

Bioguided Fractionation of Local Plants against Matrix Metalloproteinase9 and Its Cytotoxicity against Breast Cancer Cell Models: *In Silico* and *In Vitro* Study

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Table S1: The binding affinity of published PEX9 inhibitors predicted by molecular docking compared to their experimental dissociation constant upon PEX9 inhibition.

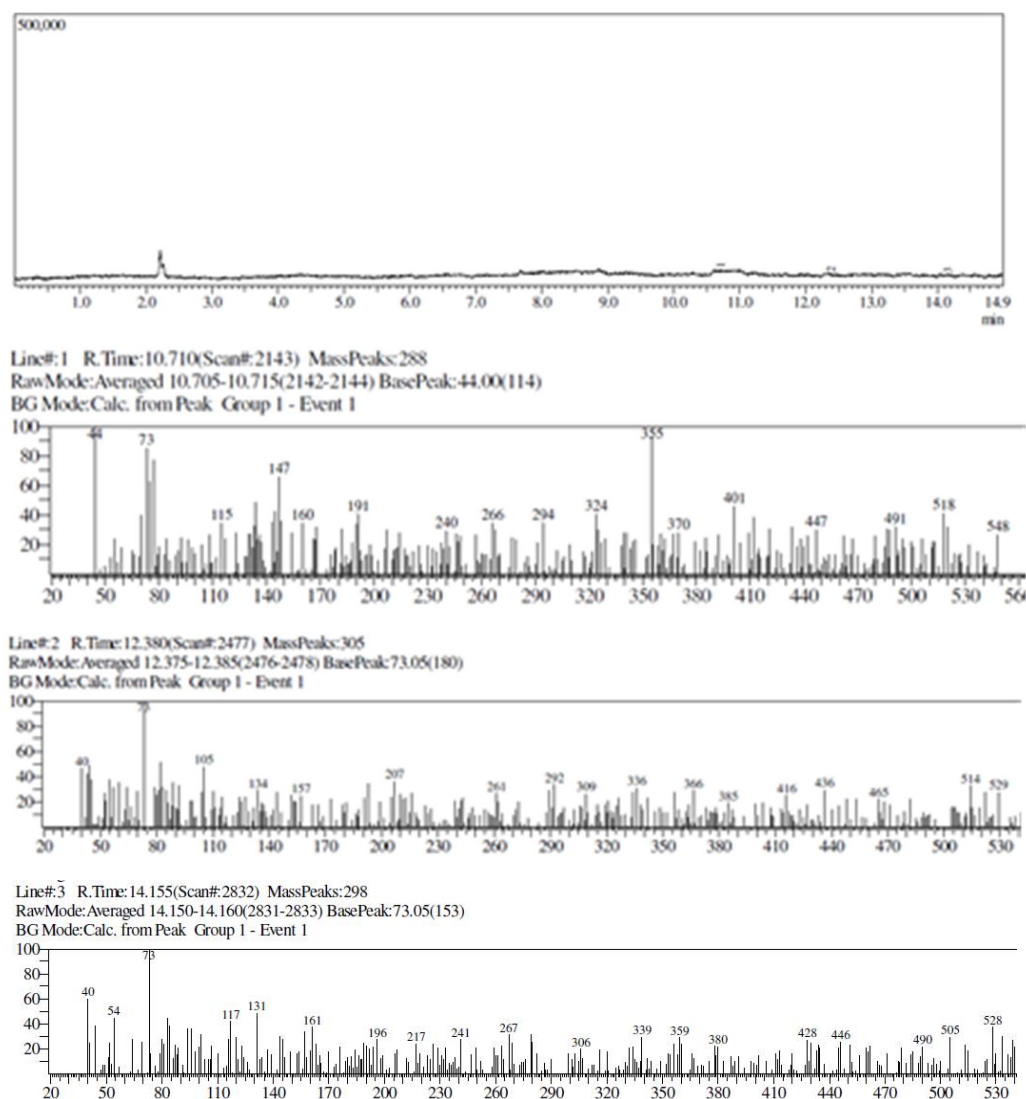
Ligand	Free Energy of Binding (kcal/mol)	K _d ^{18,19} (μM)	Activity Classification
alford_3d	-8.70	0.49	TP
alford_4d	-8.60	0.31	TP
dufour_2	-7.90	2.00	FP
alford_4c	-7.70	0.65	TP
alford_3a	-7.60	0.56	TP
alford_1d	-7.60	1.33	uncertain
alford_3b	-7.50	0.49	TP
alford_4a	-7.40	0.42	TP
alford_1c	-7.00	4.22	FP
alford_1a	-7.00	1.33	uncertain
alford_2c	-6.80	0.87	TP
alford_2a	-6.70	1.15	uncertain
alford_3c	-6.70	0.32	TP
alford_4b	-6.60	0.87	TP
alford_1b	-6.50	4.87	FP
alford_1f	-5.90	0.49	TP
alford_4e	-5.70	0.87	TP

Uncertain = moderately active

Table S2: The yield of *Ageratum conyzoides* and *Ixora coccinea* fractions of ethylacetate and *n*-hexane, respectively.

Plants	Yield (%)			
	Fraction 1	Fraction 2	Fraction 3	Fraction 4
<i>Ageratum conyzoides</i>	8.8	15.8	7.0	7.0
<i>Ixora coccinea</i>	6.8	0.3	0.9	NA

Figure S1. The mass spectra of three peaks identified from GC chromatogram of *Ixora* fraction 1. The three GC chromatogram peaks with Rt 10.709 min, 12.380 min, and 14.153 min are detected as compounds having mass/ ion: 548 (base peak 355), 529 (base peak 73), and 528 (base peak 73), respectively. The base peak informs the most stable fragment during electron impact in MS characterization.





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