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**Table 1. MOLECULAR DOCKING OF CADAMBA PHYTOCHEMICALS WITH 6M2N SARS COV-2 PROTEIN**

| SR. NO. | LIGAND | DOCKING SCORE | RMSD VALUE | INTERACTION BETWEEN LIGAND AND PROTEIN | |
|---|---|---|---|---|---|
| | | | | HYDROGEN BOND INTERACTION | HYDROPHOBIC INTERACTION |
| 1 | Native ligand | -7.2 | 2.446 | MET-49 | CYS-145, CYS-44, MET-165, ASN-142, HIS-41 |
| 2 | Remdesivir | -7.1 | 3.333 | PHE-140, LEU-141, GLN-189 | GLU-166, CYS-145, ASN-142, HIS-163, HIS-164, ,THR-25, MET-49 |
| 3 | Naringenin | -7.5 | 3.48 | ASP-187, GLY-143, SER-144 | HIS-41, HIS-163, ASN-142, CYS-145, MET-165 |
| 4 | Palmitic Acid | -4.6 | 5.136 | SER-144, CYS-145, ASN-142, GLY-143 | MET-165, HIS-41, CYS-44, MET-49 |
| 5 | Emodine | -7.8 | 2.228 | ASP-187, ASN-142 | HIS-41, CYS-145, MET-49, CYS-44 |
| 6 | Linalool | -4.4 | 1.941 | ----- | CYS-44, MET-49, HIS-41 |
| 7 | Camphene | -4.3 | 1.41 | ----- | HIS-41, MET-49, MET-165 |
| 8 | P-Cymol | -4.6 | 1.698 | ----- | PRO-52, MET-49, CYS-44, HIS-41 |
| 9 | Linalyl Acetate | -4.8 | 2.54 | GLN-189 | MET-165, HIS-41, HIS-163, CYS-145 |
| 10 | Catechin | -7.6 | 2.572 | GLU-166, GLN-189 | MET-165, CYS-145, ASN-142, HIS-41, HIS-163 |
| 11 | Chrysophanol | -7.5 | 2.721 | MET-49, GLN-189 | MET-165, CYS-44 |
| 12 | Physcion | -7.5 | 2.426 | CYS-44, ASP-187, | MET-49, HIS-41, MET-165 |
| 13 | B-Phellandrene | -4.5 | 1.991 | ----- | HIS-41, MET-165, GLN-189, PRO-52, TYR-54, CYS-44, GLU-166, ARG-188, ASP-187, HIS-164 |
| 14 | Terpinolene | -5 | 1.987 | ----- | HIS-41 |
| 15 | 2-Nonanol | -3.7 | 3.051 | ----- | MET-165, MET-49, CYS-44, HIS-41 |
| 16 | Myrcene | -4.1 | 1.561 | ----- | MET-49, MET-165, HIS-41 |
| 17 | Ursolic Acid | -5.6 | 3.607 | ----- | ASN-142 |
| 18 | Leucocyanidine | -7.8 | 2.777 | GLN-189, LEU-141 | HIS-41, HIS-164, HIS-163, ASN-142, MET-49, CYS-145 |
| 19 | Epicatechine | -7.5 | 2.903 | GLU-166, GLN-189 | MET-165, CYS-145, ASN-142, HIS-41, GLY-143 |
| 20 | Dihydrotectochrysin | -7 | 2.619 | GLU-166, GLN-143 | CYS-44, CYS-145, MET-49, LEU-27, HIS-41 |
| 21 | Sakuranetin | -7.2 | 3.352 | GLU-166 | CYS-44, CYS-145, HIS-41, MET-49 |
| 22 | Alpha-Curcumene | -5.7 | 2.381 | ----- | HIS-41, CYS-145, HIS-163 |
| 23 | Quinovic Acid | -5.6 | 2.998 | ----- | GLN-189 |
| 24 | Aromadendrin | -7.7 | 3.046 | MET-49, GLU-166 | CYS-44, CYS-145 |
| 25 | Beta-Sitosterol | -6.3 | 3.38 | ARG-188 | MET-49, MET-165, HIS-41 |
| 26 | Lupeol | -5.7 | 3.303 | ----- | HIS-41 |
