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Role of substituents on resonance assisted hydrogen bonding *vs.* intermolecular hydrogen bonding

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1. Materials and instrumentation

^{1}H and ^{13}C NMR spectra were recorded at room temperature on a Bruker Avance II + 300 (UltraShield^{TM} Magnet) spectrometer operating at 300.130 and 75.468 MHz for proton and carbon-13, respectively. The chemical shifts are reported in ppm using tetramethylsilane as the internal reference. The infrared spectra (4000–400 cm^{-1}) were recorded on a Bruker Vertex 70 instrument in KBr pellets. 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.

2. Synthesis of 1−5

(*Z*)-2-(2-(*para*-substitutedphenyl)hydrazineylidene)-*N*,*N*-diethyl-3-oxobutanamides were synthesized via the Japp−Klingemann reaction between *para*-substituted phenyldiazonium chloride and *N*,*N*-diethyl-3-oxobutanamide (*N*,*N*-dimethyl-3-oxobutanamide in the case of **5**) in water solution containing sodium hydroxide.

2.1. Diazotization

0.025 mol of *para*-substituted aniline was dissolved in 30 mL of water. The solution was cooled in an ice bath to 273 K and then 0.025 mol of $NaNO_2$ was added; after that 5.00 mL (33 %) HCl were added in portions for 1 h. The temperature of the mixture should not exceed 278 K. The resulting diazonium solution was used directly in the following coupling procedure.

2.2. Coupling

0.025 mol of NaOH was added to a mixture of 0.025 mol of *N*,*N*-diethyl-3-oxobutanamide with 20 mL of water. The solution was cooled in an ice bath to *ca*. 273 K, and a suspension of *para*-substituted phenyldiazonium chloride (see above) was added in three portions under vigorous stirring for 1 h.

The identity of (*E*/*Z*)-2-(2-(*para*-substitutedphenyl)hydrazineylidene)-*N*,*N*-diethyl-3-oxobutanamides was demonstrated by element analysis, ESI-MS, ^{1}H and ^{13}C NMR spectrometry.

1: yield, 78 % (based on *N*,*N*-diethyl-3-oxobutanamide), yellow powder, soluble in methanol, ethanol, chloroform and insoluble in water. Anal. Calcd for $C_{16}H_{23}N_3O_2$ (*M* = 289.38): C, 66.41; H, 8.01; N, 14.52. Found: C, 66.36; H, 7.97; N, 14.48 %. ESI-MS: *m/z*: 290.29 $[M+H]^+$. ^{1}H NMR of a mixture of *Z*-hydrazone-I and *E*-hydrazone-II (300.13 MHz, $CDCl_3$). *E*-hydrazone-II, *δ*: 1.11-1.28 (9H, $3CH_3$),

2.32, (3H, CH_3), 2.58−2.63 (2H, CH_2), 3.13−3.59 (4H, $2CH_2$), 7.11−7.20 (4H, C_6H_4), 14.04 (1H, N−H). *Z*-hydrazone-I, *δ*: 1.11-1.28 (9H, $3CH_3$), 2.36, (3H, CH_3), 2.58−2.63 (2H, CH_2), 3.13−3.59 (4H, $2CH_2$), 7.11−7.20 (4H, C_6H_4), 9.51 (1H, N−H). ^{13}C NMR of a mixture of *Z*-hydrazone-I and *E*-hydrazone-II (300.13 MHz, $CDCl_3$) *δ*: 12.98, 13.05, 14.14, 14.23, 15.91, 24.61, 24.64, 28.33, 28.39, 28.62, 38.99, 42.79, 114.77, 115.29, 128.85, 128.93, 130.29, 136.70, 139.55, 140.16, 140.34, 140.52, 163.22, 167.02, 194.85, 195.28. ^{1}H NMR of a mixture of *Z*-hydrazone-I and *E*-hydrazone-II (300.13 MHz, DMSO-d_6). *E*-hydrazone-II, *δ*: 0.99-1.19 (9H, $3CH_3$), 2.23, (3H, CH_3), 2.54−2.60 (2H, CH_2), 3.05−3.36 (4H, $2CH_2$), 7.17−7.35 (4H, C_6H_4), 13.63 (1H, N−H). *Z*-hydrazone-I, *δ*: 0.99-1.19 (9H, $3CH_3$), 2.39, (3H, CH_3), 2.54−2.60 (2H, CH_2), 3.05−3.36 (4H, $2CH_2$), 7.17−7.35 (4H, C_6H_4), 10.50 (1H, N−H). ^{13}C NMR *Z*-hydrazone-I (300.13 MHz, DMSO-d_6) *δ*: 12.61, 12.78, 14.05, 14.24, 15.70, 15.86, 24.37, 27.52, 37.98, 41.64, 114.61, 128.46, 137.83, 141.29, 162.98, 194.23.

2: yield, 84 % (based on *N*,*N*-diethyl-3-oxobutanamide), yellow powder, soluble in methanol, ethanol, chloroform and insoluble in water. Anal. Calcd for $C_{14}H_{19}N_3O_2$ (*M* = 261.33): C, 64.35; H, 7.33; N, 16.08. Found: C, 64.30; H, 7.28; N, 16.01 %. ESI-MS: *m/z*: 262.24 $[M+H]^+$. ^{1}H NMR of a mixture of *Z*-hydrazone-I and *E*-hydrazone-II (300.13 MHz, $CDCl_3$). *E*-hydrazone-II, *δ*: 1.12-1.28 (6H, $2CH_3$) 2.33, (3H, CH_3), 3.15−3.59 (4H, $2CH_2$), 7.03−7.35 (5H, C_6H_5), 13.97 (1H, N−H). *Z*-hydrazone-I, *δ*: 1.12-1.28 (6H, $2CH_3$), 2.45 (3H, CH_3), 3.15−3.59 (4H, $2CH_2$), 7.03−7.35 (5H, C_6H_5), 9.41 (1H, N−H). ^{13}C NMR of a mixture of *Z*-hydrazone-I and *E*-hydrazone-II (300.13 MHz, $CDCl_3$) *δ*: 24.78, 39.09, 42.92, 114.71, 115.26, 123.49, 124.25, 129.58, 130.78, 137.33, 142.37, 162.87, 166.89, 194.89, 195.57. ^{1}H NMR of a mixture of *Z*-hydrazone-I and *E*-hydrazone-II (300.13 MHz, DMSO-d_6). *E*-hydrazone-II, *δ*: 0.97-1.15 (6H, $2CH_3$), 2.22, (3H, CH_3), 3.03−3.36 (4H, $2CH_2$), 6.97−7.42 (5H, C_6H_5), 13.53 (1H, N−H). *Z*-hydrazone-I, *δ*: 0.97-1.15 (6H, $2CH_3$), 2.38 (3H, CH_3), 3.03−3.36 (4H, $2CH_2$), 6.97−7.42 (4H, C_6H_4), 10.55 (1H, N−H). ^{13}C NMR *Z*-hydrazone-I, (300.13 MHz, DMSO-d_6) *δ*: 12.60, 12.77, 14.05, 14.24, 38.00, 41.66, 114.55, 122.34, 129.23, 138.31, 143.39, 162.89, 194.42.

3: yield, 81 % (based on *N*,*N*-diethyl-3-oxobutanamide), yellow powder, soluble in methanol, ethanol and chloroform. Anal. Calcd for $C_{15}H_{19}N_3O_4$ (*M* = 305.33): C, 59.01; H, 6.27; N, 13.76. Found: C, 58.89; H, 6.21; N, 13.74 %. ESI-MS: *m/z*: 306.29 $[M+H]^+$. ^{1}H NMR of a mixture of *Z*-hydrazone-I and *E*-hydrazone-II (300.13 MHz, $CDCl_3$). *E*-hydrazone-II, *δ*: 1.14-1.30 (6H, $2CH_3$) 2.36, (3H, CH_3), 3.17−3.61 (4H, $2CH_2$), 7.29−7.35 (4H, C_6H_4), 8.06 (1H, O−H), 13.88 (1H, N−H). *Z*-hydrazone-I, *δ*: 1.14-1.30 (6H, $2CH_3$), 2.48 (3H, CH_3), 3.17−3.61 (4H, $2CH_2$), 7.29−7.35 (4H, C_6H_4), 8.08 (1H, O−H), 9.90 (1H, N−H). ^{13}C NMR of a mixture of *Z*-hydrazone-I and *E*-hydrazone-II (300.13 MHz, $CDCl_3$) *δ*: 24.87, 39.34, 40.10, 40.45, 42.85, 43.10, 43.43, 50.14, 114.31, 114.59, 123.92, 132.05, 132.13, 146.75, 146.97, 163.46, 166.33, 170.82, 194.99, 196.22, 203.05. ^{1}H NMR of a mixture of *Z*-hydrazone-I and *E*-hydrazone-II (300.13 MHz, DMSO-d_6). *E*-hydrazone-II, *δ*: 0.97-1.15 (6H, $2CH_3$), 2.13, (3H, CH_3), 3.03−3.09 (4H, $2CH_2$), 7.44−7.98 (4H, C_6H_4), 13.45 (1H, N−H). *Z*-hydrazone-I, *δ*:

0.97-1.15 (6H, $2CH_3$), 2.41 (3H, CH_3), 3.03−3.09 (4H, $2CH_2$), 7.44−7.98 (4H, C_6H_4), 10.83 (1H, N−H). ^{13}C NMR *Z*-hydrazone-I and *E*-hydrazone-II, (300.13 MHz, DMSO-d_6) δ: 12.60, 12.76, 14.04, 14.22, 24.60, 38.06, 41.72, 41.96, 48.89, 112.59, 113.90, 126.08, 128.13, 129.23, 130.77, 130.86, 131.23, 139.71, 146.52, 162.66, 166.02, 167.75, 167.95, 194.70, 203.37.

4: yield, 89 % (based on *N*,*N*-diethyl-3-oxobutanamide), yellow powder, soluble in methanol, ethanol, chloroform and insoluble in water. Anal. Calcd for $C_{15}H_{18}N_4O_2$ (*M* = 286.34): C, 62.92; H, 6.34; N, 19.57. Found: C, 62.88; H, 6.30; N, 19.52 %. ESI-MS: *m/z*: 287.30 $[M+H]^+$. ^{1}H NMR of a mixture of *Z*-hydrazone-I and *E*-hydrazone-II (300.13 MHz, $CDCl_3$). *E*-hydrazone-II, δ: 1.10-1.29 (6H, $2CH_3$) 2.35 (3H, CH_3), 3.11−3.60 (4H, $2CH_2$), 7.23−7.68 (4H, C_6H_4), 13.79 (1H, N−H). *Z*-hydrazone-I, δ: 1.10-1.29 (6H, $2CH_3$), 2.28 (3H, CH_3), 3.11−3.60 (4H, $2CH_2$), 7.23−7.68 (4H, C_6H_4), 9.94 (1H, N−H). ^{13}C NMR of a mixture of *Z*-hydrazone-I and *E*-hydrazone-II (300.13 MHz, $CDCl_3$) δ: 12.03, 12.79, 12.83, 12.89, 12.94, 14.00, 14.10, 24.65, 24.69, 28.94, 39.06, 42.79, 105.65, 106.45, 114.90, 115.15, 119.11, 119.20, 132.95, 133.75, 133.85, 139.74, 145.91, 146.09, 162.85, 165.93, 194.86, 196.40. ^{1}H NMR of a mixture of *Z*-hydrazone-I and *E*-hydrazone-II (300.13 MHz, DMSO-d_6). *E*-hydrazone-II, δ: 0.96-1.15 (6H, $2CH_3$), 2.25 (3H, CH_3), 3.03−3.35 (4H, $2CH_2$), 7.52−7.77 (4H, C_6H_4), 13.27 (1H, N−H). *Z*-hydrazone-I, δ: 0.96-1.15 (6H, $2CH_3$), 2.42 (3H, CH_3), 3.03−3.35 (4H, $2CH_2$), 7.52−7.77 (4H, C_6H_4), 10.94 (1H, N−H). ^{13}C NMR *Z*-hydrazone-I, (300.13 MHz, DMSO-d_6) δ: 12.51, 12.68, 13.78, 13.97, 14.16, 37.98, 40.20, 41.64, 103.49, 114.83, 119.40, 133.73, 140.79, 147.15, 162.35, 194.81.

5: yield, 93 % (based on *N*,*N*-dimethyl-3-oxobutanamide), orange powder soluble in DMSO, methanol, ethanol, acetone and insoluble in water. Anal. Calcd for $C_{12}H_{14}ClN_3O_2$ (*M* = 267.71): C, 53.84; H, 5.27; N, 15.70. Found: C, 53.80; H, 5.24; N, 15.66 %. ESI-MS: *m/z*: 268.65 $[M+H]^+$.

^{1}H NMR of a mixture of *Z*-hydrazone-I and E-hydrazone-II (300.13 MHz, $CDCl_3$). *E*-hydrazone-II, δ: 2.84-3.09 (6H, $2CH_3$) 2.33 (3H, CH_3), 7.10−7.26 (4H, C_6H_4), 13.94 (1H, N−H). *Z*-hydrazone-I, δ: 2.84-3.09 (6H, $2CH_3$), 2.26 (3H, CH_3), 7.10−7.26 (4H, C_6H_4), 10.17 (1H, N−H). ^{13}C NMR of a mixture of *Z*-hydrazone-I and *E*-hydrazone-II (300.13 MHz, $CDCl_3$) δ: 24.48, 28.79, 34.57, 35.47, 37.82, 39.25, 115.95, 116.31, 128.15, 129.18, 129.30, 129.48, 130.28, 136.26, 140.84, 141.14, 163.91, 166.86, 194.78, 195.94. ^{1}H NMR *Z*-hydrazone-I (300.13 MHz, DMSO-d_6) δ: 2.39 (3H, CH_3), 2.76 (3H, CH_3), 2.96 (3H, CH_3), 7.35−7.43 (4H, C_6H_4), 10.68 (1H, N−H). ^{13}C NMR *Z*-hydrazone-I, (300.13 MHz, DMSO-d_6) δ: 24.45, 33.67, 36.41, 116.07, 125.98, 129.11, 138.43, 142.38, 163.29, 194.35.

