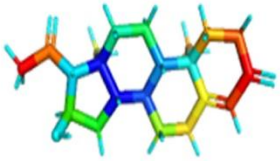
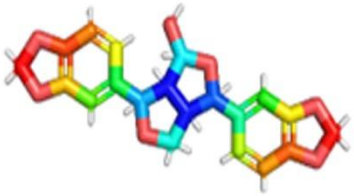
Supplementary Information



16alpha- Hydroxyprogesterone



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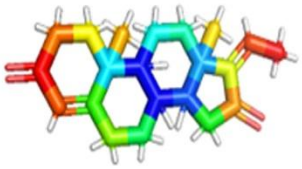

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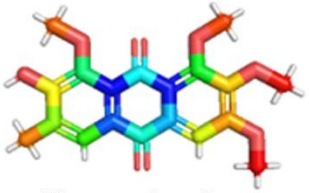
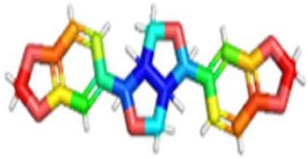


Chryso-obtusin

Obtusifolin



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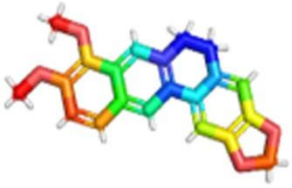

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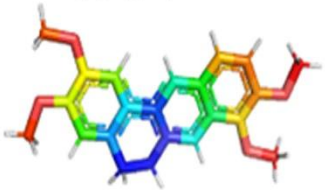

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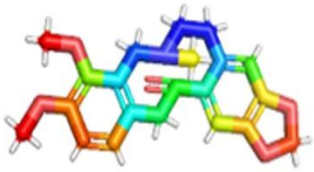
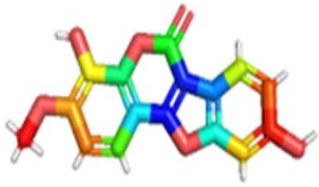
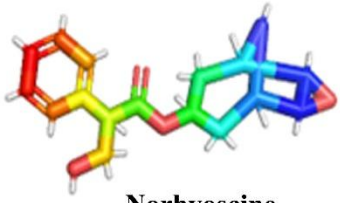


Alpha- Allocryptopine

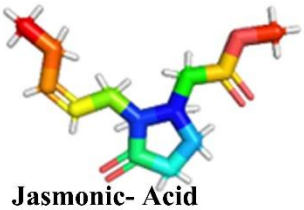
Chrysophanol



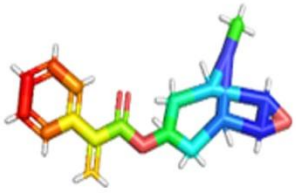
Sativol



Norhyoscine



Jasmonic- Acid



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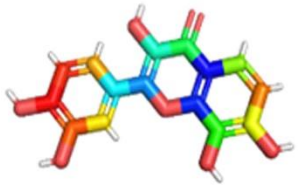

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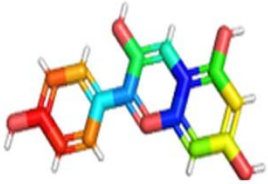
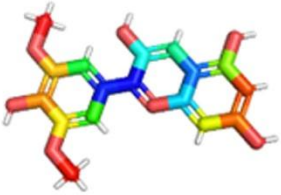


Pelargonidin



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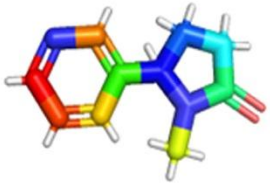

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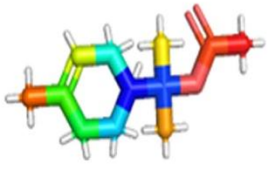
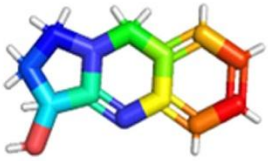
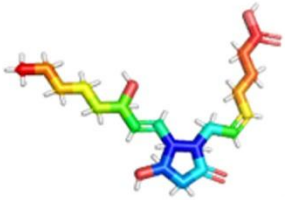


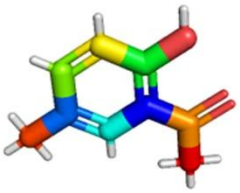
Alpha- Terpinyl-Acetate



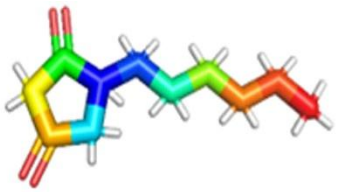
Vasicine



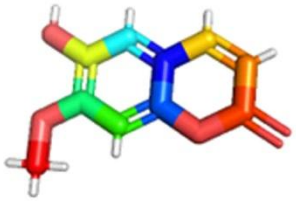
Prostaglandin-E-2



1-hydroxy-2-acetyl-4-methylbenzene



5-Hexyl-cyclopenta-1,3-Dione



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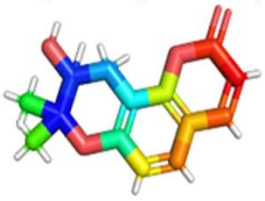

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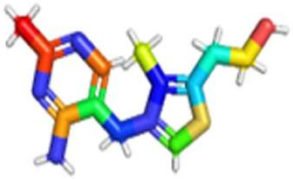
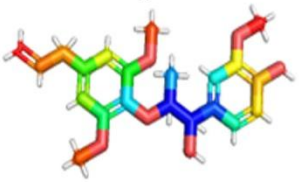
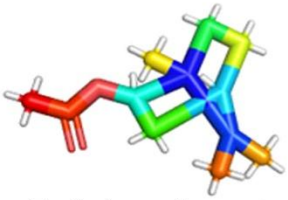


