One–Step Synthesis of Fully Functionalized Pyrazolo[3,4-*b*]pyridines *via* Isobenzofuranone Ring Opening

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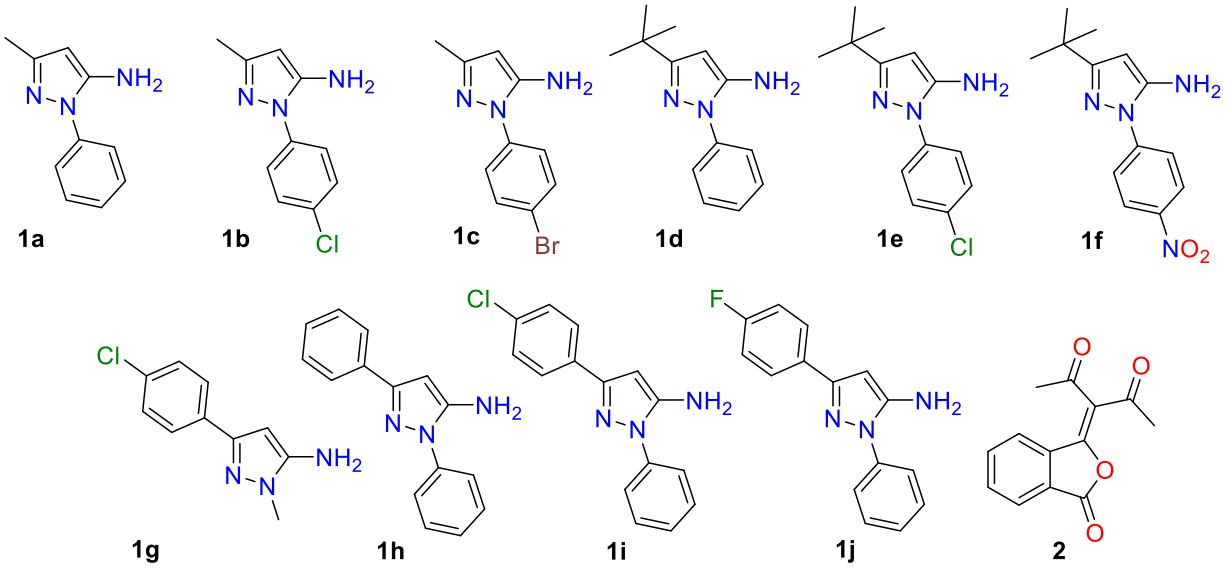
SUPPORTING INFORMATION

Content:

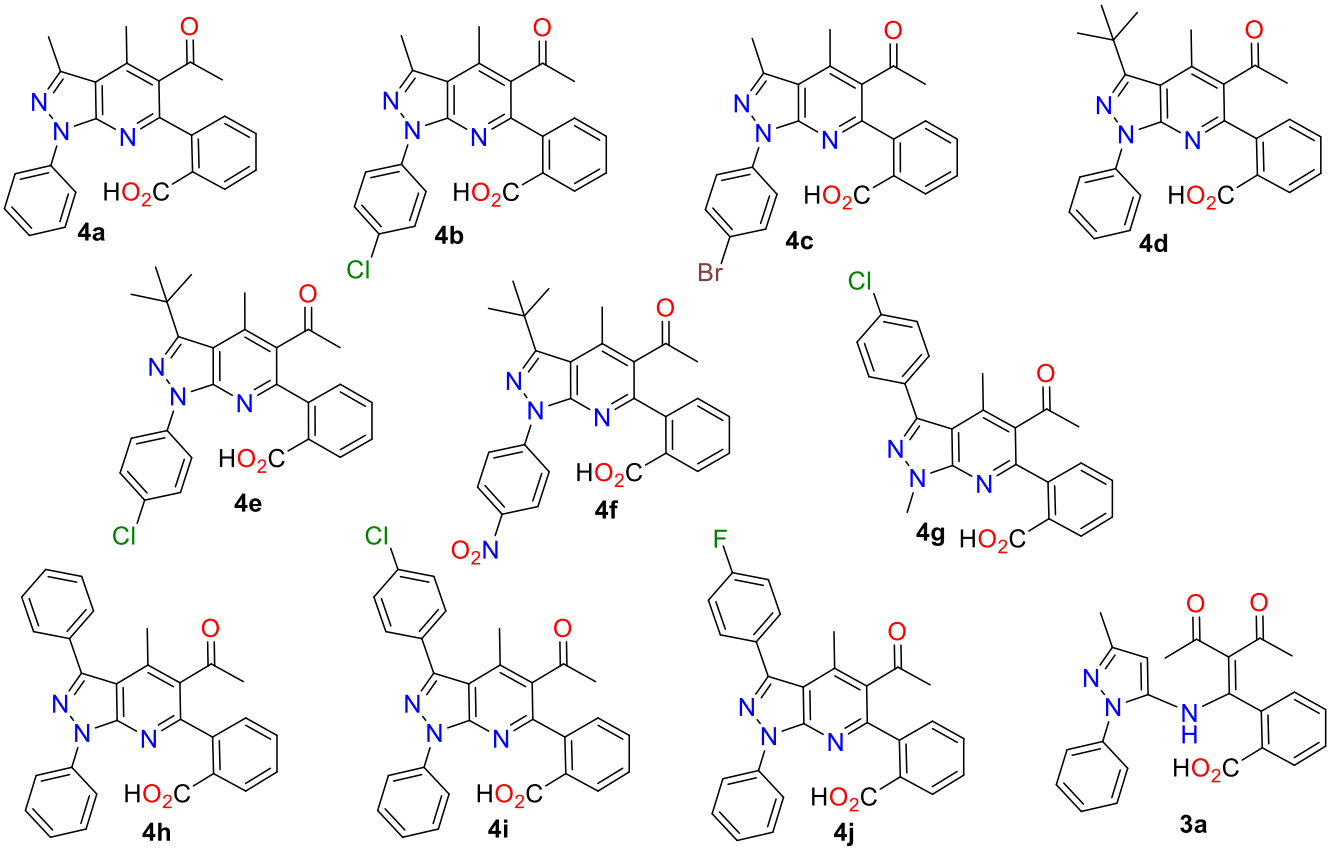
1. Overview of substrates and products numbering

***N*-Substituted 5-aminopyrazoles 1a-j and 3-(3-oxo-2-benzofuran-1(3*H*)-ylidene)pentane-2,4-dione 2**



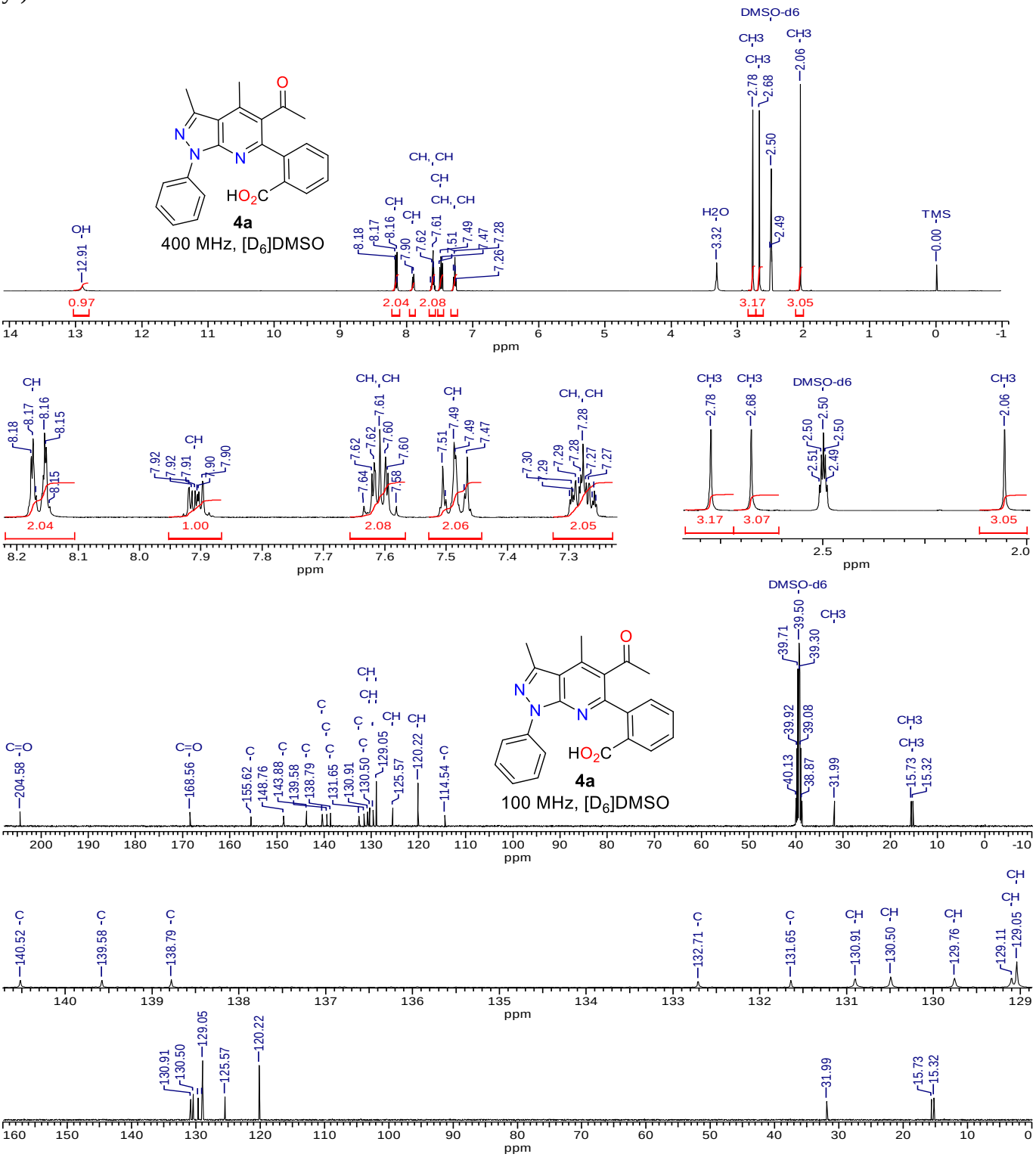
Products 4a-j and intermediate 3a

2-(5-Acetyl-1,3,4-triR-1*H*-pyrazolo[3,4-*b*]pyridin-6-yl)benzoic acid **4a-j** and 2-(2-acetyl-1-((3-methyl-1-phenyl-1*H*-pyrazol-5-yl)amino)-3-oxobut-1-en-1-yl)benzoic acid **3a**

