



## IN SILICO SEARCH OF POTENT PHYTOECDYSTEROIDS TARGETING DIFFERENT CANCER PROTEINS

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### SUPPLEMENTARY

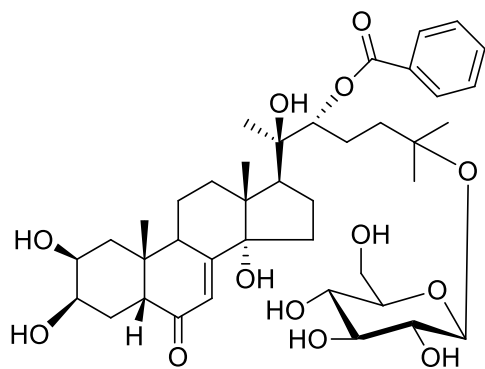
**Table S1.** List of phytoecdysteroid selected for molecular docking calculations

Code	Compound name	Reference
PES 1	Ecdysterone 22-benzoate 25-O-β-D-glycoside	(Girault et al., 2004)
PES 2	25-Deoxyecdysone 22-β-D-glucoside	(Snogan et al., 2007)
PES 3	2,22-Dideoxy-20-hydroxyecdysone-25-O-β-D-glucopyranoside	(Wang et al., 2009)
PES 4	Pterosterone-24-O-β-D-glucopyranoside	(Nishimoto et al., 1988a)
PES 5	Polypodine B 2-β-D-glucoside	(Simon et al., 2011)
PES 6	2-Deoxyecdysone-22β-D-glucoside	(Meng et al., 2001)
PES 7	Ecdysterone 25-O-β-D-glycoside	(Nishimoto et al., 1988a)
PES 8	2,22-Deoxyecdysone-25-O-β-D-glucopyranoside	(Wang et al., 2009)
PES 9	2-Deoxy-20-hydroxyecdysone-25-glucoside	(Zibareva et al., 2009)
PES 10	Castasterone	(Yokota et al., 1982)
PES 11	Makisterone A	(Baltaev, 2000)
PES 12	Pfaffiaglycosides E	(Nakamura et al., 2010)
PES 13	15-Hydroxyponasterone A	(Budesinky et al., 2009)
PES 14	2-Deoxy-20-hydroxyecdysone-22-O-β-D-glucopyranoside	(Báthori et al., 2002)
PES 15	Shidasterone 3-acetate	(Hunyadi et al., 2016)
PES 16	Polyroid B	(Simon et al., 2011)
PES 17	Sileneoside C	(Maria et al., 2005)
PES 18	Fiberaurecdyside A	(Su et al., 2007)
PES 19	Pfaffiaglycosides C	(Nakamura et al., 2010)
PES 20	Pfaffiaglycosides D	(Nakamura et al., 2010)
PES 21	20-Hydroxyecdysone-2-O-β-D-galactopyranoside	(Zhang et al., 2017)
PES 22	Silenoside H	(Yusupova et al., 2022)
PES 23	Sphenocentroside A	(Ajayi et al., 2019)
PES 24	5α-Polypodine B 3-O-β-D-glycoside	(Das et al., 2021b)

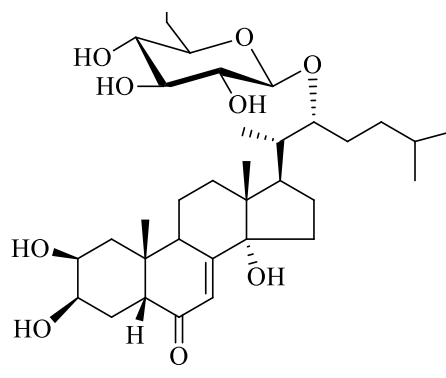
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PES 25	Makisterone B	(Baltaev, 2000)
PES 26	5 $\beta$ -Hydroxy-24(28)-dehydromakisterone	(Kumpun et al., 2011)
PES 27	septanoecdysone	(Ben Nejma et al., 2015)
PES 28	Brainesteroide D	(Wu et al., 2010)
PES 29	Podecdysone B 25-O- $\beta$ -D-glycoside	(Nishimoto et al., 1988b)
PES 30	Sidasterone A	(Baltaev, 2000)
PES 31	3-O- $\beta$ -D-Glucopyranaosyl-3 $\beta$ ,25-dihydroxy-5 $\beta$ -cholest-7-en-6-one-25-O- $\beta$ -D-glucopyranoside	(Kılınç et al., 2019)
PES 32	Ecdysone-3-O- $\beta$ -D-glucopyranoside	(Jadhav et al., 2007)
PES 33	Silenoside E	(Saatov et al., 1986)
PES 34	Ponasteroside a	(Takemoto et al., 1968)
PES 35	5 $\alpha$ -Sileneoside E	(Dzhukarova et al., 1995)
PES 36	3-O-Acetyl-20-hydroxyecdysone-2- $\beta$ -D-galactopyranoside	(Zhang et al., 2017)
PES 37	Brainesteroide C	(Wu et al., 2010)
PES 38	Brainesteroide E	(Wu et al., 2010)
PES 39	2-Deoxyecdysone 3-[4-(1- $\beta$ -D glucopyranosyl)]-ferulate	(Ho et al., 2008)
PES 40	Pterosterone-3-O- $\beta$ -D-glucopyranoside	(Jadhav et al., 2007)
PES 41	3-O-Acetyl-20-hydroxyecdysone-2- $\beta$ -D-glucopyranoside	(Zhang et al., 2017)
PES 42	Sphenocentroside B	(Ajayi et al., 2019)
PES 43	polypody B 3-O- $\beta$ -D-glycoside	(Das et al., 2021b)
PES 44	E-2-Deoxy-20-hydroxyecdysone 3-[4-(1- $\beta$ -D-glucopyranosyl)]-caffeate	(Ho et al., 2012)

