

Molecular structure, spectroscopy, quantum chemical and antibacterial activity investigations of 2-methylbenzylammonium perchlorate

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Fig. S7. Antibacterial and antifungal Activity data of $(\text{C}_8\text{H}_{12}\text{N})\text{ClO}_4$ against the different selected bacteria and fungi tested.

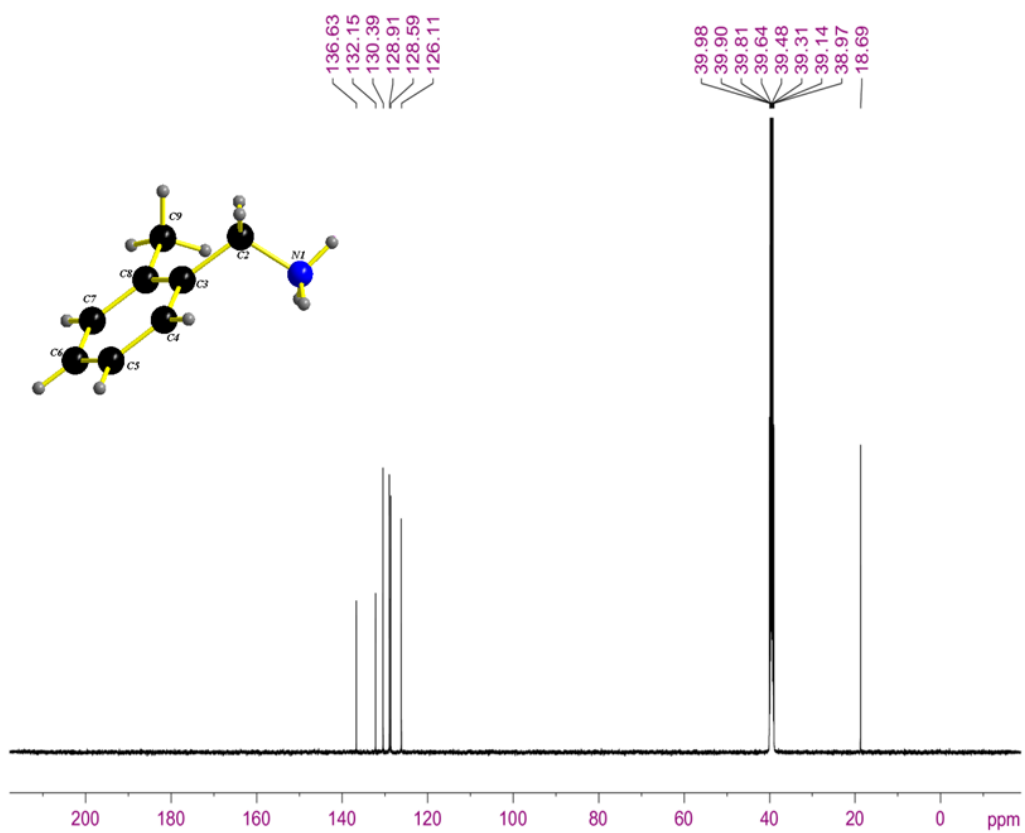


Fig. S1. The experimental ^{13}C NMR spectrum of $(\text{C}_8\text{H}_{12}\text{N})\text{ClO}_4$.

