Electronic Supplementary Information (ESI)

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Noncovalent interactions in the design of *bis*-azo dyes

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1. Materials and instrumentation

^{1}H NMR and ^{13}C NMR (300.1 and 75.5 MHz, respectively) spectra were recorded on a Bruker NMR-300 spectrometer. Chemical shifts are reported in ppm using residual signals of deuterium solvents as an internal standard ($CDCl_3$: δ 7.26 and 76.16 ppm, DMSO-d_6: δ 2.50 and 39.52 ppm for ^{1}H and ^{13}C respectively). Data are reported as follows: chemical shift, integration and multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet). Carbon, hydrogen, and nitrogen elemental analyses were carried out by the Microanalytical Service of the Instituto Superior Técnico. All of the synthetic work was performed in air and at room temperature. Electrospray mass spectra were carried out with an ion-trap instrument (Varian 500-MS LC Ion Trap Mass Spectrometer) equipped with an electrospray (ESI) ion source. The solutions in acetone were continuously introduced into the mass spectrometer source with a syringe pump at a flow rate of 10 μL/min. The drying gas temperature was maintained at 350 ºC and dinitrogen was used as nebulizer gas at a pressure of 35 psi. Scanning was performed from *m/z* = 50 to 1500. The UV-vis absorption spectra in the 200 − 700 nm region were recorded with a scan rate of 240 nm·min^{-1} by using a Lambda 35 UV-vis spectrophotometer (Perkin-Elmer) in 1.00 cm quartz cells at room temperature, with a concentration of **5**–**8** of $1.00 \cdot 10^{-6}$ mol L^{-1} in CH_2Cl_2, DMF or MeOH.

2. Synthesis of 1–4

The Schiff bases **1**–**4** were synthesized according to a reported method which was applied to the synthesis of (*E*)-1-(4-R-phenyl)-2-(2-nitrobenzylidene)hydrazones.[14] A mixture of 2,3,5,6-tetrafluoroterephthalaldehyde (10 mmol), CH_3COONa (0.82 g), ethanol (50 mL) and corresponding (*para*-substituted phenyl)hydrazine (10.2 mmol) was refluxed at 80 °C with stirring for 2 h. The reaction mixture was cooled to room temperature and water (50 mL) was added to give a precipitate of crude product, which was filtered off, washed with diluted ethanol (1:1 with water) and dried in vacuo of a rotary evaporator.

1: yellow solid (88%). Anal. Calcd for $C_{22}H_{18}F_4N_4O_2$ (*M* = 446.41): C, 59.19; H, 4.06; N, 12.55; found: C, 59.14; H, 4.01; N, 12.48 %. ^{1}H NMR (300 MHz, DMSO-d_6): δ 3.80 (s, 6H, 2OCH_3), 6.95-6.97 (m, 4H, 2Ar), 7.06-7.08 (m, 4H, 2Ar), 7.85 (s, 2H, 2CH), 10.83 (s, 2H, 2NH). ^{13}C NMR (75 MHz, DMSO-d_6): δ 60.63, 118.64, 128.94, 129.80, 135.34, 141.41, 141.99, 152.11. ESI-MS: *m/z*: 447.53 $[M+H]^+$.

2: yellow solid (87%). Anal. Calcd for $C_{22}H_{18}F_4N_4$ (*M* = 414.41): C, 63.76; H, 4.38; N, 13.52; found: C, 63.73; H, 4.34; N, 13.49 %. ^{1}H NMR (300 MHz, DMSO-d_6): δ 2.24 (s, 6H, 2CH_3), 6.98-7.01 (m, 4H, 2Ar), 7.08-7.13 (m, 4H, 2Ar), 7.87 (s, 2H, 2CH), 10.86 (s, 2H, 2NH). ^{13}C NMR (75 MHz, DMSO-d_6): δ 20.31, 112.85, 122.61, 129.81, 133.68, 138.15, 141.35, 141.94. ESI-MS: *m/z*: 415.60 $[M+H]^+$.

3: yellow solid (87%). Anal. Calcd for $C_{20}H_{14}F_4N_4$ (M = 386.35): C, 62.18; H, 3.65; N, 14.50; found: C, 62.16; H, 3.64; N, 14.49 %. ^{1}H NMR (300 MHz, DMSO-d_6): δ 6.87-6.91 (t, 3H, Ph), 7.19-7.22 (d, 4H, 2Ph), 7.27-7.33 (t, 3H, Ph), 7.97 (s, 2H, 2CH), 10.11 (s, 2H, 2NH). ^{13}C NMR (75 MHz, DMSO-d_6): δ 112.69, 114.28, 120.44, 129.20, 141.04, 142.42, 144.41. ESI-MS: *m/z*: 387.30 $[M+H]^+$.

4: yellow solid (85%). Anal. Calcd for $C_{20}H_{12}F_6N_4$ (M = 422.33): C, 56.88; H, 2.86; N, 13.27; found: C, 56.85; H, 3.00; N, 13.23 %. ^{1}H NMR (300 MHz, DMSO-d_6): δ 7.08-7.11 (m, 4H, 2Ar), 7.19-7.21 (m, 4H, 2Ar), 7.94 (s, 2H, 2CH), 10.28 (s, 2H, 2NH). ^{13}C NMR (75 MHz, DMSO-d_6): δ 124.28, 124.83, 126.09, 151.55, 153.30, 156.03, 166.85. ESI-MS: *m/z*: 423.25 $[M+H]^+$.