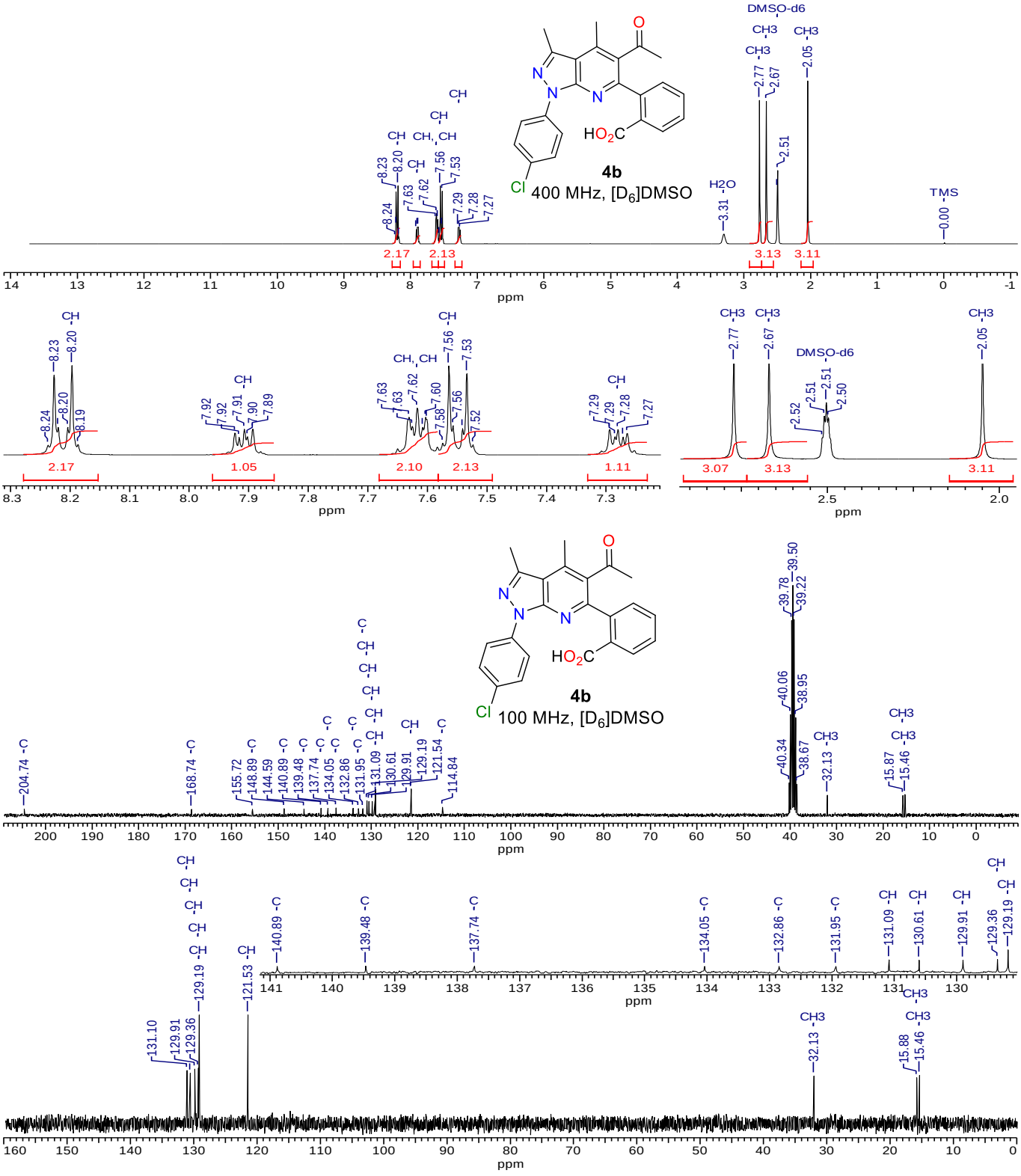


2. Copies of NMR spectra

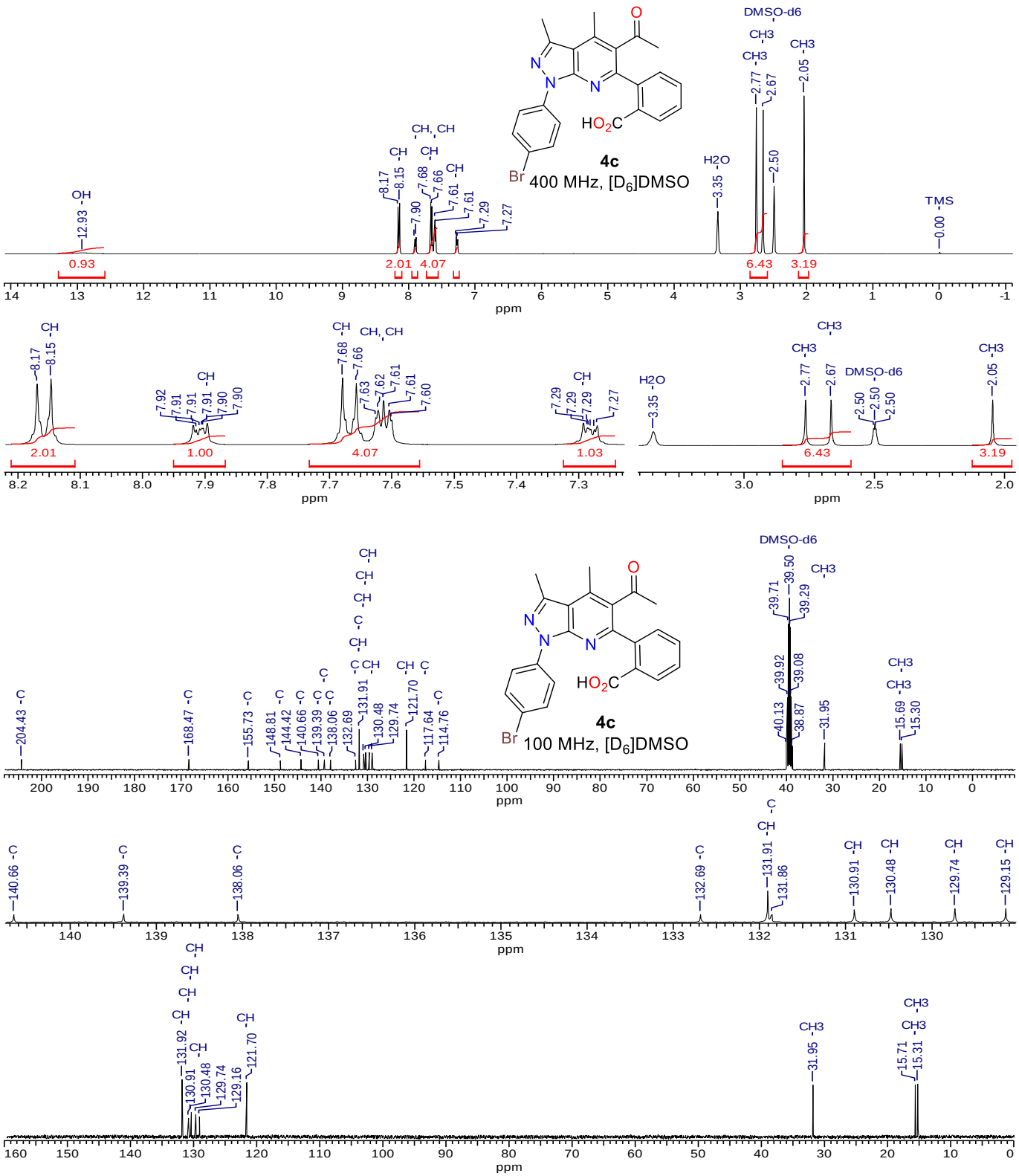
^{1}H and $^{13}C\{^{1}H\}$ NMR spectra of 2-(5-acetyl-3,4-dimethyl-1-phenyl-1*H*-pyrazolo[3,4-*b*]pyridin-6-yl)benzoic acid **4a**



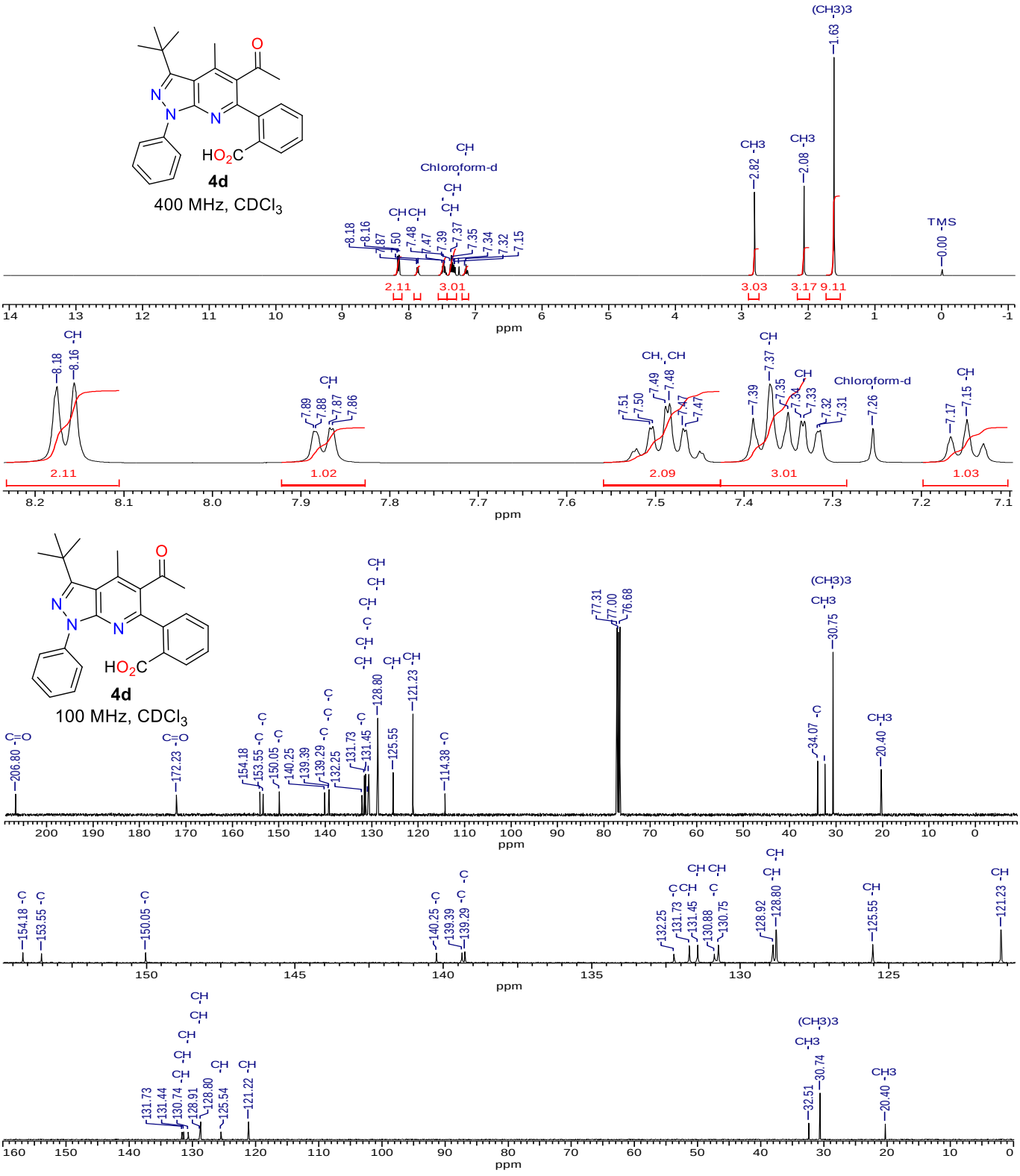
^{1}H and ^{13}C{^{1}H} NMR spectra of 2-(5-acetyl-1-(4-chlorophenyl)-3,4-dimethyl-1*H*-pyrazolo[3,4-*b*]pyridin-6-yl)benzoic acid **4b**



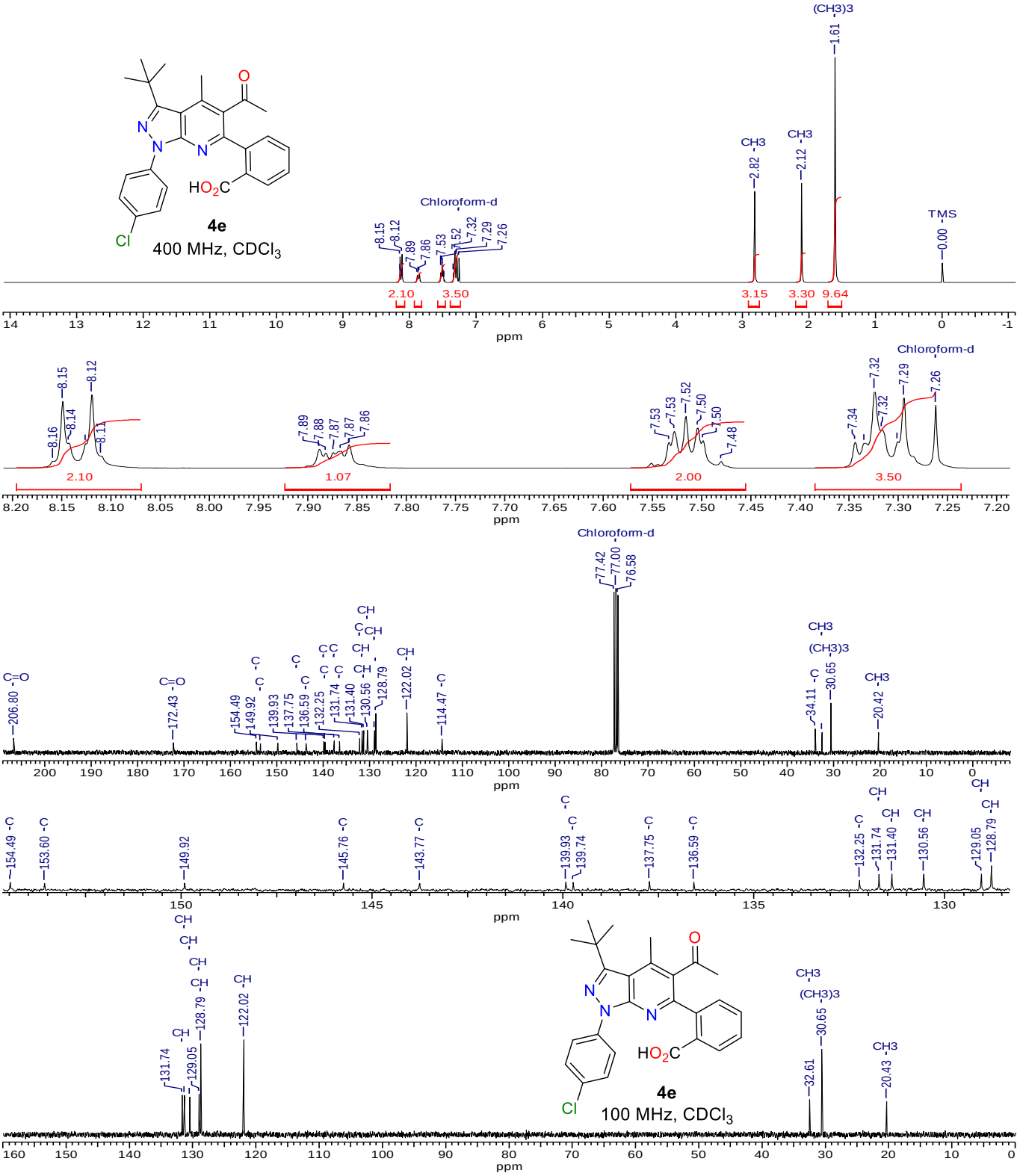
^{1}H and ^{13}C{^{1}H} NMR spectra of 2-(5-acetyl-1-(4-bromophenyl)-3,4-dimethyl-1*H*-pyrazolo[3,4-*b*]pyridin-6-yl)benzoic acid **4c**



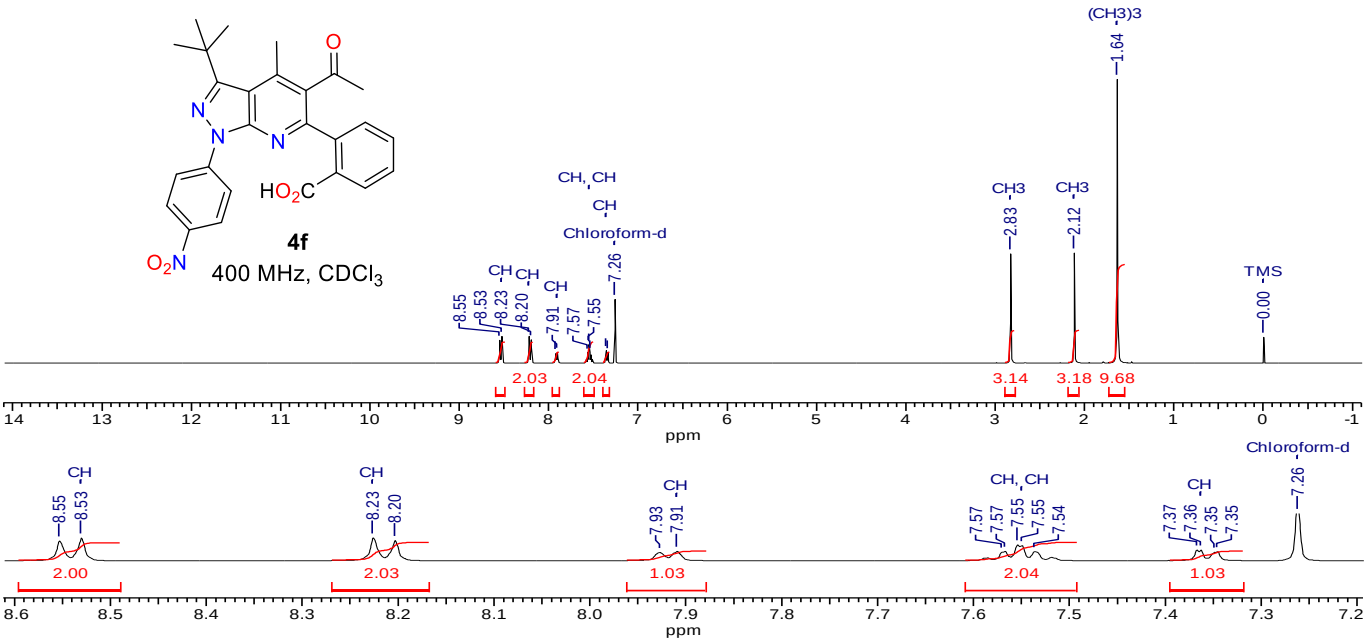
^{1}H and ^{13}C{^{1}H} NMR spectra of 2-(5-acetyl-3-(*tert*-butyl)-4-methyl-1-phenyl-1*H*-pyrazolo[3,4-*b*]pyridin-6-yl)benzoic acid **4d**

