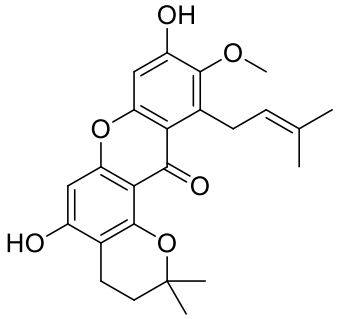
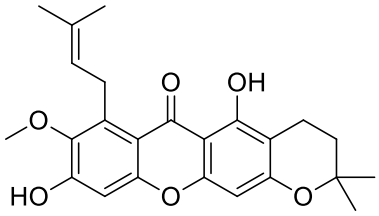
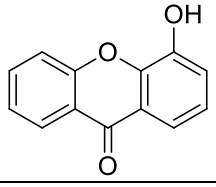
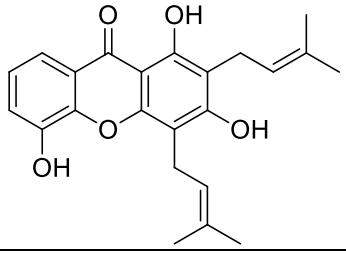
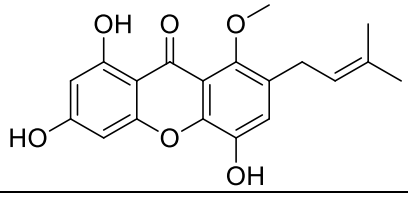
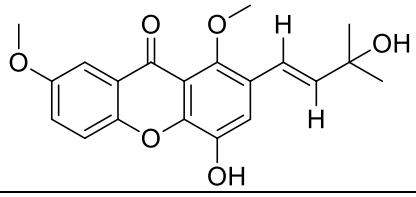
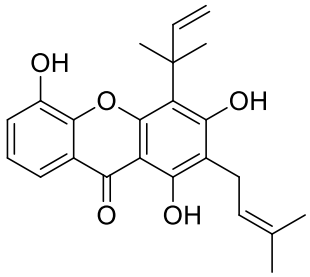
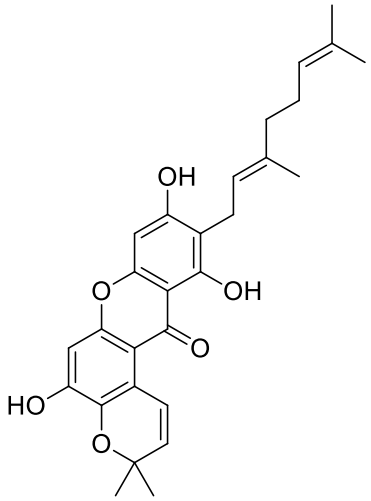
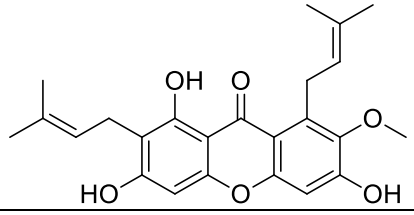
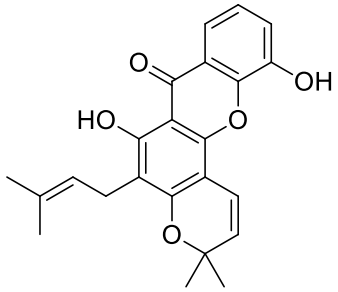
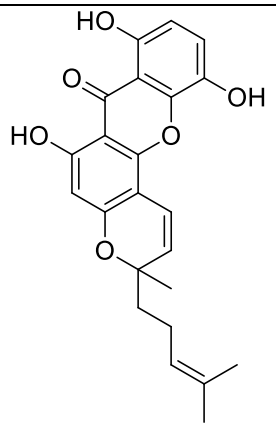
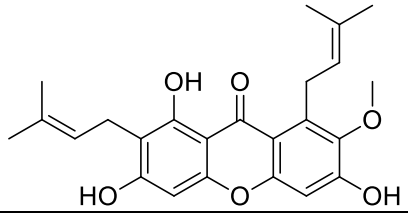
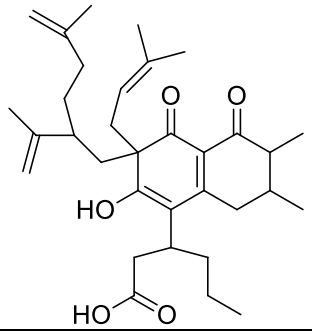
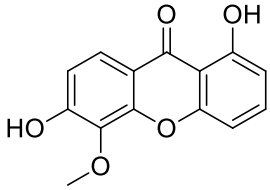
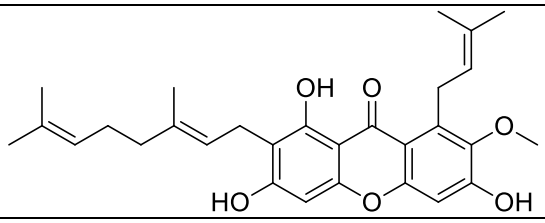
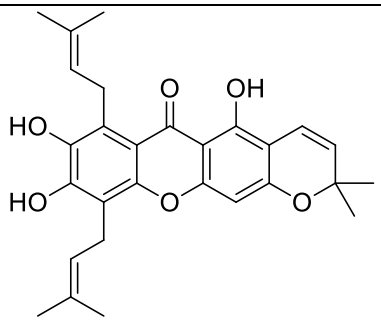
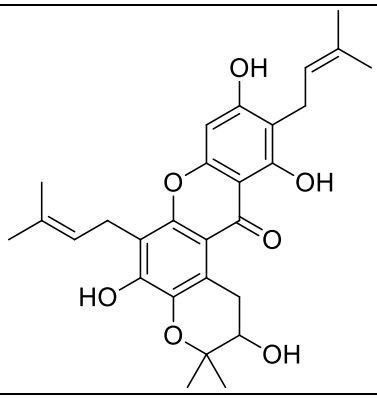
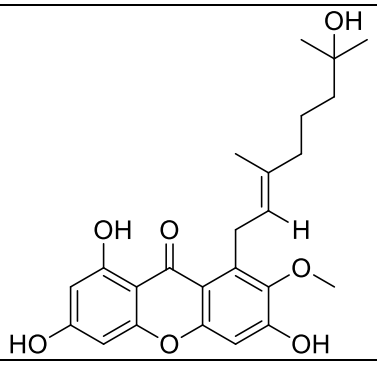
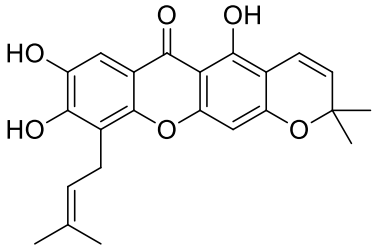
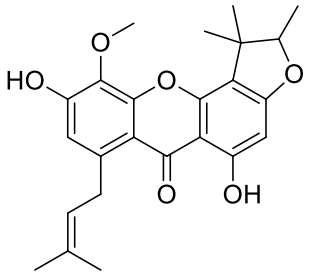
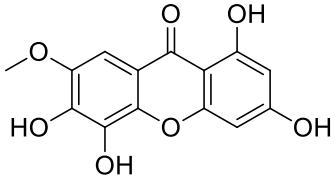
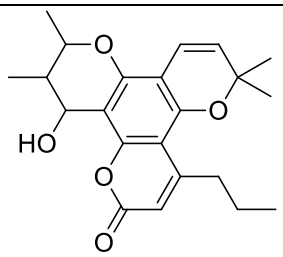
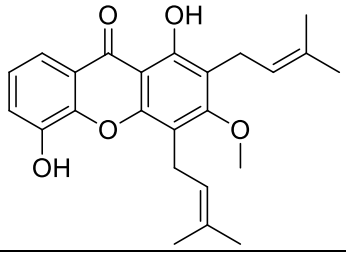
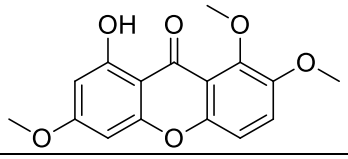
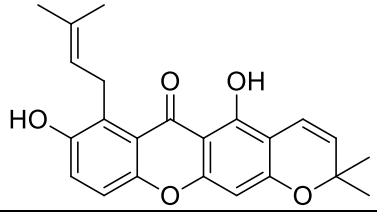
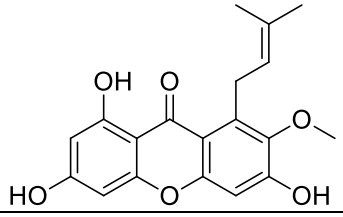
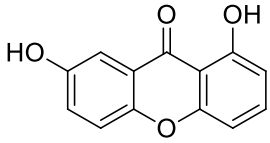
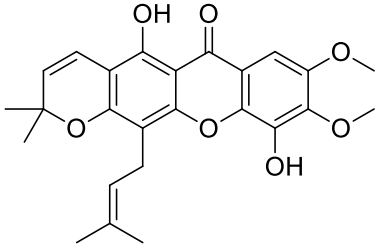
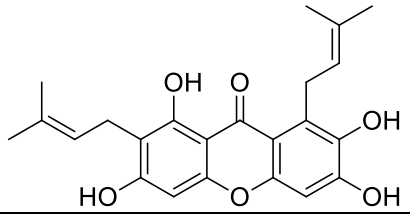
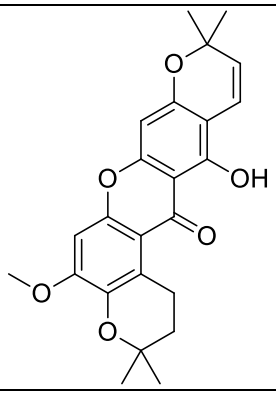
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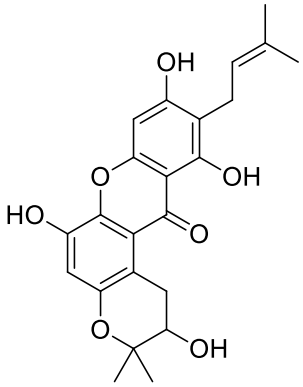
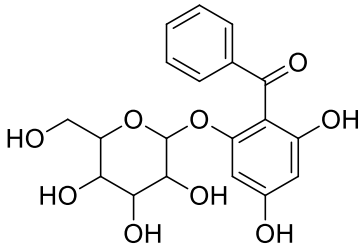
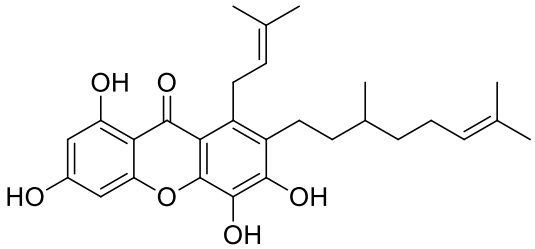
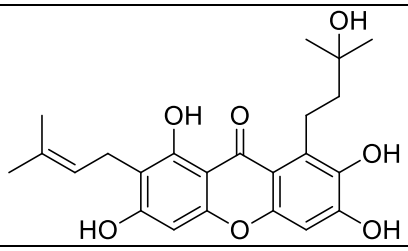
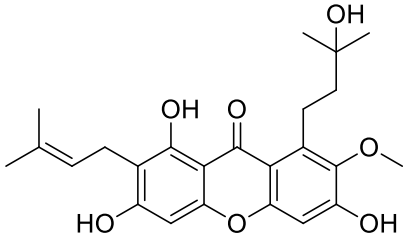
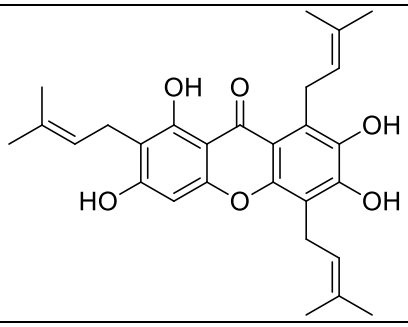
Name of compound	Pubchem ID	Chemical structure
1-Isomangostin	5281641	
3-Isomangostin	13873655	
4-hydroxyxanthone	611428	
8-Desoxygartanin	392450	
Afzeliixanthone A	11988345	
Afzeliixanthone B	102175851	

