Exploring antimicrobial feature for new imidazo[4,5-b] pyridine Derivatives based on experimental and theoretical study

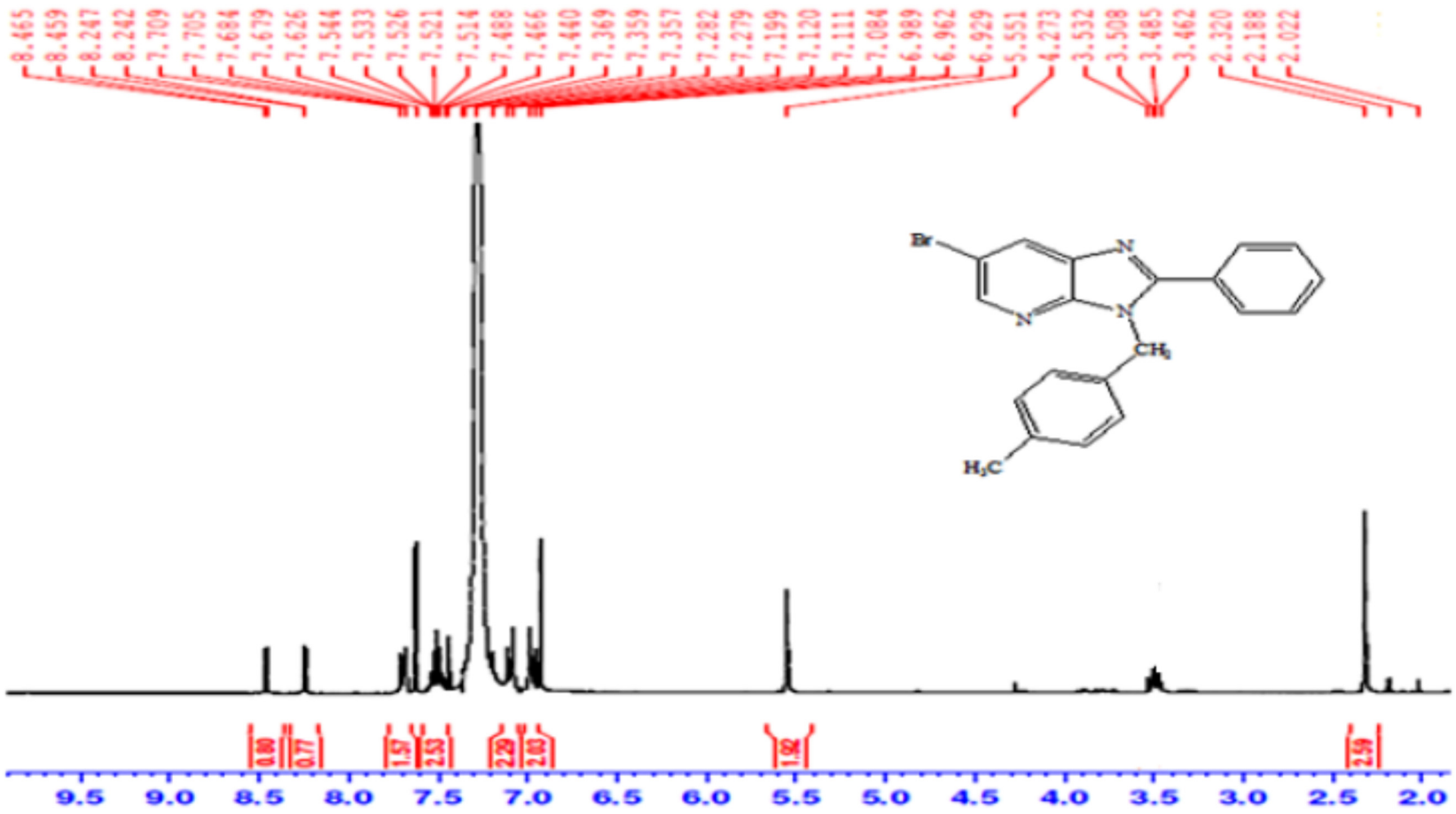


Figure S1: ^{1}H NMR spectrum of **4**

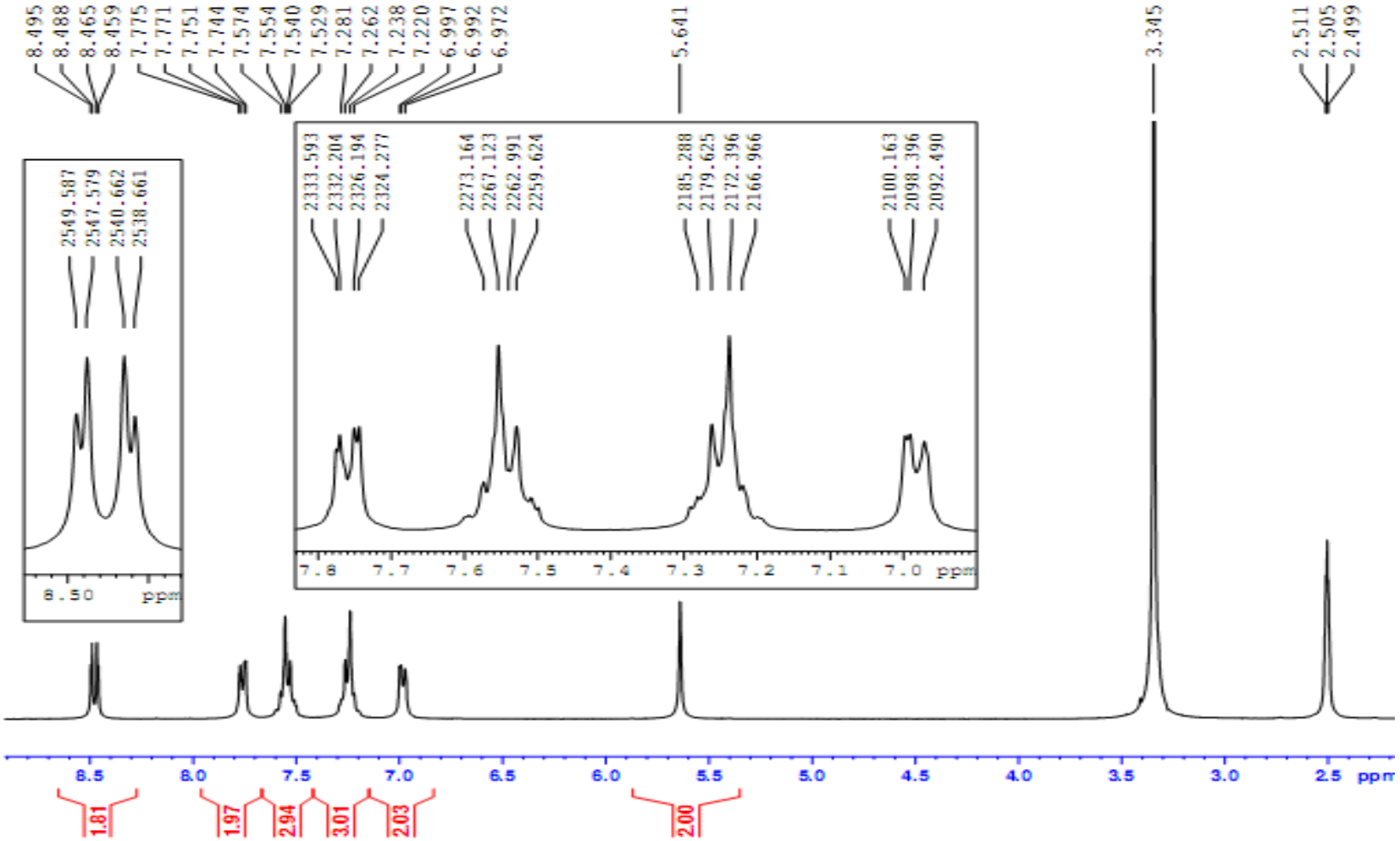


Figure S2: ^{1}H NMR spectrum of **6**

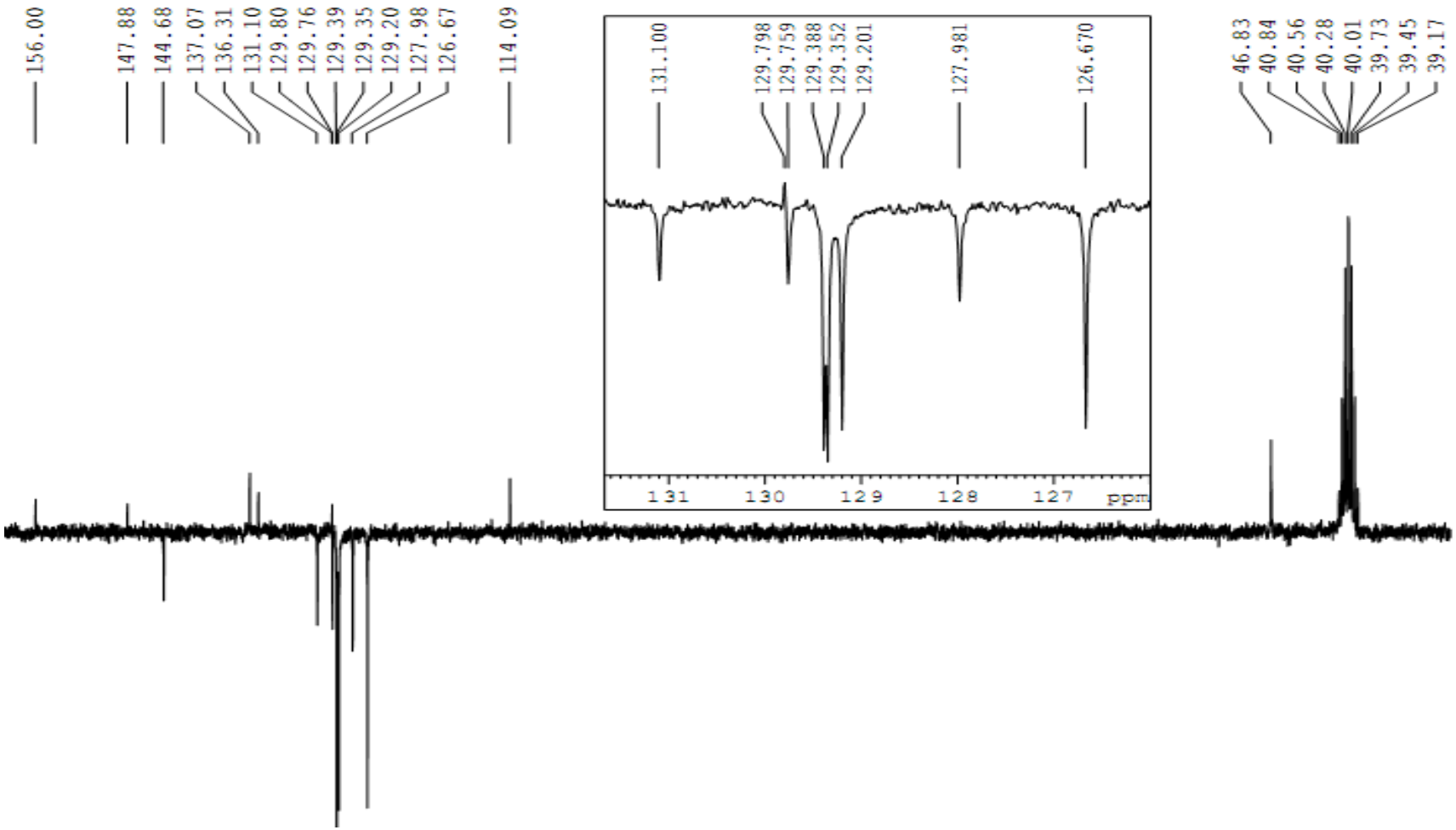


Figure S3: ^{13}C NMR spectrum of **6**

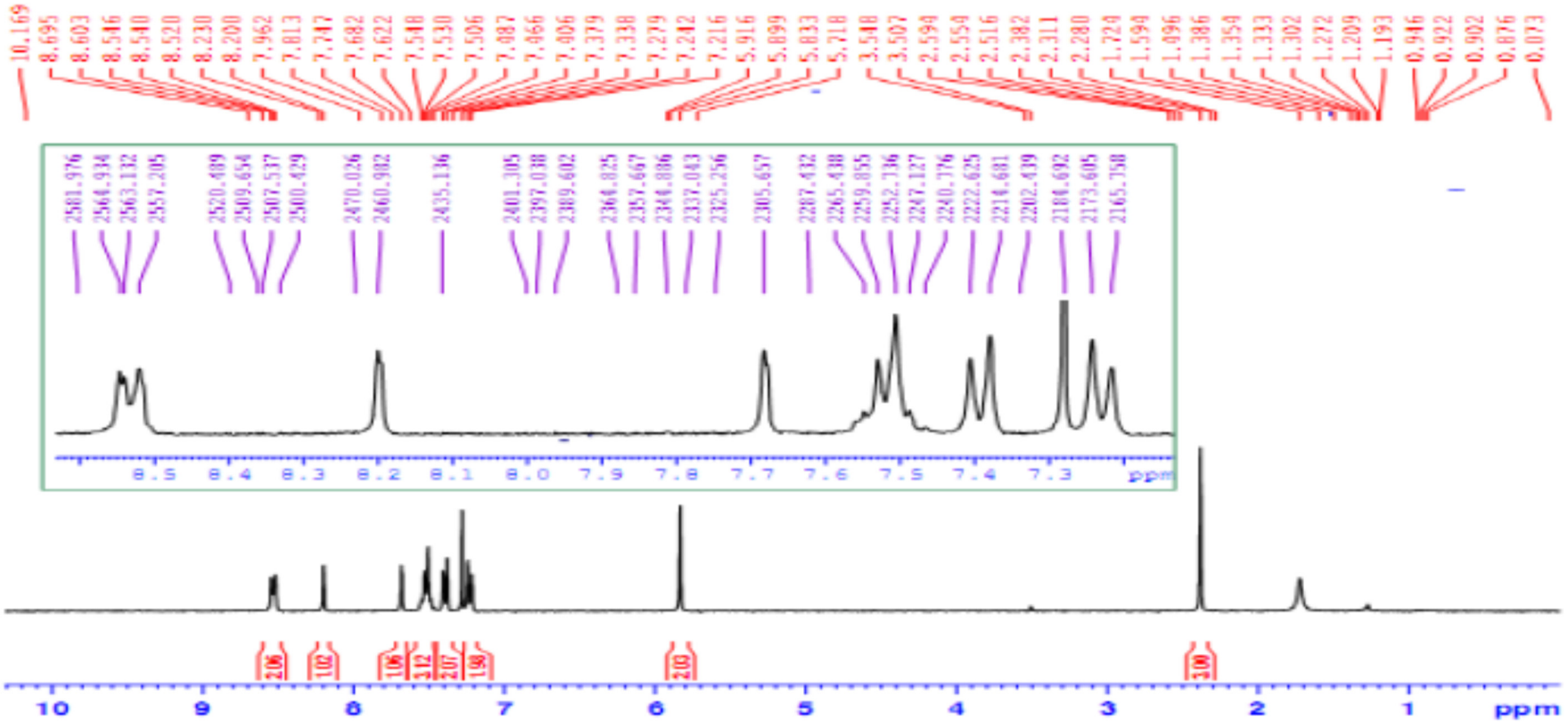