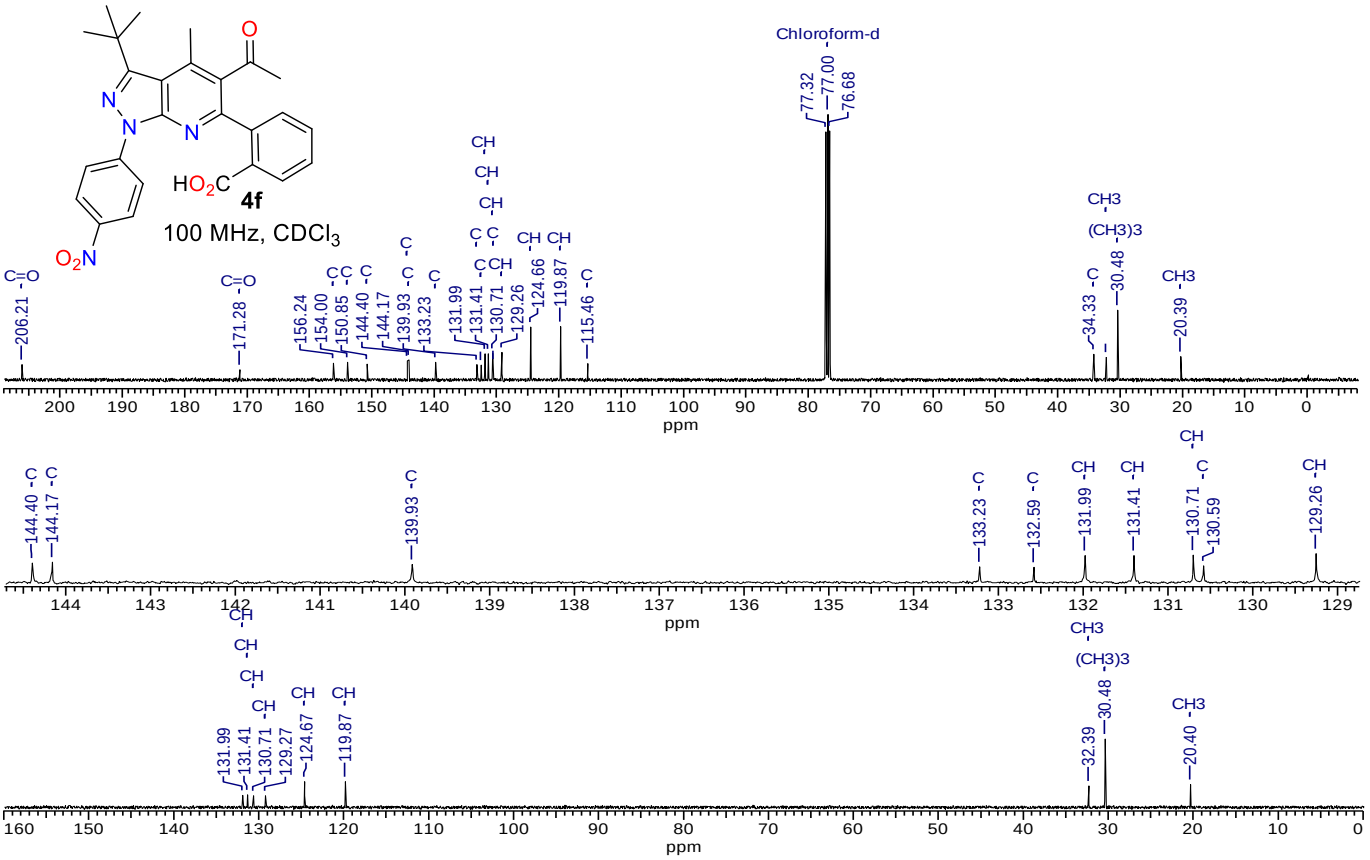


^{1}H and ^{13}C{^{1}H} NMR spectra of 2-(5-acetyl-3-(*tert*-butyl)-1-(4-chlorophenyl)-4-methyl-1*H*-pyrazolo[3,4-*b*]pyridin-6-yl)benzoic acid **4e**

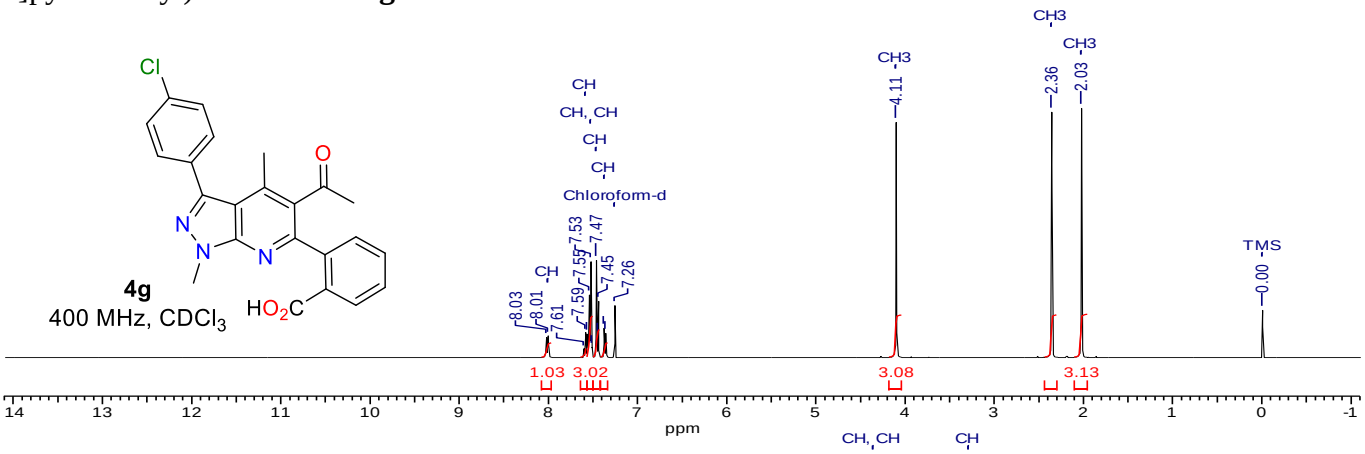


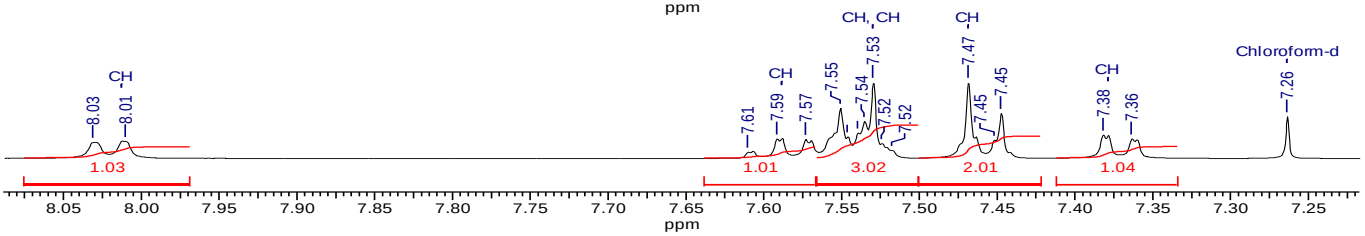
^{1}H and ^{13}C{^{1}H} NMR spectra of 2-(5-acetyl-3-(*tert*-butyl)-4-methyl-1-(4-nitrophenyl)-1*H*-pyrazolo[3,4-*b*]pyridin-6-yl)benzoic acid **4f**

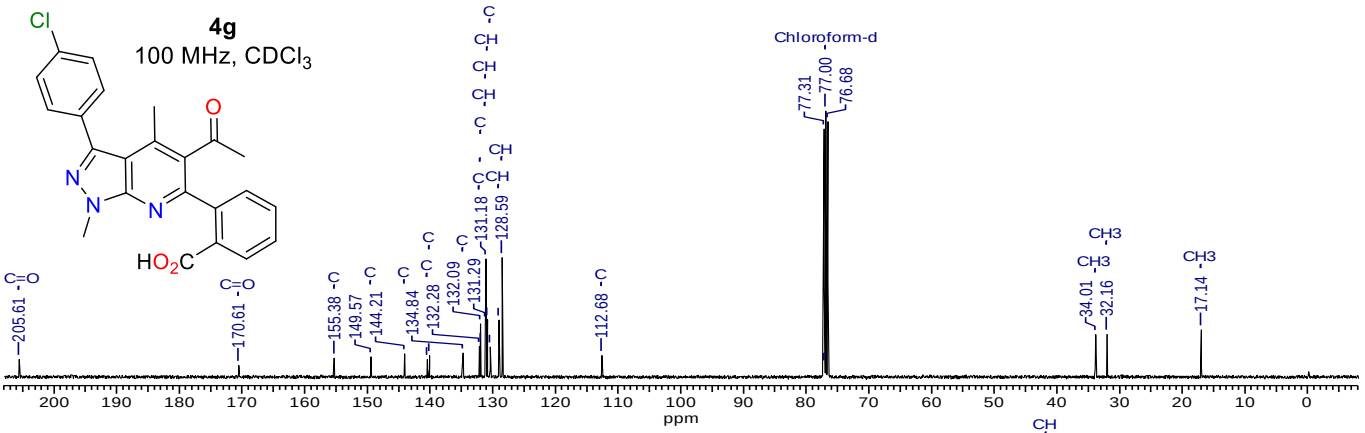


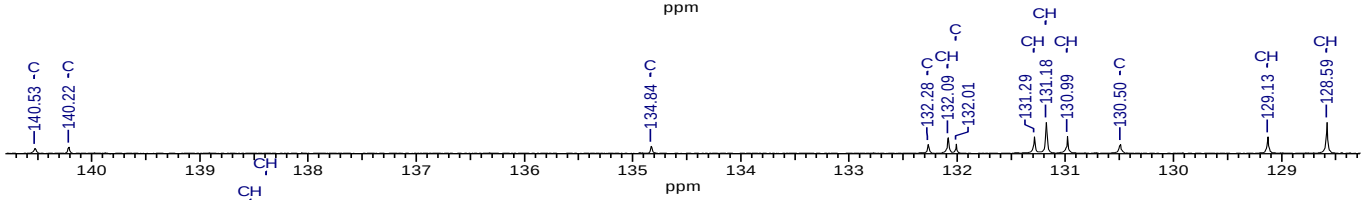


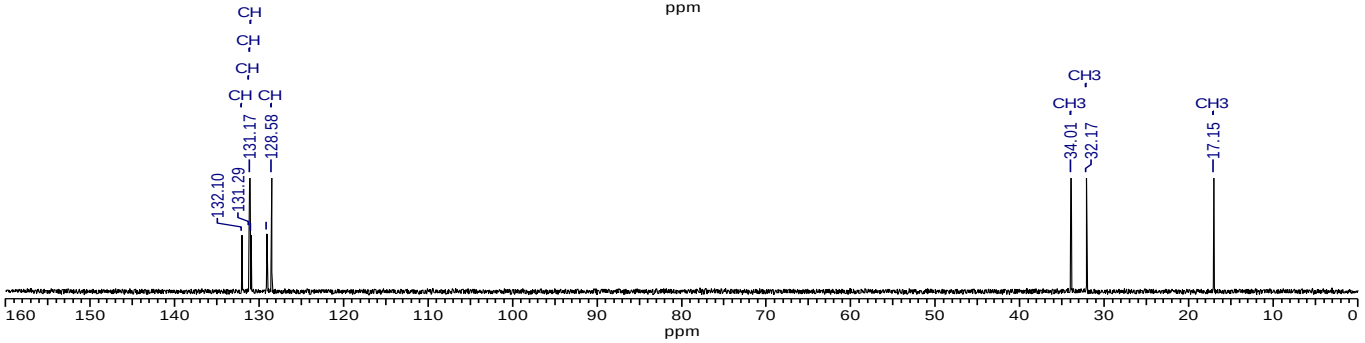
^{1}H and ^{13}C{^{1}H} NMR spectra of 2-(5-acetyl-3-(4-chlorophenyl)-1,4-dimethyl-1*H*-pyrazolo[3,4-*b*]pyridin-6-yl)benzoic acid **4g**



