**Supplementary Table S1.** Chemical compounds of Cymbopogon citratus along with molecular formula, molecular weight and chemical

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Source ID | Compound | Molecular formula | Molecular Weight (g/mol) | Reference |
| 638011 | Citral | [C10H16O](https://pubchem.ncbi.nlm.nih.gov/#query=C10H16O) | 152.23 | (Ranitha, Nour et al. 2014) |
| 8842 | Citronellol | [C10H20O](https://pubchem.ncbi.nlm.nih.gov/#query=C10H20O) | 156.26 | (Ranitha, Nour et al. 2014) |
| 527220 | Selina-6-en-4-ol | [C15H26O](https://pubchem.ncbi.nlm.nih.gov/#query=C15H26O) | 222.37 | (Amini , Costa, Pinheiro et al. 2013) |
| 519662 | Cadin-4-en-10-ol | [C15H26O](https://pubchem.ncbi.nlm.nih.gov/#query=C15H26O) | 222.37 | (Amini , Costa, Pinheiro et al. 2013) |
| 5281553 | (E)-beta-Ocimene | [C10H16](https://pubchem.ncbi.nlm.nih.gov/#query=C10H16) | 136.23 | (Amini , Costa, Pinheiro et al. 2013) |
| 8175 | Decanal | [C10H20O](https://pubchem.ncbi.nlm.nih.gov/#query=C10H20O) | 156.26 | (Amini , Costa, Pinheiro et al. 2013) |
| 931 | Naphthalene | [C10H8](https://pubchem.ncbi.nlm.nih.gov/#query=C10H8) | 128.17 | (Amini , Costa, Pinheiro et al. 2013) |
| 92138 | Elemol | [C15H26O](https://pubchem.ncbi.nlm.nih.gov/#query=C15H26O) | 222.37 | (Halabi and Sheikh 2014) |
| 91457 | beta-Eudesmol | [C15H26O](https://pubchem.ncbi.nlm.nih.gov/#query=C15H26O) | 222.37 | (Halabi and Sheikh 2014) |
| 11276107 | Cubebol | [C15H26O](https://pubchem.ncbi.nlm.nih.gov/#query=C15H26O) | 222.37 | (Halabi and Sheikh 2014) |
| 5281520 | Humulene | [C15H24](https://pubchem.ncbi.nlm.nih.gov/#query=C15H24) | 204.35 | (Halabi and Sheikh 2014) |
| 129700040 | Citral acetate (Acetyl (2E)-3,7-dimethylocta-2,6-dienoate) | [C12H18O3](https://pubchem.ncbi.nlm.nih.gov/#query=C12H18O3) | 210.27 | (Bharti, Kumar et al. 2013, Kumar, Mishra et al. 2013) |
| 5365794 | Citral diethyl acetal | [C14H26O2](https://pubchem.ncbi.nlm.nih.gov/#query=C14H26O2) | 226.35 | (Bharti, Kumar et al. 2013, Kumar, Mishra et al. 2013) |
| 29025 | Verbenone | [C10H14O](https://pubchem.ncbi.nlm.nih.gov/#query=C10H14O) | 150.22 | (Soares, Alves et al. 2013) |
| 18818 | Sabinene | [C10H16](https://pubchem.ncbi.nlm.nih.gov/#query=C10H16) | 136.23 | (Soares, Alves et al. 2013) |
| 1549026 | Geranyl acetate | [C12H20O2](https://pubchem.ncbi.nlm.nih.gov/#query=C12H20O2) | 196.29 | (Soares, Alves et al. 2013) |
| 7794 | Citronellal | [C10H18O](https://pubchem.ncbi.nlm.nih.gov/#query=C10H18O) | 154.25 | (Soares, Alves et al. 2013) |
| 527427 | (2S,4R)-p-Mentha-1(7),8-dien-2-ol | [C10H16O](https://pubchem.ncbi.nlm.nih.gov/#query=C10H16O) | 152.23 | (Amini , Nanon, Suksombat et al. 2014) |
