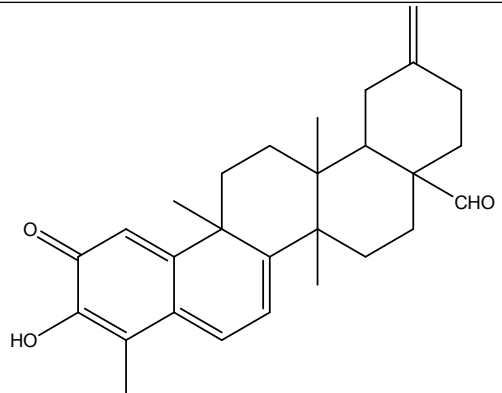
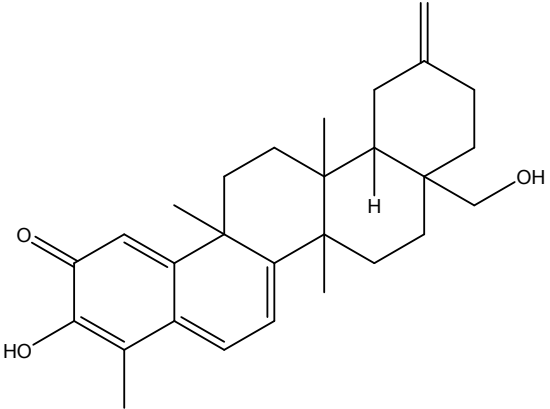
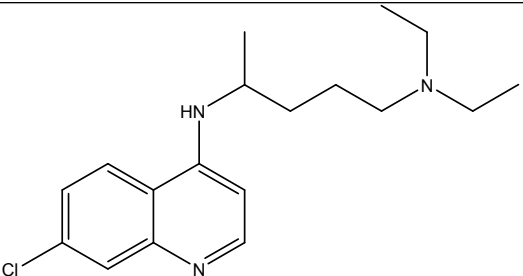
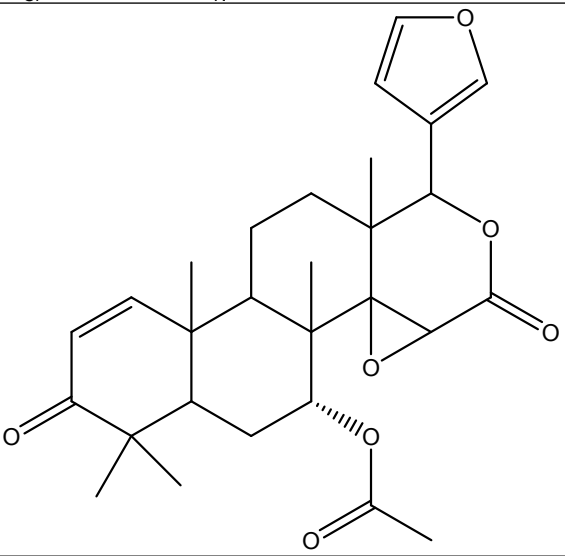
