### **Supplementary material**

### 311 ligand molecule’s structure and classification

Over the years, the chemical constituents of celery seeds, Pueraria, dandelion, artichoke, Cirsium japonicum and Periploca forrestill Schltr have been systematically studied and remarkable achievements have been made. At present, organic acids, polysaccharides, flavonoids, coumarins, terpenes, inorganic elements and trace elements have been isolated from these six plants. The molecular components of these six plants were collected from the database and literature reports. In order to distinguish the source of each molecule, repeated molecules were not removed from six plants. These 311 compounds were from *Apium graveolens* L. (57), *Puerariae Lobatae Radix* (64), *Taraxacum mongolicum* Hand. -Mazz. (63), *Cynara scolymus* (31), *Cirsium japonicum* Fisch. ex DC. (39), and *Periploca forrestii* Schltr. (57).

There were 57 compounds in celery seeds (Table s1-1), numbered 1-57 respectively, including 20 flavonoids, 19 volatile oil components, 11 terpenoids, 6 organic acids and 1 coumarin.

**Table S1-1 Statistics of small molecular compounds from celery seeds**

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Structure/Number/Name | | | | Structure/Number/Name | | | | | | | Structure/Number/Name | |
| 1. Luteolin | 2. Luteolin-3’-O-beta-D-glucoside | | | | | | | | 3. Luteolin-7-O-beta-D-glucoside | | | | |
| 4. Diosmetin -7-O-beta-D-glucoside | | | | 5. Chrysoeriol | | 6. Chrysoeriol-7-O-β-D-glucopyranoside | | | | | | |
| 7. Butylphthalide | | | | 8. 4,5-Dihydro-3-Butylphthalide | | | | | | | | 9. Fromceleryseedsoil |
| 10. Apiin | | | | 11. Apigenin | | | | | | 12. Quercetin | | |
| 13.Sudachitin | | 14. p-Hydroxybenzaldehyde | | | | | 15. 3-Hydroxy-4-isopropyl benzoic acid | | | | | |
| 16. 4-hydroxy-2-isopropyl-5-methylphenyl-1-O-β-D-glucoside | | | | 17. Vanillic acid | | | | | 18. Chlorogenic acid | | | |
| 19. Coumaroylquinic acid | | 20.Luteolin-7-(2-O-  Apiosylglucoside) | | | | | | | | 21.Chrysoeriol-7-O-  apiosylglucoside | | |
| 22. Luteolin-7-O-6’- malonylglucoside | | | | | 23.Malonylapiin | | | | | 24. 6’’-Malonylapiin | | |
| 25.Apigenin-7-O-diglucosid | | | 26.Apigenin-7-O-  caffeoylglucosid | | | | | | | 27.Luteolin-7-O-6’-  acetylglucoside | | |
| 28.Luteolin-7-O-6’-  malonylglucoside | | | 29. α-Selinene | | | | | | | 30. Cinene | | |
| 31. α-Pinene | | | 32. β-Pinene | | | | | | | 33. β-Selinene | | |
| 34. D-limonene | | | 35. α-Terpinene | | | | | | | 36. γ-Terpinene | | |
| 37. β-Myrcene | | | 38. α-Caryophyllene | | | | | | | 39. β-Caryophyllene | | |
| 40. 2-Tert-butylphenol | | | 41. γ-Elemene | | | | | | | 42. Caffeic acid | | |
| 43. Senkyunolide N | | | 44. Senkyunolide J | | | | | | | 45. Tricaprin | | |
| 46. Persicarin | | | 47. 7- Methyl Persicarin | | | | | | | 48. Coumarin | | |
| 49. Friedelin | | | 50. 5-Methoxypsoralen | | | | | | | 51. Nicotinic acid | | |
| 52. Cyclohexanehexol | | 53. Methyl[3-oxo-2-(2-pentynyl) cyclopentyl] acetate | | | | | | 54. 4-hydroxyl-5,9-dimethyl-tricyclo[6,3,0,0(1,5)]undecan-10-one | | | | |
| 55. 3-(3,4-dimethybenzoyl)-propionic acid | | | 56.p-Heptylphenol | | | | | | | 57. p-(2-aminoethyl) phenol | | |

There were 64 compounds in pueraria (Table s1-2), numbered 58-121 respectively, including 44 flavonoids and their glycosides, 3 volatile oils, 8 terpenoids and sterols, 3 organic acids, 5 coumarins and 1 other component.

