**Supplementary Table S1:** Natural components of *Nigella sativa* seeds and oil

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| --- | --- | --- | --- | --- |
| Compound | PubChem  CID | Molecular  Formula | Structure | Description |
| n-Nonane | 8141 | C9H20 | [Nonane_3D_Structure.png](https://pubchem.ncbi.nlm.nih.gov/compound/Nonane#section=3D-Conformer) | It is a clear colorless liquid having sharp smell. |
| Tricyclene | 79035 | C10H16 |  | It is a monoterpene. |
| Camphene | 6616 | C10H16 |  | It is a white to colorless crystalline solid with camphor like smell. |
| β-Pinene | 14896 | C10H16 |  | It is part of many essential oils with exocyclic double bond and a plant metabolite. |
| Sabinene | 18818 | C10H16 |  | It is a thujene and a plant metabolite. |
| Nigellicine | 11402337 | C13H14N2O3 |  | It is an alkaloid and found in many spices and herbs. |
| Nigellidine | 136828302 | C18H18N2O2 | Nigellidine_3D_Structure.png | It has indazole nucleus. |
| Nigellimine | 20725 | C12H13NO2 | 6,7-Dimethoxy-1-methylisoquinoline_3D_Structure.png | It is found in many herbs and spices. |
| Carvacrol | 10364 | C10H14O | Carvacrol_3D_Structure.png | It is a phenol and a derivative of monoterpene. It is a food additive and an inhibitor of bacterial growth. |
| Thymol | 6989 | C10H14O |  | It is a phenol and plays a role in volatile oil component. |
| Thymoquinone | 10281 | C10H12O2 |  | It is found in many herbs and spices. |
| Dithymoquinone | 398941 | C20H24O4 |  | It is anti-cancer and anti-diabetic. |
| Thymohydroquinone | 95779 | C10H14O2 |  | It is helpful in treating asthma, cough, influenza, fever, dizziness etc. |
| Oleic acid | 445639 | C18H34O2 | Oleic acid_3D_Structure.png | It is a yellowish to colorless liquid which floats on water. |
| Palmitic acid | 985 | C16H32O2 | Palmitic acid_3D_Structure.png | It is found in palm oil, butter, cheese, milk, and meat. |
| Kaempferol | 5280863 | C15H10O6 | Kaempferol_3D_Structure.png | It is an anti-oxidant and reducing oxidative stress. It is also anti-bacterial and plant metabolite. |
| Borneol | 64685 | C10H18O | Borneol_3D_Structure.png | It is a whitish lump solid having camphor like odor. It is used to make perfumes. |
| Linalool | 6549 | C10H18O | Linalool_3D_Structure.png | It is a plant metabolite and anti-microbial agent |
| Terpinolene | 11463 | C10H16 | Terpinolene_3D_Structure.png | It is used to make plastics and resins. |
| Limonene | 440917 | C10H16 | D-Limonene_3D_Structure.png | It has a lemon like smell and a colorless liquid |
| α-Thujene | 17868 | C10H16 |  | It is a natural organic compound and present in many essential oils |
| Limonene oxide | 91496 | C10H16O |  | It is a plant metabolite |
| α-Pinene | 440968 | C10H16 |  | It is used as a insect repellent and also in fragrance industry |
| Camphor | 2537 | C10H16O |  | It has same density as water and used to make moth proofing, flavorings and pharmaceuticals |
| Ledol | 92812 | C15H26O |  | It is for pain relief |
| Decanoic acid | 2969 | C10H20O2 |  | It is used to make esters for perfumes and fruit flavors |
| Linoleic acid | 5280450 | C18H32O2 |  | It is found in many plant oils and used in biosynthesis of cell membrane |
| Myristic acid | 11005 | C14H28O2 |  | It is a constituent of palm oil, butter oil and butter fat |
| Acetic acid | 176 | C2H4O2 |  | It has anti-bacterial and anti-fungal properties |
| Valencene | 9855795 | C15H24 |  | It has anti-inflammatory and anti-allergy properties |
| 4-terpineol | 11230 | C10H18O |  | It has anti-oxidant, anti-bacterial, anti-inflammatory, anti-parasitic properties. It is an apoptosis inducer |
| ρ-cymene | 7463 | C10H14 |  | It prevents cough and phlegm. It is used in fungicides and pesticides |
| *t-*butylhydroquinone | 16043 | C10H14O2 |  | It is a food additive and does not give discoloration in iron presence |
| Eicosadienoic acid | 6439848 | C20H36O2 |  | It is a long chain fatty acid |
| Myristoleic acid | 5281119 | C14H26O2 |  | It is a plant metabolite and an apoptosis inducer |
| Stearic acid | 5281 | C18H36O2 |  | It is found in many animal and plant fats and present in cocoa and shea butter |
| Thujadiene | 85582292 | C10H14 |  | It is a colorless to pale yellow liquid |
| Pinocarvone | 121719 | C10H14o |  | It is a bridged compound made from rearrangement of carvone and has a role as mouse metabolite |
| Farnesol | 445070 | C15H26o |  | It is a colorless liquid having delicate floral odor |
| Cyclohexane | 8078 | C6H12 |  | It is a clear colorless liquid having petroleum like odor |
| Longifolene | 289151 | C15H24 |  | It is a sesquiterpene |
| Ylangene | 6432119 | C15H24 |  | It is a sesquiterpenoids, which is a class of organic compounds |
| 3-Carene | 26049 | C10H16 |  | It is a colorless liquid having sweet and turpentine like odor |
| Naphthalene | 931 | C10H8 |  | It is a white, volatile, and polycyclic hydrocarbon with strong mothball odor |
| Caryophyllene | 5281515 | C15H24 |  | It is a pale yellow oily liquid |
| Methyl Stearate | 8201 | C19H38 o |  | It is a fatty acid methyl ester and have white crystals or chunky solid |