| 22311 | Limonene | [C10H16](https://pubchem.ncbi.nlm.nih.gov/#query=C10H16) | 136.23 | (Amini , Nanon, Suksombat et al. 2014) |
| 527427 | (2S,4R)-p-Mentha-1(7),8-dien-2-ol | [C10H16O](https://pubchem.ncbi.nlm.nih.gov/#query=C10H16O) | 152.23 | (Amini , Nanon, Suksombat et al. 2014) |
| 131752084 | Cymbopogonol | [C30H50O](https://pubchem.ncbi.nlm.nih.gov/#query=C30H50O) | 426.7 | (Adesegun 2013, Pinto, Sánchez et al. 2015, Zannou, Christian et al. 2015) |
| 131752135  102117096 | Cymbopogone | [C30H50O](https://pubchem.ncbi.nlm.nih.gov/#query=C30H50O) | 426.7 | (Adesegun 2013, Pinto, Sánchez et al. 2015, Zannou, Christian et al. 2015) |
| 5280445 | Luteolin | [C15H10O6](https://pubchem.ncbi.nlm.nih.gov/#query=C15H10O6) | 286.24 | (Bone, Simon Mills et al. 2012, Asif and Khodadadi 2013, Campos, Schmeda-Hirschmann et al. 2014, Roriz, Barros et al. 2014) |
| 5280863 | Kaempferol | [C15H10O6](https://pubchem.ncbi.nlm.nih.gov/#query=C15H10O6) | 286.24 | (Bone, Simon Mills et al. 2012, Asif and Khodadadi 2013, Campos, Schmeda-Hirschmann et al. 2014, Roriz, Barros et al. 2014) |
| 689043 | Caffeic acid | [C9H8O4](https://pubchem.ncbi.nlm.nih.gov/#query=C9H8O4) | 180.16 | (Bone, Simon Mills et al. 2012, Asif and Khodadadi 2013, Campos, Schmeda-Hirschmann et al. 2014, Roriz, Barros et al. 2014) |
| 289 | Catechol | [C6H6O2](https://pubchem.ncbi.nlm.nih.gov/#query=C6H6O2) | 110.11 | (Bone, Simon Mills et al. 2012, Asif and Khodadadi 2013, Campos, Schmeda-Hirschmann et al. 2014, Roriz, Barros et al. 2014) |
| 785 | Hydroquinone | [C6H6O2](https://pubchem.ncbi.nlm.nih.gov/#query=C6H6O2) | 110.11 | (Bone, Simon Mills et al. 2012, Asif and Khodadadi 2013, Campos, Schmeda-Hirschmann et al. 2014, Roriz, Barros et al. 2014) |
| 10680 | Flavone | [C15H10O2](https://pubchem.ncbi.nlm.nih.gov/#query=C15H10O2) | 222.24 | (Bone, Simon Mills et al. 2012, Asif and Khodadadi 2013, Campos, Schmeda-Hirschmann et al. 2014, Roriz, Barros et al. 2014) |
| 11349 | 3-Hydroxyflavone | [C15H10O3](https://pubchem.ncbi.nlm.nih.gov/#query=C15H10O3) | 238.24 | (Bone, Simon Mills et al. 2012, Asif and Khodadadi 2013, Campos, Schmeda-Hirschmann et al. 2014, Roriz, Barros et al. 2014) |
| 370 | Gallic acid | [C7H6O5](https://pubchem.ncbi.nlm.nih.gov/#query=C7H6O5) | 170.12 | (Bone, Simon Mills et al. 2012, Asif and Khodadadi 2013, Campos, Schmeda-Hirschmann et al. 2014, Roriz, Barros et al. 2014) |
| 5280343 | Quercetin | [C15H10O7](https://pubchem.ncbi.nlm.nih.gov/#query=C15H10O7) | 302.23 | (Bone, Simon Mills et al. 2012, Asif and Khodadadi 2013, Campos, Schmeda-Hirschmann et al. 2014, Roriz, Barros et al. 2014) |
| 3707243 | Flavan-3-ol | [C15H14O2](https://pubchem.ncbi.nlm.nih.gov/#query=C15H14O2) | 226.27 | (Bone, Simon Mills et al. 2012, Asif and Khodadadi 2013, Campos, Schmeda-Hirschmann et al. 2014, Roriz, Barros et al. 2014) |
