# Qualitative Compound Report

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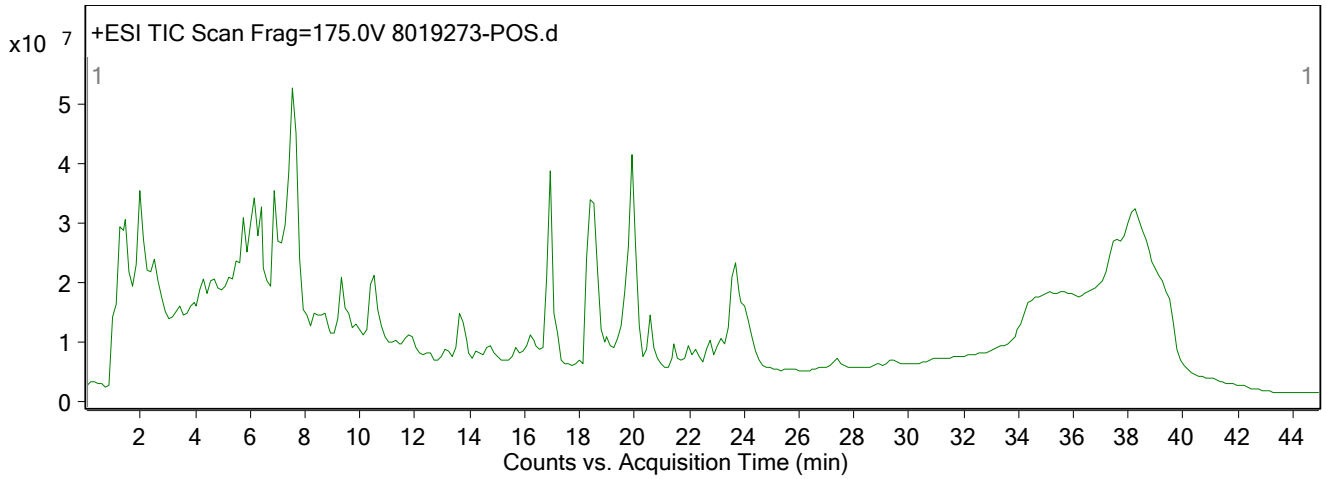
|---|---|---|---|
| **Data File** | 8019273-POS.d | **Sample Name** | 8019273-POS |
| **Sample Type** | Sample | **Position** | P1-D6 |
| **Instrument Name** | Instrument 1 | **User Name** | |
| **Acq Method** | 30min-POSi.m | **Acquired Time** | 8/19/2024 3:38:37 PM |
| **IRM Calibration Status** | Success | **DA Method** | Default.m |
| **Comment** | | | |
| **Sample Group** | | **Info.** | |
| **Stream Name** | LC 1 | **Acquisition SW Version** | 6200 series TOF/6500 series Q-TOF B.09.00 (B9044.0) |

**Fragmentor Voltage** 175 **Collision Energy** 0 **Ionization Mode** ESI




**Compound Table**

| Compound Label | RT | Mass | Abund | Name | Formula | Tgt Mass | Diff (ppm) | DB Diff (ppm) |
|---|---|---|---|---|---|---|---|---|
| Cpd 9: Boschnialactone | 0.568 | 154.0987 | 106251 | Boschnialactone | C9 H14 O2 | 154.0994 | -4.23 | 4.23 |
| Cpd 169: Watterose E | 0.955 | 1192.3456 | 13744 | Watterose E | C54 H64 O30 | 1192.3482 | -2.2 | 2.2 |
| Cpd 161: Gomphrenin III | 0.955 | 696.1793 | 16087 | Gomphrenin III | C33 H32 N2 O15 | 696.1803 | -1.43 | 1.43 |
| Cpd 34: Miserotoxin | 1.213 | 267.0969 | 1789479 | Miserotoxin | C9 H17 N O8 | 267.0954 | 5.36 | -5.36 |
| Cpd 35: Adenosine | 1.213 | 267.0969 | 1789479 | Adenosine | C10 H13 N5 O4 | 267.0968 | 0.67 | -0.67 |
| Cpd 29: Thymidine | 1.342 | 242.0904 | 1056994 | Thymidine | C10 H14 N2 O5 | 242.0903 | 0.5 | -0.5 |
| Cpd 10: (+/-)-Anabasine | 1.471 | 162.1153 | 288347 | (+/-)-Anabasine | C10 H14 N2 | 162.1157 | -2.3 | 2.3 |
| Cpd 2: 4-Hydroxymethyl-2-furaldehyde | 1.729 | 126.0316 | 588014 | 4-Hydroxymethyl-2-furaldehyde | C6 H6 O3 | 126.0317 | -1.07 | 1.07 |
| Cpd 6: Actinidine | 2.374 | 147.1048 | 298927 | Actinidine | C10 H13 N | 147.1048 | -0.22 | 0.22 |
| Cpd 67: 7-Hydroxy-3,6-bis(tigloyloxy)tropane | 2.503 | 337.1888 | 43407 | 7-Hydroxy-3,6-bis(tigloyloxy)tropane | C18 H27 N O5 | 337.1889 | -0.27 | 0.27 |
| Cpd 117: Diacetoxytetrahydroxytaxadiene | 2.631 | 452.2396 | 47312 | Diacetoxytetrahydroxytaxadiene | C24 H36 O8 | 452.241 | -3.16 | 3.16 |
| Cpd 93: Trimethyl ester dehydrochebulic acid | 2.889 | 396.0684 | 16031 | Trimethyl ester dehydrochebulic acid | C17 H16 O11 | 396.0693 | -2.16 | 2.16 |
| Cpd 107: Thamnolic acid | 3.147 | 420.0682 | 9324 | Thamnolic acid | C19 H16 O11 | 420.0693 | -2.48 | 2.48 |
| Cpd 24: Bufotenidine | 3.276 | 218.1405 | 15584 | Bufotenidine | C13 H18 N2 O | 218.1419 | -6.62 | 6.62 |
| Cpd 56: Lotusine | 3.405 | 314.1766 | 478234 | Lotusine | C19 H24 N O3 | 314.1756 | 3.27 | -3.27 |
| Cpd 134: 5-Methylcoumarin-4-cellobioside | 3.405 | 500.1528 | 123353 | 5-Methylcoumarin-4-cellobioside | C22 H28 O13 | 500.153 | -0.36 | 0.36 |
| Cpd 55: 3-Epischelhammericine | 3.405 | 313.1688 | 478234 | 3-Epischelhammericine | C19 H23 N O3 | 313.1678 | 3.3 | -3.3 |
| Cpd 160: Triptofordin F1 | 3.405 | 694.261 | 49371 | Triptofordin F1 | C37 H42 O13 | 694.2625 | -2.16 | 2.16 |
| Cpd 16: Aucubigenin | 3.405 | 184.0738 | 69864 | Aucubigenin | C9 H12 O4 | 184.0736 | 1.51 | -1.51 |
| Cpd 72: Trichodesmine | 3.534 | 349.2259 | 23600 | Trichodesmine | C20 H31 N O4 | 349.2253 | 1.82 | -1.82 |
| Cpd 127: Mingjinianuronide A | 3.534 | 478.074 | 9126 | Mingjinianuronide A | C21 H18 O13 | 478.0747 | -1.48 | 1.48 |
| Cpd 38: alpha-Obscurine | 3.663 | 274.2047 | 68296 | alpha-Obscurine | C17 H26 N2 O | 274.2045 | 0.83 | -0.83 |
| Cpd 58: L-3alpha,6beta-Ditigloyloxytropane | 3.663 | 321.195 | 462810 | L-3alpha,6beta-Ditigloyloxytropane | C18 H27 N O4 | 321.194 | 3 | -3 |
| Cpd 14: Muscarine II | 3.663 | 174.1493 | 83423 | Muscarine II | C9 H20 N O2 | 174.1494 | -0.64 | 0.64 |
| Cpd 21: Spermine | 3.921 | 202.2159 | 6977 | Spermine | C10 H26 N4 | 202.2158 | 0.97 | -0.97 |
| Cpd 19: Gentianol | 3.921 | 193.0743 | 887599 | Gentianol | C10 H11 N O3 | 193.0739 | 2.34 | -2.34 |
| Cpd 53: (2,3)trans-N-(p-Hydroxyphenethyl)ferulamide | 4.179 | 313.1325 | 438923 | (2,3)trans-N-(p-Hydroxyphenethyl)ferulamide | C18 H19 N O4 | 313.1314 | 3.64 | -3.64 |
| Cpd 33: Clavatine | 4.308 | 263.1891 | 103353 | Clavatine | C16 H25 N O2 | 263.1885 | 2.35 | -2.35 |
| Cpd 51: Fulvine | 4.308 | 309.1589 | 516868 | Fulvine | C16 H23 N O5 | 309.1576 | 3.99 | -3.99 |
| Cpd 108: 6-Methoxyl-2-acetyl-3-methyl-1,4-naphthoquinone-8-O-beta-D-glucopyranoside | 4.695 | 422.1209 | 377728 | 6-Methoxyl-2-acetyl-3-methyl-1,4-naphthoquinone-8-O-beta-D-glucopyranoside | C20 H22 O10 | 422.1213 | -1 | 1 |
| Cpd 12: Norharman | 4.824 | 168.0695 | 33880 | Norharman | C11 H8 N2 | 168.0688 | 4.58 | -4.58 |

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|---|---|---|---|---|---|---|---|---|
| Cpd 133: Strictosamide | 4.953 | 498.1998 | 150961 | Strictosamide | C26 H30 N2 O8 | 498.2002 | -0.91 | 0.91 |
| Cpd 116: (+)-Catechin-5-O-glucoside | 4.953 | 452.1316 | 88915 | (+)-Catechin-5-O-glucoside | C21 H24 O11 | 452.1319 | -0.49 | 0.49 |
| Cpd 41: N-Methyldendrobium | 5.082 | 278.2131 | 668913 | N-Methyldendrobium | C17 H28 N O2 | 278.212 | 4.01 | -4.01 |
| Cpd 39: Stenine | 5.082 | 277.2053 | 668913 | Stenine | C17 H27 N O2 | 277.2042 | 4.01 | -4.01 |
| Cpd 54: 3-Epischelhammericine | 5.211 | 313.1693 | 289489 | 3-Epischelhammericine | C19 H23 N O3 | 313.1678 | 4.74 | -4.74 |
| Cpd 129: Torachrysone-8-O-beta-D-(6'-oxayl)-glucoside | 5.469 | 480.1271 | 84837 | Torachrysone-8-O-beta-D-(6'-oxayl)-glucoside | C22 H24 O12 | 480.1268 | 0.76 | -0.76 |
| Cpd 125: Gyrophoric acid | 5.598 | 468.1057 | 57227 | Gyrophoric acid | C24 H20 O10 | 468.1057 | 0.03 | -0.03 |
| Cpd 32: 2,4,4'-Trihydroxychalcone | 5.727 | 256.0749 | 513049 | 2,4,4'-Trihydroxychalcone | C15 H12 O4 | 256.0736 | 5.31 | -5.31 |
| Cpd 126: Holantosine D | 5.727 | 475.3285 | 559769 | Holantosine D | C28 H45 N O5 | 475.3298 | -2.65 | 2.65 |
| Cpd 18: beta-Ionone | 5.727 | 192.1522 | 152955 | beta-Ionone | C13 H20 O | 192.1514 | 4.05 | -4.05 |
| Cpd 141: Ipobscurine B | 5.856 | 518.2058 | 352465 | Ipobscurine B | C29 H30 N2 O7 | 518.2053 | 0.96 | -0.96 |
| Cpd 73: Ethyl-m-digallate | 5.985 | 350.0632 | 15265 | Ethyl-m-digallate | C16 H14 O9 | 350.0638 | -1.54 | 1.54 |
| Cpd 132: 2'-(o,m-Dihydroxybenzyl) sweroside | 6.114 | 494.1433 | 41734 | 2'-(o,m-Dihydroxybenzyl) sweroside | C23 H26 O12 | 494.1424 | 1.69 | -1.69 |
| Cpd 91: Karacolidine | 6.114 | 393.2532 | 351889 | Karacolidine | C22 H35 N O5 | 393.2515 | 4.36 | -4.36 |
| Cpd 71: (S)-trans-Cyclanoline | 6.114 | 342.1718 | 126163 | (S)-trans-Cyclanoline | C20 H24 N O4 | 342.1705 | 3.82 | -3.82 |
| Cpd 69: (+)-N-Methyl laurotetanine | 6.114 | 341.164 | 98661 | (+)-N-Methyl laurotetanine | C20 H23 N O4 | 341.1627 | 3.67 | -3.67 |
| Cpd 122: 3'-Methyl eriodictyol-7-O-beta-D-glucoside | 6.372 | 464.1318 | 813446 | 3'-Methyl eriodictyol-7-O-beta-D-glucoside | C22 H24 O11 | 464.1319 | -0.06 | 0.06 |
| Cpd 1: Coumarone | 6.372 | 118.0421 | 505109 | Coumarone | C8 H6 O | 118.0419 | 1.72 | -1.72 |
| Cpd 113: 15alpha-Hydroxysoladulcidine | 6.372 | 431.3418 | 131626 | 15alpha-Hydroxysoladulcidine | C27 H45 N O3 | 431.3399 | 4.2 | -4.2 |
| Cpd 5: Coumarin | 6.372 | 146.0371 | 915913 | Coumarin | C9 H6 O2 | 146.0368 | 2.17 | -2.17 |
| Cpd 43: Zhebeiresinol | 6.372 | 280.0959 | 382133 | Zhebeiresinol | C14 H16 O6 | 280.0947 | 4.15 | -4.15 |
| Cpd 52: 19-(Z)-Taberpsychine | 6.501 | 310.204 | 14518 | 19-(Z)-Taberpsychine | C20 H26 N2 O | 310.2045 | -1.58 | 1.58 |
| Cpd 25: Armillarisin A | 6.63 | 234.0537 | 680212 | Armillarisin A | C12 H10 O5 | 234.0528 | 3.79 | -3.79 |
| Cpd 110: Ebracteolatinoside A | 6.63 | 425.0978 | 241968 | Ebracteolatinoside A | C18 H19 N O11 | 425.0958 | 4.77 | -4.77 |
| Cpd 131: 2'-(o,m-Dihydroxybenzyl) sweroside | 6.759 | 494.1426 | 54838 | 2'-(o,m-Dihydroxybenzyl) sweroside | C23 H26 O12 | 494.1424 | 0.41 | -0.41 |
| Cpd 75: Chelidonine | 6.759 | 353.128 | 155545 | Chelidonine | C20 H19 N O5 | 353.1263 | 4.72 | -4.72 |
| Cpd 82: Eckol | 6.888 | 372.0472 | 18424 | Eckol | C18 H12 O9 | 372.0481 | -2.55 | 2.55 |
| Cpd 68: Cassythidine | 7.275 | 339.1103 | 55789 | Cassythidine | C19 H17 N O5 | 339.1107 | -1.13 | 1.13 |
| Cpd 81: Allocryptopine | 7.275 | 369.1595 | 129224 | Allocryptopine | C21 H23 N O5 | 369.1576 | 5 | -5 |
| Cpd 86: Carmichaeline | 7.404 | 377.2576 | 149128 | Carmichaeline | C22 H35 N O4 | 377.2566 | 2.72 | -2.72 |
| Cpd 77: (S)-trans-N-Methyltetrahydrocolumbamine | 7.533 | 356.1881 | 269742 | (S)-trans-N-Methyltetrahydrocolumbamine | C21 H26 N O4 | 356.1862 | 5.27 | -5.27 |
| Cpd 76: (-)-Argemonine | 7.533 | 355.1802 | 269742 | (-)-Argemonine | C21 H25 N O4 | 355.1784 | 5.28 | -5.28 |
| Cpd 121: Spiropachysine | 7.92 | 462.3604 | 27113 | Spiropachysine | C31 H46 N2 O | 462.361 | -1.26 | 1.26 |
| Cpd 59: m-Digallic acid | 8.048 | 322.0309 | 7550 | m-Digallic acid | C14 H10 O9 | 322.0325 | -5 | 5 |
| Cpd 49: Angustidine | 8.177 | 301.1224 | 104989 | Angustidine | C19 H15 N3 O | 301.1215 | 2.9 | -2.9 |
| Cpd 37: 7-Methoxy-4'-hydroxyflavone | 8.306 | 268.0745 | 284650 | 7-Methoxy-4'-hydroxyflavone | C16 H12 O4 | 268.0736 | 3.54 | -3.54 |
| Cpd 105: Delavine | 8.564 | 415.3463 | 8350 | Delavine | C27 H45 N O2 | 415.345 | 3.13 | -3.13 |
| Cpd 162: Marinobufagin 3-suberoyl-L-glutamine ester | 8.693 | 718.3564 | 25363 | Marinobufagin 3-suberoyl-L-glutamine ester | C38 H54 O13 | 718.3564 | -0.07 | 0.07 |
| Cpd 28: 1,2,3,3alpha,8,8alpha-Hexahydro-2,2,8-trimethyl-5,6-azulenedimethanol | 8.693 | 236.1786 | 153913 | 1,2,3,3alpha,8,8alpha-Hexahydro-2,2,8-trimethyl-5,6-azulenedimethanol | C15 H24 O2 | 236.1776 | 4.24 | -4.24 |
| Cpd 46: Nuciferine | 8.951 | 295.1584 | 158763 | Nuciferine | C19 H21 N O2 | 295.1572 | 4.11 | -4.11 |
| Cpd 137: 5-Hydroxy-6,7,3-trimethoxyflavone-8-O-beta-D-glucoside | 8.951 | 506.1427 | 24352 | 5-Hydroxy-6,7,3-trimethoxyflavone-8-O-beta-D-glucoside | C24 H26 O12 | 506.1424 | 0.46 | -0.46 |
| Cpd 164: 7-Epi-10-deacetyltaxuyunnanine A | 9.08 | 805.3658 | 51616 | 7-Epi-10-deacetyltaxuyunnanine A | C44 H55 N O13 | 805.3673 | -1.95 | 1.95 |
| Cpd 142: 6-p-Methoxycinnamoyl catalpol | 9.209 | 522.1735 | 71733 | 6-p-Methoxycinnamoyl catalpol | C25 H30 O12 | 522.1737 | -0.52 | 0.52 |
| Cpd 66: Berberine | 9.338 | 336.125 | 713034 | Berberine | C20 H18 N O4 | 336.1236 | 4.37 | -4.37 |
| Cpd 140: 5alpha,6beta,7be8alpha-Tetraacetoxy-2-[2-(4?methoxyphenyl)ethyl]-5,6,7,8-tetrahydro-chromone (AH1a) | 9.338 | 516.1629 | 239821 | 5alpha,6beta,7be8alpha-Tetraacetoxy-2-[2-(4?methoxyphenyl)ethyl]-5,6,7,8-tetrahydro-chromone (AH1a) | C26 H28 O11 | 516.1632 | -0.41 | 0.41 |
| Cpd 163: Cinobufotoxin | 9.338 | 754.4156 | 21161 | Cinobufotoxin | C40 H58 N4 O10 | 754.4153 | 0.43 | -0.43 |
| Cpd 44: 3'-Methoxydaidzein | 9.467 | 284.0695 | 126482 | 3'-Methoxydaidzein | C16 H12 O5 | 284.0685 | 3.77 | -3.77 |
| Cpd 27: 1,2,3,3alpha,8,8alpha-Hexahydro-2,2,8-trimethyl-5,6-azulenedimethanol | 9.596 | 236.1783 | 71458 | 1,2,3,3alpha,8,8alpha-Hexahydro-2,2,8-trimethyl-5,6-azulenedimethanol | C15 H24 O2 | 236.1776 | 2.82 | -2.82 |
| Cpd 167: Kudinoside B | 9.725 | 942.4832 | 26668 | Kudinoside B | C47 H74 O19 | 942.4824 | 0.82 | -0.82 |
| Cpd 166: 26-O-beta-D-Glucopyranosyl-3beta,26-dihydroxy-choleslen-16,22-dioxo-3-O-alpha-L-rhamnopyranosyl-(1-- | 9.725 | 902.4894 | 39111 | 26-O-beta-D-Glucopyranosyl-3beta,26-dihydroxy-choleslen-16,22-dioxo-3-O-alpha-L-rhamnopyranosyl-(1-- | C45 H74 O18 | 902.4875 | 2.07 | -2.07 |
| Cpd 146: Lithospermic acid | 9.854 | 538.1105 | 53015 | Lithospermic acid | C27 H22 O12 | 538.1111 | -1.18 | 1.18 |
| Cpd 78: Tylophorinidine | 9.983 | 365.1645 | 77391 | Tylophorinidine | C22 H23 N O4 | 365.1627 | 4.87 | -4.87 |
| Cpd 79: Dehydrocorydaline | 9.983 | 366.1723 | 77391 | Dehydrocorydaline | C22 H24 N O4 | 366.1705 | 4.94 | -4.94 |
| Cpd 11: 2,4-Dimethoxybenzaldehyde | 10.499 | 166.0635 | 345315 | 2,4-Dimethoxybenzaldehyde | C9 H10 O3 | 166.063 | 3.12 | -3.12 |
| Cpd 147: Schisantherin E | 10.499 | 538.2192 | 38953 | Schisantherin E | C30 H34 O9 | 538.2203 | -2.01 | 2.01 |
| Cpd 8: 2'-Hydroxycinnamaldehyde | 10.499 | 148.0529 | 469870 | 2'-Hydroxycinnamaldehyde | C9 H8 O2 | 148.0524 | 3.14 | -3.14 |
| Cpd 152: Hupeheninoside | 10.499 | 577.4001 | 51641 | Hupeheninoside | C33 H55 N O7 | 577.3979 | 3.95 | -3.95 |
| Cpd 62: Androsin | 10.499 | 328.1172 | 150678 | Androsin | C15 H20 O8 | 328.1158 | 4.14 | -4.14 |
| Cpd 80: Methyl chlorogenate | 10.499 | 368.1101 | 36104 | Methyl chlorogenate | C17 H20 O9 | 368.1107 | -1.7 | 1.7 |
| Cpd 64: Cephalotaxinamide | 10.499 | 329.125 | 150678 | Cephalotaxinamide | C18 H19 N O5 | 329.1263 | -3.99 | 3.99 |
| Cpd 45: Lanyuamide I | 11.789 | 293.2356 | 28553 | Lanyuamide I | C18 H31 N O2 | 293.2355 | 0.3 | -0.3 |
| Cpd 168: Avenacin A1 | 11.918 | 1093.5471 | 22761 | Avenacin A1 | C55 H83 N O21 | 1093.5458 | 1.27 | -1.27 |
| Cpd 31: Aphylline | 12.821 | 248.1894 | 31949 | Aphylline | C15 H24 N2 O | 248.1889 | 2.3 | -2.3 |
| Cpd 104: Delavine | 13.079 | 415.3469 | 155758 | Delavine | C27 H45 N O2 | 415.345 | 4.42 | -4.42 |
| Cpd 136: 2alpha,3beta-Dihydroxyurs-12,19-dien-23,28-oic acid | 13.208 | 500.3157 | 32175 | 2alpha,3beta-Dihydroxyurs-12,19-dien-23,28-oic acid | C30 H44 O6 | 500.3138 | 3.76 | -3.76 |
| Cpd 124: Silandrin | 13.981 | 466.1257 | 7641 | Silandrin | C25 H22 O9 | 466.1264 | -1.4 | 1.4 |
| Cpd 36: 7-Methoxy-4'-hydroxyflavone | 14.368 | 268.0743 | 137734 | 7-Methoxy-4'-hydroxyflavone | C16 H12 O4 | 268.0736 | 2.86 | -2.86 |
| Cpd 151: Asclepin | 14.497 | 574.2795 | 28695 | Asclepin | C31 H42 O10 | 574.2778 | 2.98 | -2.98 |
| Cpd 153: (2R*,3S*,4R*,5R*,8R*,13S*,15R*)-5,8,15- | 14.497 | 596.2614 | 13398 | (2R*,3S*,4R*,5R*,8R*,13S*,15R*)-5,8,15- | C33 H40 O10 | 596.2622 | -1.32 | 1.32 |

# Qualitative Compound Report

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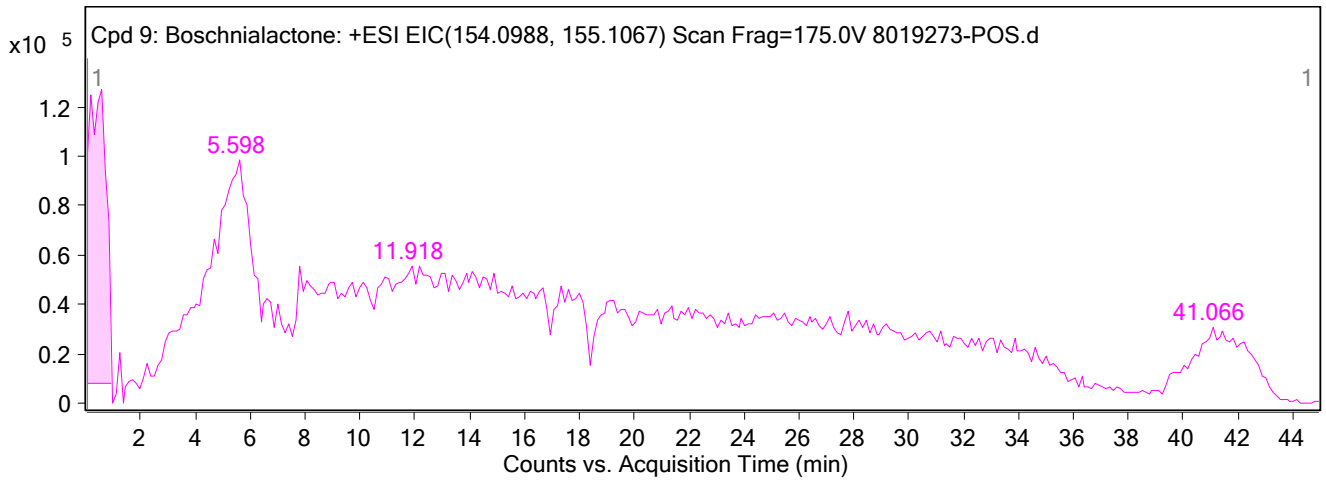
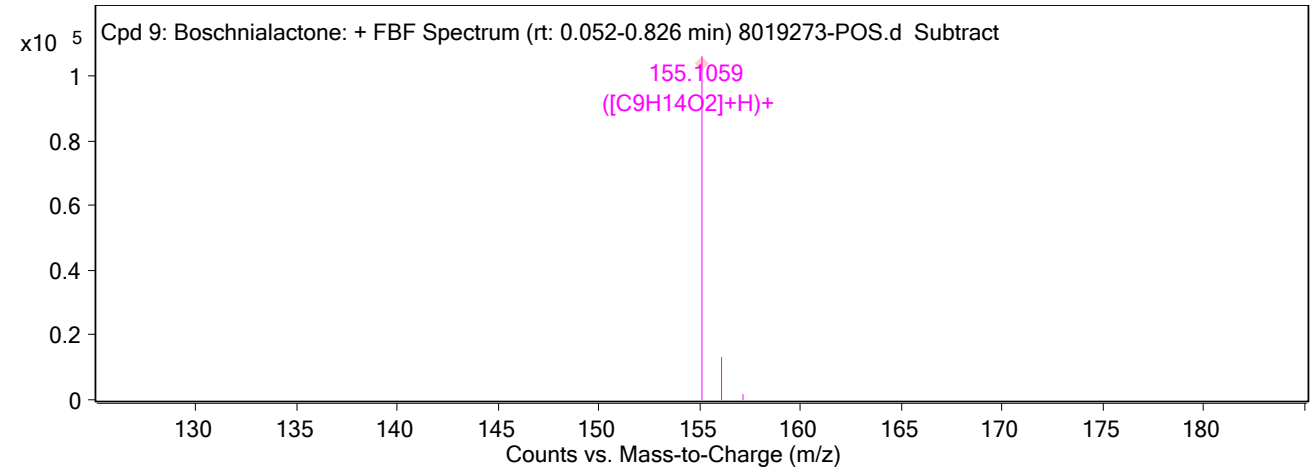
|---|---|---|---|---|---|---|---|---|
| Triacetoxy-3-benzoyloxy-9,14-dioxojatropha-6(17),11E-diene | | | | Triacetoxy-3-benzoyloxy-9,14-dioxojatropha-6(17),11E-diene | | | | |
| Cpd 60: (-)-2beta-Hydroperoxykolavelool | 14.626 | 322.2502 | 10026 | (-)-2beta-Hydroperoxykolavelool | C20 H34 O3 | 322.2508 | -1.81 | 1.81 |
| Cpd 155: Taxuspinanane B | 14.755 | 612.2566 | 137709 | Taxuspinanane B | C33 H40 O11 | 612.2571 | -0.67 | 0.67 |
| Cpd 74: 3beta,15xi,16-Trihydroxy isopimaric acid | 14.884 | 352.2244 | 153202 | 3beta,15xi,16-Trihydroxy isopimaric acid | C20 H32 O5 | 352.225 | -1.53 | 1.53 |
| Cpd 23: (-)-3,4-Di-epi-3,7-trifara-9,14-diene | 15.4 | 204.188 | 21925 | (-)-3,4-Di-epi-3,7-trifara-9,14-diene | C15 H24 | 204.1878 | 0.84 | -0.84 |
| Cpd 165: alpha-Acetyldigitoxin | 15.529 | 806.4457 | 31574 | alpha-Acetyldigitoxin | C43 H66 O14 | 806.4453 | 0.51 | -0.51 |
| Cpd 120: (+)-Pinoresinol-3-hydroxy-4-methyl-4-pentenyl ether | 15.658 | 454.1991 | 76387 | (+)-Pinoresinol-3-hydroxy-4-methyl-4-pentenyl ether | C26 H30 O7 | 454.1992 | -0.04 | 0.04 |
| Cpd 111: Sisalagenone | 16.174 | 428.2939 | 7431 | Sisalagenone | C27 H40 O4 | 428.2927 | 2.92 | -2.92 |
| Cpd 17: beta-Ionone | 16.174 | 192.1519 | 66199 | beta-Ionone | C13 H20 O | 192.1514 | 2.68 | -2.68 |
| Cpd 15: 6-Hydroxy-7-methylesculetin | 16.303 | 176.0477 | 4915 | 6-Hydroxy-7-methylesculetin | C10 H8 O3 | 176.0473 | 2.31 | -2.31 |
| Cpd 98: (3'R,4'R)-3'-Epoxyangeloyloxy-4'-acetoxy-3',4'-dihydroseselin | 16.561 | 402.133 | 117968 | (3'R,4'R)-3'-Epoxyangeloyloxy-4'-acetoxy-3',4'-dihydroseselin | C21 H22 O8 | 402.1315 | 3.86 | -3.86 |
| Cpd 158: Hernandezine | 16.561 | 652.3149 | 7000 | Hernandezine | C39 H44 N2 O7 | 652.3149 | 0.08 | -0.08 |
| Cpd 157: 9-Acetoxytaxine B | 16.819 | 625.3242 | 26912 | 9-Acetoxytaxine B | C35 H47 N O9 | 625.3251 | -1.47 | 1.47 |
| Cpd 70: Kadsurenin B | 16.948 | 342.1479 | 11363 | Kadsurenin B | C20 H22 O5 | 342.1467 | 3.45 | -3.45 |
| Cpd 97: Deoxygomisin A | 16.948 | 400.1894 | 29610 | Deoxygomisin A | C23 H28 O6 | 400.1886 | 1.9 | -1.9 |
| Cpd 119: (+)-Pinoresinol-3-hydroxy-4-methyl-4-pentenyl ether | 16.948 | 454.1988 | 928042 | (+)-Pinoresinol-3-hydroxy-4-methyl-4-pentenyl ether | C26 H30 O7 | 454.1992 | -0.86 | 0.86 |
| Cpd 123: Psychotrine | 16.948 | 464.2662 | 35458 | Psychotrine | C28 H36 N2 O4 | 464.2675 | -2.73 | 2.73 |
| Cpd 84: Fargesone A | 16.948 | 372.1585 | 22208 | Fargesone A | C21 H24 O6 | 372.1573 | 3.24 | -3.24 |
| Cpd 103: Armillaripin | 16.948 | 414.2061 | 1604171 | Armillaripin | C24 H30 O6 | 414.2042 | 4.57 | -4.57 |
| Cpd 114: Bufarenogin | 16.948 | 432.2167 | 1160208 | Bufarenogin | C24 H32 O7 | 432.2148 | 4.5 | -4.5 |
| Cpd 65: 1'-Methoxy-2'-hydroxydihydromollugin | 16.948 | 332.1263 | 23054 | 1'-Methoxy-2'-hydroxydihydromollugin | C18 H20 O6 | 332.126 | 0.81 | -0.81 |
| Cpd 100: Mammea A/AC cyclo F | 17.464 | 408.1568 | 16590 | Mammea A/AC cyclo F | C24 H24 O6 | 408.1573 | -1.27 | 1.27 |
| Cpd 88: (-)-Acetoxycollinin | 17.464 | 386.1748 | 75082 | (-)-Acetoxycollinin | C22 H26 O6 | 386.1729 | 4.93 | -4.93 |
| Cpd 92: Chinensinaphthol methyl ether | 17.98 | 394.1044 | 3867 | Chinensinaphthol methyl ether | C22 H18 O7 | 394.1053 | -2.06 | 2.06 |
| Cpd 83: 5,7,2',4',6'-Pentamethoxyflavone | 17.98 | 372.1224 | 15307 | 5,7,2',4',6'-Pentamethoxyflavone | C20 H20 O7 | 372.1209 | 4.14 | -4.14 |
| Cpd 95: 3,4-Teracrylshikonin | 18.367 | 398.1744 | 101519 | 3,4-Teracrylshikonin | C23 H26 O6 | 398.1729 | 3.74 | -3.74 |
| Cpd 26: 1,2,3,3alpha,8,8alpha-Hexahydro-2,2,8-trimethyl-5,6-azulenedimethanol | 18.754 | 236.1785 | 40040 | 1,2,3,3alpha,8,8alpha-Hexahydro-2,2,8-trimethyl-5,6-azulenedimethanol | C15 H24 O2 | 236.1776 | 3.81 | -3.81 |
| Cpd 118: (+)-Pinoresinol-3-hydroxy-4-methyl-4-pentenyl ether | 19.011 | 454.1987 | 86256 | (+)-Pinoresinol-3-hydroxy-4-methyl-4-pentenyl ether | C26 H30 O7 | 454.1992 | -1.04 | 1.04 |
| Cpd 30: (R)-4-(1,5-Dimethyl-3-oxohexyl)benzoic acid | 19.14 | 248.1423 | 175781 | (R)-4-(1,5-Dimethyl-3-oxohexyl)benzoic acid | C15 H20 O3 | 248.1412 | 4.07 | -4.07 |
| Cpd 139: Angeloylgomisin P | 19.269 | 514.2224 | 29807 | Angeloylgomisin P | C28 H34 O9 | 514.2203 | 4.06 | -4.06 |
| Cpd 90: Heteratisine | 19.656 | 391.237 | 30189 | Heteratisine | C22 H33 N O5 | 391.2359 | 2.85 | -2.85 |
| Cpd 115: Ugonin B | 19.656 | 436.1878 | 56735 | Ugonin B | C26 H28 O6 | 436.1886 | -1.89 | 1.89 |
| Cpd 109: Calopolyanolide A | 19.785 | 422.1725 | 26978 | Calopolyanolide A | C25 H26 O6 | 422.1729 | -1.1 | 1.1 |
| Cpd 130: Emetine | 19.785 | 480.2982 | 276286 | Emetine | C29 H40 N2 O4 | 480.2988 | -1.23 | 1.23 |
| Cpd 128: Bullatine C | 19.785 | 479.2904 | 276286 | Bullatine C | C26 H41 N O7 | 479.2883 | 4.35 | -4.35 |
| Cpd 96: Deoxygomisin A | 19.914 | 400.1903 | 765089 | Deoxygomisin A | C23 H28 O6 | 400.1886 | 4.39 | -4.39 |
| Cpd 159: Khekadaengoside C | 19.914 | 660.3511 | 9497 | Khekadaengoside C | C36 H52 O11 | 660.351 | 0.23 | -0.23 |
| Cpd 156: Daturametelin B | 19.914 | 616.3253 | 7283 | Daturametelin B | C34 H48 O10 | 616.3248 | 0.95 | -0.95 |
| Cpd 154: Zizyphine A | 19.914 | 611.3696 | 748331 | Zizyphine A | C33 H49 N5 O6 | 611.3683 | 2.23 | -2.23 |
| Cpd 135: Angeloylgomisin H | 20.043 | 500.2433 | 149595 | Angeloylgomisin H | C28 H36 O8 | 500.241 | 4.6 | -4.6 |
| Cpd 149: Ergosine | 20.043 | 547.2805 | 138343 | Ergosine | C30 H37 N5 O5 | 547.2795 | 1.79 | -1.79 |
| Cpd 148: Ergosine | 20.559 | 547.2806 | 635077 | Ergosine | C30 H37 N5 O5 | 547.2795 | 2.13 | -2.13 |
| Cpd 57: 2?Methoxymollugin | 20.559 | 316.1316 | 1923 | 2?Methoxymollugin | C18 H20 O5 | 316.1311 | 1.6 | -1.6 |
| Cpd 112: Armillarilin | 20.559 | 430.2011 | 664452 | Armillarilin | C24 H30 O7 | 430.1992 | 4.62 | -4.62 |
| Cpd 150: Thelephantin C | 20.946 | 558.1879 | 14303 | Thelephantin C | C32 H30 O9 | 558.189 | -1.85 | 1.85 |
| Cpd 145: Formosanatin B | 21.075 | 536.2041 | 31940 | Formosanatin B | C30 H32 O9 | 536.2046 | -1.05 | 1.05 |
| Cpd 61: Conessidine | 21.462 | 326.2707 | 15782 | Conessidine | C22 H34 N2 | 326.2722 | -4.71 | 4.71 |
| Cpd 101: Neoisostegane | 21.849 | 414.1696 | 26778 | Neoisostegane | C23 H26 O7 | 414.1679 | 4.15 | -4.15 |
| Cpd 143: Isoharringtonine | 21.849 | 531.2486 | 31487 | Isoharringtonine | C28 H37 N O9 | 531.2468 | 3.38 | -3.38 |
| Cpd 144: Formosanatin B | 21.849 | 536.2035 | 8824 | Formosanatin B | C30 H32 O9 | 536.2046 | -2.04 | 2.04 |
| Cpd 102: Armillaripin | 22.881 | 414.2057 | 28871 | Armillaripin | C24 H30 O6 | 414.2042 | 3.55 | -3.55 |
| Cpd 47: Tetrahydrobungeanool | 23.139 | 295.2524 | 936041 | Tetrahydrobungeanool | C18 H33 N O2 | 295.2511 | 4.25 | -4.25 |
| Cpd 42: (Z,Z,Z)-9,12,15-Octadecatrienoic acid | 23.139 | 278.2256 | 138490 | (Z,Z,Z)-9,12,15-Octadecatrienoic acid | C18 H30 O2 | 278.2246 | 3.7 | -3.7 |
| Cpd 48: Magnolignan A | 24.299 | 300.1348 | 35271 | Magnolignan A | C18 H20 O4 | 300.1362 | -4.54 | 4.54 |
| Cpd 50: alpha-Dichroine | 24.299 | 301.1427 | 35271 | alpha-Dichroine | C16 H19 N3 O3 | 301.1426 | 0.17 | -0.17 |
| Cpd 40: Dibutyl phthalate | 24.299 | 278.1527 | 59236 | Dibutyl phthalate | C16 H22 O4 | 278.1518 | 3.19 | -3.19 |
| Cpd 22: (Z)-5-Hydroxy-3-butylidene-phthalide | 24.428 | 204.0785 | 5090 | (Z)-5-Hydroxy-3-butylidene-phthalide | C12 H12 O3 | 204.0786 | -0.52 | 0.52 |
| Cpd 7: Phthalic anhydride | 24.428 | 148.016 | 160328 | Phthalic anhydride | C8 H4 O3 | 148.016 | -0.03 | 0.03 |
| Cpd 85: N-Methyl pachysamine A | 24.557 | 374.3646 | 19592 | N-Methyl pachysamine A | C25 H46 N2 | 374.3661 | -3.92 | 3.92 |
| Cpd 99: Cassaidine | 31.135 | 407.3029 | 12273 | Cassaidine | C24 H41 N O4 | 407.3036 | -1.71 | 1.71 |
| Cpd 138: 13beta,17beta-Epoxyalisol A | 33.457 | 506.3615 | 2274 | 13beta,17beta-Epoxyalisol A | C30 H50 O6 | 506.3607 | 1.47 | -1.47 |
| Cpd 87: Buxbodine C | 34.747 | 383.3187 | 7919 | Buxbodine C | C26 H41 N O | 383.3188 | -0.35 | 0.35 |
| Cpd 106: Maesaquinone | 35.004 | 418.3096 | 6629 | Maesaquinone | C26 H42 O4 | 418.3083 | 3.1 | -3.1 |
| Cpd 94: 4-Methyl-7-ergosta-8,24(28)-diene | 36.036 | 396.3765 | 5486 | 4-Methyl-7-ergosta-8,24(28)-diene | C29 H48 | 396.3756 | 2.15 | -2.15 |
| Cpd 3: Trigonelline | 39.777 | 137.0481 | 10340 | Trigonelline | C7 H7 N O2 | 137.0477 | 2.85 | -2.85 |
| Cpd 89: Corchoionoside C | 39.777 | 386.1938 | 11357 | Corchoionoside C | C19 H30 O8 | 386.1941 | -0.59 | 0.59 |
| Cpd 63: Rhododendrin | 40.035 | 328.1519 | 24717 | Rhododendrin | C16 H24 O7 | 328.1522 | -0.81 | 0.81 |
| Cpd 20: 6,7-Dihydroxy-1,1-dimethyl-1,2,3,4-tetrahydroisoquinoline | 40.035 | 193.1097 | 113610 | 6,7-Dihydroxy-1,1-dimethyl-1,2,3,4-tetrahydroisoquinoline | C11 H15 N O2 | 193.1103 | -3.26 | 3.26 |
| Cpd 4: Spermidine | 43.001 | 145.1583 | 9474 | Spermidine | C7 H19 N3 | 145.1579 | 2.7 | -2.7 |
| Cpd 13: L-Arginine | 43.388 | 174.1121 | 58163 | L-Arginine | C6 H14 N4 O2 | 174.1117 | 2.54 | -2.54 |

| Compound Label | Name | m/z | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 9: Boschnialactone | **Boschnialactone** | 155.1059 | 0.568 | Find By Formula | 154.0987 |

**Compound Chromatograms**




MS Zoomed Spectrum

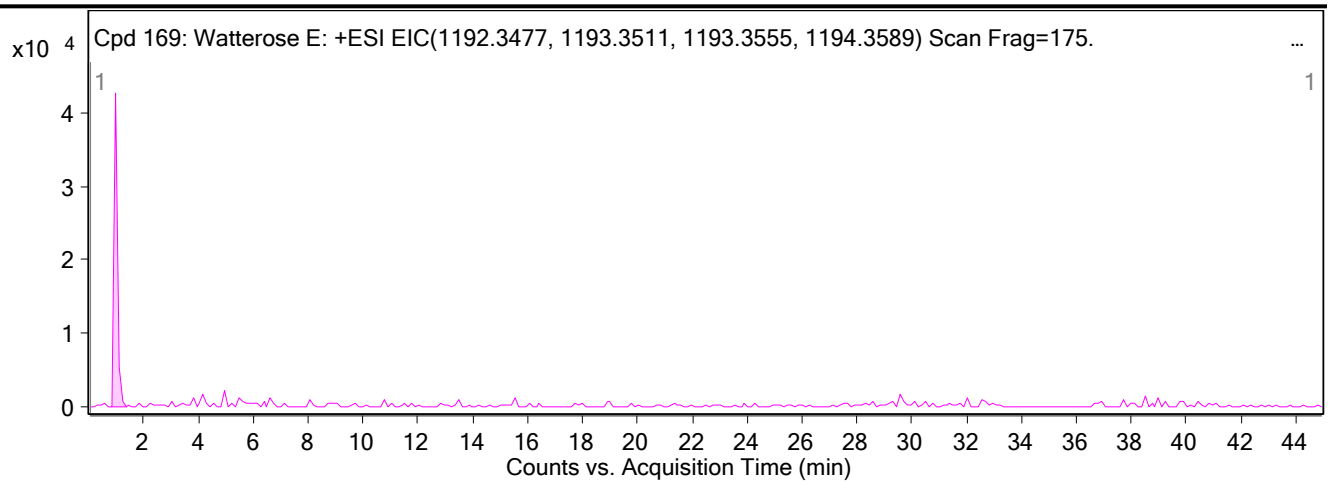



**MS Spectrum Peak List**

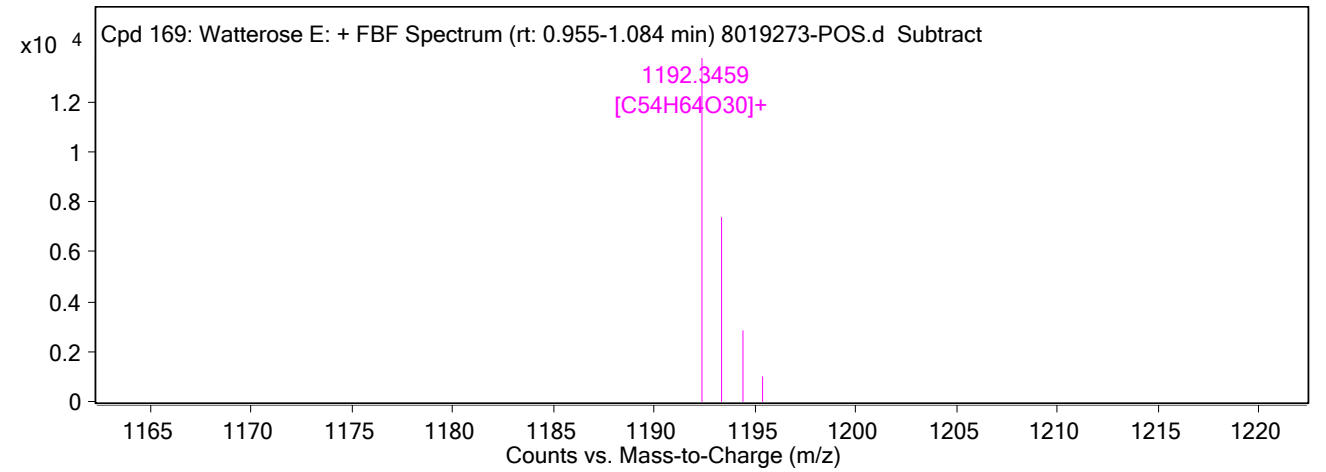
| m/z | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 155.1059 | 1 | 106251.48 | C9H14O2 | (M+H)+ |
| 156.1099 | 1 | 13322.54 | C9H14O2 | (M+H)+ |
| 157.1119 | 1 | 1685.4 | C9H14O2 | (M+H)+ |

| Compound Label | Name | m/z | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 169: Watterose E | **Watterose E** | 1192.3459 | 0.955 | Find By Formula | 1192.3456 |

**Compound Chromatograms**




MS Zoomed Spectrum

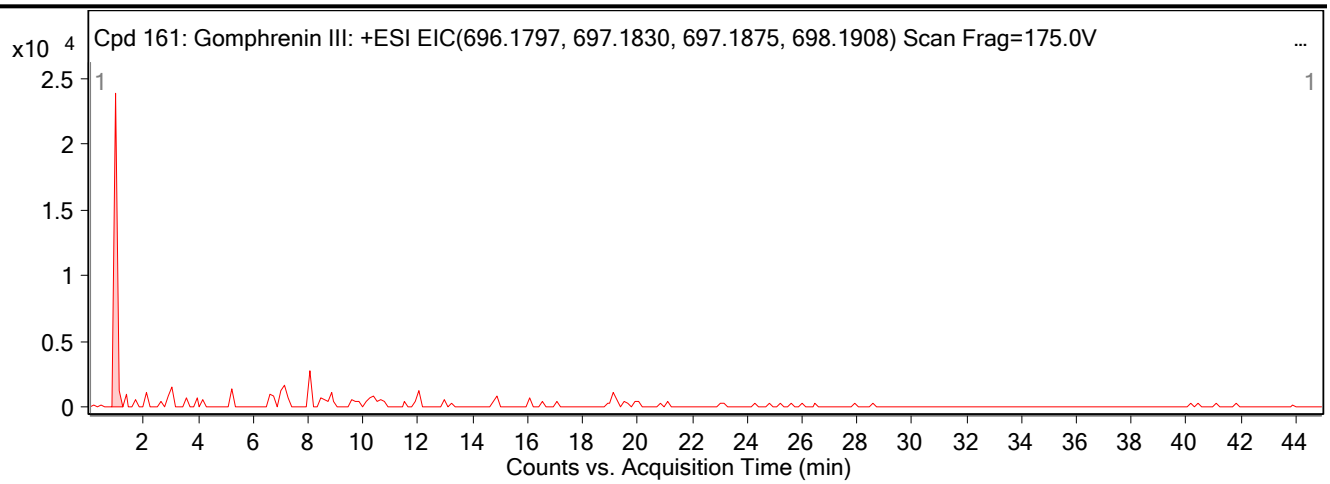



**MS Spectrum Peak List**

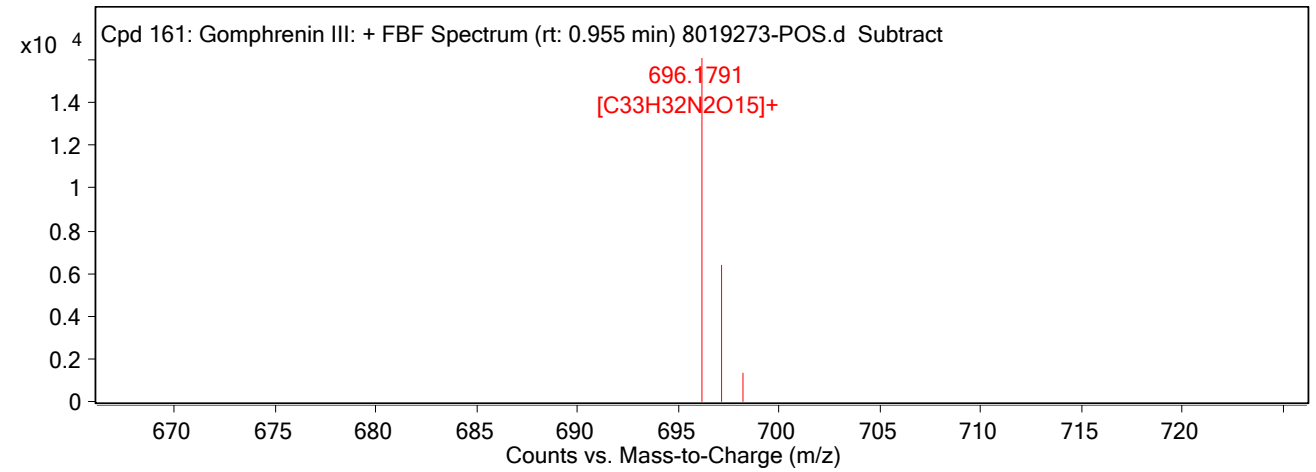
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 1192.3459 | 1 | 13743.72 | C54H64O30 | M+ |
| 1193.347 | 1 | 7336.95 | C54H64O30 | M+ |
| 1194.3499 | 1 | 2868.99 | C54H64O30 | M+ |
| 1195.3572 | 1 | 1026.7 | C54H64O30 | M+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 161: Gomphrenin III | **Gomphrenin III** | 696.1791 | 0.955 | Find By Formula | 696.1793 |

**Compound Chromatograms**




MS Zoomed Spectrum

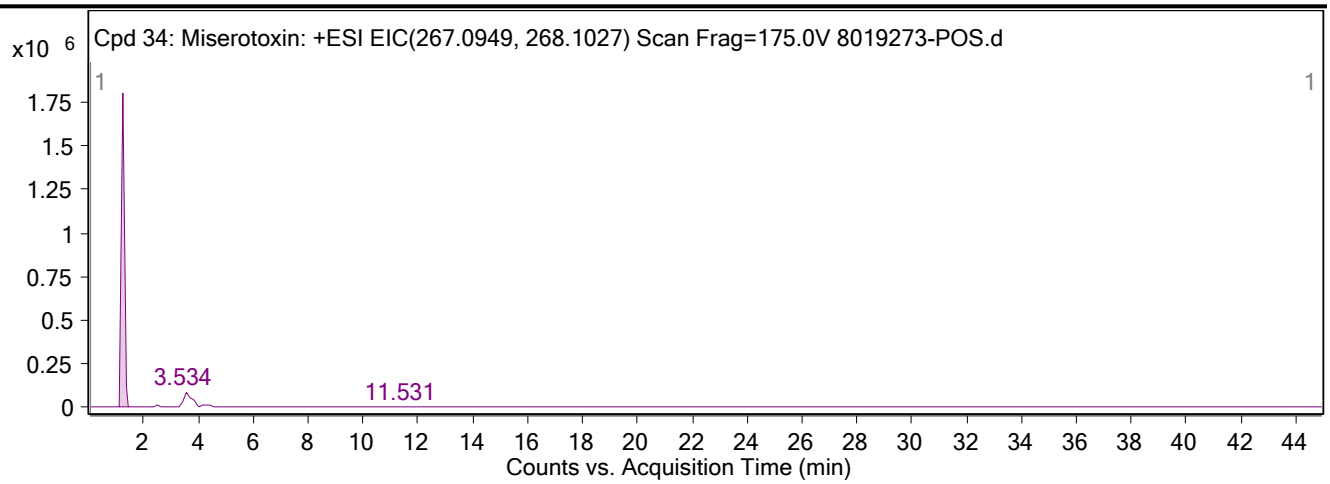



**MS Spectrum Peak List**

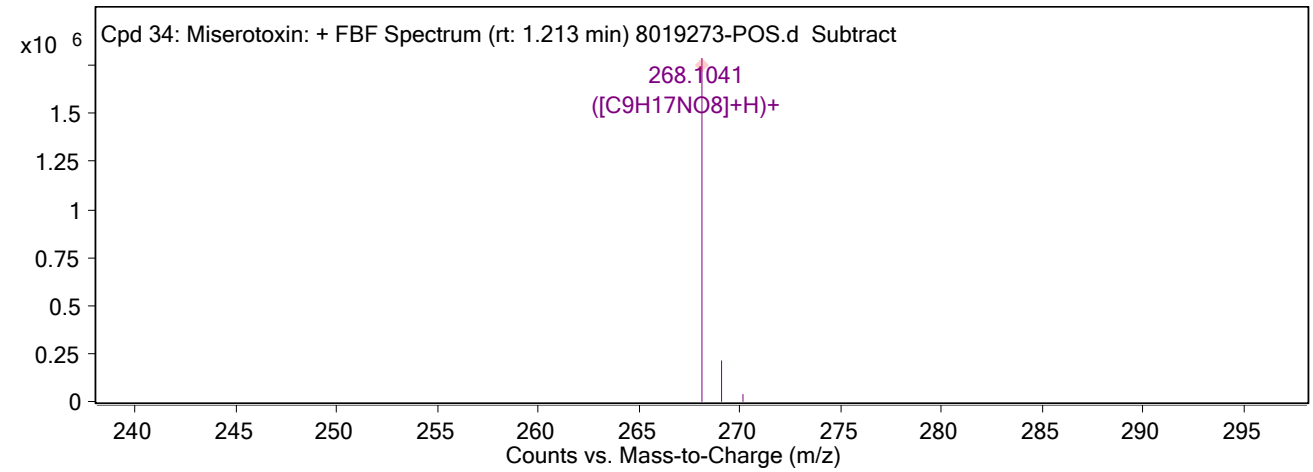
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 696.1791 | 1 | 16087.41 | C33H32N2O15 | M+ |
| 697.1817 | 1 | 6420.64 | C33H32N2O15 | M+ |
| 698.1814 | 1 | 1352.48 | C33H32N2O15 | M+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 34: Miserotoxin | **Miserotoxin** | 268.1041 | 1.213 | Find By Formula | 267.0969 |

**Compound Chromatograms**




MS Zoomed Spectrum

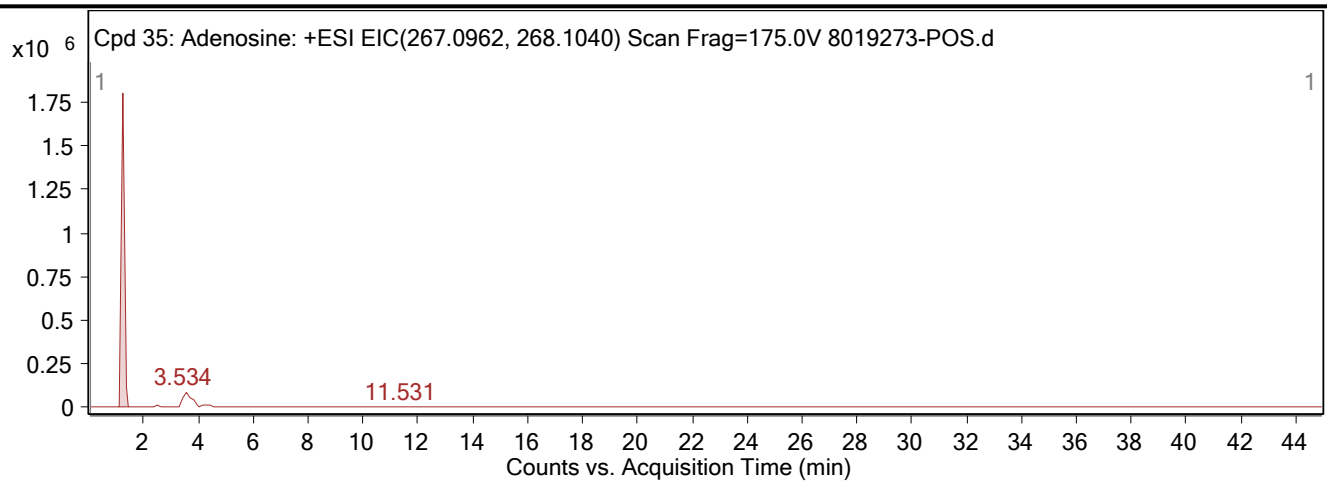



**MS Spectrum Peak List**

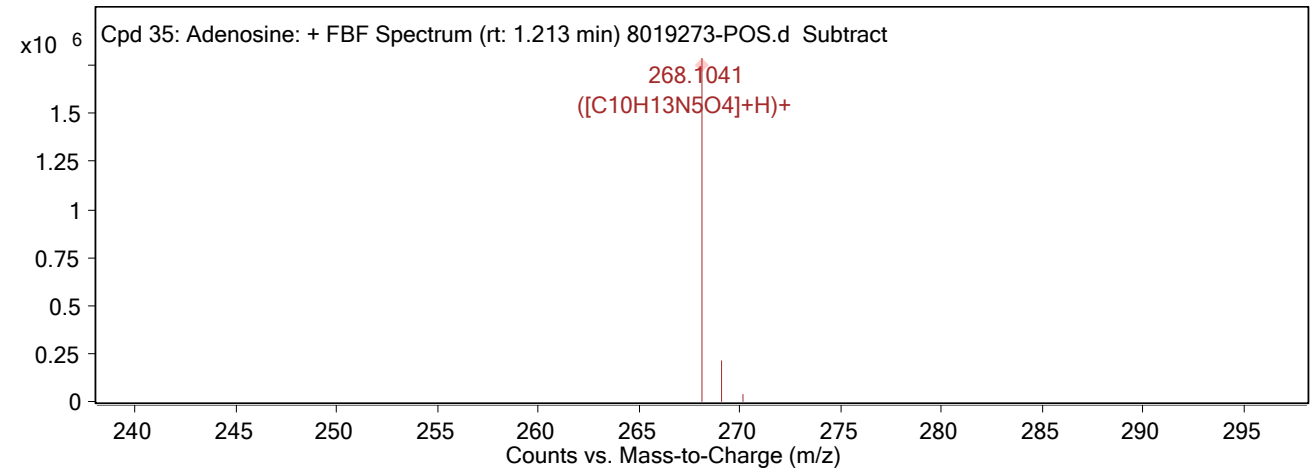
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 268.1041 | 1 | 1789478.5 | C9H17NO8 | (M+H)+ |
| 269.1082 | 1 | 215795.16 | C9H17NO8 | (M+H)+ |
| 270.1054 | 1 | 40035.41 | C9H17NO8 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 35: Adenosine | **Adenosine** | 268.1041 | 1.213 | Find By Formula | 267.0969 |

**Compound Chromatograms**




MS Zoomed Spectrum

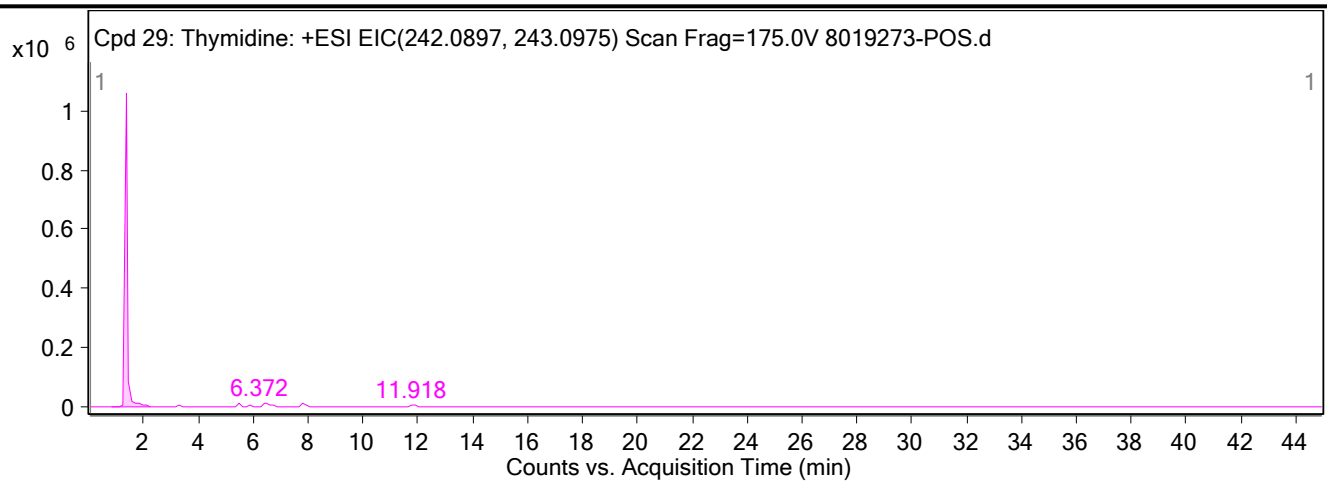



**MS Spectrum Peak List**

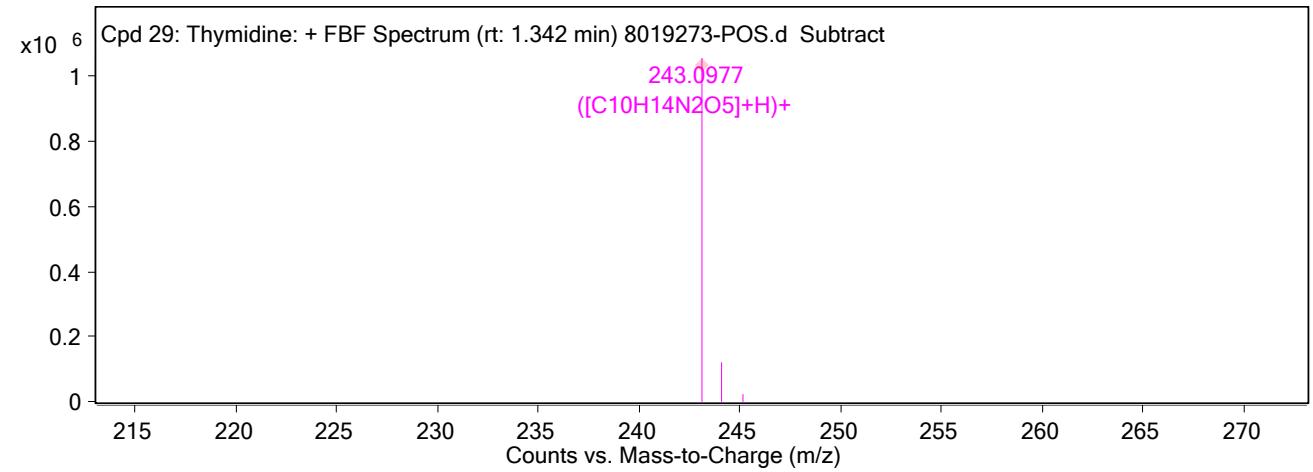
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 268.1041 | 1 | 1789478.5 | C10H13N5O4 | (M+H)+ |
| 269.1082 | 1 | 215795.16 | C10H13N5O4 | (M+H)+ |
| 270.1054 | 1 | 40035.41 | C10H13N5O4 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 29: Thymidine | **Thymidine** | 243.0977 | 1.342 | Find By Formula | 242.0904 |

**Compound Chromatograms**




MS Zoomed Spectrum

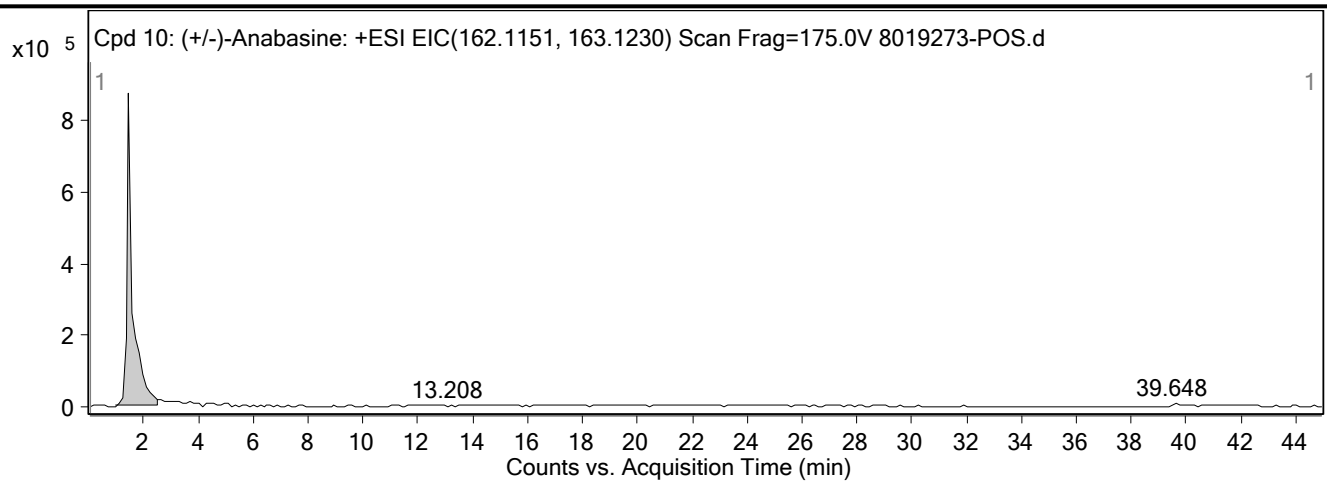



**MS Spectrum Peak List**

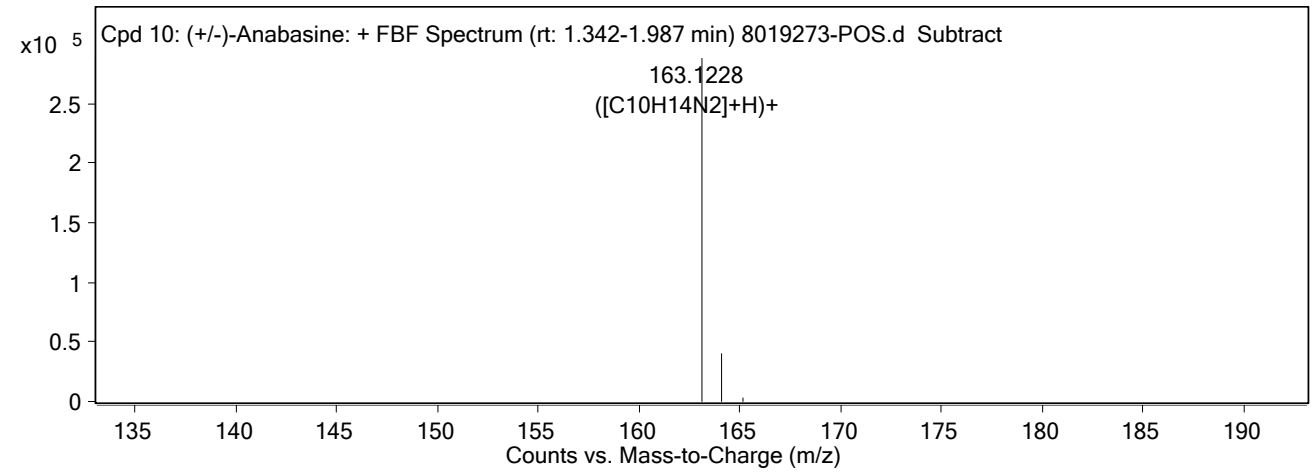
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 243.0977 | 1 | 1056994 | C10H14N2O5 | (M+H)+ |
| 244.101 | 1 | 120808.94 | C10H14N2O5 | (M+H)+ |
| 245.1014 | 1 | 23963.02 | C10H14N2O5 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 10: (+/-)-Anabasine | **(+/-)-Anabasine** | 163.1228 | 1.471 | Find By Formula | 162.1153 |

**Compound Chromatograms**




MS Zoomed Spectrum

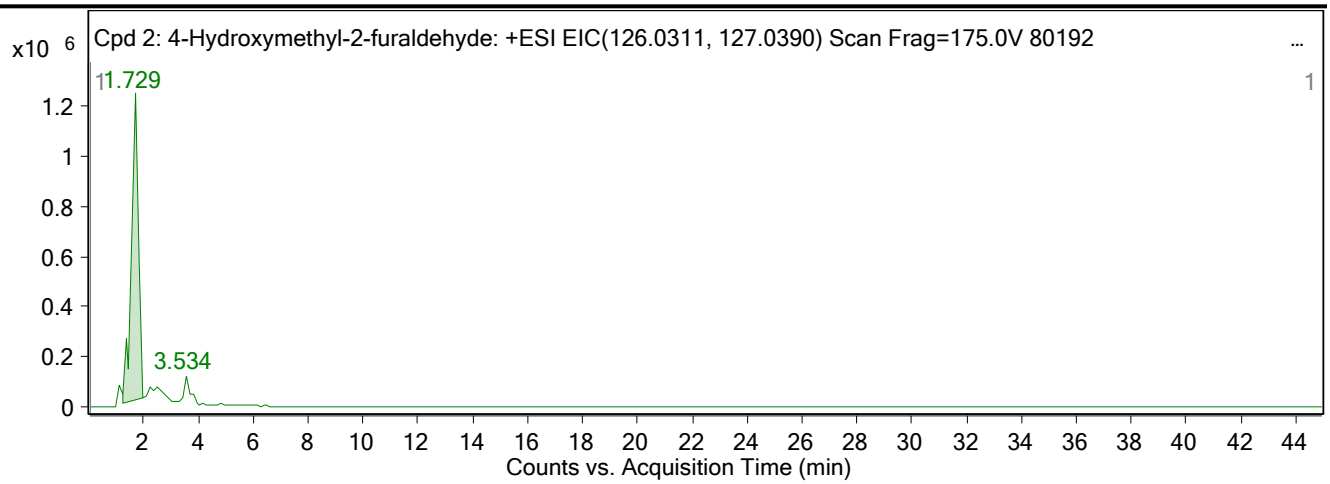



**MS Spectrum Peak List**

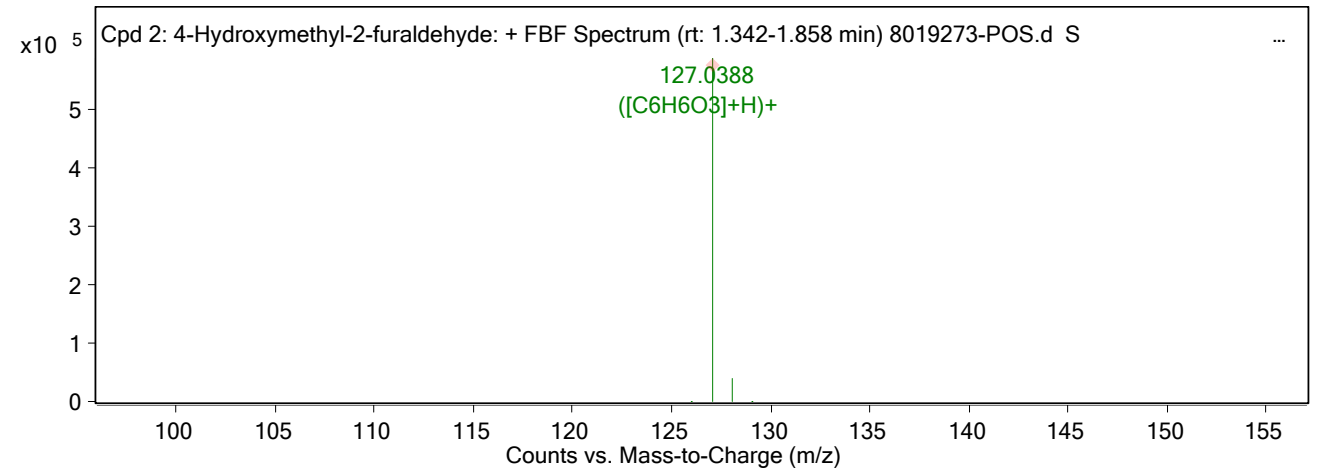
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 163.1228 | 1 | 288347.09 | C10H14N2 | (M+H)+ |
| 164.1239 | 1 | 40606.04 | C10H14N2 | (M+H)+ |
| 165.1336 | 1 | 3786.81 | C10H14N2 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 2: 4-Hydroxymethyl-2-furaldehyde | **4-Hydroxymethyl-2-furaldehyde** | 127.0388 | 1.729 | Find By Formula | 126.0316 |