3. $^{1}H/^{13}C$ NMR spectra of 1-4

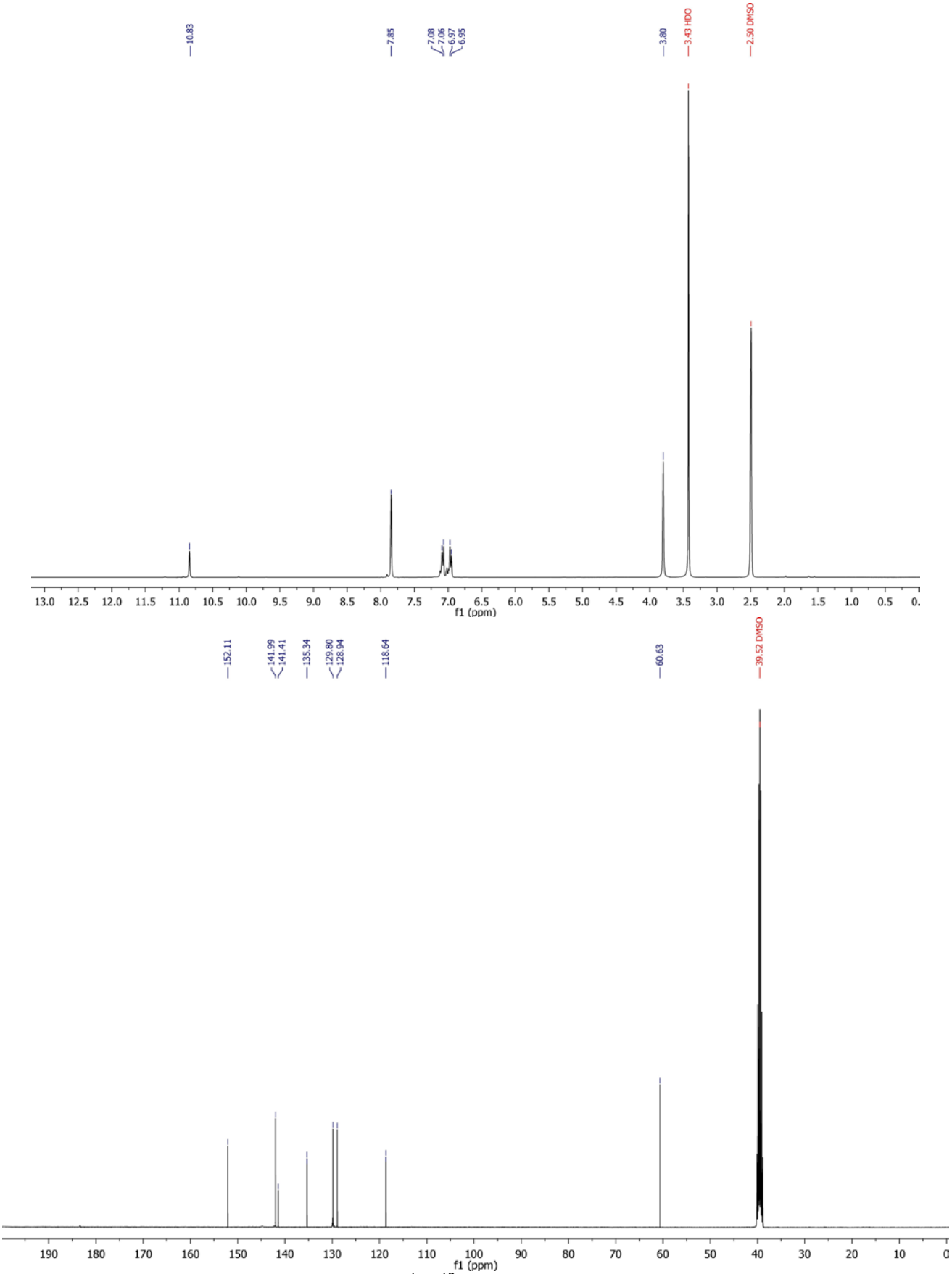


Figure S1. $^{1}H/^{13}C$ NMR spectra of **1.**

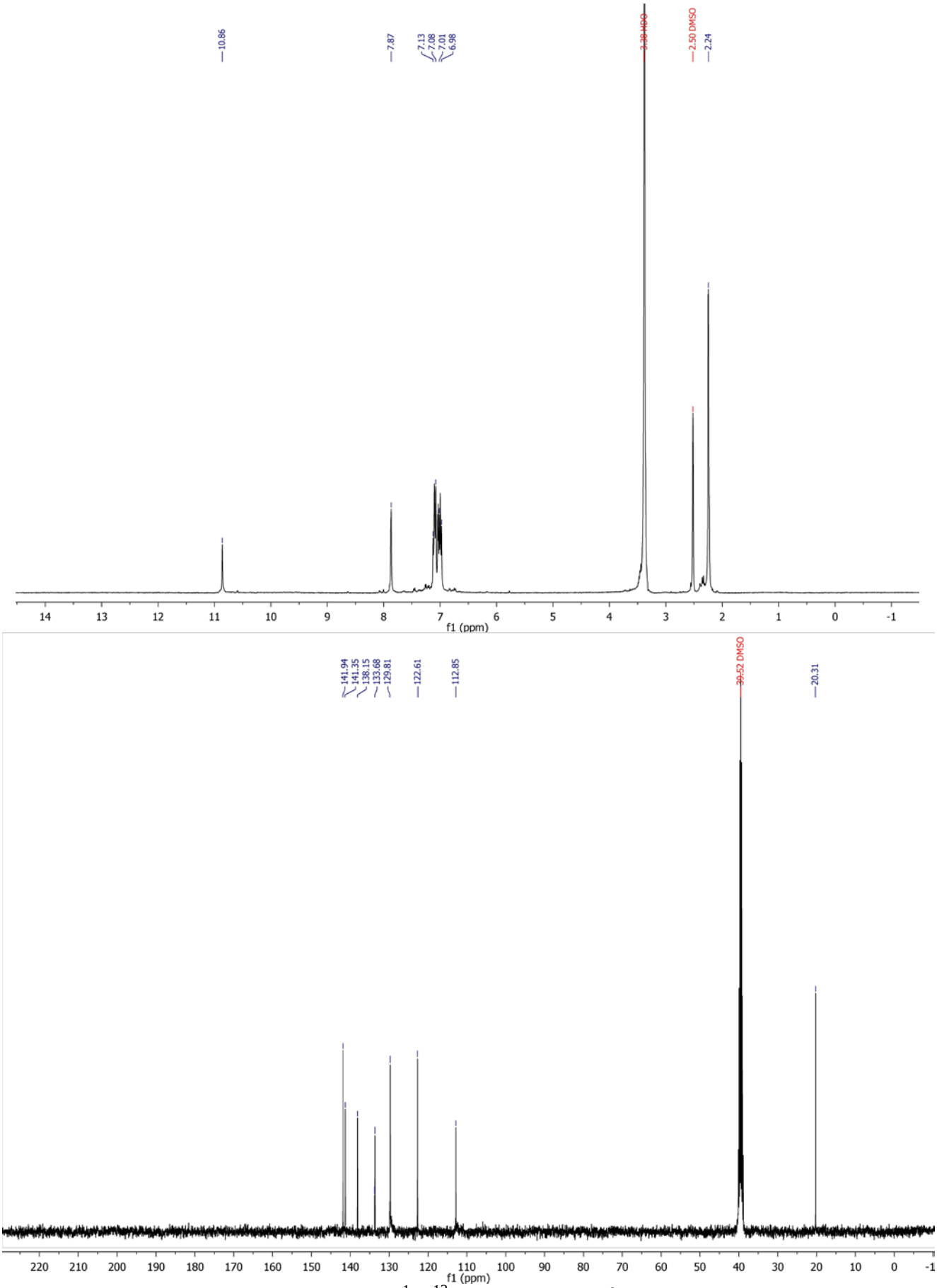


Figure S2. $^{1}H/^{13}C$ NMR spectra of **2.**

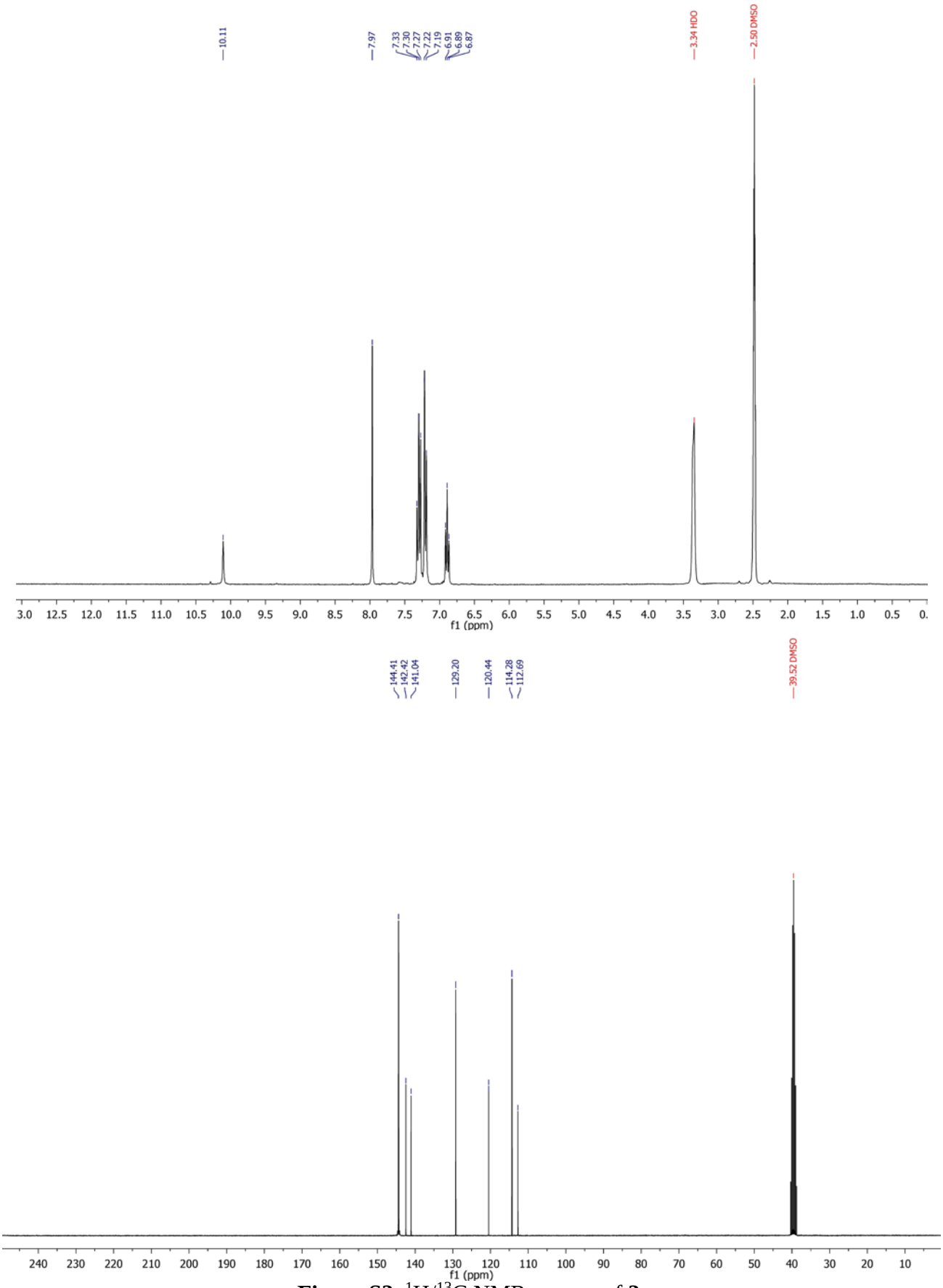


Figure S3. $^{1}H/^{13}C$ NMR spectra of **3.**

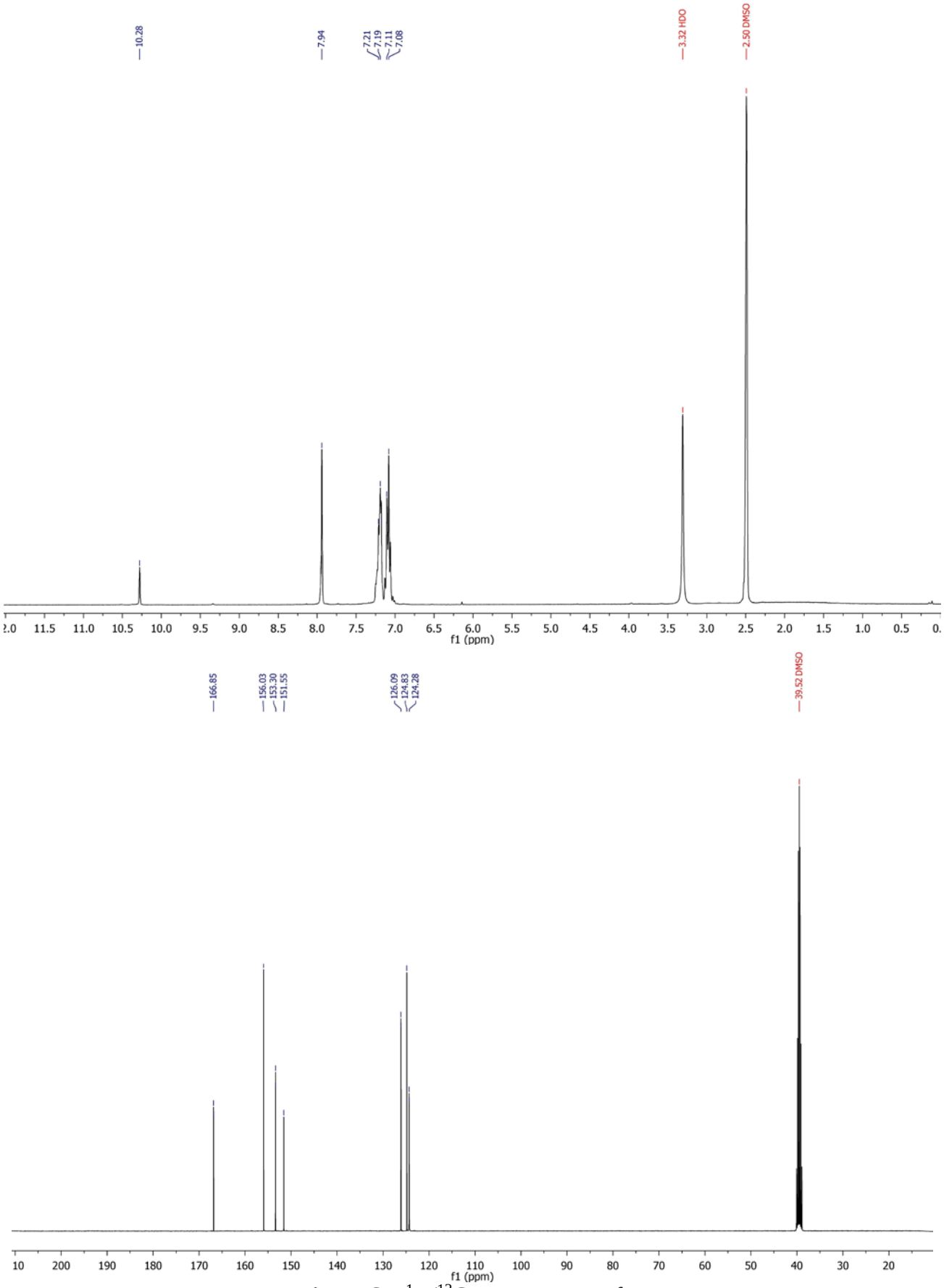


Figure S4. $^{1}H/^{13}C$ NMR spectra of **4.**

4. Synthesis of 5–8

The *bis*-azo dyes **5**–**8** were synthesized according to a reported method previously applied to (*E*)-1-(4-substituentphenyl)-2-(2,2-dichloro-1-(2-nitrophenyl)vinyl)diazene.[14] A 20 mL screw neck vial was charged with DMSO (10 mL), **1**, **2**, **3** or **4** (1 mmol), tetramethylethylenediamine (TMEDA) (295 mg, 2.5 mmol), CuCl (2 mg, 0.02 mmol) and CCl_4 (20 mmol, 10 eq.). After 1-3 h (until TLC analysis showed complete consumption of the corresponding Schiff base) the reaction mixture was poured into a ~0.01 M solution of HCl (100 mL, ~pH=2-3), and extracted with dichloromethane (3×20 mL). The combined organic phase was washed with water (3×50 mL), brine (30 mL), dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel using appropriate mixtures of hexane and dichloromethane (3/1-1/1), to give corresponding *bis*-azo dyes **5**–**8**.