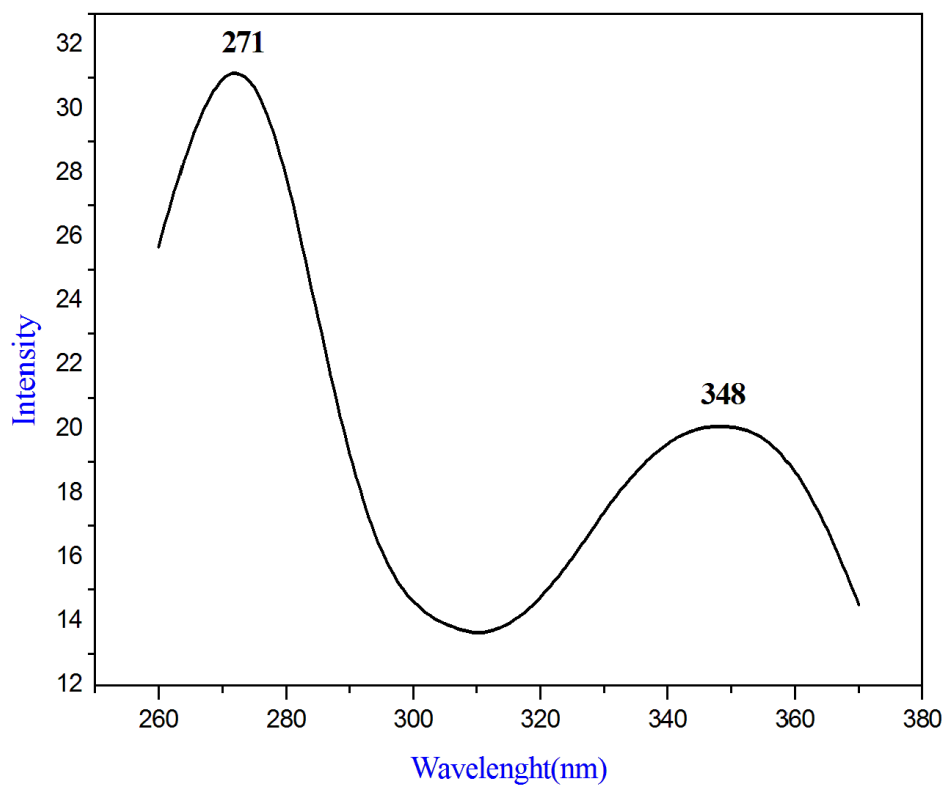


Fig. S2. Luminescence spectrum of $(C_8H_{12}N)ClO_4$.