**Compound Chromatograms**




MS Zoomed Spectrum

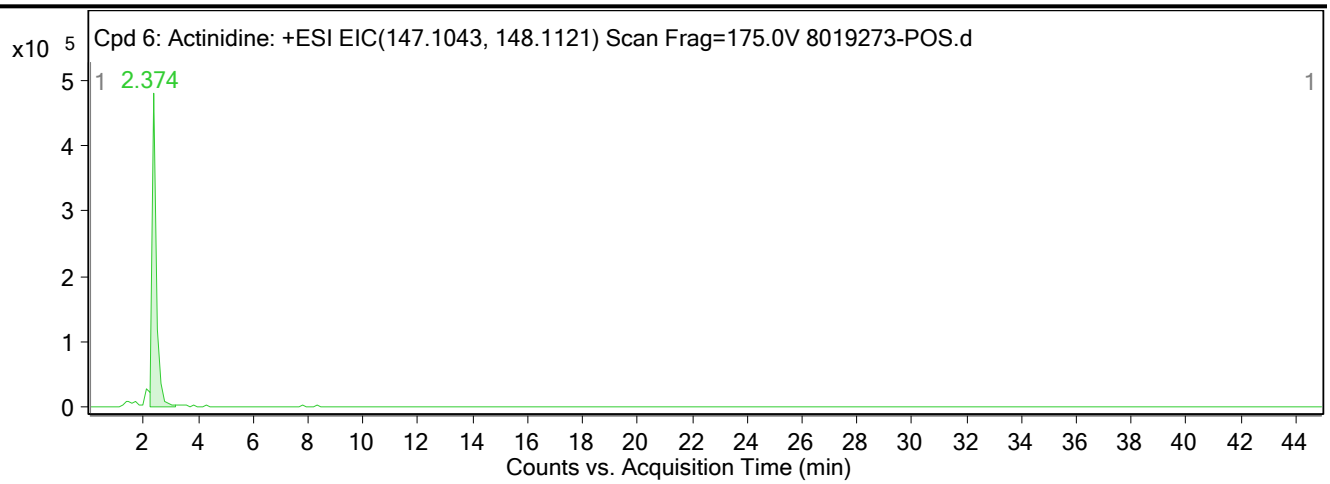



**MS Spectrum Peak List**

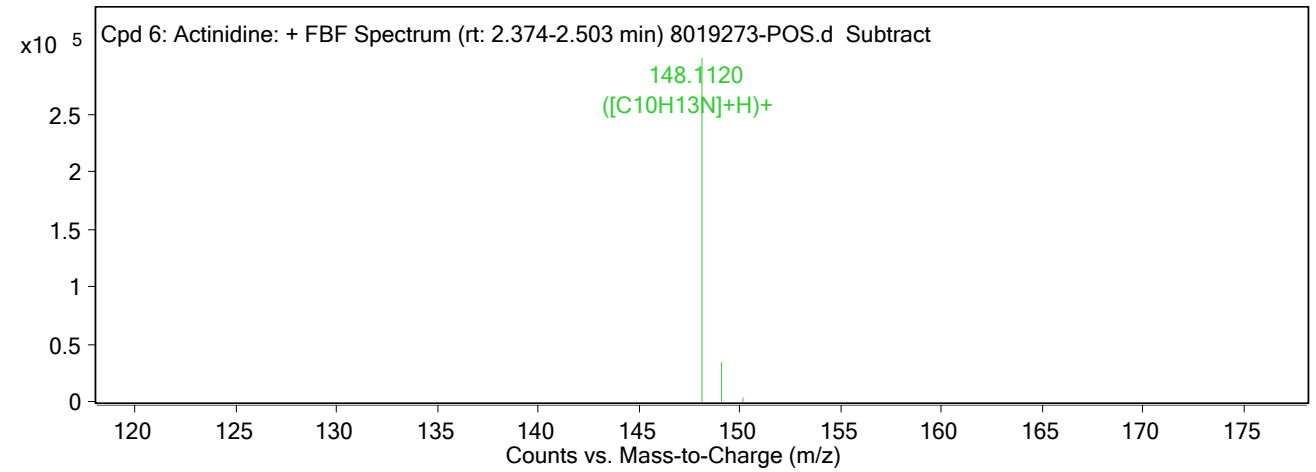
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 126.0275 | 1 | 440.19 | C6H6O3 | M+ |
| 127.0388 | 1 | 588014.19 | C6H6O3 | (M+H)+ |
| 128.0424 | 1 | 40178.77 | C6H6O3 | (M+H)+ |
| 129.0475 | 1 | 1502.77 | C6H6O3 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 6: Actinidine | **Actinidine** | 148.112 | 2.374 | Find By Formula | 147.1048 |

**Compound Chromatograms**




MS Zoomed Spectrum

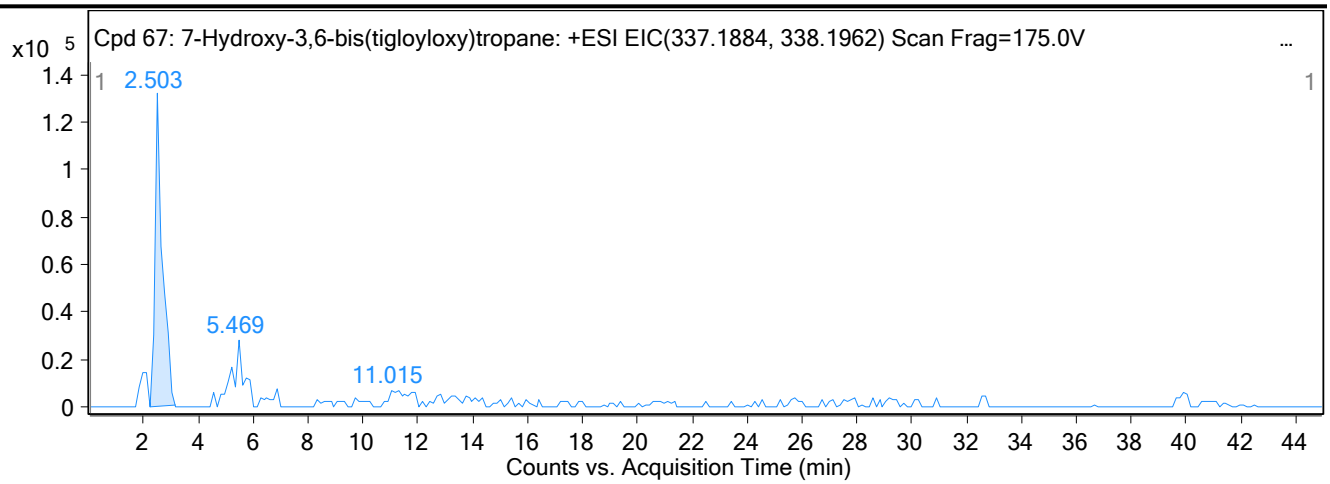



**MS Spectrum Peak List**

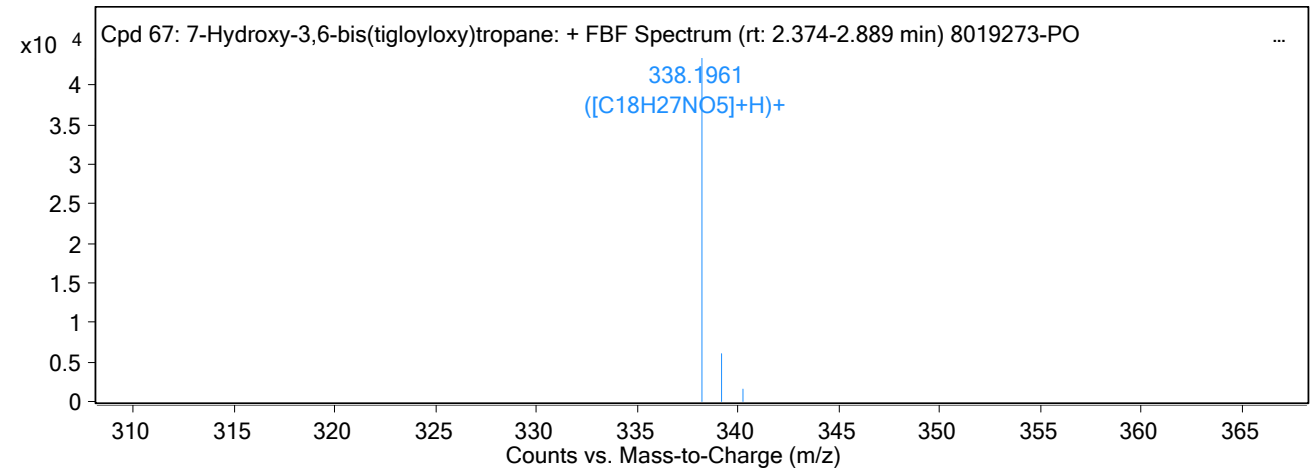
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 148.112 | 1 | 298927.22 | C10H13N | (M+H)+ |
| 149.1152 | 1 | 34281.85 | C10H13N | (M+H)+ |
| 150.1218 | 1 | 3082.36 | C10H13N | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 67: 7-Hydroxy-3,6-bis(tigloyloxy)tropane | **7-Hydroxy-3,6-bis(tigloyloxy)tropane** | 338.1961 | 2.503 | Find By Formula | 337.1888 |

**Compound Chromatograms**




MS Zoomed Spectrum

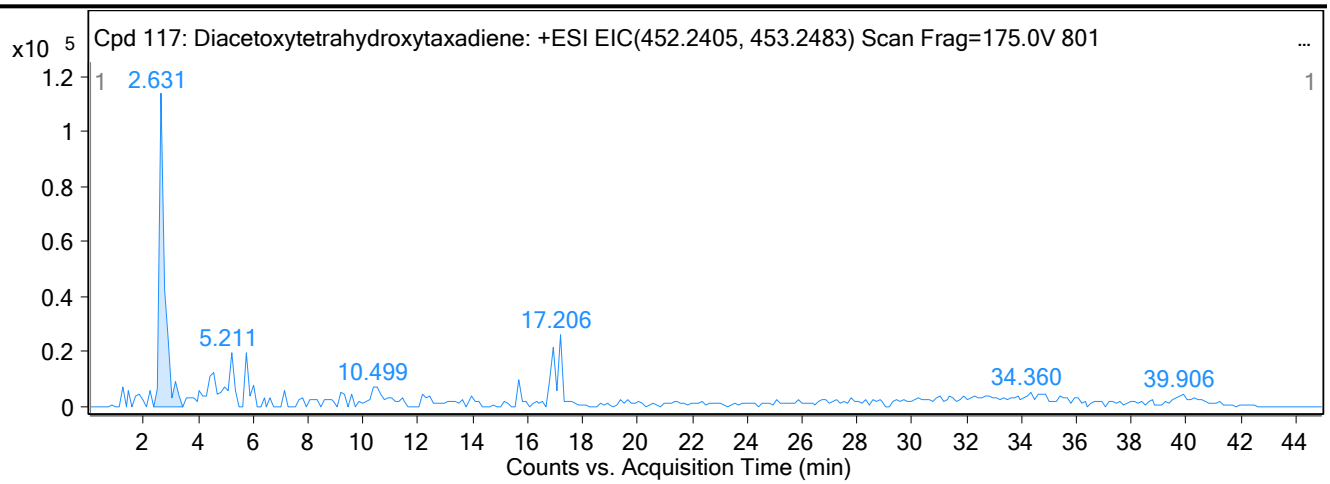



**MS Spectrum Peak List**

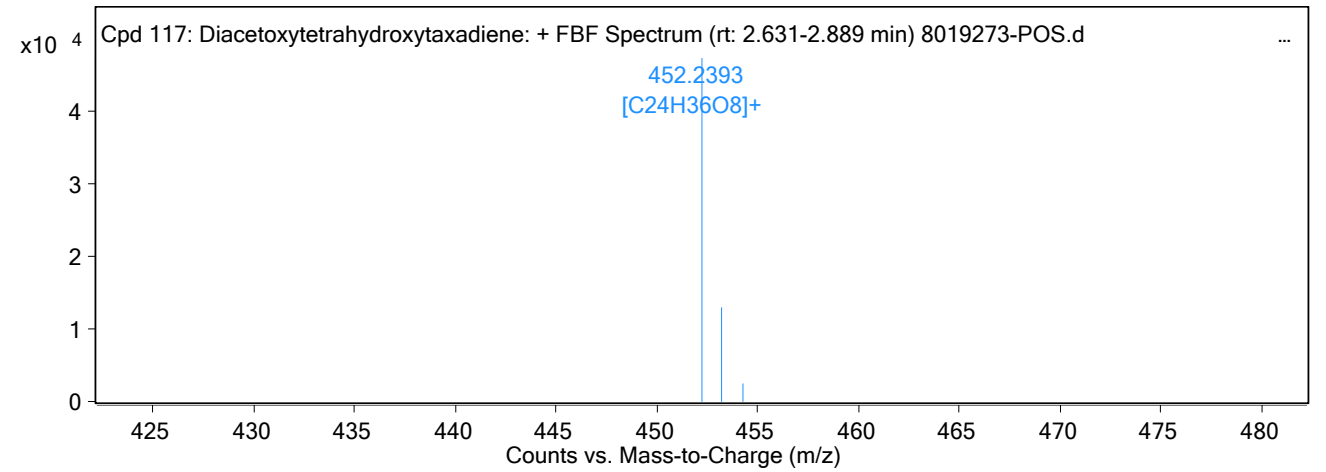
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 338.1961 | 1 | 43407.08 | C18H27NO5 | (M+H)+ |
| 339.1991 | 1 | 6104.81 | C18H27NO5 | (M+H)+ |
| 340.2034 | 1 | 1549.13 | C18H27NO5 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 117: Diacetoxytetrahydroxytaxadiene | **Diacetoxytetrahydroxytaxadiene** | 452.2393 | 2.631 | Find By Formula | 452.2396 |

**Compound Chromatograms**




MS Zoomed Spectrum

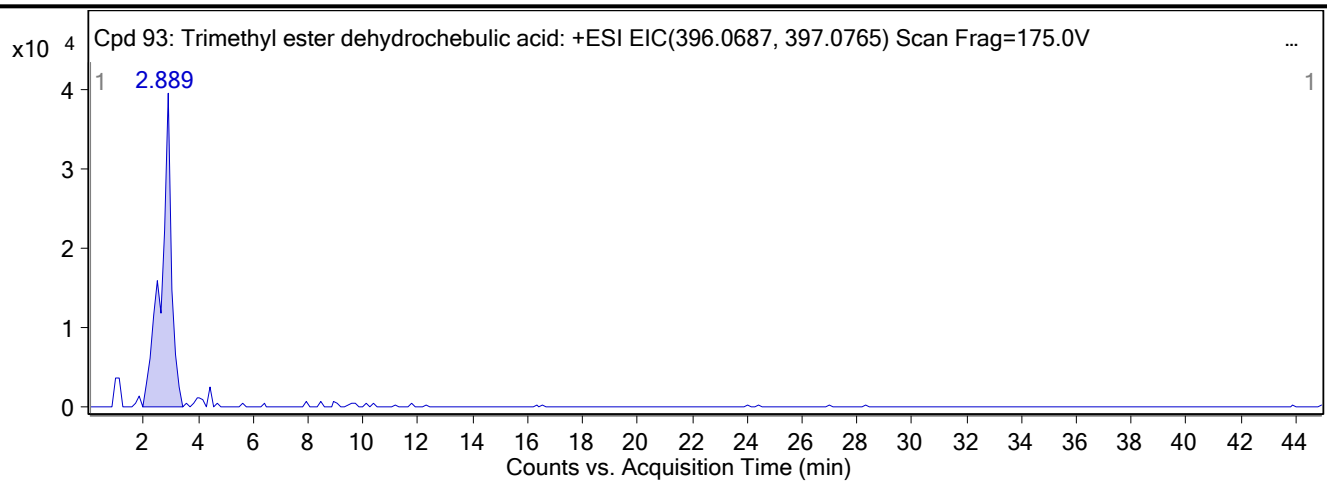



**MS Spectrum Peak List**

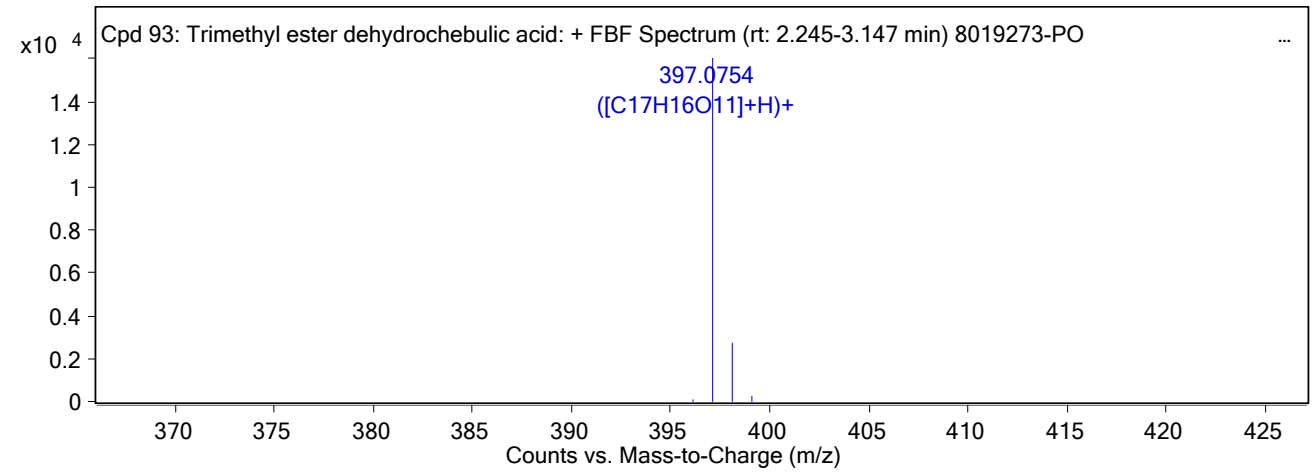
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 452.2393 | 1 | 47312.31 | C24H36O8 | M+ |
| 453.2422 | 1 | 12996.58 | C24H36O8 | M+ |
| 454.2418 | 1 | 2388.68 | C24H36O8 | M+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 93: Trimethyl ester dehydrochebulic acid | **Trimethyl ester dehydrochebulic acid** | 397.0754 | 2.889 | Find By Formula | 396.0684 |

**Compound Chromatograms**




MS Zoomed Spectrum

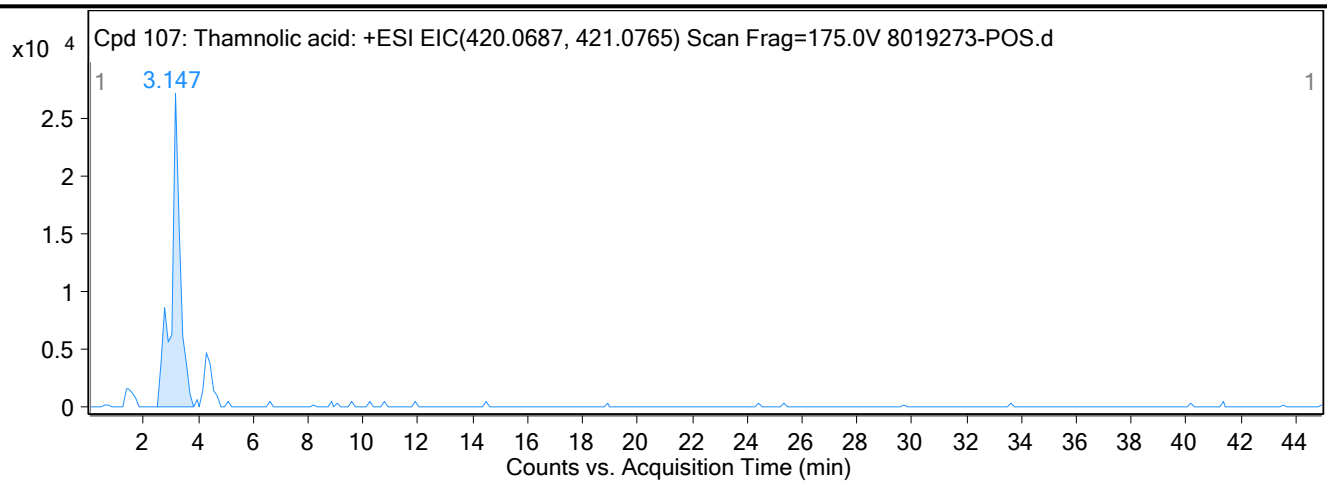



**MS Spectrum Peak List**

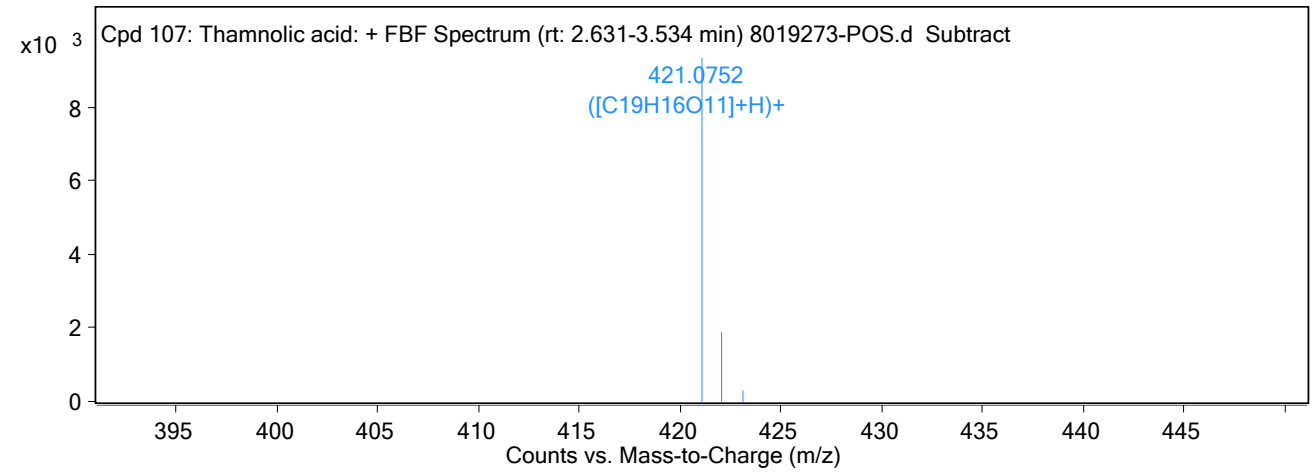
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 396.075 | 1 | 66.25 | C17H16O11 | M+ |
| 397.0754 | 1 | 16030.91 | C17H16O11 | (M+H)+ |
| 398.0792 | 1 | 2763.35 | C17H16O11 | (M+H)+ |
| 399.0949 | 1 | 292.81 | C17H16O11 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 107: Thamnolic acid | **Thamnolic acid** | 421.0752 | 3.147 | Find By Formula | 420.0682 |

**Compound Chromatograms**




MS Zoomed Spectrum

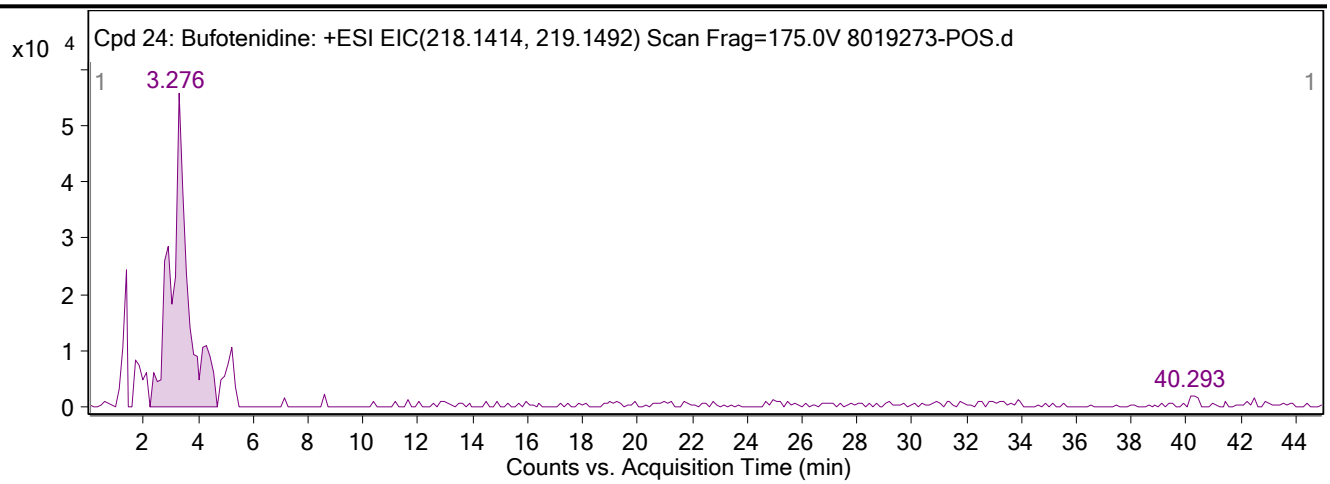



**MS Spectrum Peak List**

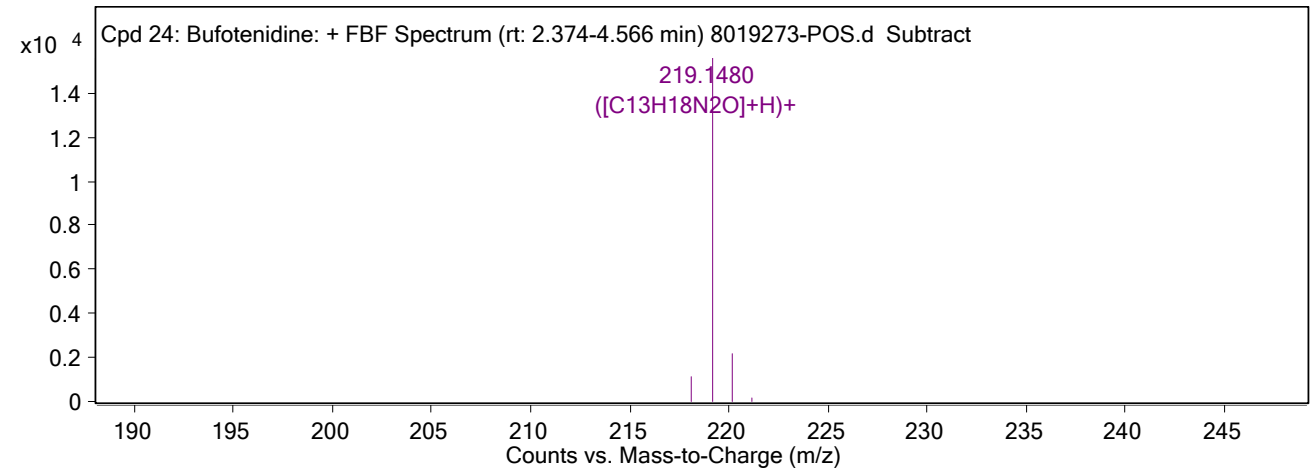
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 421.0752 | 1 | 9324.47 | C19H16O11 | (M+H)+ |
| 422.0801 | 1 | 1883.84 | C19H16O11 | (M+H)+ |
| 423.0839 | 1 | 274.03 | C19H16O11 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 24: Bufotenidine | **Bufotenidine** | 219.148 | 3.276 | Find By Formula | 218.1405 |

**Compound Chromatograms**




MS Zoomed Spectrum

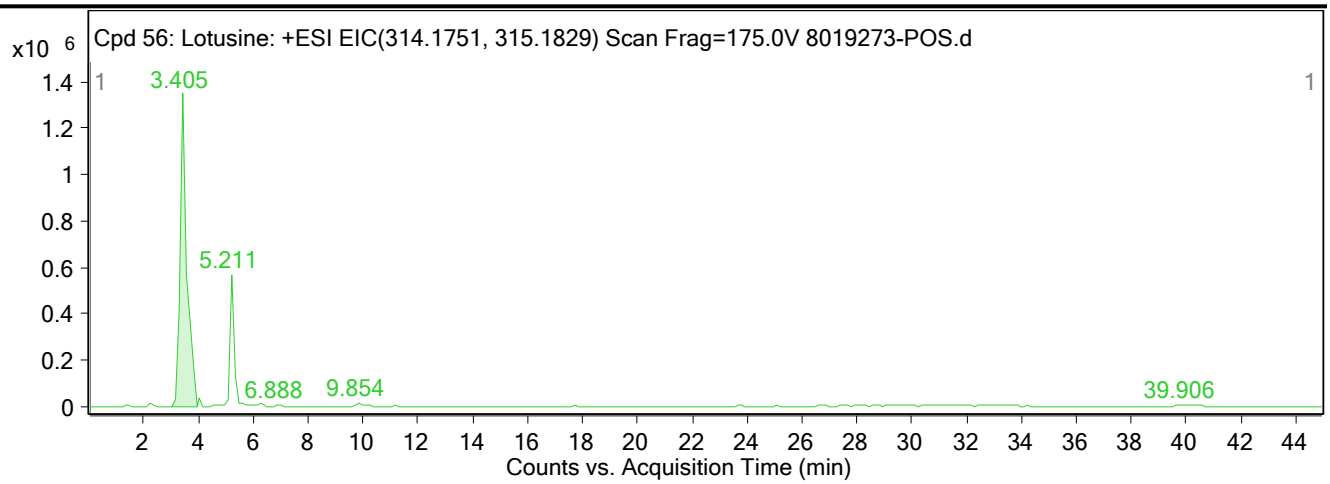



**MS Spectrum Peak List**

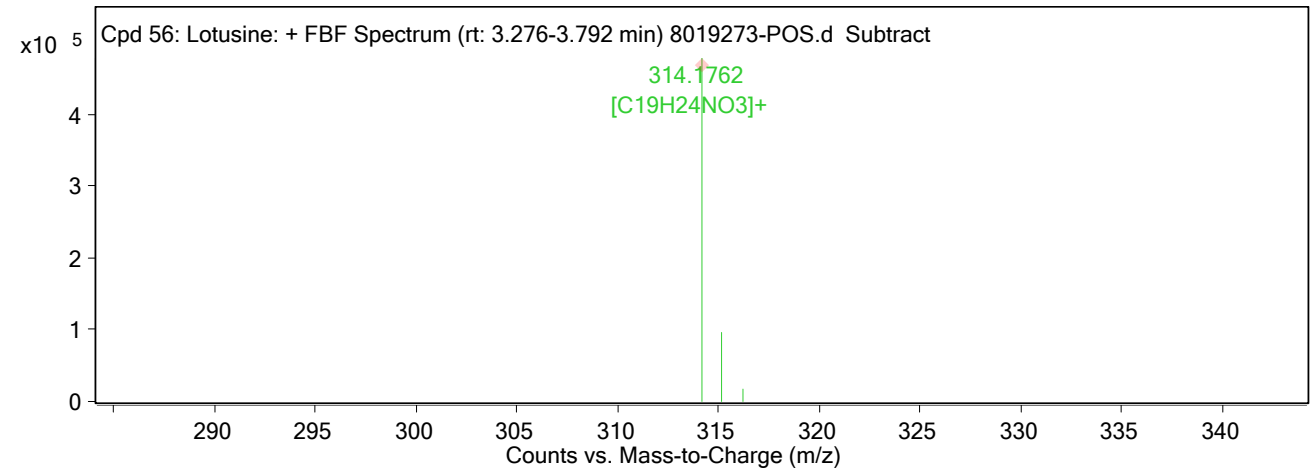
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 218.1373 | 1 | 1146.04 | C13H18N2O | M+ |
| 219.148 | 1 | 15583.72 | C13H18N2O | (M+H)+ |
| 220.151 | 1 | 2156.52 | C13H18N2O | (M+H)+ |
| 221.1452 | 1 | 201.56 | C13H18N2O | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 56: Lotusine | **Lotusine** | 314.1762 | 3.405 | Find By Formula | 314.1766 |

**Compound Chromatograms**




MS Zoomed Spectrum

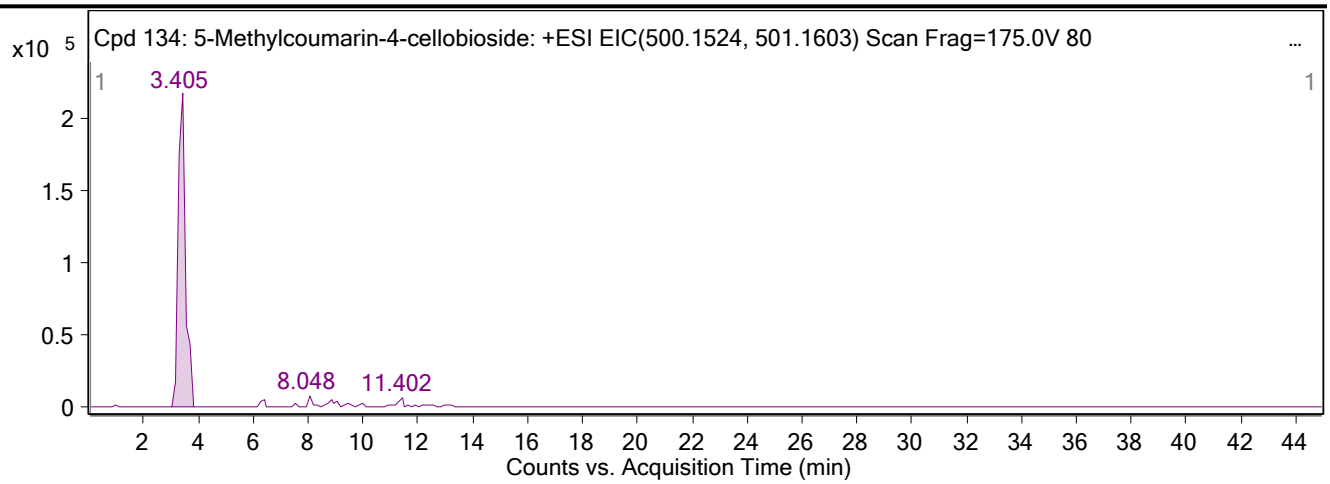



**MS Spectrum Peak List**

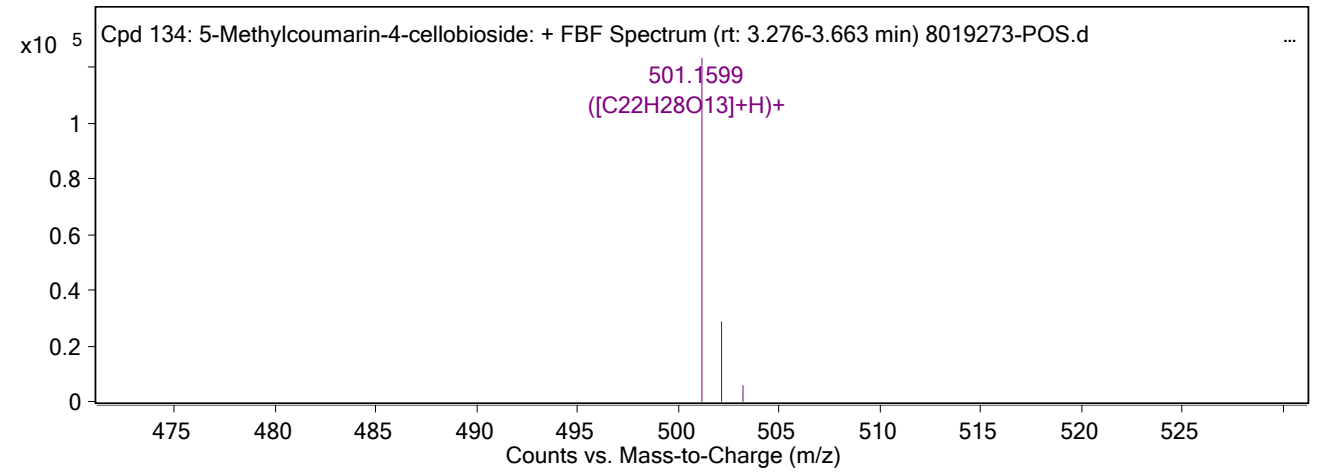
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 314.1762 | 1 | 478234.31 | C19H24NO3 | M+ |
| 315.1792 | 1 | 96022.14 | C19H24NO3 | M+ |
| 316.181 | 1 | 18459.63 | C19H24NO3 | M+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 134: 5-Methylcoumarin-4-cellobioside | **5-Methylcoumarin-4-cellobioside** | 501.1599 | 3.405 | Find By Formula | 500.1528 |

**Compound Chromatograms**




MS Zoomed Spectrum

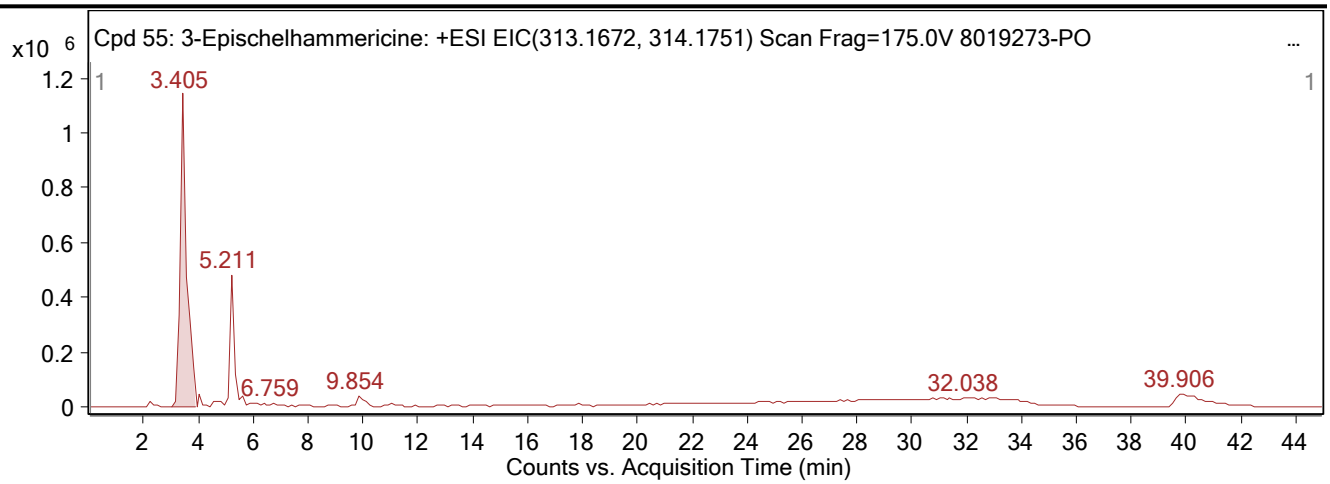



**MS Spectrum Peak List**

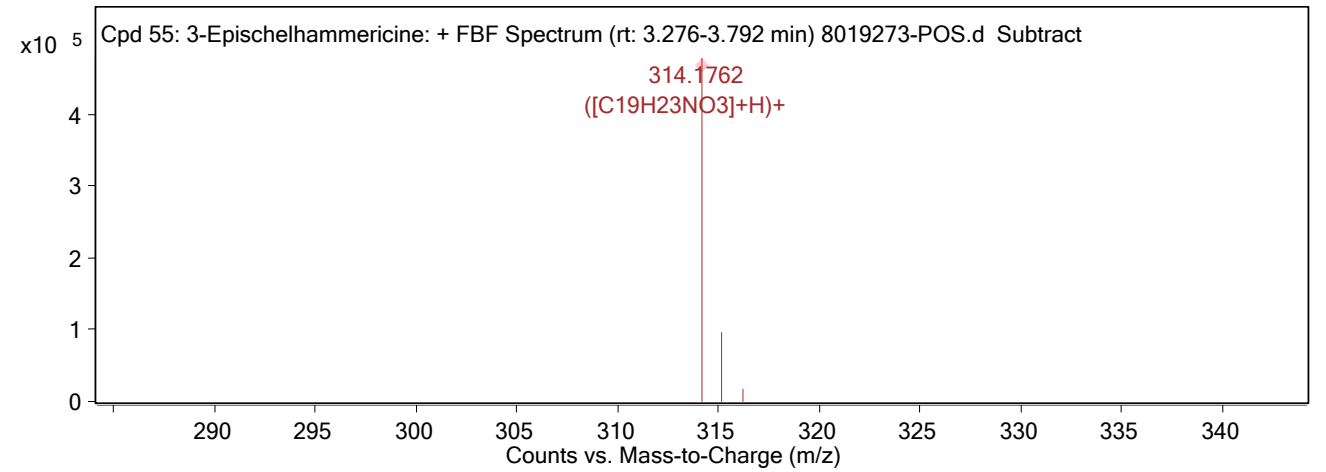
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 501.1599 | 1 | 123352.95 | C22H28O13 | (M+H)+ |
| 502.1641 | 1 | 28825.96 | C22H28O13 | (M+H)+ |
| 503.1678 | 1 | 6026.99 | C22H28O13 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 55: 3-Epischelhammericine | **3-Epischelhammericine** | 314.1762 | 3.405 | Find By Formula | 313.1688 |

**Compound Chromatograms**




MS Zoomed Spectrum

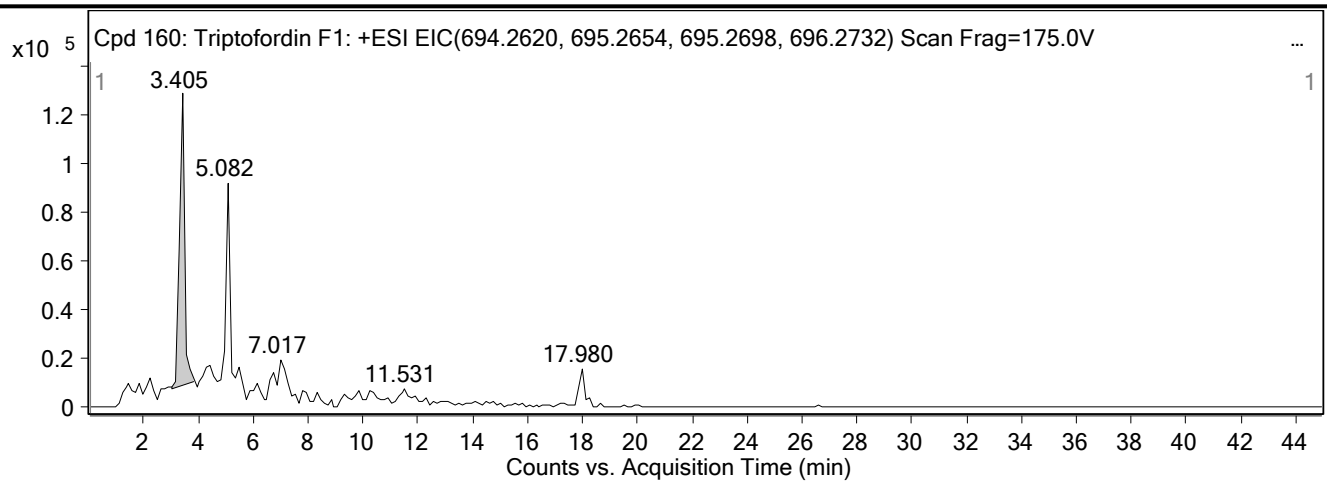



**MS Spectrum Peak List**

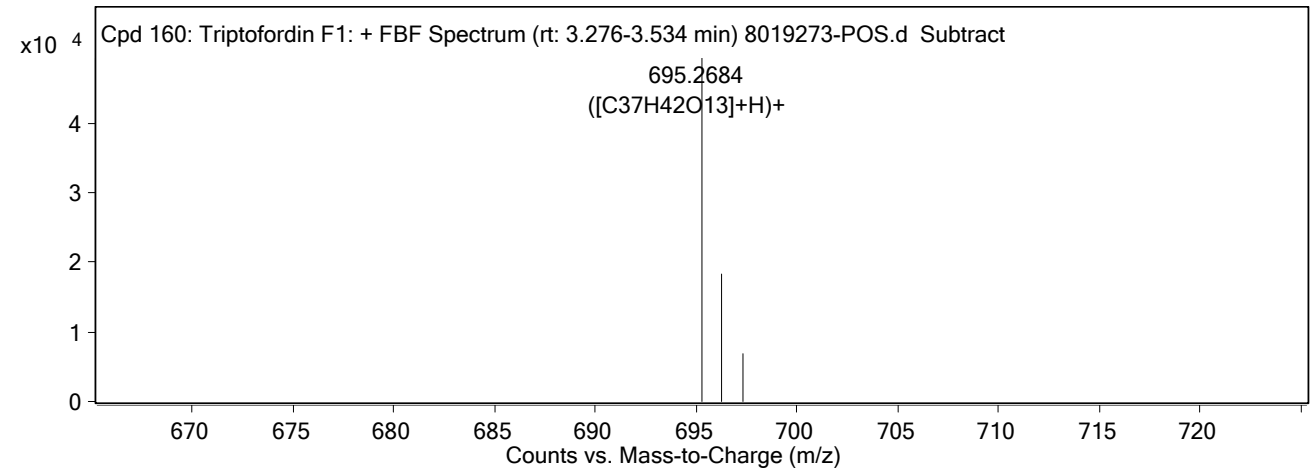
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 314.1762 | 1 | 478234.31 | C19H23NO3 | (M+H)+ |
| 315.1792 | 1 | 96022.14 | C19H23NO3 | (M+H)+ |
| 316.181 | 1 | 18459.63 | C19H23NO3 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 160: Triptofordin F1 | **Triptofordin F1** | 695.2684 | 3.405 | Find By Formula | 694.261 |

**Compound Chromatograms**




MS Zoomed Spectrum

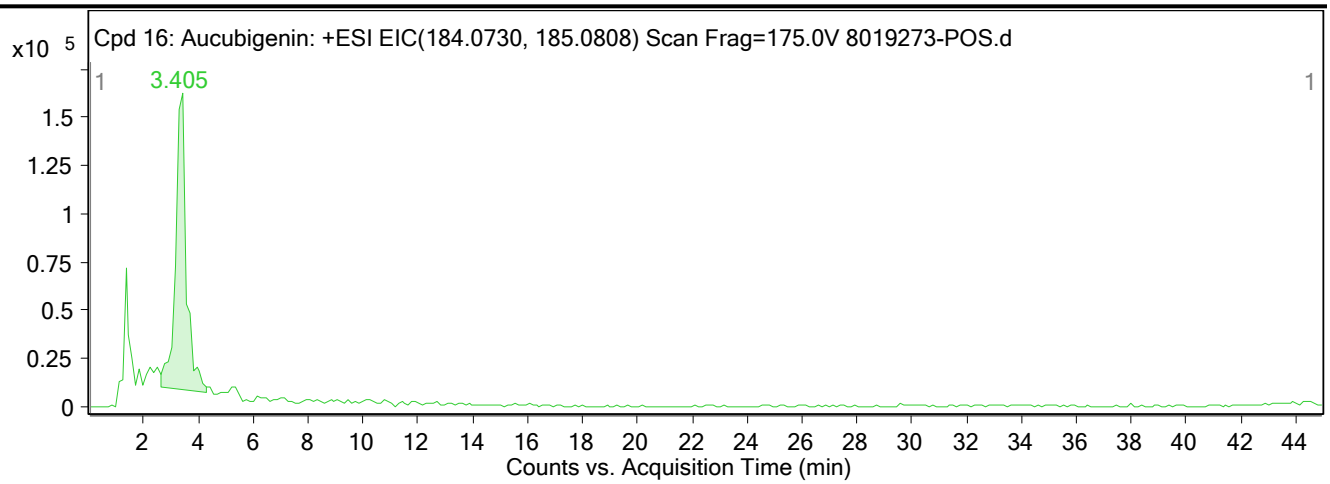



**MS Spectrum Peak List**

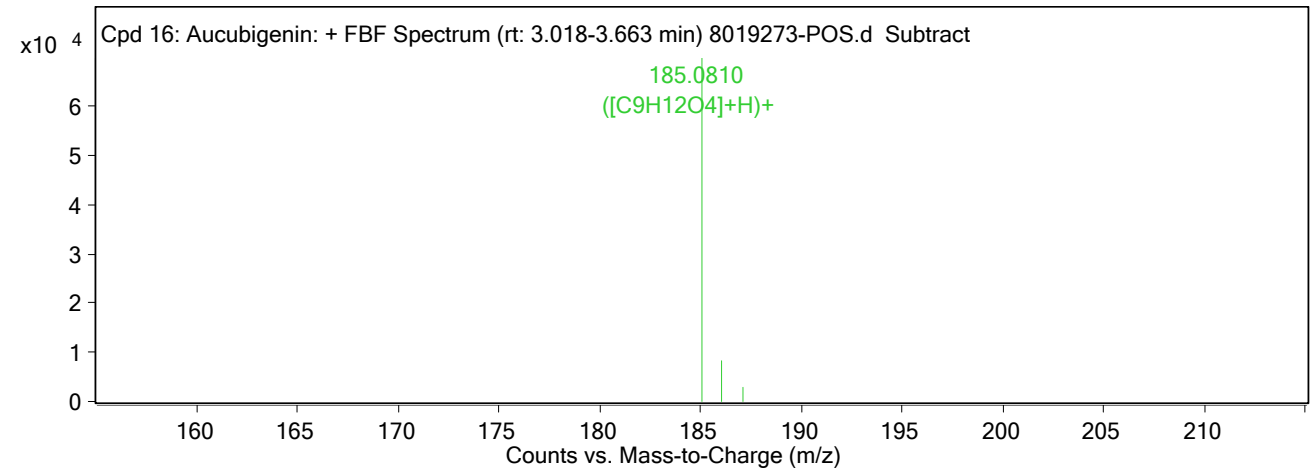
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 695.2684 | 1 | 49371.36 | C37H42O13 | (M+H)+ |
| 696.2716 | 1 | 18269.28 | C37H42O13 | (M+H)+ |
| 697.2746 | 1 | 7005.76 | C37H42O13 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 16: Aucubigenin | **Aucubigenin** | 185.081 | 3.405 | Find By Formula | 184.0738 |

**Compound Chromatograms**




MS Zoomed Spectrum

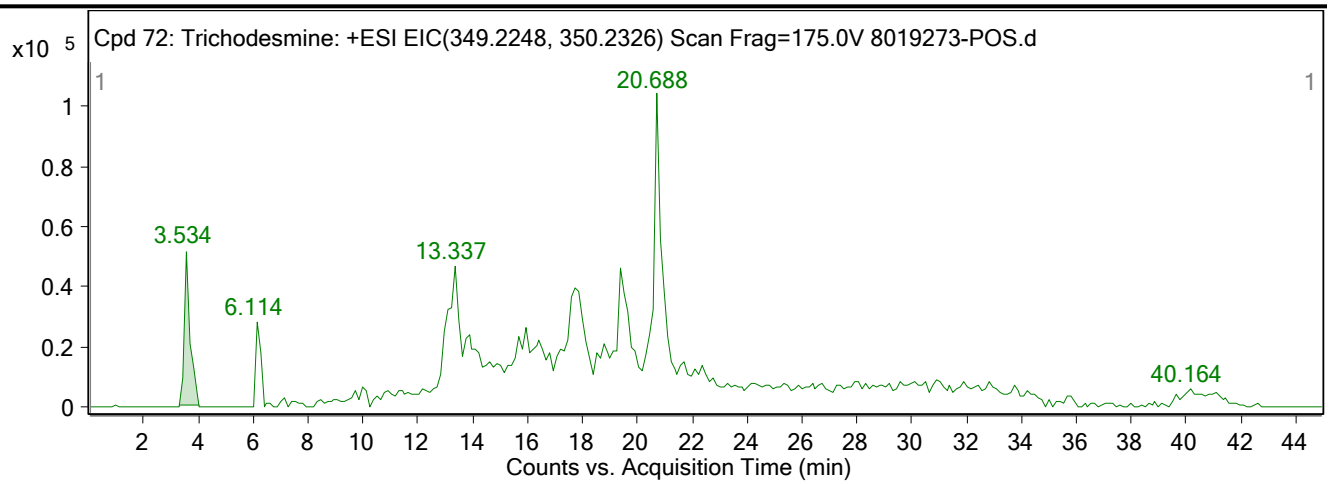



**MS Spectrum Peak List**

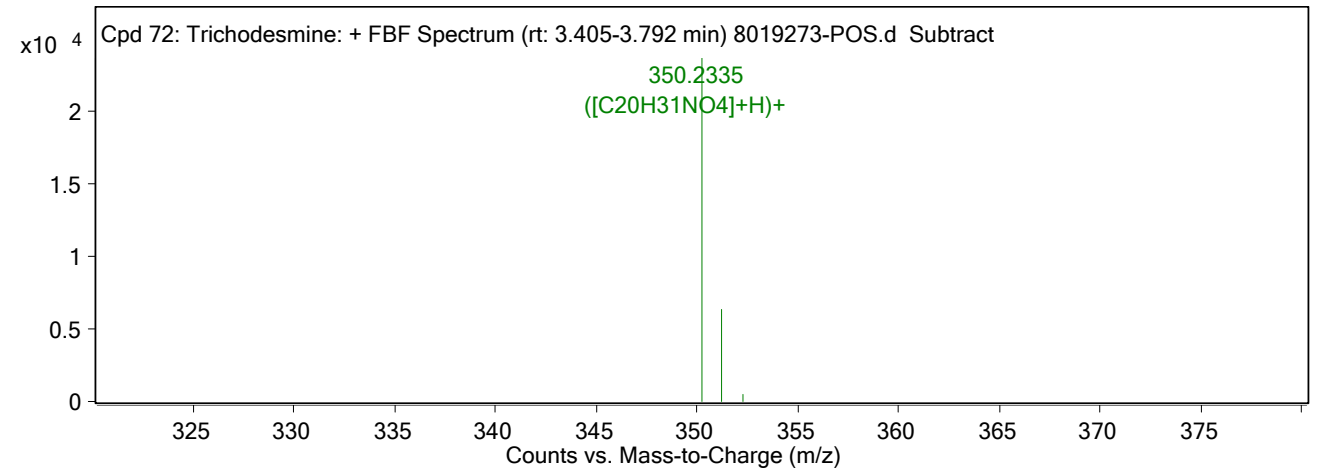
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 185.081 | 1 | 69864.02 | C9H12O4 | (M+H)+ |
| 186.0855 | 1 | 8243.22 | C9H12O4 | (M+H)+ |
| 187.0868 | 1 | 3024.08 | C9H12O4 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 72: Trichodesmine | **Trichodesmine** | 350.2335 | 3.534 | Find By Formula | 349.2259 |

**Compound Chromatograms**




MS Zoomed Spectrum

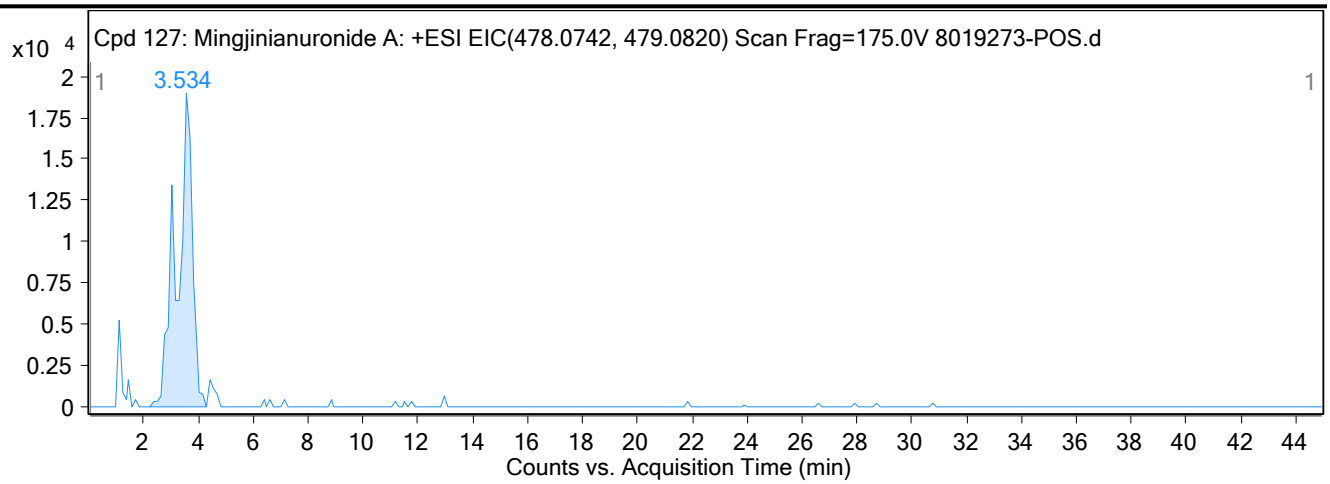



**MS Spectrum Peak List**

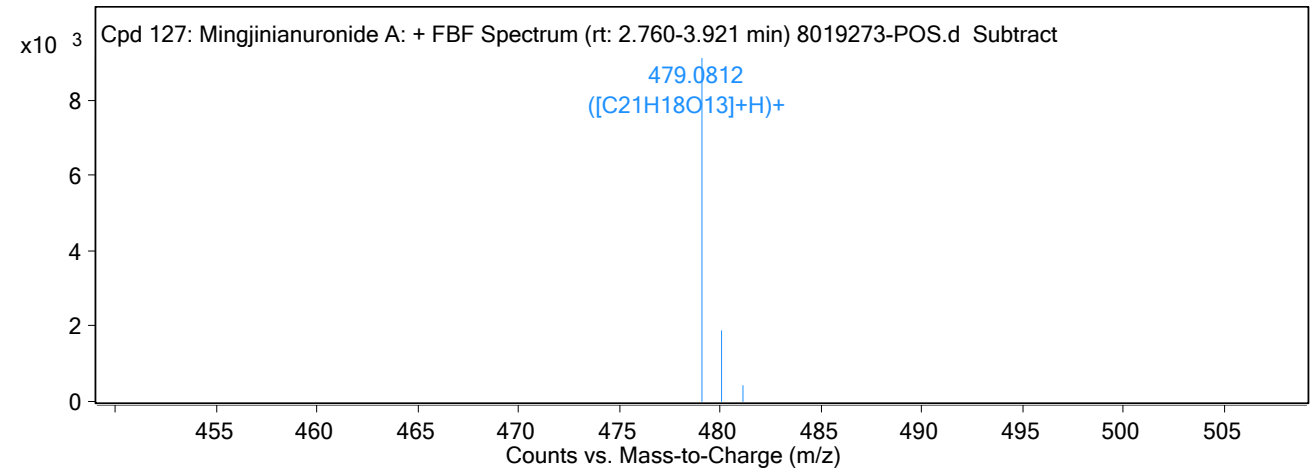
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 350.2335 | 1 | 23600.14 | C20H31NO4 | (M+H)+ |
| 351.2357 | 1 | 6370.46 | C20H31NO4 | (M+H)+ |
| 352.2359 | 1 | 533.54 | C20H31NO4 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 127: Mingjinianuronide A | **Mingjinianuronide A** | 479.0812 | 3.534 | Find By Formula | 478.074 |

**Compound Chromatograms**




MS Zoomed Spectrum

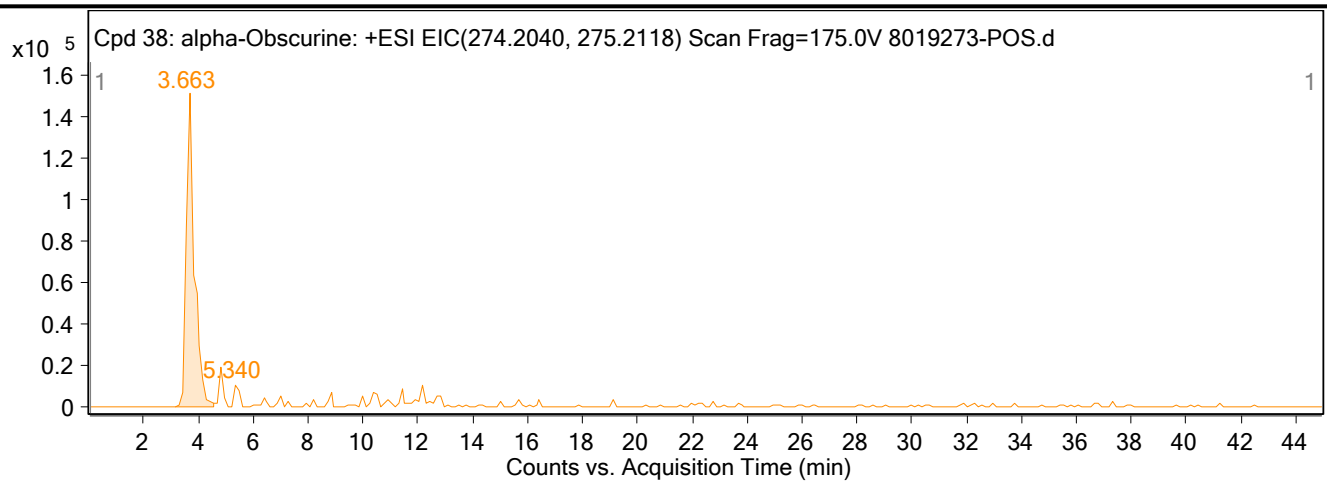



**MS Spectrum Peak List**

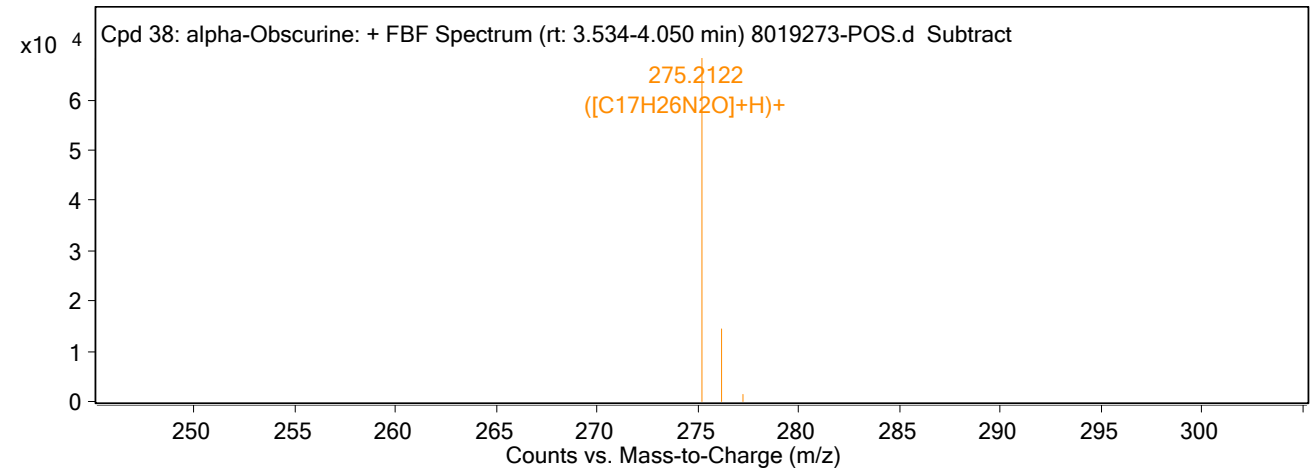
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 479.0812 | 1 | 9126.18 | C21H18O13 | (M+H)+ |
| 480.0856 | 1 | 1869.12 | C21H18O13 | (M+H)+ |
| 481.0862 | 1 | 441.7 | C21H18O13 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 38: alpha-Obscurine | **alpha-Obscurine** | 275.2122 | 3.663 | Find By Formula | 274.2047 |

**Compound Chromatograms**




MS Zoomed Spectrum

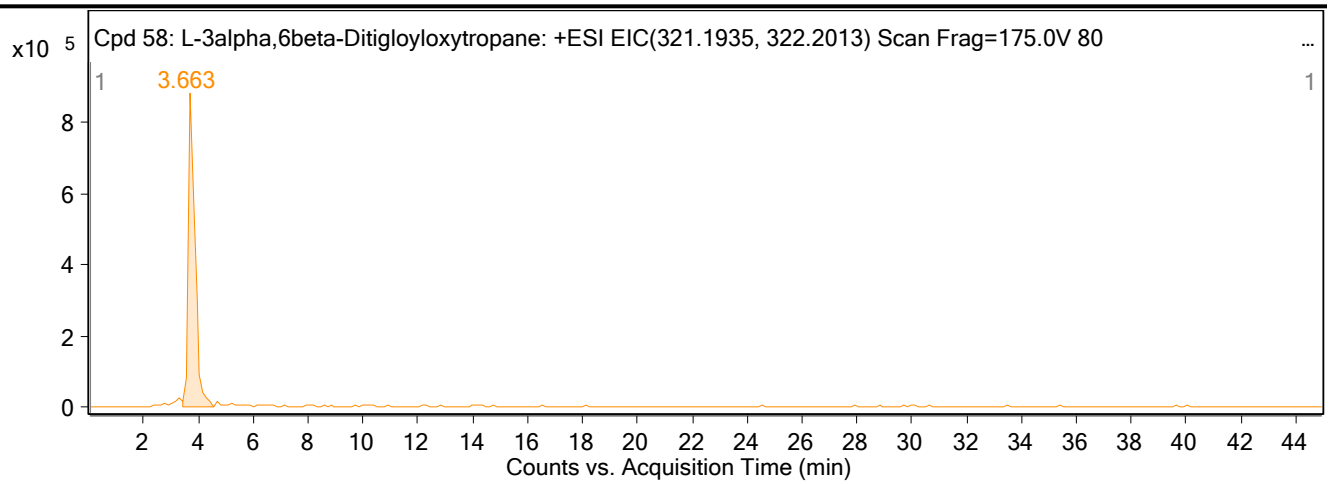



**MS Spectrum Peak List**

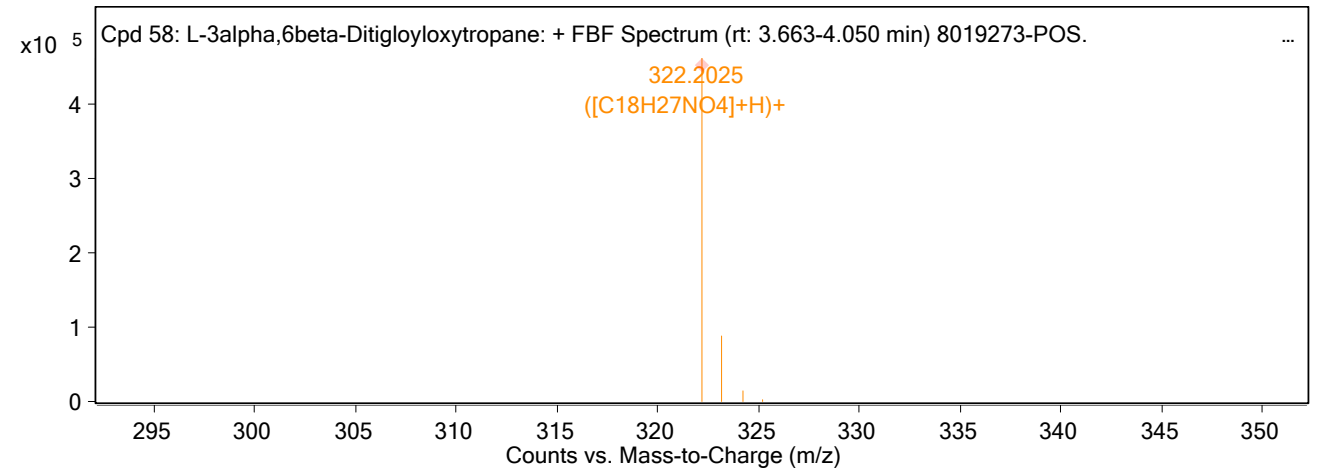
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 275.2122 | 1 | 68295.82 | C17H26N2O | (M+H)+ |
| 276.2148 | 1 | 14500.44 | C17H26N2O | (M+H)+ |
| 277.2151 | 1 | 1367.38 | C17H26N2O | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 58: L-3alpha,6beta-Ditigloyloxytropane | **L-3alpha,6beta-Ditigloyloxytropane** | 322.2025 | 3.663 | Find By Formula | 321.195 |

**Compound Chromatograms**




MS Zoomed Spectrum

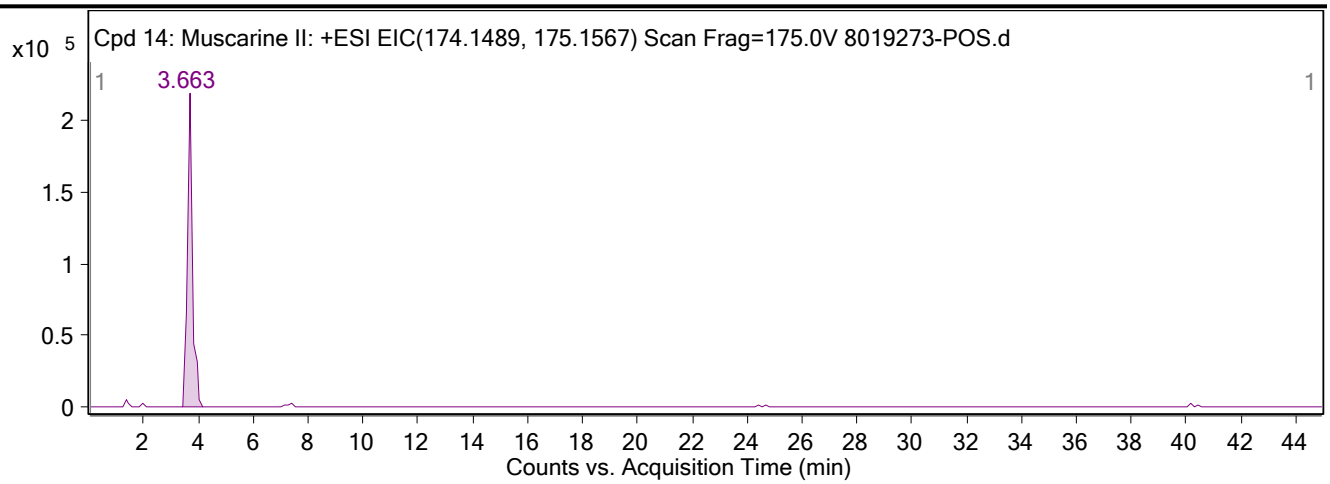



**MS Spectrum Peak List**

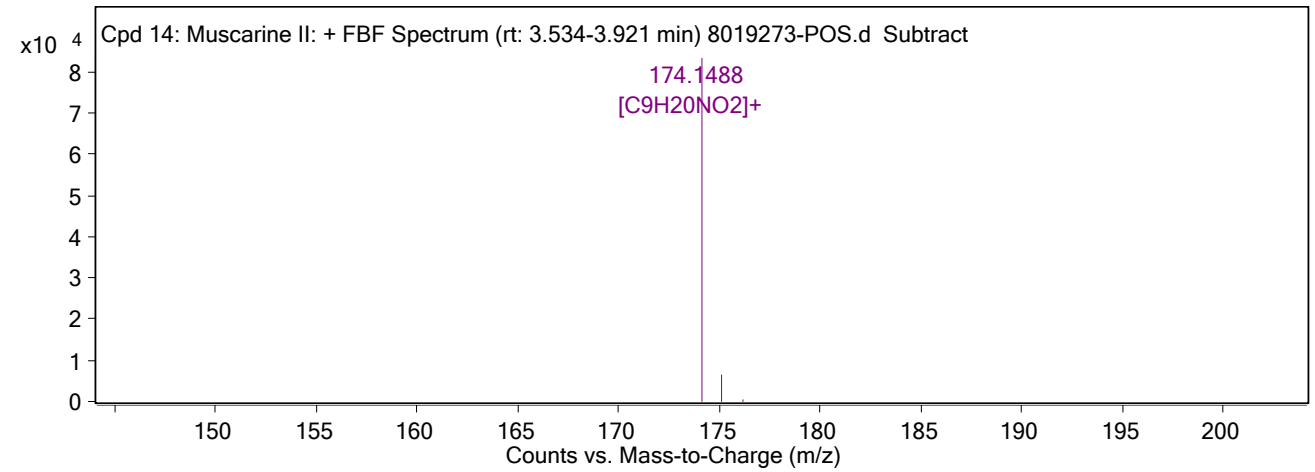
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 322.2025 | 1 | 462809.97 | C18H27NO4 | (M+H)+ |
| 323.2057 | 1 | 88109.65 | C18H27NO4 | (M+H)+ |
| 324.2021 | 1 | 15612.85 | C18H27NO4 | (M+H)+ |
| 325.2004 | 1 | 1891.26 | C18H27NO4 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 14: Muscarine II | **Muscarine II** | 174.1488 | 3.663 | Find By Formula | 174.1493 |

**Compound Chromatograms**




MS Zoomed Spectrum

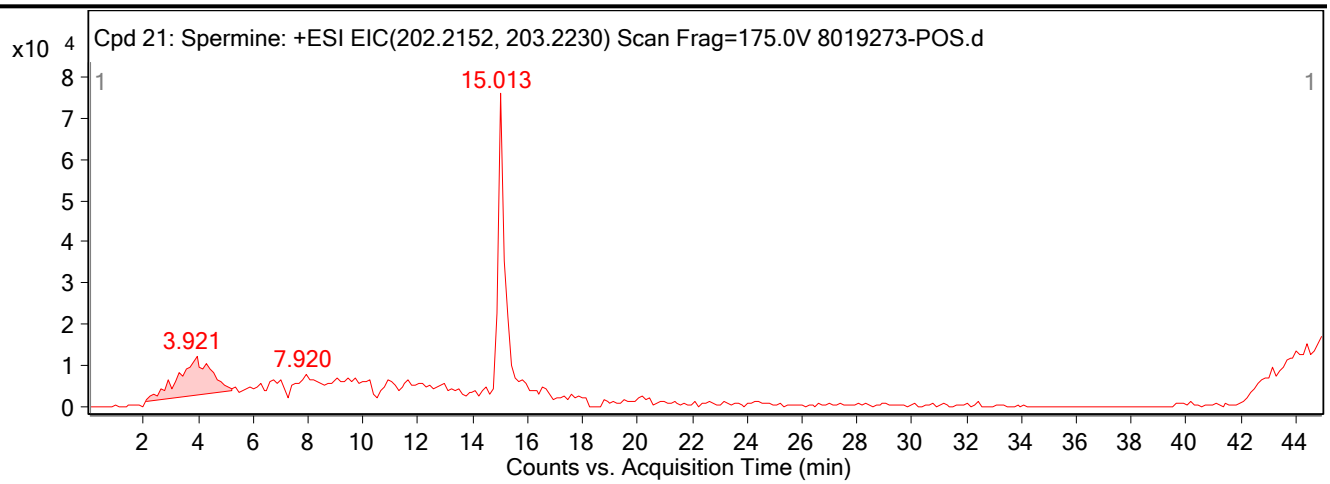



**MS Spectrum Peak List**

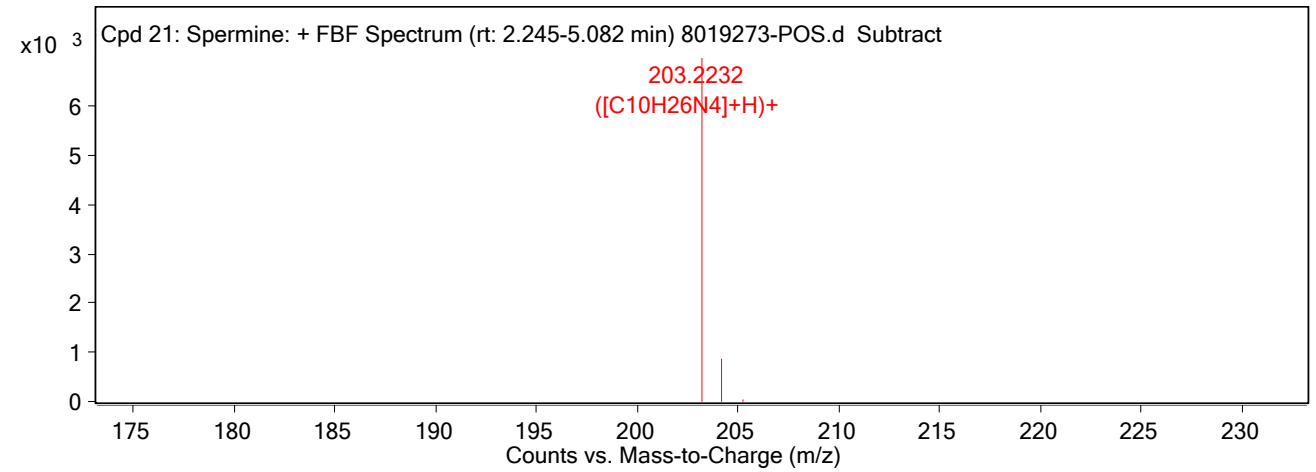
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 174.1488 | 1 | 83422.88 | C9H20NO2 | M+ |
| 175.1511 | 1 | 6396.9 | C9H20NO2 | M+ |
| 176.1523 | 1 | 556.4 | C9H20NO2 | M+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 21: Spermine | **Spermine** | 203.2232 | 3.921 | Find By Formula | 202.2159 |