5: orange solid (60%). Anal. Calcd for $C_{24}H_{14}Cl_4F_4N_4O_2$ (M = 608.20): C, 47.40; H, 2.32; N, 9.21; found: C, 47.36; H, 2.28; N, 9.16 %. ^{1}H NMR (300 MHz, $CDCl_3$): δ 3.88 (s, 6H, $2OCH_3$), 6.94-7.00 (m, 4H, 2Ar), 7.77-7.84 (m, 4H, 2Ar). ^{13}C NMR (75 MHz, $CDCl_3$): δ 54.80, 113.48, 115.06, 124.87, 124.90, 135.67, 143.95, 145.97, 162.32. ESI-MS: *m/z*: 609.14 $[M+H]^+$.

6: orange solid (58%). Anal. Calcd for $C_{24}H_{14}Cl_4F_4N_4$ (M = 576.20): C, 50.03; H, 2.45; N, 9.72; found: C, 53.55; H, 3.29; N, 12.46 %. ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.41 (s, 6H, $2CH_3$), 7.23-7.29 (m, 4H, 2Ar), 7.67-7.74 (m, 4H, 2Ar). ^{13}C NMR (75 MHz, $CDCl_3$): δ 21.80, 116.29, 123.78, 123.79, 129.98, 130.01, 138.12, 141.47, 143.44. ESI-MS: *m/z*: 577.24 $[M+H]^+$.

7: red solid (64%). Anal. Calcd for $C_{22}H_{10}Cl_4F_4N_4$ (M = 548.14): C, 48.21; H, 1.84; N, 10.22; found: C, 52.15; H, 2.78; N, 13.00 %. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.48-7.52 (d, 4H, 2Ar), 7.79-7.82 (t, 3H, Ar) 7.82-7.86 (t, 3H, 2Ar). ^{13}C NMR (75 MHz, $CDCl_3$): δ 114.19, 123.75, 129.32, 129.34, 130.04, 132.50, 141.49, 145.08. ESI-MS: *m/z*: 549.12 $[M+H]^+$.

8: orange solid (56%). Anal. Calcd for $C_{22}H_8Cl_4F_6N_4$ (M = 584.12): C, 45.24; H, 1.38; N, 9.59; found: C, 45.19; H, 1.50; N, 9.74 %. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.20-7.23 (m, 4H, 2Ar), 7.85-7.91 (m, 4H, 2Ar). ^{13}C NMR (75 MHz, $CDCl_3$): δ 112.42, 116.59, 125.84, 125.96, 130.11, 139.89, 143.05, 162.47. ESI-MS: *m/z*: 585.18 $[M+H]^+$.