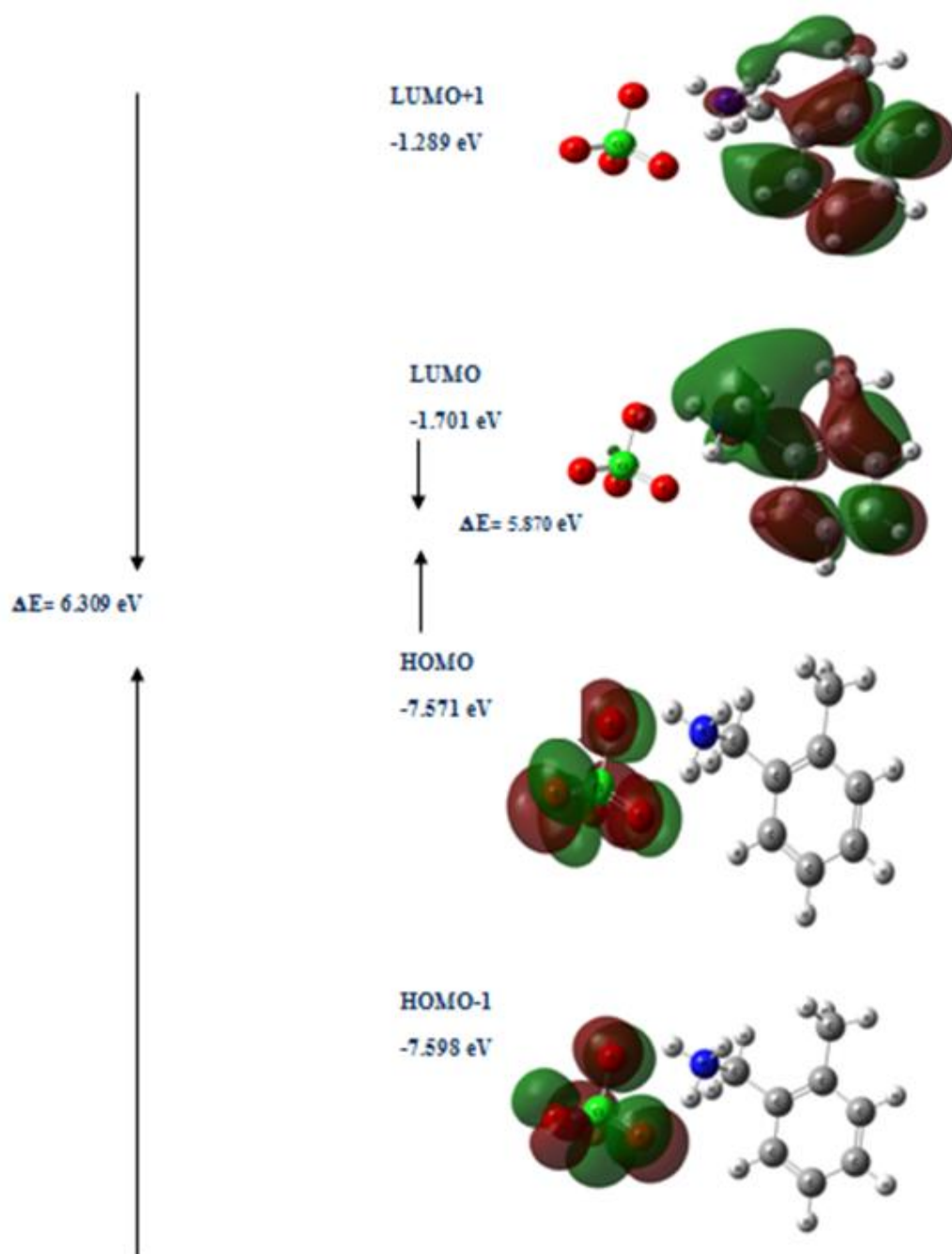


Fig. S3. Frontier molecular orbitals of $(C_8H_{12}N)ClO_4$.

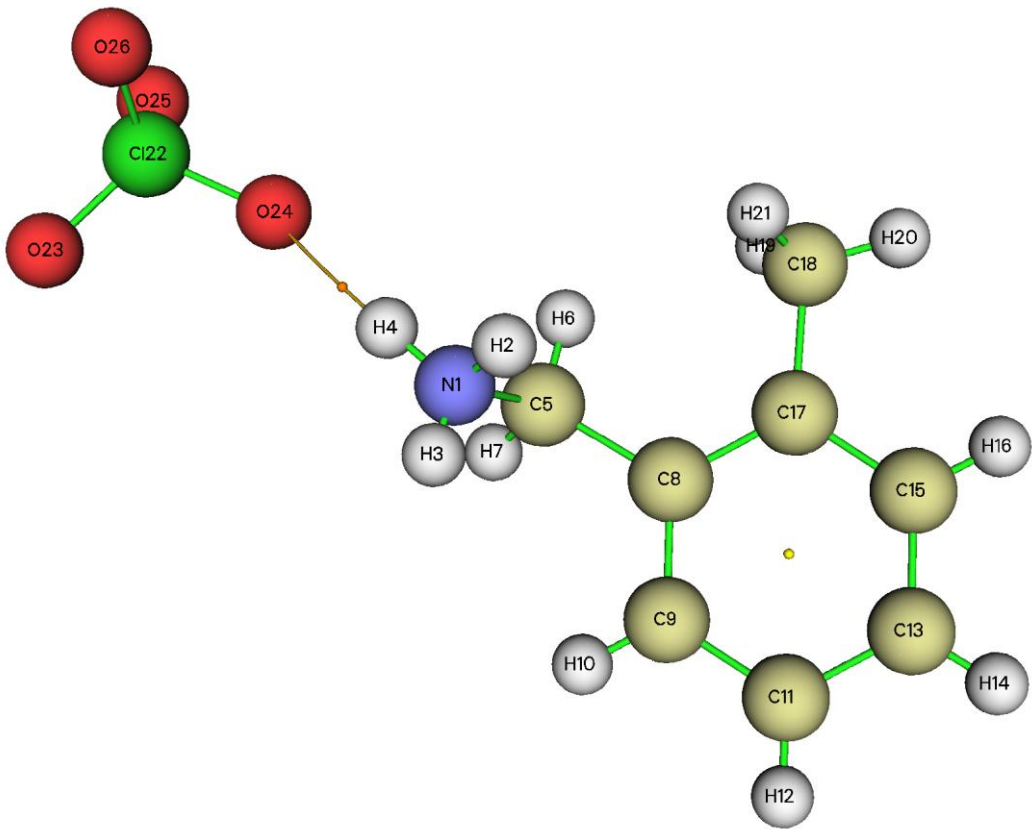


Fig. S4. Graphical representations of the AIM analysis of $(C_8H_{12}N)ClO_4$.