3. $^{1}H/^{13}C$ NMR spectra of 1−5

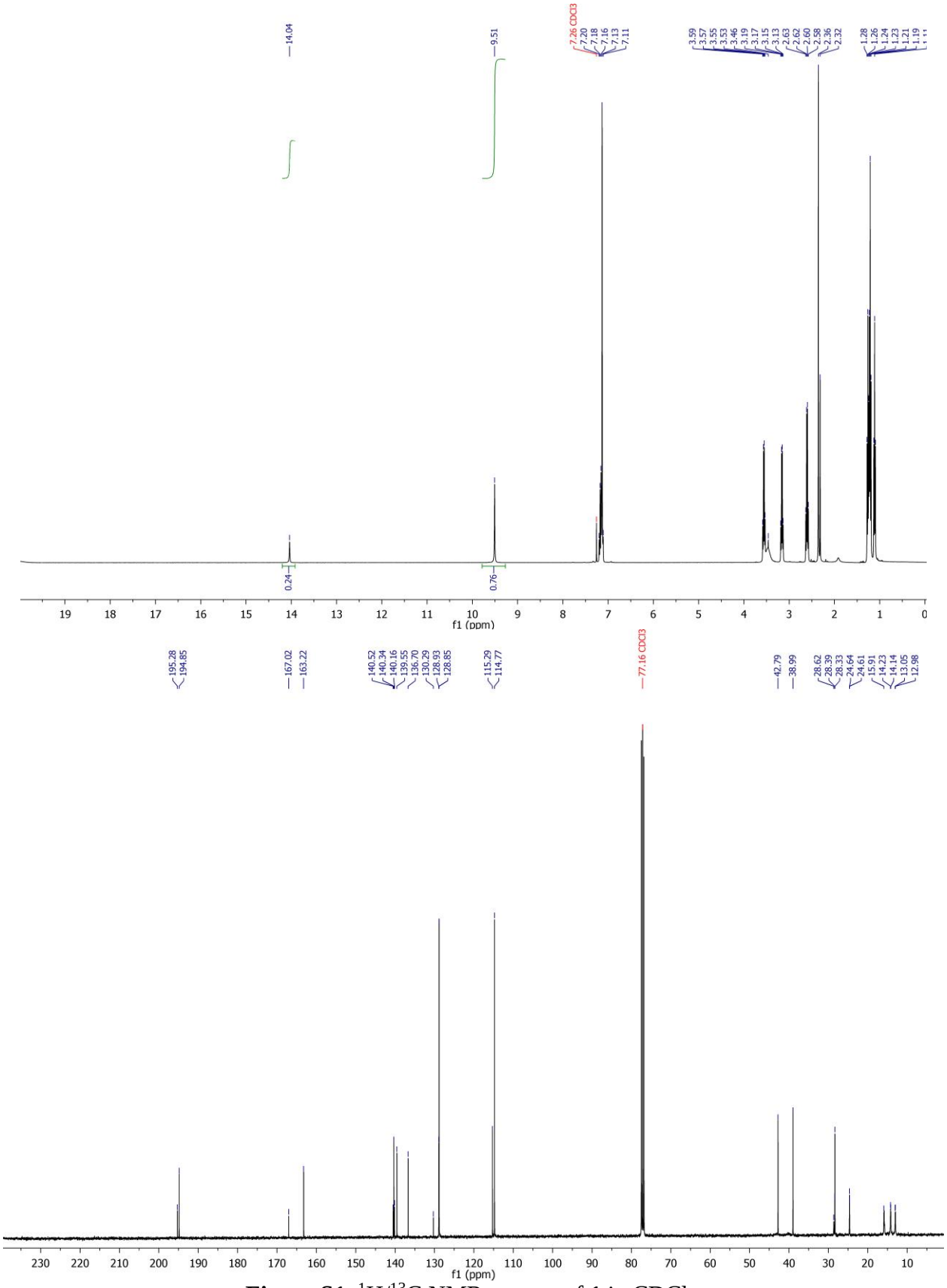


Figure S1. $^{1}H/^{13}C$ NMR spectra of **1** in $CDCl_3$.

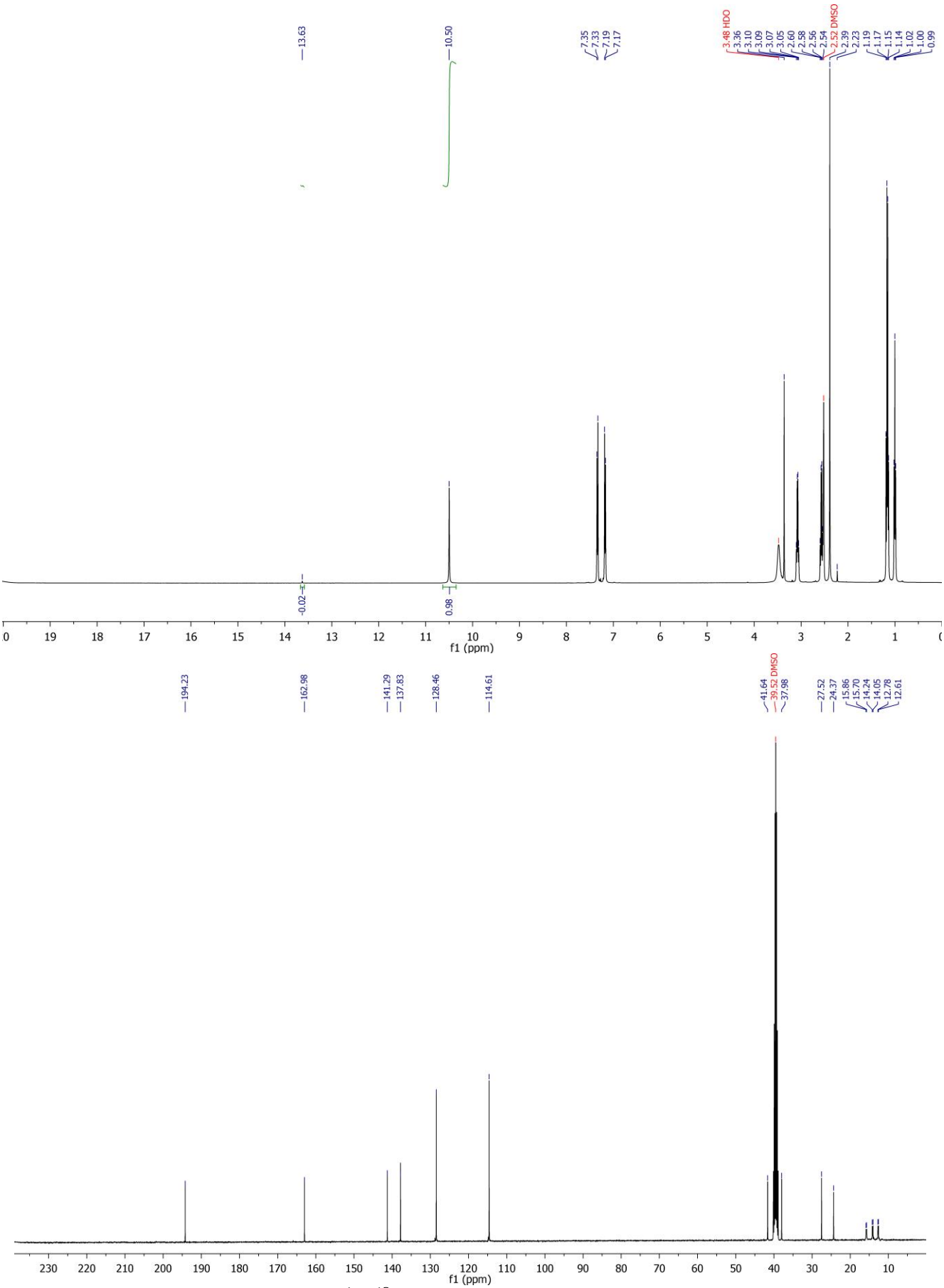


Figure S2. $^{1}H/^{13}C$ NMR spectra of **1** in DMSO-d_6.

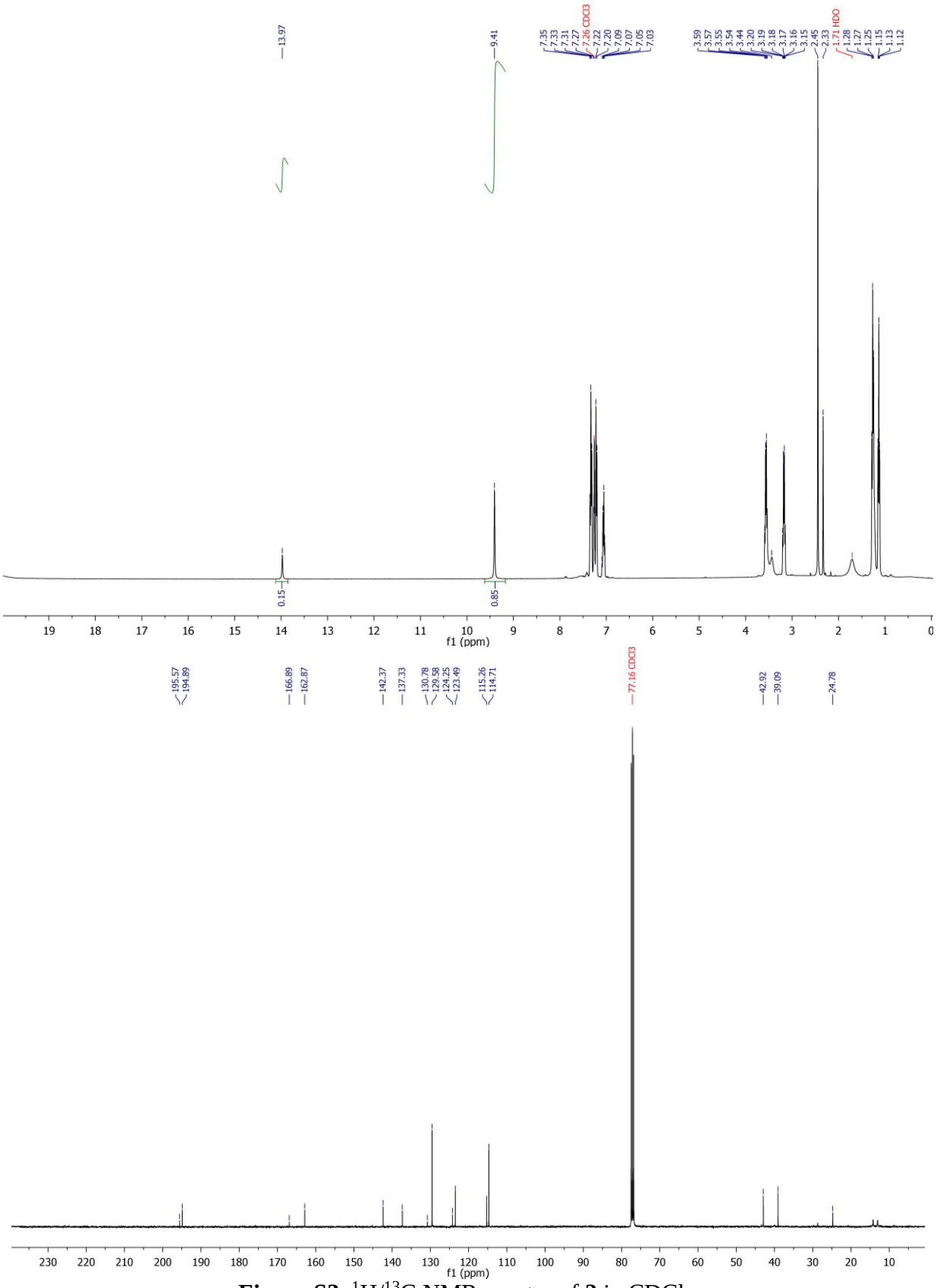


Figure S3. $^{1}H/^{13}C$ NMR spectra of **2** in $CDCl_3$.

