Article Prostaglandins Isolated from the Octocoral *Plexaura homomalla*: In Silico and In Vitro Studies Against Different Enzymes of Cancer

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Figure S1: ¹H NMR spectrum of Prostaglandin A₂-AcMe (1) in CDCl₃



Figure S2: ¹³C NMR spectrum of Prostaglandin A₂-AcMe (1) in CDCl₃



Figure S3: COSY NMR spectrum of Prostaglandin A2-AcMe (1) in CDCl3









Figure S6: ¹H NMR spectrum of Prostaglandin A₂ (2) in CDCl₃



Figure S7: ¹³C NMR spectrum of Prostaglandin A₂ (2) in CDCl₃





Figure S9: 1H NMR spectrum of derivative 3 in CDCl3



Figure S10: ¹³C NMR spectrum of derivative 3 in CDCl₃



Figure S11: ¹H NMR spectrum of derivative 4 in CDCl₃



Figure S12: ¹³C NMR spectrum of derivative 4 in CDCl₃



Figure S13: ¹H NMR spectrum of derivative 5 in CDCl₃



Figure S14: ¹³C NMR spectrum of derivative 5 in CDCl₃



Figure S15: 3D interaction models of test compounds within the active site of p38α-kinase enzyme (PDB ID: 4FA2). a) **1** (blue sticks); b) **2** (light pink sticks); c) **3** (violet sticks); d) **4** (light green sticks); and e) **5** (white sticks). Hydrogen bonds and enzyme residues in dark green lines and light brown sticks, respectively.



Figure S16: 3D interaction models of test compounds within active site of topoisomerase II*α* enzyme (PDB ID: 1ZXM). a) **1** (blue sticks); b) **2** (light pink sticks); c) **3** (violet sticks); d) **4** (light green sticks); and e) **5** (white sticks). Hydrogen bonds and enzyme residues in dark green lines and light brown sticks, respectively.



Figure S17: 3D interaction models of test compounds within the active site of Src-kinase enzyme (PDB ID: 2BDF). a) **1** (blue sticks); b) **2** (light pink sticks); c) **3** (violet sticks); d) **4** (light green sticks); and e) **5** (white sticks). Hydrogen bonds and enzyme residues in dark green lines and light brown sticks, respectively.



Table S1: Vina scores	and binding features	for the best pose of	f each test compound	within the active site of $p38\alpha$
kinase (PDB ID: 4FA2)	.)			

Commoniad	Vina Scores	Binding features		
Compound	(kcal/mol)	Residue	Type	Length (Å)
	1 -8,3	${}^{1}Gly_{110}$	H-Bond	2.0
1		1 Met ₁₀₉	H-Bond	2.0
1		${}^{1}Gly_{170}$	H-Bond	2.1
		$^{1}Leu_{171}$	H-Bond	2.3
2	<u> </u>	${}^{1}Gly_{170}$	H-Bond	2.0
Z	-8,0	$^{1}Leu_{171}$	H-Bond	2.5
3	-8,1	${}^{1}Gly_{170}$	H-Bond	2.1
4	-8,1	${}^{1}Gly_{170}$	H-Bond	2.1
5	-8,5	³ Lys ₅₃	H-Bond	2.1

¹Bonding to amide NH group; ²Bonding to amide carbonyl group; ³Bonding to side chain R

Commound	Vina Scores	Binding features		
Compound	(kcal/mol)	Residue	Туре	Length (Å)
1	0 7	${}^{1}Gly_{164}$	H-Bond	2.1
1	-8,2	³ Asn ₁₅₀	H-Bond	2.4
		³ Asn ₁₅₀	H-Bond	2.1
2	07	${}^{3}Asn_{120}$	H-Bond	2.3
2	-0,7	1 Ala 167	H-Bond	2.3
		$^{1}Ala_{167}$	H-Bond	2.3
		${}^{3}Asn_{120}$	H-Bond	1.8
2	0 5	³ Asn ₁₅₀	H-Bond	2.0
3	-0,3	1 Ala 167	H-Bond	2.1
		³ Thr ₂₁₅	H-Bond	2.2
	9.6	³ Asn ₁₂₀	H-Bond	1.8
4	-8,6	1 Ala 167	H-Bond	2.1
5	-8,0	¹ Ser ₁₄₉	H-Bond	1.8

Table S2: Vina scores and binding features for the best pose of each test compound within the active site of topoisomerase II α (PDB ID: 1ZXM)

¹Bonding to amide NH group; ²Bonding to amide carbonyl group; ³Bonding to side chain R

Commenced	Vina scores	Binding features		
Compound	(kcal/mol)	Residue	Type	Length (Å)
1	-8,3	$^{1}Asp_{404}$	H-Bond	2.3
2	8.0	$^{1}Asp_{404}$	H-Bond	2.0
2	-0,9	³ Glu ₃₁₀	H-Bond	2.2
3	-7,9	³ Lys ₂₉₅	H-Bond	2.1
4	-8,1	¹ Ser ₃₄₅	H-Bond	2.4
		³ Lys ₂₉₅	H-Bond	2.3
5	-8,1	² Asp ₄₀₄	H-Bond	2.4
		$^{3}Asp_{404}$	H-Bond	2.7

Table S3: Vina scores and binding features for the best pose of each test compound within the active site of Src-kinase (PDB ID: 2BDF)

¹Bonding to amide NH group; ²Bonding to amide carbonyl group; ³Bonding to side chain R