| 27 | Taxifolin | -7.9 | 2.105 | GLN-189, MET-49, GLU-166 | CYS-145, CYS-44 |
| 28 | Oleic Acid | -5.1 | 3.612 | LEU-141, SER-144, CYS-145 | HIS-41, MET-49, MET-165, CYS-44 |
| 29 | Geraniol | -4.6 | 2.221 | GLU-166 | MET-49, MET-165, HIS-41, CYS-145, CYS-44, PRO-52 |
| 30 | Geranyl Acetate | -5.4 | 2.167 | ASN-142, CYS-145, GLU-143, SER-144 | HIS-41, MET-49, CYS-44 |
| 31 | Apigenin | -7.5 | 3.144 | ASP-1887, GLY-143 | MET-165, HIS-41, HIS-163, LEU-141, ASN-142, CYS-145 |
| 32 | Sigmasterol | -6.6 | 3.84 | ARG-188 | MET-49, MET-165, HIS-41 |
| 33 | Quercetin-3-rhamnoglucoside | -8.7 | 2.349 | GLU-166, LEU-167, TYR-54, ASN-142, THR-26 | GLN-189, MET-49, CYS-44, HIS-41 |
| 34 | Kaempferol | -7.7 | 2.75 | HIS-41, GLN-189 | MET-49, MET-165, ASN-142 |
| 35 | Genistein | -7.8 | 2.659 | GLU-166, GLN-189 | MET-165, CYS-145, ASN-142 |
| 36 | Chrysin | -7.2 | 2.921 | MET-49, ASP-187 | HIS-41, CYS-44, THR-25 |
| 37 | Genkwanin | -7.3 | 3.428 | PHE-140, GLU-166 | CYS-44, MET-49, MET-145, HIS-41, ASN-142 |
| 38 | Tectochrysin | -7.1 | 2.451 | GLN-189, ARG-188 | HIS-41, MET-165, CYS-44, ASP-187, ASN-142, GLU-166 |
| 39 | Kaempteritrin | -7.2 | 5.074 | ASP-187, ASN-142, THR-24, THR-26 | MET-49, HIS-41, CYS-145 |
| 40 | B-Sitosterol glucoside | -6.7 | 4.443 | THR-24, ASN-119 | CYS-145, CYS-44, MET-165, HIS-41 |
| 41 | 3O'-CaffeoylSweroside | -7.6 | 3.904 | ASP-187, ASN-119, THR-25, | THR-26, ASN-142, MET-49, CYS-44, HIS-41, ARG-188 |
| 42 | Alpha-Selinene | -6.4 | 1.948 | ----- | MET-49, MET-165, CYS-44, HIS-41 |
| 43 | Dihydrocinchonine | -6.8 | 1.795 | ----- | HIS-41, MET-165 |
| 44 | Orientalone | -6.7 | 2.209 | ----- | CYS-44, MET-49, HIS-41 |
| 45 | Neosakuranin | -8.1 | 3.928 | ASN-142, THR-25, SER-144, LEU-144 | CYS-145, PRO--168, LEU-167, MET-165, MET-49 |
| 46 | 2'-hydroxy-2,4,4',5-tetramethoxy | -7.1 | 3.235 | HIS-41, GLN-189 | MET-49, MET-165, GLU-166, LEU-167, THR-25, SER-49 |

| | | | | | |
|---|---|---|---|---|---|
| 47 | Chalcone 2',4'-dihydroxy-2,4,5-trimethoxy Chalcone | -7.2 | 3.168 | HIS-41, GLN-189 | MET-165, MET-49, LEU-167, GLU-166, THR-25 |
| 48 | Puddumin B | -7.6 | 3.54 | THR-26 | ASN-142, PRO-168, LEU-167, MET-165, HIS-41 |
| 49 | Prunetinoside | -7.7 | 3.531 | ASN-142 | CYS-145, CYS-44, HIS-41, MET-49, TYR-54, ASP-187 |
| 50 | Aminocadambine A | -8 | 3.584 | GLN-189, CYS-145, ASN-142 | THR-25, MET-49 |
| 51 | Cadamine | -8.1 | 3.091 | THR-26, HIS-41 | MET-49, GLY-143, ASN-142 |
