Supplementary Material

**Supplementary Table 1.** List of natural compounds exclusively found in Sesame (*Sesamum indicum* L.)**.**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **S.No** | **Compound Name** | **PubChem ID** | **Molecular Formula** | **Molecular**  **Weight (g/mol)** | **Chemical Structure** | |
| **2D** | **3D** |
| 1. | Latifonin | [CID\_156633](https://pubchem.ncbi.nlm.nih.gov/compound/156633) | [C11H16O7](https://pubchem.ncbi.nlm.nih.gov/#query=C11H16O7) | 260.24 |  | C:\Users\Z400\Desktop\2D Structure of compounds\156633.png |
| 2. | Momor-Cerebroside I | CID\_[91895300](https://pubchem.ncbi.nlm.nih.gov/compound/91895300) | [C48H93NO10](https://pubchem.ncbi.nlm.nih.gov/#query=C48H93NO10) | 844.3 |  | C:\Users\Z400\Desktop\2D Structure of compounds\91895300.png |
| 3. | Soyacerebroside II | [CID\_6450042](https://pubchem.ncbi.nlm.nih.gov/compound/6450042) | [C40H75NO9](https://pubchem.ncbi.nlm.nih.gov/#query=C40H75NO9) | 714 |  | C:\Users\Z400\Desktop\2D Structure of compounds\6450042.png |
| 4. | Aurantiamide acetate | CID\_[9832120](https://pubchem.ncbi.nlm.nih.gov/compound/9832120) | [C27H28N2O4](https://pubchem.ncbi.nlm.nih.gov/#query=C27H28N2O4) | 444.5 |  | C:\Users\Z400\Desktop\2D Structure of compounds\9832120.png |
| 5. | Beta-sitosterol | CID\_ [222284](https://pubchem.ncbi.nlm.nih.gov/compound/222284) | [C29H50O](https://pubchem.ncbi.nlm.nih.gov/#query=C29H50O) | 414.7 |  | C:\Users\Z400\Desktop\2D Structure of compounds\222284.png |
| 6. | Daucosterol | CID\_[5742590](https://pubchem.ncbi.nlm.nih.gov/compound/5742590) | [C35H60O6](https://pubchem.ncbi.nlm.nih.gov/#query=C35H60O6) | 576.8 |  | C:\Users\Z400\Desktop\2D Structure of compounds\5742590.png |
| 7. | D-Galactitol | CID\_ [11850](https://pubchem.ncbi.nlm.nih.gov/compound/Galactitol) | [C6H14O6](https://pubchem.ncbi.nlm.nih.gov/#query=C6H14O6) | 182.17 |  | C:\Users\Z400\Desktop\2D Structure of compounds\11850.png |
| 8. | Sesamolin | CID\_[131801617](https://pubchem.ncbi.nlm.nih.gov/compound/131801617) | [C20H18O7](https://pubchem.ncbi.nlm.nih.gov/#query=C20H18O7) | 370.4 |  | C:\Users\Z400\Desktop\2D Structure of compounds\131801617.png |
| 9. | Dronabinol | CID\_ [16078](https://pubchem.ncbi.nlm.nih.gov/compound/16078) | [C21H30O2](https://pubchem.ncbi.nlm.nih.gov/#query=C21H30O2) | 314.5 |  | C:\Users\Z400\Desktop\2D Structure of compounds\16078.png |
| 10. | 1,2-Dilinoleoyl-3-Palmitoyl-Rac-Glycerol | CID\_[9544106](https://pubchem.ncbi.nlm.nih.gov/compound/9544106) | [C55H98O6](https://pubchem.ncbi.nlm.nih.gov/#query=C55H98O6) | 855.4 |  | C:\Users\Z400\Desktop\2D Structure of compounds\9544106.png |
| 11. | 1,2-Dilinoleoyl-3-Oleoyl-Rac-Glycerol | CID\_ [9544291](https://pubchem.ncbi.nlm.nih.gov/compound/9544291) | [C57H100O6](https://pubchem.ncbi.nlm.nih.gov/#query=C57H100O6) | 881.4 |  | C:\Users\Z400\Desktop\2D Structure of compounds\9544291.png |
