**Documented Phytoconstituents with Significant Therapeutic Effect against PCOS:**

| **Sl. No.** | **Residue name** | **Name of phytoconstituents** | **Source plant(s)** | **Molecular formula** | **IUPAC name** | **Chemical structure** | **Smiles code** |
| --- | --- | --- | --- | --- | --- | --- | --- |
|  | API | Apigenin | *Petroselinum crispum* (Mill.) Fuss  *Brassica oleracea* L. | C15H10O5 | 5,7-dihydroxy-2-(4-hydroxyphenyl)chromen-4-one |  | C1=CC(=CC=C1C2=CC(=O)C3=C(C=C(C=C3O2)O)O)O |
|  | CAT | Catechin | *Camellia sinensis* (L.) Kuntze | C15H14O6 | (2R,3S)-2-(3,4-dihydroxyphenyl)-3,4-dihydro-2H-chromene-3,5,7-triol |  | C1[C@@H]([C@H](OC2=CC(=CC(=C21)O)O)C3=CC(=C(C=C3)O)O)O |
|  | BER | Berberine | *Berberis* spp. | C20H18NO4+ | 16,17-dimethoxy-5,7-dioxa-13-azoniapentacyclo[11.8.0.02,10.04,8.015,20]henicosa-1(13),2,4(8),9,14,16,18,20-octaene |  | COC1=C(C2=C[N+]3=C(C=C2C=C1)C4=CC5=C(C=C4CC3)OCO5)OC |
|  | GRA | Glycyrrhizin | *Glycyrrhiza glabra* L. | C42H62O16 | (2S,3S,4S,5R,6R)-6-[(2S,3R,4S,5S,6S)-2-[[(3S,4aR,6aR,6bS,8aS,11S,12aR,14aR,14bS)-11-carboxy-4,4,6a,6b,8a,11,14b-heptamethyl-14-oxo-2,3,4a,5,6,7,8,9,10,12,12a,14a-dodecahydro-1H-picen-3-yl]oxy]-6-carboxy-4,5-dihydroxyoxan-3-yl]oxy-3,4,5-trihydroxyoxane-2-carboxylic acid |  | C[C@]12CC[C@](C[C@H]1C3=CC(=O)[C@@H]4[C@]5(CC[C@@H](C([C@@H]5CC[C@]4([C@@]3(CC2)C)C)(C)C)O[C@@H]6[C@@H]([C@H]([C@@H]([C@H](O6)C(=O)O)O)O)O[C@H]7[C@@H]([C@H]([C@@H]([C@H](O7)C(=O)O)O)O)O)C)(C)C(=O)O |
|  | MAN | Mangiferin | *Mangifera indica* L. | C19H18O11 | 1,3,6,7-tetrahydroxy-2-[(2S,3R,4R,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]xanthen-9-one |  | C1=C2C(=CC(=C1O)O)OC3=C(C2=O)C(=C(C(=C3)O)[C@H]4[C@@H]([C@H]([C@@H]([C@H](O4)CO)O)O)O)O |
|  | BAI | Baicalin | *Scutellaria baicalensis* Georgi | C21H18O11 | (2S,3S,4S,5R,6S)-6-(5,6-dihydroxy-4-oxo-2-phenylchromen-7-yl)oxy-3,4,5-trihydroxyoxane-2-carboxylic acid |  | C1=CC=C(C=C1)C2=CC(=O)C3=C(C(=C(C=C3O2)O[C@H]4[C@@H]([C@H]([C@@H]([C@H](O4)C(=O)O)O)O)O)O)O |
|  | CUR | Curcumin | *Curcuma longa* L. | C21H20O6 | (1E,6E)-1,7-bis(4-hydroxy-3-methoxyphenyl)hepta-1,6-diene-3,5-dione |  | COC1=C(C=CC(=C1)/C=C/C(=O)CC(=O)/C=C/C2=CC(=C(C=C2)O)OC)O |
|  | RES | Resveratrol | *Vitis vinifera* L.,  *Arachis hypogaea* L. | C14H12O3 | 5-[(E)-2-(4-hydroxyphenyl)ethenyl]benzene-1,3-diol |  | C1=CC(=CC=C1/C=C/C2=CC(=CC(=C2)O)O)O |
|  | SIL | Silibinin | *Silybum marianum* (L.) Gaertn. | C25H22O10 | (2R,3R)-3,5,7-trihydroxy-2-[(2R,3R)-3-(4-hydroxy-3-methoxyphenyl)-2-(hydroxymethyl)-2,3-dihydro-1,4-benzodioxin-6-yl]-2,3-dihydrochromen-4-one |  | COC1=C(C=CC(=C1)[C@@H]2[C@H](OC3=C(O2)C=C(C=C3)[C@@H]4[C@H](C(=O)C5=C(C=C(C=C5O4)O)O)O)CO)O |
|  | NAR | Naringin | *Citrus × aurantium* L. | C27H32O14 | (2S)-7-[(2S,3R,4S,5S,6R)-4,5-dihydroxy-6-(hydroxymethyl)-3-[(2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxyoxan-2-yl]oxy-5-hydroxy-2-(4-hydroxyphenyl)-2,3-dihydrochromen-4-one |  | C[C@H]1[C@@H]([C@H]([C@H]([C@@H](O1)O[C@@H]2[C@H]([C@@H]([C@H](O[C@H]2OC3=CC(=C4C(=O)C[C@H](OC4=C3)C5=CC=C(C=C5)O)O)CO)O)O)O)O)O |
|  | VIT | Vitexin | *Vitex agnus-castus*L. | C21H20O10 | 5,7-dihydroxy-2-(4-hydroxyphenyl)-8-[(2S,3R,4R,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]chromen-4-one |  | C1=CC(=CC=C1C2=CC(=O)C3=C(O2)C(=C(C=C3O)O)[C@H]4[C@@H]([C@H]([C@@H]([C@H](O4)CO)O)O)O)O |
|  | RUT | Rutin | *Fagopyrum esculentum* Moench | C27H30O16 | 2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-3-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-[[(2R,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxymethyl]oxan-2-yl]oxychromen-4-one |  | C[C@H]1[C@@H]([C@H]([C@H]([C@@H](O1)OC[C@@H]2[C@H]([C@@H]([C@H]([C@@H](O2)OC3=C(OC4=CC(=CC(=C4C3=O)O)O)C5=CC(=C(C=C5)O)O)O)O)O)O)O)O |
|  | RHA | Rhamnocitrin | *Rhamnus* spp., *Syzygium aromaticum* (L.) Merr. &L.M.Perry | C16H12O6 | 3,5-dihydroxy-2-(4-hydroxyphenyl)-7-methoxychromen-4-one |  | COC1=CC(=C2C(=C1)OC(=C(C2=O)O)C3=CC=C(C=C3)O)O |
|  | GIN | Ginsenosides | *Panax ginseng* C.A.Mey. | C30H52O2 | (3S,5R,8R,9R,10R,14R,17S)-17-(2-hydroxy-6-methylhept-5-en-2-yl)-4,4,8,10,14-pentamethyl-2,3,5,6,7,9,11,12,13,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthren-3-ol |  | CC(=CCCC(C)([C@H]1CC[C@@]2(C1CC[C@H]3[C@]2(CC[C@@H]4[C@@]3(CC[C@@H](C4(C)C)O)C)C)C)O)C |
|  | GAL | Gallic acid | *Abrus precatorius* L., *Camellia sinensis* (L.) Kuntze | C7H6O5 | 3,4,5-trihydroxybenzoic acid |  | C1=C(C=C(C(=C1O)O)O)C(=O)O |