**Table S1-2 Statistics of small molecular compounds from pueraria**

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| 58. Puerarin | | 59. 3’-Methoxypuerarin | | | | 60. 4’-O-Methoxypuerarin | | | | |
| 61. 3’-hydroxy Puerarin | | 62. Puerarin-4’-O-glucoside | | | | 63. Puerarin 6’’-O-xyloside | | | | |
| 64. Mirificin | | 65. Puerarin Xyloside | | | | 66. Daidzein | | | | |
| 67. 8-Prenyldaidzein | | 68. Malonyl-Daidzin | | | | 69. Daidzein-4,7-diglucoside | | | | |
| 70. Daidzein-7-O-methylether | | 71. 3’-Methoxy daidzein | | | | 72. 3’-Hydroxy daidzein | | | | |
| 73. Formononetin | | 74. Ononin | | | 75. 8-Methoxy formononetin 7-O-glucoside | | | | | |
| 76. 5-Hydroxy formononetin 7-O-glucoside | | 77. Genistein | | | 78. Genistin | | | | | |
| 79. Malonyl-Genistin | | 80. 8-Prenylgenistein | | | 81 Genistein-8-C-glucoside | | | | | |
| 82. Isoliquiritigenin | | 83. Neoisoliquiritin | | | 84. Biochanin A | | | | | |
| 85. β-sitosterol | 86. Sitosteryl Palmitate | | | | | | 87. Puerarol | | | |
| 88. Coumestrol | 89. Lupeol | | | | | | 90. Lupeone | | | |
| 91. Daucosterol | 92. Hesperidin | | | | | | 93. Corylin | | | |
| 94. Diisobutyl phthalate | 95. Dioctyl phthalate | | | | | | 96. Ferulic acid | | | |
| 97. Coumestrol | 98. 7-methyl-4’-Hydroxy Isoflavone | | | | | | 99. Kakkalide | | | |
| 100.5-Hydroxy-2,3,4,5-tetrahydro-1H-benzo[c]azepin-1-one | 101. Tectoridin | | | | | | 102. Tectorigenin | | | |
| 103. irisolidone | 104. 3’-methoxy daidzein-7-O-methyl ether | | | | | | | 105. 3’-methoxy formononetin | | |
| 106. Kaempferol-3-O-  robinoside-7-O-rhamnoside | | | 107. 7,4’-Dihydroxy-3’-methoxyisoflavone | | | | | | | 108. Garbanzol |
| 109. Ambocin | | | | 110. Wighteone | | | | | 111.Kaempferol-7-O-β-D-glucopyranoside | |
| 112. 6,7-dimethyl-2H-chromen-2-one | | | | 113. Sophoracoumestan A | | | | | 114. Allantoin | |
| 115. Salicylic acid | | | | 116. Quercetin | | | | | 117. Gallic acid | |
| 118. β-Sitosterol | | | | 119. Sophoradiol | | | | | 120. α-Amyrin | |
| 121. 2,3-Dihydroxypropyl hexadecanoate | | | | | | | | | | |

There were 63 compounds in dandelion (Table s1-3), numbered 122-184, including 23 flavonoids, 14 terpenoids, 14 polyphenols, 7 coumarins and 5 pigments.