**Compound Chromatograms**




MS Zoomed Spectrum

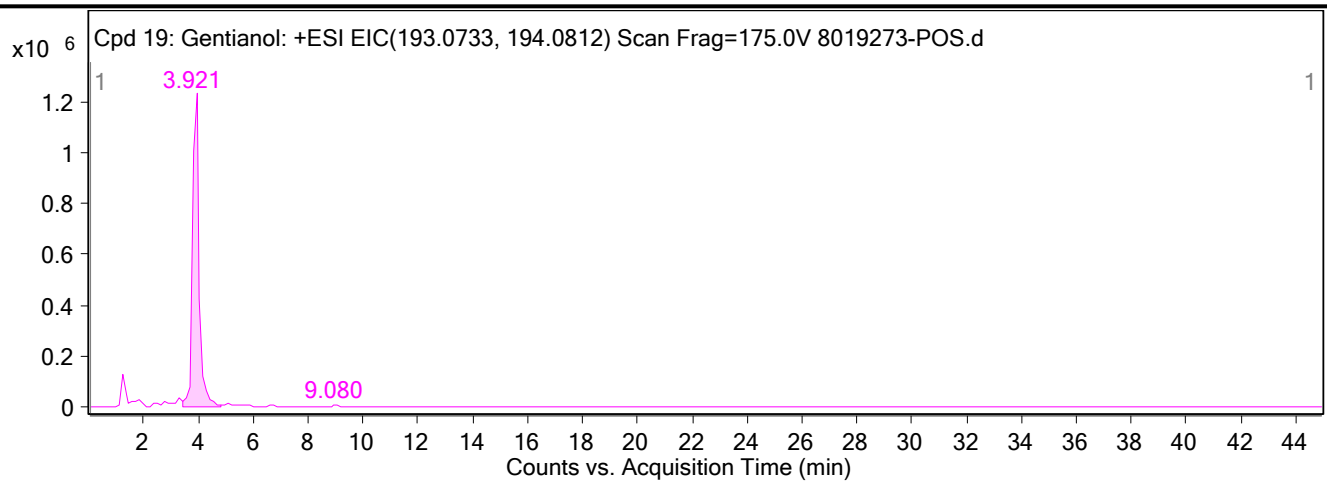



**MS Spectrum Peak List**

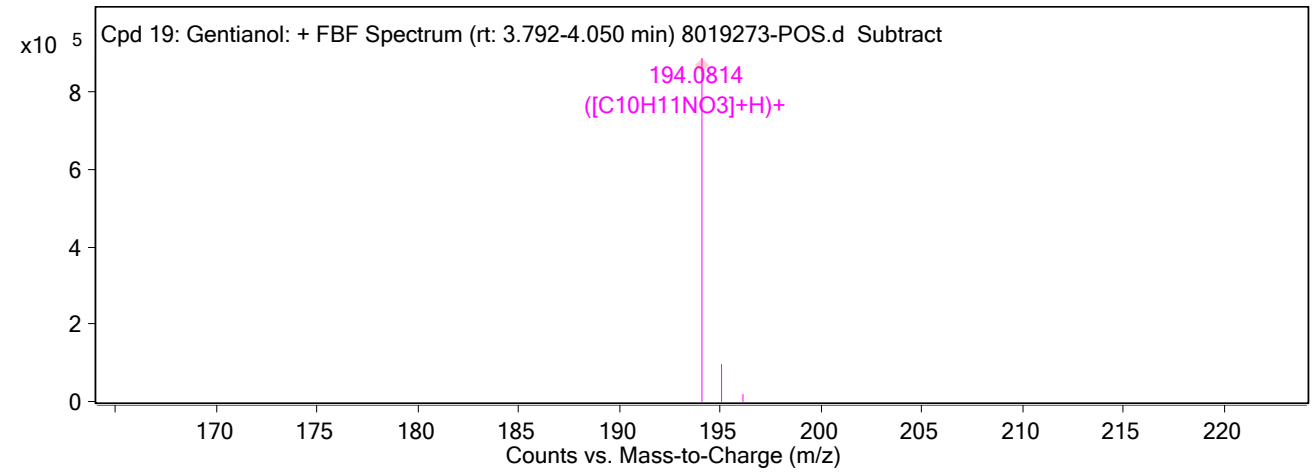
| m/z | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 203.2232 | 1 | 6977.29 | C10H26N4 | (M+H)+ |
| 204.2264 | 1 | 857.24 | C10H26N4 | (M+H)+ |
| 205.232 | 1 | 28.81 | C10H26N4 | (M+H)+ |

| Compound Label | Name | m/z | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 19: Gentianol | **Gentianol** | 194.0814 | 3.921 | Find By Formula | 193.0743 |

**Compound Chromatograms**




MS Zoomed Spectrum

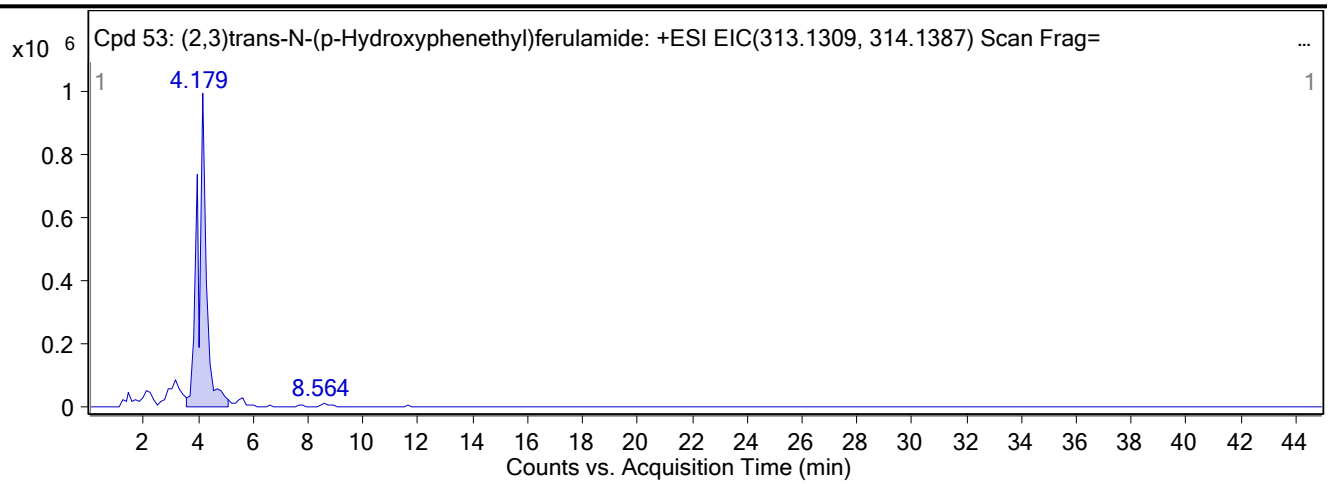



**MS Spectrum Peak List**

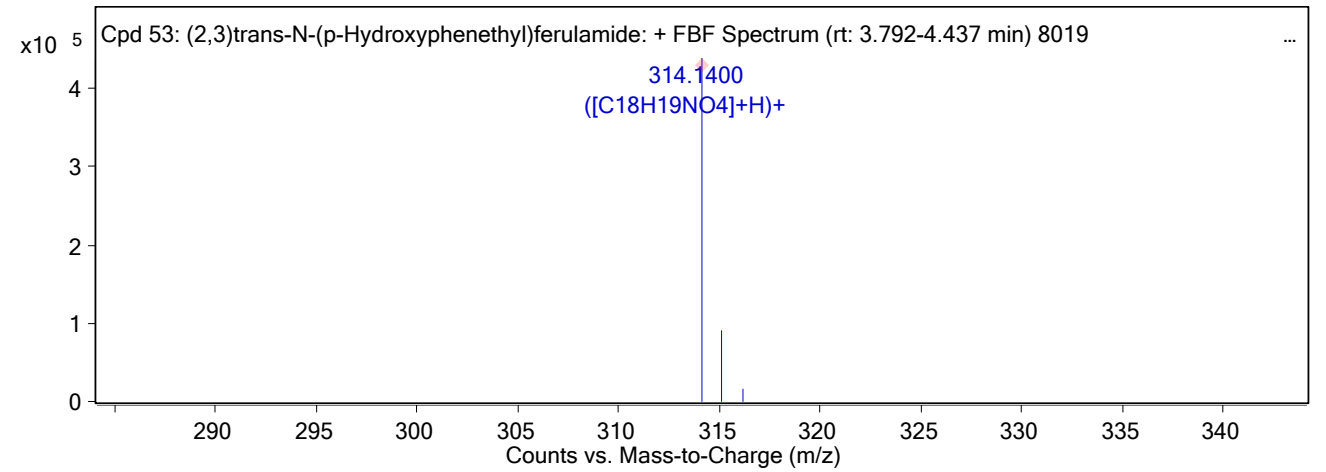
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 194.0814 | 1 | 887599.25 | C10H11NO3 | (M+H)+ |
| 195.0848 | 1 | 96263.28 | C10H11NO3 | (M+H)+ |
| 196.0946 | 1 | 19106.02 | C10H11NO3 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 53: (2,3)trans-N-(p-Hydroxyphenethyl)ferula mide | **(2,3)trans-N-(p-Hydroxyphenethyl)fer ulamide** | 314.14 | 4.179 | Find By Formula | 313.1325 |

**Compound Chromatograms**




MS Zoomed Spectrum

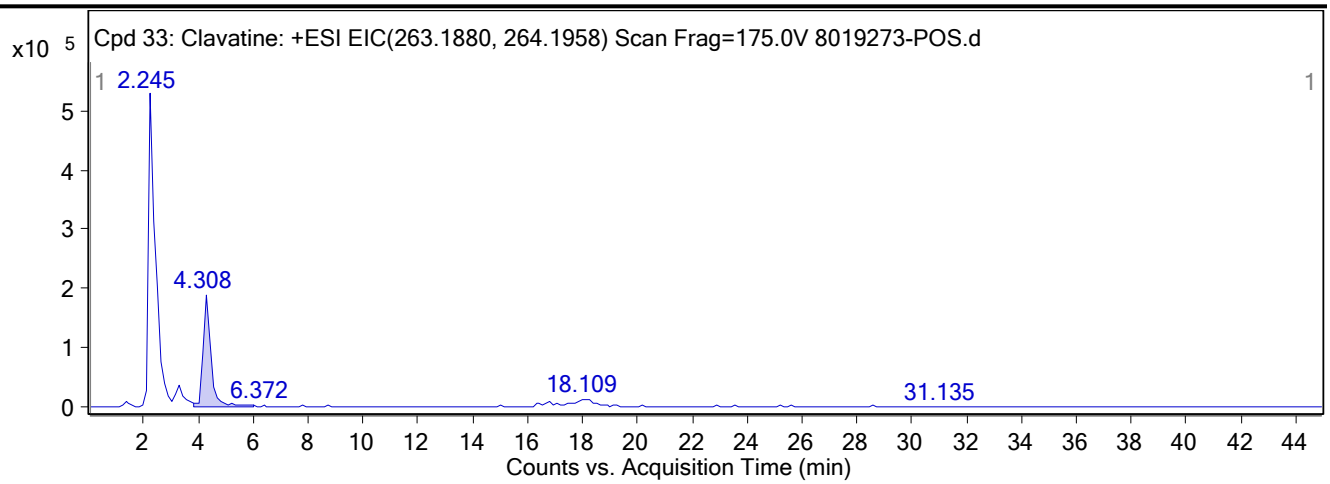



**MS Spectrum Peak List**

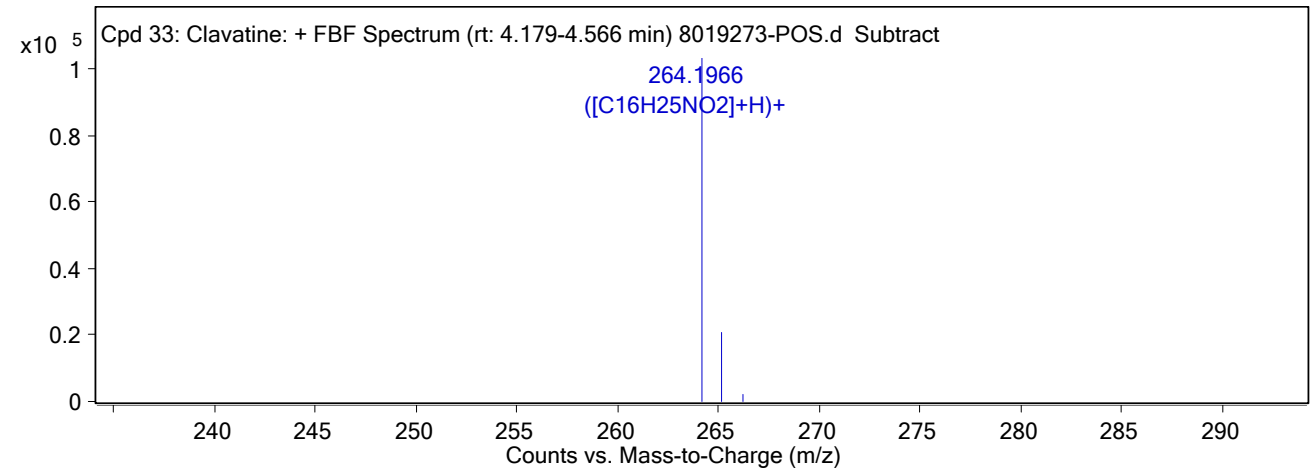
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 314.14 | 1 | 438922.78 | C18H19NO4 | (M+H)+ |
| 315.1425 | 1 | 90454.07 | C18H19NO4 | (M+H)+ |
| 316.1444 | 1 | 16171.85 | C18H19NO4 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 33: Clavatine | **Clavatine** | 264.1966 | 4.308 | Find By Formula | 263.1891 |

**Compound Chromatograms**




MS Zoomed Spectrum

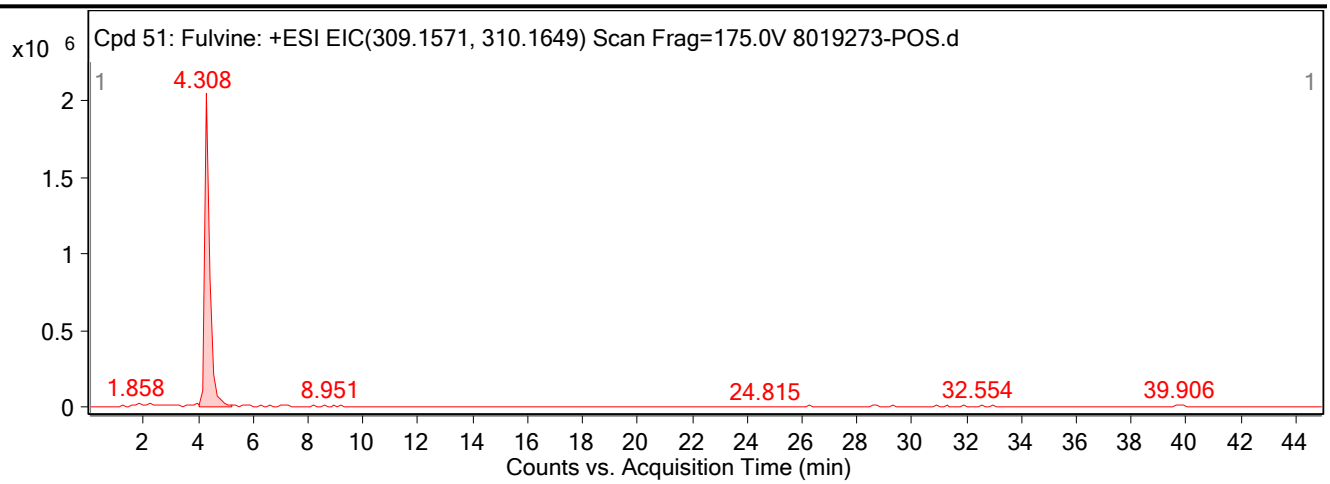



**MS Spectrum Peak List**

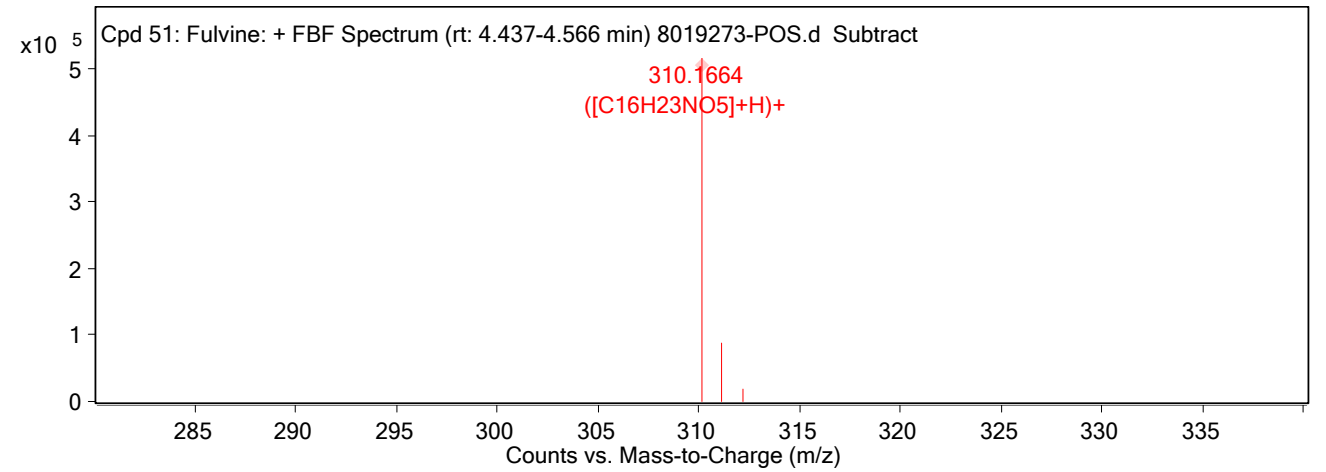
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 264.1966 | 1 | 103353.14 | C16H25NO2 | (M+H)+ |
| 265.1993 | 1 | 20601.23 | C16H25NO2 | (M+H)+ |
| 266.1997 | 1 | 1981.99 | C16H25NO2 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 51: Fulvine | **Fulvine** | 310.1664 | 4.308 | Find By Formula | 309.1589 |

**Compound Chromatograms**




MS Zoomed Spectrum

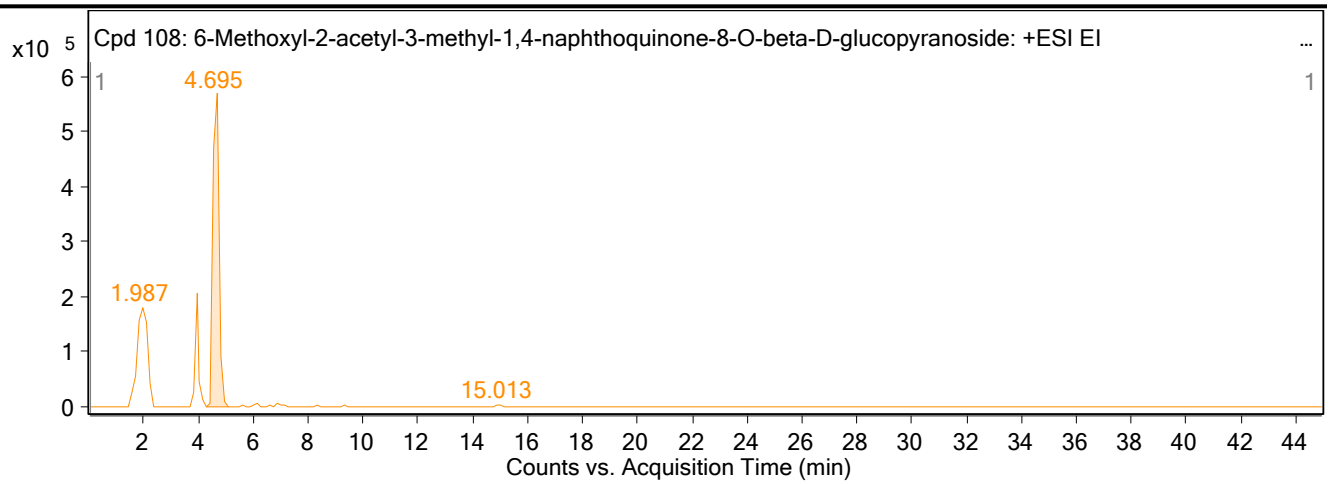



**MS Spectrum Peak List**

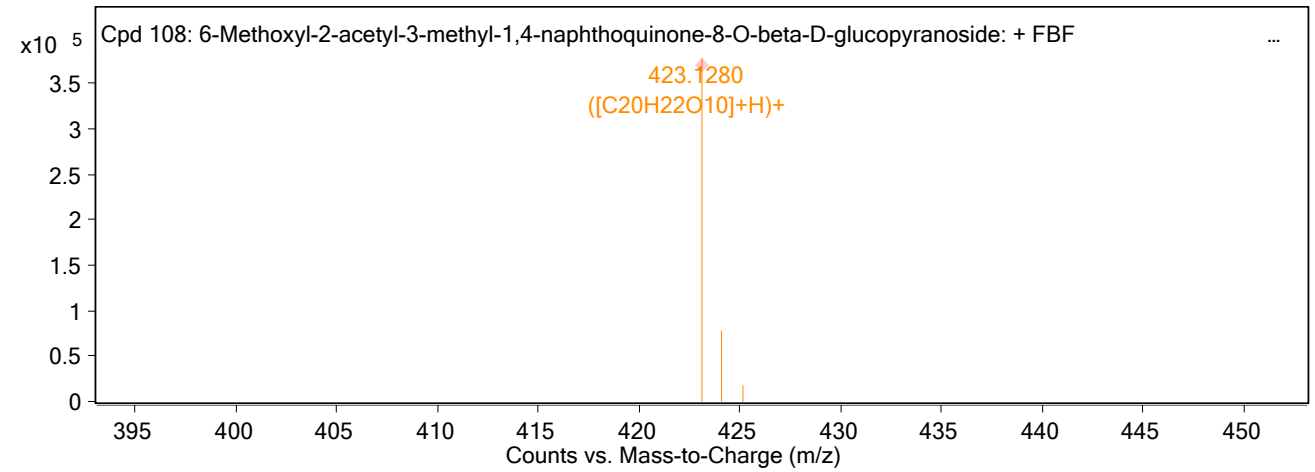
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 310.1664 | 1 | 516867.75 | C16H23NO5 | (M+H)+ |
| 311.1693 | 1 | 88731.66 | C16H23NO5 | (M+H)+ |
| 312.1658 | 1 | 18546.17 | C16H23NO5 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 108: 6-Methoxyl-2-acetyl-3-methyl-1,4-naphthoquinone-8-O-beta-D-glucopyranoside | **6-Methoxyl-2-acetyl-3-methyl-1,4-naphthoquinone-8-O-beta-D-glucopyranoside** | 423.128 | 4.695 | Find By Formula | 422.1209 |

**Compound Chromatograms**




MS Zoomed Spectrum

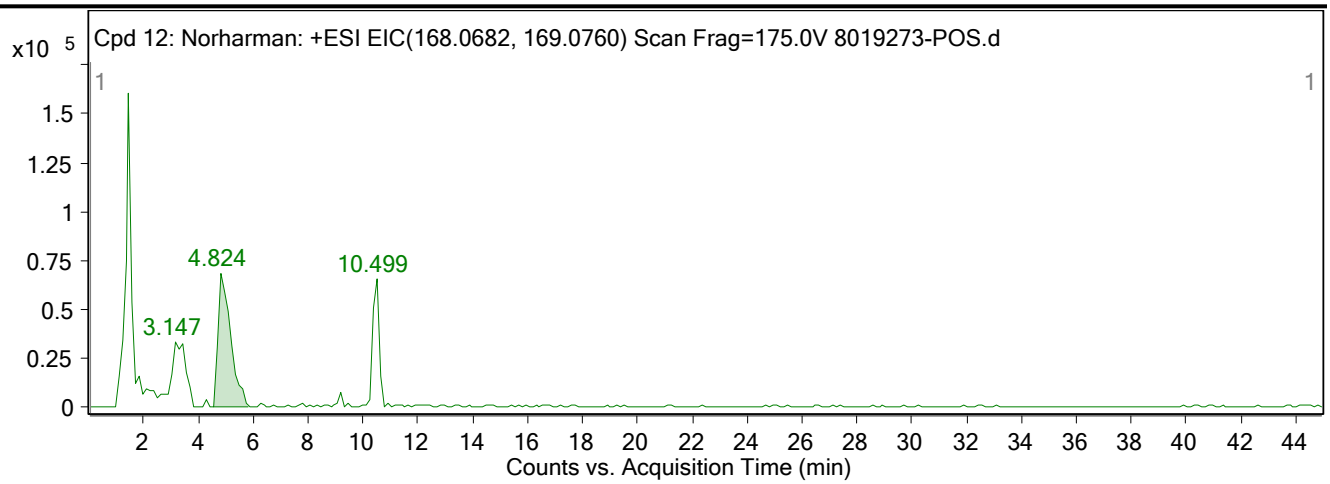



**MS Spectrum Peak List**

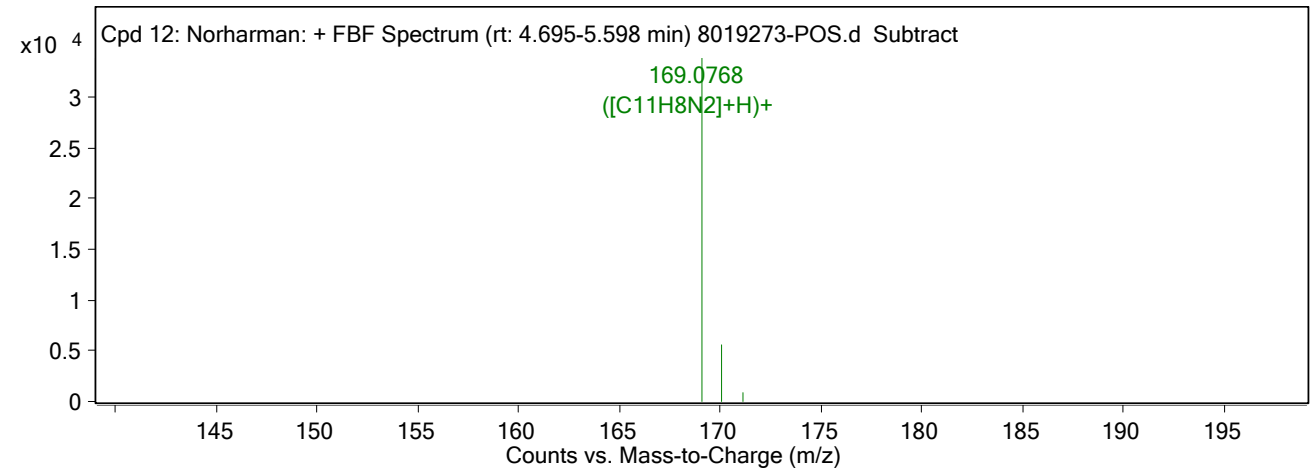
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 423.128 | 1 | 377728.13 | C20H22O10 | (M+H)+ |
| 424.1319 | 1 | 78363.66 | C20H22O10 | (M+H)+ |
| 425.1351 | 1 | 16672.11 | C20H22O10 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 12: Norharman | **Norharman** | 169.0768 | 4.824 | Find By Formula | 168.0695 |

**Compound Chromatograms**




MS Zoomed Spectrum

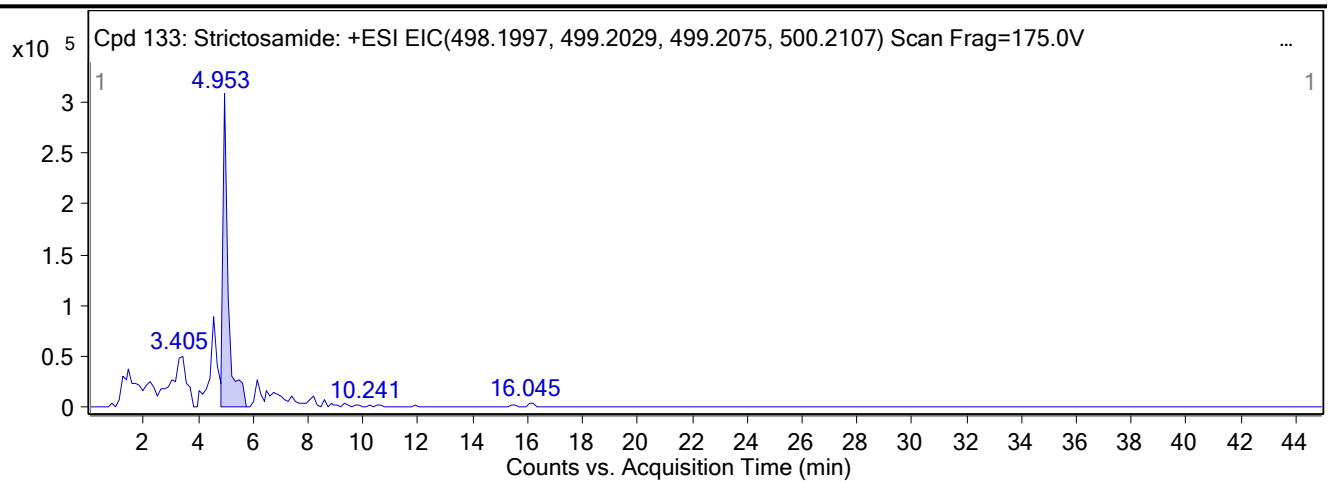



**MS Spectrum Peak List**

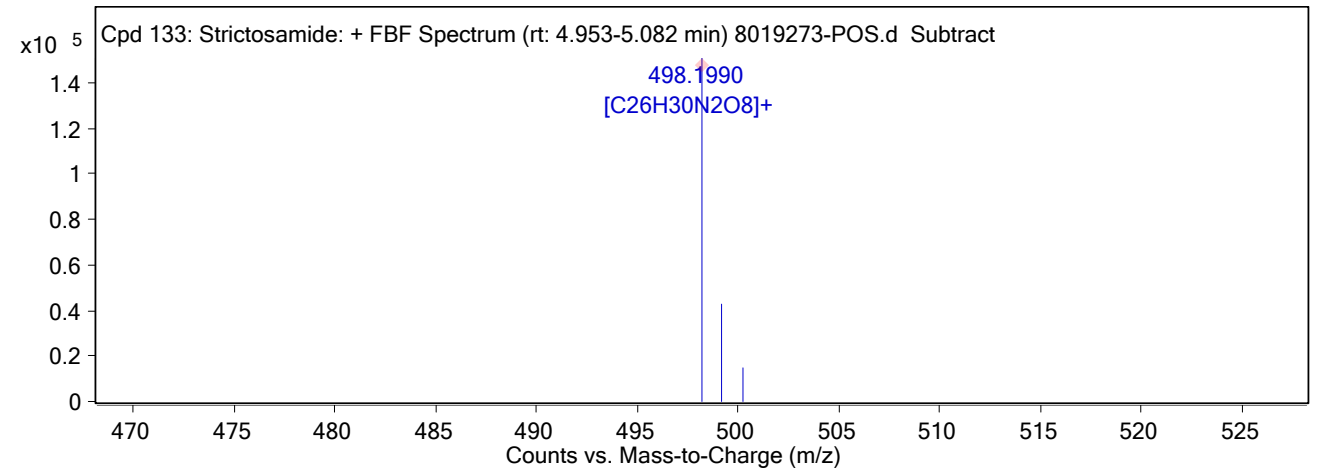
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 169.0768 | 1 | 33880.42 | C11H8N2 | (M+H)+ |
| 170.08 | 1 | 5523.41 | C11H8N2 | (M+H)+ |
| 171.0801 | 1 | 826.52 | C11H8N2 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 133: Strictosamide | **Strictosamide** | 498.199 | 4.953 | Find By Formula | 498.1998 |

**Compound Chromatograms**




MS Zoomed Spectrum

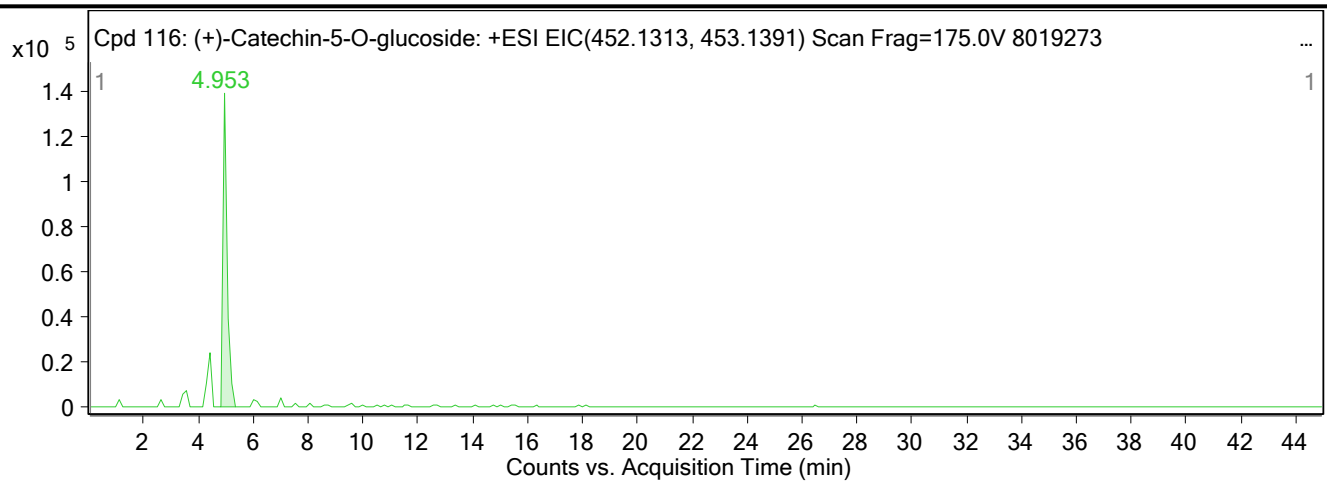



**MS Spectrum Peak List**

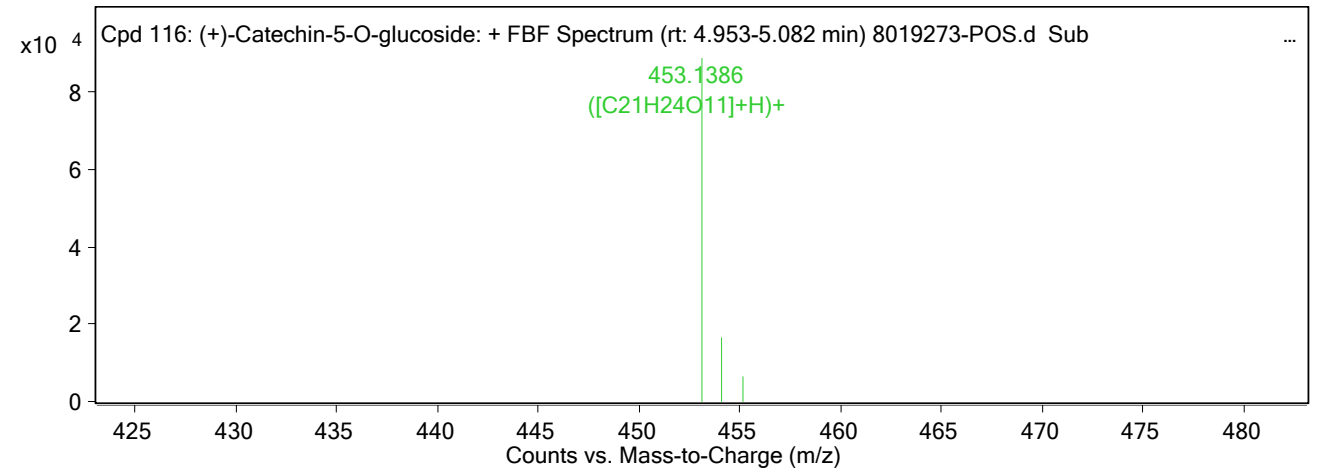
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 498.199 | 1 | 150961.47 | C26H30N2O8 | M+ |
| 499.2026 | 1 | 42970.82 | C26H30N2O8 | M+ |
| 500.2065 | 1 | 14693.53 | C26H30N2O8 | M+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 116: (+)-Catechin-5-O-glucoside | **(+)-Catechin-5-O-glucoside** | 453.1386 | 4.953 | Find By Formula | 452.1316 |

**Compound Chromatograms**




MS Zoomed Spectrum

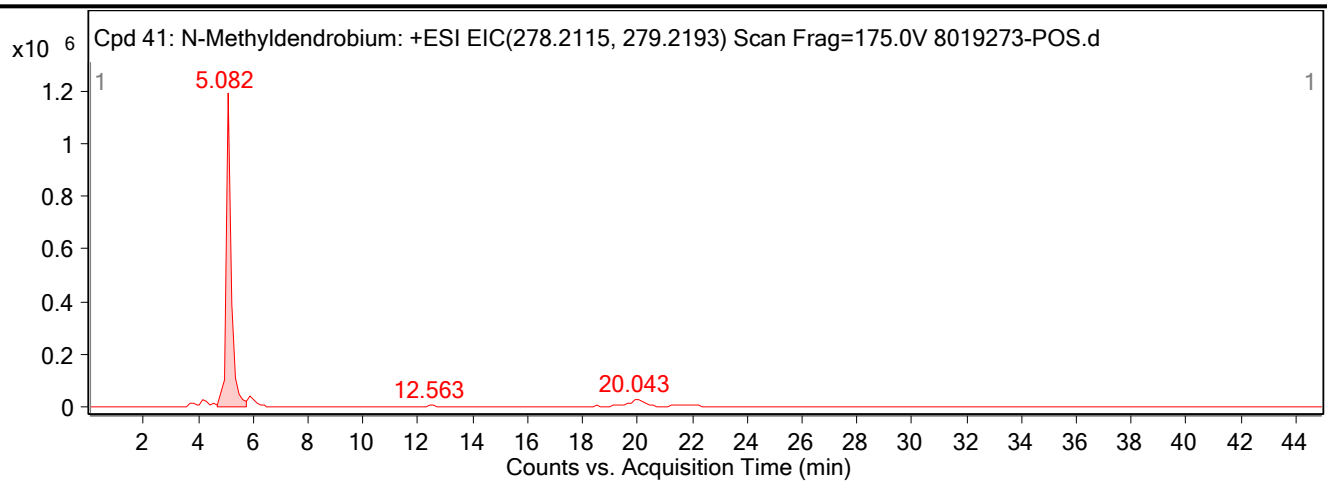



**MS Spectrum Peak List**

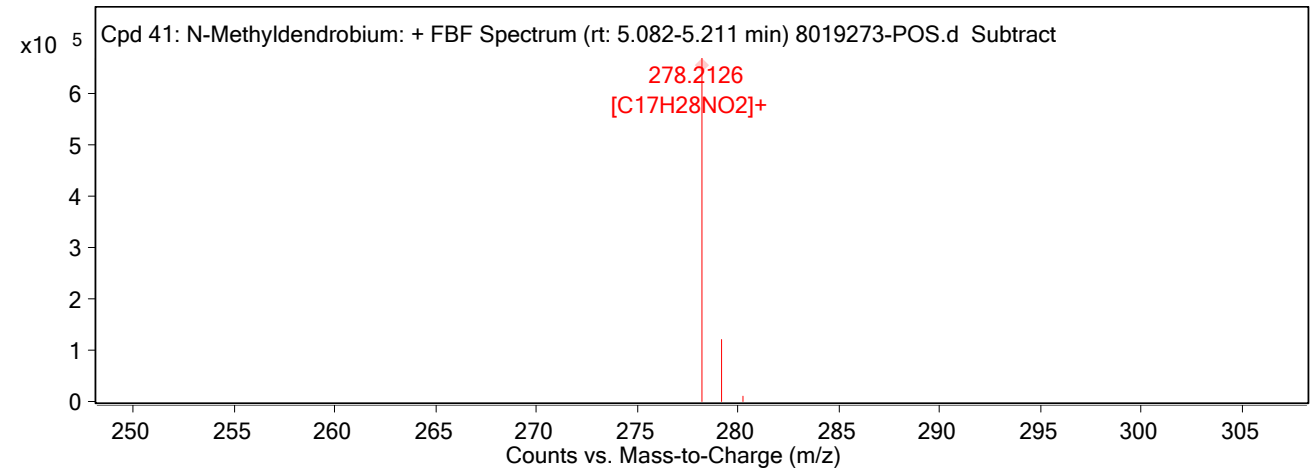
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 453.1386 | 1 | 88914.98 | C21H24O11 | (M+H)+ |
| 454.1432 | 1 | 16362.28 | C21H24O11 | (M+H)+ |
| 455.1468 | 1 | 6361.4 | C21H24O11 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 41: N-Methyldendrobium | **N-Methyldendrobium** | 278.2126 | 5.082 | Find By Formula | 278.2131 |

**Compound Chromatograms**




MS Zoomed Spectrum

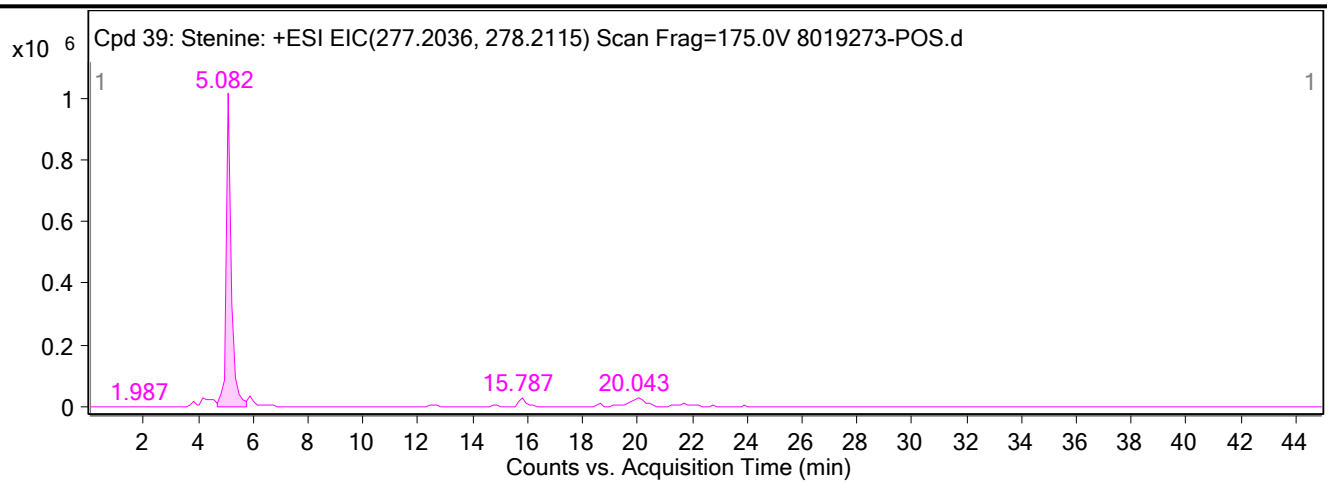



**MS Spectrum Peak List**

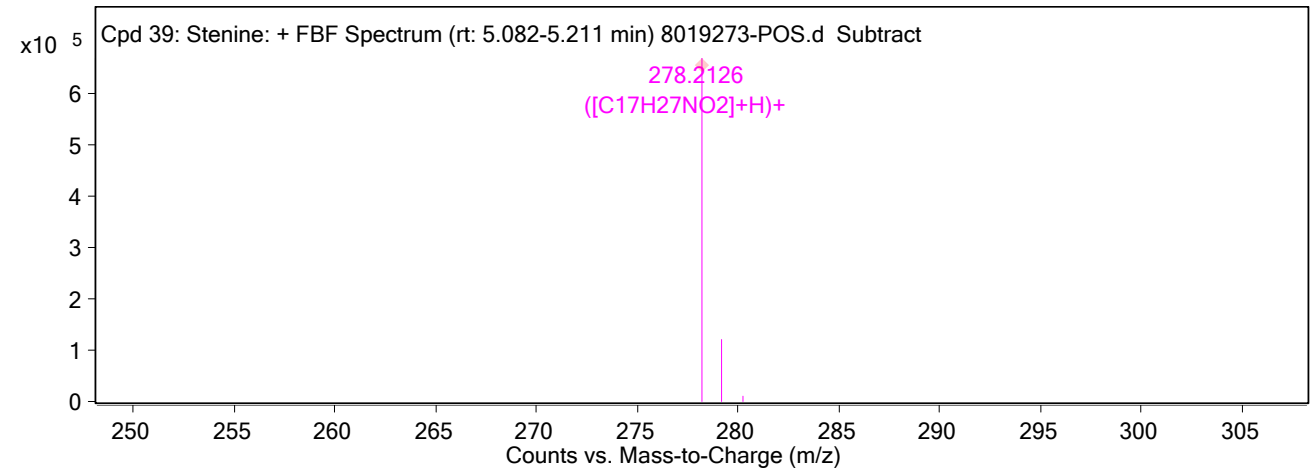
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 278.2126 | 1 | 668913.13 | C17H28NO2 | M+ |
| 279.2157 | 1 | 121851.61 | C17H28NO2 | M+ |
| 280.2178 | 1 | 11087.29 | C17H28NO2 | M+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 39: Stenine | **Stenine** | 278.2126 | 5.082 | Find By Formula | 277.2053 |

**Compound Chromatograms**




MS Zoomed Spectrum

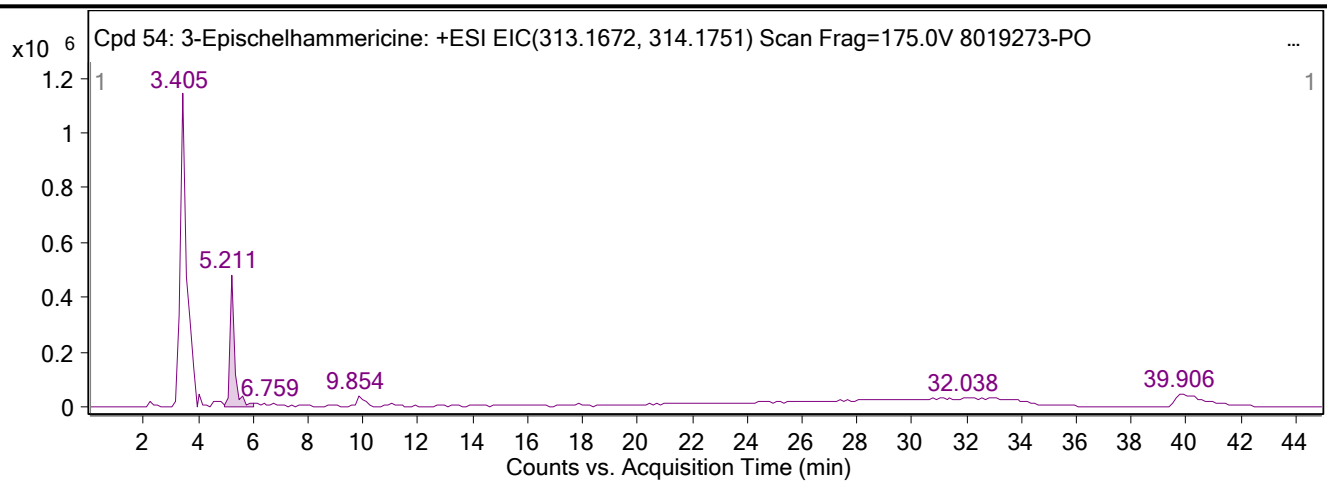



**MS Spectrum Peak List**

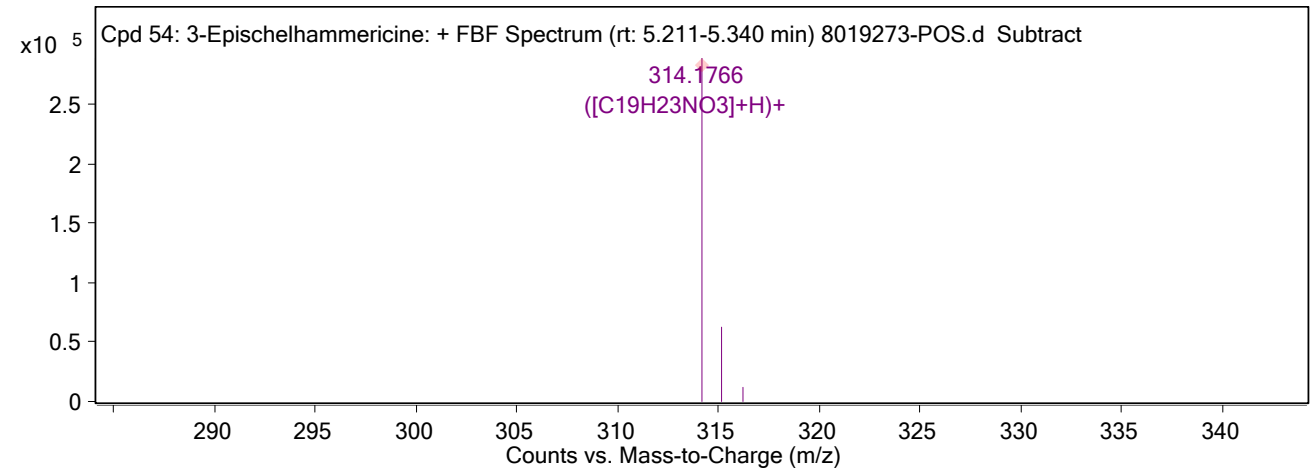
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 278.2126 | 1 | 668913.13 | C17H27NO2 | (M+H)+ |
| 279.2157 | 1 | 121851.61 | C17H27NO2 | (M+H)+ |
| 280.2178 | 1 | 11087.29 | C17H27NO2 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 54: 3-Epischelhammericine | **3-Epischelhammericine** | 314.1766 | 5.211 | Find By Formula | 313.1693 |

**Compound Chromatograms**




MS Zoomed Spectrum

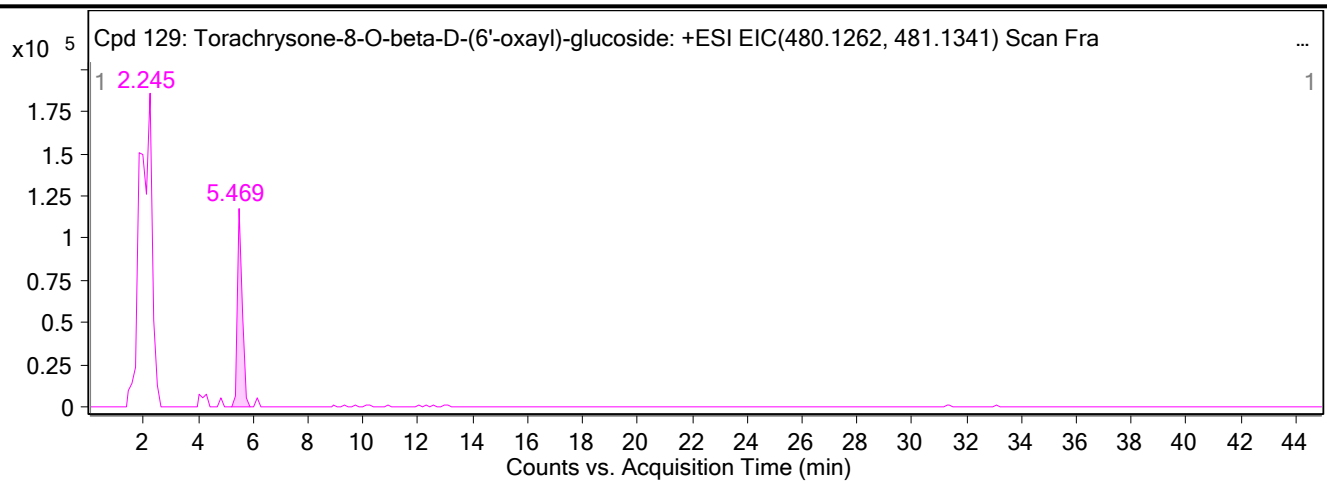



**MS Spectrum Peak List**

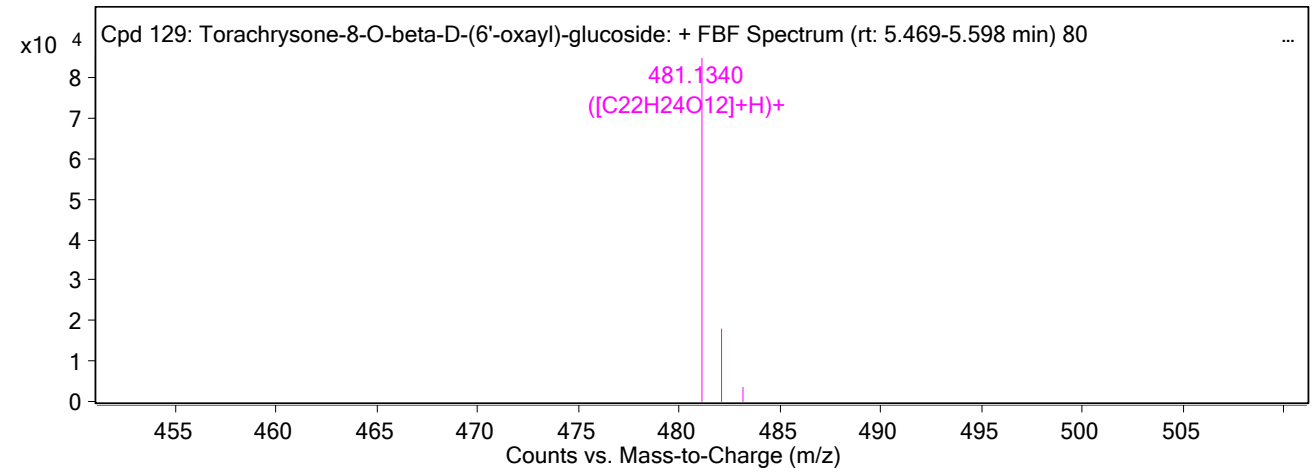
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 314.1766 | 1 | 289489.16 | C19H23NO3 | (M+H)+ |
| 315.1798 | 1 | 62062.48 | C19H23NO3 | (M+H)+ |
| 316.1811 | 1 | 11956.36 | C19H23NO3 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 129: Torachrysone-8-O-beta-D-(6'-oxayl)-glucoside | **Torachrysone-8-O-beta-D-(6'-oxayl)-glucoside** | 481.134 | 5.469 | Find By Formula | 480.1271 |

**Compound Chromatograms**




MS Zoomed Spectrum

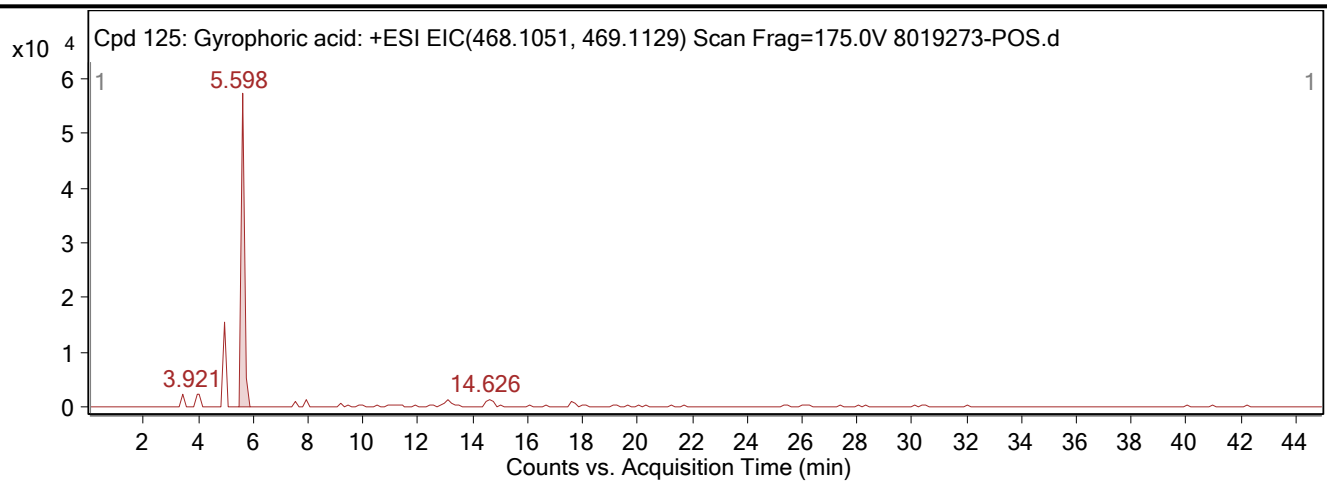



**MS Spectrum Peak List**

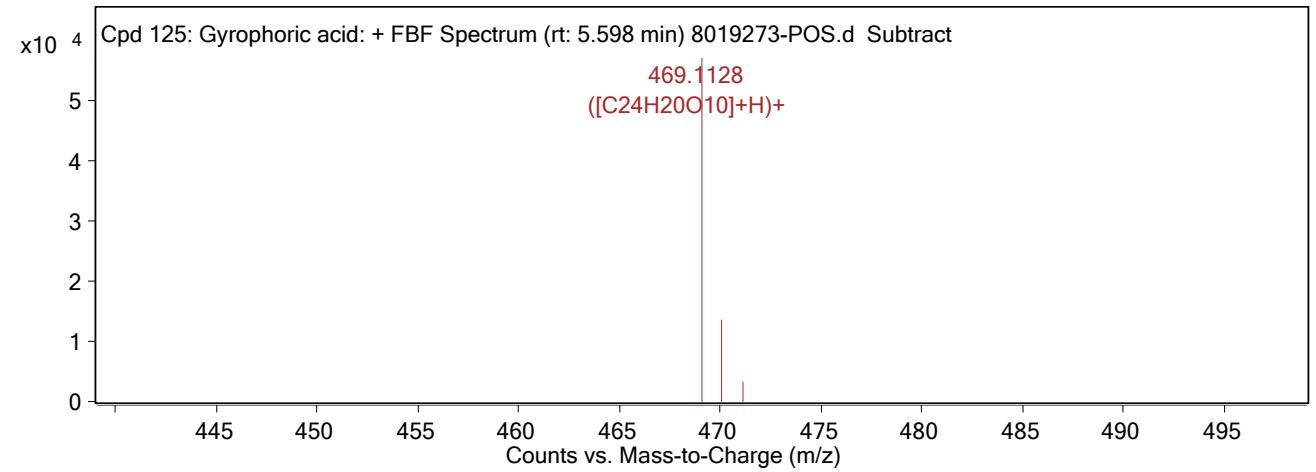
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 481.134 | 1 | 84837.48 | C22H24O12 | (M+H)+ |
| 482.1393 | 1 | 17913.11 | C22H24O12 | (M+H)+ |
| 483.1422 | 1 | 3741.5 | C22H24O12 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 125: Gyrophoric acid | **Gyrophoric acid** | 469.1128 | 5.598 | Find By Formula | 468.1057 |

**Compound Chromatograms**




MS Zoomed Spectrum

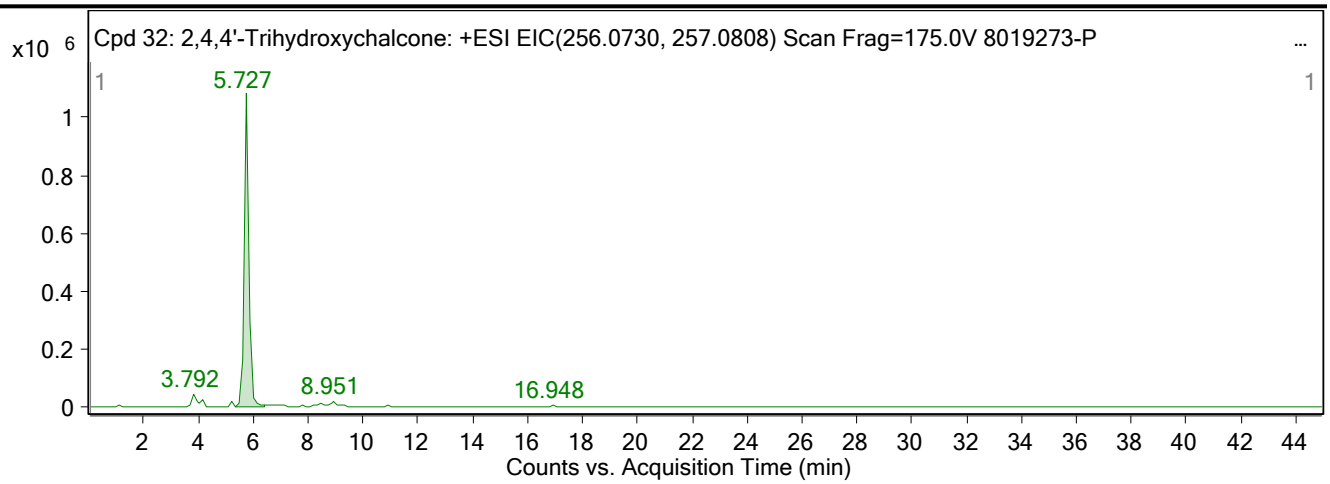



**MS Spectrum Peak List**

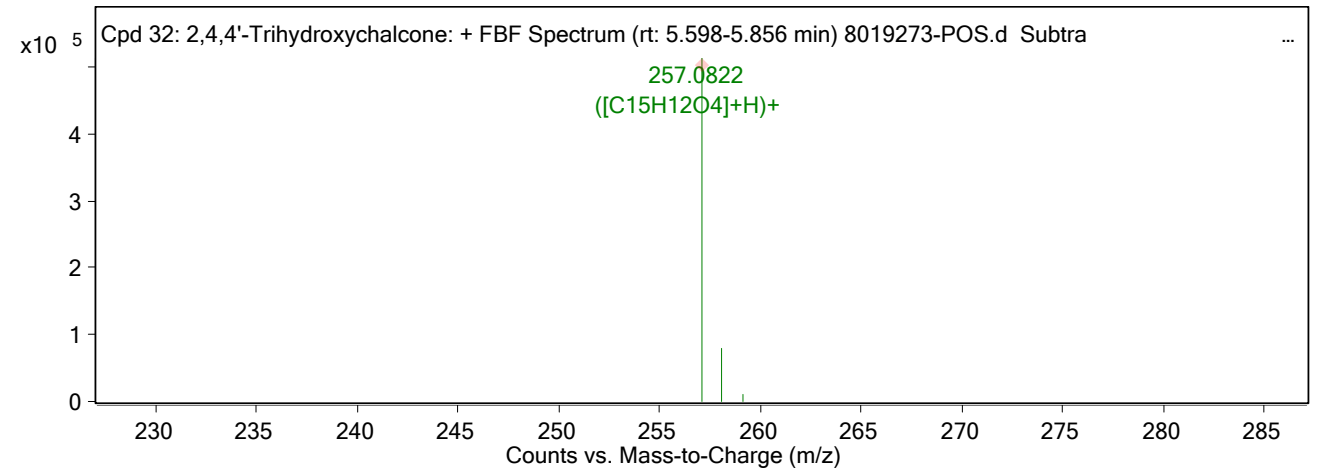
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 469.1128 | 1 | 57226.95 | C24H20O10 | (M+H)+ |
| 470.1175 | 1 | 13440.65 | C24H20O10 | (M+H)+ |
| 471.1166 | 1 | 3401.95 | C24H20O10 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 32: 2,4,4'-Trihydroxychalcone | **2,4,4'-Trihydroxychalcone** | 257.0822 | 5.727 | Find By Formula | 256.0749 |

**Compound Chromatograms**




MS Zoomed Spectrum

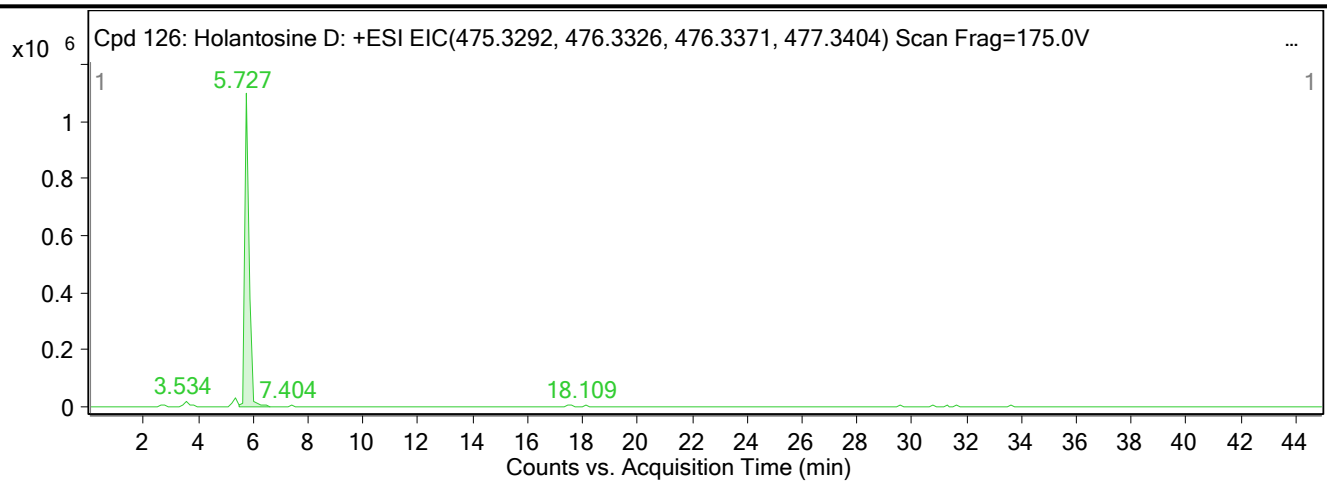



**MS Spectrum Peak List**

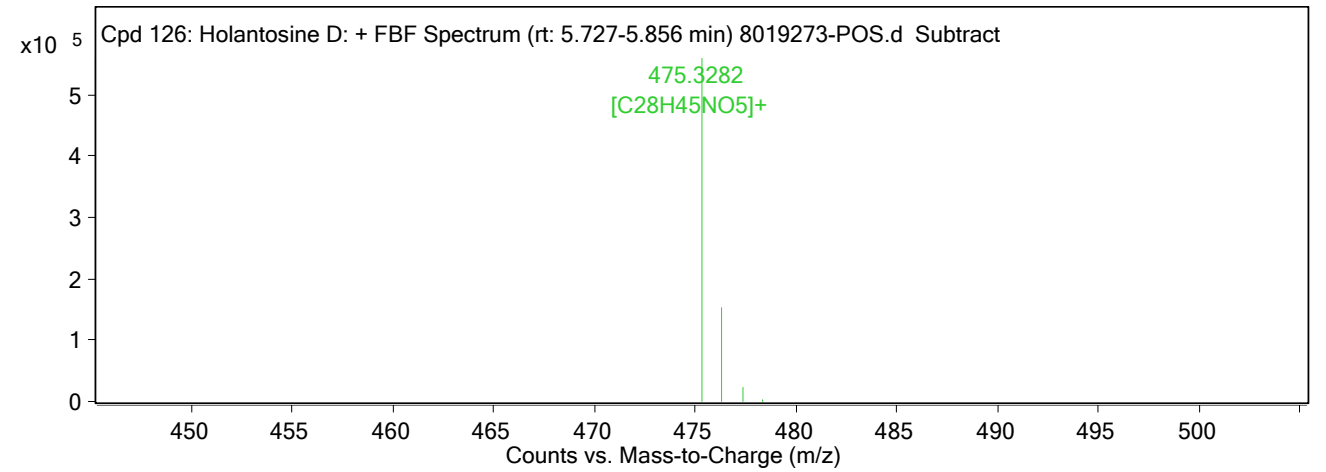
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 257.0822 | 1 | 513049.47 | C15H12O4 | (M+H)+ |
| 258.0854 | 1 | 80304.33 | C15H12O4 | (M+H)+ |
| 259.0903 | 1 | 11620.64 | C15H12O4 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 126: Holantosine D | **Holantosine D** | 475.3282 | 5.727 | Find By Formula | 475.3285 |

**Compound Chromatograms**




MS Zoomed Spectrum

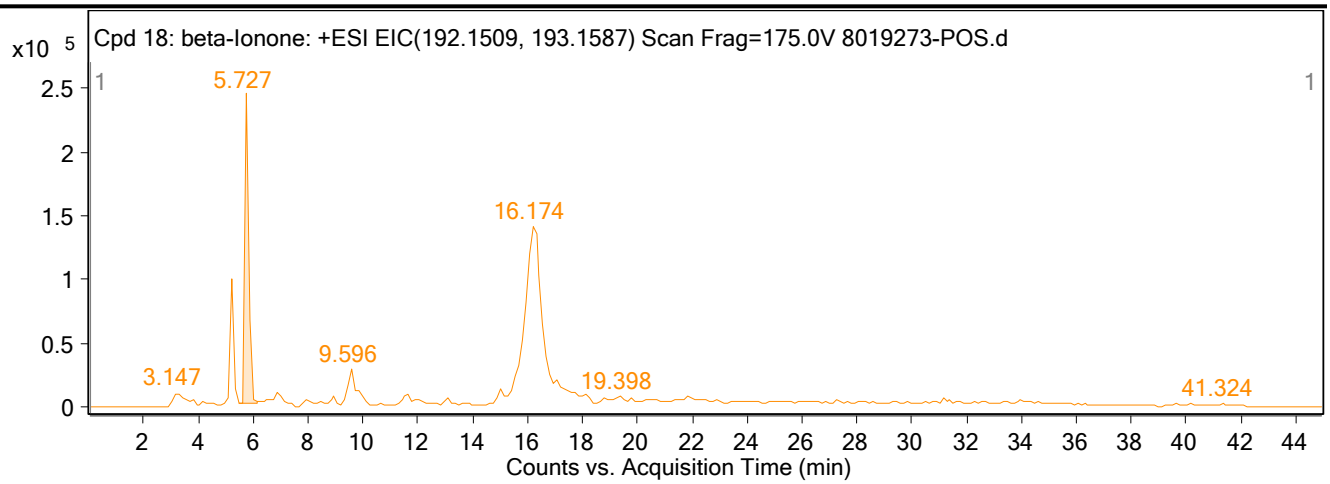



**MS Spectrum Peak List**

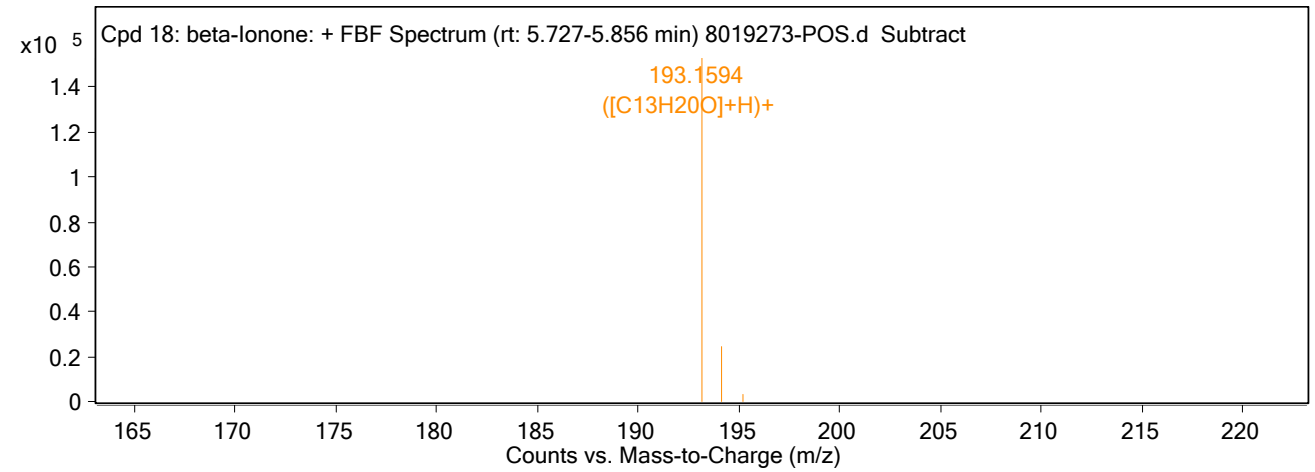
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 475.3282 | 1 | 559768.75 | C28H45NO5 | M+ |
| 476.331 | 1 | 154083.95 | C28H45NO5 | M+ |
| 477.3337 | 1 | 23460.23 | C28H45NO5 | M+ |
| 478.3247 | 1 | 4150.58 | C28H45NO5 | M+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 18: beta-Ionone | **beta-Ionone** | 193.1594 | 5.727 | Find By Formula | 192.1522 |

**Compound Chromatograms**




MS Zoomed Spectrum

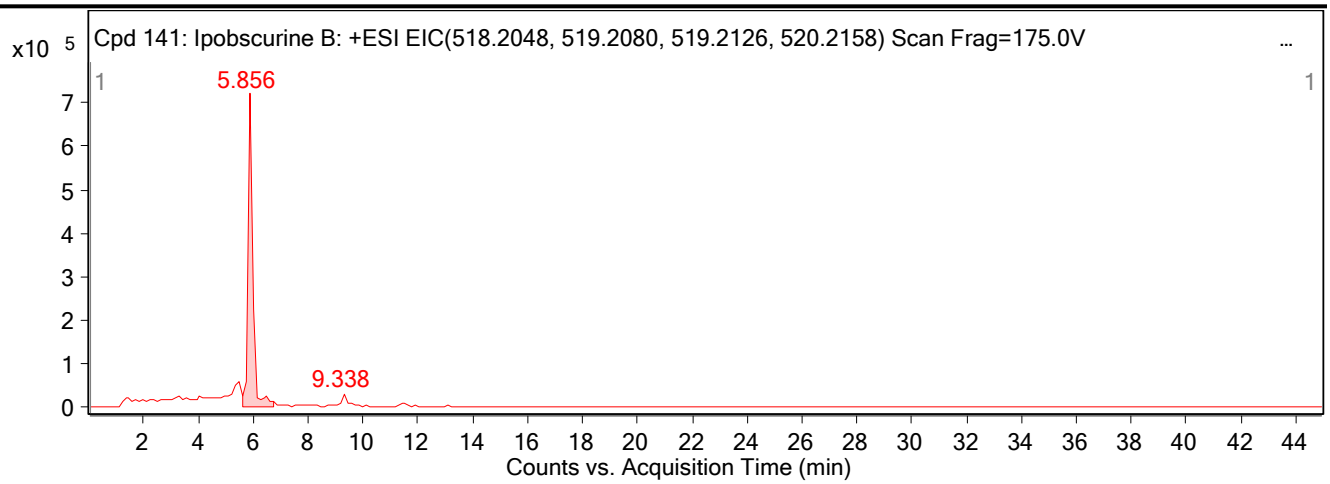



**MS Spectrum Peak List**

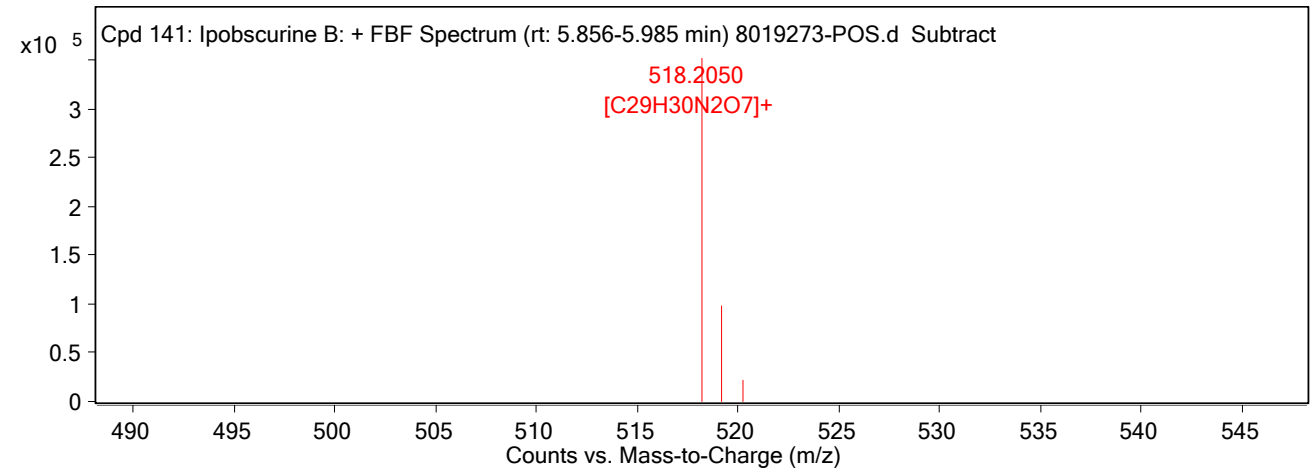
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 193.1594 | 1 | 152955.41 | C13H20O | (M+H)+ |
| 194.1627 | 1 | 24115.33 | C13H20O | (M+H)+ |
| 195.1691 | 1 | 3042.61 | C13H20O | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 141: Ipobscurine B | **Ipobscurine B** | 518.205 | 5.856 | Find By Formula | 518.2058 |