| 12. | Linoleic Acid | CID\_  [5280450](https://pubchem.ncbi.nlm.nih.gov/compound/5280450) | [C18H32O2](https://pubchem.ncbi.nlm.nih.gov/#query=C18H32O2) | 280.4 |  | C:\Users\Z400\Desktop\2D Structure of compounds\5280450.png |
| 13. | Linolenic Acid | CID\_[5280934](https://pubchem.ncbi.nlm.nih.gov/compound/5280934) | [C18H30O2](https://pubchem.ncbi.nlm.nih.gov/#query=C18H30O2) | 278.4 |  | C:\Users\Z400\Desktop\2D Structure of compounds\5280934.png |
| 14. | Oleic Acid | CID\_  [445639](https://pubchem.ncbi.nlm.nih.gov/compound/445639) | [C18H34O2](https://pubchem.ncbi.nlm.nih.gov/#query=C18H34O2) | 282.5 |  | C:\Users\Z400\Desktop\2D Structure of compounds\445639.png |
| 15. | Palmitic Acid | CID\_ [985](https://pubchem.ncbi.nlm.nih.gov/compound/985) | [C16H32O2](https://pubchem.ncbi.nlm.nih.gov/#query=C16H32O2) | 256.42 |  | C:\Users\Z400\Desktop\2D Structure of compounds\985.png |
| 16. | Pinoresinol | CID\_  [73399](https://pubchem.ncbi.nlm.nih.gov/compound/73399) | [C20H22O6](https://pubchem.ncbi.nlm.nih.gov/#query=C20H22O6) | 358.4 |  | C:\Users\Z400\Desktop\2D Structure of compounds\73399.png |
| 17. | Sesamin | CID\_ [72307](https://pubchem.ncbi.nlm.nih.gov/compound/72307) | [C20H18O6](https://pubchem.ncbi.nlm.nih.gov/#query=C20H18O6) | 354.4 |  | C:\Users\Z400\Desktop\2D Structure of compounds\72307.png |
| 18. | Sesaminol | CID\_ [94672](https://pubchem.ncbi.nlm.nih.gov/compound/94672) | [C20H18O7](https://pubchem.ncbi.nlm.nih.gov/#query=C20H18O7) | 370.4 |  | C:\Users\Z400\Desktop\2D Structure of compounds\94672.png |
| 19. | Sesamol | CID\_ [68289](https://pubchem.ncbi.nlm.nih.gov/compound/68289) | [C7H6O3](https://pubchem.ncbi.nlm.nih.gov/#query=C7H6O3) | 138.12 |  | C:\Users\Z400\Desktop\2D Structure of compounds\68289.png |
| 20. | Sesamolinol | CID\_ [443019](https://pubchem.ncbi.nlm.nih.gov/compound/443019) | [C20H20O7](https://pubchem.ncbi.nlm.nih.gov/#query=C20H20O7) | 372.4 |  | C:\Users\Z400\Desktop\2D Structure of compounds\443019.png |
| 21. | Stearic Acid | CID\_ [5281](https://pubchem.ncbi.nlm.nih.gov/compound/5281) | [C18H36O2](https://pubchem.ncbi.nlm.nih.gov/#query=C18H36O2) | 284.5 |  | C:\Users\Z400\Desktop\2D Structure of compounds\5281.png |
| 22. | Tocopherol | CID\_ [14985](https://pubchem.ncbi.nlm.nih.gov/compound/14985) | [C29H50O2](https://pubchem.ncbi.nlm.nih.gov/#query=C29H50O2) | 430.7 |  | C:\Users\Z400\Desktop\2D Structure of compounds\14985.png |
| 23. | Vitamin A Retinol | CID\_ [445354](https://pubchem.ncbi.nlm.nih.gov/compound/445354) | [C20H30O](https://pubchem.ncbi.nlm.nih.gov/#query=C20H30O) | 286.5 |  | C:\Users\Z400\Desktop\2D Structure of compounds\445354.png |