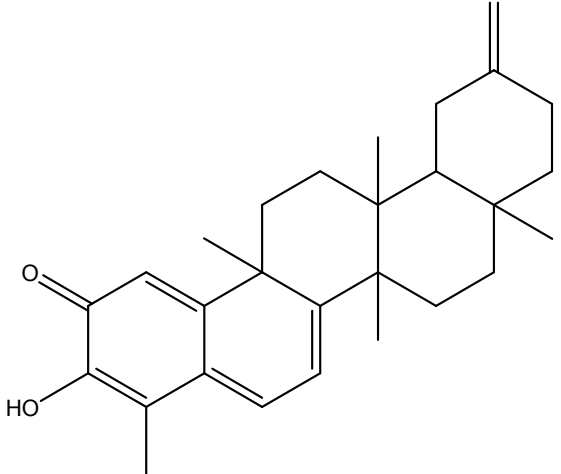
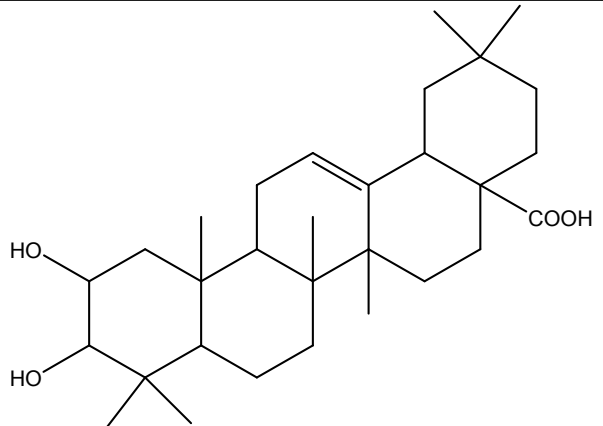
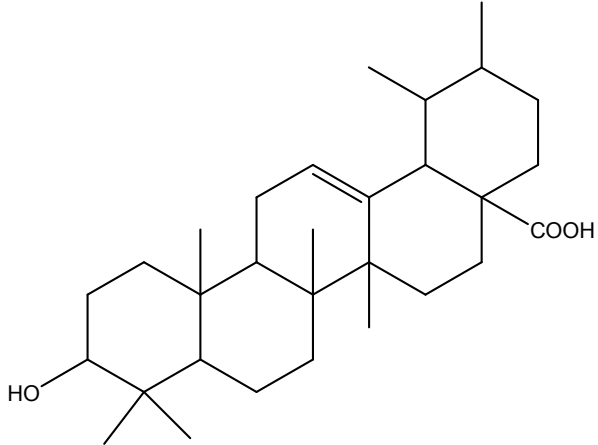
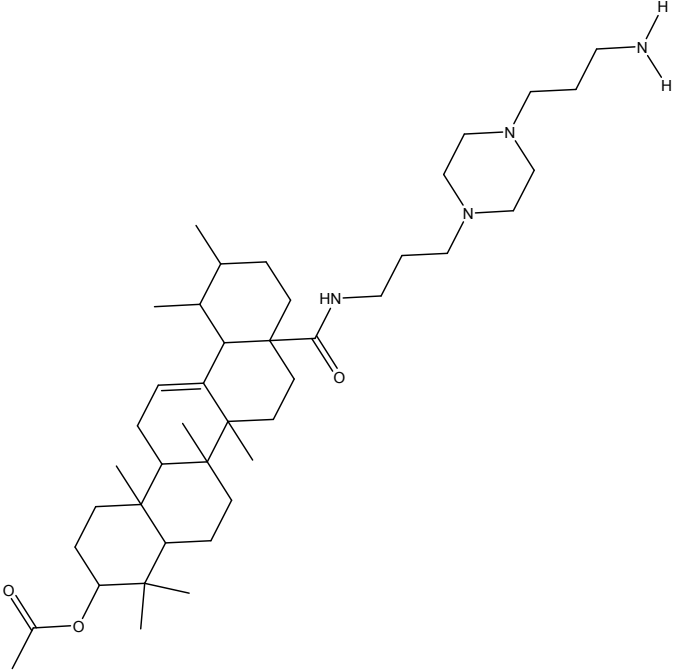


