Synthesis, Crystal structure, Thermal analysis, Spectroscopic, Optical polarizability, DFT studies, and Molecular docking approaches of novel 2-methyl-benzilamonium derivatives for a potential anti-inflammatory control

Amal Ferchichi a, Jawher Makhlouf a\*, Kelechi Chukwuemeka b, Arto Valkonen c Hatem A.

Abuelizz d, Rashad Al-Salahi d, Youness El Bakri e,\*, Wajda Smirani a

Corresponding author: yns.elbakri@gmail.com; jawhermakhlouf60@gmail.com

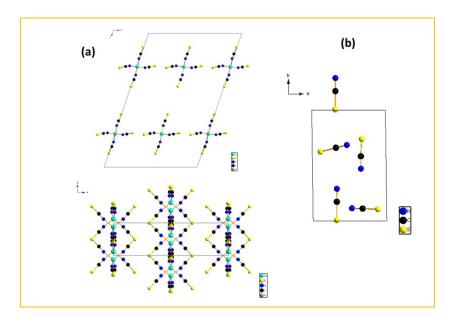
<sup>&</sup>lt;sup>a</sup> Laboratory of Material Chemistry, Faculty of Sciences of Bizerte, University of Carthage, Bizerte Zarzouna, Tunisia

<sup>&</sup>lt;sup>b</sup> Computational and Bio-Simulation Research Group, University of Calabar, Calabar, Nigeria

<sup>&</sup>lt;sup>c</sup> Department of Chemistry, University of Jyvaskyla, 40014 Jyvaskyla, Finland.

<sup>&</sup>lt;sup>d</sup> Department of Pharmaceutical Chemistry, College of Pharmacy, King Saud University, Riyadh 11451, Saudi Arabia.

<sup>&</sup>lt;sup>e</sup> Department of Theoretical and Applied Chemistry, South Ural State University, Lenin prospect 76, Chelyabinsk, 454080, Russian Federation.



 $\textbf{Fig.S1}: \label{eq:Fig.S1} Projection of the anionic part of $\left[(C_8H_{12}N)_2\operatorname{Co}(SCN)_4\right]$ (a) and $\left[(C_8H_{12}N),\operatorname{SCN}\right]$ (b) $$$ 

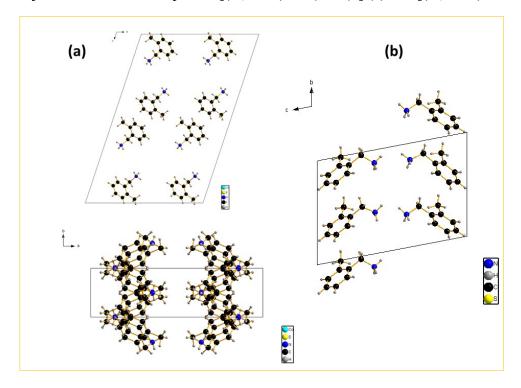


Fig. S2: Projection of the cationic part of  $[(C_8H_{12}N)_2 Co(SCN)_4]$  (a) and  $[(C_8H_{12}N), SCN]$  (b)

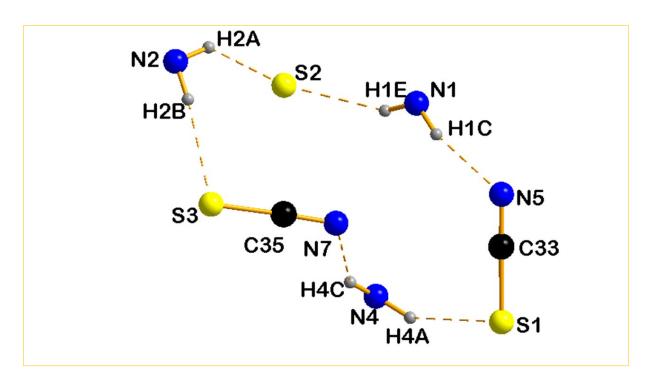
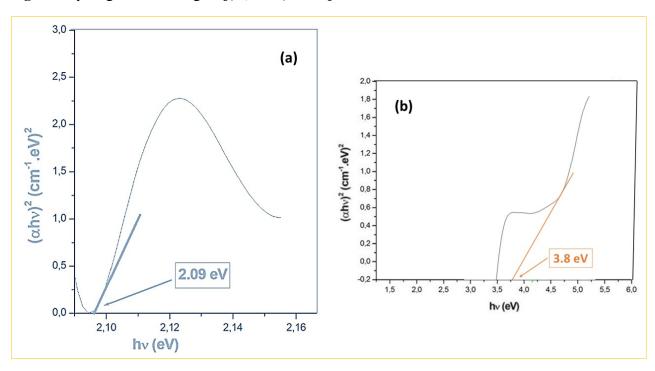


Fig. S3: Hydrogen bonds ring of  $[(C_8H_{12}N), SCN]$ 



**Fig. S4**: TAUC spectrum of (a)  $[(C_8H_{12}N)_2 Co(SCN)_4]$  (a) and  $[(C_8H_{12}N), SCN]$  (b)