

Use Case of AIDrugApp: Case studies of Virtual Screening of Inhibitors against SARS-COV-2

Divya Karade^{*1}, Vikas Karade²

¹Chemical Engineering and Process Development (CEPD) Division, CSIR-National Chemical Laboratory, Pune – 411008, India, ²Algosurg Products Pvt. Ltd., Mumbai, India

This document presents two case studies where large sets of molecules were screened by AIDrugApp to show its usefulness and application. Through this case-studies, we discovered that the Indian medicinal plant's small molecules (like Oblongine from *Tinospora cordifolia*, Acantrifoside E from *Ferula assa-foetida*, etc) and CAS COVID-19 antiviral compounds (such as CAS ID: 127047-63-6, 1174190-70-5, etc) show better results compared to clinical trial compounds (such as Remdesivir, Lopinavir, etc) included in this study. This is a very important outcome for the process of drug discovery against SARS-COV-2. We believe that if many experts contribute and collaborate using this web-platform then many such discoveries related to other diseases can help to accelerate the drug discovery process.

Web-App URL: <https://sars-covid-app.herokuapp.com/>

Case studies

In the case studies, we used the AIDRUGAPP to screen small molecules of Indian medicinal plants and CAS antiviral molecules towards Replicase polyprotein (RP)¹, Angiotensin Converting Enzyme (ACE)², 3CLpro³ and molecules related to Clinical trials (CT) for SARS-COVID-19 diseases. The screened molecules were then used for molecular docking studies and ADME (absorption, distribution, metabolism, and excretion) calculations to design an effective drug candidate molecule. The following methodology was applied in the case studies (CS1 and CS2) as also explained in Figure 1:

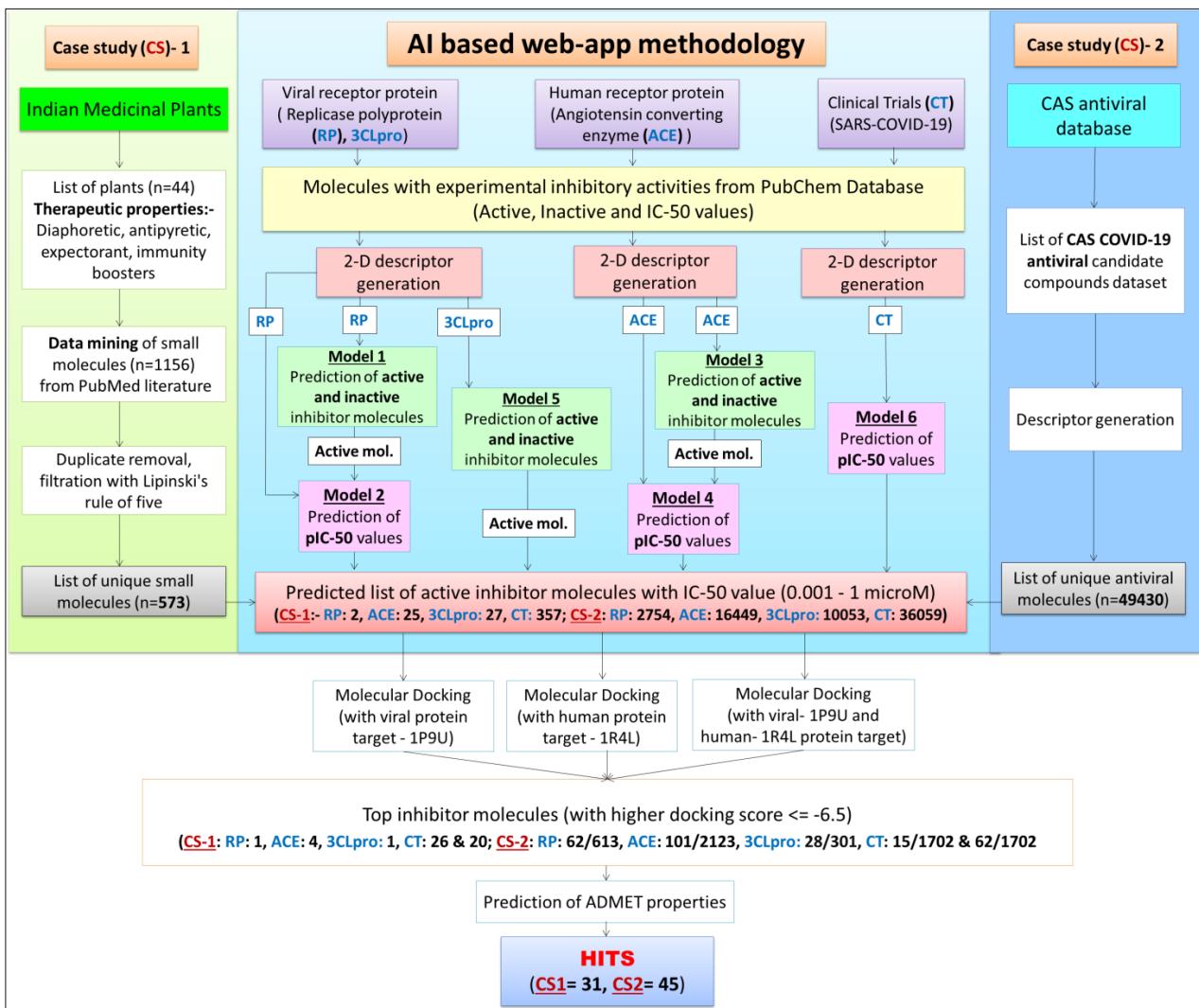


Figure 1. AI-based drug designing computational protocol against SARS-CoV-2 presented for two case studies

Methodology

CS-1:

- Collected a list of plants (n=44) with therapeutic properties: Diaphoretic, antipyretic, Expectorant and immunity boosters from databases^{4,5} related to Indian medicinal plants (Appendix 1).
- Text mined a list of chemical names of small molecules (n=1156) related to Indian medicinal plants from PubMed literature through PubTator⁶ (Appendix 2).

3. Chemical names were converted into molecular SMILES in python by using NIH/NCI Chemical Identifier Resolver (<https://cactus.nci.nih.gov/chemical/structure>) and manually from the PubChem database.
4. Molecular descriptors (hydrogen bond acceptor atoms, hydrogen bond donor atoms, number of rotatable bonds, molecular density, logP, logS, number of rings, and molecular weight) were generated by using molecular SMILES.
5. Molecules were filtered by removing duplicates and by applying “Lipinski's rule of five” to get a unique list of drug-like molecules (n= 573).
6. Input .csv file containing molecular descriptors were uploaded in web-app.
7. Molecular data were processed and statistically analyzed through the “visualize the analysis of uploaded data” section in the batch module of the web-app (Fig. 2A).
8. Active and inactive inhibitor molecules were predicted against RP, ACE and 3CLpro datasets available in the web-app.
9. Active inhibitor molecules were used to predict their pIC-50 values towards RP, ACE and SARS-COV-2 CT by uploading their molecular descriptors .csv file in web-app.
10. Molecules were selected which were tagged as “In” the applicability domain of the predictive models.
11. Active inhibitor molecules with their pIC-50 values (0.001 to 1 microM) were virtually screened for further molecular docking analysis using Schrodinger's Maestro Version 11.3.016⁷ for validating DL models.
 - a. Molecules virtually screened from web apps dataset named RP, 3CLpro and CT were used for molecular docking analysis with replicase enzyme- 3CLpro protein target (PDB ID: [1P9U](#)).

- b. Molecules virtually screened from web apps dataset named ACE and CT were used for molecular docking analysis with human ACE protein target (PDB ID: [1R4L](#)) for validating DL models.
12. Active inhibitor molecules with pIC-50 values and high docking scores (≤ -6.5) were used to evaluate pharmacokinetics, drug-likeness and medicinal chemistry friendliness by using SwissADME⁸.

CS-2:

1. CAS COVID-19 antiviral candidate compounds (n= 49,430) were collected with SMILES from the CAS database (<https://www.cas.org/covid-19-antiviral-compounds-dataset>, 2020; Online; accessed 30-11-2020).
2. Molecular descriptors (hydrogen bond acceptor atoms, hydrogen bond donor atoms, number of rotatable bonds, molecular density, logP, logS, number of rings and molecular weight) were generated by using molecular SMILES.
3. Input .csv file containing molecular descriptors were uploaded in web-app.
4. Molecular data were processed and statistically analyzed through the “visualize the analysis of uploaded data” section in the batch module of the web-app (Fig. 2B).
5. Active and inactive inhibitor molecules were predicted against RP, ACE and 3CLpro datasets available in the web-app.
6. Active inhibitor molecules were used to predict their pIC-50 values towards RP, ACE and SARS-COV-2 CT by uploading their molecular descriptors .csv file in web-app.
7. Molecules were selected which were tagged as “In” the applicability domain of the predictive models.
8. Active inhibitor molecules with their pIC-50 values (0.001 to 1 microM) were virtually screened for further molecular docking analysis using Schrodinger’s Maestro Version 11.3.016⁷ for validating DL models.

- a. Molecules virtually screened from web apps dataset named RP, 3CLpro and CT were used for molecular docking analysis with replicase enzyme- 3CLpro protein target (PDB ID: [1P9U](#)).
 - b. Molecules virtually screened from web apps dataset named ACE and CT were used for molecular docking analysis with human ACE protein target (PDB ID: [1R4L](#)) for validating DL models.
9. Active inhibitor molecules with pIC-50 values and high docking scores ($<= -6.5$) were used to evaluate pharmacokinetics, drug-likeness and medicinal chemistry friendliness by using SwissADME⁸.

Results

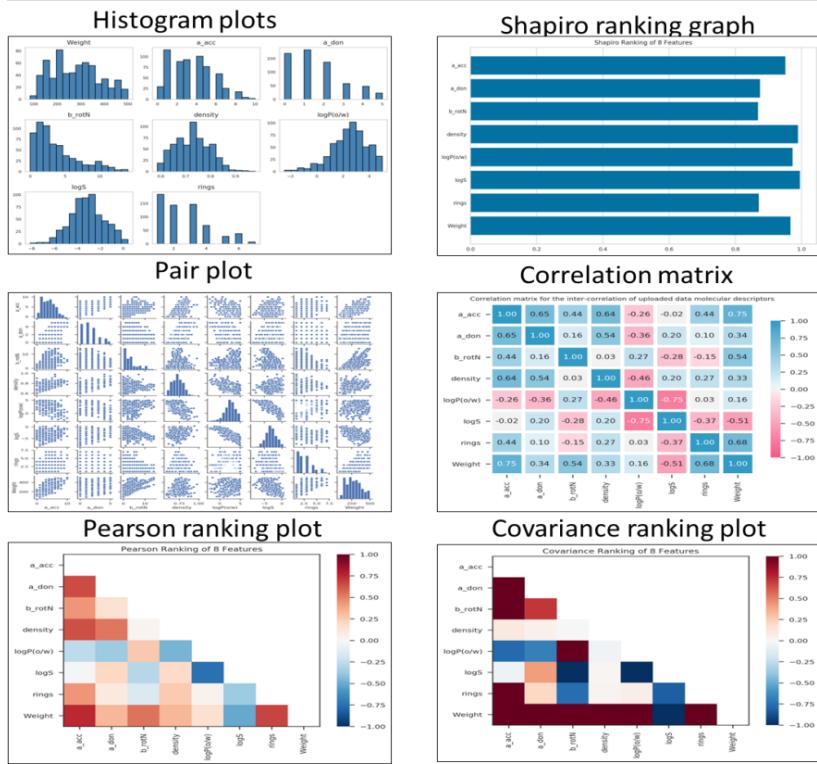
Data analysis and visualization using AIDrugApp

AIDRUGAPP was used to analyze Indian medicinal plants and CAS COVID-19 antiviral compounds data for better understanding. Files (.csv) containing molecular descriptors were uploaded in the batch section of the web-app to visualize the uploaded data analysis (Fig. 2).

CS1: Dataframes for Indian medicinal plants data can be viewed in the form of a table consisting of molecular SMILES, molecular descriptors and their bioactivities. It consists of $n = 573$ rows of molecular data and $n = 8$ columns of descriptor values. The statistical analysis of model data can be visualized in the form of a table (Fig. 2A). It contains the count of molecular data, the mean value, standard deviation, minimum value, 25% value, 50% value, 75% value and maximum value for each descriptor data. The data range value for molecular weight (85.15 - 499.60), hydrogen bond acceptor atoms (0 - 10), hydrogen bond donor atom (0 - 5), number of rotatable bonds (0 - 14), molecular density (0.59 – 0.98), logP (-2.46 – 4.98), logS (-8.13 – 0.40) and number of rings (1 - 7) were visualized in histogram plots. Shapiro ranking graphs for 8 features were generated on the scale [0,1] which shows log S with the higher ranking. All other descriptors values show a ranking of more than 0.8. Pair plots show the chemical space of diverse molecules in each descriptor range.

Data analysis of Indian medicinal plants small molecules

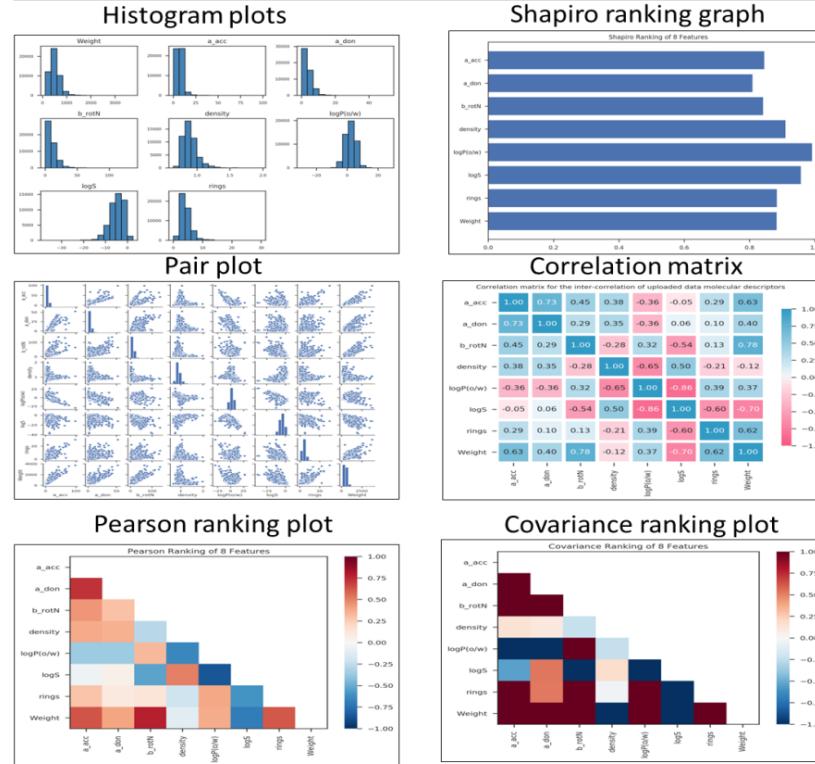
	a_acc	a_don	b_rotN	density	logP(o/w)	logS	rings	Weight
count	617	617	617	617	617	617	617	617
mean	3.4246	1.5186	3.5705	0.7274	2.4352	-3.1386	2.6029	279.0322
std	2.1338	1.3794	3.3408	0.0700	1.3750	1.4844	1.5171	100.6128
min	0	0	0	0.5860	-2.4550	-8.1345	1	85.1500
25%	2	0	1	0.6743	1.6310	-4.0792	1	198.1740
50%	3	1	2	0.7293	2.5330	-3.1367	2	276.3760
75%	5	2	5	0.7757	3.3037	-2.1555	3	354.3580
max	10	5	14	0.9780	4.9770	0.4036	7	499.6010



(A)

Data analysis of CAS COVID-19 antiviral candidate compounds

	a_acc	a_don	b_rotN	density	logP(o/w)	logS	rings	Weight
count	49430	49430	49430	49430	49430	49430	49430	49430
mean	7.0429	3.5464	10.3050	0.8921	2.0911	-4.8155	3.6944	504.1675
std	3.5526	2.8367	7.7390	0.1079	3.4931	3.2375	1.8582	205.9593
min	0	0	0	0.6493	-29.6679	-37.5642	0	110.1160
25%	5	2	5	0.8159	-0.5618	-6.6946	2	354.3580
50%	7	3	8	0.8727	2.3185	-4.5434	3	472.7100
75%	8	5	14	0.9427	4.5384	-2.2865	5	604.7945
max	98	52	137	1.9733	27.2930	2.5504	30	3,748.3879



(B)

Figure 2. Data analysis visualizations from AIDRUGAPP for (A) CS1-Indian medicinal plants small molecules and (B) CS2-CAS COVID-19 antiviral candidate compounds

Correlation matrix, Pearson ranking plots and Covariance ranking plots were generated to visualize the inter-correlation of molecular descriptors and their correlation with bioactivity. The plots show the highest positive inter-correlation (0.75) between molecular weight and hydrogen bond acceptor atoms and the lowest negative inter-correlation (-0.75) between logS and logP.

CS2: Dataframes for CAS COVID-19 antiviral compounds data can be viewed in the form of a table consisting of molecular SMILES, molecular descriptors and their bioactivities. It consists of n = 49430 rows of molecular data and n = 8 columns of descriptor values. The statistical analysis of model data can be visualized in the form of a table (Fig. 2B). It contains the count of molecular data, the mean value, standard deviation, minimum value, 25% value, 50% value, 75% value and maximum value for each descriptor data. The data range value for molecular weight (110.12 - 3748.39), hydrogen bond acceptor atoms (0 - 98), hydrogen bond donor atom (0 - 52), number of rotatable bonds (0 - 137), molecular density (0.64 – 1.97), logP (-29.67 – 27.29), logS (-37.50 – 2.55) and number of rings (0 - 30) were visualized in histogram plots. Shapiro ranking graphs for 8 features were generated on the scale [0,1] which shows log P with the higher ranking. All other descriptors values show a ranking of more than 0.8. Pair plots show the chemical space of diverse molecules in each descriptor range. Correlation matrix, Pearson ranking plots and Covariance ranking plots were generated to visualize the inter-correlation of molecular descriptors and their correlation with bioactivity. The plots show the highest positive inter-correlation (0.78) between molecular weight and number of rotatable bonds and the lowest negative inter-correlation (-0.86) between logS and logP.

Prediction using AIDrugApp - Receptor based virtual screening

Case study 1: Indian medicinal plants small molecules

The list of medicinal plant's small molecules (n = 573) was virtually screened twice each for RP and ACE and once for 3CLpro and CT DL models of AI-based web-app. The first screening was done to get active inhibitor molecules (n = 103 and 49) against RP and ACE receptor proteins

respectively. The second screening was done to get pIC-50 values (0.001 – 1 microM) for active inhibitor molecules ($n = 2$ and 25). Whereas, molecules were also screened to get active inhibitor molecules against 3CLpro ($n = 27$) and for virtual screening of chemical features related to CT associated molecular structures ($n = 361$). The screening process was finished within a few minutes. Screened molecules were then used for molecular docking analysis against ACE (PDB ID: [1R4L](#)) and replicase enzyme- 3CLpro (PDB ID: [1P9U](#)) protein targets for further validation of DL models. Active inhibitor molecules with IC-50 values ($n = 2$) screened from RP DL model were used for docking analysis with PDB ID: [1P9U](#) (Fig 3.A, Table 1 entry 1) to get $n = 1$ molecule with high docking scores (≤ -6.0). On the other hand, active inhibitor molecules with IC-50 values ($n = 25$) screened from the ACE DL model were used for docking analysis with PDB ID: [1R4L](#) (Fig 3.B, Table 1 entry 2) to get $n = 4$ molecules with high docking scores (≤ -6.5). Screened molecules with IC-50 values from CT DL models ($n = 357$) were used for docking with both PDB ID: [1P9U](#) and PDB ID: [1R4L](#) (Fig 3.C and D, Table 1 entry 3 and 4) to get $n = 20$ and 26 molecules with high docking scores (≤ -6.5) respectively. Similarly, active inhibitor molecules ($n = 27$) screened against 3CLpro were used for docking analysis with PDB ID: [1P9U](#) (Fig 3.E, Table 1 entry 5) to get $n = 1$ molecule with high docking scores (≤ -6.5). Molecular docking scores of screened molecules were also compared with drug candidates ($n = 141$) used in SARS-COV-2 CT experimental molecular docking scores to explore the interaction pattern of molecules (Fig 3. F and G, Table 2). Further, the Inhibitor molecules (total, $n = 41$) were selected for ADME properties predictions. A final list of potential drug candidate molecules ($n = 14$) was procured from Indian medicinal plants against SARS-COV-2⁹ (Fig 4. A-B, Table 3). We have also calculated ADME properties for SARS-COV-2 CT experimental molecules which possess the best docking scores (≥ 6.5) among all (Fig 4. C-D, Table 4).

Case study 2: CAS COVID-19 antiviral candidate compounds

A list of antiviral molecules (n= 49430) related to COVID-19 were virtually screened twice each for RP, ACE and once for 3CLpro and CT DL models of AI-based web-app. The first screening was done to get active inhibitor molecules (n= 44,620 and 41,537) against RP and ACE receptor proteins respectively. The second screening was done to get IC-50 values (0.001 – 1 microM) for active inhibitor molecules (n= 2754 and 10053). Whereas, molecules were also screened to get active inhibitor molecules against 3CLpro (n= 12,421) and for virtual screening of chemical features related to CT associated molecular structures (n= 36,059).

The screening process was finished within a few minutes. Screened molecules were then used for molecular docking analysis against ACE (PDB ID: [1R4L](#)) and replicase enzyme- 3CLpro (PDB ID: [1P9U](#)) protein targets for further validation of DL models. Out of n=2754 molecules screened with RP DL model, n= 613 were used for molecular docking with [1P9U](#) to get n=62 molecules with high docking scores (<= -6.5) (Fig 3.H, Table 1 entry 5). On the other hand, active inhibitor molecules with IC-50 values n= 2123 was used out of 16,449 (screened with ACE DL model) molecules for molecular docking with [1R4L](#) to get n=101 molecules with high docking scores (Fig 3.I, Table 1 entry 6). Whereas, n = 1702 molecules were used from 36,059 (screened from CT DL model) molecules for docking with both PDB ID: [1P9U](#) (Fig 3.J, Table 1 entry 7) and PDB ID: [1R4L](#) to get n = 15 and 62 molecules with high docking scores respectively (Fig 3.K, Table 1 entry 8). Similarly, n= 301 molecules were used from 10053 (screened from 3CLpro DL model) for molecular docking with [1P9U](#) to get n = 28 molecules with high docking scores (Fig 3.L, Table 1 entry 9). Molecular docking scores of screened molecules were also compared with drug candidates (n= 141) used in SARS-COV-2 CT experimental molecular docking scores to explore the interaction pattern of molecules (Fig 3. F and G, Table 2). Further, Inhibitor molecules (total, n = 248) were selected for ADME properties predictions. A final list of potential drug candidate molecules (n=45) was procured from CAS antiviral compounds against SARS-COV-2⁹

(Fig 4. E-F, Table 3). For comparison, ADME properties were also been calculated for SARS-COV-2 CT experimental molecules which possess the best docking scores (≥ 6.5) among all (Fig 4. C-D, Table 4).

DISCUSSION

We have developed and presented a web-app (AIDRUGAPP) for predicting inhibitory activities and IC-50 values of compounds towards RP, ACE and CT for SARS-COVID-19 diseases. We also presented two case studies to show the useful application of AIDRUGAPP. The results of these case-studies will simplify the development of novel drugs from the Indian medicinal plants based on the secondary metabolites, their corresponding bioactivities (reported in the scientific literature with experimental evidence) and CAS COVID-19 antiviral candidate compounds dataset.

It has been observed that the pIC-50 values and molecular docking scores of inhibitors are not correlated and one cannot conclude the result based on only one presumption. Although the drug compounds like Remdesivir, Lopinavir, etc (Table 2) used for CT experiments for SARS-COVID-19 diseases show good binding scores with RP, 3CLpro and ACE receptor proteins, they still show low efficacy in the ADME study. Other CT compounds included in this study such as Baricitinib (Fig. 3C, Table 2 entry 4, Table 4 entry 4), Formoterol (Fig. 3D, Table 2 entry 11, Table 4 entry 1) show better results in this study. However, the Indian medicinal plant's small molecules like Oblongine from *Tinospora cordifolia* (Fig. 3A, Table 3 entry 1), Acantrifoside E from *Ferula assa-foetida* (Fig. 3B, Table 3 entry 2), etc and CAS antiviral compounds such as CAS ID: 127047-63-6 (Fig. 3E, Table 3 entry 11), 1174190-70-5 (Fig. 3F, Table 3 entry 12), etc shows even better results compared to CT compounds included in this study. The case studies demonstrate how the above-mentioned computational protocol executed by using AIDRUGAPP helped to deduce an important outcome that is useful for drug designing against SARS-COVID-19 diseases.

CONCLUSION

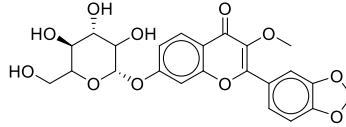
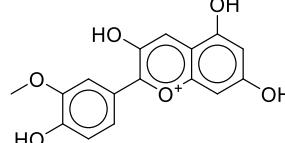
We developed and presented a simple, fast, and cost-effective computational protocol for drug designing implemented through a user-friendly web-app. We also applied and presented the two case studies for virtual screening of inhibitor molecules for SARS-COVID-19 diseases using the web-app. We believe that AIDrugApp will benefit the entire community of biologists, chemists, and even non-experts for their drug development endeavors to facilitate faster drug discovery.

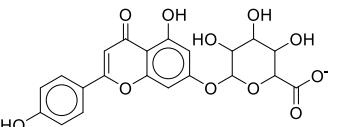
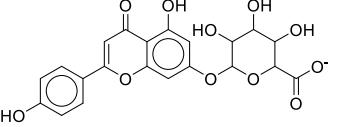
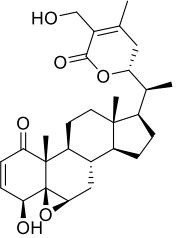
REFERENCES

1. Kumar, P.; Bhardwaj, T.; Kumar, A.; Gehi, B. R.; Kapuganti, S. K.; Garg, N.; Nath, G.; Giri, R., Reprofiling of approved drugs against SARS-CoV-2 main protease: an in-silico study. *Journal of Biomolecular Structure and Dynamics* **2020**, 1-15.
2. Chatterjee, B.; Thakur, S. S., ACE2 as a potential therapeutic target for pandemic COVID-19. *RSC Advances* **2020**, 10 (65), 39808-39813.
3. Rathnayake, A. D.; Zheng, J.; Kim, Y.; Perera, K. D.; Mackin, S.; Meyerholz, D. K.; Kashipathy, M. M.; Battaile, K. P.; Lovell, S.; Perlman, S., 3C-like protease inhibitors block coronavirus replication in vitro and improve survival in MERS-CoV-infected mice. *Science translational medicine* **2020**, 12 (557).
4. Karade, D.; Vijayasarathi, D.; Kadoo, N.; Vyas, R.; Ingle, P.; Karthikeyan, M., Design of Novel Drug-like Molecules using Informatics Rich Secondary Metabolites Analysis of Indian Medicinal and Aromatic Plants. *Combinatorial Chemistry & High Throughput Screening* **2020**.
5. Mohanraj K, K. B., Vivek-Ananth RP, Chand RPB, Aparna SR, Mangalapandi P, Samal A., IMPPAT: A curated database of Indian Medicinal Plants, Phytochemistry And Therapeutics. *Sci Rep.* **2018 Mar** **12**, 8 (1), 4329.
6. Wei, C.-H.; Kao, H.-Y.; Lu, Z., PubTator: a web-based text mining tool for assisting biocuration. *Nucleic acids research* **2013**, 41 (W1), W518-W522.
7. Release, S., 1: Maestro 019-3 SR. *Glide, LigPrep, Protein Preparation Wizard, Prime, Desmond Molecular Dynamics System, Maestro-Desmond Interoperability Tools, Schrödinger, LLC, New York, NY* **2020**.
8. Daina, A.; Michelin, O.; Zoete, V., SwissADME: a free web tool to evaluate pharmacokinetics, drug-likeness and medicinal chemistry friendliness of small molecules. *Sci Rep* 7: 42717. doi. org/10.1038/srep4 2017, 2717.
9. Daina, A.; Zoete, V., A boiled-egg to predict gastrointestinal absorption and brain penetration of small molecules. *ChemMedChem* **2016**, 11 (11), 1117.

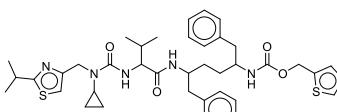
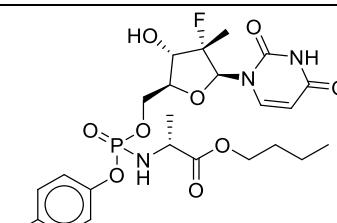
Table 1: List of inhibitor molecules (selected, n= 10) against SARS-COVID-19 diseases screened from Indian medicinal plants small molecules and CAS COVID-19 antiviral candidate compounds towards SARS-COV-2 RP, ACE (receptor for SARS-COV-2 in human) and Clinical trials for SARS-COVID-19 diseases.

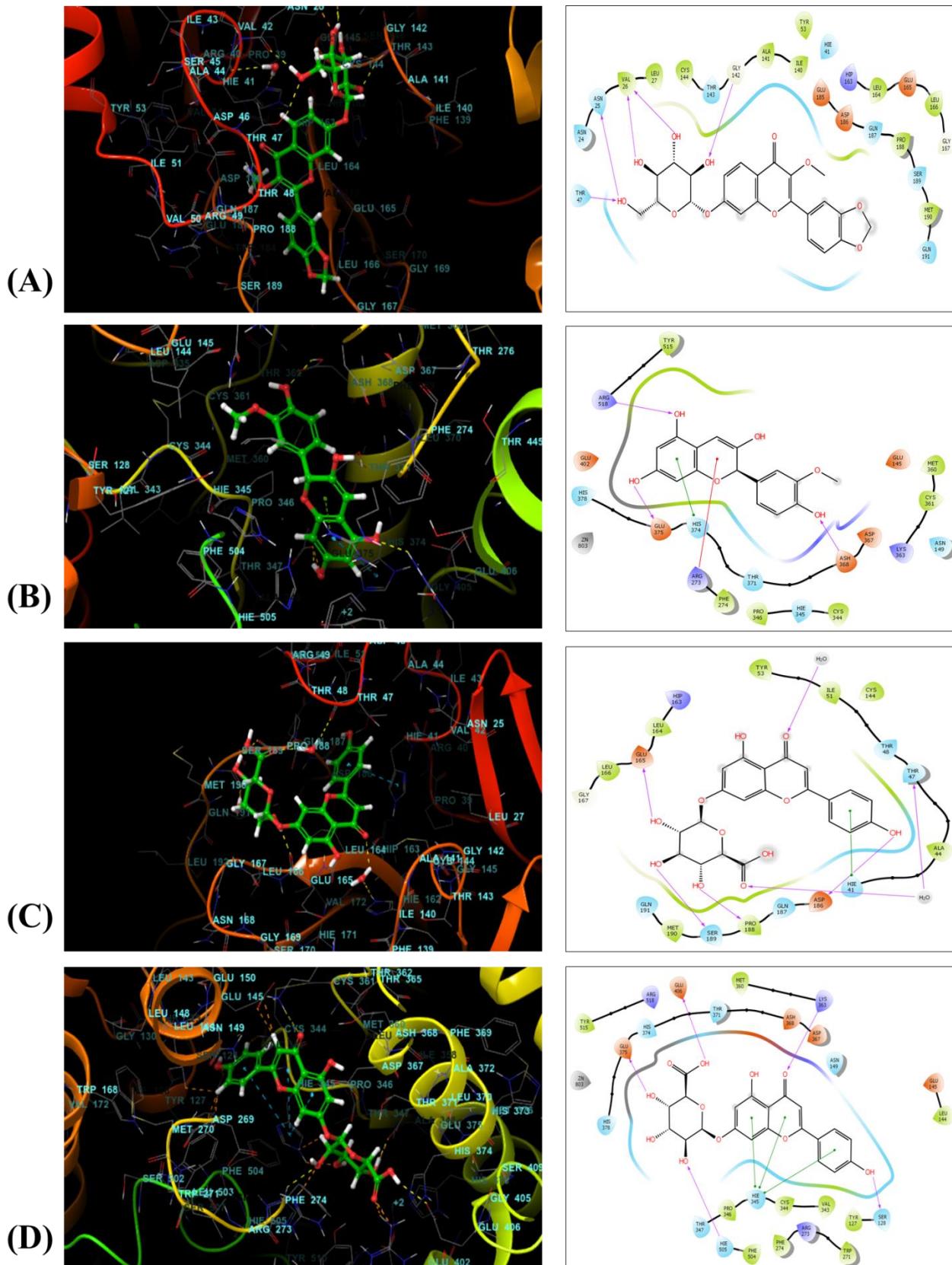
* Please refer to Figure 3 for molecular docking poses

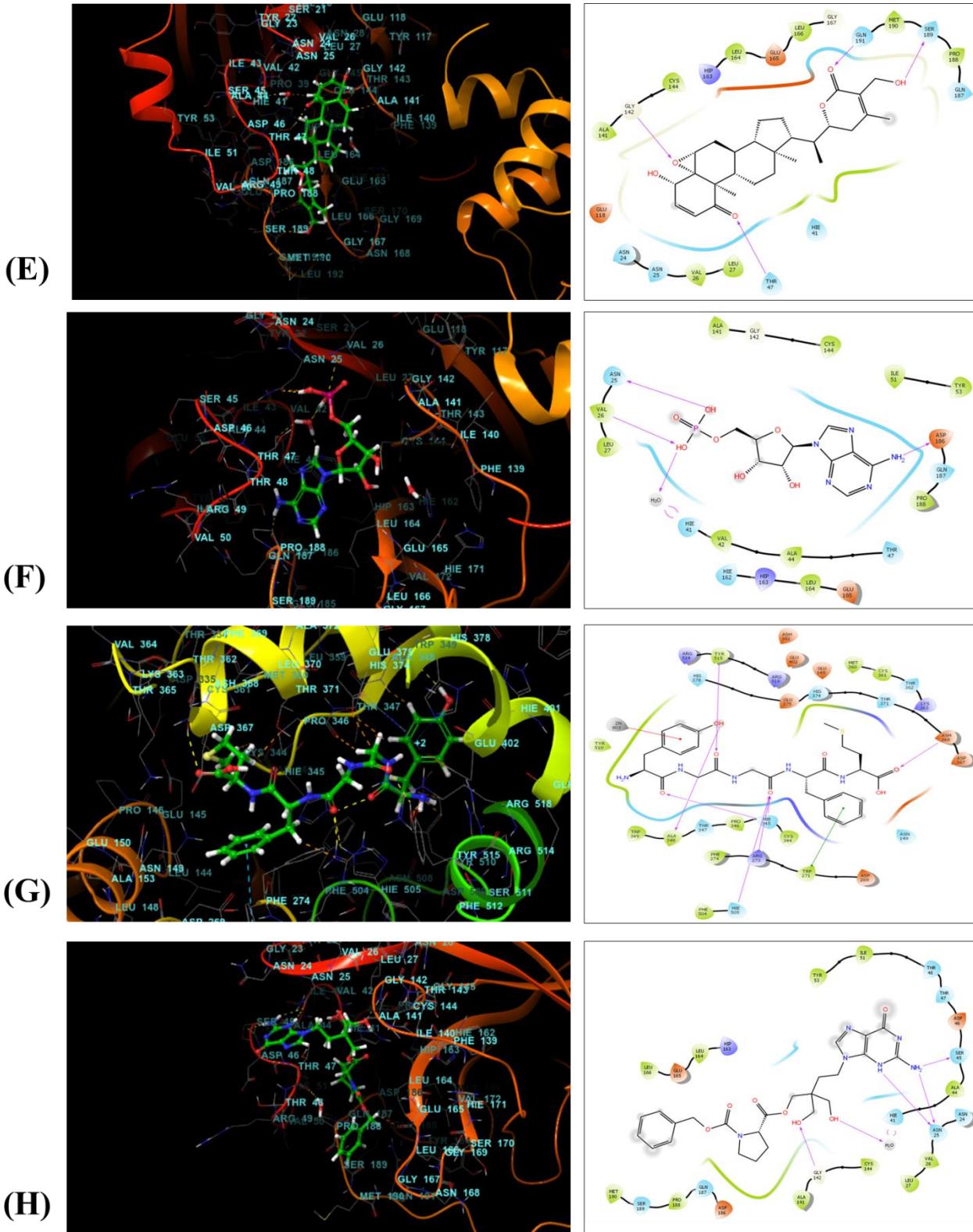
Sr. no.	DL model dataset	Receptor protein target	Molecule	Predicted IC-50 (microM) value	Glide docking score	Glide Energy (kcal/mol)	Glide emodel score	Interacting residues
Indian medicinal plants								
1	CT	1P9U	 Pongamoside D <i>(Hyoscyamus niger, PMID: 19401911)</i>	0.44	-7.947	-7.947	-80.49	THR47, ASN24, ASN25, VAL26, LEU27, CYS144, THR143, GLY142, ALA141, ILE140, GLU185, ASP186, GLN187, PRO188, SER189, MET190, GLN191 *(Fig. 3A)
2	ACE	1R4L	 Peonidin <i>(Brassica nigra, PMID: 1675200)</i>	0.47	-6.502	-6.502	-66.922	TYR515, ARG518, GLU402, HIS378, GLU375, HIS374, THR371, ASH368, ASP367, GLU145, MET360, CYS361, LYS363, CYS344, HIE345, PRO346, PHE274, ARG273 *(Fig. 3B)

			12907406)					
3	CT	1P9U	 apigenin 7-O- β -D-glucuronide <i>(Ocimum tenuiflorum or Ocimum sanctum, PMID: 30870993)</i>	0.32	-8.52	-8.52	-81.227	HIP163, LEU164, GLU165, LEU166, GLY167, GLN191, MET190, SER189, PRO188, GLN187, ASP186, HIE41, ALA44, THR47, THR48, ILE51, TYR53 *(Fig. 3C)
4	CT	1R4L	 apigenin 7-O- β -D-glucuronide <i>(Ocimum tenuiflorum or Ocimum sanctum, PMID: 30870993)</i>	0.32	-8.221	-8.221	-90.248	HIS378, GLU375, HIS374, THR371, ASH368, ASP367, ASN149, ZN803, TYR515, ARG518, GLU406, MET360, LYS363, THR347, PRO346, HIE345, CYS344, VAL343, TYR127, SER128, HIE505, PHE504, PHE274, ARG273, TRP271 *(Fig. 3D)
5	3CLpro	1P9U		-	-6.538	-6.538	-59.141	ALA141, GLY142, CYS144, HIP163, LEU164, GLU165, LEU166, GLY167, GLN191, MET190, SER189, PRO188, GLN187, HIE41, THR47, LEU27, VAL26, ASN25, ASN24, GLU118

			Withaferin A <i>(Withania Somnifera, PMID: 29661206)</i>					*(Fig. 3E)
CAS COVID-19 antiviral candidate compounds								
6	RP	1P9U	 CAS Id: 172645-42-0	0.96	-7.608	-7.608	-82.695	LEU166, GLU165, LEU164, HIP163, TYR53, ILE51, THR48, THR47, ASP46, SER45, ALA44, HIE41, ASN24, ASN25, VAL26, LEU27, CYS144, GLY142, ALA141, ASP186, GLN187, PRO188, SER189, MET190 *(Fig. 3H)
7	ACE	1R4L	 CAS Id: 170111-57-6	0.009	-9.585	-9.585	-132.92 2	LEU503, PHE504, HIE505, THR276, PHE274, ARG273, TRP271, ALA348, THR347, PRO346, HIE345, CYS344, ASN149, TYR510, LEU144, GLU145, LYS363, THR362, CYS361, MET360, ASP367, ASH368, LEU370, THR371, HIS374, GLU375, HIS378, ARG514, TYR515, ARG518 *(Fig. 3I)
8	CT	1P9U	 CAS Id: 134-46-3	0.11	-7.462	-7.462	-66.854	ASN25, VAL26, LEU27, ALA141, GLY142, HIE41, CYS144, THR47, GLU165, LEU164, HIP163, ASP186, GLN187, PRO188

									*(Fig. 3J)
9	CT	1R4L	 CAS Id: 1004318-43-7	0.10	-8.689	-8.689	-	135.67 4	HIS378, GLU375, HIS374, THR371, LEU370, ASH368, ASP367, THR445, GLU406, ASN149, ASH382, THR276, PHE274, ARG273, TRP271, ASP269, PHE504, HIE505, HIE345, PRO346, THR347, ALA348,
10	3CLpro	1P9U	 CAS Id: 1064684-54-3	-	-8.013	-8.013	-	-83.325	LEU164, GLU165, LEU166, GLY167, GLN191, MET190, SER189, PRO188, GLN187, ASP186, TYR53, ILE51, THR48, THR47, ALA44, HIE41





