|  |  |  |
| --- | --- | --- |
| Ligand Number | Phytochemicals | Binding Affinities |
| 1 | Hexadecanal | -5.4 |
| 2 | Vanillin | -5.3 |
| 3 | Eucalyptol | -5.4 |
| 4 | p-CYMENE | -6 |
| 5 | 2-Undecanone | -5.6 |
| 6 | Vanillic Acid | -5.2 |
| 7 | Terpinolene | -5.7 |
| 8 | 2-(4-Methylphenyl)propan-2-ol | -5.9 |
| 9 | 2-Undecanol | -5.9 |
| 10 | Myrcene | -5.1 |
| 11 | Cholesterol sulfate | -5.1 |
| 12 | Curlone | -7.1 |
| 13 | Cinnamic Acid | -6.7 |
| 14 | Ferulic acid | -6.1 |
| 15 | 1,5-Bis(4-hydroxy-3-methoxyphenyl)penta-1,4-dien-3-one | -6.3 |
| **16** | **(4Z,6E)-5-Hydroxy-1,7-bis(4-hydroxy-3-methoxyphenyl)-4,6-heptadie n-3-one; 5-hydroxy-1,7-bis(4-hydroxy-3-methoxyphenyl)-4,6-heptadiene-3-one** | **-7.5** |
| **17** | **Calebin A** | **-7.7** |
| **18** | **Cinnamaldehyde** | **-7.9** |
| 19 | p-Coumaric acid | -5.6 |
| 20 | (4Z,6E)-5-Hydroxy-1-(4-hydroxy-3-methoxyphenyl)-7-(4-hydroxyphenyl)hepta-4,6-dien-3-one | -6.1 |
| **21** | **Geranyl acetate** | **-7.9** |
| 22 | gamma-Bisabolene, (Z)- | -5.9 |
| 23 | Humulene | -6.5 |
| 24 | (1E,4Z,6E)-5-hydroxy-1,7-bis(4-hydroxy-3-methoxyphenyl)hepta-1,4,6-trien-3-one | -5.0 |
| **25** | **(1E,4Z,6E)-5-hydroxy-1,7-bis(4-hydroxy-3-methoxyphenyl)hepta-1,4,6-trien-3-one** | **-7.9** |
| 26 | 9,12-Octadecadienoic acid, (E,Z)- | -5.7 |
| **27** | **Bisdemethoxycurcumin** | **-7.6** |
| 28 | beta-Farnesene, (6Z)- | -5.9 |
| 29 | Isofuranodiene | -6.5 |
| 30 | (3Z,7E)-3,7-dimethyl-10-propan-2-ylidenecyclodeca-3,7-dien-1-one | -5.6 |
| **31** | **Demethoxycurcumin** | **-7.7** |
| **32** | **[(E)-4-(4-hydroxy-3-methoxyphenyl)-2-oxobut-3-enyl] (E)-3-(4-hydroxyphenyl)prop-2-enoate** | **-7.9** |
| **33** | **Tauroursodeoxycholic acid** | **-7.4** |
| 34 | Curcumanolides A | -6.3 |
| 35 | Epiprocurcumenol | -6.8 |
| 36 | 2-Cyclohexen-1-one, 6-(1,5-dimethyl-4-hexenyl)-3-methyl- | -6.2 |
| 37 | (E,6S)-2-methyl-6-(4-methylphenyl)hept-2-en-1-ol | -6.6 |
| 38 | (1S,4S,6R)-1-Methyl-4-((Z)-6-methylhepta-2,5-dien-2-yl)-7-oxabicyclo[4.1.0]heptane | -7.1 |
| 39 | Turmeronol A | -6.8 |
| 40 | (R,R)-1-isopropyl-4-methyl-3-(prop-1-en-2-yl)-4-vinylcyclohexene | -6.7 |
| **41** | **(1E)-7-Hydroxy-1,7-bis(4-hydroxy-3-methoxyphenyl)-1-heptene-3,5-dione** | **-7.6** |
| 42 | Curcumanolides B | -6.5 |
| 43 | Bisacurone A | -6.7 |
| 44 | Bisacurone C | -6.5 |
| 45 | Bisacurone B | -6.6 |
| 46 | 3-Hydroxybisabola-1,10-dien-9-one | -6.9 |
| 47 | 5-Hydroxy-4-methoxybisabola-2,10-dien-9-one | -6.9 |
| 48 | 5-(6-Methylhept-5-en-2-yl)cyclohex-2-ene-1,4-diol | -6.7 |
| 49 | Aromadendrene oxide 2 | -5.9 |
| 50 | Caffeic Acid | -6.3 |
| Standard | Topotecan | 7.4 |