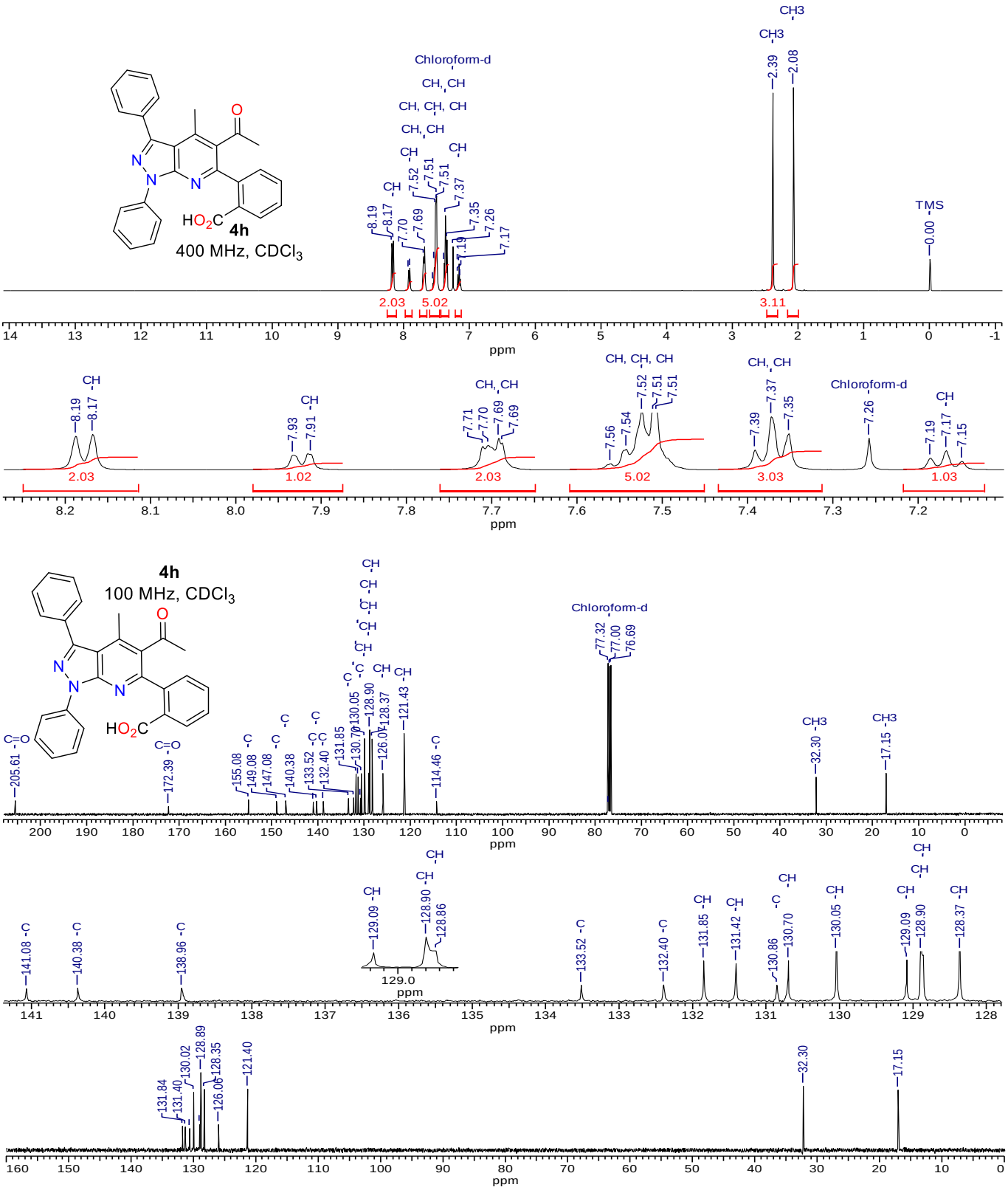




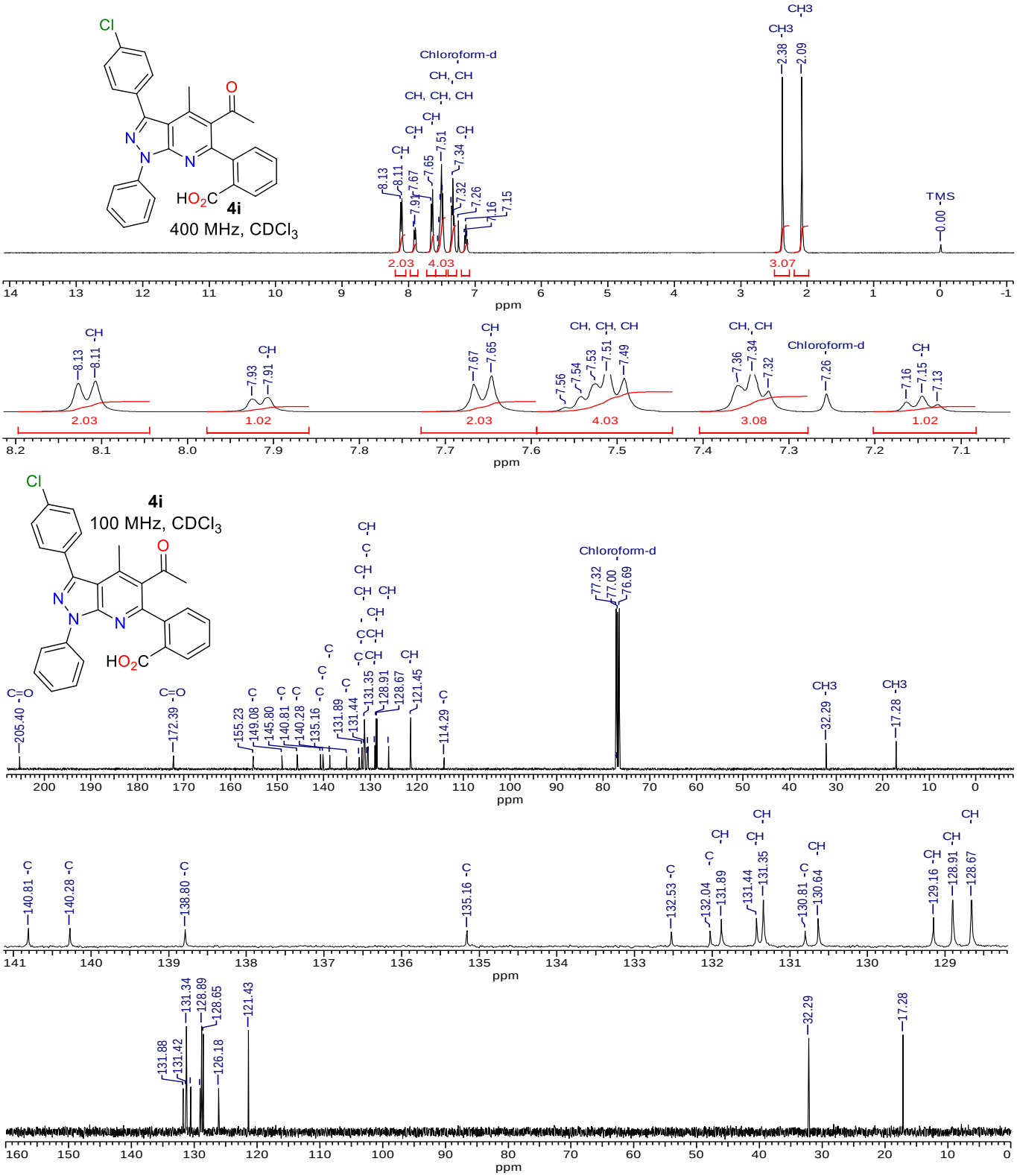




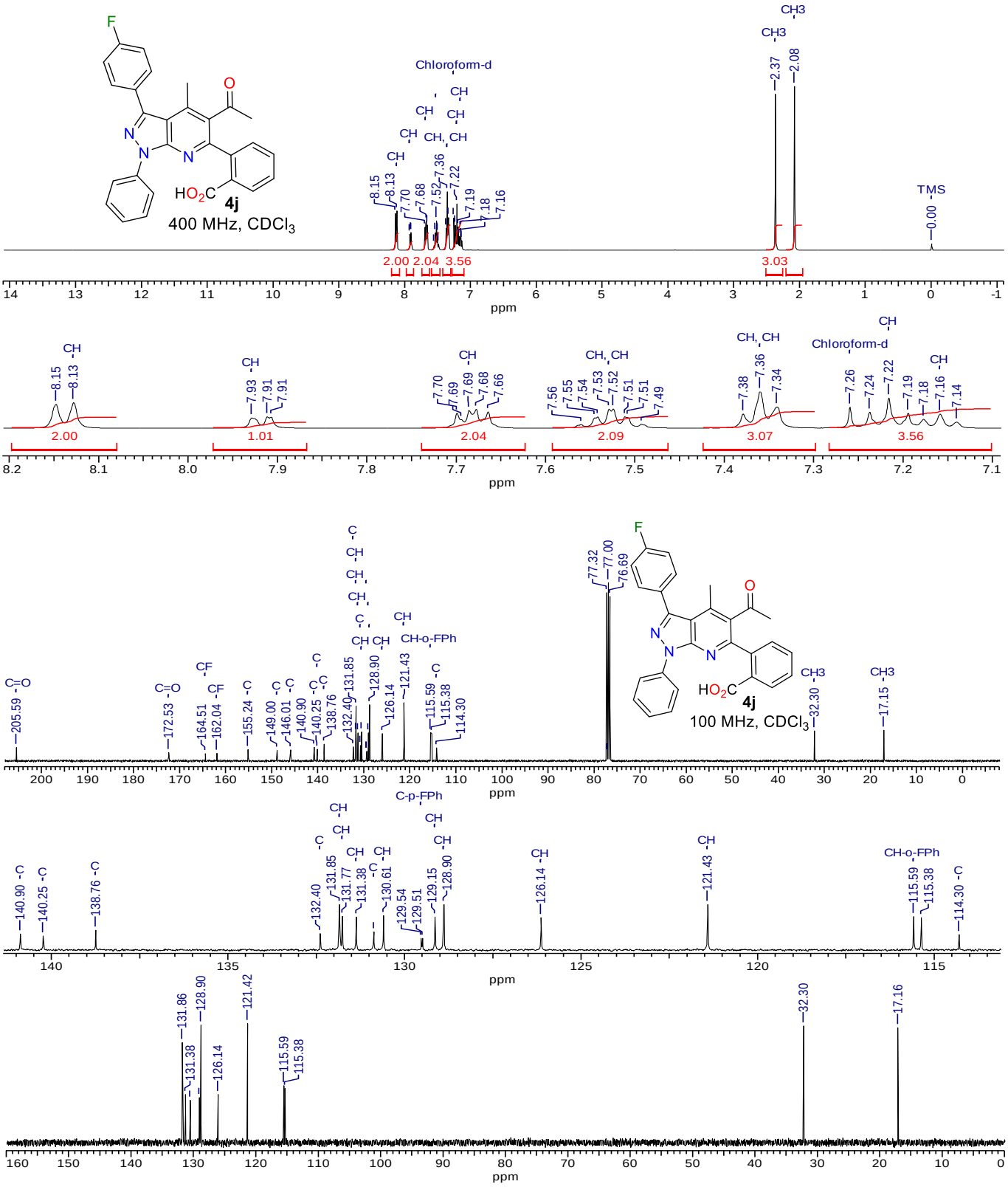
^{1}H and $^{13}C\{^{1}H\}$ NMR spectra of 2-(5-acetyl-4-methyl-1,3-diphenyl-1*H*-pyrazolo[3,4-*b*]pyridin-6-yl)benzoic acid **4h**



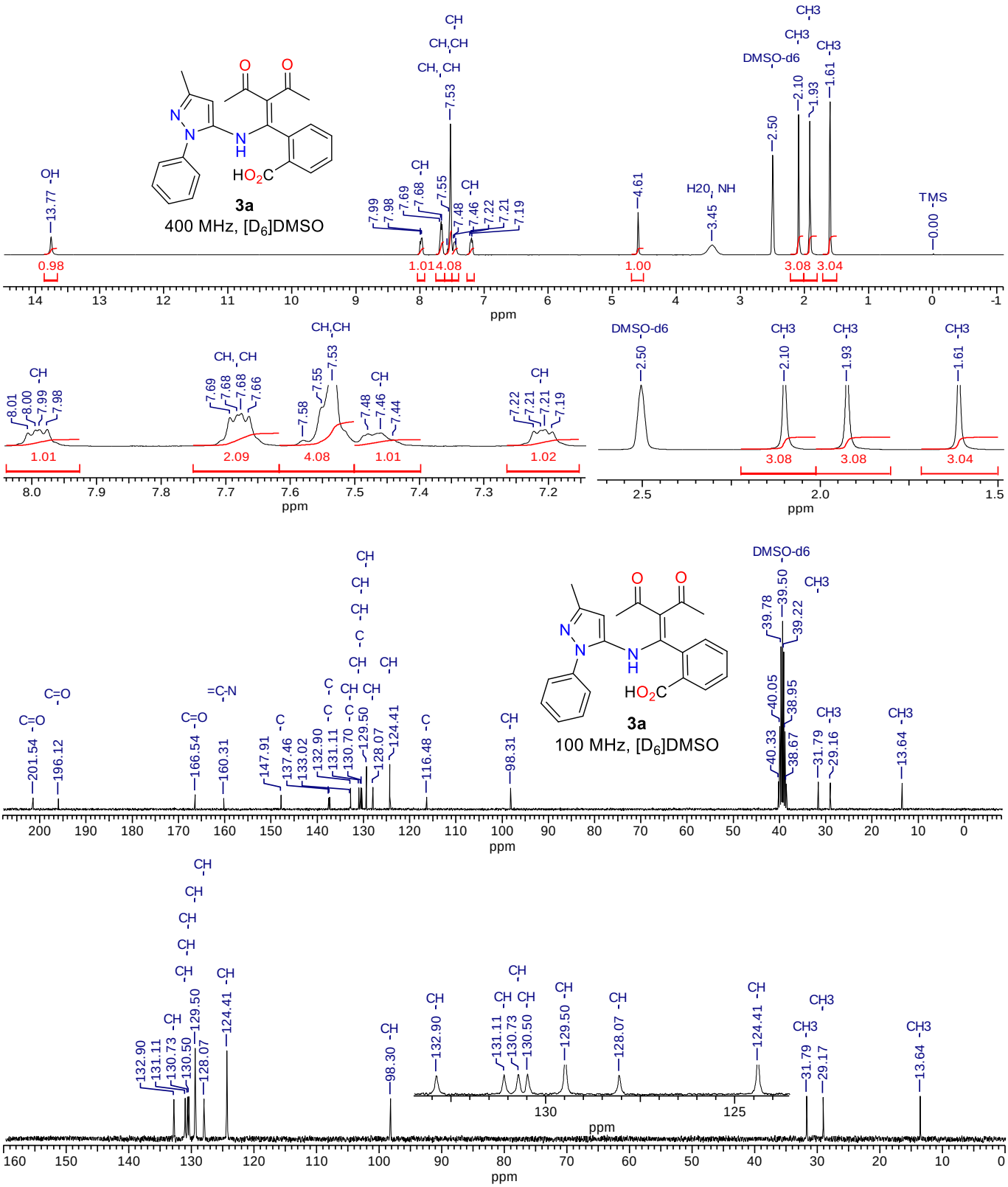
^{1}H and ^{13}C{^{1}H} NMR spectra of 2-(5-acetyl-3-(4-chlorophenyl)-4-methyl-1-phenyl-1*H*-pyrazolo[3,4-*b*]pyridin-6-yl)benzoic acid **4i**



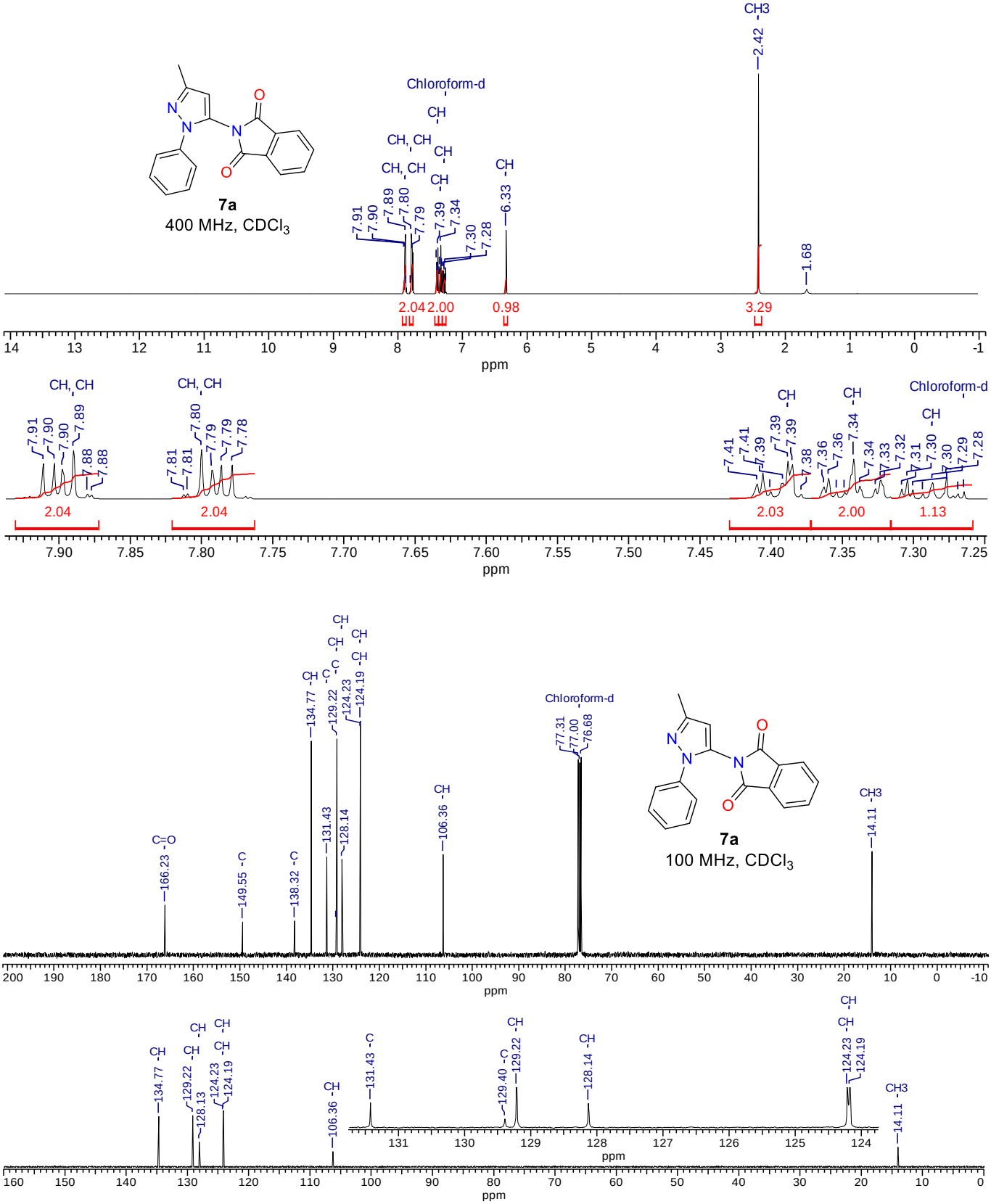
^{1}H and ^{13}C{^{1}H} NMR spectra of 2-(5-acetyl-3-(4-fluorophenyl)-4-methyl-1-phenyl-1*H*-pyrazolo[3,4-*b*]pyridin-6-yl)benzoic acid **4j**



