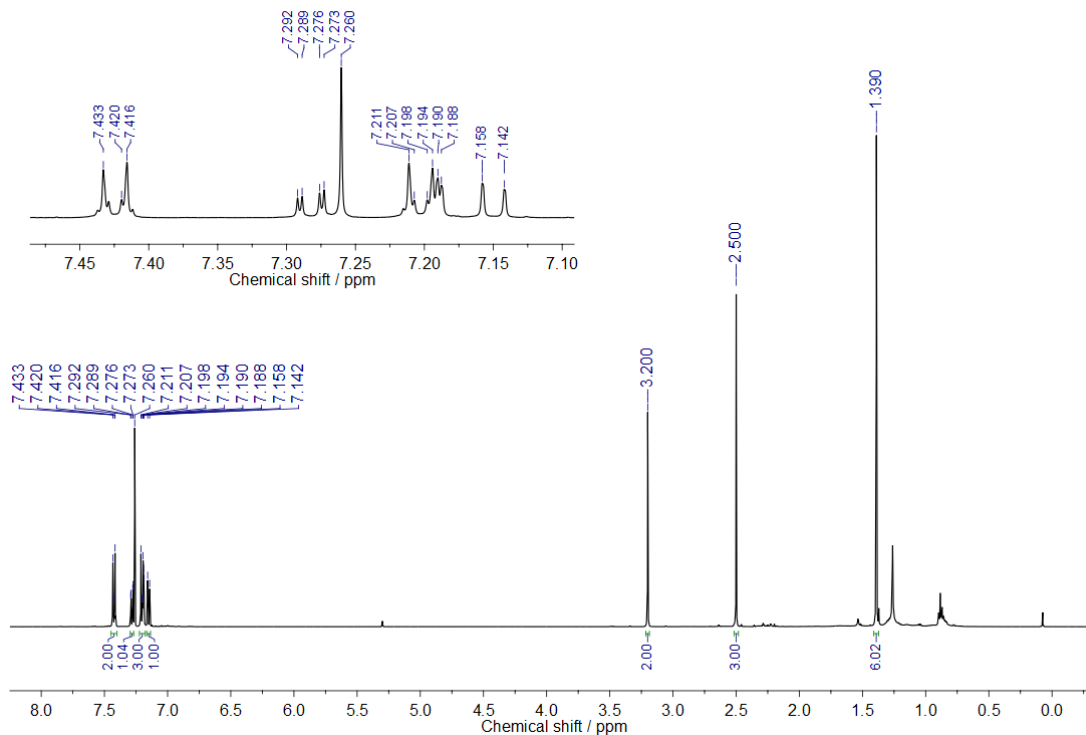
Figure S7. *¹H NMR spectrum of **5** recorded in CDCl₃.*

Figure S8. *¹³C{¹H} NMR spectrum of **5** recorded in CDCl₃.*

Figure S9. *^{1}H NMR spectrum of* **6** *recorded in CDCl$_3$.*

Figure S10. *^{13}C{^{1}H} NMR spectrum of* **6** *recorded in CDCl$_3$.*

500 MHz, CDCl3

7.406
7.393
7.331
7.317
7.260
7.196
7.182
6.638
6.625
2.491
3.812

2.00
2.00
2.00
2.00
2.00
3.00

Figure S11. ¹H NMR spectrum of **7** recorded in CDCl₃.

500 MHz, CDCl3

77.414
77.160
76.906
146.733
138.532
133.050
131.782
126.149
120.481
114.903
112.823
90.326
87.233
15.683