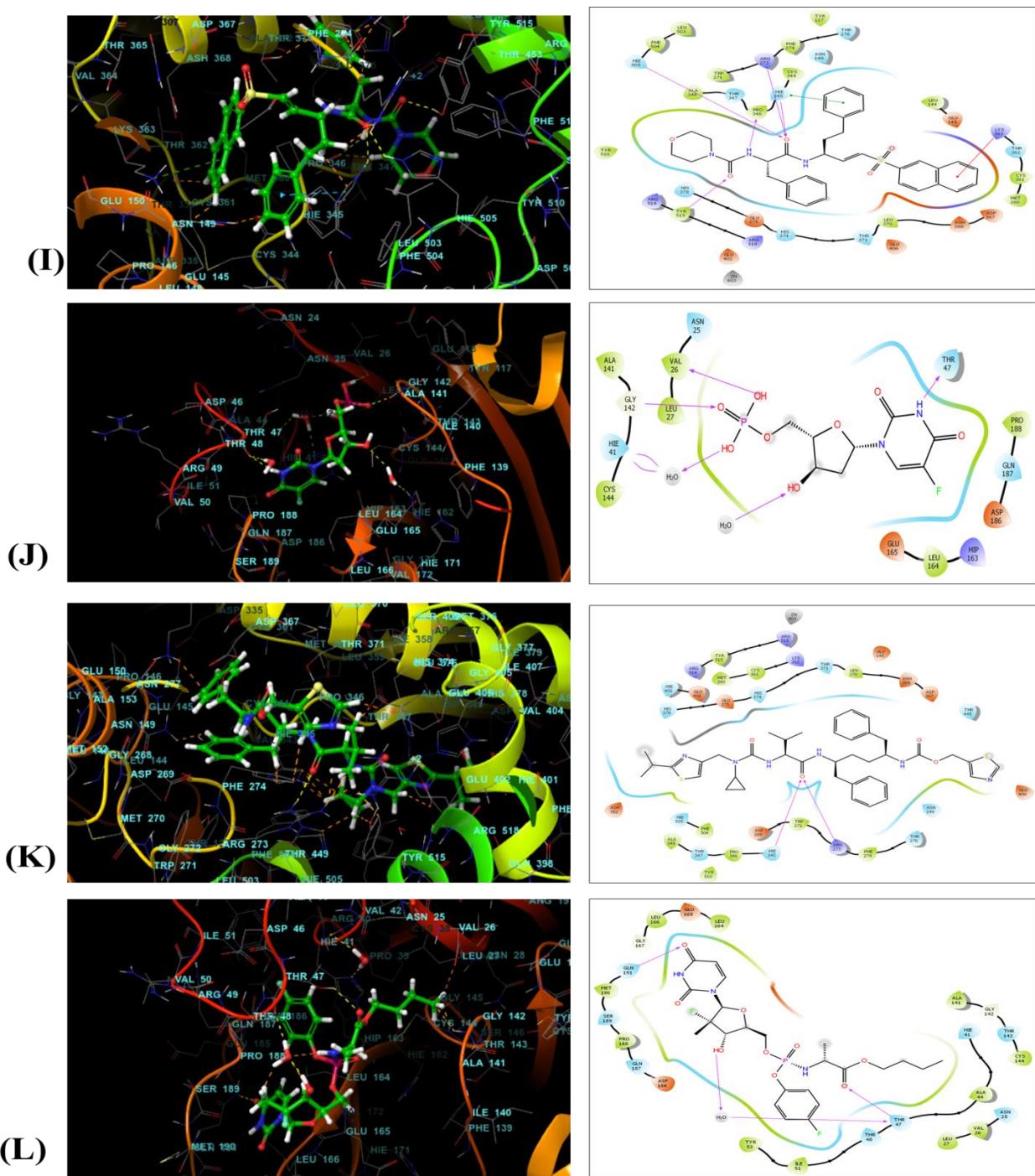
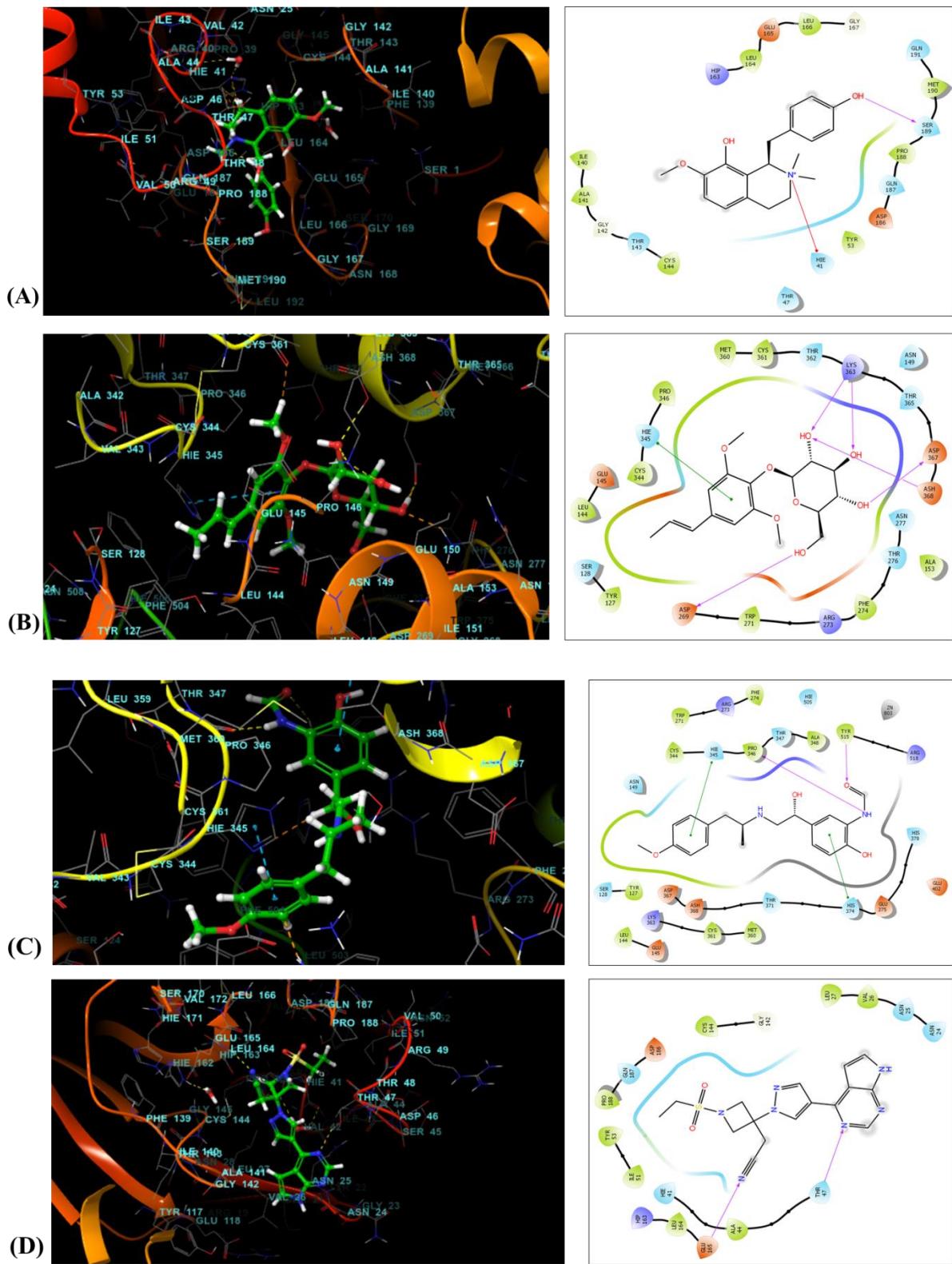


Figure 3. The best docking pose of top compounds against SARS-CoV-2 diseases screened by AIDRUGAPP from Indian medicinal plants small molecules (A-E), SARS COVID-19 clinical trial experimental compounds (F-G) and CAS COVID-19 antiviral candidate compounds (H-L) generated using Schrodinger.

* Please refer to Table 1 and 2 for more information



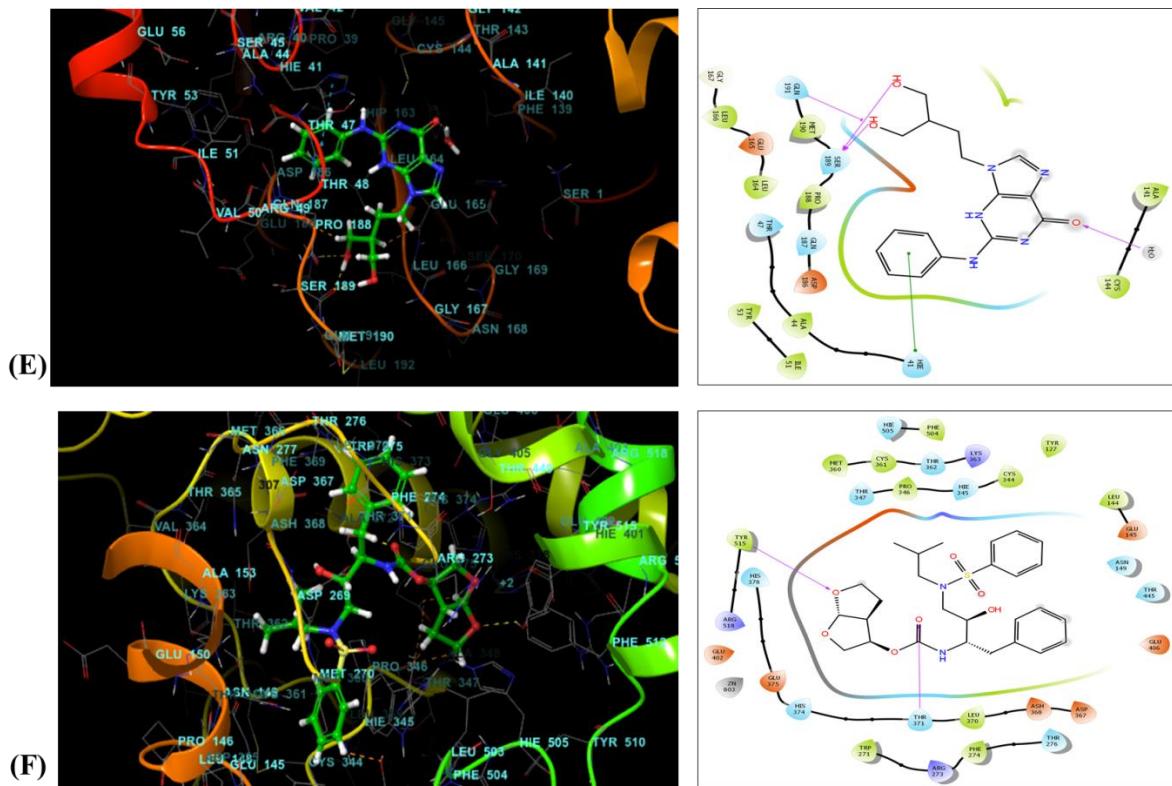
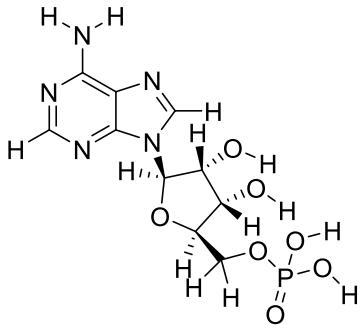
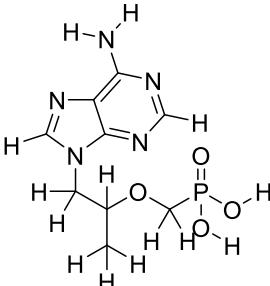
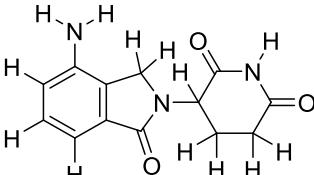
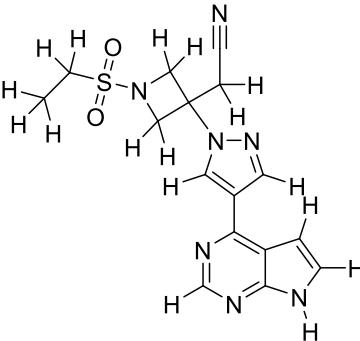
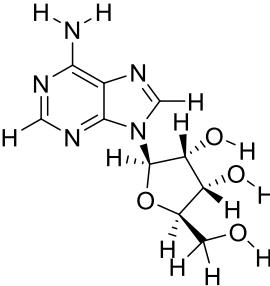
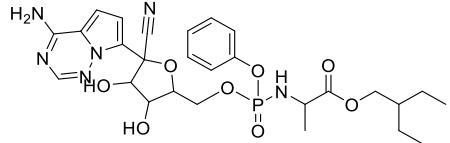
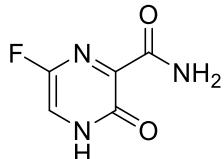


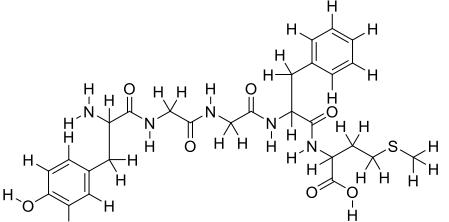
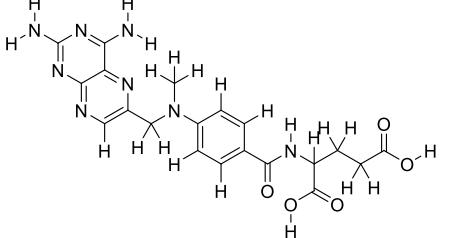
Figure 4. Docking pose of top compounds against SARS-CoV-2 main protease. The figure consists of two panels, (E) and (F), showing the binding site of the enzyme with various amino acid residues labeled. Panel (E) shows a green stick model of a compound docked into the active site, with residues like GLU 56, TYR 53, ILE 51, THR 47, ASP 95, THR 48, VAL 50, MET 90, SER 189, MET 190, LEU 192, GLU 10, PRO 108, ILE 140, PHE 139, CYS 144, ALA 141, GLU 145, THR 143, GLU 142, ILE 140, GLY 169, LEU 166, GLY 167, ASN 168, and SER 1. Panel (F) shows a similar view with different residues labeled, including MET 365, THR 276, ASN 277, GLU 369, ILE 368, ARG 273, TYR 416, HIE 401, ARG 518, PHE 519, GLU 150, ALA 153, YS 363, ASP 269, PRO 346, MET 361, HIE 345, LEU 503, PHE 504, TYR 510, and GLU 145. A yellow ribbon indicates the protein backbone. (* Please refer to Table 3 for more information)

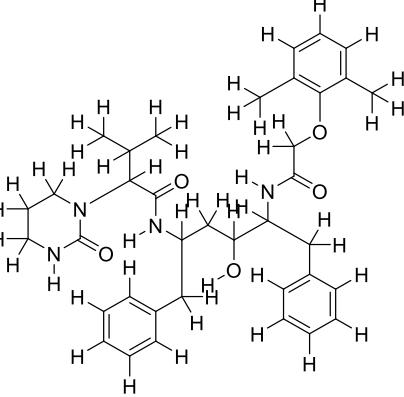
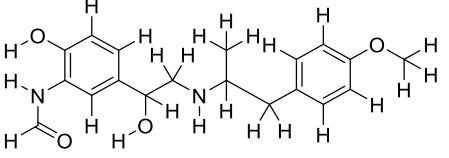
Table 2: List of selected drug candidate molecules (n=14) used against SARS-COV-2 clinical trial experiments (** Please refer to Figure 6 for molecular docking poses)

Sr. no.	Receptor protein target	CT Drug molecule	Experimental IC-50 (microM) value	Glide docking score	Glide Energy (kcal/mol)	Glide emodel score	Interacting residues
1	1P9U	 PubChem ID: 6083 (Adenosine monophosphate)	0.1	-8.052	-8.052	-74.324	ALA141, GLY142, CYS144, ILE51, TYR53, ASP186, GLN187, PRO188, ASN25, VAL26, LEU27, HIE41, VAL42, ALA44, THR47, HIE162, HIP163, LEU164, GLU165 *(Fig. 3F)
2	1P9U		0.38	-7.207	-7.207	-65.095	HIE41, ALA141, GLY142, THR143, CYS144, ASN25, VAL26, LEU27, THR47, ILE51, SER189, PRO188, GLN187, LEU164, GLU165

		PubChem ID: 464205 (Tenovovir)					
3	1P9U		0.1	-7.191	-7.191	-49.454	HIE41, ALA44, THR47, ASP186, GLN187, PRO188, SER189, GLN191
		PubChem ID: 216326 (Lenalidomide)					
4	1P9U		0.0008	-7.075	-7.075	-64.968	THR47, ALA44, HIE41, ILE51, TYR53, PRO188, GLN187, ASP186, CYS144, GLY142, LEU27, VAL26, ASN25, ASN24
		PubChem ID: 44205240 (Baricitinib)					

5	1P9U	 PubChem ID: 60961 (Adenosine)	0.001148	-7.009	-7.009	-53.374	THR47, HIE41, GLN191, MET190, SER189, PRO188, GLN187, ASP186, LEU164, GLU165, LEU166, GLY167
6	1P9U	 PubChem ID: 121304016 (Remdesivir)	0.987	-5.556	-5.556	-62.358	CYS144, THR143, GLY142, ALA141, GLN191, MET190, SER189, PRO188, GLN187, ASP186, THR47, THR48, ILE51, TYR53
7	1P9U	 PubChem ID: 492405 (Favipiravir)	0.044	-5.64	-5.64	-35.501	GLU165, LEU164, PRO188, GLN187, ASP186, ILE51, TYR53, HIE41, THR47

8	1R4L	 PubChem ID: 443363 (MET-enkephalin)	0.001	-9.695	-9.695	141.39 1	ARG514, TYR515, ARG518, HIS378, GLU375, HIS374, THR371, ASH368, ASP367, ZN803, TYR510, TRP349, ALA348, THR347, PRO346, HIE345, CYS344, ASN149, PHE274, ARG273, TRP271, ASP269, PHE504, HIE505 *(Fig. 3G)
9	1R4L	 PubChem ID: 126941 (Methotrexate)	2.00e-08	-8.216	-8.216	111.34 1	GLU145, CYS344, HIE345, PRO346, THR347, ALA348, TYR515, ARG518, PHE504, HIE505, PHE274, ARG273, TRP271, ASP269, HIS378, GLU375, HIS374, THR371, ASH368, ASP367, THR365, LYS363, CYS361

10	1R4L	 <p>PubChem ID: 92727 (Lopinavir)</p>	0.001	-8.189	-8.189	121.00 9	HIE505, PHE504, TYR515, ARG518, THR276, PHE274, ARG273, TRP271, ASP269, ASN149, TYR510, HIS378, GLU375, HIS374, THR371, LEU370, ASH368, ASP367
11	1R4L	 <p>PubChem ID: 3410 (Formoterol)</p>	0.0004	-7.816	-7.816	-82.382	ASN149, CYS344, HIE345, PRO346, THR347, ALA348, TYR515, ARG518, SER128, TYR127, ASP367, ASH368, THR371, HIS374, GLU375, HIS378

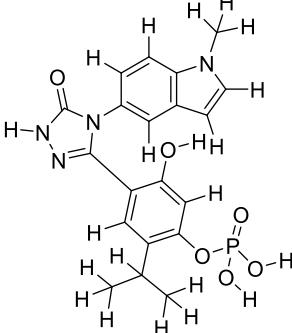
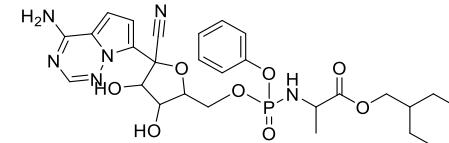
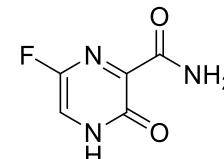
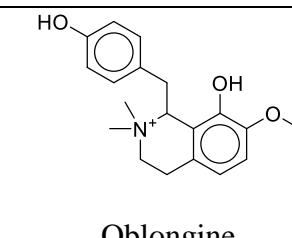
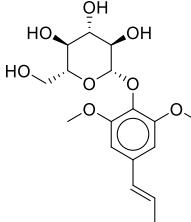
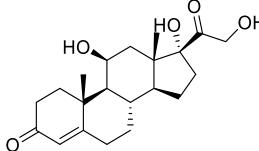
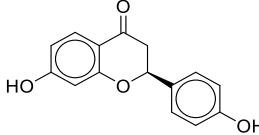
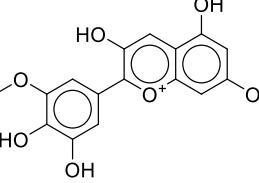
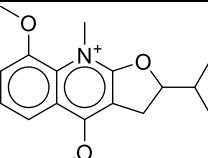
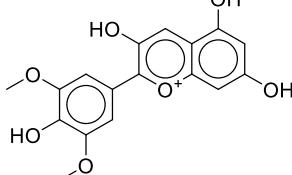
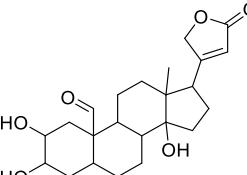
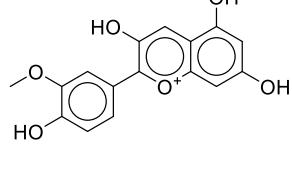
12	1R4L	 PubChem ID: 135565962 (Defibrotide sodium)	0.088	-7.524	-7.524	101.26 ₆	PHE274, ARG273, TRP271, ASP269, ASN149, ZN803, HIS378, GLU375, HIS374, THR371, ASH368, ASP367, THR347, PRO346, HIE345, CYS344, LYS363, THR362, CYS361, MET360, GLU145
13	1R4L	 PubChem ID: 121304016 (Remdesivir)	0.987	-7.488	-7.488	101.18 ₈	TYR127, ASN149, CYS344, HIE345, PRO346, THR347, ALA348, TYR510, PHE504, HIE505, MET360, CYS361, THR362, LYS363, ASP367, ASH368, THR371, HIS374, GLU375, HIS378, GLU402
14	1R4L	 PubChem ID: 492405 (Favipiravir)	0.044	-6.692	-6.692	-51.736	GLU402, TYR515, ALA348, THR347, PRO346, HIE345, PHE504, HIE505, TYR510

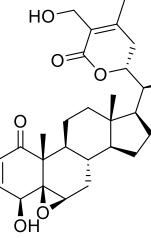
Table 3: List of selected top potential drug candidate molecules (n=20) against SARS-COVID-19 diseases screened with ADME study from Indian medicinal plants small molecules and CAS COVID-19 antiviral candidate compounds towards SARS-COV-2 RP, ACE (receptor for SARS-COV-2 in human) and Clinical trials for SARS-COVID-19 diseases. (* For more information please refer to Figure 3 for molecular docking poses)

BBB permeant: permeability to Blood-brain barrier, Pgp substrate: a substrate for permeability glycoprotein, GI absorption: passively absorbed by the gastrointestinal tract

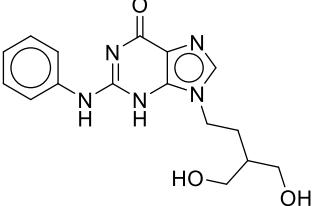
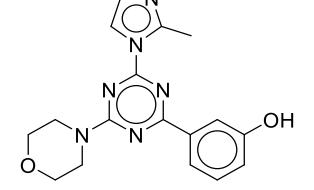
Sr. no.	Receptor protein/ Dataset	Molecule	Source	Predict ed IC- 50 (micro M)	Glide docki ng score	Molec ular weigh t	TPSA	logP	*BBB perm eant	*Pgp subst rate	*GI absorpti on	Synt hetic Acce ssibil ity
Indian medicinal plants												
1	CT (1P9U)	 Oblongine	IMP (Tinospora cordifolia, PMID: 26627195)	0.20	-7.556 *(Fig. 4A)	314.4	49.69	2.87	Yes	Yes	High	3.18

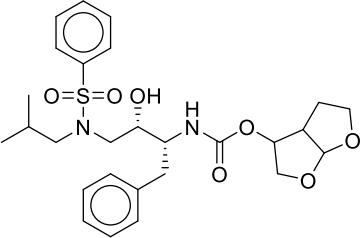
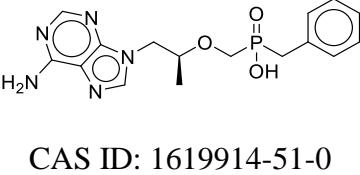
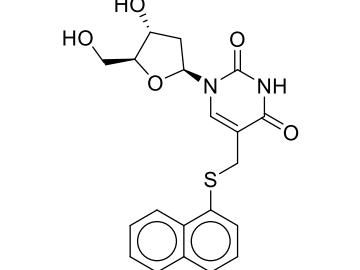
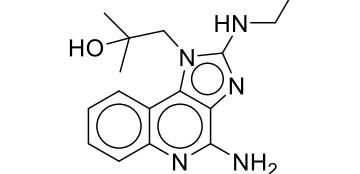
2	ACE(1R4 L)	 <p>Acantrifoside E</p>	IMP (<i>Ferula assa-foetida</i> , PMID: 23701832)	0.92	-7.188 *(Fig. 4B)	356.3 7	117.8 4	- 0.24	No	Yes	High	4.71
3	CT (1R4L)	 <p>Cortisol</p>	IMP (<i>Aconitum napellus</i> , PMID: 29288825)	0.29	-6.726 6	362.4 6	94.83 4	1.01	No	Yes	High	5.16
4	CT (1P9U)	 <p>Liquiritigenin</p>	IMP (<i>Aconitum napellus</i> , PMID: 25889555)	0.04	-6.927 5	256.2 5	66.76	2.65	Yes	Yes	High	2.95
5	ACE(1R4 L)	 <p>Petunidin</p>	IMP (<i>Crocus sativus</i> , PMID: 29484754)	0.67	-6.875 7	317.2 2	123.5	2.94	No	Yes	High	3.23

6	CT (1R4L)	 Lunasin	IMP (<i>Solanum nigrum</i> , PMID: 20083341)	0.39	-6.657	288.3 6	31.57	4.6	Yes	Yes	High	3.51
7	ACE(1R4 L)	 Malvidin	IMP (<i>Brassica nigra</i> , PMID: 12907406)	0.31	-6.634	331.3 2	112.5	3.2	No	Yes	High	3.33
8	CT (1P9U)	 Calotropagenin	IMP (<i>Calotropis gigantea</i> , PMID: 20460804)	0.45	-6.634	404.5 6	104.0	1.78	No	Yes	High	5.49
9	ACE(1R4 L)	 Peonidin	IMP (<i>Brassica nigra</i> , PMID: 12907406)	0.47	-6.502	301.2 7	103.2 9	3.20 9	No	Yes	High	3.18

10	3CLpro (1P9U)	 Withaferin A	IMP (<i>Withania Somnifera</i> , PMID: 29661206)	-	-6.538	470.6	96.36	3.19	No	Yes	High	6.83
----	------------------	---	--	---	--------	-------	-------	------	----	-----	------	------

CAS COVID-19 antiviral candidate compounds

11	RP(1P9U)	 CAS ID: 127047-63-6	CAS COVID-19 antiviral candidate compounds	0.22	-7.332 *(Fig. 4E)	329.3 5	116.0 6	1.13	No	Yes	High	2.8
12	RP(1P9U)	 CAS ID: 1174190-70-5	CAS COVID-19 antiviral candidate compounds	0.85	-7.116	338.3 6	89.19 4	0.52	No	Yes	High	3

13	CT (1R4L)	 CAS ID: 799269-48-0	CAS COVID-19 antiviral candidate compounds	0.07	-6.704 *(Fig. 4F)	397.3 6	110.4 7	3.11	No	Yes	High	3.6
14	3CLpro (1P9U)	 CAS ID: 1619914-51-0	CAS COVID-19 antiviral candidate compounds	-	-6.734	361.3 4	125.9 6	0.49	No	Yes	High	
15	3CLpro (1P9U)	 CAS ID: 828921-87-5	CAS COVID-19 antiviral candidate compounds	-	-6.979	400.4 5	129.8 5	1.51 3	No	Yes	High	4.46
16	RP(1P9U)	 CAS ID: 879000-78-9	CAS COVID-19 antiviral candidate compounds	0.94	-6.964	299.3 7	88.99	2.33	No	Yes	High	2.81

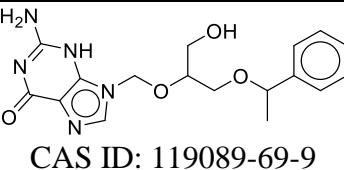
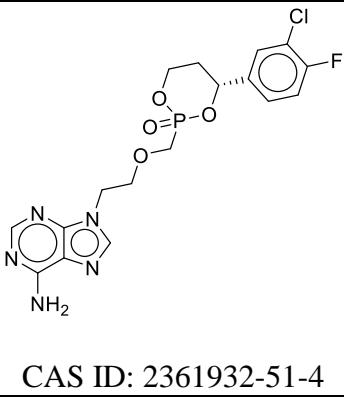
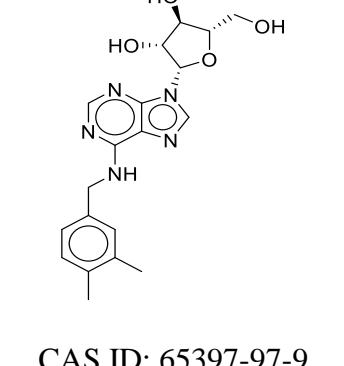
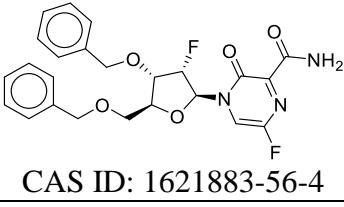
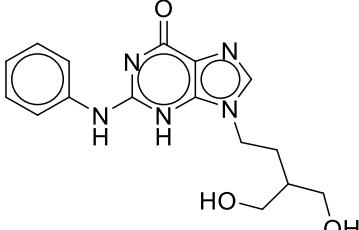
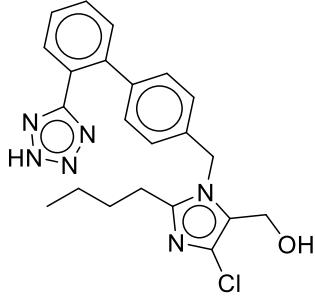
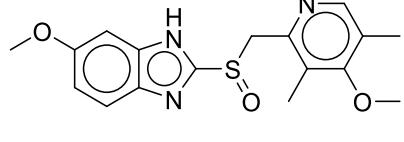
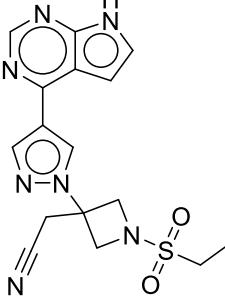
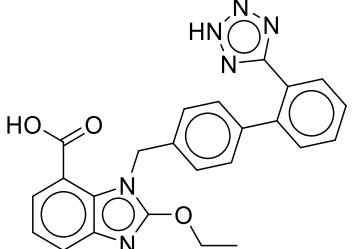
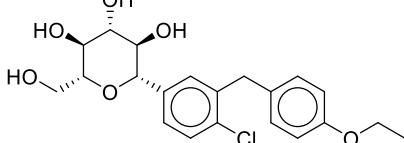
17	RP(1P9U)		CAS COVID-19 antiviral candidate compounds CAS ID: 119089-69-9	0.85	-6.784	359.3 8	128.2 8	1.11	No	Yes	High	3.89
18	3CLpro (1P9U)		CAS COVID-19 antiviral candidate compounds CAS ID: 2361932-51-4	-	-6.977	441.7 8	124.1 9	1.61	No	Yes	High	4
19	RP(1P9U)		CAS COVID-19 antiviral candidate compounds CAS ID: 65397-97-9	0.34	-6.769	385.4 2	125.5 5	0.42	No	Yes	High	4.41
20	RP(1P9U)		CAS COVID-19 antiviral candidate compounds CAS ID: 1621883-56-4	0.28	-6.653	471.4 5	105.6 7	1.95	No	Yes	High	5.03

Table 4: List of top best drug candidate molecules (n=6) used against SARS-CoV-2 clinical trial experiments with ADME properties predictions. (* For more information please refer to Figure 3 for molecular docking poses)

BBB permeant: permeability to Blood-brain barrier, Pgp substrate: substrate for permeability glycoprotein, GI absorption: passively absorbed by the gastrointestinal tract

Sr . no .	Recept or protein	Molecule	Source	Experi mental IC-50 (micro M)	Glide dockin g score	Molec ular weigh t	TPSA	logP	*BBB perm eant	*Pgp subst rate	*GI absor ption	Synt hetic Acce ssibil ity
1	1R4L	 PubChem CID: 3410 (Formoterol)	PubChem Compounds used in SARS-CoV-2 clinical trials	0.0004	-7.816 *(Fig. 4D)	344.4	116.0 6	2.40	No	Yes	High	3.08

2	1R4L	 PubChem CID: 3961 (Losartan)	PubChem Compounds used in SARS-CoV-2 clinical trials	0.0003 3	-7.496	422.9 1	92.51	5.42	No	Yes	High	3.45
3	1R4L	 PubChem CID: 4594 (Omeprazole)	PubChem Compounds used in SARS-CoV-2 clinical trials	0.0955	-7.352	345.4 2	96.31	1.32	No	Yes	High	3.58
4	1P9U	 PubChem CID: 44205240 (Baricitinib)	PubChem Compounds used in SARS-CoV-2 clinical trials	0.0008	-7.075 *(Fig. 4C)	371.4 2	128.9 4	-1.36	No	Yes	High	3.07

5	1P9U, 1R4L	 <p>PubChem CID: 2541 (Candesartan)</p>	PubChem Compounds used in SARS-CoV-2 clinical trials	0.0002	-6.82, -7.454	440.4 5	118.8 1	5.28	No	Yes	High	3.33
6	1P9U, 1R4L	 <p>PubChem CID: 9887712 (Dapagliflozin)</p>	PubChem Compounds used in SARS-CoV-2 clinical trials	0.0004 9	-6.5, -7.43	408.8 7	99.38	2.45	No	Yes	High	4.52

Appendix 1: List of Indian medicinal plants (n= 44) with their common names and botanical families

Sr No	Botanical plant_name	Common name	Botanical family
1	<i>Abrus precatorius</i>	coral pea, crab s eye, indian liquorice, jequerity seed, jumbie beans, lucky or paternoster bean, rati, rosary pea	Fabaceae
2	<i>Aconitum ferox</i>	bachhnag, bachnak, bis, bish, mahoar, mitha-zahar, mithazahar, singya, singya-bis, singyabis, teliya-bis	Ranunculaceae
3	<i>Aconitum napellus</i>	bachnag, mithavis, mithazahar	Ranunculaceae
4	<i>Allium sativum</i>	garlic, poor-mans-treacle	Amaryllidaceae
5	<i>Apium graveolens</i>	celery, marsh parsley, smallage, wild celery	Apiaceae
6	<i>Bacopa monnieri</i>	water hyssop	Plantaginaceae
7	<i>Brassica nigra</i>	black mustard, black or brown mustard	Brassicaceae
8	<i>Caesalpinia bonduc</i>	bonduc nut, nicker bean	Caesalpiniaceae
9	<i>Calotropis gigantea</i>	wara, yercum	Apocynaceae
10	<i>Capsicum annuum</i>	paprika	Solanaceae
11	<i>Coccinia grandis</i>	bhimb, bimb, gol, golan, golenda, kaduri, kandaroi, kanduri, kanduri-kebel, kanduri-ki-bel;, kanduriki-bel, kanturi, kunderi, kundru, shiv lingi, teedor, tidori	Cucurbitaceae
12	<i>Crocus sativus</i>	saffron, saffron cress	Iridaceae
13	<i>Croton tiglium</i>	croton oil	Euphorbiaceae
14	<i>Cymbopogon khasianus</i>	Lemon grass	Poaceae
15	<i>Cymbopogon martini</i>	palmarosa, Indian geranium, gingergrass and rosha or rosha grass.	Poaceae
16	<i>Cymbopogon winterianus</i>	Java citronella	Poaceae
17	<i>Datura stramonium</i>	apple-of-peru, devil s-apple, jamestown weed, jimson or jamestown weed, jimsonweed, mad apple, stinkweed, stramonium, thorn weed, thorn-apple	Solanaceae
18	<i>Desmodium gangeticum</i>	chirpat, chuppa, salpalnu, salpan, salpani, salun, salvian, salwan, sarivan	Fabaceae
19	<i>Ferula assa-foetida</i>	himg, hing, hingra	Apiaceae

20	<i>Ficus religiosa</i>	bo-tree, peepul, pipal, pipul	Moraceae
21	<i>Hyoscyamus niger</i>	black henbane, devil s-eye, henbane, hog bean, jupiter s bean, poison tobacco, stinking nightshade	Solanaceae
22	<i>Justicia adhatoda</i>	adhatoda	Acanthaceae
23	<i>Mallotus philippensis</i>	kamala	Euphorbiaceae
24	<i>Mentha arvensis</i>	field mint, wild mint, or corn mint	Lamiaceae
25	<i>Mentha piperita</i>	Peppermint	Lamiaceae
26	<i>Monarda citriodora</i>	lemon beebalm, lemon mint and purple horsemint.	Lamiaceae
27	<i>Ocimum tenuiflorum or Ocimum sanctum</i>	Tulsi	Lamiaceae
28	<i>Papaver somniferum</i>	gear, maw seed, opium poppy, scag, smack	Papaveraceae
29	<i>Phyllanthus emblica</i>	amla	Phyllanthaceae
30	<i>Pimpinella anisum</i>	anise, aniseed, pastis, raki, sweet cumin	Apiaceae
31	<i>Piper cubeba</i>	cubeb, java pepper	Piperaceae
32	<i>Ruta graveolens</i>	common rue, countryman s-treacle, garden rue, german rue, herb-of-grace, rue	Rutaceae
33	<i>Santalum album</i>	indian sandalwood	Santalaceae
34	<i>Semecarpus anacardium</i>	marking nut	Anacardiaceae
35	<i>Solanum nigrum</i>	black nightshade	Solanaceae
36	<i>Solanum virginianum</i>	adkuntali, bhatkatai, bhatkatya, bhuiakhanderi, bhumiringani, bhur hingani, bhuringni, bhutkatya, choto-baigan, dhaturi, dorlika-phal, gulari, jangli-baigan, katai, kataikhuadda, kateli, kattay, kutia, raingani, remgani, rengni, ringni, satyanasi	Solanaceae
37	<i>Swertia chirayita</i>	charaita, charayatah, chiraitu, chirata, chirayata, cirayata, kiryat-charayatah, nepalinim	Gentianaceae
38	<i>Tagetes minuta</i>	muster John Henry, southern marigold, stinking roger, wild marigold, or black mint	Asteraceae

39	<i>Terminalia bellirica</i>	bahera or beleric or bastard myrobalan	Combretaceae
40	<i>Tinospora cordifolia</i>	adharvela, amrta, gilai, giloe, giloy, gul-bel, gulanca, gulancha, gulbel, gulj-gloe, guluncha, gurach, gurch, gurcha, gurja, neem gilol, neem-giloj, neem-gilol, nim giloy, ushwa	Menispermaceae
41	<i>Valeriana jatamansi</i>	garden valerian	Caprifoliaceae
42	<i>Vetiveria zizanioides</i>	cucus, khuskhus, sandalwood fan, sevendra (grass), vetiver	Poaceae
43	<i>Withania Somnifera</i>	Ashwagandha	Solanaceae
44	<i>Zingiber officinale</i>	ginger	Zingiberaceae

Appendix 2: List of small molecules (n= 1156) related to Indian medicinal plants text mined from PubMed literature with their SMILES

Sr. no.	Plant source	PMID	Molecule	SMILES
1	<i>Abrus precatorius</i>	30105196	7,12-Dimethylbenz[a]anthracene	c12c(ccc3c1cccc3)c(c1c(cccc1)c2C)C
2	<i>Abrus precatorius</i>	7537681	abruquinone A	CO C1=C(OC)C=C2OC C(CC2=C1)C1=CC(=O)C(OC)=C(OC)C1=O
3	<i>Abrus precatorius</i>	26283803	bhilawanol	CCCCCC=CCCCCCC CC1=C(C(=CC=C1)O)O
4	<i>Abrus precatorius</i>	22262933	glycyrrhizin	CC1(C)[C@H](CC[C@H]2C[C@H]1CC[C@H]1C[C@H]2C(=O)C=C2[C@H]3C[C@H]2C(=O)C[C@H]3(C)CC[C@H]2C(=O)O)O[C@H]1O[C@H](C[C@H](O)[C@H](O)[C@H]1O[C@H]2O[C@H](C[C@H](O)[C@H](O)[C@H]2O)C(O)=O)C(O)=O
5	<i>Abrus precatorius</i>	12168762	sophoradiol	CC1(C)C[C@H](O)[C@H]2C(C)CC[C@H]3(C)C(=CC[C@H]4C[C@H]5C(C)CC[C@H](O)C(C)C[C@H]5CC[C@H]3C4C)[C@H]2C1

6	<i>Abrus precatorius</i>	26283803	strychnine	O=C1C[C@@@H]2OCC=C3CN4CC[C@@@]56[C@@@H]4C[C@@@H]3[C@@@H]2[C@@@H]5N1C1=CC=CC=C61
7	<i>Abrus precatorius</i>	25010655	Abrin	CN[C@@H](Cc1c[nH]c2ccccc12)C(O)=O
8	<i>Aconitum ferox</i>	24023444	aconitine	CCN1C[C@@@]2(COC)[C@@H]3[C@@H](OC)[C@@H]4C1[C@@@]3([C@@H]1C[C@@@]3(O)[C@@H](OC(=O)C5=CC=CC=C5)[C@@H]1[C@]4(OC(C)=O)[C@@H](O)[C@@H]3OC)[C@H](C[C@H]2O)OC
9	<i>Aconitum ferox</i>	5037482	indaconitine	CCN1C[C@@]2(COC)[C@@H]3[C@@H](OC)[C@@H]4[C@@H]1[C@]3([C@@H]1C[C@]3(O)[C@@H](OC(=O)C5=CC=CC=C5)[C@@H]1[C@]4(C[C@@H]3OC)OC(C)=O)[C@H](C[C@H]2O)OC
10	<i>Aconitum ferox</i>	24023444	pseudoaconitine	CCN1C[C@@@]2(COC)[C@@H]3[C@@H](OC)[C@@H]4[C@@H]1[C@@]3([C@@H]1C[C@@]3(O)[C@@H](OC(=O)C5=CC=C(OC)C(OC)=C5)[C@@H]1[C@@@]4(C[C@@H]3OC)OC(C)=O)[C@H](C[C@H]2O)OC
11	<i>Aconitum napellus</i>	16462027	12-O-tetradecanoylphorbol 13-acetate	CCCCCCCCCC(=O)OC1C(C2(C(C=C(C3(C2=C(C3=O)C)O)CO)C4C1(C4(C)C)OC(=O)C)O)C
12	<i>Aconitum napellus</i>	20846913	1-octanol	CCCCCCCO
13	<i>Aconitum napellus</i>	11076560	3-hydroxy-2-methyl-4H-pyran-4-one	CC1=C(O)C(=O)C=CO1
14	<i>Aconitum napellus</i>	26895385	acetaminophen	CC(=O)NC1=CC=C(O)C=C1

