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SUPPLEMENTARY MATERIAL TO

# GC–MS characterisation and chemometric differentiation of volatile fractions from inflorescences of selected *Echinacea* and *Rudbeckia* species

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TABLE SI. Content of volatiles (%) from inflorescences of *Echinacea* and *Rudbeckia* spp.

| Compound | RI | RI Library | Content, % | | | | |
|---|---|---|---|---|---|---|---|
| | | | *E. purpurea* | *E. paradoxa* | *R. hirta* | *R. fulgida* | *R. laciniata* |
| Hexanal | 799 | 801 | 0.15 ± 0.01 | 0.29 ± 0.02 | 0.05 ± 0.00 | 0.10 ± 0.01 | 0.10 ± 0.01 |
| *(E)*-2-Hexenal | 848 | 854 | 0.04 ± 0.00 | 0.08 ± 0.00 | 0.05 ± 0.00 | 0.11 ± 0.02 | 0.03 ± 0.00 |
| **α-Pinene** | **932** | **932** | **9.28 ± 0.67** | **0.40 ± 0.02** | **0.13 ± 0.00** | **0.45 ± 0.05** | **0.62 ± 0.05** |
| **Camphene** | **947** | **952** | **9.28 ± 0.67** | **1.08 ± 0.06** | **0.35 ± 0.00** | **0.45 ± 0.06** | **0.89 ± 0.06** |
| 2,4-Thujadiene | 947 | 956 | 0.42 ± 0.02 | 0.36 ± 0.02 | 0.12 ± 0.00 | 0.15 ± 0.02 | 0.30 ± 0.02 |
| Methyl isohexyl ketone | 953 | 956 | 0.27 ± 0.01 | 0.14 ± 0.01 | 0.05 ± 0.00 | 0.01 ± 0.00 | 0.04 ± 0.00 |
| α-Sabinene | 972 | 974 | 1.38 ± 0.07 | 0.82 ± 0.05 | 0.41 ± 0.01 | 0.39 ± 0.06 | 3.49 ± 0.28 |
| **β-Pinene** | **975** | **978** | **1.98 ± 0.13** | **1.11 ± 0.07** | **0.46 ± 0.01** | **0.54 ± 0.07** | **5.51 ± 0.26** |
| Methyl heptenone | 986 | 986 | 0.04 ± 0.00 | 0.16 ± 0.01 | 0.06 ± 0.00 | 0.02 ± 0.00 | 0.05 ± 0.00 |
| β-Myrcene | 990 | 991 | 1.56 ± 0.60 | 0.23 ± 0.01 | 0.55 ± 0.01 | 0.61 ± 0.10 | 8.17 ± 0.65 |
| 2-Pentylfuran | 991 | 993 | 0.55 ± 0.02 | 1.64 ± 0.09 | 0.87 ± 0.01 | 0.57 ± 0.09 | 0.87 ± 0.07 |
| *(E)*-2-(1-Pentenyl)furan | 1001 | 1000 | 0.24 ± 0.02 | 0.06 ± 0.00 | 0.03 ± 0.00 | 0.02 ± 0.00 | 0.07 ± 0.00 |
| *(E,E)*-2,4-Heptadienal | 1009 | 1012 | 0.12 ± 0.01 | 0.31 ± 0.03 | 0.10 ± 0.00 | 0.07 ± 0.01 | 0.05 ± 0.00 |
| α-Terpinene | 1016 | 1017 | 0.40 ± 0.02 | 0.23 ± 0.19 | 0.26 ± 0.00 | 0.09 ± 0.13 | 0.15 ± 0.01 |