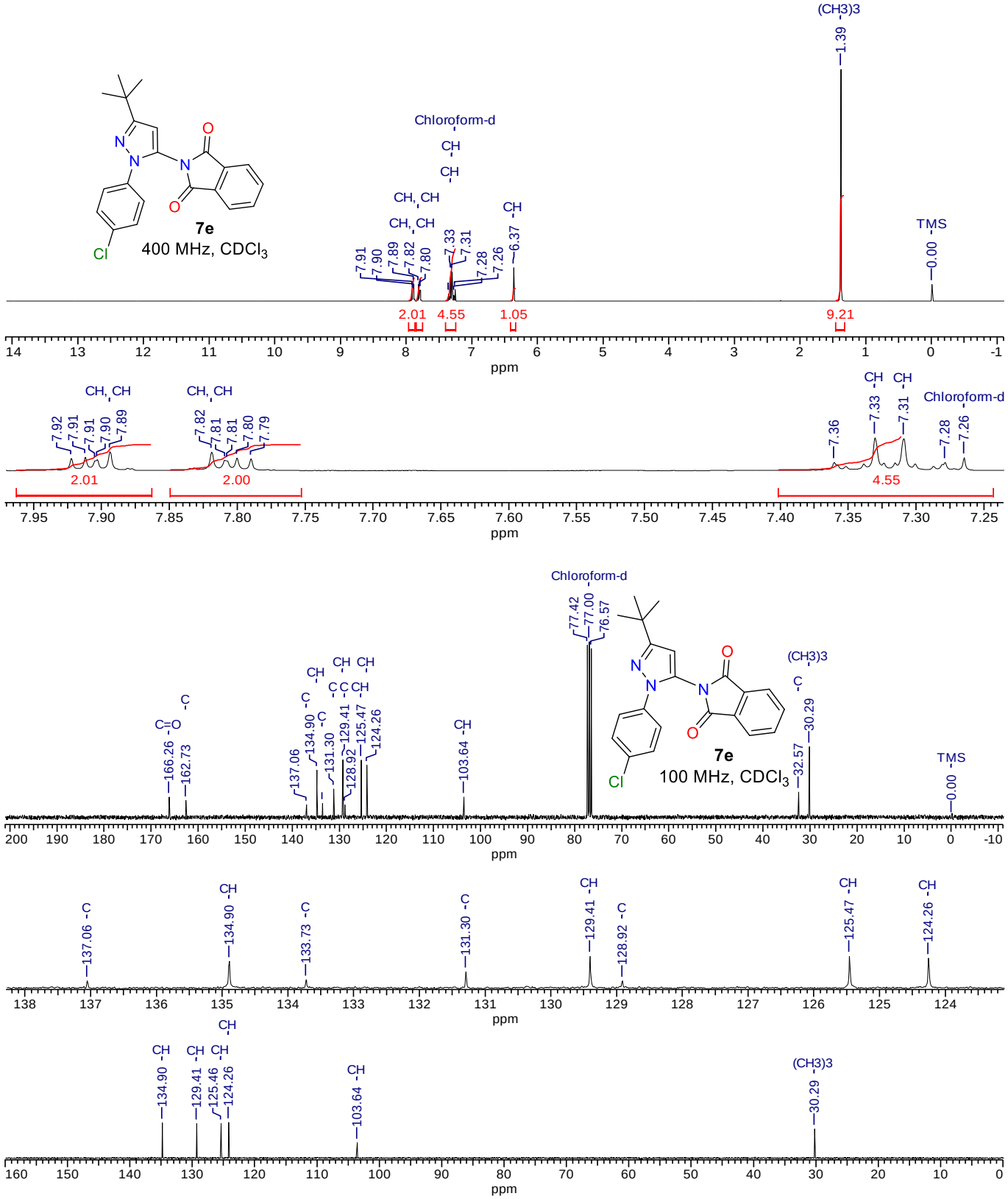
^{1}H and ^{13}C{^{1}H} NMR spectra of 2-(2-acetyl-1-((3-methyl-1-phenyl-1*H*-pyrazol-5-yl)amino)-3-oxobut-1-en-1-yl)benzoic acid **3a**



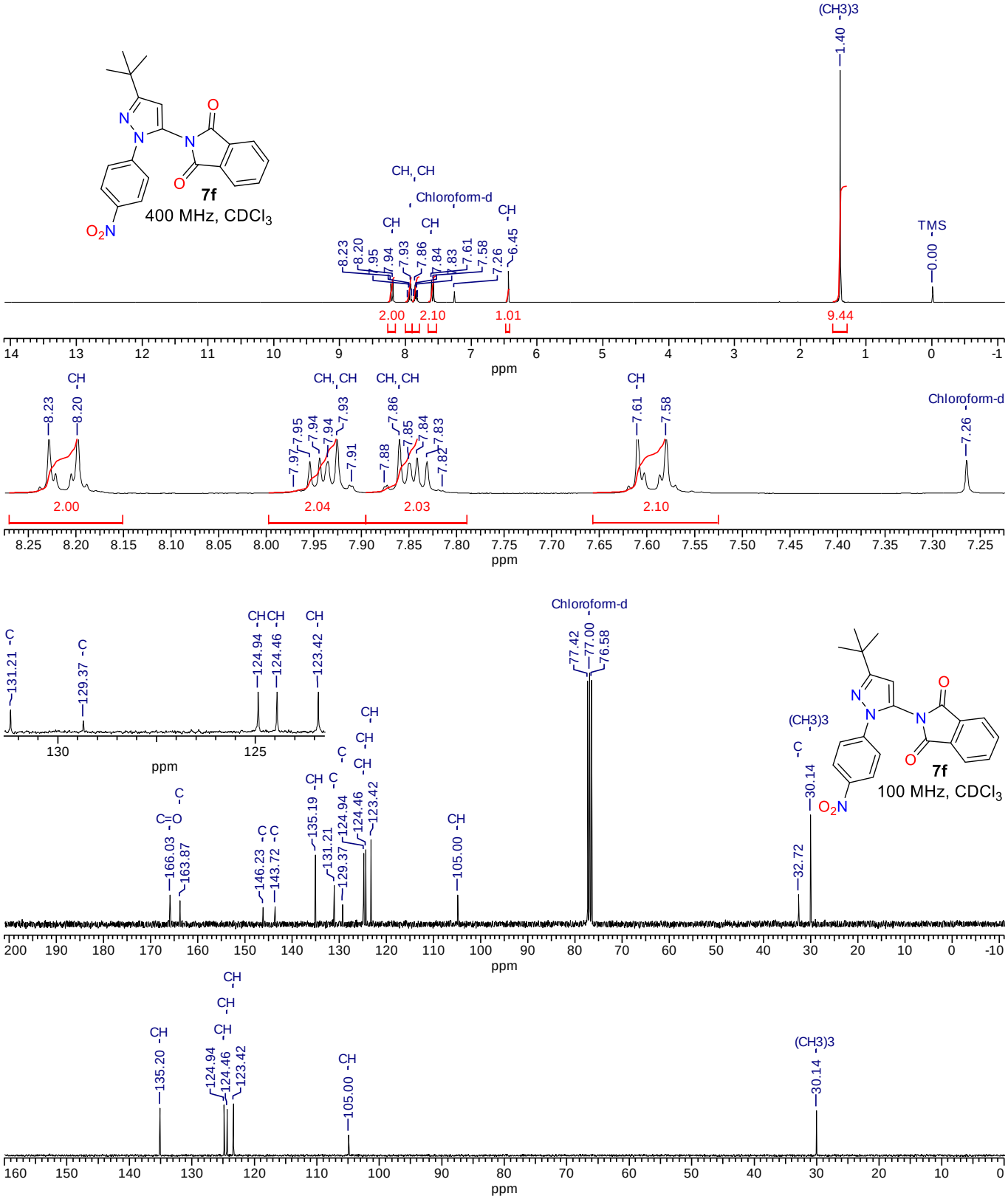
^{1}H and ^{13}C{^{1}H} NMR spectra of 2-(3-methyl-1-phenyl-1*H*-pyrazol-5-yl)isoindoline-1,3-dione **7a**



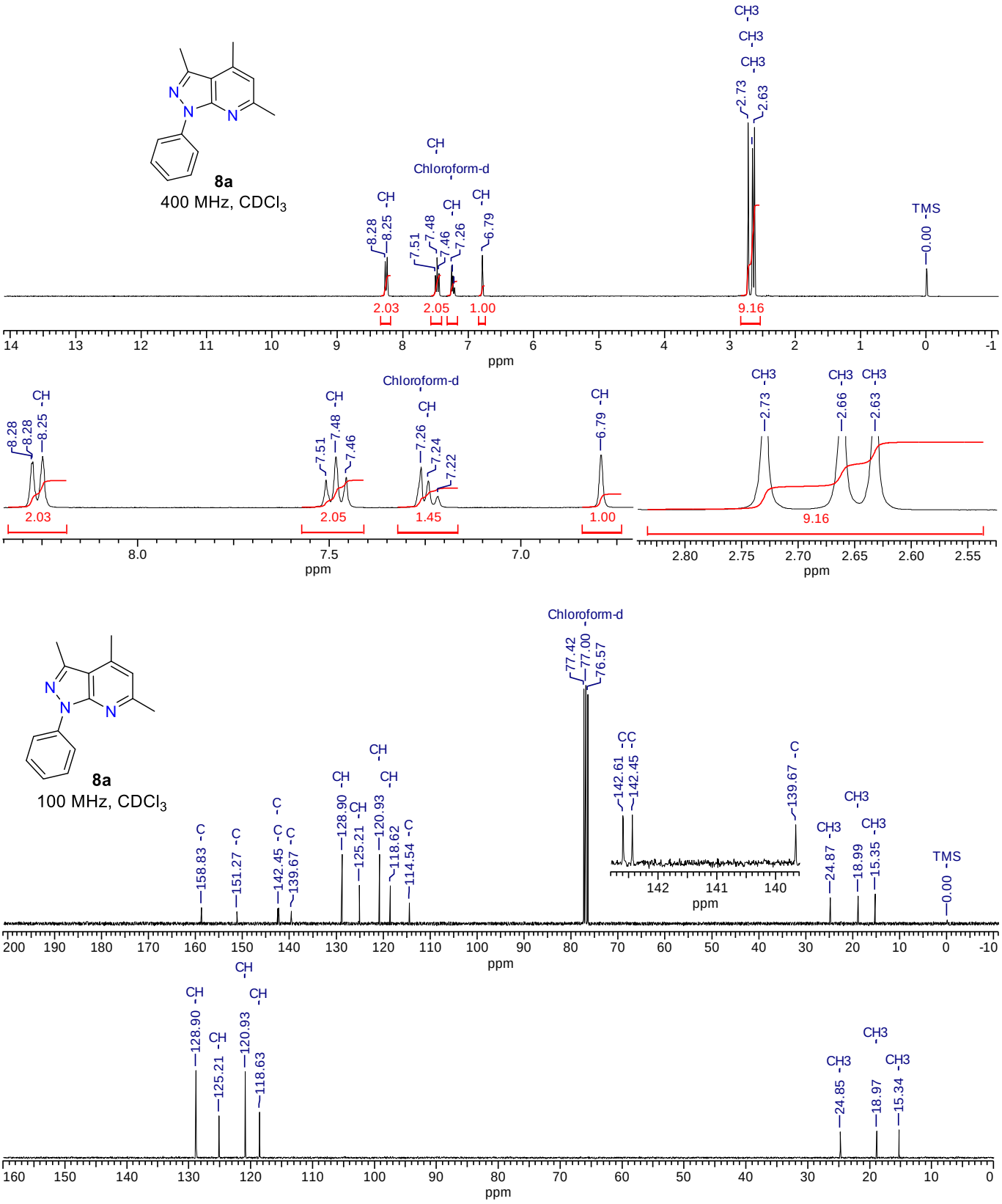
^{1}H and ^{13}C{^{1}H} NMR spectra of 2-(3-(*tert*-butyl)-1-(4-chlorophenyl)-1*H*-pyrazol-5-yl)isoindoline-1,3-dione **7e**



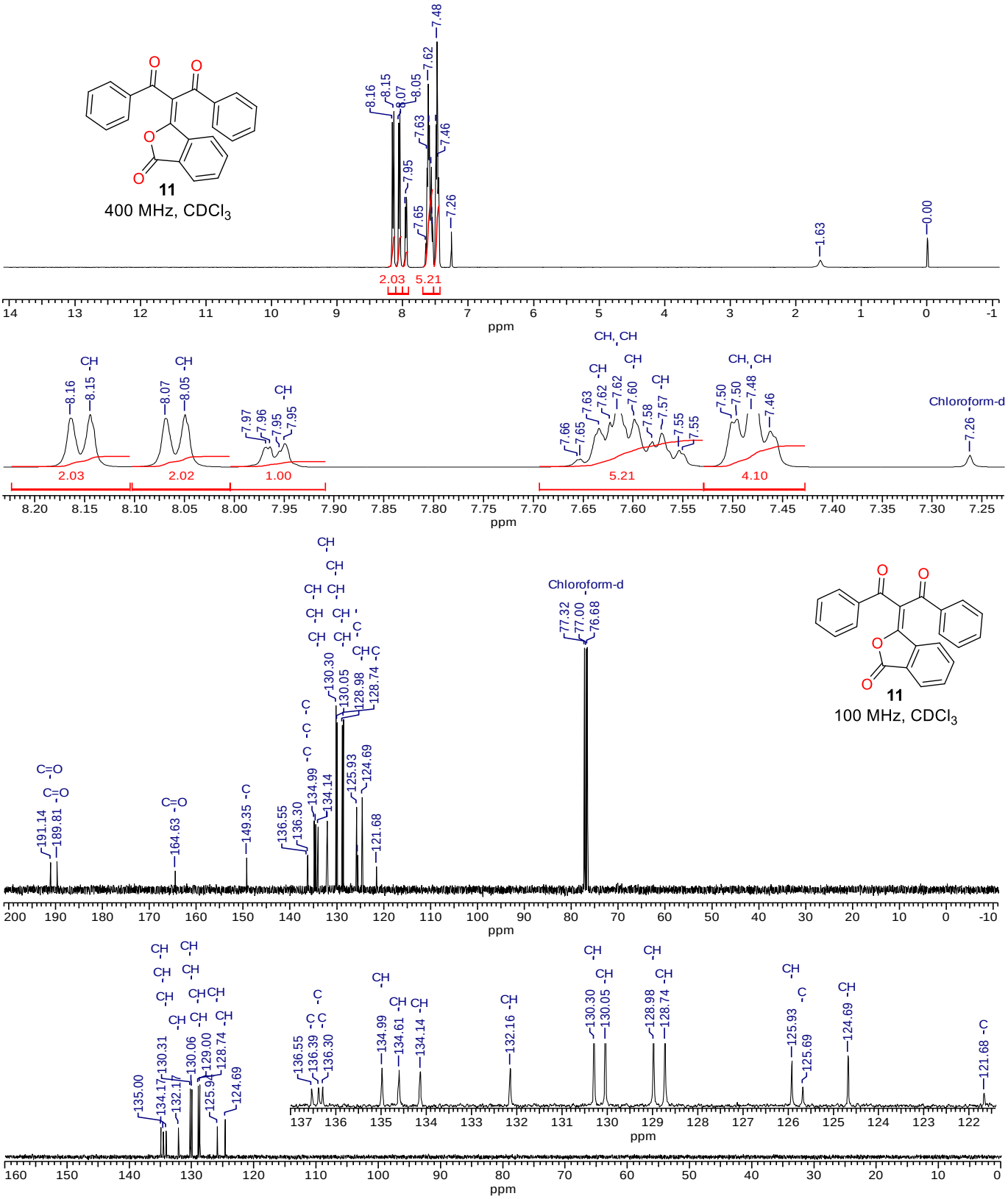
^{1}H and ^{13}C{^{1}H} NMR spectra of 2-(3-(*tert*-butyl)-1-(4-nitrophenyl)-1*H*-pyrazol-5-yl)isoindoline-1,3-dione **7f**