5. $^{1}H/^{13}C$ NMR spectra of 5-8

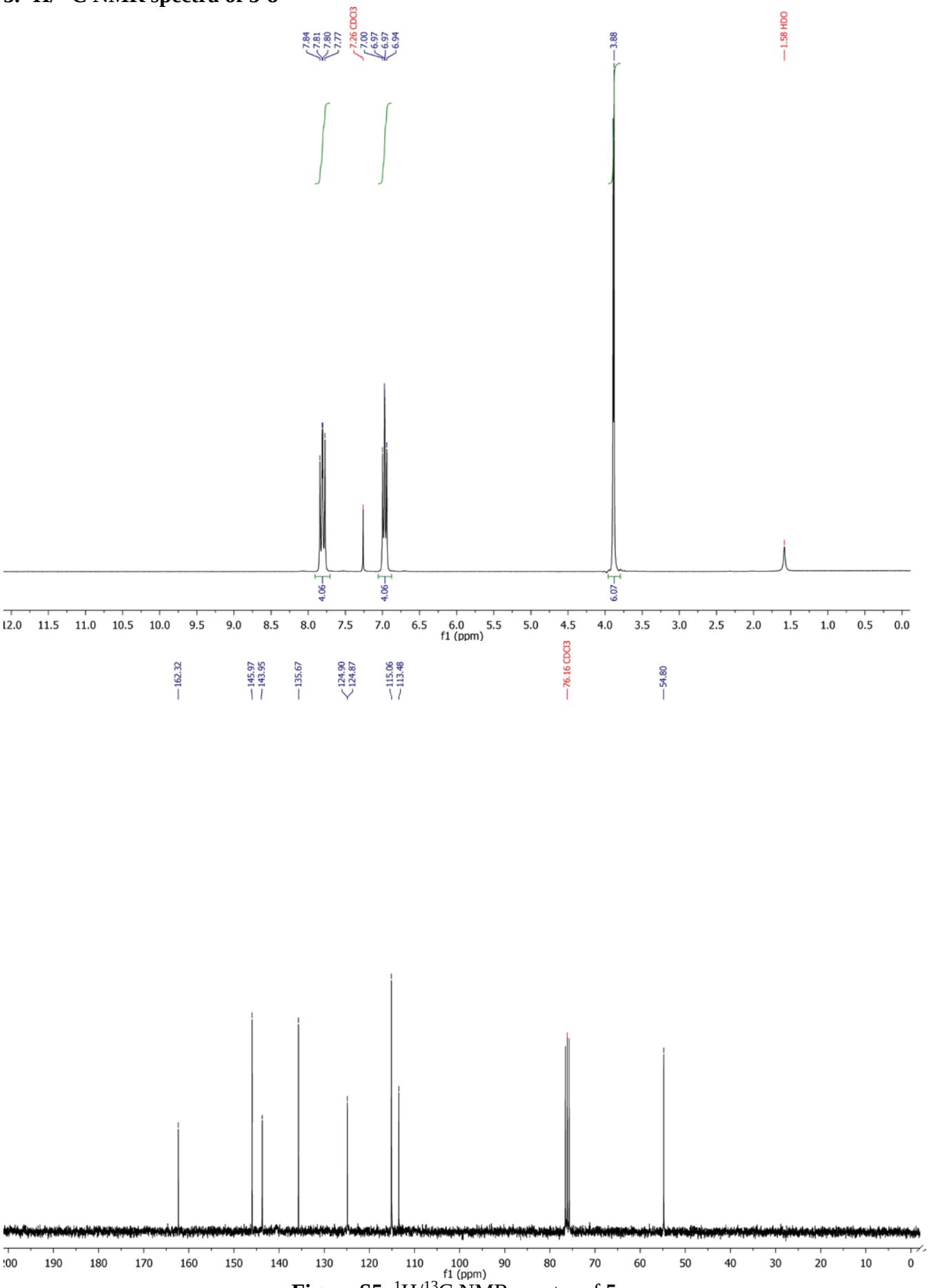


Figure S5. $^{1}H/^{13}C$ NMR spectra of **5.**

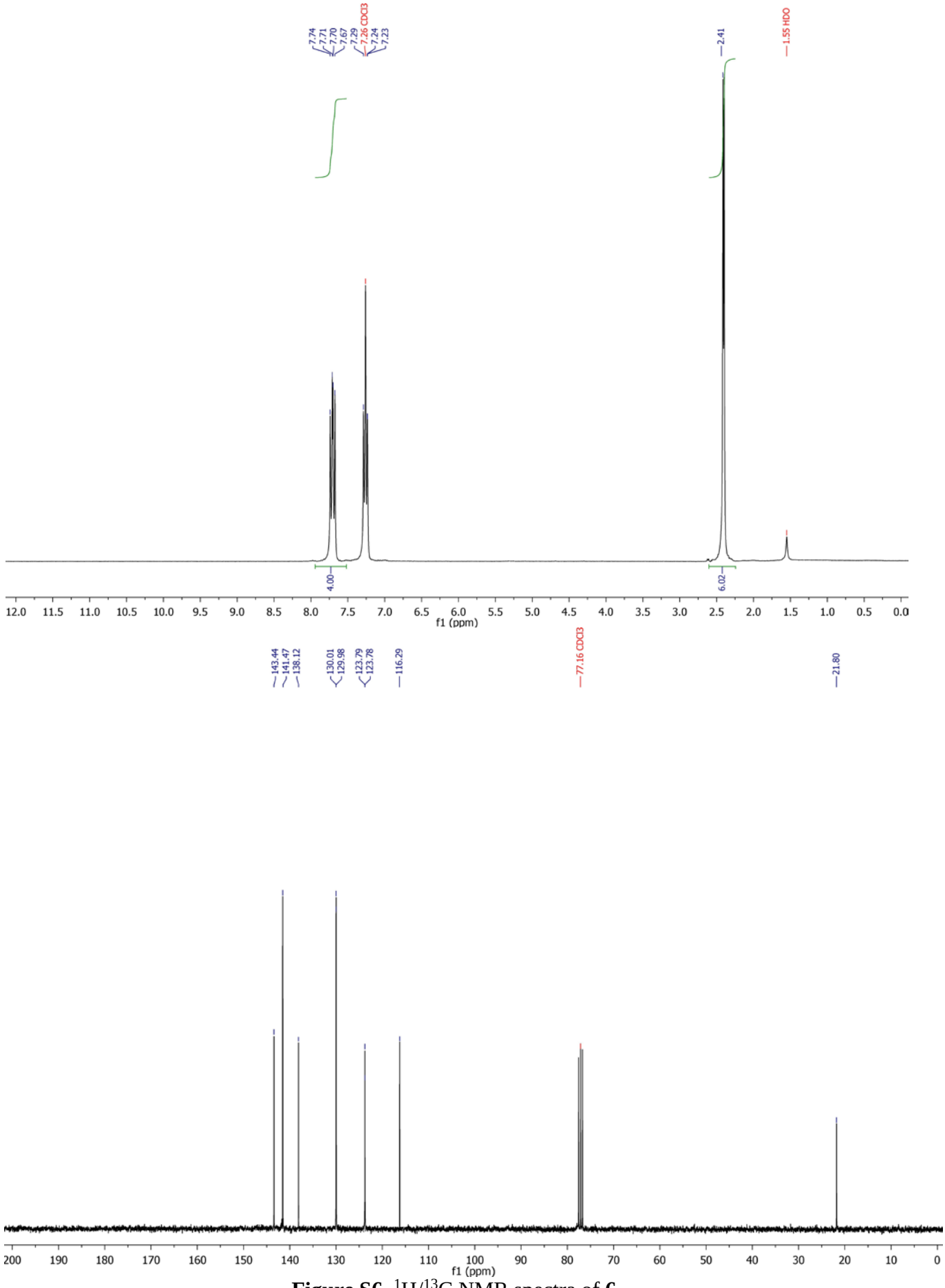


Figure S6. $^{1}H/^{13}C$ NMR spectra of **6.**

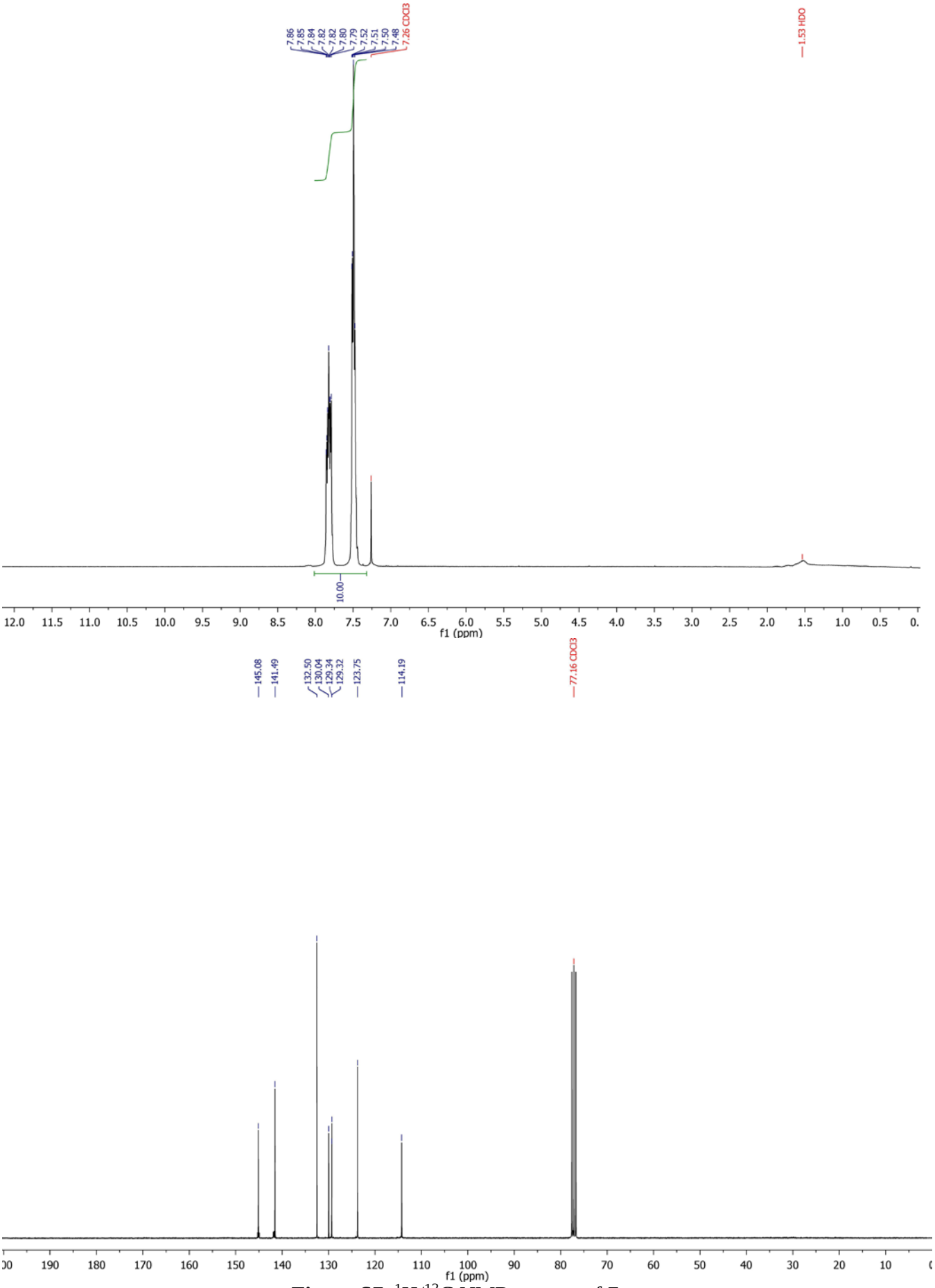


Figure S7. $^{1}H/^{13}C$ NMR spectra of **7.**

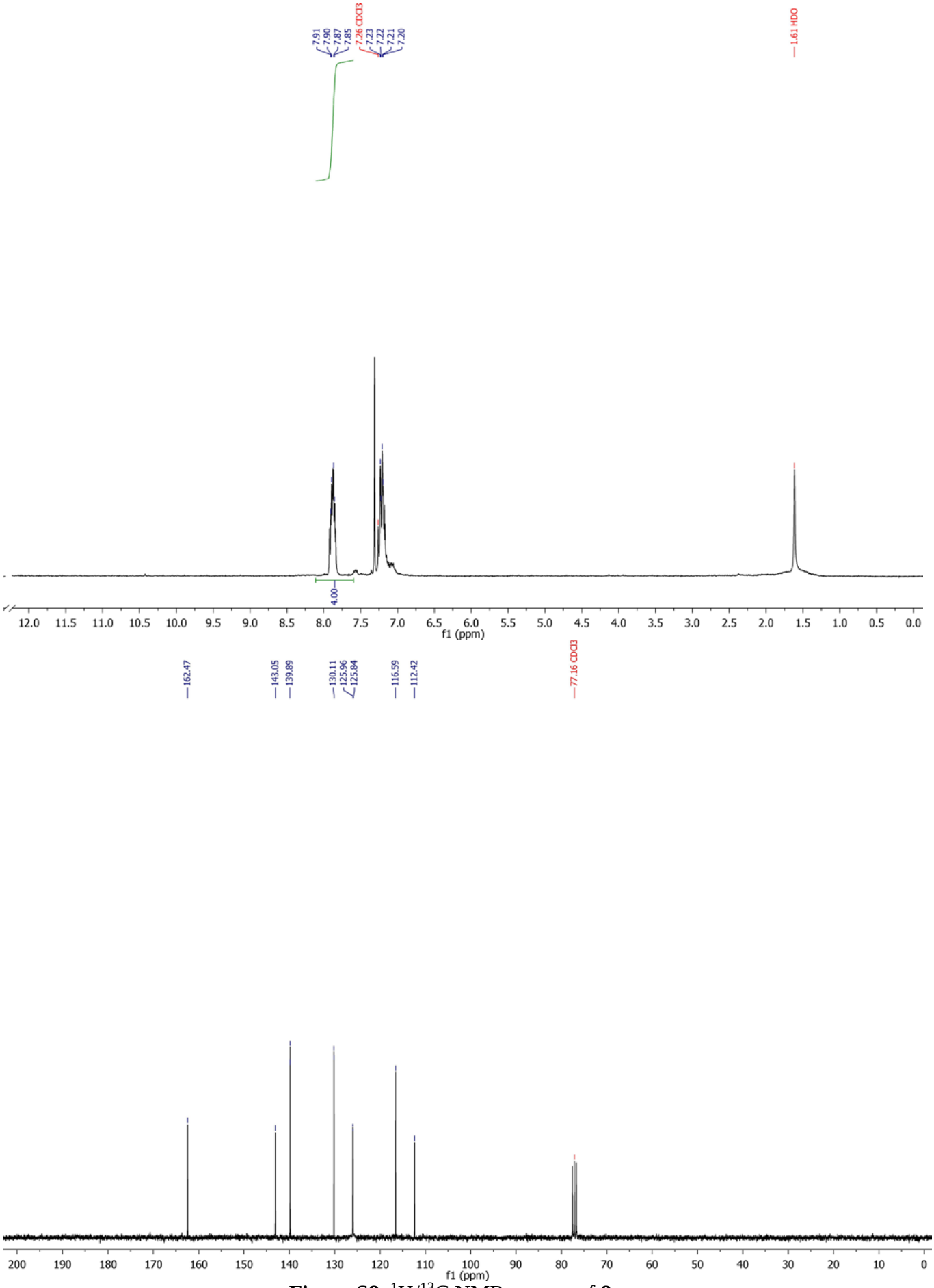


Figure S8. $^{1}H/^{13}C$ NMR spectra of **8.**

6. X-ray analysis

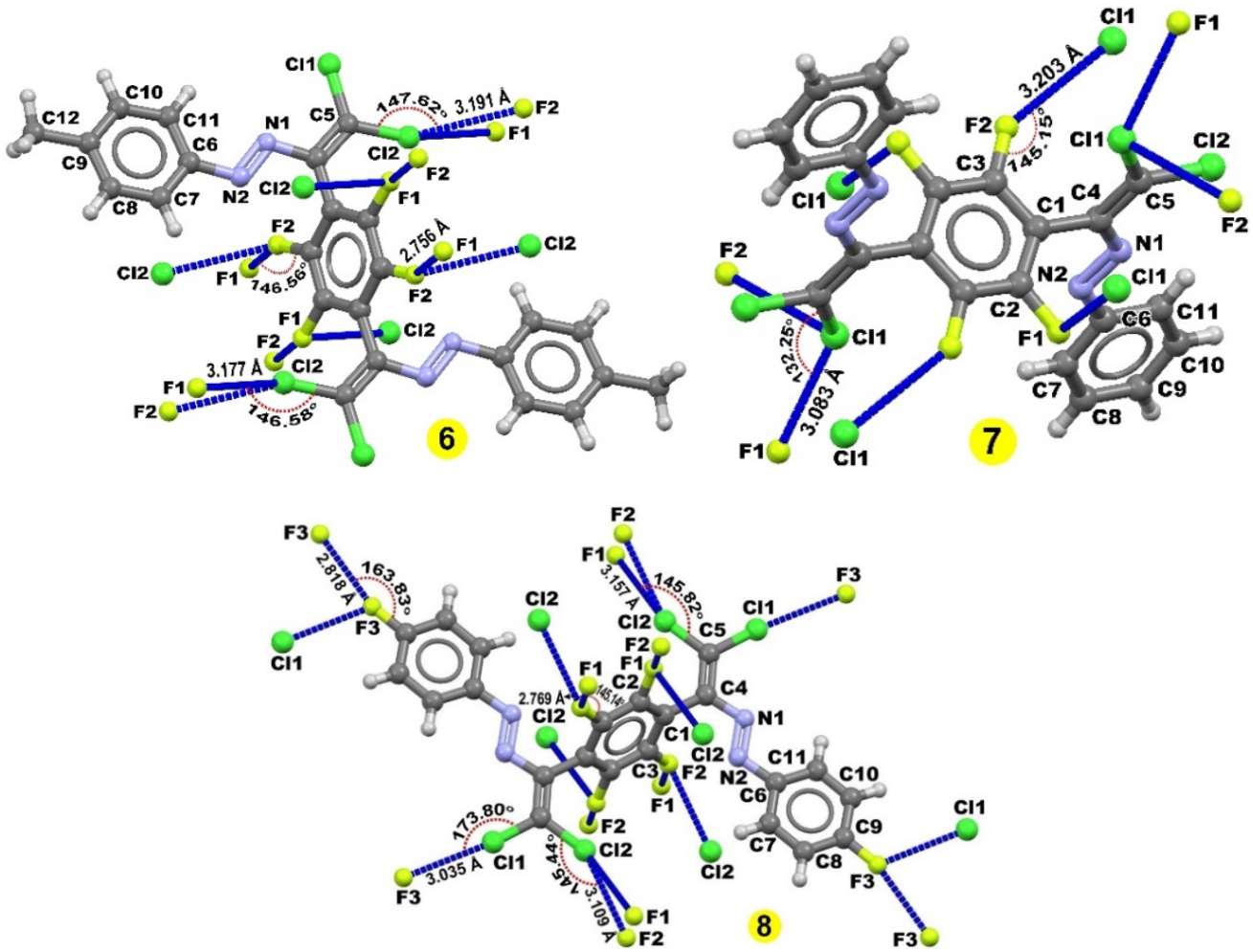