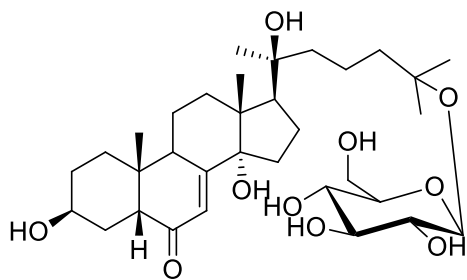
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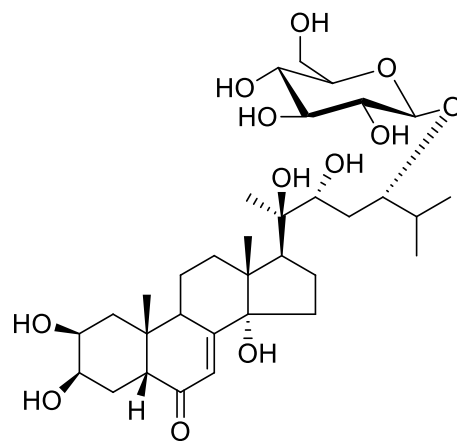
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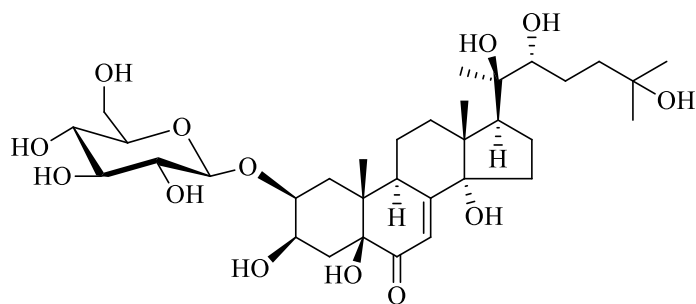
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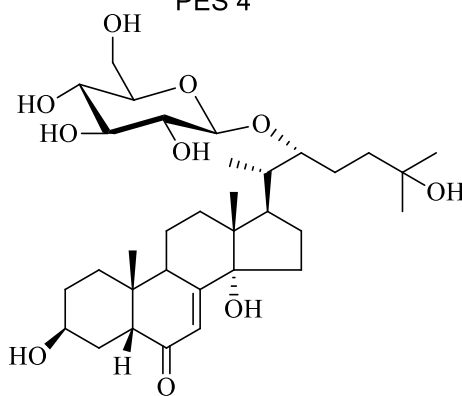
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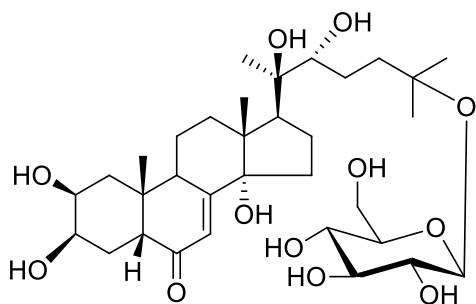
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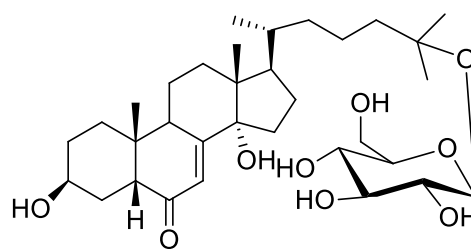
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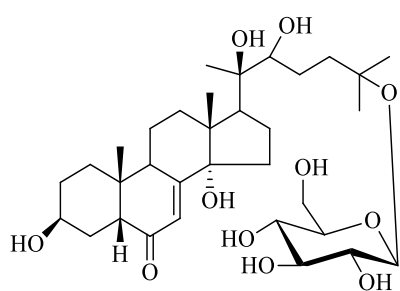
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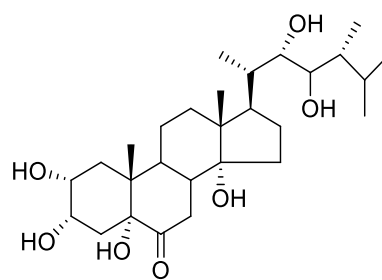
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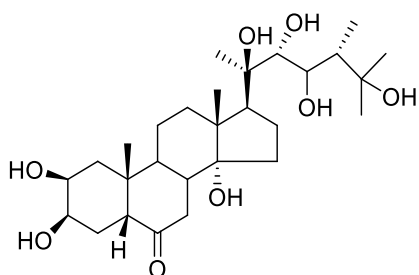
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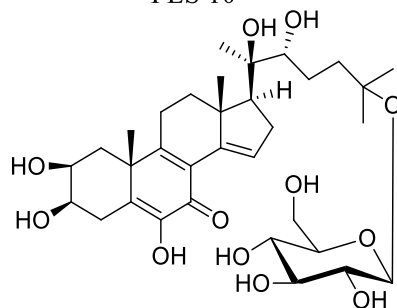