Figure S4: ^{1}H NMR spectrum of **7**

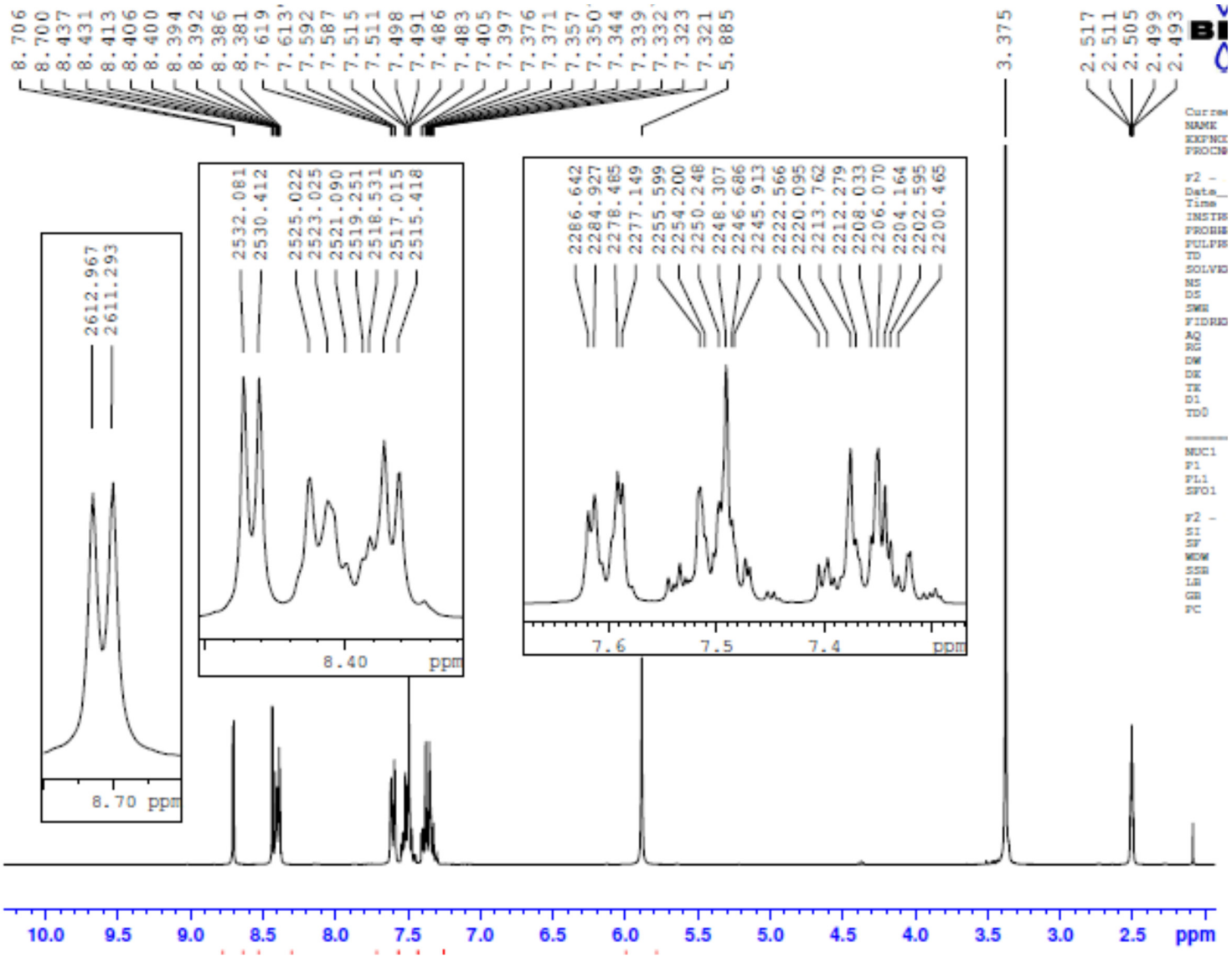


Figure S5: ^{1}H NMR spectrum of **8**

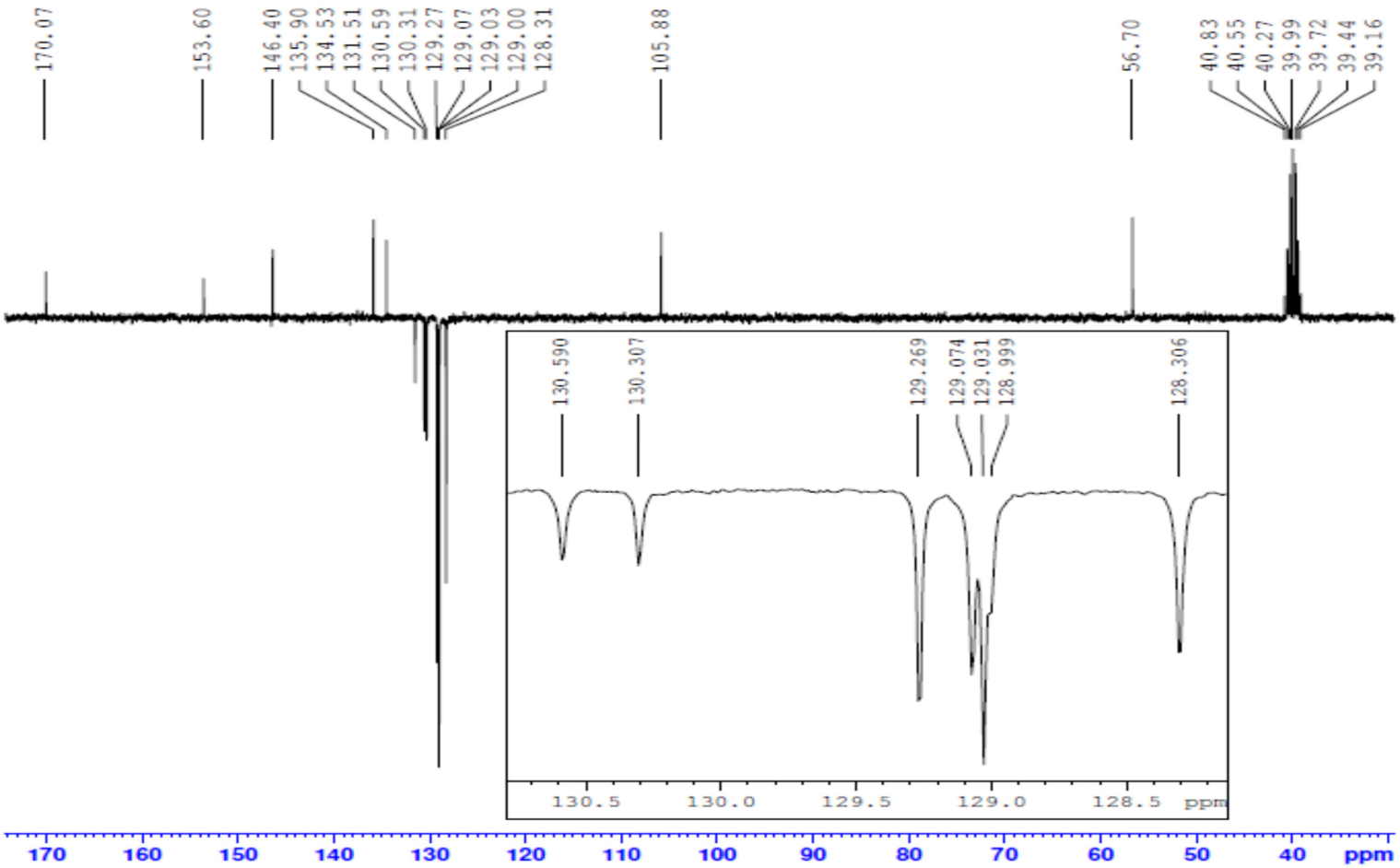


Figure S6: ^{13}C NMR spectrum of **8**

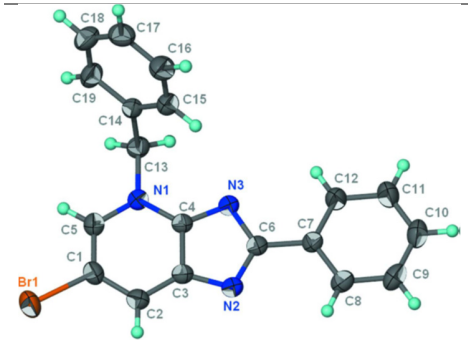
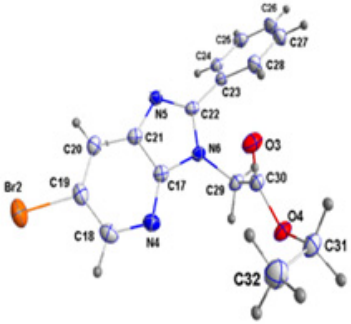
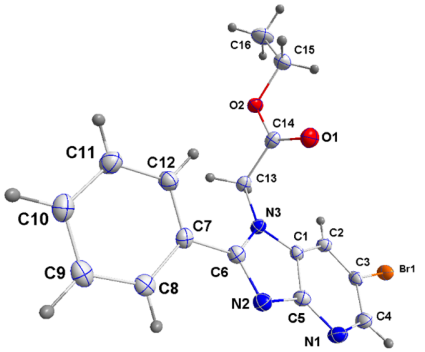
3	6	8
		

Figure S7: Oretp view of **3, 6 and 8**

Table S1. Sample, Data collection and structure refinement crystal data for 3.