| **o-Cymene** | **1023** | **1022** | **11.98 ± 0.63** | **0.12 ± 0.01** | **0.08 ± 0.00** | **0.02 ± 0.00** | **0.64 ± 0.06** |
| β-Phellandrene | 1028 | 1031 | nd | 3.46 ± 0.31 | 2.44 ± 0.01 | 2.78 ± 0.40 | nd |
| **Limonene** | **1028** | **1031** | **1.43 ± 0.12** | **nd** | **nd** | **nd** | **14.63 ± 0.64** |
| Hyacinthin | 1042 | 1045 | 0.31 ± 0.02 | 0.92 ± 0.07 | 0.19 ± 0.01 | nd | nd |
| γ-Terpinene | 1057 | 1060 | nd | 0.04 ± 0.00 | 0.02 ± 0.00 | nd | nd |
| α-Terpinolene | 1087 | 1088 | 0.04 ± 0.01 | 0.01 ± 0.00 | 1.16 ± 0.03 | 0.01 ± 0.00 | 0.06 ± 0.00 |
| Linalool | 1098 | 1099 | 0.04 ± 0.00 | 0.20 ± 0.01 | 4.04 ± 0.10 | 0.02 ± 0.00 | 0.43 ± 0.03 |
| Perillene | 1100 | 1101 | 0.10 ± 0.01 | 0.07 ± 0.01 | 1.67 ± 0.04 | 0.02 ± 0.00 | 0.58 ± 0.04 |
| Pelargonaldehyde | 1103 | 1104 | 0.07 ± 0.00 | 0.49 ± 0.02 | 0.10 ± 0.01 | 0.30 ± 0.04 | 0.10 ± 0.01 |
| *(Z)*-p-Menthen-2-en-1-ol | 1119 | 1122 | 0.04 ± 0.00 | 0.04 ± 0.00 | 2.13 ± 0.03 | 0.02 ± 0.00 | 0.15 ± 0.01 |
| α-Campholenal | 1124 | 1125 | 1.08 ± 0.09 | 0.02 ± 0.00 | 0.01 ± 0.00 | nd | 0.03 ± 0.00 |
| *(E)*-p-2-Menthen-1-ol | 1137 | 1140 | 0.34 ± 0.02 | 0.03 ± 0.00 | 0.01 ± 0.00 | nd | 0.14 ± 0.01 |
| *(Z)*-Verbenol | 1139 | 1140 | 0.25 ± 0.02 | nd | 0.01 ± 0.00 | nd | 0.01 ± 0.00 |
| *(E)*-Verbenol | 1143 | 1144 | 1.65 ± 0.10 | 0.02 ± 0.00 | 0.01 ± 0.00 | nd | 0.04 ± 0.00 |
| Cucumber aldehyde | 1151 | 1155 | 0.54 ± 0.07 | 0.12 ± 0.00 | 0.07 ± 0.00 | 0.07 ± 0.01 | 0.12 ± 0.00 |
| *(E)*-2-Nonenal | 1158 | 1162 | 0.02 ± 0.00 | 0.15 ± 0.01 | 0.08 ± 0.00 | 0.06 ± 0.01 | 0.08 ± 0.00 |
| Pinocarvone | 1161 | 1162 | 0.31 ± 0.02 | 0.03 ± 0.00 | 0.01 ± 0.00 | nd | 0.14 ± 0.01 |
| p-Mentha-1,5-dien-8-ol | 1165 | 1167 | 0.30 ± 0.03 | 0.01 ± 0.00 | 0.01 ± 0.00 | nd | 0.04 ± 0.00 |
| Terpinen-4-ol | 1175 | 1177 | 0.09 ± 0.00 | 0.04 ± 0.00 | 0.02 ± 0.00 | 0.01 ± 0.00 | 0.40 ± 0.02 |
| Melilotal | 1182 | 1183 | 0.08 ± 0.01 | 0.23 ± 0.01 | 0.05 ± 0.00 | 0.01 ± 0.00 | 0.02 ± 0.00 |
| Dill ether | 1184 | 1185 | 0.01 ± 0.00 | 0.01 ± 0.00 | 0.27 ± 0.00 | nd | 0.01 ± 0.00 |