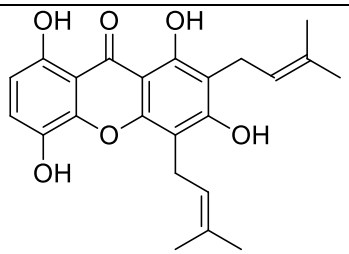
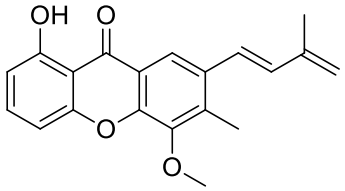
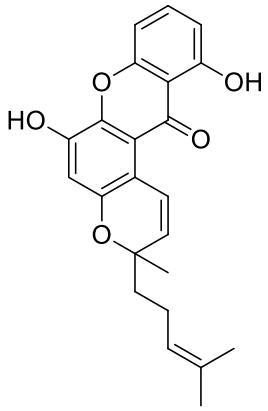
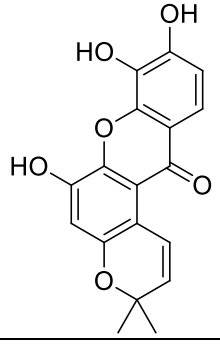
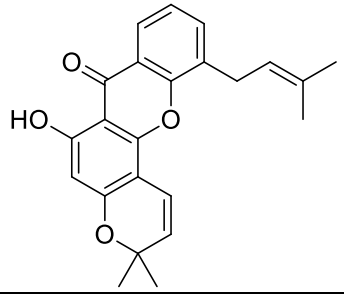
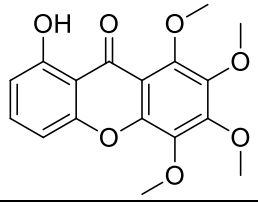
Allanxanthone A	636851	
Allanxanthone B	11328706	
Alpha-Mangostin	5281650	
Ananixanthone	493305	
Bangangxanthone A	11524043	