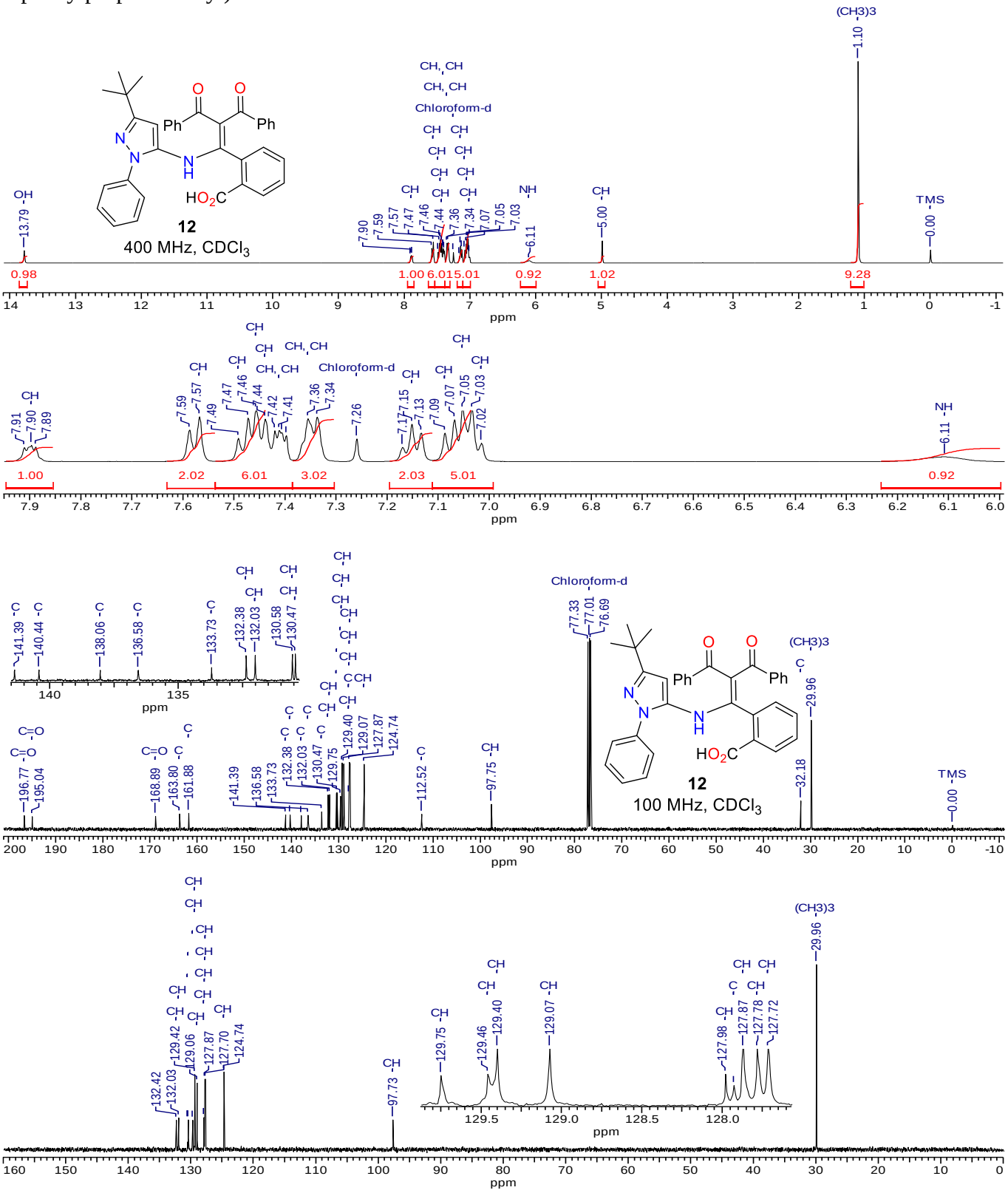
^{1}H and ^{13}C{^{1}H} NMR spectra of 3,4,6-trimethyl-1-phenyl-1*H*-pyrazolo[3,4-*b*]pyridine **8a**



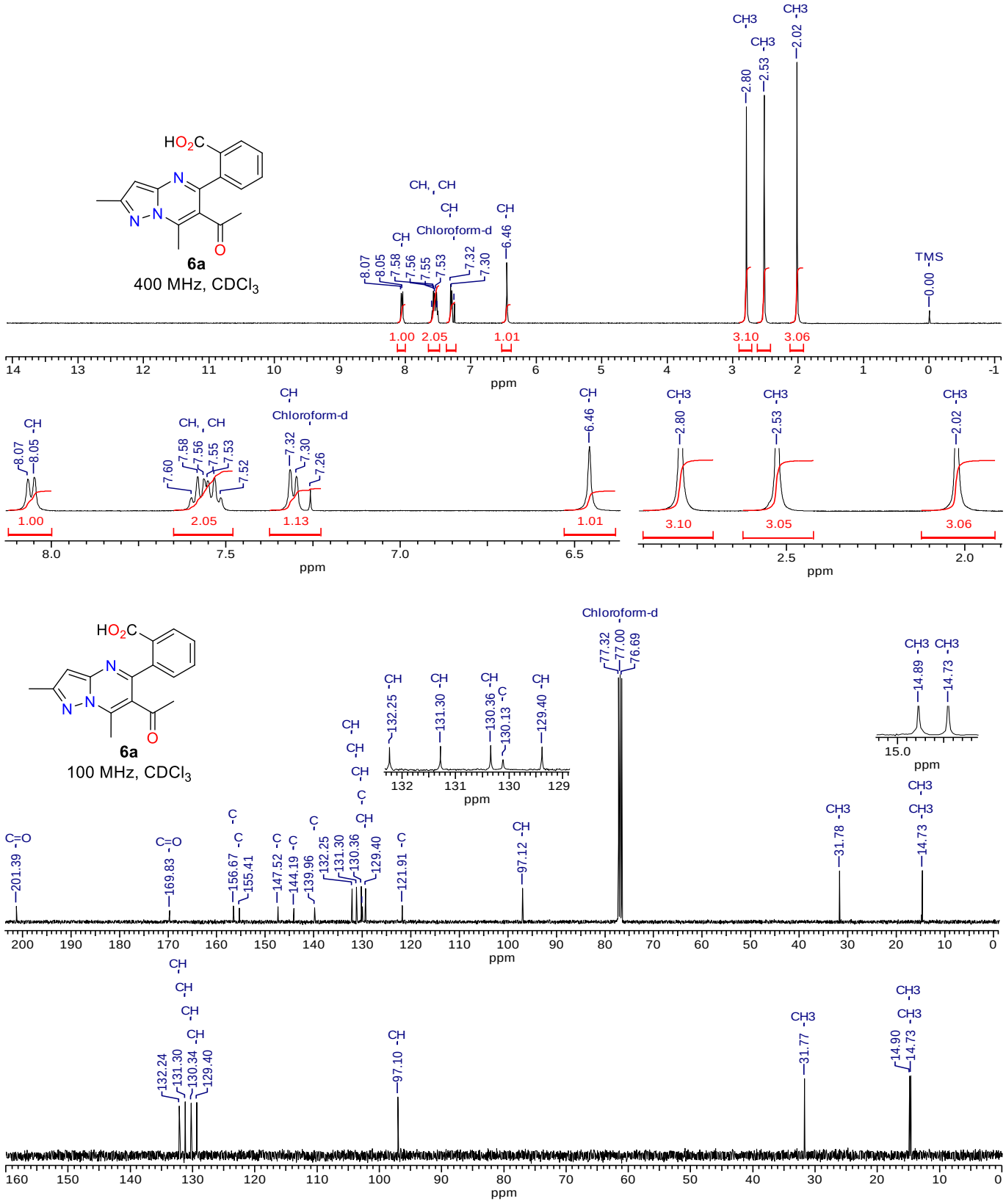
^{1}H and $^{13}C\{^{1}H\}$ NMR spectra of 2-(3-oxoisobenzofuran-1(3*H*)-ylidene)-1,3-diphenylpropane-1,3-dione **11**



^{1}H and ^{13}C{^{1}H} NMR spectra of 2-(2-benzoyl-1-((3-(tert-butyl)-1-phenyl-1*H*-pyrazol-5-yl)amino)-3-oxo-3-phenylprop-1-en-1-yl)benzoic acid **12**

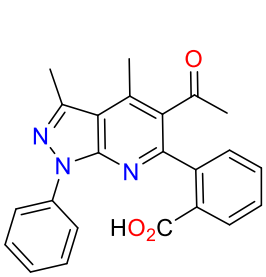


^{1}H and ^{13}C{^{1}H} NMR spectra of 2-(6-acetyl-2,7-dimethylpyrazolo[1,5-*a*]pyrimidin-5-yl)benzoic acid **6a**

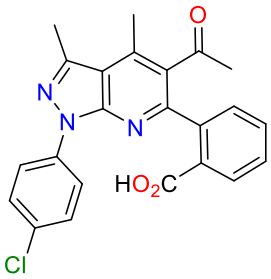


3. ORTEP drawing for structures of 4a, 4b, 4g and 4j

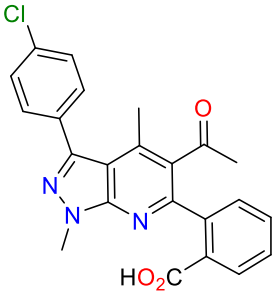
Displacement ellipsoids are drawn at the 30% probability level.



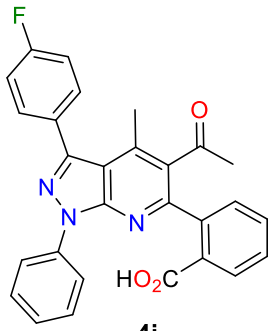
4a



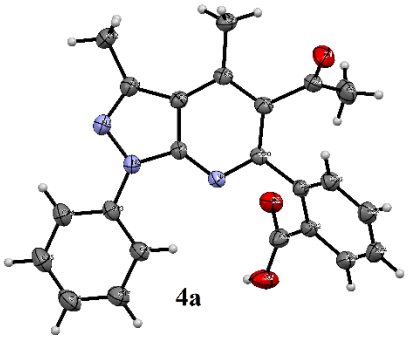
4b



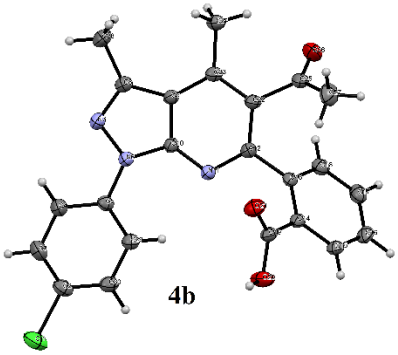
4g



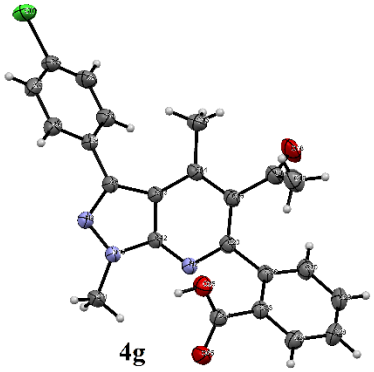
4j



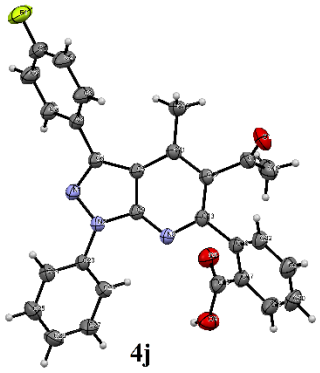
4a



4b



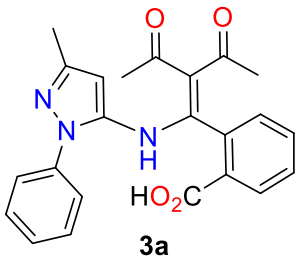
4g



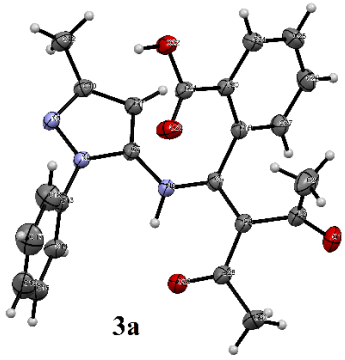
4j

4. ORTEP drawing for structure of intermediate 3a

Displacement ellipsoids are drawn at the 30% probability level.



3a



3a

5. Structural and Supramolecular information of 4a

Table S1. Crystal data and experimental details.

Crystal data	
Chemical formula	$C_{26}H_{25}N_4O_4$
M_r	457.50
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	298(2)
a, b, c (Å)	7.1294 (7), 32.835 (3), 10.2161 (9)
β (°)	96.947 (9)
V (Å^3)	2374.0 (4)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.09
Crystal size (mm)	0.24 × 0.13 × 0.10
Data collection	
Diffractometer	SuperNova, Dual, Cu at zero, Atlas diffractometer
Absorption correction	Multi-scan
T_{min}, T_{max}	0.811, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	44624, 4339, 3594
R_{int}	0.064
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.602
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.060, 0.164, 1.00
No. of reflections	4339
No. of parameters	324
No. of restraints	21
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.32, −0.43

Structural and supramolecular features

Figure S1a shows the molecule of **4a**. In this structure, the pyrazole (N2-N3-C7-C8-C11) and pyridyl (N1-C4-C5-C7-C8-C20) rings are nearly coplanar between them with a dihedral angle of 3.05(12)° introducing strain in this system of fused rings. The least-square plane that contains the benzene ring (C13-C14-C15-C16-C17-C18) have a dihedral angle of 2.51(15)° with the pyrazole ring which leave these atoms nearly in the same plane. However, the six-membered ring (C21-C22-C23-C24-C25-C26) that is substituting the pyridyl fragment have a different conformation out of the main plane that contains the fused ring system with a dihedral angle of 49.75(10)°. The asymmetric unit also contains one molecule of solvent which have two different orientations refined with an occupancy ratio of 0.289(5)/0.711(5) in the O4/O5 atoms, respectively. Both solvent orientations are consistent with the double presence of hydrogen atoms (observed in the difference Fourier maps) in O2 and O3, O(2, 3)–H(2, 3)···O(4, 5)^{i} [symmetry code: (i) −x, −y+1, −z+1], which were assigned with the same occupancy ratio of the O4/O5 atoms (see Figure S1b). In the supramolecular structure (Figure S1c), pairs of solvent molecules are connected by C1–H1C···O5^{ii} [symmetry code: (ii) −x+1, −y+1, −z+2] hydrogen bonds which are further connected to molecules of **4a** through O(2, 3)–H(2, 3)···O(4, 5) hydrogen bonds. The three-dimensional molecular assembly is

completed by C6–H6B···O1^{iii} [symmetry code: (iii) *x*,1/2-*y*,1/2+*z*] and C25–H25···Cg$_2^{iv}$ [Cg$_2$ being the centroid of N1–C8–C7–C5–C4–C20, symmetry code: (iv) *x*,1/2-*y*,-1/2+*z*] hydrogen interactions.

