

## Supplementary Information

**Supplementary Table 1: Bioactive Compounds, Plant Sources, and Chemical Classification**

| S. No | Compounds (1bvr)                   | Plants                                                            | Plant Family                | Plant Part              | Class of Compounds               |
|-------|------------------------------------|-------------------------------------------------------------------|-----------------------------|-------------------------|----------------------------------|
| 1.    | Chryso-obtusin                     | <i>Cassia tora</i> (Chakunda)                                     | Fabaceae                    | Seed                    | Polyketides                      |
| 2.    | Episesamin                         | <i>Cinnamomum camphora</i> (camphor tree)                         | Lauraceae                   | Leaves                  | Phenylpropanoids                 |
| 3.    | Norhyoscyne                        | <i>Datura metel</i> (Thornapple)                                  | Solanaceae                  | Root                    | Tropane alkaloid                 |
| 4.    | Apohyoscyne                        | <i>Datura metel</i> (Thornapple)                                  | Solanaceae                  | Root                    | Tropane alkaloid                 |
| 5.    | Melanoxetin                        | <i>Albizia lebbeck</i> (Indian siris)                             | Fabaceae                    | Wood                    | Flavonoids                       |
| 6.    | Pelargonidin                       | <i>Punica granatum</i> (Dalim)                                    | Punicaceae                  | Fruit                   | Flavonoids                       |
| 7.    | Malvidin                           | <i>Punica granatum</i> (Dalim)                                    | Punicaceae                  | Fruit                   | Flavonoids                       |
| 8.    | Cotinine                           | <i>Allium cepa</i>                                                | Solanaceae                  | Leaf                    | Alkaloid                         |
| 9.    | Alpha- Terpinyl-Acetate            | <i>Cinnamomum camphora</i> (Kapoor)                               | Lauraceae                   | Leaf                    | Menthane monoterpenoids          |
| 10.   | Vasicine                           | <i>Justicia adhatoda</i> (Arusha)                                 | Acanthaceae                 | Plant                   | Quinazoline alkaloid             |
| 11.   | Prostaglandin-E-2                  | <i>Allium sativum</i> (Lehsun, Garlic)                            | Amaryllida<br>Cae           | Essential oil           | Eicosanoids                      |
| 12.   | 1-hydroxy-2-acetyl-4-methylbenzene | <i>Ageratum conyzoides</i> (Jangli pudina)                        | Asteraceae                  | Shoot                   | Acetophenones                    |
| 13.   | 5-Hexyl-cyclopenta-1,3-Dione       | <i>Allium cepa</i> (Pyaz)                                         | Amaryllidaceae              | Bulb                    | Beta-diketone                    |
| 14.   | Thiamin                            | <i>Punica granatum</i> (Dalim)                                    | Punicaceae                  | Fruit                   | Diazines                         |
| 15.   | (Rac)- Myrsilignan                 | <i>Myristica fragrans</i> (Jaifal, Nutmeg)                        | Myristicaceae               | Leaf, seed, Plant<br>EO | Phenylpropanoids.                |
| 16.   | Borneol-acetate                    | <i>Cannabis sativa</i> (Ganja)                                    | Pinaceae                    | Plant                   | bicyclic monoterpenoids          |
| 17.   | Endo-bornyl-acetate                | <i>Ageratum conyzoides</i> (Visadoori)                            | Pinaceae,                   | Plant                   | bicyclic monoterpenoid           |
| 18.   | Trans-sinapic-acid                 | <i>Allium cepa</i> (Pyaz)                                         | Amaryllidaceae              | Seed                    | Phenylpropanoids                 |
