

Understanding the Molecular Mechanisms that Govern Opioid Potency Through a Course-embedded Computational Research Project

Keegan Gunderson*, Faith Oldenburg, Sudeep Bhattacharyay, & Sanchita Hati*

Department of Chemistry and Biochemistry, University of Wisconsin - Eau Claire, Eau Claire, WI

<https://doi.org/10.33697/ajur.2025.137>

Students: gunderker8370@uwec.edu*, oldenbfa6097@uwec.edu

Mentors: bhattas@uwec.edu, batis@uwec.edu*

APPENDIX

	Electronegativity (eV)	Hardness (eV)
Codeine	2.253	6.038
Fentanyl	3.055	6.612
Hydrocodone	2.345	5.945
Hydromorphone	2.476	5.910
Meperidine	2.699	6.430
Methadone	2.363	5.654
Morphine	2.336	6.065
Oxycodone	2.333	6.024
Oxymorphone	2.553	5.994
Imitrex	2.104	5.121

Table S1. The computed molecular properties (electronegativity and chemical hardness) of the nine opioids and Imitrex.

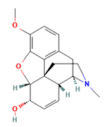
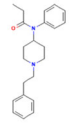
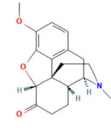
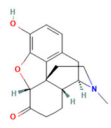
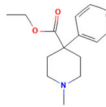
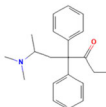
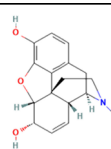
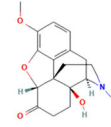
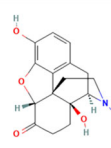
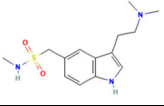
Opioid	Chemical Structure	Makeup
Codeine		Natural
Fentanyl		Synthetic
Hydrocodone		Semi-synthetic
Hydromorphone		Semi-synthetic
Meperidine		Synthetic
Methadone		Synthetic
Morphine		Natural
Oxycodone		Semi-synthetic
Oxymorphone		Semi-synthetic
Imitrex		Pain reliever

Table S2. Chemical structure, obtained from *PubChem*, of the nine opioids and Imitrex