| 52 | Phelasingenin | -5.8 | 3.816 | ASN-142, GLU-166, GLN-189 | ----- |
| 53 | Cadambagenic acid | -6 | 3.177 | GLN-189, CYS-145, ASN-142 | MET-165 |
| 54 | Cadambine | -7.6 | 2.934 | GLU-166, ASN-142 | LEU-141, CYS-145, HIS-164 |
| 55 | Feruloylquinic Acid | -7.6 | 3.7 | ASP-187, ASN-142, GLU-166, GLN-189, LEU-141, GLY-143 | HIS-41, MET-49, CYS-44 |
| 56 | Cadambine Acid | -7.7 | 3.628 | GLN-1989, GLU-166, ASN-142 | ET-49, ASP-187, TYR-54 |
| 57 | B-Sitosterol-3O-galactopyranoside | -7.1 | 3.094 | THR-26 | HIS-41, THR-25, ASN-119 |
| 58 | Amygdalin | -7.7 | 3.366 | GLN-189, GLY-143 | THR-26, CYS-145, MET-49, HIS-41 |
| 59 | Pinocembrin | -7.1 | 2.643 | ASP-187, GLN-189, MET-49 | HIS-41, CYS-145, CYS-44 |
| 60 | Quercetin | -7.9 | 2.515 | GLN-189, GLU-166, PHE-140, HIS-41 | MET-49, MET-165, ASN-142 |
| 61 | 3-Dihydro Cadambine | -8.3 | 3.243 | HIS-41, MET-49, GLN-189 | HIS-163, PHE-140, GLU-166 |
| 62 | 3-Beta-Dihydro Cadambine | -8.2 | 2.134 | HIS-41, MET-49, GLY-163 | PHE-140, ASN-142, GLU-166 |
| 63 | Kaempferol-3O-glucoside | -8.1 | 2.63 | THR-26, CYS-145, ASN-142, ASP-48 | MET-49, CYS-44, HIS-41 |
| 64 | Chlorogenic Acid | -7.3 | 3.827 | MET-49, THR-25, CYS-145, GLY-143 | THR-26, HIS-41 |
| 65 | Dihydrowogonin | -7.4 | 2.88 | HIS-41, GLN-189, ASP-187 | MET-49, MET-165, CYS-44, CYS-145, ARG-188 |
| 66 | 3-Beta-Isodihydro Cadambine | -8.3 | 3.152 | HIS-41, GLU-166, GLN-189, GLY-143 | MEET-145, ASN-142, PHE-140 |
| 67 | Aminocadambine B | -8.4 | 3.71 | GLN-192, ARG-188, MET-49 | HIS-41, THR-25 |
| 68 | Afzelin | -8.5 | 3.281 | GLU-166, LEU-141, CYS-44, TYR-54 | MET-449, CYS-145, HIS-163 |
| 69 | Padmakastein | -8 | 2.873 | GLU-166, GLN-189, PHE-140 | MET-165, MET-49, CYS-44, CYS-145, ASN-142 |

**Table 2. Physiochemical properties of Phytochemicals**

| Sr. No. | Ligands | Docking Score (Kcal/mol) | Molecular Weight (g/mol) | No. of Rotatable bonds | H-bond Acceptor | H-bond Donor | TPSA (Å²) | Log P | Follows Lipinski Rule | No. of Violations |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | Native ligand | -7.2 | 270.24 | 1 | 5 | 3 | 90.90 | 2.24 | Yes | 0 |
| 2 | Remdesivir | -7.1 | 602.58 | 14 | 12 | 14 | 213.36 | 1.50 | No | 2 |
| 3 | Naringenin | -7.5 | 272.25 | 1 | 5 | 3 | 86.99 | 1.84 | Yes | 0 |
| 4 | Palmitic acid | -4.6 | 256.42 | 14 | 2 | 1 | 37.3 | 5.2 | No | 1 |
| 5 | Emodin | -7.8 | 270.24 | 0 | 5 | 3 | 94.83 | 1.87 | Yes | 0 |
| 6 | Linalool | -4.4 | 154.25 | 4 | 1 | 1 | 20.23 | 2.66 | Yes | 0 |