Thiamin



(Rac)- Myrislignan

Borneol-acetate



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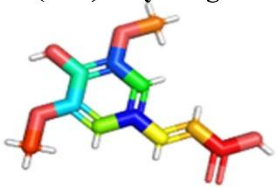
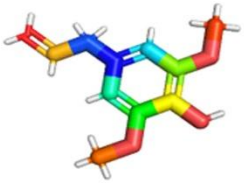
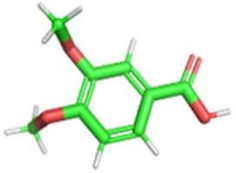


Trans-sinapic-acid

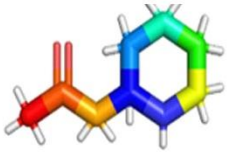
Vanillic- Acid-4-Beta-D-Glucoside



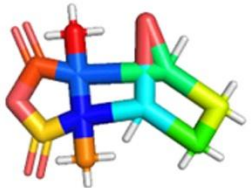
5- Methoxyeugenol



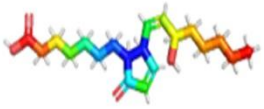
Veratric-acid



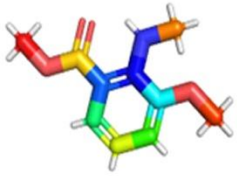
Pelletierine



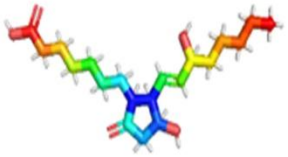
Cantharidin



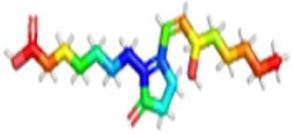
Prostaglandin-A-1



Damascenine

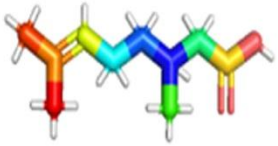


Prostaglandin-E-1

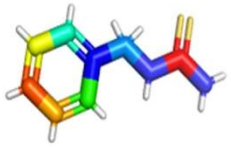


Prostaglandin-B-1

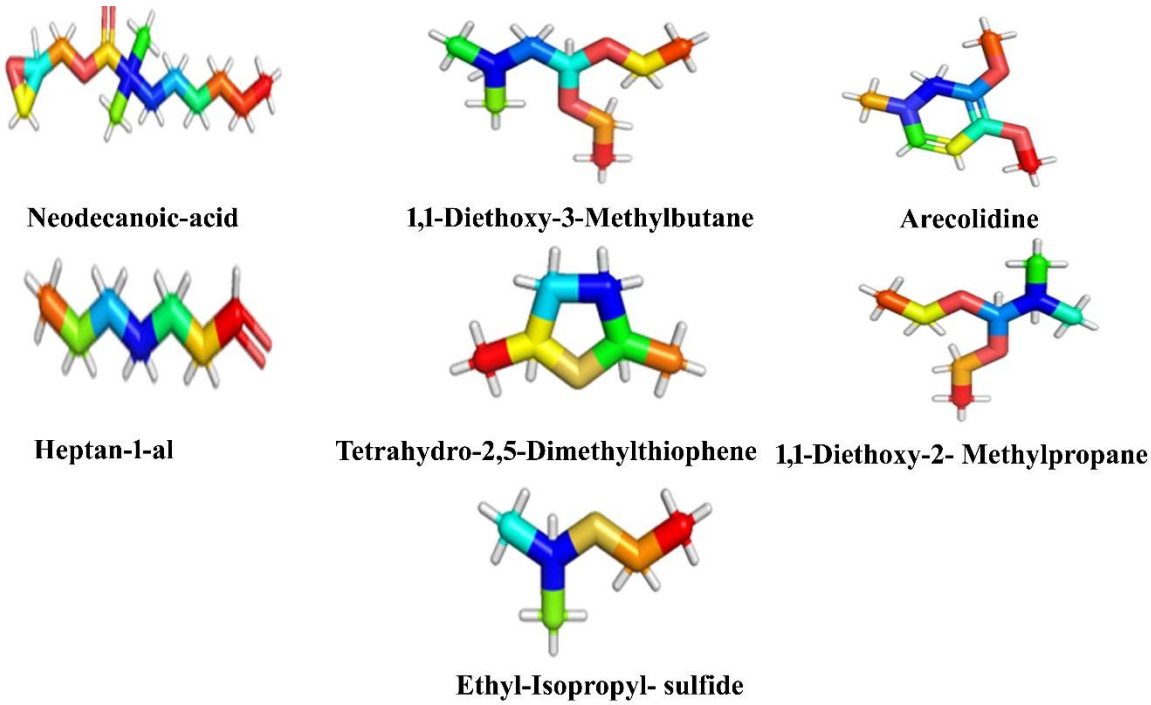