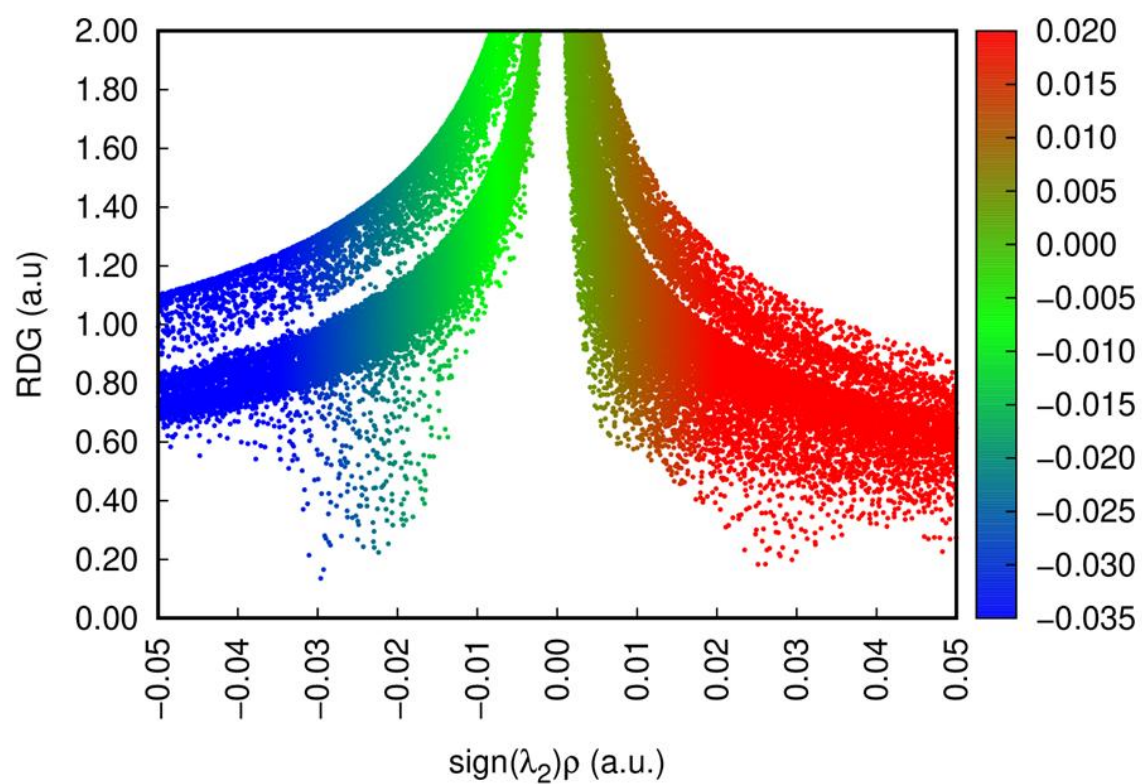


Fig. S5. Graphical representation of RDG versus the electron density multiplied by the sign of the second Hessian eigenvalue for $(\text{C}_8\text{H}_{12}\text{N})\text{ClO}_4$.