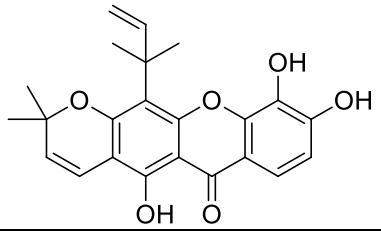
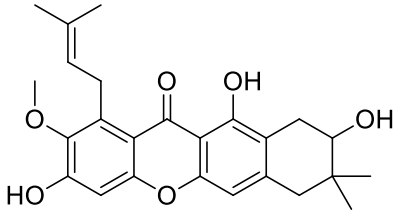
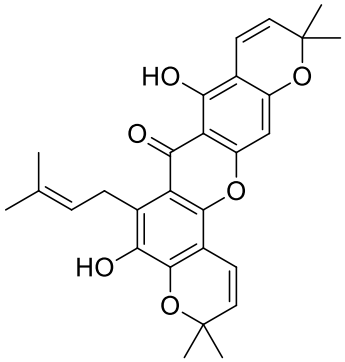
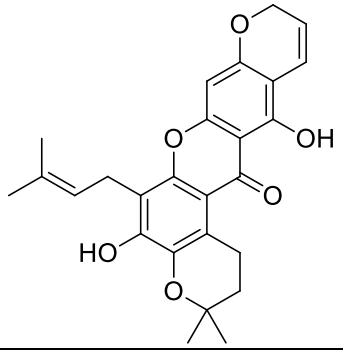
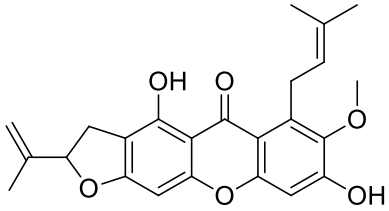
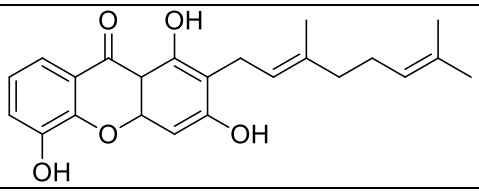
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Brasiliensic acid	71436711	
Buchanaxanthone	5481840	
Butyraxanthone A	44138727	
Butyraxanthone B	25073518	
Butyraxanthone C	44138728	