Delta-octalactone



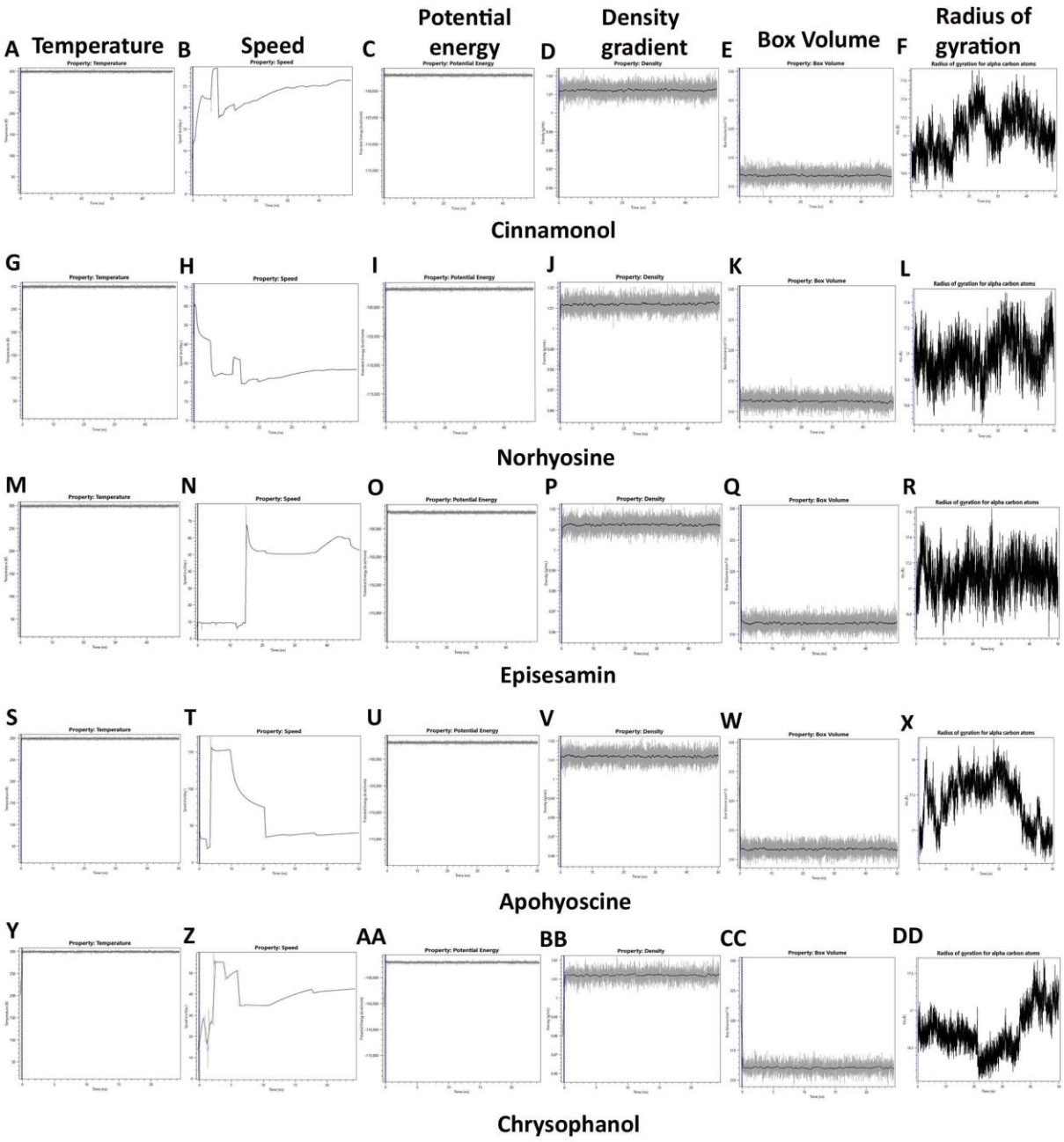
Citronellic- Acid



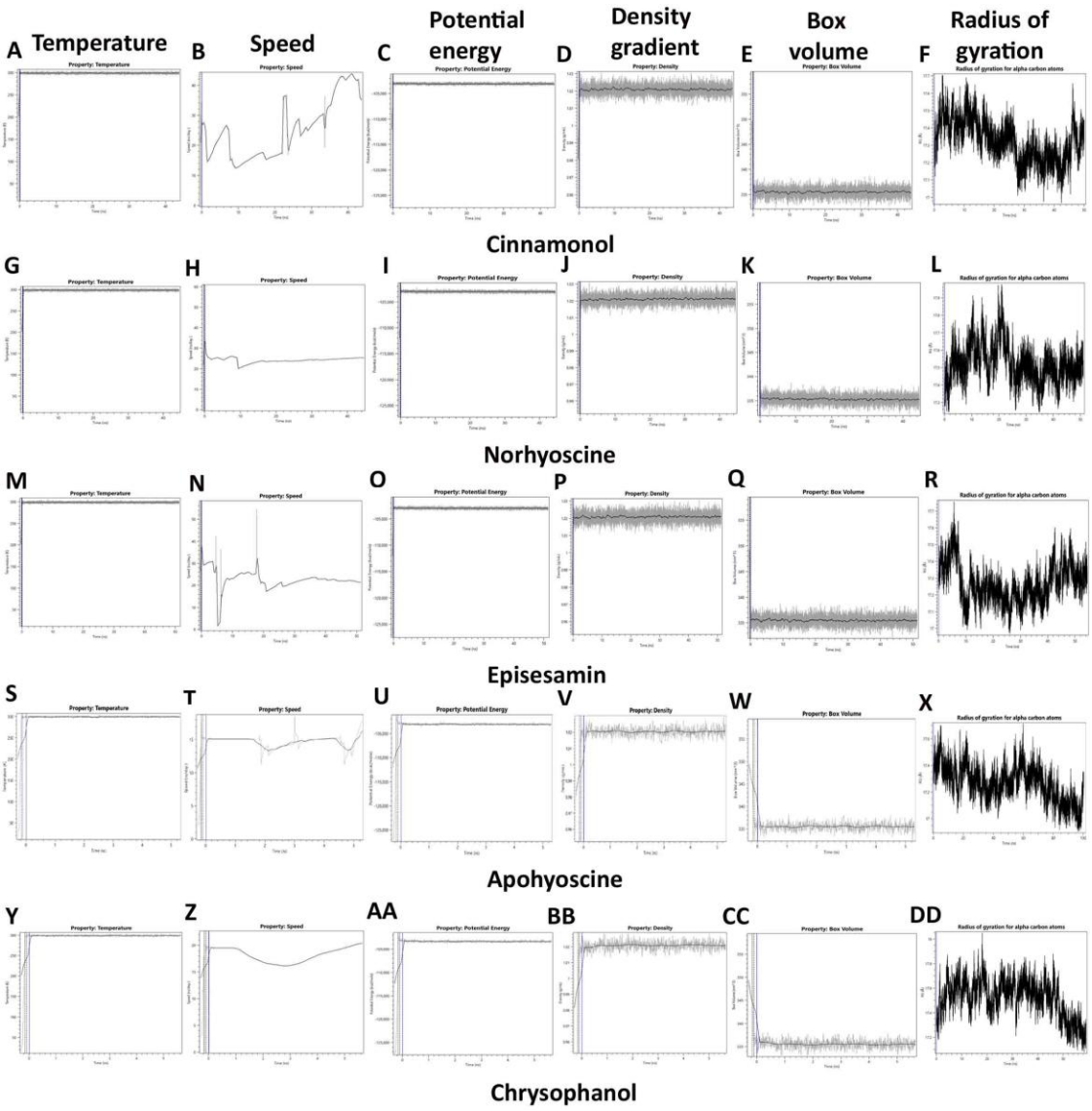
Carpasemine



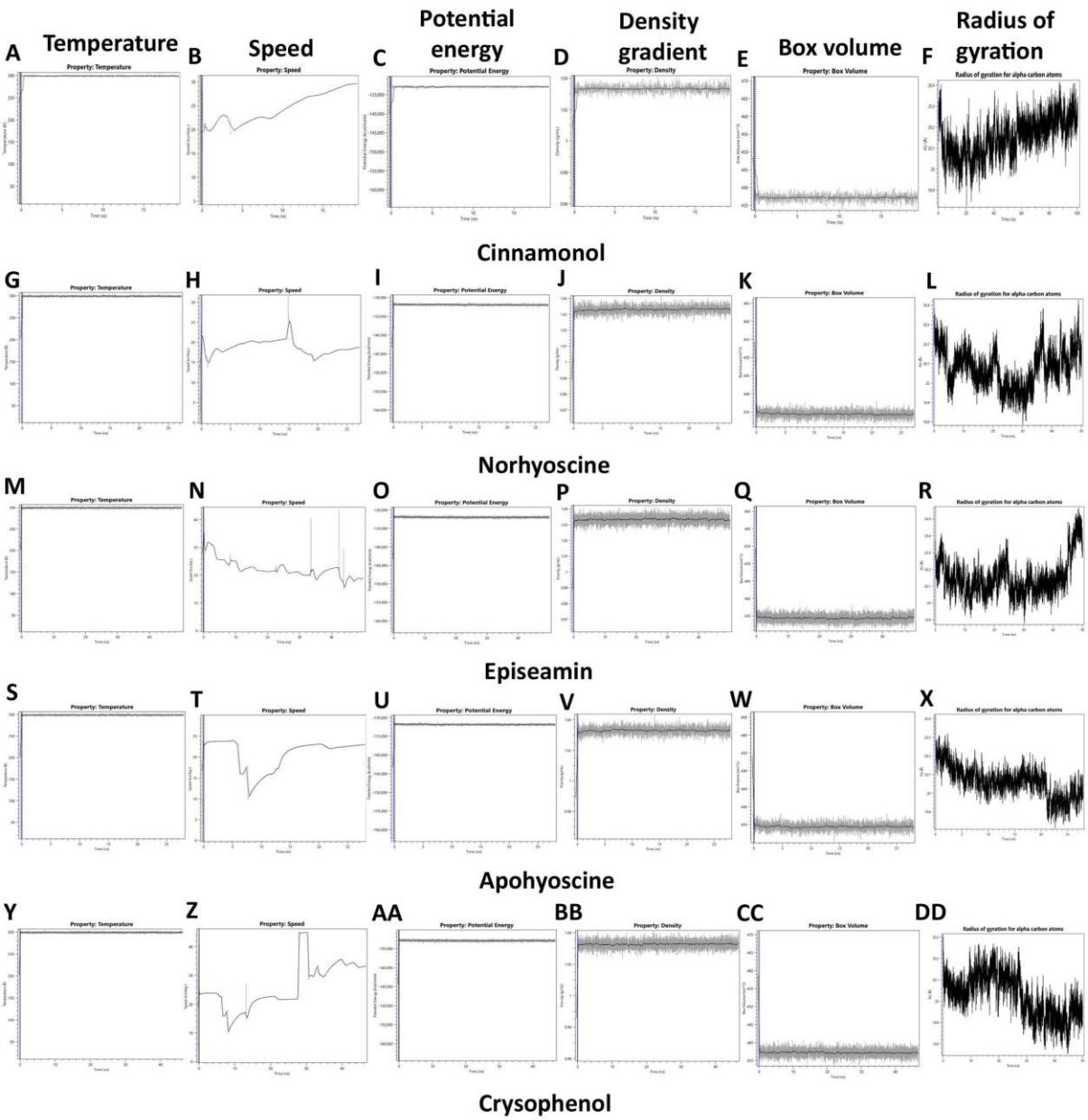
Supplementary figure 1: Two-dimensional structures forty-nine phytochemicals shortlisted for molecular docking.



Supplementary figure 2: Molecular dynamics simulation analysis of HadAB–ligand complexes for selected phytocompounds. Each row corresponds to a different ligand: (A–F) Cinnamomol; (G–L) Norhyoscine; (M–R) Episesamin; (S–X) Apohyoscine; (Y–DD) Chrysophanol. The parameters analyzed include Temperature (A, G, M, S, Y), Speed (B, H, N, T, Z), Potential Energy (C, I, O, U, AA), Density Gradient (D, J, P, V, BB), Box Volume (E, K, Q, W, CC), and Radius of Gyration (F, L, R, X, DD) over the 50 ns simulation period. The stability of each system was assessed to evaluate conformational behavior, compactness, and system equilibration.



Supplementary figure 3: Molecular dynamics simulation analysis of protein FabG1–ligand complexes for selected phytocompounds. Each row corresponds to a different ligand: (A–F) Cinnamomol; (G–L) Norhyoscine; (M–R) Episesamin; (S–X) Apohyoscine; (Y–DD) Chrysophanol. The parameters analyzed include Temperature (A, G, M, S, Y), Speed (B, H, N, T, Z), Potential Energy (C, I, O, U, AA), Density Gradient (D, J, P, V, BB), Box Volume (E, K, Q, W, CC), and Radius of Gyration (F, L, R, X, DD) over the 50 ns simulation period. The stability of each system was assessed to evaluate conformational behavior, compactness, and system equilibration.