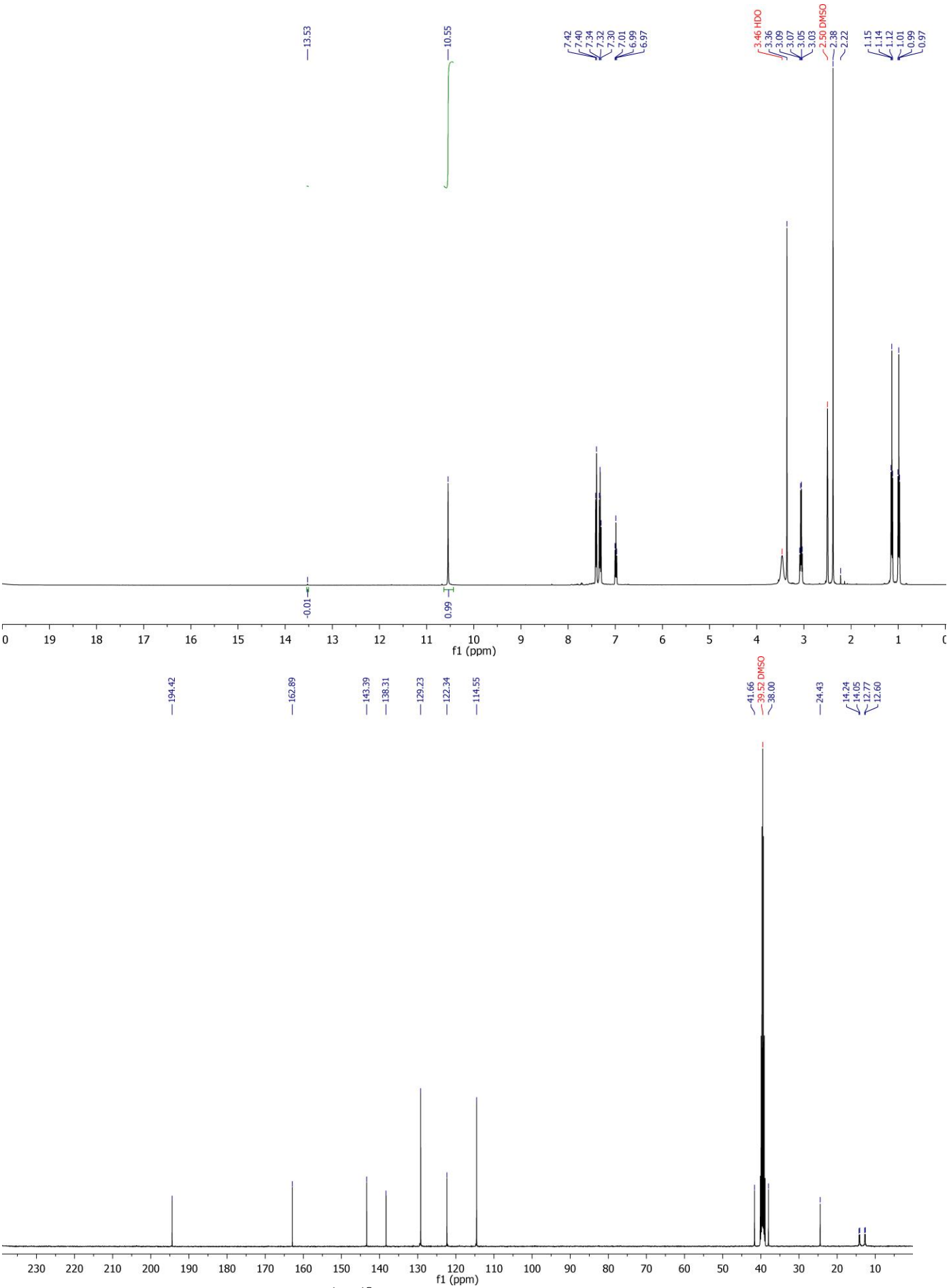


Figure S4. $^{1}H/^{13}C$ NMR spectra of **2** in DMSO-d_6.

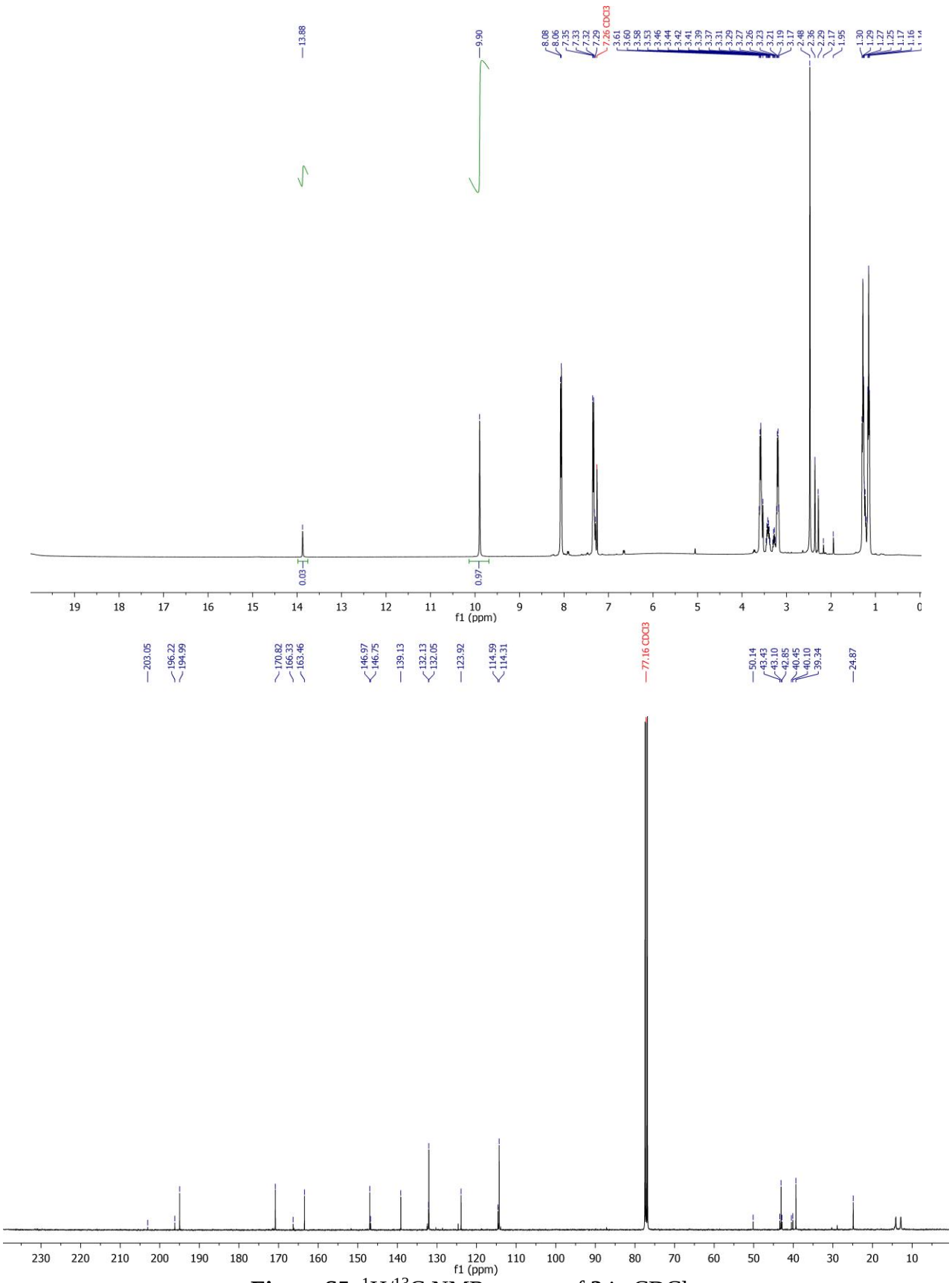


Figure S5. $^{1}H/^{13}C$ NMR spectra of **3** in $CDCl_3$.

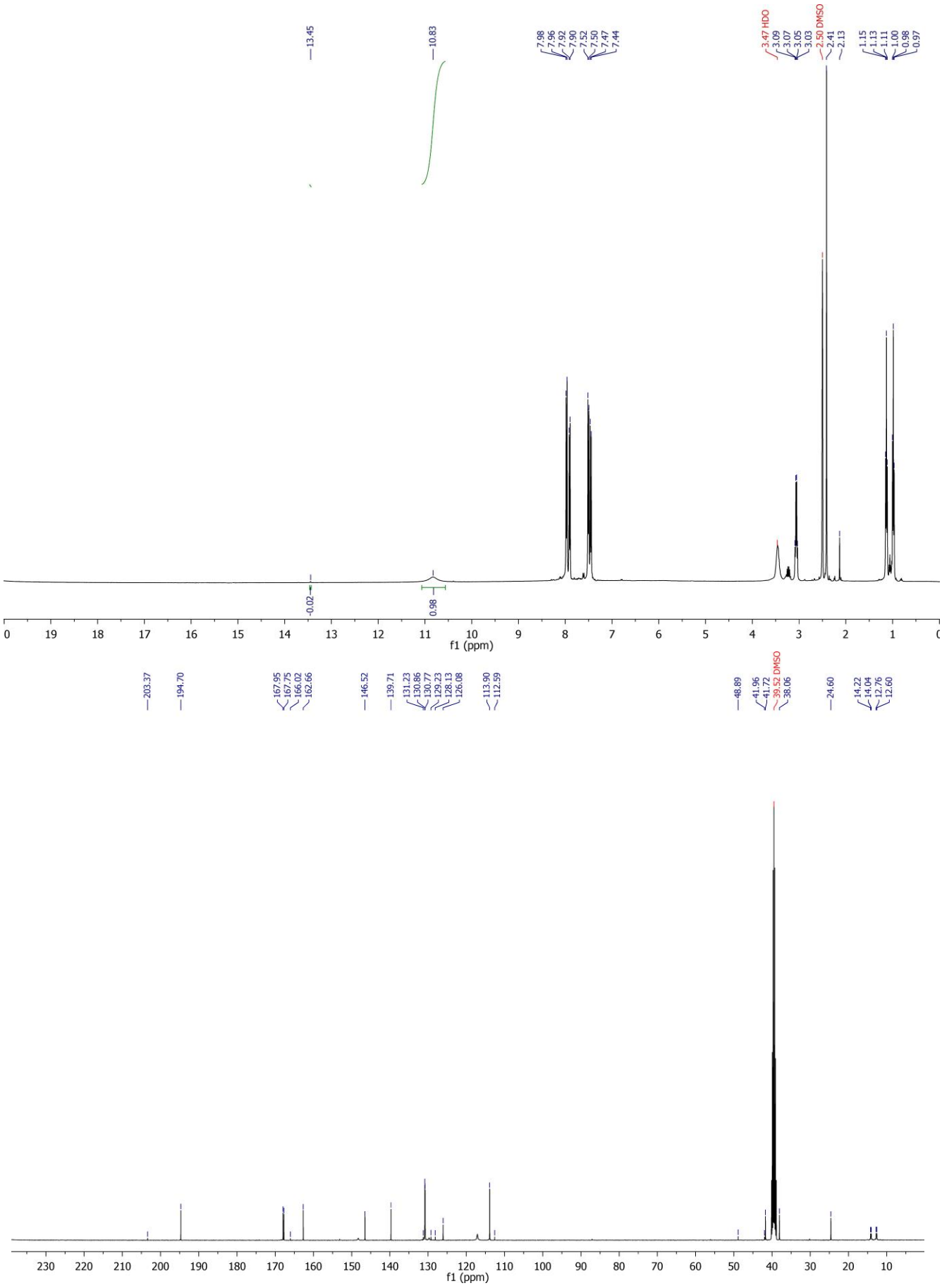


Figure S6. $^{1}H/^{13}C$ NMR spectra of **3** in DMSO-d_6.

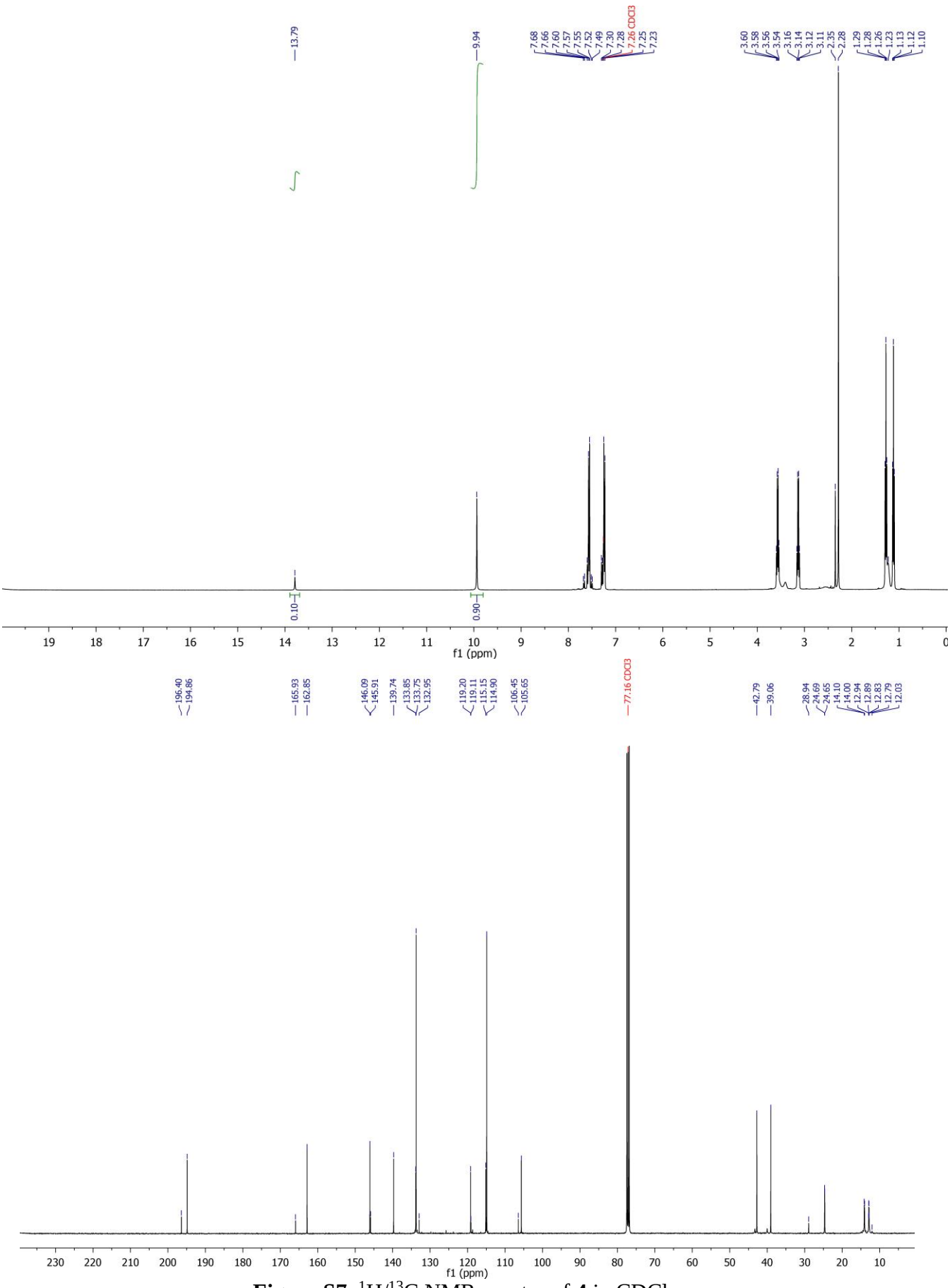


Figure S7. $^{1}H/^{13}C$ NMR spectra of **4** in $CDCl_3$.