| 19.   | Vanillic- Acid-4-Beta-D-Glucoside  | <i>Capsicum annuum</i> (chili pepper)                             | Solanaceae                  | Fruit                   | Hydrolyzable tannins             |
| 20.   | 5- Methoxyeugenol                  | <i>Myristica fragrans</i> (Javitri)                               | Myristicaceae               | Essential oil           | Methoxyphenols                   |
| 21.   | Veratric-acid                      | <i>Verbascum Thapsus</i> (Mullein)                                | Scrophulariaceae            | Fruit                   | Phenolic                         |
| 22.   | Pelletierine                       | <i>Punica granatum</i> (Dalim)                                    | Punicaceae                  | Plant                   | Alkaloid                         |
| 23.   | Cantharidin                        | <i>Butea Monosperma</i> (Dhaak)                                   | Fabaceae                    | Plant                   | Terpenoid                        |
| 24.   | Prostaglandin-A-1                  | <i>Allium sativum</i> (Lehsun, Garlic)                            | Liliaceae                   | Seed                    | Eicosanoids                      |
| 25.   | Damascenine                        | <i>Nigella sativa</i> (kala jeera)                                | Ranunculaceae               | Plant                   | Alkaloids                        |
| 26.   | Prostaglandin-E-1                  | <i>Allium sativum</i> (Lehsun, Garlic)                            | Liliaceae                   | Bulb                    | Eicosanoids                      |
| 27.   | Prostaglandin-B-1                  | <i>Allium sativum</i> (Lehsun, Garlic)                            | Liliaceae                   | Bulb                    | Eicosanoids                      |
| 28.   | Delta-octalactone                  | <i>Allium cepa</i>                                                | Liliaceae                   | Fruit                   | Organic compounds                |
| 29.   | Citronellic- Acid                  | <i>Cinnamomum camphora</i> / <i>Elettaria cardamomum</i> (Kapoor) | Lauraceae/<br>Zingiberaceae | EO/Fruit                | Acyclic monoterpenoid            |
| 30.   | Carpasemine                        | <i>Carica papaya</i> (Papita)                                     | Caricaceae                  | Seed                    | Alkaloids                        |
| 31.   | Neodecanoic-acid                   | <i>Allium cepa</i> (Pyaz)                                         | Liliaceae                   | Bulb                    | Medium-chain FA                  |
| 32.   | 1,1-Diethoxy-3-Methylbutane        | <i>Capsicum annuum</i> (chili pepper)                             | Solanaceae                  | Fruit                   | Acyclic monoterpenoids           |
| 33.   | Arecolidine                        | <i>Areca catechu</i> Tiger grass,                                 | Arecaceae                   | Seed                    | Alkaloid ester                   |
| 34.   | Heptan-1-al                        | <i>Centella asiatica</i> (Gotu kola,)                             | Apiaceae                    | Shoot                   | Organic compounds                |
| 35.   | Tetrahydro-2,5-Dimethylthiophene   | <i>Allium sativum</i> (Lehsun, Garlic)                            | Amaryllidaceae              | Bulb                    | Organic compounds/<br>thiophenes |
| 36.   | 1,1-Diethoxy-2- Methylpropane      | <i>Capsicum annuum</i> (Chili pepper)                             | Solanaceae                  | Fruit                   | Organic compound                 |
| 37.   | Ethyl-Isopropyl- sulfide           | <i>Zingiber officinale</i> (Soont/zinger)                         | Zingiberaceae               | Essential oil           | dialkylthioethers                |

**Supplementary Table-2: Drug-like properties of 37 compounds**

| S.No. | Compounds                          | Molecular Mass(g/mol) | Xlog P3(<5) | H donar (≤5) | H acceptor (≤10) | Molar Refractivity |