| 9064 | Cianidanol (catechin) | [C15H14O6](https://pubchem.ncbi.nlm.nih.gov/#query=C15H14O6) | 290.27 | (Bone, Simon Mills et al. 2012, Asif and Khodadadi 2013, Campos, Schmeda-Hirschmann et al. 2014, Roriz, Barros et al. 2014) |
| 6780 | Anthraquinone | [C14H8O2](https://pubchem.ncbi.nlm.nih.gov/#query=C14H8O2) | 208.21 | (Akande, Samuel et al. 2011, Ekpenyong, Akpan et al. 2015) |
| 54678486 | Warfarin (coumarins) | [C19H16O4](https://pubchem.ncbi.nlm.nih.gov/#query=C19H16O4) | 308.3 | (Akande, Samuel et al. 2011, Ekpenyong, Akpan et al. 2015) |
| 250395 | Tannic acid | [C27H24O18](https://pubchem.ncbi.nlm.nih.gov/#query=C27H24O18) | 636.5 | (Akande, Samuel et al. 2011, Ekpenyong, Akpan et al. 2015) |
| 638011 | Citral (GERANIAL) | [C10H16O](https://pubchem.ncbi.nlm.nih.gov/#query=C10H16O) | 152.23 | (Soares, Alves et al. 2013) |
| 643779 | Neral | [C10H16O](https://pubchem.ncbi.nlm.nih.gov/#query=C10H16O) | 152.23 | (Soares, Alves et al. 2013) |
| 7439 | Carvone | [C10H14O](https://pubchem.ncbi.nlm.nih.gov/#query=C10H14O) | 150.22 | (Sepúlveda-Arias, Veloza et al. 2013) |
| 8843 | 3,7-Dimethyl-2,6-octadienal | [C10H16O](https://pubchem.ncbi.nlm.nih.gov/#query=C10H16O) | 152.23 | (Melariri 2010, Arrey Tarkang, Franzoi et al. 2014, Kpoviessi, Bero et al. 2014) |
| 1794427 | Chlorogenic acid  (3-O-Caffeoylquinic acid) | [C16H18O9](https://pubchem.ncbi.nlm.nih.gov/#query=C16H18O9) | 354.31 | (Campos, Schmeda-Hirschmann et al. 2014) |
| 442659 | Swertiajaponin | [C22H22O11](https://pubchem.ncbi.nlm.nih.gov/#query=C22H22O11) | 462.4 | (Campos, Schmeda-Hirschmann et al. 2014) |
| 114776 | Isoorientin | [C21H20O11](https://pubchem.ncbi.nlm.nih.gov/#query=C21H20O11) | 448.4 | (Campos, Schmeda-Hirschmann et al. 2014) |
| 12172380 | alpha-Pinene | C10H16 | 136.23 | NA |
| 14896 | Beta-Pinene | C10H16 | 136.23 | ––〃–– |
| 2758 | Eucalyptol | C10H18O | 154.25 | ––〃–– |
| 10582 | Myrtenol | C10H16O | 152.23 | ––〃–– |
| 68316 | Perillene | C10H14O | 150.22 | ––〃–– |
| 6549 | Linalool | C10H18O | 154.25 | ––〃–– |
| 165266 | Myrtanal | C10H16O | 152.23 | ––〃–– |
| 102684 | Photocitral A | C10H16O | 152.23 | ––〃–– |
| 164888 | cis-Verbenol | C10H16O | 152.23 | ––〃–– |
| 643820 | trans-Carveol (Nerol) | C10H18O | 154.25 | ––〃–– |

**Supplementary Table S2**. The crystallographic properties of COVID-19 main protease with its native ligand N3 (PDB ID: 6LU7)

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| PDB ID | Enzyme | Classification | Organism | Expression System | Method | Resolution | Total Structure Weight | Atom Count |
| 6LU7 | Main Protease | Viral Protein | SARS Corona Virus 2 | Escherichia coli BL21 (DE3) | X-Ray Diffraction | 2.16 Å | 34.51 kDa | 2500 |