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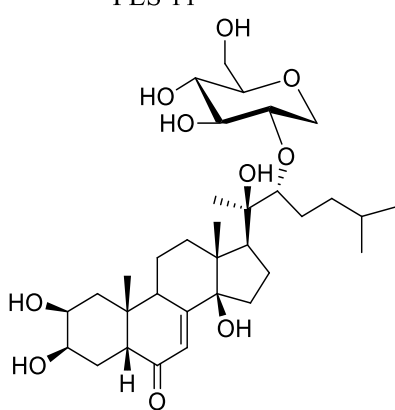
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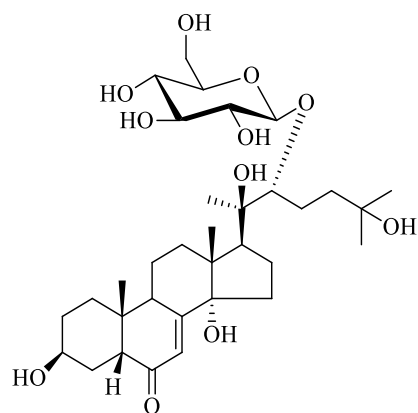
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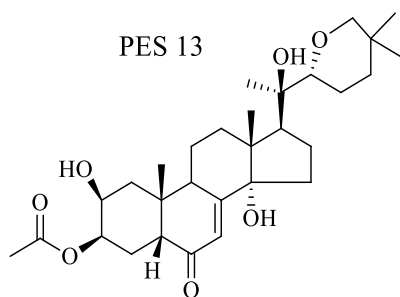
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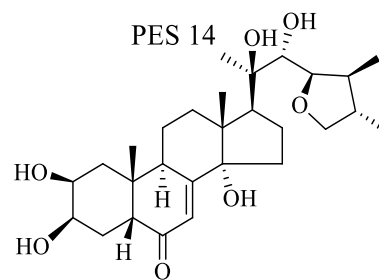
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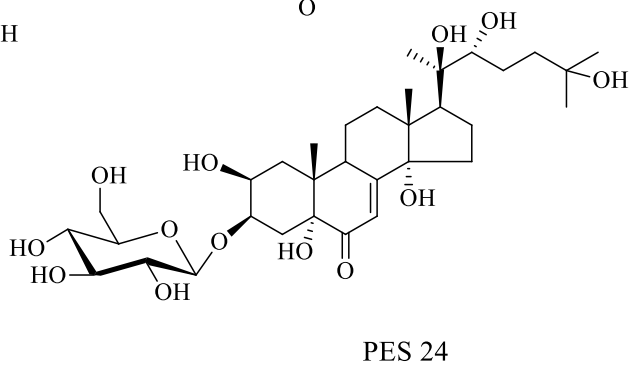
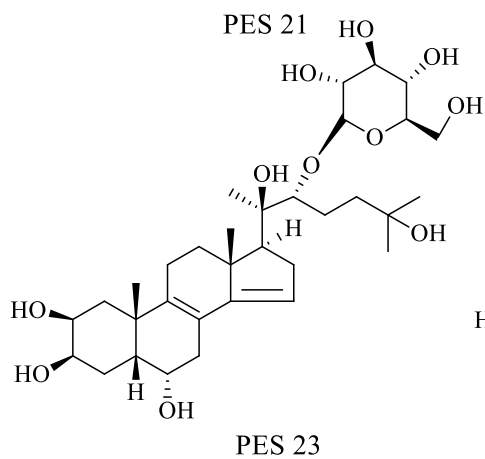
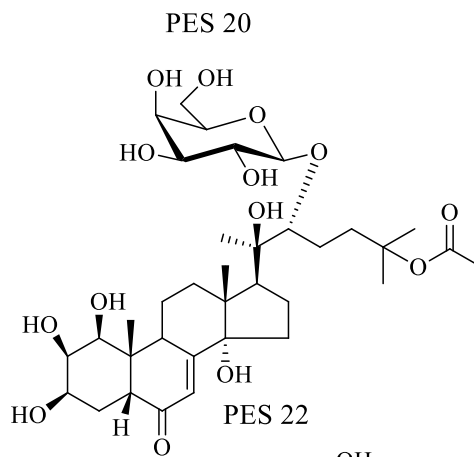
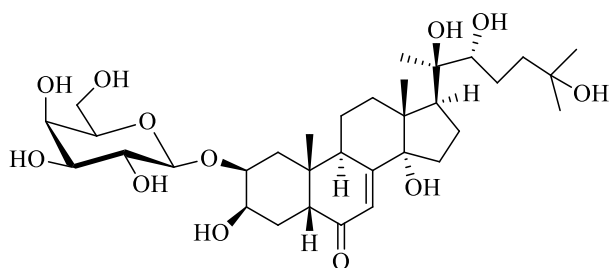
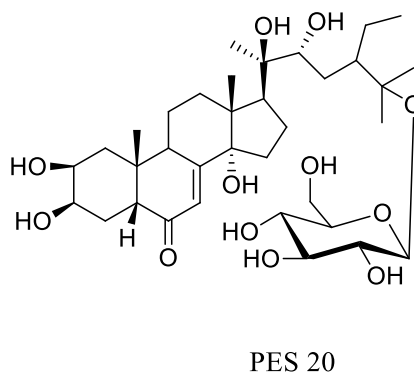
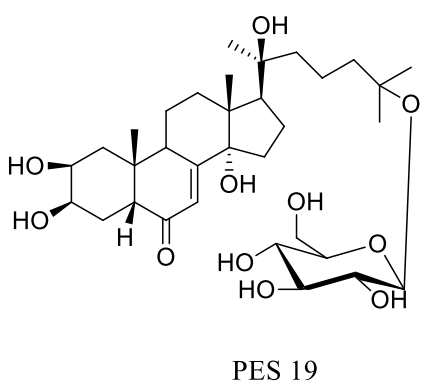
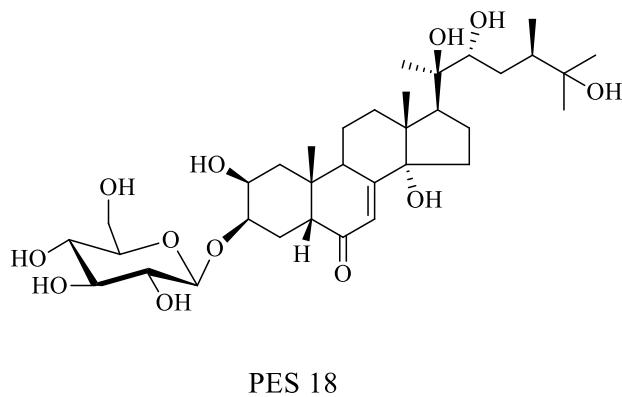
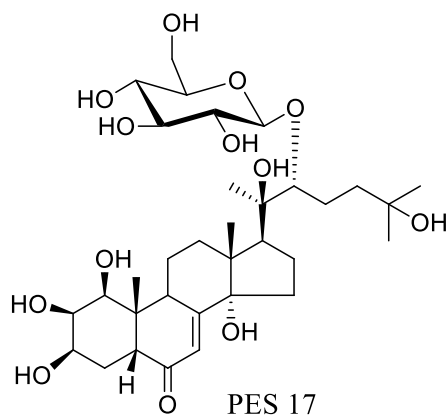
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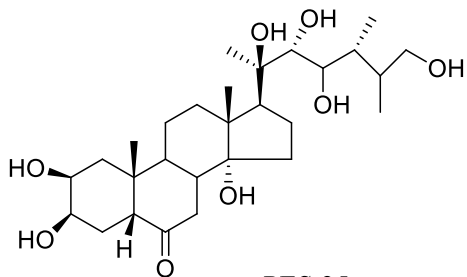