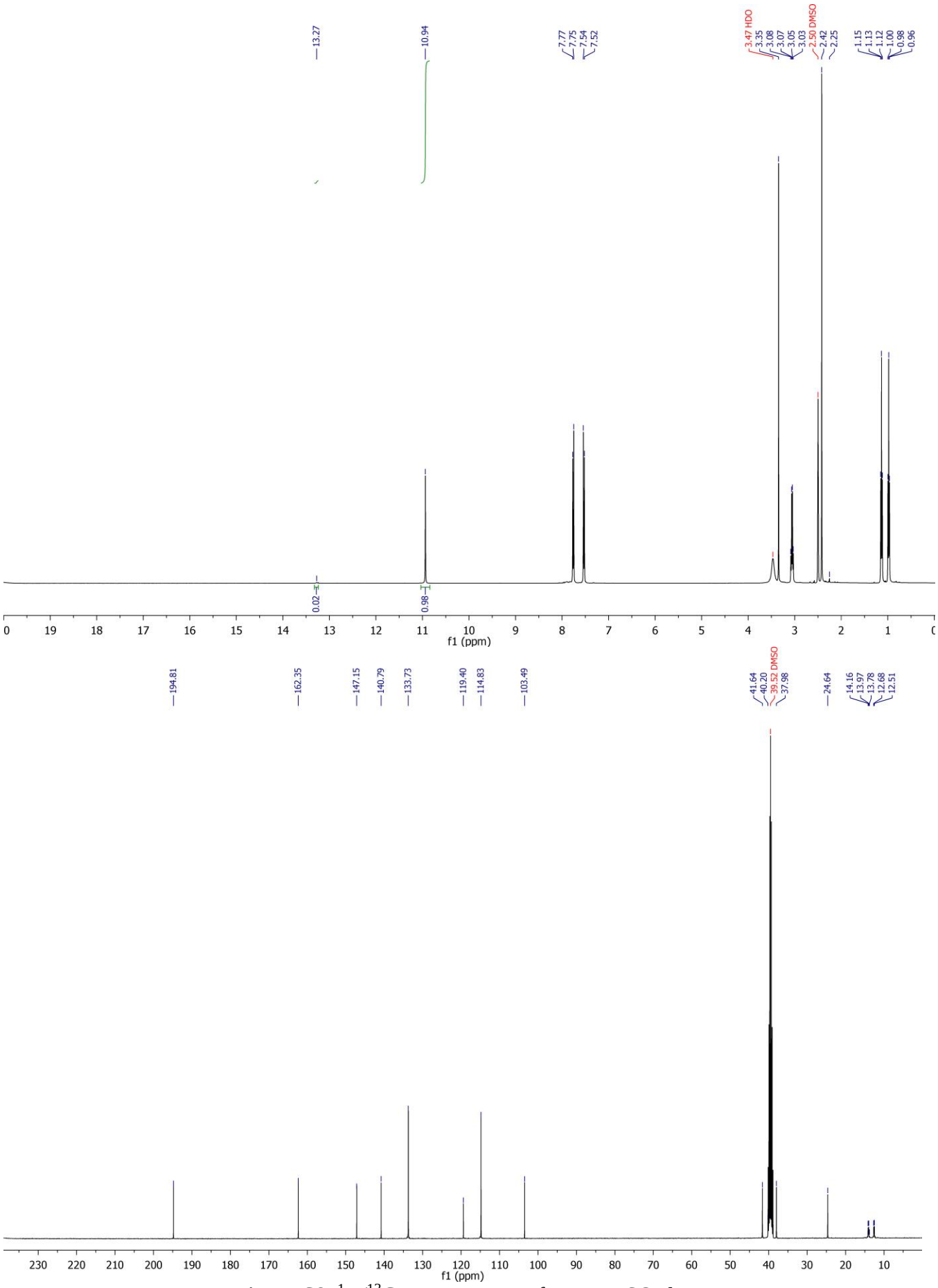


Figure S8. $^{1}H/^{13}C$ NMR spectra of **4** in DMSO-d_6.

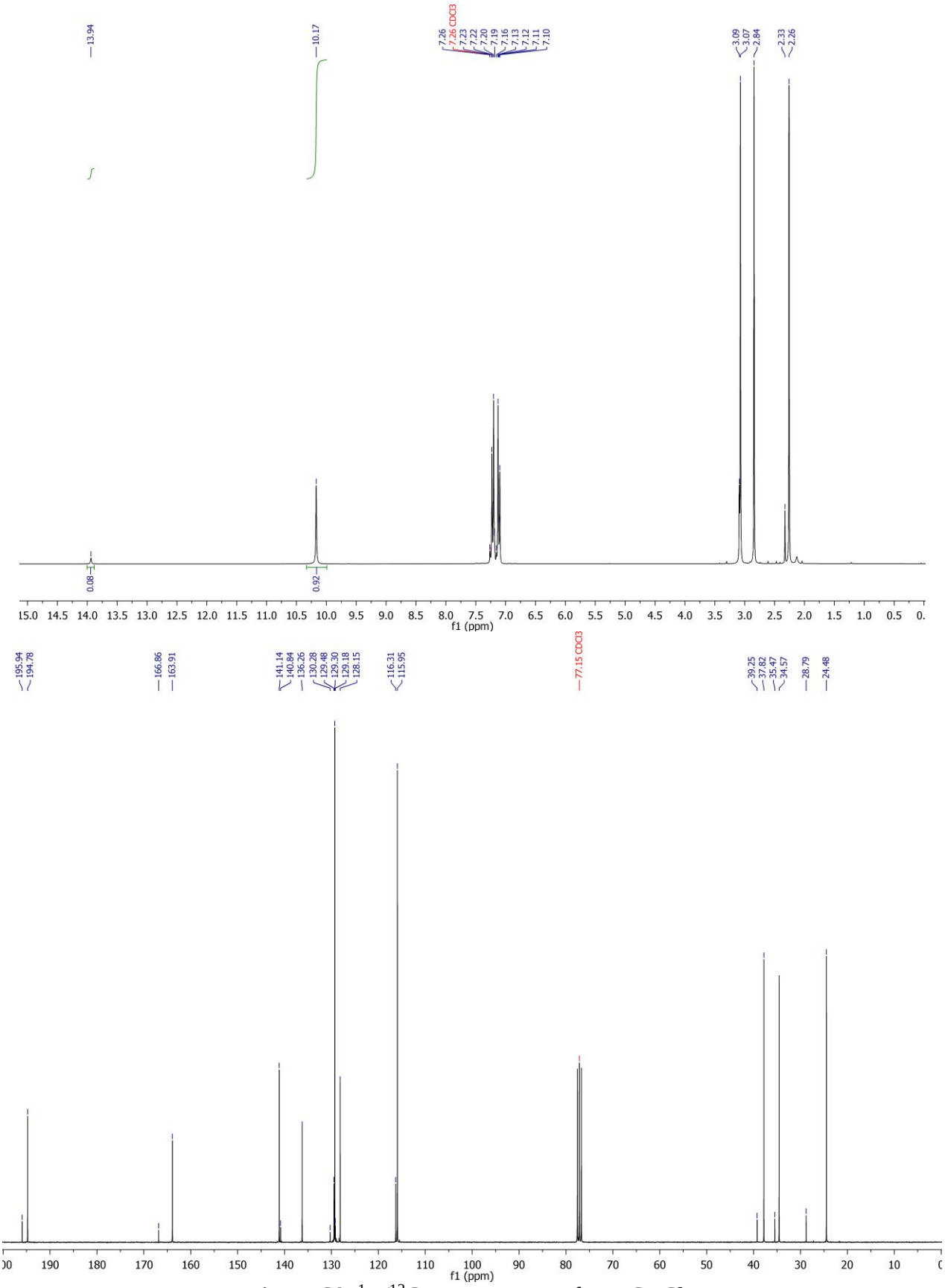


Figure S9. $^{1}H/^{13}C$ NMR spectra of **5** in $CDCl_3$.

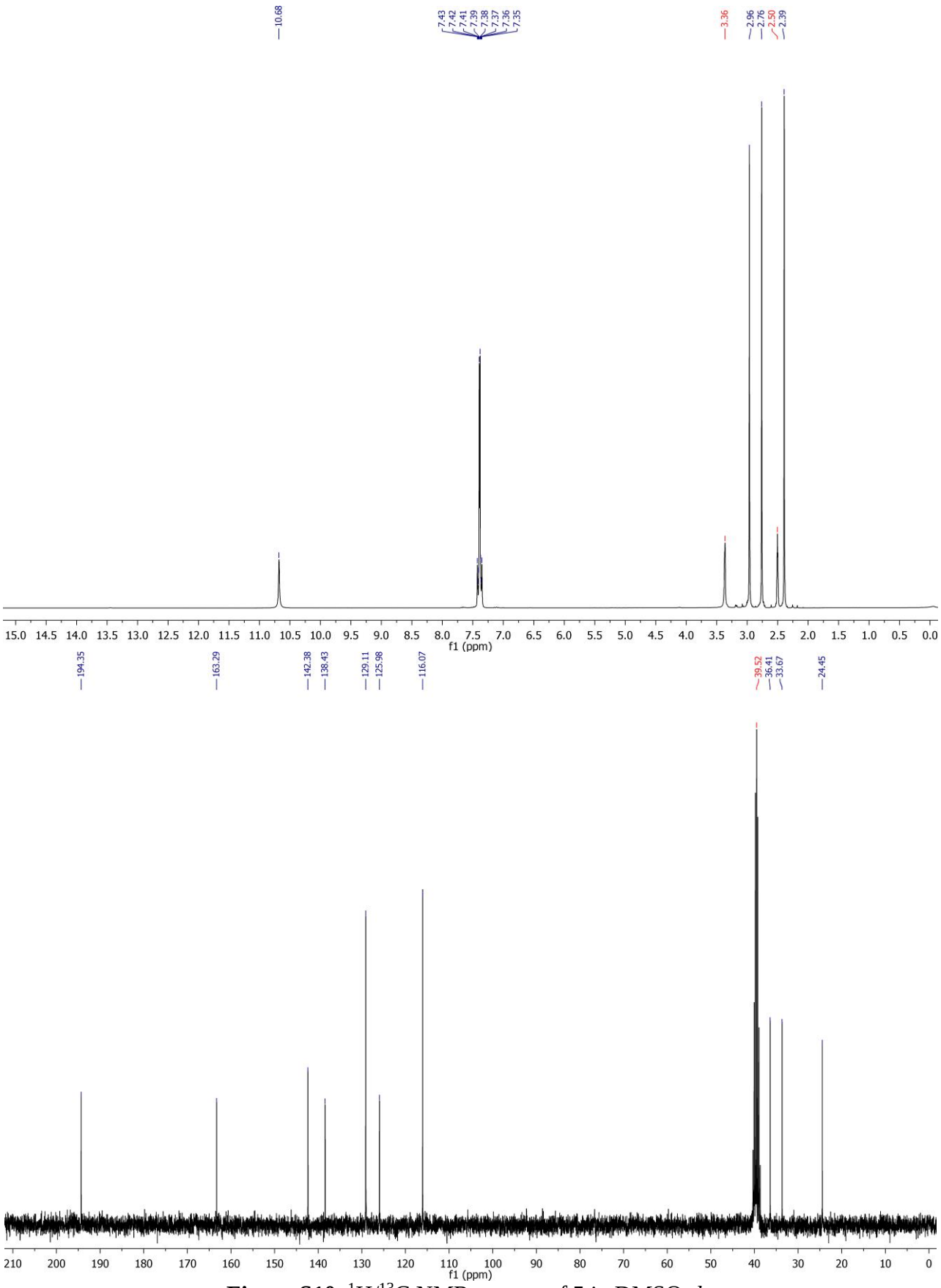


Figure S10. $^{1}H/^{13}C$ NMR spectra of **5** in DMSO-d_6.

4. X-ray analysis

X-ray diffraction patterns of **1**–**5** were collected using a Bruker SMART APEX-II CCD area detector equipped with graphite-monochromated Mo-Kα radiation (λ = 0.71073 Å) at 100(2), 150(2) or 296(2) K (Table S1). Absorption correction was applied by SADABS [s1,s2]. The structures were solved by direct methods and refined on F^2 by full-matrix least-squares using Bruker's SHELXTL-97 [s3]. Structure **3** seems to have a partially occupied phenol oxygen attached to C6. Only about 8% occupancy. All non-hydrogen atoms were refined anisotropically. The hydrogen atoms were inserted at calculated positions. The details of the crystallographic data and H-bonds for **1**–**5** are summarized in Table S1 and S2, respectively. Crystallographic data for the structural analysis have been deposited to the Cambridge Crystallographic Data Center (CCDC 1963600 for **1**, 1963601 for **2**, 1963602 for **3**, 1963603 for **4** and 1963604 for **5**). Copy of this information can be obtained free of charge from The Director, CCDC, 12 Union Road, Cambridge CB2 1EZ, UK (Fax: (+44) 1223-336033; E-mail: deposit@ccdc.cam.ac.uk or www.ccdc.cam.ac.uk/data_request/cif).