| 7 | Camphene | -4.3 | 136.23 | 0 | 0 | 0 | 0 | 3.43 | No | 1 |
| 8 | p-Cymol | -4.6 | 134.22 | 1 | 0 | 0 | 0 | 3.5 | No | 1 |
| 9 | Linalyl acetate | -4.8 | 196.29 | 6 | 2 | 0 | 26.3 | 3.24 | Yes | 0 |
| 10 | Catechin | -7.6 | 290.27 | 1 | 6 | 5 | 110.38 | 0.85 | Yes | 0 |
| 11 | Chrysophenol | -7.5 | 254.24 | 0 | 4 | 2 | 74.6 | 2.38 | Yes | 0 |
| 12 | Physcion | -7.5 | 284.26 | 1 | 5 | 2 | 83.83 | 2.27 | Yes | 0 |
| 13 | Beta-Phellandrene | -4.5 | 136.23 | 1 | 0 | 0 | 0 | 3.07 | Yes | 0 |
| 14 | Terpinolene | -5.0 | 136.23 | 0 | 0 | 0 | 0 | 3.4 | Yes | 0 |
| 15 | 2-Nonanol | -3.7 | 144.25 | 6 | 1 | 1 | 20.23 | 2.77 | Yes | 0 |
| 16 | Myrcene | -4.1 | 136.23 | 4 | 0 | 0 | 0 | 3.43 | Yes | 0 |
| 17 | Ursolic acid | -5.6 | 456.7 | 1 | 3 | 2 | 57.53 | 5.88 | No | 1 |
| 18 | Leucocyanidin | -7.8 | 306.27 | 1 | 7 | 6 | 130.61 | 0.07 | No | 1 |
| 19 | Epicatechin | -7.5 | 290.27 | 1 | 6 | 5 | 110.38 | 0.85 | Yes | 0 |
| 20 | Dihydrotectochrysin | -7.0 | 270.28 | 2 | 4 | 1 | 55.76 | 2.66 | Yes | 0 |
| 21 | Sakuranetin | -7.2 | 286.28 | 2 | 5 | 2 | 75.99 | 2.25 | Yes | 0 |
| 22 | Curcumene | -5.7 | 202.34 | 4 | 0 | 0 | 0 | 4.86 | No | 1 |
| 23 | Quinovic acid | -5.6 | 486.68 | 2 | 5 | 3 | 94.83 | 4.85 | No | 1 |
| 24 | Aromadendrin | -7.7 | 288.25 | 1 | 6 | 4 | 107.22 | 0.99 | Yes | 0 |
| 25 | β-sitosterol | -6.3 | 414.71 | 6 | 1 | 1 | 20.23 | 7.19 | No | 1 |
| 26 | Lupeol | -5.7 | 426.72 | 1 | 1 | 1 | 20.23 | 7.26 | No | 1 |
| 27 | Taxifolin | -7.9 | 304.25 | 1 | 7 | 5 | 127.45 | 0.63 | Yes | 0 |
| 28 | Oleic acid | -5.1 | 282.46 | 15 | 2 | 1 | 37.3 | 5.71 | No | 1 |
| 29 | Geraniol | -4.6 | 154.25 | 4 | 1 | 1 | 20.23 | 2.78 | Yes | 0 |
| 30 | Geranyl acetate | -5.4 | 196.29 | 6 | 2 | 0 | 26.3 | 3.21 | Yes | 0 |
| 31 | Apigenin | -7.5 | 270.24 | 1 | 5 | 3 | 90.9 | 2.11 | Yes | 0 |
| 32 | Stigmasterol | -6.6 | 412.69 | 5 | 1 | 1 | 20.23 | 6.97 | No | 1 |
| 33 | Rutin | -8.7 | 610.52 | 6 | 16 | 10 | 269.43 | -1.12 | No | 3 |
| 34 | Kaempferol | -7.7 | 286.24 | 1 | 6 | 4 | 111.13 | 1.58 | Yes | 0 |
| 35 | Genistein | -7.8 | 270.24 | 1 | 5 | 3 | 90.9 | 2.04 | Yes | 0 |
| 36 | Chrysin | -7.2 | 254.24 | 1 | 4 | 2 | 70.67 | 2.55 | Yes | 0 |
| 37 | Genkwanin | -7.3 | 284.26 | 2 | 5 | 2 | 79.9 | 2.5 | Yes | 0 |
| 38 | Tectochrysin | -7.1 | 268.26 | 2 | 4 | 1 | 59.67 | 2.95 | Yes | 0 |
| 39 | Kaempteritrin | -7.2 | 578.52 | 5 | 14 | 8 | 228.97 | -0.46 | No | 3 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| 40 | β-sitosterol glucoside | -6.7 | 576.85 | 9 | 6 | 4 | 99.38 | 5.51 | No | 1 |
