AICIng
Associazione Italiana di Chimica per Ingegneria

POLITECNICO MILANO 1863

Società Chimica Italiana
Divisione di Chimica per le Tecnologie

XIII Congresso Nazionale AICIng e II Congresso Nazionale della Divisione di Chimica per le Tecnologie della SCI

ATTI DEL CONVEGNO

25-28 giugno 2023
Politecnico di Milano

XIII Congresso Nazionale AICIng e II Congresso Nazionale della Divisione di Chimica per le Tecnologie della Società Chimica Italiana

ATTI DEL CONVEGNO
25-28 Giugno 2023 - Milano

a cura di:
Giuseppina Raffaini, Fabio Ganazzoli

ISBN 978 88 3623 147 8

www.edisesuniversita.it
assistenza.edises.it

- **P14** GALLO, Vito — Food analysis by Community-Built NMR Analytical Systems
- **P15** MAURIELLO, Francesco — The full valorization of anchovy fillet leftovers: a prospective life cycle assessment
- **P16** DIRÈ, Sandra — Biostar-Pack: preparation of starch nanocomposites towards the valorization of organic food waste for sustainable packaging
- **P17** RAOS, Guido — CO_2 sequestration and storage in seawater: experimental and modelling approaches
- **P18** PILIA, Luca — Cyclopentadienyl-phenylendiamino-cobalt complexes as homogeneous selective electrocatalysts for CO_2 reduction.
- **P19** DEPERO, Laura Eleonora — Exploring the Circular Economy's Potential for Foundry Sands
- **P20** MARZORATI, Stefania — Targeting phenolics through supercritical CO_2 technology: valorization of coffee silverskin for functional extracts production
- **P21** RAOS, Guido — Squalane: a test case for computational rheology of molecular and complex fluids
- **P22** PICARELLI, Chiara — Study on Perampanel for drug sensing by DFT and Raman spectroscopy
- **P23** FINOCCHIO, Elisabetta — A close look at the catalyst surface: Oxygenated and Chlorinated VOCs conversion over Fe-Ceria catalyst through FT-IR spectroscopy
- **P24** FAMULARI, Antonino — Unusual properties of M12L8 poly-[n]-catenanes: a QM/X-ray study
- **P25** CAPPELLO, Miriam — Waste oil/water emulsions as absorbents for volatile organic solvents abatement
- **P26** PETRUCCI, Rita — Blood-Brain Barrier (BBB) permeability of new miconazole-like scaffold compounds by HPLC-ESI-MS/MS
- **P27** LOTTI, Nadia — Hydrogel-like PBS-based thermoplastic copolymer for biomedical applications
- **P28** GIANNITELLI, Sara Maria — Printability assessment of a thermosensitive photocurable biomaterial ink

Study on Perampanel for drug sensing by DFT and Raman spectroscopy

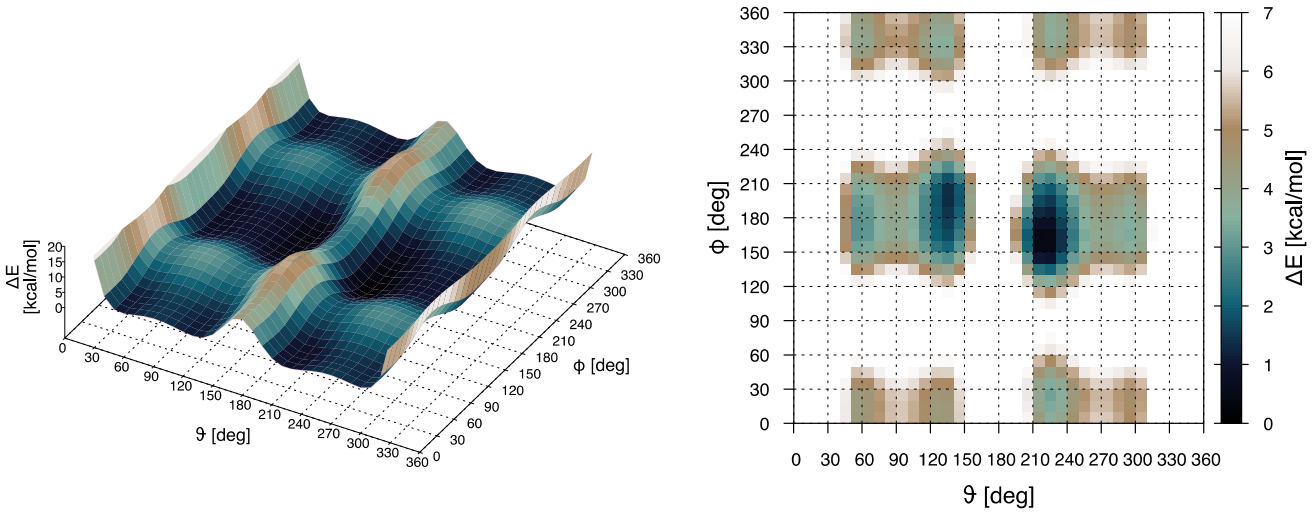
Chiara Picarelli[1], Nicolò Simone Villa[1], Giuseppina Raffaini[1], Matteo Tommasini[1]

