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Molecular Docking Studies Of Natural Phenolic Compound and Derivates With Phospholipase A2

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Introduction

The enzym phospholipase A2 (PLA2) catalyzes the conversion of membrane phospholipids in the inflammatory mediators, such as prostaglandins and leukotrienes. Because of this role, substances with inhibitory activity of PLA2 enzyme, has gained prominence in the scientific community like possible anti-inflammatory. Several studies have shown that phenolic compounds such as flavonoids, phenolic acids and other, has, among various biological activities, anti-inflammatory activity by inhibition of the enzyme PLA2. Based on this context, this study aimed to conduct a molecular docking study of various natural phenolic compounds and some of their derivatives forward to the enzyme PLA2.

Results and Discussion

It was observed that among the phenolic compounds included in the study, those with better interaction with the enzyme were rosmarinic acid 3'-O-beta-glucoside, 4-nerolidylcatechol, rosmarinic acid methyl ester, quercetin 3-O-malonylglucoside, quercetin pentaacetate and rosmarinic acid, respectively (Figure 1 and 2) (Table 1).

Table 1. Docking energies of phenolic compounds against the enzyme phospholipase A2

Compound	ΔG Binding (Kcal/mol)[a]	ΔG vdw_hb_desolv	ΔG Eletrostatic	ΔG Total Internal	ΔG Unbound energy	ΔG Energy torsional
Quercetin	-7.06	-8.42	-0.42	-1.12	-1.12	1.79
4-Nerolidylcatechol	-9.44	-11.96	-0.46	-1.09	-1.09	2.98
Caffeic Acid	-5.75	-6.95	-0.29	-0.47	-0.47	1.49
Ferulic Acid	-5.54	-5.82	-1.21	-0.48	-0.48	1.49
Sinapic Acid	-5.95	-6.48	-1.26	-0.85	-0.85	1.79
Rosmarinic Acid	-8.13	-10.92	-0.79	-1.24	-1.24	3.58
rosmarinic acid 3'-O-beta-glucoside	-9.68	-14.17	-0.58	-4.17	-4.17	5.07
Rosmarinic Acid Methyl Ester	-8.87	-12.12	-0.03	-0.92	-0.92	3.28
Rosmarinyl glucoside	-7.62	-12.74	-0.25	-1.97	-1.97	5.37
Quercetin 3-Methil Ether	-7.30	-8.6	-0.49	-0.88	-0.88	1.79
Rutin	-2.87	-7.21	-0.42	-2.01	-2.01	4.77
Retusin	-7.71	-9.08	-0.42	-0.65	-0.65	1.79
Amentoflavone	-5.62	-7.9	-0.4	-1.63	-1.63	2.68
Gallic Acid	-4.43	-5.18	-0.74	-0.74	-0.74	1.49
Quercimeritrin	-7.76	-10.97	-0.37	-0.48	-0.48	3.58
Quercetin pentaacetate	-8.79	-11.9	-0.17	-0.24	-0.24	3.28
Isoquercetin	-7.24	-10.49	-0.33	-1.14	-1.14	3.58
Quercetin 3-O-malonylglucoside	-8.81	-13.23	-0.35	-0.67	-0.67	4.77

[a] ΔG binding = ΔG vdW+hb+desolv + ΔG elec + ΔG total + ΔG tor - ΔG unb.