|-------|------------------------------------|-----------------------|-------------|--------------|------------------|--------------------|
| 1.    | Chryso-obtusin                     | 358                   | 2.6         | 1            | 7                | 85.5               |
| 2.    | Episesamin                         | 354                   | 3.0         | 0            | 6                | 87.3               |
| 3.    | Norhyosine                         | 289                   | 1.4         | 2            | 5                | 73.6               |
| 4.    | Apohyosine                         | 285                   | 1.8         | 0            | 3                | 74.5               |
| 5.    | Melanoxetin                        | 302                   | 0.7         | 5            | 7                | 65.0               |
| 6.    | Pelargonidin                       | 271                   | 0.8         | 4            | 5                | 63.1               |
| 7.    | Malvidin                           | 331                   | 1.5         | 4            | 7                | 74.8               |
| 8.    | Cotinine                           | 176                   | 1.4         | 0            | 1                | 47.6               |
| 9.    | Alpha- Terpinyl-Acetate            | 196                   | 3.0         | 0            | 2                | 62.3               |
| 10.   | Vasicine                           | 188                   | 1.3         | 1            | 2                | 51.6               |
| 11.   | Prostaglandin-E-2                  | 352                   | 3.9         | 3            | 5                | 103.3              |
| 12.   | 1-hydroxy-2-acetyl-4-methylbenzene | 150                   | 1.5         | 1            | 2                | 41.5               |
| 13.   | 5-Hexyl-cyclopenta-1,3-Dione       | 182                   | 2.6         | 0            | 2                | 57.0               |
| 14.   | Thiamin                            | 265                   | 1.6         | 3            | 1                | 68.5               |
| 15.   | (Rac)- Myrislignan                 | 374                   | 3.8         | 2            | 6                | 98.7               |
| 16.   | Borneol-acetate                    | 196                   | 3.0         | 0            | 2                | 60.5               |
| 17.   | Endo-bornyl-acetate                | 196                   | 3.0         | 0            | 2                | 60.5               |
| 18.   | Trans-sinapic-acid                 | 224                   | 0.7         | 2            | 5                | 50.8               |
| 19.   | Vanillic- Acid-4-Beta-D-Glucoside  | 330                   | 1.1         | 5            | 9                | 70.7               |
| 20.   | 5- Methoxyeugenol                  | 196                   | 2.3         | 1            | 3                | 53.9               |
| 21.   | Veratric-acid                      | 182                   | 1.1         | 1            | 4                | 40.9               |
| 22.   | Pelletierine                       | 141                   | 1.8         | 1            | 1                | 45.2               |
| 23.   | Cantharidin                        | 196                   | 1.4         | 0            | 4                | 47.0               |
| 24.   | Prostaglandin-A-1                  | 336                   | 4.2         | 2            | 4                | 102.5              |
| 25.   | Damascenine                        | 195                   | 1.6         | 0            | 3                | 48.7               |
| 26.   | Prostaglandin-E-1                  | 354                   | 4.1         | 3            | 5                | 105.6              |
| 27.   | Prostaglandin-B-1                  | 336                   | 4.2         | 2            | 4                | 102.6              |
| 28.   | Delta-octalactone                  | 142                   | 1.9         | 0            | 2                | 42.8               |