15	<i>Aconitum napellus</i>	21582830	aconifine	<chem>CCN1C[C@@@]2(COC)[C@H]3[C@@@H](OC)[C@H]4C1[C@]3([C@H](C[C@H]2O)OC)[C@]1(O)C[C@@]2(O)[C@H](OC(=O)C3=CC=C C=C3)[C@@@H]1[C@]4(OC(C)=O)[C@@@H](O)[C@@@H]2OC</chem>
16	<i>Aconitum napellus</i>	29404034	aconine	<chem>CCN1C[C@@@]2(COC)[C@H]3[C@@@H](OC)[C@H]4[C@@@H]1[C@@@]3([C@@@H]1C[C@@@]3(O)[C@H](O)[C@@@H]1[C@]4(O)[C@@@H](O)[C@@@H]3OC)[C@H](C[C@H]2O)OC</chem>
17	<i>Aconitum napellus</i>	6084153	actinomycin D	<chem>CC(C)C1NC(=O)C(NC(=O)C2=C3N=C4C(OC3=C(C)C=C2)=C(C)C(=O)C(N)=C4C(=O)NC2C(C)OC(=O)C(C(C)C)N(C)C(=O)CN(C)C(=O)C3CCCC3C(=O)C(NC2=O)C(C)C(C)OC(=O)C(C(C)C)N(C)C(=O)CN(C)C(=O)C2CCCN2C1=O</chem>
18	<i>Aconitum napellus</i>	50847	ajmaline	<chem>CC[C@H]1[C@@@H]2C[C@H]3[C@@@H]4N(C)C5=CC=CC=C5[C@]44C[C@@H](C2[C@H]4O)N3[C@@@H]1O</chem>
19	<i>Aconitum napellus</i>	24469098	aloe-emodin	<chem>OCC1=CC(O)=C2C(=O)C3=C(O)C=CC=C3C(=O)C2=C1</chem>
20	<i>Aconitum napellus</i>	28886613	amiodarone	<chem>CCCCCC1=C(C(=O)C2=CC(I)=C(OCCN(CC)CC)C(I)=C2)C2=CC=CC=C2O1</chem>
21	<i>Aconitum napellus</i>	25594733	anisodamine	<chem>CN1[C@H]2C[C@H](O)[C@@H]1C[C@H](C2)OC(=O)[C@H](CO)C1=CC=CC=C1</chem>
22	<i>Aconitum napellus</i>	7765001	anthocyanin	<chem>C1=CC=C(C=C1)C1=[O+]C2=CC=CC=C2=C1</chem>
23	<i>Aconitum napellus</i>	29200734	ascorbate	<chem>OC[C@H](O)[C@H]1OC(=O)C1=O</chem>

24	<i>Aconitum napellus</i>	28330176	atisine	C[C@@@]12CCC[C@]3(C4OCCN4C1)[C@@H]2CC[C@@]12CC[C@H](C[C@@H]31)C(=C)[C@H]2O
25	<i>Aconitum napellus</i>	24216273	atropine	CN1[C@H]2CC[C@@H]1C[C@@H](C2)OC(=O)C(CO)C1=CC=CC=C1
26	<i>Aconitum napellus</i>	23629873	baicalein	OC1=CC2=C(C(O)=C1O)C(=O)C=C(O2)C1=CC=CC=C1
27	<i>Aconitum napellus</i>	24469098	baicalin	O[C@@H]1[C@@H](O)[C@H](OC2=C(O)C(=O)=C3C(=O)C=C(OC3=C2)C2=CC=CC=C2)O[C@@H]([C@H]1O)C(=O)=O
28	<i>Aconitum napellus</i>	30050591	Benazepril	CCOC(=O)[C@H](CCC1=CC=CC=C1)N[C@H]1CCC2=CC=CC=C2N(CC(O)=O)C1=O
29	<i>Aconitum napellus</i>	30404196	bergapten	COC1=C2C=COC2=CC2=C1C=CC(=O)O2
30	<i>Aconitum napellus</i>	12686443	beta-carotene	C\C(\C=C\ C=C(\C)\C=C\ C1=C(C)CCCC1(C)C)=C/C=C/C=C(\C)/C=C/C=C\ C1=C(C)CCCC1(C)C
31	<i>Aconitum napellus</i>	24791539	beta-sitosterol	CC[C@H](CC[C@@H](C)[C@H]1CC[C@H]2[C@@H]3CC=C4C[C@@H](O)CC[C@]4(C)[C@H]3CC[C@]12C)C(C)C
32	<i>Aconitum napellus</i>	9374271	bicuculline	CN1CCC2=CC3=C(OC(=O)C=C2[C@H]1[C@@H]1OC(=O)C2=C1C=CC1=C2OCO1
33	<i>Aconitum napellus</i>	24216273	brucine	CO[C@H]1CC2=C(C=C1O)C[C@@@]13CCN4CC5=CCO[C@H]6CC(=O)N2[C@H]1[C@H]6[C@H]5C[C@@H]34
34	<i>Aconitum napellus</i>	28925115	caffeic acid	OC(=O)\C=C\ C1=CC=C(O)C(O)=C1
35	<i>Aconitum napellus</i>	28981338	caffeine	CN1C=NC2=C1C(=O)N(C)C(=O)N2C

36	<i>Aconitum napellus</i>	30404196	capnoidine	CN1CCC2=CC3=C(OC O3)C=C2[C@@H]1[C @@H]1OC(=O)C2=C1 C=CC1=C2OCO1
37	<i>Aconitum napellus</i>	26320055	capsaicin	CO[C@H]1CC(CNC(=O)C CCC\ C=C\ C(C)C)=CC=C1O
38	<i>Aconitum napellus</i>	30132593	chlorogenic acid	O[C@@H]1C[C@](O)(C[C@@H](OC(=O)\ C=C\ C2=CC=C(O)C(O)=C2)[C@@H]1O)C(O)=O
39	<i>Aconitum napellus</i>	25597888	chrysophanol	CC1=CC(O)=C2C(=O)C3=C(O)C=CC=C3C(=O)C2=C1
40	<i>Aconitum napellus</i>	28925115	cinnamic acid	OC(=O)\ C=C\ C1=CC=CC=C1
41	<i>Aconitum napellus</i>	4576411	cis-aconitate	[O-]C(=O)C\ C(=C\ C([O-])=O)C([O-])=O
42	<i>Aconitum napellus</i>	6103050	cocaine	CO[C@H]1CC[C@H](C[C@H]1OC(=O)C1=CC=CC=C1)N2C
43	<i>Aconitum napellus</i>	24216273	colchicine	CO[C@H]1CC2=C(C(OC)=C1OC)C1=CC=C(OC)C(=O)C=C1[C@H](CC2)NC(C)=O
44	<i>Aconitum napellus</i>	16724552	condelphine	CCN1C[C@]2(COC)C[C@H](O)[C@@]34[C@@H]5C[C@H]6[C@H](OC(C)=O)[C@@H]5[C@](O)(C[C@H]6OC)[C@@H](C[C@H]23)C14
45	<i>Aconitum napellus</i>	29288825	cortisol	C[C@]12C[C@H](O)[C@H]3[C@@H](CCC4=CC(=O)CC[C@]34C)[C@@H]1CC[C@]2(O)C(=O)CO
46	<i>Aconitum napellus</i>	28681583	creatine	CN(CC(O)=O)C(N)=N
47	<i>Aconitum napellus</i>	26715569	creatinine	CN1CC(=O)N=C1N
48	<i>Aconitum napellus</i>	23451494	CTAB	[Br-].CCCCCCCCCCCCCCC CC[N+](C)(C)C
49	<i>Aconitum napellus</i>	25719303	curcumin	CO[C@H]1CC(\ C=C\ C(=O)CC(=O)\ C=C\ C2=CC=C(O)C(OC)=C2)=CC=C1O

50	<i>Aconitum napellus</i>	25878466	cyperene	C[C@@H]1CC[C@@H]2CC3=C(C)CC[C@]13C2(C)C
51	<i>Aconitum napellus</i>	24216273	cytisine	O=C1C=CC=C2[C@H]3CNC[C@H](C3)CN12
52	<i>Aconitum napellus</i>	9459571	delcorine	CCN1C[C@@]2(COC)CC[C@H](OC)[C@]34[C@@H]5C[C@H]6[C@H](OC)[C@@H]5[C@]5(C[C@@H]6OC)O CO[C@]5([C@@H](O)[C@H]23)[C@@H]14
53	<i>Aconitum napellus</i>	24452459	delcosine	CCN1C[C@@]2(COC)CC[C@H](O)[C@]34[C@@H]5C[C@H]6[C@H](O)[C@@H]5[C@@J](O)(C[C@@H]6OC)[C@](O)([C@@H](OC)[C@H]23)[C@@H]14
54	<i>Aconitum napellus</i>	14443271	delphinine	CO[C@@]12CC[C@H](OC)[C@@]34[C@@H]5C[C@H]6(O)[C@H](OC(=O)C7=CC=C C=C7)[C@@H]5[C@@J](C[C@@H]6OC)(OC(C)=O)[C@@H](OC)[C@H]13)C4N(C)C2
55	<i>Aconitum napellus</i>	15797610	delsoline	CCN1C[C@]2(COC)CC[C@H](O)[C@@]34C5C[C@H]6[C@H](OC)[C@@H]5[C@](O)(C[C@@H]6OC)[C@@J](O)([C@@H](OC)[C@H]23)[C@@H]14
56	<i>Aconitum napellus</i>	8368077	denudatine	CCN1C[C@@]2(C)CC[C@@]34[C@@H]1[C@@H](C[C@H]23)[C@@]12CC[C@@H](OC)[C@@H]41)C(=C)[C@H]2O
57	<i>Aconitum napellus</i>	29484902	dexamethasone	C[C@@H]1C[C@H]2[C@@H]3CCC4=CC(=O)C=C[C@]4(C)[C@@]3(F)[C@@H](O)C[C@]2(C)[C@@]1(O)C(=O)CO
58	<i>Aconitum napellus</i>	6086363	diethylthiocarbamate	CCN(CC)C([S-])=S

59	<i>Aconitum napellus</i>	6086363	disulfiram	CCN(CC)C(=S)SSC(=S)N(CC)CC
60	<i>Aconitum napellus</i>	27139035	doxorubicin	COCl=CC=CC2=C1C(=O)C1=C(O)C3=C(C[C@]O)(C[C@@H]3O[C@H]3C[C@H](N)[C@H](O)[C@H](C)O3)C(=O)CO)C(O)=C1C2=O
61	<i>Aconitum napellus</i>	26910236	emodin	CC1=CC(O)=C2C(=O)C3=C(O)C=C(O)C=C3C(=O)C2=C1
62	<i>Aconitum napellus</i>	29758520	ent-kaurene	CC1(C)CCC[C@@]2(C)[C@@H]3CC[C@@H]4C[C@]3(CC4=C)CC[C@H]12
63	<i>Aconitum napellus</i>	27912193	ephedrine	CN[C@@H](C)[C@H](O)C1=CC=CC=C1
64	<i>Aconitum napellus</i>	13926071	eserine	CNC(=O)OC1=CC=C2N(C)[C@H]3N(C)CC[C@@]3(C)C2=C1
65	<i>Aconitum napellus</i>	28925115	ferulic acid	COCl=C(C=CC(=C1)C=CC(=O)O)O
66	<i>Aconitum napellus</i>	15844518	formononetin	COCl=CC=C(C=C1)C1=COC2=CC(O)=CC=C2C1=O
67	<i>Aconitum napellus</i>	19945676	gelsemine	CN1C[C@]2(C=C)[C@@H]3C[C@H]4OC[C@@H]3[C@@H]1[C@@H]2[C@]41C(O)=NC2=CC=CC=C12
68	<i>Aconitum napellus</i>	25904478	geranyl diphosphate	CC(C)=CCC\ C(C)=C\ COP(O)(=O)OP(O)(O)=O
69	<i>Aconitum napellus</i>	23126187	gingerol	CCCCC[C@H](O)CC(=O)CCC1=CC=C(O)C(O)C=C1
70	<i>Aconitum napellus</i>	24205074	ginsenoside	O1[C@H](CO)[C@@H](O)[C@H](O)[C@@H](O)[C@@H]1O[C@@H]1[C@@H]2[C@@H]([C@H]3C[C@@H](O)[C@H]4[C@@H](CC[C@@H]4[C@@H](O[C@@H]4O[C@H](CO)[C@@H](O)[C@H]4O)(CCC=C(C)C)C)(C)[C@@]3(C1)C)(CC[C@H](O)C2(C)C)C

71	<i>Aconitum napellus</i>	27818926	ginsenoside Rc	<chem>CC(C)=CCC[C@](C)(O[C@@H]1O[C@H](CO[C@@H]2O[C@H](O)[C@H]2O)[C@H](O)[C@H]1O)[C@H]1CC[C@]2(C)[C@@H]1[C@H](O)C[C@@H]1[C@@]3(C)CC[C@H](O[C@@H]4O[C@H](CO[C@@H](O)[C@H](O)[C@H]4O)[C@@H]4O[C@H](CO)[C@@H](O)[C@H](O)[C@H]4O)C(C)(C)[C@@H]3CC[C@@]21C</chem>
72	<i>Aconitum napellus</i>	28911382	Ginsenoside Rg1	<chem>C[C@@H]1C[C@H](O)C(C)(C)[C@@H]2[C@H](C[C@]3(C)[C@H](C[C@@H](O)[C@@H]4[C@H](CC[C@@]34C)[C@](C)(CCC=C(C)C)O[C@@H]3O[C@H](CO)[C@@H](O)[C@H]3O)C12O[C@@H]1O[C@H](CO)[C@@H](O)[C@H](O)[C@H]1O</chem>
73	<i>Aconitum napellus</i>	30892884	hetisine	<chem>C[C@@]12CN3C4C[C@@]5CC(=C)[C@H]7[C@H](O)C5C3[C@@](C[C@@H](O)C1)([C@@H]24)[C@@H]6[C@@H]7O</chem>
74	<i>Aconitum napellus</i>	24846827	hippurate	<chem>[O-]C(=O)CNC(=O)C1=C C=CC=C1</chem>
75	<i>Aconitum napellus</i>	30597748	hypaconitine	<chem>CO[C@@]12CC[C@H](OC)[C@@]34[C@@H]5C[C@@]6(O)[C@H](OC(=O)C7=CC=C C=C7)[C@@H]5[C@@](OC(C)=O)([C@@H](C[C@H](OC)[C@H]13)C4N(C)C2)[C@@H](O)[C@@H]6OC</chem>
76	<i>Aconitum napellus</i>	29200734	hypotaurine	<chem>NCCS(O)=O</chem>
77	<i>Aconitum napellus</i>	12233816	indomethacin	<chem>COC1=CC=C2N(C(=O)C3=CC=C(Cl)C=C3)C</chem>

				C)=C(CC(O)=O)C2=C1
78	<i>Aconitum napellus</i>	24791539	inosine	OC[C@H]1O[C@H]([C@H](O)[C@@H]1O)N1C=NC2=C(O)N=CN=C12
79	<i>Aconitum napellus</i>	25889555	isoliquiritigenin	OC1=CC=C(\C=C\ C(=O)C2=CC=C(O)C=C2O)C=C1
80	<i>Aconitum napellus</i>	9489612	isoprenaline	CC(C)NCC(O)C1=CC=C(O)C(O)=C1
81	<i>Aconitum napellus</i>	24469098	jatrorrhizine	CO C1=CC2=C(CC[N+]3=C2C=C2C=CC(OC)=C(OC)C2=C3)C=C1O
82	<i>Aconitum napellus</i>	30863932	jesaconitine	CCN1C[C@]2(COC)[C@H]3[C@@H](OC)[C@H]4[C@@H]1[C@]3([C@@H]1C[C@]3(O)[C@H](OC(=O)C5=CC=C(OC)C=C5)[C@@H]1[C@@]4(OC(C)=O)[C@@H](O)[C@@H]3OC)[C@H](C[C@H]2O)OC
83	<i>Aconitum napellus</i>	25322557	karakoline	CCN1C[C@]2(C)CC[C@H](O)[C@@]34[C@@H]5C[C@H]6[C@H](O)[C@@H]5[C@](O)(C[C@H]6OC)[C@@H](C[C@H]23)C14
84	<i>Aconitum napellus</i>	21277363	ketoconazole	CC(=O)N1CCN(CC1)C1=CC=C(OCC2COCC(N3C=CN=C3)O2)C2=CC=C(Cl)C=C2Cl)C=C1
85	<i>Aconitum napellus</i>	4191693	k-strophanthoside	CO[C@H]1C[C@H](O[C@H]2CC[C@@]3(C=O)[C@H]4CC[C@@]5(C)[C@H](CC[C@@]5(O)[C@@H]4CC[C@@]3(O)C2)C2=CC(=O)OC2O[C@H](C)[C@H]1O[C@H]1O[C@H](CO)[C@@H](O)[C@H](O)[C@H]2O[C@H](CO)[C@@H](O)[C@H](O)[C@H]2O)[C@H](O)[C@H]1O

86	<i>Aconitum napellus</i>	30723741	Lappaconitine	<chem>CCN1C[C@]2(CC[C@H](OC)[C@]34[C@@H]5C[C@H]6[C@H](OC)[C@@]5(O)[C@@H](O)(C[C@@H]6OC)[C@@H](C[C@H]23)[C@@H]14)OC(=O)C1=CC=CC=C1N=C(C)O</chem>
87	<i>Aconitum napellus</i>	28839367	licochalcone A	<chem>COC1=CC(O)=C(C=C1\ C=C\ C(=O)C1=CC=C(O)C=C1)C(C)(C)C=C</chem>
88	<i>Aconitum napellus</i>	12686443	linoleic acid	<chem>CCCCC\ C=C/C\ C=C/C\CCCCCCC(O)=O</chem>
89	<i>Aconitum napellus</i>	25889555	liquiritigenin	<chem>OC1=CC=C(C=C1)[C@@H]1CC(=O)C2=CC=C(O)C=C2O1</chem>
90	<i>Aconitum napellus</i>	23892202	liquiritin	<chem>OC[C@H]1O[C@@H](OC2=CC=C(C=C2)[C@@H]2CC(=O)C3=CC=C(O)C=C3O2)[C@H](O)[C@@H](O)[C@@H]1O</chem>
91	<i>Aconitum napellus</i>	30404196	luteolin	<chem>OC1=CC(O)=C2C(=O)C=C(OC2=C1)C1=CC=C(O)C(O)=C1</chem>
92	<i>Aconitum napellus</i>	12407981	lycaconitine	<chem>CCN1C[C@@]2(COC(=O)C3=CC=CC=C3N3C(=O)CCC3=O)CC[C@H](OC)[C@]34[C@@H]5C[C@H]6[C@H](OC)[C@@H]5[C@@](O)(C[C@@H]6OC)[C@@](O)([C@@H](OC)[C@@H]23)[C@@H]14</chem>
93	<i>Aconitum napellus</i>	24452459	lycoctonine	<chem>CCN1C[C@]2(CO)CC[C@H](OC)[C@@]34[C@@H]5C[C@H]6[C@H](OC)[C@@H]5[C@@](O)(C[C@@H]6OC)[C@@](O)([C@@H](OC)[C@@H]23)C14</chem>
94	<i>Aconitum napellus</i>	24216273	matrine	<chem>O=C1CCC[C@@H]2[C@H]3CCCN4CCC[C@@H](CN12)[C@@H]34</chem>

95	<i>Aconitum napellus</i>	30892884	mesaconitine	<chem>COC[C@H]12CN(C)[C@@H]3[C@@H]4[C@H](OC)[C@H]1[C@@]3([C@@H]1C[C@]3(O)[C@H](OC(=O)C5=C C=CC=C5)[C@@H]1[C@@]4(OC(C)=O)[C@@H](O)[C@@H]3OC)[C@H](C[C@H]2O)OC</chem>
96	<i>Aconitum napellus</i>	16770829	methyllycaconitine	<chem>CCN1CC2(COC(=O)C3=CC=CC=C3N3C(=O)CC(C)C3=O)CCC(OC)C34C5CC6C(OC)C5C(OC)(CC6OC)C(O)(C(OC)C23)C14</chem>
97	<i>Aconitum napellus</i>	25904478	mevalonate	<chem>CC(O)(CCO)CC([O-])=O</chem>
98	<i>Aconitum napellus</i>	25904478	mevalonate diphosphate	<chem>C[C@H](O)(CCO)CC(=O)OP([O-])(=O)OP([O-])([O-])=O</chem>
99	<i>Aconitum napellus</i>	30180777	morphine	<chem>CN1CC[C@H]23[C@H]4OC5=C2C(C[C@H]1[C@@H]3C=C[C@H]4O)=CC=C5O</chem>
100	<i>Aconitum napellus</i>	24143362	napelline	<chem>CCN1C[C@H]2(C)CC[C@H](O)[C@@]34[C@H]1[C@H](C[C@H]23)[C@]12C[C@H]([C@@H](O)C[C@H]41)C(=C)[C@H]2O</chem>
101	<i>Aconitum napellus</i>	3338564	nicotine	<chem>CN1CCCC1C1=CC=N1</chem>
102	<i>Aconitum napellus</i>	2518340	nifedipine	<chem>COC(=O)C1=C(C)NC(C)=C(C1C1=CC=CC=C1[N+](O-))=O)C(=O)OC</chem>
103	<i>Aconitum napellus</i>	23213736	Nonacosane	<chem>CCCCCCCCCCCCCCCCCCCCCC</chem>
104	<i>Aconitum napellus</i>	28850863	norcoclaurine	<chem>OC1=CC=C(CC2[NH2+]CCC3=CC(O)=C(O)C=C23)C=C1</chem>
105	<i>Aconitum napellus</i>	25324527	norpseudoephedrine	<chem>C[C@H](N)[C@@H](O)C1=CC=CC=C1</chem>
106	<i>Aconitum napellus</i>	20848395	oleic acid	<chem>CCCCCCCC\ C=C/CCC CCCCC(O)=O</chem>
107	<i>Aconitum napellus</i>	15844518	ononin	<chem>CO[C@H]1=CC=C(C=C1)C1=COC2=CC(O[C@H]3O[C@H](CO)[C@H]23)C=C1</chem>

				<chem>]([O])[C@H](O)[C@H]3O)=CC=C2C1=O</chem>
108	<i>Aconitum napellus</i>	9833644	ouabain	<chem>C[C@@H]1O[C@@H](O[C@H]2C[C@@H](O)[C@]3(CO)[C@H]4[C@@H](O)C[C@]5(C)[C@H](CC[C@]5(O)[C@@H]4CC[C@]3(O)C2)C2=CC(=O)OC2)[C@H](O)[C@H](O)[C@H]1O</chem>
109	<i>Aconitum napellus</i>	30974202	paclitaxel	<chem>CC(=O)O[C@@H]1C2=C(C)[C@H](C[C@@H](O)[C@@H](OC(=O)C3=CC=CC=C3)[C@@H]3[C@@H]4(CO[C@@H]4C[C@H](O)[C@@H]3(C)C1=O)OC(C)=O)C2(C)COC(=O)[C@H](O)[C@@H](NC(=O)C1=CC=CC=C1)C1=CC=CC=C1</chem>
110	<i>Aconitum napellus</i>	12569436	palmitic acid	<chem>CCCCCCCCCCCCCCCCC</chem> <chem>CC(O)=O</chem>
111	<i>Aconitum napellus</i>	16386798	peroxynitrite	<chem>[O-]ON=O</chem>
112	<i>Aconitum napellus</i>	28681583	phosphatidylinositol	<chem>CCCCCCCCCCCCCCCC</chem> <chem>CCCCC(=O)OC[C@H](COP(=O)(=O)OC1C(O)C(O)C(O)[C@@H](O)C1O)OC(=O)CCCCC\ C=C/C\ C=C/C\ C=C/C\ C=C/CC</chem>
113	<i>Aconitum napellus</i>	27912193	pseudoephedrine	<chem>CN[C@@H](C)[C@@H](O)C1=CC=CC=C1</chem>
114	<i>Aconitum napellus</i>	25719303	Psoralidin	<chem>CC(C)=CCC1=CC2=C(OC(=O)C3=C2OC2=C3C=CC(O)=C2)C=C1O</chem>
115	<i>Aconitum napellus</i>	2573715	putrescine	<chem>NCCCCN</chem>
116	<i>Aconitum napellus</i>	28925115	quinic acid	<chem>O[C@@H]1C[C@@H](O)[C@@H](O)C(=O)C1</chem>
117	<i>Aconitum napellus</i>	21277363	quinidine	<chem>CO[C@H]1C2=C(C=CN=C2C=C1)[C@H](O)[C@H]1C[C@@H]2CCN1C[C@H]2C=C</chem>

118	<i>Aconitum napellus</i>	2403008	reserpine	<chem>CO[C@H]1[C@@@H](C[C@@H]2CN3CCC4=C(NC5=CC(OC)=CC=C45)[C@H]3C[C@@H]2[C@@H]1C(=O)OC)OC(=O)C1=CC(OC)=C(OC)C(OC)=C1</chem>
119	<i>Aconitum napellus</i>	24469098	rhein	<chem>OC(=O)C1=CC(O)=C2C(=O)C3=C(O)C=CC=C3C(=O)C2=C1</chem>
120	<i>Aconitum napellus</i>	15997105	ruscogenin	<chem>C[C@H]1[C@@H]2[C@H](C[C@H]3[C@@H]4CC=C5C[C@@H](O)C[C@@H](O)[C@]5(C)[C@H]4CC[C@]23C)O[C@]11CC[C@@H](C)CO1</chem>
121	<i>Aconitum napellus</i>	30410440	ryanodine	<chem>CC(C)[C@@@]1(O)[C@@H](OC(=O)C2=CC=CN2)[C@@]2(O)[C@@]3(C)C[C@]4(O)O[C@@@]5([C@H](O)[C@@H](C)CC[C@]35O)[C@@]2(O)[C@@@]14C</chem>
122	<i>Aconitum napellus</i>	25011247	salidroside	<chem>OC[C@H]1O[C@@H](OCCC2=CC=C(O)C=C2)[C@H](O)[C@@H](O)[C@@H]1O</chem>
123	<i>Aconitum napellus</i>	6132517	salsolinol	<chem>C[C@@H]1NCCCC2=C(C(O)=C(O)C=C12</chem>
124	<i>Aconitum napellus</i>	25315049	saponins	<chem>CC=C(C)C(=O)OC1C(C2(C(CC1(C)C)C3=CC4C5(CCC(C(C5CCC4(C3(CC2O)C)C)CO)OC6C(C(C(C(O6)C(=O)O)OC7C(C(C(C(O7)CO)O)O)OC8C(C(C(O8)CO)O)O)C)CO(=O)C</chem>
125	<i>Aconitum napellus</i>	30404196	scoulerine	<chem>COCl=CC2=C(C=C1O)[C@@H]1CC3=C(CN1CC2)C(O)=C(OC)C=C3</chem>
126	<i>Aconitum napellus</i>	24452459	septentriodine	<chem>CCN1CC2(CCC(C34C2C(C(C31)C5(CC(C6CC4C5C6OC)OC)O)OC)CO)COCl=CC7=CC=C7NC(=O)CCC(=O)OC</chem>

127	<i>Aconitum napellus</i>	17405023	septentrionine	<chem>CCN1C[C@@@]2(COC(=O)C3=CC=CC=C3N=C(O)CCC(=O)OC)CC[C@H](OC)[C@]34[C@@H]5C[C@H]6[C@H](OC)[C@@H]5[C@](C[C@@H]6OC)(OC)[C@](O)([C@@H](OC)[C@H]23)[C@@H]14</chem>
128	<i>Aconitum napellus</i>	30926314	Songorine	<chem>CCN1C[C@@@]2(C)CC[C@H](O)[C@]34[C@@H]2C[C@@H]([C@@H]13)[C@@]12C[C@@H](C(=C)[C@H]1O)C(=O)C[C@@H]42</chem>
129	<i>Aconitum napellus</i>	4408029	sparteine	<chem>C1CCN2C[C@@H]3[C@@H](CN4CCCC[C@H]34)[C@@H]2C1</chem>
130	<i>Aconitum napellus</i>	24791539	stearic acid	<chem>CCCCCCCCCCCCCCCCCC(=O)=O</chem>
131	<i>Aconitum napellus</i>	28330176	steviol	<chem>C[C@@]12CCC[C@](C)([C@H]1CC[C@@]13CC(=C)[C@@](O)(C1)CC[C@@H]23)C(O)=O</chem>
132	<i>Aconitum napellus</i>	27746335	taurine	<chem>NCCS(O)(=O)=O</chem>
133	<i>Aconitum napellus</i>	25371696	testosterone	<chem>C[C@]12CC[C@H]3[C@@H](CCC4=CC(=O)CC[C@]34C)[C@@H]1CC[C@H]2O</chem>
134	<i>Aconitum napellus</i>	29783906	tetrodotoxin	<chem>OC[C@@]11(O)[C@H]2O[C@@]3(O)O[C@@H]1[C@@H]1[C@@H](O)NC(=N)N[C@]1([C@@H]2O)[C@@H]3O</chem>
135	<i>Aconitum napellus</i>	11858801	thapsigargin	<chem>CCCCCC(=O)O[C@@H]1[C@@H](OC(=O)C(\C)=C/C)C(C)=C2[C@@H]3OC(=O)[C@@](C)(O)[C@@]3(O)[C@H](C[C@](C)(OC(C)=O)[C@@H]12)OC(=O)C2C</chem>
136	<i>Aconitum napellus</i>	2984017	theophylline	<chem>CN1C2=C(NC=N2)C(=O)N(C)C1=O</chem>
137	<i>Aconitum napellus</i>	9489612	timolol	<chem>CC(C)(C)NC[C@H](O)COCl=NSN=C1N1CCOCC1</chem>

138	<i>Aconitum napellus</i>	5664138	Trans-aconitate	[O-]C(=O)C\C(=C/C([O-])=O)C([O-])=O
139	<i>Aconitum napellus</i>	26946628	tubeimoside I	C[C@@H]1O[C@H]2O[C@@H]3[C@@H](O)[C@@H](O)CO[C@H]3OC(=O)[C@]34CCC(C)(C)C[C@H]3C3=CC[C@@H]5[C@@]6(C)C[C@H](O)[C@H](O)[C@@H]7O[C@H](CO)[C@@H](O)[C@H]7O[C@@H]7OC[C@H](OC(=O)O[C@@H]1[C@@H](O[C@@H]1OC[C@@H](O)[C@H](O)[C@H]1O)[C@H]2O)[C@H](O)[C@H]7O[C@@H]6CC[C@@]5(C)[C@J3(C)CC4
140	<i>Aconitum napellus</i>	469553	umbelliferone	OC1=CC=C2C=CC(=O)OC2=C1
141	<i>Aconitum napellus</i>	27898008	valine	CC(C)[C@H](N)C(O)=O
142	<i>Aconitum napellus</i>	19408253	veatchine	C[C@@]12CCC[C@]3([C@@H]4OCCN4C1)[C@H]1CC[C@H]4C[C@@]1(CC[C@@H]23)[C@@H](O)C4=C
143	<i>Aconitum napellus</i>	9833644	veratridine	CO C1=CC=C(C=C1OC(=O)O[C@H]1CC[C@@]2(C)[C@@H]3CC[C@H]4[C@]5(O)C[C@H](O)[C@@]6(O)[C@@H](CN7C[C@H](C)CC[C@H]7[C@@]6(C)O)[C@]5(O)C[C@]24O[C@]13O
144	<i>Aconitum napellus</i>	9875455	vincristine	CC[C@]1(O)C[C@H]2CN(C1)CCC1=C(NC3=CC=CC=C13)[C@@](C2)(C(=O)OC)C1=CC2=C(C=C1OC)N(C=O)[C@@H]1[C@]22CCN3CC=C[C@](CC)([C@@H]23)[C@@H](OC(C)=O)[C@]1(O)C(=O)OC

145	<i>Aconitum napellus</i>	24469098	wogonin	<chem>COC1=C(O)C=C(O)C2=C1OC(=CC2=O)C1=C C=CC=C1</chem>
146	<i>Aconitum napellus</i>	9548384	yohimbine	<chem>CO[C@H]1[C@H](O)CC[C@H]2CN3CCC4=C(NC5=CC=C C=C45)[C@H]3C[C@H]12</chem>
147	<i>Aconitum napellus</i>	19401984	Physostigmine	<chem>CNC(=O)Oc1ccc2N(C)[C@H]3N(C)CC[C@@]3(C)c2c1</chem>
148	<i>Allium sativum</i>	21906328	(+)-alliin	<chem>C=CCS(=O)CC(C(=O)O)N</chem>
149	<i>Allium sativum</i>	25819001	1,8-cineole	<chem>C[C@@]12CC[C@@H](CC1)C(C)(C)O2</chem>
150	<i>Allium sativum</i>	1382365	Ajoene	<chem>C=CCSS\ C=C\ CS(=O)C=C</chem>
151	<i>Allium sativum</i>	31009577	allicin	<chem>C=CCSS(=O)CC=C</chem>
152	<i>Allium sativum</i>	10193205	Alliin	<chem>N[C@@H](C[S@@](=O)C(=O)CC=C)C(O)=O</chem>
153	<i>Allium sativum</i>	27056828	allyl methyl trisulfide	<chem>CSSSCC=C</chem>
154	<i>Allium sativum</i>	25639557	cyanidin	<chem>OC1=CC2=[O+]C(=C(O)C=C2C(O)=C1)C1=C C=C(O)C(O)=C1</chem>
155	<i>Allium sativum</i>	2713853	D-carvone	<chem>CC(=C)[C@H]1CC=C(C)C(=O)C1</chem>
156	<i>Allium sativum</i>	2504484	Diallyl sulfide	<chem>C=CCSCC=C</chem>
157	<i>Allium sativum</i>	25373222	D-limonene	<chem>CC(=C)[C@@H]1CCC(C)=CC1</chem>
158	<i>Allium sativum</i>	10588342	ethiin or S-ethylcysteine sulfoxide	<chem>N[C@@H](CS(CC)=O)C(O)=O</chem>
159	<i>Allium sativum</i>	16320201	kaempferol 3- O-beta-D-glucopyranosyl-(1-->4)-glucopyranoside	<chem>O1[C@H](CO)[C@@H](O[C@@H]2O[C@H](CO)[C@@H](O)[C@H](O)[C@H]2O)[C@H](O)[C@@H](O)C1OC1=C(Oc2c(C1=O)c(O)cc(O)c2)c1ccc(O)cc1</chem>
160	<i>Allium sativum</i>	16320201	kaempferol 3- O-beta-D-rhamnopyranosyl-(1-->2)-glucopyranoside	<chem>O1[C@H](CO)[C@@H](O)[C@H](O)[C@@H](O[C@@H]2O[C@H](C)[C@@H](O)[C@H](O)[C@H]2O)C1OC1=C(Oc2c(C1=O)c(O)cc(O)c2)c1ccc(O)cc1</chem>
161	<i>Allium sativum</i>	16320201	kaempferol 3-O-glucopyranoside	<chem>O1[C@H](CO)[C@@H](O)[C@H](O)[C@@H](O)C1OC1=C(Oc2c(C1=O)c(O)cc(O)c2)c1ccc(O)cc1</chem>

				=O)c(O)cc(O)c2)c1ccc(O)cc1
162	<i>Allium sativum</i>	16320201	kaempferol 7-O-glucopyranoside	OC1=C(C2=CC=C(O)C=C2)OC3=C(C(O)=CC(OC4[C@@H]([C@H]([C@@H]([C@@H](CO)O)O)O)=C3)C1=O
163	<i>Allium sativum</i>	19768983	kaempferol-3-O-beta-D-glucopyranoside or astragalin	C1=CC(=CC=C1C2=C(C(=O)C3=C(C=C(C=C3O2)O)O)OC4C(C(C(C(=O)CO)O)O)O)
164	<i>Allium sativum</i>	19768983	kaempferol-3-O-beta-D-glucopyranosyl-7-O-beta-D-glucopyranoside	O1C(CO)C(O)C(O)C(O)C(O)C1OC1=C(Oc2c(C1=O)c(O)cc(OC1OC(CO)C(O)C(O)C1O)c2)c1ccc(O)cc1
165	<i>Allium sativum</i>	25819001	nerolidol	CC(C)=CCC\ C(C)=C\ C C[C@](C)(O)C=C
166	<i>Allium sativum</i>	973445	quercetin-4'-glucoside	O1C(CO)C(O)C(O)C(O)C(O)C1Oc1ccc(cc1O)C=1Oc2c(C(=O)C=1O)c(O)cc(O)c2
167	<i>Allium sativum</i>	2684627	retinol	C\ C(=C/CO)\ C=C\ C=C(/C)\ C=C\ C1=C(C)CCC1(C)C
168	<i>Allium sativum</i>	2712320	sorbic acid	C\ C=C\ C=C\ C(O)=O
169	<i>Allium sativum</i>	25819001	squalene	CC(C)=CCC\ C(C)=C\ C C\ C(C)=C\ CC\ C=C(/C)CC\ C=C(/C)CCC=C(C)C
170	<i>Allium sativum</i>	25819001	terpinolene	CC(C)=C1CCC(C)=CC1
171	<i>Allium sativum</i>	2684627	tocopherol	CC(C)CCC[C@@H](C)CCC[C@@H](C)CCC[C@]1(C)CCC2=C(C)C(O)=C(C)C(C)=C2O1
172	<i>Allium sativum</i>	8053972	vinyldithiine	C=CC1=CSC=CS1
173	<i>Apium graveolens</i>	19777835	(9Z) 1,9-heptadecadiene-4,6-diyne-3,8,11-triol	CCCCCCC(O)\ C=C/C(O)C#CC#CC(O)C=C
174	<i>Apium graveolens</i>	8446516	3-n-butyl phthalide	CCCCC1OC(=O)C2=C(C=CC=C12
175	<i>Apium graveolens</i>	19777835	5,8-dimethoxy psoralen	O=C1OC2=C(OC)C3=C(C=CO3)C(OC)=C2C=C1
176	<i>Apium graveolens</i>	4080514	alpha-pinene	CC1=CCC2CC1C2(C)C
177	<i>Apium</i>	26500081	a-phellandrene	CC(C)C1CC=C(C)C=C

	<i>graveolens</i>			1
178	<i>Apium graveolens</i>	29923397	apigenin	<chem>OC1=CC=C(C=C1)C1=CC(=O)C2=C(O)C=C(O)C=C2O1</chem>
179	<i>Apium graveolens</i>	23790931	Apigenin 7-O-glucoside	<chem>OCC1O[C@H](OC2=CC(O)=C3C(=O)C=C(OC3=C2)C2=CC=C(O)C=C2)C(O)[C@H](O)[C@H]1O</chem>
180	<i>Apium graveolens</i>	26500081	apiol	<chem>COC1=CC(CC=C)=C(O)C)C2=C1OCO2</chem>
181	<i>Apium graveolens</i>	19777835	benzolic acid	<chem>OC(=O)C1=CC=CC=C1</chem>
182	<i>Apium graveolens</i>	20136461	beta-pinene	<chem>CC1(C)C2CC1C(=C)C2</chem>
183	<i>Apium graveolens</i>	18766378	beta-selinene	<chem>CC(=C)[C@@H]1CC[C@H]2(C)CCCC(=C)[C@@H]2C1</chem>
184	<i>Apium graveolens</i>	22934666	camphene	<chem>CC1(C)C2CCC(C2)C1=C</chem>
185	<i>Apium graveolens</i>	26500081	carotol	<chem>CC(C)[C@H]1CC[C@H]2(C)CC=C(C)CC[C@H]1O</chem>
186	<i>Apium graveolens</i>	26500081	Carvacrol	<chem>CC(C)C1=CC=C(C)C(=O)=C1</chem>
187	<i>Apium graveolens</i>	15553907	catechol	<chem>OC1=CC=CC=C1O</chem>
188	<i>Apium graveolens</i>	4080514	cis-allo-ocimene	<chem>CC=C(C)C=CC=C(C)C</chem>
189	<i>Apium graveolens</i>	22934666	cumene	<chem>CC(C)C1=CC=CC=C1</chem>
190	<i>Apium graveolens</i>	26500081	cuminaldehyde	<chem>CC(C)C1=CC=C(C=O)C=C1</chem>
191	<i>Apium graveolens</i>	19777835	eugenic acid	<chem>COC1=CC(CC=C)=CC=C1O</chem>
192	<i>Apium graveolens</i>	4080514	gamma-terpinene	<chem>CC(C)C1=CCC(C)=CC1</chem>
193	<i>Apium graveolens</i>	4080514	humulene	<chem>C\ C1=C/CC(C)(C)\ C=C\ C(C)=C\ CC1</chem>
194	<i>Apium graveolens</i>	19777835	isofraxidin	<chem>COCC1=C(O)C(OC)=C2OC(=O)C=CC2=C1</chem>
195	<i>Apium graveolens</i>	15553907	L-DOPA	<chem>N[C@H](CC1=CC=C(O)C(=O)=C1)C(=O)=O</chem>
196	<i>Apium graveolens</i>	4080514	limonene	<chem>CC(=C)C1CCC(C)=CC1</chem>
197	<i>Apium graveolens</i>	19777835	lunularic acid	<chem>OC(=O)C1=C(O)C=CC=C1CCC1=CC=C(O)C=C1</chem>