| 24. | Vitamin K Phylloquinone | CID\_ [5284607](https://pubchem.ncbi.nlm.nih.gov/compound/5284607) | [C31H46O2](https://pubchem.ncbi.nlm.nih.gov/#query=C31H46O2) | 450.7 |  | C:\Users\Z400\Desktop\2D Structure of compounds\5284607.png |
| 25. | Arachidic acid | CID\_ [10467](https://pubchem.ncbi.nlm.nih.gov/compound/10467) | [C20H40O2](https://pubchem.ncbi.nlm.nih.gov/#query=C20H40O2) | 312.5 |  | C:\Users\Z400\Desktop\2D Structure of compounds\10467.png |
| 26. | Myristic acid | CID\_ [11005](https://pubchem.ncbi.nlm.nih.gov/compound/11005) | [C14H28O2](https://pubchem.ncbi.nlm.nih.gov/#query=C14H28O2) | 228.37 |  | C:\Users\Z400\Desktop\2D Structure of compounds\11005.png |
| 27. | Behenic acid | CID\_ [8215](https://pubchem.ncbi.nlm.nih.gov/compound/8215) | [C22H44O2](https://pubchem.ncbi.nlm.nih.gov/#query=C22H44O2) | 340.6 |  | C:\Users\Z400\Desktop\2D Structure of compounds\8215.png |
| 28. | Octanoic acid | CID\_ [379](https://pubchem.ncbi.nlm.nih.gov/compound/379) | [C8H16O2](https://pubchem.ncbi.nlm.nih.gov/#query=C8H16O2) | 144.21 |  | C:\Users\Z400\Desktop\2D Structure of compounds\379.png |
| 29. | Decanoic acid | CID\_ [2969](https://pubchem.ncbi.nlm.nih.gov/compound/2969) | [C10H20O2](https://pubchem.ncbi.nlm.nih.gov/#query=C10H20O2) | 172.26 |  | C:\Users\Z400\Desktop\2D Structure of compounds\2969.png |
| 30. | Lauric acid | CID\_ [3893](https://pubchem.ncbi.nlm.nih.gov/compound/3893) | [C12H24O2](https://pubchem.ncbi.nlm.nih.gov/#query=C12H24O2) | 200.32 |  | C:\Users\Z400\Desktop\2D Structure of compounds\3893.png |
| 31. | Eicosenoic acid | CID\_ [5282768](https://pubchem.ncbi.nlm.nih.gov/compound/5282768) | [C20H38O2](https://pubchem.ncbi.nlm.nih.gov/#query=C20H38O2) | 310.5 |  | C:\Users\Z400\Desktop\2D Structure of compounds\5282768.png |
| 32. | Lariciresinol | CID\_ [332427](https://pubchem.ncbi.nlm.nih.gov/compound/332427) | [C20H24O6](https://pubchem.ncbi.nlm.nih.gov/#query=C20H24O6) | 360.4 |  | C:\Users\Z400\Desktop\2D Structure of compounds\332427.png |
| 33. | Campesterol | CID\_ [173183](https://pubchem.ncbi.nlm.nih.gov/compound/173183) | [C28H48O](https://pubchem.ncbi.nlm.nih.gov/#query=C28H48O) | 400.7 |  | C:\Users\Z400\Desktop\2D Structure of compounds\173183.png |
| 34. | Δ5‐Avenasterol | CID\_[5281326](https://pubchem.ncbi.nlm.nih.gov/compound/5281326) | [C29H48O](https://pubchem.ncbi.nlm.nih.gov/#query=C29H48O) | 412.7 |  | C:\Users\Z400\Desktop\2D Structure of compounds\5281326.png |
| 35. | Δ7‐Stigmasterol | CID\_[131751494](https://pubchem.ncbi.nlm.nih.gov/compound/131751494) | [C29H46O](https://pubchem.ncbi.nlm.nih.gov/#query=C29H46O) | 410.7 |  | C:\Users\Z400\Desktop\2D Structure of compounds\131751494.png |
| 36. | Δ7‐Avenasterol | CID\_[12795736](https://pubchem.ncbi.nlm.nih.gov/compound/12795736) | [C29H48O](https://pubchem.ncbi.nlm.nih.gov/#query=C29H48O) | 412.7 |  | C:\Users\Z400\Desktop\2D Structure of compounds\12795736.png |