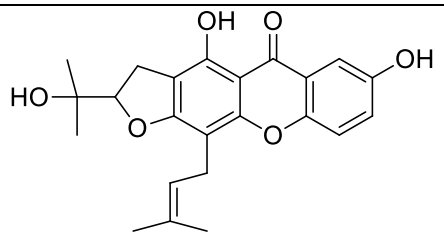
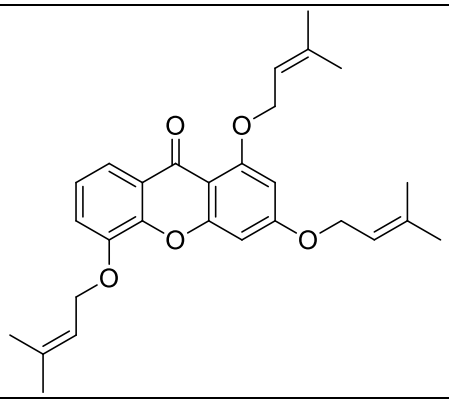
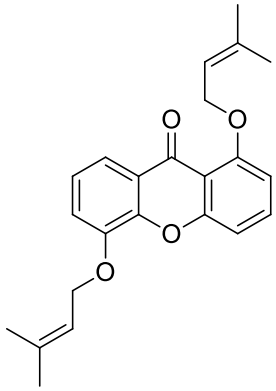
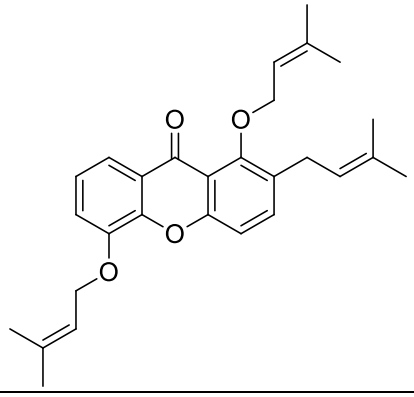
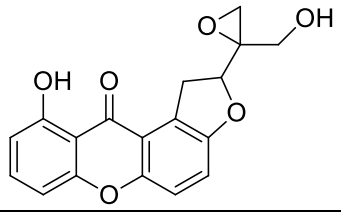
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Costatolide	461128	
Cudraxanthone G	42645953	

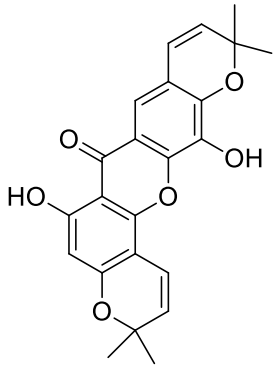
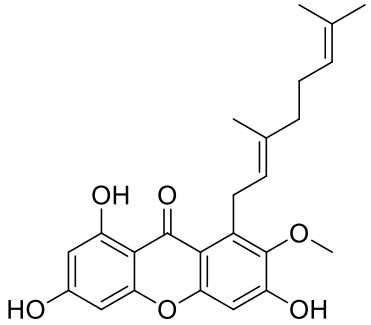
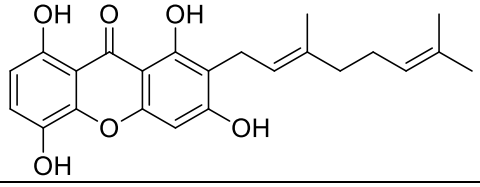
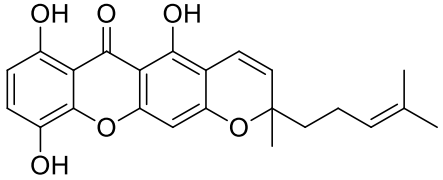
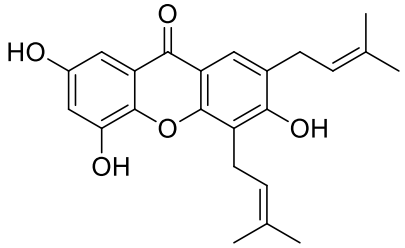
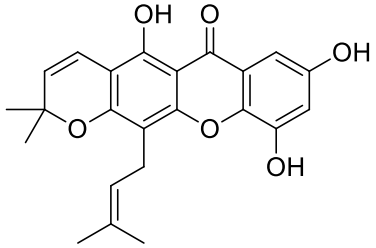
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Euxanthone	5281631	
Gaboxanthone	11704807	
Gamma-mangostin	5464078	
Garcimangosone B	11143989	

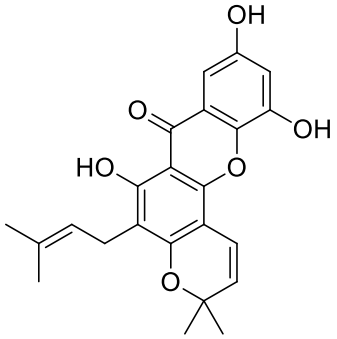
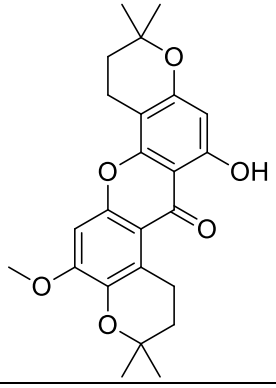
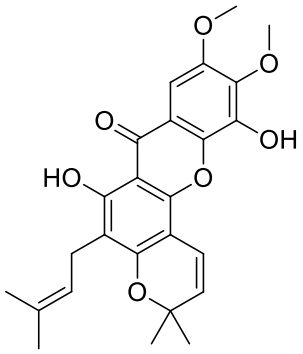
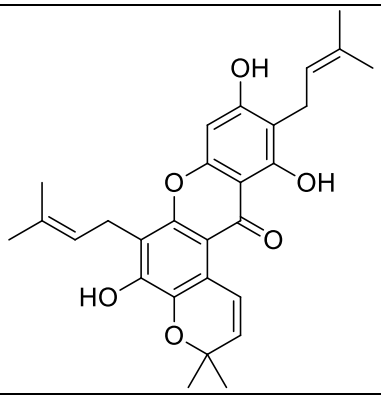
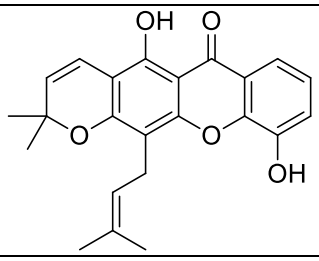
Garcimangosone C	10916629	
Garcimangosone D	11003703	
Garciniaxanthone E	10457167	
Garcinone C	44159808	
Garcinone D	5495926	
Garcinone E	10298511	