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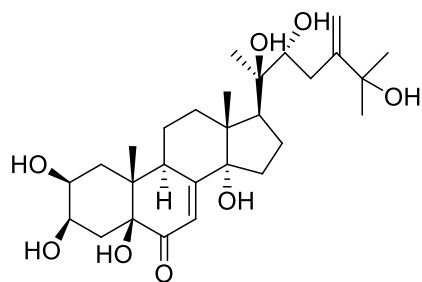


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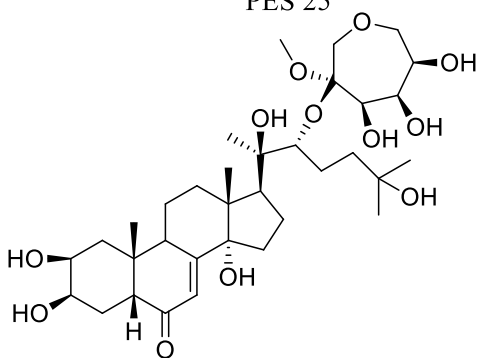




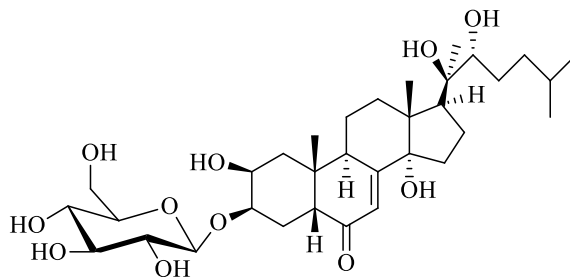
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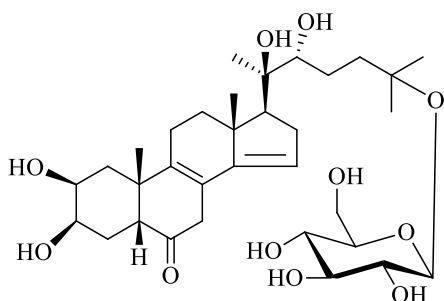
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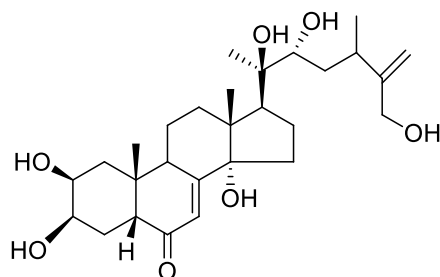
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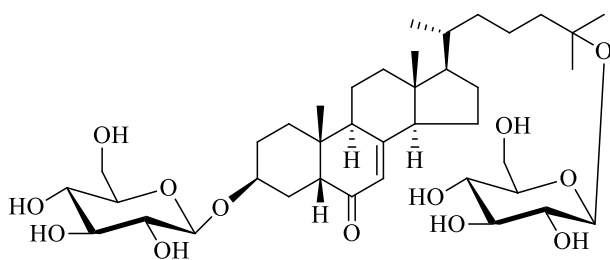
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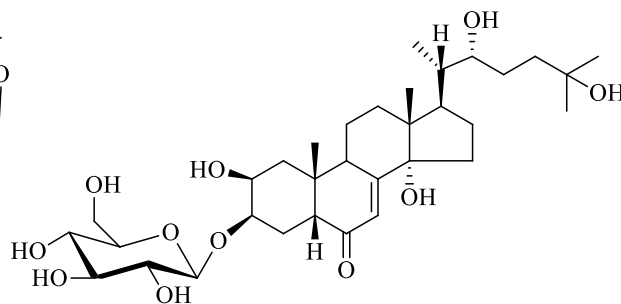
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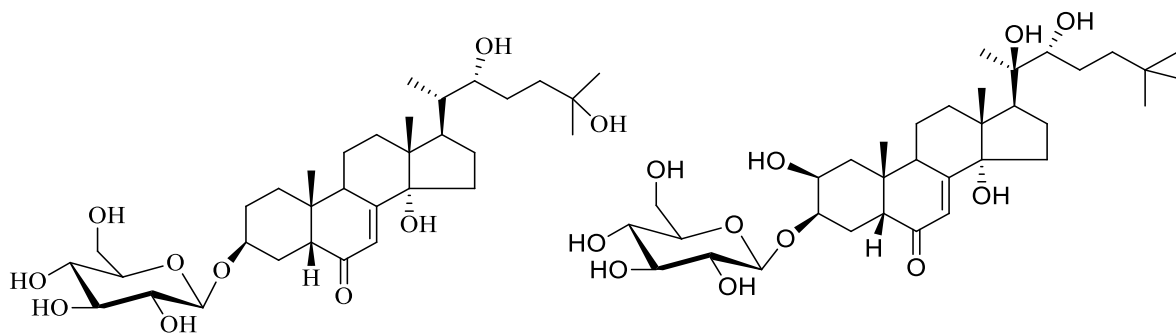
PES 30