Table S1. Crystallographic data and structure refinement details for **1**–**5**.

	1	**2**	**3**	**4**	**5**
Empirical formula	$C_{16}H_{23}N_3O_2$	$C_{14}H_{19}N_3O_2$	$C_{15}H_{19}N_3O_4$	$C_{15}H_{18}N_4O_2$	$C_{12}H_{14}ClN_3O_2$
fw	289.37	261.32	305.33	286.33	267.71
Temperature (K)	150(2)	296(2)	150(2) K	296(2)	100(2)
Cryst. Syst.	Monoclinic	Triclinic	Monoclinic	Monoclinic	Monoclinic
Space group	*P2₁/n*	*P-1*	*P2₁/c*	*P2₁*	*P2₁/n*
a (Å)	7.3955(5)	7.4907(6)	7.5227(3)	7.6003(4)	17.998(2)
b (Å)	9.6559(7)	9.7684(8)	15.5942(6)	19.5864(12)	7.5198(9)
c (Å)	22.6536(15)	10.3754(10)	13.0925(5)	10.5405(6)	18.740(2)
α, °	90	88.424(3)	90	90	90
β, °	96.448(2)	75.466(3)	94.426(2)	93.758(2)	97.185(3)
γ, °	90	86.310(3)	90	90	90
V (Å^3)	1607.47(19)	733.32(11)	1531.31(10)	1565.71(15)	2516.4(5)
Z	4	2	4	4	8
ρ_{calc} (g cm^{-3})	1.196	1.183	1.324	1.215	1.413
μ(Mo Kα) (mm^{-1})	0.080	0.081	0.097	0.084	0.302
F (000)	624	280	648	608	1120
R1[a] (I ≥ 2σ)	0.0508	0.0467	0.0478	0.0379	0.0489
wR2[b] (I ≥ 2σ)	0.1354	0.1271	0.1372	0.0910	0.1075
GOOF	1.017	1.050	1.054	1.027	1.047

[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. Hydrogen bond interactions in **1**−**5**.

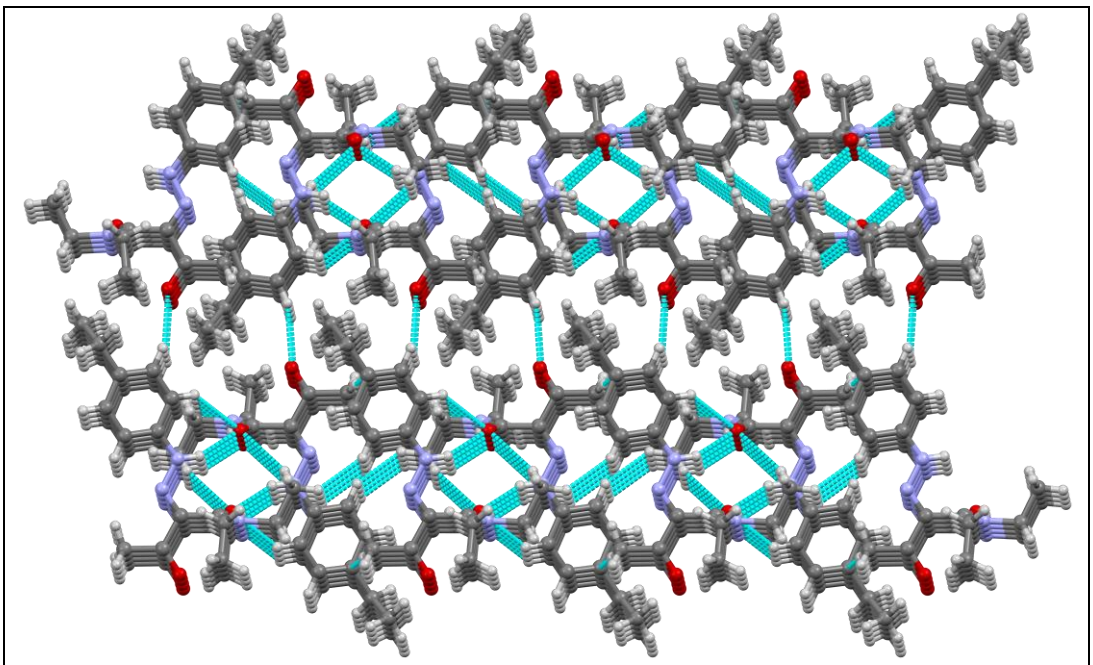
Compound	D−H···A	Distances (Å)			Angles (º)
		D−H	H···A	D···A	D−H···A
1	N(1)-H(1N)...O(1)	0.90	2.08	2.9251(19)	155
	C(5)-H(5A)...O(2)	0.95	2.53	3.433(2)	158
	C(6)-H(6A)...O(1)	0.95	2.58	3.338(2)	137
	C(9)-H(9A)...N(2)	0.98	2.34	2.814(2)	109
	C(14)-H(14C)...O(1)	0.98	2.57	3.483(2)	155
2	N(1)-H(1N)...O(3)	0.90	1.99	2.848(3)	160
	N(5)-H(5N)...O(1)	0.90	1.96	2.818(3)	158
	C(11)-H(11B)...N(8)	0.97	2.61	3.508(5)	154
	C(20)-H(20A)...O(4)	0.93	2.55	3.335(4)	142
	C(24)-H(24B)...N(6)	0.96	2.46	2.787(4)	100
	C(28)-H(28B)...O(3)	0.97	2.29	2.727(4)	107
	C(28)-H(28A)...N(8)	0.97	2.63	3.597(5)	174
	C(6)-H(6A)...O(3)	0.93	2.61	3.302(4)	132
	C(5)-H(5A)...O(2)	0.93	2.70	3.446(4)	138
	C(11)-H(11A)...O(4)	0.97	2.72	3.524(4)	141
	C(27)-H(27A)...O(3)	0.96	2.70	3.422(4)	132
3	O(4)-H(4O)...O(2)	0.86(3)	1.73(3)	2.5780(16)	168(2)
	N(1)-H(1N)...O(3)	0.90	2.26	3.0986(16)	155.1
	C(9)-H(9B)...N(2)	0.98	2.62	3.555(2)	160.6
	C(12)-H(12B)...O(1)#4	0.98	2.51	3.241(2)	131.6
4	N(1)-H(1N)...O(1)	0.90	2.08	2.9504(15)	161
	C(5)-H(5A)...O(2)	0.93	2.61	3.415(2)	146
	C(6)-H(6A)...O(1)	0.93	2.62	3.348(2)	136
	C(12)-H(12B)...O(1)	0.96	2.68	3.585(3)	157
	C(14)-H(14C)...O(2)	0.96	2.67	3.619(3)	168
5	N(1)-H(1N)...O(1)	0.90	2.34	2.897(2)	120.3
	N(1)-H(1N)...O(2)	0.90	2.15	2.947(2)	146.7
	N(4)-H(4N)...O(3)	0.90	2.28	2.841(2)	120.6
	N(4)-H(4N)...O(4)	0.90	2.21	2.983(2)	143.5
	C(2)-H(2A)...O(2)	0.95	2.50	3.217(2)	132.7
	C(3)-H(3A)...O(3)	0.95	2.38	3.314(2)	169.3
	C(10)-H(10A)...Cl(2)	0.98	2.80	3.494(2)	128.1
	C(14)-H(14A)...O(4)	0.95	2.50	3.149(2)	125.4
	C(21)-H(21B)...N(5)	0.98	2.61	3.407(3)	138.1

References

[s1] SMART & SAINT Software Reference Manuals, Version 6.22, Bruker AXS Analytic X-ray Systems, Inc., Madison, WI, 2000.

[s2] Sheldrick GM. SADABS Software for Empirical Absorption Correction, University of Göttingen, Germany, 2000.

[s3] Sheldrick GM. SHELXTL V5.1, Software Reference Manual, Bruker AXS Inc., Madison, Wisconsin, 1997.



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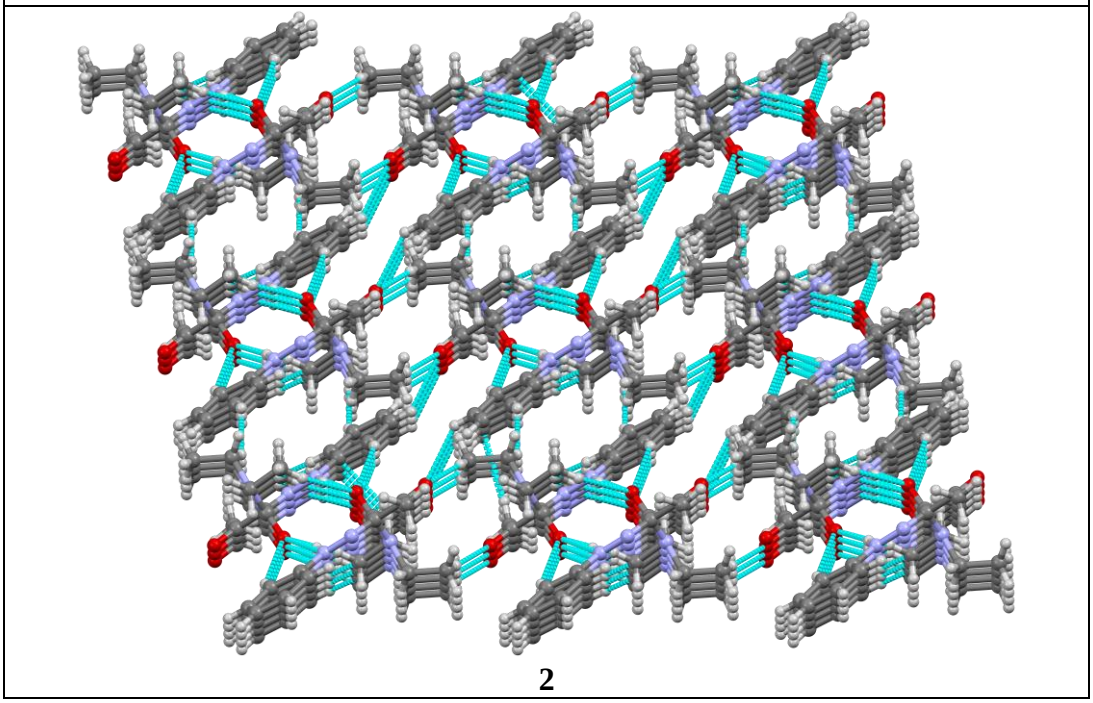

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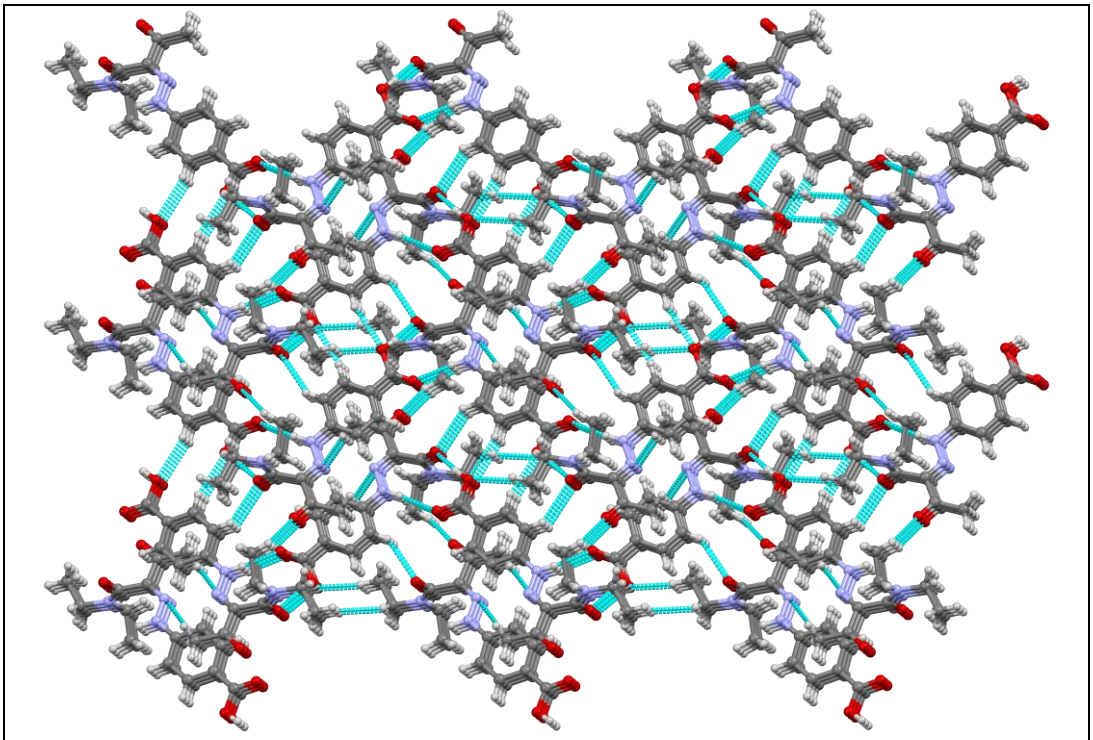