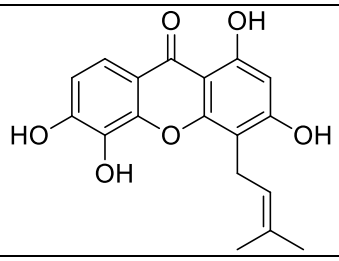
Gartanin	5281633	
Globulixanthone A	5323527	
Globulixanthone B	10452251	
Globulixanthone C	5317656	
Laurentixanthone A	10681685	
Laurentixanthone B	16081684	

Macluraxanthone	5281646	
Mangostanol	10048103	
Mangostenone A	509267	
Mangostenone B	21672078	
Mangostenone F	49866102	
Mangostinone	6478778	

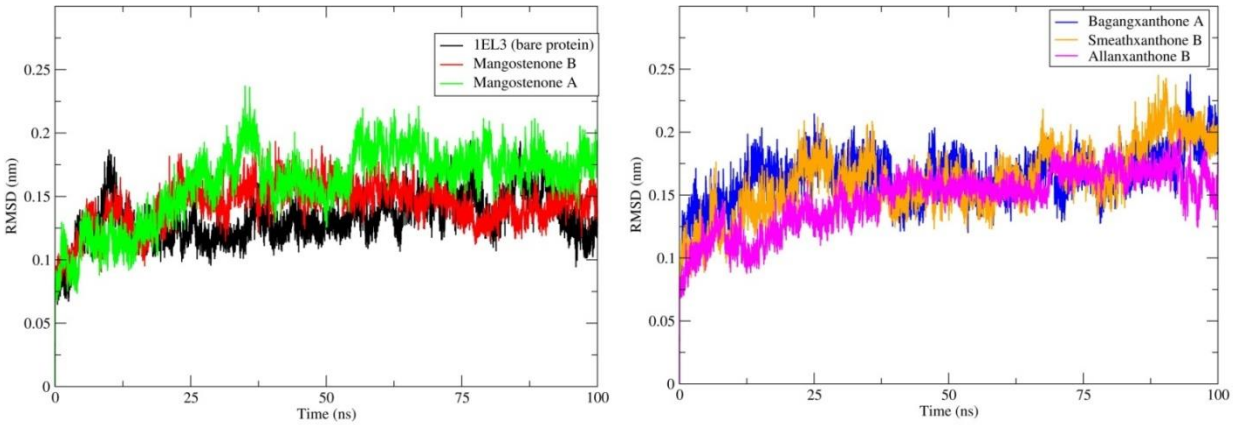
Mangoxanthone	101763994	
Polyanxanthone A	24814164	
Polyanxanthone B	24814165	
Polyanxanthone C	101844608	
Psoroxanthin	24854052	

Rheediaxanthone A	102060338	
Rubraxanthone	9953366	
Smeathxanthone A	11509473	
Smeathxanthone B	11625362	
Staudtiixanthone A	44517666	
Staudtiixanthone B	44517672	

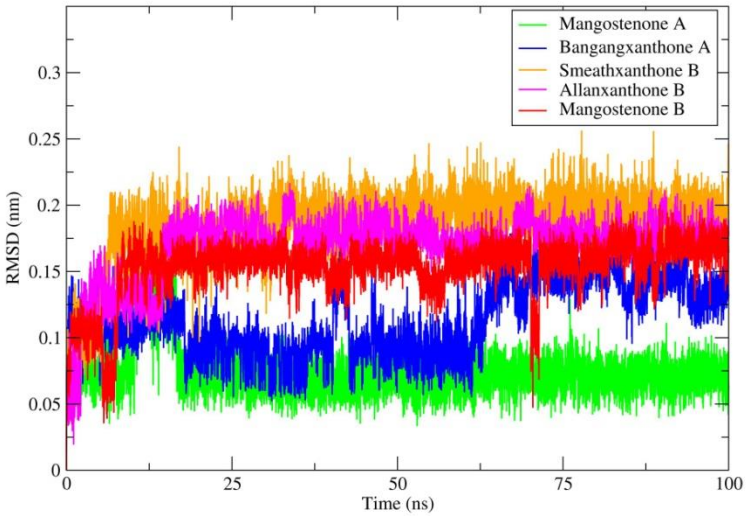
Staudtiixanthone C	44517665	
Staudtiixanthone D	44517673	
Symphonin	11561251	
Tovophyllin A	42645954	
Trapezifolixanthone	188341	