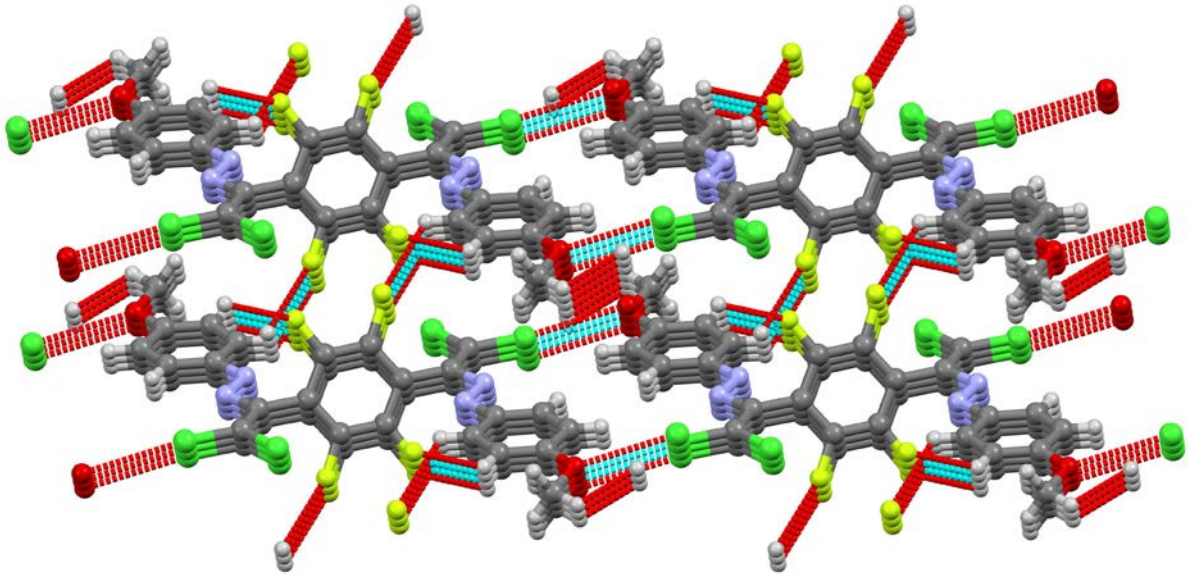
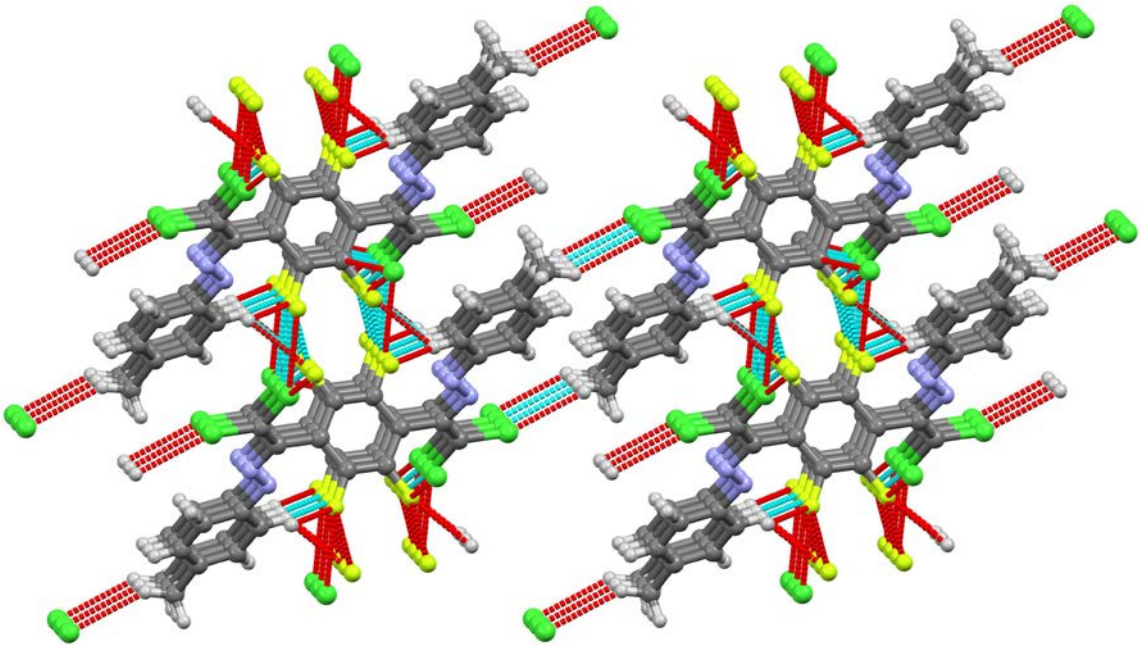


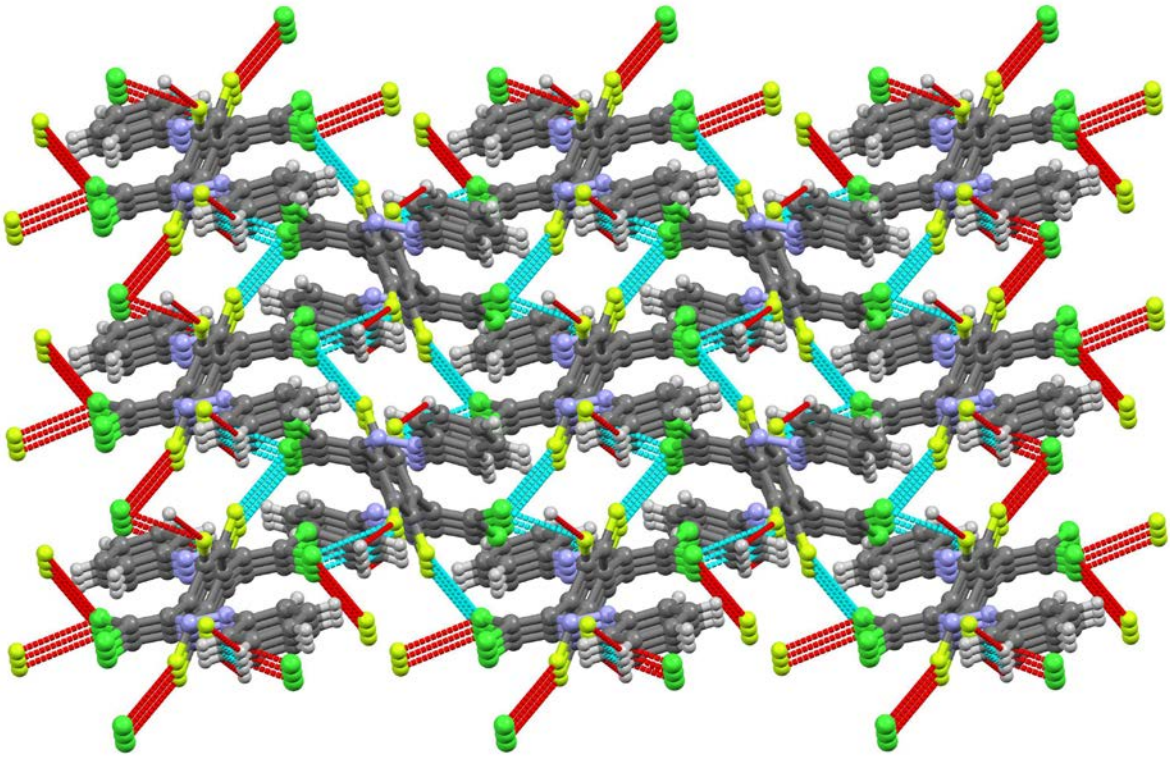
Figure S9. Weak intermolecular interactions in **6**, **7** and **8**.



5



6



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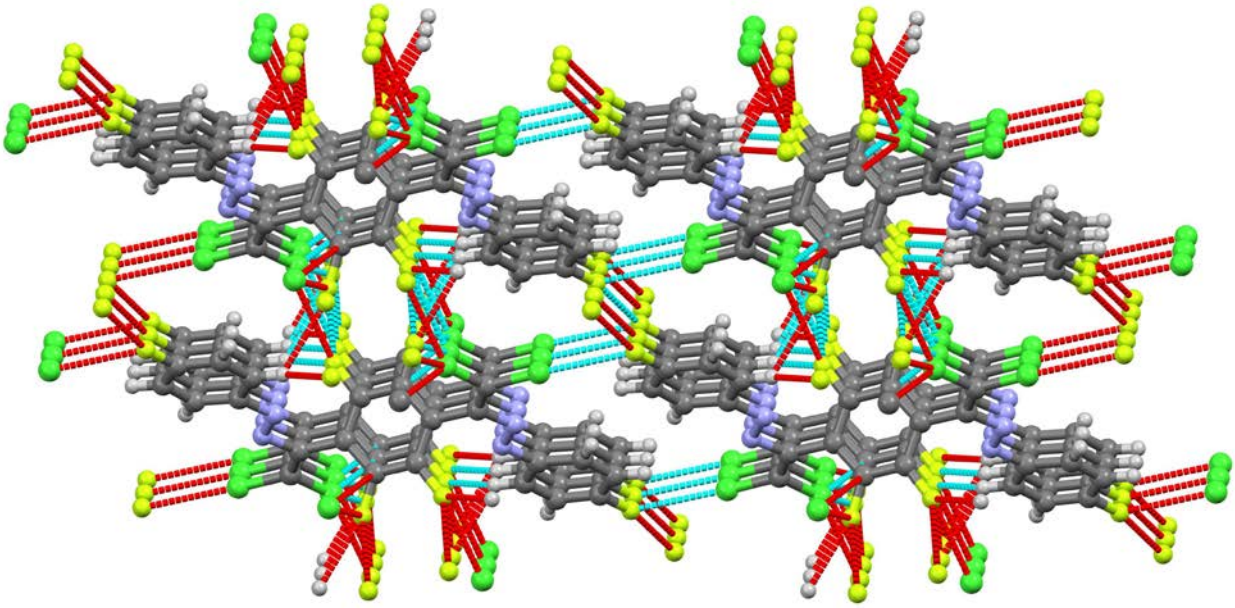

8

Figure S10. Packing diagrams of **5**–**8**.

Table S1. Crystallographic data and structure refinement details for **5-8**.