198	<i>Apium graveolens</i>	19777835	lunularin	OC1=CC=C(CCC2=CC=CC(O)=C2)C=C1
199	<i>Apium graveolens</i>	26500081	myristicin	COC1=CC(CC=C)=CC2=C1OCO2
200	<i>Apium graveolens</i>	22974401	neocnidilide	CCCCC1C2CCCC=C2C(=O)O1
201	<i>Apium graveolens</i>	26500081	neral	CC(C)=CCC\ C(C)=C/C=O
202	<i>Apium graveolens</i>	19777835	oplopandiol	CCCCCC\ C=C/[C@H](O)C#CC#C[C@@H](O)CC
203	<i>Apium graveolens</i>	22934666	p-cymene	CC(C)C1=CC=C(C)C=C1
204	<i>Apium graveolens</i>	19777835	p-hydroxyphenylethanol ferulate	COC1=CC(C=CC(=O)OCCC2=CC=C(O)C=C2)=CC=C1O
205	<i>Apium graveolens</i>	8446516	p-mentha-2,8-dien-1-ol	CC(=C)C1CCC(C)(O)C=C1
206	<i>Apium graveolens</i>	8446516	p-mentha-8(9)-en-1,2-diol	CC(=C)C1CCC(C)(O)C(O)C1
207	<i>Apium graveolens</i>	15553907	resorcinol	OC1=CC(O)=CC=C1
208	<i>Apium graveolens</i>	22934666	sabinene	CC(C)C12CC1C(=C)C C2
209	<i>Apium graveolens</i>	8446516	sedanolide	CCCCC1OC(=O)C2=CCCC12
210	<i>Apium graveolens</i>	4080514	senkyunolide	O1C(C2=C(C=CCC2)C1=O)CCCC
211	<i>Apium graveolens</i>	19777835	succinic acid	OC(=O)CCC(O)=O
212	<i>Apium graveolens</i>	26500081	thymol	CC(C)C1=CC=C(C)C=C1O
213	<i>Apium graveolens</i>	19777835	trans-cinnamic acid	C1=CC=C(C=C1)C=CC(=O)O
214	<i>Apium graveolens</i>	4080514	trans-farnesene	CC(C)=CCC\ C(C)=C\ CC(C)=C=C
215	<i>Apium graveolens</i>	26500081	γ -terpinene	C1C=C(CC=C1C(C)C)C
216	<i>Apium graveolens</i>	26500081	α -terpinene	CC1=CC=C(CC1)C(C)C
217	<i>Apium graveolens</i>	22934666	β -pinene	CC1(C2CCC(=C)C1C2)C
218	<i>Apium graveolens</i>	22934666	γ -terpinene	CC1=CCC(=CC1)C(C)C
219	<i>Apium graveolens</i>	4080514	cis-beta-ocimene	CC(C)=CC/C=C(/C)C=C
220	<i>Apium graveolens</i>	4080514	myrcene	CC(C)=CCCC(=C)C=C

221	<i>Apium graveolens</i>	26500081	terpinen-4-ol	CC1=C2CC(CC1C3(CC4CC(=C3C)C4(C)C)C5C(O)C6CC(=C5C)C6(C)C)C2(C)C
222	<i>Apium graveolens</i>	26500081	trans-anethole	COc1ccc(\C=C\ C)cc1
223	<i>Apium graveolens</i>	26500081	a-pinene	C12CC(CC=C1C)C2(C)C
224	<i>Apium graveolens</i>	26500081	carvone	O=C1CC(CC=C1C)C(C)=C
225	<i>Bacopa monnieri</i>	27729727	bacopasaponin C	CC(=CC1COC23CC4(CO2)C(C3C1(C)O)CCC5C4(CCC6C5(CCC(C6(C)C)OC7C(C(C(CO7)O)OC8C(C(C(C(O8)CO)O)O)OC9C(C(C(O9)CO)O)O)C)C
226	<i>Bacopa monnieri</i>	22733208	Bacopasaponin D	CC(=CC1COC23CC4(CO2)C(C3C1(C)O)CCC5C4(CCC6C5(CCC(C6(C)C)OC7C(C(C(CO7)CO)O)OC8C(C(C(C(O8)CO)O)O)OC9C(C(C(O9)CO)O)O)C)C
227	<i>Bacopa monnieri</i>	27907870	bacopaside I	CC(=CC1COC23CC4(CO2)C(C3C1(C)O)CCC5C4(CCC6C5(CCC(C6(C)C)OC7C(C(C(CO7)O)OC8C(C(C(C(O8)CO)O)O)OC9C(C(C(O9)CO)O)O)C)C
228	<i>Bacopa monnieri</i>	30073654	bacopaside II	CC(=CC1COC23CC4(CO2)C(C3C1(C)O)CCC5C4(CCC6C5(CCC(C6(C)C)OC7C(C(C(CO7)CO)OC8C(C(C(C(O8)CO)O)O)OC9C(C(C(O9)CO)O)O)C)C
229	<i>Bacopa monnieri</i>	22733208	bacopaside III	CC(=CC1COC23CC4(CO2)C(C3C1(C)O)CCC5C4(CCC6C5(CCC(C6(C)C)OC7C(C(C(CO7)O)OC8C(C(C(C(O8)CO)O)O)OC9C(C(C(O9)CO)O)O)C)C
230	<i>Bacopa monnieri</i>	22733208	bacopaside V	CC(=CC1CC(C2C3CC4C5(CCC(C(C5CCC4(C36CC2(O1)OC6)C)(C)OC7C(C(C(CO7)O)OC8C(C(C(C(O8)CO)O)O)C)C

)O)O)O)C)(C)O)C
231	<i>Bacopa monnieri</i>	19606439	bacopaside X	CC(=CC1CC(C2C3CC C4C5(CCC(C(C5CCC4 (C36CC2(O1)OC6)C)(C)C)OC7C(C(C(CO7)O) OC8C(C(C(C(O8)CO)O)O)O)OC9C(C(C(O9)C O)O)O)C)(C)O)C
232	<i>Bacopa monnieri</i>	29414544	bacoside A	CC(C)=CCCC(C)(O)C1 C2CCC3C(C)(CCC4C(C)(C)C(CCC34CO)OC3 OC(CO)C(OC4OCC(O) C(O)C4O)C(O)C3O)C2 (C)CC1=O
233	<i>Bacopa monnieri</i>	29142420	bacoside B	CC(=CCCC(C)(C1C2C CC3C(C2(CC1=O)C)(C CC4C3(CCC(C4(C)C)O C5C(C(C(C(O5)CO)OC 6C(C(C(CO6)O)O)O)O) O)CO)C)O)C
234	<i>Bacopa monnieri</i>	27441247	bacoside-A3	CC(=CC1CC(C2C3CC C4C5(CCC(C(C5CCC4 (C36CC2(O1)OC6)C)(C)C)OC7C(C(C(C(O7)C O)O)OC8C(C(C(C(O8) CO)O)O)OC9C(C(C(O9)CO)O)O)C)(C)O)C
235	<i>Bacopa monnieri</i>	29142420	cucurbitacin B	CC(=O)OC(C)(C)\C=C\ C(=O)[C@](C)(O)[C@H]1[C@H](O)C[C@@]2(C)[C@@H]3CC=C4[C@@H](C[C@H](O)C(=O)C4(C)C)[C@]3(C)C(=O)C[C@]12C
236	<i>Bacopa monnieri</i>	29142420	cucurbitacin E	CC(=O)OC(C)(C)\C=C\ C(=O)[C@](C)(O)[C@H]1[C@H](O)C[C@@]2(C)[C@@H]3CC=C4[C@@H](C=C(O)C(=O)C4(C)C)[C@]3(C)C(=O)C[C@]12C
237	<i>Bacopa monnieri</i>	27046025	neochlorogenic acid	O[C@@H]1C[C@@](O)(C[C@@H](OC(=O)\C=C\ C2=CC=C(O)C(O)=C2)[C@H]1O)C(O)=O

238	<i>Bacopa monnieri</i>	24396246	Piperine	O=C(\C=C\C=C\ C1=CC=C2OCOC2=C1)N1CCCCC1
239	<i>Bacopa monnieri</i>	27784187	stigmasterol	CC[C@H](\C=C\[C@@H](C)[C@H]1CC[C@H]2[C@@H]3CC=C4C[C@@H](O)CC[C@@]4(C)[C@H]3CC[C@@]12C)C(C)C
240	<i>Brassica nigra</i>	20180576	3-butenyl isothiocyanate	C=CCN=C=S
241	<i>Brassica nigra</i>	17828429	4-hydroxyglucobrassicin	OC[C@H]1O[C@@H](SC(CC2=CNC3=CC=C C(O)=C23)=NOS(O)(=O)=O)[C@H](O)[C@@H](O)[C@H](O)[C@@H]1O
242	<i>Brassica nigra</i>	17828429	4-methoxyglucobrassicin	COCl=C2C(CC(S[C@@H]3O[C@H](CO)[C@@H](O)[C@H](O)[C@H]3O)=NOS(O)(=O)=O)=CNC2=CC=C1
243	<i>Brassica nigra</i>	18082143	allyl isothiocyanate	C=CCN=C=S
244	<i>Brassica nigra</i>	26555822	bisphenol F	OC1=CC=C(CC2=CC=C(O)C=C2)C=C1
245	<i>Brassica nigra</i>	17467751	brassinin	CSC(=S)NCC1=CNC2=CC=CC=C12
246	<i>Brassica nigra</i>	22040386	capric acid	CCCCCCCCCC(O)=O
247	<i>Brassica nigra</i>	12907406	delphinidin	OC1=CC2=[O+]C(=C(O)C=C2C(O)=C1)C1=CC(O)=C(O)C(O)=C1
248	<i>Brassica nigra</i>	17828429	glucobrassicin	OC[C@H]1O[C@@H](SC(CC2=CNC3=CC=C C=C23)=NOS(O)(=O)=O)[C@H](O)[C@@H](O)[C@@H]1O
249	<i>Brassica nigra</i>	27052706	malic acid	OC(CC(O)=O)C(O)=O
250	<i>Brassica nigra</i>	12907406	malvidin	COCl=CC(=CC(OC)=C1O)C1=[O+]C2=CC(O)=CC(O)=C2C=C1O
251	<i>Brassica nigra</i>	12907406	peonidin	COCl=CC(=CC=C1O)C1=[O+]C2=CC(O)=CC(O)=C2C=C1O
252	<i>Brassica nigra</i>	28787461	sinapine	COCl=CC(\C=C\C(=O)OCC[N+](C)(C)C)=CC(OC)=C1O
253	<i>Brassica nigra</i>	17828429	sinigrin	OC[C@H]1O[C@@H](SC(CC=C)=NOS([O-])(=O)=O)[C@H](O)[C@@H](O)[C@H](O)[C@@H]1O

254	<i>Brassica nigra</i>	24377653	sulphoraphane	CS(=O)CCCCN=C=S
255	<i>Caesalpinia bonduc</i>	26756595	3-acetoxy-a-caesalpin	o1c2c(cc1)C(O)(C1C(C2)C2(C)C(O)(C(C)(C)C(OC(=O)C)CC2=O)C(OC(=O)C)C1OC(=O)C)C
256	<i>Caesalpinia bonduc</i>	30670919	4,4'-dihydroxy-2'-methoxy-chalcone	COC1=CC(O)=CC=C1C(=O)\C=C\C1=CC=C(O)C=C1
257	<i>Caesalpinia bonduc</i>	26756595	6-deacetoxybonducellpin B	o1c2c(cc1)C(C1C(C2)C2(C)C(O)(C(O)C1O)C(CCC2=O)(C)C)C(OC)=O
258	<i>Caesalpinia bonduc</i>	19413105	bonducellpin E	o1c2c(cc1)C(C1C(C2)C2(C)C(O)(C(O)C1OC(=O)C)C(CCC2=O)(C)C)C(OC)=O
259	<i>Caesalpinia bonduc</i>	29979518	caesalmin C	o1c2c(cc1)C(C1C(C2)C2(C)C(O)(C(OC(=O)C)C1OC(=O)C)C(CCC2O)C(=O)C)(C)C)=C
260	<i>Caesalpinia bonduc</i>	19413105	caesalpinin B	o1c2c(cc1)C(O)(C1C(C2)C2(C)C(O)(C(OC(=O)C)C1OC(=O)C)C(CC2O)=C(C)C)C
261	<i>Caesalpinia bonduc</i>	29979518	caesalpinin MJ	o1c2c(cc1)C(C1C(C2)C2(C)C(O)(CC1OC(=O)C)C(CCC2OC(=O)C)(C)C)=C
262	<i>Caesalpinia bonduc</i>	19413105	caesalpinolide A	O1C2(O)C(=CC1=O)C(O)(C1C(C2)C2(C(C(CC2)(C)C)C(OC(=O)C)C1)C)C
263	<i>Caesalpinia bonduc</i>	19413105	cordylane A	o1c2c(cc1)C(C1C(C2)C2(C(C(CC2)(CO)C(OC(=O)C)C1)C)C
264	<i>Caesalpinia bonduc</i>	30670919	kaempferol-3-O-a-L-rhamnopyranosyl-(1>2)-b-D-xylopyranoside	O1c2c(C(=O)C(O[C@H]3OC[C@@H](O)[C@H](O)[C@H]3O[C@@H]3O[C@@H](C)[C@H](O)[C@@H](O)[C@H]3O)=C1c1ccc(O)cc1)c(O)cc(O)c2
265	<i>Caesalpinia bonduc</i>	30670919	kaempferol-3-O-b-D-xylopyranoside	O1c2c(C(=O)C(O[C@H]3OC[C@@H](O)[C@H](O)[C@H]3O)=C1c1ccc(O)cc1)c(O)cc(O)c2

266	<i>Caesalpinia bonduc</i>	19413105	neocaesalpin H	O1C2(O)C(=CC1=O)C(C1C(C2)C2(C(CC1)C(CCC2)(C(=O)[O-])C)C)C
267	<i>Caesalpinia bonduc</i>	19413105	neocaesalpin P	O1C=2C(=CC1)C(C1C(C=2)C2(CCCC(C)(C)C2(O)C(OC(=O)C=Cc2ccccc2)C1O)C)C
268	<i>Caesalpinia bonduc</i>	30670919	quercetin-3-methyl	[CH2]OC1=C(OC2=C(C(O)=CC(O)=C2)C1=O)C1=CC(O)=C(O)C=C1
269	<i>Calotropis gigantea</i>	26937251	9,11-dehydroergosterol peroxide	O1OC23C4CCC(C(C=CC(C(C)C)C)C)C4(CC=C2C2(C1(CC(O)CC2)C=C3)C)C
270	<i>Calotropis gigantea</i>	21815415	(24R)-24-ethylcholest-4-en-3-one	CC[C@H](CC[C@H](C)[C@H]1CC[C@H]2[C@H]3CCC4=CC(=O)CC[C@]4(C)[C@H]3CC[C@]12C)C(C)C
271	<i>Calotropis gigantea</i>	21815415	(24R)-3beta-hydroxy-24-ethylcholest-5-en-7-one	CC[C@H](CC[C@H](C)[C@H]1CC[C@H]2[C@H]3[C@H](CC[C@]12C)[C@H]1(C)CC[C@H](O)CC1=CC3=O)C(C)C
272	<i>Calotropis gigantea</i>	21815415	(24S)-24-ethylcholest-4,22-dien-3-one	CC[C@H](C=C[C@@H](C)[C@H]1CC[C@H]2[C@H]3CCC4=CC(=O)CC[C@]4(C)[C@H]3CC[C@]12C)C(C)C
273	<i>Calotropis gigantea</i>	20460804	12beta-hydroxycoroglaucigenin	O1CC(=CC1=O)C1CC2(O)C3C(CC(O)C12C)C1(C(CC(O)CC1)CC3)CO
274	<i>Calotropis gigantea</i>	21815415	3,5,8-trihydroxy-24-methylcholest-6,22-diene	CC(C)C(C)C=C[C@@H](C)[C@H]1CC[C@H]2[C@H]3[C@H]1(C)CC[C@H]1[C@H]2(O)C=CC2(O)CC(O)CC[C@]12C
275	<i>Calotropis gigantea</i>	28495081	5-hydroxymethylfurfurals	o1c(ccc1C=O)CO
276	<i>Calotropis gigantea</i>	21815415	6beta-hydroxy-24-ethylcholest-4,22-dien-3-one	CCC(C=C[C@@H](C)[C@H]1CC[C@H]2[C@H]3C[C@H](O)C4=CC(=O)CC[C@]4(C)[C@H]3CC[C@]12C)C(C)C

277	<i>Calotropis gigantea</i>	20460804	calotropagenin	O1CC(=CC1=O)C1CC C2(O)C3C(CCC12C)C1 (CC(O)C(O)CC1CC3)C =O
278	<i>Calotropis gigantea</i>	9549894	calotropin	C[C@H]1C[C@H](O)[C@@]2(O)O[C@H]3C[C@]4(C=O)[C@@H](CC[C@H]5[C@@H]4CC[C@]4(C)[C@H](CC[C@]5O)C4=CC(=O)OC4)C[C@H]3O[C@H]2O1
279	<i>Calotropis gigantea</i>	29936715	Calotroposide A	CC1C(C(CC(O1)OC2C(OC(CC2OC)OC3C(OC(CC3OC)OC4C(OC(CC4OC)OC5C(OC(CC5OC)OC6CCC7(C8CC(C9(C(CCC9(C8(CC=C7C6)O)O)C(=O)C)C)OC(=O)C1=CC=CC=C1)C)C)C)OC)O
280	<i>Calotropis gigantea</i>	29237703	cardenolide	CC12CCC3C(CCC4CC CCC34C)C1C=CC2C1 COC(=O)C1
281	<i>Calotropis gigantea</i>	29484762	Coroglaucigenin	O1CC(=CC1=O)C1CC C2(O)C3C(CCC12C)C1 (C(CC(O)CC1)CC3)CO
282	<i>Calotropis gigantea</i>	26937251	ergosterol peroxide	CC(C)[C@H](C)\C=C[C@H](C)[C@H]1CC[C@H]2[C@]1(C)CC[C@H]1[C@]3(C)CC[C@H](O)C[C@H]3OO[C@H]21C=C3
283	<i>Calotropis gigantea</i>	20460804	frugoside	O1C(C)C(O)C(O)C(O) C1OC1CC2CCC3C(CC C4(C)C(CCC34O)C3=C C(OC3)=O)C2(CC1)CO
284	<i>Calotropis gigantea</i>	1368420	isorhamnetin-3-O-[2-O-beta-D-galactopyranosyl-6-O-alpha-L-rhamnopyranosyl]- beta-D-glucopyranoside	O1c2c(C(=O)C(O[C@H]3O[C@H](CO[C@H]4O[C@H](C)[C@H](O)[C@H](O)[C@H](O)[C@H]4O)[C@H](O)[C@H](O)[C@H](O)[C@H]3O[C@H](CO)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H]3O)=C1c1cc(OC)c(O)cc1c(O)cc(O)c2

285	<i>Calotropis gigantea</i>	1368420	isorhamnetin-3-O-glucopyranoside	O1[C@H](CO)[C@@H](O)[C@@H](O)C1OC1=C(Oc2c(C1=O)c(O)cc(O)c2)c1cc(OC)c(O)cc1
286	<i>Calotropis gigantea</i>	1368420	isorhamnetin-3-O-rutinoside	O1C(COC2OC(C)C(O)C(O)C(O)C(O)C1OC1=C(Oc2c(C1=O)c(O)cc(O)c2)c1cc(OC)c(O)cc1
287	<i>Calotropis gigantea</i>	20460804	R-(-)-mevalonolactone	C[C@H]1(O)CCOC(=O)C1
288	<i>Calotropis gigantea</i>	1368420	taraxasteryl acetate	CC1C2C3CCC4C5(CC C(C)C5CCC4(C3(CC2(CCC1=C)C)C)(C)C)OC(=O)C)C
289	<i>Capsicum annuum</i>	29934165	isoquercetin	OC[C@H]1O[C@H](OC2=C(OC3=CC(O)=CC(O)=C3C2=O)C2=CC=C(O)C(O)=C2)[C@H](O)[C@@H](O)[C@@H]1O
290	<i>Capsicum annuum</i>	11556809	1-deoxycapsidiol	C[C@H]1[C@H](O)CCC2=CC[C@H](C[C@]12C)C(C)=C
291	<i>Capsicum annuum</i>	31022566	6-gingerol	CCCCCC(O)CC(=O)C CC1=CC=C(OC)C(O)=C1
292	<i>Capsicum annuum</i>	31022566	6-shogaol	CCCCC\ C=C/C/C(=O)CC C1=CC=C(O)C(OC)=C1
293	<i>Capsicum annuum</i>	24065101	alpha-carotene	C\C(\ C=C\ C=C(/C)\ C=C\ C1C(C)=CCCC1(C)C)=C/C=C/C=C(\ C)/C=C/C1=C(C)CCCC1(C)C
294	<i>Capsicum annuum</i>	27517345	altenuene	CO C1=CC(O)=C2C(=O)O[C@]3(C)C[C@H](O)[C@H](O)C=C3C2=C1
295	<i>Capsicum annuum</i>	17587684	caffeoyleputrescine	Oc1cc(ccc1O)C=CC(=O)NCCCC[NH3+]
296	<i>Capsicum annuum</i>	31027574	capsaicin (8-methyl-N-vanillyl-6-nonenamide)	O(C)c1cc(ccc1O)CNC(=O)CCCC=CC(C)C
297	<i>Capsicum annuum</i>	30820539	capsanthin	C\C(\ C=C\ C=C(/C)\ C=C\ C(=O)[C@]1(C)C[C@H](O)CC1(C)C)=C/C=C/C=C(\ C)/C=C/C=C/

				C(\C)/C=C/C1=C(C)C[C@@H](O)CC1(C)C
298	<i>Capsicum annuum</i>	24065101	capsanthin-5,6-epoxide	O1C2(C=CC(=CC=CC(=CC=CC=C(C=CC(=O)C3(CC(O)CC3(C)C)C)C)C(CC(O)CC12C)(C)C
299	<i>Capsicum annuum</i>	7765694	Capsicoside A	C[C@H](CC[C@]1(O)O[C@H]2C[C@H]3[C@@H]4CC[C@H]5C[C@@H](O[C@@H]6O[C@H](CO)[C@@H](O)[C@H](O[C@@H]7O[C@H](CO)[C@@H](O)[C@H]8O[C@H](CO)[C@@H](O)[C@H]9O[C@H](CO)[C@@H](O)[C@H]9O)[C@H]8O[C@@H]8O[C@H](CO)[C@@H](O)[C@H](O)[C@H]8O)[C@H](O)[C@H]7O)[C@H]6O)[C@H](O)C[C@]5(C)[C@H]4CC[C@]3(C)[C@H]2[C@H]1C)CO[C@H]1O[C@H](CO)[C@@H](O)[C@H](O)[C@H]1O
300	<i>Capsicum annuum</i>	24065101	capsorubin	C\C(\C=C\ C=C(\C)\C=C\ C(=O)[C@]1(C)C[C@@H](O)CC1(C)C)=C/C=C/C=C(\C)/C=C/C=C\ C(=O)[C@]1(C)C[C@@H](O)CC1(C)C
301	<i>Capsicum annuum</i>	28721659	Coumarin	O=C1OC2=CC=CC=C2C=C1
302	<i>Capsicum annuum</i>	18222931	delphinidin-3-p-coumaroyl-rutinoside-5-glucoside	CC1C(C(C(C(O1)OCC2C(C(C(C(O2)OC3=C([O+])=C4C=C(C=C(C4=C3)OC5C(C(C(C(O5)CO)O)O)O)O)C6=CC(=C(C(=C6)O)O)O)O)O)O)O)OC(=O)C=CC7=C=C(C=C7)O

303	<i>Capsicum annuum</i>	31022566	dihydrocapsaicin	<chem>COc1=CC(CNC(=O)CCCCC(C)C)=CC=C1O</chem>
304	<i>Capsicum annuum</i>	20826626	Dihydrocapsiate	<chem>COc1=CC(COC(=O)CCCCC(C)C)=CC=C1O</chem>
305	<i>Capsicum annuum</i>	30449166	homocapsaicin	<chem>CCC(C)\C=C\CCCCC(=O)NCC1=CC=C(O)C(OC)=C1</chem>
306	<i>Capsicum annuum</i>	30449166	homodihydrocapsaicin I	<chem>O(C)c1cc(ccc1O)CNC(=O)CCCCCCCC(C)C</chem>
307	<i>Capsicum annuum</i>	30449166	homodihydrocapsaicin II	<chem>CCC(C)CCCCCCC(=O)NCC1=CC(=C(C=C1)O)OC</chem>
308	<i>Capsicum annuum</i>	29934165	kaempferol-3-glucoside	<chem>OC[C@H]1O[C@H](OC2=C(OC3=CC(O)=CC(O)=C3C2=O)C2=CC=C(O)C=C2)[C@H](O)[C@@H](O)[C@@H]1O</chem>
309	<i>Capsicum annuum</i>	30724264	lutein	<chem>C/C(\C=C\C=C(/C)\C=C\C[C@H]1C(C)=C[C@H](O)CC1(C)C)=C/C=C(\C)/C=C/C=C(\C)/C=C/C1=C(C)C[C@H](O)CC1(C)C</chem>
310	<i>Capsicum annuum</i>	29934165	myricetin	<chem>OC1=CC(O)=C2C(OC(=C(O)C2=O)C2=CC(O)=C(O)C(O)=C2)=C1</chem>
311	<i>Capsicum annuum</i>	18222931	neoxanthin	<chem>C/C(\C=C\C=C(/C)\C=C\C[C@H]12O[C@H]1(C)C[C@H](O)CC2(C)C)=C/C=C/C=C(\C)/C=C/C=C(\C)C=C=C1C(C)(C)C[C@H](O)C[C@H]1(C)O</chem>
312	<i>Capsicum annuum</i>	30449166	nordihydrocapsaicin	<chem>COc1=CC(CNC(=O)CCCC(C)C)=CC=C1O</chem>
313	<i>Capsicum annuum</i>	30449166	N-vanillyl-4,8-dimethylnonanamide	<chem>COc1=CC(CNC(=O)CC(C)CCCC(C)C)=CC=C1O</chem>
314	<i>Capsicum annuum</i>	30449166	N-vanillyl-4E,6E-dien-8-methylnonanamide	<chem>CC(C)CCCCCCC(NCC1=CC=C(O)C(OC)=C1)=O</chem>
315	<i>Capsicum annuum</i>	30449166	N-vanillyldecanamide	<chem>CCCCCC(=O)NCC1=CC=C(O)C(OC)=C1</chem>

316	<i>Capsicum annuum</i>	30449166	N-vanillyloctanamide	CCCCCCCC(=O)NCC1=CC=C(O)C(OC)=C1
317	<i>Capsicum annuum</i>	30724264	p-hydroxybenzoic acid	OC(=O)C1=CC=C(O)C=C1
318	<i>Capsicum annuum</i>	22417420	phytic acid	OP(O)(=O)O[C@H]1[C@H](OP(O)(O)=O)[C@H](OP(O)(O)=O)[C@H](OP(O)(O)=O)[C@H](OP(O)(O)=O)[C@H](OP(O)(O)=O)[C@H]1OP(O)(O)=O
319	<i>Capsicum annuum</i>	30724264	phytoene	CC(C)=CCC\ C(C)=C\ C C\ C(C)=C\ CC\ C(C)=C\ C=C\ C=C(/C)CC\ C=C(/C)CC\ C=C(/C)CCC=C(C)C
320	<i>Capsicum annuum</i>	27283607	quercetin 3-O-rhamnoside	C[C@@H]1O[C@@H](OC2=C(OC3=CC(O)=CC(O)=C3C2=O)C2=C C=C(O)C(O)=C2)[C@H](O)[C@H](O)[C@H]1O
321	<i>Capsicum annuum</i>	27283607	quercetin 3-O-rhamnoside-7-O-glucoside	O1C(CO)C(O)C(O)C(O)C(O)C1Oc1cc(O)c2c(OC(=C(OC3OC(C)C(O)C(O)C3O)C2=O)c2cc(O)c(O)cc2)c1
322	<i>Capsicum annuum</i>	30724264	quercetin-3-glucoside	OC[C@@H](O)[C@H]1O[C@@H](OC2=C(O)C3=CC(O)=CC(O)=C3C2=O)C2=CC=C(O)C(O)=C2)[C@H](O)[C@H]1O
323	<i>Capsicum annuum</i>	30724264	sinapic acid	COCl=CC(\ C=C\ C(O)=O)=CC(OC)=C1O
324	<i>Capsicum annuum</i>	27517345	tentoxin	CC(C)C[C@@H]1NC(=O)[C@H](C)N(C)C(=O)CNC(=O)\ C(=C\ C2=CC=CC=C2)N(C)C1=O
325	<i>Capsicum annuum</i>	27517345	tenuazonic acid	CC[C@H](C)[C@@H]1NC(=O)C(C(C)=O)=C1O
326	<i>Capsicum annuum</i>	18222931	violaxanthin	C\ C(\ C=C\ C=C(/C)\ C=C\ C[C@@]12O[C@H]1(C)C[C@H](O)CC2(C)C)=C/C=C/C=C(\ C)/C=C/C=C(\ C)/C=C/[C@@]12O[C@H]1(C)C[C@H](O)CC2(C)C

327	<i>Capsicum annuum</i>	29934165	vitexin	<chem>OC[C@H]1O[C@H]([C@H](O)[C@@H](O)[C@@H]1O)C1=C2OC(=CC(=O)C2=C(O)C=C1O)C1=CC=C(O)C=C1</chem>
328	<i>Capsicum annuum</i>	24065101	zeaxanthin	<chem>C\C(\C=C\C=C(\C)\C=C\CC1=C(C)C[C@@H](O)CC1(C)C)=C/C=C/C=C(\C)/C=C/C1=C(C)C[C@@H](O)CC1(C)C</chem>
329	<i>Capsicum annuum</i>	24065101	β -carotene	<chem>CC1=C(C(CCC1)(C)C)C=CC(=CC=CC(=CC=CC=C(C)C=CC2=C(CCCC2(C)C)C)C)C</chem>
330	<i>Capsicum annuum</i>	30724264	β -cryptoxanthin	<chem>CC1=C(C(CCC1)(C)C)C=CC(=CC=CC(=CC=CC=C(C)C=CC2=C(CC(CC2(C)C)O)C)C)C</chem>
331	<i>Coccinia grandis</i>	29062847	7-octadecanal	<chem>CCCCCCCCCC(=O)CCCC</chem>
332	<i>Coccinia grandis</i>	29062847	n-eicosane	<chem>CCCCCCCCCC(=O)CCCC</chem>
333	<i>Coccinia grandis</i>	29062847	n-tetracosane	<chem>CCCCCCCCCC(=O)CCCC</chem>
334	<i>Coccinia grandis</i>	29062847	tricosane	<chem>CCCCCCCCCC(=O)CCCC</chem>
335	<i>Crocus sativus</i>	19473679	2,2,2-trimethyl-2-cyclohexene-1,4-dione (4-oxoisophorone)	<chem>O=C1C(C)(C)(C)=CC(CC1)=O</chem>
336	<i>Crocus sativus</i>	26922339	2,2,6-trimethyl-1,4-cyclohexanedione	<chem>CC1CC(=O)CC(C)(C)C1=O</chem>
337	<i>Crocus sativus</i>	26922339	2,6,6-trimethyl-4-hydroxy-1-cyclohexene-1-carbaldehyde (HTCC))	<chem>O=CC1=C(C)CC(O)CC1(C)C</chem>
338	<i>Crocus sativus</i>	26922339	2,6,6-trimethyl-4-oxo-2-cyclohexen-1-carbaldehyde	<chem>CC1=CC(=O)CC(C)(C)C1=O</chem>
339	<i>Crocus sativus</i>	22079266	4-hydroxydihydro-2(3H)-furanone	<chem>OC1COC(=O)C1</chem>
340	<i>Crocus sativus</i>	26922339	alpha-isophorone	<chem>O=C1CC(CC(=C1)C)(C)C</chem>
341	<i>Crocus sativus</i>	19473679	beta-cyclocitral	<chem>CC1=C(C=O)C(C)(C)C1</chem>
342	<i>Crocus sativus</i>	19473679	beta-ionone	<chem>CC(=O)\C=C\C1=C(C)</chem>

				CCCC1(C)C
343	<i>Crocus sativus</i>	30599111	crocetin	C\ C(\ C=C\ C=C(/C)C(O)=O)=C/C=C/C=C(\ C)/C=C/C=C(\ C)C(O)=O
344	<i>Crocus sativus</i>	30599111	crocin	C\ C(\ C=C\ C=C(/C)C(=O)O[C@@H]1O[C@H](CO[C@@H]2O[C@H](CO)[C@@H](O)[C@H](O)[C@H]2O)[C@@H](O)[C@H](O)[C@H]1O)=C/C=C/C=C(\ C)/C=C/C=C(\ C)C(=O)O[C@@H]1O[C@H](CO[C@@H]2O[C@H](CO)[C@@H](O)[C@H](O)[C@H]2O)[C@@H](O)[C@H](O)[C@H]1O
345	<i>Crocus sativus</i>	19473679	hydroxy-beta-ionone	CC1=C(\ C=C\ C(=O)CO)C(C)(C)CCC1
346	<i>Crocus sativus</i>	26922339	ketoisophorone	O=C1C(CC(=O)C=C1C)(C)C
347	<i>Crocus sativus</i>	21639689	lauric acid	CCCCCCCCCC(O)=O
348	<i>Crocus sativus</i>	18401844	naringenin	OC1=CC=C(C=C1)[C@@H]1CC(=O)C2=C(O)C=C(O)C=C2O1
349	<i>Crocus sativus</i>	29484754	petunidin	CO C1=CC(=CC(O)=C1O)C1=[O+]C2=CC(O)=CC(O)=C2C=C1O
350	<i>Crocus sativus</i>	26922339	phenylethyl alcohol	OCCC1=CC=CC=C1
351	<i>Crocus sativus</i>	30575987	picrocrocin	CC1=C(C=O)C(C)(C)C[C@@H](C1)O[C@@H]1O[C@H](CO)[C@@H](O)[C@H](O)[C@H](O)[C@H]1O
352	<i>Crocus sativus</i>	26922339	safranal	CC1=C(C=O)C(C)(C)C=C1
353	<i>Croton tiglium</i>	28925158	methyl (9S,10R,11E,13R)-9,10,13-trihydroxyoctadec-11-enoate	CCCCC[C@@H](O)\C=C\[C@@H](O)[C@@H](O)CCCCCCCC(=O)OC
354	<i>Croton tiglium</i>	28925158	(9S,10R,11E,13R)-9,10,13-trihydroxyoctadec-11-enoic acid	CCCCC[C@@H](O)\C=C\[C@@H](O)[C@@H](O)CCCCCCCC(=O)O

355	<i>Croton tiglum</i>	28499304	12-O-(2-methyl)-butyrylphorbol-13-aetate	O=C1[C@]2(O)[C@@H](C=C1C)[C@]1(O)[C@H]([C@H]3[C@@](OC(=O)C4=NC=C4)([C@H](OC(=O)C(CC)C)[C@H]1C)C3(C)C)C=C(C2)CO
356	<i>Croton tiglum</i>	28925158	12-O-(a-methyl)butyrylphorbol-13-decanoate	O=C1[C@]2(O)[C@@H](C=C1C)[C@]1(O)[C@H]([C@H]3[C@@](OC(=O)CCCCCCCC)([C@H](OC(=O)C(CC)C)[C@H]1C)C3(C)C)C=C(C2)CO
357	<i>Croton tiglum</i>	28499304	12-O-Tiglylphorbol-13-acetate	O=C1[C@]2(O)[C@@H](C=C1C)[C@]1(O)[C@H]([C@H]3[C@@](OC(=O)C)([C@H](OC(=O)\C(=C\CC)\C)[C@H]1C)C3(C)C)C=C(C2)CO
358	<i>Croton tiglum</i>	28925158	12-O-tiglylphorbol-13-decanoate	O=C1[C@]2(O)[C@@H](C=C1C)[C@]1(O)[C@H]([C@H]3[C@@](OC(=O)CCCCCCCC)([C@H](OC(=O)\C(=C\CC)\C)[C@H]1C)C3(C)C)C=C(C2)CO
359	<i>Croton tiglum</i>	28499304	12-O-tiglylphorbol-13-isobutyrate	O(C(=O)C(C)C)C12C(C3C=C(CC4(O)C(C=C(C)C4=O)C3(O)C(C)C1OC(=O)C(=CC)C)CO)C2(C)C
360	<i>Croton tiglum</i>	28925158	4(1H)-quinolinone	O=C1C=CNC2=C1C=C C=C2
361	<i>Croton tiglum</i>	28925158	5-hydroxy-2-pyridinemethanol	OCC1=NC=C(O)C=C1
362	<i>Croton tiglum</i>	28925158	bis(2,3-dihydroxypropyl)nonanedioate	OCC(O)COC(=O)CCCCCCC(=O)OCC(O)CO
363	<i>Croton tiglum</i>	25538350	crotonic acid	C C=C C(O)=O
364	<i>Croton tiglum</i>	17701561	crotonine or 2-(furan-2-yl)-5-(2,3,4-trihydroxy-butyl)-1,4-diazine	o1cccc1- c1ncc(nc1)CC(O)C(O)CO
365	<i>Croton tiglum</i>	30534799	crotonol B	CC=CCO
366	<i>Croton tiglum</i>	23252276	eicosenoic acid	CCCCCCCCCCCCCC CCC C=C/C(O)=O

367	<i>Croton tiglum</i>	23252276	fenchyl alcohol	CC1(C)[C@@@H]2CC[C@@](C)(C2)[C@@@H]1O
368	<i>Croton tiglum</i>	23252276	isoborneol	CC1(C)[C@@@H]2CC[C@]1(C)[C@@H](O)C2
369	<i>Croton tiglum</i>	24948847	Phorbol 12-myristate 13-acetate (PMA)	O(C(=O)C)C12C(C3C=C(CC4(O)C(C=C(C)C4=O)C3(O)C(C)C1OC(=O)CCCCCCCCCCCC)CO)C2(C)C
370	<i>Croton tiglum</i>	12816455	Phorbol 12-octanoate-13-acetate	O=C1[C@]2(O)[C@@H](C=C1C)[C@]1(O)[C@H]([C@H]3[C@@](OC(=O)C)([C@H](OC(=O)CCCCCCC)[C@H]1C)C3(C)C)C=C(C2)CO
371	<i>Cymbopogon martini</i>	21893402	cinnamaldehyde	O=C\ C=C\ C1=CC=CC=C1
372	<i>Cymbopogon martini</i>	21893402	citral	CC(C)=CCC\ C(C)=C\ C=O
373	<i>Cymbopogon martini</i>	30277563	geraniol	CC(C)=CCC\ C(C)=C\ C O
374	<i>Cymbopogon martini</i>	17987504	nerol	CC(C)=CCC\ C(C)=C/C O
375	<i>Cymbopogon martini</i>	17987504	piperitone	CC(C)C1CCC(C)=CC1=O
376	<i>Cymbopogon martini</i>	21893402	eugenol	O(C)c1cc(ccc1O)CC=CC=C
377	<i>Cymbopogon winterianus</i>	29205073	citronella	CC(CCC=C(C(C)C)CC=O
378	<i>Cymbopogon winterianus</i>	30097258	citronellol	CC(CCO)CCC=C(C)C
379	<i>Cymbopogon winterianus</i>	30097258	linalool	CC(C)=CCCC(C)(O)C=C
380	<i>Datura stramonium</i>	22568232	1-Acetyl-7-hydrox-beta-carbol-ine	Oc1cc2[nH]c3c(c2cc1)cnc3C(=O)C
381	<i>Datura stramonium</i>	20858536	3-(3'-methoxytropoyloxy)tropane	O(C(=O)C(CO)c1cc(OC)ccc1)C1CC2[NH+](C(C1)CC2)C
382	<i>Datura stramonium</i>	20858536	3,7-dihydroxy-6-(2'-methylbutyryloxy)tropane	O(C(=O)C(CC)C)C1C2[NH+]((C(CC(O)C2)C1)O)C
383	<i>Datura stramonium</i>	20858536	3,7-dihydroxy-6-propionyloxytropane	O(C(=O)CC)C1[C@H]2[NH+]([C@H])(CC(O)C2)C1O)C
384	<i>Datura stramonium</i>	20858536	3b-tropoyloxy-6b-isovaleroyloxytropane	[H][C@@@]12C[C@@H](OC(C(C3=CC=CC=C3)CO)=O)C[C@@@]([C]