| 29.   | Citronellic- Acid                  | 170                   | 2.4         | 1            | 2                | 53.7               |
| 30.   | Carpasemine                        | 166                   | -0.4        | 3            | 0                | 43.3               |
| 31.   | Neodecanoic-acid                   | 172                   | 2.5         | 1            | 2                | 55.3               |
| 32.   | 1,1-Diethoxy-3-Methylbutane        | 160                   | 2.7         | 0            | 2                | 52.5               |
| 33.   | Arecolidine                        | 155                   | 1.5         | 0            | 2                | 42.3               |
| 34.   | Heptan-1-al                        | 114                   | 2.1         | 0            | 1                | 38.5               |
| 35.   | Tetrahydro-2,5-Dimethylthiophene   | 116                   | 1.8         | 0            | 0                | 40.0               |
| 36.   | 1,1-Diethoxy-2- Methylpropane      | 146                   | 2.4         | 0            | 2                | 47.1               |
| 37.   | Ethyl-Isopropyl- sulfide           | 104                   | 1.7         | 0            | 0                | 36.7               |

**Supplementary Table-3: List of 37 compounds that successfully satisfy all ADMET analysis**

| S.No | Compounds (1bvr)                   | Mutagenicity | Carcinogenicity Mouse | Carcinogenicity Rat | HIA % | Pcaco-2(nm/s) | Pmdc k(nm/s) | Pskin(nm/s) | PPB%  | BBB% | Cyp2d6    |
|------|------------------------------------|--------------|-----------------------|---------------------|-------|---------------|--------------|-------------|-------|------|-----------|
| 1.   | Chryso-obtusin                     | Mutagen      | -                     | +                   | 96.19 | 22.34         | 175.63       | -3.72       | 85.69 | 0.01 | Non       |
| 2.   | Episesamin                         | Mutagen      | -                     | -                   | 97.95 | 57.02         | 20.60        | -4.41       | 83.12 | 0.05 | Non       |
| 3.   | Norhyoscinine                      | Mutagen      | +                     | -                   | 92.06 | 20.49         | 1.41         | -4.66       | 18.72 | 0.02 | Non       |
| 4.   | Apoxyoscinine                      | Mutagen      | +                     | -                   | 98.02 | 53.50         | 49.45        | -3.96       | 35.00 | 0.02 | Non       |
| 5.   | Melanoxetin                        | Mutagen      | -                     | +                   | 63.46 | 12.71         | 63.71        | -4.42       | 90.54 | 0.18 | Non       |
| 6.   | Pelargonidin                       | Mutagen      | -                     | -                   | 83.58 | 1.29          | 59.76        | -3.99       | 100   | 0.53 | Substrate |
| 7.   | Malvidin                           | Mutagen      | -                     | +                   | 83.10 | 1.75          | 109.94       | -4.20       | 94.94 | 0.05 | Weakly    |
| 8.   | Cotinine                           | Mutagen      | -                     | -                   | 99.79 | 30.28         | 5.47         | -2.85       | 57.20 | 0.99 | Non       |
| 9.   | Alpha-Terpinyl-Acetate             | Mutagen      | -                     | -                   | 100   | 37.76         | 262.08       | -1.29       | 98.53 | 0.89 | Non       |
| 10.  | Vasicine                           | Mutagen      | -                     | -                   | 95.47 | 29.31         | 278.64       | -3.86       | 80.33 | 0.54 | Weakly    |
| 11.  | Prostaglandin-E-2                  | Mutagen      | -                     | +                   | 89.18 | 18.66         | 0.09         | -1.92       | 89.69 | 0.19 | Non       |
| 12.  | 1-hydroxy-2-acetyl-4-methylbenzene | Mutagen      | +                     | -                   | 94.50 | 20.02         | 61.39        | -1.72       | 85.71 | 0.74 | Non       |
| 13.  | 5-Hexyl-cyclopenta-1,3-Dione       | Mutagen      | +                     | +                   | 98.92 | 14.80         | 54.18        | -1.61       | 100   | 0.86 | Non       |