Table S2: Training set compounds used to develop a QSAR model for antimalarial activity

S. No.	Sample	Structure	Activity IC ₅₀ (µg/ml)	Reference
1	1		0.0799	Figueiredo et. al., 1998
3	2		0.1402	

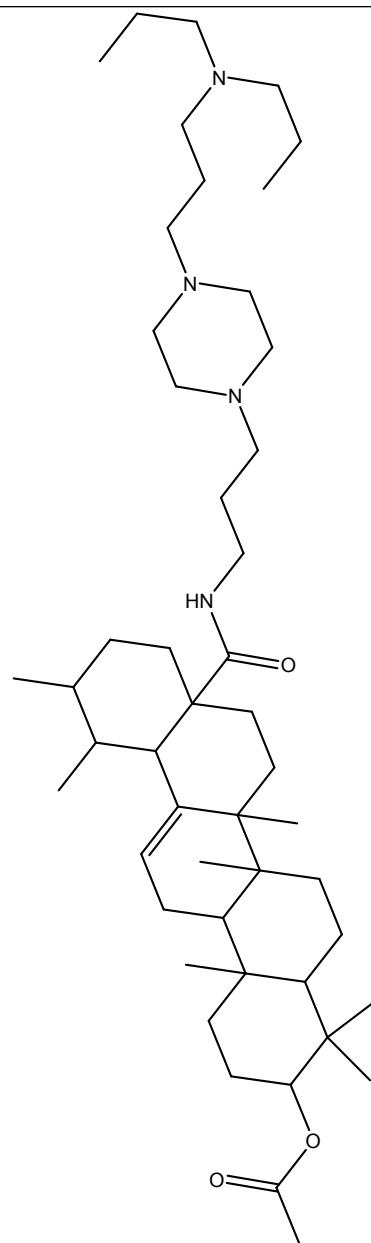
7	3		0.0046	
9	4		1.496	Lee et. al., 2008

10	5		0.2	Thiem et. al., 2005
15	6		9.974	Ma et. al., 2006

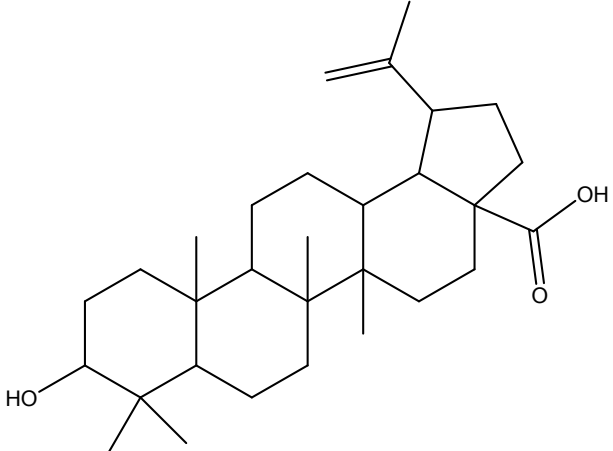
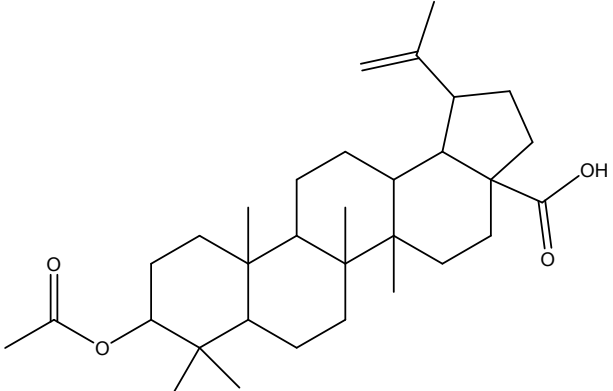
16	7	 <p>The structure shows a complex polycyclic system with three fused six-membered rings. It features a hydroxyl group (HO) on the leftmost ring and a carboxylic acid group (COOH) on the rightmost ring. There are several methyl groups attached to the rings, and a double bond is present in the middle ring.</p>	12.7	Baren et. al., 2006
20	8	 <p>The structure shows a complex polycyclic system with three fused six-membered rings. It features an acetate ester group (CH₃COO-) on the leftmost ring and a long-chain amide group (-NH-) on the rightmost ring. The amide group is connected to a piperazine ring, which is further linked to a terminal primary amine group (-NH₂).</p>	0.3133	Gnoatto et. al., 2008