PES 31

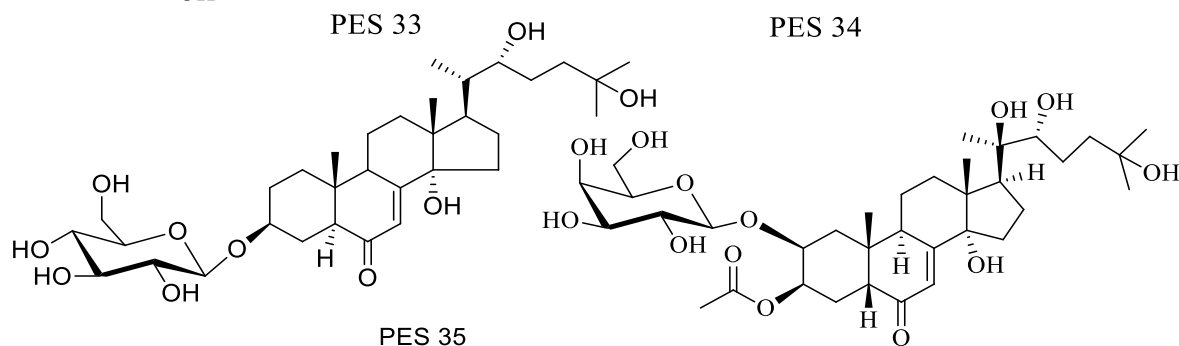


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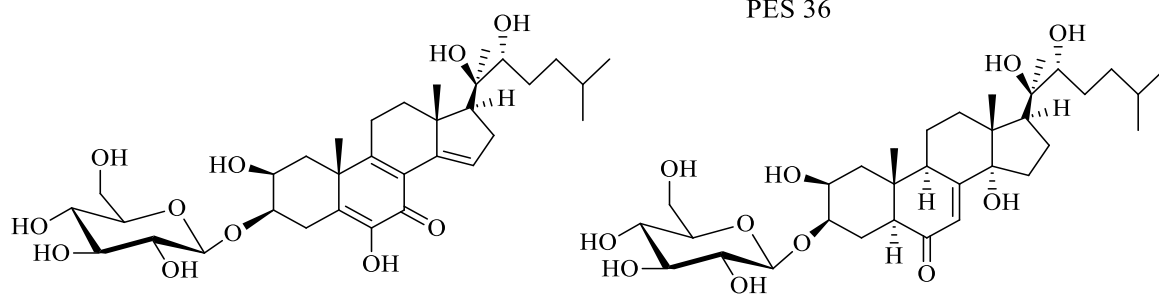
PES 33