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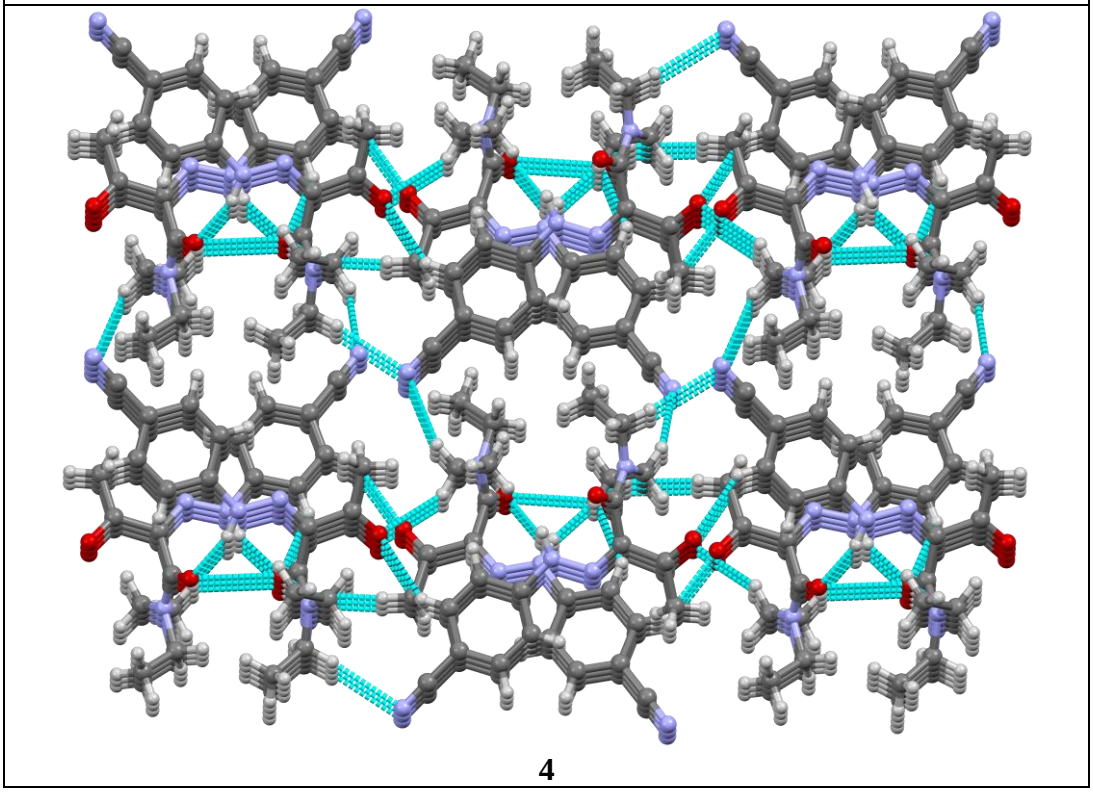

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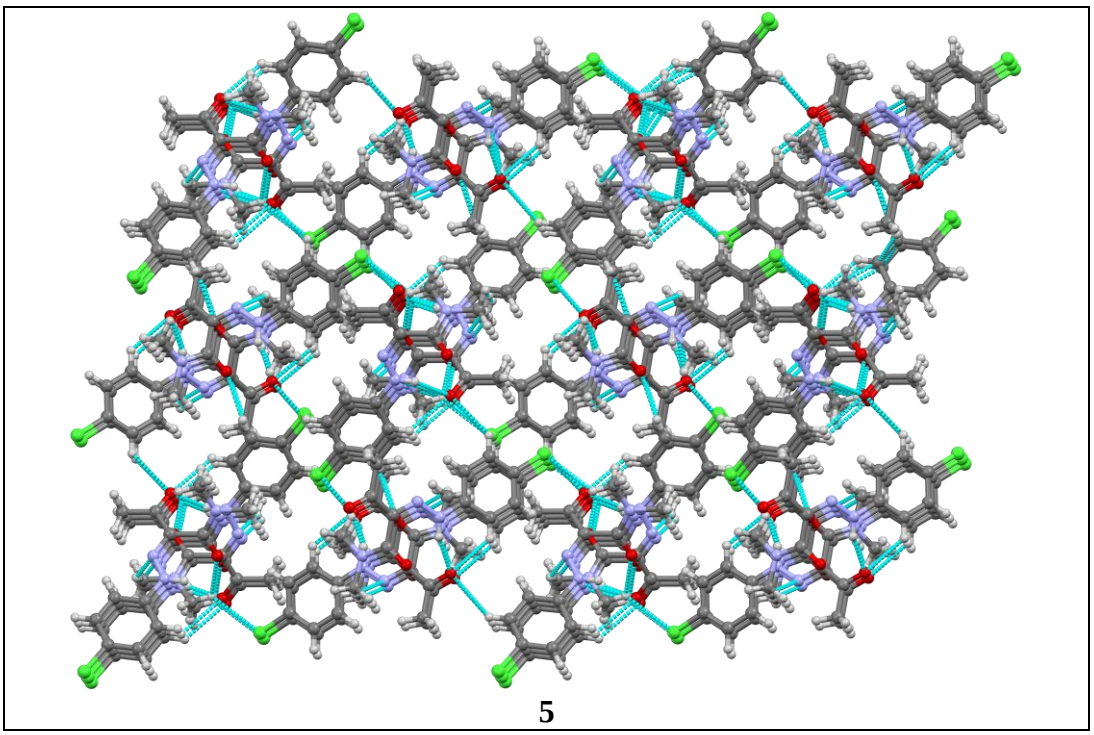

5

Figure S11. Packing diagrams of **1**−**5**.

5. Computational details

The full geometry optimization of all structures has been carried out at the DFT level of theory using the M06-2X[S4] functional with the help of the Gaussian-09[S5] program package. The 6-31+G* basis set was used for the calculations of the molecular structures. The solvent effects were taken into account in single-point calculations using the Solvation Model based on Density (SMD) model[S6] with chloroform taken as solvent. The Gibbs free energies in solution (G_s) were calculated as $G_s = E_s - E_g + G_g$ where E_g and G_g are total and Gibbs free energies in gas phase and E_s is total energy in solution. No symmetry operations have been applied in calculations. The Hessian matrix was calculated analytically for the optimized structures to prove the location of correct minima (no imaginary frequencies were found) and to estimate the thermodynamic parameters, the latter calculated at 25 °C. The topological analysis of the electron density distribution with help of the AIM method of Bader[S7] was performed using the program AIMAll.[S8]

References

[S4] Y. Zhao and D. G. Truhlar, *Theor. Chem. Acc.*, 2008, **120**, 215.

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[S6] A. V. Marenich, C. J. Cramer and D. G. Truhlar, *J. Phys. Chem. B*, 2009, **113**, 6378.

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[S8] T. A. Keith and T. K. Gristmill, AIMAll (Version 13.01.27), Software, Overland Park KS, USA, 2013 (aim.tkgristmill.com).

Table S3. Calculated total and Gibbs free energies in gas phase and chloroform solution (in Hartree).

Structure	E_g	E_s	G_g
X = Et			
***E*-hydrazone-I**	-1875.723662	-1875.763873	-1875.057431
***Z*-hydrazone-I**	-1875.753657	-1875.793157	-1875.086457
***E*-hydrazone-II**	-937.860328	-937.883602	-937.537355
***Z*-enol-azo-III**	-937.845023	-937.867046	-937.521722
***Z*-hydrazone-II**	-937.860651	-937.884925	-937.538355
X = H			
***Z*-hydrazone-I**	-1718.573220		-1718.011657
X = COOH			
***Z*-hydrazone-I**	-2095.612198		-2095.025611
X = CN			
***Z*-hydrazone-I**	-1903.011914		-1902.453890
Model structures			
Acetyl derivatives			
R = H	-780.707579		-780.490796
R = Et	-859.293161		-859.023239
Methyl derivatives			
R = H	-667.403924		-667.194824
R = Et (conformer 1)	-745.988841		-745.727437
R = Et (conformer 2)	-745.989541		-745.726238

Table S4. Cartesian atomic coordinates (in Å) of the equilibrium structures (either atomic symbol or nuclear charge is indicated in the first column).

***E*-hydrazone-I (X = Et)**

O	0.032882	1.245235	-0.646477
O	-1.066867	4.233187	0.522876
N	-2.737720	-0.012411	0.410454
H	-1.794207	-0.403044	0.500004
N	-2.950834	1.290678	0.308654
C	0.134919	1.630034	1.719575
C	-3.806686	-0.917357	0.375382
C	-5.127342	-0.502343	0.187678
H	-5.348444	0.552881	0.071165
C	-6.143637	-1.452531	0.158698
H	-7.170452	-1.120065	0.016220
C	-5.882128	-2.817543	0.306324
C	-4.552417	-3.208565	0.488661
H	-4.316438	-4.264023	0.609173
C	-3.520139	-2.278366	0.526354
H	-2.492737	-2.600009	0.681924
C	-1.957254	2.109283	0.289048
C	-2.092194	3.594355	0.255209
N	-3.262293	4.213272	-0.036441
C	-4.486367	3.587395	-0.533777
C	-3.264873	5.675702	0.038451
C	-0.513138	1.645672	0.367706
C	-6.989329	-3.838879	0.210124
H	-7.916356	-3.416448	0.615826
H	-6.741093	-4.708275	0.830291
C	-7.225135	-4.293786	-1.235386
H	-8.026612	-5.037659	-1.291211
H	-7.501332	-3.443033	-1.867187
H	-6.314994	-4.736601	-1.653230
O	-0.134287	-1.382615	0.761775
O	1.146879	-4.316497	-0.335021
N	2.681307	-0.037235	-0.392690
H	1.729792	0.333097	-0.487802
N	2.915712	-1.324181	-0.173732
C	-0.092477	-1.718268	-1.614174
C	3.732494	0.888972	-0.404752
C	5.058260	0.514105	-0.175749
H	5.297884	-0.526288	0.013713
C	6.055616	1.484743	-0.199276
H	7.086929	1.183893	-0.023333
C	5.769781	2.830888	-0.441875
C	4.434584	3.182246	-0.663439
H	4.179566	4.222432	-0.856485
C	3.421228	2.231215	-0.648930
H	2.388970	2.521240	-0.832700
C	1.934845	-2.152417	-0.085868

C	2.106700	-3.630616	0.035379
N	3.247485	-4.190964	0.506470
C	3.333011	-5.652375	0.421868
C	4.361293	-3.485259	1.135951
C	0.483308	-1.731526	-0.229473
C	6.855022	3.879272	-0.407264
H	7.805501	3.434127	-0.724965
H	6.622701	4.672462	-1.128042
C	7.018783	4.491739	0.989136
H	7.806156	5.252628	0.997688
H	7.278436	3.719630	1.721168
H	6.084741	4.959933	1.317086
H	-2.648183	5.974554	0.888454
H	-4.296113	5.985595	0.239086
C	-2.743278	6.316979	-1.243951
H	-4.911452	4.277087	-1.273096
C	-5.494677	3.320607	0.579194
H	-4.237091	2.665665	-1.059339
H	-2.792400	7.408299	-1.173097
H	-3.337396	6.004401	-2.109499
H	-1.702992	6.024490	-1.407755
H	-5.741072	4.244651	1.112879
H	-5.083847	2.605035	1.296959
H	-6.423170	2.911424	0.166195
H	0.110239	2.645279	2.127511
H	1.160940	1.259791	1.660088
H	-0.448585	0.980086	2.384052
C	5.568469	-3.354948	0.213380
H	4.632201	-4.052551	2.034673
H	4.020993	-2.504167	1.462878
H	2.408382	-6.076064	0.825646
H	4.161169	-5.958545	1.068340
C	3.554355	-6.151884	-1.003342
H	5.292558	-2.806411	-0.692447
H	5.949045	-4.339510	-0.078937
H	6.378877	-2.818657	0.718927
H	2.712675	-5.863315	-1.637365
H	3.632536	-7.243973	-1.010405
H	4.474654	-5.737260	-1.426475
H	0.537435	-1.099368	-2.264747
H	-1.112340	-1.327069	-1.613956
H	-0.069136	-2.744196	-1.997268

***Z*-hydrazone-I (X = Et)**

O	-0.852548	1.088403	0.724274
O	-0.590217	4.337001	1.331533
N	2.417400	1.267390	-0.295488
H	1.703204	0.571982	-0.553341
N	2.100560	2.354408	0.377465
N	-0.731973	2.166142	-1.279059
C	3.760227	0.862630	-0.387545

C	4.796364	1.594717	0.196969
H	4.569308	2.502997	0.744251
C	6.107452	1.146856	0.062486
H	6.910372	1.723747	0.517897
C	6.418785	-0.021188	-0.639507
C	5.363707	-0.737809	-1.212355
H	5.575397	-1.650619	-1.765752
C	4.046107	-0.309015	-1.097207
H	3.234580	-0.875371	-1.548182
C	0.863130	2.708570	0.494862
C	0.559275	3.934559	1.268349
C	1.701911	4.642514	1.958646
H	2.498398	4.878641	1.247470
H	1.318663	5.554456	2.417959
H	2.136903	3.992169	2.724198
C	-0.319496	1.916675	-0.025151
C	-0.064969	3.116102	-2.171294
H	-0.105848	2.687783	-3.178927
H	0.991512	3.173394	-1.897671
C	-0.707862	4.499878	-2.146968
H	-0.187434	5.166098	-2.842314
H	-1.759269	4.452208	-2.447195
H	-0.663380	4.928680	-1.142352
C	-1.936712	1.503970	-1.784535
H	-2.481765	2.236681	-2.389730
H	-2.564424	1.259916	-0.925806
C	-1.618123	0.253943	-2.599287
H	-2.543289	-0.284066	-2.833185
H	-1.122721	0.508034	-3.542825
H	-0.952307	-0.408270	-2.039638
C	7.838994	-0.524411	-0.728999
H	8.531717	0.325277	-0.708481
H	7.989016	-1.030366	-1.690119
C	8.179189	-1.488979	0.413560
H	9.211242	-1.846241	0.335901
H	8.057948	-0.996027	1.383890
H	7.513202	-2.358156	0.396285
O	0.852525	-1.088577	-0.724460
O	0.590087	-4.336938	-1.332261
N	-2.417329	-1.267689	0.295710
H	-1.703019	-0.572330	0.553452
N	-2.100616	-2.354554	-0.377565
N	0.731784	-2.166256	1.278905
C	-3.760113	-0.862779	0.387834
C	-4.796363	-1.594832	-0.196513
H	-4.569442	-2.503195	-0.743712
C	-6.107402	-1.146825	-0.061985
H	-6.910409	-1.723685	-0.517280
C	-6.418568	0.021317	0.639908
C	-5.363375	0.737885	1.212622

