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Molecular Docking of new eugenol derivatives with selenium like Catechol O-methyltransferase inhibitors

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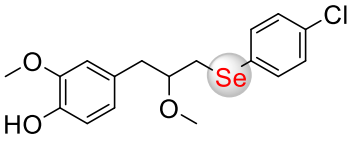
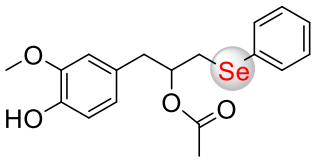
ABSTRACT

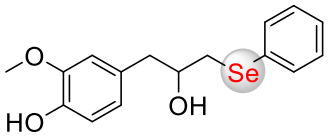
Parkinson's Disease is the second neurodegenerative disease most frequent in people over 60 years old. Tremors, rigidity, and postural instability are common symptoms of the disease, in addition to emotional disturbs, due to a decrease of dopamine levels in the brain.[1,2] The combination of L-Dopa with Dopa decarboxylase and catechol O-methyltransferase (COMT) inhibitors is used to repair the dopamine level. Tolcapone, Entacapone, and Opicapone are COMT inhibitors approved by FDA, however have some problems like hepatotoxicity and less potential.[3] To initialize the studies of new inhibitors of COMT, molecular docking is an important tool in drug discovery, due to less necessity of investment, fast results, and support for the synthesis of the compounds more important for the study.[4] This work realized the docking study of eugenol derivatives with selenium like COMT inhibitors. Software used for molecular docking was MOPAC 22.0.6, AutoDock Tools 1.5.7., Biovia Discovery Studio 2021 and PyMol.



3a



3b



3c

Compound	ΔG (kcal-mol^{-1})	Distance (Å)
Tolcapone	-6.16	2.92
Entacapone	-5.59	3.58
3a	-6.19	2.86
3b	-6.60	3.02
3c	-6.63	2.84

Compounds **3a**, **3b,** and **3c** showed excellent results, acquiring good binding energy and approximation of the cofactor SAM and Mg^{2+} in Molecular Docking. As a result, these compounds show potential to advance for *in vitro* and *in vivo* tests.

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