Table S2. Hydrogen-bond geometry (Å, °)

D—H···A	D—H	H···A	D···A	D—H···A
C18—H18···N1	0.93	2.35	2.996 (3)	126.6
O3—H3···O5^{i}	0.82	1.77	2.576 (8)	166.3
O2—H2···O4^{i}	0.82	1.77	2.591 (3)	173.6
C1—H1C···O5^{ii}	0.96	2.40	3.053 (8)	124.7
C6—H6B···O1^{iii}	0.96	2.49	3.358 (4)	150.0
C25—H25···Cg$_2^{iv}$	0.93	2.79	3.627 (3)	150.0

Symmetry codes: (i) −x, −y+1, −z+1; (ii) −x+1, −y+1, −z+2; (iii) x, −y+1/2, z+1/2; (iv) x, −y+1/2, z−1/2.

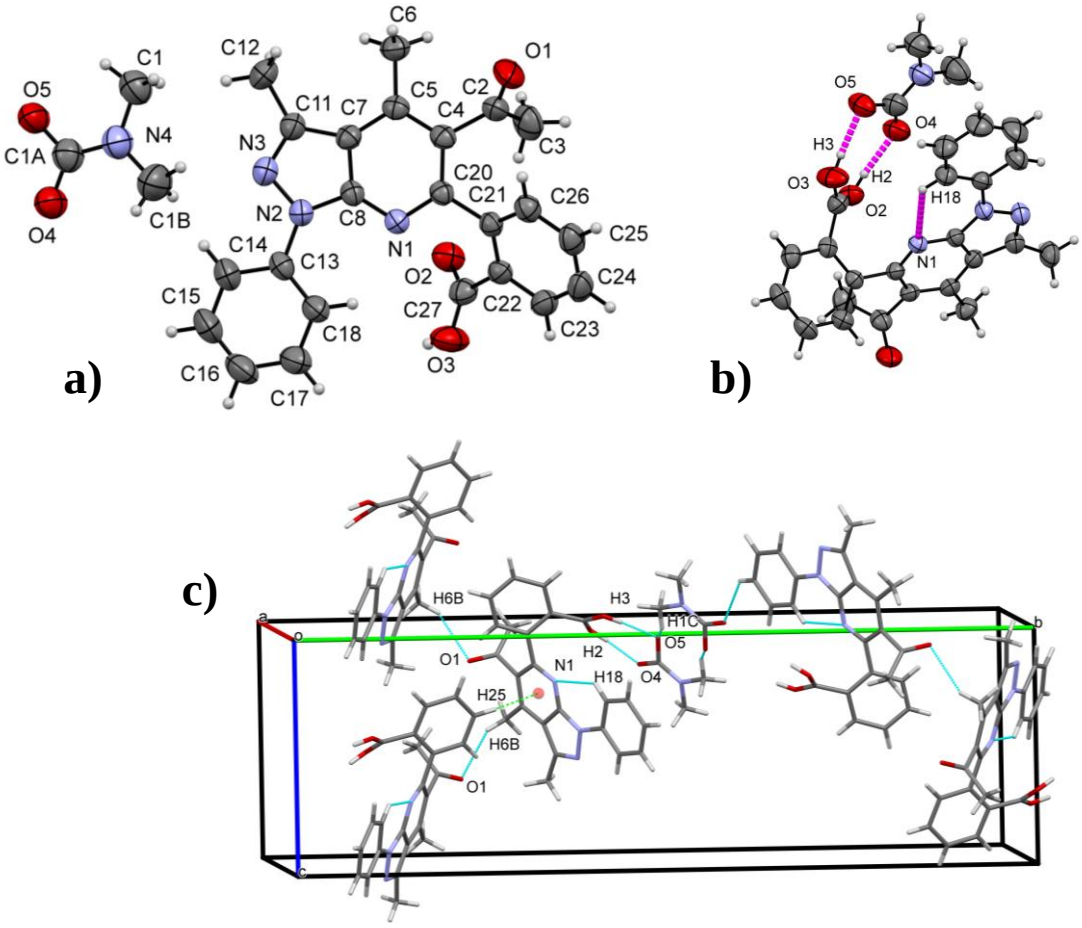


Figure S1. a) The molecular structure of **4a**, showing anisotropic displacement ellipsoids drawn at the 50% probability level. **b)** The molecular structure showing the solvent-molecule interaction and the intramolecular O–H···N contact. **c)** The crystal structure of the title compound, showing the O–H···O and C–H···(O, Cg$_2$) hydrogen-bonding interactions (dotted lines).

6. Structural and Supramolecular information of 4b

Table S3. Crystal data and experimental details.

Crystal data	
Chemical formula	$C_{26}H_{25}ClN_4O_4$
M_r	492.95
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	298(2)
a, b, c (Å)	7.0920 (15), 34.990 (8), 9.922 (3)
β (°)	98.12 (3)
V (Å^3)	2437.5 (11)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.20
Crystal size (mm)	0.25 × 0.16 × 0.08
Data collection	
Diffractometer	SuperNova, Dual, Cu at zero, Atlas diffractometer
Absorption correction	Multi-scan
T_{min}, T_{max}	0.611, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	23890, 4581, 3196
R_{int}	0.107
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.610
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.091, 0.254, 1.03
No. of reflections	4581
No. of parameters	323
No. of restraints	15
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.53, −0.48

Structural and supramolecular features

Figure S2a shows the molecule of **4b**. In this structure, the pyrazole (N6-N7-C8-C9-C10) and pyridyl (N11-C10-C9-C23-C22-C12) rings are forming a fused ring and are nearly coplanar between them with a dihedral angle of 2.33(19)° making this fragment less strained as compared with **4a**. The least-square plane that contains the benzene (C5-C4-C3-C2-C30-C29) ring substituted in the N6 atom of the pyrazole fragment has a dihedral angle of 14.0(2)° with this ring leaving this structure with less planar tendency as compared with **4a**. The main plane that contains the fused ring have a dihedral angle of 50.74(15)° with the benzene ring (C13-C14-C15-C16-C17-C18), a value very close to the observed in **4a** giving approximately the same conformation of this moiety regarding to the main body of the molecule. The asymmetry unit also contains a solvent molecule as observed in **4a**, however, in this case, only one orientation was observed. This molecular conformation allows the formation of the intramolecular C29–H29···N11 hydrogen bond (Table S4). In the supramolecular structure (Figure S2b), the solvent molecules are connected to **4b** through the O20–H20···O31 and C35–H35C···O21^{i} [symmetry code: (i) -*x*,1-*y*,2-*z*] hydrogen bonds. A combination of these interactions with the C24–H24C···O26^{ii} [symmetry code: (ii) *x*,3/2-*y*,-1/2+*z*]

hydrogen bonds and the weaker C17–H17···Cg2^{iii} [Cg2 being the centroid of N11–C10–C9–C23–C22–C12, symmetry code: (iii) *x*,3/2-*y*,1/2+*z*] interactions keep the molecules joint in the supramolecular assembly of the crystal.

Table S4. Hydrogen-bond geometry (Å, °)

D—H···A	D—H	H···A	D···A	D—H···A
C29—H29···N11	0.93	2.41	3.036 (5)	124.7
O20—H20···O31	0.82	1.83	2.622 (5)	162.2
C35—H35C···O21^{i}	0.96	2.47	3.387 (7)	160.3
C24—H24C···O26^{ii}	0.96	2.46	3.417 (6)	174.0
C17—H17···Cg$_2^{iii}$	0.93	2.88	3.704 (5)	148.0

Symmetry codes: (i) −x, −y+1, −z+2; (ii) x, −y+3/2, z−1/2; (iii) x, −y+3/2, z+1/2.

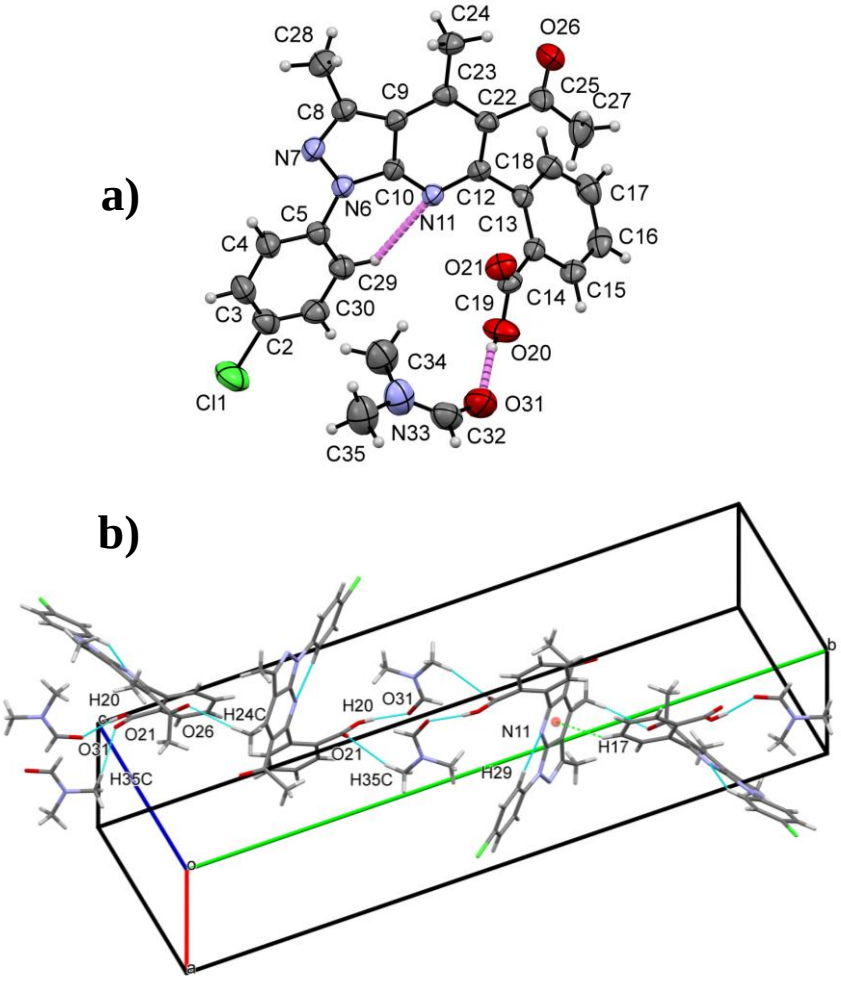


Figure S2. a) The molecular structure of **4b**, showing anisotropic displacement ellipsoids drawn at the 50% probability level, the solvent-molecule interaction and the intramolecular C–H···N contact. **b)** The crystal structure of the title compound, showing the O–H···O and C–H···(O, Cg$_2$) hydrogen-bonding interactions (dotted lines).

7. Structural and Supramolecular information of 4g

Table S5. Crystal data and experimental details.

Crystal data	
Chemical formula	$C_{23}H_{18}ClN_3O_3$
M_r	419.85
Crystal system, space group	Monoclinic, *C*2/*c*
Temperature (K)	298 (2)
a, *b*, *c* (Å)	16.130 (2), 17.057 (3), 15.338 (2)
β (°)	106.066 (14)
V (Å^3)	4055.2 (11)
Z	8
Radiation type	Mo *K*α
μ (mm^{-1})	0.22
Crystal size (mm)	0.40 × 0.28 × 0.10
Data collection	
Diffractometer	SuperNova, Dual, Cu at zero, Atlas diffractometer
Absorption correction	Multi-scan
T_{min}, T_{max}	0.584, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	21420, 4140, 3203
R_{int}	0.045
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.625
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.056, 0.159, 1.09
No. of reflections	4140
No. of parameters	289
No. of restraints	14
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.24, −0.34

Structural and supramolecular features

Figure S3a shows the molecule of **4g**. In this structure, the pyrazole (N10-N9-C8-C13-C12) and pyridyl (N21-C12-C13-C14-C16-C20) rings have a dihedral angle of 3.49(12)° between their least-square planes making of this structure a more strained one compared with **4a** and **4b**. The benzene rings (C2-C3-C4-C5C6-C7) and (C22-C23-C27-C28-C29-C30) have dihedral angles of 58.64(10)° and 44.77(10)°, respectively, with the mean plane that contains the fused ring. The conformation of these molecules does not allow the formation of intramolecular hydrogen contacts as observed in previous cases. In the supramolecular structure (Figure S3b), pairs of inversion-related molecules are connected by two equivalent O26–H1···O25^{i} [symmetry code: (i) 1-*x*,1-*y*,1-*z*] hydrogen bonds to form slabs of infinite chains that run along [-110]. These chains are further connected through C11–H11A···Cl2^{ii} [symmetry code: (ii) -1/2+*x*,1/2-*y*,1/2+*z*] hydrogen bonds along [001] direction. In the crystal, additional van de Waals forces help to define the three-dimensional array.

Table S6. Hydrogen-bond geometry (Å, °)

D—H···A	D—H	H···A	D···A	D—H···A
O26—H1···O25^{i}	0.830 (10)	1.870 (12)	2.696 (2)	173 (4)
C11—H11A···Cl2^{ii}	0.96	2.82	3.553 (4)	134.3

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1; (ii) *x*−1/2, −*y*+1/2, *z*+1/2.