| 14.  | Thiamin                            | Mutagen      | -                     | -                   | 91.10 | 5.44          | 0.54         | -4.57       | 9.07  | 0.02 | Substrate |
| 15.  | (Rac)-Myrislignan                  | Non-Mutagen  | -                     | +                   | 93.93 | 39.36         | 1.58         | -2.38       | 89.24 | 0.69 | Non       |
| 16.  | Borneol-acetate                    | Mutagen      | -                     | -                   | 100   | 37.67         | 148.16       | -2.00       | 83.32 | 0.80 | Non       |
| 17.  | Endobornyl-acetate                 | mutagen      | -                     | +                   | 100   | 37.67         | 148.16       | -2.00       | 83.32 | 0.80 | Non       |
| 18.  | Trans-sinapic-acid                 | Mutagen      | -                     | +                   | 88.55 | 19.85         | 270.19       | -2.28       | 47.50 | 0.72 | Non       |
| 19.  | Vanillic-Acid-4-Beta-D-Glucoside   | Mutagen      | -                     | -                   | 86.48 | 15.37         | 0.56         | -4.68       | 36.88 | 0.01 | Non       |

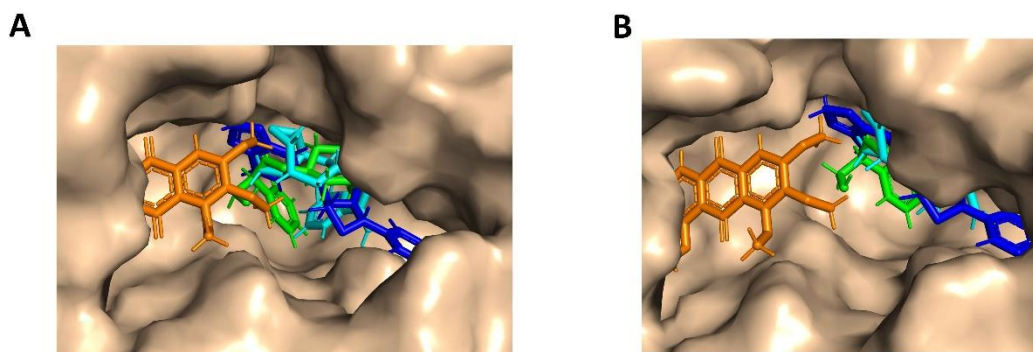
|     |                                  |         |   |   |       |       |        |       |       |       |        |
|-----|----------------------------------|---------|---|---|-------|-------|--------|-------|-------|-------|--------|
| 20. | 5-Methoxy eugenol                | Mutagen | + | - | 94.57 | 50.53 | 43.31  | -2.10 | 91.47 | 0.55  | Non    |
| 21. | 5-Methoxy eugenol                | Mutagen | + | - | 94.57 | 50.53 | 43.31  | -2.10 | 91.47 | 0.55  | Non    |
| 22. | Veratric-acid                    | Mutagen | - | + | 92.68 | 20.57 | 52.15  | -2.08 | 77.89 | 1.05  | Non    |
| 23. | Pelletierine                     | Mutagen | + | - | 94.19 | 35.77 | 6.84   | -3.65 | 0.80  | 0.45  | weakly |
| 24. | Cantharidin                      | mutagen | - | + | 92.21 | 21.02 | 23.04  | -4.33 | 42.48 | 0.87  | Non    |
| 25. | Prostaglandin-A-1                | Mutagen | - | + | 95.51 | 20.74 | 0.09   | -1.80 | 100   | 0.89  | Non    |
| 26. | Damascenine                      | Mutagen | + | + | 94.33 | 25.56 | 42.51  | -2.33 | 63.20 | 0.59  | Non    |
| 27. | Prostaglandin-E-1                | Mutagen | + | + | 87.29 | 18.66 | 0.07   | -1.67 | 100   | 0.33  | Non    |
| 28. | Prostaglandin-B-1                | Mutagen | - | + | 95.51 | 20.70 | 0.09   | -1.07 | 100   | 0.97  | Non    |
| 29. | Delta-octalactone                | Mutagen | + | + | 100   | 50.71 | 60.92  | -1.97 | 100   | 0.79  | Weakly |
| 30. | Citronellc- Acid                 | mutagen | + | + | 96.57 | 5.69  | 240.57 | -1.11 | 100   | 0.85  | Non    |
| 31. | Carpasemine                      | Mutagen | - | - | 93.81 | 21.02 | 61.30  | -2.55 | 39.93 | 0.59  | Non    |
| 32. | Neodecanoic-acid                 | Mutagen | - | - | 95.67 | 8.09  | 189.63 | -1.22 | 100   | 0.82  | Non    |
| 33. | 1,1-Diethoxy-3-Methylbutane      | Mutagen | + | + | 100   | 49.97 | 59.45  | -1.79 | 100   | 0.89  | Non    |
| 34. | Arecolidine                      | Mutagen | + | - | 100   | 56.41 | 241.98 | -3.30 | 74.49 | 0.80  | Non    |
| 35. | Heptan-1-al                      | Mutagen | - | - | 100   | 37.21 | 164.12 | -1.61 | 97.42 | 1.02  | Non    |
| 36. | Tetrahydro-2,5-Dimethylthiophene | Mutagen | - | + | 100   | 21.98 | 0.88   | -2.28 | 88.86 | 0.789 | Non    |
| 37. | 1,1-Diethoxy-2-Methylpropane     | Mutagen | + | + | 100   | 48.67 | 92.59  | -2.04 | 100   | 0.82  | Non    |
| 38. | Ethyl-Isopropyl-sulfide          | Mutagen | - | + | 100   | 21.65 | 0.84   | -1.77 | 82.60 | 0.80  | Non    |

**Supplementary Table 4: Binding energy, inhibition constant score, and interacting amino acid information of selected four compounds**

| S. No | Compounds (1bvr)                   | B.E. (kcal/mol) | Ki        | Interacting amino acid                                                                                                              |
|-------|------------------------------------|-----------------|-----------|-------------------------------------------------------------------------------------------------------------------------------------|