**Compound Chromatograms**




MS Zoomed Spectrum

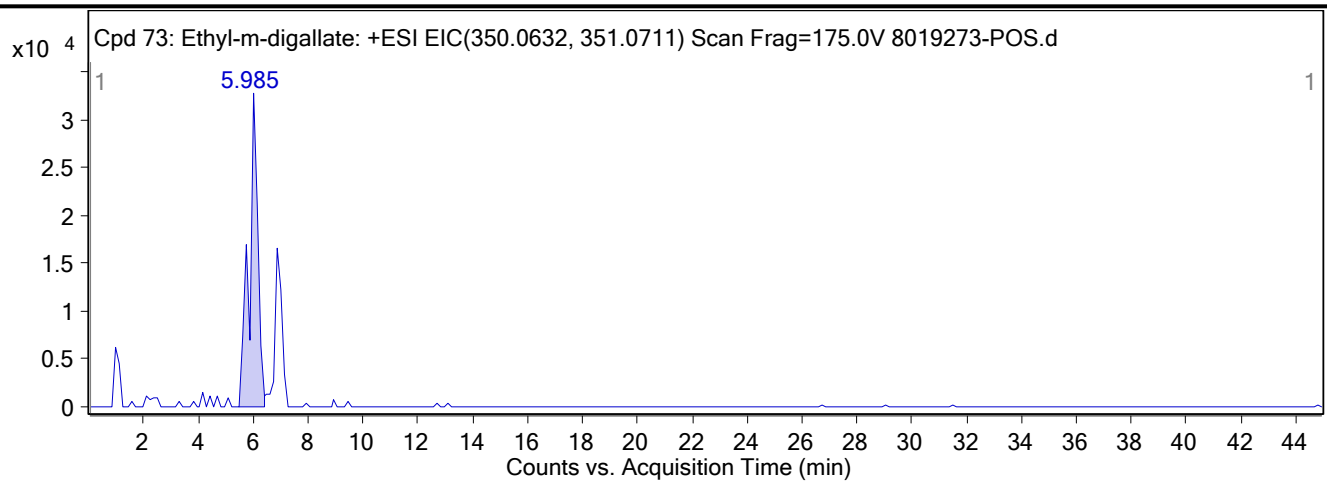



**MS Spectrum Peak List**

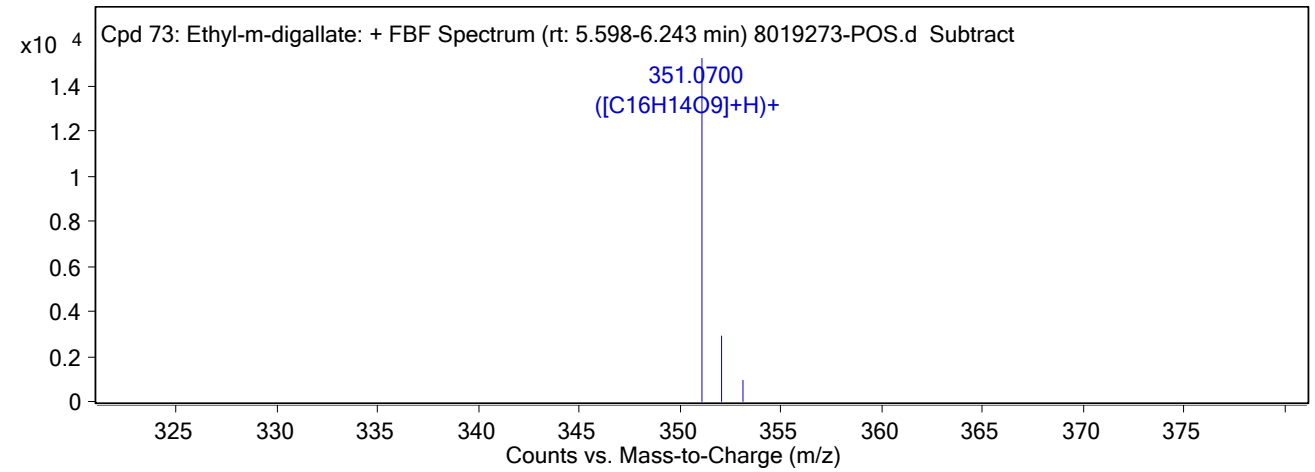
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 518.205 | 1 | 352465.03 | C29H30N2O7 | M+ |
| 519.208 | 1 | 97353.2 | C29H30N2O7 | M+ |
| 520.2176 | 1 | 22383.1 | C29H30N2O7 | M+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 73: Ethyl-m-digallate | **Ethyl-m-digallate** | 351.07 | 5.985 | Find By Formula | 350.0632 |

**Compound Chromatograms**




MS Zoomed Spectrum

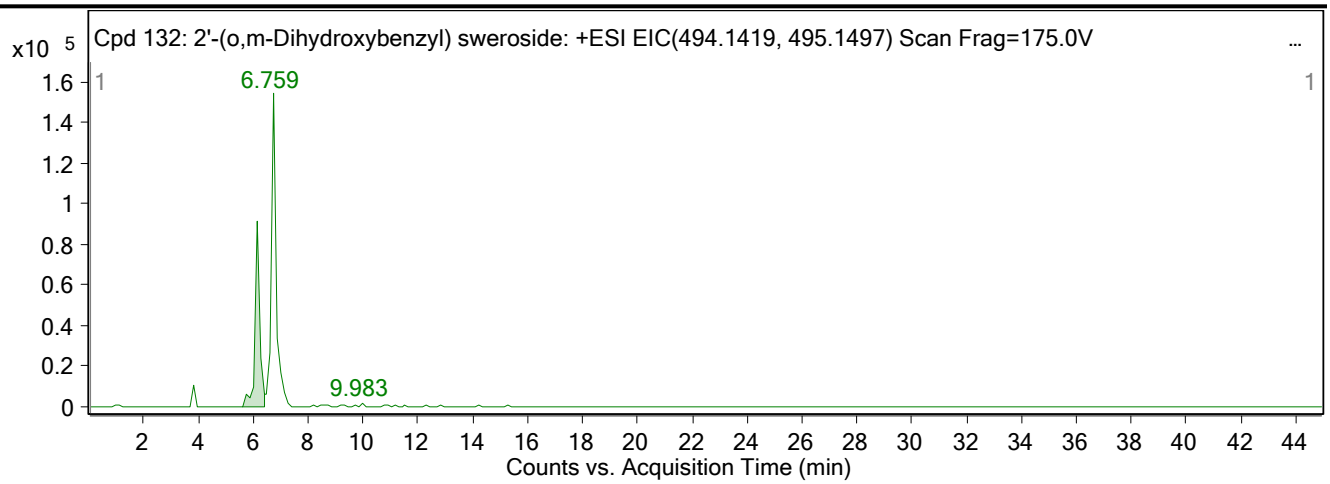



**MS Spectrum Peak List**

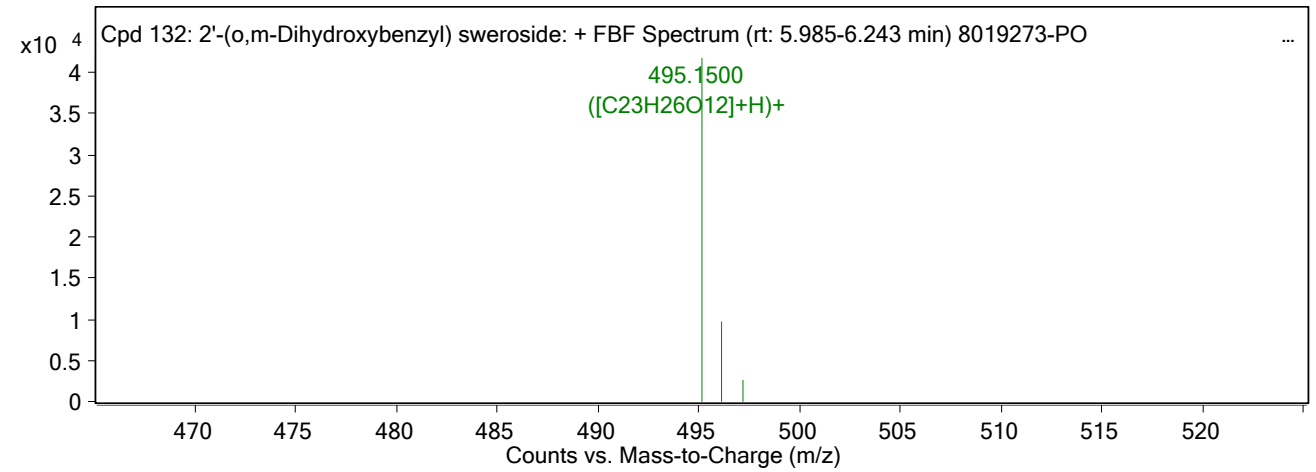
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 351.07 | 1 | 15264.54 | C16H14O9 | (M+H)+ |
| 352.0754 | 1 | 2880.52 | C16H14O9 | (M+H)+ |
| 353.0791 | 1 | 960.11 | C16H14O9 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 132: 2'-(o,m-Dihydroxybenzyl) sweroside | **2'-(o,m-Dihydroxybenzyl) sweroside** | 495.15 | 6.114 | Find By Formula | 494.1433 |

**Compound Chromatograms**




MS Zoomed Spectrum

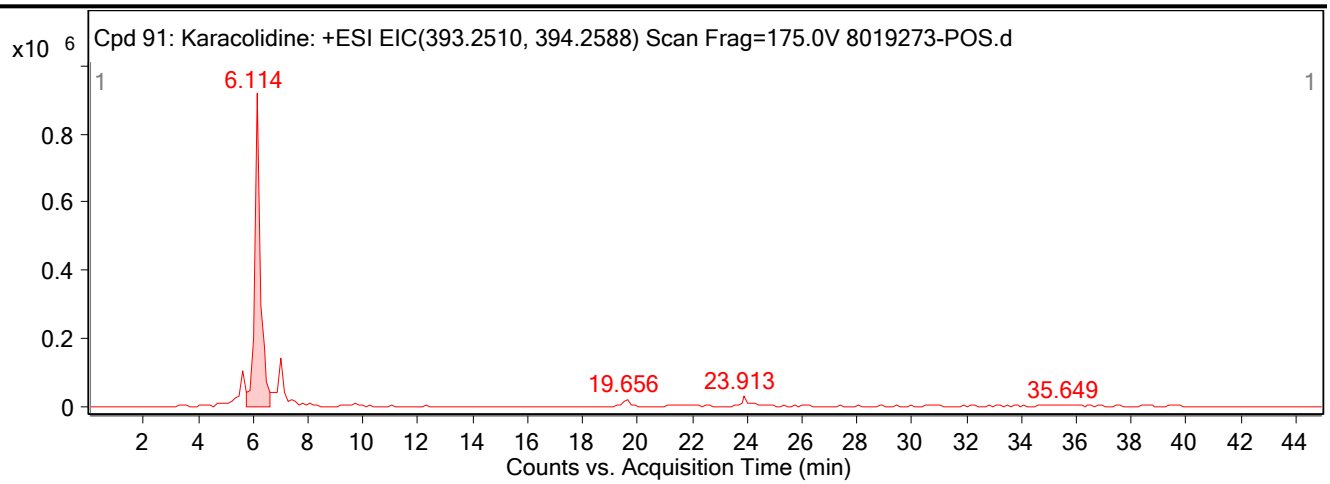



**MS Spectrum Peak List**

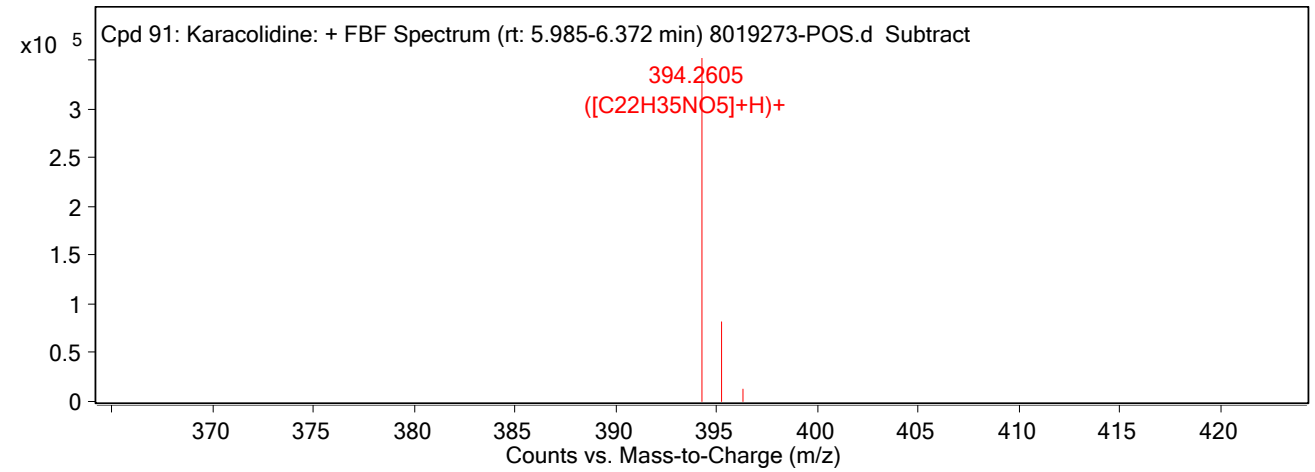
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 495.15 | 1 | 41734.04 | C23H26O12 | (M+H)+ |
| 496.1544 | 1 | 9797.91 | C23H26O12 | (M+H)+ |
| 497.1627 | 1 | 2668.68 | C23H26O12 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 91: Karacolidine | **Karacolidine** | 394.2605 | 6.114 | Find By Formula | 393.2532 |

**Compound Chromatograms**




MS Zoomed Spectrum

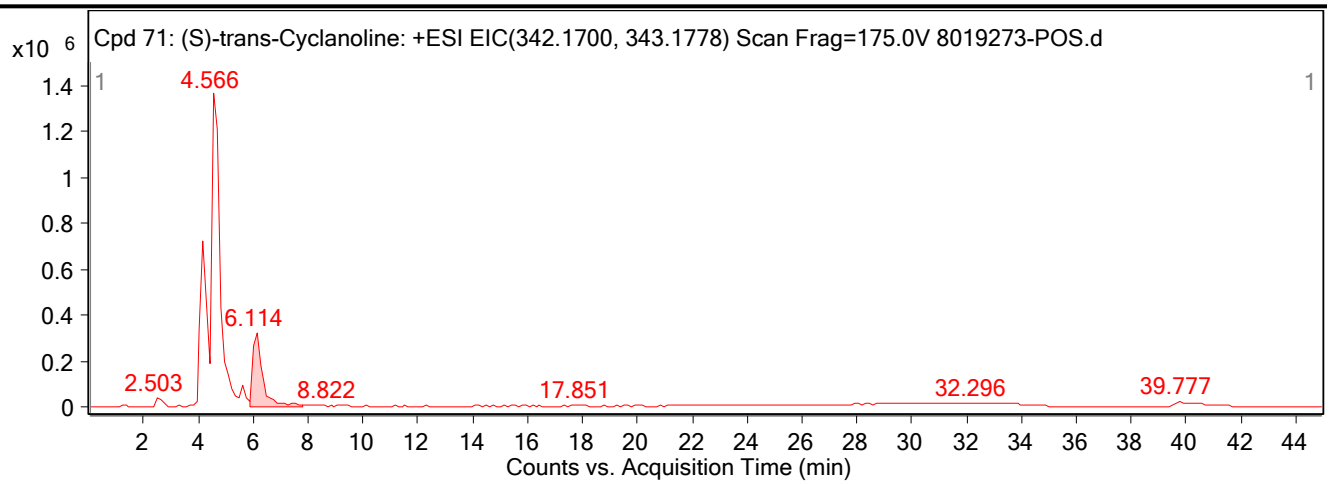



**MS Spectrum Peak List**

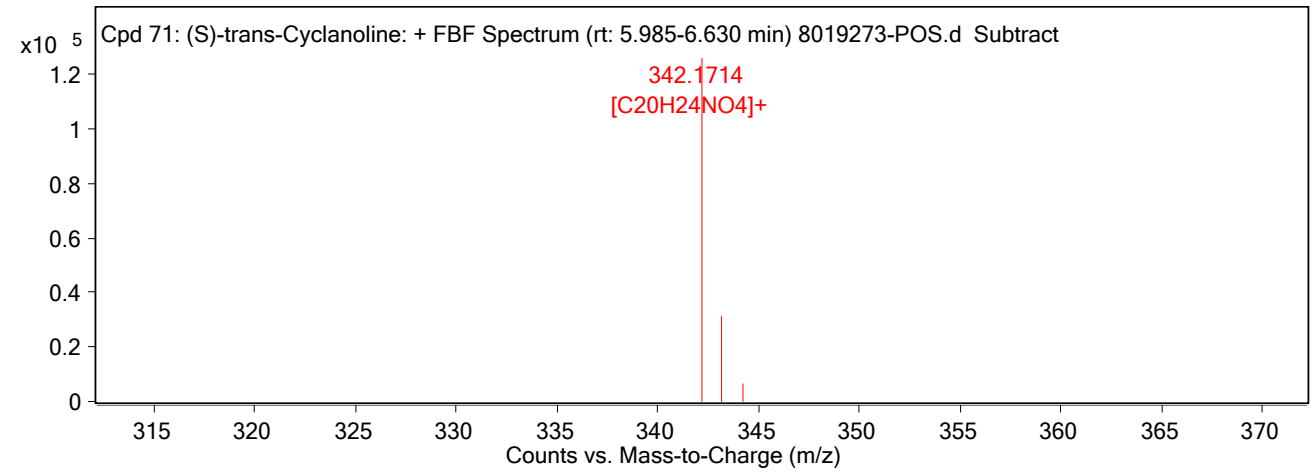
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 394.2605 | 1 | 351889.28 | C22H35NO5 | (M+H)+ |
| 395.2637 | 1 | 81331.63 | C22H35NO5 | (M+H)+ |
| 396.2674 | 1 | 13604.86 | C22H35NO5 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 71: (S)-trans-Cyclanoline | **(S)-trans-Cyclanoline** | 342.1714 | 6.114 | Find By Formula | 342.1718 |

**Compound Chromatograms**




MS Zoomed Spectrum

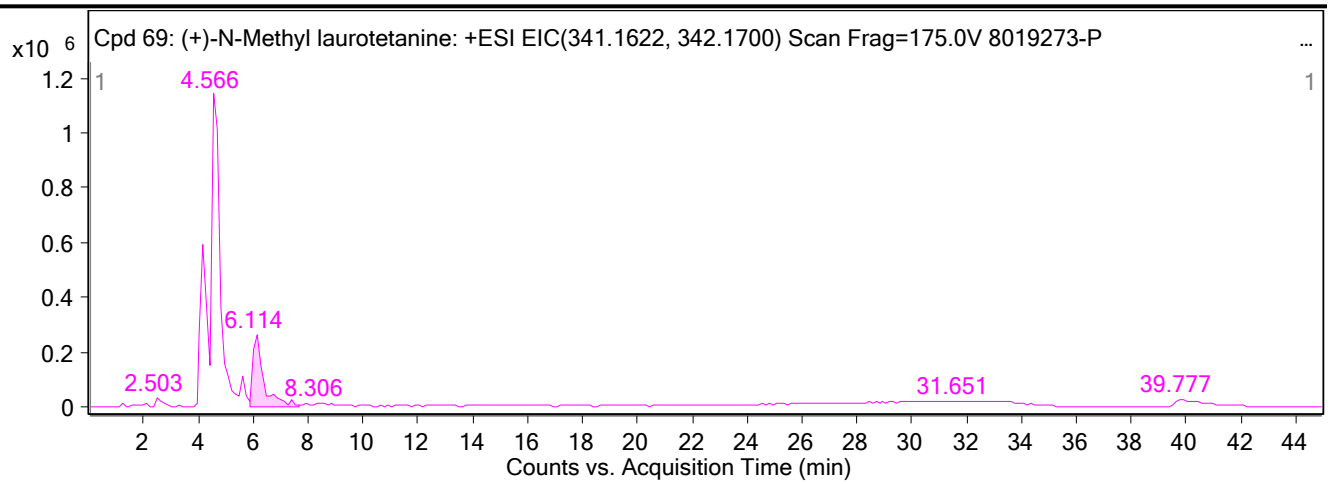



**MS Spectrum Peak List**

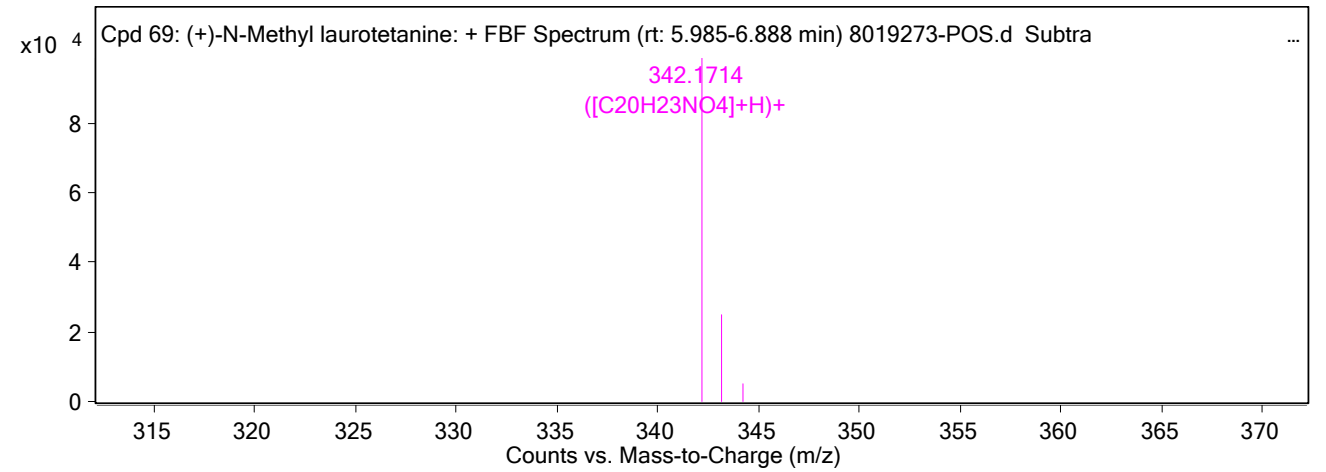
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 342.1714 | 1 | 126163.34 | C20H24NO4 | M+ |
| 343.1743 | 1 | 31127.19 | C20H24NO4 | M+ |
| 344.1758 | 1 | 6371.7 | C20H24NO4 | M+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 69: (+)-N-Methyl laurotetanine | **(+)-N-Methyl laurotetanine** | 342.1714 | 6.114 | Find By Formula | 341.164 |

**Compound Chromatograms**




MS Zoomed Spectrum

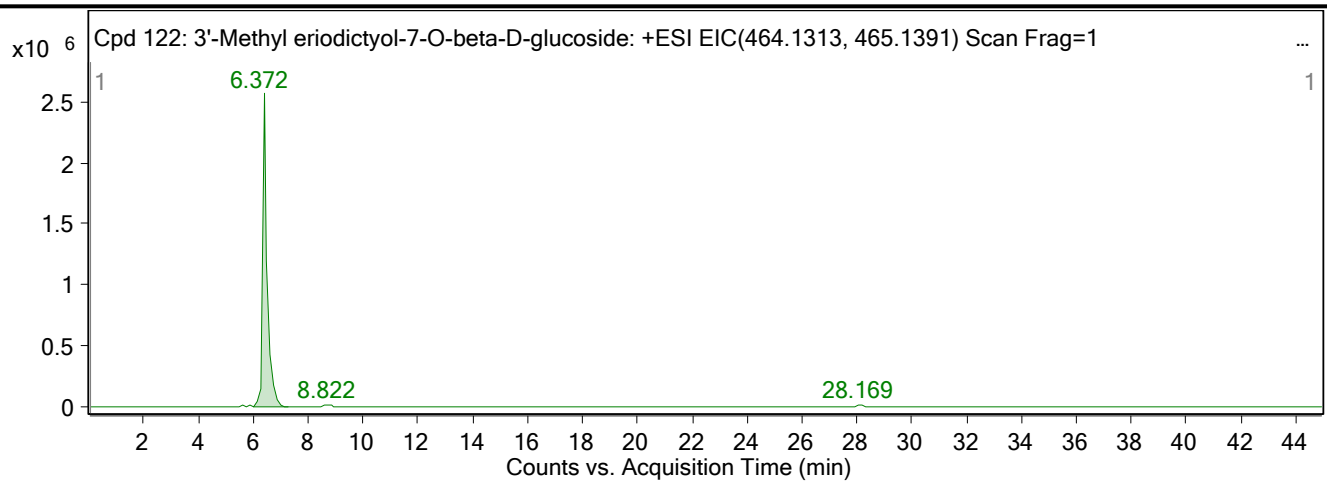



**MS Spectrum Peak List**

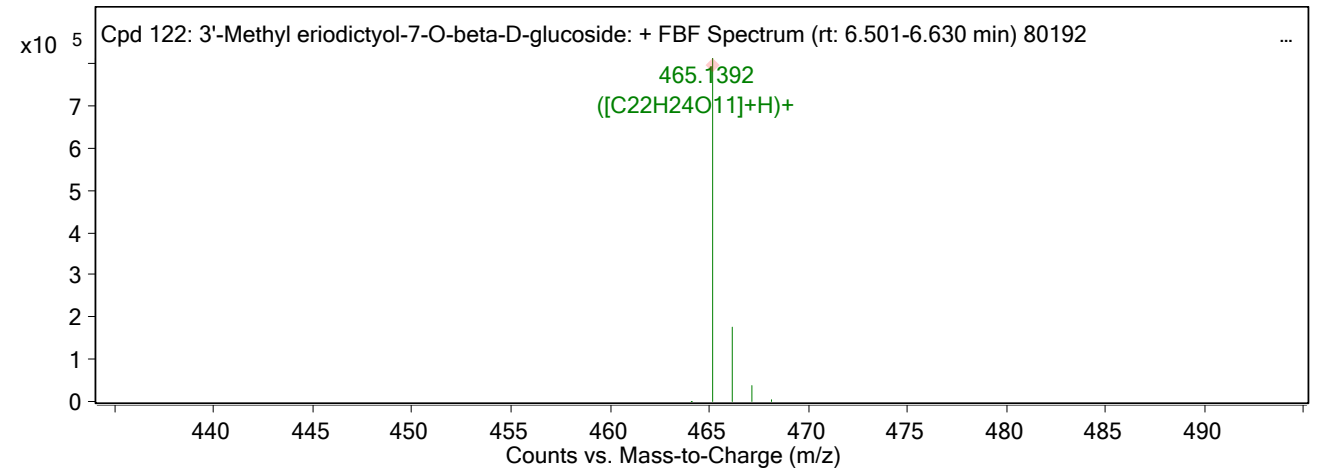
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 342.1714 | 1 | 98660.51 | C20H23NO4 | (M+H)+ |
| 343.1743 | 1 | 25062.71 | C20H23NO4 | (M+H)+ |
| 344.1757 | 1 | 5254.66 | C20H23NO4 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 122: 3'-Methyl eriodictyol-7-O-beta-D-glucoside | **3'-Methyl eriodictyol-7-O-beta-D-glucoside** | 465.1392 | 6.372 | Find By Formula | 464.1318 |

**Compound Chromatograms**




MS Zoomed Spectrum

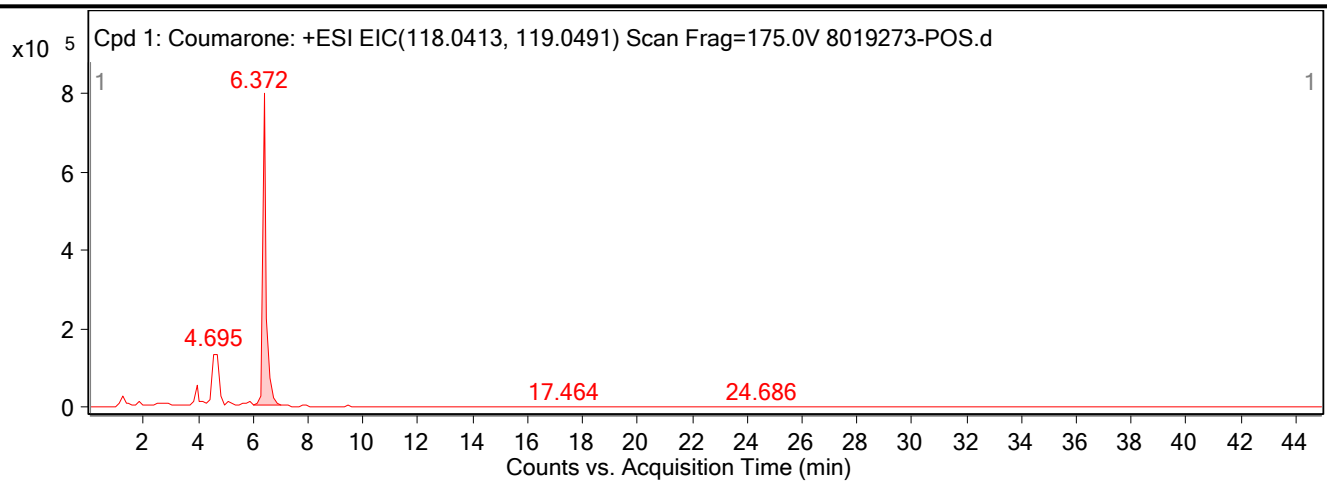



**MS Spectrum Peak List**

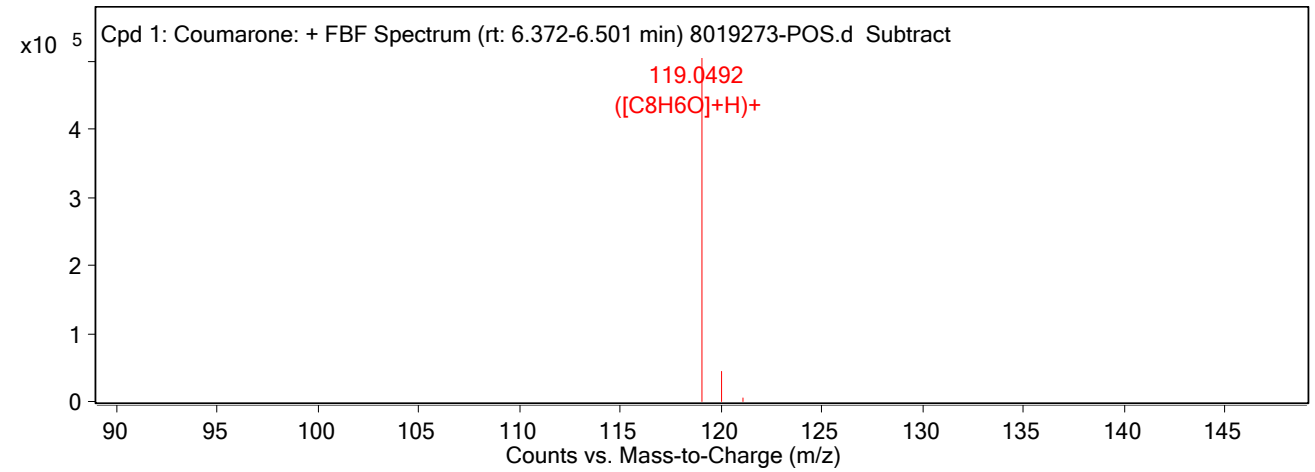
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 464.1288 | 1 | 769.54 | C22H24O11 | M+ |
| 465.1392 | 1 | 813445.88 | C22H24O11 | (M+H)+ |
| 466.1423 | 1 | 174456.2 | C22H24O11 | (M+H)+ |
| 467.1444 | 1 | 35936.08 | C22H24O11 | (M+H)+ |
| 468.1502 | 1 | 4622.56 | C22H24O11 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 1: Coumarone | **Coumarone** | 119.0492 | 6.372 | Find By Formula | 118.0421 |

**Compound Chromatograms**




MS Zoomed Spectrum

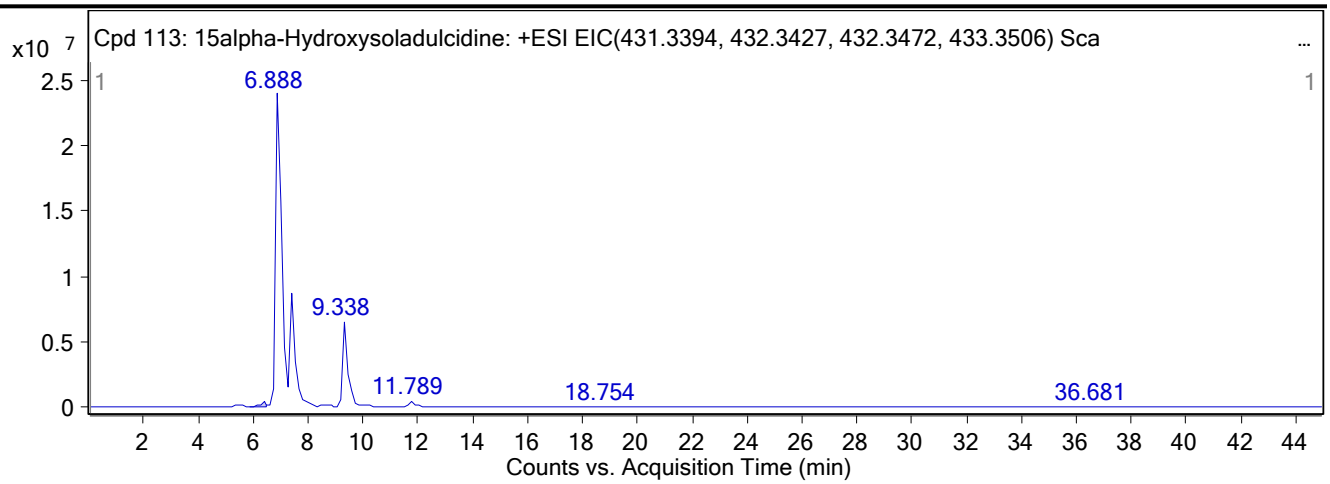



**MS Spectrum Peak List**

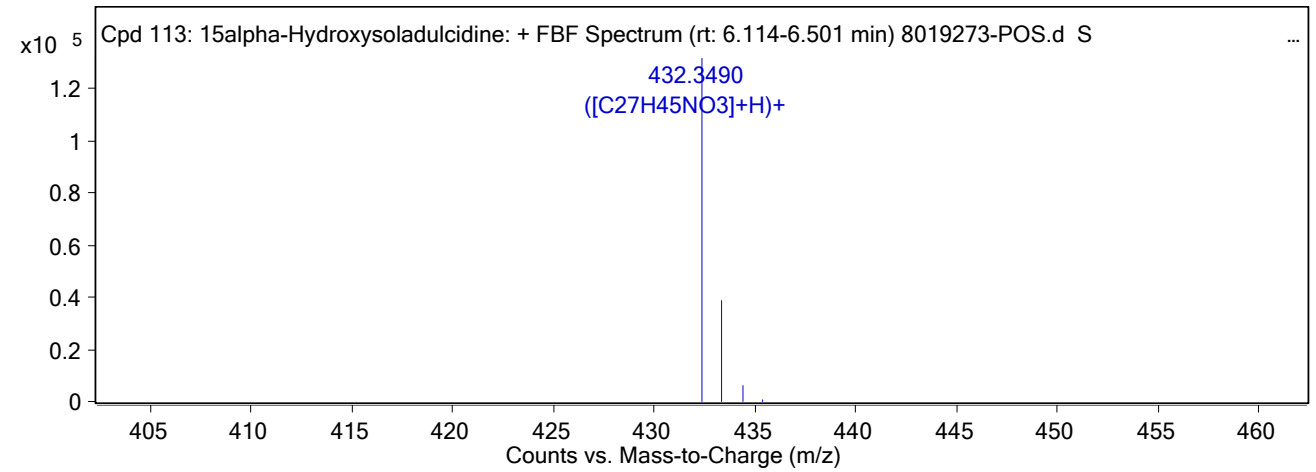
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 119.0492 | 1 | 505108.63 | C8H6O | (M+H)+ |
| 120.0525 | 1 | 43734.12 | C8H6O | (M+H)+ |
| 121.0645 | 1 | 6144.72 | C8H6O | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 113: 15alpha-Hydroxysoladulcidine | **15alpha-Hydroxysoladulcidine** | 432.349 | 6.372 | Find By Formula | 431.3418 |

**Compound Chromatograms**




MS Zoomed Spectrum

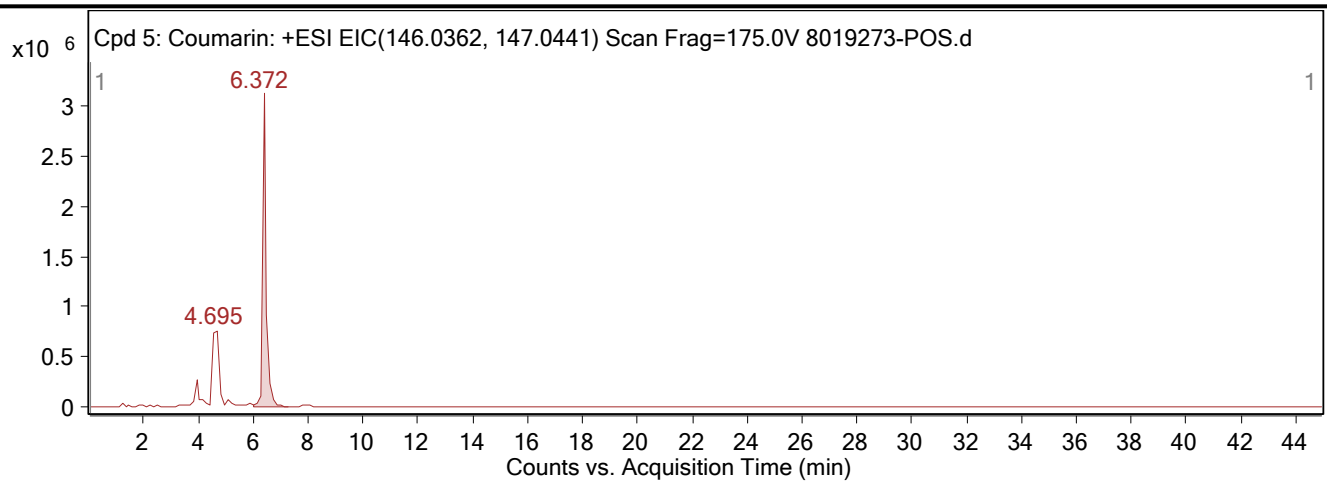



**MS Spectrum Peak List**

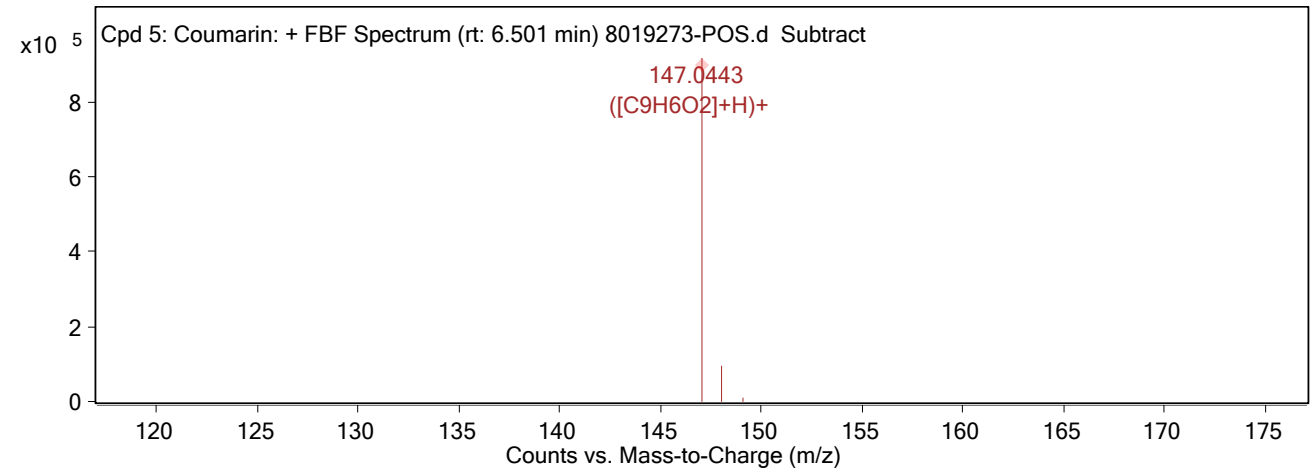
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 432.349 | 1 | 131625.81 | C27H45NO3 | (M+H)+ |
| 433.3525 | 1 | 38493.54 | C27H45NO3 | (M+H)+ |
| 434.355 | 1 | 5850.42 | C27H45NO3 | (M+H)+ |
| 435.3564 | 1 | 1027.26 | C27H45NO3 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 5: Coumarin | **Coumarin** | 147.0443 | 6.372 | Find By Formula | 146.0371 |

**Compound Chromatograms**




MS Zoomed Spectrum

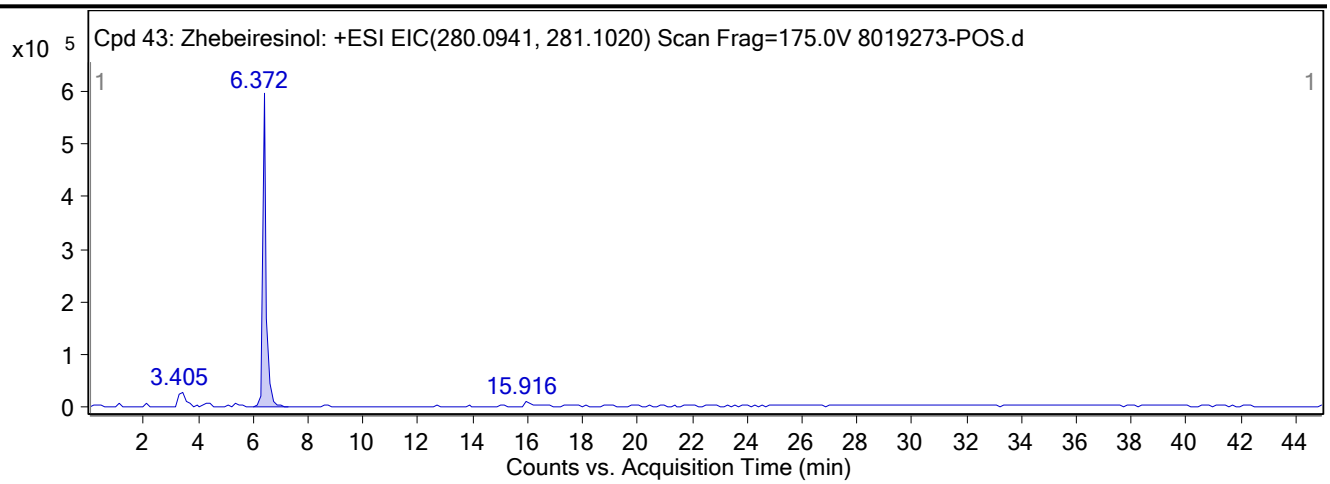



**MS Spectrum Peak List**

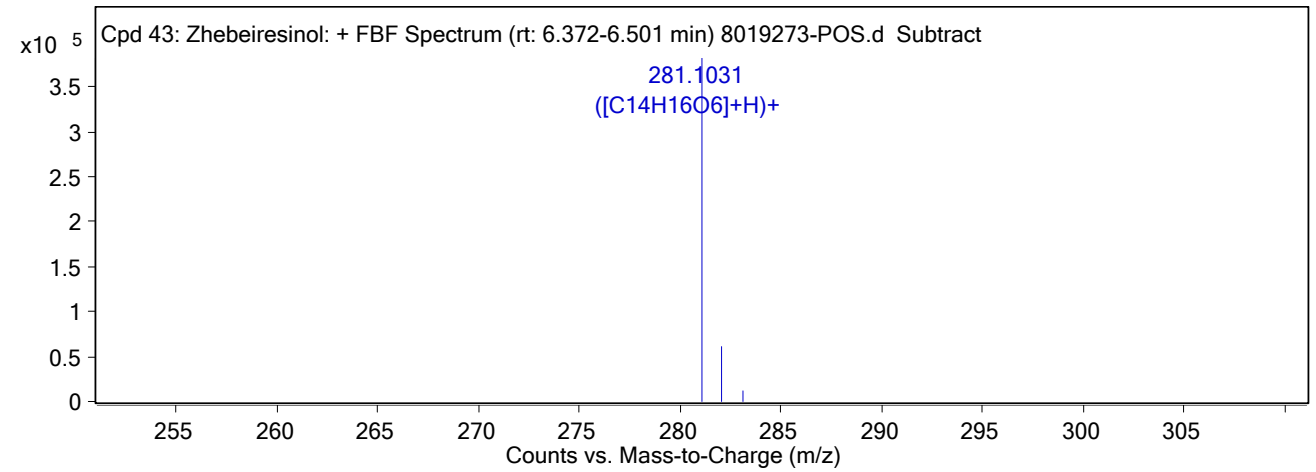
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 147.0443 | 1 | 915913.38 | C9H6O2 | (M+H)+ |
| 148.0477 | 1 | 92560.2 | C9H6O2 | (M+H)+ |
| 149.0574 | 1 | 10421.19 | C9H6O2 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 43: Zhebeiresinol | **Zhebeiresinol** | 281.1031 | 6.372 | Find By Formula | 280.0959 |

**Compound Chromatograms**




MS Zoomed Spectrum

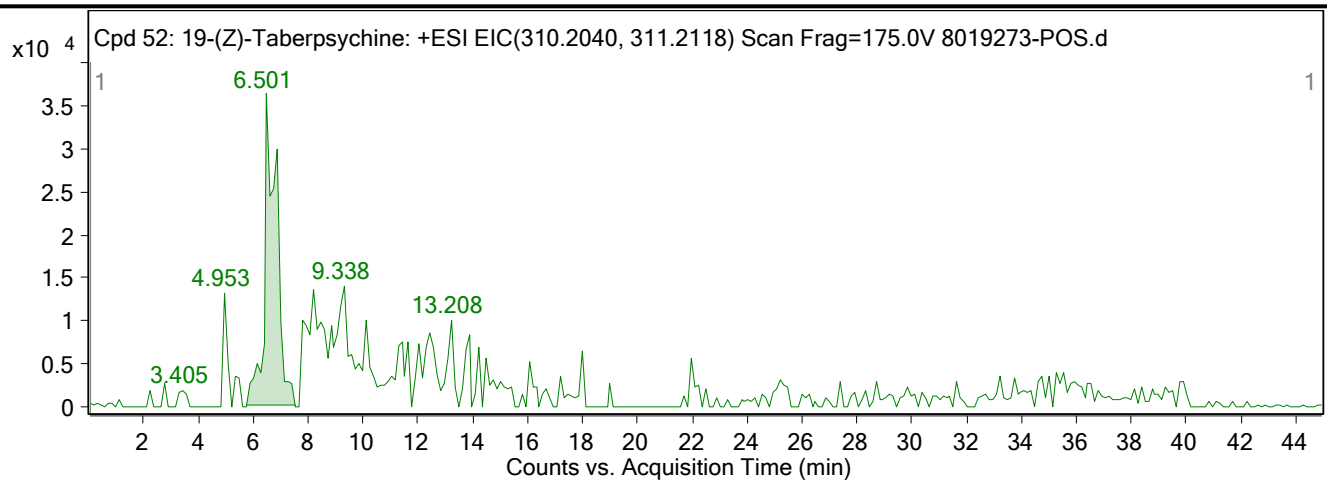



**MS Spectrum Peak List**

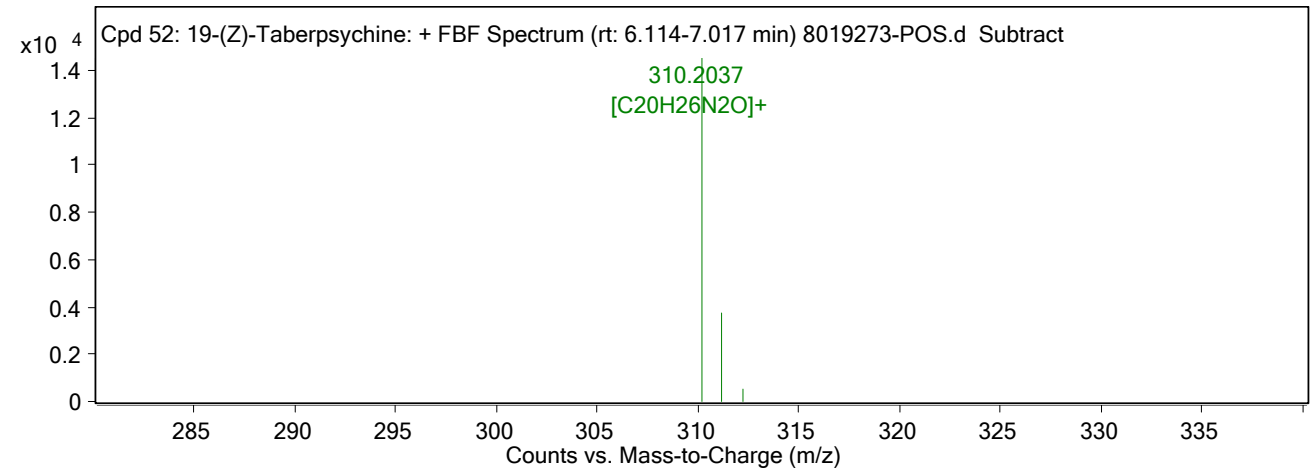
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 281.1031 | 1 | 382133.31 | C14H16O6 | (M+H)+ |
| 282.1066 | 1 | 60711.88 | C14H16O6 | (M+H)+ |
| 283.1098 | 1 | 11287.43 | C14H16O6 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 52: 19-(Z)-Taberpsychine | **19-(Z)-Taberpsychine** | 310.2037 | 6.501 | Find By Formula | 310.204 |

**Compound Chromatograms**




MS Zoomed Spectrum

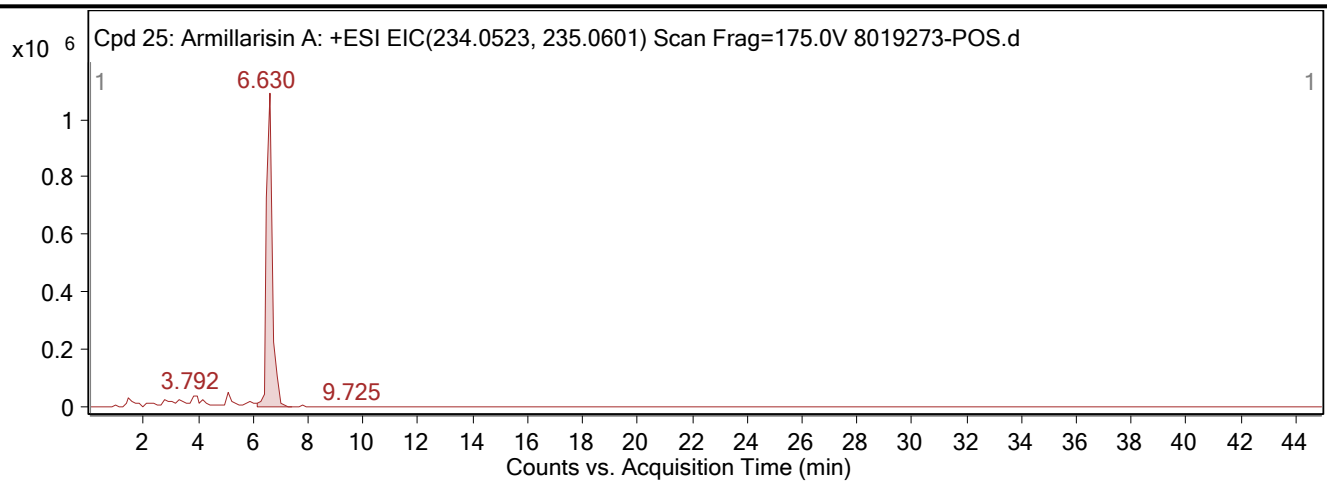



**MS Spectrum Peak List**

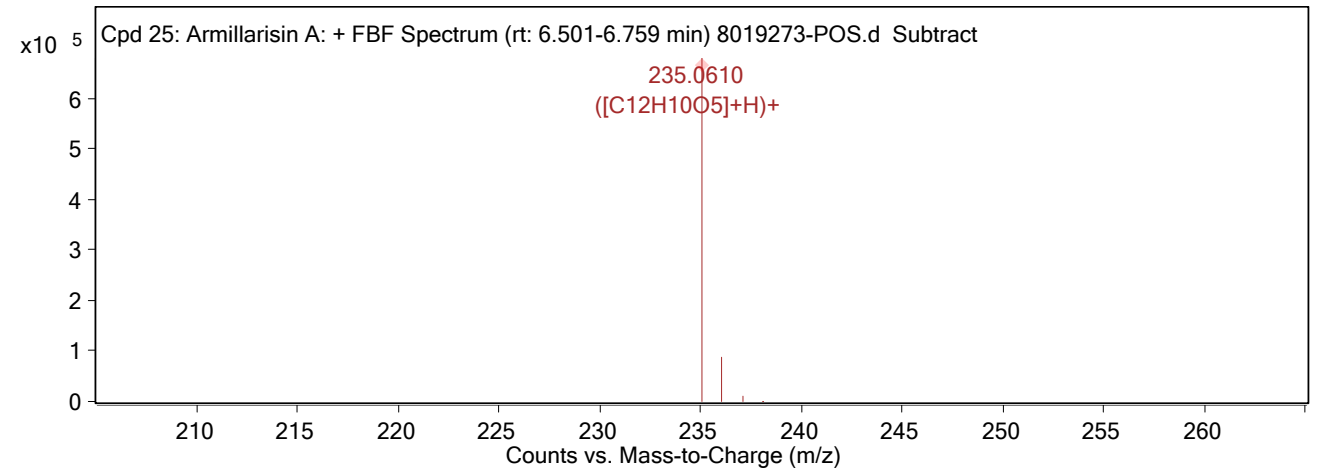
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 310.2037 | 1 | 14518.44 | C20H26N2O | M+ |
| 311.2051 | 1 | 3713.01 | C20H26N2O | M+ |
| 312.2144 | 1 | 512.61 | C20H26N2O | M+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 25: Armillarisin A | **Armillarisin A** | 235.061 | 6.63 | Find By Formula | 234.0537 |

**Compound Chromatograms**




MS Zoomed Spectrum

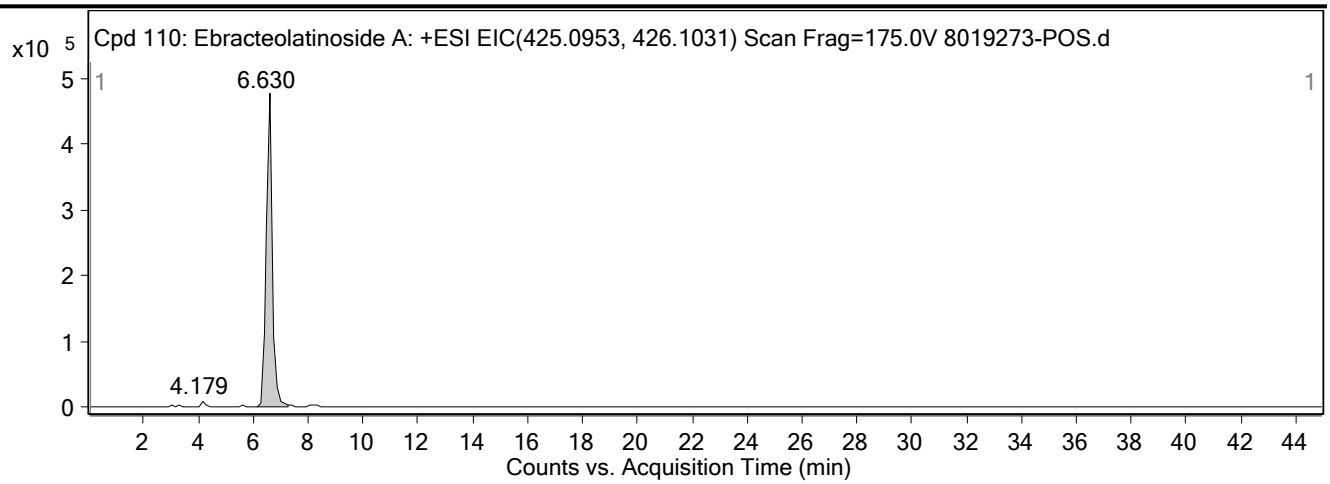



**MS Spectrum Peak List**

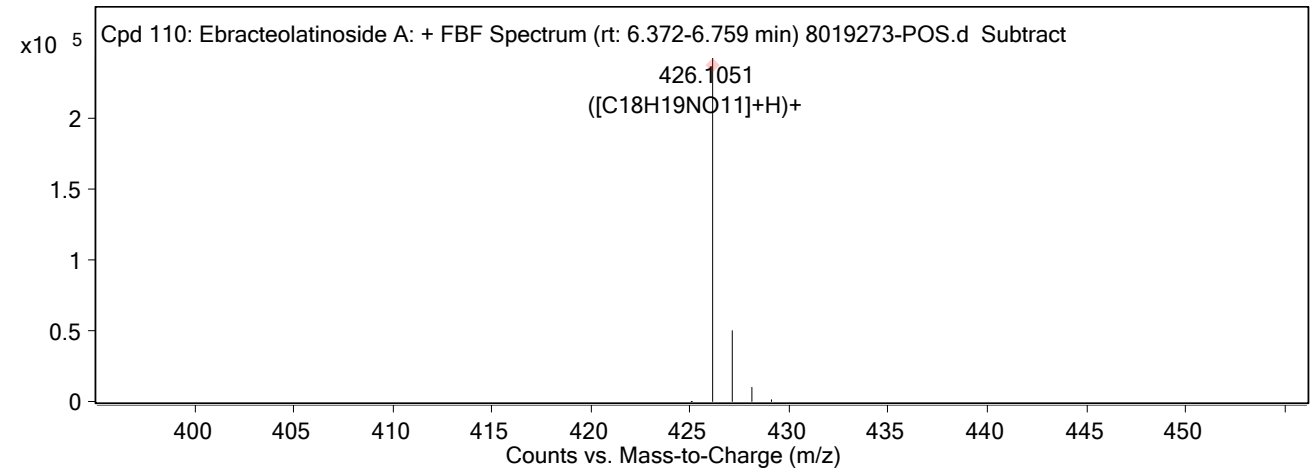
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 235.061 | 1 | 680212.13 | C12H10O5 | (M+H)+ |
| 236.0643 | 1 | 88020.91 | C12H10O5 | (M+H)+ |
| 237.0669 | 1 | 12245.05 | C12H10O5 | (M+H)+ |
| 238.0697 | 1 | 702.89 | C12H10O5 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 110: Ebracteolatinoside A | **Ebracteolatinoside A** | 426.1051 | 6.63 | Find By Formula | 425.0978 |

**Compound Chromatograms**




MS Zoomed Spectrum

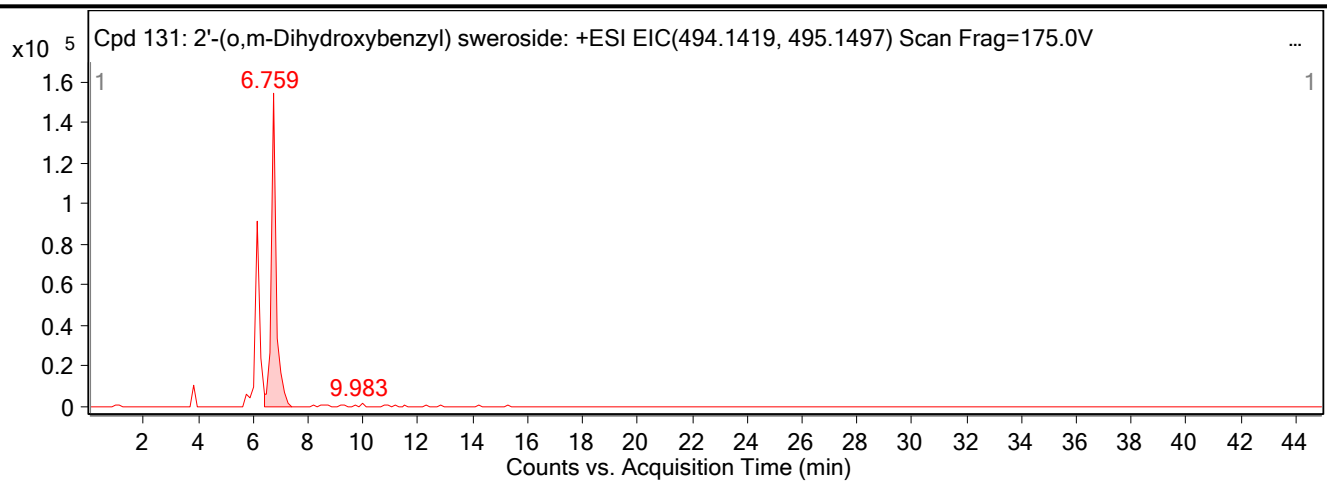



**MS Spectrum Peak List**

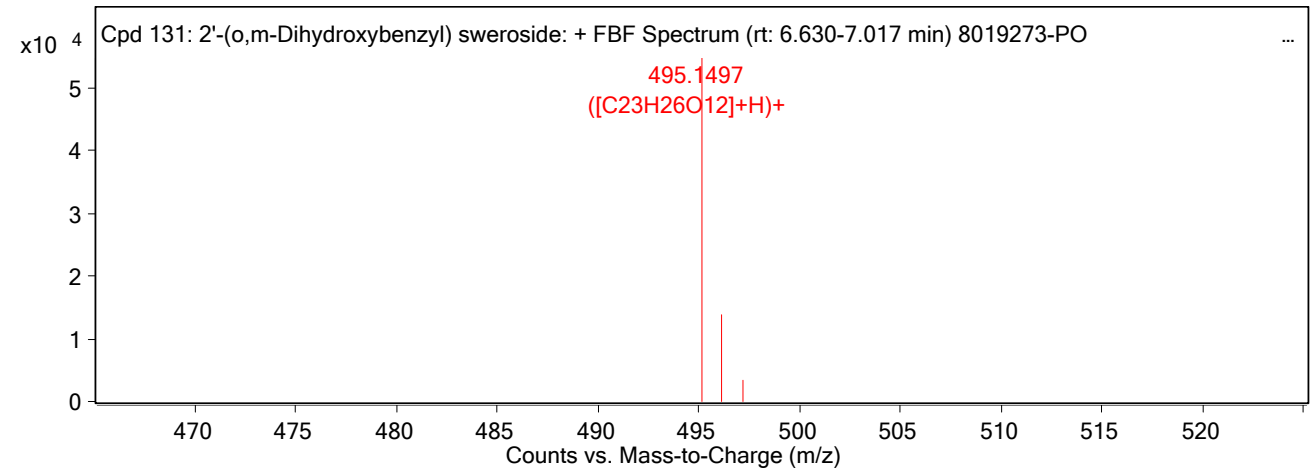
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 425.0857 | 1 | 302.19 | C18H19NO11 | M+ |
| 426.1051 | 1 | 241968.11 | C18H19NO11 | (M+H)+ |
| 427.1082 | 1 | 49902.07 | C18H19NO11 | (M+H)+ |
| 428.111 | 1 | 10256.25 | C18H19NO11 | (M+H)+ |
| 429.1188 | 1 | 1674.74 | C18H19NO11 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 131: 2'-(o,m-Dihydroxybenzyl) sweroside | **2'-(o,m-Dihydroxybenzyl) sweroside** | 495.1497 | 6.759 | Find By Formula | 494.1426 |

**Compound Chromatograms**




MS Zoomed Spectrum

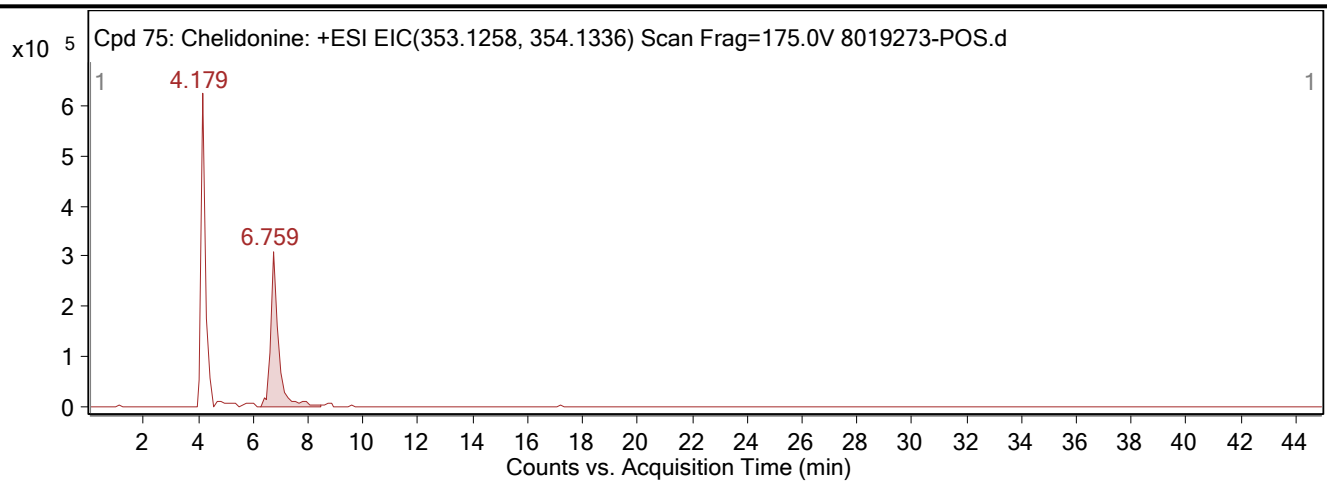



**MS Spectrum Peak List**

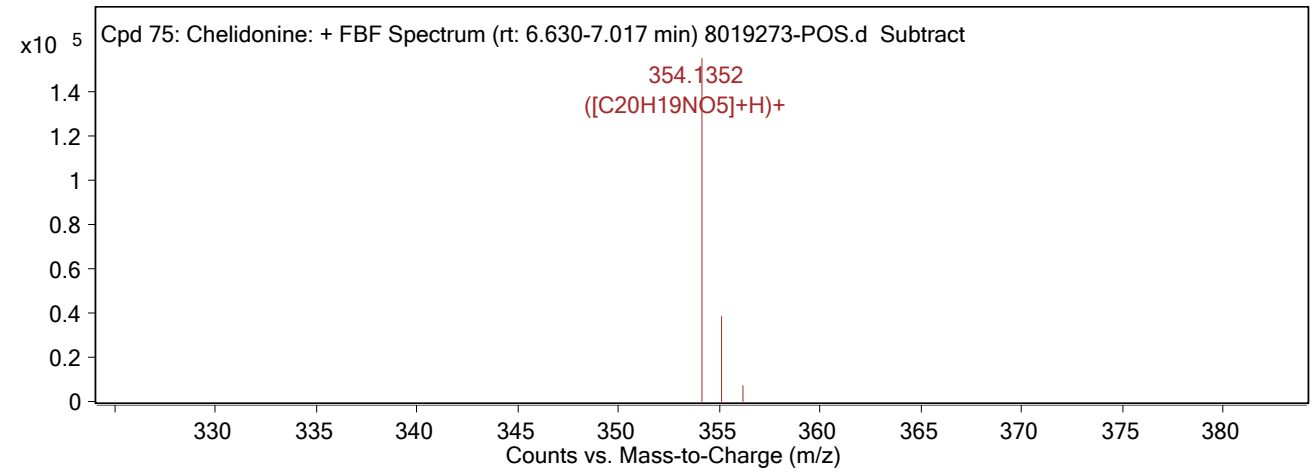
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 495.1497 | 1 | 54838.34 | C23H26O12 | (M+H)+ |
| 496.1544 | 1 | 13959.98 | C23H26O12 | (M+H)+ |
| 497.155 | 1 | 3478.86 | C23H26O12 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 75: Chelidonine | **Chelidonine** | 354.1352 | 6.759 | Find By Formula | 353.128 |

**Compound Chromatograms**




MS Zoomed Spectrum

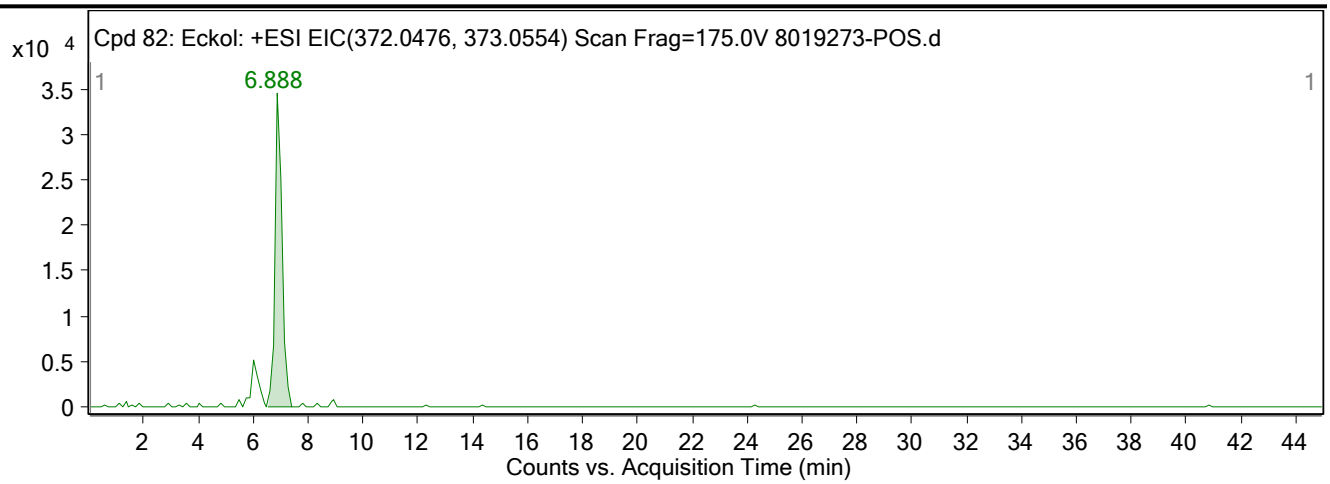



**MS Spectrum Peak List**

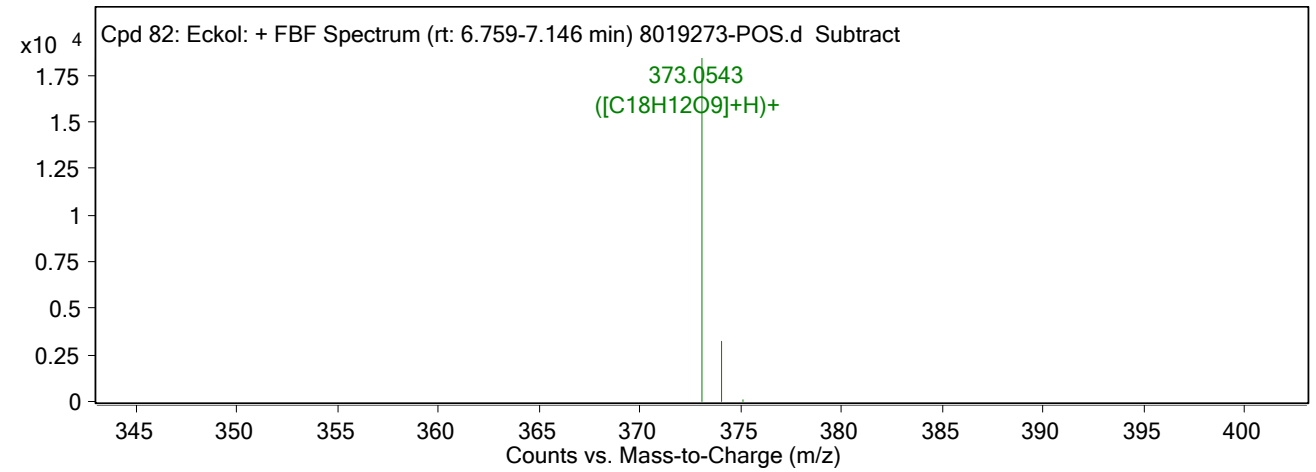
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 354.1352 | 1 | 155545.3 | C20H19NO5 | (M+H)+ |
| 355.1385 | 1 | 38315.52 | C20H19NO5 | (M+H)+ |
| 356.143 | 1 | 7088.83 | C20H19NO5 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 82: Eckol | **Eckol** | 373.0543 | 6.888 | Find By Formula | 372.0472 |