Supplementary figure 4: Molecular dynamics simulation analysis of KasA–ligand complexes for selected phytocompounds. Each row corresponds to a different ligand: (A–F) Cinnamomol; (G–L) Norhyoscine; (M–R) Episesamin; (S–X) Apohyoscine; (Y–DD) Chrysophanol. The parameters analyzed include Temperature (A, G, M, S, Y), Speed (B, H, N, T, Z), Potential Energy (C, I, O, U, AA), Density Gradient (D, J, P, V, BB), Box Volume (E, K, Q, W, CC), and Radius of Gyration (F, L, R, X, DD) over the 50 ns simulation period. The stability of each system was assessed to evaluate conformational behavior, compactness, and system equilibration.

Supplementary Table-1: Bioactive Compounds, Plant Sources, and Chemical Classification

S.No.	Phytochemicals	Plant Name	Plants Family	Plants Part	Class of Compounds
1.	16alpha-Hydroxyprogesterone	*Commiphore mukul* (Guggul)	*Burseraceae*	Stem	Steroid
2.	Guggulsterone Z	*Commiphore mukul* (Guggul)	*Burseraceae*	Stem	Steroid
3.	Cinnamonol	*Cinnamomum camphora* (camphor tree)	*Lauraceae*	Leaves	NA
4.	Episesamin	*Cinnamomum camphora* (camphor tree)	*Lauraceae*	Leaves	Phenylpropanoids
5.	Sativol	Crocus sativus (kesar)	*Iridaceae*	Essential Oil	Pterocarpan
6.	Norhyoscine	*Datura metel* (Thornapple)	*Solanaceae*	Root	Tropane alkaloid
7.	Berberine chloride	Berberis aristata (Daru Haldi)	*Berberidaceae*	Bark	alkaloids
8.	Melanoxetin	*Albizia lebbeck* (Indian siris)	*Fabaceae*	Wood	Flavonoids
9.	Pelargonidin	*Punica granatum* (Dalim)	*Punicaceae*	Fruit	Flavonoids
10.	Thiamin	*Punica granatum* (Dalim)	*Punicaceae*	Fruit	Diazines
11.	Apohyoscine	*Datura metel* (Thornapple)	*Solanaceae*	Root	Tropane alkaloid
12.	Alpha-Allocryptopine	Argemone mexicana (Satyanashi)	*Berberidaceae*	Root	Magnoliopsida
13.	Obtusifolin	Cassia tora(Chakunda)	*Fabaceae*	Seed	Anthraquinone
14.	Lomatin	Nardostachys jatamansi (Jatamamsi)	*Valerianaceae*	Rhizome	NA
15.	Palmatine chloride	Berberis aristata (Daru Haldi)	*Berberidaceae*	Bark	Alkaloids
16.	Chrysophanol	*Cassia tora* (Chakunda)	*Fabaceae*	Leaf/fruit	Anthraquinone
17.	5-Hexyl-Cyclopenta-1,3-Dione	*Allium cepa* (Pyaz)	*Amaryllidaceae*	Bulb	Beta-diketone
18.	Chryso-obtusin	*Cassia tora* (Chakunda)	*Fabaceae*	Seed	Polyketides
19.	Alpha- Terpinyl-Acetate	*Cinnamomum camphora* (Kapoor)	*Lauraceae*	Leaf	Menthane monoterpenoids
20.	(Rac)- Myrislignan	*Myristica fragrans* (Jaifal, Nutmeg)	*Myristicaceae*	Leaf, seed	Phenylpropanoids .
21.	Malvidin	*Punica granatum* (Dalim)	*Punicaceae*	Fruit	Flavonoids
22.	Borneol-acetate	*Cannabis sativa* (Ganja)	*Pinaceae*	Plant	Bicyclic monoterpenoids
23.	Endo-bornyl-acetate	*Ageratum conyzoides* (Visadoori)	*Pinaceae,*	Plant	bicyclic monoterpenoid
24.	Isoscopoletin	*Althaea officinalis* (Khatmi)	*Magnoliopsida*	Shoot/Root	hydroxycoumarin
25.	Cantharidin	*Butea Monosperma* (Dhaak)	*Fabaceae*	Plant	Terpenoid
26.	Trans-sinapic-acid	*Allium cepa* (Pyaz)	*Amaryllidaceae*	Seed	Phenylpropanoids
27.	5- Methoxyeugenol	*Myristica fragrans* (Javitri)	*Myristicaceae*	Essential oil	Methoxyphenols