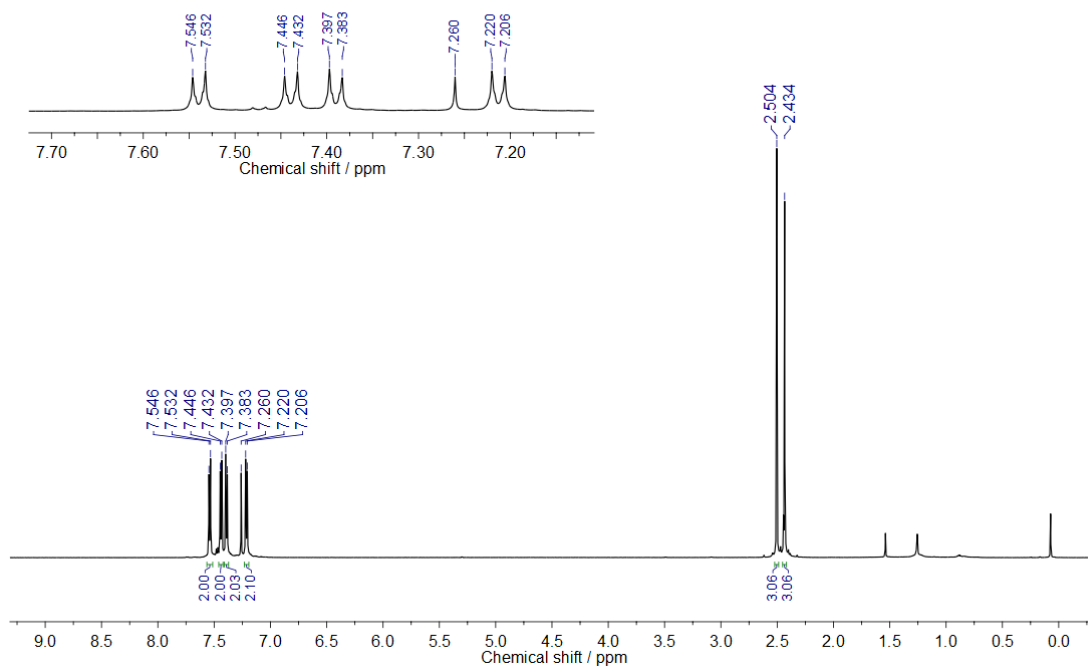**Figure S12**. ¹³C{¹H} NMR spectrum of **7** recorded in CDCl₃.

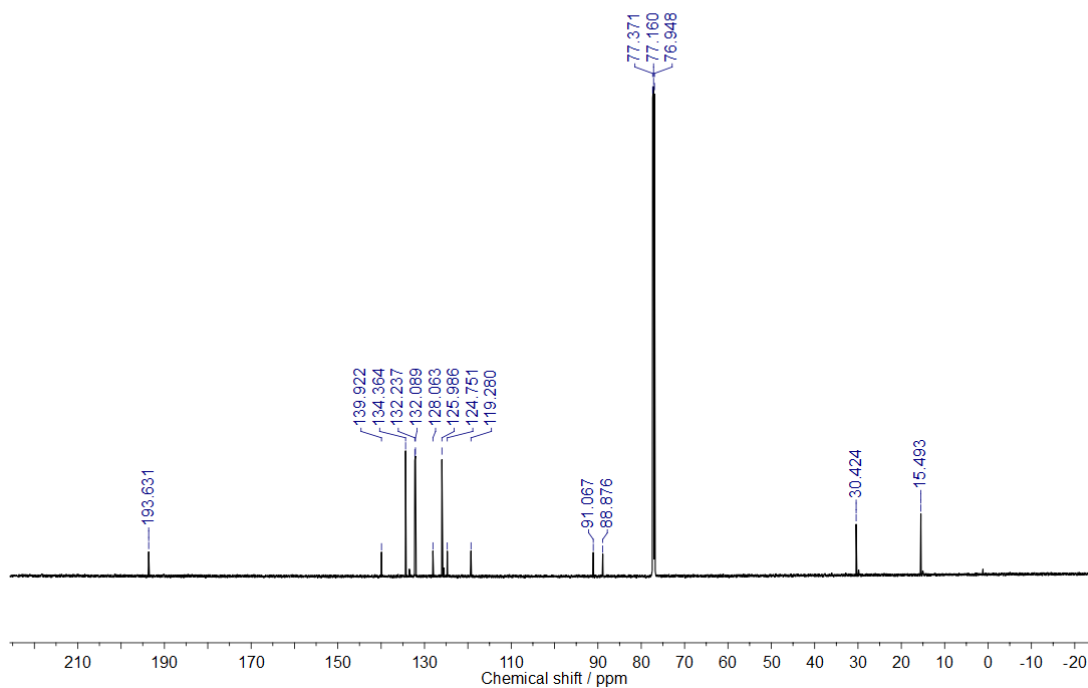**Figure S13**. ¹H NMR spectrum of **8** recorded in CDCl₃.

Figure S14. ¹³C{¹H} NMR spectrum of **8** recorded in CDCl₃.