				$\text{@ @ H]}(\text{OC}(\text{CC}(\text{C})\text{C})=\text{O})\text{C1})(\text{N2C})[\text{H}]$
385	<i>Datura stramonium</i>	27450719	3-piperidinemethanol	OCC1CCCNC1
386	<i>Datura stramonium</i>	20858536	3-tigloyloxy-6,7-epoxytropane	O1C2C3[NH+](C(CC(O C(=O)C(=CC)C)C3)C12)C
387	<i>Datura stramonium</i>	20858536	3-tigloyloxy-6-isobutyryloxy-7-hydroxytropane	O(C(=O)C(C)C)C1C2[NH+](C(CC(OC(=O)C(=CC)C)C2)C1O)C
388	<i>Datura stramonium</i>	20858536	3-tropoyloxy-6-isobutyryloxytropane	O(C(=O)C(C)C)C1C2[NH+](C(C1)CC(OC(=O)C(CO)c1ccccc1)C2)C
389	<i>Datura stramonium</i>	20858536	6,7-dehydro-3-tigloyloxytropane	O(C(=O)C(=CC)C)C1C2[NH+](C(C1)C=C2)C
390	<i>Datura stramonium</i>	20858536	6,7-dehydrohyoscyamine	O(C(=O)C(CO)c1ccccc1)C1CC2[NH+](C(C1)C=C2)C
391	<i>Datura stramonium</i>	20858536	6,7-dehydrotropine	OC1CC2[NH+](C(C1)C=C2)C
392	<i>Datura stramonium</i>	22568232	7-hydroxy-beta-carbolinel-propionic acid	Oc1cc2[nH]c3c(c2cc1)ccn3 C=C\ C(=O)[O-]
393	<i>Datura stramonium</i>	27450719	amphetamine	CC(N)CC1=CC=CC=C1
394	<i>Datura stramonium</i>	29359500	apoatropine	CN1C2CCC1CC(C2)OC(=O)C(=C)C1=CC=C C=C1
395	<i>Datura stramonium</i>	22568232	cleomiscosin A	COCl=CC(=CC=C1O)[C@H]1OC2=C(OC)C=C3C=CC(=O)OC3=C2O[C@H]1CO
396	<i>Datura stramonium</i>	20858536	cyclotropine	O1C2CC3[NH+](C(C2)CC3)C1
397	<i>Datura stramonium</i>	22568232	daturadiol	OC1CCC2(C(C1(C)C)C(O)CC1(C2CC=C2C3C C(CCC3(CCC12C)C)(C)C)C)C
398	<i>Datura stramonium</i>	22568232	daturaolone	OC1C2C(C)(C)C(=O)CC2(C2CC=C3C4CC(C CC4(CCC3(C)C2(C1)C)C)C)C
399	<i>Datura stramonium</i>	22568232	fraxetin	COCl=C(O)C(O)=C2OC(=O)C=CC2=C1
400	<i>Datura stramonium</i>	23506688	hyoscamine	O(C(=O)C(CO)c1ccccc1)C1CC2[NH+](C(C1)CC2)C

401	<i>Datura stramonium</i>	22568232	hyoscyamilactol	CC(C1CCC2C1(CCC3C2C4C(O4)C5(C3(C(=O)C=CC5)C)OC)C6C7(C(O7)(C(O6)O)C)C)
402	<i>Datura stramonium</i>	30560886	hyoscyamine	CN1[C@H]2CC[C@@H]1C[C@@H](C2)OC(=O)[C@H](CO)C1=CC=C1
403	<i>Datura stramonium</i>	24197002	Lubimin	C[C@@H]1C[C@H](O)C[C@H](C=O)[C@]1CC[C@H](C1)C(C)=C
404	<i>Datura stramonium</i>	22568232	N-trans-feruloyl tryptamine	O(C)c1cc(ccc1O)C=CC(=O)NCCc1c2c([nH]c1)cccc2
405	<i>Datura stramonium</i>	29359500	physoperuvine	CN1C2CCC1(O)CCC2
406	<i>Datura stramonium</i>	29359500	pseudotropine	CN1[C@H]2CC[C@@H]1C[C@@H](O)C2
407	<i>Datura stramonium</i>	31020486	scopolamine	CN1[C@H]2C[C@H](C[C@@H]1[C@H]1O[C@@H]2)OC(=O)[C@H](CO)C1=CC=CC=C1
408	<i>Datura stramonium</i>	22568232	scopoletin	CO C1=C(O)C=C2OC(=O)C=CC2=C1
409	<i>Datura stramonium</i>	27450719	spermine	NCCCNCCCCNCCCN
410	<i>Datura stramonium</i>	29359500	tropine	CN1[C@H]2CC[C@@H]1C[C@H](O)C2
411	<i>Datura stramonium</i>	22568232	umckalin	O1c2c(C=CC1=O)c(OC)c(OC)c(O)c2
412	<i>Ferula assa-foetida</i>	23497874	(E)-1-propenyl sec-butyl disulfide	CCC(SS/C=C/C)C
413	<i>Ferula assa-foetida</i>	12444696	(E)-3-methylsulfinyl-2-propenyl sec-butyl disulfide (foetisulfide A)	CCC(C)SSCC=CS(=O)C
414	<i>Ferula assa-foetida</i>	23497874	(Z)-1-propenyl sec-butyl disulfide	CCC(SS/C=C\C)C
415	<i>Ferula assa-foetida</i>	23320824	1, 2-dithiolane	C1CSSC1
416	<i>Ferula assa-foetida</i>	23497874	10-epi- γ -eudesmol	OC(C)(C)[C@H]1CC2=C(C)CCC[C@@]2(C)C C1
417	<i>Ferula assa-foetida</i>	21404434	2,3,4-trimethylthiophene	CC1=C(C)C(C)=CS1
418	<i>Ferula assa-foetida</i>	12444696	3,4,5-trimethyl-2-(methylsulfinyloxymethoxythyl)thiophene	s1c(COS(=O)C)c(C)c(C)c1C

			(foetithiophene B)	
419	<i>Ferula assa-foetida</i>	12444696	3,4,5-trimethyl-2-thiophenecarboxylic acid (foetithiophene A)	s1c(C(=O)[O-])c(C)c(C)c1C
420	<i>Ferula assa-foetida</i>	21425676	7-(((E)-5-((1S,3S,6S)-3,6-dihydroxy-2,2,6-trimethylcyclohexyl)-3-methylpent-2-en-1-yl)oxy)-2H-chromen-2-one (asimafoetidnol)	O1c2cc(OC\ C=C(\ CC[C@@H]3[C@@](O)(CC[C@H](O)C3(C)C)C)/C)ccc2C=CC1=O
421	<i>Ferula assa-foetida</i>	23701832	7-isopentenyloxycoumarin	O1c2cc(OCCC(C)=C)cccc2C=CC1=O
422	<i>Ferula assa-foetida</i>	23701832	acantrifoside E	COCl=CC(\ C=C\ C)=C C(OC)=C1O[C@@H]1O[C@H](CO)[C@@H](O)[C@H](O)[C@H]1O
423	<i>Ferula assa-foetida</i>	21404434	a-terpinyl acetate	CC(=O)OC(C)(C)C1CC(C(C)=CC1=O
424	<i>Ferula assa-foetida</i>	25237347	badrakemin acetate	CC(=O)OC1CCC2(C(C1(C)C)CCC(=C)C2COCC3=CC4=C(C=C3)C=CC(=O)O4)C
425	<i>Ferula assa-foetida</i>	23701832	conferone	O1c2cc(OCC3C4(C(CC=C3)C(C)(C)C(=O)CC4)C)ccc2C=CC1=O
426	<i>Ferula assa-foetida</i>	23701832	diversin	O1c2cc(OCCC(=CC(=O)CC(C)=C)C)ccc2C=CC1=O
427	<i>Ferula assa-foetida</i>	23701832	farnesiferol A	CC1(C)[C@H](O)CC[C@@]2(C)[C@@H](COCC3=CC=C4OC(=O)C=CC4=C3)C(=C)CC[C@H]12
428	<i>Ferula assa-foetida</i>	21749391	ferulsinaic acid	O1c2cc(OCC3C(CCC(=O)[O-])(C)C(CC3C)C=C(C)C)ccc2C=CC1=O
429	<i>Ferula assa-foetida</i>	25753585	Galbanic acid	C[C@H]1CCC([C@H](CCC(=O)O)[C@@]1(C)COCC1=CC=C2OC(=O)C=CC2=C1)=C(C)C
430	<i>Ferula assa-foetida</i>	25237347	kellerin	O1c2cc(OCC3C4(C(CC3(O)C)C(C)(C)C(OC(=O)C)CC4)C)ccc2C=CC1=O
431	<i>Ferula assa-foetida</i>	23701832	mogoltadone	O1c2cc(OCC3C4(C(CC3=C)C(C)(C)C(=O)C)CC4)C)ccc2C=CC1=O

				C4)C)ccc2C=CC1=O
432	<i>Ferula assa-foetida</i>	23701832	tschimgine	CC1(C2CCC1(C(C2)OC(=O)C3=CC=C(C=C3)OC)C
433	<i>Ferula assa-foetida</i>	27703798	umbelliprenin	CC(C)=CCC\ C(C)=C\ C C\ C(C)=C\ COC1=CC=C2C=CC(=O)OC2=C1
434	<i>Ferula assa-foetida</i>	21404434	verbenone	CC1=CC(=O)[C@H]2[C[C@H]1C2(C)C
435	<i>Ferula assa-foetida</i>	23701832	herniarin	COc1ccc2C=CC(=O)Oc2c1
436	<i>Ficus religiosa</i>	29142437	a-amyrin acetate	C[C@H]1CC[C@]2(C)CC[C@]3(C)C(=CC[C@H]4[C@H]5(C)C C[C@H](OC(C)=O)C(C)(C)[C@H]5CC[C@H]34C)[C@H]2[C@H]1C
437	<i>Ficus religiosa</i>	29142437	bergaptol	OC1=C2C=CC2=CC2=C1C=CC(=O)O2
438	<i>Ficus religiosa</i>	29142437	Ergost-5-en-3beta-ol	CC(C)C(C)CC[C@H]1(C)[C@H]1CC[C@H]2[C@H]3CC=C4C[C@H](O)CC[C@H]4(C)[C@H]3CC[C@H]12C
439	<i>Ficus religiosa</i>	29142437	germacrene	CC(C)[C@H]1CC\ C(C)=C\ CC\ C(C)=C\ C1
440	<i>Ficus religiosa</i>	29142437	lanosterol	C[C@H](CCC=C(C)C)[C@H]1CC[C@H]2(C)C3=C(CC[C@H]12C)[C@@H]1(C)CC[C@H](O)C(C)(C)[C@H]1CC3
441	<i>Ficus religiosa</i>	14998314	oxalic acid	OC(=O)C(O)=O
442	<i>Ficus religiosa</i>	20837125	pentylenetetrazole	C1CCN2N=NN=C2CC1
443	<i>Ficus religiosa</i>	20837125	picrotoxin	CC(=C)[C@H]1C2OC(=O)C1[C@H]1CC[C@H]2(C)C3=C(CC[C@H]12C)[C@@H]1(C)CC[C@H](O)C(C)(C)[C@H]1CC3
444	<i>Hyoscyamus niger</i>	11858758	1,24-tetracosanediol diferulate	COc1=CC(C=CC(=C1)C=CC(=O)OCCCCCCCCCCCCCCCC=CCOC(=O)C=CC2=CC(=C(C=C2)O)OC)O

445	<i>Hyoscyamus niger</i>	10543915	16alpha-acetoxyhyoscymilactol	CC(C1CC2(C(O2)(C(O1)O)C)C)C3(CC4C3(CCC5C4C6C(O6)C7(C5(C(=O)C=CC7)C)O)C)OC(=O)C
446	<i>Hyoscyamus niger</i>	11858758	1-O-(9Z,12Z-octadecadienoyl)glycerol	CCCCC\ C=C/C\C=C/C/C=CCCCC(=O)OCC(O)CO
447	<i>Hyoscyamus niger</i>	11858758	1-O-(9Z,12Z-octadecadienoyl)-2-O-(9Z,12Z-octadecadienoyl)glycerol	CCCCC\ C=C/C\C=C/C/C=CCCCCCC(=O)OCC(CO)OC(=O)CCCCCCC\ C=C/C\C=C/C/CCCCC
448	<i>Hyoscyamus niger</i>	11858758	1-O-(9Z,12Z-octadecadienoyl)-3-O-(9Z-octadecenoyl)glycerol	CCCCCCCC\ C=C/CCC CCCCC(=O)OCC(O)C OC(=O)CCCCCCC\ C=C/C\C=C/CCCCC
449	<i>Hyoscyamus niger</i>	11858758	1-O-(9Z,12Z-octadecadienoyl)-3-O-nonadecanoyl glycerol	OC(COC(CCCCCC)CCCCCCCC)=O)C OC(CCCCCC/C=C\C/C=C\CCCC)=O
450	<i>Hyoscyamus niger</i>	11858758	1-O-octadecanoyl glycerol	CCCCCCCCCCCCCC CCCC(=O)OCC(O)CO
451	<i>Hyoscyamus niger</i>	19401911	balanophonin	O[C@H]1[C@H](CO[C@H]2CC(=O)C3=C2C2=C(O)C(O)=C(O)C=C2C(=O)O3)O[C@H](OC(=O)\ C=C\ C2=CC=C(O)C(O)=C2)[C@H](O)[C@H]1O
452	<i>Hyoscyamus niger</i>	11858758	cannabisin D	O(C)c1cc(ccc1O)C1c2cc(O)c(OC)cc2C=C(C(=O)NCCc2ccc(O)cc2)C1C(=O)NCCc1ccc(O)cc1
453	<i>Hyoscyamus niger</i>	11858758	cannabisin G	COC1=C(C=CC(=C1)C=C(C=CC2=CC(=C(C=C2)O)OC)C(=O)NCC3=CC=C(C=C3)O)C(=O)NCCC4=CC=C(C=C4)O)O
454	<i>Hyoscyamus niger</i>	19720117	cleomiscosin B	O1c2c(OC(CO)C1c1cc(OC)c(O)cc1)c(OC)cc1C=CC(Oc12)=O
455	<i>Hyoscyamus niger</i>	24322778	cuscohygrine	CN1CCC[C@H]1CC(=O)C[C@H]1CCCN1C
456	<i>Hyoscyamus niger</i>	10543915	daturalactone-4	CC(C1CCC2C1(CCC3C2C4C(O4)C5(C3(C(=O)C=CC5)O)C)C6C

				C7(C(O7)(C(=O)O6)C)C
457	<i>Hyoscyamus niger</i>	11858758	grossamide	COCl=CC(\C=C\ C(=O)NCCC2=CC=C(O)C=C2)=CC2=C1O[C@H]([C@H]2C(=O)NCCC1=CC=C(O)C=C1)C1=CC=C(O)C(OC)=C1
458	<i>Hyoscyamus niger</i>	19401911	hyoscyamal	O(C(=O)C(CO)c1cccc1)C1CC2([NH+](C(C1)CC2)C)C=O
459	<i>Hyoscyamus niger</i>	11858758	hyoscyamide	O(C)c1cc(ccc1O)C=C(C=Cc1cc(OC)c(O)cc1)C(=O)NCCc1ccc(O)cc1)C(=O)NCCc1ccc(O)cc1
460	<i>Hyoscyamus niger</i>	16595960	Hyosgerin	O1c2c(OC(COC(=O)C)C1c1cc(OC)c(O)cc1)c(OC)cc1C=CC(Oc12)=O
461	<i>Hyoscyamus niger</i>	19693762	littorine	CN1[C@H]2CC[C@@H]1C[C@H](C2)OC(=O)[C@H](O)CC1=CC=CC=C1
462	<i>Hyoscyamus niger</i>	11858758	N-trans-feruloyl tyramine	COCl=C(C=CC(=C1)C=CC(=O)NCCC2=CC=C(C=C2)O)O
463	<i>Hyoscyamus niger</i>	19401911	pongamoside C	COCl=C(OC2=C(C=C(O[C@@H]3OC(CO)[C@@H](O)[C@H](O)C3)O)C3=C2C=CO3)C1=O)C1=CC=CC=C1
464	<i>Hyoscyamus niger</i>	19401911	pongamoside D	COCl=C(OC2=CC(O[C@@H]3OC(CO)[C@@H](O)[C@H](O)C3O)=CC=C2C1=O)C1=CC=C2OCOC2=C1
465	<i>Hyoscyamus niger</i>	16653065	Tropinone	CN1[C@H]2CC[C@@H]1CC(=O)C2
466	<i>Hyoscyamus niger</i>	24322778	anisodamine	O(C(=O)[C@H](CO)c1cccc1)[C@@H]1C[C@H]2[NH+]([C@H](C1)C[C@@H]2O)C
467	<i>Justicia adhatoda</i>	22899014	anisotine	CNC1=CC=C(C=C1C(=O)OC)C1CCN2C1=NC1=CC=CC=C1C2=O
468	<i>Justicia adhatoda</i>	26632438	vasicine	OC1CCN2CC3=CC=C(C=C3N=C12

469	<i>Justicia adhatoda</i>	26632438	vasicinone	O[C@H]1CCN2C1=NC 1=CC=CC=C1C2=O
470	<i>Justicia adhatoda</i>	22899014	vasicoline	N12C(=Nc3c(C1)cccc3) C(CC2)c1ccccc1N(C)C
471	<i>Justicia adhatoda</i>	22899014	vasicolinone	O=C1N2C(=Nc3c1cccc 3)C(CC2)c1ccccc1N(C) C
472	<i>Justicia adhatoda</i>	22899014	adhatodine	CNc1ccc(cc1C(=O)OC) C2CCN3Cc4cccc4N=C C23
473	<i>Mallotus philippensis</i>	24099509	1-(5,7-dihydroxy-2,2,6-trimethyl-2H-1-benzopyran-8-yl)-3-phenyl-2-propen-1-one	CC1=C(O)C(C(=O)C=C C2=CC=CC=C2)=C2O C(C)(C)C=CC2=C1O
474	<i>Mallotus philippensis</i>	26998192	11-O-galloylbergenin	O1C2C(OC(=O)c3c2c(O)c(O)c(O)c3)C(O)C(OC1COc(=O)c1cc(O)c(O)c(O)c1
475	<i>Mallotus philippensis</i>	24099509	4'-hydroxyrottlerin	O1c2c(C=CC1(C)C)c(O)c(Cc1c(O)c(C(=O)C)c(O)c(C)c1O)c(O)c2C(=O)C=Cc1ccc(O)cc1
476	<i>Mallotus philippensis</i>	20420321	4-O-galloylbergenin	O1C2C(OC(=O)c3c2c(O)c(O)c(O)c3)C(OC(=O)c2cc(O)c(O)c(O)c2)C(OC)C1CO
477	<i>Mallotus philippensis</i>	20334129	8-cinnamoyl-2,2-dimethyl-7-hydroxy-5-methoxychromene	COCl=C2C=CC(C)(C)OC2=C(C(=O)\C=C\ C2=CC=CC=C2)C(O)=C1
478	<i>Mallotus philippensis</i>	20334129	8-cinnamoyl-5,7-dihydroxy-2,2,6-trimethylchromene	CC1=C(O)C(C(=O)\C=C\ C2=CC=CC=C2)=C2OC(C)(C)C=CC2=C1O
479	<i>Mallotus philippensis</i>	30276553	bergenin	COCl=C(O)C=C2C(=O)O[C@@H]3[C@@H](O)[C@H](O)[C@@H](CO)O[C@H]3C2=C1O
480	<i>Mallotus philippensis</i>	18484534	betulin	CC(=C)[C@@H]1CC[C@]2(CO)CC[C@]3(C)[C@H](CC[C@H]4[C@H]5(C)CC[C@H](O)C(C)(C)[C@@H]5CC[C@H]34C)[C@@H]12
481	<i>Mallotus philippensis</i>	20420321	dihydromyricetin	O[C@@H]1[C@H](OC2=CC(O)=CC(O)=C2C1=O)C1=CC(O)=C(O)C(O)=C1

482	<i>Mallotus philippensis</i>	18484534	friedelin	C[C@H]1C(=O)CC[C@@H]2[C@]1(C)CC[C@H]1[C@@@]2(C)CC[C@@]2(C)[C@@@H]3CC(C)(C)CC[C@]3(C)CC[C@]12C
483	<i>Mallotus philippensis</i>	25105119	isocoumarins	O1C=Cc2c(cccc2)C1=O
484	<i>Mallotus philippensis</i>	20420321	isovitexin	OC[C@H]1O[C@H]([C@H](O)[C@@H](O)[C@@H]1O)C1=C(O)C=C2OC(=CC(=O)C2=C1O)C1=CC=C(O)C=C1
485	<i>Mallotus philippensis</i>	18484534	lupeol	CC(=C)[C@@@H]1CC[C@]2(C)CC[C@]3(C)[C@H](CC[C@@H]4[C@@@]5(C)CC[C@H](O)C(C)(C)[C@@H]5CC[C@@]34C)[C@@@H]12
486	<i>Mallotus philippensis</i>	29054523	mallotophilippen A	CCC(C)C(=O)C1=C(O)C(CC2=C(O)C(C)=C(O)C(C(=O)C(C)C)=C2O)=C(O)C2=C1OC(C)(C)C=C2
487	<i>Mallotus philippensis</i>	29054523	mallotophilippen B	CCC(C)C(=O)C1=C(O)C(CC2=C(O)C(C)=C(O)C(C(=O)=C2O)=C(O)C2=C1OC(C)(C)C=C2
488	<i>Mallotus philippensis</i>	20334129	mallotophilippen F or 8-cinnamoyl-5,7-dihydroxy-2,2-dimethyl-6-geranylchromene	O1c2c(C=CC1(C)C)c(O)c(C\ C=C(\ CC\ C=C(\ C)/C)/C)c(O)c2C(=O)\ C=C\ c1cccc1
489	<i>Mallotus philippensis</i>	15516755	mallotophilippens C	O1c2c(C=CC1(C)C)c(O)c(CC=C(CCC=C(C)C)C)c(O)c2C(=O)C=Cc1cc(O)cc1
490	<i>Mallotus philippensis</i>	15516755	mallotophilippens D	O1c2c(C=CC1(C)C)c(O)c(CC=C(CCC=C(C)C)C)c(O)c2C(=O)C=Cc1cc(O)cc1
491	<i>Mallotus philippensis</i>	15516755	mallotophilippens E	O1c2c(C=CC1(CCC=C(C)C)C)c(O)c(CC=C(C)C)c(O)c2C(=O)C=Cc1cc(O)cc1
492	<i>Mallotus philippensis</i>	24041234	Mallotus B	O1c2c(c(O)c(CC=C(C)C)c(O)c2Cc2c(O)c(C(=O)c(O)c(C)c2O)C(=O))CC1c1cccc1

493	<i>Mallotus philippensis</i>	20420321	pachysandiol A	<chem>OC1C(C)C2(C(CC1O)C1(C(CC2)C2(CCC3(C(CC(CC3)(C)C)C2(CC1)C)C)C)C)C</chem>
494	<i>Mallotus philippensis</i>	20420321	platanoside	<chem>CC1O[C@H](OC2=CC(OC)=CC(O)=C3C2=O)C2=CC=C(O)C=C2)[C@H](OC(=O)\C=C\CC=C(O)C=C2)C(OC(=O)\C=C\CC=C(O)C=C2)=CC=C(O)C=C2)[C@H]1O</chem>
495	<i>Mallotus philippensis</i>	29054523	Rottlerin	<chem>CC(=O)C1=C(O)C(C)=C(O)C(CC2=C(O)C3=C(OC(C)C)C=C3)C(C(=O)\C=C\CC=C(O)C=C3)=C2O)=C1O</chem>
496	<i>Mallotus philippensis</i>	25105119	isorottlerin	<chem>CC(=O)c1c(O)c(C)c(O)c(Cc2c(O)c3C=CC(C)(C)Oc3c4C(=O)CC(Oc24)c5cccc5)c1O</chem>
497	<i>Mentha arvensis</i>	30150845	isomenthone	<chem>CC(C)C1CCC(C)CC1=O</chem>
498	<i>Mentha arvensis</i>	16815640	Linarin (acacetin-7-O-beta-d-rutinoside)	<chem>O1C(COC2OC(C)C(O)C(O)C2O)C(O)C(O)C(O)C1Oc1cc(O)c2c(OC(=CC2=O)c2ccc(OC)cc2)c1</chem>
499	<i>Mentha arvensis</i>	29031422	l-menthol	<chem>CC(C)[C@H]1CC[C@H](C)C[C@H]1O</chem>
500	<i>Mentha arvensis</i>	29031422	l-menthone	<chem>CC(C)[C@@H]1CC[C@@H](C)CC1=O</chem>
501	<i>Mentha arvensis</i>	30150845	menthol	<chem>CC(C)[C@@H]1CC[C@@H](C)C[C@H]1O</chem>
502	<i>Mentha arvensis</i>	24279749	morin	<chem>OC1=CC=C(C(O)=C1)C1=C(O)C(=O)C2=C(O)C=C(O)C=C2O1</chem>
503	<i>Mentha arvensis</i>	30150845	neomenthyl acetate	<chem>CC(C)[C@@H]1CC[C@@H](C)C[C@@H]1OC(=O)</chem>
504	<i>Mentha arvensis</i>	29031422	rosmarinic acid	<chem>OC(=O)C(CC1=CC=C(O)C(O)=C1)OC(=O)\C=C\CC=C(O)C(O)=C1</chem>
505	<i>Mentha arvensis</i>	30150845	menthone	<chem>O=C1C[C@@H](CC[C@H]1C(C)C)C</chem>
506	<i>Mentha piperita</i>	15734920	(-)-trans-isopiperitenol	<chem>CC(=C)[C@H]1CCC(C)=C[C@H]1O</chem>
507	<i>Mentha piperita</i>	28334238	carvol	<chem>CC(=C)C1CC=C(C)C(=O)C=C1</chem>

				O)C1
508	<i>Mentha piperita</i>	28250658	caryophyllene	C\ C1=C/CCC(=C)[C@H]2CC(C)(C)[C@@H]2CC1
509	<i>Mentha piperita</i>	30319836	catechin	O[C@H]1CC2=C(O)C=C(O)C=C2O[C@@H]1C1=CC=C(O)C(O)=C1
510	<i>Mentha piperita</i>	11853178	diosmin	CO C1=CC=C(C=C1O)C1=CC(=O)C2=C(O)C=C(O[C@@H]3O[C@H](CO[C@@H]4O[C@@H](C)[C@H](O)[C@@H](O)[C@H](O)[C@H]4O)[C@@H](O)[C@H](O)[C@H]3O)C=C2O1
511	<i>Mentha piperita</i>	16662335	d-neomenthol	CC(C)C1CCC(C)CC1O
512	<i>Mentha piperita</i>	16662329	d-neomenthyl glucoside	O1[C@H](CO)[C@@H](O)[C@H](O)[C@H](O)C1OC1CC(CCC1C(C)C)C
513	<i>Mentha piperita</i>	16662335	d-neomenthyl-beta-d-glucoside	O1[C@H](CO)[C@@H](O)[C@H](O)[C@H](O)[C@@H]1OC1CC(CCC1C(C)C)C
514	<i>Mentha piperita</i>	16402541	eriocitrin	C[C@@H]1O[C@@H](OC[C@H]2O[C@@H](OC3=CC(O)=C4C(=O)C[C@H](OC4=C3)C3=CC=C(O)C(O)=C3)[C@H](O)[C@@H](O)[C@@H]2O)[C@H](O)[C@@H](O)[C@H](O)[C@H]1O
515	<i>Mentha piperita</i>	11853178	hesperidin	CO C1=CC=C(C=C1O)[C@@H]1CC(=O)C2=C(O)C=C(O[C@@H]3O[C@H](CO[C@@H]4O[C@@H](C)[C@H](O)[C@@H](O)[C@H]4O)[C@@H](O)[C@H](O)[C@H]3O)C=C2O1
516	<i>Mentha piperita</i>	30867394	iso-menthone	O=C1CC(CCC1C(C)C)C
517	<i>Mentha piperita</i>	15734920	isopiperitenol	CC(=C)C1CCC(C)=CC1O
518	<i>Mentha piperita</i>	9666476	isopiperitenone	CC(=C)C1CCC(C)=CC1O

519	<i>Mentha piperita</i>	16402541	isorhoifolin	C[C@@H]1O[C@@H](OC[C@H]2O[C@H](OC3=CC(O)=C4C(=O)C=C(OC4=C3)C3=CC=C(O)C=C3)[C@H](O)[C@@H](O)[C@@H]2O)[C@H](O)[C@H](O)[C@H]1O
520	<i>Mentha piperita</i>	18052102	lithospermic acid	OC(=O)[C@@H](CC1=CC=C(O)C(O)=C1)OC(=O)\C=C\ C1=CC=C(O)C2=C1C(C(O2)C1=CC=C(O)C(O)=C1)C(O)=O
521	<i>Mentha piperita</i>	18052102	luteolin 7-O-beta-glucuronide	O1c2c(C(=O)C=C1c1cc(O)c(O)cc1)c(O)cc(O[C@@H]1O[C@H](C(=O)[O-])[C@@H](O)[C@H](O)[C@H]1O)c2
522	<i>Mentha piperita</i>	16402541	luteolin-7-O-rutinoside	O1C(COC2OC(CO)C(O)C(O)C2O)C(O)C(O)C(O)C1Oc1cc(O)c2c(OC(=CC2=O)c2cc(O)c(O)cc2)c1
523	<i>Mentha piperita</i>	28795021	menthofuran	C[C@@H]1CCC2=C(C1)OC=C2C
524	<i>Mentha piperita</i>	28250658	menthol acetate	CC(C)[C@@H]1CC[C@H](C)C[C@H]1OC(C)=O
525	<i>Mentha piperita</i>	16402541	narirutin	C[C@@H]1O[C@@H](OC[C@H]2O[C@H](OC3=CC(O)=C4C(=O)C=C(OC4=C3)C3=CC=C(O)C=C3)[C@H](O)[C@@H](O)[C@@H]2O)[C@H](O)[C@H](O)[C@H]1O
526	<i>Mentha piperita</i>	30319840	p-anisidine	COCl=CC=C(N)C=C1
527	<i>Mentha piperita</i>	31032736	pheophorbide a	CCC1=C(C)C2=NC1=C C1=C(C)C3=C(N1)C([C@@H](C(=O)OC)C3=O)=C1N=C(C=C3NC(=C2)C(C=C)=C3C)[C@H](C)[C@@H]1CCC(O)=O
528	<i>Mentha piperita</i>	28250658	pulegone	C[C@@H]1CCC(=C(CC)C(=O)C1

529	<i>Mentha piperita</i>	16402541	rosmarinic acids	Oc1cc(ccc1O)CC(OC(=O)C=Cc1cc(O)c(O)cc1)C(=O)[O-]
530	<i>Mentha piperita</i>	30319840	a-tocopherol	O1c2c(CC[C@]1(CCC[C@@H](CCC[C@H](CCCC(C)C)C)C)c(C)c(O)c(C)c2C
531	<i>Mentha piperita</i>	17390896	Methanol	OC1CC(CCC1C(C)C)C
532	<i>Mentha piperita</i>	28795021	menthyl acetate	O(C(=O)C)[C@@H]1C[C@@H](CC[C@H]1C(C)C)C
533	<i>Monarda citriodora</i>	21328358	L-carvone	CC(=C)[C@@H]1CC=C(C(C)C(=O)C1
534	<i>Ocimum tenuiflorum or Ocimum sanctum</i>	19252314	1-(4-hydroxy-3-methoxyphenyl)-1,2,3-tris(4-allyl-2-methoxyphenoxy)propane	O(C(C(Oc1ccc(cc1OC)CC=C)COc1ccc(cc1OC)CC=C)c1cc(O)cc1)c1ccc(cc1OC)CC=C
535	<i>Ocimum tenuiflorum or Ocimum sanctum</i>	19252314	1,2-bis(4-allyl-2-methoxyphenoxy)-3-(4-hydroxy-3-methoxyphenyl)-3-methoxypropane	O(C(C(OC)c1cc(O)cc1)COc1ccc(cc1OC)CC=C)c1ccc(cc1OC)CC=C
536	<i>Ocimum tenuiflorum or Ocimum sanctum</i>	19252314	1-allyl-4-(5-allyl-2-hydroxy-3-methoxyphenoxy)-3-(4-allyl-2-methoxyphenoxy)-5-methoxybenzene	O(c1c(Oc2ccc(cc2OC)CC=C)cc(cc1OC)CC=C)c1cc(cc(OC)c1O)CC=C
537	<i>Ocimum tenuiflorum or Ocimum sanctum</i>	30870993	3-(3,4-dihydroxyphenyl) lactic acid	Oc1cc(ccc1O)CC(O)C(=O)[O-]
538	<i>Ocimum tenuiflorum or Ocimum sanctum</i>	19252314	3-(5-allyl-2-hydroxy-3-methoxyphenyl)-1-(4-hydroxy-3-methoxyphenoxy)-prop-1-ene	O(C)c1cc(cc(CC=COc2cc(OC)c(O)cc2)c1O)CC=C
539	<i>Ocimum tenuiflorum or Ocimum sanctum</i>	19252314	5-allyl-3-(4-allyl-2-methoxyphenoxy)methyl-2-(4-hydroxy-3-methoxyphenyl)-7-methoxy-2,3-dihydrobenzofuran	O1c2c(cc(cc2OC)CC=C)C(COc2ccc(cc2OC)CC=C)C1c1cc(OC)c(O)cc1
540	<i>Ocimum tenuiflorum or Ocimum sanctum</i>	19252314	6-allyl-3-(4-allyl-2-methoxyphenoxy)-3',8-dimethoxyflavan-4'-ol	O1c2c(CC(Oc3ccc(cc3OC)CC=C)C1c1cc(OC)c(O)cc1)cc(cc2OC)CC=C

541	<i>Ocimum tenuiflorum or Ocimum sanctum</i>	19252314	6-allyl-3',8-dimethoxy-flavan-3,4'-diol	O1c2c(CC(O)C1c1cc(O C)c(O)cc1)cc(cc2OC)C C=C
542	<i>Ocimum tenuiflorum or Ocimum sanctum</i>	30870993	apigenin 7-O-beta-D-glucuronide	O1C(C(=O)[O-]C(O)C(O)C(O)C1Oc1cc(O)c2c(OC(=CC2=O)c2ccc(O)cc2)c1
543	<i>Ocimum tenuiflorum or Ocimum sanctum</i>	17850106	apigenin-7-O-beta-D-glucuronic acid	O1c2c(C(=O)C=C1c1cc(O)c(O)cc(OC(=O)[C@H]1O[C@H](O)[C@H](O)[C@H](O)[C@@H]1O)c2
544	<i>Ocimum tenuiflorum or Ocimum sanctum</i>	30870993	b-caryophyllene oxide	C[C@H]12CC[C@H]3[C@H](CC3(C)C)C(=C)CC[C@H]1O2
545	<i>Ocimum tenuiflorum or Ocimum sanctum</i>	21409717	b-elemene	C1[C@H](C(C)=C)[C@@](CC[C@H]1C(C)=C)(C=C)C
546	<i>Ocimum tenuiflorum or Ocimum sanctum</i>	15553132	beta-elemene	CC(=C)[C@@H]1CC[C@H](C(C)=C)[C@H](C1)C(C)=C
547	<i>Ocimum tenuiflorum or Ocimum sanctum</i>	30804629	borneol	OC1CC2CCC1(C)C2(C)C
548	<i>Ocimum tenuiflorum or Ocimum sanctum</i>	30804629	camphor	CC1(C)C2CCC1(C)C(=O)C2
549	<i>Ocimum tenuiflorum or Ocimum sanctum</i>	23682780	carnosic acid	Oc1c(cc2c(c1O)C1(C(C)C2)C(CCC1)C)C(=O)[O-]C(C)C
550	<i>Ocimum tenuiflorum or Ocimum sanctum</i>	25676726	epicatechin	O1c2c(C[C@H](O)[C@H]1c1cc(O)c(O)cc1)c(O)cc(O)c2
551	<i>Ocimum tenuiflorum or Ocimum sanctum</i>	25676726	eupalitin	O1c2c(C(=O)C(O)=C1c1ccc(O)cc1)c(O)c(OC)c(OC)c2
552	<i>Ocimum tenuiflorum or Ocimum sanctum</i>	21409717	germacrene D	CC(C)C1CC\ C(C)=C\ CC(=C)\ C=C\ 1

553	<i>Ocimum tenuiflorum or Ocimum sanctum</i>	21305853	Linolenic acid	CC\ C=C/C\ C=C/C\ C=C /CCCCCCCC(O)=O
554	<i>Ocimum tenuiflorum or Ocimum sanctum</i>	17850106	luteolin-5-O-beta-D-glucopyranoside	O1c2c(C(=O)C=C1c1cc(O)c(O)cc1)c(O[C@H]1O[C@H](CO)[C@@H](O)[C@H](O)[C@H]1O)cc(O)c2
555	<i>Ocimum tenuiflorum or Ocimum sanctum</i>	17850106	luteolin-7-O-beta-D-glucopyranoside	O1c2c(C(=O)C=C1c1cc(O)c(O)cc1)c(O)cc(O[C@H]1O[C@H](CO)[C@@H](O)[C@H](O)[C@H]1O)c2
556	<i>Ocimum tenuiflorum or Ocimum sanctum</i>	17850106	luteolin-7-O-beta-D-glucuronic acid 6"-methyl ester	O1C(C(OC)=O)C(O)C(O)C1Oc1cc(O)c2c(OC(=CC2=O)c2cc(O)c(O)cc2)c1
557	<i>Ocimum tenuiflorum or Ocimum sanctum</i>	24302801	methyleugenol	O(C)c1cc(ccc1OC)CC=C
558	<i>Ocimum tenuiflorum or Ocimum sanctum</i>	17850106	ocimarin	O1c2c(ccc(O)c2)C(C)=C(CCO)C1=O
559	<i>Ocimum tenuiflorum or Ocimum sanctum</i>	27396915	Orientin	OC[C@H]1O[C@H]([C@H](O)[C@@H](O)[C@@H]1O)C1=C2OC(=CC(=O)C2=C(O)C=C1O)C1=CC=C(O)C(O)=C1
560	<i>Ocimum tenuiflorum or Ocimum sanctum</i>	23677922	p-coumaric acid	Oc1ccc(cc1)C=CC(=O)[O-]
561	<i>Ocimum tenuiflorum or Ocimum sanctum</i>	30870993	protocatechuic acid	OC(=O)C1=CC=C(O)C(O)=C1
562	<i>Ocimum tenuiflorum or Ocimum sanctum</i>	30870993	Rabdosiin	Oc1cc(ccc1O)C1c2cc(O)c(O)cc2C=C(C(OC(Cc2cc(O)c(O)cc2)C(=O)[O-])=O)C1C(OC(Cc1cc(O)c(O)cc1)C(=O)[O-])=O
563	<i>Ocimum tenuiflorum or Ocimum sanctum</i>	30804629	selinene	CC(=C)[C@@@H]1CC[C@@@]2(C)CCC=C(C)[C@@@H]2C1

564	<i>Ocimum tenuiflorum or Ocimum sanctum</i>	26315624	urosolic acid	OC1CCC2(C(CCC3(C2 CC=C2C4C(C)C(CCC4 (CCC23C)C(=O)[O-]C)C)C1(C)C)C
565	<i>Ocimum tenuiflorum or Ocimum sanctum</i>	26471526	vanillic acids	COCl=C(C=CC(=C1)C(=O)O)O
566	<i>Ocimum tenuiflorum or Ocimum sanctum</i>	26471526	vanillin	O(C)c1cc(ccc1O)C=O
567	<i>Ocimum tenuiflorum or Ocimum sanctum</i>	27396915	vicenin	O1C(C(O)C(O)C(O)C1 CO)c1c(O)c(c2OC(=CC(=O)c2c1O)c1ccc(O)cc1)C1OC(CO)C(O)C(O)C1O
568	<i>Ocimum tenuiflorum or Ocimum sanctum</i>	18095647	methylchavicol	Cc1cc(CC=C)ccc1O
569	<i>Ocimum tenuiflorum or Ocimum sanctum</i>	22664506	ocimumoside A	CCCCCCCCCC(=O)OC(COC1C(C(C(C(O1)CN)O)O)OCOC(=O)CCCCCCCC
570	<i>Ocimum tenuiflorum or Ocimum sanctum</i>	22664506	ocimumoside B	CCCCCCCCCC(=O)OCC(COC1C(C(C(C(O1)CO)O)O)O)OC(=O)CCCCCCCC
571	<i>Papaver somniferum</i>	9988096	(-)Thebaine	O1C2C34C(C([NH+](CC3)Cc3c4c1c(OC)cc3)=CC=C2OC
572	<i>Papaver somniferum</i>	3459191	(+)-salutaridine	O(C)C1=CC23c4c(CC([NH+](CC2)C)C3=CC1=O)ccc(OC)c4O
573	<i>Papaver somniferum</i>	22535422	(S)-laudanosine	O(C)c1cc(ccc1OC)CC1[NH+](CCc2c1cc(OC)c(OC)c2)C
574	<i>Papaver somniferum</i>	22535422	(S)-tetrahydropapaverine	O(C)c1cc(ccc1OC)CC1[NH2+]CCc2c1cc(OC)c(OC)c2
575	<i>Papaver somniferum</i>	15921406	10-hydroxydihydrosanguinarine	CN1CC2=C3OCOC3=C(C(O)=C2C2=C1C1=CC3=C(OCO3)C=C1C=C2
576	<i>Papaver somniferum</i>	17765420	3,4-diacetyl-6-methoxyphenanthrene	COCl=CC2=C(C=C1)C=CC1=C2C(C(C)=O)=C(C=C1)C(C)=O