**Supplementary Table S2:** Docking Score of Nigella sativa compounds with spike protein

|  |  |  |
| --- | --- | --- |
| No. | Compounds | Docking Score |
| 1 | n-Nonane | -4.9746 |
| 2 | Tricyclene | -4.6558 |
| 3 | Camphene | -4.5584 |
| 4 | β-Pinene | -4.3128 |
| 5 | Sabinene | -4.6257 |
| 6 | Nigellicine | -5.5418 |
| 7 | Nigellidine | -5.9424 |
| 8 | Nigellimine | -5.3960 |
| 9 | Carvacrol | -4.9105 |
| 10 | Thymol | -4.8852 |
| 11 | Thymoquinone | -4.8633 |
| 12 | Dithymoquinone | -5.7371 |
| 13 | Thymohydroquinone | -5.0080 |
| 14 | Oleic acid | -7.0120 |
| 15 | Palmitic acid | -6.3564 |
| 16 | Kaempferol | -5.8171 |
| 17 | Borneol | -4.3367 |
| 18 | Linalool | -5.1225 |
| 19 | Terpinolene | -4.8497 |
| 20 | Limonene | -4.8588 |
| 21 | α-Thujene | -4.8781 |
| 22 | Limonene oxide | -4.8070 |
| 23 | α-Pinene | -4.3473 |
| 24 | Camphor | -4.2822 |
| 25 | Ledol | -5.1227 |
| 26 | Decanoic acid | -5.6697 |
| 27 | Linoleic acid | -6.9182 |
| 28 | Myristic acid | -6.2906 |
| 29 | Acetic acid | -3.5985 |
| 30 | Valencene | -4.8395 |
| 31 | 4-terpineol | -4.7617 |
| 32 | ρ-cymene | -4.6655 |
| *33* | *t-*butylhydroquinone | -4.7617 |
| 34 | Eicosadienoic acid | -7.4234 |
| 35 | Myristoleic acid | -6.4648 |
| 36 | Stearic acid | -7.0729 |
| 37 | Thujadiene | -4.7222 |
| 38 | Pinocarvone | -4.6306 |
| 39 | Farnesol | -6.1679 |
| 40 | Cyclohexan | -3.7914 |
| 41 | Longifolene | -4.8889 |
| 42 | Ylangene | -4.4748 |
| 43 | 3-Carene | -4.8296 |
| 44 | Naphthalene | -4.4270 |
| 45 | Caryophyllene | -4.9035 |
| 46 | Methyl Stearate | -7.4506 |