| Cryptone | 1184 | 1184 | 0.02 ± 0.00 | 0.15 ± 0.01 | 0.05 ± 0.00 | 0.01 ± 0.00 | 1.16 ± 0.05 |
| α-Terpineol | 1189 | 1190 | 0.12 ± 0.01 | 0.02 ± 0.00 | 0.03 ± 0.00 | nd | 0.14 ± 0.01 |
| Myrtenal | 1194 | 1193 | 0.79 ± 0.04 | 0.07 ± 0.00 | 0.04 ± 0.00 | nd | 0.34 ± 0.03 |
| β-Safranal | 1198 | 1201 | 0.13 ± 0.16 | 0.25 ± 0.01 | 0.23 ± 0.00 | 0.02 ± 0.00 | 0.18 ± 0.01 |
| Caprinaldehyde | 1204 | 1206 | 0.04 ± 0.00 | 0.18 ± 0.01 | 0.08 ± 0.00 | 0.07 ± 0.01 | 0.21 ± 0.01 |
| *(E)*-Carveol | 1217 | 1217 | 0.43 ± 0.03 | 0.05 ± 0.00 | 0.07 ± 0.00 | nd | 0.03 ± 0.00 |
| Cuminaldehyde | 1238 | 1239 | 0.04 ± 0.00 | 0.10 ± 0.01 | 0.05 ± 0.00 | nd | 1.62 ± 0.10 |
| Carvone | 1242 | 1242 | 0.40 ± 0.03 | 0.07 ± 0.00 | 0.56 ± 0.01 | 0.01 ± 0.00 | 0.10 ± 0.00 |
| Piperitone | 1253 | 1253 | 0.05 ± 0.00 | 0.01 ± 0.00 | 0.56 ± 0.01 | nd | 0.04 ± 0.00 |
| Phellandral | 1273 | 1276 | 0.01 ± 0.00 | 0.05 ± 0.00 | 0.02 ± 0.00 | 0.06 ± 0.01 | 0.79 ± 0.07 |

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|---|---|---|---|---|---|---|---|
| | | | *E. purpurea* | *E. paradoxa* | *R. hirta* | *R. fulgida* | *R. laciniata* |
| Bornyl acetate | 1285 | 1285 | nd | 1.53 ± 0.07 | 0.71 ± 0.01 | 0.44 ± 0.04 | 2.55 ± 0.18 |
| *(E,Z)*-2,4-Decadienal | 1292 | 1295 | 0.05 ± 0.00 | 0.22 ± 0.01 | 0.07 ± 0.00 | 0.08 ± 0.01 | 0.05 ± 0.00 |
| Carvacrol | 1300 | 1299 | 0.95 ± 0.03 | 0.02 ± 0.00 | 0.03 ± 0.00 | nd | 0.04 ± 0.00 |
| Undecyl aldehyde | 1305 | 1307 | nd | 0.03 ± 0.00 | 0.01 ± 0.00 | 0.01 ± 0.00 | 0.03 ± 0.00 |
| *(E,E)*-2,4-Decadienal | 1315 | 1317 | 0.21 ± 0.02 | 0.73 ± 0.02 | 0.25 ± 0.00 | 0.28 ± 0.04 | 0.28 ± 0.02 |
| δ-Eiemene | 1337 | 1338 | 0.59 ± 0.02 | 0.67 ± 0.02 | 0.96 ± 0.01 | 4.76 ± 0.81 | 0.26 ± 0.01 |
| α-Cubebene | 1350 | 1351 | 0.11 ± 0.01 | 0.04 ± 0.00 | 0.06 ± 0.00 | 1.64 ± 0.29 | 0.26 ± 0.01 |
| Ylangene | 1372 | 1372 | 0.03 ± 0.00 | 0.19 ± 0.01 | 0.17 ± 0.01 | 0.07 ± 0.01 | 0.10 ± 0.01 |
| α-Copaene | 1376 | 1376 | 0.45 ± 0.03 | 0.16 ± 0.02 | 0.13 ± 0.00 | 0.09 ± 0.02 | 0.12 ± 0.01 |
| Daucene | 1380 | 1380 | 0.45 ± 0.03 | 0.08 ± 0.01 | 0.16 ± 0.00 | 0.10 ± 0.02 | 0.12 ± 0.01 |