| 1.    | Chryso-obtusin                     | -8.92           | 289.31 nM | VAL65, LEU63, ASP64, PHE41, ILE95, ILE122, GLY96, ILE16, PHE97, GLN66, SER94, GLY14                                                 |
| 2.    | Episesamin                         | -8.74           | 395.09 nM | ALA157, TYR158, PRO193, PHE149, ILE21, THR196, SER94, ILE194, MET199, LEU218, PRO156                                                |
| 3.    | Norhyoscyne                        | -7.84           | 1.78 uM   | TYR158, ASP148, MET147, PRO193, PHE149, MET199, ILE194, ILE21, GLY192, ALA191                                                       |
| 4.    | Apoxyhyoscyne                      | -7.74           | 2.13 uM   | PRO156, ALA157, MET155, TYR158, ILE215, LEU218, MET103, GLY192, ILE194, MET199, PHE149, PRO193                                      |
| 5.    | Melanoxetin                        | -7.66           | 2.43 uM   | PHE41, ILE15, GLY14, GLY40, THR39, SER13, LEU63, VAL65, ILE95, ILE122, GLY96, PHE97                                                 |
| 6.    | Pelargonidin                       | -7.49           | 3.25 uM   | LEU63, VAL65, SER13, GLY14, THR39, GLY40, ILE95, PHE41, GLY96, PHE97, ILE122, ASP64                                                 |
| 7.    | Malvidin                           | -7.34           | 4.15 uM   | ILE95, SER94, GLY14, ILE15, ILE16, SER20, ALA22, THR196, SER19, ILE21, MET199, ILE194, PRO193, GLY192, ALA191, PHE149, GLY96, PHE97 |
| 8.    | Cotinine                           | -7.27           | 4.70 uM   | THR39, GLY40, GLY14, ILE122, ILE95, PHE41, VAL65, ASP64, LEU63, SER13                                                               |
| 9.    | Alpha- Terpinyl-Acetate            | -7.06           | 6.70 uM   | GLY96, ILE122, ILE95, VAL65, SER13, PHE41, GLY40, LEU63, THR39, GLY14, SER94                                                        |
| 10.   | Vasicine                           | -6.99           | 7.87 uM   | PHE41, ASP64, LEU63, THR39, GLY40, GLY14, ILE122, VAL65, PHE41                                                                      |
| 11.   | Prostaglandin-E-2                  | -6.96           | 7.94 uM   | MET103, MET199, PHE149, TYR158, PRO193, ALA191, ILE21, THR196, ILE194, SER20, GLY192, ASP148, LYS165, ALA22, SER94, GLY14           |
| 12.   | 1-hydroxy-2-acetyl-4-methylbenzene | -6.82           | 10.03 uM  | ILE95, SER13, GLY14, THR39, ILE15, GLY40, PHE41, LEU63, VAL65                                                                       |
| 13.   | 5-Hexyl-cyclopenta-1,3-Dione       | -6.82           | 10.09 uM  | LEU63, VAL65, SER13, THR39, GLY40, GLY14, SER94, ILE16, ILE95, ILE15, PHE41, ASP64                                                  |
| 14.   | Thiamin                            | -6.75           | 11.20 uM  | SER13, GLY14, LEU63, VAL65, ILE95, ILE122, GLY96, THR39, GLY40, PHE41, PHE97                                                        |
| 15.   | (Rac)- Myrislignan                 | -6.67           | 12.81 uM  | GLY96, PHE97, ILE15, PHE41, GLY40, THR39, SER13, LEU63, GLY14, ASP64, ILE95, VAL65, ILE122, SER94                                   |
| 16.   | Borneol-acetate                    | -6.58           | 15.03 uM  | GLY96, ILE15, LEU63, SER13, GLY14, THR39, ILE95, PHE41, GLY40, ILE16, SER94                                                         |
| 17.   | Endo-bornyl-acetate                | -6.56           | 15.61 uM  | TYR158, ASP148, ILE194, PRO193, MET199, PHE149, MET147, GLY192, ALA191, ILE21                                                       |
| 18.   | Trans-sinapic-acid                 | -6.56           | 15.57 uM  | GLN66, LYS118, PHE41, ILE122, VAL65, LEU63, GLY14, SER94, GLY96, PHE97, ILE95                                                       |
| 19.   | Vanillic- Acid-4-Beta-D-Glucoside  | -6.53           | 16.28 uM  | LEU63, VAL65, ILE95, ASP64, ILE122, SER94, ILE16, ILE15, ILE47, PHE41, GLY14, GLY40, THR39, SER13                                   |