H	-5.574934	1.650771	1.765945
C	-4.045827	0.308955	1.097420
H	-3.234209	0.875287	1.548257
C	-0.863192	-2.708685	-0.495140
C	-0.559388	-3.934469	-1.268953
C	-1.702088	-4.642382	-1.959203
H	-2.497022	-4.881414	-1.247224
H	-1.318247	-5.552776	-2.421083
H	-2.139382	-3.990980	-2.722516
C	0.319420	-1.916824	0.024944
C	0.064743	-3.116250	2.171082
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H	-0.991791	-3.173339	1.897624
C	0.707458	-4.500103	2.146470
H	0.187046	-5.166375	2.841777
H	1.758913	-4.452583	2.446559
H	0.662809	-4.928751	1.141795
C	1.936496	-1.504107	1.784462
H	2.481499	-2.236847	2.389674
H	2.564267	-1.260050	0.925775
C	1.617876	-0.254098	2.599229
H	2.543031	0.283919	2.833150
H	1.122458	-0.508218	3.542751
H	0.952065	0.408118	2.039576
C	-7.838703	0.524741	0.729445
H	-8.531570	-0.324814	0.708371
H	-7.988792	1.030228	1.690802
C	-8.178539	1.489961	-0.412672
H	-9.210528	1.847400	-0.334975
H	-8.057261	0.997468	-1.383230
H	-7.512376	2.358993	-0.394868

***Z*-hydrazone-I (X = H)**

8	-0.462955	-1.302957	-0.739606
8	0.815065	-4.286251	-1.318193
7	2.701649	-0.433291	0.330499
1	1.804724	0.006324	0.580576
7	2.742343	-1.563763	-0.347345
7	-0.025058	-2.262459	1.280504
6	3.853248	0.364289	0.432298
6	5.071386	-0.026387	-0.131647
1	5.137179	-0.966915	-0.666948
6	6.181781	0.801773	0.004527
1	7.127078	0.494152	-0.433885
6	6.092862	2.012985	0.690043
6	4.872340	2.392667	1.247786
1	4.786023	3.333344	1.783982
6	3.752717	1.575963	1.126933
1	2.797915	1.870350	1.556375
6	1.678020	-2.283519	-0.476323
6	1.778006	-3.541236	-1.255601

6	3.084453	-3.847355	-1.949413
1	3.913543	-3.839228	-1.236213
1	3.003480	-4.824495	-2.426973
1	3.298383	-3.080014	-2.700165
6	0.299604	-1.905245	0.027216
6	0.904538	-2.936008	2.189331
1	0.712854	-2.538210	3.191911
1	1.924984	-2.645368	1.927330
6	0.751196	-4.454352	2.171867
1	1.451899	-4.908703	2.879319
1	-0.261691	-4.752761	2.459603
1	0.947046	-4.850909	1.172167
6	-1.388132	-2.032526	1.764552
1	-1.672568	-2.905330	2.362225
1	-2.046185	-2.006548	0.894348
6	-1.511012	-0.749927	2.581342
1	-2.565835	-0.541140	2.790566
1	-0.983272	-0.833577	3.537700
1	-1.081701	0.094201	2.035432
1	6.964196	2.652950	0.788262
8	0.462976	1.302791	0.739767
8	-0.815126	4.286466	1.317565
7	-2.701628	0.433162	-0.330378
1	-1.804700	-0.006500	-0.580379
7	-2.742326	1.563669	0.347414
7	0.025157	2.262331	-1.280321
6	-3.853278	-0.364334	-0.432297
6	-5.071441	0.026430	0.131533
1	-5.137211	0.966952	0.666848
6	-6.181891	-0.801637	-0.004765
1	-7.127204	-0.493948	0.433564
6	-6.093007	-2.012836	-0.690307
6	-4.872465	-2.392598	-1.247952
1	-4.786176	-3.333265	-1.784171
6	-3.752786	-1.575991	-1.126967
1	-2.797973	-1.870438	-1.556341
6	-1.677992	2.283406	0.476391
6	-1.778039	3.541394	1.255226
6	-3.084482	3.847671	1.948977
1	-3.913655	3.838923	1.235885
1	-3.003658	4.825110	2.425950
1	-3.298152	3.080742	2.700227
6	-0.299568	1.905075	-0.027070
6	-0.904394	2.935996	-2.189097
1	-0.712617	2.538438	-3.191755
1	-1.924837	2.645234	-1.927222
6	-0.751180	4.454343	-2.171215
1	-1.451873	4.908829	-2.878591
1	0.261702	4.752923	-2.458791
1	-0.947147	4.850602	-1.171415

6	1.388246	2.032382	-1.764316
1	1.672740	2.905199	-2.361941
1	2.046258	2.006342	-0.894079
6	1.511118	0.749804	-2.581141
1	2.565940	0.541010	-2.790361
1	0.983389	0.833482	-3.537502
1	1.081797	-0.094337	-2.035254
1	-6.964385	-2.652727	-0.788626

***Z*-hydrazone-I (X = COOH)**

8	0.857867	1.121265	-0.640656
8	0.582657	4.389631	-1.151285
7	-2.440506	1.216111	0.226594
1	-1.724852	0.524046	0.491017
7	-2.113696	2.336135	-0.398943
7	0.656619	2.157377	1.379176
6	-3.771384	0.792622	0.242943
6	-4.788801	1.531504	-0.374227
1	-4.546061	2.457302	-0.882686
6	-6.094779	1.062868	-0.328355
1	-6.888321	1.627762	-0.806588
6	-6.398590	-0.135235	0.325359
6	-5.376226	-0.865407	0.939950
1	-5.624505	-1.793663	1.445635
6	-4.068418	-0.409047	0.904815
1	-3.267587	-0.973356	1.375837
6	-0.882098	2.714081	-0.441069
6	-0.562231	3.974449	-1.160761
6	-1.681155	4.688629	-1.879537
1	-2.510037	4.895488	-1.196720
1	-1.290054	5.617687	-2.295534
1	-2.074648	4.055696	-2.681233
6	0.291111	1.927330	0.108765
6	-0.045796	3.088140	2.265587
1	-0.062443	2.629528	3.260612
1	-1.085946	3.165726	1.939223
6	0.610110	4.465085	2.315975
1	0.054780	5.116730	2.997738
1	1.641040	4.399649	2.676884
1	0.628095	4.921292	1.322664
6	1.847026	1.491034	1.913832
1	2.354920	2.207328	2.568174
1	2.515351	1.286210	1.075518
6	1.507877	0.209194	2.668849
1	2.428376	-0.324797	2.928877
1	0.965256	0.424740	3.595626
1	0.879014	-0.442158	2.056255
6	-7.778828	-0.668031	0.391838
8	-0.857880	-1.121179	0.640783
8	-0.582658	-4.389652	1.151173
7	2.440496	-1.216039	-0.226500

1	1.724844	-0.523952	-0.490881
7	2.113687	-2.336071	0.399024
7	-0.656658	-2.157284	-1.379042
6	3.771391	-0.792602	-0.242930
6	4.788815	-1.531527	0.374175
1	4.546067	-2.457315	0.882650
6	6.094810	-1.062946	0.328225
1	6.888357	-1.627872	0.806411
6	6.398632	0.135143	-0.325510
6	5.376262	0.865354	-0.940043
1	5.624549	1.793598	-1.445747
6	4.068437	0.409050	-0.904828
1	3.267602	0.973389	-1.375809
6	0.882085	-2.714003	0.441164
6	0.562226	-3.974460	1.160708
6	1.681144	-4.688691	1.879443
1	2.510023	-4.895509	1.196609
1	1.290037	-5.617777	2.295371
1	2.074645	-4.055818	2.681182
6	-0.291123	-1.927237	-0.108642
6	0.045729	-3.088070	-2.265448
1	0.062323	-2.629511	-3.260499
1	1.085894	-3.165619	-1.939123
6	-0.610144	-4.465034	-2.315711
1	-0.054830	-5.116710	-2.997457
1	-1.641094	-4.399650	-2.676571
1	-0.628062	-4.921173	-1.322367
6	-1.847072	-1.490931	-1.913671
1	-2.354993	-2.207221	-2.567996
1	-2.515373	-1.286092	-1.075339
6	-1.507926	-0.209097	-2.668701
1	-2.428426	0.324890	-2.928730
1	-0.965308	-0.424650	-3.595478
1	-0.879063	0.442262	-2.056114
6	7.778888	0.667880	-0.392073
8	-8.680491	0.112904	-0.244771
8	-8.101712	-1.692648	0.948472
8	8.680554	-0.113081	0.244500
8	8.101780	1.692490	-0.948716
1	-9.545352	-0.320057	-0.143705
1	9.545425	0.319850	0.143395

***Z*-hydrazone-I (X = CN)**

8	0.818668	1.149070	-0.648338
8	0.408929	4.380933	-1.228405
7	-2.482801	1.115105	0.205796
1	-1.737314	0.454959	0.469328
7	-2.207656	2.238486	-0.441061
7	0.553488	2.210069	1.350511
6	-3.794570	0.641252	0.248538
6	-4.852782	1.343500	-0.342417

1	-4.656835	2.279527	-0.852237
6	-6.139208	0.830229	-0.268211
1	-6.964671	1.367064	-0.725169
6	-6.384694	-0.381040	0.390466
6	-5.321623	-1.077750	0.979867
1	-5.510567	-2.016823	1.490231
6	-4.033432	-0.571061	0.913292
1	-3.203054	-1.107738	1.364880
6	-0.992996	2.665922	-0.490404
6	-0.720100	3.924993	-1.233187
6	-1.862967	4.584468	-1.965270
1	-2.697696	4.777105	-1.285240
1	-1.504767	5.517888	-2.400620
1	-2.235372	3.922287	-2.753286
6	0.209578	1.942217	0.082167
6	-0.190804	3.130940	2.213557
1	-0.197023	2.691847	3.217390
1	-1.230614	3.162344	1.878932
6	0.413167	4.532092	2.240171
1	-0.170175	5.175872	2.905554
1	1.443538	4.512489	2.607928
1	0.420281	4.969185	1.238222
6	1.765378	1.602815	1.907409
1	2.234309	2.349694	2.556377
1	2.451524	1.413743	1.079602
6	1.470604	0.319761	2.678444
1	2.408953	-0.165261	2.968552
1	0.898439	0.526761	3.589129
1	0.886197	-0.371641	2.065643
6	-7.721247	-0.905376	0.462311
8	-0.818692	-1.149048	0.648504
8	-0.408977	-4.380658	1.229007
7	2.482787	-1.115111	-0.205766
1	1.737291	-0.454956	-0.469252
7	2.207664	-2.238454	0.441165
7	-0.553496	-2.210028	-1.350339
6	3.794572	-0.641315	-0.248675
6	4.852816	-1.343575	0.342206
1	4.656883	-2.279563	0.852103
6	6.139258	-0.830367	0.267831
1	6.964746	-1.367212	0.724733
6	6.384728	0.380851	-0.390946
6	5.321626	1.077571	-0.980279
1	5.510557	2.016602	-1.490724
6	4.033418	0.570945	-0.913533
1	3.203017	1.107630	-1.365070
6	0.993001	-2.665871	0.490587
6	0.720115	-3.924872	1.233492
6	1.862953	-4.584185	1.965767
1	2.697719	-4.776947	1.285820

1	1.504739	-5.517517	2.401295
1	2.235306	-3.921838	2.753670
6	-0.209587	-1.942190	-0.081991
6	0.190799	-3.130868	-2.213417
1	0.197019	-2.691730	-3.217230
1	1.230609	-3.162288	-1.878794
6	-0.413178	-4.532016	-2.240106
1	0.170160	-5.175762	-2.905527
1	-1.443550	-4.512387	-2.607861
1	-0.420294	-4.969166	-1.238184
6	-1.765398	-1.602774	-1.907212
1	-2.234337	-2.349651	-2.556177
1	-2.451532	-1.413710	-1.079392
6	-1.470645	-0.319712	-2.678247
1	-2.409001	0.165319	-2.968318
1	-0.898513	-0.526707	-3.588953
1	-0.886212	0.371678	-2.065459
6	7.721298	0.905120	-0.462970
7	-8.798349	-1.327531	0.519621
7	8.798413	1.327222	-0.520423