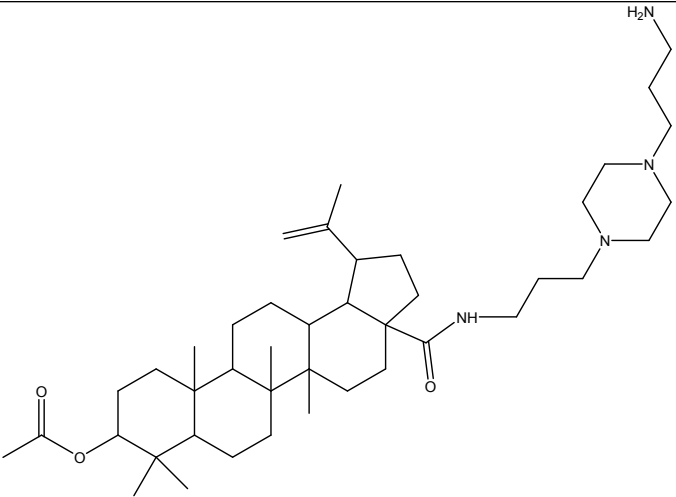
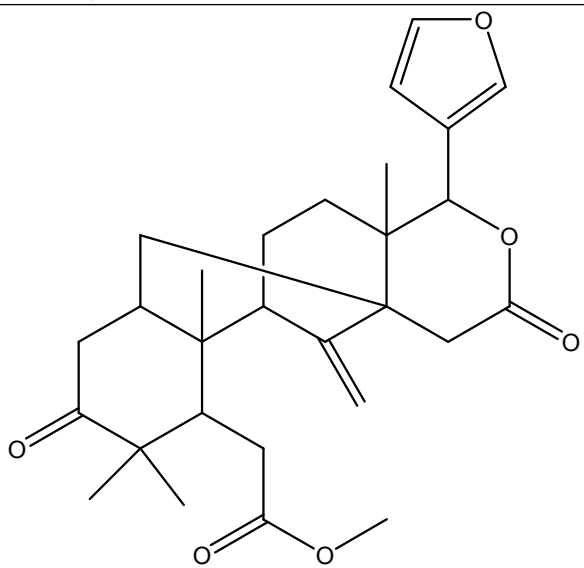
24

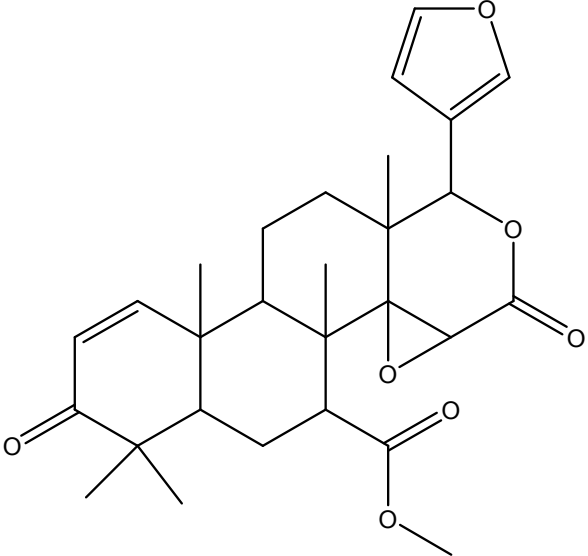
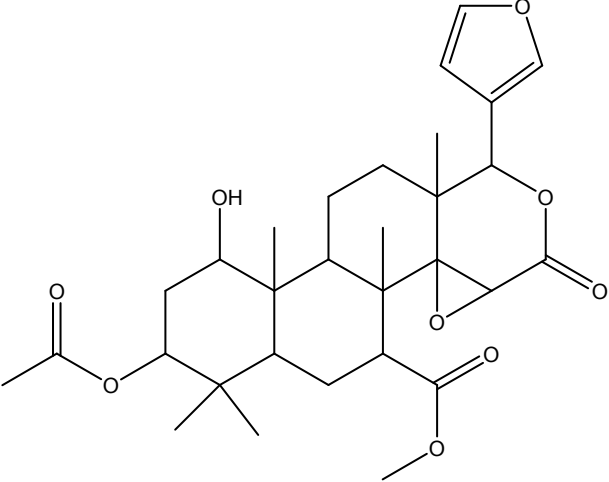
9