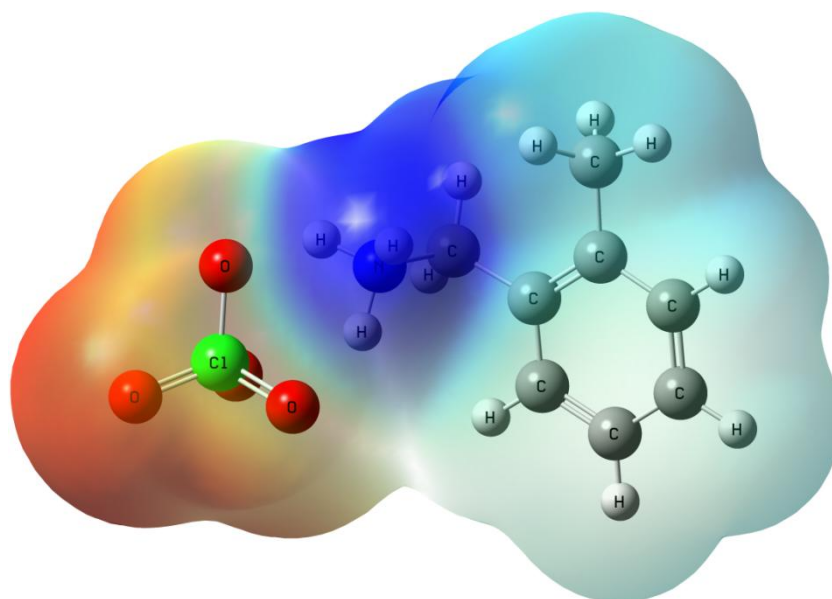


Fig. S6. Molecular electrostatic potential for (C₃H₁₂N)ClO₄ calculated at the B3LYP/6-311++G(d,p) level of theory.