PES 34



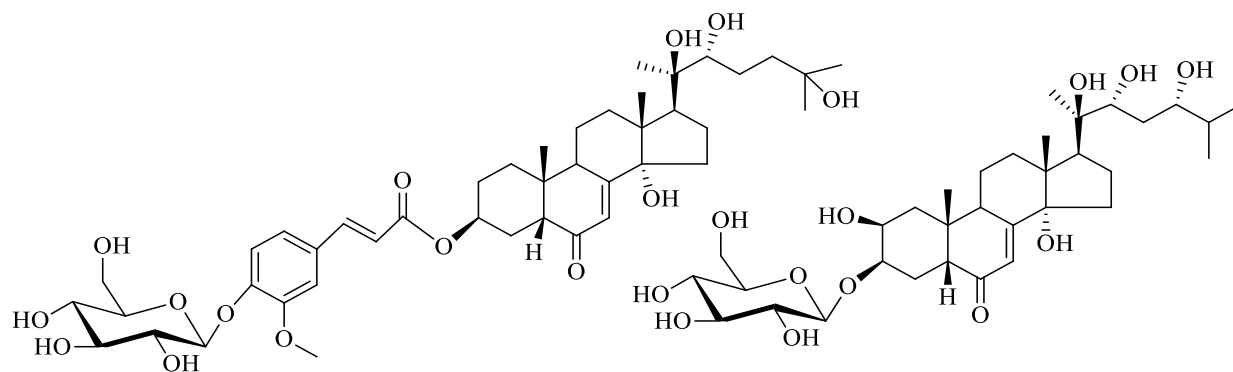
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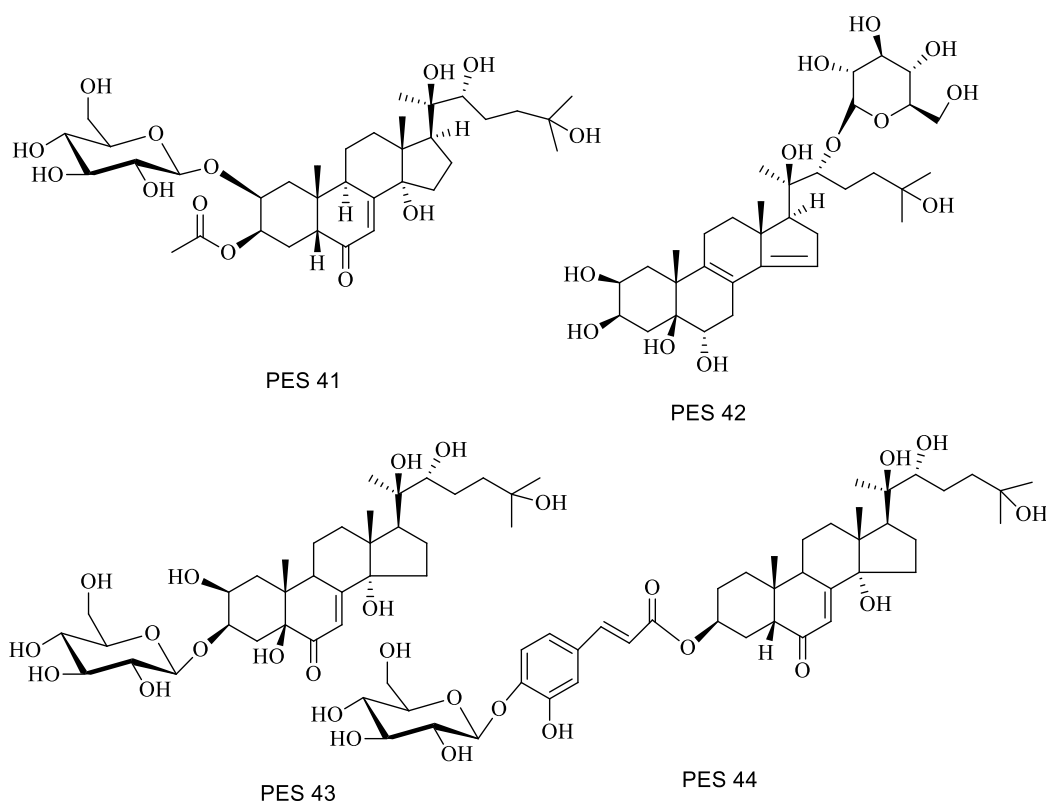
PES 37

PES 38



PES 39

PES 40



**Figure S1.** Molecular structure of screened phytoecdysteroid

**Table S2.** Ramachandran plot analysis of different receptors

	<b>3L3M</b>	<b>2A0C</b>	<b>8H7H</b>
Residues in most favoured regions	265	235	219
Residues in additional allowed regions	36	23	23
Residues in generously allowed regions	3	2	2
Residues in disallowed regions	3	0	1
No. of non-glycine and non-proline residues	307	260	245
No. of end-residues	2	2	1
No. of glycine residues	23	16	16
No. of proline residues	16	19	12
Total no. of residues	348	297	274