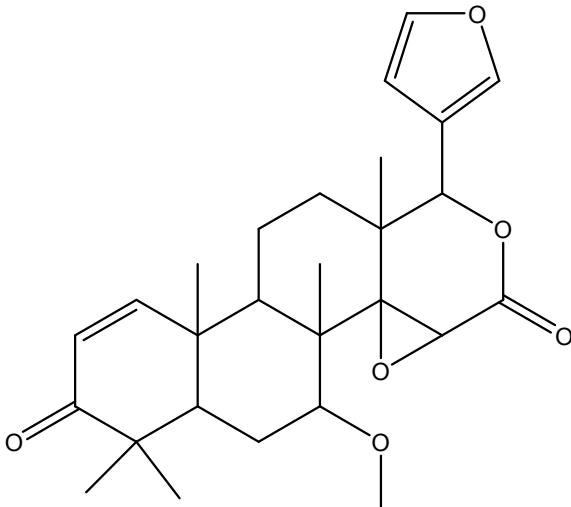
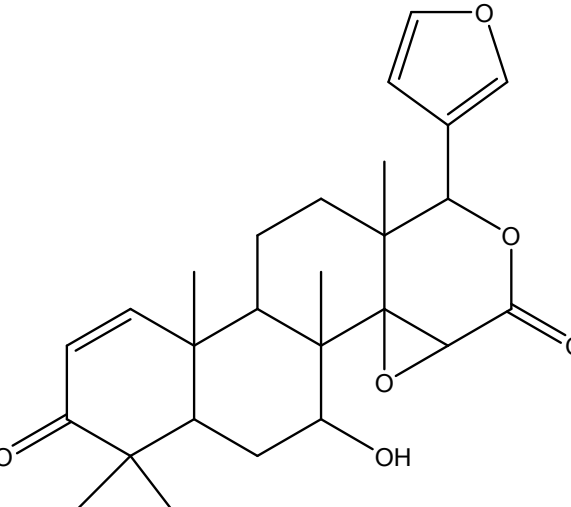


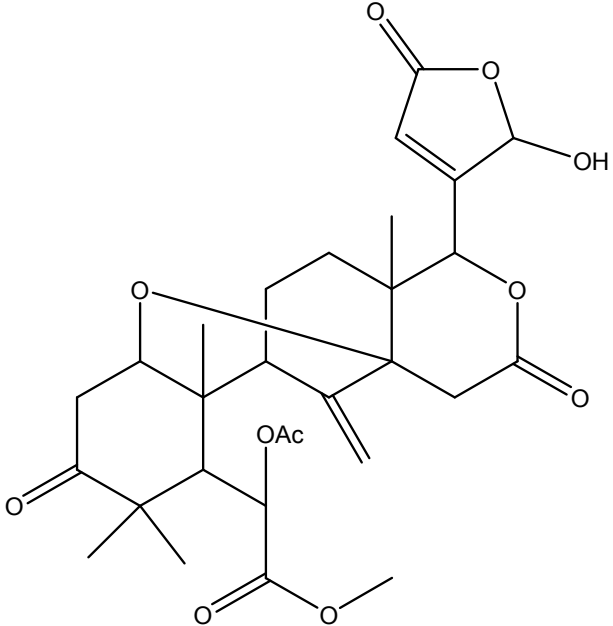
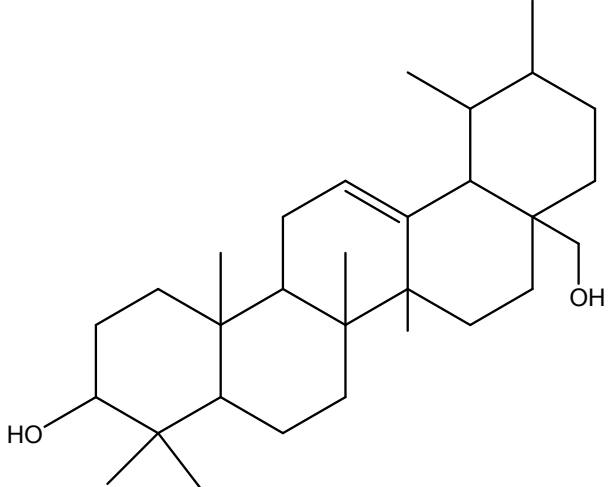
0.7652