[1]Department of Chemistry, Materials, and Chemical Engineering "Giulio Natta", Politecnico di Milano, Piazza L. Da Vinci 32, 20131 Milano, Italy

Email: chiara.picarelli@polimi.it

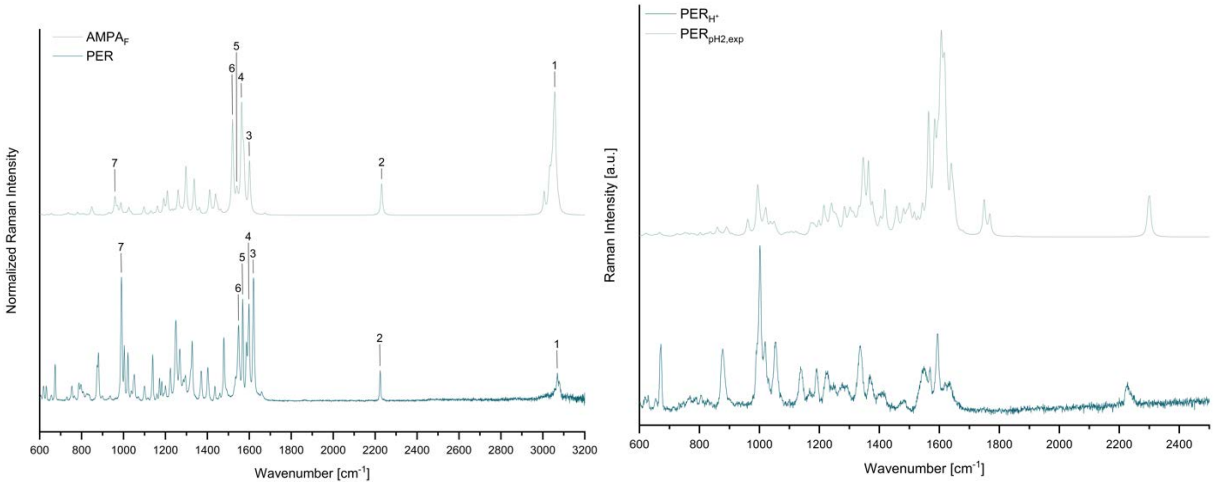
Keywords: Perampanel, Raman spectroscopy, Density Functional Theory

Perampanel (PER) is an anti-epilepsy drug used to treat and prevent the onset of seizures. Given the seriousness of the treating disease and the potential collateral effects of PER, only a narrow dosage range can effectively treat the patients [1]. Therapeutic Drug Monitoring (TDM) is thus used to control the presence of PER in the patients' biological fluids, *e.g.*, blood plasma [2].
In recent years, to improve the patient's quality of life, non-invasive alternative techniques have been investigated to accompany and complement TDM. Specifically, Raman spectroscopy and SERS can detect Perampanel in its protonated forms [3][4]. But a detailed theoretical model of both the molecular and vibrational structure of PER is still lacking.
In such context, the work presented here is the computational effort aimed to produce a thorough model of the chemical and vibrational structure of PER. Using the B3LYP/6-31G(d,p) method, the Potential Energy Surface (PES) of PER was systematically investigated. The exploration of the PES brought up the equilibrium PER conformers, among which one matches the structure of PER within its target receptor as reported in the Protein Data Bank [5].



PES (left) and PES map (right) of PER.

From the equilibrium structures of PER, we could simulate the theoretical Raman spectra. Furthermore, since SERS analyses are performed in acidic conditions, by protonating such structures also the theoretical SERS spectrum could be determined. Comparing the theoretical Raman and SERS spectra with the experimental data [4] gave a promisingly good match, which validates this model as a benchmark for future vibrational spectroscopy studies on PER.



Comparison between theoretical (top) and experimental (bottom) Raman (left) and SERS (right) spectra.

A conformational study based on Molecular Mechanics (MM) and Molecular Dynamics (MD) simulations of PER in vacuo and in explicit water is ongoing [6]. The adsorption process on the gold surface will be investigated for comparison with experimental data [7].

Acknowledgements

C.P., G.F., and M.T. have been partially funded by European Union - Next Generation EU.

References

[1] T. Hanada, Expert opinion on drug discovery, vol. *9*, no. 4, pp. 449–458, **2014**.
[2] J.-S. Kang and M.-H. Lee, The Korean Journal of internal medicine, vol. *24*, no. 1, pp. 1–10, **2009**.
[3] D.-Y. Kim, J. Moon, Y.-W. Shin, et al., Epilepsia, vol. *61*, no. 6, pp. 1120–1128, May **2020**.
[4] N.S. Villa, M.S. Thesis, Politecnico di Milano, **2018**.
[5] M.V. Yelshanskaya, A.K. Singh, J.M. Sampson, C. Narangoda, M. Kurnikova, and A.I. Sobolevsky, Neuron, vol. *91*, no. 6, pp. 1305–1315, Sep. **2016**.
[6] Materials Studio BIOVIA. Accelrys Inc. InsightII 2000; Accelrys Inc.: San Diego, CA, USA, 2000.
[7] G. Raffaini, M. Catauro, *Materials* **2022**, *15*, 2759.