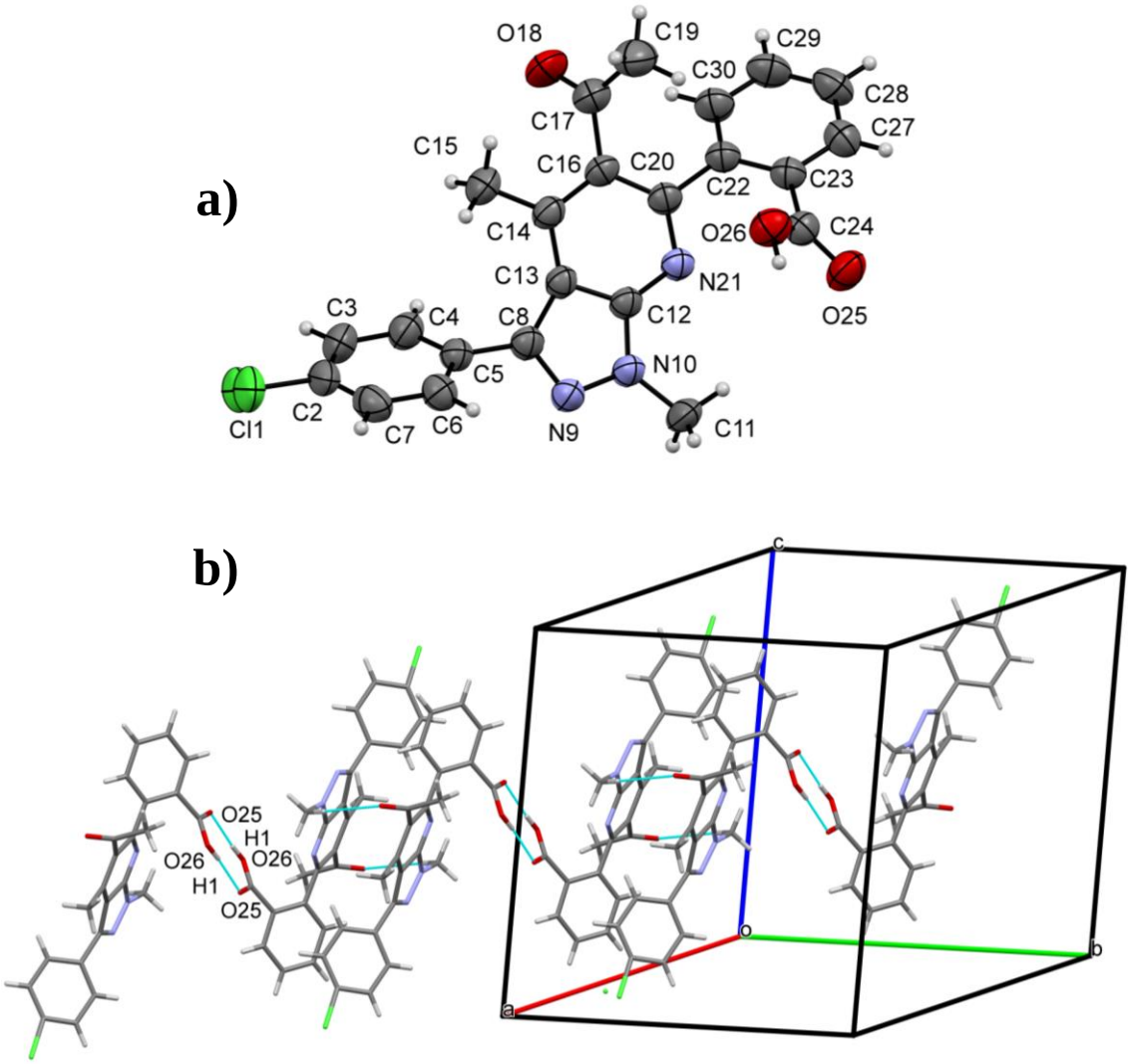


Figure S3. a) The molecular structure of **4g**, showing anisotropic displacement ellipsoids drawn at the 50% probability level. **b)** The crystal structure of the title compound, showing the O–H· · · O and C–H· · · O hydrogen-bonding interactions (dotted lines).

8. Structural and Supramolecular information of 4f

Table S7. Crystal data and experimental details.

Crystal data	
Chemical formula	$C_{28}H_{20}FN_3O_3 \cdot C_3H_7NO$
M_r	538.56
Crystal system, space group	Triclinic, *P-1*
Temperature (K)	298(2)
a, *b*, *c* (Å)	10.8530 (15), 12.0931 (16), 12.7462 (12)
α, β, γ (°)	111.386 (10), 93.203 (10), 111.842 (13)
V (Å^3)	1409.9 (3)
Z	2
Radiation type	Mo *K*α
μ (mm^{-1})	0.09
Crystal size (mm)	0.17 × 0.16 × 0.08
Data collection	
Diffractometer	SuperNova, Dual, Cu at zero, Atlas diffractometer
Absorption correction	Multi-scan
T_{min}, T_{max}	0.677, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	28985, 5753, 3751
R_{int}	0.071
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.625
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.074, 0.235, 1.02
No. of reflections	5753
No. of parameters	418
No. of restraints	158
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.65, −0.27

Structural and supramolecular features

Figure S4a shows the molecule of **4f**. In this structure, the pyrazole (N2-N1-C7-C8-C9) and pyridyl (N3-C9-C8-C11-C12-C13) rings are forming a fused ring forming a dihedral angle of 4.52(16)° between them, which leave this molecule as the most strained structure. In this case, three benzene rings are part of the molecule substituting the principal fused ring and making dihedral angles of 54.78(18)° for C1-C2-C3-C4-C5-C5, 53.09(16)° for C16-C17-C19-C20-C21-C22 and 34.99(16)° for C23-C24-C25-C26-C27-C28 with the mean least-square plane that contains the fused ring. The compound crystallized with a solvent molecule in the asymmetric unit which was refined with a model assuming a discrete disorder (not shown in Figure S4 for clarity). In the supramolecular structure (Figure S4b), the molecules are connected by C6–H6···O1^{i} [symmetry code: (i) 1+*x*, *y*, *z*] hydrogen bonds to form chains that run along [100] direction. The solvent molecules help to define the crystal structure through C31A–H31C···Cg1^{ii} [Cg_1 being the centroid of N1–N2–C9–C8–C7, symmetry code: (ii) 1-*x*, 1-*y*, 1-*z*] and O3–HO3···O4A hydrogen bonds in the [001] direction.

Table S8. Hydrogen-bond geometry (Å, °)

D—H···A	D—H	H···A	D···A	D—H···A
C28—H28···N3	0.93	2.53	3.008 (4)	112.3
O3—HO3···O4A	0.809 (19)	1.83 (3)	2.584 (16)	154 (5)
C6—H6···O1^{i}	0.93	2.48	3.317 (5)	149.5
C31A—H31C···Cg1^{ii}	0.93	2.84	3.444 (12)	122.0

Symmetry codes: (i) *x*+1, *y*, *z*; (ii) −*x*+1, −*y*+1, −*z*+1.

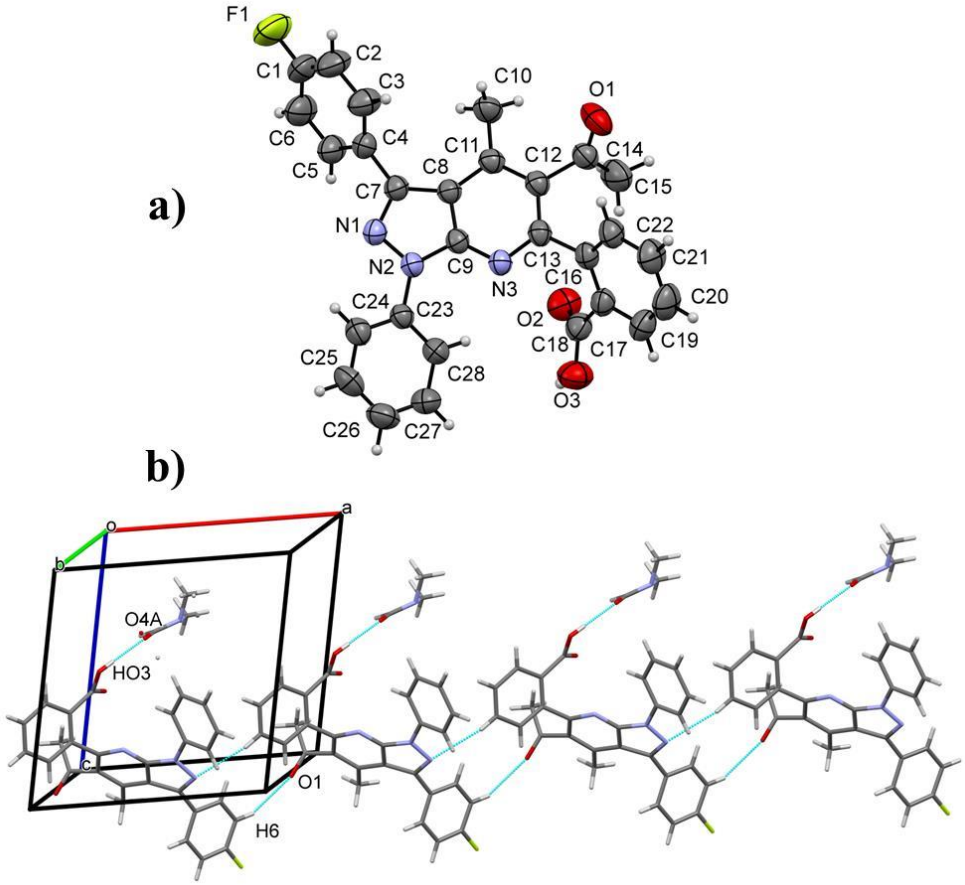


Figure S4. a) The molecular structure of **4f**, showing anisotropic displacement ellipsoids drawn at the 50% probability level. **b)** The crystal structure of the title compound, showing the C–H···N and O–H···O hydrogen-bonding interactions (dotted lines).

9. Structural and Supramolecular information of 3a

Table S9. Crystal data and experimental details.

Crystal data	
Chemical formula	$C_{23}H_{21}N_3O_4$
M_r	403.43
Crystal system, space group	Triclinic, *P*-1
Temperature (K)	298(2)
a, *b*, *c* (Å)	10.0379 (13), 10.2812 (13), 10.6299 (13)
α, β, γ (°)	73.378 (11), 83.687 (10), 80.048 (11)
V (Å^3)	1033.2 (2)
Z	2
Radiation type	Mo *K*α
μ (mm^{-1})	0.09
Crystal size (mm)	0.24 × 0.15 × 0.12
Data collection	
Diffractometer	SuperNova, Dual, Cu at zero, Atlas diffractometer
Absorption correction	Multi-scan
T_{min}, T_{max}	0.765, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	19845, 5490, 3549
R_{int}	0.047
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.713
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.063, 0.181, 1.07
No. of reflections	5490
No. of parameters	284
No. of restraints	61
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.29, −0.24

Structural and supramolecular features

Figure S5a shows the molecule of **3a**. In this structure, the pyrazole ring (N8-N9-C7-C10-C11) has dihedral angles of 77.58(13)° and 56.57(11)° with the benzene rings C13-C14-C15-C16-C17-C18 and C19-C20-C24-C25-C26-C27, respectively, which leave the five and six-membered rings in a non-coplanar conformation which allows the formation of the intramolecular N6–H3···O29 and C30–H30C···O1 hydrogen bonds as observed in Table S10. In the supramolecular structure (Figure S5b), pairs of inversion-related molecules, connected by two equivalent strong O22–H22···N9^{i} [symmetry code: (i) -*x*, 1-*y*, 1-*z*] hydrogen bonds form slabs of infinite chains of molecules running along [011] by weaker C26–H26···O1^{ii} [symmetry code: (ii) -*x*, 2-*y*, 2-*z*] hydrogen interactions keeping the slabs joint in the diagonal of the *bc* plane. Parallel chains are further connected by C16–H16···O23^{iii} [symmetry code: (iii) 1-*x*, 1-*y*, 1-*z*] hydrogen bonds to build the crystal structure in the [100] direction. Additional weaker C–H···O/C–H··· π interactions and van de Waals forces help to define the three-dimensional array.

Table S10. Hydrogen-bond geometry (Å, °)

D—H···A	D—H	H···A	D···A	D—H···A
N6—H3···O29	0.97 (2)	1.72 (2)	2.554 (2)	141.7 (19)
C30—H30C···O1	0.96	2.60	2.966 (3)	103.0
O22—H22···N9^{i}	0.93 (3)	1.81 (3)	2.710 (2)	161 (3)
C26—H26···O1^{ii}	0.93	2.53	3.359 (3)	149.0
C16—H16···O23^{iii}	0.93	2.51	3.389 (4)	158.0

Symmetry codes: (i) −*x*, −*y*+1, −*z*+1; (ii) −*x*, −*y*+2, −*z*+2; (iii) −*x*+1, −*y*+1, −*z*+1.

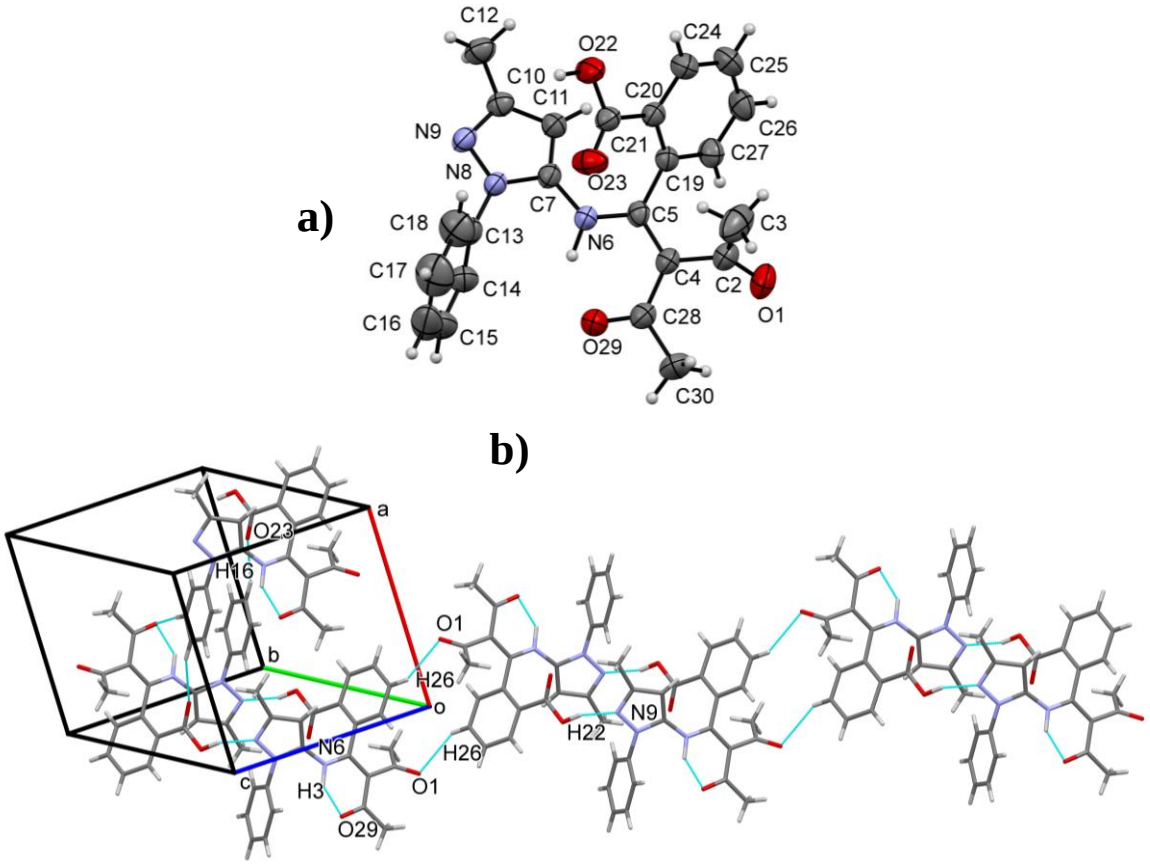


Figure S5. a) The molecular structure of **3a**, showing anisotropic displacement ellipsoids drawn at the 50% probability level. **b)** The crystal structure of the title compound, showing the O–H · · · N and C–H · · · O hydrogen-bonding interactions (dotted lines).