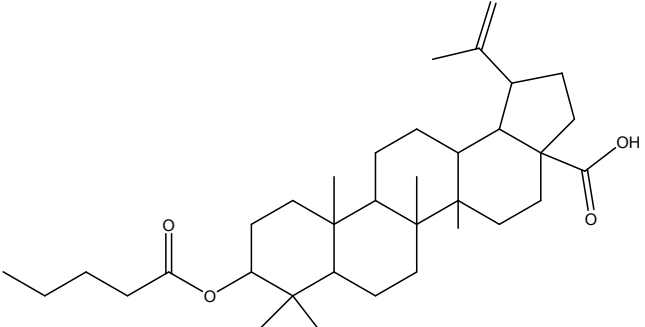
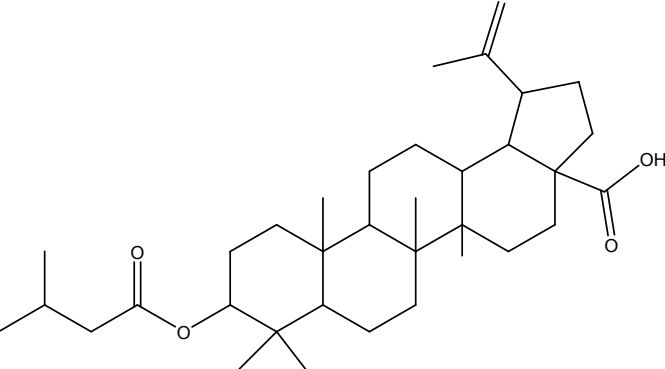
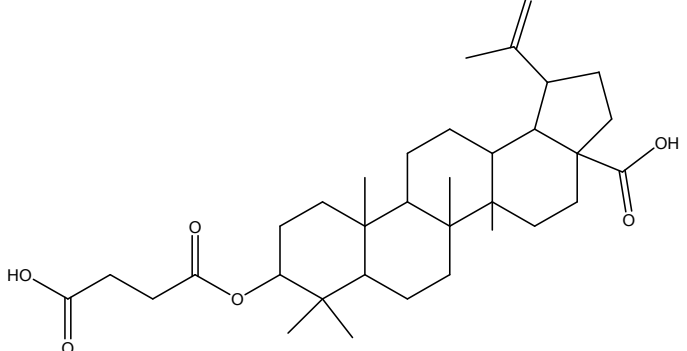
27	10	 <p>The structure shows a complex polycyclic system consisting of several fused six-membered rings. A hydroxyl group (HO) is attached to one of the rings. A carboxylic acid group (-COOH) is attached to another ring. A vinyl group (-CH=CH₂) is attached to a five-membered ring fused to the system.</p>	10.2758	Dom'inguez-Carmona et. Al., 2010
28	11	 <p>The structure is similar to the one above, but instead of a hydroxyl group, it features an acetate group (-COOCH₃) attached to one of the rings. The carboxylic acid group and the vinyl group are also present.</p>	5.8851	