C19H14BrN3	**F(000) = 736**
Mr = 364.24	Dx = 1.530 Mg m−3
Monoclinic, P21/c	Mo Kα radiation, λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 9876 reflections
a = 8.6613 (6) Å	θ = 2.4–27.2°
b = 19.7631 (13) Å	μ = 2.60 mm−1
c = 9.3683 (6) Å	T = 293 K
β = 99.647 (3)°	Prism, brown
V = 1580.93 (18) Å3	0.28 × 0.24 × 0.20 mm
Z = 4	
Bruker X8 APEXII diffractometer	4613 independent reflections
Radiation source: fine-focus sealed tube	3492 reflections with I > 2σ(I)
graphite	Rint = 0.035
φ and ω scans	θmax = 30.1°, θmin = 2.4°
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −12→11
Tmin = 0.529, Tmax = 0.624	k = −27→27
57936 measured reflections	l = −13→13
Refinement on F^2	Primary atom site location: structure invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map

R[F2> 2σ(F2)] = 0.032	Hydrogen site location: inferred from neighbouring sites
wR(F2) = 0.098	H-atom parameters constrained
S = 1.00	w = 1/[σ2(Fo2) + (0.0518P)2+ 0.5269P] where P = (Fo2 + 2Fc2)/3
4613 reflections	(Δ/σ)max = 0.001
208 parameters	Δρmax = 0.63 e Å^{-3}
0 restraints	Δρmin = −0.51 e Å^{-3}

Table S2. Sample, Data collection and structure refinement crystal data for 6.

Chemical formula	$C_{16}H_{14}BrN_3O_2$	
Formula weight	360.21 g/mol	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal size	0.156 x 0.244 x 0.364 mm	
Crystal habit	colorless block	
Crystal system	monoclinic	
Space group	P 1 21/c 1	
Unit cell dimensions	a = 21.1444(14) Å	α = 90°
	b = 7.6970(5) Å	β = 118.0730(10)°
	c = 21.2671(14) Å	γ = 90°
Volume	3054.0(3) $Å^3$	
Z	8	
Density (calculated)	1.567 g/cm^3	
Absorption coefficient	2.702 mm^{-1}	
F(000)	1456	
Diffractometer	Bruker Smart APEX CCD	
Radiation source	fine-focus sealed tube, MoKα	
Theta range for data collection	1.92 to 28.80°	
Index ranges	-28<=h<=28, -10<=k<=10, -28<=l<=28	
Reflections collected	56392	
Independent reflections	7958 [R(int) = 0.0369]	
Coverage of independent reflections	99.6%	
Absorption correction	numerical	
Max. and min. transmission	0.6780 and 0.4400	
Structure solution technique	direct methods	
Structure solution program	*SHELXT* (Sheldrick, 2015)	