Ugaxanthone	5321880	

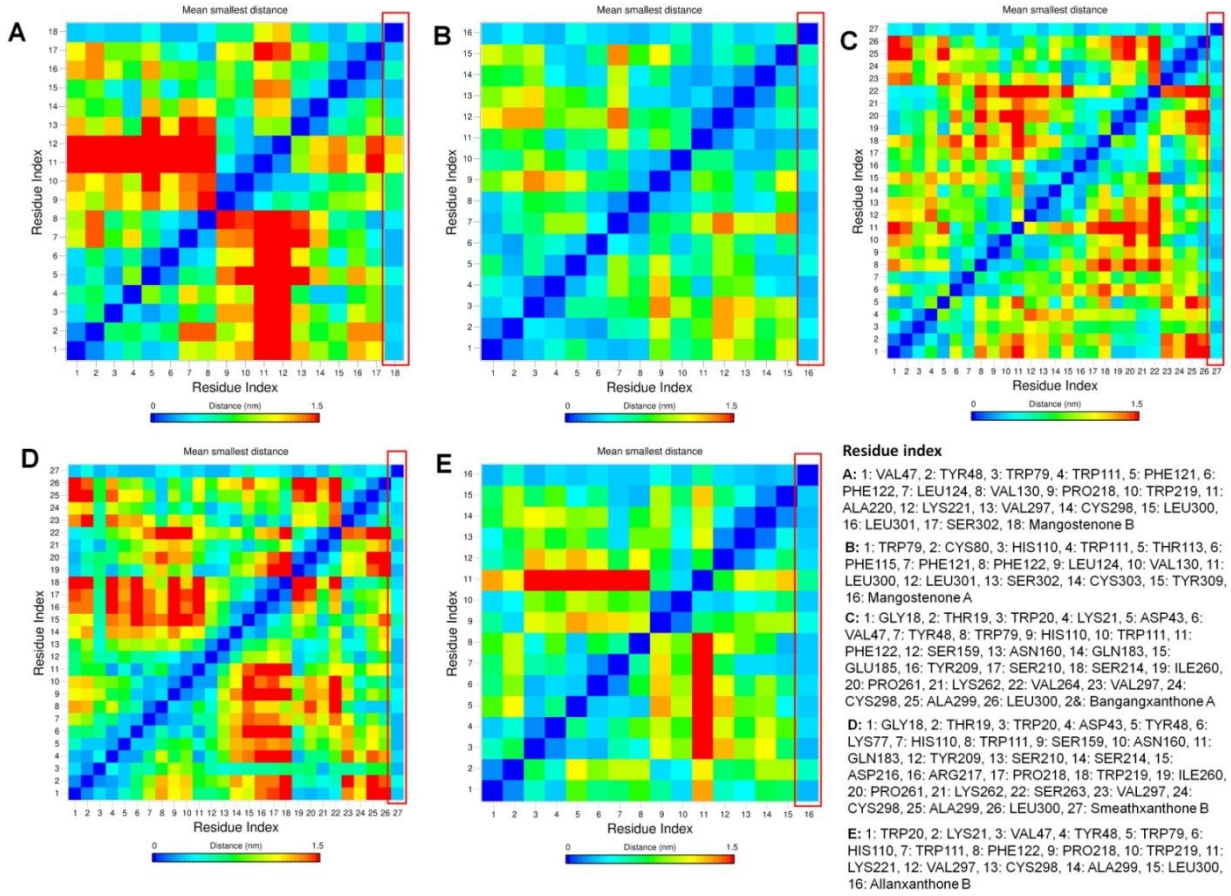
Supplementary information, Figure S1: RMSD in AR backbone atoms when bound to xanthones.



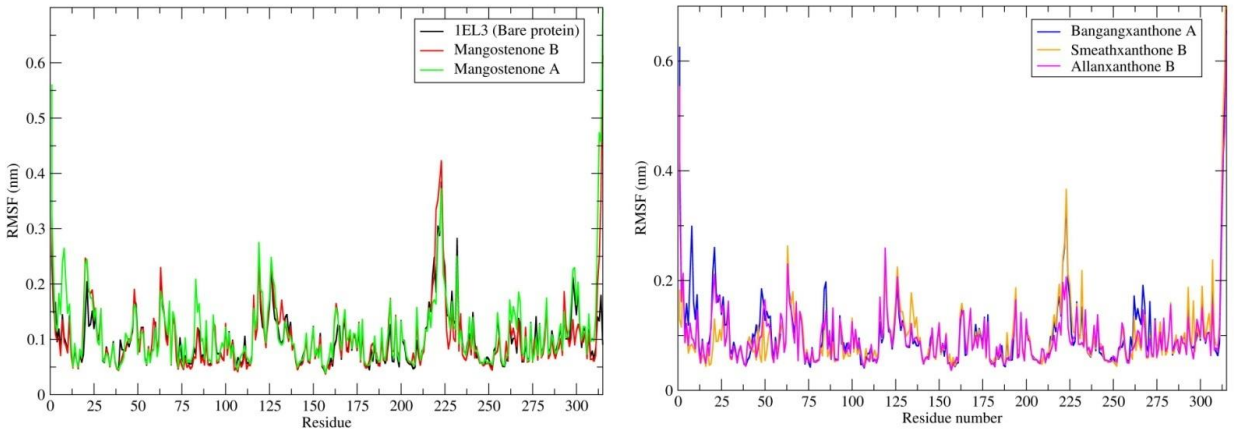
Supplementary information, Figure S2: RMSD in ligand atoms when bound to AR.