28.	Pelletierine	*Punica granatum* (Dalim)	*Punicaceae*	Plant	Alkaloid
29.	Delta-octalactone	*Allium cepa* (Payaz)	*Liliaceae*	Fruit	Organic compounds
30.	Vasicine	*Justicia adhatoda* (Arusha)	*Acanthaceae*	Plant	Quinazoline alkaloid
31.	Cotinine	*Allium cepa*	*Solanaceae*	Leaf	Alkaloid
32.	1-hydroxy-2-acetyl-4-methylbenzene	*Allium cepa* (Pyaz)	*Asteraceae*	Shoot	Acetophenones
33.	Veratric-acid	*Verbascum Thapsus* (Mullein)	*Scrophulariaceae*	Fruit	Phenolic
34.	Damascenine	*Nigella sativa* (kala jeera)	*Ranunculaceae*	Plant	Alkaloids
35.	Prostaglandin-E-1	*Allium sativum* (Lehsun, Garlic)	*Liliaceae*	Bulb	Eicosanoids
36.	Carpasemine	*Carica papaya* (Papita)	*Caricaceae*	Seed	Alkaloids
37.	Neodecanoic- Acid	*Allium cepa* (Pyaz)	*Liliaceae*	Bulb	Medium-chain fatty acid
38.	Heptan-1-al	*Centella asiatica* (Gotu kola)	*Apiaceae*	Shoot	Organic compounds
39.	Prostaglandin-E-2	*Allium sativum* (Lehsun, Garlic)	*Amaryllida ceae*	Essential oil	Eicosanoids
40.	Prostaglandin-A-1	*Allium sativum* (Lehsun, Garlic)	*Liliaceae*	Seed	Eicosanoids
41.	Citronellic- Acid	*Cinnamomum camphora /Elettaria cardamomum* (Kapoor)	*Lauraceae/ Zingiberaceae*	EO/Fruit	Acyclic monoterpenoid
42.	Tetrahydro-2,5-Dimethylthiophene	*Allium sativum* (Lehsun, Garlic)	*Amaryllidaceae*	Bulb	Organic compounds/ thiophenes
43.	Prostaglandin-B-1	*Allium sativum* (Lehsun, Garlic)	*Liliaceae*	Bulb	Eicosanoids
44.	1,1-Diethoxy-3-Methylbutane	*Capsicum annuum* (chili pepper)	*Solanaceae*	Fruit	Acyclic monoterpenoids
45.	1,1-Diethoxy-2-Methylpropane	*Capsicum annuum* (chili pepper)	*Solanaceae*	Fruit	Organic compound
46.	Arecolidine	*Areca catechu* (Supari)	*Arecaceae*	fruit	Alkaloid
47.	Jasmonic- Acid	*Allium sativum* (Lehsun, Garlic)	*Valerianaceae*	Root	Iasmonate
48.	Vanillic- Acid-4-Beta-D-Glucoside	*Capsicum annuum* (chili pepper)	*Solanaceae*	Fruit	Hydrolyzable tannins
49.	Ethyl-Isopropyl-sulfide	Zingiber officinale (Soont/zinger)	*Zingiberaceae*	Essential oil, Rhizome	Dialkylthioethers

Supplementary Table-2: Drug-like properties of forty-nine compounds those satisfied lipinski rule five/ Lipinski rule of five drug-likeness properties of potential compounds

S.No.	Compounds	Molecular Mass(g/mol)	Xlog P3(<5)	H donar (≤5)	H acceptor (≤10)	Molar Refractivity
1.	16alpha- Hydroxyprogesterone	330	4.0	1	3	102.4
2.	Guggulsterone Z	312	4.1	0	2	98.7
3.	Cinnamonol	370	2.7	1	7	88.1
4.	Episesamin	354	3.0	0	6	87.3
5.	Sativol	298	1.1	2	6	64.4
6.	Norhyoscine	289	1.4	2	5	73.6
7.	Berberine chloride	371	1.8	0	4	85.1
8.	Melanoxetin	302	0.7	5	7	65.0
9.	Pelargonidin	271	0.8	4	5	63.1
10	Thiamin	265	1.6	3	1	68.5
11	Apohyoscine	285	1.8	0	3	74.5
12	Alpha- Allocryptopine	369	3.3	0	5	98.2
13	Obtusifolin	284	1.8	2	5	67.9
14	Lomatin	246	1.9	1	4	62.8
15	Palmatine chloride	387	2.2	0	4	92.5
16	Chrysophanol	254	1.6	2	4	61.7
17	5-Hexyl-cyclopenta-1,3-Dione	182	2.6	0	2	57.0
18	Chryso-obtusin	358	2.6	1	7	85.5
19	Alpha- Terpinyl-Acetate	196	3.0	0	2	62.3
20	(Rac)- Myrislignan	374	3.8	2	6	98.7
21	Malvidin	331	1.5	4	7	74.8
22	Borneol-acetate	196	3.0	0	2	60.5
23	Endo-bornyl-acetate	196	3.0	0	2	60.5
24	Isoscopoletin	192	0.9	1	4	42.6
25	Cantharidin	196	1.4	0	4	47.0
26	Trans-sinapic-acid	224	0.7	2	5	50.8
27	5- Methoxyeugenol	196	2.3	1	3	53.9
28	Pelletierine	141	1.8	1	1	45.2
29	Delta-octalactone	142	1.9	0	2	42.8
30	Vasicine	188	1.3	1	2	51.6
31	Cotinine	176	1.4	0	1	47.6
32	1-hydroxy-2-acetyl-4-methylbenzene	150	1.5	1	2	41.5
33	Veratric-acid	182	1.1	1	4	40.9
34	Damascenine	195	1.6	0	3	48.7
35	Prostaglandin-E-1	354	4.1	3	5	105.6
36	Carpasemine	166	-0.4	3	0	43.3
37	Neodecanoic-acid	172	2.5	1	2	55.3
38	Heptan-1-al	114	2.1	0	1	38.5
39	Prostaglandin-E-2	352	3.9	3	5	103.3
40	Prostaglandin-A-1	336	4.2	2	4	102.5
41	Citronellic- Acid	170	2.4	1	2	53.7
42	Tetrahydro-2,5-Dimethylthiophene	116	1.8	0	0	40.0
43	Prostaglandin-B-1	336	4.2	2	4	102.6

44	1,1-Diethoxy-3-Methylbutane	160	2.7	0	2	52.5
45	1,1-Diethoxy-2- Methylpropane	146	2.4	0	2	47.1
46	Arecolidine	155	1.5	0	2	42.3
47	Jasmonic- Acid	224	3.0	0	3	65.5
48	Vanillic- Acid-4-Beta-D-Glucoside	330	1.1	5	9	70.7
49	Ethyl-Isopropyl- sulfide	104	1.7	0	0	36.7

Supplementary Table-3: Result of forty-nine compounds that successfully satisfy all ADMET analysis / List of ADMET properties of herbal compounds evaluated by PreADMET tool