577	<i>Papaver somniferum</i>	17765420	3-acetyl-6-methoxy-4,5-epoxyphenanthrene	COC1=C2OC3=C(C=C C4=C3C2=C(C=C1)C=C4)C(C)=O
578	<i>Papaver somniferum</i>	9333895	3-monoacetylmorphine	CN1CC[C@@]23[C@H]4OC5=C2C(C[C@@H]1[C@@H]3C=C[C@@H]4O)=CC=C5OC(C)=O
579	<i>Papaver somniferum</i>	11900600	6-monoacetylmorphine	CN1CC[C@@]23[C@H]4OC5=C2C(C[C@@H]1[C@@H]3C=C[C@@H]4O)=C(C=C5O)C(C)=O
580	<i>Papaver somniferum</i>	9333895	acetylcodeine	O1C2C34C(C([NH+](C3)C)Cc3c4c1c(OC)cc3)C=CC2OC(=O)C
581	<i>Papaver somniferum</i>	29607619	aporphine	CN1CCC2=CC=CC3=C2C1CC1=CC=CC=C31
582	<i>Papaver somniferum</i>	29607619	benzophenanthridine	n1c2c(c3c4c(ccc3c1)ccc4)cccc2
583	<i>Papaver somniferum</i>	29607619	benzylisoquinoline	C(C1=CC=CC=C1)C1=NC=CC2=CC=CC=C12
584	<i>Papaver somniferum</i>	12880320	bismorphine A	C[NH+]1CCC23C4C1C C5=C2C(=C(C=C5C6=CC(=C7C8=C6CC9C1C8(CC[NH+]9C)C(O7)C(C=C1)O)O)O)OC3C(C=C4)O
585	<i>Papaver somniferum</i>	12880320	bismorphine B	CN1CCC23C4C1CC5=C2C(=C(C=C5)OC6=C(C=C7C8=C6CC9C1C8(CC[NH+]9C)C(O7)C(C=C1)O)O)OC3C(C=C4)O
586	<i>Papaver somniferum</i>	15966752	buprenorphine N	CC(C)(C)C(C)(C1CC23CCC1(C4C25CCN(C3C6=C5C(=C(C=C6)O)O)4)CC7CC7)OC)O
587	<i>Papaver somniferum</i>	22535422	canadine	COCC1=CC=C2CC3N(CC4=CC5=C(OCO5)C=C34)CC2=C1OC
588	<i>Papaver somniferum</i>	16566764	codamine	COCC1=CC=C(C[C@@H]2N(C)CCC3=CC(OC)=C(O)C=C23)C=C1OC
589	<i>Papaver somniferum</i>	29779229	codeine	COCC1=CC=C2C[C@@H]3[C@@H]4C=C[C@H](O)[C@@H]5OC1=C2[C@]45CCN3C

590	<i>Papaver somniferum</i>	29779229	codeinone	<chem>COC1=CC=C2C[C@@H]3[C@@H]4C=CC(=O)[C@@H]5OC1=C2[C@]4CCN3C</chem>
591	<i>Papaver somniferum</i>	15921406	dihydrosanguinarine	<chem>CN1CC2=C3OCOC3=C C=C2C2=C1C1=CC3=C(OC(OC)C=C1C=C2</chem>
592	<i>Papaver somniferum</i>	16566764	laudanine	<chem>CO[C@H]1CC=C(CC2N(C)CCC3=CC(OC)=C(OC)C=C23)C=C1O</chem>
593	<i>Papaver somniferum</i>	16566764	Laudanosine	<chem>CO[C@H]1CC=C(C[C@@H]2N(C)CCC3=CC(OC)=C(OC)C=C23)C=C1O</chem>
594	<i>Papaver somniferum</i>	27634038	magnoflorine	<chem>CO[C@H]1CC=C2C[C@H]3C4=C(CC[N+]3(C)C)C=C(OC)C(O)=C4C2=C1O</chem>
595	<i>Papaver somniferum</i>	11900600	meconine	<chem>O1Cc2c(c(OC)c(OC)cc2)C1=O</chem>
596	<i>Papaver somniferum</i>	22535422	N-methylcanadine	<chem>O1c2c(OC1)cc1CC[N+]3(C(Cc4c(C3)c(OC)c(O)C)cc4)c1c2)C</chem>
597	<i>Papaver somniferum</i>	26909086	noscapine	<chem>CO[C@H]1CC=C2C[C@H](OC(=O)C2=C1OC)[C@@H]1N(C)CCC2=CC3=C(OCO3)C(OC)=C12</chem>
598	<i>Papaver somniferum</i>	29408320	oripavine	<chem>CO[C@H]1CC=C2C[C@H]3CC4=CC=C(O)C5=C4[C@@]2(CCNC3)C[C@H]1O5</chem>
599	<i>Papaver somniferum</i>	26264169	palaudine	<chem>O(C)c1ccc(cc1O)Cc1nc cc2c1cc(OC)c(OC)c2</chem>
600	<i>Papaver somniferum</i>	28754627	Papaverine	<chem>CO[C@H]1CC=C(CC2=NC=CC3=CC(OC)=C(OC)C=C23)C=C1OC</chem>
601	<i>Papaver somniferum</i>	29607619	protoberberine	<chem>[n+]12c(-c3c(CC1)cccc3)cc1c(cc1c)c2</chem>
602	<i>Papaver somniferum</i>	16566764	reticuline	<chem>CO[C@H]1CC=C(C[C@@H]2N(C)CCC3=CC(OC)=C(OC)C=C23)C=C1O</chem>
603	<i>Papaver somniferum</i>	15921406	sanguinarine	<chem>C[N+]1=CC2=C(C=CC3=C2OCO3)C2=C1C1=C(C=C2)C=C2OCOC2=C1</chem>
604	<i>Papaver somniferum</i>	11900600	thebaine	<chem>CO[C@H]1CC=C2C[C@H]3CC4=CC=C(O)C5=C4[C@@]2(CCNC3)C[C@H]1O</chem>

				H]1O5
605	<i>Phyllanthus emblica</i>	22485126	β -glucogallin	C1=C(C=C(C(=C1O)O)O)C(=O)OC2C(C(C(C(O2)CO)O)O)O
606	<i>Phyllanthus emblica</i>	19374435	4'-hydroxyphyllaemblicin B	CC1COC2(CC1OC(=O)C3=CC=C(C=C3)O)C(=O)C4(C(CC(CC4O2)C(=O)OC5C(C(C(C(O5)CO)O)O)OC6C(C(C(C(O6)CO)O)O)O)O
607	<i>Phyllanthus emblica</i>	17999342	apigenin-7-O-(6"-butyryl-beta-glucopyranoside	CCCC(=O)C(O)[C@H]1O[C@@H](OC2=CC(O)=C3C(=O)C=C(OC3=C2)C2=CC=C(O)C=C2)[C@H](O)[C@@H](O)[C@@H]1O
608	<i>Phyllanthus emblica</i>	26415402	Betulinic acid	CC(=C)[C@@H]1CC[C@H]2(CC[C@]3(C)[C@H](CC[C@@H]4[C@@H]5(C)CC[C@H](O)C(C)(C)[C@@H]5CC[C@@]34C)[C@@H]12)C(=O)=O
609	<i>Phyllanthus emblica</i>	26415402	Betulonic acid	CC(=C)C1CCC2(C1C3CCC4C5(CCC(=O)C(C5CCC4(C3(CC2)C)C)C)C(=O)O
610	<i>Phyllanthus emblica</i>	26415402	Daucosterol	CC[C@H](CC[C@H](C)[C@H]1CC[C@H]2[C@@H]3CC=C4C[C@H](CC[C@@H]4(C)[C@H]3CC[C@@H]12)O[C@@H]1O[C@H](CO)[C@@H](O)[C@H](O)[C@H]1O)C(C)C
611	<i>Phyllanthus emblica</i>	22889097	digalloylglucose	C1=C(C=C(C(=C1O)O)O)C(=O)C(C(C(C(C(O)O)O)O)O)(C(=O)C2=CC(=C(C(=C2O)O)O)O)O
612	<i>Phyllanthus emblica</i>	23935377	emblicanin B	C1C2C(C3=C(C(=O)O2)OC(=O)C4=CC(=C(C=C4C5=C(C(=C(C=C5C(=O)O3)O)O)O)O)O)OC(=O)C6=CC(=C(C(=C6C7=C(C(=C(C=C7C(=O)O1)O)O)O)O)O)O

613	<i>Phyllanthus emblica</i>	19063633	emblicanins A	C1C2C(C(=C(C(=O)O2)OC(=O)C3=CC(=C(C(=C3)O)O)OC(=O)C4=CC(=C(C(=C4)O)O)OC(=O)C5=CC(=C(C(=C5C6=C(C(=C(C=C6C(=O)O1)O)O)O)O)O
614	<i>Phyllanthus emblica</i>	24066235	epigallocatechin	O[C@ @H]1CC2=C(O)C=C(O)C=C2O[C@ @H]1C1=CC(O)=C(O)C(O)=C1
615	<i>Phyllanthus emblica</i>	24066235	epigallocatechin gallate	O1c2c(C[C@ @H](OC(=O)c3cc(O)c(O)c(O)c3)[C@H]1c1cc(O)c(O)c(O)c1)c(O)cc(O)c2
616	<i>Phyllanthus emblica</i>	21317655	geraniin	OC1=CC(=CC(O)=C1O)C(=O)O[C@ @H]1O[C@ @H]2COC(=O)C3=C C(O)=C(O)C(O)=C3C3=C(O)C(O)=C(O)C=C3C(=O)O[C@H]3[C@ @H]2OC(=O)C2=CC(=O)[C@]4(O)OC5=C(O)C(O)=CC(=C5[C@H]2C4(O)O)C(=O)O[C@ @H]13
617	<i>Phyllanthus emblica</i>	25268491	glochicoccin D	CC1COCC2(CC1OC(=O)C3=CC=C(C=C3)O)C(=O)C4(C(CC(CC4O2)C(=O)O)O)O
618	<i>Phyllanthus emblica</i>	26050007	isocorilagin	C1C2C(C(C(C(O2)OC(=O)C3=CC(=C(C(=C3)O)O)O)OC(=O)C4=C C(=C(C(=C4C5=C(C(=C(C=C5C(=O)O1)O)O)O)O)O
619	<i>Phyllanthus emblica</i>	26050007	kaempferol	OC1=CC=C(C=C1)C1=C(O)C(=O)C2=C(O)C=C(O)C=C2O1
620	<i>Phyllanthus emblica</i>	26050007	kaempferol 3-b-d-glucopyranoside	O=C1C(O[C@H]2[C@ @H]([C@H]([C@ @H]([C@ @H](CO)O2)O)O)O)=C(C3=CC=C(O)C=C3)OC4=C1C(O)=CC(O)=C4

621	<i>Phyllanthus emblica</i>	26415402	Lupeol acetate	O(C(=O)C)[C@H]1CC[C@]2([C@@H](CC[C@@]3([C@@H]2CC[C@@H]2[C@@H]4[C@@J](CC[C@]23C)(CC[C@H]4C(C)=C)C)C)C1(C)C)
622	<i>Phyllanthus emblica</i>	17999342	methyl gallate	Oc1c(O)cc(cc1O)C(OC)=O
623	<i>Phyllanthus emblica</i>	26415402	Oleanolic acid	CC1(C)CC[C@@]2(CC[C@]3(C)C(=CC[C@@H]4[C@@]5(C)CC[C@H](O)C(C)(C)[C@@H]5CC[C@@]34C)[C@@H]2C1)C(O)=O
624	<i>Phyllanthus emblica</i>	23935377	pedunculagin	OC1O[C@@H]2COC(=O)C3=CC(O)=C(O)C(O)=C3C3=C(O)C(O)=C(O)C=C3C(=O)O[C@H]2[C@@H]2OC(=O)C3=CC(O)=C(O)C(O)=C3C3=C(O)C(O)=C(O)C=C3C(=O)O[C@@H]12
625	<i>Phyllanthus emblica</i>	19374435	phyllaemblicin A	CC1COC2(CC1OC(=O)C3=CC=CC=C3)C(=O)C4(C(CC(CC4O2)C(=O)OC5C(C(C(C(O5)CO)O)O)O)O)O
626	<i>Phyllanthus emblica</i>	19374435	phyllaemblicin B	CC1COC2(CC1OC(=O)C3=CC=CC=C3)C(=O)C4(C(CC(CC4O2)C(=O)OC5C(C(C(C(O5)CO)O)O)OC6C(C(C(C(O6)CO)O)O)O)O)O
627	<i>Phyllanthus emblica</i>	19374435	phyllaemblicin C	CC1COC2(CC1OC(=O)C3=CC=CC=C3)C(=O)C4(C(CC(CC4O2)C(=O)OC5C(C(C(C(O5)CO)O)O)OC6C(C(C(C(O6)CO)O)O)OC7C(C(C(C(O7)O)O)O)O)O
628	<i>Phyllanthus emblica</i>	19374435	phyllaemblicins E	CC1COC2(CC1OC(=O)C3=CC=CC=C3)C(=O)C4(C(CC(CC4O2)C(=O)OC5C(C(C(C(O5)CO)O)O)OC6C(C(C(C(O6)CO)O)O)OC7C(C(C(C(O7)O)O)O)O)O

629	<i>Phyllanthus emblica</i>	19374435	phyllaemblicins F	CC1COC2(CC1OC(=O)C3=CC=CC=C3)C(=O)C4(C(CC(CC4O2)C(=O)OCC5C(C(C(C(O5)OC6C(C(C(OC6OC(=O)C7CC(C8(C(C7)OC9(C8=O)CC(C(CO9)C)OC(=O)C1=CC=CC=C1)O)O)CO)O)O)O)O)O
630	<i>Phyllanthus emblica</i>	21073944	Progallin A	CCOC(=O)C1=CC(=C(C(=C1)O)O)O
631	<i>Phyllanthus emblica</i>	23935377	puniguconin	O[C@H]1COC(=O)C2=CC(O)=C(O)C(O)=C2C=C(O)C(O)=C(O)C=C2C(=O)O[C@H]1[C@H](OC(=O)C1=CC(O)=C(O)C(O)=C1)[C@@H](OC(=O)C1=CC(O)=C(O)C(O)=C1)C(O)=O
632	<i>Phyllanthus emblica</i>	21317655	pyrogallol	OC1=CC=CC(O)=C1O
633	<i>Phyllanthus emblica</i>	26050007	quercetin	OC1=CC2=C(C(O)=C1)C(=O)C(O)=C(O2)C1=CC(O)=C(O)C(O)=C1C(O)=C1
634	<i>Phyllanthus emblica</i>	26050007	quercetin 3-b-d-glucopyranoside	OC[C@H]1O[C@H](O)(OC2=C(OC3=C(C(O)=CC(O)=C3)C2=O)C2=CC(O)=C(O)C=C2)[C@@H](O)[C@H](O)[C@H]1O
635	<i>Phyllanthus emblica</i>	20506691	rutin	CC1OC(OCC2OC(OC3=C(OC4=CC(O)=CC(O)=C4C3=O)C3=CC=C(O)C(O)=C3)C(O)C(O)C2O)C(O)C(O)C1O
636	<i>Phyllanthus emblica</i>	20506691	tannin	OC1=CC(=CC(O)=C1O)C(=O)OC1=CC(=CC(O)=C1O)C(=O)OCC1OC(OC(=O)C2=CC(O)=C(O)C(OC(=O)C3=CC(O)=C(O)C(O)=C3)=C2)C(OC(=O)C2=CC(O)=C(O)C(OC(=O)C3=CC(O)=C(O)C(O)=C3)=C2)C(OC(=O)C2=CC(O)=C(O)C(OC(=O)C3=CC(O)=C(O)C(O)=C3)=C2)C1OC(=O)C1=CC(O)=C(O)C(OC(=O)C2=CC(O)=C(O)C(O)=C2)=C1

637	<i>Phyllanthus emblica</i>	26415402	Triacontanoic acid	CCCCCCCCCC CCCCCCCCCC CC(O)=O
638	<i>Phyllanthus emblica</i>	26415402	Triacontanol	CCCCCCCCCC CCCCCCCCCC CCO
639	<i>Phyllanthus emblica</i>	26415402	Ursolic acid	C[C@H]1CC[C@H] 2(CC[C@H]3(C)C(=CC[C@H]4[C@@H]5(C)C C[C@H](O)C(C)(C)[C@@H]5CC[C@H]4C) [C@@H]2[C@H]1C)C(O)=O
640	<i>Phyllanthus emblica</i>	24053418	vanillic acid	COCC1=CC(=CC=C1O) C(O)=O
641	<i>Phyllanthus emblica</i>	21317655	elaeocarpusin	O[C@H]1COC2(O)[C@@H]1OC(=O)[C@H]2 3OC4(O)C(=O)CC35[C@H]6c7c(O[C@H]4 O)c(O)c(O)cc7C(=O)O[C@H]8[C@@H](O[C@H]9 COCC(=O)c%10cc(O)c(O)c(O)c%10c%11c (O)c(O)c(O)cc%11C(=O)O[C@H]8[C@@H]9 OC5=O)OC(=O)c%12c(O)c(O)c(O)c%12
642	<i>Phyllanthus emblica</i>	22889097	monogalloylglucose	OC[C@@H](O)[C@@H](O)[C@@H](O)C(=O)C(=O)c1cc(O)c(O)c(O)c1
643	<i>Pimpinella anisum</i>	12809723	(E)-1'-(2-hydroxy-5-methoxyphenyl)propane beta-D-glucopyranoside	COCC1=CC(CCC[C@H]2 2(O)O[C@H](CO)[C@@H](O)[C@H](O)[C@H]2O)=C(O)C=C1
644	<i>Pimpinella anisum</i>	12809723	(E)-3-hydroxyanethole beta-D-glucopyranoside	COCC1=CC(O[C@@H]2 O[C@H](CO)[C@@H](O)[C@H](O)[C@H]2O)=C(\C=C\C)C=C1
645	<i>Pimpinella anisum</i>	12419910	1'-(4-hydroxyphenyl)propane-1',2'-diol 2'-O-beta-D-glucopyranoside	O1[C@H](CO)[C@@H](O)[C@H](O)[C@@H](O)[C@@H]1OC(C(O)c1ccc(O)cc1)C
646	<i>Pimpinella anisum</i>	12809723	1-deoxy-L-erythritol 3-O-beta-D-glucopyranoside	O1[C@H](CO)[C@@H](O)[C@H](O)[C@@H](O)[C@@H]1OC@H(O)C)CO
647	<i>Pimpinella anisum</i>	12809723	3-hydroxyestragole beta-D-glucopyranoside	O1C(CO)C(O)C(O)C(O)C(O)C1Oc1cc(ccc1OC)CC=C

648	<i>Pimpinella anisum</i>	29185164	5-hydroxy-7-methoxy-2-methylchromen-4-one	COC1=CC2=C(C(O)=C1)C(=O)C=C(C)O2
649	<i>Pimpinella anisum</i>	18266152	alpha-farnesene	CC(C)=CCC\ C(C)=C\ C\ C=C(/C)C=C
650	<i>Pimpinella anisum</i>	30689411	anethole	CO C1=CC=C(\ C=C\ C)C=C1
651	<i>Pimpinella anisum</i>	910554	apigenin 7-glucoside	O1C(CO)C(O)C(O)C(O)C1Oc1cc(O)c2c(OC(=CC2=O)c2ccc(O)cc2)c1
652	<i>Pimpinella anisum</i>	23749680	a-terpineol	CC1=CCC(CC1)C(C)(C)O
653	<i>Pimpinella anisum</i>	29185164	bergapten or 4-methoxyfuro[3,2-g]chromen-7-one	CO C1=C2C=CC(=O)OC2=CC3=C1C=CO3
654	<i>Pimpinella anisum</i>	18266152	beta-Bourbonene	CC(C)[C@H]1CC[C@H]2(C)[C@H]3CC[C(=C)[C@H]3[C@@H]12
655	<i>Pimpinella anisum</i>	22926042	cis-isoeugenol	CO C1=CC(\ C=C/C)=C C=C1O
656	<i>Pimpinella anisum</i>	21391475	cis-vaccenic acid	CCCCC\ C=C/CCCCC CCCCC(O)=O
657	<i>Pimpinella anisum</i>	6999244	dianethole	CO C1=CC=C(C=CCC(C)C2=CC=C(OC)C=C2)C=C1
658	<i>Pimpinella anisum</i>	21817824	ergosterol	CC(C)[C@H](C)\ C=C\ C[C@H](C)[C@H]1CC[C@H]2C3=CC=C4C[C@H](O)CC[C@]4(C)[C@H]3CC[C@]12C
659	<i>Pimpinella anisum</i>	22848853	estragole	CO C1=CC=C(CC=C)C=C1
660	<i>Pimpinella anisum</i>	23749680	foeniculin	O(CC=C(C)C)c1ccc(cc1)C=CC
661	<i>Pimpinella anisum</i>	18266152	gamma-himachalene	CC1=CC2C(CC1)C(C)=CCCC2(C)C
662	<i>Pimpinella anisum</i>	12809723	hexane-1,5-diol 1-O-beta-D-glucopyranoside	O1[C@H](CO)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H]1OCCCCCC(O)C
663	<i>Pimpinella anisum</i>	910554	isoorientin	OC[C@H]1O[C@H](C[C@H](O)[C@H](O)[C@H](O)[C@H]1O)C1=C(O)C=C2OC(=CC(=O)C2=C1O)C1=CC=C(O)C(O)=C1

664	<i>Pimpinella anisum</i>	12809723	methyl syringate 4-O-beta-D-glucopyranoside	O1C(CO)C(O)C(O)C(O)C1Oc1c(OC)cc(cc1OC)C(OC)=O
665	<i>Pimpinella anisum</i>	23749680	p-anisaldehyde	COCl=CC=C(C=O)C=C1
666	<i>Pimpinella anisum</i>	6999244	photoanethole	COCl=CC=C(\C=C\ C2=CC=C(OC)C=C2)C=C1
667	<i>Pimpinella anisum</i>	7581216	pseudoisoeugenol	COCl=CC=C(O)C(C=C)C=C1
668	<i>Pimpinella anisum</i>	910554	Quercetin 3-glucuronide	O1[C@H](C(=O)[O-])[C@@H](O)[C@H](O)[C@@H](O)C1OC1=C(Oc2c(C1=O)c(O)cc(O)c2)c1cc(O)c(O)cc1
669	<i>Pimpinella anisum</i>	18266152	trans-pseudoisoeugenyl 2-methylbutyrate	O(C(=O)C(CC)C)c1ccc(OC)cc1C=CC
670	<i>Pimpinella anisum</i>	22926042	y-himachalene	C12C(CCC(=C1)C)C(=CCCC2(C)C)C
671	<i>Pimpinella anisum</i>	22848853	para-anisaldehyde	COc1ccc(C=O)cc1
672	<i>Piper cubeba</i>	30335227	(-) -5-methoxyatein	O1CC(Cc2cc(OC)c3OC Oc3c2)C(Cc2cc(OC)c(OC)c(OC)c2)C1=O
673	<i>Piper cubeba</i>	30583698	(-) -clusin	O1CC(Cc2cc3OCOc3cc2)C(Cc2cc(OC)c(OC)c(OC)c2)C1O
674	<i>Piper cubeba</i>	15748631	(-) -dihydroclusin	COCl=CC(=CC(=C1OC)OC)CC(CO)C(CC2=CC3=C(C=C2)OCO3)CO
675	<i>Piper cubeba</i>	15748631	(-) -dihydrocubebin	C1OC2=C(O1)C=C(C=C2)CC(CO)C(CC3=CC4=C(C=C3)OCO4)CO
676	<i>Piper cubeba</i>	30583698	(-) -haplomyrfolin	O1CC(Cc2cc(OC)c(O)c2)C(Cc2cc3OCOc3cc2)C1=O
677	<i>Piper cubeba</i>	30583698	(-) -yatein	O1CC(Cc2cc3OCOc3cc2)C(Cc2cc(OC)c(OC)c(OC)c2)C1=O
678	<i>Piper cubeba</i>	15679319	(1 alpha,2 beta,5 alpha,8 alpha 10 alpha)-1,10-epoxy-2-hydroxy-3,7(11)-guaiadien-12,8-olide	O1[C@H]2C(C[C@@H]3[C@@]4(O[C@]4(C2)C)[C@H](O)C=C3C)=C(C)C1=O
679	<i>Piper cubeba</i>	15679319	(5 alpha,8 alpha)-2-oxo-1(10),3,7(11)-guaiatrien-12,8-olide	O1[C@@H]2CC(=C3[C@@H](CC2=C(C)C1=O)C(=CC3=O)C)C

680	<i>Piper cubeba</i>	22006194	4-terpineol	CC(C)C1(O)CCC(C)=C C1
681	<i>Piper cubeba</i>	29973507	alpha-cubebene	CC(C)[C@@H]1CC[C@H](C)C23CC=C(C)[C@@H]2[C@@H]13
682	<i>Piper cubeba</i>	15748631	clusin	COC1=CC(=CC(=C1O)OC)CC2C(COC2O)CC3=CC4=C(C=C3)OCO4
683	<i>Piper cubeba</i>	30583698	cubebin	O[C@H]1OC[C@H](CC2=CC=C3OCOC3=C2)[C@H]1CC1=CC=C2OCOC2=C1
684	<i>Piper cubeba</i>	30022310	cubebinin	O1CC(Cc2cc(OC)c(OC)c(OC)c2)C(Cc2cc(OC)c(OC)c(OC)c2)C1O
685	<i>Piper cubeba</i>	30012946	cubebol	CC1CCC(C2C13C2C(CC3)(C)O)C(C)C
686	<i>Piper cubeba</i>	30012946	d-germacrene	CC1=CCCC(=C)C=CC(CC1)C(C)C
687	<i>Piper cubeba</i>	30012946	dihydroclusin	O1c2cc(ccc2OC1)CC(C(Cc1cc(OC)c(OC)c(OC)c1)CO)CO
688	<i>Piper cubeba</i>	30335227	dihydrocubebin	OC[C@H](CC1=CC=C2OCOC2=C1)[C@H](CO)CC1=CC=C2OCOC2=C1
689	<i>Piper cubeba</i>	15679319	ethoxyclusin	O1CC(Cc2cc(OCC)c3OCOC3=c2)C(Cc2cc(OC)c(OC)c(OC)c2)C1O
690	<i>Piper cubeba</i>	22006194	eucalyptol	CC12CCC(CC1)C(C)(C)O2
691	<i>Piper cubeba</i>	30335227	hinokinin	O=C1OC[C@H](CC2=CC=C3OCOC3=C2)[C@H]1CC1=CC=C2OCOC2=C1
692	<i>Piper cubeba</i>	30012946	ledol	CC1CCC2C1C3C(C3(C)C)CCC2(C)O
693	<i>Piper cubeba</i>	30022310	magnosalin	COCC1=CC(OC)=C(C=C1OC)[C@@H]1[C@H](C)[C@@H](C)[C@H]1C1=CC(OC)=C(OC)C=C1OC
694	<i>Piper cubeba</i>	30012946	piperidine	C1CCNCC1
695	<i>Piper cubeba</i>	30019519	yatein	COCC1=CC(C[C@@H]2[C@@H](CC3=CC=C4OCOC4=C3)COC2=O)=CC(OC)=C1OC
696	<i>Piper cubeba</i>	22006194	δ-3-carene	CC1=CCC2C(C1)C2(C)

				C
697	<i>Piper cubeba</i>	31454974	beta-asarone	<chem>COC1=CC(OC)=C(\C=C/C)C=C1OC</chem>
698	<i>Ruta graveolens</i>	28093914	(-)-chalepin	<chem>O1c2c(C=C(C(C=C)(C)C1=O)cc1CC(Oc1c2)C(O)(C)C</chem>
699	<i>Ruta graveolens</i>	28093914	(-)-rutamarin	<chem>CC(=O)OC(C)(C)[C@H]1CC2=C(O1)C=C1OC(=O)C(=CC1=C2)C(C)(C)C=C</chem>
700	<i>Ruta graveolens</i>	17345275	1-hydroxyrutacridone epoxide	<chem>O1c2c(c3N(c4c(ccc4)C(=O)c3c(O)c2)C)C(O)C1C1(OC1)C</chem>
701	<i>Ruta graveolens</i>	10869689	2-Nonanone	<chem>CCCCCC(C)=O</chem>
702	<i>Ruta graveolens</i>	10869689	2-undecanone	<chem>CCCCCCCCCCC(C)=O</chem>
703	<i>Ruta graveolens</i>	17292351	3-(1'-1'-dimethylallyl)-6-hydroxy-7-methoxy-coumarin	<chem>O1c2cc(OC)c(O)cc2C=C(C(C=C)(C)C)C1=O</chem>
704	<i>Ruta graveolens</i>	5711895	3-(3-1',1'-dimethylallyl)-6-(3',3'-dimethylallyl)-umbelliferone (gravelliferone)	<chem>O1c2cc(O)c(cc2C=C(C(C=C)(C)C)C1=O)CC=C(C)C</chem>
705	<i>Ruta graveolens</i>	11473445	3',6-disinapoylsucrose	<chem>O1C(OC2OC(COC(=O)C=Cc3cc(OC)c(O)c(OC)c3)C(O)C(O)C2O)(CO)C(OC(=O)C=Cc2cc(OC)c(O)c(OC)c2)C(O)C1CO</chem>
706	<i>Ruta graveolens</i>	12568545	4-hydroxycoumarin	<chem>OC1=CC(=O)OC2=CC=CC=C12</chem>
707	<i>Ruta graveolens</i>	12568545	7-methoxycoumarin	<chem>CO C1=CC=C2C=CC(=O)OC2=C1</chem>
708	<i>Ruta graveolens</i>	10869689	chalepensin	<chem>CC(C)(C=C)C1=CC2=CC3=C(OC=C3)C=C2O C1=O</chem>
709	<i>Ruta graveolens</i>	11473445	cnidioside A	<chem>O1C(CO)C(O)C(O)C(O)C1Oc1cc2occc2cc1CC C(=O)[O-]</chem>
710	<i>Ruta graveolens</i>	17345275	furoacridone	<chem>o1c2c(c3c(nc4C=CC(=O)Cc4c3)cc2)cc1</chem>
711	<i>Ruta graveolens</i>	10869689	geijerene	<chem>C1CC=CC(C(C)=C)C1(C=C)C</chem>
712	<i>Ruta graveolens</i>	16271733	gravacridondiol	<chem>CC(CO)(C1CC2=C(O1)C=C(C3=C2N(C4=CC=CC=C4C3=O)C)O)O</chem>
713	<i>Ruta graveolens</i>	27272785	gravacridonediol	<chem>O1c2cc(O)c3c(N(c4c(ccc4)C3=O)C)c2CC1C(O)(CO)C</chem>

714	<i>Ruta graveolens</i>	27272785	gravacridonetriol	O1c2cc(O)c3c(N(c4c(cc4)C3=O)C)c2CC1C(O)(CO)CO
715	<i>Ruta graveolens</i>	17345275	gravacridonol	O1c2cc(O)c3c(N(c4c(cc4)C3=O)C)c2CC1C(CO)=C
716	<i>Ruta graveolens</i>	2062959	isogravacridonchlorine	CC(CCl)(C1CC2=C(O1)C=C(C3=C2N(C4=CC=CC=C4C3=O)C)O)O
717	<i>Ruta graveolens</i>	27272785	isogravacridone chlorine	C1CC(O)(C)C1Oc2cc(O)c3c(N(c4c(ccc4)C3=O)C)c2C1
718	<i>Ruta graveolens</i>	30078970	kokusaginine	CO C1=C(OC)C=C2C(OC)=C3C=COC3=NC2=C1
719	<i>Ruta graveolens</i>	11473445	methylpicraquassioside A	O1C(CO)C(O)C(O)C(O)C1Oc1cc2occc2c(OC)c1CCC(OC)=O
720	<i>Ruta graveolens</i>	11473445	picraquassioside A	O1C(CO)C(O)C(O)C(O)C1Oc1cc2occc2c(OC)c1CCC(=O)[O-]
721	<i>Ruta graveolens</i>	27272785	rutacridone	CN1C2=CC=CC=C2C(=O)C2=C(O)C=C3OC(CC3=C12)C(C)=C
722	<i>Ruta graveolens</i>	30078970	y-fagarine	o1c2nc3c(ccc3OC)c(OC)c2cc1
723	<i>Santalum album</i>	30922222	(E)-a-bergamotene	C12CC(CC=C1C)C2(CC=C(C)C)C
724	<i>Santalum album</i>	30922222	(E)-nerolidol	CC(C)=CCC\ C(C)=C/C[C@@](C)(O)C=C
725	<i>Santalum album</i>	15974602	(Z)-1beta-hydroxy-2-hydrolanceol	OC1(CCC(CC1)C(CCC=C(CO)C)=C)C
726	<i>Santalum album</i>	15974602	(Z)-2beta-hydroxy-14-hydro-beta-santalol	OC1(C2CC(CC2)C1(CC=C(CO)C)C)C
727	<i>Santalum album</i>	15974602	(Z)-7-hydroxynuciferol	OC(CCC=C(CO)C)(C)c1ccc(cc1)C
728	<i>Santalum album</i>	15974602	(Z)-alpha-santalol	C\ C(CO)=C\ CC[C@]1(C)[C@H]2CC3C(C2)[C@]1C
729	<i>Santalum album</i>	15974602	(Z)-beta-santalol	CC(=CCCC1(C2CCC(C2)C1=C)C)CO
730	<i>Santalum album</i>	15974602	(Z)-campherene-2beta,13-diol	CC(=CCCC1(C2CCC1(C(C2)O)C)C)CO
731	<i>Santalum album</i>	15974602	(Z)-lanceol	CC1=CCC(CC1)C(=C)CCC=C(C)CO
732	<i>Santalum album</i>	15974602	2R-(Z)-campherene-2,13-diol	OC1CC2CCC1(C)C2(CC=C(CO)C)C
733	<i>Santalum album</i>	17045624	alpha-bisabolol	CC(C)=CCCC(C)(O)C1CCC(C)=CC1

734	<i>Santalum album</i>	15974602	alpha-santadiol	OCC(=CCCC1(C2CC3C(C2)C13C)C)CO
735	<i>Santalum album</i>	30922222	a-santalene	CC(C)=CCC[C@]1(C)[C@H]2C[C@@H]3[C@@H](C2)[C@]13C
736	<i>Santalum album</i>	30922222	b-bisabolene	CC(C)=CCCC(=C)C1C CC(C)=CC1
737	<i>Santalum album</i>	22951817	bergamotene	CC(=CCCC1(C2CCC(=C)C1C2)C)C
738	<i>Santalum album</i>	17045624	beta-curcumene	CC(CCC=C(C)C)C1=C CC(C)=CC1
739	<i>Santalum album</i>	15974602	beta-santadiol	CC1(C2CCC(C2)C1=C) CCC=C(CO)CO
740	<i>Santalum album</i>	25450628	b-santadiol	OCC(=CCCC1(C2CC(C)C2)C1=C)CO
741	<i>Santalum album</i>	30922222	b-santalene	CC(C)=CCC[C@]1(C)[C@H]2CC[C@H](C2)C1=C
742	<i>Santalum album</i>	30922222	b-santalol	C\CC(CO)=C\CC[C@]1(C)[C@H]2CC[C@H](C2)C1=C
743	<i>Santalum album</i>	22375392	chrysin-6-C-beta-D-glucopyranoside	OC[C@H]1O[C@H](OC2=C(O)C=C3OC(=CC(=O)C3=C2O)C2=CC=CC=C2)[C@H](O)[C@@H](O)[C@@H]1O
744	<i>Santalum album</i>	22375392	chrysin-8-C-beta-D-glucopyranoside	OC[C@H]1O[C@H](OC2=C3OC(=CC(=O)C3=C(O)C=C2O)C2=CC=CC=C2)[C@H](O)[C@@H](O)[C@@H]1O
745	<i>Santalum album</i>	30922222	epi-b-santalene	C12CC(CC1)C(=C)C2(=CCC=C(C)C)C
746	<i>Santalum album</i>	22951817	exo-b-bergamotene	C12CC(CCC1=C)C2(C=CC=C(C)C)C
747	<i>Santalum album</i>	17045624	gamma-curcumene	C[C@H](CCC=C(C)C)C1=CC=C(C)CC1
748	<i>Santalum album</i>	22375392	isorhamnetin	COCC1=CC(=CC=C1O)C1=C(O)C(=O)C2=C(O)C=C(O)C=C2O1
749	<i>Santalum album</i>	30922222	santalene	C12CC3C(C1)C3(C)C2(=CCC=C(C)C)C
750	<i>Santalum album</i>	30922222	santalol	CC(CO)=CCCC1(C)C2(=CCC=C(C)C)C1=C
751	<i>Santalum album</i>	30977996	sesquisabinene	C12CC1(CCC2=C)C(C=CC=C(C)C)C

752	<i>Santalum album</i>	22375392	vicenin-2	OC[C@H]1O[C@H](C[C@H](O)[C@@H](O)[C@@H]1O)C1=C(O)C([C@@H]2O[C@H](CO)[C@@H](O)[C@H](O)[C@H]2O)=C2OC(=CC(=O)C2=C1O)C1=CC=C(O)C=C1
753	<i>Santalum album</i>	23860319	α -santalene	CC(=CCCC1(C2CC3C1(C3C2)C)C)C
754	<i>Santalum album</i>	17045624	beta-bisabolene	CC(C)=CCCC(=C)[C@H]1CCC(=CC1)C
755	<i>Santalum album</i>	30922222	a-santalol	OC C(=C/CC[C@@H]1(C2CC3C(C2)C13C)C)\C
756	<i>Santalum album</i>	22375392	isovitexin	O1c2c(c(O)c([C@@H]3O[C@H](CO)[C@H](O)[C@H](O)[C@H]3O)c(O)c2)C(=O)C=C1c1cc(O)cc1
757	<i>Semecarpus anacardium</i>	19429311	3-(8'(Z),11'(Z)-pentadecadienyl) catechol	CCC\ C=C/C\ C=C/CCC CCCCC1=C(O)C(O)=C C=C1
758	<i>Semecarpus anacardium</i>	15305321	3,4,2',4'-tetrahydroxychalcone (butein)	Oc1cc(O)ccc1C(=O)C=Cc1cc(O)c(O)cc1
759	<i>Semecarpus anacardium</i>	27680742	3-O-methyl quercetin	COCl=C(OC2=C(C(O)=CC(O)=C2)C1=O)C1=CC(O)=C(O)C=C1
760	<i>Semecarpus anacardium</i>	15305321	7,3',4'-trihydroxy fl avone	OC1=CC=C2C(=O)C=C(OC2=C1)C1=CC(O)=C(O)C=C1
761	<i>Semecarpus anacardium</i>	23559802	anacardic acid	OC(=O)C1=C(O)C=CC=C1CCCCCCC\ C=C/C\ C=C/CC=C
762	<i>Semecarpus anacardium</i>	23559802	Bhilawanol A	Oc1c(cccc1O)CCCCCCC CC=CCCCCC
763	<i>Semecarpus anacardium</i>	23559802	Bhilawanol B	Oc1c(cccc1O)CCCCCCC C=CCC=CCCCCC
764	<i>Semecarpus anacardium</i>	26267092	pyrocatechol	Oc1cccc1O
765	<i>Solanum nigrum</i>	20845784	(+)-medioresinol	O1CC2C(COC2c2cc(O)C)c(O)cc2)C1c1cc(OC)c(O)c(OC)c1
766	<i>Solanum nigrum</i>	17944186	3, 4-dihydroxbenzoic acid	Oc1cc(ccc1O)C(=O)[O-]
767	<i>Solanum nigrum</i>	17944186	3-methoxy-4-hydroxyienzoic acid	O(C)c1cc(ccc1O)C(=O)[O-]

768	<i>Solanum nigrum</i>	17944186	adenosine	NC1=C2N=CN([C@@H]3O[C@H](CO)[C@@H](O)[C@H]3O)C2=NC=N1
769	<i>Solanum nigrum</i>	30076759	a-Solanine	CC1C2CCC(C)CN2C2 CC3C4CC=C5CC(CCC5(C)C4CCC3(C)C12)O C1OC(CO)C(O)C(OC2OC(CO)C(O)C2O) C1OC1OC(C)C(O)C(O)C1O
770	<i>Solanum nigrum</i>	30179424	benzoiisovanillin	O(C)c1c2c(cccc2)c(cc1O)C=O
771	<i>Solanum nigrum</i>	16768003	citric acids	C(C(=O)O)C(CC(=O)O)(C(=O)O)O
772	<i>Solanum nigrum</i>	30643798	degalactotigonin	CC1CCC2(C(C3C(O2)CC4C3(CCC5C4CCC6C5(CCC(C6)OC7C(C(C(C(O7)CO)OC8C(C(C(C(O8)CO)O)OC9C(C(C(CO9)O)O)OC2C(C(C(C(O2)CO)O)O)O)O)O)C)C)OC1
773	<i>Solanum nigrum</i>	20681660	gentisic acid	OC(=O)C1=CC(O)=CC=C1O
774	<i>Solanum nigrum</i>	17944186	hydroxybenzoic acid	OC1=CC=C(C=C1)C([O-])=O
775	<i>Solanum nigrum</i>	22388971	inunigroside A (5 α ,22S,23S,25R)- 3 β ,23-dihydroxyspirostane 3-O- β -lycotetraoside)	CC1CC(C2(C(C3C(O2)CC4C3(CCC5C4CCC6C5(CCC(C6)OC7C(C(C(C(O7)CO)OC8C(C(C(C(O8)CO)O)OC9C(C(C(CO9)O)O)OC2C(C(C(C(O2)CO)O)O)O)O)O)C)C)OC1)O
776	<i>Solanum nigrum</i>	20083341	lunasin	O1c2[n+](c3c(cccc3OC)c(OC)c2CC1C(C)C)C
777	<i>Solanum nigrum</i>	20681660	m-coumaric acid	OC(=O)\C=C\ C1=CC(O)=CC=C1
778	<i>Solanum nigrum</i>	30627484	nigrumnin-I	CC1CCC2(C(C3C(O2)CC4C3(CCC5C4CCC6C5(CCC(C6)OC7C(C(C(C(O7)CO)OC8C(C(C(C(O8)CO)O)OC9C(C(C(CO9)O)O)OC2C(C(C(C(C(O2)CO)O)O)O)O)O)C)C)OC1