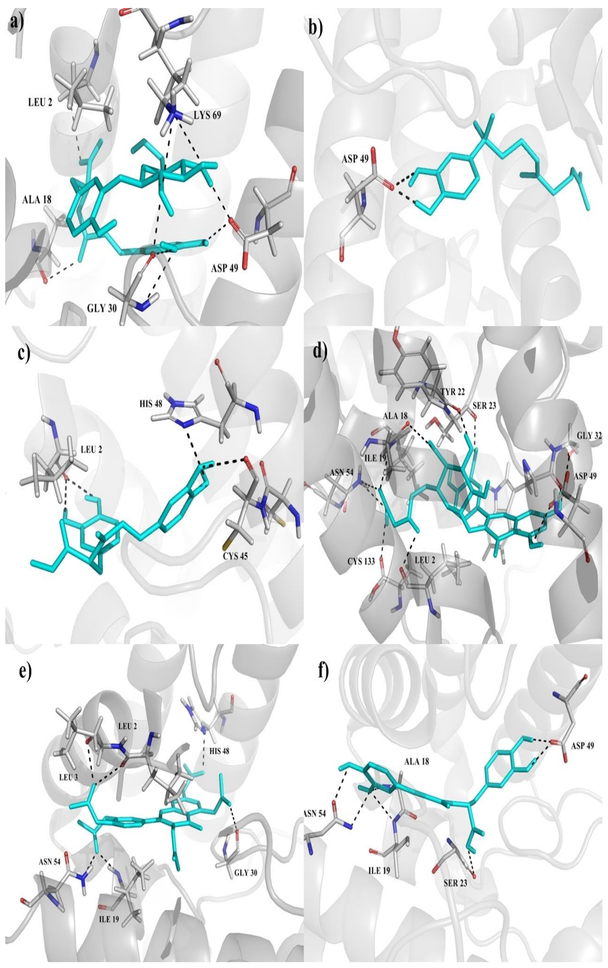

Figure 1 Hydrogen bonds of phenolic compounds **a)** rosmarinic acid 3'-O-beta-glucoside, **b)** 4-nerolidylcatechol, **c)** rosmarinic acid methyl ester, **d)** quercetin 3-O-malonylglucoside, **e)** quercetin pentaacetate e **f)** rosmarinic acid with amino acids at the active site of PLA2

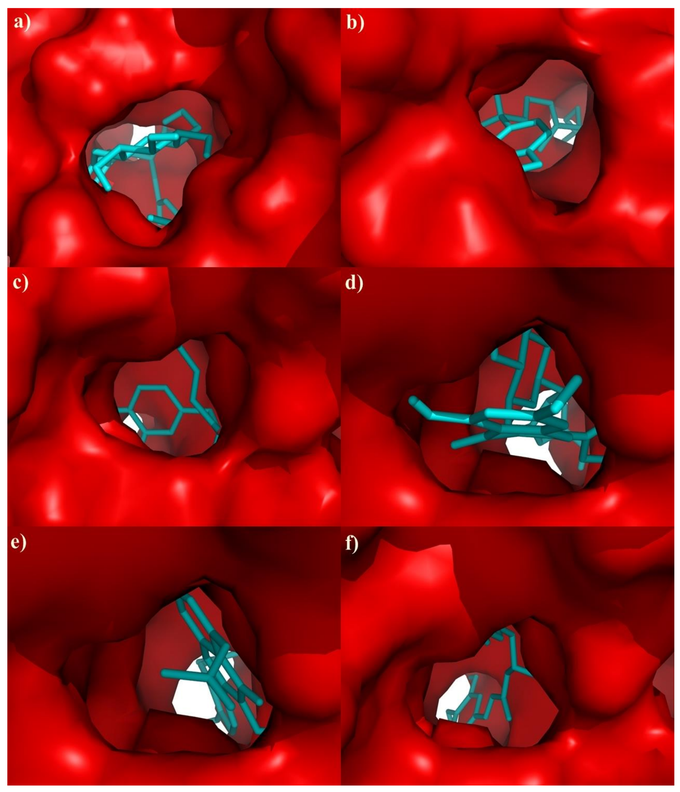

Figure 2. Compounds **a)** rosmarinic acid 3'-O-beta-glucoside, **b)** 4-nerolidylcatechol, **c)** rosmarinic acid methyl ester, **d)** quercetin 3-O-malonylglucoside, **e)** quercetin pentaacetate e **f)** rosmarinic acid in active site of PLA2.

Materials and Methods

The crystallographic structure of PLA 2 was obtained from Target Database Protein Data Bank [PDB ID: 1KPM] and the ligands were obtained from PubChem Database. The docking was performed using the AutoDock 4.0 software. .

Conclusion

The present study provides a better understanding of the inhibition of PLA2 by phenolic compounds, which may contribute to the development of new anti-inflammatories.

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