S. No.	Compounds	Mutagenicity	Carcinogenicity Mouse	Carcinogenicity Rat	HIA %	Pcaco-2(nm/s)	Pmdck(nm/s)	Pskin (nm/s)	PPB %	BBB%	Cyp2d6
1.	16alpha-Hydroxyprogesterone	NM	+	+	95.57	20.21	79.99	-3.29	100	0.33	Non
2.	Guggulsterone Z	NM	+	+	99.06	28.17	160.5	-2.12	100	0.91	Non
3.	Cinnamonol	Mutagen	-	-	96.71	37.30	17.95	-4.43	78.45	0.02	Non
4.	Episesamin	Mutagen	-	-	97.95	57.02	20.60	-4.41	83.12	0.05	Non
5.	Sativol	Mutagen	-	+	93.86	3.08	51.96	-3.80	96.55	0.03	Non
6.	Norhyoscine	Mutagen	+	-	92.06	20.49	1.41	-4.66	18.72	0.02	Non
7.	Berberine chloride	Mutagen	-	-	98.09	21.09	0.47	-4.76	27.03	0.20	Inhibitor
8.	Melanoxetin	Mutagen	-	+	63.46	12.71	63.71	-4.42	90.54	0.18	Non
9.	Pelargonidin	Mutagen	-	-	83.58	1.29	59.76	-3.99	100	0.53	Substrate
10.	Thiamin	Mutagen	-	-	91.10	5.44	0.54	-4.57	9.07	0.02	Substrate
11.	Apohyoscine	Mutagen	+	-	98.02	53.50	49.45	-3.96	35.00	0.02	Non
12.	Alpha-Allocryptopine	Mutagen	-	-	97.91	50.37	10.44	-4.00	69.01	0.02	Non
13.	Obtusifolin	Mutagen	-	+	94.03	15.49	70.38	-3.51	95.45	0.72	Non
14.	Lomatin	Mutagen	-	-	95.36	4.30	88.42	-3.20	69.50	0.68	Non
15.	Palmatine chloride	Mutagen	-	-	98.13	21.10	0.32	-4.63	28.59	0.24	Inhibitor
16.	Chrysophanol	Mutagen	-	+	93.74	16.33	43.05	-3.46	100	0.71	Non
17.	5-Hexyl-cyclopenta-1,3-Dione	Mutagen	+	+	98.92	14.80	54.18	-1.61	100	0.86	Non
18.	Chryso-obtusin	Mutagen	-	+	96.19	22.34	175.63	-3.72	85.69	0.01	Non
19.	Alpha- Terpinyl-Acetate	Mutagen	-	-	100	37.76	262.08	-1.29	98.53	0.89	Non
20.	(Rac)-Myrislignan	Non-Mutagen	-	+	93.93	39.36	11.58	-2.38	889.24	00.69	Non
21.	Malvidin	Mutagen	-	+	83.10	1.75	109.94	-4.20	94.94	0.05	Weakly
22.	Borneol-acetate	Mutagen	-	-	1100	337.67	1148.16	-2.00	883.32	00.80	Non
23.	Endo-bornyl-acetate	Mutagen	- -	+ +	1100	337.67	148.16	-2.00	83.32	0.80	Non
24.	Isoscopoletin	Mutagen	-	+	93.92	18.84	67.45	-3.13	48.82	0.64	Non
25.	Cantharidin	Mutagen	-	+	92.21	21.02	23.04	-4.33	42.48	0.87	Non

26.	Trans-sinapic-acid	Mutagen	-	+	888.55	119.85	2270.19	-2.28	447.50	00.72	Non
27.	5-Methoxyeugenol	Mutagen	+	-	94.57	50.53	43.31	-2.10	91.47	0.55	Non
28.	Pelletierine_	Mutagen	+	-	94.19	35.77	6.84	-3.65	0.80	0.45	Weakly
29.	Delta-octalactone	Mutagen	+	+	100	50.71	60.92	-1.97	100	0.79	Weakly
30.	Vasicine	Mutagen	-	-	95.47	29.31	278.64	-3.86	80.33	0.54	Weakly
31.	Cotinine	Mutagen	-	-	99.79	30.28	5.47	-2.85	57.20	0.99	Non
32.	1-hydroxy-2-acetyl-4-methylbenzene	Mutagen	+	-	94.50	20.02	61.39	-1.72	85.71	0.74	Non
33.	Veratric-acid	Mutagen	-	+	92.68	0.57	52.15	-2.08	77.89	1.05	Non
34.	Damascene	Mutagen	+	+	94.33	25.56	42.51	-2.33	63.20	0.59	Non
35.	Prostaglandin-E-1	Mutagen	+	+	87.29	18.66	0.07	-1.67	100	0.33	Non
36.	Carpasemine	Mutagen	-	-	93.81	21.02	61.30	-2.55	39.93	0.59	Non
37.	Neodecanoic-acid	Mutagen	-	-	95.67	8.09	189.63	-1.22	100.00	0.82	Non
38.	Heptan-1-al	Mutagen	-	-	100	37.21	164.12	-1.61	97.42	1.02	Non
39.	Prostaglandin-E-2	Mutagen	-	+	89.18	18.66	0.09	-1.92	89.69	0.19	Non
40.	Prostaglandin-A-1	Mutagen	-	+	95.51	20.74	0.09	-1.80	100	0.89	Non
41.	Citronellic- Acid	Mutagen	+	+	96.57	5.69	40.57	-1.11	100	0.85	Non
42.	Tetrahydro-2,5-Dimethylthiophene	Mutagen	-	+	100	21.98	0.88	-2.28	88.86	0.78	Non
43.	Prostaglandin-B-1	Mutagen	-	+	95.51	20.70	0.09	-1.07	100	0.97	Non
44.	1,1-Diethoxy-3-Methylbutane	Mutagen	+	+	100	49.97	59.45	-1.79	100	0.89	Non
45.	1,1-Diethoxy-2-Methylpropane	Mutagen	+	+	100	48.67	92.59	-2.04	100	0.82	Non
46.	Arecolidine	Mutagen	+	-	100	56.41	241.98	-3.30	74.49	0.80	Non
47.	Jasmonic- Acid	Non-Mutagen	+	+	97.61	22.15	69.58	-1.58	78.02	0.27	Non
48.	Vanillic- Acid-4-Beta-D-Glucoside	Mutagen	-	-	86.48	15.37	0.56	-4.68	36.88	0.01	Non
49.	Ethyl-Isopropyl-sulfide	Mutagen	-	+	100	21.65	0.84	-1.77	82.60	0.80	Non