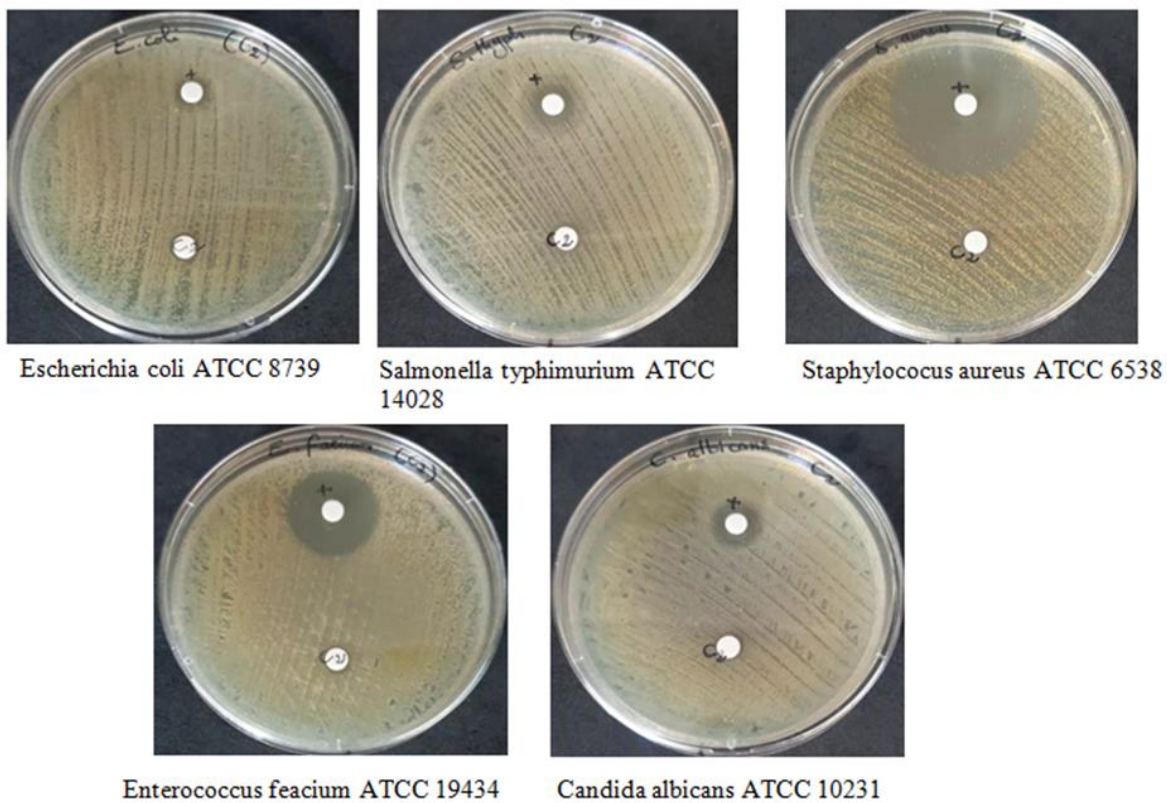


Fig. S7. Antibacterial and antifungal Activity data of $(C_8H_{12}N)ClO_4$ against the different selected bacteria and fungi tested.

Table Captions

Table S1. Enrichment ratio of different inter-contact and percentage of each atom on the surface Hirshfeld in $(C_8H_{12}N)ClO_4$.

Table S2. Theoretically computed and Experimental carbon NMR chemical shifts.

Table S3. Global reactivity descriptors the computed for the title compound.

Table S4. Topological parameters of $(C_8H_{12}N)ClO_4$.

Table S1. Enrichment ratio of different inter-contact and percentage of each atom on the surface Hirshfeld in $(C_8H_{12}N)ClO_4$.

Enrichment ratio	H	C	O
H	0.85	1.42	1.22
C		-	
O			-
% Surface	63.4	8.1	28.4

Table S2. Theoretically computed and Experimental carbon NMR chemical shifts.

Atoms	Experimental chemical shift in ppm	Calculated chemical shift in ppm	
		TMS B3LYP/6-311+G(2d,p)	GIAO (ppm)
C2	38.97		29.386
C3	136.63		147.51
C4	130.39		129.159
C5	128.59		129.159
C6	126.11		126.033
C7	128.91		129.159
C8	132.15		134.868
C9	18.69		29.386

Table S3. Global reactivity descriptors the computed for the title compound.

Parameters (eV)	Values
E_{HOMO}	-7.571
E_{LUMOMO}	-1.701
Energy band gap $ E_{\text{HOMO}}-E_{\text{LUMO}} $	5.870
$E_{\text{HOMO-1}}$	-7.598
$E_{\text{LUMO+1}}$	-1.289
Energy band gap $ E_{\text{HOMO-1}}-E_{\text{LUMO+1}} $	6.309
Ionization potential ($I = -E_{\text{HOMO}}$)	7.571
Electron affinity ($A = -E_{\text{LUMO}}$)	1.701
Chemical hardness ($\eta = (I-A)/2$)	2.935
Chemical softness ($S = 1/2\eta$)	0.170
Electronegativity ($\chi = (I+A)/2$)	4.636
Chemical potential ($\mu = -(I+A)/2$)	-4.636
Electrophilicity index $\omega = \mu^2/2\eta$	3.661
Maximum charge transfer index ($\Delta N_{\text{max.}} = -\mu/\eta$)	1.579

Table S4. Topological parameters of (C₈H₁₂N)ClO₄.

	H₄...O₂₄
Density of all electrons $\rho(\mathbf{r})$ (a.u.)	$1.748532675 \cdot 10^{-2}$
Lagrangian kinetic energy $G(\mathbf{r})$ (a.u.)	$2.494707156 \cdot 10^{-2}$
Potential energy density $V(\mathbf{r})$ (a.u.)	$-2.090168563 \cdot 10^{-2}$
Energy density $E(\mathbf{r})$ or $H(\mathbf{r})$ (a.u.)	$4.045385929 \cdot 10^{-3}$
Laplacian of electron density $\nabla^2\rho(\mathbf{r})$ (a.u.)	$1.159698300 \cdot 10^{-1}$
Reduced density gradient (RDG)	$1.612136507 \cdot 10^{-15}$
Eigen values of Hessian	$1.597841151 \cdot 10^{-1}$ $-2.104380311 \cdot 10^{-2}$ $-2.277048204 \cdot 10^{-2}$
Ellipticity of electron density(ϵ)	$8.2052 \cdot 10^{-2}$
Eta index(ζ)	$1.42508 \cdot 10^{-1}$