**Compound Chromatograms**




MS Zoomed Spectrum

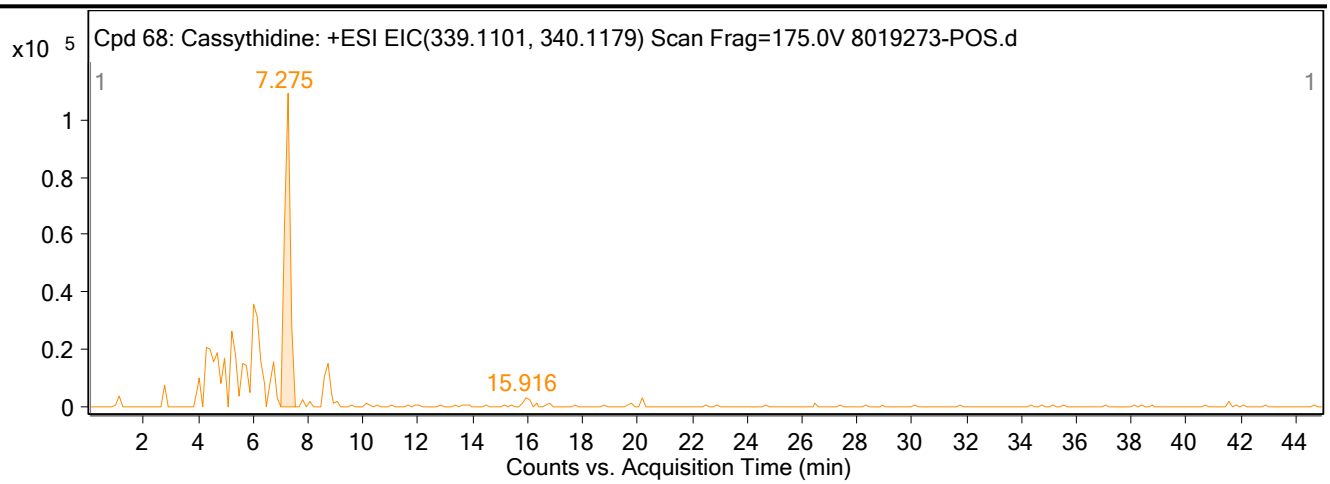



**MS Spectrum Peak List**

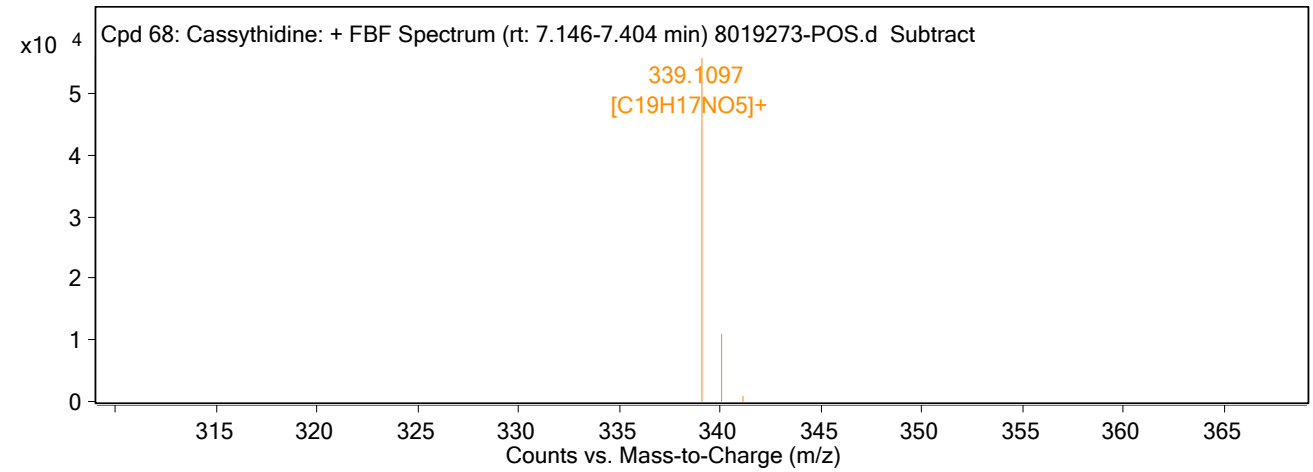
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 373.0543 | 1 | 18424.12 | C18H12O9 | (M+H)+ |
| 374.0591 | 1 | 3244.48 | C18H12O9 | (M+H)+ |
| 375.0563 | 1 | 97.74 | C18H12O9 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 68: Cassythidine | **Cassythidine** | 339.1097 | 7.275 | Find By Formula | 339.1103 |

**Compound Chromatograms**




MS Zoomed Spectrum

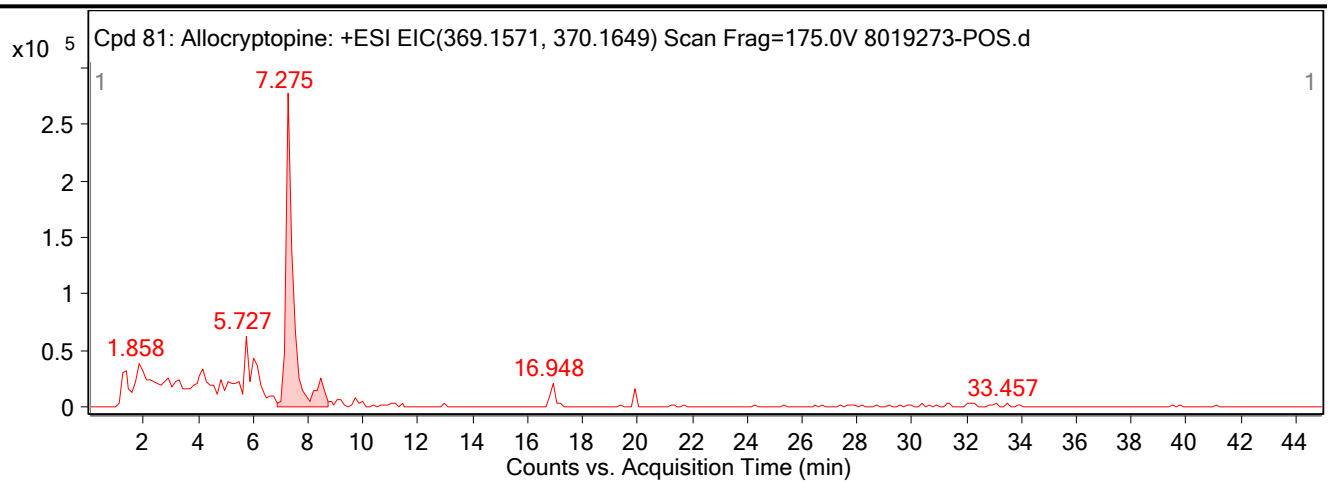



**MS Spectrum Peak List**

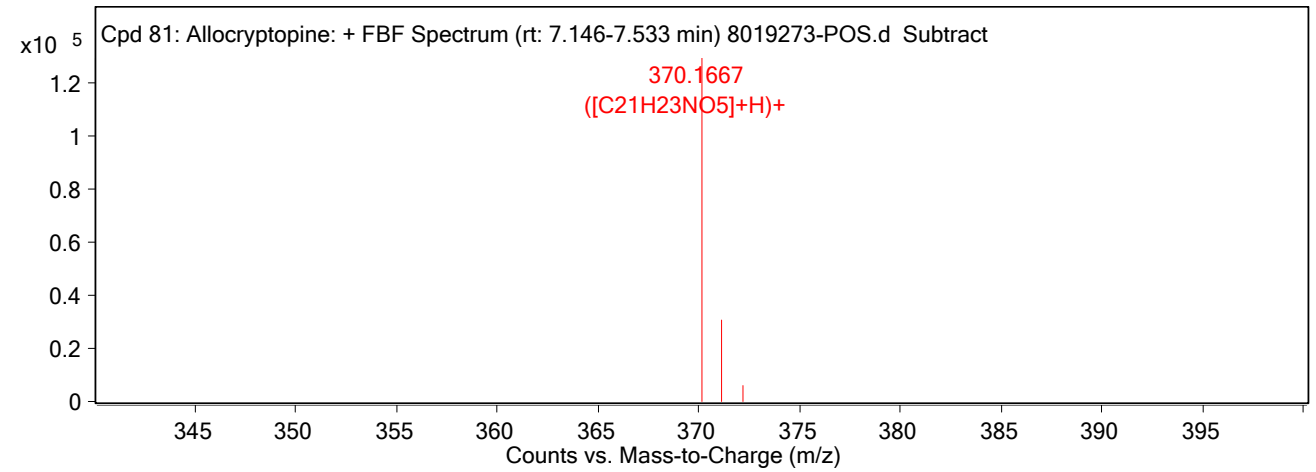
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 339.1097 | 1 | 55789.3 | C19H17NO5 | M+ |
| 340.1134 | 1 | 10888.98 | C19H17NO5 | M+ |
| 341.1158 | 1 | 915.45 | C19H17NO5 | M+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 81: Allocryptopine | **Allocryptopine** | 370.1667 | 7.275 | Find By Formula | 369.1595 |

**Compound Chromatograms**




MS Zoomed Spectrum

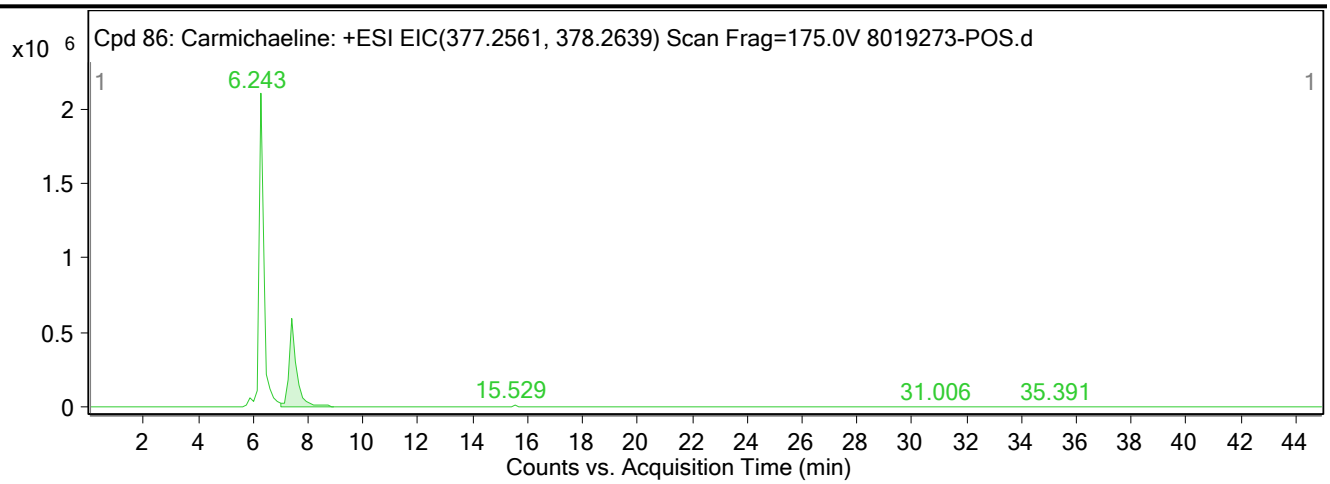



**MS Spectrum Peak List**

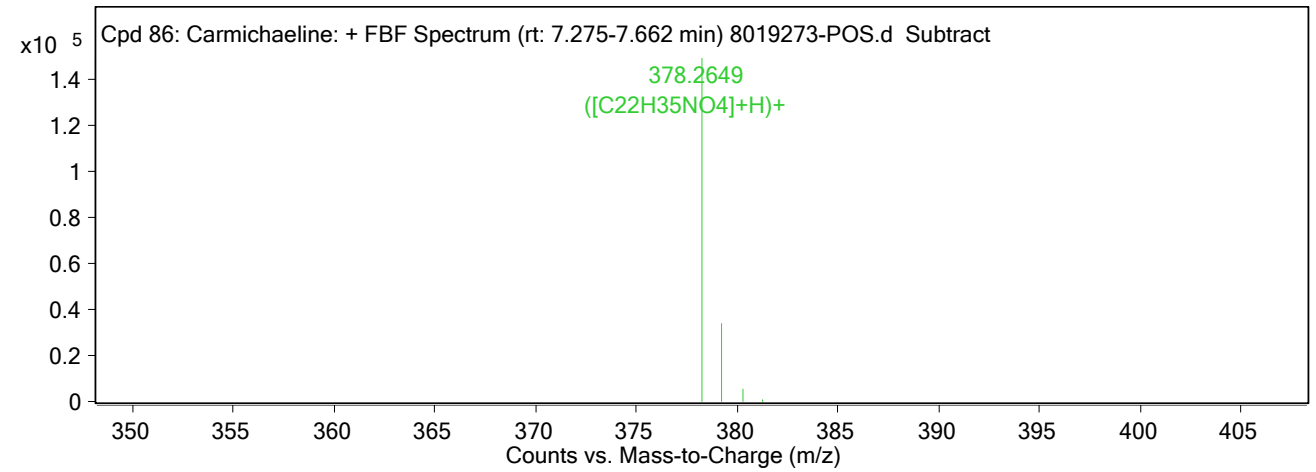
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 370.1667 | 1 | 129223.75 | C21H23NO5 | (M+H)+ |
| 371.1698 | 1 | 30420.85 | C21H23NO5 | (M+H)+ |
| 372.175 | 1 | 5705.48 | C21H23NO5 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 86: Carmichaeline | **Carmichaeline** | 378.2649 | 7.404 | Find By Formula | 377.2576 |

**Compound Chromatograms**




MS Zoomed Spectrum

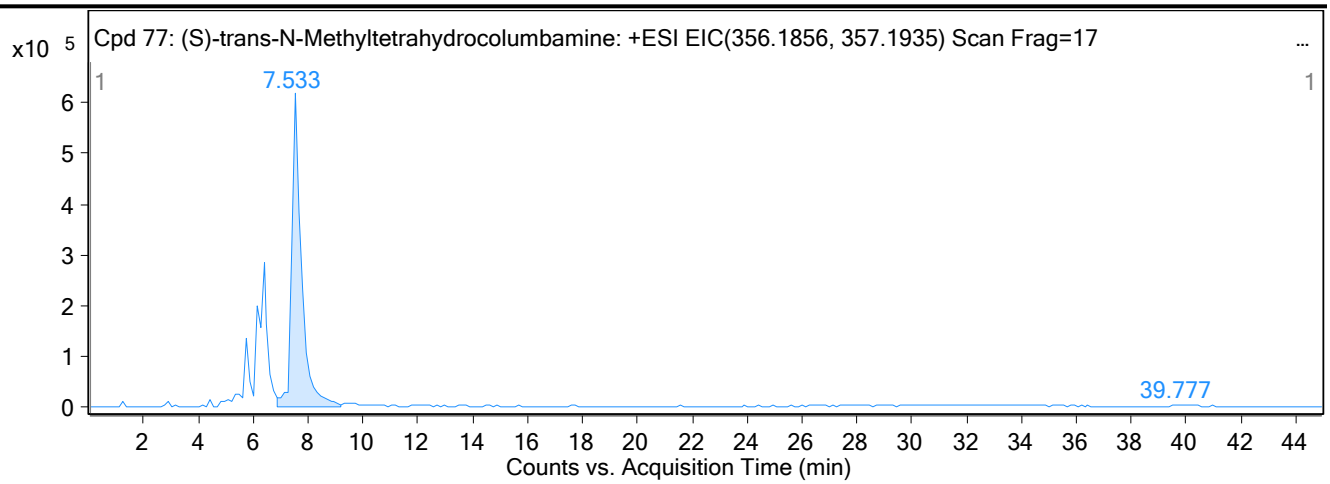



**MS Spectrum Peak List**

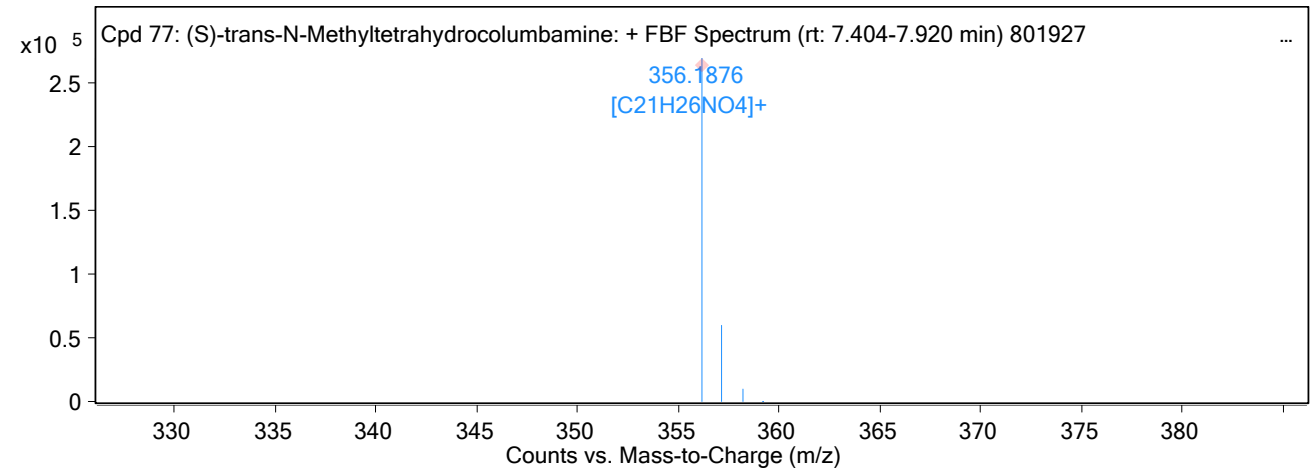
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 378.2649 | 1 | 149127.72 | C22H35NO4 | (M+H)+ |
| 379.2682 | 1 | 33571.8 | C22H35NO4 | (M+H)+ |
| 380.2703 | 1 | 5420.13 | C22H35NO4 | (M+H)+ |
| 381.2738 | 1 | 837.34 | C22H35NO4 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 77: (S)-trans-N-Methyltetrahydrocolumbamine | **(S)-trans-N-Methyltetrahydrocolumbamine** | 356.1876 | 7.533 | Find By Formula | 356.1881 |

**Compound Chromatograms**




MS Zoomed Spectrum

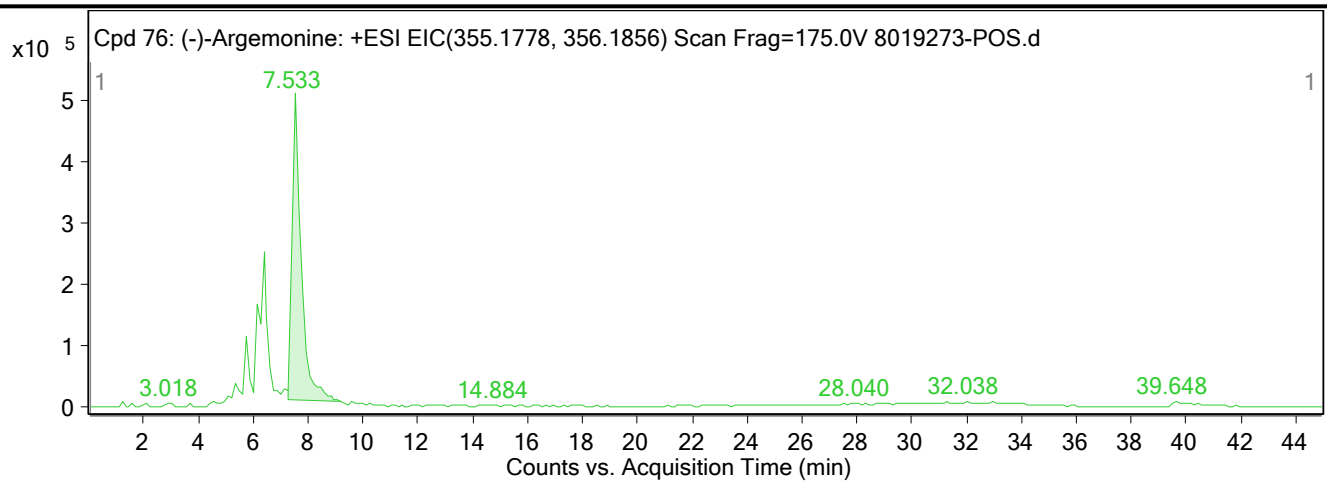



**MS Spectrum Peak List**

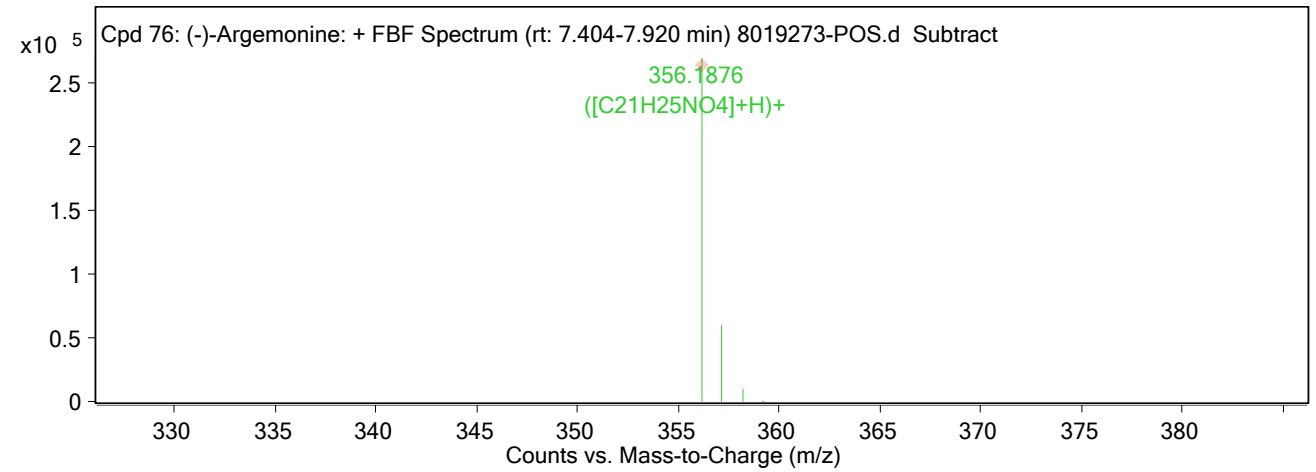
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 356.1876 | 1 | 269741.81 | C21H26NO4 | M+ |
| 357.1905 | 1 | 60494.3 | C21H26NO4 | M+ |
| 358.1933 | 1 | 9409.66 | C21H26NO4 | M+ |
| 359.1957 | 1 | 507.53 | C21H26NO4 | M+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 76: (-)-Argemonine | **(-)-Argemonine** | 356.1876 | 7.533 | Find By Formula | 355.1802 |

**Compound Chromatograms**




MS Zoomed Spectrum

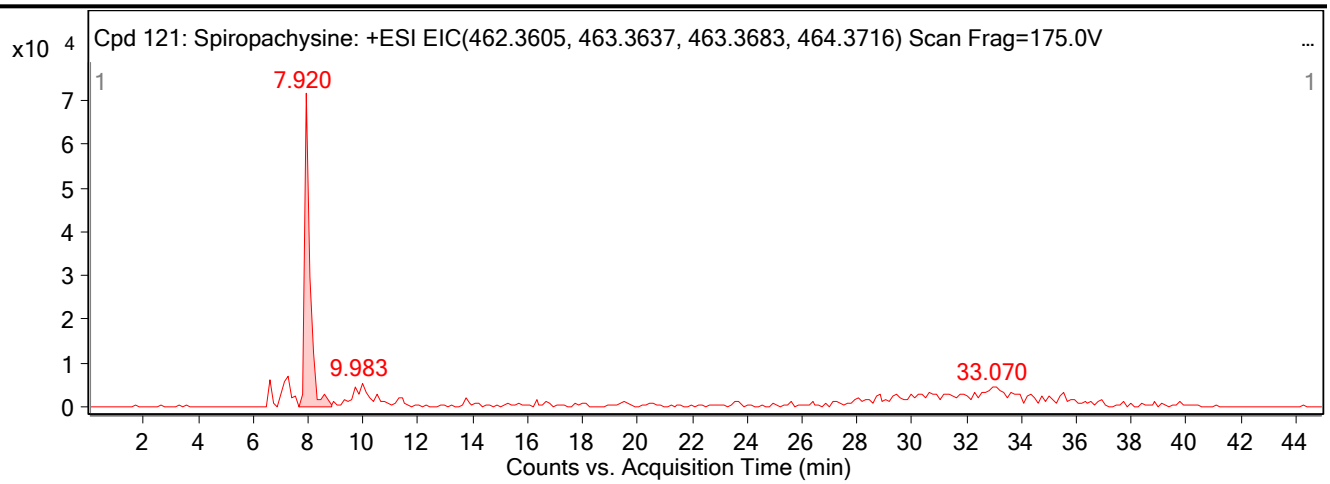



**MS Spectrum Peak List**

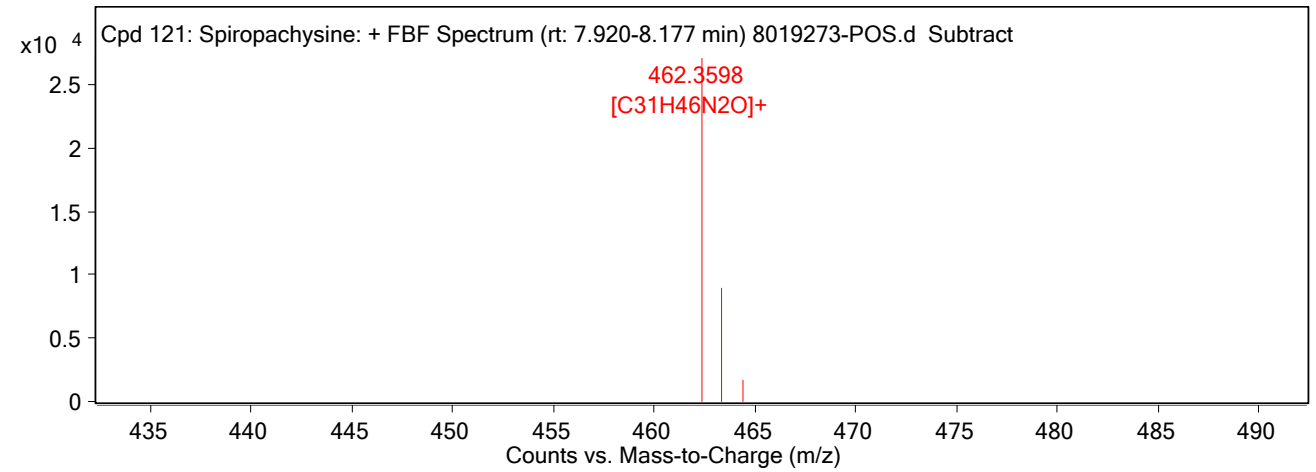
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 356.1876 | 1 | 269741.81 | C21H25NO4 | (M+H)+ |
| 357.1905 | 1 | 60494.3 | C21H25NO4 | (M+H)+ |
| 358.1933 | 1 | 9409.66 | C21H25NO4 | (M+H)+ |
| 359.1957 | 1 | 507.53 | C21H25NO4 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 121: Spiropachysine | **Spiropachysine** | 462.3598 | 7.92 | Find By Formula | 462.3604 |

**Compound Chromatograms**




MS Zoomed Spectrum

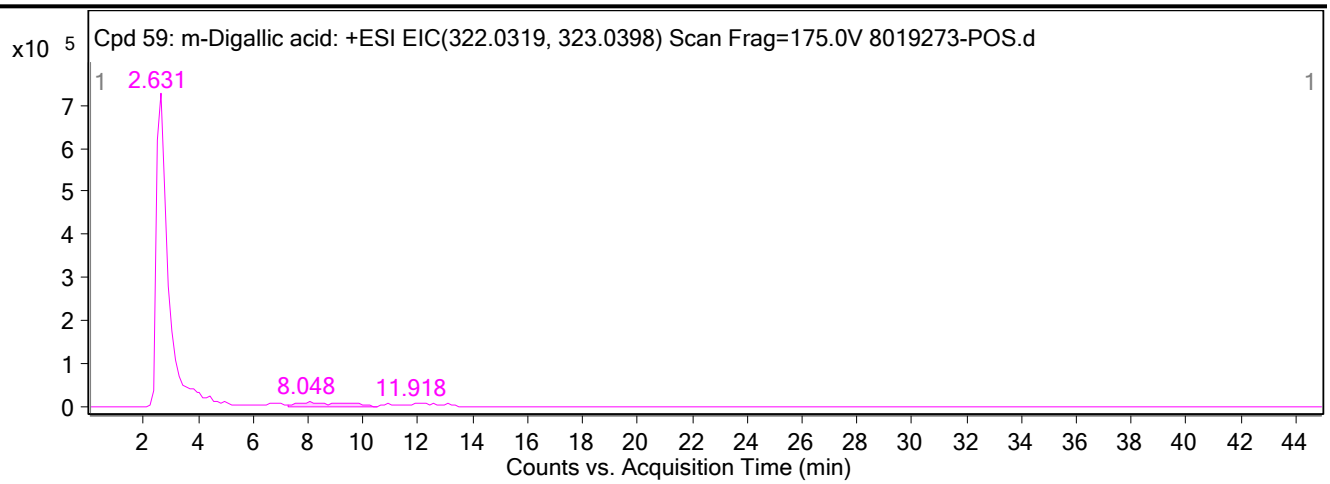



**MS Spectrum Peak List**

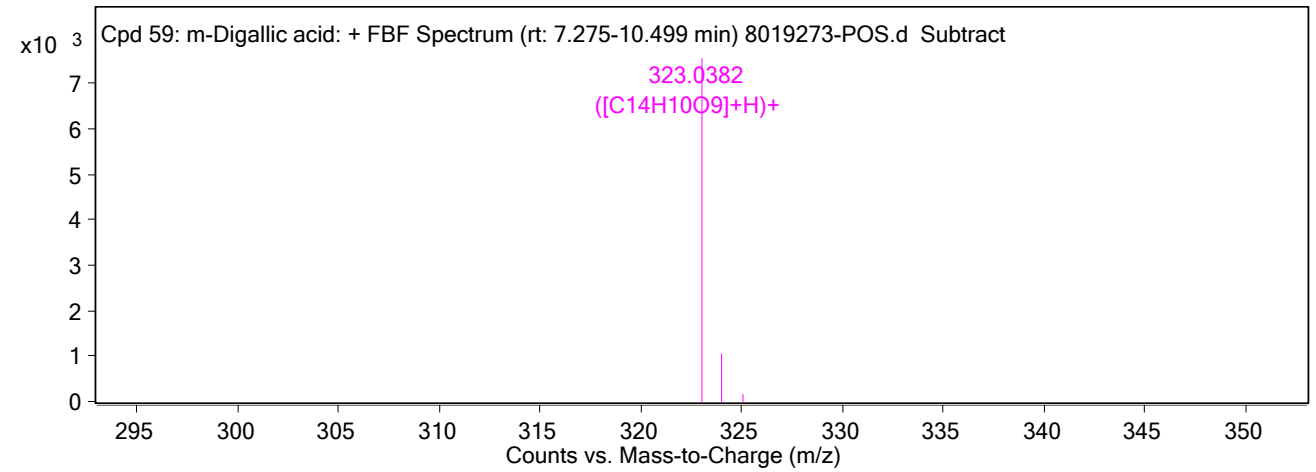
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 462.3598 | 1 | 27112.86 | C31H46N2O | M+ |
| 463.3634 | 1 | 8985.67 | C31H46N2O | M+ |
| 464.3669 | 1 | 1688.62 | C31H46N2O | M+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 59: m-Digallic acid | **m-Digallic acid** | 323.0382 | 8.048 | Find By Formula | 322.0309 |

**Compound Chromatograms**




MS Zoomed Spectrum

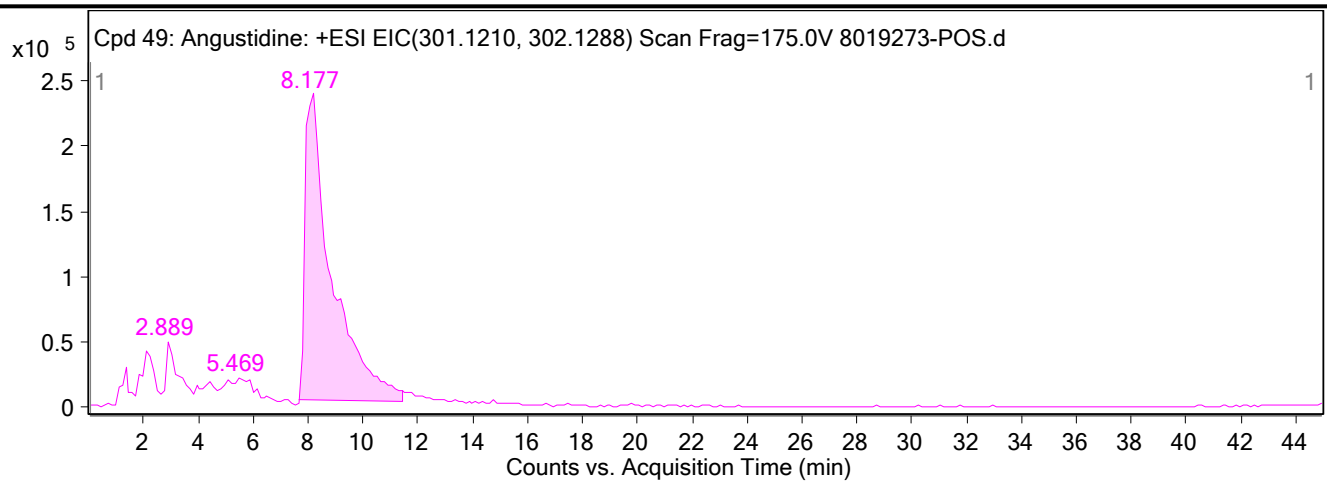



**MS Spectrum Peak List**

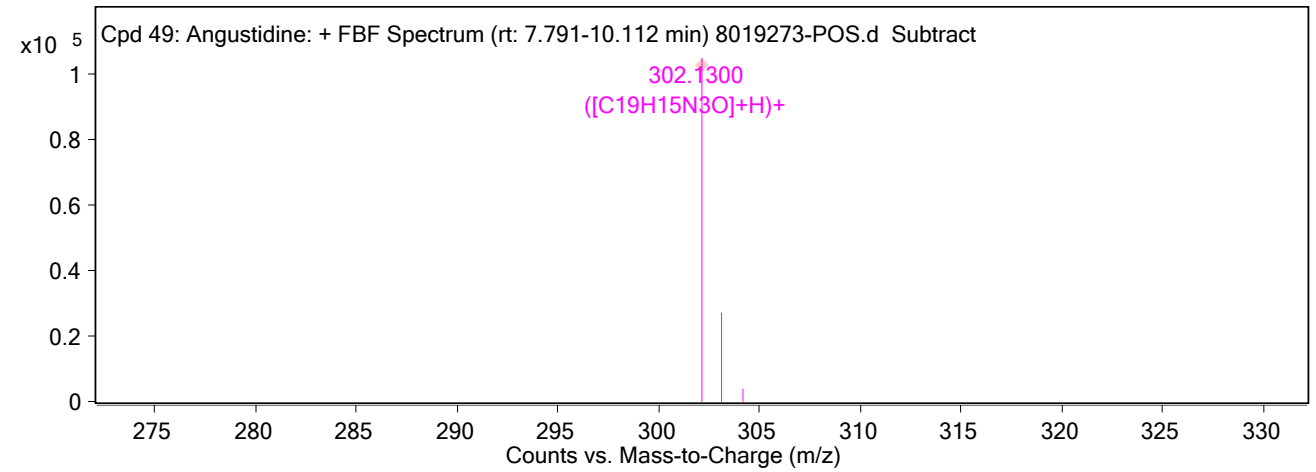
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 323.0382 | 1 | 7550.21 | C14H10O9 | (M+H)+ |
| 324.0414 | 1 | 1046.28 | C14H10O9 | (M+H)+ |
| 325.0401 | 1 | 154.94 | C14H10O9 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 49: Angustidine | **Angustidine** | 302.13 | 8.177 | Find By Formula | 301.1224 |

**Compound Chromatograms**




MS Zoomed Spectrum

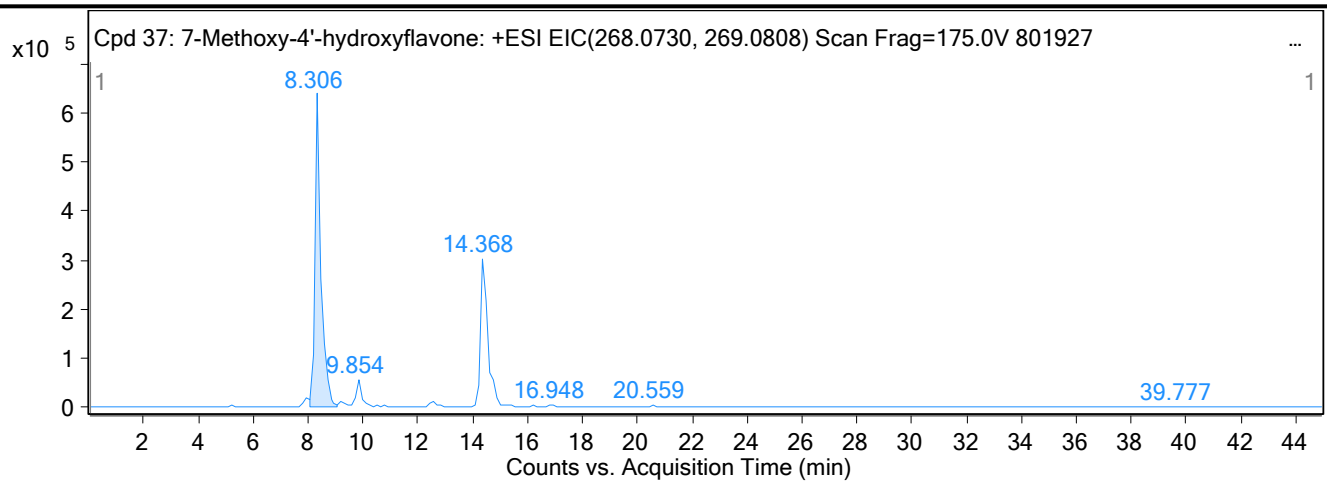



**MS Spectrum Peak List**

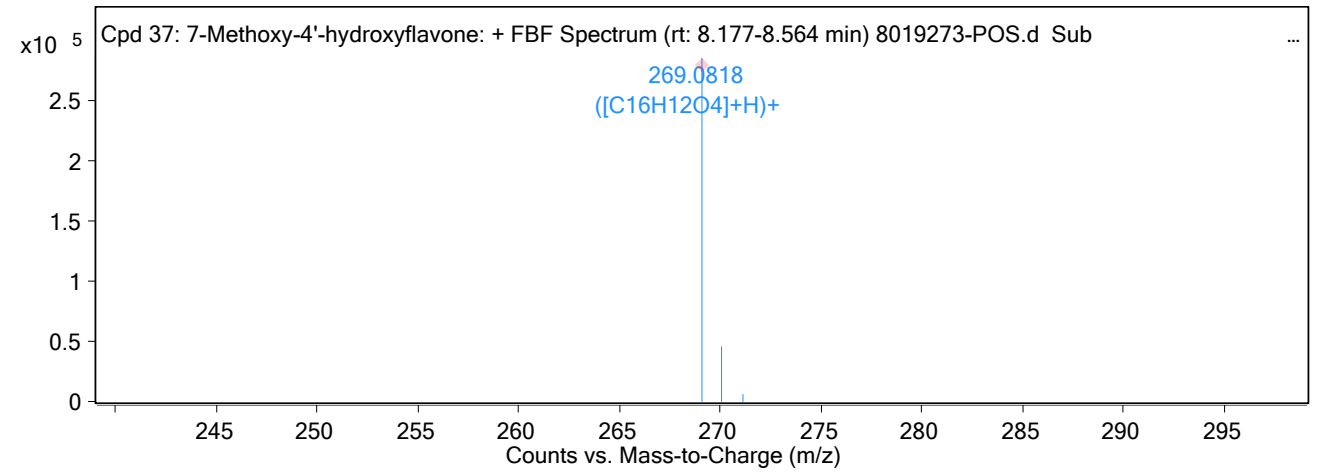
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 302.13 | 1 | 104988.56 | C19H15N3O | (M+H)+ |
| 303.1312 | 1 | 26934.63 | C19H15N3O | (M+H)+ |
| 304.1375 | 1 | 3923.29 | C19H15N3O | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 37: 7-Methoxy-4'-hydroxyflavone | **7-Methoxy-4'-hydroxyflavone** | 269.0818 | 8.306 | Find By Formula | 268.0745 |

**Compound Chromatograms**




MS Zoomed Spectrum

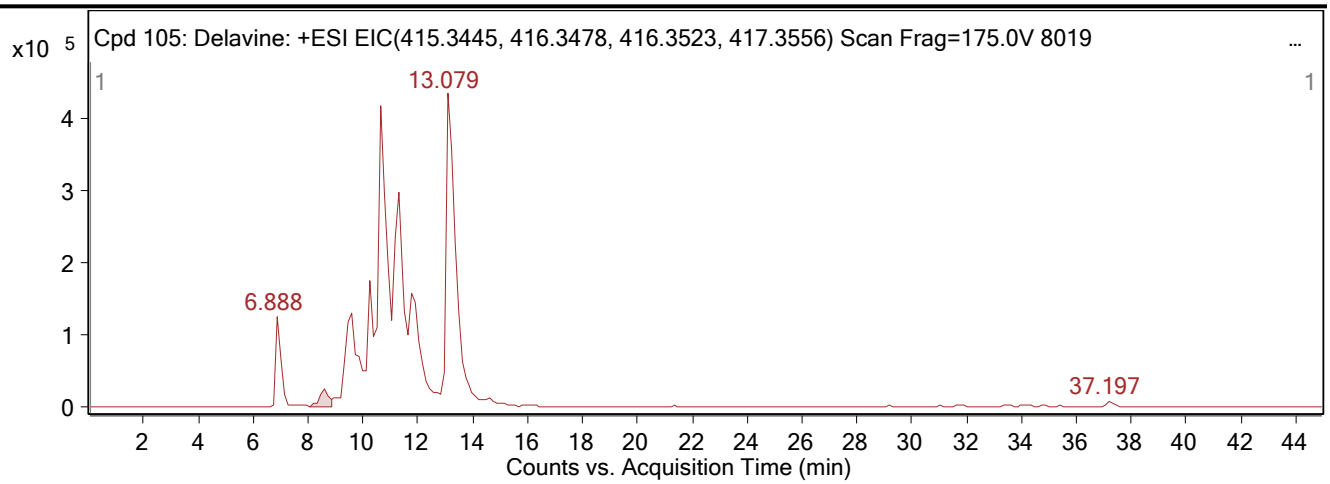



**MS Spectrum Peak List**

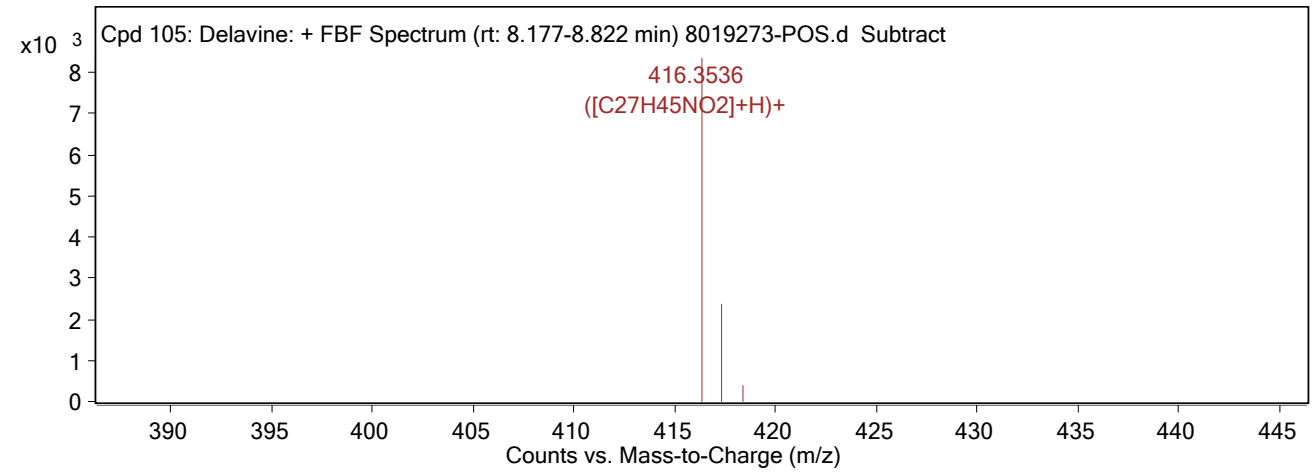
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 269.0818 | 1 | 284649.72 | C16H12O4 | (M+H)+ |
| 270.085 | 1 | 45870.05 | C16H12O4 | (M+H)+ |
| 271.0889 | 1 | 5489.79 | C16H12O4 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 105: Delavine | **Delavine** | 416.3536 | 8.564 | Find By Formula | 415.3463 |

**Compound Chromatograms**




MS Zoomed Spectrum

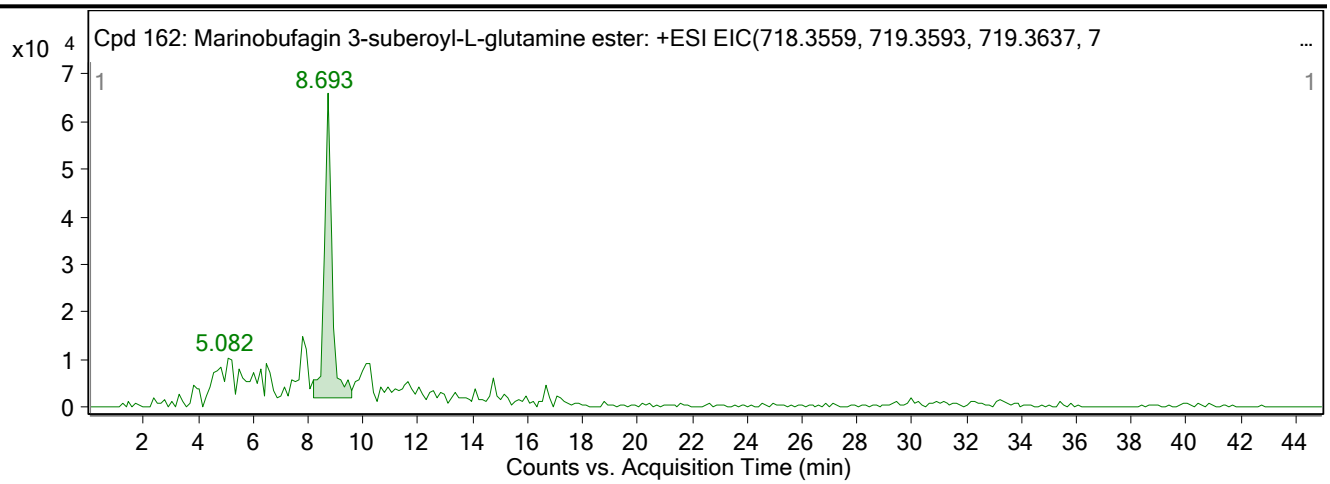



**MS Spectrum Peak List**

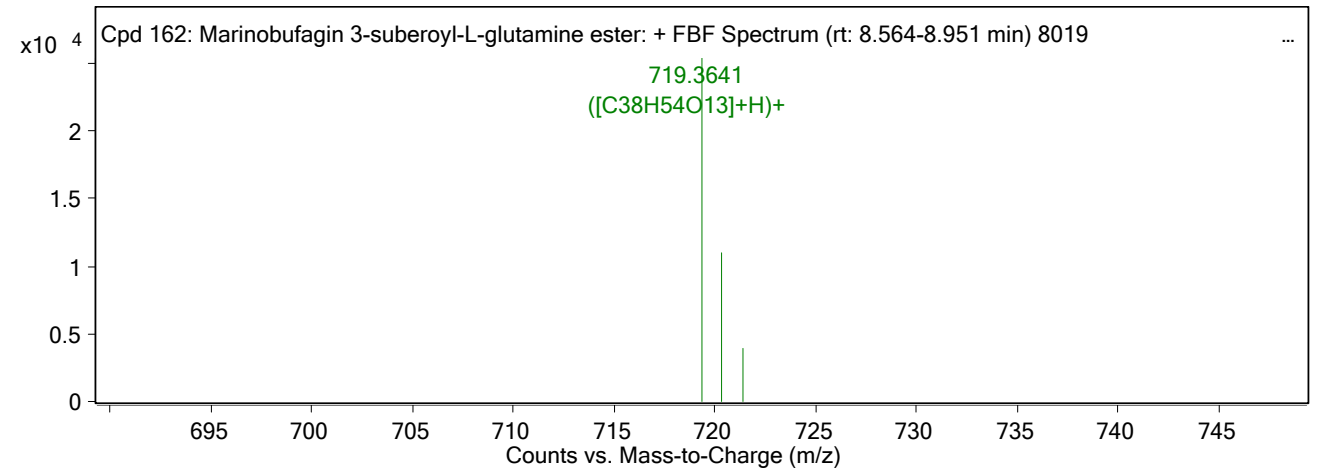
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 416.3536 | 1 | 8349.75 | C27H45NO2 | (M+H)+ |
| 417.357 | 1 | 2378.21 | C27H45NO2 | (M+H)+ |
| 418.3599 | 1 | 379.9 | C27H45NO2 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 162: Marinobufagin 3-suberoyl-L-glutamine ester | **Marinobufagin 3-suberoyl-L-glutamine ester** | 719.3641 | 8.693 | Find By Formula | 718.3564 |

**Compound Chromatograms**




MS Zoomed Spectrum

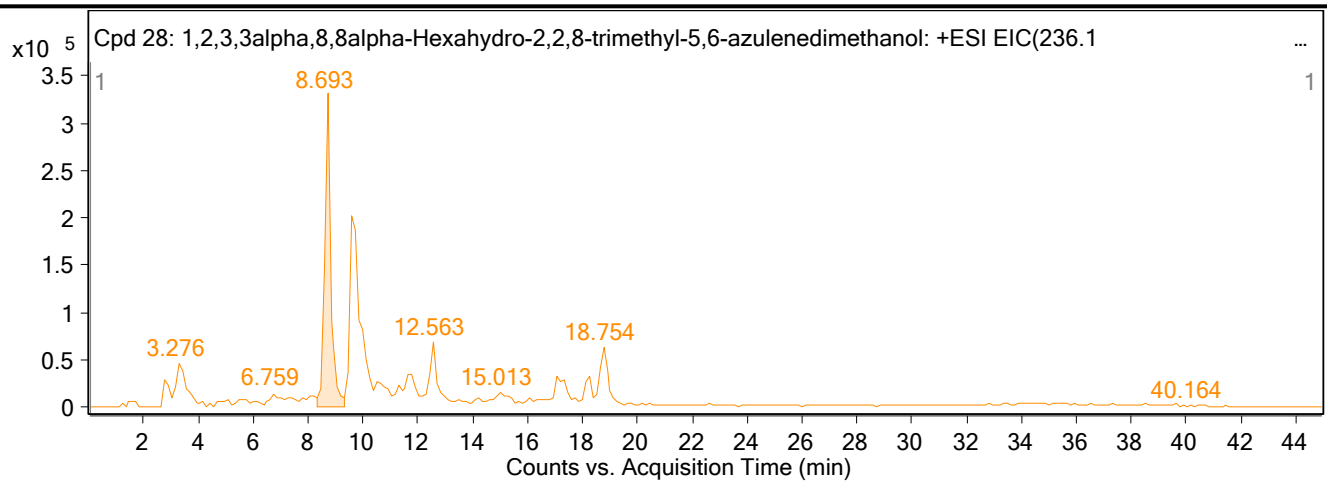



**MS Spectrum Peak List**

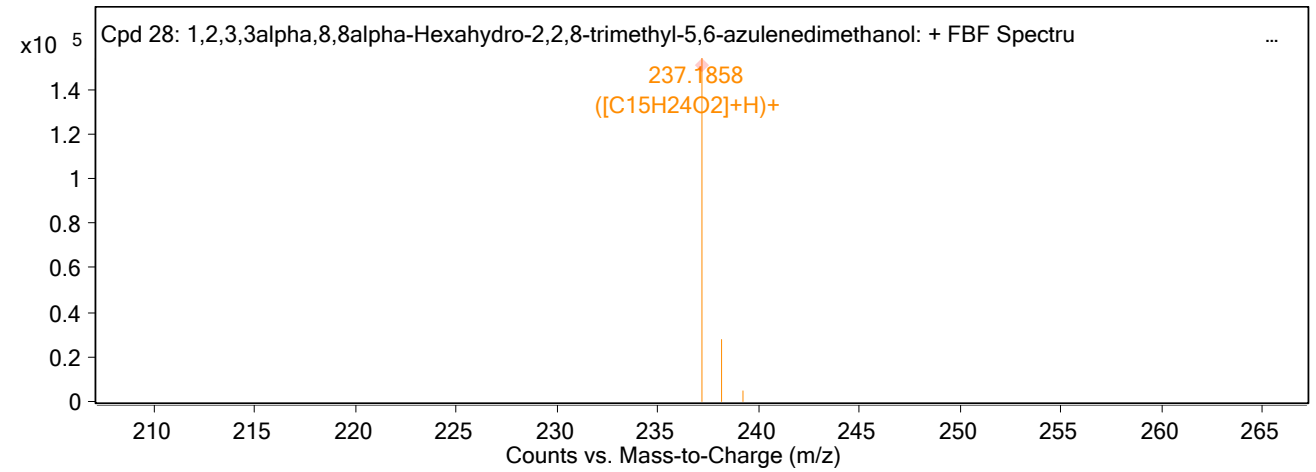
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 719.3641 | 1 | 25362.54 | C38H54O13 | (M+H)+ |
| 720.3673 | 1 | 10928.96 | C38H54O13 | (M+H)+ |
| 721.3665 | 1 | 3975.33 | C38H54O13 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 28: 1,2,3,3alpha,8,8alpha-Hexahydro-2,2,8-trimethyl-5,6-azulenedimethanol | **1,2,3,3alpha,8,8alpha-Hexahydro-2,2,8-trimethyl-5,6-azulenedimethanol** | 237.1858 | 8.693 | Find By Formula | 236.1786 |

**Compound Chromatograms**




MS Zoomed Spectrum

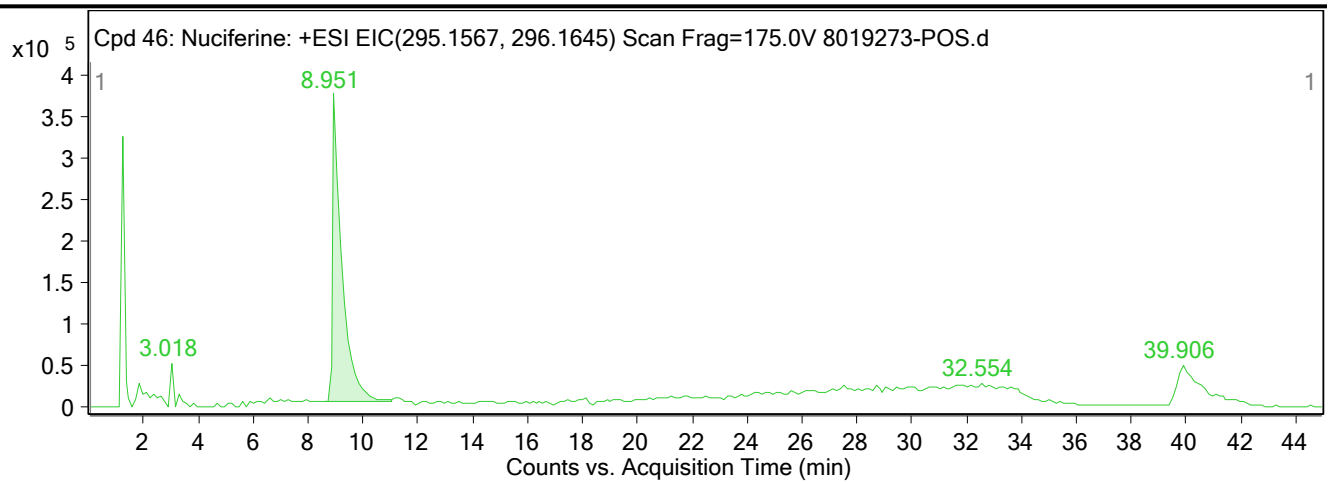



**MS Spectrum Peak List**

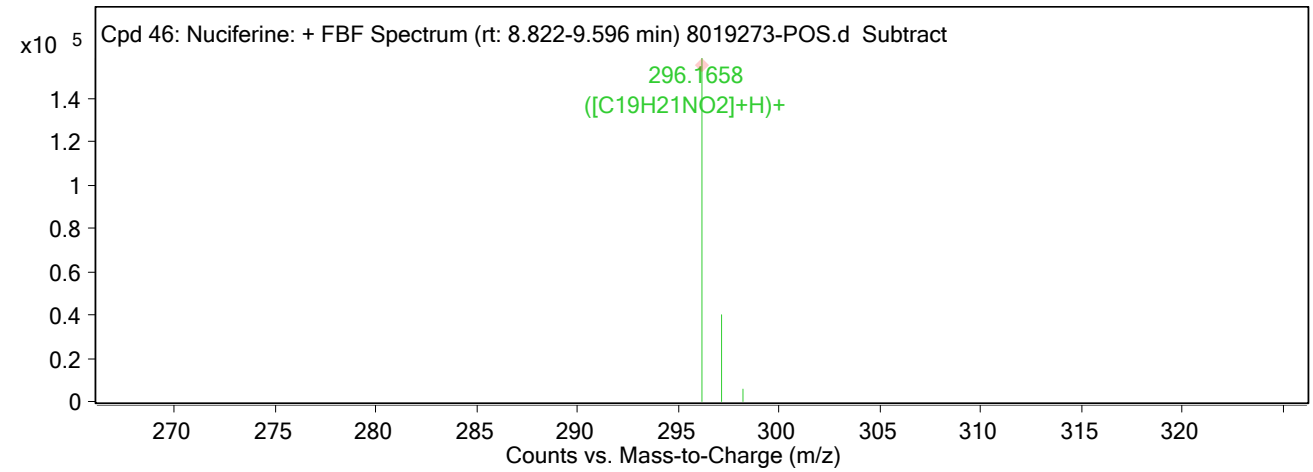
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 237.1858 | 1 | 153913.02 | C15H24O2 | (M+H)+ |
| 238.189 | 1 | 27999.61 | C15H24O2 | (M+H)+ |
| 239.1967 | 1 | 4601.68 | C15H24O2 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 46: Nuciferine | **Nuciferine** | 296.1658 | 8.951 | Find By Formula | 295.1584 |

**Compound Chromatograms**




MS Zoomed Spectrum

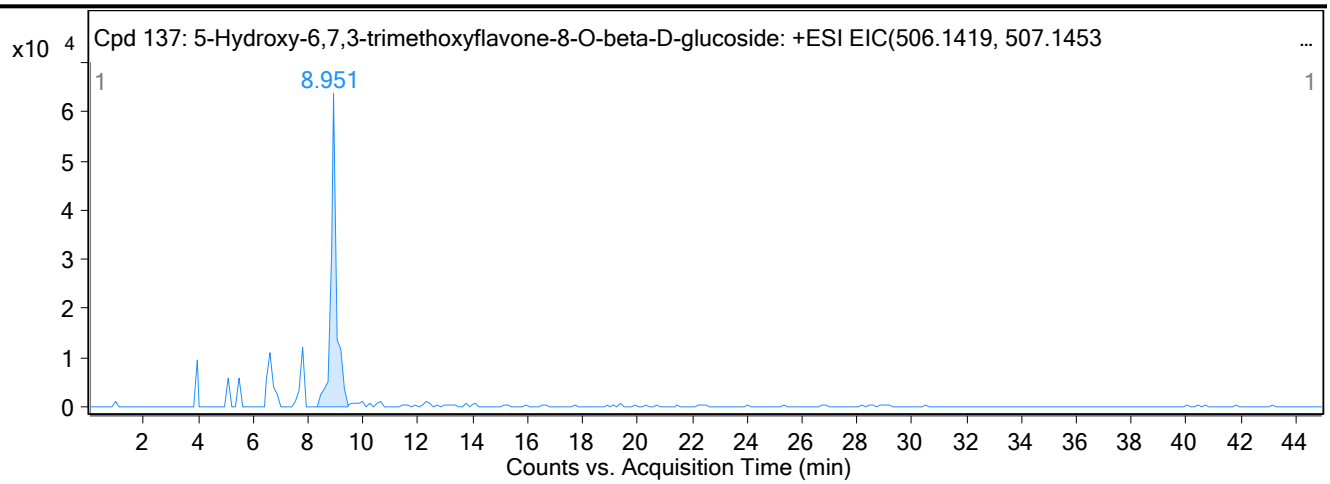



**MS Spectrum Peak List**

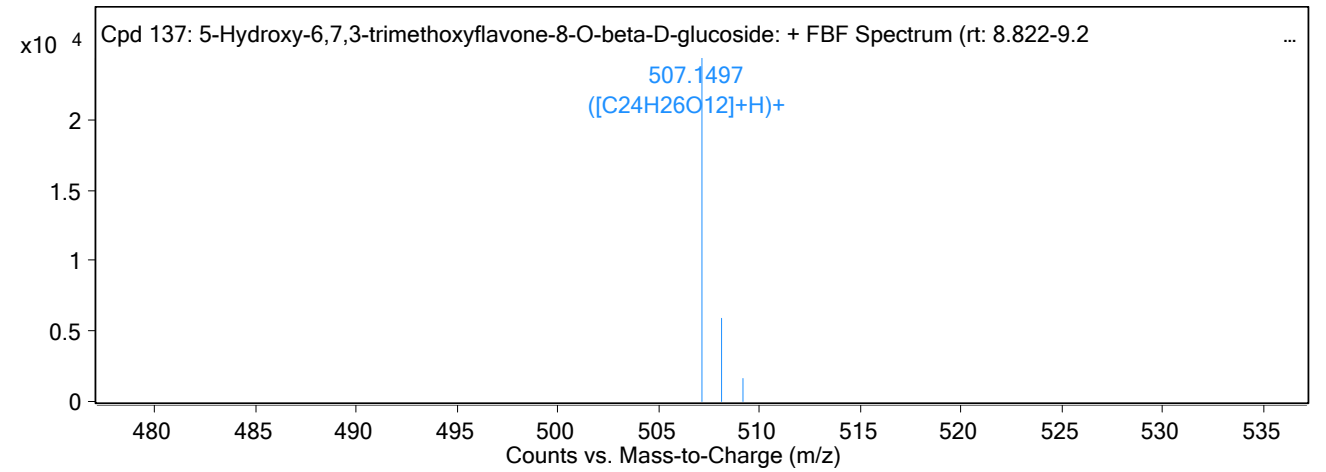
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 296.1658 | 1 | 158763.48 | C19H21NO2 | (M+H)+ |
| 297.1687 | 1 | 40355.57 | C19H21NO2 | (M+H)+ |
| 298.1729 | 1 | 5676.44 | C19H21NO2 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 137: 5-Hydroxy-6,7,3-trimethoxyflavone-8-O-beta-D-glucoside | **5-Hydroxy-6,7,3-trimethoxyflavone-8-O-beta-D-glucoside** | 507.1497 | 8.951 | Find By Formula | 506.1427 |

**Compound Chromatograms**




MS Zoomed Spectrum

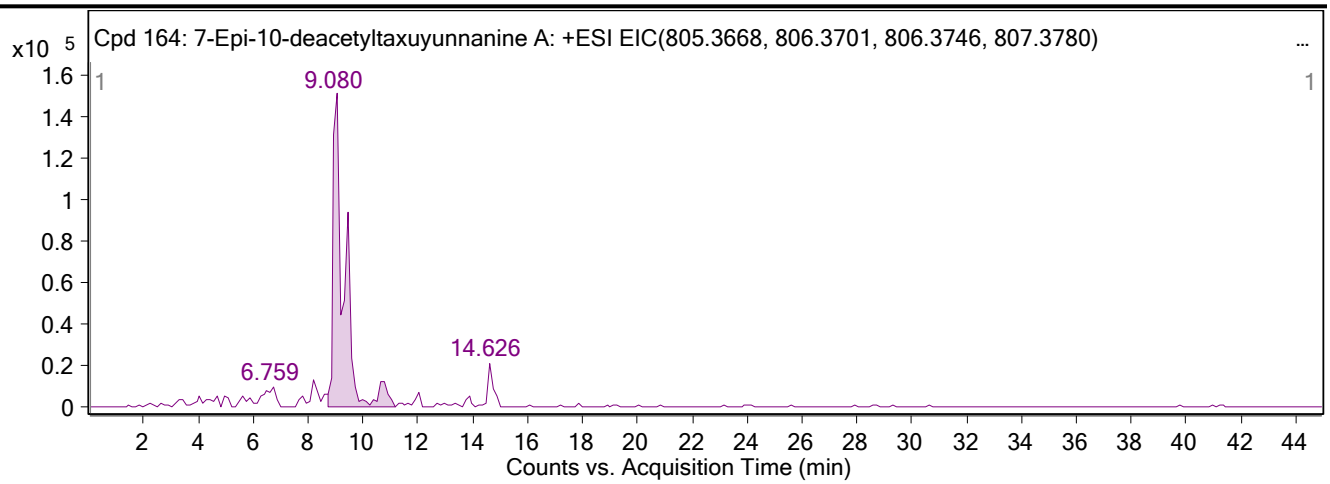



**MS Spectrum Peak List**

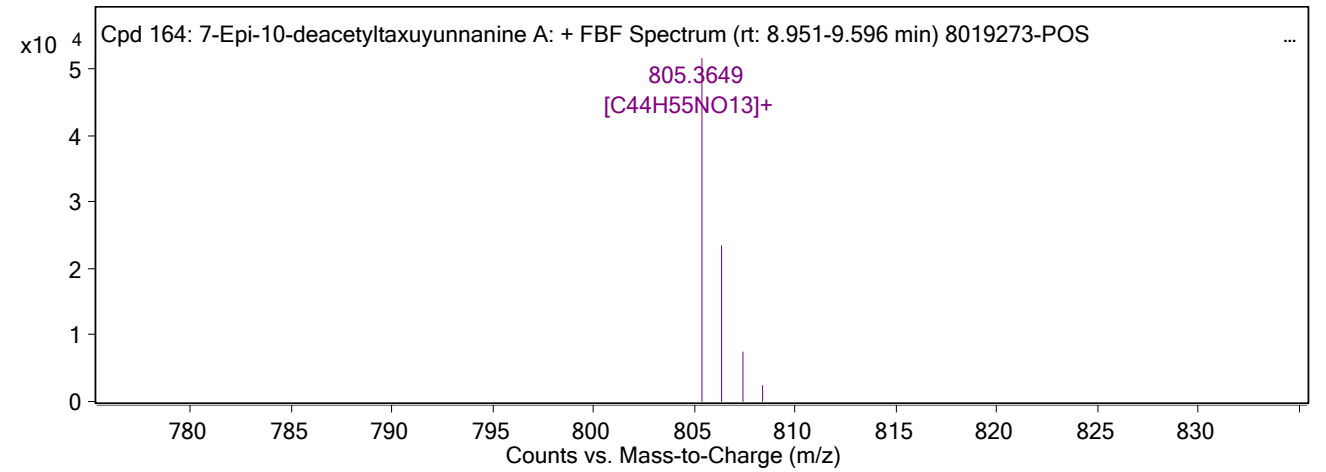
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 507.1497 | 1 | 24351.73 | C24H26O12 | (M+H)+ |
| 508.1535 | 1 | 5962.2 | C24H26O12 | (M+H)+ |
| 509.1592 | 1 | 1679.92 | C24H26O12 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 164: 7-Epi-10-deacetyltaxuyunnanine A | **7-Epi-10-deacetyltaxuyunnanine A** | 805.3649 | 9.08 | Find By Formula | 805.3658 |

**Compound Chromatograms**




MS Zoomed Spectrum

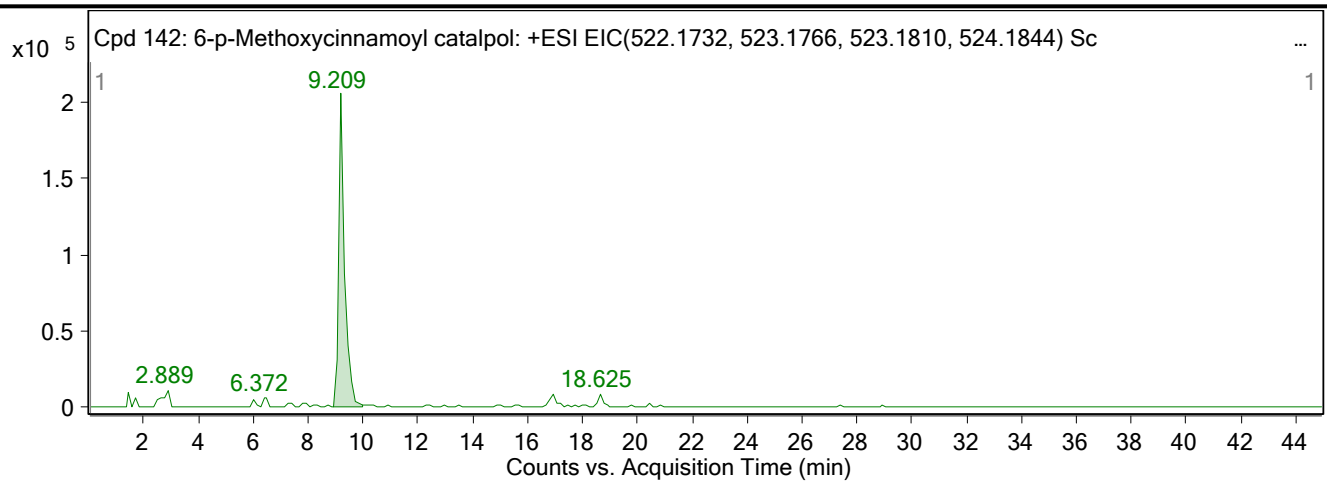



**MS Spectrum Peak List**

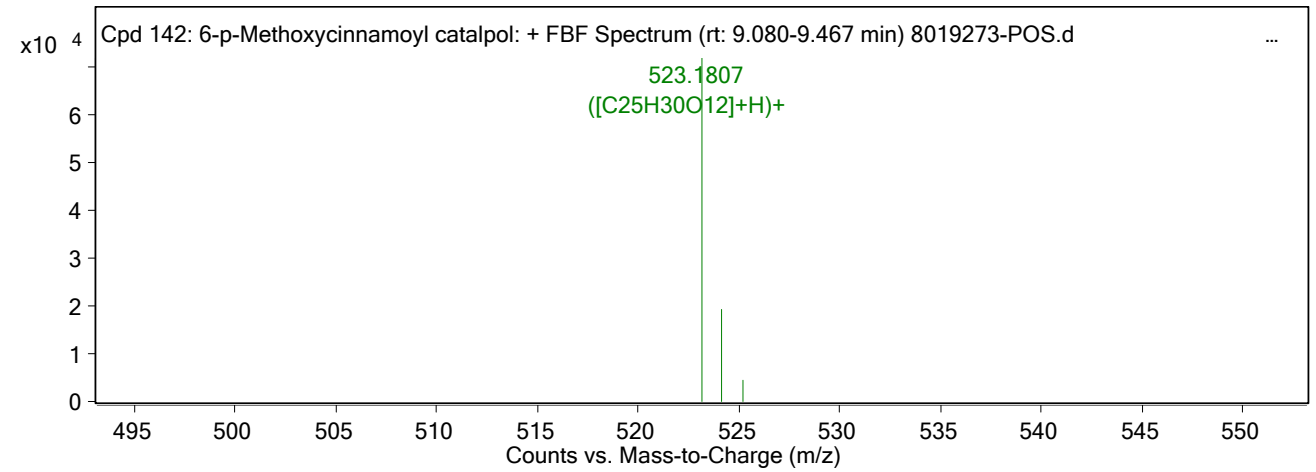
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 805.3649 | 1 | 51615.89 | C44H55NO13 | M+ |
| 806.368 | 1 | 23538.52 | C44H55NO13 | M+ |
| 807.3723 | 1 | 7439.96 | C44H55NO13 | M+ |
| 808.3846 | 1 | 2436.34 | C44H55NO13 | M+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 142: 6-p-Methoxycinnamoyl catalpol | **6-p-Methoxycinnamoyl catalpol** | 523.1807 | 9.209 | Find By Formula | 522.1735 |

**Compound Chromatograms**




MS Zoomed Spectrum

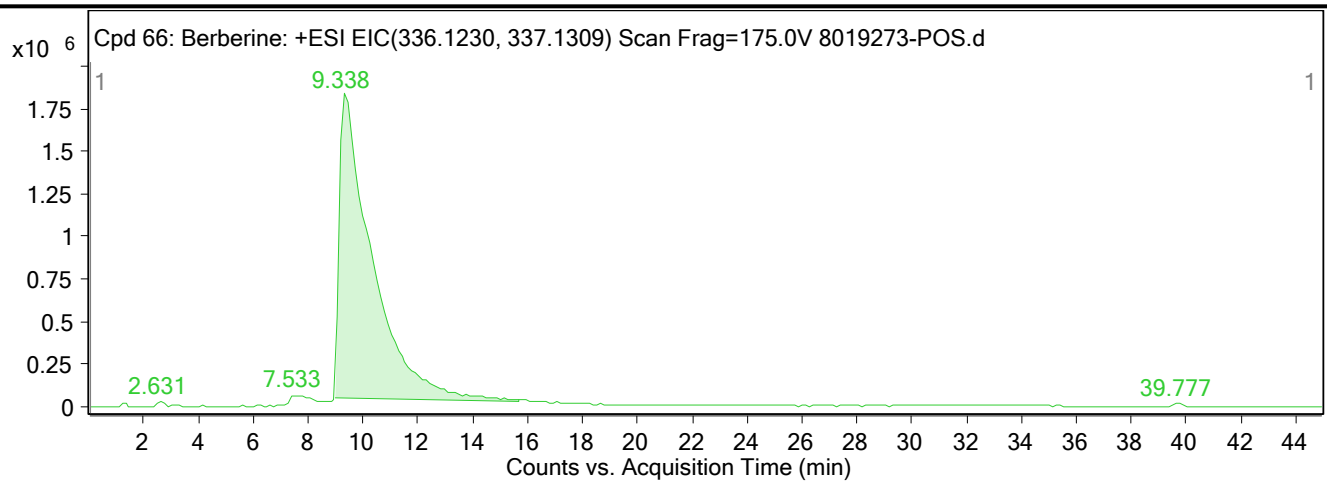



**MS Spectrum Peak List**

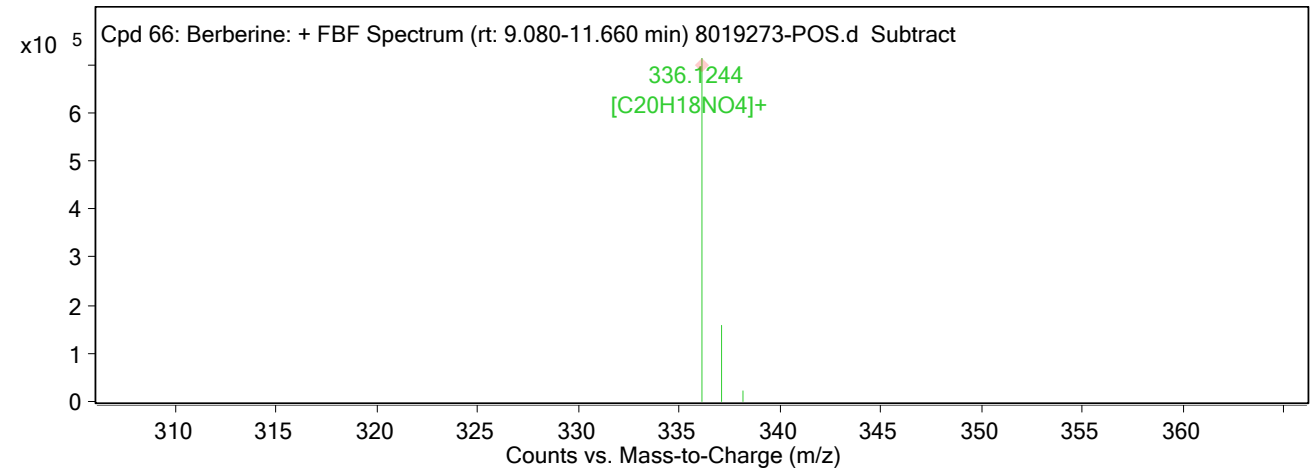
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 523.1807 | 1 | 71732.57 | C25H30O12 | (M+H)+ |
| 524.1839 | 1 | 19296.21 | C25H30O12 | (M+H)+ |
| 525.1884 | 1 | 4289.58 | C25H30O12 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 66: Berberine | **Berberine** | 336.1244 | 9.338 | Find By Formula | 336.125 |