**Table S1-3 Statistics of small molecular compounds from dandelion**

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| 122. Luteolin | | | | 123. Quercetin | | | | | | 124. Isorhamnetin | |
| 125. Luteolin-7-O-β-D-glucoside | | 126. Luteolin-4’-O-β-D-glucoside | | | | | | 127. Luteolin-3’-O-β-D-glucoside | | | |
| 128. Luteolin- 7-O-β-D  -gentiobioside | | | 129. Luteolin-7-O-β-D- galactoside | | | | | | 130. Quercetin-3-O-β-D-  glucoside | | |
| 131. Quercetin-7-O-β-D- glucoside | | | 132. Quercetin-7,3’,4’- trimethyl ether | | | | | 133. Isorhamnetin-3-O-β-D -glucoside | | | |
| 134. Isorhamnetin-7-O-β-  D-glucoside | | | 135. Isorhamnetin-3,7-O-β-  D-diglucoside | | | | | | | | 136. Apigenin |
| 137. Diosmetin | | | 138. Rutinum | | | | | | | | 139. Hesperetin |
| 140. Hesperidin | | | 141. Genkwanin | | | | | | | | 142. Alquds |
| 143. Absinthin | | | 144. Artemetin | | | | | 145. Apigenin-7-O-β-D-glucoside | | | |
| 146. p-Hydroxybenzoic acid | | | 147. Protocatechuric acid | | | | | 148. Vanillic acid | | | |
| 149. 2,4-Dihyroxybenzoic acid | | | 150. Syringic acid | | | | | 151. p-Coumaric acid | | | |
| 152. Caffeic acid | 153. Ferulic acid | | | | | 154. Chicoric acid | | | | | |
| 155. Monocaffeoyltartaric acid | | 156. p-Hydorxyphenylacetic acid | | | | | 157. Chlorogenic acid | | | | |
| 158. Gallic acid | 159. Methyl gallate | | | | | | | 160. Esculetin | | | |
| 161. Taraxasteryl Acetate | 162. Lupeol acetate | | | | | | | 163. Taraxasterol | | | |
| 164. Stigmasterol | 165. Arnidiol | | | | | | | 166. φ-taraxasterol | | | |
| 167. φ-taraxasteryl acetate | 168. Lupenol | | | | | | | 169. Tarolupenol | | | |
| 170. Scopooletin | 171. Umbelliferone | | | | | | | 172. Cihoriin | | | |
| 173. Esculin | 174. Daphnetin | | | | | | | 175. Coumestrol | | | |
| 176. Sonchuside A | 177. Deacetylmatricarin | | | | | | | 178. Lettucenin A | | | |
| 179. Taraxacin | 180. Antheraxanthin | | | | | | | | | | |
| 181. Crytoxanthin | | | | | 182. Zeaxanthin | | | | | | |
| 183. Neoxanthin | | | | | 184. Deepoxyneoxanthin | | | | | | |

There are 31 compounds in artichoke (Table s1-4), numbered 185-215 respectively. Among them, 8 are flavonoids, 10 are terpenoids, and 13 are polyphenols.

**Table S1-4 Statistics of small molecular compounds from artichoke**

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| 185. Luteolin | 186. Apigenin | | | | 187. Luteolin-7-O-glucoside | | |
| 188. Narirutin | 189. Apigenin-7-O-rutinoside | | | | 190. Luteolin-7-O-beta-rutinoside | | |
| 191. Cyanidin-3-O-glucoside | 192. Cyanidin 3,5-O-diglucoside | | | | 193. Cynaropicrin | | |
| 194. Aguerin A | 195. Aguerin B | | | | 196. Grosheimin | | |
| 197. Cynartriol | 198. Cynaracoloside C | | | | 199. Cynarinin A | | |
| 200. Cynarinin B | 201. Ethyl Caffeate | | | | 202. Caffeic acid | | |
| 203. 1,3-Dicaffeoylquinic acid | | 204. 3,4-Dicaffeoylquinic acid | | 205. 3,5-Dicaffeoylquinic acid | | | |
| 206. 4,5-Dicaffeoylquinic acid | 207. 1,5-Dicaffeoylquinic acid | | | | | 208. Chlorogenic acid | |
| 209. Vanillic acid | 210. Protocatechuic aldehyde | | | | | 211. β-Sitosterol | |
| 212. Piresil-4-O-beta-D-glucopyraside | | | 213. Syringaresinol | | | | 214. 3-Hydroxy-2-naphthoic acid | |
| 215. Loganin | | | | | | | |

There are 39 compounds in Cirsium japonicum (Table s1-5), numbered 216-254, including 17 flavonoids and flavonoid glycosides, 6 terpenoids and sterols, and 16 long-chain enols and volatile oils.