Supplementary Table 4: Binding energy and inhibition constant scores of all forty-nine phytochemicals

S.No.	Phytochemicals	B.E HadAB (kcal/mol)	Ki (μM)	B.E FabG1 (kcal/mol)	Ki (μM)	B.E KasA (kcal/mol)	Ki (μM)
1.	16alpha-Hydroxyprogesterone	-10.8	0.01	-7.94	1.51	-8.83	0.33
2.	Guggulsterone Z	-10.0	0.04	-8.65	0.45	-8.18	1.01
3.	Cinnamonol	-9.25	0.15	-7.95	1.48	-7.59	2.72
4.	Episesamin	-8.96	0.27	-7.70	2.26	-8.32	0.80
5.	Sativol	-8.91	0.29	-7.75	2.08	-8.13	1.10
6.	Norhyoscine	-8.74	0.39	-6.78	10.7	-9.95	0.05
7.	Berberine chloride	-8.61	0.49	-7.10	6.23	-7.98	1.40
8.	Melanoxetin	-8.29	0.83	-8.21	0.95	-7.42	3.62
9.	Pelargonidin	-8.11	1.13	-6.24	26.7	-8.44	0.65
10.	Thiamin	-7.95	1.48	-6.38	21.0	-7.17	5.57
11.	Apohyoscine	-7.94	1.51	-7.30	4.42	-9.70	0.07
12.	Alpha-Allocryptopine	-7.91	1.58	-7.33	4.24	-8.42	0.67
13.	Obtusifolin	-7.83	1.82	-7.30	4.44	-7.79	1.96
14.	Lomatin	-7.47	3.34	-7.07	6.61	-8.59	0.50
15.	Palmatine chloride	-7.45	3.45	-6.16	30.7	-7.62	2.58
16.	Chrysophanol	-7.19	5.40	-7.11	6.14	-7.94	1.51
17.	5-Hexyl-Cyclopenta-1,3-Dione	-7.14	5.82	-5.28	134.83	-6.85	9.46
18.	Chryso-obtusin	-7.10	6.22	-6.56	15.6	-6.50	17.18
19.	Alpha- Terpinyl-Acetate	-7.05	6.83	-6.82	10.0	-7.41	3.70
20.	(Rac)- Myrislignan	-6.94	8.25	-6.24	26.4	-6.62	13.99
21.	Malvidin	-6.84	9.67	-6.06	36.2	-7.58	2.77
22.	Borneol-acetate	-6.68	12.74	-6.73	21.4	-7.19	5.39
23.	Endo-bornyl-acetate	-6.66	13.02	-6.10	34.0	-7.19	5.34
24.	Isoscopoletin	-6.64	13.67	-5.07	192.52	-6.64	13.49
25.	Cantharidin	-6.44	19.13	-5.84	52.5	-6.76	11.02
26.	Trans-sinapic-acid	-6.37	21.33	-6.20	28.3	-5.26	140.54
27.	5- Methoxyeugenol	-6.37	21.43	-5.26	138.51	-6.07	35.48
28.	Pelletierine	-6.36	21.95	-4.56	457.18	-6.56	15.59
29.	Delta-octalactone	-6.20	28.42	-4.94	239.76	-6.32	23.16
30.	Vasicine	-6.18	29.48	-6.06	36.00	-6.35	22.03
31.	Cotinine	-6.18	29.32	-6.18	29.57	-6.52	16.58
32.	1-hydroxy-2-acetyl-4-methylbenzene	-6.14	31.67	-5.63	74.63	-6.08	34.90
33.	Veratric-acid	-5.65	72.11	-4.91	253.49	-7.20	5.27
34.	Damascenine	-5.54	87.40	-6.38	21.05	-5.40	110.97
35.	Prostaglandin-E-1	-5.45	101.73	-6.86	9.42	-6.05	36.53
36.	Carpasemine	-5.41	108.22	-5.17	161.65	-5.73	62.65
37.	Neodecanoic- Acid	-5.37	115.86	-5.51	92.01	-5.02	207.68
38.	Heptan-1-al	-5.34	122.03	-3.49	2.78	-4.61	414.30
39.	Prostaglandin-E-2	-5.25	141.78	-6.88	8.99	-5.57	82.40
40.	Prostaglandin-A-1	-5.29	131.68	-6.64	13.62	-5.58	81.09
41.	Citronellic- Acid	-5.17	163.13	-5.60	79.14	-5.44	102.31
42.	Tetrahydro-2,5-Dimethylthiophene	-5.09	185.35	-4.71	352.46	-5.11	178.11

43.	Prostaglandin-B-1	-5.02	207.85	-6.50	17.33	-5.57	137.46
44.	1,1-Diethoxy-3-Methylbutane	-4.89	261.31	-3.93	1310	-4.56	455.95
45.	1,1-Diethoxy-2-Methylpropane	-4.83	286.67	-3.47	2860	-4.14	930.49
46.	Arecolidine	-4.73	340.26	-4.20	840.68	-5.17	162.88
47.	Jasmonic- Acid	-4.68	370.75	-6.56	15.63	-7.84	1.80
48.	Vanillic- Acid-4-Beta-D-Glucoside	-4.49	512.00	-6.26	25.86	-5.54	86.63
49.	Ethyl-Isopropyl-sulfide	-3.94	1300	-5.34	121.42	-4.05	1080