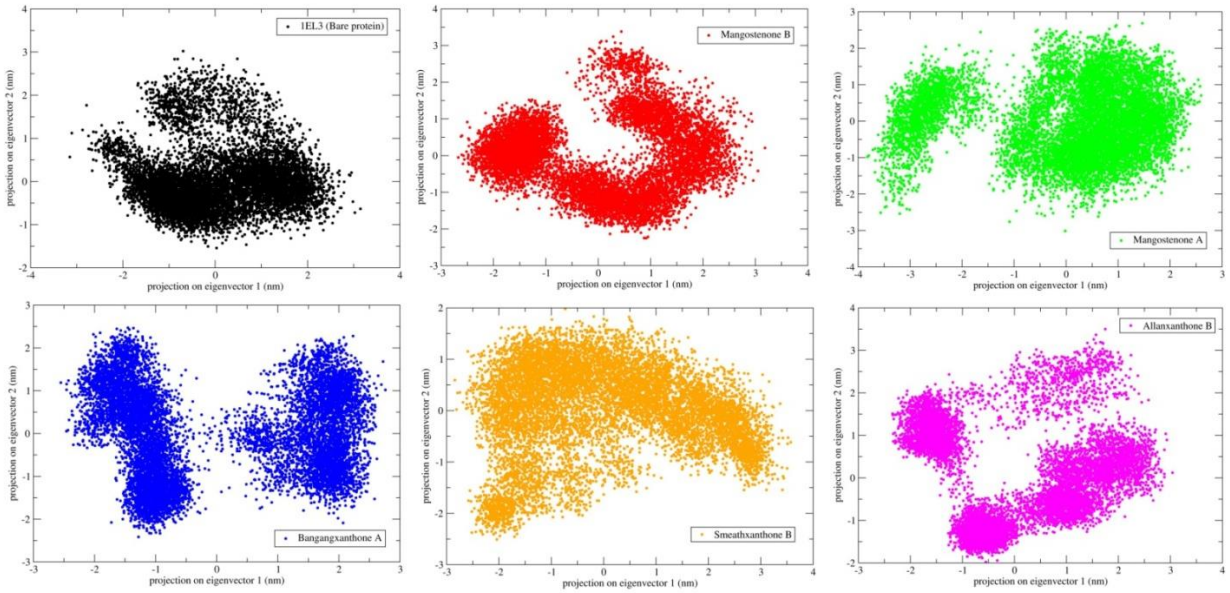
Supplementary information, Figure S3: Contact map analysis between ligands and residues within 1.5 nm contact distance during MD simulation.



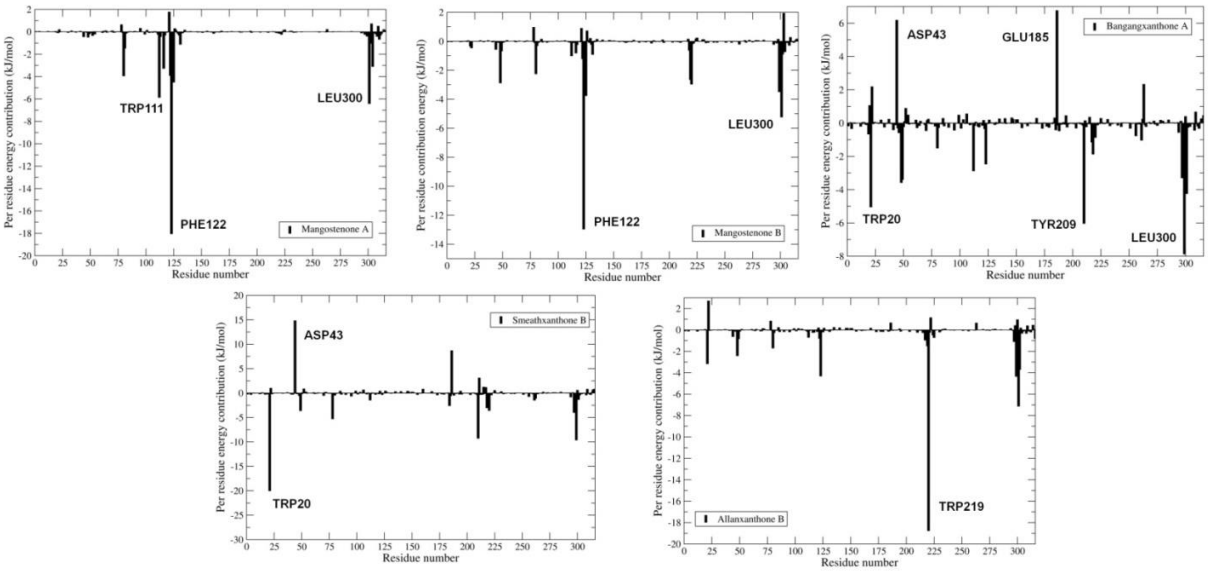
Supplementary file, Figure S4: Root mean square fluctuations in AR residues in bare protein and when bound toxanthones under study.