**Table S1-5 Statistics of small molecular compounds from Cirsium japonicum**

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| 216. Hispidulin | | | | | | 217. Apigenin | | | | 218. Iuteolin | |
| 219. Pectolinarin | | | | | | 220. Acacetin | | | | 221. Quercetin | |
| 222. Tilianin | | | | | 223. Diosmetin | | | | 224. Linarin | | |
| 225. Pectolinarigenin | | | | | 226. Scrophulein | | | | 227. Tachioside | | |
| 228. Cirsimarin | | | | | 229. Ciryneol A | | | | 230.Ciryneol C | | |
| 231.Ciryneol B | | | | | 232.Ciryneol D | | | | 233.Ciryneol E | | |
| 234. Stigmasterol | | | | | 235. β-sitosterol | | | | 236. Daucosterol | | |
| 237. Pectolinarigenin | | | | | 238. Quercitrin | | | | 239. α-Amyrine | | |
| 240. β-Amyrine | | | | 241. Aplotaxene | | | | | | | 242. Cyperene |
| 243. β-Caryophyllene | | 244. Cedrene | | | | | | 245. 1-Pentadecene | | | |
| 246. Inulolide | | 247. α-Elemene | | | | | | 248. (-)-Germacrene D | | | |
| 249. α-Cadinene | 250. Lupenol acetate | | | | | | 251. cis-8,9-epoxy-heptadeca-1-ene-  11,13-diyne-10-ol | | | | |
| 252. 8,9,10-triacetoxy-heptadeca-1-ene-11,13-diyne | | | 253. Tilianin | | | | | | 254. Tracheloside | | |

There are 57 compounds in periploca forrestii schltr (Table s1-6), numbered 255-311, including 6 flavonoids and flavonoid glycosides, 20 terpenoids and sterols, 8 polyphenols, 3 cardiac glycosides, 3 coumarins, 4 anthraquinones, 3 fatty acids, 4 oligosaccharides and 6 others.

**Table S1-6 Statistics of small molecular compounds from periploca forrestii schltr**

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| 255. α-Amyrine | 256. α-Amyrin acetate | | | | | 257. β-Amyrin | | | |
| 258. β-Amyrin acetate | 259. Ursolic Acid | | | | | 260. β-sitosterol | | | |
| 261. Daucosterol | 262. Emodin | | | | | 263. Periplocymarin | | | |
| 264. Periplogenin | 265. Periplocin | | | | | 266. Emodinmono methyl ether | | | |
| 267. N-(4-ethoxy phenyl)-Acetamide | | | 268. 3-Propyl anisole | | | 269. Oleanolic acid | | | |
| 270. Scopoletin | 271. Kaempferol | | | | | 272. Quercetin | | | |
| 273. Palmitic acid | | 274. Cleomiscosin A | | | | | | | 275. Cleomiscosin B |
| 276. Vanillic acid | 277. Syringic acid | | | | | 278. (+)-Syringaresinol | | | |
| 279. Methyl 2,4-dihydroxybenzoate | 280. Emodin-8-O-β-D-  glucopyranoside | | | | | | 281. Physcion-8- glucoside | | |
| 282. Kaempferol-3-O-  galactoside | 283. Juglalin | | | | | | 284. Quercetin-3-O-β-  D-glucoside | | |
| 285. Guaijaverin | 286 Jacoumaric acid | | | | | | | 287. TanshinoneⅡA | |
| 288. Ethyl caffeate | 289. p-Cymene | | | | | | | 290. Linalool | |
| 291. Camphor | 292. Isomenthone | | | | | | | 293. Borneol | |
| 294. Menthol | 295. Terpinen-4-ol | | | | | | | 296. α-terpineol | |
| 297. Estragole | 298. Pulegone | | | | | | | 299. E-anethole | |
| 300. Eugenol | 301. Paeonal | | | | | | | 302. Myristicin | |
| 303. Nerolidol | 304. α-cedrol | | | | 305. 1-(3-methyl-2-butenoxy)-4-(1-propenyl)benzene | | | | |
| 306. Myristicacid | | | | 307. 9,12,15-Octadecatrienol | | | | | |
| 308. Periperoxide B | | | | 309. Periperoxide C | | | | | |
| 310. Periperoxide D | | | | 311. Periperoxide E | | | | | |