| 41 | 3'O-caffeoylsweroside | -7.6 | 520.48 | 8 | 12 | 5 | 181.44 | 0.49 | No | 2 |
| 42 | Alpha-Selinene | -6.4 | 204.35 | 1 | 0 | 0 | 0 | 4.4 | No | 1 |
| 43 | Dihydrocinchonine | -6.8 | 296.41 | 3 | 3 | 1 | 36.36 | 2.85 | Yes | 0 |
| 44 | Orientalone | -6.7 | 260.24 | 2 | 5 | 1 | 80.67 | 1.54 | Yes | 0 |
| 45 | Neosakuranin (2, 4′-dihydroxy-4-methoxy-6-glucosidoxychalcone) | -8.1 | 448.42 | 7 | 10 | 6 | 166.14 | 0.52 | No | 1 |
| 46 | 2′-hydroxy 2, 4, 4′, 6′-tetramethoxycha_ lcone | -7.1 | 344.36 | 7 | 6 | 1 | 74.22 | 3.13 | Yes | 0 |
| 47 | 2′, 4′ dihydroxy-2, 4, 6′-trimethoxychalcon | -7.2 | 330.33 | 6 | 6 | 2 | 85.22 | 2.72 | Yes | 0 |
| 48 | Puddumin B | -7.6 | 448.42 | 5 | 10 | 5 | 155.14 | 0.52 | Yes | 0 |
| 49 | Prunetinoside | -7.7 | 446.4 | 5 | 10 | 5 | 159.05 | 0.69 | Yes | 0 |
| 50 | Aminocadambine A | -8.0 | 437.49 | 4 | 6 | 2 | 95.1 | 1.37 | Yes | 0 |
| 51 | Cadamine | -8.1 | 363.41 | 3 | 5 | 2 | 78.45 | 1.99 | Yes | 0 |
| 52 | Phelasingenin | -5.8 | 486.68 | 2 | 5 | 3 | 94.83 | 5.07 | No | 1 |
| 53 | Cadambagenic acid | -6.0 | 486.68 | 2 | 5 | 3 | 94.83 | 5.04 | No | 1 |
| 54 | Cadambine | -7.6 | 544.55 | 5 | 11 | 5 | 163.17 | 0.06 | No | 2 |
| 55 | Feruloyquinic acid | -7.6 | 368.34 | 6 | 9 | 5 | 153.75 | 0.01 | Yes | 0 |
| 56 | Cadambine acid | -7.7 | 544.55 | 5 | 11 | 5 | 163.17 | 0.06 | No | 2 |
| 57 | β-sitosterol-3-O-D-galactopyranoside | -7.1 | 576.85 | 9 | 6 | 4 | 99.38 | 5.51 | No | 1 |
| 58 | Amygdalin | -7.7 | 457.43 | 7 | 12 | 7 | 202.32 | -2.32 | No | 2 |
| 59 | Pinocembrin | -7.1 | 256.25 | 1 | 4 | 2 | 66.76 | 2.26 | Yes | 0 |
| 60 | Quercetin | -7.9 | 302.24 | 1 | 7 | 5 | 131.36 | 1.23 | Yes | 0 |
| 61 | 3 Dihydrocadambin | -8.3 | 546.57 | 5 | 11 | 6 | 174.17 | -0.36 | No | 3 |
| 62 | 3-Beta Dihydrocadambin | -8.2 | 546.57 | 5 | 11 | 6 | 174.17 | -0.36 | No | 3 |
| 63 | Kaempferol-3O-glucoside | -8.1 | 448.38 | 4 | 11 | 7 | 190.28 | -0.25 | No | 2 |
| 64 | Chlorogenic Acid | -7.3 | 354.31 | 5 | 9 | 6 | 164.75 | -0.38 | No | 1 |
| 65 | Dihydrowogonin | -7.4 | 286.28 | 2 | 5 | 2 | 75.99 | 2.23 | Yes | 0 |
| 66 | 3-Beta Iso Dihydrocadambin | -8.3 | 546.57 | 6 | 11 | 6 | 174.17 | -0.24 | No | 3 |
| 67 | Aminocadambine B | -8.4 | 451.51 | 6 | 6 | 2 | 95.1 | 1.64 | Yes | 0 |
| 68 | Afzelin | -8.5 | 432.32 | 3 | 10 | 6 | 170.05 | 0.6 | No | 1 |
| 69 | Padmakastein | -8.0 | 284.26 | 2 | 5 | 2 | 79.9 | 2.43 | Yes | 0 |