***E*-hydrazone-II (X = Et)**

O	-3.140036	-0.673932	2.256681
O	-1.627814	2.701708	0.391597
N	0.539718	1.228861	0.590184
H	0.150018	2.161660	0.441661
N	-0.279641	0.237647	0.825476
N	-2.240267	-1.973639	0.630573
C	1.927174	1.014277	0.568386
C	2.483824	-0.238709	0.834694
H	1.835250	-1.072788	1.078689
C	3.865755	-0.390880	0.796979
H	4.294509	-1.368217	1.009771
C	4.717826	0.677607	0.501168
C	4.137236	1.922377	0.242096
H	4.774549	2.774166	0.013447
C	2.758084	2.097415	0.272477
H	2.323223	3.073507	0.070811
C	-1.572255	0.397179	0.861223
C	-2.271876	1.681898	0.632353
C	-3.778297	1.712994	0.661448
H	-4.204282	0.879435	0.092939
H	-4.125355	1.597671	1.692378
H	-4.114104	2.665754	0.250164
C	-2.377499	-0.799030	1.300351
C	-1.491323	-2.146529	-0.614611
H	-1.234371	-3.209053	-0.681655
H	-0.550429	-1.599504	-0.559754
C	-2.300676	-1.715827	-1.834918
H	-1.745841	-1.911148	-2.758111
H	-3.253322	-2.254030	-1.883096

H	-2.517244	-0.642683	-1.786823
C	-3.029878	-3.111266	1.104142
H	-3.251888	-3.741140	0.235888
H	-3.974401	-2.731101	1.499349
C	-2.289874	-3.903518	2.176889
H	-2.887483	-4.760310	2.504400
H	-1.332069	-4.276160	1.797973
H	-2.096860	-3.263387	3.042100
C	6.211415	0.481382	0.409892
H	6.517431	-0.321010	1.091454
H	6.723794	1.391454	0.743492
C	6.657413	0.138179	-1.016900
H	7.741301	-0.007000	-1.067310
H	6.170678	-0.779561	-1.363071
H	6.385749	0.941077	-1.710295

***E*-enol-azo-II (X = Et)**

O	-3.002285	1.135568	1.153061
O	-3.080311	-2.902767	2.184863
N	-0.523555	0.672534	1.208356
H	-2.010843	1.336491	1.167522
N	-0.727784	-0.572386	1.238435
C	-4.565349	-0.623738	1.244890
C	0.836347	1.073532	1.246355
C	1.905196	0.184270	1.408370
H	1.703485	-0.875629	1.522496
C	3.203407	0.675595	1.433678
H	4.032908	-0.016596	1.565529
C	3.471449	2.045253	1.303473
C	2.391778	2.918105	1.148039
H	2.576293	3.985894	1.050860
C	1.084884	2.441060	1.121514
H	0.245001	3.120944	1.005912
C	-2.039238	-1.011589	1.226477
C	-2.223343	-2.486993	1.407303
N	-1.391319	-3.327348	0.718947
C	-1.333488	-4.727473	1.132495
C	-0.567433	-2.926466	-0.420393
C	-3.141277	-0.173033	1.207251
C	4.891309	2.554871	1.280590
H	5.516287	1.929848	1.928915
H	4.923662	3.570723	1.691154
C	5.470771	2.557648	-0.139799
H	6.500861	2.927613	-0.143415
H	5.467291	1.546897	-0.561044
H	4.873565	3.195764	-0.799248
C	0.078375	-5.147271	1.534194
H	-1.710187	-5.367362	0.325181
H	-2.019238	-4.832286	1.973180
H	0.486855	-2.859066	-0.120920
H	-0.873249	-1.926264	-0.725478

C	-0.721401	-3.868311	-1.613163
H	0.453692	-4.501705	2.334652
H	0.781031	-5.095836	0.695661
H	0.070312	-6.179290	1.898117
H	-0.320482	-4.866604	-1.414178
H	-0.175962	-3.457773	-2.468401
H	-1.775002	-3.969993	-1.893362
H	-4.692242	-1.618584	0.819618
H	-5.176560	0.111537	0.716381
H	-4.894974	-0.674503	2.288059

***Z*-hydrazone-II (X = Et)**

O	-5.278579	-1.312178	0.836517
O	-5.932300	-4.824932	-0.664208
N	-2.764047	-1.513534	-0.254171
H	-3.418505	-0.878963	0.207290
N	-3.186047	-2.707362	-0.591619
N	-6.603771	-1.811603	-0.927110
C	-1.394371	-1.208471	-0.266670
C	-0.444655	-2.104942	-0.763084
H	-0.765159	-3.068201	-1.144252
C	0.899266	-1.748666	-0.749907
H	1.634579	-2.454289	-1.132019
C	1.330946	-0.512757	-0.257168
C	0.362027	0.368258	0.229838
H	0.667004	1.335631	0.623348
C	-0.987660	0.032278	0.228767
H	-1.726595	0.728288	0.618774
C	-4.454053	-2.996862	-0.596859
C	-4.783843	-4.432657	-0.785301
C	-3.648576	-5.386519	-1.086870
H	-3.062943	-5.041746	-1.943556
H	-2.967261	-5.443869	-0.232816
H	-4.073503	-6.371044	-1.285754
C	-5.496080	-1.987119	-0.179003
C	-6.843323	-2.400353	-2.240801
H	-7.863006	-2.803490	-2.246615
H	-6.176968	-3.247312	-2.382283
C	-6.642206	-1.386181	-3.364463
H	-6.855809	-1.849980	-4.332654
H	-7.299419	-0.517982	-3.254664
H	-5.606567	-1.031146	-3.372611
C	-7.642294	-0.929940	-0.388136
H	-8.271489	-0.618178	-1.226555
H	-7.164120	-0.040420	0.029555
C	-8.472627	-1.643031	0.674818
H	-9.269229	-0.987636	1.040805
H	-8.926856	-2.550303	0.264101
H	-7.837379	-1.924117	1.518516
C	2.788955	-0.125382	-0.303286
H	3.409643	-1.008167	-0.108798

H	3.002818	0.592293	0.497428
C	3.178324	0.484731	-1.655202
H	4.237882	0.759522	-1.674286
H	2.993695	-0.225870	-2.467761
H	2.586094	1.383059	-1.858465

Model structures

Acetyl derivatives

R = H

8	-3.449933	2.702993	0.328603
8	-4.576958	-1.322572	-0.031696
7	-1.061732	1.690146	0.201344
1	-1.659545	2.521337	0.284671
7	-1.639096	0.534608	0.104647
7	-5.201830	1.281278	0.224359
6	0.340557	1.796070	0.192520
6	1.166263	0.673985	0.099246
1	0.723996	-0.313984	0.032213
6	2.545978	0.845395	0.099728
1	3.186782	-0.031378	0.029915
6	3.131148	2.112742	0.191942
6	2.282839	3.219413	0.284771
1	2.709765	4.217163	0.360119
6	0.900103	3.071481	0.285869
1	0.253163	3.942078	0.362186
6	-2.942893	0.389333	0.108905
6	-3.390001	-1.019171	-0.014318
6	-2.331483	-2.095553	-0.118830
1	-1.689656	-1.925997	-0.987640
1	-1.687478	-2.090217	0.764993
1	-2.837760	-3.057241	-0.207822
6	-3.883043	1.546223	0.228643
1	-5.535539	0.326825	0.137867
1	-5.835629	2.064141	0.304509
6	4.629603	2.282180	0.134217
1	5.115284	1.416814	0.600304
1	4.922600	3.161932	0.718889
6	5.132042	2.435316	-1.307019
1	6.219504	2.557260	-1.334356
1	4.869665	1.555202	-1.903272
1	4.675764	3.308888	-1.784243

R = Et

8	-1.689365	2.488026	0.557919
8	-3.428336	-1.337824	0.373733
7	0.504455	1.102461	0.643988
1	0.043911	2.020706	0.637243
7	-0.247619	0.048018	0.577995
7	-3.643295	1.359720	0.414273
6	1.902447	0.982243	0.725251
6	2.536546	-0.261782	0.755966

1	1.941557	-1.167723	0.718189
6	3.923051	-0.315271	0.840534
1	4.412361	-1.286961	0.867899
6	4.703382	0.844849	0.896009
6	4.045265	2.076845	0.864394
1	4.626114	2.995714	0.908656
6	2.658938	2.154071	0.780143
1	2.162197	3.121048	0.759685
6	-1.555142	0.111248	0.505166
6	-2.210268	-1.217456	0.439318
6	-1.329262	-2.448026	0.456943
1	-0.627095	-2.434489	-0.381068
1	-0.736027	-2.484558	1.374918
1	-1.974816	-3.324441	0.392486
6	-2.303314	1.408461	0.496590
1	-4.077615	0.441026	0.388032
6	-4.439152	2.577911	0.422886
1	-5.407106	2.333122	-0.022835
1	-3.943131	3.310268	-0.220707
6	-4.615417	3.148563	1.827595
1	-5.222473	4.059060	1.795083
1	-5.111862	2.424505	2.481017
1	-3.640337	3.397281	2.254786
6	6.209994	0.764522	0.930878
1	6.517929	-0.105341	1.523175
1	6.613280	1.649503	1.436582
6	6.810245	0.661750	-0.476942
1	7.902487	0.601444	-0.436141
1	6.435951	-0.228778	-0.992590
1	6.535830	1.534625	-1.078416

Methyl derivatives

R = H

8	-3.069004	2.239616	1.566893
7	-0.714131	1.211211	0.952774
1	-1.254008	2.048887	1.174041
7	-1.333368	0.048478	0.918997
7	-4.796394	0.793949	1.691695
6	0.657389	1.289580	0.688546
6	1.424832	0.158174	0.397306
1	0.951884	-0.816634	0.376409
6	2.785115	0.300988	0.144751
1	3.374659	-0.586967	-0.076972
6	3.415935	1.548623	0.172979
6	2.629915	2.665940	0.467674
1	3.091051	3.651148	0.500391
6	1.268500	2.547211	0.723354
1	0.674853	3.429008	0.953085
6	-2.602684	-0.072848	1.152179
6	-3.177056	-1.462972	1.075567
6	-3.482328	1.080599	1.480441

1	-5.181683	-0.132657	1.602426
1	-5.417370	1.563849	1.898009
6	4.881355	1.690622	-0.159758
1	5.420094	0.792774	0.166002
1	5.305748	2.532884	0.399851
6	5.112806	1.908145	-1.660097
1	6.179642	2.008791	-1.885564
1	4.717420	1.065936	-2.237676
1	4.602014	2.814402	-2.002110
1	-2.372831	-2.161657	0.838960
1	-3.940473	-1.549644	0.291376
1	-3.627870	-1.774285	2.026590

R = Et (conformer 1)

8	-2.694486	2.294773	0.529121
7	-0.565806	0.745880	0.730413
1	-0.940469	1.692661	0.657251
7	-1.411135	-0.267993	0.743917
7	-4.691700	1.256160	0.470726
6	0.810938	0.522756	0.816739
6	1.355504	-0.761290	0.913962
1	0.694858	-1.620521	0.924976
6	2.735700	-0.914270	0.999567
1	3.149636	-1.918097	1.077908
6	3.603667	0.181560	0.992077
6	3.037836	1.456034	0.894250
1	3.685908	2.330524	0.890150
6	1.661884	1.633068	0.807524
1	1.240630	2.633206	0.737262
6	-2.693345	-0.101166	0.663765
6	-3.538980	-1.347271	0.689312
6	-3.337050	1.237466	0.550547
1	-5.214817	0.392619	0.487919
6	-5.411925	2.516229	0.360214
6	5.100929	-0.006646	1.031236
1	5.343224	-0.902238	1.615937
1	5.563964	0.842045	1.549008
6	5.703432	-0.137024	-0.372920
1	6.789338	-0.270798	-0.326952
1	5.273308	-0.995443	-0.899519
1	5.492538	0.757658	-0.968189
1	-2.881863	-2.213490	0.784893
1	-4.123918	-1.466494	-0.231995
1	-4.235123	-1.355510	1.538037
6	-6.909890	2.263117	0.294644
1	-5.062948	3.044911	-0.533585
1	-5.155904	3.144658	1.220407
1	-7.169873	1.652144	-0.576603
1	-7.448883	3.210354	0.211887
1	-7.264517	1.753057	1.196761

R = Et (conformer 2)

8	-2.552969	1.991573	0.033360
7	-0.221285	0.759884	-0.077088
1	-0.727231	1.635825	0.060808
7	-0.911702	-0.334556	-0.336702
7	-4.382556	0.720607	-0.334457
6	1.172472	0.713282	0.015507
6	1.890999	-0.478774	-0.119127
1	1.358722	-1.405340	-0.300321
6	3.277442	-0.457634	-0.010481
1	3.826415	-1.392356	-0.111907
6	3.983451	0.724912	0.231411
6	3.245634	1.904244	0.363712
1	3.764116	2.842022	0.553948
6	1.859304	1.907268	0.258524
1	1.303940	2.836105	0.366216
6	-2.204643	-0.336824	-0.418566
6	-2.857622	-1.658668	-0.727692
6	-3.038052	0.881270	-0.217934
1	-4.763253	-0.203573	-0.473221
6	-5.293675	1.831557	-0.095657
1	-6.237462	1.594526	-0.594982
1	-4.867395	2.714604	-0.578843
6	-5.511918	2.099298	1.390907
1	-6.196076	2.942290	1.530704
1	-5.940461	1.222161	1.886277
1	-4.559217	2.342332	1.868612
6	5.491724	0.733816	0.289269
1	5.847944	-0.197380	0.746181
1	5.829810	1.551390	0.937112
6	6.120593	0.891475	-1.100674
1	7.214093	0.898321	-1.042381
1	5.816431	0.069396	-1.757107
1	5.794628	1.826951	-1.567403
1	-3.525345	-1.988231	0.079305
1	-2.079131	-2.413955	-0.847227
1	-3.439864	-1.621617	-1.657254