	5	**6**	**7**	**8**
Empirical formula	$C_{24}H_{14}Cl_4F_4N_4O_2$	$C_{24}H_{14}Cl_4F_4N_4$	$C_{22}H_{10}Cl_4F_4N_4$	$C_{22}H_8Cl_4F_6N_4$
fw	608.19	576.19	548.14	584.12
Temperature (K)	150(2)	150(2)	296(2)	150(2)
Cryst. Syst.	Triclinic	Triclinic	Monoclinic	Triclinic
Space group	P-1	P-1	$P2_1/c$	P-1
a (Å)	6.9129(9)	5.9278(9)	12.2519(4)	5.9287(4)
b (Å)	7.2480(9)	7.2851(11)	7.2378(3)	7.2856(5)
c (Å)	14.7369(19)	15.889(3)	13.8051(5)	14.8040(9)
α, °	76.471(5)	97.953(5)	90	97.067(2)
β, °	81.089(5)	97.431(5)	112.020(10)	95.028(2)
γ, °	64.077(5)	111.124(4)	90	112.098(2)
V (Å^3)	644.50(15)	621.87(17)	1134.89(7)	581.70(7)
Z	1	1	2	1
ρ_{calc} *(g cm^{-3})*	1.567	1.539	1.604	1.667
μ(Mo Kα) (mm^{-1})	0.519	0.528	0.574	0.577
F (000)	306	290	548	290
R1[a] *($I \geq 2\sigma$)*	0.0418	0.0390	0.0310	0.0324
wR2[b] *($I \geq 2\sigma$)*	0.0966	0.0812	0.0875	0.0766
GOOF	1.007	1.007	1.064	1.034

[a] $R1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$. [b] $wR2 = [\Sigma[w(F_o^2 - F_c^2)^2]/ \Sigma[w(F_o^2)^2]]^{1/2}$.

Table S2. Dihedral angles in **5-8**.

5	F···Cl repulsive <C2C1C4C5 69.9(3)	<C2 C1 C4 N1 -110.9(3)
	F···N repulsive <C3C1C4N1 65.6(4)	<C3C1C4C5 -113.5(3)
6	F···Cl repulsive <C2C1C4C5 -64.7(4)	<C2C1C4N1 115.4(3)
	F···N repulsive <C3C1C4N1 -61.8(3)	<C3C1C4C5 118.1(3)
7	F···Cl repulsive <C3 1 4 5 -64.50(19)	<C3C1C4N1 117.35(15)
	F···N repulsive <C2 1 4 1 -64.28(19)	<C2C1C4C5 113.88(16
8	F···Cl repulsive <C2C1C4C5 -66.0(2)	<C2C1C4N1 114.16(18)
	F···N repulsive <C3C1C4N1 -62.3(2)	<C3C1C4C5 117.56(19)

Table S3. Hydrogen bond interactions in **5-8**.

Compound	D−H···A	Distances (Å)			Angles (º)
		D−H	H···A	D···A	D−H···A
5	C(8)-H(8)...F(2)	0.95	2.50	3.255(3)	137.4
	C(2)-H(7)...F(1)	0.95	2.55	3.177 (3)	157.2
6	C(7)-H(7)...F(1)	0.95	2.60	3.265(3)	127.1
	C(7)-H(7)...F(2)	0.95	2.59	3.389(3)	141.5
	C(12)-H(12A)...Cl(1)	0.98	2.87	3.734(3)	148.0
7	C(9)-H(9)...Cl(1)	0.93	3.09	3.814(2)	136.5
	C(7)-H(7)...Cl(2)	0.93	3.07	3.694(2)	125.6
	C(9)-H(9)...F(2)	0.93	2.74	3.612(2)	156.6
	C(10)-H(10)…F(1)	0.93	2.63	3.364(3)	136.5
8	C(10)-H(10)…Cl(1)	0.95	3.02	3.731(2)	132.4
	C(7)-H(7)...F(1)	0.95	2.57	3.241(2)	127.4
	C(7)-H(7)...F(2)	0.95	2.54	3.302(2)	137.5

Table S4. Halogen bonding parameters for **5**-**8**.

Compound	*D*···*A*	*D*···*A* (Å)	*D*−C···*A* (°)
5	Cl(1) .... O(1)^{i}	3.140(19)	169.49 (11) (C5)
6	Cl(2) .... F(1)^{ii}	3.177(2)	146.58 (11) (C5)
	Cl(2) .... F(2)^{iii}	3.191 (17)	147.62 (10) (C5)
	F(1) .... F(2)^{iv}	2.756(2)	138.19(15) (C2)
7	Cl(1) .... F(1)^{v}	3.083(10)	132.25(6) (C5)
	F(2) .... Cl(1)^{v}	3.203(10)	145.15(8) (C3)
8	Cl(2) .... F(1)^{vi}	3.1572(13)	145.82(7) (C5)
	Cl(2) .... F(2)^{vii}	3.109(11)	145.44(7) (C5)
	Cl(1) .... F(3)^{i}	3.035(14)	173.80(8) (C5)
	F(1) … F(2)^{viii}	2.769(15)	138.79(10) (C2)
	F(3) … F(3)^{ix}	2.818(2)	163.83(13) (C9)

Symmetry code(s): (i) 1-x, 1-y, -z; (ii) -1+x, y, z; (iii) -1+x, -1+y, z; (iv) x, -1+y, z; (v) 2-x, 1/2+y, 3/2-z; (vi) 1+x, y, z; (vii) 1+x, 1+y, z; (viii) x, 1+y, z; (ix) -1-x, -y, 2-z

7. UV-vis spectroscopy

Table S5. Absorption maxima (λ_{max}) of **5**−**8** in CH_2Cl_2, DMF and MeOH.

	CH_2Cl_2	DMF	MeOH	σ_p[11]
5	231/316/345	211/263/338	222/325/351	−0.27
6	231/325/361	225/326/364	221/321/358	−0.17
7	222/308/364	233/319/366	214/325/341	0.00
8	220/327/358	220/327/381	217/324/366	0.06
ε^{a} [12]	41	44	55	
α^{b} [12]	0.13	0.00	0.98	
β^{c} [12]	0.10	0.69	0.66	

[a] Electric permittivity of solvent; [b] H-bond donating ability of solvent; [c] H-bonding acceptor ability of solvent.

8. Computational details

The full geometry optimization of all structures has been carried out at the DFT level of theory using the M06-2X[S1] functional with the help of the Gaussian-09[S2] program package. The Def2-TZVP basis set was used for the calculations of the molecular structures **5**, while the 6-31+G* basis set was applied for the dimers and for the monomers calculated to estimate the binding energies. No symmetry operations have been applied in calculations. The basis set superposition error (BSSE) was corrected using the counterpoise method.[S3] The topological analysis of the electron density distribution with help of the AIM method of Bader[S4] was performed using the program AIMAll.[S5] The Hirshfeld molecular surfaces were generated using the CrystalExplorer 17.5 program[S6] based on the X-ray structures. The normalized contact distances[S7] based on van der Waals radii were mapped onto the Hirshfeld surface. Initial structures of the dimers selected for the optimization corresponded to the experimental X-ray structures.

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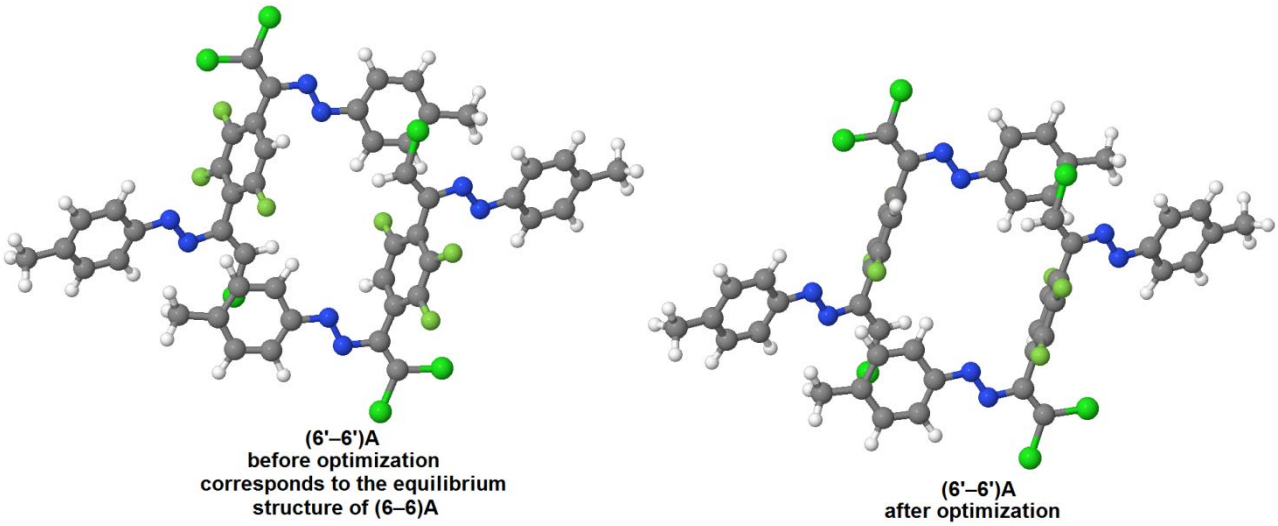

Figure S11. Initial and optimized structures of the model dimer **(6'–6')A** without the Cl...F bonds.

Table S6. Contributions of the intermolecular contacts in the Hirshfeld surface (in %).

Inside atoms	Outside atoms					
	Cl	F	N	C	H	O
Structure **5**						
C	5.9	0.2	0.1	3.8	4.1	0.3
Cl		3.5	1.3	6.0	10.3	1.7
F	2.8	4.3			7.5	
H	7.7	7.2	3.2	2.6	16.6	1.7
N	1.3			0.1	3.7	
O	1.4			0.1	2.6	
Structure **6**						
C	6.4		1.0	2.2	5.6	
Cl		4.6	2.0	6.4	10.2	
F	3.7	4.3			6.5	
H	6.9	6.2	1.9	3.9	22.9	
N	1.9			1.0	2.3	
Structure **7**						
C	5.8	0.2	1.3	1.6	9.3	
Cl	2.9	5.2	1.6	5.7	9.2	
F	3.7	3.7			8.2	
H	6.2	7.5	1.8	7.2	12.8	
N	1.6	0.2		1.3	2.9	
Structure **8**						
C	7.3	0.8	1.2	2.8	4.4	
Cl	0.1	8.3	2.1	7.3	7.3	
F	6.2	6.8	0.1	0.3	10.7	
H	5.4	10.1	1.7	2.7	8.7	
N	2.0			1.3	2.3	

Table S7. Cartesian atomic coordinates (in Å) of the calculated equilibrium structures.