**Compound Chromatograms**




MS Zoomed Spectrum

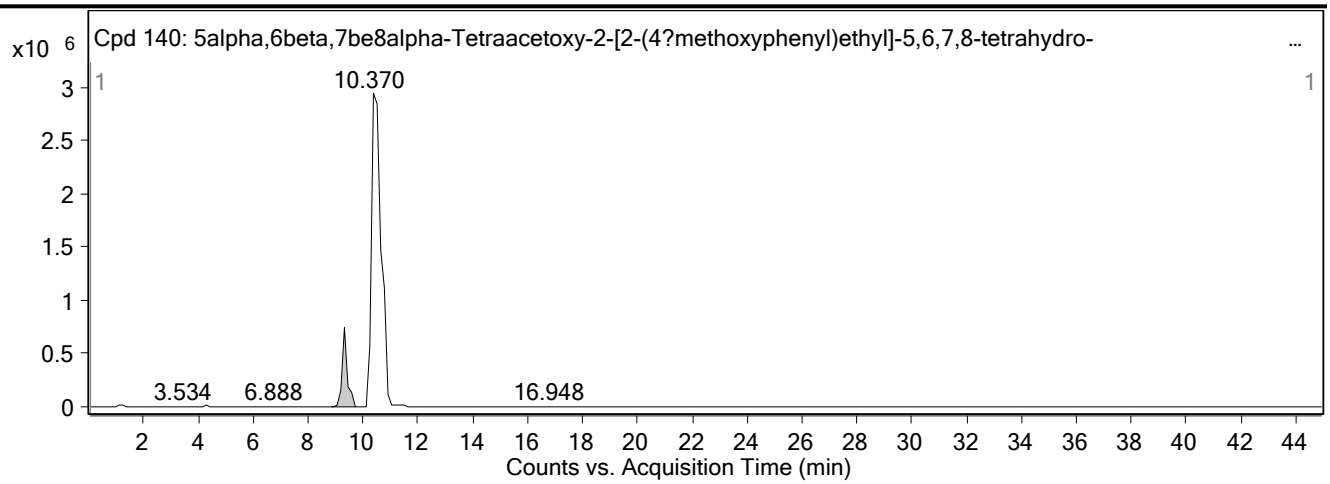



**MS Spectrum Peak List**

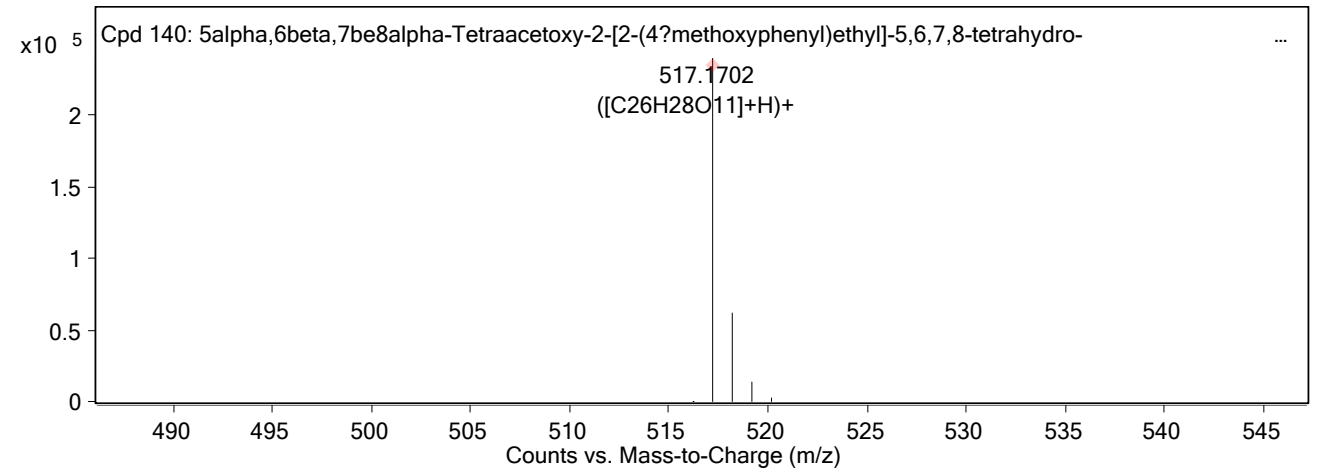
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 336.1244 | 1 | 713034.13 | C20H18NO4 | M+ |
| 337.1278 | 1 | 157465.14 | C20H18NO4 | M+ |
| 338.1321 | 1 | 23511.25 | C20H18NO4 | M+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 140: 5alpha,6beta,7be8alpha-Tetraacetoxy-2-[2-(4?methoxyphenyl)ethyl]-5,6,7,8-tetrahydro-chromone (AH1a) | **5alpha,6beta,7be8alpha-Tetraacetoxy-2-[2-(4?methoxyphenyl)ethyl]-5,6,7,8-tetrahydro-chromone (AH1a)** | 517.1702 | 9.338 | Find By Formula | 516.1629 |

**Compound Chromatograms**




MS Zoomed Spectrum

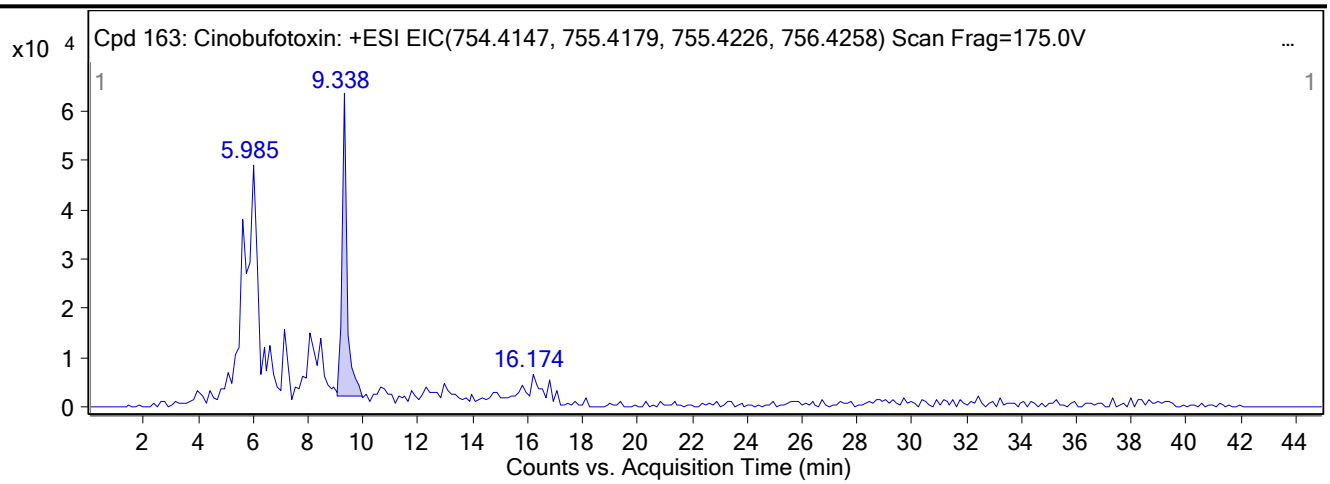



**MS Spectrum Peak List**

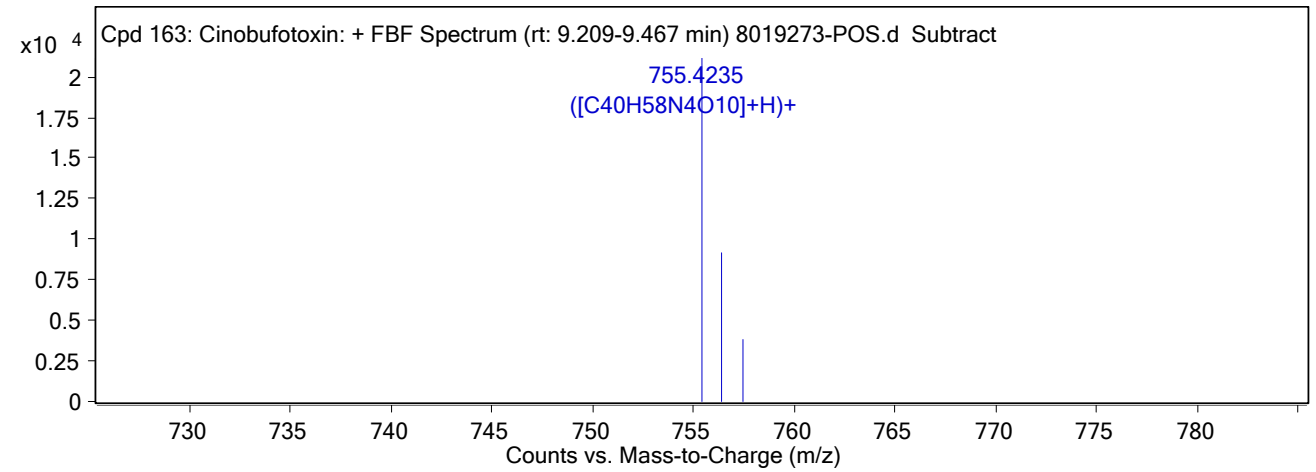
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 516.172 | 1 | 306.42 | C26H28O11 | M+ |
| 517.1702 | 1 | 239820.75 | C26H28O11 | (M+H)+ |
| 518.1735 | 1 | 62433.11 | C26H28O11 | (M+H)+ |
| 519.1767 | 1 | 13276.63 | C26H28O11 | (M+H)+ |
| 520.1772 | 1 | 2033.42 | C26H28O11 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 163: Cinobufotoxin | **Cinobufotoxin** | 755.4235 | 9.338 | Find By Formula | 754.4156 |

**Compound Chromatograms**




MS Zoomed Spectrum

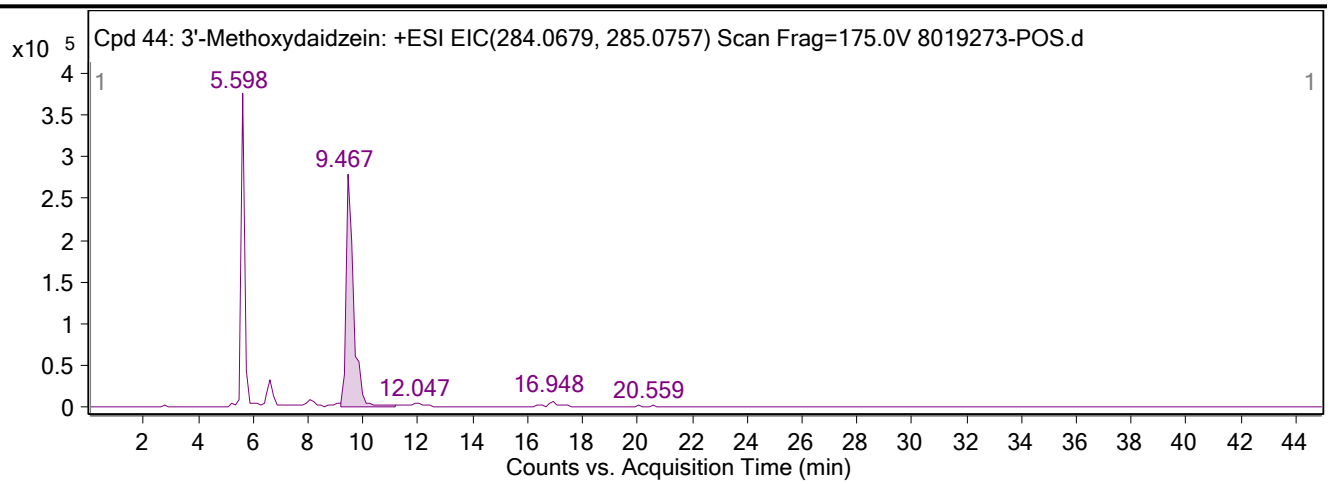



**MS Spectrum Peak List**

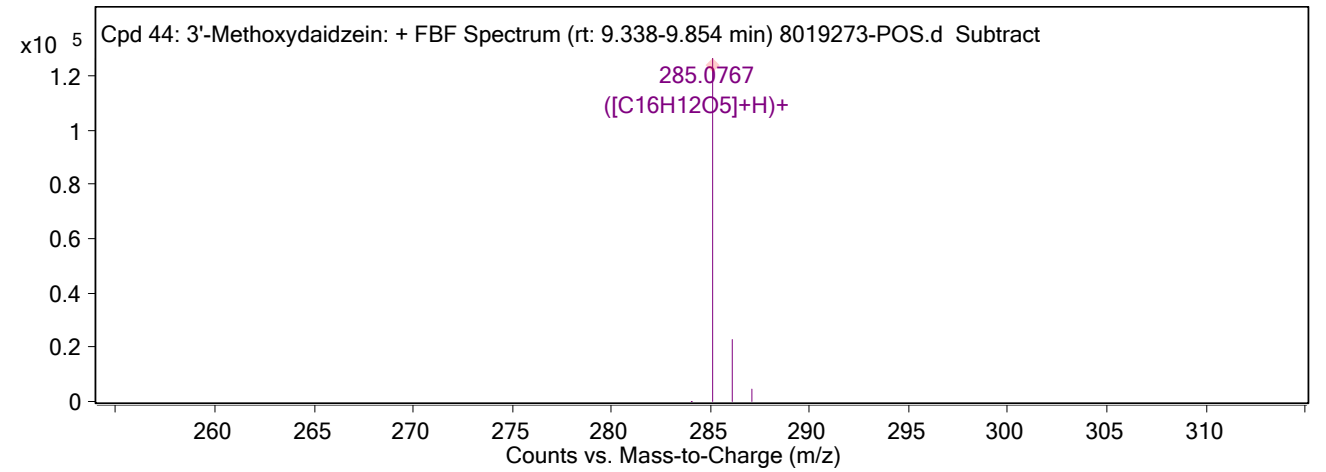
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 755.4235 | 1 | 21161.11 | C40H58N4O10 | (M+H)+ |
| 756.4252 | 1 | 9209.61 | C40H58N4O10 | (M+H)+ |
| 757.4277 | 1 | 3807.05 | C40H58N4O10 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 44: 3'-Methoxydaidzein | **3'-Methoxydaidzein** | 285.0767 | 9.467 | Find By Formula | 284.0695 |

**Compound Chromatograms**




MS Zoomed Spectrum

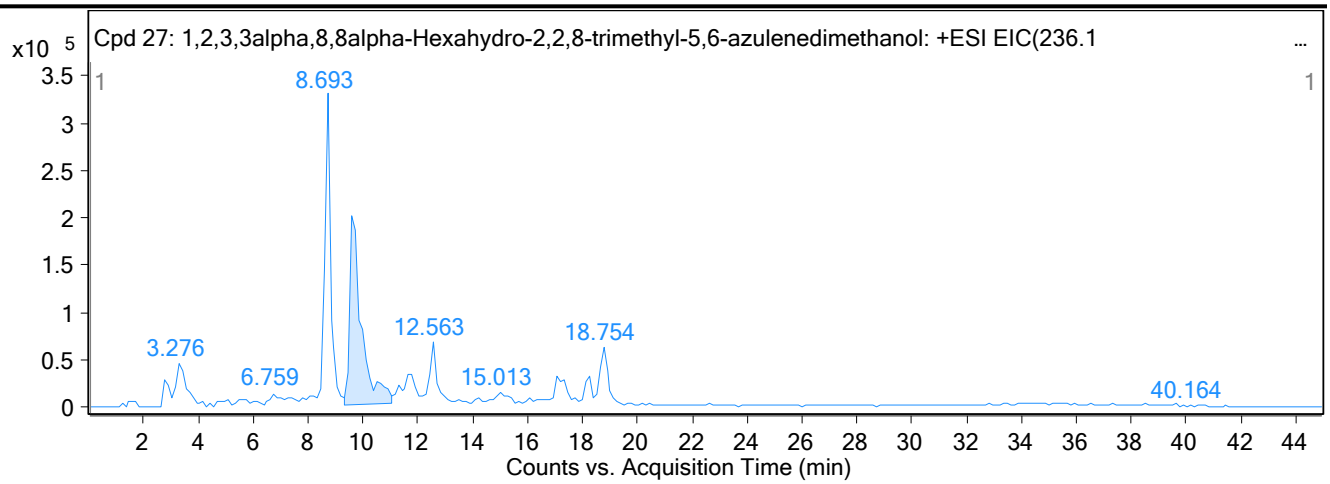



**MS Spectrum Peak List**

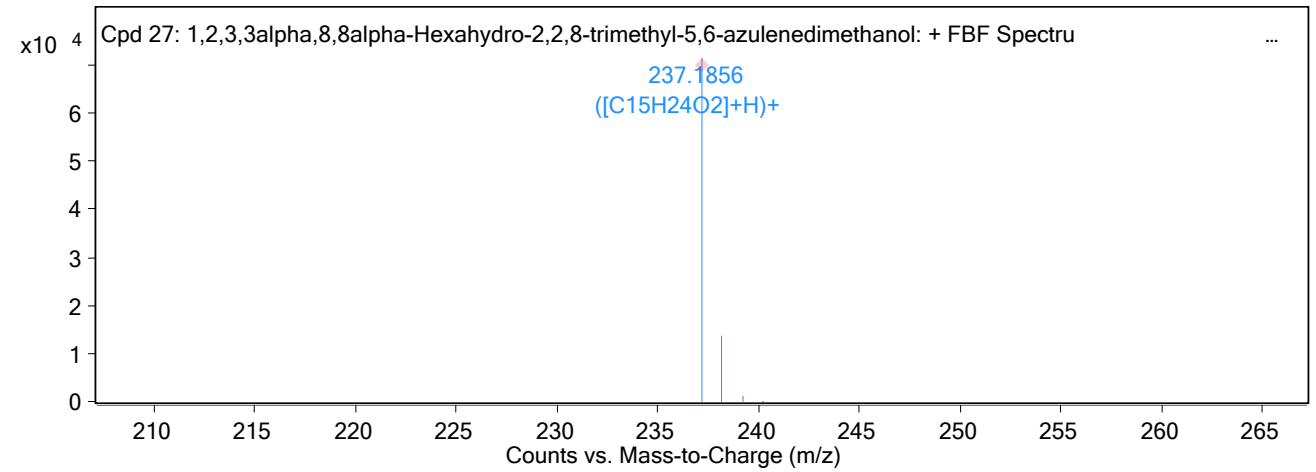
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 284.0666 | 1 | 148.69 | C16H12O5 | M+ |
| 285.0767 | 1 | 126482.42 | C16H12O5 | (M+H)+ |
| 286.08 | 1 | 22593.9 | C16H12O5 | (M+H)+ |
| 287.0873 | 1 | 4303.96 | C16H12O5 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 27: 1,2,3,3alpha,8,8alpha-Hexahydro-2,2,8-trimethyl-5,6-azulenedimethanol | **1,2,3,3alpha,8,8alpha-Hexahydro-2,2,8-trimethyl-5,6-azulenedimethanol** | 237.1856 | 9.596 | Find By Formula | 236.1783 |

**Compound Chromatograms**




MS Zoomed Spectrum

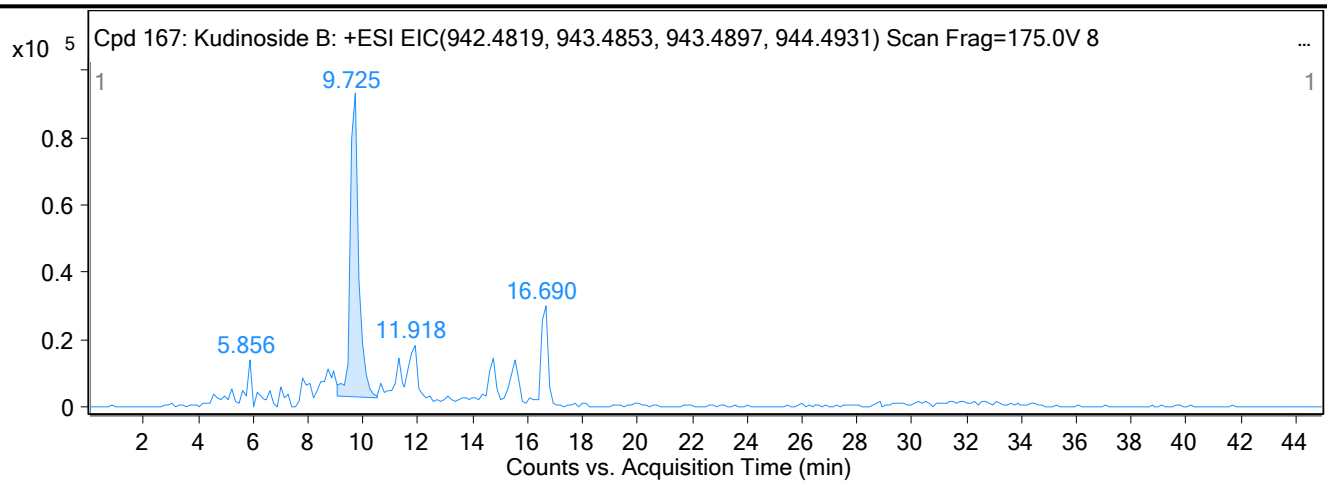



**MS Spectrum Peak List**

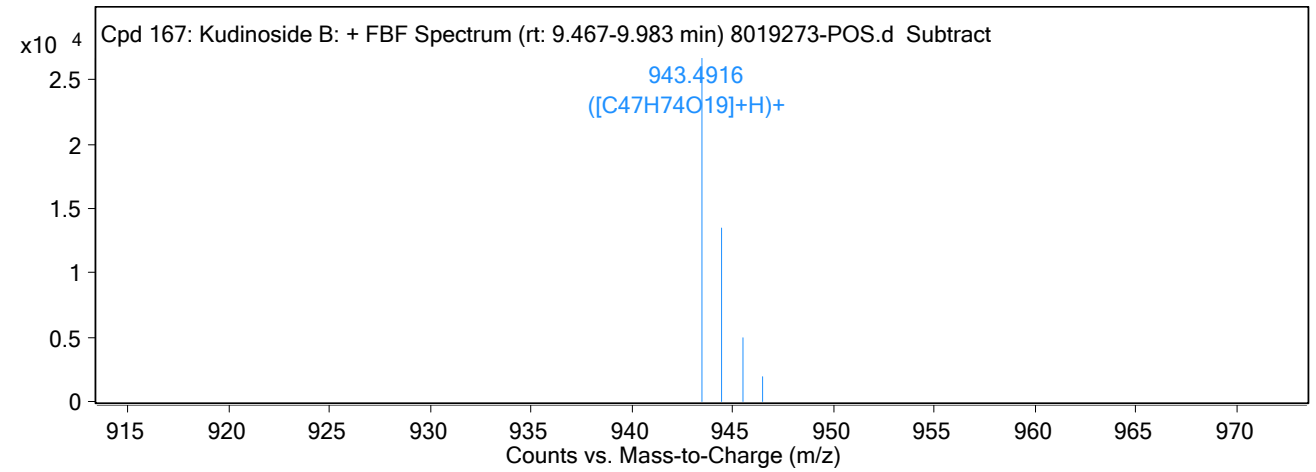
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 237.1856 | 1 | 71458.36 | C15H24O2 | (M+H)+ |
| 238.1889 | 1 | 13522.44 | C15H24O2 | (M+H)+ |
| 239.1905 | 1 | 1222.94 | C15H24O2 | (M+H)+ |
| 240.1907 | 1 | 98.53 | C15H24O2 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 167: Kudinoside B | **Kudinoside B** | 943.4916 | 9.725 | Find By Formula | 942.4832 |

**Compound Chromatograms**




MS Zoomed Spectrum

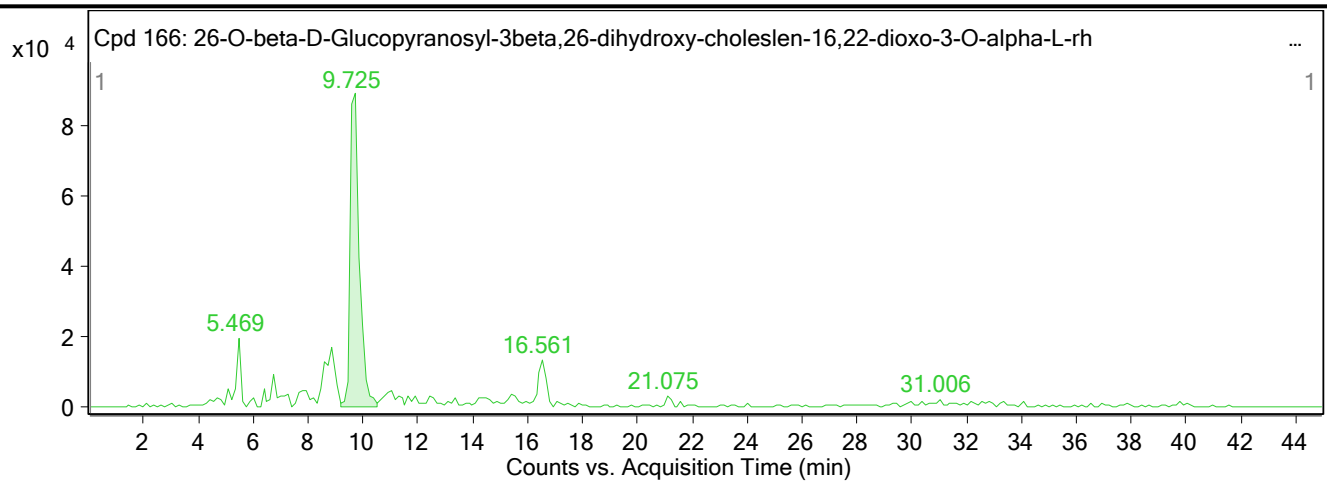



**MS Spectrum Peak List**

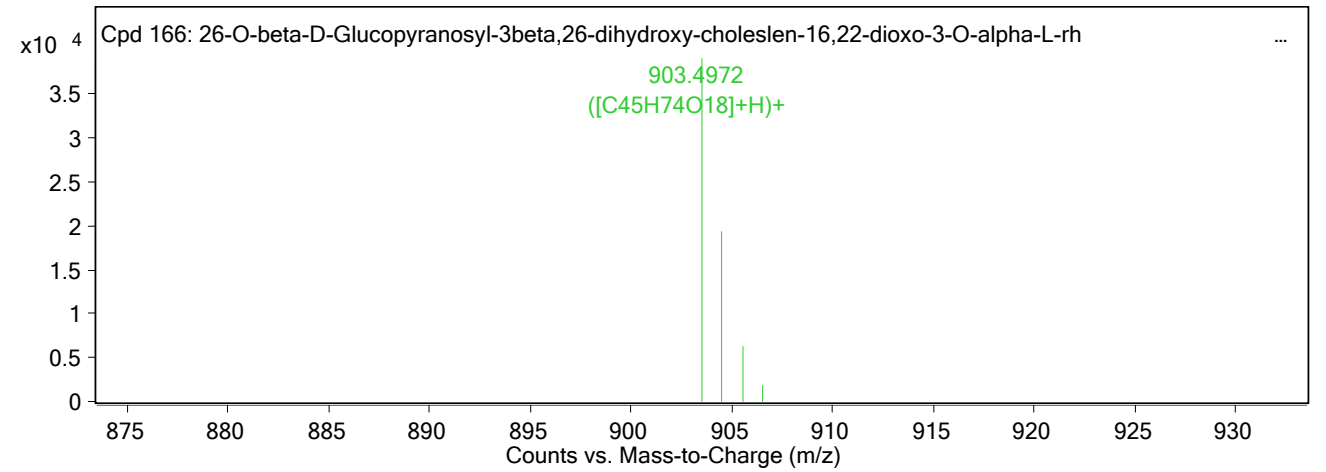
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 943.4916 | 1 | 26667.79 | C47H74O19 | (M+H)+ |
| 944.4931 | 1 | 13486.42 | C47H74O19 | (M+H)+ |
| 945.4975 | 1 | 4995.8 | C47H74O19 | (M+H)+ |
| 946.4877 | 1 | 1999.18 | C47H74O19 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 166: 26-O-beta-D-Glucopyranosyl-3beta,26-dihydroxy-cholesten-16,22-dioxo-3-O-alpha-L-rhamnopyranosyl-(1-- | **26-O-beta-D-Glucopyranosyl-3beta,26-dihydroxy-cholesten-16,22-dioxo-3-O-alpha-L-rhamnopyranosyl-(1--** | 903.4972 | 9.725 | Find By Formula | 902.4894 |

**Compound Chromatograms**




MS Zoomed Spectrum

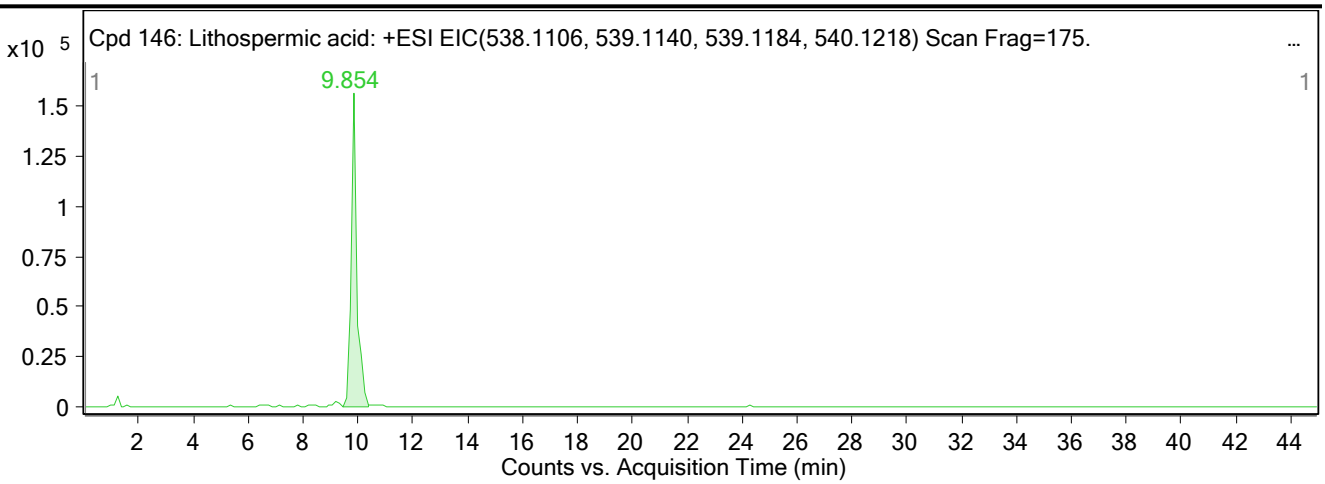



**MS Spectrum Peak List**

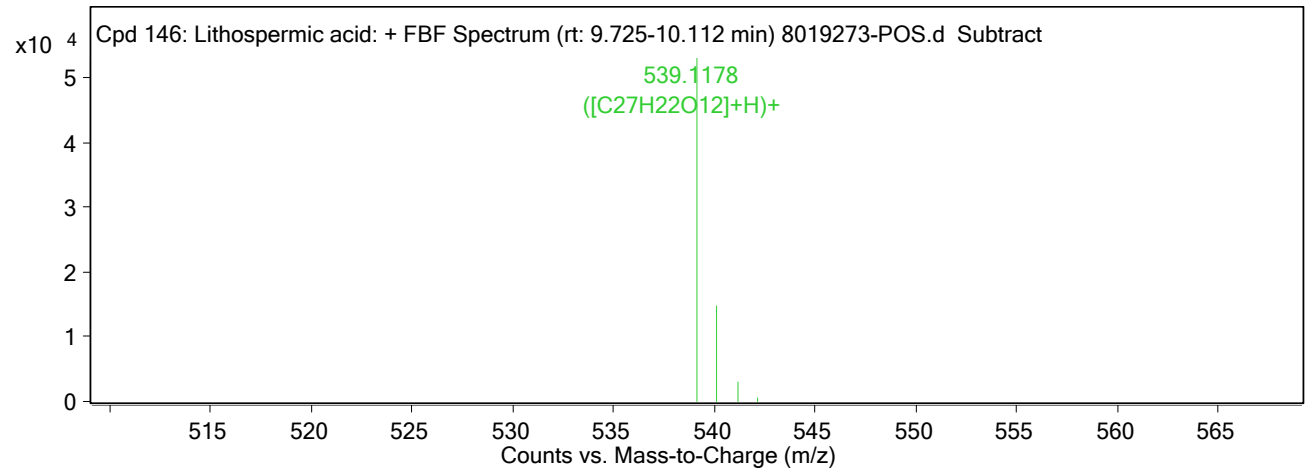
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 903.4972 | 1 | 39110.53 | C45H74O18 | (M+H)+ |
| 904.5003 | 1 | 19265.32 | C45H74O18 | (M+H)+ |
| 905.5027 | 1 | 6277.63 | C45H74O18 | (M+H)+ |
| 906.4925 | 1 | 1905.14 | C45H74O18 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 146: Lithospermic acid | **Lithospermic acid** | 539.1178 | 9.854 | Find By Formula | 538.1105 |

**Compound Chromatograms**




MS Zoomed Spectrum

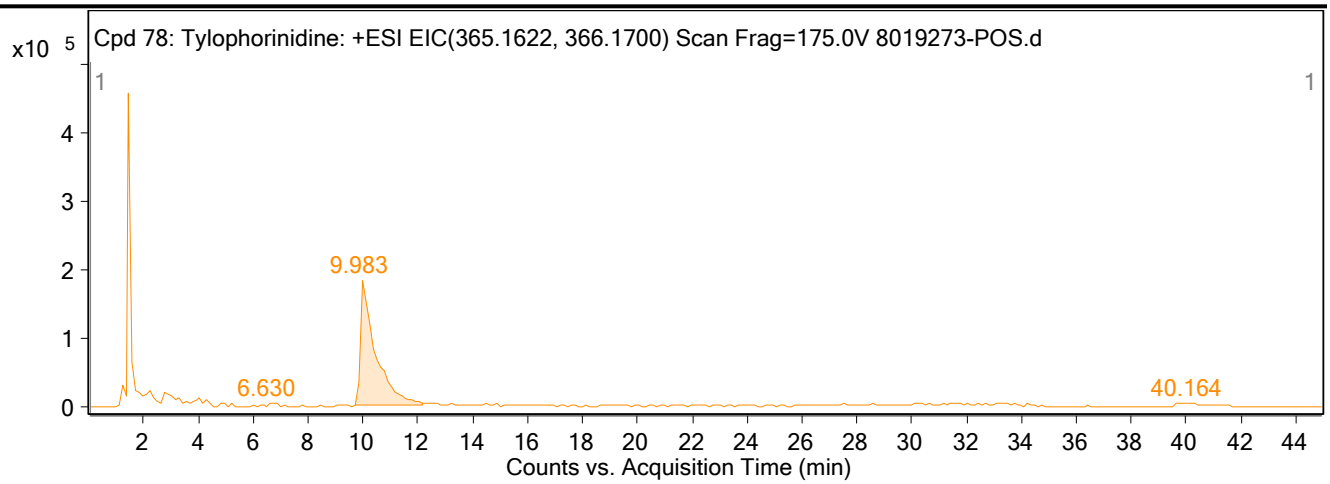



**MS Spectrum Peak List**

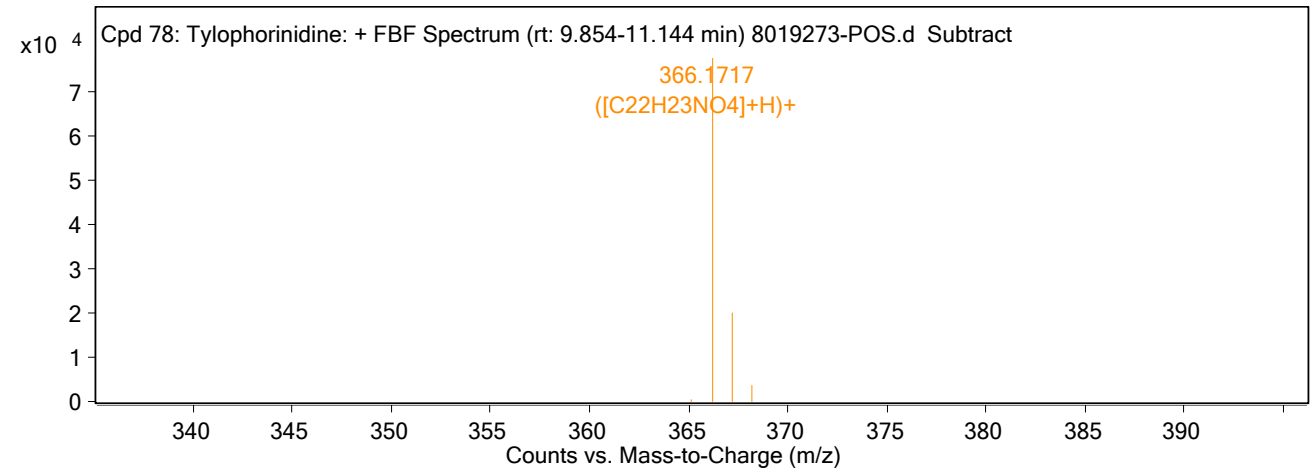
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 539.1178 | 1 | 53014.91 | C27H22O12 | (M+H)+ |
| 540.121 | 1 | 14817.17 | C27H22O12 | (M+H)+ |
| 541.1241 | 1 | 2933.51 | C27H22O12 | (M+H)+ |
| 542.1247 | 1 | 441.47 | C27H22O12 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 78: Tylophorinidine | **Tylophorinidine** | 366.1717 | 9.983 | Find By Formula | 365.1645 |

**Compound Chromatograms**




MS Zoomed Spectrum

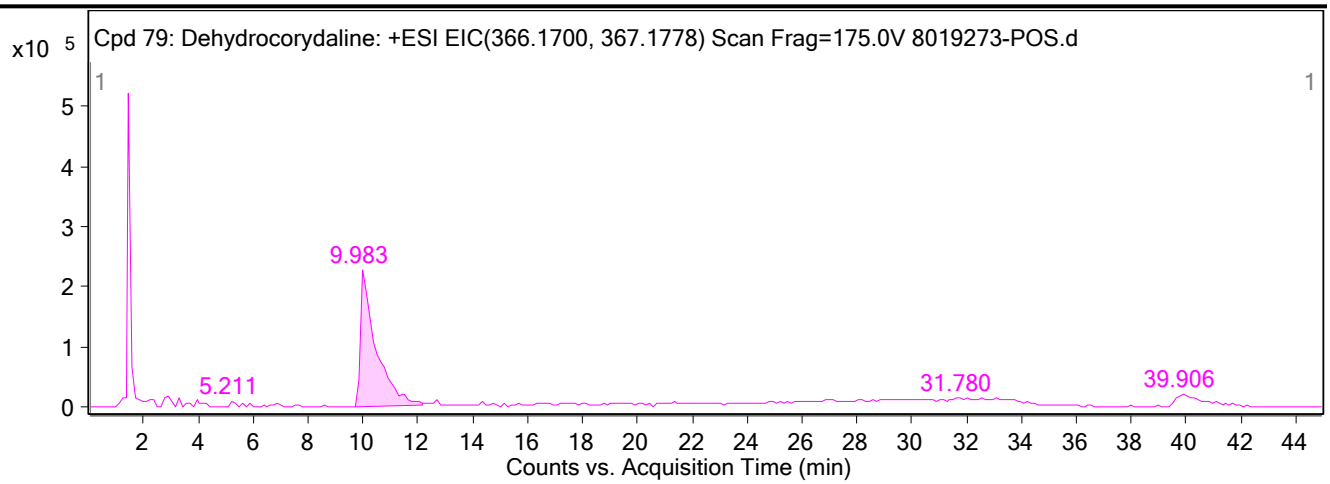



**MS Spectrum Peak List**

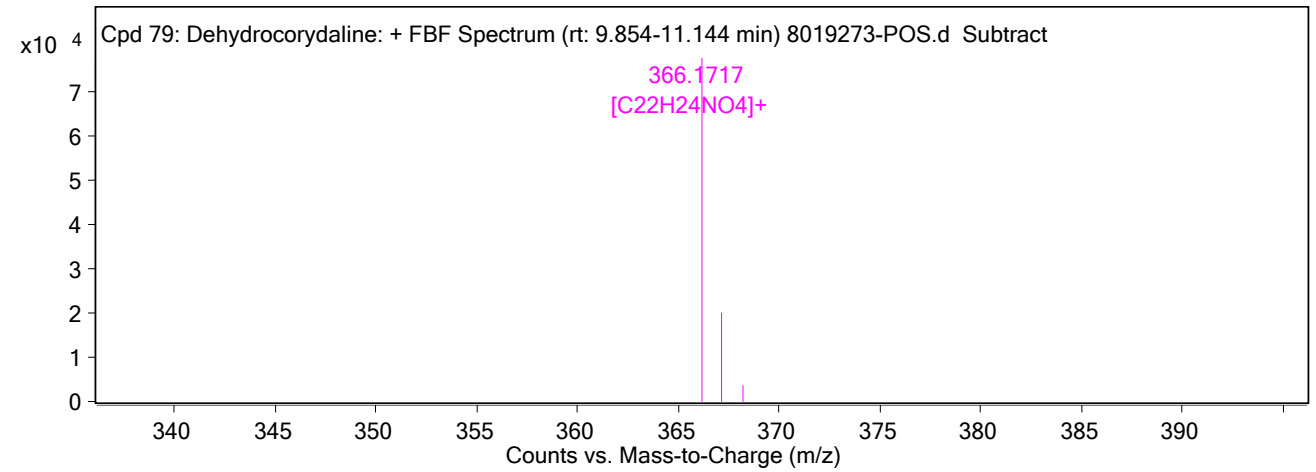
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 365.1576 | 1 | 426.18 | C22H23NO4 | M+ |
| 366.1717 | 1 | 77390.84 | C22H23NO4 | (M+H)+ |
| 367.1754 | 1 | 20027.29 | C22H23NO4 | (M+H)+ |
| 368.1786 | 1 | 3634.84 | C22H23NO4 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 79: Dehydrocorydaline | **Dehydrocorydaline** | 366.1717 | 9.983 | Find By Formula | 366.1723 |

**Compound Chromatograms**




MS Zoomed Spectrum

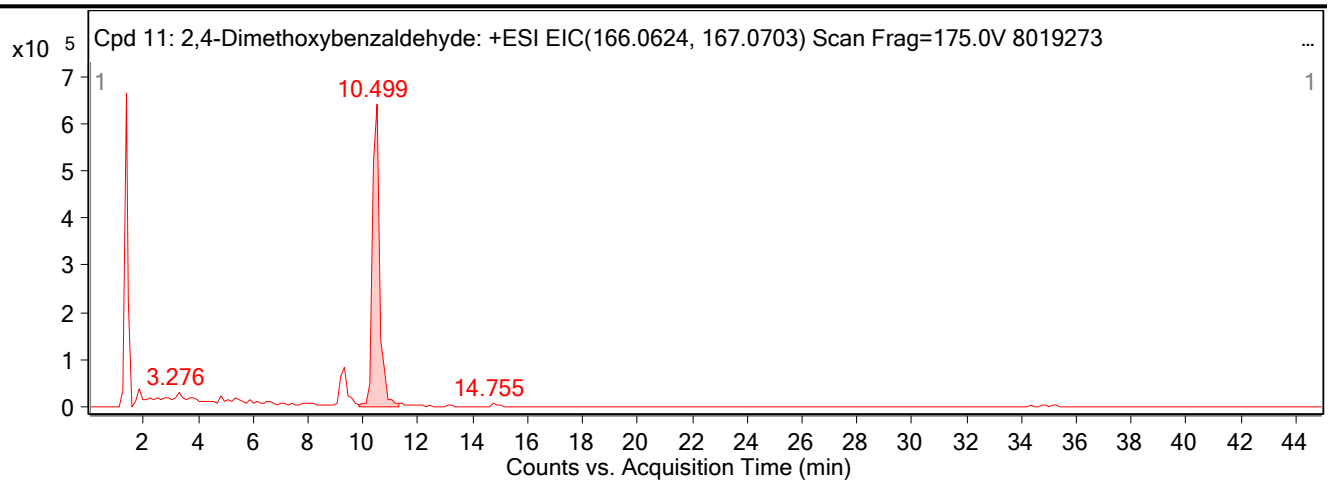



**MS Spectrum Peak List**

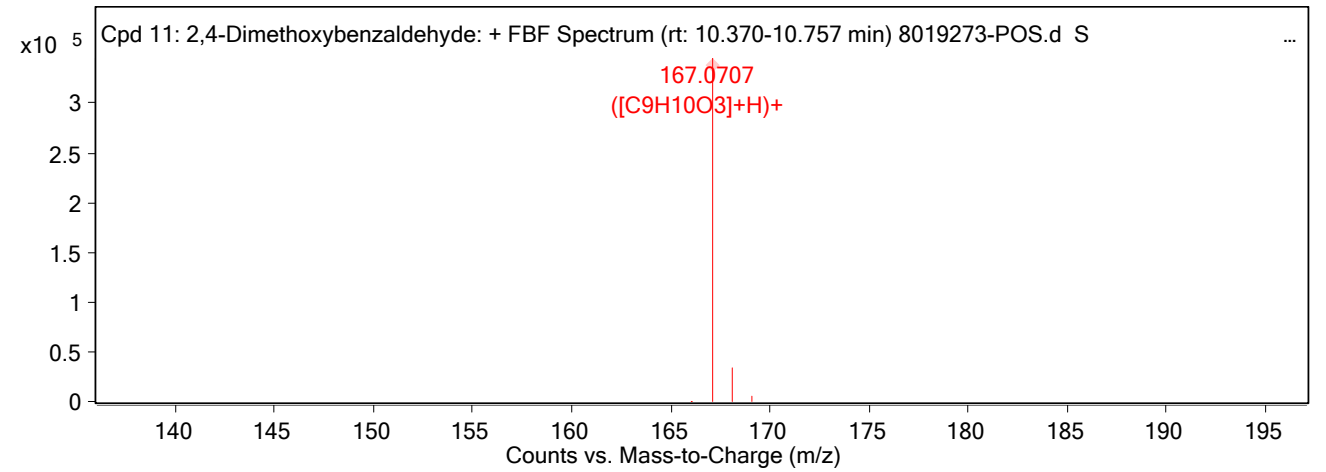
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 366.1717 | 1 | 77390.84 | C22H24NO4 | M+ |
| 367.1754 | 1 | 20027.29 | C22H24NO4 | M+ |
| 368.1786 | 1 | 3634.84 | C22H24NO4 | M+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 11: 2,4-Dimethoxybenzaldehyde | 2,4-Dimethoxybenzaldehyde | 167.0707 | 10.499 | Find By Formula | 166.0635 |

**Compound Chromatograms**




MS Zoomed Spectrum

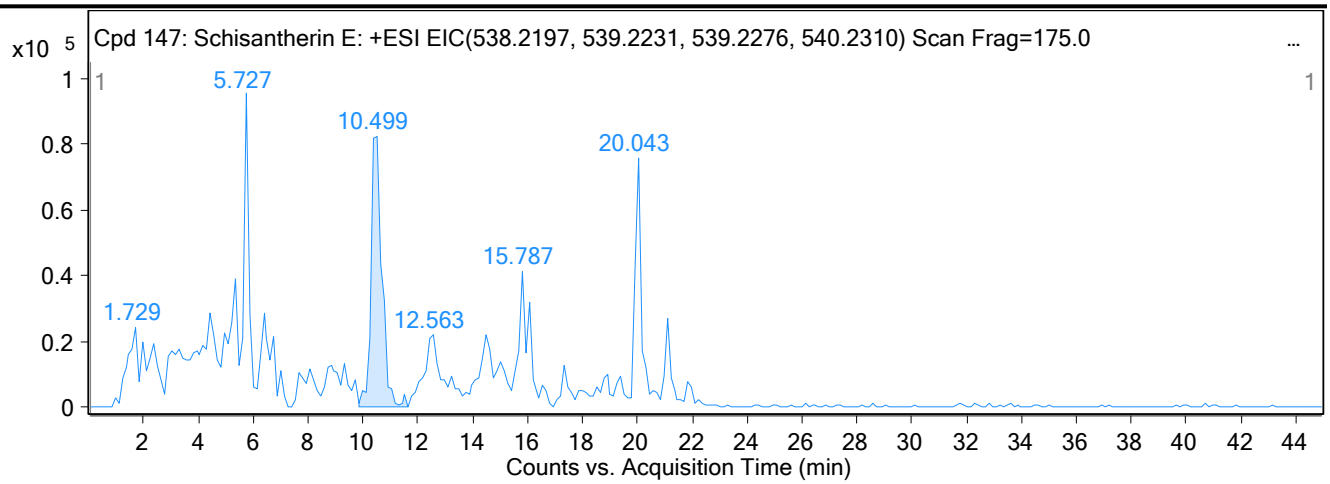



**MS Spectrum Peak List**

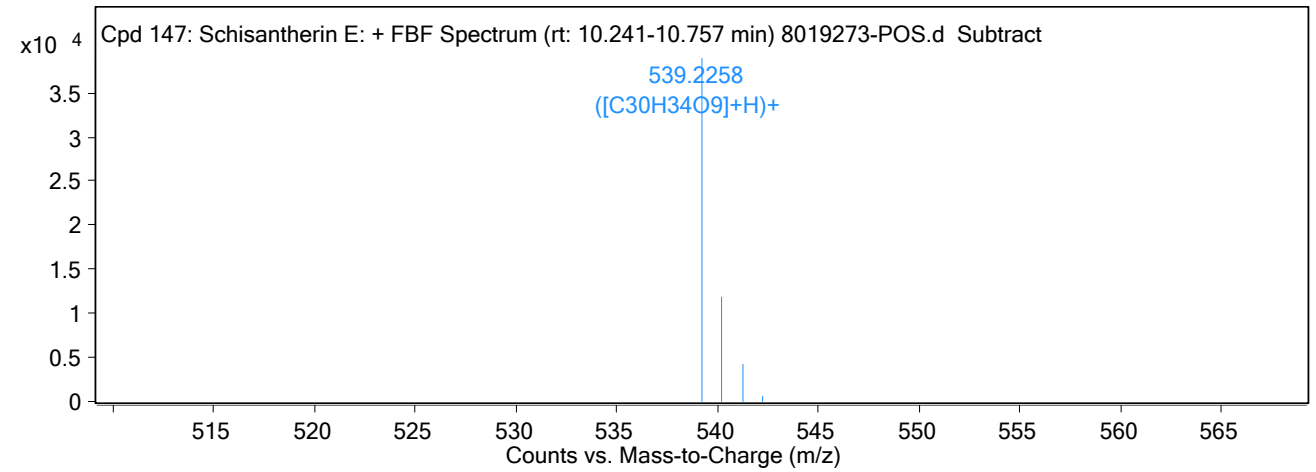
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 166.0593 | 1 | 93.19 | C9H10O3 | M+ |
| 167.0707 | 1 | 345314.69 | C9H10O3 | (M+H)+ |
| 168.0738 | 1 | 34139.33 | C9H10O3 | (M+H)+ |
| 169.0849 | 1 | 6185.4 | C9H10O3 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 147: Schisantherin E | **Schisantherin E** | 539.2258 | 10.499 | Find By Formula | 538.2192 |

**Compound Chromatograms**




MS Zoomed Spectrum

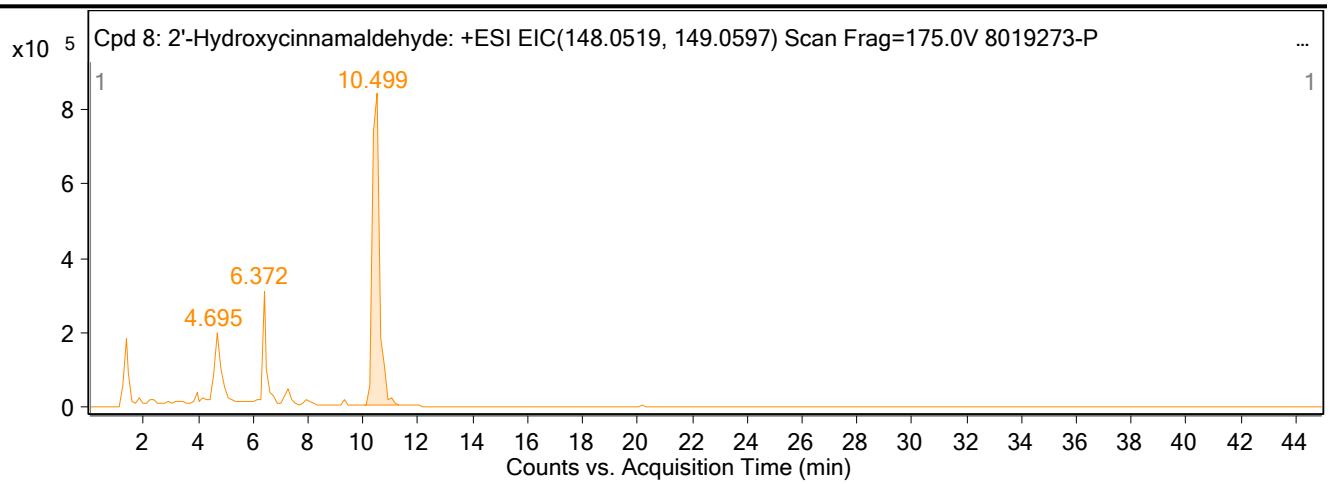



**MS Spectrum Peak List**

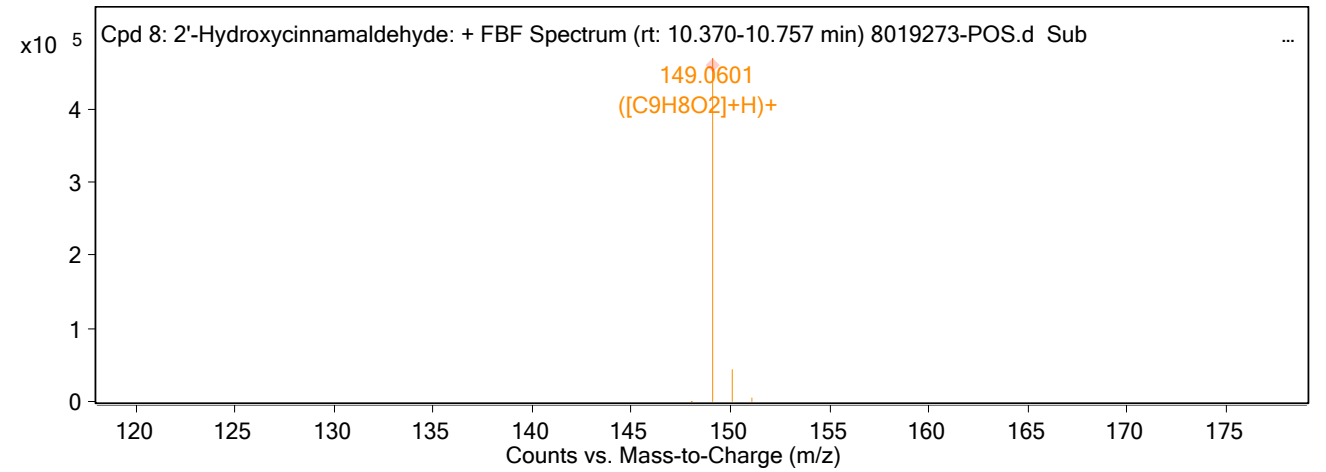
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 539.2258 | 1 | 38952.71 | C30H34O9 | (M+H)+ |
| 540.2309 | 1 | 11957.71 | C30H34O9 | (M+H)+ |
| 541.2337 | 1 | 4211.29 | C30H34O9 | (M+H)+ |
| 542.2479 | 1 | 691.97 | C30H34O9 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 8: 2'-Hydroxycinnamaldehyde | **2'-Hydroxycinnamaldehyde** | 149.0601 | 10.499 | Find By Formula | 148.0529 |

**Compound Chromatograms**




MS Zoomed Spectrum

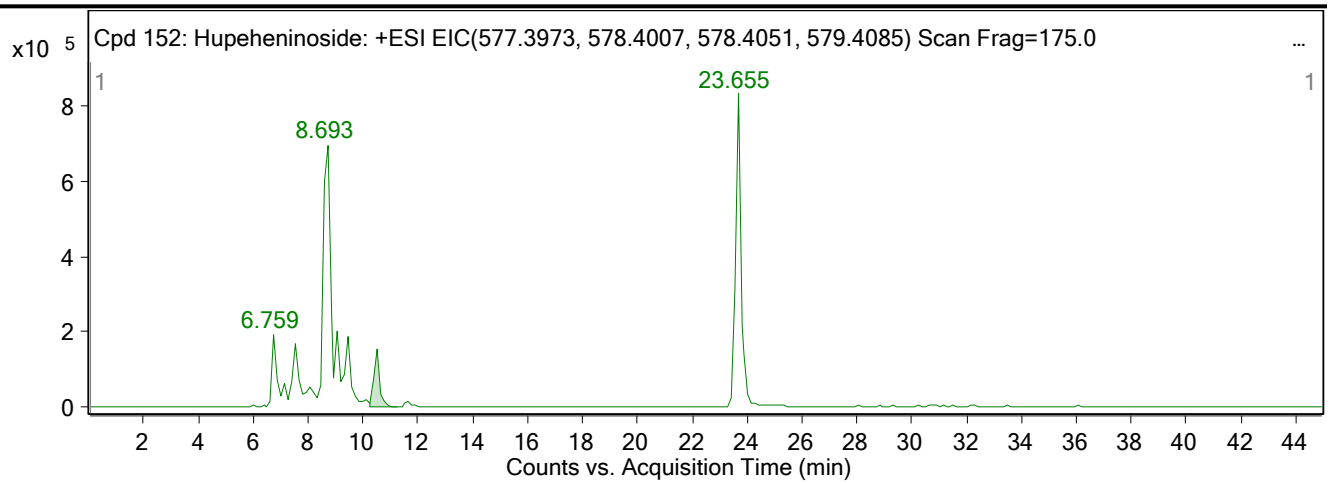



**MS Spectrum Peak List**

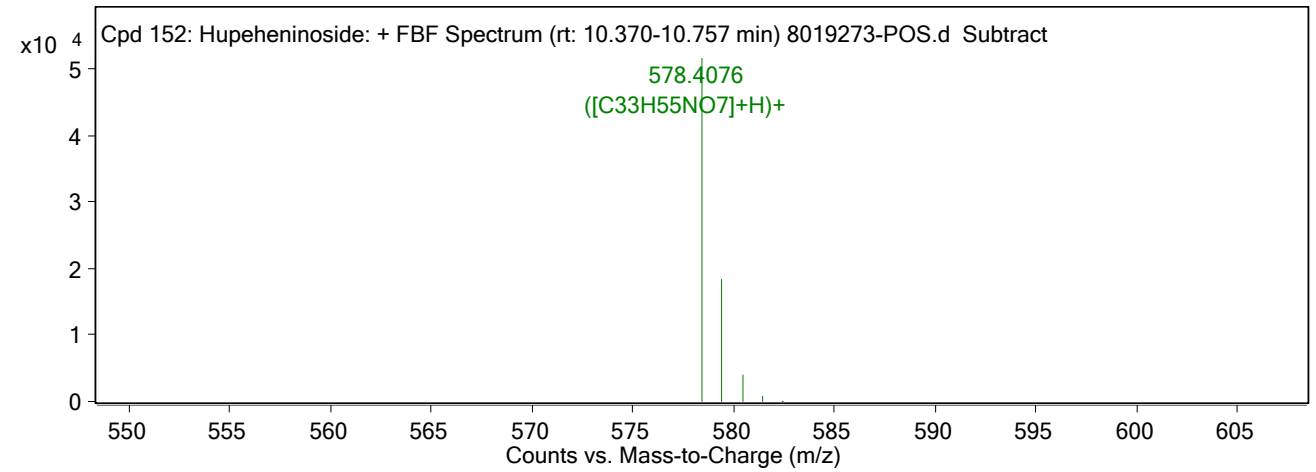
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 148.051 | 1 | 586.8 | C9H8O2 | M+ |
| 149.0601 | 1 | 469869.91 | C9H8O2 | (M+H)+ |
| 150.0634 | 1 | 43981.39 | C9H8O2 | (M+H)+ |
| 151.071 | 1 | 4291.43 | C9H8O2 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 152: Hupeheninoside | **Hupeheninoside** | 578.4076 | 10.499 | Find By Formula | 577.4001 |

**Compound Chromatograms**




MS Zoomed Spectrum

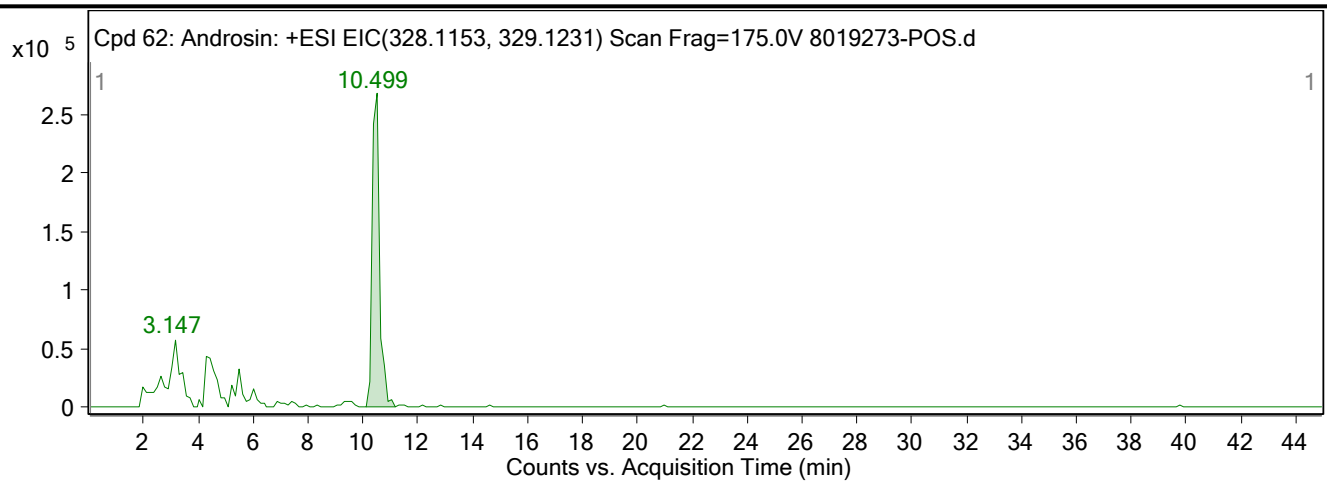



**MS Spectrum Peak List**

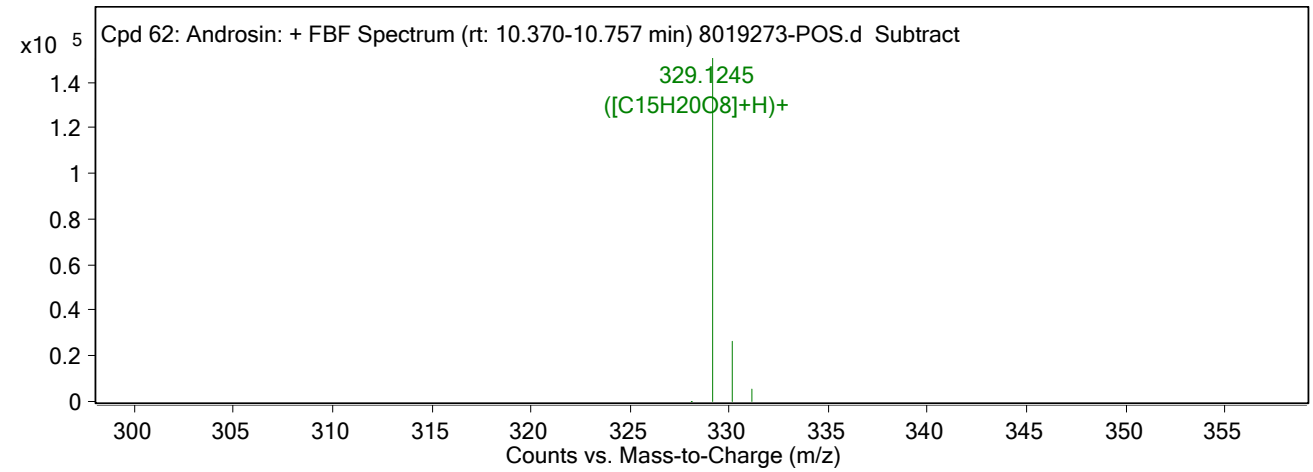
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 578.4076 | 1 | 51640.72 | C33H55NO7 | (M+H)+ |
| 579.4107 | 1 | 18487.63 | C33H55NO7 | (M+H)+ |
| 580.4126 | 1 | 4034.52 | C33H55NO7 | (M+H)+ |
| 581.4128 | 1 | 808.71 | C33H55NO7 | (M+H)+ |
| 582.4204 | 1 | 123.97 | C33H55NO7 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 62: Androsin | **Androsin** | 329.1245 | 10.499 | Find By Formula | 328.1172 |

**Compound Chromatograms**




MS Zoomed Spectrum

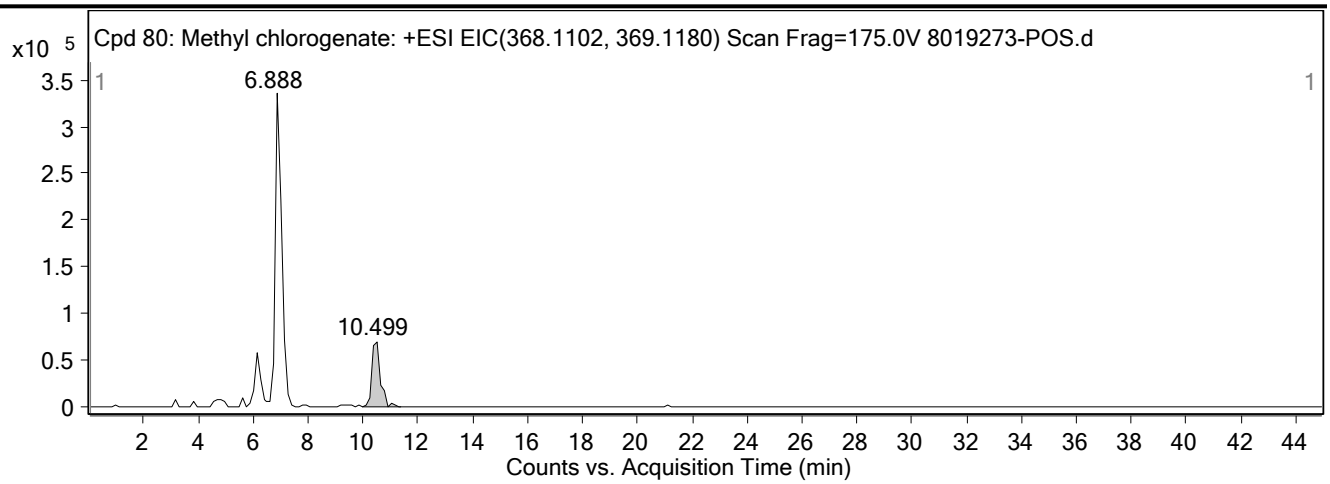



**MS Spectrum Peak List**

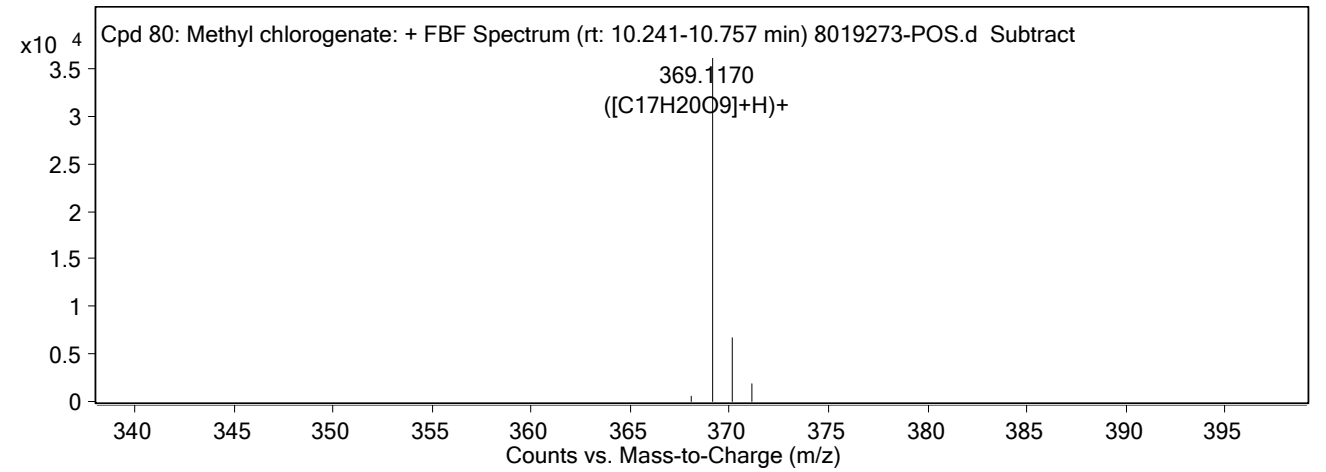
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 328.1197 | 1 | 335.21 | C15H20O8 | M+ |
| 329.1245 | 1 | 150677.69 | C15H20O8 | (M+H)+ |
| 330.1277 | 1 | 26748.48 | C15H20O8 | (M+H)+ |
| 331.1293 | 1 | 5834.38 | C15H20O8 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 80: Methyl chlorogenate | **Methyl chlorogenate** | 369.117 | 10.499 | Find By Formula | 368.1101 |

**Compound Chromatograms**




MS Zoomed Spectrum

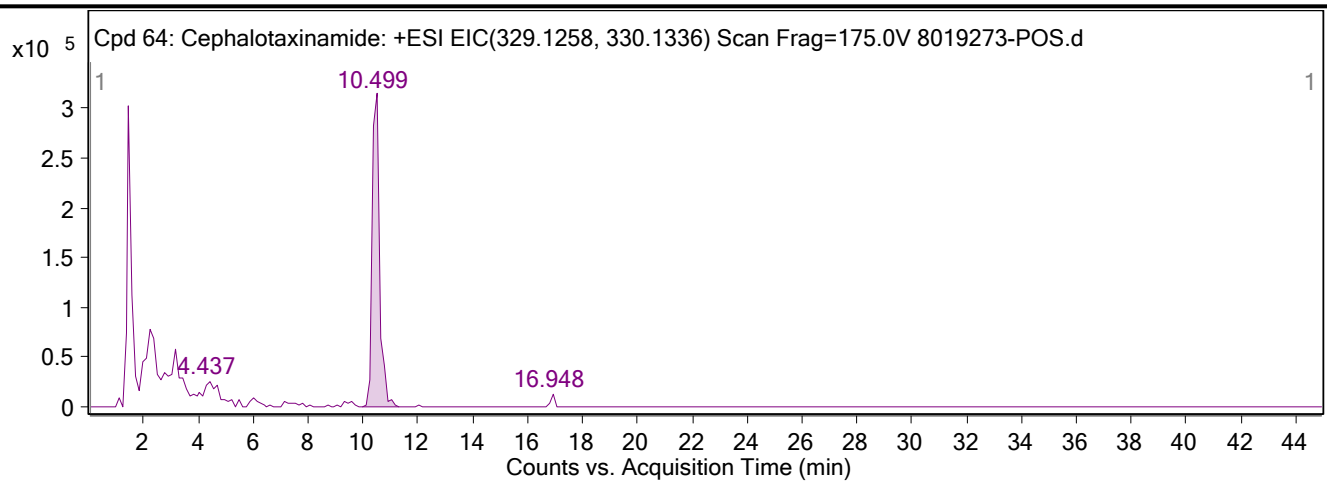



**MS Spectrum Peak List**

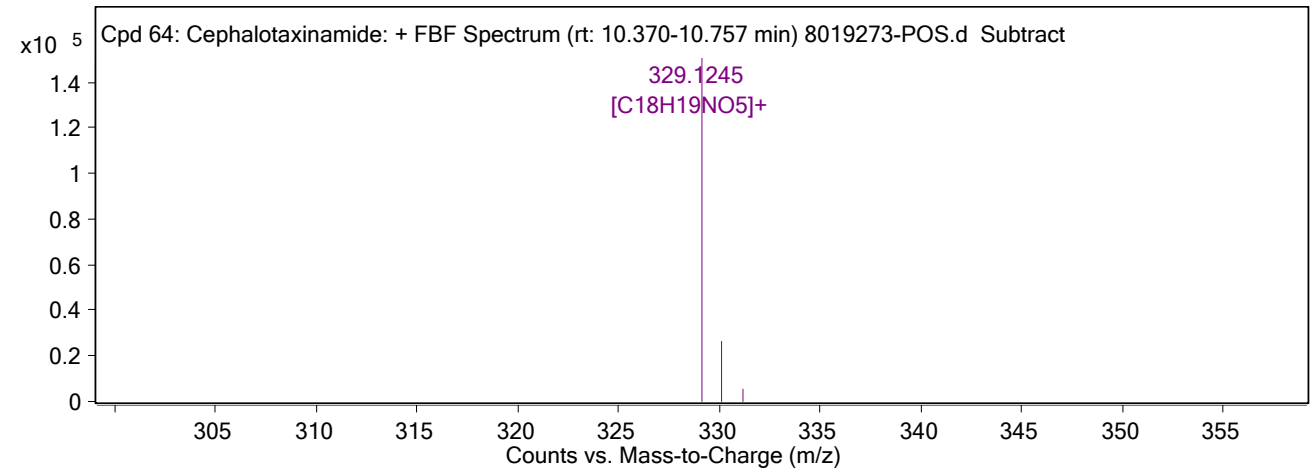
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 368.1143 | 1 | 642.55 | C17H20O9 | M+ |
| 369.117 | 1 | 36103.91 | C17H20O9 | (M+H)+ |
| 370.1213 | 1 | 6663.63 | C17H20O9 | (M+H)+ |
| 371.1269 | 1 | 1805.97 | C17H20O9 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 64: Cephalotaxinamide | **Cephalotaxinamide** | 329.1245 | 10.499 | Find By Formula | 329.125 |