PROCHECK

# Ramachandran Plot

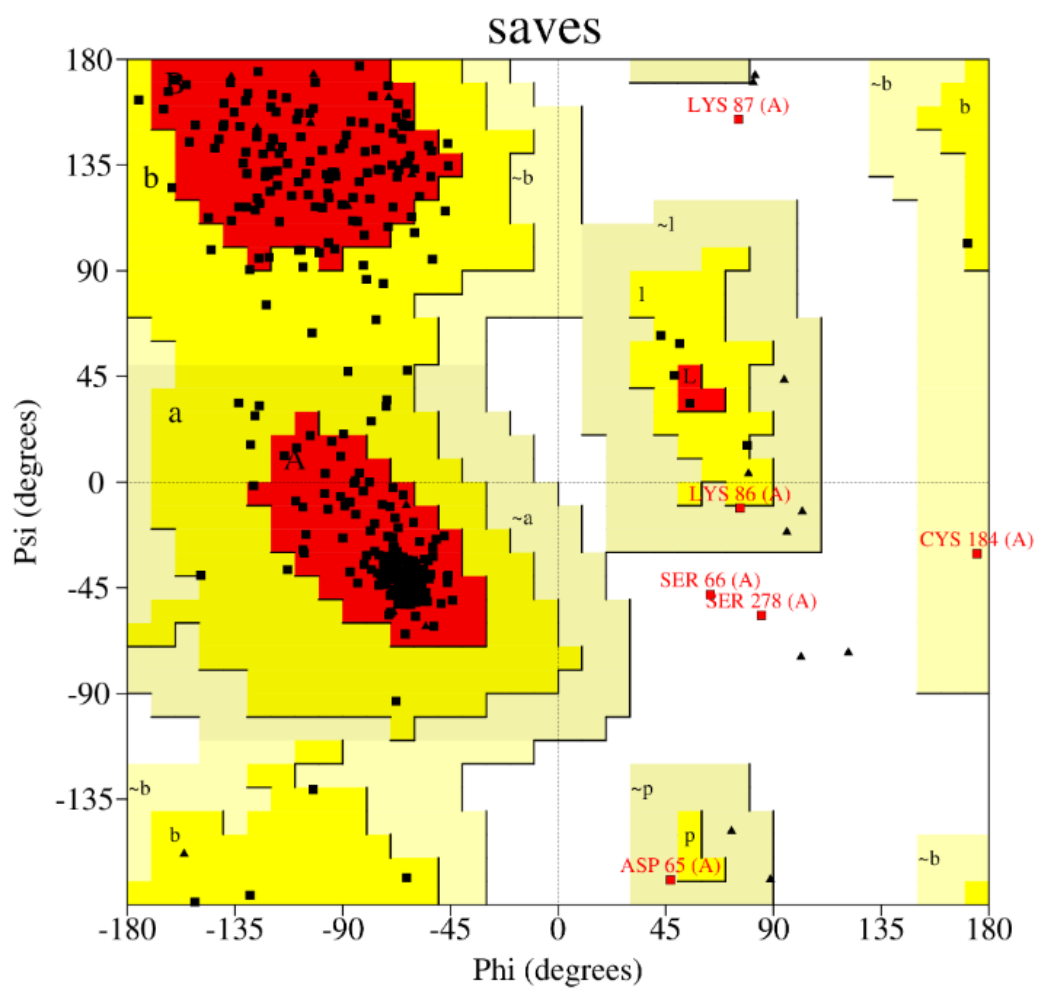
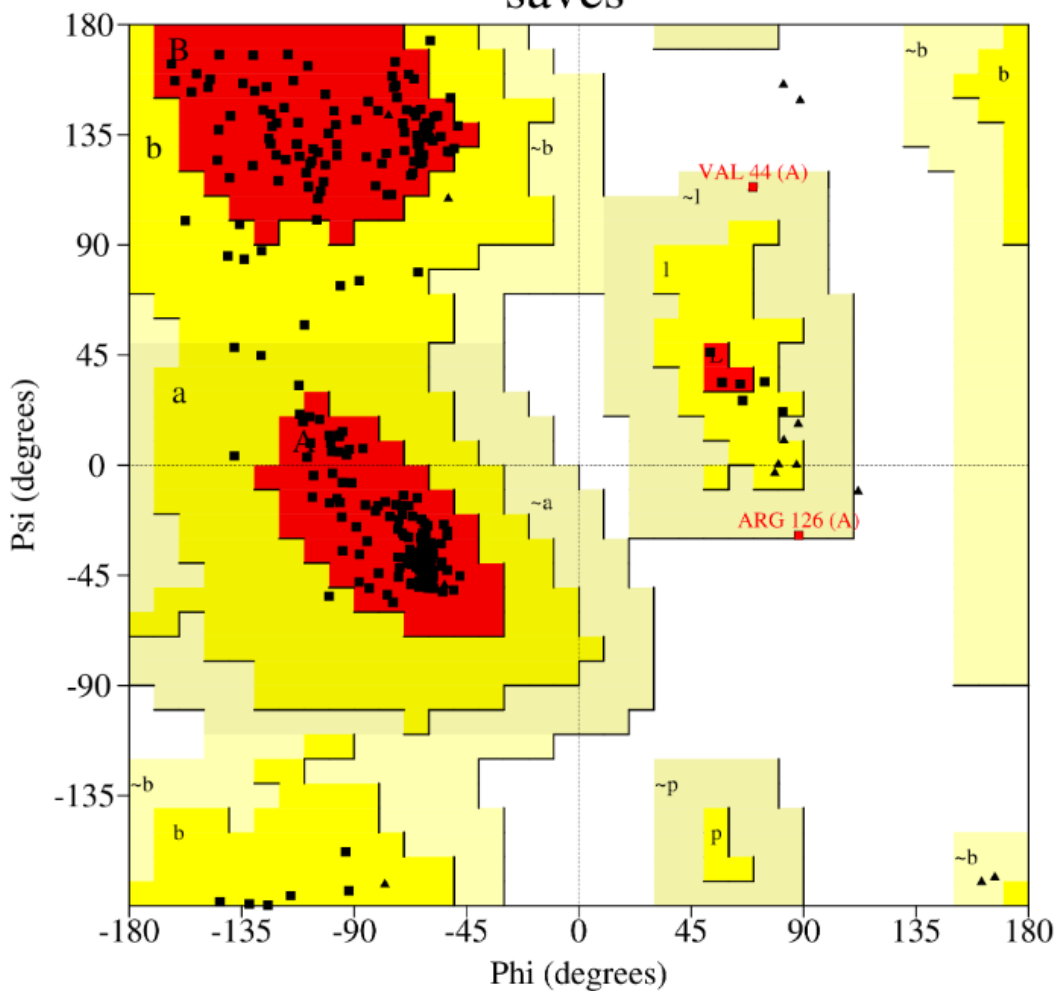