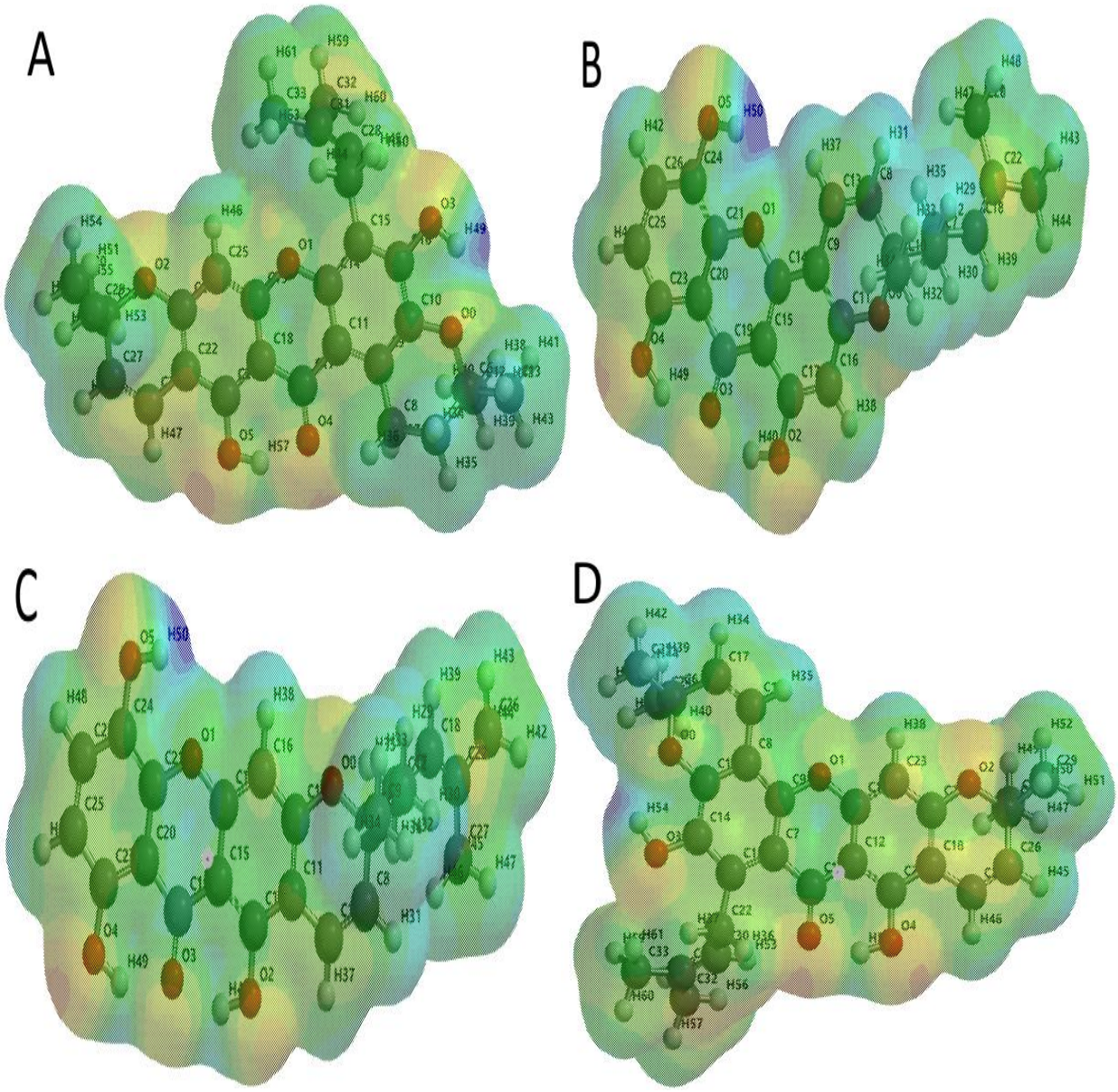
Supplementary file Figure S5: 2D projection of eigenvector 1 and eigenvector 2 for all the systems under study



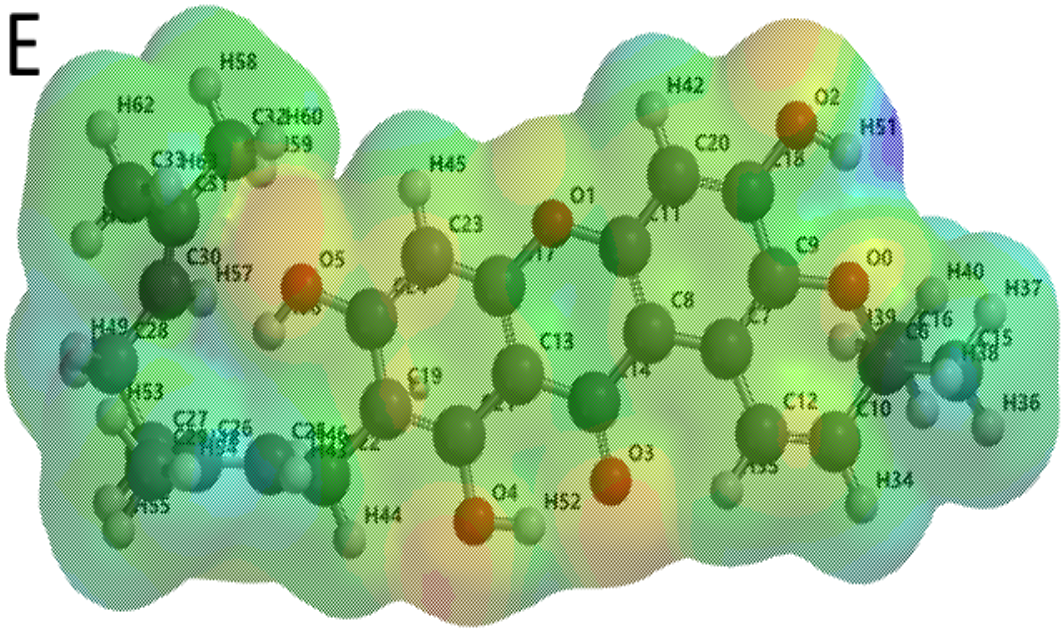
Supplementary file Figure S6: Results of per-residue domain decompostion study



Supplementary Figure S7: Illustration diagram of the MESP of mangostenone B (A), bangangxanthone A (B), smeathxanthone B (C), mangostenone A (D) and allanxanthone B (E).



E


H58
H62
C32
H60
H59
C33
H63
C31
C30
H57
O5
H49
C28
H53
C27
C29
C25
C26
H55
H44
H45
C23
O1
C24
C19
C13
C14
O3
O4
H52
H42
O2
H51
C20
C18
C11
C9
O0
C8
C7
H40
H37
H39
C16
C6
C15
H38
C12
C10
H36
H34