| β-Elemene | 1393 | 1391 | 0.56 ± 0.05 | 0.81 ± 0.04 | 0.85 ± 0.02 | 1.00 ± 0.15 | 0.23 ± 0.02 |
| **β-Copaene** | **1431** | **1432** | **4.18 ± 0.31** | **2.18 ± 0.13** | **3.96 ± 0.02** | **8.89 ± 1.39** | **4.22 ± 0.32** |
| γ-Elemene | 1435 | 1434 | 0.42 ± 0.02 | 0.29 ± 0.04 | 0.35 ± 0.01 | 1.19 ± 0.35 | 0.14 ± 0.01 |
| ***(E)*-α-Bergamotene** | **1439** | **1435** | **0.18 ± 0.01** | **8.51 ± 0.45** | **4.17 ± 0.09** | **4.64 ± 0.71** | **0.65 ± 0.03** |
| Isogermacrene D | 1447 | 1448 | 0.93 ± 0.03 | 0.36 ± 0.02 | 0.78 ± 0.03 | 2.06 ± 0.29 | 0.87 ± 0.05 |
| β-Santalene | 1462 | 1461 | 0.02 ± 0.00 | 0.54 ± 0.04 | 0.10 ± 0.01 | 0.32 ± 0.04 | 0.25 ± 0.01 |
| *(Z)*-Muurola-4(15),5-diene | 1467 | 1463 | 0.84 ± 0.38 | 0.57 ± 0.02 | 1.15 ± 0.08 | 1.29 ± 0.22 | 1.02 ± 0.36 |
| **Germacrene D** | **1486** | **1489** | **9.98 ± 5.53** | **8.94 ± 0.28** | **16.55 ± 0.03** | **16.39 ± 5.70** | **12.49 ± 4.66** |
| **Eremophilene** | **1485** | **1494** | **0.79 ± 0.54** | **2.33 ± 3.22** | **9.22 ± 0.06** | **10.23 ± 1.47** | **7.75 ± 0.35** |
| α-Muurolene | 1501 | 1499 | 0.86 ± 0.06 | 0.55 ± 0.03 | 0.85 ± 0.02 | 5.71 ± 3.47 | 0.88 ± 0.08 |
| Cubebol | 1497 | 1493 | 1.50 ± 0.10 | 0.05 ± 0.00 | 0.07 ± 0.00 | 0.04 ± 0.01 | 0.11 ± 0.00 |
| γ-Amorphene | 1501 | 1496 | 1.11 ± 0.16 | 0.56 ± 0.03 | 0.85 ± 0.02 | 2.03 ± 0.36 | 0.88 ± 0.08 |
| γ-Cadinene | 1517 | 1513 | 1.01 ± 0.21 | 0.75 ± 0.02 | 0.85 ± 0.01 | 2.08 ± 0.33 | 0.88 ± 0.08 |
| Tridecane aldehyde | 1511 | 1512 | 0.35 ± 0.27 | 0.50 ± 0.02 | 0.22 ± 0.00 | 0.14 ± 0.02 | 0.02 ± 0.00 |
| δ-Cadinene | 1526 | 1524 | 0.17 ± 0.01 | 1.15 ± 0.04 | 0.56 ± 0.03 | 0.09 ± 0.00 | 0.09 ± 0.01 |
| α-Amorphene | 1526 | 1526 | 3.54 ± 0.19 | 0.64 ± 0.04 | 0.68 ± 0.02 | 0.53 ± 0.07 | 0.69 ± 0.04 |
| α-Cadinene | 1540 | 1538 | 0.12 ± 0.01 | 0.16 ± 0.02 | 0.09 ± 0.00 | 0.04 ± 0.00 | 0.08 ± 0.00 |
| α-Calacorene | 1546 | 1542 | 0.35 ± 0.02 | 0.66 ± 0.04 | 0.43 ± 0.02 | 0.07 ± 0.01 | 0.09 ± 0.01 |