779	<i>Solanum nigrum</i>	30643798	O-acetyl solasodine	O1C2C(C(C)C13[NH2+]CC(CC3)C)C1(C(C3C(CC1)C1(C(CC(OC(=O)C)CC1)=CC3)C)C2)C
780	<i>Solanum nigrum</i>	30076759	physalin	O(C(=O)CCCCCCCCCCC)C1CC(C)(C)C(C=CC(=CC=CC(=CC=CC=C(C=CC=C(C=C2C(CC(OC(=O)CCC)CCCCCCCCCCC)CC=2C)(C)C)C)C)C)=C(C1)C
781	<i>Solanum nigrum</i>	24454566	physalin G	C[C@@]12OC(=O)[C@]3(O)CC[C@H]4[C@@H](C[C@H](O)C5=C C=CC(=O)[C@]45C)[C@@]45O[C@@@]13[C@@@H](C4=O)[C@]1(C)C[C@H]2OC(=O)[C@H]1CO5
782	<i>Solanum nigrum</i>	24454566	physalin H	CC12CC3C4(C56C1C(=O)C(O5)(C7CC(C8(CC=CC(=O)C8(C7CCC6(C(=O)O4)O)C)Cl)O)O CC2C(=O)O3)C
783	<i>Solanum nigrum</i>	20845784	pinoresinol	COCl=CC(=CC=C1O)[C@H]1OC[C@H]2[C@@H]1CO[C@@H]2C1=CC=C(O)C(OC)=C1
784	<i>Solanum nigrum</i>	30643798	soladulcoside A	CC1CC(C2(C(C3C(O2)C(C4C3(CCC5C4CCC6C5(CCC(C6)OC7C(C(C(O7)CO)O)O)OC8C(C(C(C(O8)C)O)O)O)C)C)O)OC1=O)O
785	<i>Solanum nigrum</i>	30076759	solamargine	C[C@H]1[C@H]2[C@H](C[C@H]3[C@@@H]4CC=C5C[C@H](CC[C@]5(C)[C@H]4CC[C@]23C)O[C@@@H]2O[C@H](CO)[C@@H](O)[C@@H]3O[C@@@H](C)[C@H](O)[C@@H](O)[C@H]3O)[C@H](O)[C@H]2O[C@@@H]2O[C@H](C)[C@H](O)[C@@H](O)[C@H](O)[C@H]2O[C@@@H]2O[C@H](C)[C@H](O)[C@@H](O)[C@H]11CC[C@H](C)CN1

786	<i>Solanum nigrum</i>	17885838	solanigroside A (5alpha-pregn-16-en-3beta-ol-20-one 3-O-beta-D-xylopyranosyl-(1 --> 3)-O-[alpha-L-arabinopyranosyl-(1 --> 2)]-O-beta-D-glucopyranosyl-(1 --> 4)-O-[alpha-L-rhamnopyranosyl-(1 --> 2)]-O-beta-D-galactopyranoside)	CC(C1=CC[C@@]2([H])[C@]3([H])CC[C@@]4([H])C[C@@H](O[C@H]5[C@@H]([C@H]([C@H])([C@@H](CO)O5)O[C@H]6[C@@H]([C@H]([C@H](CO)O6)O)[C@H]7[C@@H]([C@H]([C@H](CO7)O)O)O[C@H]8[C@@H]([C@H]([C@H](CO8)O)O)O)[C@H]9[C@@H]([C@H]([C@H]([C@H](C)O9)O)O)O)CC[C@]4(C)[C@@]3([H])CC[C@]12C)=O
787	<i>Solanum nigrum</i>	17885838	solanigroside B (5alpha-pregn-16-en-3beta-ol-20-one 3-O-beta-D-glucopyranosyl-(1 --> 2)-O-[beta-D-glucopyranosyl-(1 --> 3)]-O-beta-D-glucopyranosyl-(1 --> 4)-O-beta-D-galactopyranoside)	CC(C1=CC[C@@]2([H])[C@]3([H])CC[C@@]4([H])C[C@@H](O[C@H]5[C@@H]([C@H]([C@H])([C@@H](CO)O5)O[C@H]6[C@@H]([C@H]([C@H](CO)O6)O)[C@H]7[C@@H]([C@H]([C@H]([C@H](CO)O7)O)O)O[C@H]8[C@@H]([C@H]([C@H]([C@H](CO)O8)O)O)O)O)CC[C@]4(C)[C@@]3([H])CC[C@]12C)=O
788	<i>Solanum nigrum</i>	23790901	solanigroside P	CC1CCC2(C(C3C(O2)CC4C3(C(CC5C4CC=C6C5(CC(C6)OC7C(C(C(C(O7)CO)OC8C(C(C(C(O8)C)O)O)O)O)C)O)C)NC1
789	<i>Solanum nigrum</i>	29890469	Solanine A	CC1CCC2(C(C3C(N2C1)CC4C3(CC5C4CC=C6C5(CC(C6)OC7C(C(C(C(O7)CO)O)OC8C(C(C(C(O8)CO)O)O)O)O)C9C(C(C(C(O9)C)O)O)O)C)C)C
790	<i>Solanum nigrum</i>	30643798	solasodine	C[C@H]1[C@H]2[C@H](C[C@H]3[C@@H]4CC=C5C[C@@H](O)CC[C@]5(C)[C@H]4CC[

				C@]23C)O[C@]11CC[C@@H](C)CN1
791	<i>Solanum nigrum</i>	23790901	solasonine	C[C@H]1[C@H]2[C@H](C[C@H]3[C@@H]4CC=C5C[C@H](CC[C@]5(C)[C@H]4CC[C@]23C)O[C@@H]2O[C@H](CO)[C@H](O)[C@H](O[C@@H]3O[C@H](CO)[C@@H](O)[C@H](O)[C@H]3O)[C@H]2O[C@@H]2O[C@@H](C)[C@H](O)[C@@H](O)[C@H]2O)OC[C@]11CC[C@@H](C)CN1
792	<i>Solanum nigrum</i>	20845784	syringaresinol	CO C1=CC(=CC(OC)=C1O)C1OCC2C1COC2C1=CC(OC)=C(O)C(OC)=C1
793	<i>Solanum nigrum</i>	30179424	syringic acid (4-hydroxy-3, 5-dimethoxybenzoic acid)	CO C1=CC(=CC(=C1O)OC)C(=O)O
794	<i>Solanum nigrum</i>	16768003	tartaric acid	OC(C(O)C(O)=O)C(O)=O
795	<i>Solanum nigrum</i>	20845784	tetracosanoic acid	CCCCCCCCCCCCCC CCCCCCCCCC(O)=O
796	<i>Solanum nigrum</i>	30076759	uttroside B	CC1C2C(CC3C2(CCC4C3CCC5C4(CCC(C5)OC6C(C(C(C(O6)CO)OC7C(C(C(C(O7)CO)O)OC8C(C(C(CO8)O)O)OC9C(C(C(C(O9)CO)O)O)O)O)O)O)C)OC1(CC(C)COC1C(C(C(C(O1)CO)O)O)O)O
797	<i>Solanum nigrum</i>	17290784	luteine	CC(=O)[C@H]1CC[C@H]2[C@@H]3CCC4=CC(=O)CC[C@]4(C)[C@H]3CC[C@]12C
798	<i>Swertia chirayita</i>	25622657	1,3,6,7-tetrahydroxy-9H-xanthen-9-one	OC1=CC(O)=C2C(OC3=CC(O)=C(O)C=C3C2=O)=C1
799	<i>Swertia chirayita</i>	24013889	1,5,8-trihydroxy-3-methoxy xanthone	CO C1=CC(O)=C2C(=O)C3=C(O)C=CC(O)=C3OC2=C1

800	<i>Swertia chirayita</i>	29235293	1,8-dihydroxy-3,5,7-trimethoxyxanthone	<chem>CO[C@H]1C(=O)C=C2C(=O)C3=C(O)C(OC)=CC(O)C=C3OC2=C1</chem>
801	<i>Swertia chirayita</i>	31076338	12-hydroxyoleanolic lactone	<chem>O1CC2(CC[C@H]3[C@H](C2)C=2[C@H](CC3)(C)[C@H]3[C@H](CC=2O)[C@H]2[C@@H](CC3)C(C)(C)[C@@H](O)CC2)C)C1=O)C</chem>
802	<i>Swertia chirayita</i>	24013889	1-hydroxy-2,3,4,6-tetramethoxyxanthone	<chem>CO[C@H]1C(=O)C=C2C(=O)C3=C(O)C(OC)=C(OC)C(OC)=C3OC2=C1</chem>
803	<i>Swertia chirayita</i>	29235293	1-hydroxy-3, 7-dimethoxyxanthone	<chem>CO[C@H]1C(=O)C=C2OC3=CC(OC)=CC(O)=C3C(=O)C2=C1</chem>
804	<i>Swertia chirayita</i>	29235293	1-hydroxy-3,5,7,8-tetramethoxyxanthone	<chem>CO[C@H]1C(=O)C=C2C(=O)C3=C(OC)C(OC)=CC(OC)=C3OC2=C1</chem>
805	<i>Swertia chirayita</i>	31076338	1-hydroxy-3,5-dimethoxyxanthone	<chem>CO[C@H]1C(=O)C=C2C(=O)C3=CC=CC(OC)=C3OC2=C1</chem>
806	<i>Swertia chirayita</i>	30210007	Amarogentin	<chem>OC[C@H]1O[C@H](O[C@H]2OC=C3[C@@H](CCOC3=O)[C@H]2C=C)[C@H](OC(=O)C2=C(O)C=C(O)C=C2C2=CC=CC(O)=C2)[C@@H](O)[C@@H]1O</chem>
807	<i>Swertia chirayita</i>	25622657	amaronitidin	<chem>O1C(CO)C(O)C(O)C(O)c2c(cc(O)cc2O)-c2cc(O)ccc2C1OC1OC=C2C(=CCOC2=O)C1C=C</chem>
808	<i>Swertia chirayita</i>	25622657	amaroswerin	<chem>OC[C@H]1O[C@H](O[C@H]2OC=C3[C(=O)OCC[C@@H]3(O)[C@H]2C=C)[C@H](OC(=O)C2=C(O)C=C(O)C=C2C2=CC=CC(O)=C2)[C@@H](O)[C@@H]1O</chem>
809	<i>Swertia chirayita</i>	25622657	deoxyloganic acid	<chem>O1C(CO)C(O)C(O)C(O)C1OC1OC=C(C2C1C(CC2)C)C(=O)[O-]</chem>
810	<i>Swertia chirayita</i>	29235293	erythrodiol	<chem>CC1(C)CC[C@H]2(CO)CC[C@H]3(C)C(=CC[C@H]4[C@@H]5(C)CC[C@H](O)C(C)(C)[C@@H]5CC[C@@H]34C)C</chem>

				@H]2C1
811	<i>Swertia chirayita</i>	23275688	Gentianine	C=CC1=CN=CC2=C1C COC2=O
812	<i>Swertia chirayita</i>	30210007	gentiopicroside	OC[C@H]1O[C@@H](O[C@@H]2OC=C3C(=O)OCC=C3[C@H]2C=C[C@H](O)[C@@H](O)[C@@H]1O
813	<i>Swertia chirayita</i>	25622657	iriflophenone	Oc1cc(O)cc(O)c1C(=O)c1ccc(O)cc1
814	<i>Swertia chirayita</i>	30210007	isogentisin	CO C1=CC=C2OC3=CC(O)=CC(O)=C3C(=O)C2=C1
815	<i>Swertia chirayita</i>	25622657	loganic acid	C[C@H]1[C@@H](O)C[C@H]2[C@@H]1[C@H](O)[C@@H](CO)[C@@H](O)[C@H](O)[C@H]1O)OC=C2C(O)=O
816	<i>Swertia chirayita</i>	25622657	maclurin	OC1=CC(O)=C(C(=O)C2=CC=C(O)C(O)=C2)C(O)=C1
817	<i>Swertia chirayita</i>	27041855	mangiferin	OC[C@H]1O[C@H]([C@H](O)[C@@H](O)[C@@H]1O)C1=C(O)C=C2OC3=CC(O)=C(O)C=C3C(=O)C2=C1O
818	<i>Swertia chirayita</i>	31076338	methylswertianin	CO C1=CC(O)=C2C(=O)C3=C(O)C(OC)=CC=C3OC2=C1
819	<i>Swertia chirayita</i>	29235293	sinapaldehyde	CO C1=CC(C=CC=O)=CC(OC)=C1O
820	<i>Swertia chirayita</i>	23275688	Swerchirin	CO C1=CC(O)=C2C(=O)C3=C(O)C=CC(OC)=C3OC2=C1
821	<i>Swertia chirayita</i>	30210007	swertiamarin	OC[C@H]1O[C@@H](O[C@@H]2OC=C3C(=O)OCC[C@@]3(O)[C@H]2C=C)[C@H](O)[C@@H](O)[C@@H]1O
822	<i>Swertia chirayita</i>	29235293	syringaldehyde	CO C1=CC(C=O)=CC(OC)=C1O
823	<i>Swertia chirayita</i>	23275688	Xanthone	O=C1C2=CC=CC=C2OC2=CC=C12

824	<i>Swertia chirayita</i>	31076338	bellidifolin	O1c2c(C(=O)c3c1cc(O C)cc3O)c(O)ccc2O
825	<i>Tagetes minuta</i>	24693417	cis-ocimene	CC(=CCC=C(C)C=C)C
826	<i>Tagetes minuta</i>	30496680	(E)-ocimenone	CC(=CC(=O)C=C(C)C=C)C
827	<i>Tagetes minuta</i>	24689306	(Z)-beta-ocimene	CC(C)=CC\ C=C(\ C)C=C
828	<i>Tagetes minuta</i>	24689306	(Z)-tagetone	CC(C)CC(=O)\ C=C(\ C)C=C
829	<i>Tagetes minuta</i>	8551298	2,2',5',2"-terthiophene	C1(C2=CC=C(C3=CC=CS3)S2)=CC=CS1
830	<i>Tagetes minuta</i>	30295511	5-(4-hydroxybut-1-ynyl)-2,2'-bithiophene	OCCC#CC1=CC=C(S1)C1=CC=CS1
831	<i>Tagetes minuta</i>	8551298	5-(but-3-ene-1-ynyl)-2,2'-bithiophene	C=CC#CC1=CC=C(S1)C1=CC=CS1
832	<i>Tagetes minuta</i>	8551298	5-(but-3-ene-1-ynyl)-5'-methyl-2,2'-bithiophene	CC1=CC=C(S1)C1=CC=C(S1)C#CC=C
833	<i>Tagetes minuta</i>	24599122	5-methyl-2,2',5',2",5",2",5",2"-quinquethiophene	s1c(ccc1-c1sc(cc1)-c1sc(cc1)-c1sc(cc1)C
834	<i>Tagetes minuta</i>	26441652	6-hydroxykaempferol 7-O-beta-glucopyranoside	O1c2c(C(=O)C(O)=C1c1ccc(O)cc1)c(O)c(O)c(O[C@H]1O[C@H](C O)[C@H](O)[C@H](O)[C@H](O)[C@H]1O)c2
835	<i>Tagetes minuta</i>	24693417	cis-tagetone	CC(C)CC(=O)C=C(C)C=C
836	<i>Tagetes minuta</i>	29670846	dihydrotagetone	CC(C)CC(=O)CC(C)C=C
837	<i>Tagetes minuta</i>	29288025	protocatechuic acid methyl ester	COC(=O)C1=CC(=C(C=C1)O)O
838	<i>Tagetes minuta</i>	24599122	quercetin-3,6-dimethyl ether	O.COC1=C(OC2=C(C(O)=C(C)C(O)=C2)C1=O)C1=CC(O)=C(O)C=C1.COC1=C(OC2=C(C(O)=C(C)C(O)=C2)C1=O)C1=CC(O)=C(O)C=C1
839	<i>Tagetes minuta</i>	29670846	spathulenol	CC1(C)[C@H]2CCC(=C)[C@H]3CC[C@](C)(C)O[C@H]3[C@H]12
840	<i>Tagetes minuta</i>	30295511	tagetnoic acid ([4-((3S,6S)-6-((3E,8E)-octadeca-3,8-dien-1-yl)-3,6-dihydro-1,2-dioxin-3-yl)butanoic acid])	O1O[C@H](C=C[C@H]1CCCC(=O)[O-])CC\ C=C\ CCC\ C=C\ CCCCCCCC
841	<i>Tagetes minuta</i>	24689306	(Z)-ocimenone	CC(C)=CC(=O)\ C=C(\ C)

)C=C
842	<i>Tagetes minuta</i>	30295511	22,23-dihydrospinasterone	CC[C@H](CC[C@H]2(C3=CC[C@H]4CC(=O)CC[C@]4(C)[C@H]3CC[C@]12C)C(C)C)
843	<i>Tagetes minuta</i>	24693417	3,9-epoxy-p-mentha-1,8(10)diene	CC1=CC2OCC(=C)C2CC1
844	<i>Tagetes minuta</i>	25182441	tagetone	CC(C)CC(=O)\C=C(/C)C=C
845	<i>Tagetes minuta</i>	25182441	limonene	C1CC(=CCC1C(C)=C)C
846	<i>Terminalia bellirica</i>	23299756	1,2,3,4,6-penta-O-galloyl-b-D-glucose	OC1=CC(C(OC[C@@H](O2)[C@@H](OC(C3=CC(O)=C(O)C(O)=C3)=O)[C@H](OC(C4=C(C(O)=C(O)C(O)=C4)=O)[C@@H](OC(C5=C(C(O)=C(O)C(O)=C5)=O)[C@@H]2OC(C6=C(C(O)=C(O)C(O)=C6)=O)=CC(O)=C1O
847	<i>Terminalia bellirica</i>	23299756	1,2,3,6-tetra-O-galloyl-b-D-glucose	O[C@H]([C@@H](CO C(C1=CC(O)=C(O)C(O)=C1)=O)O2)[C@H](OC(C3=CC(O)=C(O)C(O)=C3)=O)[C@@H](OC(C4=CC(O)=C(O)C(O)=C4)=O)[C@@H]2OC(C5=CC(O)=C(O)C(O)=C5)=O
848	<i>Terminalia bellirica</i>	23299756	arjunetin	O1C(CO)C(O)C(O)C(O)C1OC(=O)C12C(C3=CC4C(CCC5C(C)(C)C(O)C(O)CC45C)(C)C3(C(C1)C)C(O)C(CC2)C)C
849	<i>Terminalia bellirica</i>	23299756	arjunglucoside-I	CC1(CCC2(CCC3(C(=CCC4C3(CCC5C4(CC(C(C5(C)CO)O)O)C)C)C2C1O)C)C(=O)OC6C(C(C(C(O6)CO)O)O)O)C
850	<i>Terminalia bellirica</i>	23299756	arjunglucoside-II	CC1(CCC2(CCC3(C(=CCC4C3(CCC5C4(CC(C(C5(C)CO)O)O)C)C)C2C1)C)C(=O)OC6C(C(C(C(O6)CO)O)O)O)C

851	<i>Terminalia bellirica</i>	23299756	arjunglucoside-III	<chem>CC1(CCC2(CCC3(C(=CC(=O)C4C3(CCC5C4(CC(C(C5(C)C)O)O)C)C)C)C2C1O)C)C(=O)OC6C(C(C(C(O6)CO)O)O)OC</chem>
852	<i>Terminalia bellirica</i>	23299756	bellericoside	<chem>CC1(CCC2(CCC3(C(=CCC4C3(CCC5C4(CC(C(C5(CO)CO)O)O)C)C)C)C2C1)C)C(=O)OC6C(C(C(C(O6)CO)O)O)OC</chem>
853	<i>Terminalia bellirica</i>	23299756	chebulagic acid	<chem>O[C@H]1[C@H]2[C@H](CC(O)=O)C(=O)O[C@@H]3[C@H]4COC(=O)C5=CC(O)=C(O)C(O)=C5C5=C(O)C(O)=C(O)C=C5C(=O)O[C@@H]3[C@@H](OC(=O)C3=CC(O)=C(O)C(OC1=O)=C23)[C@H](OC(=O)C1=CC(O)=C(O)C(O)=C1)O4</chem>
854	<i>Terminalia bellirica</i>	23299756	chebulinic acid	<chem>O[C@H]1[C@H]2[C@H](CC(O)=O)C(=O)O[C@@H]3[C@@H](CO C(=O)C4=CC(O)=C(O)C(O)=C4)O[C@@H](OC(=O)C4=CC(O)=C(O)C(O)=C4)[C@H](OC(=O)C4=CC(O)=C(O)C(O)=C1=O)=C24)[C@H]3O C(=O)C1=CC(O)=C(O)C(O)=C1</chem>
855	<i>Terminalia bellirica</i>	23299756	chebuloside II	<chem>CC1(CCC2(CCC3(C(=CCC4C3(CC(C5(C)CO)O)O)C)O)C)C2C1)C)C(=O)OC6C(C(C(C(O6)CO)O)O)OC</chem>
856	<i>Terminalia bellirica</i>	23299756	corilagin	<chem>O[C@@H]1[C@H]2CO C(=O)C3=CC(O)=C(O)C(O)=C3C3=C(O)C(O)=C(O)C=C3C(=O)O[C@@H]1[C@@H](O)[C@H](OC(=O)C1=CC(O)=C(O)C(O)=C1)O2</chem>
857	<i>Terminalia bellirica</i>	23299756	ellagic acid	<chem>OC1=CC2=C3C(OC(=O)C4=C3C(OC2=O)=C(O)C(O)=C4)=C1O</chem>

858	<i>Terminalia bellirica</i>	22105160	gallic acid	OC(=O)C1=CC(O)=C(O)C(O)=C1
859	<i>Terminalia bellirica</i>	23299756	gallic acid methyl ester	CO[C@H]1CC2=C(O)C=C(CO)C=C1
860	<i>Terminalia bellirica</i>	25190275	trifluoroacetic acid	OC(=O)C(F)(F)F
861	<i>Tinospora cordifolia</i>	24425954	(-) epicatechin	O[C@H]1CC2=C(O)C=C(CO)C=C1
862	<i>Tinospora cordifolia</i>	29034429	1-docosene	CCCCCCCCCCCCCCCCC CCCCCCC=C
863	<i>Tinospora cordifolia</i>	29034429	1-eicosanol	CCCCCCCCCCCCCCCCC CCCCCCCO
864	<i>Tinospora cordifolia</i>	29034429	1-eicosene	CCCCCCCCCCCCCCCCC CCCC=C
865	<i>Tinospora cordifolia</i>	29050549	1-hexadecanol	CCCCCCCCCCCCCCCCC CCO
866	<i>Tinospora cordifolia</i>	29050549	1-hexadecene	CCCCCCCCCCCCCCCCC C=C
867	<i>Tinospora cordifolia</i>	29034429	1-octadecanol	CCCCCCCCCCCCCCCCC CCCCO
868	<i>Tinospora cordifolia</i>	29034429	1-octadecene	CCCCCCCCCCCCCCCCC CCC=C
869	<i>Tinospora cordifolia</i>	29034429	1-tetradecene	CCCCCCCCCCCCCCCCC=C
870	<i>Tinospora cordifolia</i>	29034429	2,4-di-tert-butylphenol	CC(C)(C)C1=CC(=C(O)C=C1)C(C)(C)C
871	<i>Tinospora cordifolia</i>	30166229	b-ecdysone	CC(C)(O)CC[C@H](O)[C@@](C)(O)[C@H]1CC[C@]2(O)C3=CC(=O)[C@H]4C[C@H](O)[C@@H](O)C[C@H]4(C)[C@H]3CC[C@H]12C
872	<i>Tinospora cordifolia</i>	29142429	behenic alcohol	CCCCCCCCCCCCCC CCCCCCCCCO
873	<i>Tinospora cordifolia</i>	29460537	berberine	CO[C@H]1C2=C(N+)[C@H](C=C2C=C1)C1=CC2=C(OC(=O)C=C1)CC3
874	<i>Tinospora cordifolia</i>	20496230	cleroda-1(10)-en-6beta-ol	O[C@H]1C[C@H](C)[C@](C2=CCC[C@H](C)[C@@]12C)(CC[C@H](CC)C)C
875	<i>Tinospora cordifolia</i>	22946632	columbin	C[C@H]12C[C@H](OC(=O)[C@H]1CC[C@H]1(C)[C@H]2[C@H]2OC(=O)[C@H]1(O)C=C2)C1=CO=C1

876	<i>Tinospora cordifolia</i>	22497272	cordifolide A	S(CCOC1OC(CO)C(O)C(O)C1O)C1CCC2C3(C(OC(=O)C13O)CC1C2(CC(OC1=O)c1ccoc1)C)C
877	<i>Tinospora cordifolia</i>	28962889	cordifolioside A (β -D-Glucopyranoside,4-(3-hydroxy-1-propenyl)-2,6-dimethoxyphenyl 3-O-D-apio- β -D-furanosyl)	CO C1=CC(=CC(=C1O)C2C(C(C(C(O2)CO)O)OC3C(C(CO3)(CO)O)O)OC)C=CCO
878	<i>Tinospora cordifolia</i>	29034429	cyclotetradecane	C1CCCCCCCCCC1
879	<i>Tinospora cordifolia</i>	28962889	ecdysterone	CC(C)(O)CCC(O)[C@](C)(O)C1CCC2(O)C3=CC(=O)[C@@H]4C[C@@H](O)[C@@H](O)C[C@]4(C)C3CC[C@]12C
880	<i>Tinospora cordifolia</i>	21976812	isocolumbin	C[C@]12C[C@@H](O)C(=O)[C@@H]1CC[C@@]1(C)[C@@H]2[C@H]2OC(=O)[C@]1(O)C=C2)C1=CO C=C1
881	<i>Tinospora cordifolia</i>	26627195	isocorydine	CO C1=CC=C2C[C@@H]3N(C)CCC4=CC(OC)=C(OC)C(=C34)C2=C1O
882	<i>Tinospora cordifolia</i>	22430503	N-methyl-2-pyrrolidone	CN1CCCC1=O
883	<i>Tinospora cordifolia</i>	26627195	oblongine	O(C)c1ccc2c(c1O)C([N+](CC2)(C)C)Cc1ccc(O)cc1
884	<i>Tinospora cordifolia</i>	26627195	palmatine	CO C1=CC2=C(C=C1O)C1C1=[N+]([CC2)C=C2C(OC)=C(OC)C=CC2=C1
885	<i>Tinospora cordifolia</i>	18951283	saponarin (apigenin-6-C-glucosyl-7-O-glucoside)	O1C(C(O)C(O)C(O)C1CO)c1c(O)c2c(OC(=CC2=O)c2ccc(O)cc2)cc1OC1OC(CO)C(O)C(O)C1O
886	<i>Tinospora cordifolia</i>	22472109	syringin	CO C1=CC(\C=C\CO)=CC(OC)=C1O[C@@H]1O[C@H](CO)[C@@H](O)[C@H](O)[C@H]1O
887	<i>Tinospora cordifolia</i>	26627195	tetrahydropalmatine	CO C1=CC2=C(C=C1O)C1C1=[N+]([CC2)C=C2C(OC)=C(OC)N1CC2)C(OC)=C(OC)

				C=C3
888	<i>Tinospora cordifolia</i>	26253577	tinocordiside	O1C(CO)C(O)C(O)C(O)C1OC(C)(C)C1C2C3C(C2C(=O)C=C3C)(CC1)C
889	<i>Tinospora cordifolia</i>	31035042	tinosponone	O1C(CC2(C3C(CCC2C1=O)(C)C(O)C=CC3=O)C)c1ccoc1
890	<i>Tinospora cordifolia</i>	22946632	tinosporide	C[C@]12C[C@@H](OC(=O)[C@H]1CC[C@H]1(C)[C@H]2[C@@H]2OC(=O)[C@]1(O)[C@H]1O[C@@H]21)C1=CO=C1
891	<i>Tinospora cordifolia</i>	21976812	tinosporin	CC12CCC3(C(=O)OC(CC3(C1CC4C(C2(C(=O)OC)O)O4)C)C5=CO=C5)O
892	<i>Tinospora cordifolia</i>	26253577	yangambin	CO C1=CC(=CC(OC)=C1OC)[C@H]1OC[C@H]2[C@@H]1CO[C@@H]2C1=CC(OC)=C(OC)C(OC)=C1
893	<i>Tinospora cordifolia</i>	28962889	β -Sitosterol	CCC(CCC(C)C1CCC2C1(CCC3C2CC=C4C3(CCC(C4)O)C)C)C(C)C
894	<i>Tinospora cordifolia</i>	20171072	beta-Ecdysone	CC(C)(O)CC[C@@H](O)[C@](C)(O)[C@H]1CC[C@H]2(O)C3=CC(=O)[C@@H]4C[C@@H](O)[C@@H](O)C[C@]4(C)[C@H]3CC[C@H]1C
895	<i>Tinospora cordifolia</i>	29460537	isoquinolone	O=C1NC=Cc2cccc12
896	<i>Valeriana jatamansi</i>	21366063	methyl linoleate	CCCCC\ C=C/C\ C=C/C\ CCCCC(=O)OC
897	<i>Valeriana jatamansi</i>	20151678	(+)-9'-isovaleroxylariciresinol	O1CC(Cc2cc(OC)c(O)cc2)C(COC(=O)CC(C)C)C1c1cc(OC)c(O)cc1
898	<i>Valeriana jatamansi</i>	28623738	(4b,8b)-8-methoxy-3-methoxy-10-methylene-2,9-dioxatricyclo[4.3.1.0(3,7)]decan-4-ol	O1C2O[C@@H](OC)C3C(C[C@@H](O)C)C13OC2=C
899	<i>Valeriana jatamansi</i>	20853876	1,5-dihydroxy-3,8-epoxyvaledichlorine	ClCC12OC3OC(O)C1C(O)(CC2OC(=O)C)C3

900	<i>Valeriana jatamansi</i>	12502349	1-homoacevaltrate	O1CC12C1C(=CC2OC(=O)CC(OC(=O)C)(C)C)C(=COC1OC(=O)CC(C)C)COC(=O)C
901	<i>Valeriana jatamansi</i>	12502349	1-homoisoacevaltrate	O1CC12C1C(=CC2OC(=O)C)C(=COC1OC(=O)CC(CC)C)COC(=O)C(OC(=O)C)C(C)C
902	<i>Valeriana jatamansi</i>	18666542	2-butanone,4-(2,6,6-trimethyl-2-cyclohexen-1-yl)	O=C(CCC1C(CCC=C1C)(C)C)C
903	<i>Valeriana jatamansi</i>	26983241	3'(S)-acetoxy-4'(R)-angeloyloxy-3',4'-dihydroxanthyletin	O1c2c(cc3C=CC(Oc3c2)=O)[C@@@H](OC(=O)\C(=C/C)\C)[C@H](OC(=O)C)C1(C)C
904	<i>Valeriana jatamansi</i>	26009656	7-epi-a-selinene	C12CC(CCC1(CCC=C2C)C(C)=C
905	<i>Valeriana jatamansi</i>	28623738	8-methoxy-4-acetoxy-3-chlormethyl-10-methylen-2,9-dioxa-tricyclo[4.3.1.0(3,7)]decan	ClCC12OC3OC(OC)C1C(CC2OC(=O)C)C3=C
906	<i>Valeriana jatamansi</i>	29232391	acevaltrate	CC(C)CC(=O)O[C@@@H]1OC=C(COC(C)=O)C2=C[C@H](OC(=O)C)C(C)(C)OC(C)=O)[C@]3(CO3)[C@@H]12
907	<i>Valeriana jatamansi</i>	26009656	a-guaiene	C[C@H]1CCC2=C1C[C@@H](CC[C@@H]2C)C(C)=C
908	<i>Valeriana jatamansi</i>	21366063	a-gurjunene	C12C(CCC(C3C1=C(C)C3)C)C2(C)C
909	<i>Valeriana jatamansi</i>	24804225	a-muurolene	CC(C)[C@@@H]1CC=C(C)[C@H]2CCC(C)=C[C@@H]12
910	<i>Valeriana jatamansi</i>	18666542	aristolene	C12C(CC=C3CCCC(C)C13)C2(C)C
911	<i>Valeriana jatamansi</i>	16276973	baldrinal	CC(=O)OCC1=COC=C2C(C=O)=CC=C12
912	<i>Valeriana jatamansi</i>	24804225	b-guaiene	C[C@H]1CCC2=C1CC(C[C@@H]2C)=C(C)C
913	<i>Valeriana jatamansi</i>	24804225	b-gurjunene	C[C@@@H]1CC[C@@H]2[C@H]([C@H]3[C@@H]1CCC3=C)C2(C)C
914	<i>Valeriana jatamansi</i>	26009656	bornyl acetate	CC(=O)OC1CC2CCC1(C)C2(C)C
915	<i>Valeriana jatamansi</i>	24804225	b-patchoulene	CC1CCC2=C1CC3CCC2(C3(C)C)C

916	<i>Valeriana jatamansi</i>	24804225	b-vatirenene	CC1CC=CC2=CCC(CC12C)=C(C)C
917	<i>Valeriana jatamansi</i>	18666542	cadinol	CC1=CC2C(CCC(C2CC1)(C)O)C(C)C
918	<i>Valeriana jatamansi</i>	26009656	calarene/β-gurjunene	C12C(CCC3=CCCC(C)C13C)C2(C)C
919	<i>Valeriana jatamansi</i>	18666542	caryophyllene oxide	CC12CCC3C(CC3(C)C)C(=C)CCC1O2
920	<i>Valeriana jatamansi</i>	28623738	chlorovaltrate A	ClCC12OC3OC(OC(=O)CC(C)C)C1C(O)(CC2OC(=O)C)C3=C
921	<i>Valeriana jatamansi</i>	16276973	coniferin	COCC1=CC(\C=C\CO)=CC=C1O[C@H]1O[C@H](CO)[C@H](O)[C@H](O)[C@H]1O
922	<i>Valeriana jatamansi</i>	18666542	cubenol	OC12C(C=C(CC1)C)C(CCC2)C(C)C
923	<i>Valeriana jatamansi</i>	21366063	cuparene	CC1=CC=C(C=C1)[C@]1(C)CCCC1(C)C
924	<i>Valeriana jatamansi</i>	26983241	decursidin	O1c2c(cc3C=CC(Oc3c2)=O)C(OC(=O)C=C(C)C)C(OC(=O)C=C(C)C)C1(C)C
925	<i>Valeriana jatamansi</i>	26983241	decursitin A	O1c2c(cc3C=CC(Oc3c2)=O)C(OC(=O)C(=CC)C)C(OC(=O)C(=CC)C)C1(C)C
926	<i>Valeriana jatamansi</i>	26983241	decursitin B	O1c2c(cc3C=CC(Oc3c2)=O)C(OC(=O)C(=CC)C)C(OC(=O)C=C(C)C)C1(C)C
927	<i>Valeriana jatamansi</i>	24804225	dehydroaromadendrene	C12C(CC=C(C3C1C(CC3)C)C2(C)C
928	<i>Valeriana jatamansi</i>	26983241	dibutyl phthalate	CCCCOC(=O)C1=CC=CC=C1C(=O)OCCCC
929	<i>Valeriana jatamansi</i>	22006721	guaiol	C[C@H]1CCC2=C1C[C@H](CC[C@H]2C)C(C)(C)O
930	<i>Valeriana jatamansi</i>	16276973	hexacosanic acid	CCCCCCCCCCCCCCCCCC(O)=O
931	<i>Valeriana jatamansi</i>	30213112	isochlorogenic acid A	O(C(=O)C=Cc1cc(O)c(O)cc1)C1CC(O)(CC(O)C(=O)C=Cc2cc(O)c(O)cc2)C1O)C(=O)[O-]
932	<i>Valeriana jatamansi</i>	30213112	isochlorogenic acid B	O(C(=O)C=Cc1cc(O)c(O)cc1)C1C(OC(=O)C=Cc2cc(O)c(O)cc2)CC(O)(CC1O)C(=O)[O-]

933	<i>Valeriana jatamansi</i>	30213112	isochlorogenic acid C	C1C(C(C(CC1(C(=O)O)O)OC(=O)C=CC2=CC(=C(C=C2)O)O)OC(=O)C=CC3=CC(=C(C=C3)O)O)
934	<i>Valeriana jatamansi</i>	16724553	IVHD-valtrate	O1CC12C1C(O)(CC2O C(=O)C)C=COC1OC(=O)CC(C)C)COCC(=O)C(OC(=O)CC(C)C)C(C)C
935	<i>Valeriana jatamansi</i>	20151678	Jatamanins H	CC12C(CC3C1C(=O)OCC3C(O2)OC)O
936	<i>Valeriana jatamansi</i>	26009656	kessane	O1C(C2CC3C(CCC3C)C1(CC2)C)(C)C
937	<i>Valeriana jatamansi</i>	26009656	maaliol	OC1(C2C3C(CCC2(CC1)C)C3(C)C)C
938	<i>Valeriana jatamansi</i>	25469856	nardostachin	O1C=C(C2C(C(C)C(O)C2)C1OC(=O)CC(C)C)COCC(=O)CC(C)C
939	<i>Valeriana jatamansi</i>	22006721	seychellene	CC1CCC2(C(=C)C3CC2(C1C3)C)C
940	<i>Valeriana jatamansi</i>	26009656	seychellene	C12CC3CCCC1(C)C(CC2C)C)C3=C
941	<i>Valeriana jatamansi</i>	26009656	β -patchoulene	C12CC3=C(CCC3C)C(CC1)C)C2(C)C
942	<i>Valeriana jatamansi</i>	21366063	valeracetate	CCCCCC([O-])=O
943	<i>Valeriana jatamansi</i>	26971960	valerenic acid	CC1CCC(C=C(/C)C(O)=O)C2=C(C)CCC12
944	<i>Valeriana jatamansi</i>	16724553	valeriotetrate A	CC(C)CC(=O)OC1C2C(CC(C2(COC(=O)C(C)C)OC(=O)CC(C)C)O)OC(=O)C)(C(=CO1)COC(=O)C(C(C)C)OC(=O)CC(C)C)O
945	<i>Valeriana jatamansi</i>	20853876	Valeriotetrate C	CC(C)CC(=O)CO[C@H](C(C)C)C(=O)OC[C@]1(O)[C@H](C[C@]2(O)[C@H]1[C@@H](OC(=O)CC(C)C)OC=C2CO[C@H](OC(=O)CC(C)C)C(C)C)OC(C)=O
946	<i>Valeriana jatamansi</i>	16724553	valerosidate	O1C(CO)C(O)C(O)C(O)C1OCC=1C2C(C(O)(C)C(O)C2)C(OC=1)OC(=O)CC(C)C

947	<i>Valeriana jatamansi</i>	30638055	Valtrate	CC(C)CC(=O)O[C@H]1C=C2[C@H](C[C@H](OC(=O)CC(C)C)OC=C2CO[C@H]1C[C@H]11CO1
948	<i>Valeriana jatamansi</i>	26009656	viridiflorol	C[C@H]1CC[C@H]2[C@H]1[C@H]1[C@@H](CC[C@]2(C)O)C1(C)C
949	<i>Valeriana jatamansi</i>	23036722	volvaltrate B	CC(C)CC(=O)O[C@H](C(C)C)C(=O)OCC1=C O[C@H](OC(=O)CC(C)C)C2[C@H](O)(CCl)[C@H](C[C@]12O)OC(C)=O
950	<i>Valeriana jatamansi</i>	26009656	α -bulnesene/ δ -guaiene	CC1CCC2=C(CCC(CC12)C(=C)C)C
951	<i>Valeriana jatamansi</i>	26009656	α -patchoulene	CC1CCC23C1CC(C2(C)C)CC=C3C
952	<i>Valeriana jatamansi</i>	23036722	chlorovaltrate A	CC(C)CC(=O)OC1C2C3(CC(C2(OC(C3=C)O1)CCl)OC(=O)C)O
953	<i>Valeriana jatamansi</i>	23036722	chlorovaltrates E	CC(C)CC(=O)OC1C2C(CC(C2(CCl)O)O)(C(=CO1)COC(=O)C(C(C)C)OC(=O)CC(C)C)O
954	<i>Valeriana jatamansi</i>	23036722	Chlorovaltrates K	CC(C)CC(=O)OCC1=C OC(C2C1CC(C2(CCl)O)OC(=O)C)OC(=O)CC(C)C
955	<i>Valeriana jatamansi</i>	23036722	Chlorovaltrates L	CC(C)CC(=O)OC1C=C2(C(C1(CCl)O)C(OC=C2CO[C@H]1C[C@H]11CO1)COC(=O)C(C(C)C)OC(=O)C(C)C
956	<i>Valeriana jatamansi</i>	23036722	Chlorovaltrates M	CC(C)CC(=O)OC1C2C(=CC(C2(CCl)O)OCCC(C)(C)OC(=O)C)C(=CO1)COC(=O)C
957	<i>Valeriana jatamansi</i>	23036722	Chlorovaltrates N	CCC(C)CC(=O)OC1C=C2(C(C1(CCl)O)C(OC=C2CO[C@H]1C[C@H]11CO1)COC(=O)CC(C)C
958	<i>Valeriana jatamansi</i>	25665939	jatamanin A	CC1(C(CC2C1C(=O)OCC2=C)O)O
959	<i>Valeriana jatamansi</i>	25665939	jatamanvaltrate A	CC(C)CC(=O)OC1C2C(CC(C2(COC(=O)CC(C)(C)OC(=O)C)C(=CO1)COC(=O)C(C(C)C)OC(=O)CC(