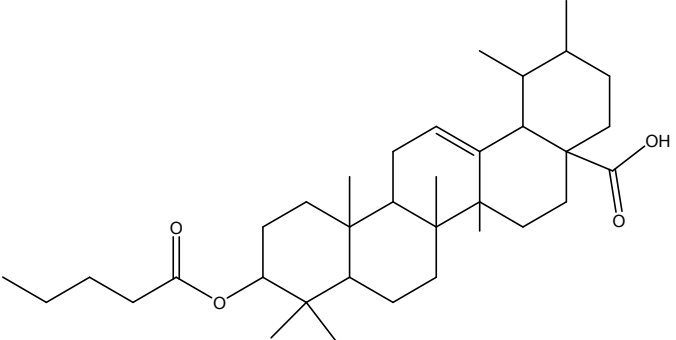
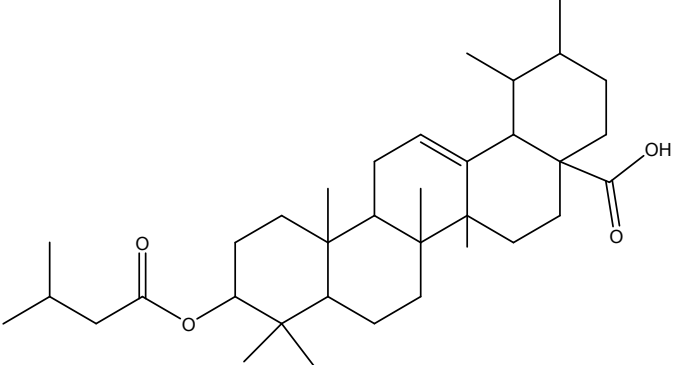
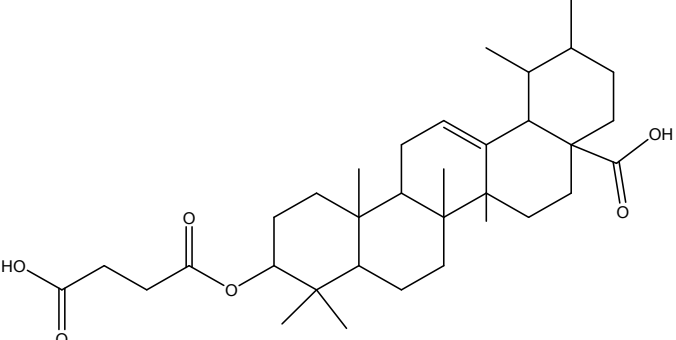
30	12	 <p>The structure shows a complex polycyclic system consisting of several fused six-membered rings. A piperazine ring is attached to the system via a propyl chain, with a primary amine group (-NH₂) extending from the piperazine ring. There are also methyl and isopropenyl substituents on the polycyclic core.</p>	0.1498	Innocente et. al 2012
36	13	 <p>The structure features a complex polycyclic core with multiple fused rings. It includes a furan ring (five-membered oxygen-containing ring) and a lactone ring (six-membered ring with an internal ester group). There are also methyl and isopropenyl substituents on the polycyclic system.</p>	5.39	Bickii et. al., 2000

38	14	 <p>Chemical structure of compound 38: A complex polycyclic molecule featuring a decalin core. It has a methyl group on the leftmost ring, a double bond on the rightmost ring, and a methyl group on the bridgehead carbon. A side chain is attached to the rightmost ring, containing a furfuryl group, a carbonyl group, and a methoxy group.</p>	1.25	
40	15	 <p>Chemical structure of compound 40: A complex polycyclic molecule similar to compound 38, but with a hydroxyl group (OH) on the leftmost ring and an acetate group (CH₃COO-) on the bridgehead carbon. The side chain is identical to compound 38, containing a furfuryl group, a carbonyl group, and a methoxy group.</p>	9.63	

42	16		0.783	Omar et. al., 2003
43	17		1.828	

47	18	 <p>The structure shows a complex polycyclic system with a furan ring attached to one of the rings. It features a methyl group, a vinyl group, and an acetate (OAc) group. A lactone ring is also present, fused to the main structure.</p>	6.9	Saewan et. al., 2006
53	19	 <p>The structure shows a complex polycyclic system with two hydroxyl (HO) groups. It features a methyl group and a vinyl group. The rings are interconnected in a complex manner.</p>	3.3	Filho et. al., 2009

54	20		15.6838	Silva et. al., 2013
55	21		23.7961	
59	22		36.7468	

61	23		38.3982	
62	24		38.939	
64	25		32.2927	