**Compound Chromatograms**




MS Zoomed Spectrum

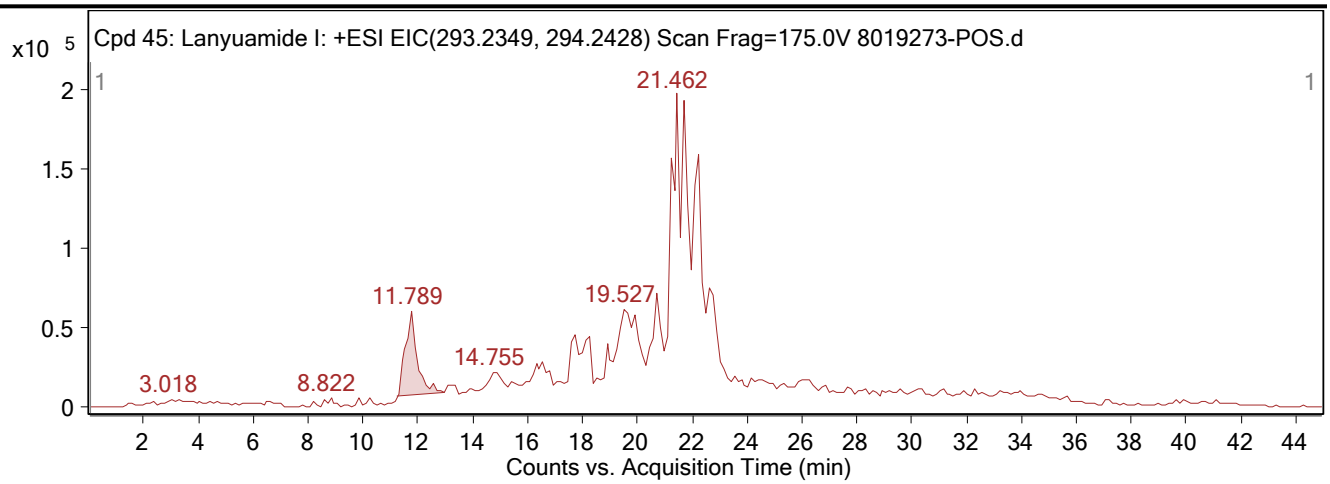



**MS Spectrum Peak List**

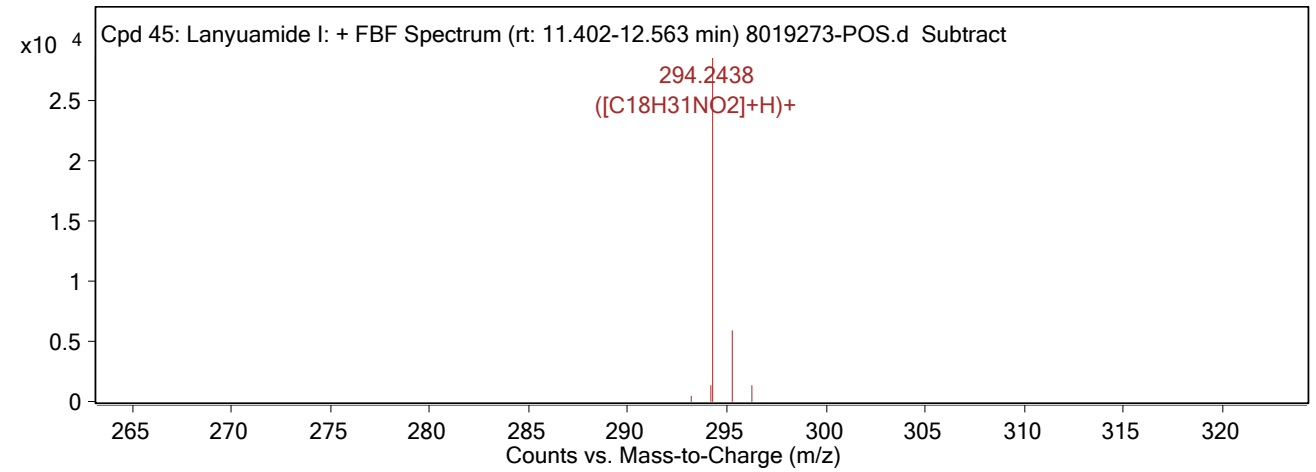
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 329.1245 | 1 | 150677.69 | C18H19NO5 | M+ |
| 330.1277 | 1 | 26748.48 | C18H19NO5 | M+ |
| 331.1293 | 1 | 5834.38 | C18H19NO5 | M+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 45: Lanyuamide I | **Lanyuamide I** | 294.2438 | 11.789 | Find By Formula | 293.2356 |

**Compound Chromatograms**




MS Zoomed Spectrum

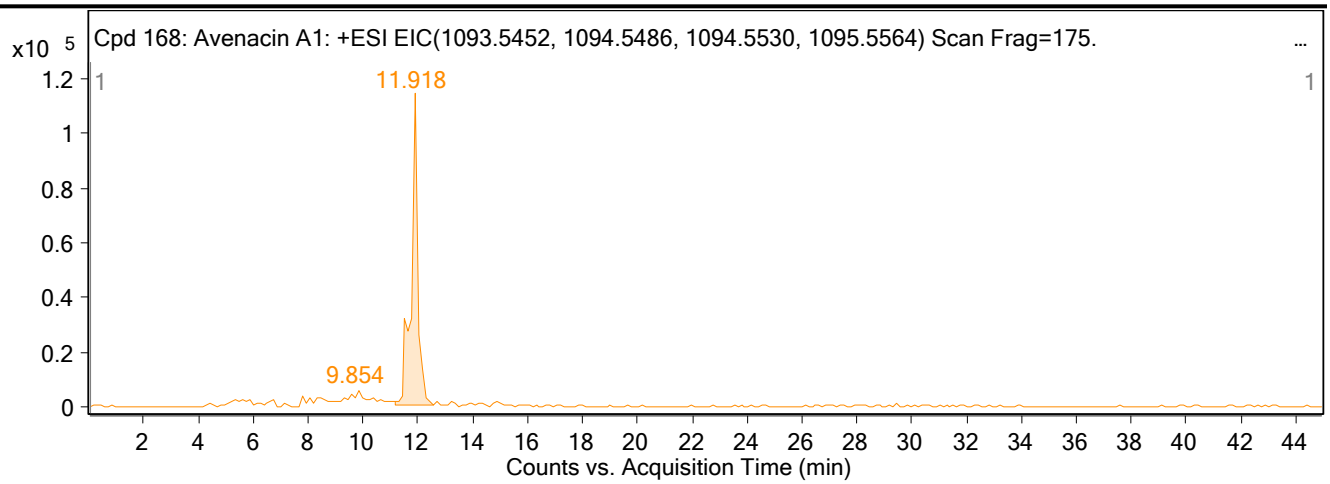



**MS Spectrum Peak List**

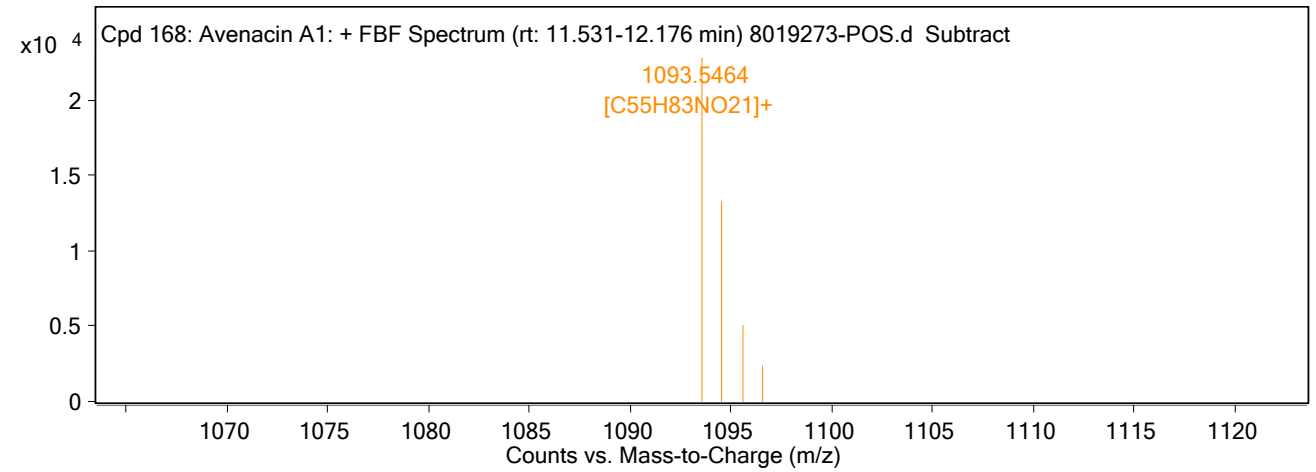
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 293.2307 | 1 | 469.69 | C18H31NO2 | M+ |
| 294.2148 | 1 | 1406.27 | C18H31NO2 | M+ |
| 294.2438 | 1 | 28553.2 | C18H31NO2 | (M+H)+ |
| 295.2463 | 1 | 5848.24 | C18H31NO2 | (M+H)+ |
| 296.2538 | 1 | 1268.14 | C18H31NO2 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 168: Avenacin A1 | **Avenacin A1** | 1093.5464 | 11.918 | Find By Formula | 1093.5471 |

**Compound Chromatograms**




MS Zoomed Spectrum

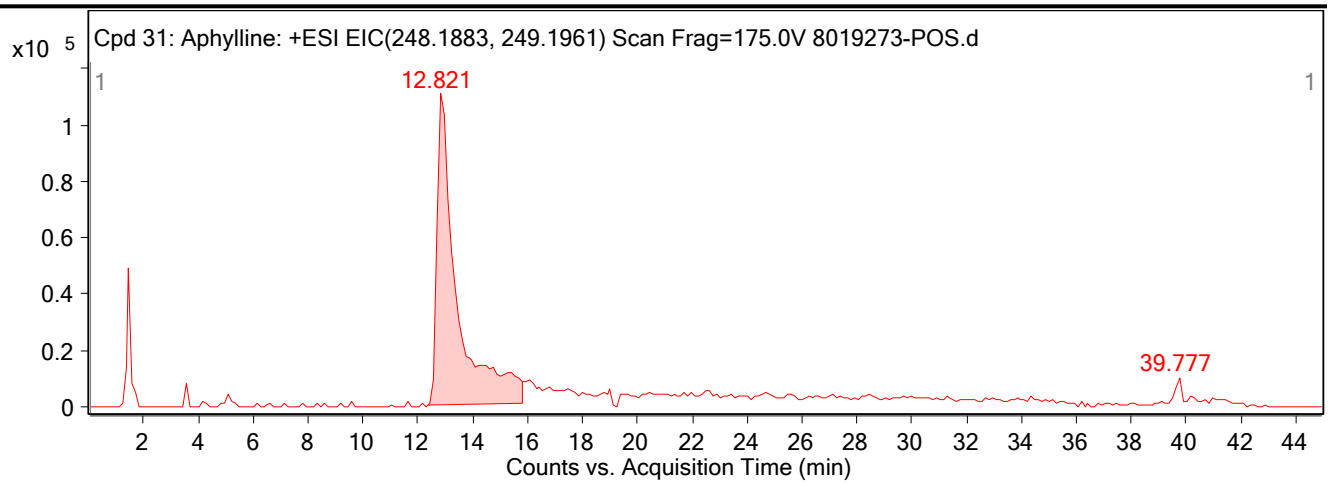



**MS Spectrum Peak List**

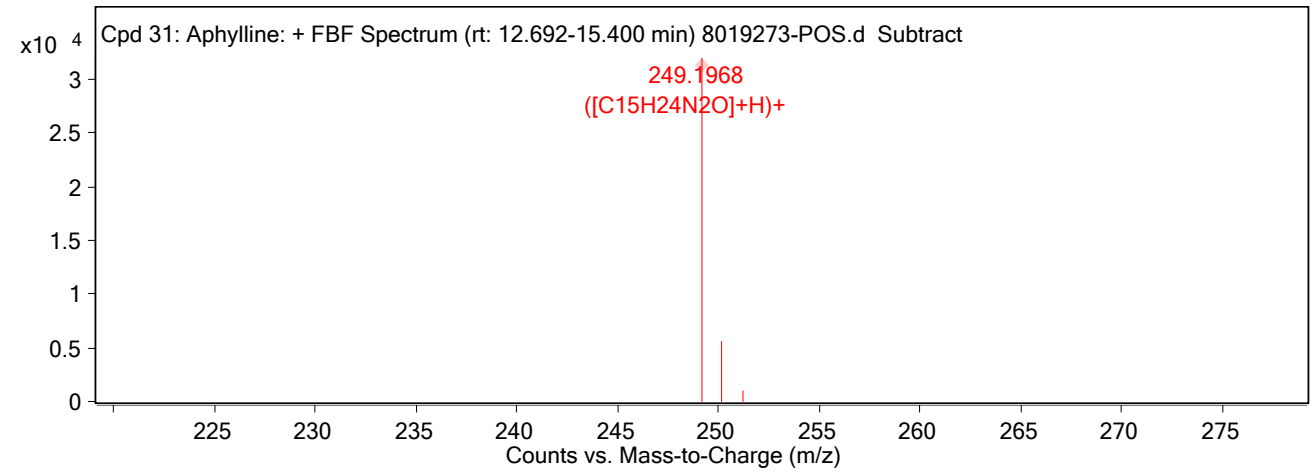
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 1093.5464 | 1 | 22761.4 | C55H83NO21 | M+ |
| 1094.5502 | 1 | 13234.81 | C55H83NO21 | M+ |
| 1095.5544 | 1 | 5000.07 | C55H83NO21 | M+ |
| 1096.5535 | 1 | 2352.6 | C55H83NO21 | M+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 31: Aphylline | **Aphylline** | 249.1968 | 12.821 | Find By Formula | 248.1894 |

**Compound Chromatograms**




MS Zoomed Spectrum

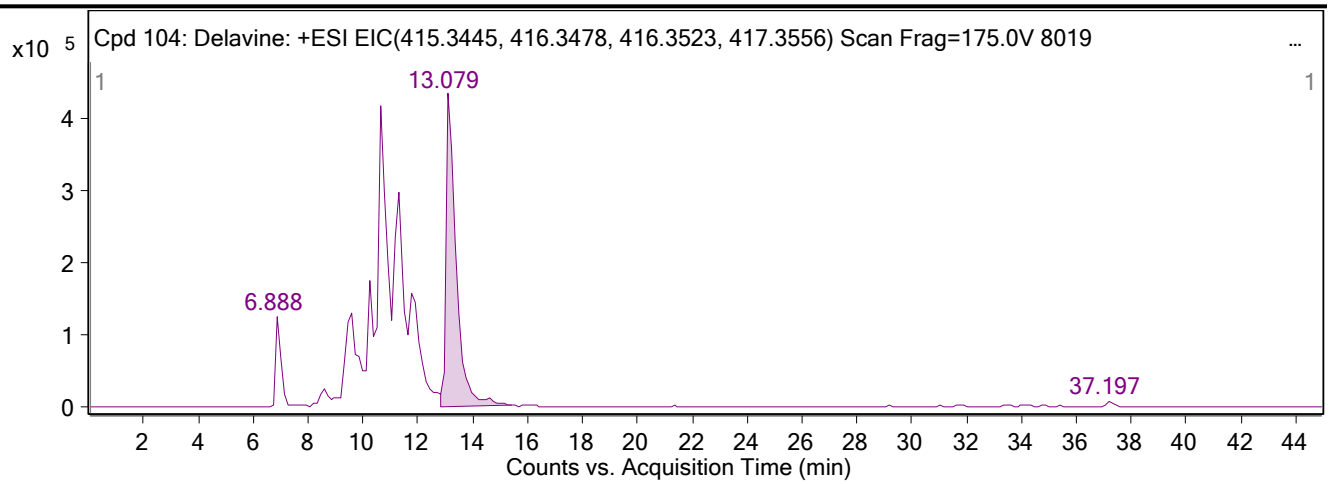



**MS Spectrum Peak List**

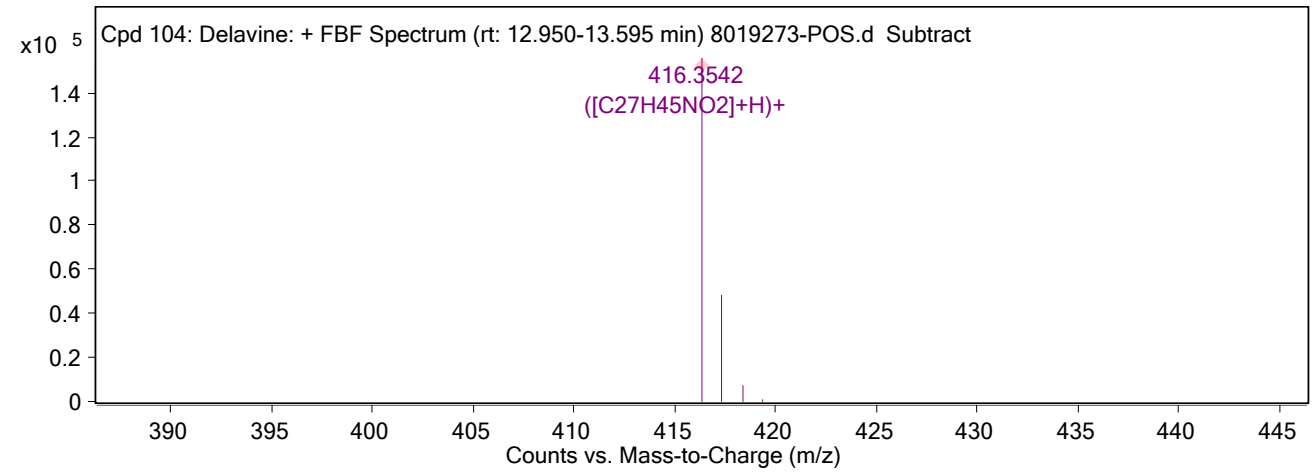
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 249.1968 | 1 | 31949.31 | C15H24N2O | (M+H)+ |
| 250.1996 | 1 | 5660.41 | C15H24N2O | (M+H)+ |
| 251.201 | 1 | 1072.49 | C15H24N2O | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 104: Delavine | **Delavine** | 416.3542 | 13.079 | Find By Formula | 415.3469 |

**Compound Chromatograms**




MS Zoomed Spectrum

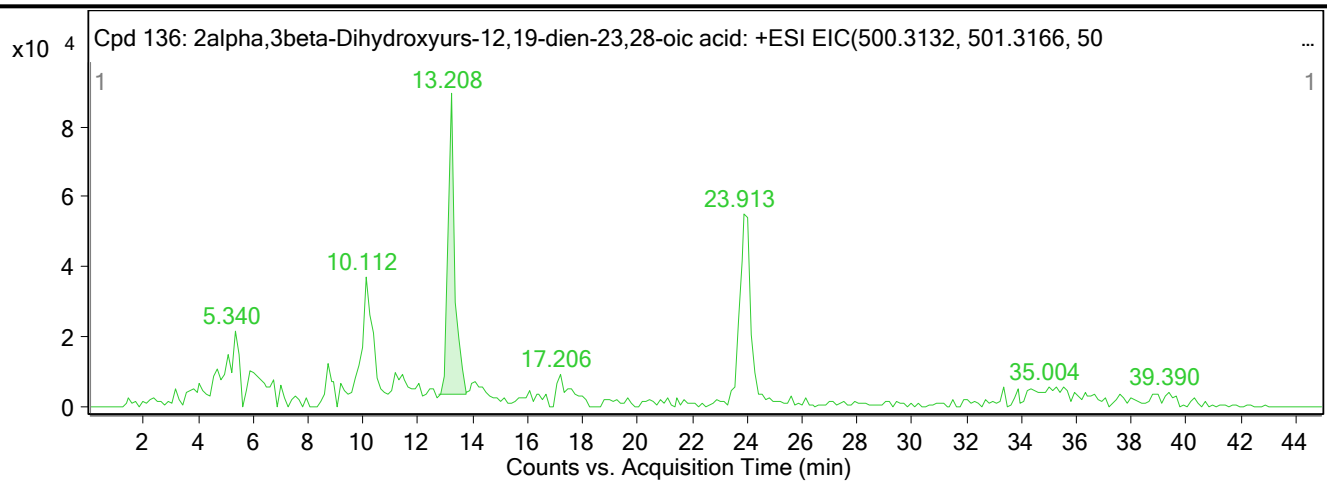



**MS Spectrum Peak List**

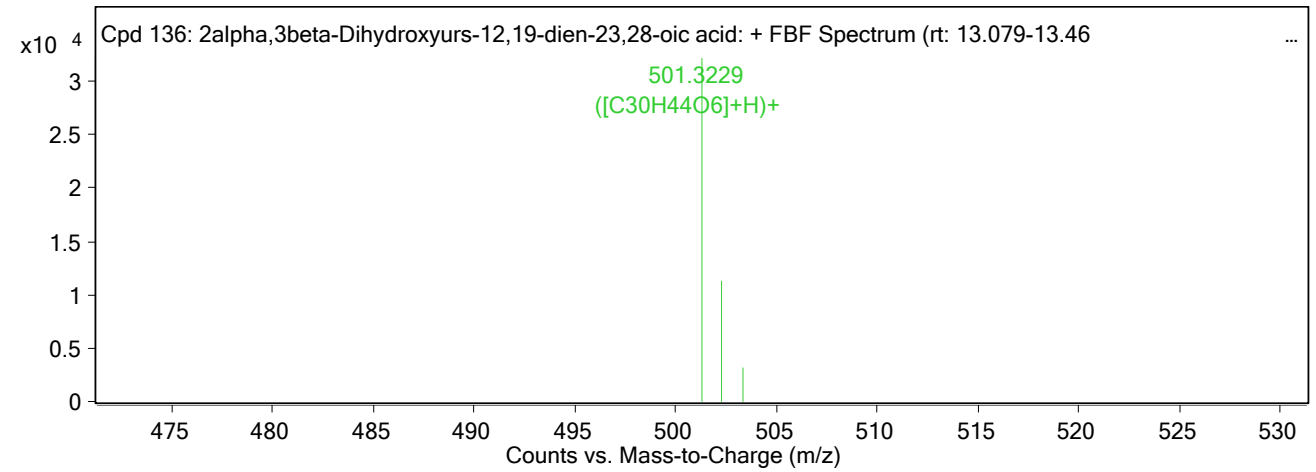
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 416.3542 | 1 | 155757.77 | C27H45NO2 | (M+H)+ |
| 417.3574 | 1 | 48610.63 | C27H45NO2 | (M+H)+ |
| 418.3603 | 1 | 7177.84 | C27H45NO2 | (M+H)+ |
| 419.3635 | 1 | 756.91 | C27H45NO2 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 136: 2alpha,3beta-Dihydroxyurs-12,19-dien-23,28-oic acid | **2alpha,3beta-Dihydroxyurs-12,19-dien-23,28-oic acid** | 501.3229 | 13.208 | Find By Formula | 500.3157 |

**Compound Chromatograms**




MS Zoomed Spectrum

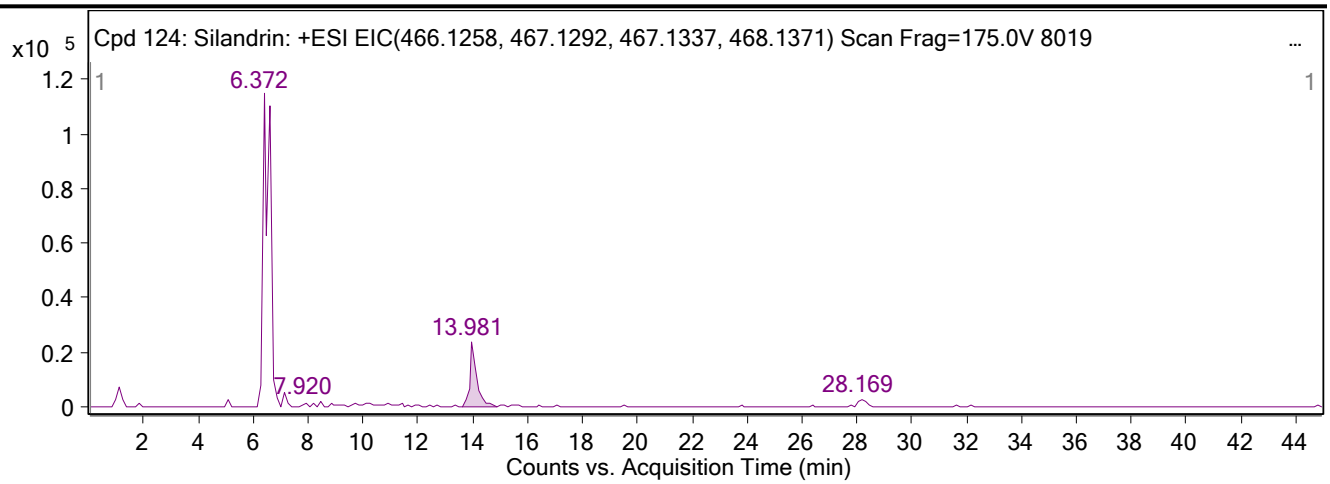



**MS Spectrum Peak List**

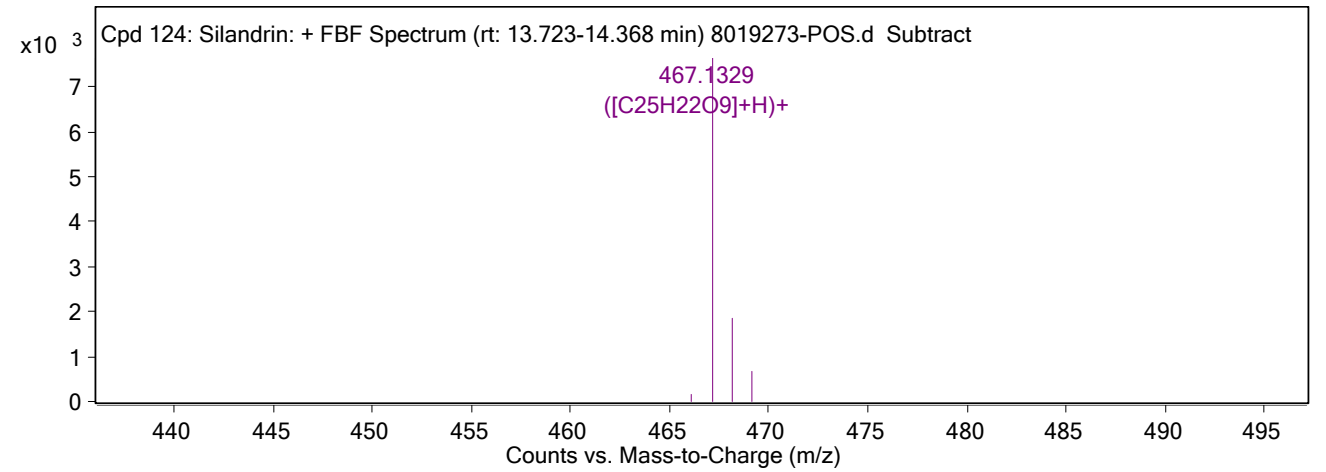
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 501.3229 | 1 | 32174.75 | C30H44O6 | (M+H)+ |
| 502.3263 | 1 | 11270.96 | C30H44O6 | (M+H)+ |
| 503.3301 | 1 | 3170.62 | C30H44O6 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 124: Silandrin | **Silandrin** | 467.1329 | 13.981 | Find By Formula | 466.1257 |

**Compound Chromatograms**




MS Zoomed Spectrum

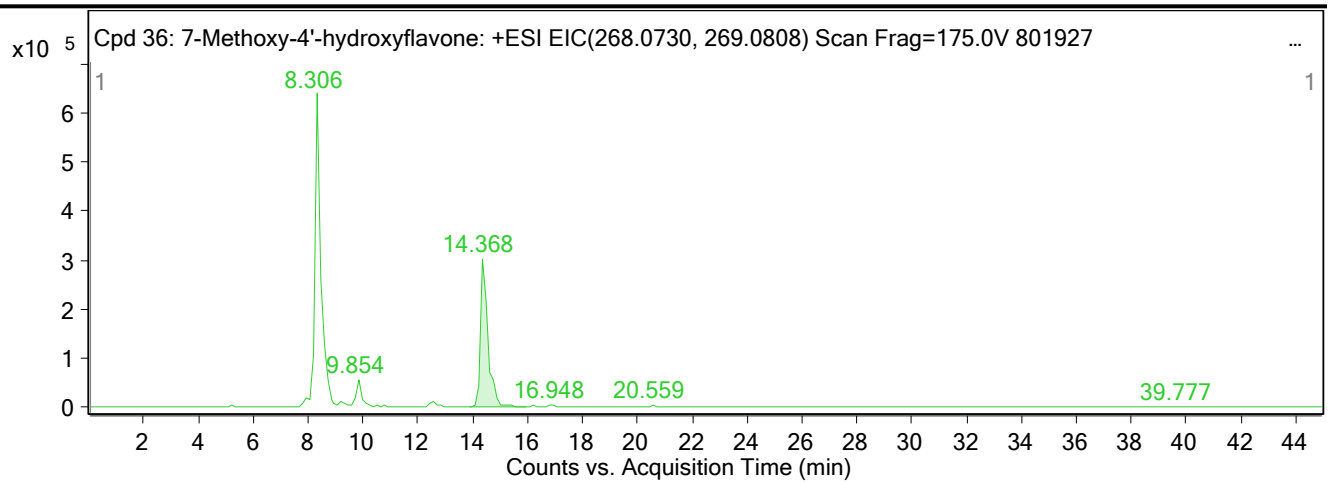



**MS Spectrum Peak List**

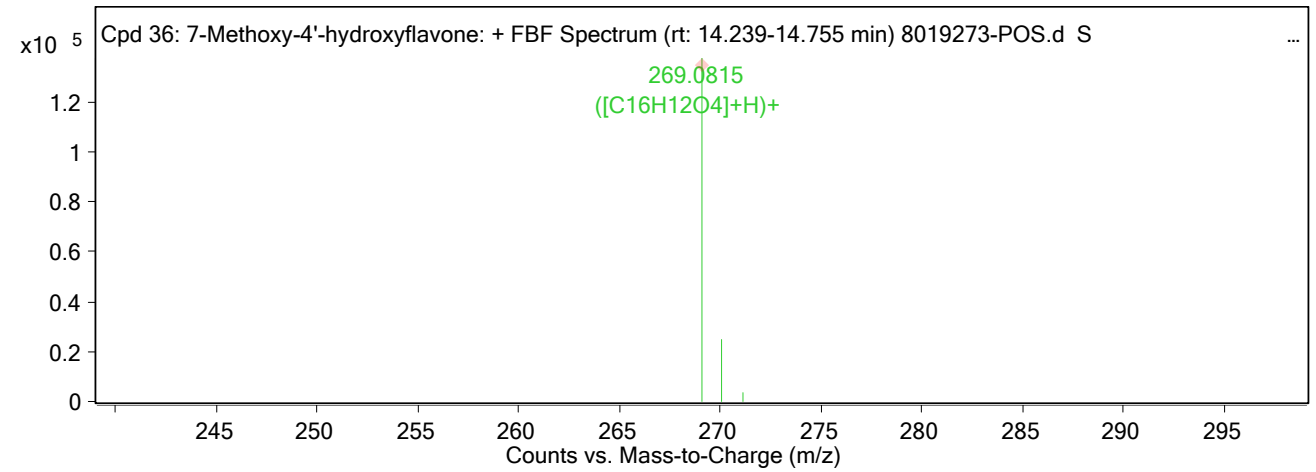
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 466.1323 | 1 | 165.38 | C25H22O9 | M+ |
| 467.1329 | 1 | 7641.21 | C25H22O9 | (M+H)+ |
| 468.1362 | 1 | 1845.69 | C25H22O9 | (M+H)+ |
| 469.1384 | 1 | 671.22 | C25H22O9 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 36: 7-Methoxy-4'-hydroxyflavone | **7-Methoxy-4'-hydroxyflavone** | 269.0815 | 14.368 | Find By Formula | 268.0743 |

**Compound Chromatograms**




MS Zoomed Spectrum

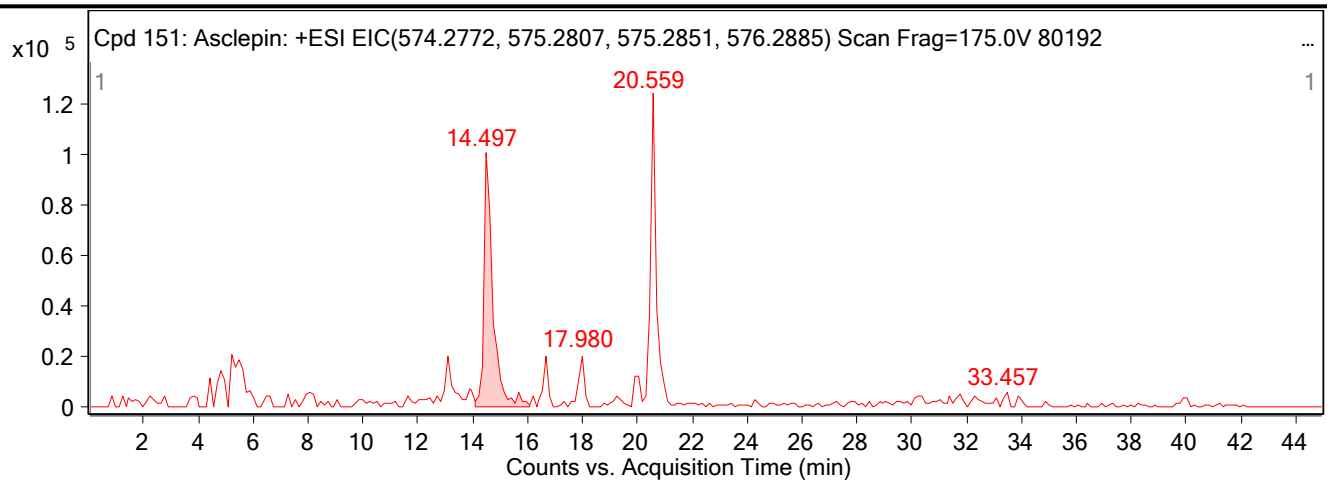



**MS Spectrum Peak List**

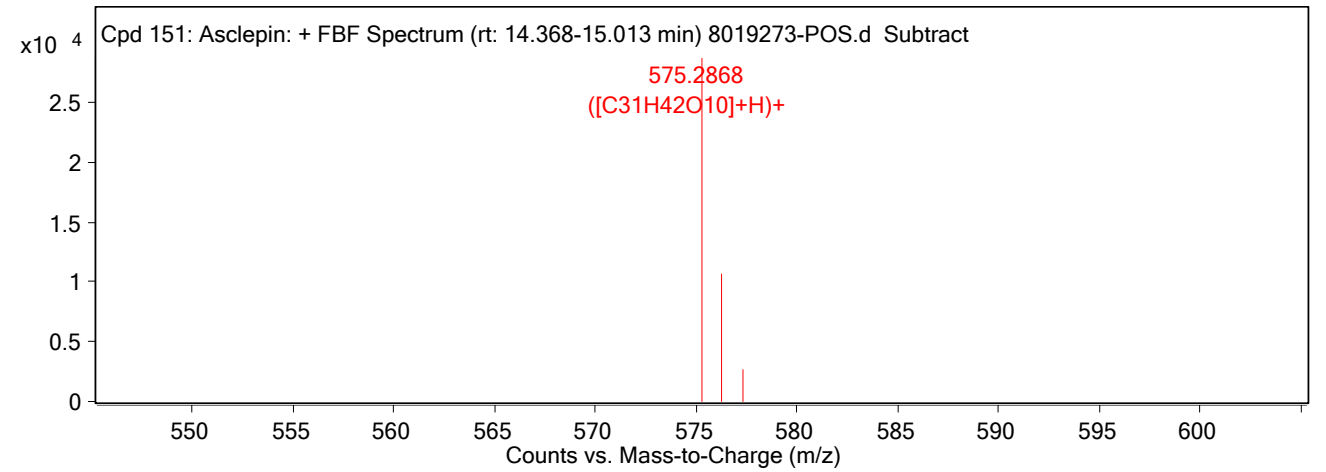
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 269.0815 | 1 | 137734.09 | C16H12O4 | (M+H)+ |
| 270.0849 | 1 | 25127.63 | C16H12O4 | (M+H)+ |
| 271.0908 | 1 | 3298.62 | C16H12O4 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 151: Asclepin | **Asclepin** | 575.2868 | 14.497 | Find By Formula | 574.2795 |

**Compound Chromatograms**




MS Zoomed Spectrum

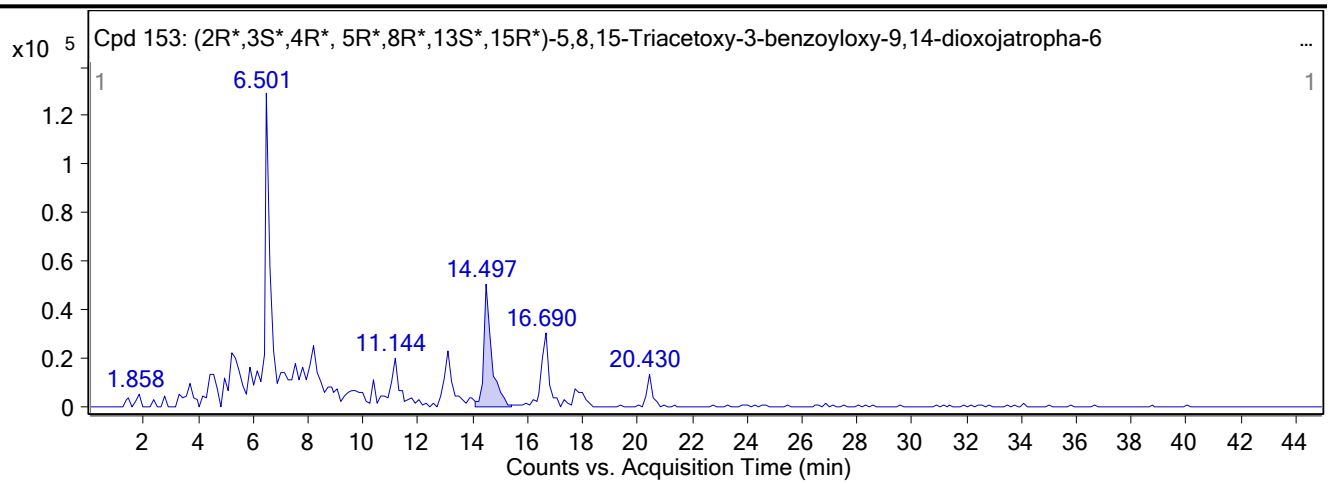



**MS Spectrum Peak List**

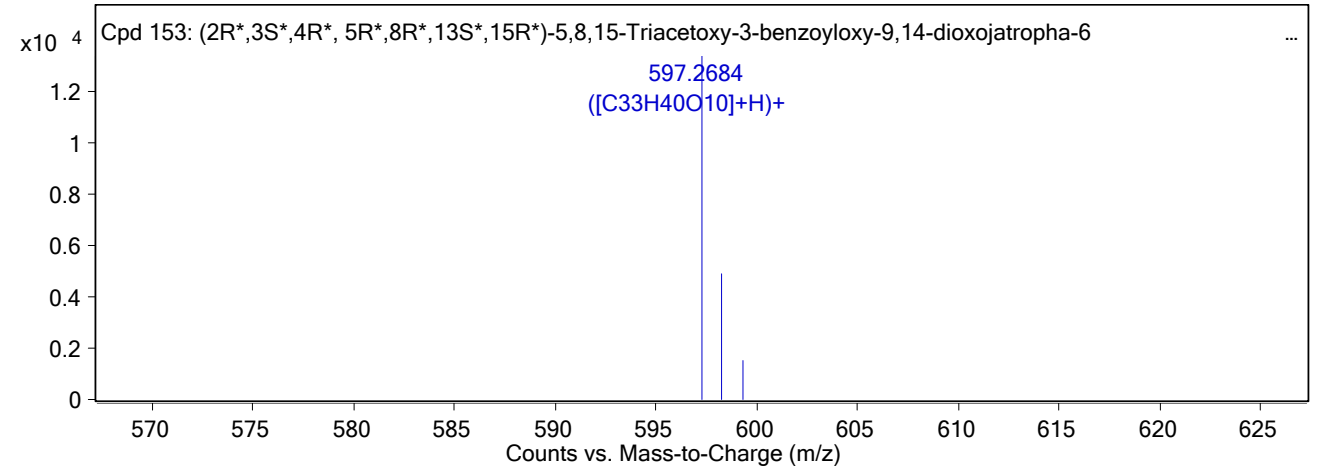
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 575.2868 | 1 | 28695.45 | C31H42O10 | (M+H)+ |
| 576.2901 | 1 | 10660.58 | C31H42O10 | (M+H)+ |
| 577.2928 | 1 | 2607.26 | C31H42O10 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 153: (2R*,3S*,4R*,5R*,8R*,13S*,15R*)-5,8,15-Triacetoxy-3-benzoyloxy-9,14-dioxojatropha-6(17),11E-diene | **(2R*,3S*,4R*,5R*,8R*,13S*,15R*)-5,8,15-Triacetoxy-3-benzoyloxy-9,14-dioxojatropha-6(17),11E-diene** | 597.2684 | 14.497 | Find By Formula | 596.2614 |

**Compound Chromatograms**




MS Zoomed Spectrum

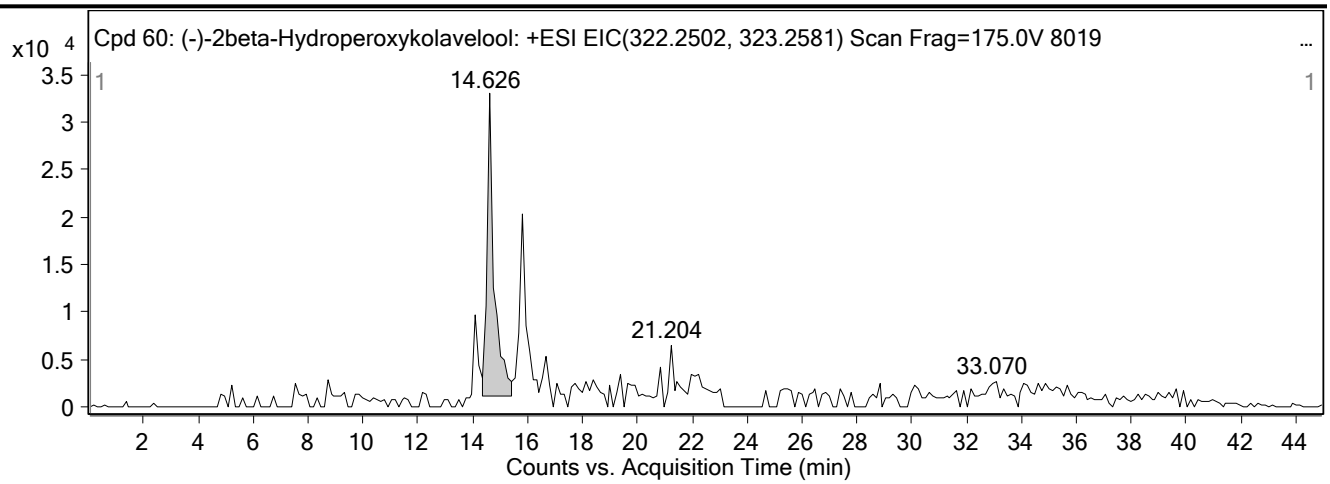



**MS Spectrum Peak List**

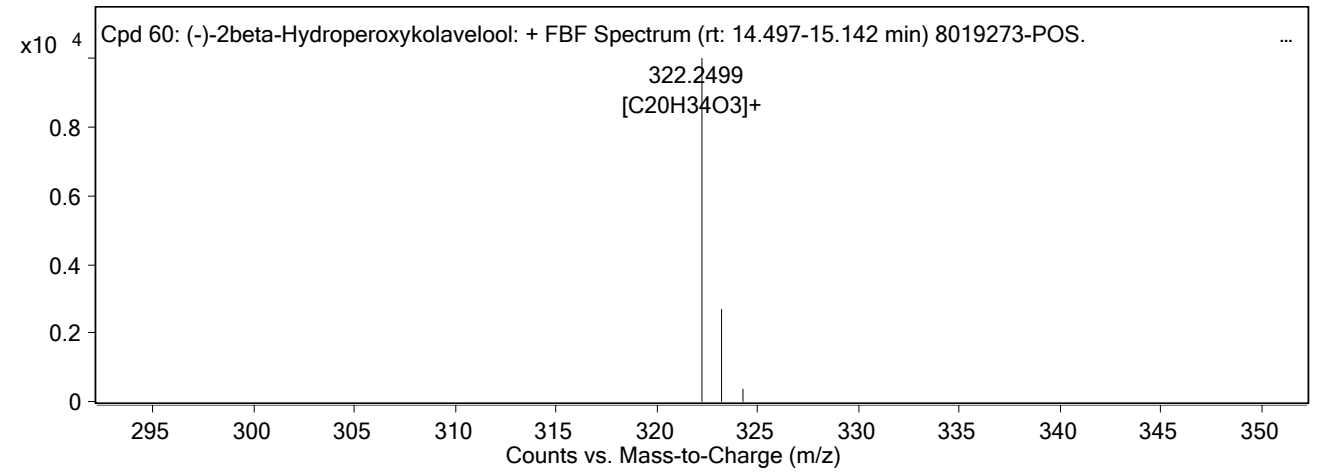
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 597.2684 | 1 | 13397.51 | C33H40O10 | (M+H)+ |
| 598.2726 | 1 | 4930.3 | C33H40O10 | (M+H)+ |
| 599.2749 | 1 | 1502.42 | C33H40O10 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 60: (-)-2beta-Hydroperoxykolavelool | **(-)-2beta-Hydroperoxykolavelool** | 322.2499 | 14.626 | Find By Formula | 322.2502 |

**Compound Chromatograms**




MS Zoomed Spectrum

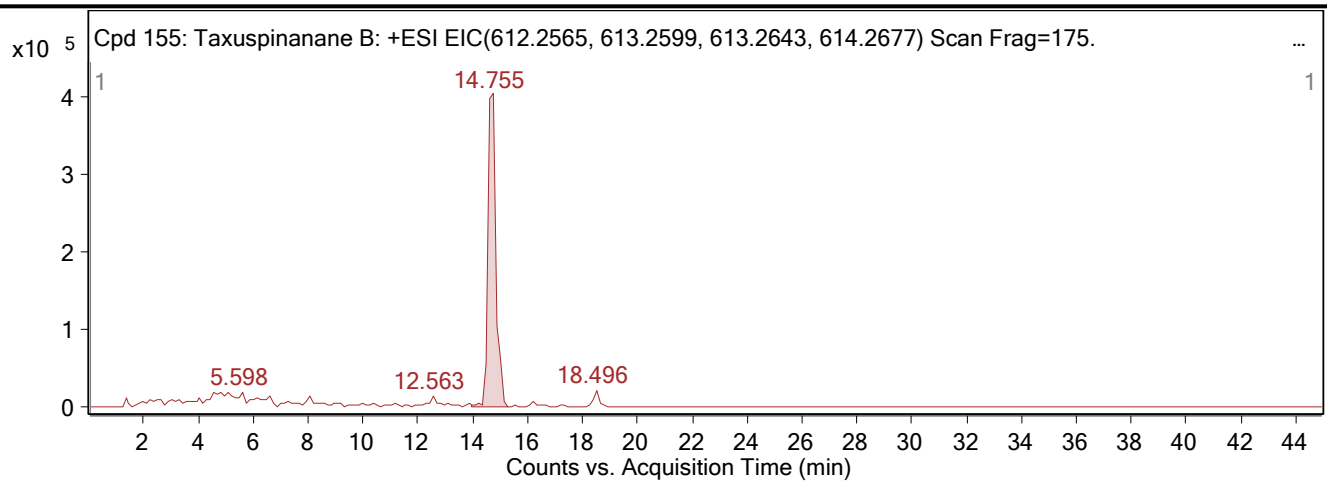



**MS Spectrum Peak List**

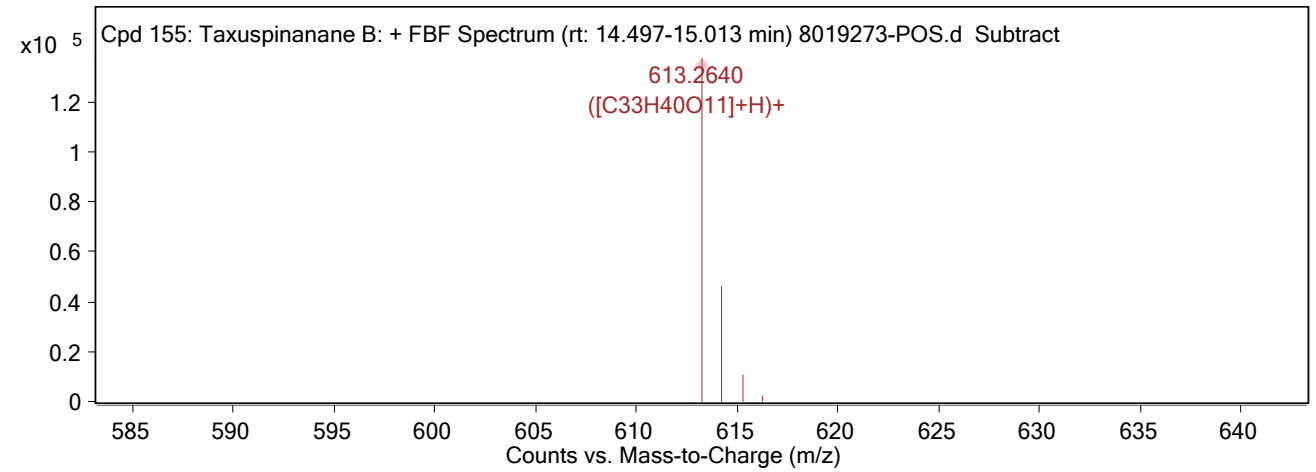
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 322.2499 | 1 | 10025.83 | C20H34O3 | M+ |
| 323.2522 | 1 | 2665.98 | C20H34O3 | M+ |
| 324.2551 | 1 | 364.03 | C20H34O3 | M+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 155: Taxuspinanane B | **Taxuspinanane B** | 613.264 | 14.755 | Find By Formula | 612.2566 |

**Compound Chromatograms**




MS Zoomed Spectrum

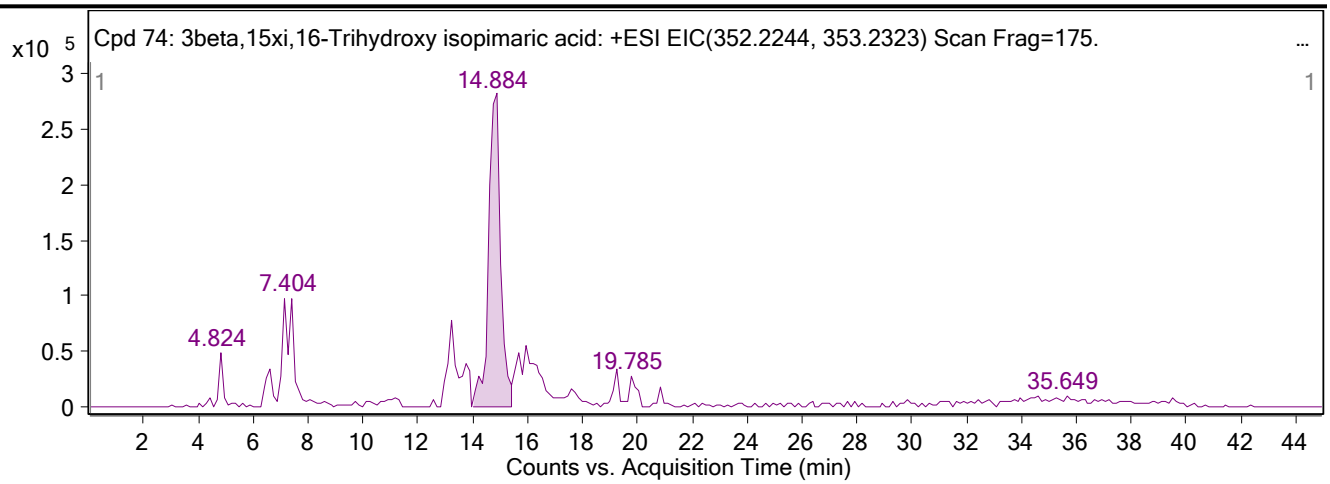



**MS Spectrum Peak List**

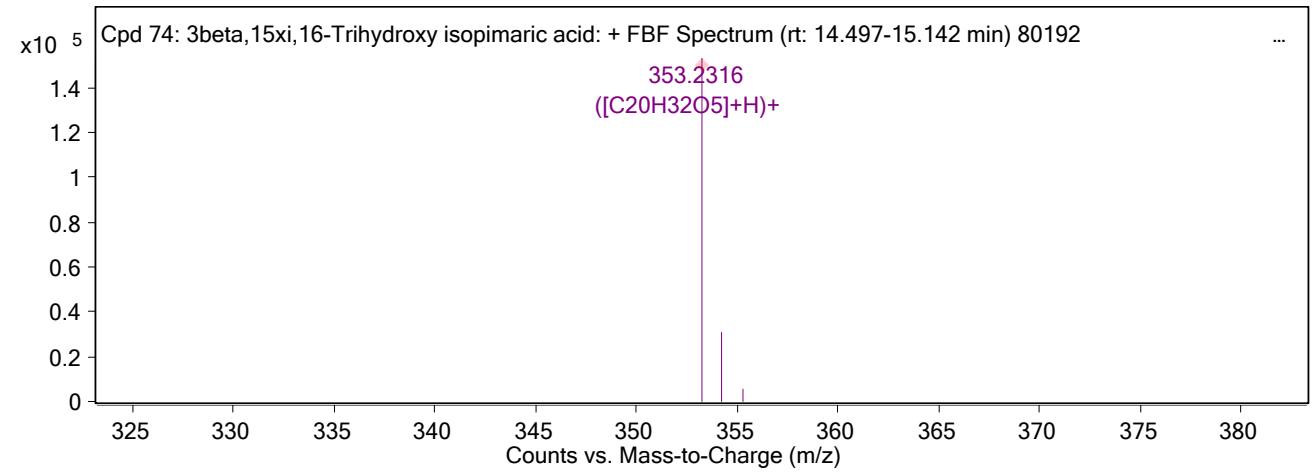
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 613.264 | 1 | 137708.92 | C33H40O11 | (M+H)+ |
| 614.2671 | 1 | 45975.23 | C33H40O11 | (M+H)+ |
| 615.2699 | 1 | 10632.29 | C33H40O11 | (M+H)+ |
| 616.2741 | 1 | 1945.42 | C33H40O11 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 74: 3beta,15xi,16-Trihydroxy isopimaric acid | **3beta,15xi,16-Trihydroxy isopimaric acid** | 353.2316 | 14.884 | Find By Formula | 352.2244 |

**Compound Chromatograms**




MS Zoomed Spectrum

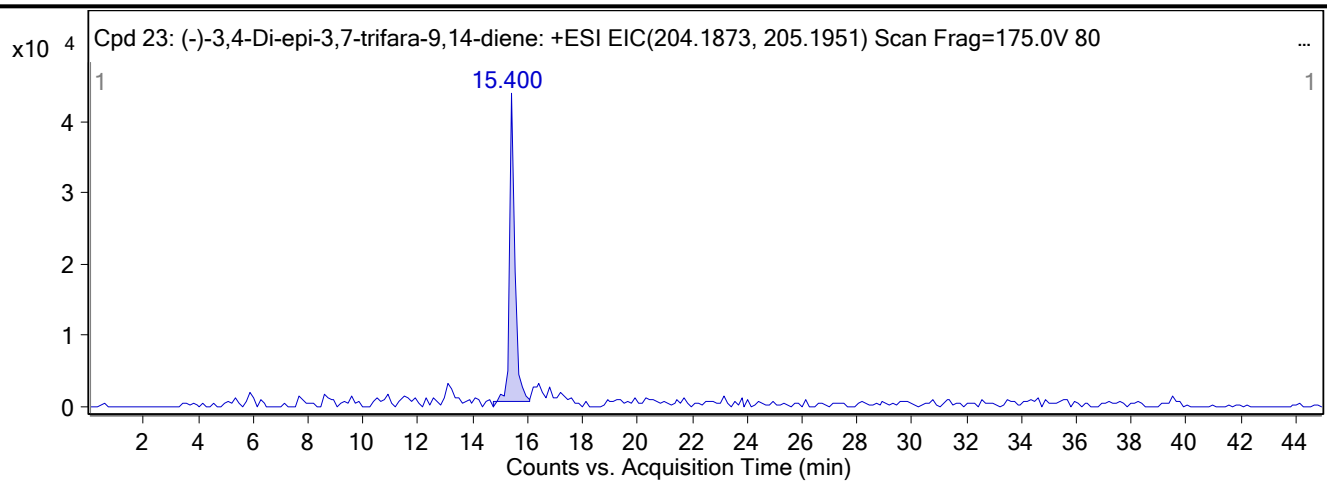



**MS Spectrum Peak List**

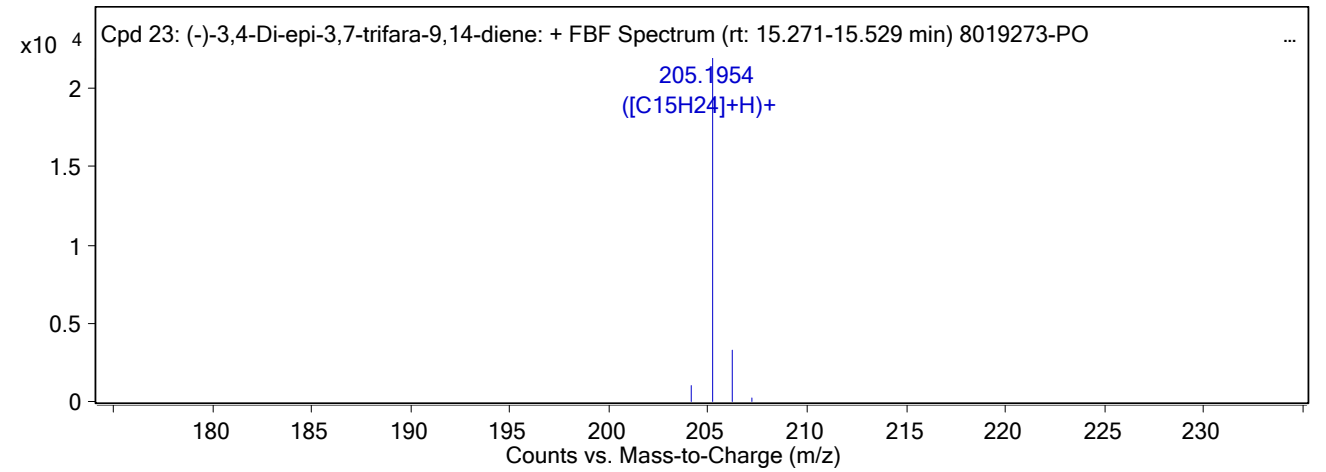
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 353.2316 | 1 | 153202.45 | C20H32O5 | (M+H)+ |
| 354.235 | 1 | 30536.82 | C20H32O5 | (M+H)+ |
| 355.2416 | 1 | 5320.18 | C20H32O5 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 23: (-)-3,4-Di-epi-3,7-trifara-9,14-diene | **(-)-3,4-Di-epi-3,7-trifara-9,14-diene** | 205.1954 | 15.4 | Find By Formula | 204.188 |

**Compound Chromatograms**




MS Zoomed Spectrum

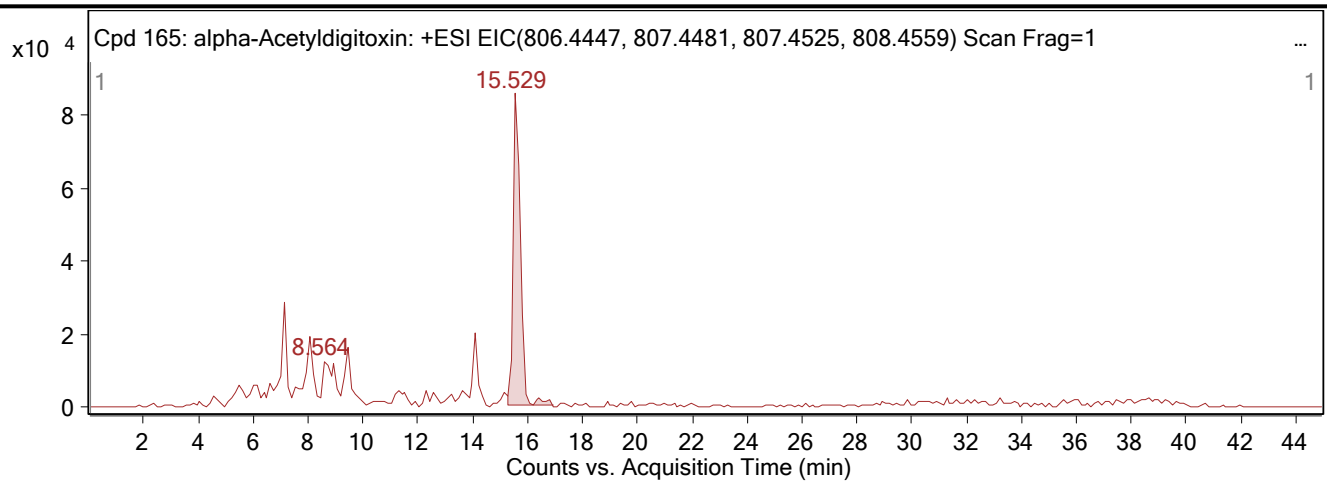



**MS Spectrum Peak List**

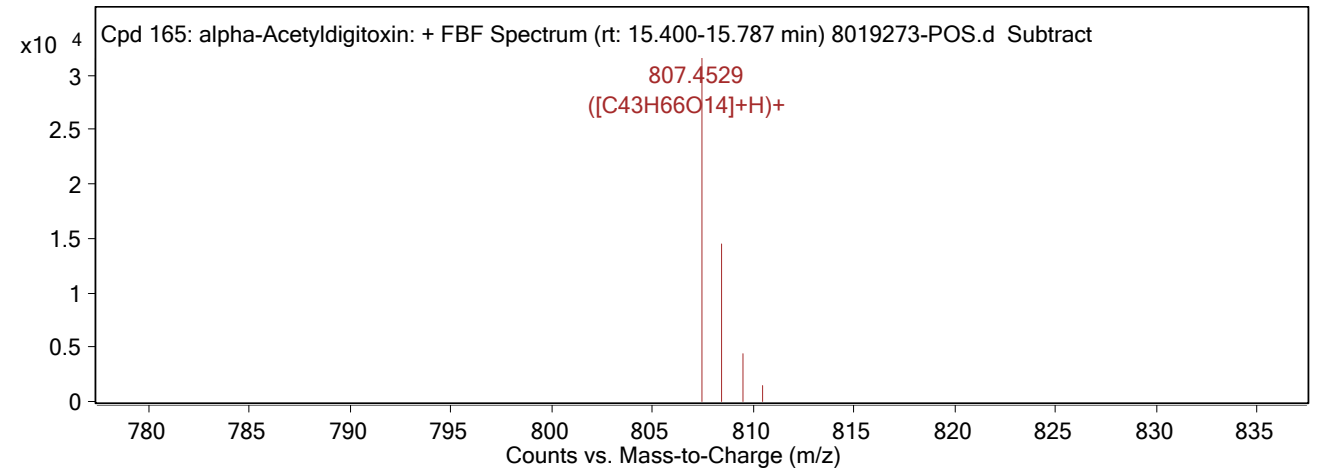
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 204.1831 | 1 | 1027.7 | C15H24 | M+ |
| 205.1954 | 1 | 21924.81 | C15H24 | (M+H)+ |
| 206.199 | 1 | 3268.4 | C15H24 | (M+H)+ |
| 207.2033 | 1 | 213.42 | C15H24 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 165: alpha-Acetyldigitoxin | **alpha-Acetyldigitoxin** | 807.4529 | 15.529 | Find By Formula | 806.4457 |

**Compound Chromatograms**




MS Zoomed Spectrum

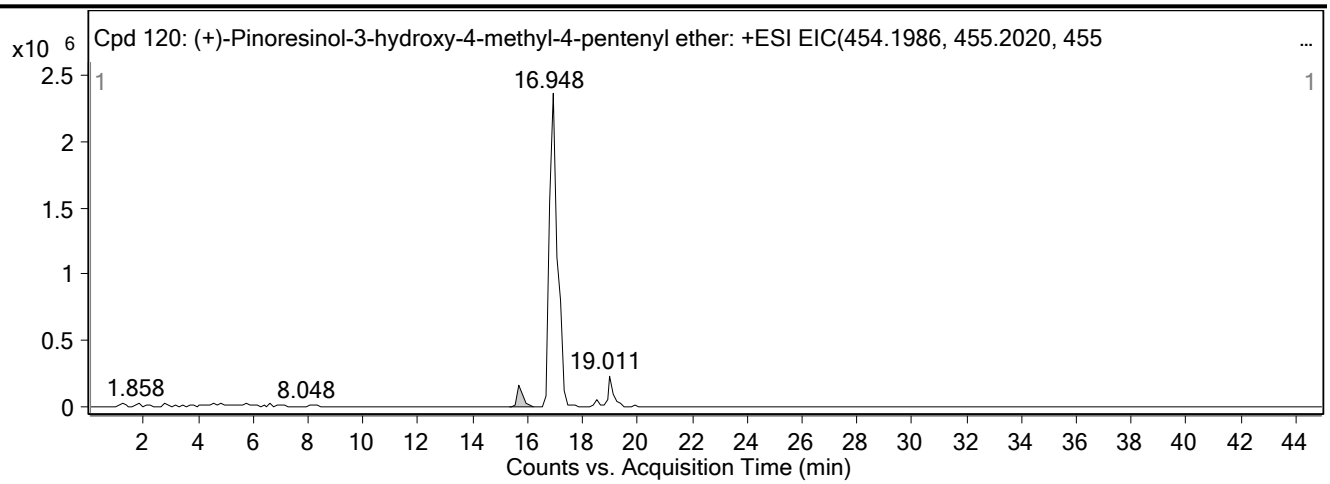



**MS Spectrum Peak List**

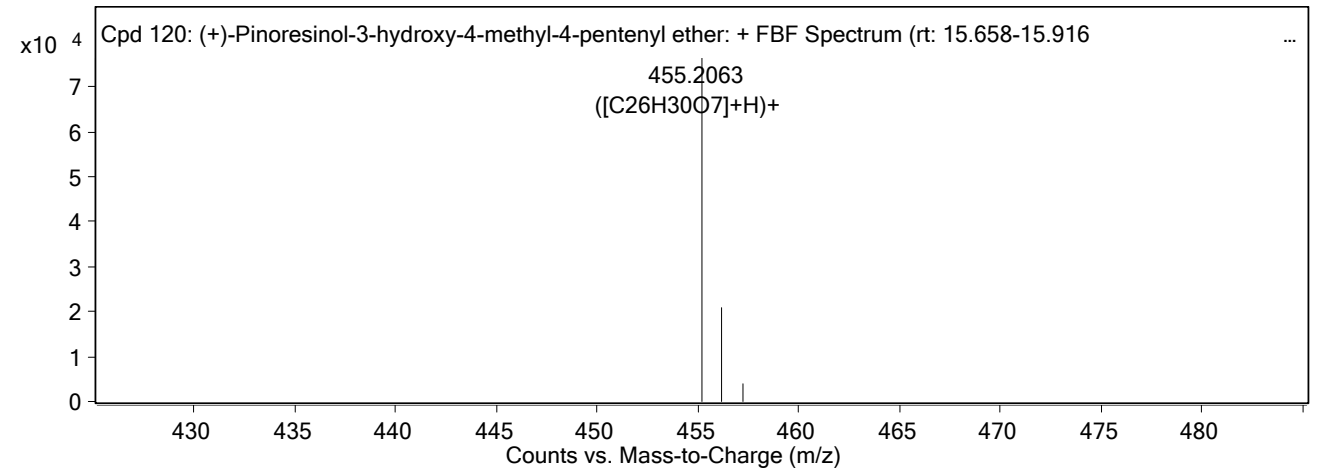
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 807.4529 | 1 | 31574.05 | C43H66O14 | (M+H)+ |
| 808.4569 | 1 | 14485.26 | C43H66O14 | (M+H)+ |
| 809.4591 | 1 | 4455.94 | C43H66O14 | (M+H)+ |
| 810.4587 | 1 | 1425.04 | C43H66O14 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 120: (+)-Pinoresinol-3-hydroxy-4-methyl-4-pentenyl ether | **(+)-Pinoresinol-3-hydroxy-4-methyl-4-pentenyl ether** | 455.2063 | 15.658 | Find By Formula | 454.1991 |

**Compound Chromatograms**




MS Zoomed Spectrum

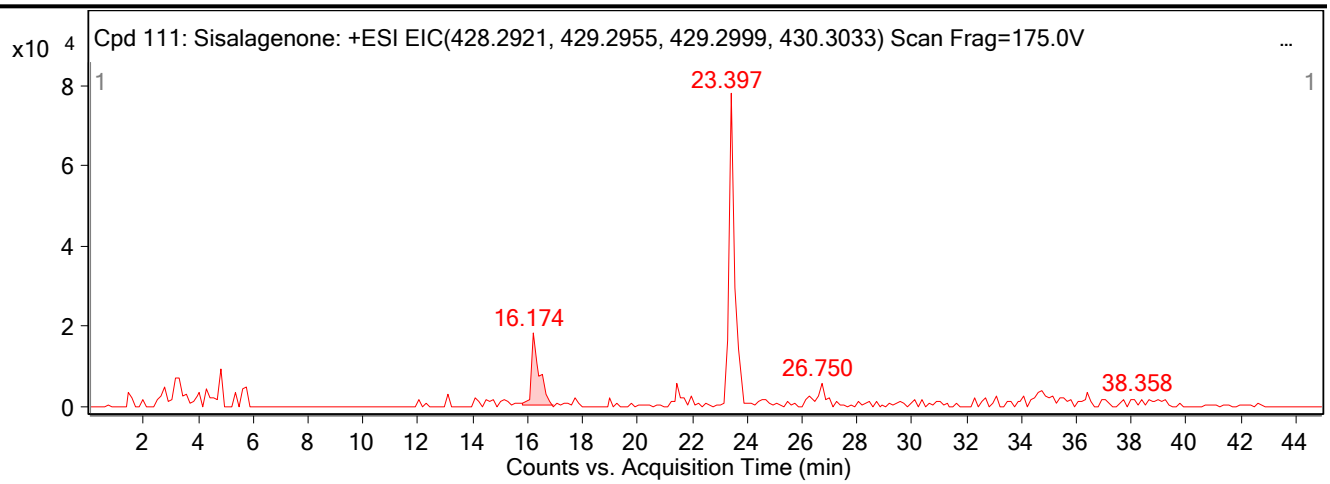



**MS Spectrum Peak List**

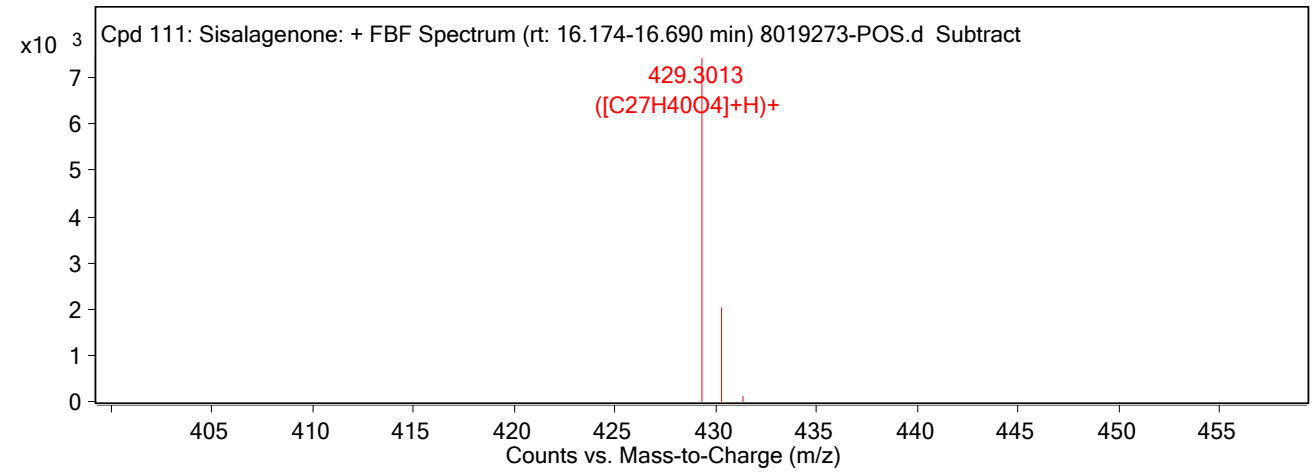
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 455.2063 | 1 | 76386.72 | C26H30O7 | (M+H)+ |
| 456.2099 | 1 | 20924.44 | C26H30O7 | (M+H)+ |
| 457.2144 | 1 | 3943.76 | C26H30O7 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 111: Sisalagenone | **Sisalagenone** | 429.3013 | 16.174 | Find By Formula | 428.2939 |

**Compound Chromatograms**




MS Zoomed Spectrum

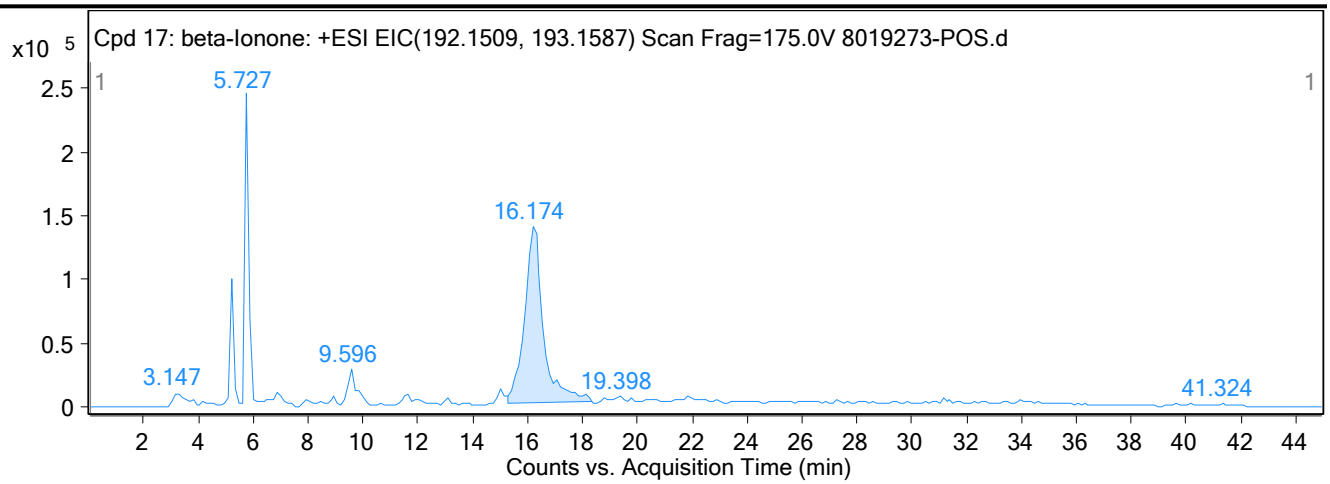



**MS Spectrum Peak List**

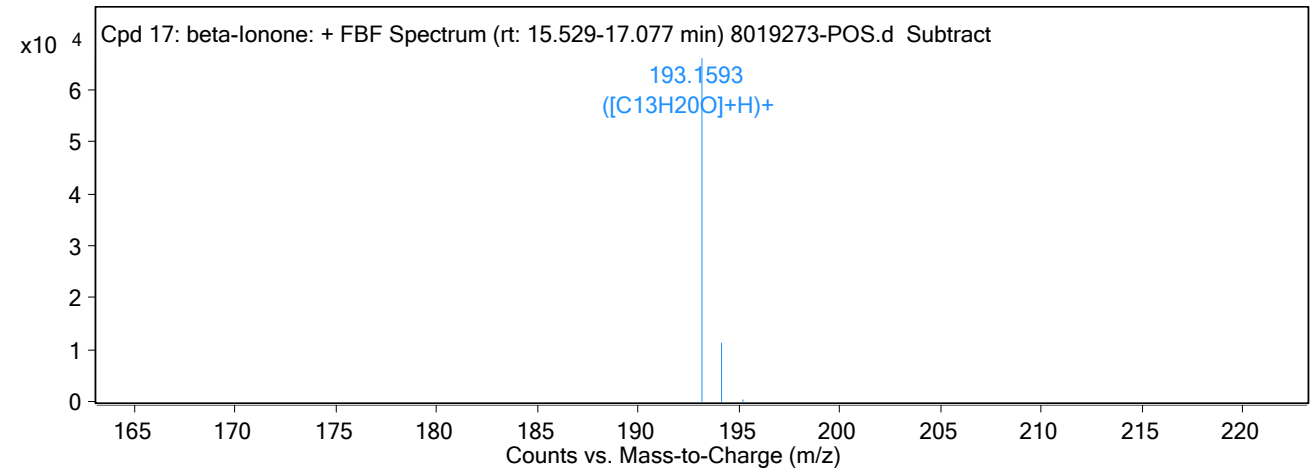
| m/z | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 429.3013 | 1 | 7430.79 | C27H40O4 | (M+H)+ |
| 430.3043 | 1 | 2018.01 | C27H40O4 | (M+H)+ |
| 431.3028 | 1 | 99.64 | C27H40O4 | (M+H)+ |

| Compound Label | Name | m/z | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 17: beta-Ionone | **beta-Ionone** | 193.1593 | 16.174 | Find By Formula | 192.1519 |