				C)C)O
960	<i>Valeriana jatamansi</i>	25665939	valeriandoid D	CC(C)CC(=O)OCC1=C 2C=CC(C2C(OC1OC)O C(=O)CC(C)C)(COC(=O) C(C(C)C)OC(=O)CC (C)C)O
961	<i>Valeriana jatamansi</i>	25665939	valeriandoid E	CC(C)CC(=O)OC(C(C) C)C(=O)OCC1(C=CC2 =C(C(OC(C21)OC)OC) COC(=O)C)O
962	<i>Valeriana jatamansi</i>	25665939	valeriandoid F	CC(C)CC(=O)OC1C=C 2C(C1(COC)O)C(OC=C C2COC(=O)C)OC(=O) CC(C)C
963	<i>Valeriana jatamansi</i>	25665939	valeriandoids B	CC(C)CC(=O)OC1C2C (=CC(C2(CCl)O)OC(=O) CC(C)(C)OC(=O)C C(=CO1)COC(=O)C
964	<i>Vetiveria zizanioides</i>	22474964	trans-eudesma-4(15),7-dien-12-ol (vetiselinol)	OCC(C)C=1CC2C(CC=1)(CCCC2=C)C
965	<i>Vetiveria zizanioides</i>	18618805	(-)khusimone	CC1(C2CCC3(C2)C(C1 =C)CCC3=O)C
966	<i>Vetiveria zizanioides</i>	18618805	(-)patchoulol	C[C@H]1CC[C@@]2(O)C(C)(C)[C@@H]3C C[C@@]2(C)[C@H]1C3
967	<i>Vetiveria zizanioides</i>	22474964	(E)-eremophila-1(10),7(11)-12-ol (isovalencenol)	OCC(C)C1=CC2(C(CC 1)=CCCC2C)C
968	<i>Vetiveria zizanioides</i>	22474964	(E)-opposita-4(15),7(11)-dien-12-ol	OCC(=CC1C2C(CC1)(CCCC2=C)C)C
969	<i>Vetiveria zizanioides</i>	22474964	11-dien-2alpha-ol (nootkatol)	OC1CC(C)C2(CC(CCC 2=C1)C(C)=C)C
970	<i>Vetiveria zizanioides</i>	22474964	13-nor-trans-eudesma-4(15),7-dien-11-one	O=C(C)C=1CC2C(CC=1)(CCCC2=C)C
971	<i>Vetiveria zizanioides</i>	30451435	3,3,8,8-tetramethyltricyclo[5.1.0.0(2,4)]oct-5-ene-5-propanoic acid	O=C([O-])CCC=1C2C(C3C(C=1)C3(C)C)C2(C)C
972	<i>Vetiveria zizanioides</i>	30451435	6-isopropenyl-4,8a-dimethyl-1,2,3,5,6,7,8,8a-octahydronaphthalen-2-ol	CC(=C)C1CCC2(C)CC(O)CC(C)=C2C1

973	<i>Vetiveria zizanioides</i>	22474964	alpha-vetivone	C[C@@H]1CC(=O)C=C2CCC(C[C@@]12C)=C(C)C
974	<i>Vetiveria zizanioides</i>	22474964	amorph-4-en-10-ol	OC1(C2C(C=C(CC2)C)C(CC1)C(C)C)C
975	<i>Vetiveria zizanioides</i>	22474964	beta-vetispirene	C1C2(CCC1=C(C)C)C(CC=CC2=C)C
976	<i>Vetiveria zizanioides</i>	22474964	beta-vetivenene	C1C2(C(=CCC1=C(C)C)C=CCC2C)C
977	<i>Vetiveria zizanioides</i>	22474964	beta-vetivone	C[C@@H]1CC(=O)C=C(C)[C@@]11CCC(C1)=C(C)C
978	<i>Vetiveria zizanioides</i>	22474964	bisabolane	CC(C)CCCC(C)C1CCC(C)CC1
979	<i>Vetiveria zizanioides</i>	24772013	cedr-8-en-13-ol	OCC1(C2CC3(C1CCC3C)CC=C2C)C
980	<i>Vetiveria zizanioides</i>	22474964	cedrane	C[C@@H]1CC[C@H]2C(C)(C)[C@H]3C[C@]12CC[C@H]3C
981	<i>Vetiveria zizanioides</i>	22474964	delta-selinene	CC(C)C1=CC2=C(C)C CCC2(C)CC1
982	<i>Vetiveria zizanioides</i>	22474964	eremophilane	CC(C)[C@@H]1CC[C@H]2CCC[C@H](C)[C@@]2(C)C1
983	<i>Vetiveria zizanioides</i>	22474964	eudesma-4,6-diene (delta-selinene)	CC1=C2C=C(CCC2(CC1)C)C(C)C
984	<i>Vetiveria zizanioides</i>	22474964	eudesmane	CC(C)[C@@H]1CC[C@H]2(C)CCC[C@H](C)(C)[C@@H]2C1
985	<i>Vetiveria zizanioides</i>	22474964	isovalencenol	CC1CCC=C2C1(C=C(C2)C(C)CO)C
986	<i>Vetiveria zizanioides</i>	23841574	khusenic acid	CC1(C2CCC3(C2)C(C1)=C)CCC3C(=O)O)C
987	<i>Vetiveria zizanioides</i>	26345879	khusimol	CC1(C)[C@@H]2CC[C@]3(C2)[C@@H](CO)CC[C@H]3C1=C
988	<i>Vetiveria zizanioides</i>	22474964	khusimone	O=C1C23C(CC1)C(=C)C(C(C2)CC3)(C)C
989	<i>Vetiveria zizanioides</i>	26810796	Prometryn	CSC1=NC(NC(C)C)=N C(NC(C)C)=N1
990	<i>Vetiveria zizanioides</i>	22474964	vetiselinol	CC(CO)C1=CCC2(CCC(=C)C2C1)C
991	<i>Vetiveria zizanioides</i>	22474964	ziza-6(13)-en-12-ol (khusimol)	CC1(C2CCC3(C2)C(CCC3C1=C)CO)C
992	<i>Vetiveria zizanioides</i>	26359641	zizanoic acid	CC1(C)[C@@H]2CC[C@]3(C2)[C@@H](CC[C@H]3C1=C)C(O)=O
993	<i>Vetiveria zizanioides</i>	22474964	zizaane	C[C@H]1CCC2C(=C)C(C)(C)[C@@H]3CC[C@H]23C

				@]12C3
994	<i>Withania Somnifera</i>	24467542	12-deoxy withastramonolide	CC1=C(C(=O)OC(C1)C(C)C2CCC3C2(CCC4C3C5C(O5)C6(C4(C(=O)C=CC6)C)O)C)CO
995	<i>Withania Somnifera</i>	29945694	12-deoxywithastromonolide	O1C(=O)C(CO)=C(CC1C(C)C1CCC2C3C(CCC12C)C1(C(C2OC23)C(O)C=CC1=O)C)C
996	<i>Withania Somnifera</i>	22125584	2,3-didehydrosomnifericin	O1C(=O)C(CO)=C(CC1C(C)C1CCC2C3C(CCC12C)C1(C)C(O)(C(O)C3)C(O)C=CC1=O)C
997	<i>Withania Somnifera</i>	22125584	2,3-dihydrowithaferin A	O1C(=O)C(CO)=C(CC1C(C)C1CCC2C3C(CCC12C)C1(C2(OC2C3)C(O)CCC1=O)C)C
998	<i>Withania Somnifera</i>	15520512	2,3-dihydrowithaferin-A	CC1=C(C(=O)OC(C1)C(C)C2CCC3C2(CCC4C3CC5C6(C4(C(=O)CCC6O)C)O5)C)CO
999	<i>Withania Somnifera</i>	17879227	27-deoxywithaferin A	O1C(=O)C(C)=C(CC1C(C)C1CCC2C3C(CCC12C)C1(C2(OC2C3)C(O)C=CC1=O)C)C
1000	<i>Withania Somnifera</i>	24422976	27-hydroxy withanone	O1C(=O)C(CO)=C(CC1C(C)C1(O)CCC2C3C(CC12C)C1(C)C(O)(C2OC23)CC=CC1=O)C
1001	<i>Withania Somnifera</i>	30677568	27-Hydroxywithanolide B	O1C(=O)C(CO)=C(CC1C(C)C1CCC2C3C(CCC12C)C1(C)C(O)(C2OC23)CC=CC1=O)C
1002	<i>Withania Somnifera</i>	22125584	3-methoxy-2,3-dihydrowithaferin A	O1C(=O)C(CO)=C(CC1C(C)C1CCC2C3C(CCC12C)C1(C2(OC2C3)C(O)C(OC)CC1=O)C)C
1003	<i>Withania Somnifera</i>	14575818	4, 16-dihydroxy-5beta, 6beta-epoxyphysagulin D	CC1=C(C(=O)OC(C1)C(C)C2(CC3C2(CCC4C3CC5C6(C4(C(CC(C6O)OC7C(C(C(C(O7)CO)O)O)O)O)C)O5)C)O)C
1004	<i>Withania Somnifera</i>	27605335	4-B-hydroxy-withanolide E	O1C(=O)C(C)=C(CC1C(O)(C)C1(O)CCC2(O)C3(CCC12C)C1(C2(OC2C3)C(O)C=CC1=O)C)C

1005	<i>Withania Somnifera</i>	12210769	aesculetin	O1c2cc(O)c(O)cc2C=C C1=O
1006	<i>Withania Somnifera</i>	12210769	Beta-amyrin	O[C@H]1CC[C@]2([C @@H](CC[C@@@]3([C @@H]2CC=C2[C@@ H]4CC(CC[C@@@]4(CC [C@]23C)C)(C)C)C1(C)C)C
1007	<i>Withania Somnifera</i>	18061221	beta-sitosterol glucoside	O1[C@H](CO)[C@@H](O)[C@H](O)[C@@H](O)[C@@H]1O[C@@ H]1CC2=CC[C@H]3[C@@H]4CC[C@H]([C@@H](CC[C@H](C(C)C)CC)C)[C@]4(CC[C@@H]3[C@@H]3[C@]2(CC1)C)C
1008	<i>Withania Somnifera</i>	25809293	campesterol	O[C@@H]1CC2=CC[C@H]3[C@@H]4CC[C@H]([C@@H](CC[C@H](C(C)C)C)C)[C@]4(CC[C@@H]3[C@]2(C C1)C)C
1009	<i>Withania Somnifera</i>	12045329	coagulin Q	O1C(CO)C(O)C(O)C(O)C1OC1CC(O)C2(C3C(C4CCC(C(O)(C)C5OC(=O)C(C)=C(C5)C)C4(C C3)C)CC=C2C1)C
1010	<i>Withania Somnifera</i>	30998355	docosanyl ferulate	O(C)c1cc(ccc1O)C=CC (OCCCCCCCCCC=O)CCCCCCCC=O
1011	<i>Withania Somnifera</i>	14032282	isopelletierine	O=C(CC1[NH2+]CCCC 1)C
1012	<i>Withania Somnifera</i>	27743505	ixocarpalactone A	O1C(C(O)C(O)(C)C2C 3(C(CC2O)C2C(CC3)C 3(C4(OC4C2)C(O)C=C C3=O)C)C(C)C(C)C1 =O
1013	<i>Withania Somnifera</i>	30677568	Morusin	O1c2c(C(=O)C(CC=C(C)C)=C1c1ccc(O)cc1O) c(O)cc1OC(C=Cc12)(C) C
1014	<i>Withania Somnifera</i>	14575818	physagulin D	CC1=C(C(=O)OC(C1)C (C)C2CCC3C2(CCC4C 3CC=C5C4(C(CC(C5)O C6C(C(C(C(O6)CO)O) O)O)O)C)C)CO
1015	<i>Withania Somnifera</i>	19475989	Physagulin D	O1C(CO)C(O)C(O)C(O)C1OC1CC(O)C2(C3C(C4CCC(C(C)C5OC(=O)C(CO)=C(C5)C)C4(CC

				3)C)CC=C2C1)C
1016	<i>Withania Somnifera</i>	14575818	sitoindoside IX	C[C@@H]([C@H]1CC [C@H]2[C@@H]3C[C @H]4O[C@]44[C@@ H](O)C=CC(=O)[C@]4 (C)[C@H]3CC[C@]12 C)[C@H]1CC(C)=C(C O[C@@H]2O[C@H](C O)[C@@H](O)[C@H](O)[C@H]2O)C(=O)O1
1017	<i>Withania Somnifera</i>	27146059	sitosterol	O[C@@H]1CC2=CC[C @H]3[C@@H]4CC[C @H]([C@@H](CC[C@ H](C(C)C)CC)C)[C@]4 (CC[C@@H]3[C@]2(C C1)C)C
1018	<i>Withania Somnifera</i>	18061221	stigmasterol glucoside	O1C(CO)C(O)C(O)C(O)C1OC1CC2=CCC3C4 CCC(C(C=CC(C(C)C)C C)C)C4(CCC3C2(CC1) C)C
1019	<i>Withania Somnifera</i>	14575818	Viscosalactone B	O1C(=O)C(CO)=C(CC1 C(C)C1CCC2C3C(CCC 12C)C1(C2(OC2C3)C(O)C(O)CC1=O)C)C
1020	<i>Withania Somnifera</i>	27605335	withafastuosin D diacetate	O1C(=O)C(COC(=O)C) =C(CC1C(COC(=O)C) C1CCC2C3C(CCC12C) C1(C2(OC2C3)CC=CC 1=O)C)C
1021	<i>Withania Somnifera</i>	27605335	withafastuosin E	O1C(=O)C(CO)=C(CC1 C(CO)C1CCC2C3C(CC C12C)C1(C)C(O)(CC= CC1=O)C(O)C3)C
1022	<i>Withania Somnifera</i>	27605335	withaferin A diacetate	O1C(=O)C(COC(=O)C) =C(CC1C(C)C1CCC2C 3C(CCC12C)C1(C2(OC 2C3)C(OC(=O)C)C=CC 1=O)C)C
1023	<i>Withania Somnifera</i>	29661206	Withaferin-A	O1C(=O)C(CO)=C(CC1 C(C)C1CCC2C3C(CCC 12C)C1(C2(OC2C3)C(O)C=CC1=O)C)C

1024	<i>Withania Somnifera</i>	31090025	withanolide	O1[C@H](CC(C)=C(C)C1=O)[C@@@](O)(C)[C@H]1CC[C@H]2[C@H]3[C@H](CC[C@]12C)[C@@@]1([C@@@]2(O[C@H]2C3)[C@@@H](O)C=CC1=O)C
1025	<i>Withania Somnifera</i>	30403672	Withanolide A	O1C(=O)C(C)=C(CC1C(O)(C)C1CCC2C3C(CC12C)C1(C)C(O)(C2OC23)CC=CC1=O)C
1026	<i>Withania Somnifera</i>	30403672	Withanolide B	O1C(=O)C(=CCC1C(C)C1CCC2C3C(CC12C)C1(C)C(O)(C2OC23)C=CC1=O)C
1027	<i>Withania Somnifera</i>	27743505	withanolide D	CC1=C(C)C(=O)O[C@H](C1)[C@@@](C)(O)[C@H]1CC[C@H]2[C@H]3C[C@H]4O[C@@]4[C@@H](O)C=CC(=O)[C@@@]4(C)[C@H]3CC[C@@]12C
1028	<i>Withania Somnifera</i>	20836852	Withanolide D (C4 β -C5 β ,C6 β -epoxy-1-oxo-,20 β , dihydroxy-20S,22R-witha-2,24-dienolide)	CC1=C(C(=O)OC(C1)C(C)C2CCC3C2(CC4C3CC5C6(C4(C(=O)C=CC6O)C)O5)C)O)C
1029	<i>Withania Somnifera</i>	29115713	withanolide S	O1C(=O)C(C)=C(CC1C(O)(C)C1(O)CCC2(O)C3(CCC12C)C1(C)C(O)(CC=CC1=O)C(O)C3)C
1030	<i>Withania Somnifera</i>	28447311	withanolide-A	CC1=C(C(=O)OC(C1)C(C)C2CCC3C2(CC4C3CC5C(O5)C6(C4(C(=O)C=CC6)C)O)C)O)C
1031	<i>Withania Somnifera</i>	30776236	withanone	O1C(=O)C(C)=C(CC1C(C)C1(O)CCC2C3C(CC12C)C1(C)C(O)(C2OC23)CC=CC1=O)C
1032	<i>Withania Somnifera</i>	30403672	Withanoside IV	CC1=C(C(=O)OC(C1)C(C)C2CCC3C2(CC4C3CC5C4(C(CC(C5)OC6C(C(C(C(O7)CO)O)O)O)O)O)O)C)CO

1033	<i>Withania Somnifera</i>	30403672	Withanoside V	<chem>CC1=C(C(=O)OC(C1)C(C)C2CCC3C2(CCC4C3CC=C5C4(C(CC(C5)OC6C(C(C(C(O6)CO)COC7C(C(C(C(O7)CO)O)O)O)O)O)O)O)C)C</chem>
1034	<i>Withania Somnifera</i>	19475989	Withanoside VI	<chem>CC1=C(C(=O)OC(C1)C(C)C2CCC3C2(CCC4C3CC=C5C4(C(CC(C5)OC6C(C(C(C(O6)CO)O)O)O)C)C)C)O)C</chem>
1035	<i>Withania Somnifera</i>	22125584	withanoside X	<chem>CC1=C(C(=O)OC(C1)C(C)C2CCC3C2(CCC4C3CC=C5C4(C(CC(C5)OC6C(C(C(C(O6)CO)O)O)O)C)C)COC7C(C(C(C(O7)CO)O)O)O</chem>
1036	<i>Withania Somnifera</i>	11408168	withanosides II	<chem>CC1=C(C(=O)OC(C1)C(C)C2CCC3C2(CCC4C3C5C(O5)C6(C4(C(CC(C6)OC7C(C(C(C(O7)COC8C(C(C(C(O8)CO)O)O)O)O)O)O)C)C)C</chem>
1037	<i>Withania Somnifera</i>	11408168	withanosides III	<chem>CC1=C(C(=O)OC(C1)C(C)C2CCC3C2(CCC4C3C5C(O5)C6(C4(C(CC(C6)OC7C(C(C(C(O7)COC8C(C(C(C(O8)CO)O)O)O)O)O)C)C)CO</chem>
1038	<i>Withania Somnifera</i>	27605335	withaperuvin	<chem>O1C(=O)C(C)=C(CC1C(O)(C)C1(O)CCC2(O)C3(CCC12C)C1(C)C(O)(C(O)C3)C(O)C=CC1=O)C</chem>
1039	<i>Withania Somnifera</i>	25572656	Z-guggulsterone	<chem>O=C1CC2C3C(CCC2(C)C1=CC)C1(C(=CC(=O)CC1)CC3)C</chem>
1040	<i>Zingiber officinale</i>	15110695	(3R,5S)-3,5-dihydroxy-1-(4-hydroxy-3,5-dimethoxyphenyl)-7-(4-hydroxy-3-methoxyphenyl)heptane	<chem>O(C)c1cc(cc(OC)c1O)CC[C@@H](O)C[C@@H](O)CCc1cc(OC)c(O)c1</chem>
1041	<i>Zingiber officinale</i>	15110695	(3R,5S)-3-acetoxy-5-hydroxy-1,7-bis(4-hydroxy-3-methoxyphenyl)heptane	<chem>O(C)c1cc(ccc1O)CC[C@@H](OC(=O)C)C[C@@H](O)CCc1cc(OC)c(O)cc1</chem>

1042	<i>Zingiber officinale</i>	26606508	(3R,6R,7S)-1,10-bisaboladien-3-ol	OC1(CCC(C=C1)C(CC C=C(C)C)C)
1043	<i>Zingiber officinale</i>	15110695	(3S,5S)-3,5-diacetoxy-1,7-bis(4-hydroxy-3-methoxyphenyl)heptane	O(C)c1cc(ccc1O)CC[C@H](OC(=O)C)C[C@H](OC(=O)C)CCc1cc(OC)c(O)cc1
1044	<i>Zingiber officinale</i>	1469612	(3S,5S)-dihydroxy 1-(4'-hydroxy-3',5'-dimethoxyphenyl)-7-(4"-hydroxy-3"-methoxyphenyl)heptane	O(C)c1cc(cc(OC)c1O)CC[C@H](O)C[C@@H](O)CCc1cc(OC)c(O)cc1
1045	<i>Zingiber officinale</i>	26606508	(3S,6R,7S)-1,10-bisaboladien-3-ol	CC1[C@H](O)C=C(C(CCCC(C)C)=C)CC1
1046	<i>Zingiber officinale</i>	21954969	(5R)-5-acetoxy-1,7-bis(4-hydroxy-3-methoxyphenyl)heptan-3-one	O(C)c1cc(ccc1O)CCC(=O)C[C@H](OC(=O)C)CCc1cc(OC)c(O)cc1
1047	<i>Zingiber officinale</i>	15110695	(5S)-5-acetoxy-1,7-bis(4-hydroxy-3-methoxyphenyl)heptan-3-one	O(C)c1cc(ccc1O)CCC(=O)C[C@@H](OC(=O)C)CCc1cc(OC)c(O)cc1
1048	<i>Zingiber officinale</i>	22370785	(E)-geranylferulic acid	COCl=CC(/C=C(C/C=C(CC/C=C(C)/C)/C)/C(O)=O)=CC=C1O
1049	<i>Zingiber officinale</i>	24428842	(S)-[6]-gingerol	O(C)c1ccc(cc1O)CCC(=O)CC(O)CCCC
1050	<i>Zingiber officinale</i>	22370785	(Z)-geranylferulic acid	COCl=CC(/C=C(C/C=C(CC/C=C(C)/C)/C)/C(O)=O)=CC=C1O
1051	<i>Zingiber officinale</i>	22370785	[10]-gingerdione	O(C)c1cc(ccc1O)CCC(=O)CC(=O)CCCCCCCC
1052	<i>Zingiber officinale</i>	25063389	[10]-shogaol	CCCCCCCCCCCC=CC(=O)CCCl=CC(=C(C=C1)O)OC
1053	<i>Zingiber officinale</i>	21497863	[10]-zingerines	CCCCCCCCCCCC(CC(=O)CCCl=CC(=C(C=C1)O)OC)N2C=NC3=C(N=CN=C32)N
1054	<i>Zingiber officinale</i>	18814211	[12]-gingerol	CCCCCCCCCCCC(CC(=O)CCCl=CC(=C(C=C1)O)OC)O
1055	<i>Zingiber officinale</i>	26396335	[4]gingerol	O(C)c1cc(ccc1O)CCC(=O)CC(O)CCC
1056	<i>Zingiber officinale</i>	25063389	[4]-shogaol	O(C)c1cc(ccc1O)CCC(=O)C=CCCC

1057	<i>Zingiber officinale</i>	25063389	[6]-dehydrogingerdione	O(C)c1cc(ccc1O)C=CC(=O)CC(=O)CCCCC
1058	<i>Zingiber officinale</i>	26396335	[6]-gingediacetate	O(C)c1cc(ccc1O)CCC(OC(=O)C)CC(OC(=O)C)CCCCC
1059	<i>Zingiber officinale</i>	30091159	[6]-gingerol	CCCCCC(CC(=O)CCC1=CC(=C(C=C1)O)OC)O
1060	<i>Zingiber officinale</i>	15996695	[6]-isoshogaol	O(C)c1cc(ccc1O)CCC=CC(=O)CCCCC
1061	<i>Zingiber officinale</i>	25063389	[6]-shogaol	O(C)c1cc(ccc1O)CCC(=O)C=CCCCC
1062	<i>Zingiber officinale</i>	21497863	[6]-zingerines	CCCCCC(CC(=O)CCC1=CC(=C(C=C1)O)OC)N2C=NC3=C(N=CN=C32)N
1063	<i>Zingiber officinale</i>	22370785	[8]-paradol	CCCCCC(=O)CC C1=CC(=C(C=C1)O)OC
1064	<i>Zingiber officinale</i>	21497863	[8]-zingerines	CCCCCC(CC(=O)CC1=CC(=C(C=C1)O)OC)N2C=NC3=C(N=CN=C32)N
1065	<i>Zingiber officinale</i>	21240763	1-(4',5'-dihydroxy-3'-methoxy-phenyl)-dec-4-en-3-one	O(C)c1cc(cc(O)c1O)CC(=O)C=CCCCC
1066	<i>Zingiber officinale</i>	15996695	1-(4'-hydroxy-3'-methoxyphenyl)-2-nonadecen-1-one	O(C)c1cc(ccc1O)C(=O)C=CCCCCCCCCCCCCCCC
1067	<i>Zingiber officinale</i>	15110695	1,5-epoxy-3-hydroxy-1-(4-hydroxy-3,5-dimethoxyphenyl)-7-(4-hydroxy-3-methoxyphenyl)heptane	O1C(CC(O)CC1CCc1cc(OC)c(O)c(OC)c1
1068	<i>Zingiber officinale</i>	19031369	1,7-bis-(4' hydroxyl-3' methoxyphenyl)-5-methoxyheptan-3-one	O(C)c1cc(ccc1O)CCC(OC(=O)CCc1cc(OC)c(O)c1
1069	<i>Zingiber officinale</i>	15996695	1,7-bis-(4'-hydroxy-3'-methoxyphenyl)-3-hydroxy-5-acetoxyheptane	O(C)c1cc(ccc1O)CCC(OC(=O)C)CC(O)CCc1cc(OC)c(O)c1
1070	<i>Zingiber officinale</i>	15996695	1,7-bis-(4'-hydroxy-3'-methoxyphenyl)-5-methoxyheptan-3-one	CO(CCC1=CC(OC)=C(O)C=C1)CC(=O)CC C1=CC(OC)=C(O)C=C1
1071	<i>Zingiber officinale</i>	27393063	1,8-epoxy-p-menthan-3-ol	O1C(C2CCC1(CC2O)C)(C)C

1072	<i>Zingiber officinale</i>	30708987	10-gingerol	O(C)c1cc(ccc1O)CCC(=O)CC(O)CCCCCCCCC
1073	<i>Zingiber officinale</i>	30708987	10-shogaol	O(C)c1cc(ccc1O)CCC(=O)C=CCCCCC
1074	<i>Zingiber officinale</i>	20837112	12-gingerol	O(C)c1cc(ccc1O)CCC(=O)CC(O)CCCCCCCC
1075	<i>Zingiber officinale</i>	22370785	1-dehydro-[6]-gingerdione	O(C)c1cc(ccc1O)C=CC([O-])=CC(=O)CCCC
1076	<i>Zingiber officinale</i>	22370785	1-dehydro-[8]-gingerdione	O(C)c1cc(ccc1O)C=CC(=O)CC(=O)CCCC
1077	<i>Zingiber officinale</i>	20363635	1-dehydro-6-gingerdione	CCCCCCC(=O)CC(=O)C=CC1=CC(=C(C=C1)O)OC
1078	<i>Zingiber officinale</i>	27393063	2-heptanol	CCCCCC(C)O
1079	<i>Zingiber officinale</i>	11455660	3-hydroxy-1-(4-hydroxy-3-methoxyphenyl)butane	O(C)c1cc(ccc1O)CCC(O)C
1080	<i>Zingiber officinale</i>	22370785	4a,5b-dihydroxybisabola-2,10-diene	O[C@]1(C=CC(C[C@H]1O)C(CCCC(C)C)=C)C
1081	<i>Zingiber officinale</i>	18618523	4-gingerol	CCCC(CC(=O)CCC1=CC(=C(C=C1)O)OC)O
1082	<i>Zingiber officinale</i>	15996695	5-(4'-hydroxy-3'-methoxyphenyl)-3-hydroxy-1-pentanal	O(C)c1cc(ccc1O)CCC(=O)CC=O
1083	<i>Zingiber officinale</i>	15996695	5-(4'-hydroxy-3'-methoxyphenyl)-pent-2-en-1-al	O(C)c1cc(ccc1O)CCC=CC=O
1084	<i>Zingiber officinale</i>	28554232	5,9-dihydroxy borneol 2-O-b-D-glucopyranoside	O1[C@H](CO)[C@@H](O)[C@H](O)[C@@H](O)C1OC1CC2C(CO)(C)C1(CC2O)C
1085	<i>Zingiber officinale</i>	18177011	5-[4-hydroxy-6-(4-hydroxyphenethyl)tetrahydro-2 H-pyran-2-yl]-3-methoxybenzene-1,2-diol	O1C(CC(O)CC1CCc1cc(O)cc1)c1cc(OC)c(O)c(O)c1
1086	<i>Zingiber officinale</i>	29253614	5-gingerol	O(C)c1cc(ccc1O)CCC(=O)CC(O)CCCC
1087	<i>Zingiber officinale</i>	15110695	5-hydroxy-1-(3,4-dihydroxy-5-methoxyphenyl)-7-(4-hydroxy-3-methoxyphenyl)hepta	O(C)c1cc(cc(O)c1O)CC(=O)CC(O)CCc1cc(O)C)c(O)cc1

			n-3-one	
1088	<i>Zingiber officinale</i>	21240763	5-hydroxy-1-(4',5'-dihydroxy-3'-methoxy-phenyl)-decan-3-one	O(C)c1cc(cc(O)c1O)CC C(=O)CC(O)CCCC
1089	<i>Zingiber officinale</i>	15110695	5-hydroxy-1-(4-hydroxy-3-methoxyphenyl)-7-(3,4-dihydroxy-5-methoxy-phenyl)heptan-3-one	O(C)c1cc(cc(O)c1O)CC C(O)CC(=O)CCc1cc(O C)c(O)cc1
1090	<i>Zingiber officinale</i>	15996695	6-(4'-hydroxy-3'-methoxyphenyl)-2-nonyl-2-hydroxytetrahydropyran	O1C(CCCC1(O)CCCC CCCC)c1cc(OC)c(O)c c1
1091	<i>Zingiber officinale</i>	30638524	6-dehydroshogaol	O(C)c1cc(ccc1O)C=CC (=O)C=CCCCCC
1092	<i>Zingiber officinale</i>	26396335	6-gingediol	O(C)c1cc(ccc1O)CCC (O)CC(O)CCCC
1093	<i>Zingiber officinale</i>	20837112	6-gingerdione	O(C)c1cc(ccc1O)CCC (=O)CC(=O)CCCC
1094	<i>Zingiber officinale</i>	28106738	6-Paradol	O(C)c1cc(ccc1O)CCC (=O)CCCCCCC
1095	<i>Zingiber officinale</i>	20837112	8-gingerdione	O(C)c1cc(ccc1O)CCC (=O)CC(=O)CCCCCCC
1096	<i>Zingiber officinale</i>	30708987	8-gingerol	O(C)c1cc(ccc1O)CCC (=O)CC(O)CCCCCCC
1097	<i>Zingiber officinale</i>	26404226	8-paradol	O(C)c1cc(ccc1O)CCC (=O)CCCCCCCC
1098	<i>Zingiber officinale</i>	30708987	8-shogaol	O(C)c1cc(ccc1O)CCC (=O)C=CCCCCC
1099	<i>Zingiber officinale</i>	26672336	a-cedrene	[C@H]12C[C@H]3([C@H](CC[C@H]3C)C1(C)C)CC=C2C
1100	<i>Zingiber officinale</i>	29844252	a-citronellal	CC(CCCC(C)=C)CC=O
1101	<i>Zingiber officinale</i>	17511060	alpha-copaene	C12C3C(CC=C1C)[C@]2(CCC3C(C)C)C
1102	<i>Zingiber officinale</i>	19253546	alpha-curcumene	c1cc(ccc1C)[C@H](CC C=C(C)C)C
1103	<i>Zingiber officinale</i>	17511060	alpha-phellandrene	CC1=CCC(C=C1)C(C) C
1104	<i>Zingiber officinale</i>	21366054	alpha-terpineol	OC(C)(C)C1CCC(=CC1))C
1105	<i>Zingiber officinale</i>	30381960	ar-curcumene	CC1=CC=C(C=C1)C(C)CCC=C(C)C

1106	<i>Zingiber officinale</i>	30381960	ar-turmerone	O=C(CC(C)c1ccc(cc1)C)C=C(C)C
1107	<i>Zingiber officinale</i>	30381960	a-zingiberene	C1=C[C@H](CC=C1C)[C@H](CCC=C(C)C)C
1108	<i>Zingiber officinale</i>	26672336	b-bisabolol	OC1(CCC(=CC1)C)C(C CC=C(C)C)C
1109	<i>Zingiber officinale</i>	25190894	b-carotene	C1CCC(C)=C(\C=C\ C(=C\ C(=C\ C=C\ C(=C\ C=C\ C(=C\ C=C\ C=2 C(CCCC=2C)(C)C)/C)/C)(C)C1(C)C
1110	<i>Zingiber officinale</i>	21954969	bisgingerdione A	O(C)c1cc(ccc1O)CCC(=O)C(C(=O)CCCCC)C C(C(=O)CCc1cc(OC)c(O)cc1)C(=O)CCCCCCCC
1111	<i>Zingiber officinale</i>	21954969	bisgingerdione B	O(C)c1cc(ccc1O)CCC(=O)C(C(=O)CCCCCCCC CC)CC(C(=O)CCc1cc(OC)c(O)cc1)C(=O)CCCCCCCC
1112	<i>Zingiber officinale</i>	30381960	b-phellandrene	C1CC(C=CC1C(C)C)=C
1113	<i>Zingiber officinale</i>	30381960	b-sesquiphellandrene	C1CC(C=CC1C(CCC=C(C)C)C)=C
1114	<i>Zingiber officinale</i>	26672336	cubebene	C123C(C1C(=CC2)C)C(CCC3C)C(C)C
1115	<i>Zingiber officinale</i>	30979347	Curcumene	c1cc(ccc1C(CCC=C(C)C)C)C
1116	<i>Zingiber officinale</i>	26672336	decanal	CCCCCCCCCC=O
1117	<i>Zingiber officinale</i>	27816008	dehydroshogaol	CCCCCCC=CC(=O)C=C C1=CC(=C(C=C1)O)OC
1118	<i>Zingiber officinale</i>	30108729	dehydrozingeron	O(C)c1cc(ccc1O)C=CC(=O)C
1119	<i>Zingiber officinale</i>	20229191	D-mevalonolactone	O1CC[C@ @](O)(CC1=O)C
1120	<i>Zingiber officinale</i>	21060298	fisetin	O1c2c(ccc(O)c2)C(=O)C(O)=C1c1cc(O)c(O)cc1
1121	<i>Zingiber officinale</i>	26404226	galanganol C	O1CC(CC(CC=Cc2ccc(O)cc2)C1c1ccc(O)cc1)C(O)c1ccc(O)cc1
1122	<i>Zingiber officinale</i>	22370785	galanolactone	O1CC12CCC1C(CCCC1(C)C)(C)C2CC=C1CCOC1=O
1123	<i>Zingiber officinale</i>	29844252	geranyl acetate	CC(C)=CCC\ C(C)=C\ C OC(C)=O

1124	<i>Zingiber officinale</i>	26404226	gingerenone A	O(C)c1cc(ccc1O)CCC(=O)\C=C\CCc1cc(OC)c(O)cc1
1125	<i>Zingiber officinale</i>	26384019	Gingerenone B	O(C)c1cc(cc(OC)c1O)C CC=CC(=O)CCc1cc(OC)c(O)cc1
1126	<i>Zingiber officinale</i>	26384019	Gingerenone C	O(C)c1cc(ccc1O)CCC(=O)C=CCCCc1ccc(OC)cc1
1127	<i>Zingiber officinale</i>	29609660	gingerenone-A	O(C)c1cc(ccc1O)CCC(=O)C=CCCCc1cc(OC)c(O)cc1
1128	<i>Zingiber officinale</i>	8069973	gingerglycolipids A	CCC=CCC=CCC=CCC CCCCCC(=O)OCC(CO C1C(C(C(CO1)COC2C(C(C(C(O2)CO)O)O)O)O)O)O
1129	<i>Zingiber officinale</i>	8069973	gingerglycolipids B	CCCCCC=CCC=CCCC CCCCC(=O)OCC(COC1C(C(C(CO1)COC2C(C(C(C(O2)CO)O)O)O)O)O)O
1130	<i>Zingiber officinale</i>	8069973	gingerglycolipids C	CCCCCC=CCCC CCCC(=O)OCC(COC1C(C(C(CO1)COC2C(C(C(C(O2)CO)O)O)O)O)O)O
1131	<i>Zingiber officinale</i>	25063389	hexahydrocurcumin	COCl=CC(CCC(O)CC(=O)CC2=CC=C(O)C(OC)=C2)=CC=C1O
1132	<i>Zingiber officinale</i>	29844252	isobornyl acetate	O(C(=O)C)C1C[C@H]2CC[C@@]1(C)C2(C)C
1133	<i>Zingiber officinale</i>	29253614	methyl 6- gingerol	O(C)c1cc(ccc1OC)CCC(=O)CC(O)CCCC
1134	<i>Zingiber officinale</i>	16189817	methylgingerols	CCCCCC(CC(=O)CCC1=CC(=C(C=C1)OC)OC)O
1135	<i>Zingiber officinale</i>	21060298	morin	O1c2c(C(=O)C(O)=C1c1ccc(O)cc1O)c(O)cc(O)c2
1136	<i>Zingiber officinale</i>	26672336	murolan-3, 9 (11)-diene-10-peroxy	O(O)C1C2C(CCC1=C)C(C=CC2C(C)C)C
1137	<i>Zingiber officinale</i>	27771925	paradol	CCCCCC(=O)CCC1=CC(=C(C=C1)O)OC
1138	<i>Zingiber officinale</i>	20590154	pentadecanoic acid	CCCCCCCCCCCCCCCC C(O)=O
1139	<i>Zingiber officinale</i>	29609660	shogaol	CCCCCC=CC(=O)CCC1=CC(=C(C=C1)O)OC

1140	<i>Zingiber officinale</i>	18177011	sodium (E)-7-hydroxy-1,7-bis(4-hydroxyphenyl)hept-5-ene-3 R-sulfonate	S(=O)(=O)([O-])C(C[C@H](S(=O)(=O))[O-])C C=C\ C(O)c1ccc(O)c1c1ccc(O)cc1
1141	<i>Zingiber officinale</i>	18177011	sodium (E)-7-hydroxy-1,7-bis(4-hydroxyphenyl)hept-5-ene-3 S-sulfonate	S(=O)(=O)([O-])C(C[C@ @H](S(=O)(=O))[O-])C C=C\ C(O)c1ccc(O)c1c1ccc(O)cc1
1142	<i>Zingiber officinale</i>	21060298	tannic acid	C1=C(C=C(C(=C1O)O)O)C(=O)OC2=CC(=CC(=C2O)O)C(=O)OCC3C(C(C(C(O3)OC(=O)C4=CC(=C(C(=C4)OC(=O)C5=CC(=C(C(=C5)O)O)O)O)O)OC(=O)C6=CC(=C(C(=C6)OC(=O)C7=CC(=C(C(=C7)O)O)O)O)O)OC(=O)C8=CC(=C(C(=C8)OC(=O)C9=CC(=C(C(=C9)O)O)O)O)OC(=O)C1=CC(=C(C(=C1)OC(=O)C1=C C(=C(C(=C1)O)O)O)O)O
1143	<i>Zingiber officinale</i>	26404226	tetrahydrocurcumin	COCl=C(C=CC(=C1)CC(=O)CC(=O)CCC2=CC(=C(C=C2)O)OC)O
1144	<i>Zingiber officinale</i>	21366054	trans-linalool oxide acetate	CC(C)=CCCC(C)(OC(C)=O)C=C
1145	<i>Zingiber officinale</i>	22370785	trans-sesquipiperitol	OC1C=C(CCC1C(CCC=C(C(C)C)C)C
1146	<i>Zingiber officinale</i>	26672336	y-elemene	C1C(C(C)=C)C(CCC1=C(C(C)C)(C=C)C
1147	<i>Zingiber officinale</i>	21476200	Zerumbone	O=C/1\ C=C\ C(C\ C=C(\ CC\ C=C\ 1/C)/C)(C)C
1148	<i>Zingiber officinale</i>	30936626	zingerone	O(C)c1cc(ccc1O)CCC(=O)C
1149	<i>Zingiber officinale</i>	29844252	α -zingiberene	CC1=CCC(C=C1)C(C)CCC=C(C)C
1150	<i>Zingiber officinale</i>	30549623	β -bisabolene	CC1=CCC(CC1)C(=C)CCC=C(C)C
1151	<i>Zingiber officinale</i>	26672336	β -sesquiphellandrene	CC(CCC=C(C)C)C1CC(=C)C=C1
1152	<i>Zingiber officinale</i>	21366054	(Z)-dimethoxycitral	COCl=CC(C=C)C=CCC(C)=CC=O
1153	<i>Zingiber officinale</i>	22370785	[6]-paradol	CCCCCC(=O)CCc1ccc(O)c(OC)c1

1154	<i>Zingiber officinale</i>	24267247	10-dehydrogingerdione	<chem>CCCCCCCCC(=O)C=C(O)C=C/c1ccc(O)c(OC)c1</chem>
1155	<i>Zingiber officinale</i>	20837112	10-gingerdione	<chem>CCCCCCCCC(=O)C=C(O)CCc1ccc(O)c(OC)c1</chem>
1156	<i>Zingiber officinale</i>	19253546	alpha-zingiberene	<chem>C[C@H](CCC=C(C)C)[C@H]1CC=C(C)C=C1</chem>