| Trimethylbicycloheptyl butenone | 1557 | 1558 | 0.62 ± 0.05 | 0.51 ± 0.02 | 0.51 ± 0.00 | 0.11 ± 0.02 | 0.48 ± 0.04 |
| Mint oxide | 1570 | 1573 | 0.42 ± 0.03 | 0.69 ± 0.03 | 0.48 ± 0.01 | 0.11 ± 0.02 | 0.23 ± 0.02 |
| *(E)*-Nerolidol | 1569 | 1564 | 1.78 ± 0.20 | 0.19 ± 0.01 | 0.11 ± 0.01 | 0.03 ± 0.01 | 0.05 ± 0.01 |
| Spathulenol | 1583 | 1577 | 1.15 ± 0.07 | 2.58 ± 0.02 | 0.76 ± 0.00 | 0.17 ± 0.02 | 0.46 ± 0.03 |
| Caryophyllene oxide | 1588 | 1581 | 0.69 ± 0.48 | 1.36 ± 0.10 | 1.04 ± 0.17 | 0.21 ± 0.03 | 0.85 ± 0.05 |
| Salvial-4(14)-en-1-one | 1599 | 1595 | 1.98 ± 0.16 | 7.08 ± 0.23 | 6.21 ± 0.08 | 1.87 ± 0.31 | 1.27 ± 0.09 |
| Junenol | 1623 | 1620 | 0.31 ± 0.07 | 0.09 ± 0.01 | 0.11 ± 0.05 | 0.05 ± 0.01 | 0.10 ± 0.01 |
| Isospathulenol | 1635 | 1638 | 0.48 ± 0.07 | 1.29 ± 0.25 | 0.63 ± 0.15 | 0.32 ± 0.04 | 0.07 ± 0.02 |
| epi-α-Cubenol | 1632 | 1627 | 0.48 ± 0.07 | 1.29 ± 0.25 | 0.59 ± 0.10 | 0.32 ± 0.04 | 0.05 ± 0.03 |
| 1,7-Diepi-α-cedrenol | 1648 | 1639 | 0.13 ± 0.04 | 0.73 ± 0.52 | 0.11 ± 0.05 | 0.05 ± 0.00 | 0.21 ± 0.05 |
| t-Cadinol | 1646 | 1640 | 1.69 ± 0.13 | 1.13 ± 0.04 | 0.44 ± 0.02 | 1.08 ± 0.16 | 0.32 ± 0.01 |
| α-Muurolol | 1652 | 1645 | 0.39 ± 0.08 | 0.18 ± 0.03 | 0.14 ± 0.01 | 0.07 ± 0.01 | 0.16 ± 0.01 |
| **α–Cadinol** | **1660** | **1653** | **0.80 ± 0.12** | **7.34 ± 0.21** | **5.34 ± 0.10** | **0.65 ± 0.08** | **0.29 ± 0.05** |
| ent-Germacra-4(15),5,10(14)-trien-1β-ol | 1692 | 1690 | 0.33 ± 0.13 | 1.96 ± 0.11 | 1.76 ± 0.06 | 0.61 ± 0.09 | 1.55 ± 0.14 |
| Shyobunol | 1697 | 1699 | 0.58 ± 0.03 | 0.10 ± 0.04 | 0.07 ± 0.00 | 0.01 ± 0.01 | nd |
| n-Pentadecanal | 1715 | 1715 | 0.05 ± 0.00 | 0.27 ± 0.01 | 0.15 ± 0.03 | 0.10 ± 0.01 | 0.03 ± 0.00 |

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| Compound | RI | RI Library | Content, % | | | | |
|---|---|---|---|---|---|---|---|
| | | | *E. purpurea* | *E. paradoxa* | *R. hirta* | *R. fulgida* | *R. laciniata* |
| α-Mintsulfide | 1742 | 1742 | 0.08 ± 0.01 | 0.12 ± 0.01 | 0.10 ± 0.03 | 0.12 ± 0.02 | 0.89 ± 0.06 |
| Isobicyclogermacrenal | 1745 | 1737 | 0.22 ± 0.01 | 0.19 ± 0.03 | 0.16 ± 0.01 | 0.04 ± 0.01 | 0.05 ± 0.00 |