Figure S2. Ramchandan plot of 3L3M receptor

PROCHECK

# Ramachandran Plot

saves



**Figure S3.** Ramchandran plot of 2A0C receptor

PROCHECK

# Ramachandran Plot

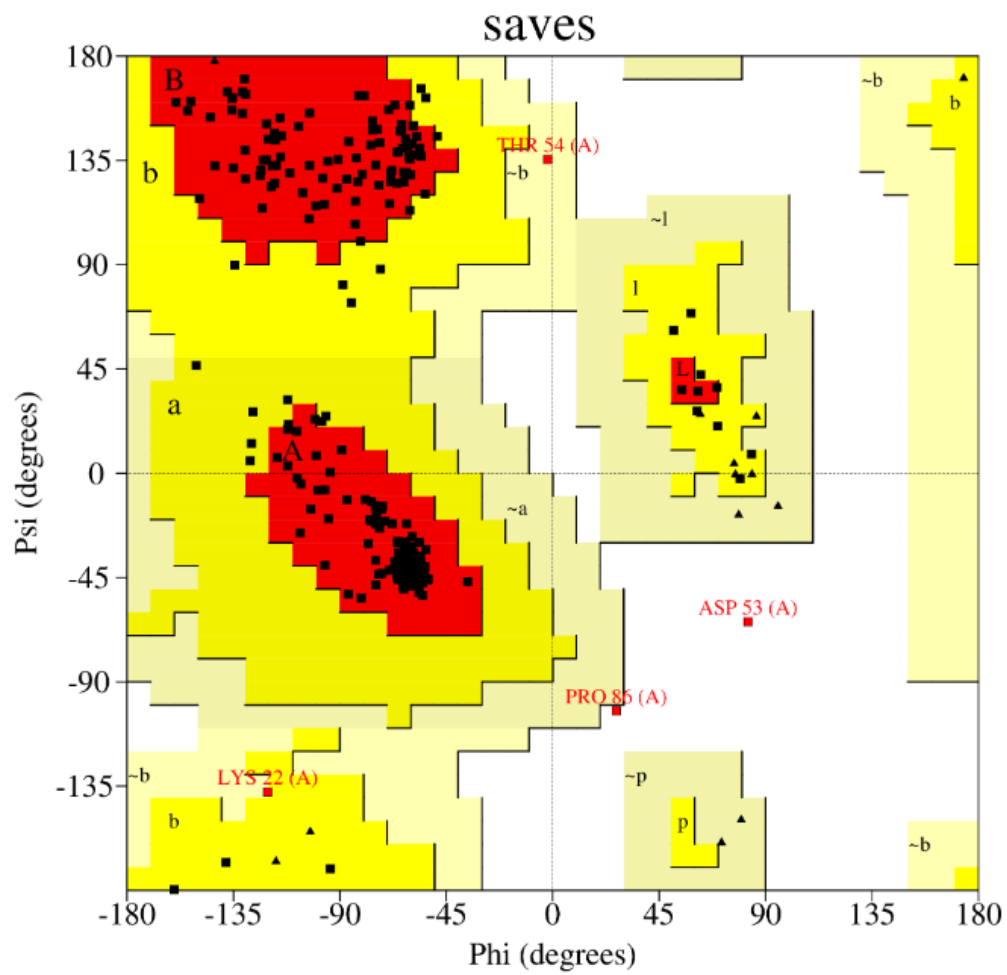


Figure S4. Ramchandran plot of 8H7H

**Table S3.** Toxicity results from PRO-tox II server

<b>Compounds</b>	<b>Hepatotoxicity</b>	<b>Carcinogenicity</b>	<b>Immunotoxicity</b>	<b>Mutagenicity</b>	<b>Cytotoxicity</b>
<b>PES 1</b>	Inactive	Inactive	Active	Inactive	Inactive
<b>PES 2</b>	Inactive	Inactive	Active	Inactive	Inactive
<b>PES 3</b>	Inactive	Inactive	Active	Inactive	Inactive
<b>PES 4</b>	Inactive	Inactive	Active	Inactive	Inactive
<b>PES 5</b>	Inactive	Inactive	Active	Inactive	Inactive
<b>PES 6</b>	Inactive	Inactive	Active	Inactive	Inactive
<b>PES 7</b>	Inactive	Inactive	Active	Inactive	Inactive
<b>PES 8</b>	Inactive	Inactive	Inactive	Inactive	Inactive
<b>PES 9</b>	Inactive	Inactive	Active	Inactive	Inactive
<b>PES 10</b>	Inactive	Inactive	Active	Inactive	Inactive
<b>PES 11</b>	Inactive	Inactive	Active	Inactive	Inactive
<b>PES 12</b>	Inactive	Inactive	Active	Inactive	Inactive
<b>PES 13</b>	Inactive	Inactive	Active	Inactive	Inactive
<b>PES 14</b>	Inactive	Inactive	Active	Inactive	Inactive
<b>PES 15</b>	Inactive	Inactive	Active	Inactive	Inactive
<b>PES 16</b>	Inactive	Inactive	Inactive	Inactive	Inactive
<b>PES 17</b>	Inactive	Inactive	Active	Inactive	Inactive
<b>PES 18</b>	Inactive	Inactive	Active	Inactive	Inactive
<b>PES 19</b>	Inactive	Inactive	Active	Inactive	Inactive
<b>PES 20</b>	Inactive	Inactive	Active	Inactive	Inactive
<b>PES 21</b>	Inactive	Inactive	Active	Inactive	Inactive
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<b>PES 23</b>	Inactive	Inactive	Active	Inactive	Inactive
<b>PES 24</b>	Inactive	Inactive	Active	Inactive	Inactive
<b>PES 25</b>	Inactive	Inactive	Active	Inactive	Inactive
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<b>PES 43</b>	Inactive	Inactive	Active	Inactive	Inactive
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