5 (Def2-TZVP)

Cl	1.34262	-2.40302	0.38054
Cl	4.20834	-2.47243	0.60762
F	1.72894	0.75456	3.47777
N	4.01296	0.34898	1.36853
N	4.59523	0.82761	0.38177
C	1.52062	0.53768	1.14818
C	1.06417	1.03007	2.36037
C	2.77435	-0.24844	1.07419
C	7.63586	2.12658	2.08587
H	8.11014	2.20135	3.05529
C	8.29975	2.67908	0.98141
O	9.48786	3.26061	1.24576
C	2.78005	-1.54554	0.72849
C	6.41868	1.51127	1.92828
H	5.89859	1.08283	2.77398
C	7.72771	2.60622	-0.28519
H	8.22251	3.02581	-1.14819
C	6.49766	1.98190	-0.43474
H	6.02831	1.91073	-1.40764
C	5.83840	1.43510	0.65581
F	1.18856	0.40863	-1.17688
C	0.78720	0.84733	0.01337
Cl	-0.64023	5.04469	2.06972
Cl	-3.50593	5.11401	1.84236
F	-0.48587	2.23329	3.62647
N	-3.31026	2.29271	1.08092
N	-3.23961	1.08529	0.79991
C	-0.81795	2.10423	1.30140
C	-0.08449	1.79458	2.43620
C	-2.07177	2.89021	1.37540
C	-6.85040	0.42571	0.19683
H	-7.82126	0.90294	0.19604
C	-6.78346	-0.93581	-0.13121
O	-7.96190	-1.52479	-0.42112
C	-2.07756	4.18726	1.72129
C	-5.70888	1.12226	0.50782
H	-5.75015	2.17264	0.76137
C	-5.55604	-1.59165	-0.14277
H	-5.48319	-2.63936	-0.39303
C	-4.40795	-0.87958	0.17352
H	-3.43940	-1.36310	0.17221
C	-4.47094	0.46721	0.49771
F	-1.02626	1.88733	-1.02817
C	-0.36147	1.61185	0.08924
C	-7.95382	-2.89682	-0.75410
C	10.20259	3.82901	0.16892
H	10.45239	3.07230	-0.57919

H	11.11640	4.23549	0.59298
H	9.63014	4.63223	-0.30227
H	-7.35480	-3.08027	-1.64988
H	-8.98791	-3.16758	-0.94765
H	-7.56736	-3.49892	0.07223

5 (6-31+G*)

Cl	-2.77550	2.72075	0.73948
Cl	-5.64659	2.70046	1.13078
F	-6.31617	1.21845	-1.60508
F	-4.95795	-1.68318	1.85735
O	1.40626	-4.04840	-1.78581
N	-3.07062	-0.09232	-0.04791
N	-3.20581	-1.25249	-0.48975
C	-5.57606	-0.19191	0.13873
C	-6.52919	0.16719	-0.80984
C	-5.84159	-1.30446	0.93247
C	-4.29178	0.54145	0.26343
C	-4.23742	1.82802	0.66421
C	-1.99843	-1.92048	-0.78987
C	-2.13660	-3.15430	-1.42089
H	-3.13731	-3.51848	-1.63436
C	-1.01847	-3.90280	-1.77968
H	-1.14972	-4.85661	-2.27661
C	0.25309	-3.40575	-1.48470
C	0.39871	-2.16924	-0.82835
H	1.40183	-1.82356	-0.59336
C	-0.71534	-1.43007	-0.48572
H	-0.61364	-0.47960	0.02958
C	1.32842	-5.30815	-2.42600
H	2.35881	-5.63755	-2.55949
H	0.84030	-5.22188	-3.40349
H	0.78958	-6.03083	-1.80281
F	-7.23362	-3.08394	1.57449
F	-8.60000	-0.16387	-1.86831
C	-7.96849	-1.65466	-0.15248
C	-7.01999	-2.02237	0.78915
C	-7.71003	-0.55060	-0.94745
H	-8.88936	-2.21593	-0.26251

7 (6-31+G*)

Cl	5.522364	-3.120000	1.657845
Cl	8.055514	-1.892487	1.003150
F	4.267648	1.150213	2.213315
N	6.475209	0.426242	0.135510
N	5.805208	1.388468	-0.288696
C	4.211841	-0.566351	0.599463
C	3.559299	0.367873	1.397045
C	5.692669	-0.653698	0.595830
C	8.616891	3.685051	-1.179469
H	9.701171	3.740406	-1.152449
C	7.877573	4.758633	-1.686996
H	8.390903	5.643105	-2.052790
C	6.347301	-1.751075	1.027501

C	7.973501	2.548891	-0.707056
H	8.530856	1.707755	-0.308477
C	6.486171	4.697112	-1.721859
H	5.911540	5.530382	-2.114453
C	5.832689	3.561990	-1.249391
H	4.749579	3.482300	-1.261656
C	6.574213	2.492254	-0.745368
F	4.004461	-2.266840	-1.025460
C	3.427561	-1.363149	-0.229193
Cl	0.083818	2.250342	-0.510954
Cl	-2.449256	1.022653	0.143708
F	1.338663	-2.019921	-1.066318
N	-0.868825	-1.296013	1.011285
N	-0.198749	-2.258201	1.435459
C	1.394485	-0.303275	0.547439
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C	-0.086341	-0.215976	0.551060
C	-3.010213	-4.555097	2.326115
H	-4.094487	-4.610551	2.299142
C	-2.270783	-5.628663	2.833516
H	-2.784033	-6.513211	3.199240
C	-0.741040	0.881355	0.119383
C	-2.366939	-3.418841	1.853779
H	-2.924373	-2.577717	1.455292
C	-0.879385	-5.567037	2.868324
H	-0.304669	-6.400298	3.260811
C	-0.226020	-4.431813	2.395945
H	0.857082	-4.352021	2.408162
C	-0.967652	-3.362097	1.892039
F	1.601862	1.397169	2.172418
C	2.178763	0.493505	1.376121

8 (6-31+G*)

Cl	4.060726	-0.257879	-0.619970
Cl	2.170892	1.924387	-0.781651
F	0.287954	0.906906	1.609727
F	-0.480381	-1.239771	-2.518220
F	1.617012	-8.177110	-0.004276
N	1.712065	-2.005177	-0.418568
N	0.721182	-2.752000	-0.292560
C	-0.022081	-0.184463	-0.461043
C	-0.521438	0.553324	0.608185
C	-0.912788	-0.537532	-1.469414
C	1.390687	-0.635363	-0.501957
C	2.417221	0.232495	-0.615384
C	1.031969	-4.133817	-0.218505
C	-0.066140	-4.989665	-0.112591
H	-1.062181	-4.557940	-0.092781
C	0.121146	-6.366075	-0.039801
H	-0.709740	-7.058419	0.039883
C	1.420130	-6.849841	-0.072780
C	2.532726	-6.019778	-0.174820
H	3.524777	-6.458244	-0.194713

C	2.335728	-4.649435	-0.249242
H	3.175643	-3.967795	-0.331940
Cl	-6.827433	0.652985	-0.188803
Cl	-4.937649	-1.529350	-0.027365
F	-3.054685	-0.511881	-2.418516
F	-2.286334	1.634853	1.709377
F	-4.383338	8.572246	-0.802950
N	-4.478718	2.400251	-0.390010
N	-3.487780	3.147034	-0.515829
C	-2.744636	0.579475	-0.347753
C	-2.245277	-0.158298	-1.416990
C	-1.853929	0.932557	0.660608
C	-4.157394	1.030407	-0.306834
C	-5.183948	0.162565	-0.193508
C	-3.798499	4.528884	-0.589634
C	-2.700348	5.384692	-0.695449
H	-1.704336	4.952916	-0.715454
C	-2.887571	6.761128	-0.767944
H	-2.056660	7.453449	-0.847568
C	-4.186528	7.244957	-0.734755
C	-5.299158	6.414923	-0.632797
H	-6.291186	6.853440	-0.612724
C	-5.102229	5.044553	-0.558676
H	-5.942166	4.362933	-0.476012

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F	8.192522	2.623025	-1.354829
F	8.599565	0.317423	2.740348
C	8.448381	1.500655	0.704575
C	7.756918	1.711189	-0.478195
C	7.963457	0.549638	1.586705
H	9.345402	2.064779	0.932850
Cl	3.415575	-2.940771	-0.637797
Cl	6.293689	-2.989855	-0.339006
F	6.374791	-1.068459	2.184417
F	5.980579	1.211668	-1.927838
O	-0.863615	4.276012	-0.505930
N	3.636995	-0.027113	-0.297103
N	3.723000	1.192271	-0.040038
C	6.118500	0.027797	0.107591
C	6.812398	-0.171594	1.297348
C	6.610301	0.988038	-0.773097
C	4.867105	-0.711677	-0.192606
C	4.854670	-2.048531	-0.372348
C	2.521562	1.922358	-0.171044
C	2.579551	3.248557	0.251021
H	3.517463	3.624195	0.649450
C	1.462551	4.076013	0.167257
H	1.529268	5.103433	0.504833
C	0.277016	3.561395	-0.362306
C	0.214364	2.225493	-0.799978
H	-0.721267	1.863007	-1.216746
C	1.325075	1.411190	-0.705777

H	1.291217	0.385184	-1.058664
C	-0.867306	5.630282	-0.094019
H	-1.872450	5.999813	-0.296563
H	-0.653949	5.714767	0.977838
H	-0.137545	6.214549	-0.666300
Cl	-3.319464	2.941513	0.081473
Cl	-6.190550	3.023196	0.464696
F	-6.860129	0.883589	-1.794366
F	-5.501907	-1.023027	2.301077
O	0.862296	-4.250574	-0.605780
N	-3.614576	0.020507	0.048989
N	-3.749768	-1.214486	-0.077514
C	-6.120025	-0.027384	0.255053
C	-7.073147	0.073971	-0.754141
C	-6.385552	-0.896591	1.309696
C	-4.835744	0.713267	0.185691
C	-4.781377	2.059725	0.239830
C	-2.542388	-1.937389	-0.194522
C	-2.680563	-3.292486	-0.484702
H	-3.681266	-3.699509	-0.596641
C	-1.562426	-4.108352	-0.637542
H	-1.693678	-5.158273	-0.870682
C	-0.290870	-3.551886	-0.481265
C	-0.145247	-2.187638	-0.167309
H	0.857873	-1.792915	-0.029793
C	-1.259298	-1.384969	-0.027669
H	-1.157602	-0.333519	0.224072
C	0.784455	-5.633091	-0.898108
H	1.814855	-5.985816	-0.941800
H	0.296341	-5.802758	-1.864619
H	0.245616	-6.169857	-0.109108
F	-7.777577	-2.449271	2.390395
F	-9.143961	-0.519762	-1.690864
C	-8.512447	-1.515660	0.352351
C	-7.563955	-1.627128	1.357060
C	-8.253990	-0.654973	-0.701282
H	-9.433322	-2.086279	0.391339