**Supplementary Table S3.** The binding energies (ΔG) and Root Mean Square Deviation (RMSD) values of 50 compounds of C. citratus obtained by docking with the main protease (PDB ID: 6LU7)

|  |  |  |  |
| --- | --- | --- | --- |
| **Sr No.** | **Compounds** | **Docking Scores** | **RMSD** |
| 1 | Tannic acid | -8.12501907 | 2.34577584 |
| 2 | Isoorientin | -7.38438511 | 1.20860994 |
| 3 | Swertiajaponin | -7.33355188 | 1.17815518 |
| 4 | Chlorogenic acid | -6.88325262 | 1.04582047 |
| 5 | Cymbopogonol | -6.48206711 | 1.68587506 |
| 6 | Warfarin | -6.32509041 | 1.81630361 |
| 7 | Citral diethyl acetal | -6.30906057 | 2.42593336 |
| 8 | Citral acetate | -6.18121672 | 2.32145476 |
| 9 | Luteolin | -6.17798948 | 1.84351552 |
| 10 | Kaempferol | -6.13175917 | 0.958073258 |
| 11 | Cianidanol | -6.02349663 | 1.5389291 |
| 12 | beta-Eudesmol | -5.81402826 | 0.971954167 |
| 13 | Cadin-4-en-10-ol | -5.81395149 | 1.36495137 |
| 14 | Geranyl acetate | -5.79436111 | 1.47860849 |
| 15 | Quercetin | -5.7830286 | 1.17935121 |
| 16 | Elemol | -5.61480951 | 1.32408929 |
| 17 | Cymbopogone | -5.55722237 | 1.62206423 |
| 18 | Flavone | -5.52629042 | 1.56045115 |
| 19 | Decanal | -5.48819351 | 1.75112987 |
| 20 | Flavan-3-ol | -5.43162203 | 2.85422325 |
| 21 | 3-Hydroxyflavone | -5.42190647 | 1.11565185 |
| 22 | Citronellal | -5.30528688 | 1.23379385 |
| 23 | Selina-6-en-4-ol | -5.33551025 | 0.924315631 |
| 24 | Humulene | -5.23563194 | 2.76302195 |
| 25 | Linalool | -5.21370268 | 1.39594388 |
| 26 | Citronellol | -5.17844391 | 1.15874279 |
| 27 | (E)-beta-Ocimene | -5.09972286 | 0.817325652 |
| 28 | 3,7-Dimethyl-2,6-octadienal | -5.08053541 | 0.688222706 |
| 29 | Citral | -5.05754709 | 0.938642025 |
| 30 | Neral | -5.03121805 | 1.05498183 |
| 31 | Anthraquinone | -5.0276432 | 1.33883202 |
| 32 | Photocitral A | -5.00530052 | 1.35120523 |
| 33 | Perillene | -4.93853951 | 1.44400418 |
| 34 | Caffeic acid | -4.91639042 | 3.28890371 |
| 35 | Beta-Pinene | -4.88864183 | 1.29854524 |
| 36 | Myrtenol | -4.76467848 | 1.04850042 |
| 37 | Carvone | -4.72771168 | 2.77521348 |
| 38 | Sabinene | -4.7263341 | 0.966760218 |
| 39 | cis-Verbenol | -4.65629148 | 0.422109783 |
| 40 | Verbenone | -4.62157583 | 1.00992298 |
| 41 | Limonene | -4.61773252 | 2.00403094 |
| 42 | (2S,4R)-p-Mentha-1(7),8-dien-2-ol | -4.56072235 | 1.81909704 |
| 43 | Eucalyptol | -4.55217218 | 0.764431655 |
| 44 | Gallic acid | -4.51160526 | 2.92548108 |
| 45 | trans-Carveol | -4.43248081 | 3.31258917 |
| 46 | Myrtanal | -4.37368965 | 1.71577668 |
| 47 | Naphthalene | -4.28574181 | 3.52768898 |
| 48 | Hydroquinone | -4.15826368 | 2.92524552 |
| 49 | Catechol | -4.04190731 | 1.45527864 |
| 50 | alpha-Pinene | -4.43521023 | 0.854688048 |