Refinement method	Full-matrix least-squares on F^2	
Refinement program	SHELXL-2014/7 (Sheldrick, 2014)	
Function minimized	$\Sigma\ w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	7958 / 0 / 399	
Goodness-of-fit on F^2	1.035	
Δ/σ_{max}	0.002	
Final R indices	6411 data; $I>2\sigma(I)$	R1 = 0.0307, wR2 = 0.0755
	all data	R1 = 0.0430, wR2 = 0.0803
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0421P)^2+0.9304P]$ where $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	0.782 and -0.639 eÅ^{-3}	
R.M.S. deviation from mean	0.063 eÅ^{-3}	

Table S3. Sample, crystal data, data collection and structure refinement for 8

Chemical formula	**$C_{16}H_{14}BrN_3O_2$**
Formula weight	360.21 g/mol
Temperature	150(2) K
Wavelength	0.71073 Å
Crystal size	0.060 x 0.150 x 0.210 mm
Crystal habit	colorless plate
Crystal system	monoclinic
Space group	P 1 21/n 1
Unit cell dimensions	a = 14.6923(8) Å α = 90°
	b = 6.1988(3) Å β = 92.9110(10)°
	c = 16.2254(8) Å γ = 90°
Volume	1475.82(13) $Å^3$
Z	4
Density (calculated)	1.621 g/cm^3
Absorption coefficient	2.796 mm^{-1}
F(000)	728
Diffractometer	Bruker Smart APEX CCD
Radiation source	fine-focus sealed tube, MoKα
Theta range for data collection	1.82 to 29.18°
Index ranges	-20<=h<=20, -8<=k<=8, -22<=l<=21
Reflections collected	27419
Independent reflections	3981 [R(int) = 0.0436]
Coverage of independent reflections	99.7%
Absorption correction	multi-scan
Max. and min. transmission	0.8500 and 0.5910
Structure solution technique	direct methods
Structure solution program	*SHELXT* (Sheldrick, 2015)

Refinement method	Full-matrix least-squares on F^2
Refinement program	SHELXL-2014/7 (Sheldrick, 2014)
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$
Data / restraints / parameters	3981 / 0 / 200
Goodness-of-fit on F^2	1.064
Δ/σ_{max}	0.001
Final R indices	3236 data; $I>2\sigma(I)$ R1 = 0.0307, wR2 = 0.0781
	all data R1 = 0.0414, wR2 = 0.0814
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0468P)^2]$ where $P=(F_o^2+2F_c^2)/3$
Largest diff. peak and hole	0.758 and -0.349 $eÅ^{-3}$
R.M.S. deviation from mean	0.079 $eÅ^{-3}$

Table S4: the H-bond geometry (Å, °) in **3,6 and 8** molecules.

		3		
D*—H *A	*D*—H	H *A*	D *A*	*D*—H *A*
H24— O1H15B [i]	0.117	2.603	2.939	110
H28—O3H31 A[ii]	0.136	2.652	2.311	119
C13—N5 H13 A[i]	0.546	2.652	3.165	135.5
Symmetry codes: (i) −*x*+1, *y*+1/2, −*z*+3/2; (ii) *x*, −*y*+1/2, *z*−1/2.				
		6		
D*—H *A	*D*—H	H *A*	D *A*	*D*—H *A*
C14—O1 H16A[i]	0.119	2.601	1.206	124
C5—N2 H13A[ii]	0.440	2.310	1.338	125
C4—N1H4[i]	0.150	2.600	1.331	118.2
Symmetry codes: (i) x,-1+y,z (ii) *1-x,-y,1-z*.				
		8		
D*—H *A	*D*—H	H *A*	D *A*	*D*—H *A*
C13—C14 H13A[i]	0.252	2.148	1.385	109.3
C15—C16 H10B[ii]	0.95	1.370	1.370	109.6
Symmetry codes: (i) 1-x,1-y,1-z (ii) 1/2-x,-1/2+y,1/2-z				