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Cl	-1.012009	2.314114	4.347839
Cl	-1.215670	1.586505	1.560187
F	2.088834	1.052996	1.047421
F	0.534555	5.504973	1.024263
N	1.436683	3.755834	3.571507
N	2.539767	4.249943	3.257366
C	1.272313	3.268657	1.104652
C	1.888605	2.222860	0.427942
C	1.108775	4.464699	0.414846
C	0.771315	3.135978	2.497334
C	-0.350665	2.439415	2.773527
C	3.220560	4.885927	4.326527
C	4.567930	5.168043	4.106505
H	5.008511	4.896092	3.151458

C	5.322711	5.777267	5.105822
H	6.375316	5.986192	4.933016
C	4.740963	6.132607	6.324208
C	3.376647	5.862277	6.519784
H	2.909026	6.150389	7.459037
C	2.616101	5.244600	5.539670
H	1.559561	5.044573	5.688697
C	5.542110	6.805111	7.408612
H	5.536507	6.207908	8.326751
H	5.121472	7.786351	7.653598
H	6.581954	6.949018	7.103988
Cl	3.584756	4.482873	-5.280395
Cl	4.293042	5.392990	-2.625419
F	1.269597	5.749320	-1.539265
F	2.849273	1.307286	-1.501988
N	1.591166	2.774207	-3.930496
N	0.708037	2.117420	-3.342240
C	2.082985	3.534372	-1.596333
C	1.496956	4.593245	-0.911471
C	2.282499	2.351137	-0.893073
C	2.349715	3.587171	-3.055371
C	3.289398	4.388427	-3.593128
C	-0.072781	1.265483	-4.157484
C	-1.063890	0.555880	-3.478283
H	-1.173729	0.713349	-2.409562
C	-1.873847	-0.341539	-4.165970
H	-2.637489	-0.899736	-3.628809
C	-1.698462	-0.552170	-5.535093
C	-0.714871	0.191556	-6.209387
H	-0.578395	0.040938	-7.278173
C	0.096848	1.093530	-5.538496
H	0.866540	1.655080	-6.058264
C	-2.489942	-1.609697	-6.255121
H	-2.705525	-1.321550	-7.288507
H	-1.916081	-2.544861	-6.277638
H	-3.434788	-1.822587	-5.745925
Cl	-3.584756	-4.482873	5.280395
Cl	-4.293042	-5.392990	2.625419
F	-1.269597	-5.749320	1.539265
F	-2.849273	-1.307286	1.501988
N	-1.591166	-2.774207	3.930496
N	-0.708037	-2.117420	3.342240
C	-2.082985	-3.534372	1.596333
C	-1.496956	-4.593245	0.911471
C	-2.282499	-2.351137	0.893073
C	-2.349715	-3.587171	3.055371
C	-3.289398	-4.388427	3.593128
C	0.072781	-1.265483	4.157484
C	1.063890	-0.555880	3.478283
H	1.173729	-0.713349	2.409562
C	1.873847	0.341539	4.165970
H	2.637489	0.899736	3.628809

C	1.698462	0.552170	5.535093
C	0.714871	-0.191556	6.209387
H	0.578395	-0.040938	7.278173
C	-0.096848	-1.093530	5.538496
H	-0.866540	-1.655080	6.058264
C	2.489942	1.609697	6.255121
H	2.705525	1.321550	7.288507
H	1.916081	2.544861	6.277638
H	3.434788	1.822587	5.745925
Cl	1.012009	-2.314114	-4.347839
Cl	1.215670	-1.586505	-1.560187
F	-2.088834	-1.052996	-1.047421
F	-0.534555	-5.504973	-1.024263
N	-1.436683	-3.755834	-3.571507
N	-2.539767	-4.249943	-3.257366
C	-1.272313	-3.268657	-1.104652
C	-1.888605	-2.222860	-0.427942
C	-1.108775	-4.464699	-0.414846
C	-0.771315	-3.135978	-2.497334
C	0.350665	-2.439415	-2.773527
C	-3.220560	-4.885927	-4.326527
C	-4.567930	-5.168043	-4.106505
H	-5.008511	-4.896092	-3.151458
C	-5.322711	-5.777267	-5.105822
H	-6.375316	-5.986192	-4.933016
C	-4.740963	-6.132607	-6.324208
C	-3.376647	-5.862277	-6.519784
H	-2.909026	-6.150389	-7.459037
C	-2.616101	-5.244600	-5.539670
H	-1.559561	-5.044573	-5.688697
C	-5.542110	-6.805111	-7.408612
H	-5.536507	-6.207908	-8.326751
H	-5.121472	-7.786351	-7.653598
H	-6.581954	-6.949018	-7.103988

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Cl	-6.920760	1.507472	-2.236720
Cl	-7.664593	-1.219744	-2.829170
F	-5.556233	-0.374012	1.664129
N	-5.551555	-1.994000	-0.955997
N	-4.626808	-2.346170	-0.197828
C	-4.734092	0.327795	-0.432040
C	-4.692493	0.358886	0.958884
C	-5.652412	-0.597933	-1.138678
C	-5.113464	-6.045543	-0.409112
H	-5.681262	-6.789912	-0.959545
C	-4.226722	-6.448073	0.595042
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C	-1.848680	8.245421	0.954380
H	-1.101452	8.909924	1.378162
C	-2.882382	8.770216	0.171881
H	-2.933254	9.839924	-0.009352
C	-0.910673	2.227453	2.458945
C	-1.771187	6.879907	1.192871
H	-0.976003	6.454515	1.796268
C	-3.845740	7.924934	-0.374666
H	-4.648087	8.331431	-0.982804
C	-3.776467	6.554183	-0.139248
H	-4.510400	5.867715	-0.551054
C	-2.742661	6.034646	0.640943
F	-3.804131	1.154598	2.971919
C	-3.782042	1.154179	1.636676
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Cl	9.232216	-0.655879	-0.335381
F	4.806810	0.545351	1.641410
N	6.852252	1.031348	-0.666415
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C	5.146584	-0.772190	-0.283117
C	4.313272	-0.277894	0.714531
C	6.555526	-0.318127	-0.379192
C	7.550756	4.996170	-1.517317
H	8.544270	5.431216	-1.573531
C	6.426657	5.795703	-1.748700
H	6.552441	6.848765	-1.983208
C	7.597017	-1.156850	-0.205689
C	7.405224	3.648437	-1.217284
H	8.265449	3.012969	-1.034262
C	5.148466	5.245599	-1.679161
H	4.275377	5.865218	-1.859703
C	4.993216	3.895019	-1.378210
H	4.011095	3.435454	-1.314839
C	6.117611	3.100456	-1.149993
F	5.337822	-2.120539	-2.210509
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F	2.748764	-2.795788	-2.098974

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C	0.617120	-8.037322	0.912144
H	0.400199	-9.090373	1.066673
C	-0.013158	-0.977927	-0.297291
C	-0.127902	-5.826228	0.272774
H	-0.901956	-5.146694	-0.070856
C	1.902973	-7.551194	1.140985
H	2.688777	-8.221157	1.476276
C	2.180666	-6.202768	0.931136
H	3.174265	-5.794167	1.090943
C	1.165740	-5.343071	0.507871
F	2.219976	-0.130727	1.755362
C	2.974417	-0.630531	0.773954

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Cl	1.683028	-0.190592	11.969544
Cl	2.168149	0.503088	9.206236
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C	-0.318871	-1.146114	8.537372
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C	-0.297183	-2.365172	7.867787
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C	-2.334487	-3.032493	11.563134
C	-3.430772	-3.771266	11.113173
H	-3.650857	-3.780571	10.049978
C	-4.217538	-4.479653	12.015366
H	-5.074555	-5.064542	11.700018
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C	-2.794216	-3.693947	13.835103
H	-2.581310	-3.688724	14.898841
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F	-1.670504	0.943031	5.900919
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C	-0.724559	-2.472103	6.552837
C	-1.221651	-0.146593	6.526685

C	-1.600871	-1.448362	4.430729
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H	1.020148	1.807457	-0.218637
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C	1.600871	1.448362	-4.430729
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C	-3.011036	-1.670995	-2.548927
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C	-0.495869	-0.811011	-1.635680
H	0.486463	-0.486176	-1.306792
Cl	-1.683028	0.190592	-11.969544
Cl	-2.168149	-0.503088	-9.206236
F	0.850795	-1.152159	-8.441210
F	-0.163173	3.453008	-8.487605
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C	0.297183	2.365172	-7.867787
C	-0.105505	1.053818	-9.955973
C	-1.181274	0.334183	-10.336096
C	2.334487	3.032493	-11.563134
C	3.430772	3.771266	-11.113173
H	3.650857	3.780571	-10.049978
C	4.217538	4.479653	-12.015366
H	5.074555	5.064542	-11.700018
C	3.879918	4.423206	-13.358824

C	2.794216	3.693947	-13.835103
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Cl	5.065586	0.996454	4.907317
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C	4.678149	0.837580	3.244750
C	1.017151	-1.753567	4.267417
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C	-0.997683	-3.050321	4.598451
H	-1.881508	-3.558164	4.224500
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H	2.135339	-1.225309	6.032349
Cl	0.646548	-1.134508	-4.880431
Cl	-0.029723	-1.773478	-2.149635
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F	2.153294	2.213806	-1.337565
F	6.690069	4.099489	-6.934378
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C	2.508890	1.093580	-0.699572
C	2.083698	-0.224109	-2.788465
C	1.031788	-0.954055	-3.219765
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C	5.643567	2.507359	-3.872522
H	5.920847	2.421771	-2.826101
C	6.394911	3.277779	-4.753810
H	7.281099	3.817627	-4.438515
C	5.977514	3.352549	-6.074343
C	4.848496	2.691780	-6.548924
H	4.562067	2.799913	-7.589598
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H	3.221974	1.389925	-5.993077
Cl	-0.646698	1.134127	4.880971
Cl	0.030135	1.772643	2.150197
F	-2.846737	2.457327	1.203949

F	-2.153664	-2.214241	1.338149
F	-6.692347	-4.098514	6.933692
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C	-2.835410	1.255494	0.624066
C	-2.508751	-1.093955	0.699982
C	-2.083688	0.223776	2.788885
C	-1.031732	0.953595	3.220272
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C	-5.644385	-2.506813	3.872111
H	-5.921312	-2.421152	2.825602
C	-6.396257	-3.276970	4.753178
H	-7.282522	-3.816536	4.437613
C	-5.979286	-3.351844	6.073838
C	-4.850193	-2.691436	6.548744
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C	-4.112391	-1.919008	5.665061
H	-3.223092	-1.390121	5.993435
Cl	-5.064445	-0.996712	-4.907315
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F	-3.580507	2.269165	-1.349231
F	1.598188	3.619143	-6.801166
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C	-4.677136	-0.837899	-3.244709
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C	0.099425	2.411640	-3.749923
H	0.254241	2.406132	-2.676114
C	0.998272	3.050390	-4.598861
H	1.882256	3.558138	-4.225145
C	0.738882	3.014502	-5.959794
C	-0.375546	2.378740	-6.502660
H	-0.525139	2.392363	-7.577195
C	-1.261482	1.741829	-5.648031
H	-2.135110	1.225471	-6.032072