| 20.   | 5- Methoxyeugenol                  | -6.51           | 16.84 uM  | SER13, GLY14, LEU63, PHE41, SER94, ILE95, GLY96, THR39, GLY40, ILE47, ILE16, ILE15                                                  |
| 21.   | Veratric-acid                      | -6.31           | 23.51 uM  | VAL65, ILE95, GLY14, SER13, THR39, GLY40, SER13, THR39, GLY40, LEU63, PHE41, ILE122, VAL65                                          |
| 22.   | Pelletierine                       | -6.23           | 26.90 uM  | PHE41, ILE122, ILE95, ASP64, VAL65, LEU63, THR39, GLY40                                                                             |
| 23.   | Cantharidin                        | -6.18           | 29.49 uM  | ILE95, SER94, VAL65, GLY14, SER13, GLY40, LEU63, PHE41, THR39, VAL65                                                                |
| 24.   | Prostaglandin-A-1                  | -6.03           | 38.10 uM  | ASP148, GLY192, LYS165, MET199, THR196, VAL189, MET147, VAL238, ALA191, ILE21, PHE149, PRO193, ILE194, TYR158                       |
| 25.   | Damascenine                        | -5.84           | 52.11 uM  | ILE122, VAL65, ASP64, LEU63, SER13, THR13, GLY14, GLY40, ILE15, ILE95, PHE41                                                        |
| 26.   | Prostaglandin-E-1                  | -5.78           | 57.54 uM  | GLY96, ILE95, PHE97, LEU197, ILE16, THR17, THR196, ALA198, SER20, ALA22, ILE21, GLY14, SER94                                        |
| 27.   | Prostaglandin-B-1                  | -5.74           | 61.77 uM  | ILE15, GLY40, THR39, PHE41, GLY14, ILE95, SER94, ILE16, GLY96, PHE97                                                                |
| 28.   | Delta-octalactone                  | -5.68           | 68.16 uM  | SER94, PHE41, GLY40, THR39, SER13, GLY14, LEU63, VAL65, ILE95                                                                       |
| 29.   | Citronellic- Acid                  | -5.61           | 77.63 uM  | ILE95, ILE15, GLY40, LEU63, THR39, SER13, ASP64, VAL65, GLY14, ILE47, PHE41, ILE16                                                  |

|     |                                  |       |           |                                                                             |
|-----|----------------------------------|-------|-----------|-----------------------------------------------------------------------------|
| 30. | Carpasemine                      | -5.59 | 80.28 uM  | ILE95, LEU63, ASP64, ILE122, VAL65, PHE41, THR39, GLY14, GLY40, ILE15       |
| 31. | Neodecanoic-acid                 | -5.31 | 127.82 uM | ILE16, ASP64, PHE41, GLY40, LEU63, THR39, GLY14, SER13, ILE95, ILE47, ILE15 |
| 32. | 1,1-Diethoxy-3-Methylbutane      | -5.06 | 194.33 uM | THR39, SER13, GLY40, GLY14, LEU63, ILE15, ASP64, ILE95, PHE41, VAL65        |
| 33. | Arecolidine                      | -4.91 | 250.02 uM | ILE16, ILE15, PHE41, ILE95, THR39, LEU63, SER13, GLY40, GLY14               |
| 34. | Heptan-1-al                      | -4.66 | 386.95 uM | SER13, THR39, GLY40, GLY14, LEU63, ASP64, ILE95, ILE122, VAL65, PHE41       |
| 35. | Tetrahydro-2,5-Dimethylthiophene | -4.59 | 430.05 uM | GLY40, GLY14, THR39, ILE15, SER13, ILE95, LEU63, PHE41, VAL65               |
| 36. | 1,1-Diethoxy-2-Methylpropane     | -4.58 | 438.28 uM | ILE95, ILE15, PHE41, GLY40, GLY14, VAL65, SER13, LEU63, THR39               |
| 37. | Ethyl-Isopropyl- sulfide         | -3.53 | 2.57 mM   | PHE41, ILE95, VAL65, ASP64, GLY40, GLY14, THR39, SER13, LEU63               |





**Supplementary Figure S2:** Superimposition of docked phytochemicals within the binding pocket of the InhA protein. Four phytochemicals Episeasmin (blue), Norhoscience (green), Apohyoscience (cyan), and Cryso-obtusin (orange) were docked into the active site of InhA and visualized within the protein's surface representation. Panel A shows a straight view of the docking site, illustrating the overall alignment and overlap of the ligands. Panel B provides a rotated perspective, highlighting that Cryso-obtusin (orange) occupies a distinct binding region compared to the other three compounds, suggesting a potentially unique binding mode or allosteric interaction.