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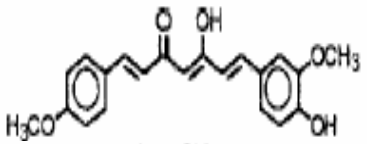
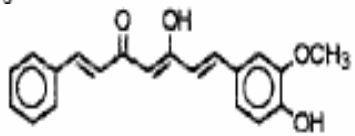
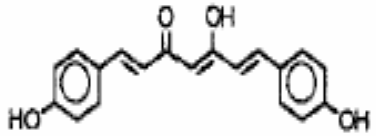
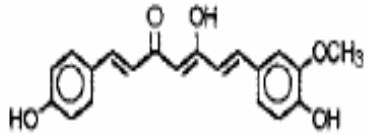
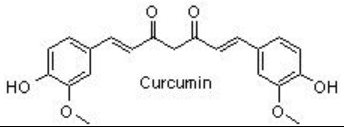
www.bioinformation.net **Hypothesis**

Supplementary material

S. NO	Structure	Chemical formula	Binding energies	
			HAT Enzyme	SERCA Enzyme
1		DAH1 - 5-hydroxy-7-(4-hydroxy-3-methoxyphenyl)-1-(4-methoxyphenyl)-1,4,6-heptatrien-3-one	(i) -29.18 (ii) -164.279 (iii) 19.2593 (iv) -144.562	(i) -30.2461 (ii) -106.192 (iii) 17.5476 (iv) -88.1829
2		DAH2 - 5-hydroxy-7-(4-hydroxy-3-methoxyphenyl)-1-phenyl-1,4,6-heptatrien-3-one	(i) -26.2266 (ii) -158.909 (iii) 14.3788 (iv) -144.468	(i) -25.6674 (ii) -93.8525 (iii) 5.5588 (iv) -88.0193
3		DAH3 - 5-hydroxy-1,7-di(4-hydroxyphenyl)-1,4,6-heptatrien-3-one	(i) -24.7644 (ii) -157.339 (iii) 10.5144 (iv) -146.824	(i) -22.4891 (ii) -94.5298 (iii) 1.3044 (iv) -93.2254
4		DAH4 - 5-hydroxy-7-(4-hydroxy-3-methoxyphenyl)-1-(4-hydroxyphenyl)-1,4,6-heptatrien-3-one	(i) -26.5945 (ii) -161.974 (iii) 15.9454 (iv) -145.986	(i) -29.1099 (ii) -98.3877 (iii) 0.068099 (iv) -98.4211
5		CURCUMIN - 1E,6E)-1,7-bis(4-hydroxy-3-methoxyphenyl)hepta-1,6-diene-3,5-dione	(i) -17.0122 (ii) -166.369 (iii) 10.8862 (iv) -112.07	(i) -20.03916 (ii) -108.678 (iii) 12.3604 (iv) -81.7927

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S.No	Energy total	Compound
1	-182.4	5388781
2	-182	5317600
3	-181	167551
4	-170	528158
5	-161	5318148
6	-146	ZINC 02243778
7	-141	ZINC 05023674
8	-135	ZINC 1045599
9	-133	ZINC 057722412
10	-112	Curcumin

Table 2: The results of top 10 best docking compounds on Histone acetyltransferase enzyme

S.No	Compound	E. Tot (Curcumin unbound)	E. Tot (Curcumin bound)
1	DAH1	-88.182	-88.36
2	DAH2	-88.01	-97.05
3	DAH3	-93.22	-99.08
4	DAH4	-98.42	-107.66

Table 3: Showing comparative docking energies of diarylheptanoids when they are docked to SERCA enzyme and to curcumin bound SERCA enzyme

S No.	Compound	SERCA enzyme	Curcumin bound SERCA enzyme
1	DAH1	Ser610	Ile931
		Asn330	Arg325
2	DAH2	Arg325	Ser610
3	DAH3	Arg325	Ser610
		Trp932	Trp932
4	DAH4	Arg325	Ser610
		Trp932	

Table 4: Showing residues forming hydrogen bond interactions at the active site.

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