| Xanthorrhizol | 1754 | 1752 | 0.03 ± 0.01 | 1.38 ± 0.13 | 0.30 ± 0.01 | 0.35 ± 0.06 | 0.05 ± 0.01 |
| Myristic acid | 1770 | 1768 | 0.14 ± 0.01 | nd | nd | nd | 0.61 ± 0.04 |
| α-Muurolene-14-ol | 1780 | 1777 | 0.27 ± 0.02 | 0.30 ± 0.01 | 0.25 ± 0.01 | 0.10 ± 0.02 | 0.16 ± 0.01 |
| 14-Hydroxy-δ-cadinene | 1805 | 1803 | 0.55 ± 0.03 | 0.53 ± 0.02 | 0.47 ± 0.01 | 0.19 ± 0.04 | 0.21 ± 0.02 |
| **Perhydrofarnesyl acetone** | **1850** | **1844** | **0.38 ± 0.02** | **6.62 ± 0.32** | **2.16 ± 0.03** | **2.00 ± 0.28** | **0.39 ± 0.03** |
| Benzyl salicylate | 1878 | 1871 | 0.59 ± 0.04 | 0.08 ± 0.00 | 0.07 ± 0.00 | 0.07 ± 0.01 | 0.19 ± 0.01 |
| Heptadecanal | 1926 | 1921 | 0.37 ± 0.03 | 0.30 ± 0.01 | 0.13 ± 0.00 | 0.06 ± 0.01 | 0.04 ± 0.00 |
| n-Hexadecanoic acid | 1970 | 1968 | 1.63 ± 1.41 | 0.77 ± 0.19 | 1.43 ± 0.05 | 0.39 ± 0.05 | 1.44 ± 1.18 |
| Geranyllinalool | 2030 | 2034 | 0.02 ± 0.00 | 0.06 ± 0.00 | 0.34 ± 0.00 | 0.11 ± 0.02 | 0.22 ± 0.02 |
| Kaurene | 2042 | 2040 | 0.01 ± 0.00 | 0.04 ± 0.00 | 0.59 ± 0.01 | 0.21 ± 0.03 | nd |
| Stearyl alcohol | 2083 | 2082 | 0.01 ± 0.00 | 0.17 ± 0.01 | 0.06 ± 0.04 | 0.24 ± 0.03 | 0.02 ± 0.02 |
| Phytol | 2113 | 2114 | 0.19 ± 0.01 | 1.92 ± 0.05 | 1.05 ± 0.02 | 0.70 ± 0.09 | 0.10 ± 0.01 |
| Hexacosane | 2594 | 2600 | 0.79 ± 0.05 | 3.42 ± 0.09 | 2.70 ± 0.03 | 0.75 ± 0.12 | 1.32 ± 0.07 |
| Monoterpene hydrocarbons | | | 37.85 | 7.93 | 7.65 | 5.51 | 35.04 |
| Oxygenated monoterpenes | | | 7.50 | 3.38 | 9.38 | 0.76 | 7.09 |
| Sesquiterpene hydrocarbons | | | 26.69 | 30.14 | 38.75 | 63.22 | 32.07 |
| Oxygenated sesquiterpenes | | | 13.14 | 27.58 | 18.40 | 6.12 | 5.91 |
| Other compounds* | | | 7.36 | 17.33 | 9.05 | 6.01 | 8.10 |
| Yield of volatile fractions, % (v/w) | | | 0.62 | 0.18 | 0.53 | 0.12 | 0.12 |

Values represent mean ± SD (n = 3). Bold - 5% and more; nd - not detected; *Including aliphatic aldehydes, ketones, furans, fatty acids, diterpenoids, long-chain hydrocarbons and other minor non-terpenoid constituents.

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