**Compound Chromatograms**




MS Zoomed Spectrum

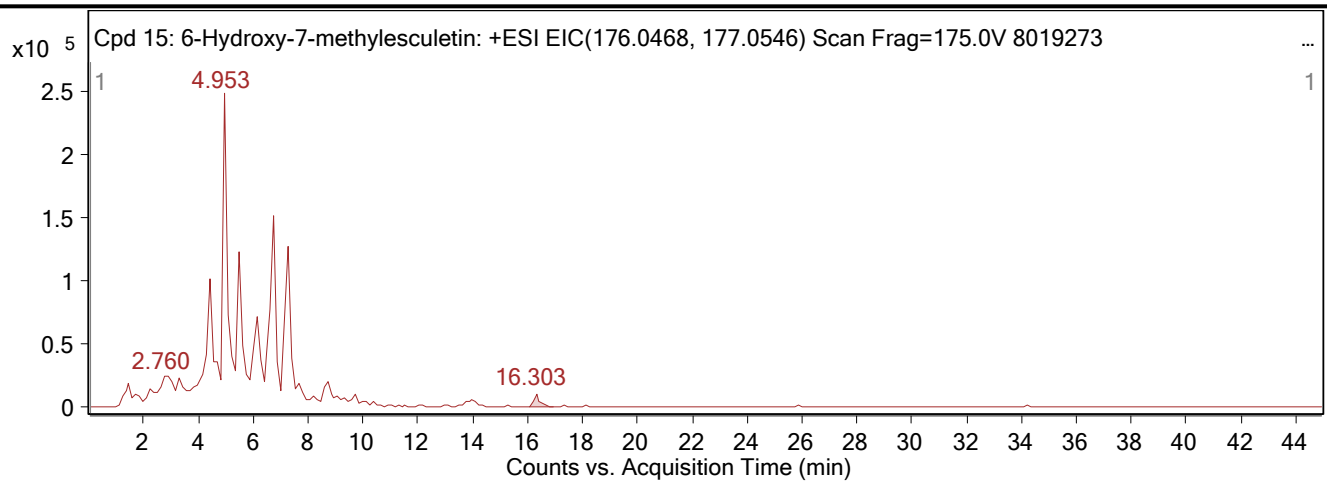



**MS Spectrum Peak List**

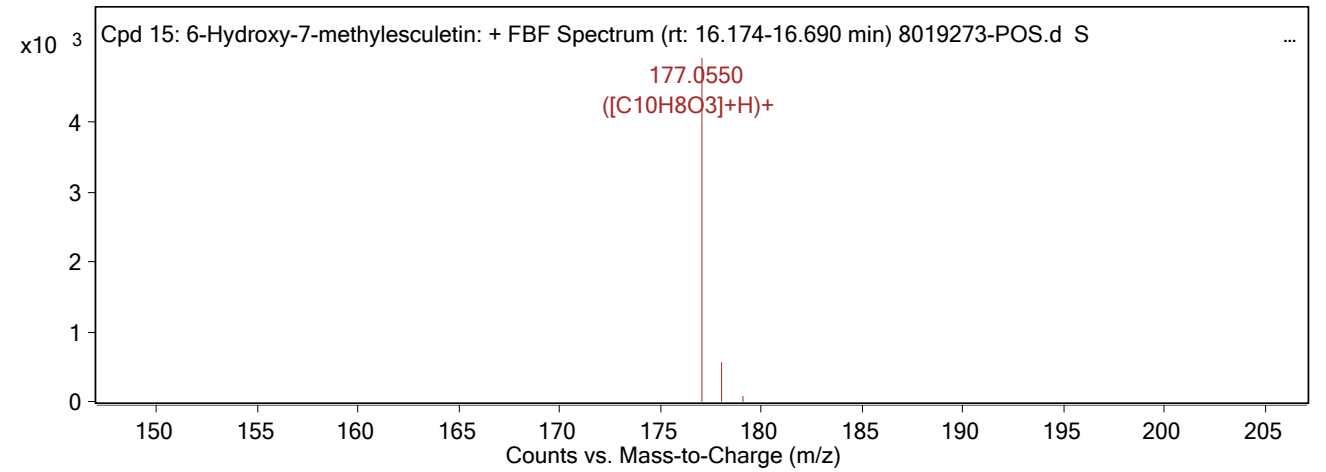
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 193.1593 | 1 | 66198.55 | C13H20O | (M+H)+ |
| 194.1619 | 1 | 11148.27 | C13H20O | (M+H)+ |
| 195.1658 | 1 | 513.24 | C13H20O | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 15: 6-Hydroxy-7-methylesculetin | **6-Hydroxy-7-methylesculetin** | 177.055 | 16.303 | Find By Formula | 176.0477 |

**Compound Chromatograms**




MS Zoomed Spectrum

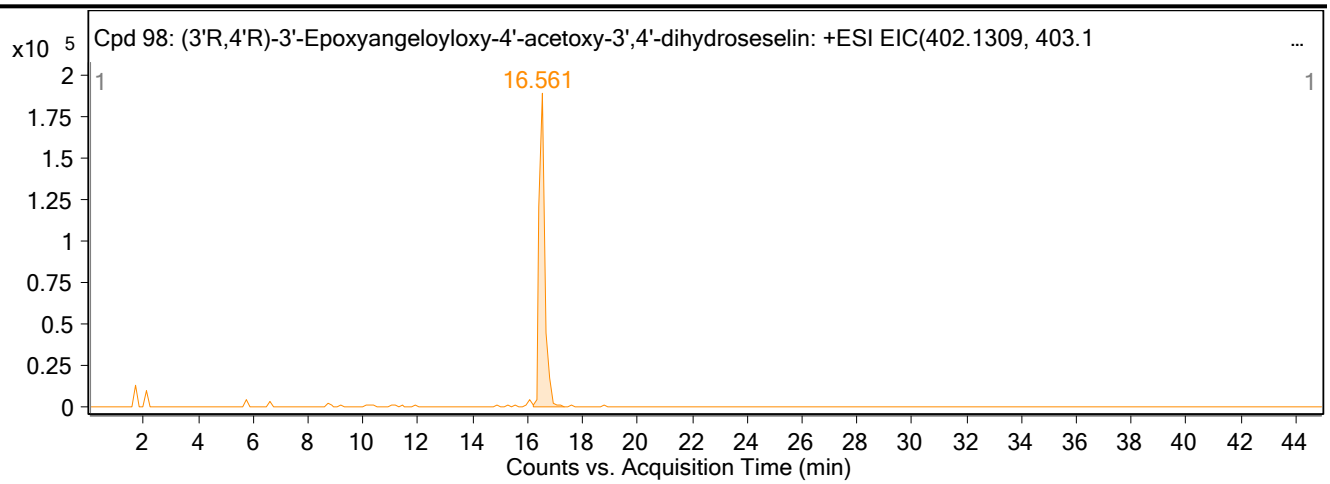



**MS Spectrum Peak List**

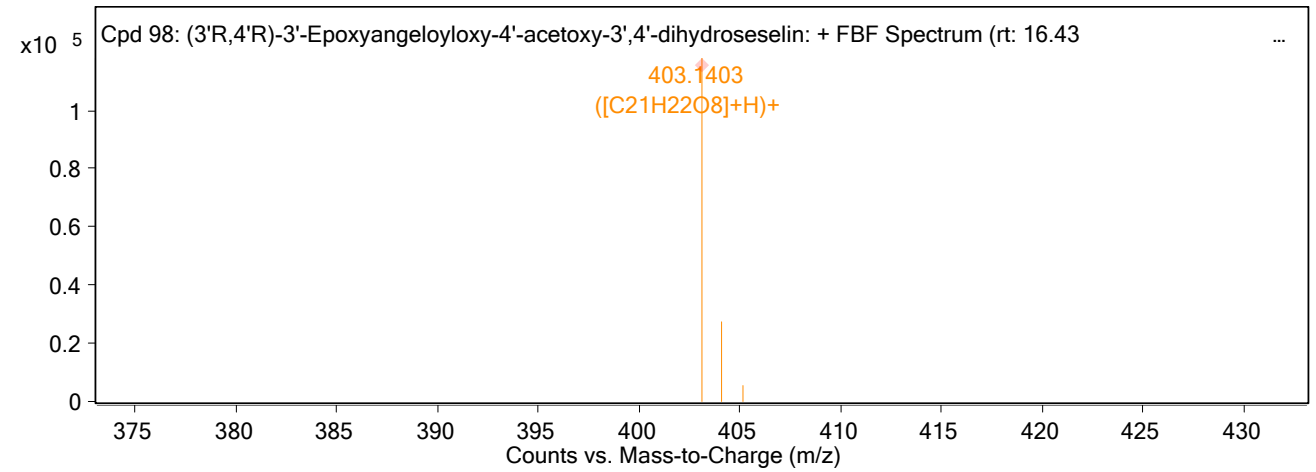
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 177.055 | 1 | 4914.76 | C10H8O3 | (M+H)+ |
| 178.058 | 1 | 559.25 | C10H8O3 | (M+H)+ |
| 179.0673 | 1 | 78.56 | C10H8O3 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 98: (3'R,4'R)-3'-Epoxyangeloyloxy-4'-acetoxy-3',4'-dihydroselin | **(3'R,4'R)-3'-Epoxyangeloyloxy-4'-acetoxy-3',4'-dihydroselin** | 403.1403 | 16.561 | Find By Formula | 402.133 |

**Compound Chromatograms**




MS Zoomed Spectrum

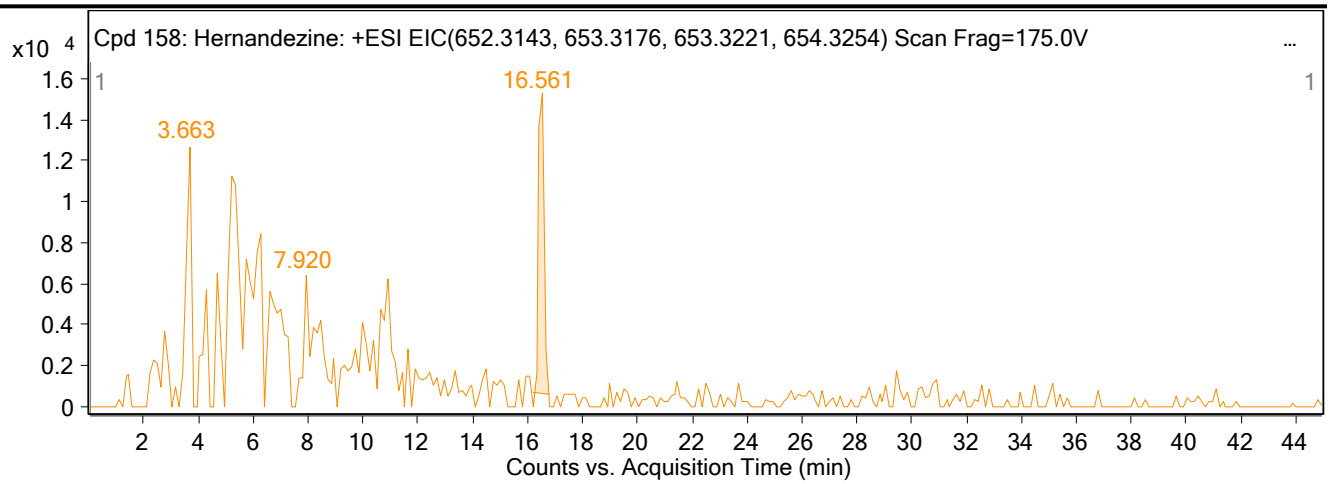



**MS Spectrum Peak List**

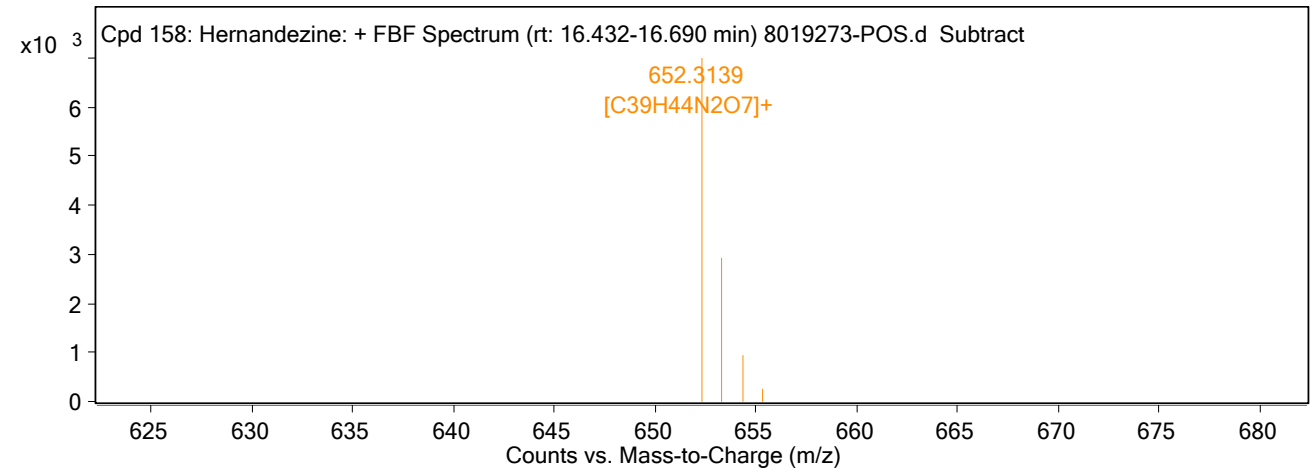
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 403.1403 | 1 | 117968.35 | C21H22O8 | (M+H)+ |
| 404.1434 | 1 | 27180.91 | C21H22O8 | (M+H)+ |
| 405.147 | 1 | 5286.14 | C21H22O8 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 158: Hernandezine | **Hernandezine** | 652.3139 | 16.561 | Find By Formula | 652.3149 |

**Compound Chromatograms**




MS Zoomed Spectrum

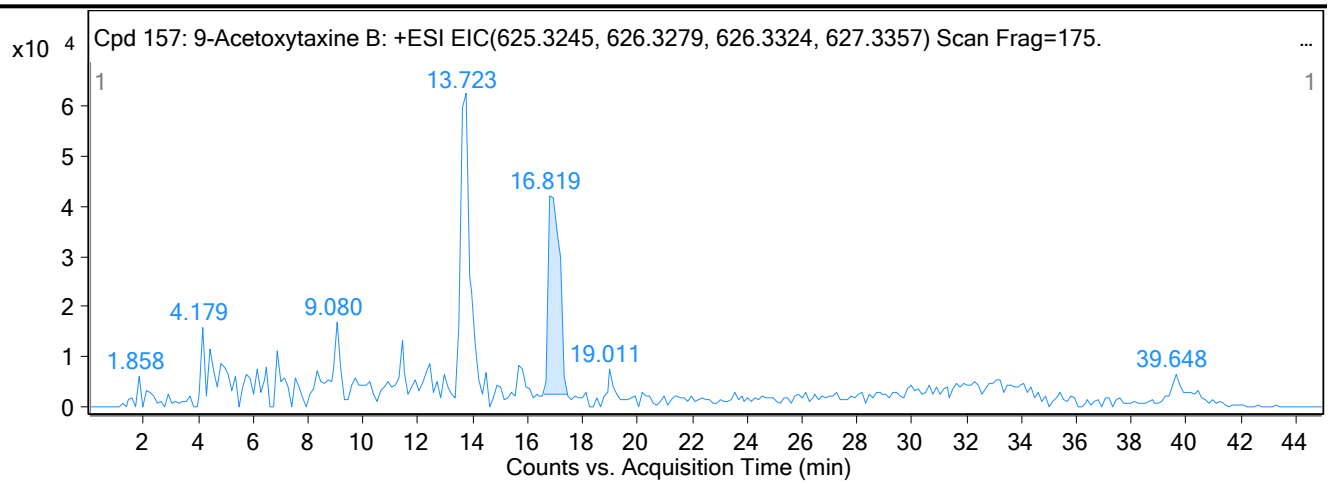



**MS Spectrum Peak List**

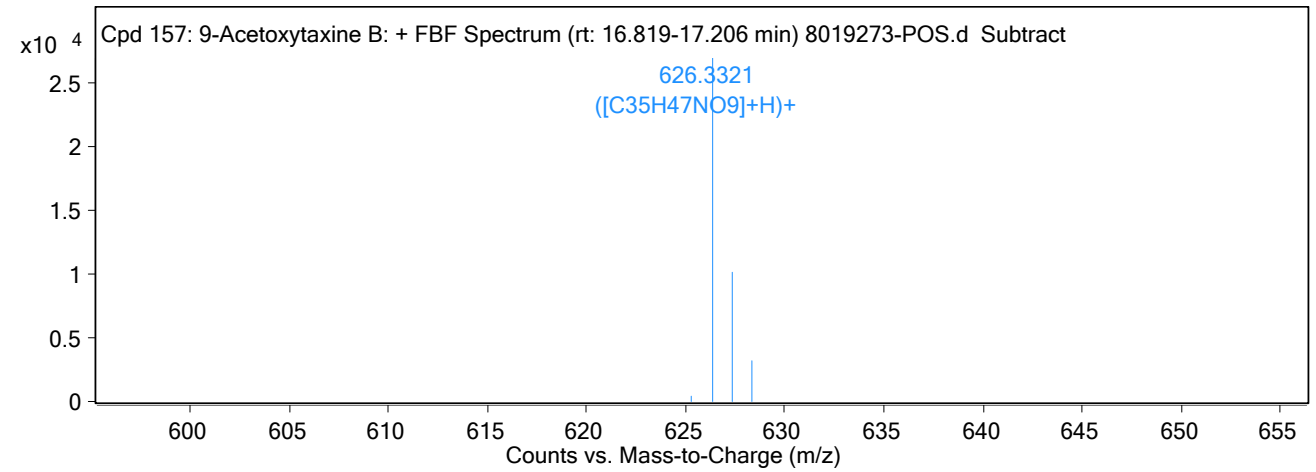
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 652.3139 | 1 | 7000.13 | C39H44N2O7 | M+ |
| 653.3192 | 1 | 2941.48 | C39H44N2O7 | M+ |
| 654.3186 | 1 | 934.35 | C39H44N2O7 | M+ |
| 655.3264 | 1 | 252.95 | C39H44N2O7 | M+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 157: 9-Acetoxytaxine B | **9-Acetoxytaxine B** | 626.3321 | 16.819 | Find By Formula | 625.3242 |

**Compound Chromatograms**




MS Zoomed Spectrum

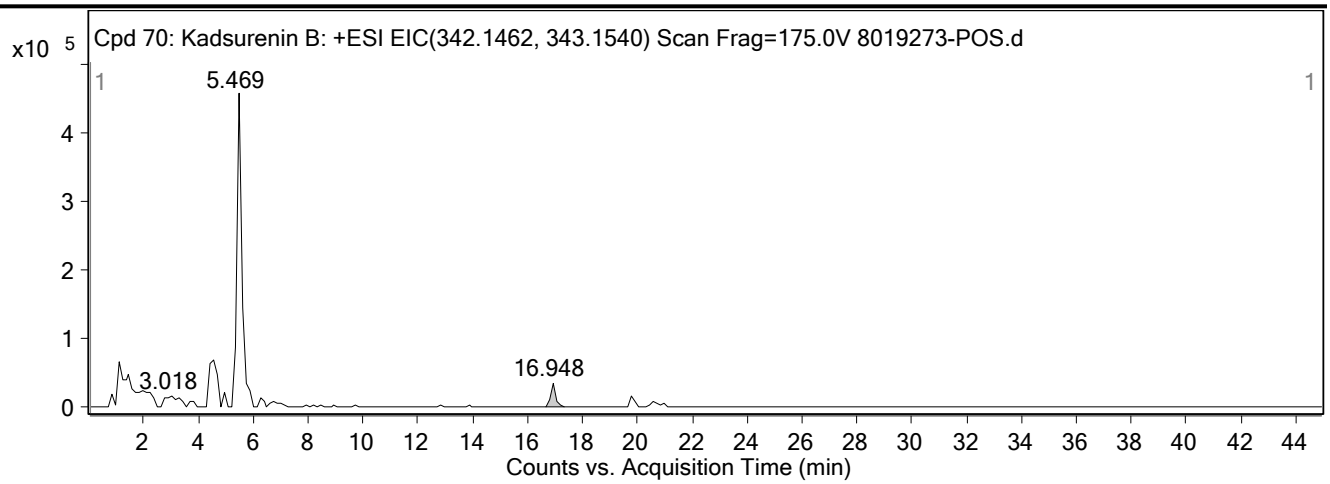



**MS Spectrum Peak List**

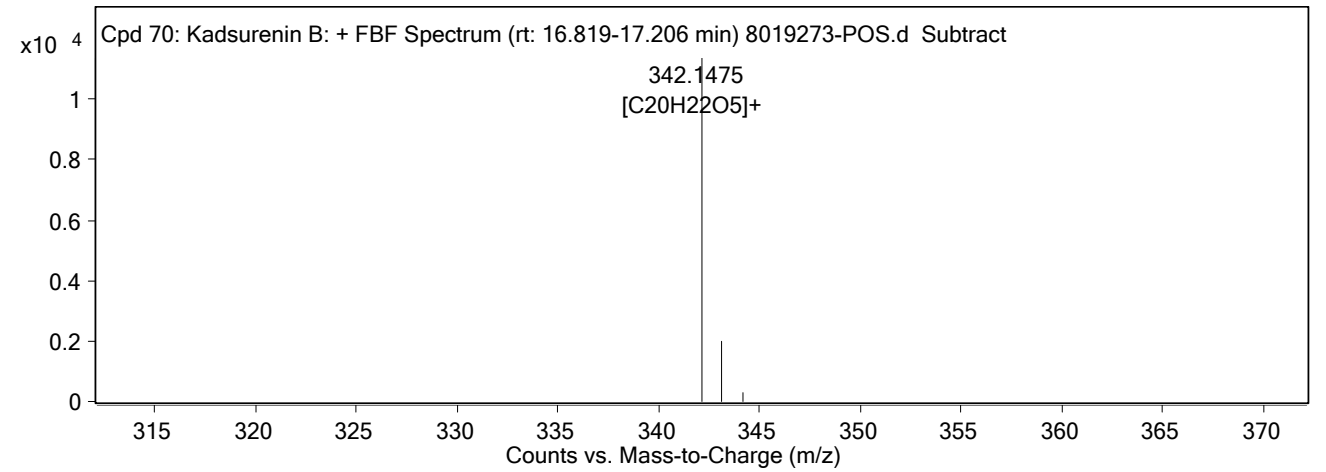
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 625.3125 | 1 | 425.05 | C35H47NO9 | M+ |
| 626.3321 | 1 | 26912.14 | C35H47NO9 | (M+H)+ |
| 627.335 | 1 | 10069.46 | C35H47NO9 | (M+H)+ |
| 628.3326 | 1 | 3162.12 | C35H47NO9 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 70: Kadsurenin B | **Kadsurenin B** | 342.1475 | 16.948 | Find By Formula | 342.1479 |

**Compound Chromatograms**




MS Zoomed Spectrum

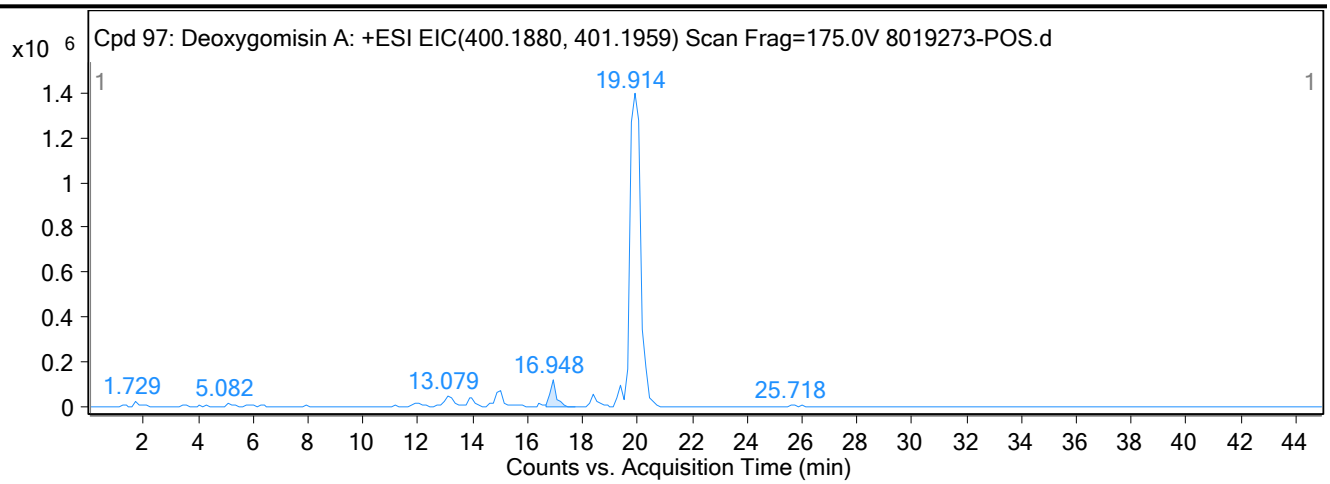



**MS Spectrum Peak List**

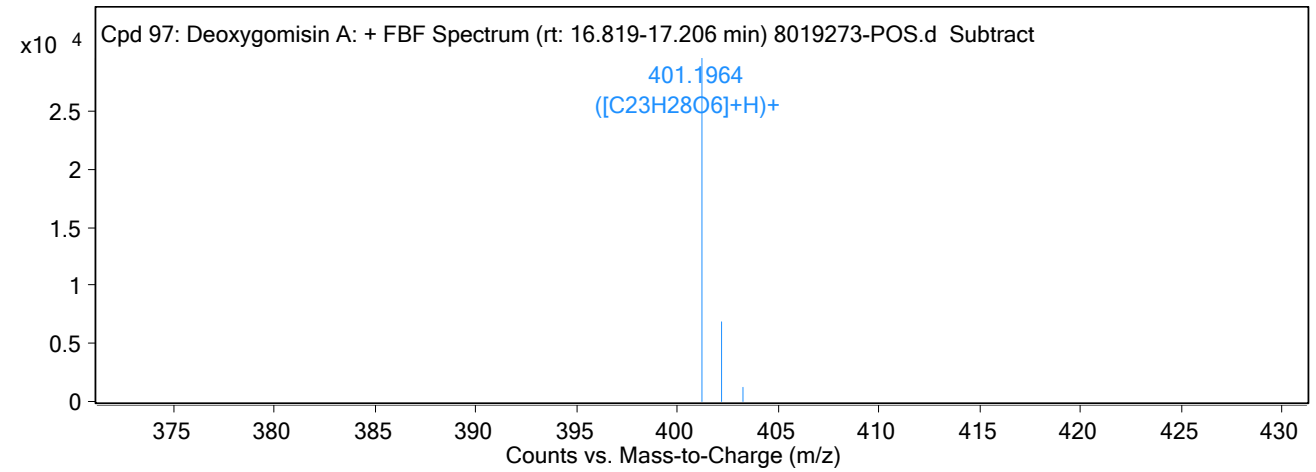
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 342.1475 | 1 | 11363 | C20H22O5 | M+ |
| 343.1505 | 1 | 1995.55 | C20H22O5 | M+ |
| 344.1494 | 1 | 303.09 | C20H22O5 | M+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 97: Deoxygomisin A | **Deoxygomisin A** | 401.1964 | 16.948 | Find By Formula | 400.1894 |

**Compound Chromatograms**




MS Zoomed Spectrum

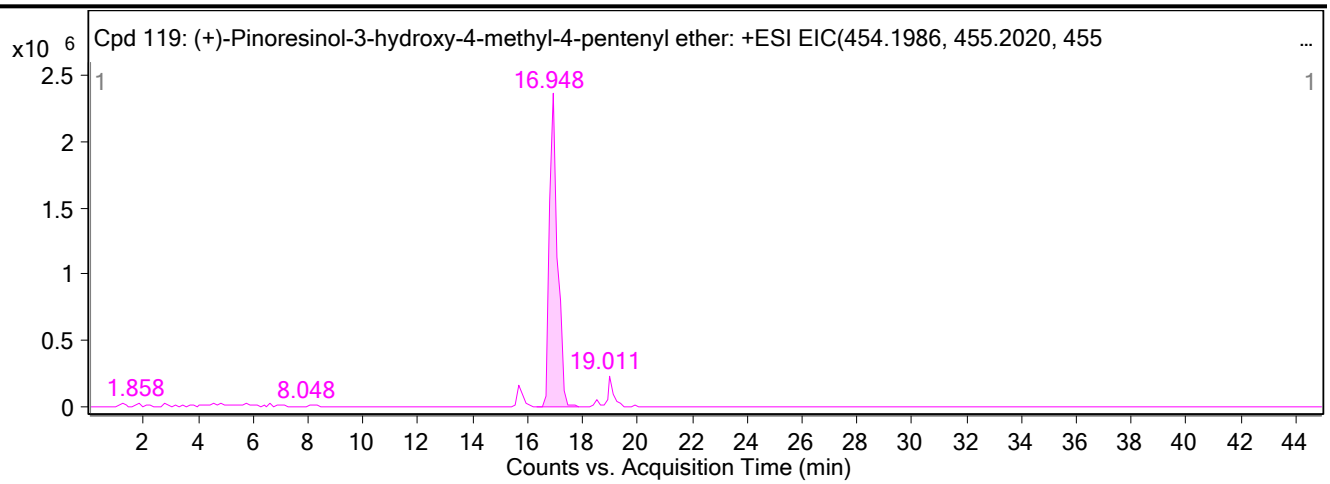



**MS Spectrum Peak List**

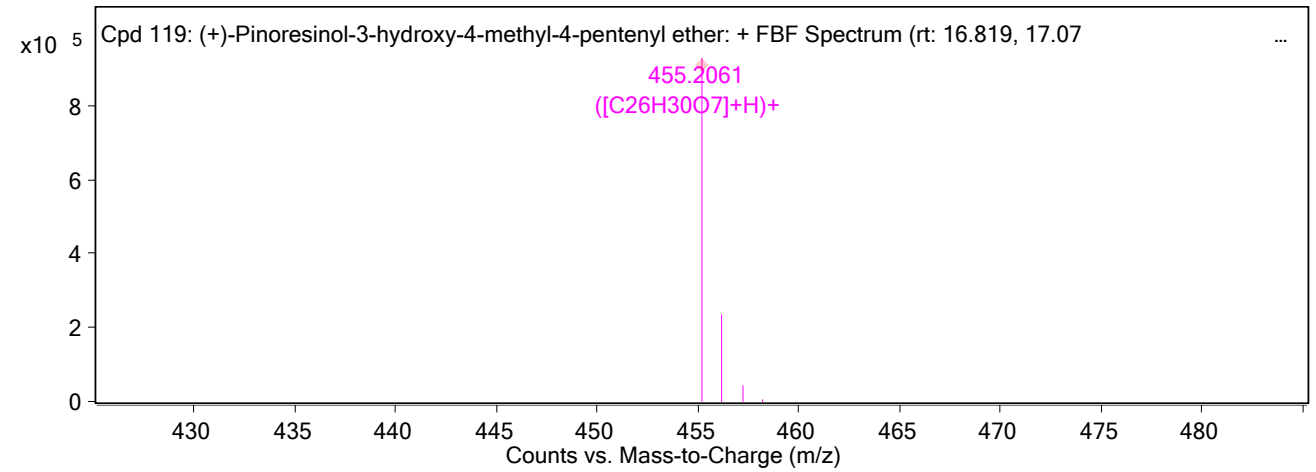
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 401.1964 | 1 | 29610.11 | C23H28O6 | (M+H)+ |
| 402.201 | 1 | 6832.47 | C23H28O6 | (M+H)+ |
| 403.2024 | 1 | 1187.05 | C23H28O6 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 119: (+)-Pinoresinol-3-hydroxy-4-methyl-4-pentenyl ether | **(+)-Pinoresinol-3-hydroxy-4-methyl-4-pentenyl ether** | 455.2061 | 16.948 | Find By Formula | 454.1988 |

**Compound Chromatograms**




MS Zoomed Spectrum

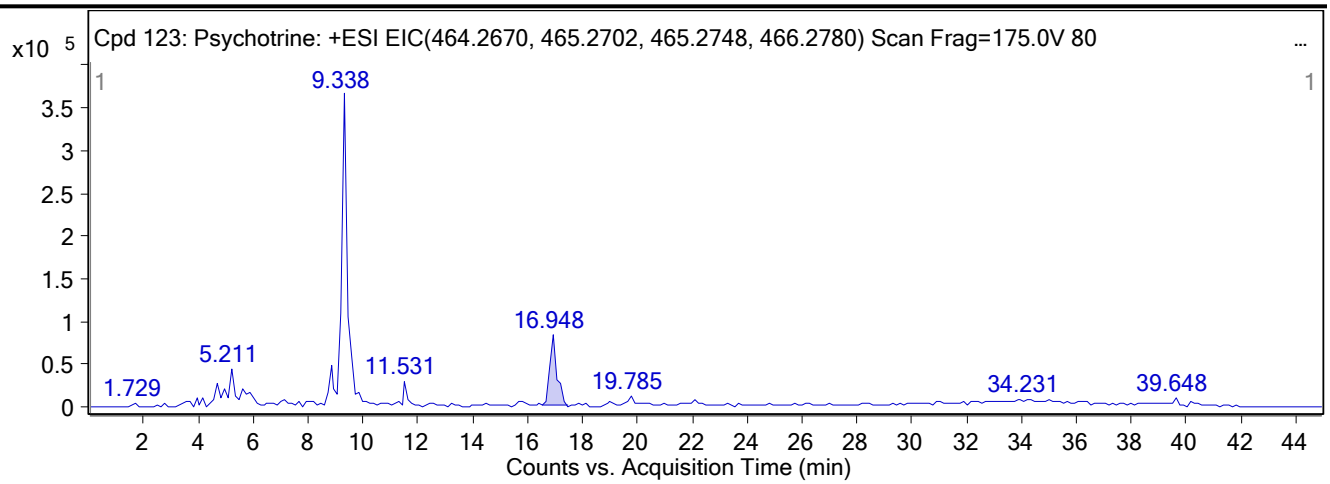



**MS Spectrum Peak List**

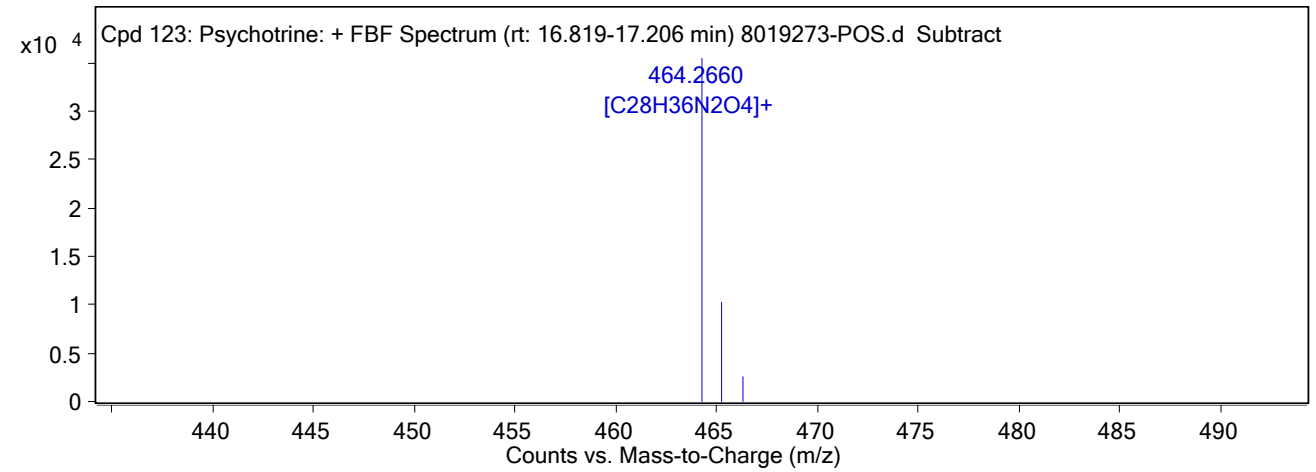
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 455.2061 | 1 | 928042 | C26H30O7 | (M+H)+ |
| 456.2094 | 1 | 232645.5 | C26H30O7 | (M+H)+ |
| 457.212 | 1 | 41896.75 | C26H30O7 | (M+H)+ |
| 458.2143 | 1 | 6107.61 | C26H30O7 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 123: Psychotrine | **Psychotrine** | 464.266 | 16.948 | Find By Formula | 464.2662 |

**Compound Chromatograms**




MS Zoomed Spectrum

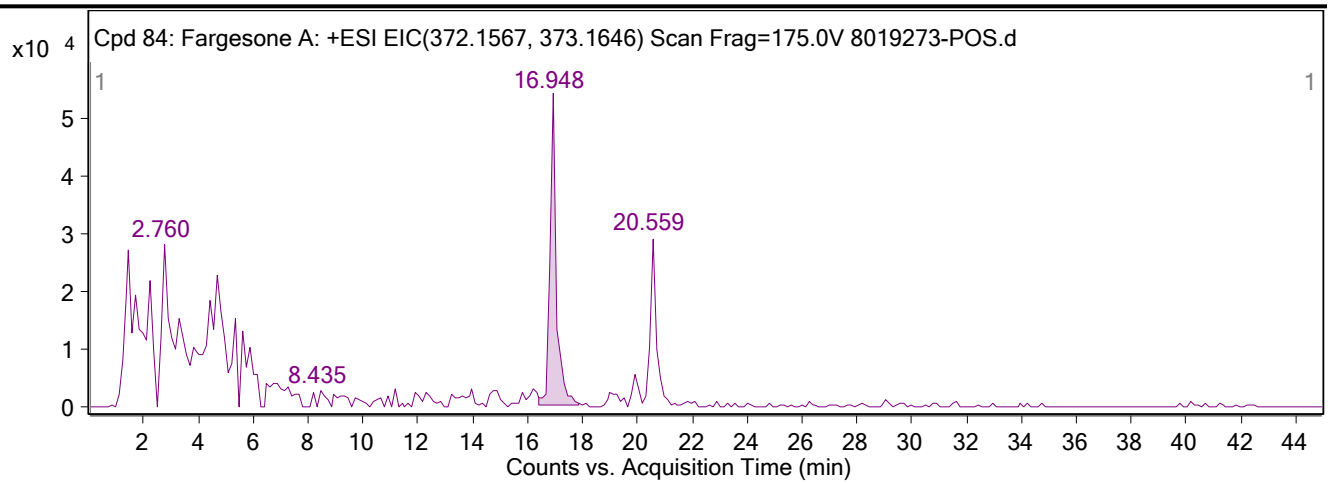



**MS Spectrum Peak List**

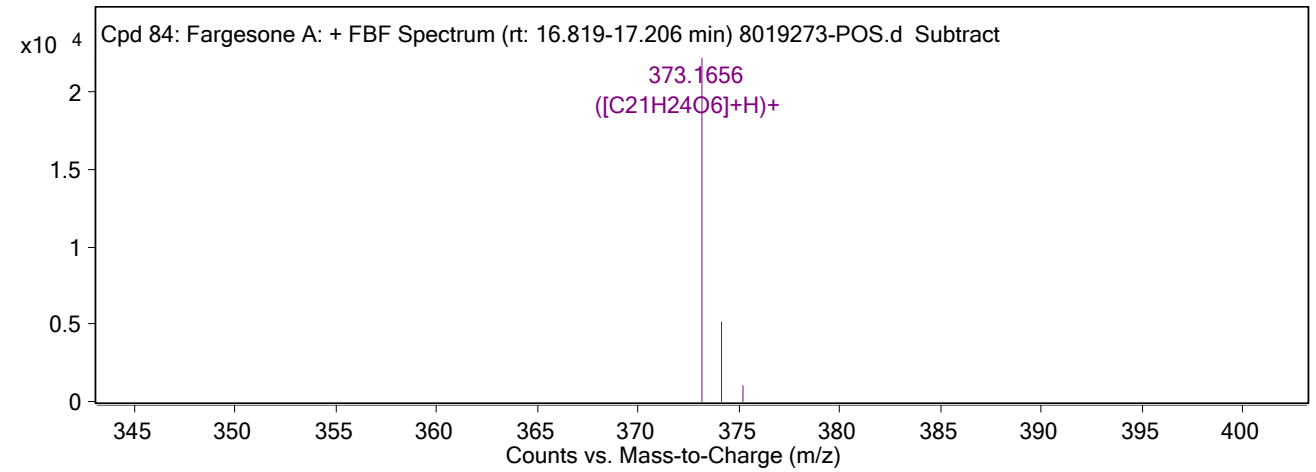
| m/z | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 464.266 | 1 | 35458.43 | C28H36N2O4 | M+ |
| 465.2688 | 1 | 10202.28 | C28H36N2O4 | M+ |
| 466.2688 | 1 | 2604.36 | C28H36N2O4 | M+ |

| Compound Label | Name | m/z | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 84: Fargesone A | **Fargesone A** | 373.1656 | 16.948 | Find By Formula | 372.1585 |

**Compound Chromatograms**




MS Zoomed Spectrum

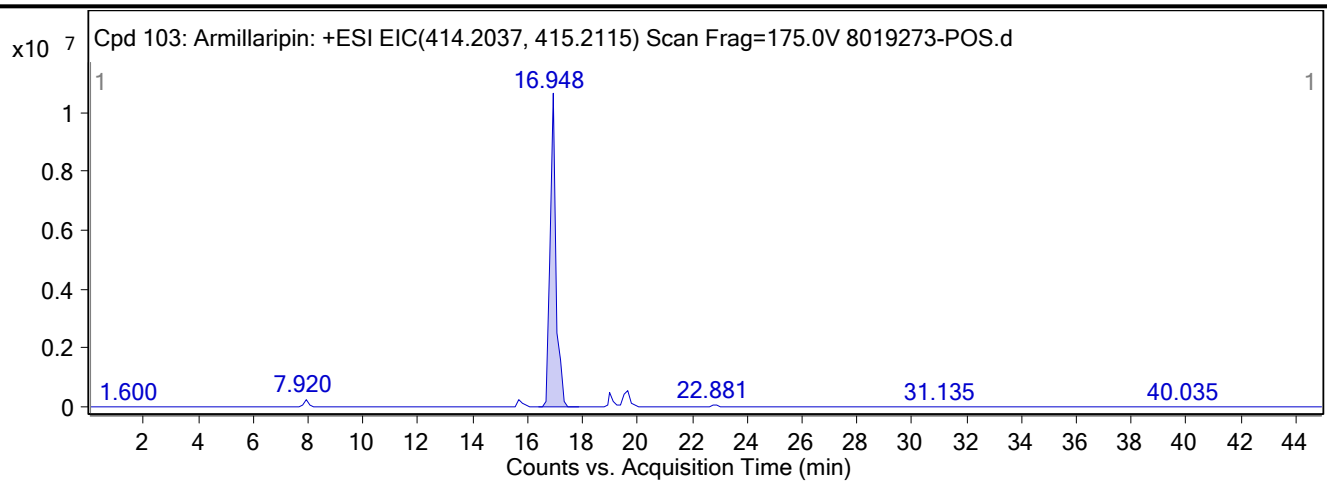



**MS Spectrum Peak List**

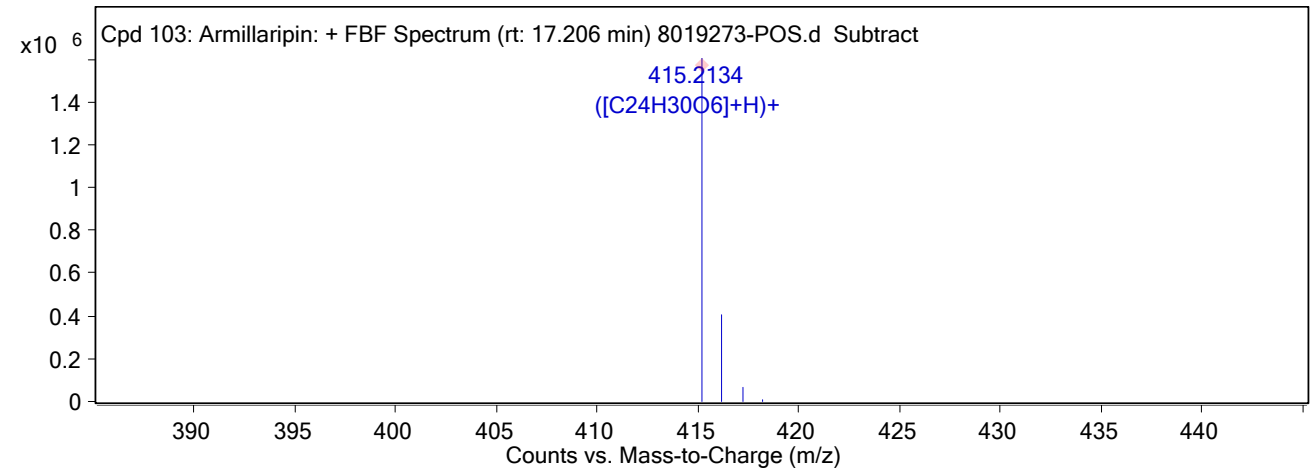
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 373.1656 | 1 | 22207.85 | C21H24O6 | (M+H)+ |
| 374.1696 | 1 | 5193.72 | C21H24O6 | (M+H)+ |
| 375.1743 | 1 | 1055.28 | C21H24O6 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 103: Armillaripin | **Armillaripin** | 415.2134 | 16.948 | Find By Formula | 414.2061 |

**Compound Chromatograms**




MS Zoomed Spectrum

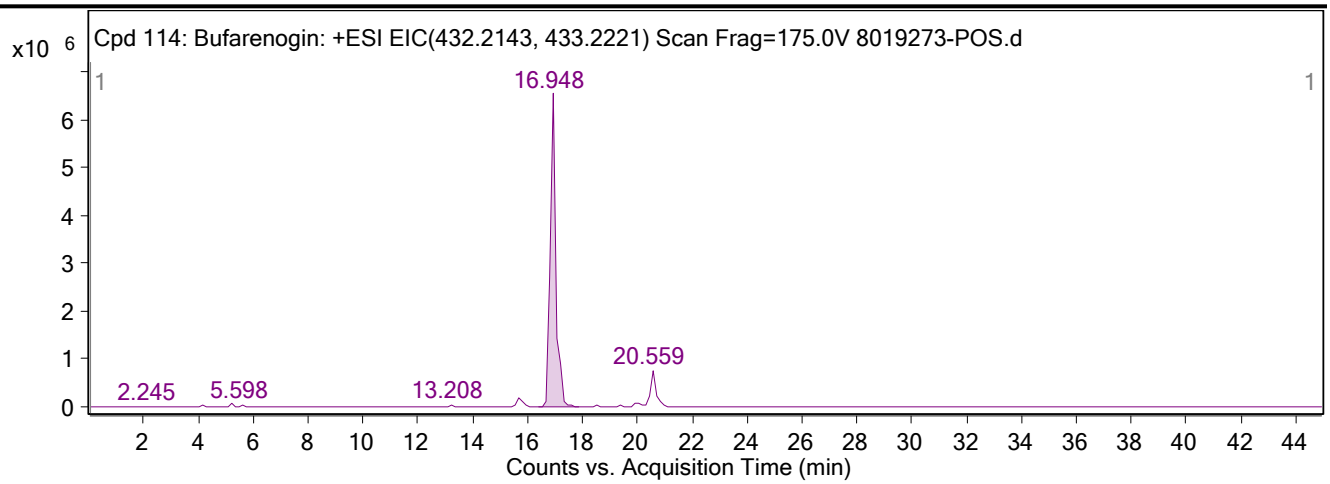



**MS Spectrum Peak List**

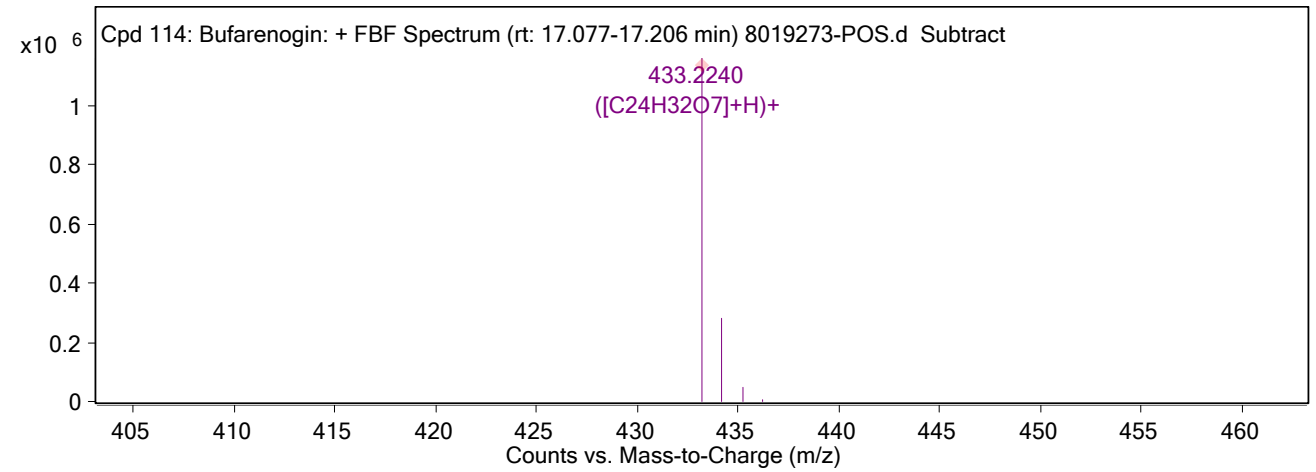
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 415.2134 | 1 | 1604171.25 | C24H30O6 | (M+H)+ |
| 416.2168 | 1 | 404719 | C24H30O6 | (M+H)+ |
| 417.2189 | 1 | 68838.15 | C24H30O6 | (M+H)+ |
| 418.2221 | 1 | 7480.43 | C24H30O6 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 114: Bufarenogin | **Bufarenogin** | 433.224 | 16.948 | Find By Formula | 432.2167 |

**Compound Chromatograms**




MS Zoomed Spectrum

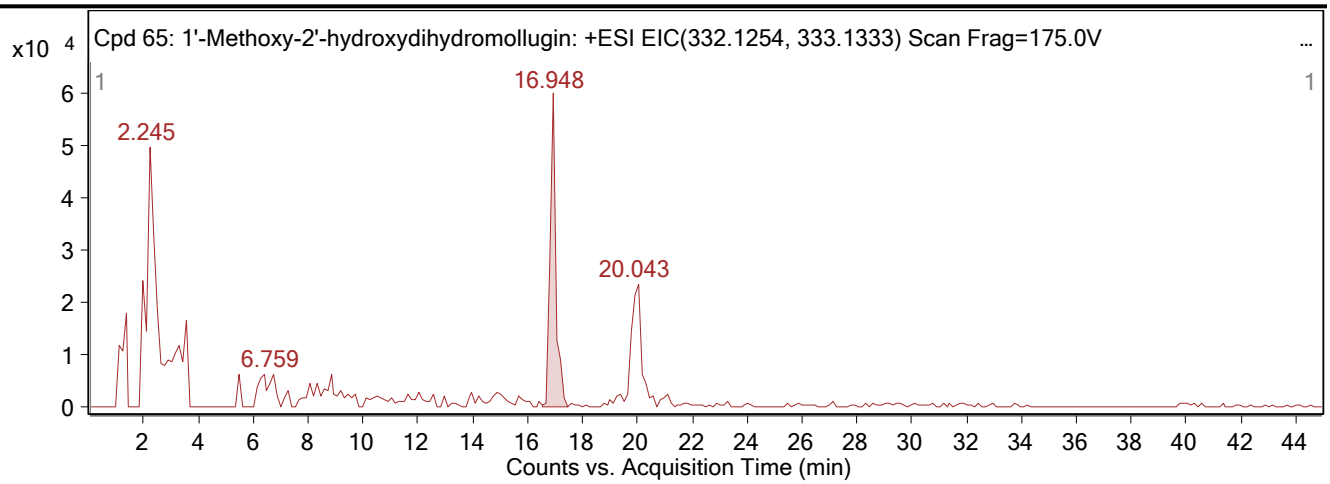



**MS Spectrum Peak List**

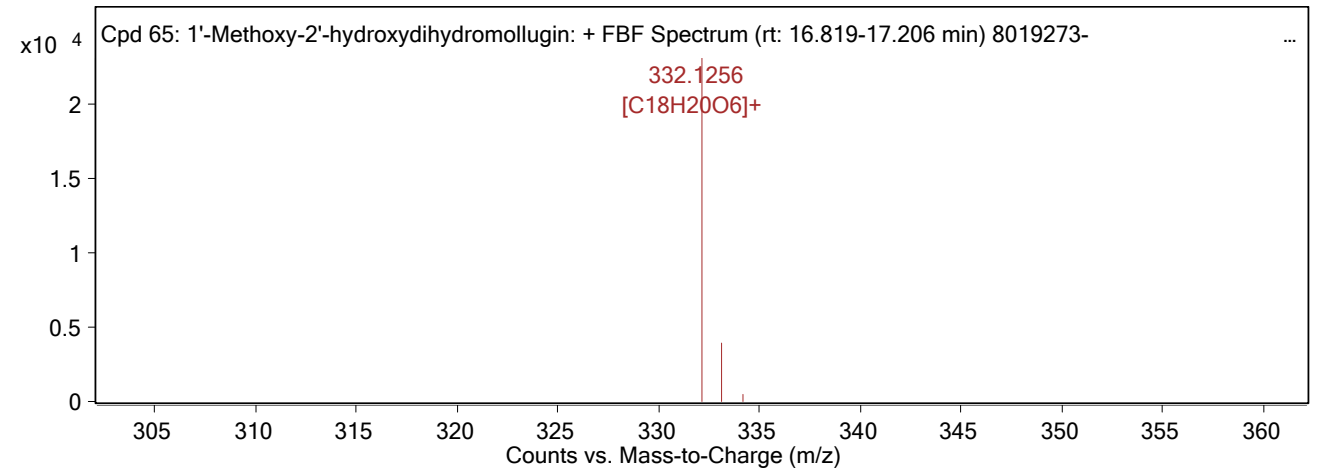
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 433.224 | 1 | 1160208.25 | C24H32O7 | (M+H)+ |
| 434.2274 | 1 | 281244.78 | C24H32O7 | (M+H)+ |
| 435.23 | 1 | 50656.12 | C24H32O7 | (M+H)+ |
| 436.2336 | 1 | 7840.25 | C24H32O7 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 65: 1'-Methoxy-2'-hydroxydihydromollugin | **1'-Methoxy-2'-hydroxydihydromollugin** | 332.1256 | 16.948 | Find By Formula | 332.1263 |

**Compound Chromatograms**




MS Zoomed Spectrum

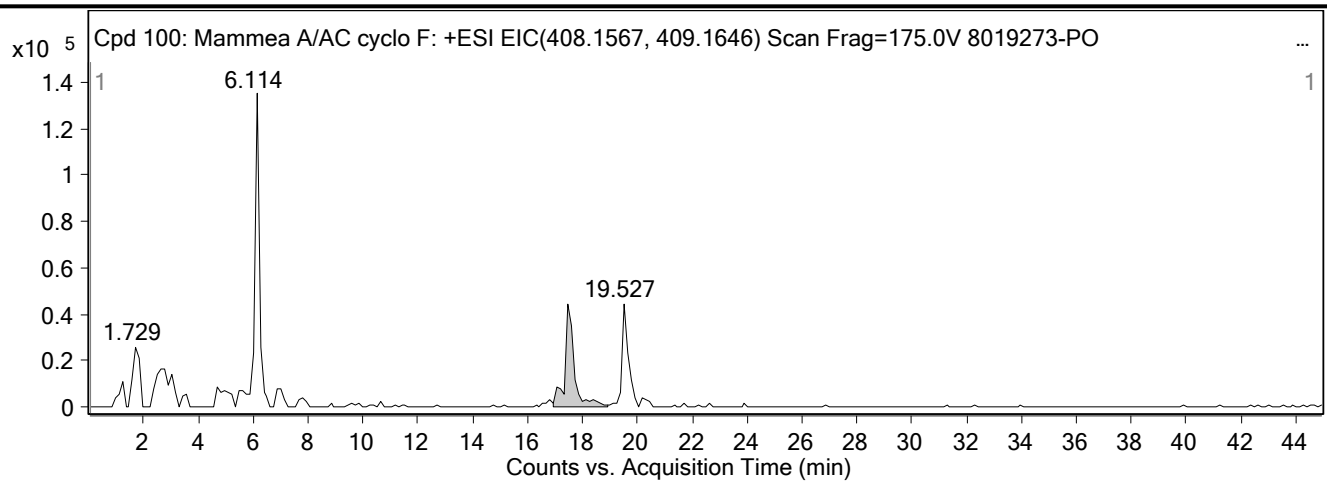



**MS Spectrum Peak List**

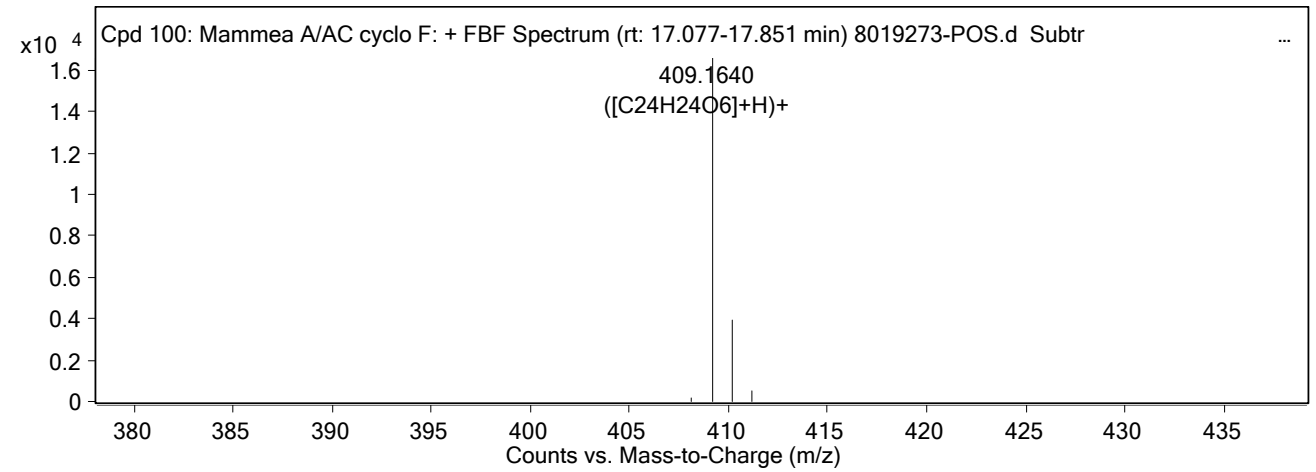
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 332.1256 | 1 | 23054.3 | C18H20O6 | M+ |
| 333.1297 | 1 | 3987.73 | C18H20O6 | M+ |
| 334.1332 | 1 | 514.13 | C18H20O6 | M+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 100: Mammea A/AC cyclo F | **Mammea A/AC cyclo F** | 409.164 | 17.464 | Find By Formula | 408.1568 |

**Compound Chromatograms**




MS Zoomed Spectrum

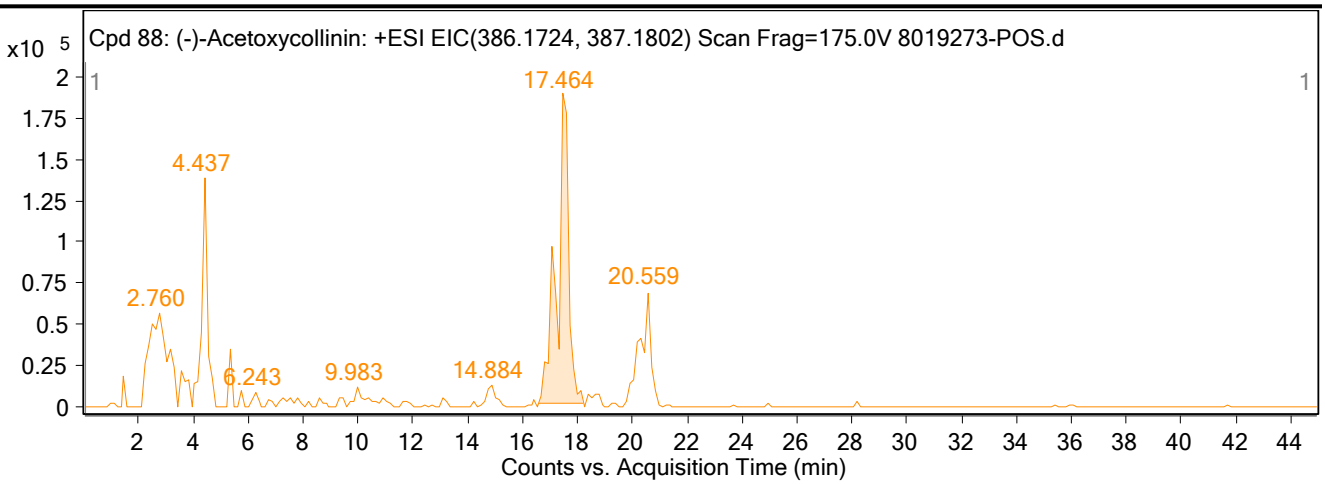



**MS Spectrum Peak List**

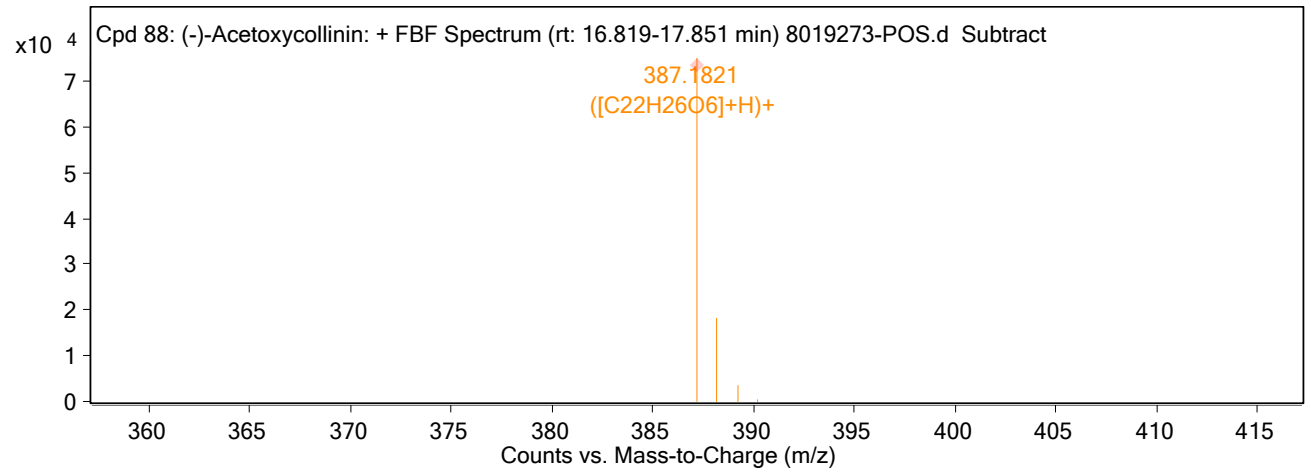
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 408.1507 | 1 | 167.72 | C24H24O6 | M+ |
| 409.164 | 1 | 16589.86 | C24H24O6 | (M+H)+ |
| 410.1679 | 1 | 3960.84 | C24H24O6 | (M+H)+ |
| 411.1696 | 1 | 537.78 | C24H24O6 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 88: (-)-Acetoxycollinin | **(-)-Acetoxycollinin** | 387.1821 | 17.464 | Find By Formula | 386.1748 |

**Compound Chromatograms**




MS Zoomed Spectrum

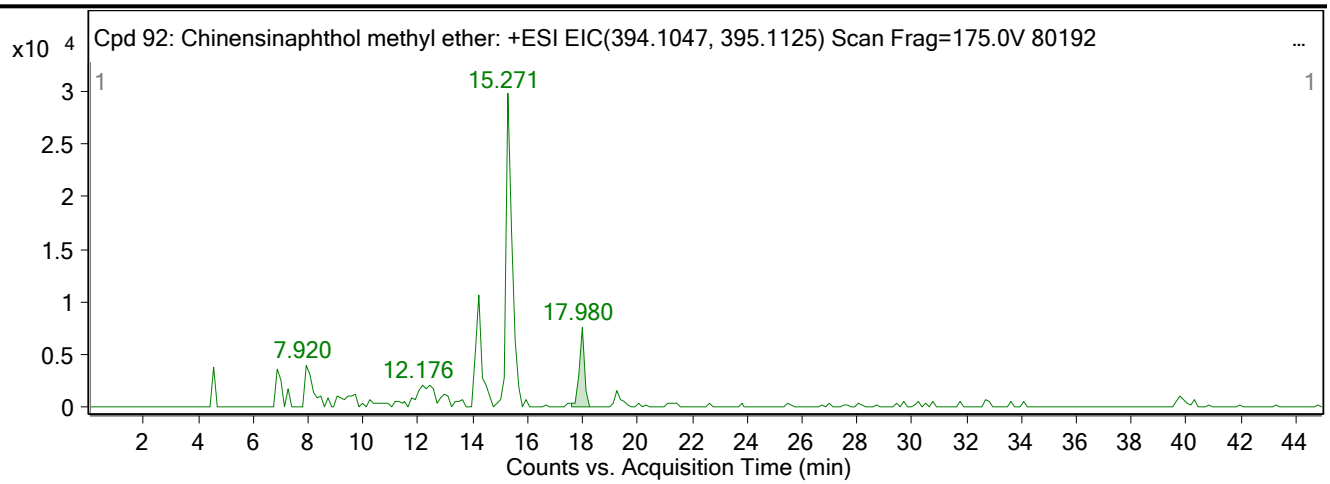



**MS Spectrum Peak List**

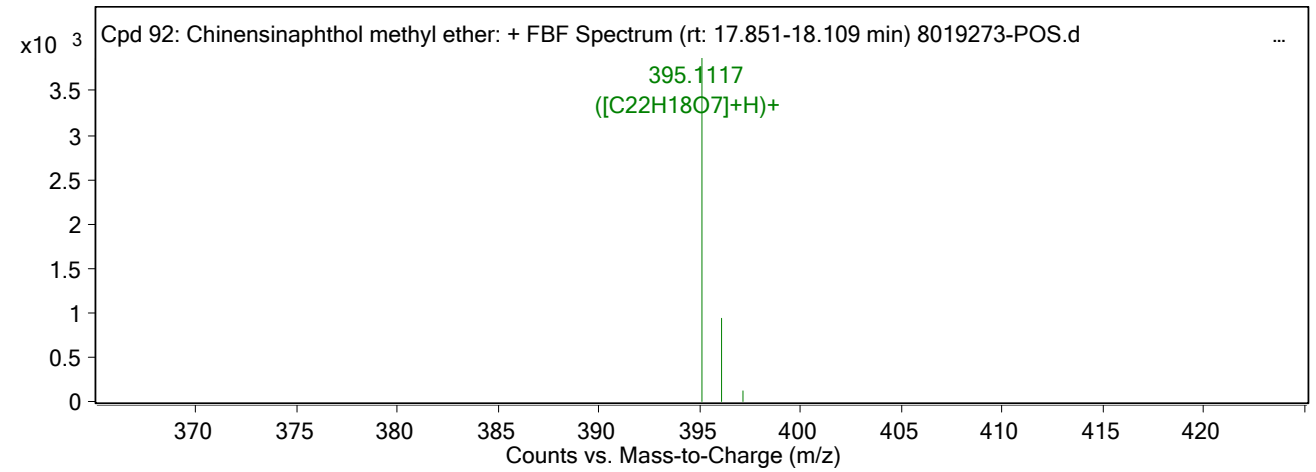
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 387.1821 | 1 | 75082.48 | C22H26O6 | (M+H)+ |
| 388.1856 | 1 | 18026.15 | C22H26O6 | (M+H)+ |
| 389.1884 | 1 | 3554.09 | C22H26O6 | (M+H)+ |
| 390.1928 | 1 | 360.73 | C22H26O6 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 92: Chinensinaphthol methyl ether | **Chinensinaphthol methyl ether** | 395.1117 | 17.98 | Find By Formula | 394.1044 |

**Compound Chromatograms**




MS Zoomed Spectrum

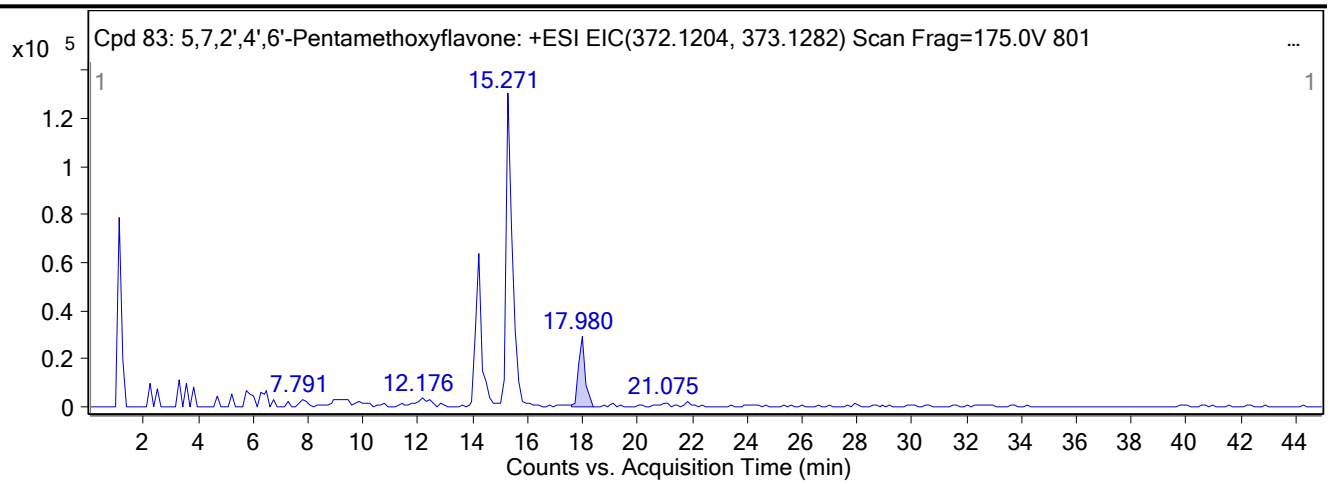



**MS Spectrum Peak List**

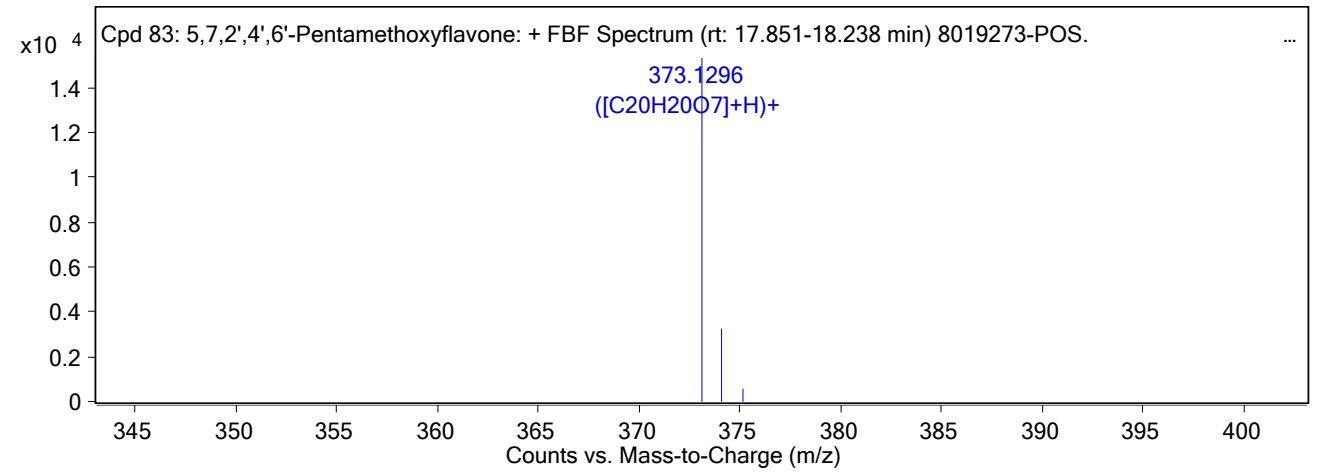
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 395.1117 | 1 | 3867.15 | C22H18O7 | (M+H)+ |
| 396.1157 | 1 | 931.14 | C22H18O7 | (M+H)+ |
| 397.1149 | 1 | 118.92 | C22H18O7 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 83: 5,7,2',4',6'-Pentamethoxyflavone | **5,7,2',4',6'-Pentamethoxyflavone** | 373.1296 | 17.98 | Find By Formula | 372.1224 |

**Compound Chromatograms**




MS Zoomed Spectrum

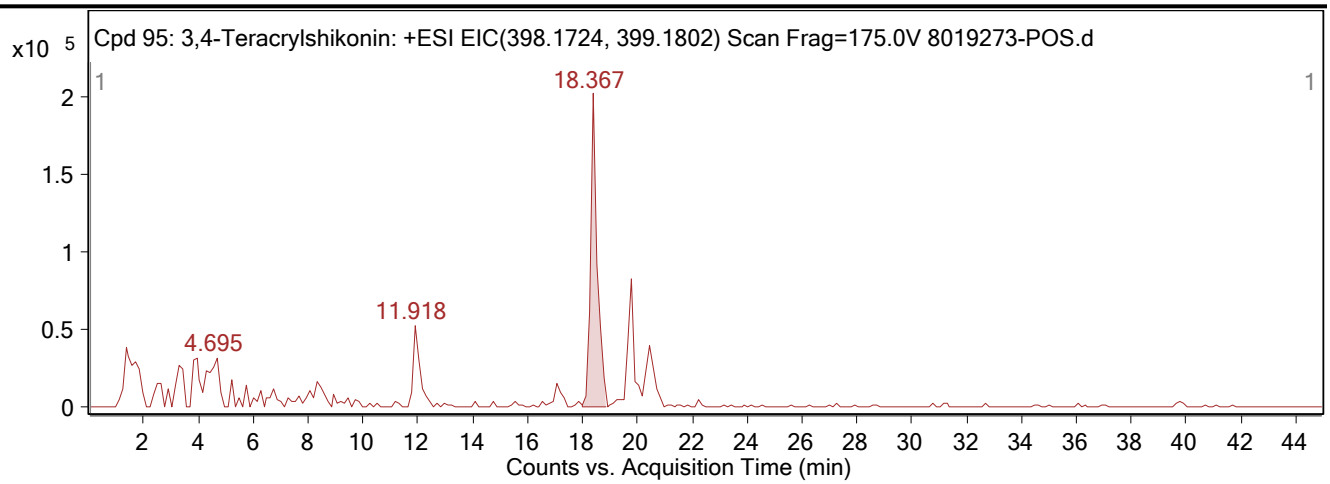



**MS Spectrum Peak List**

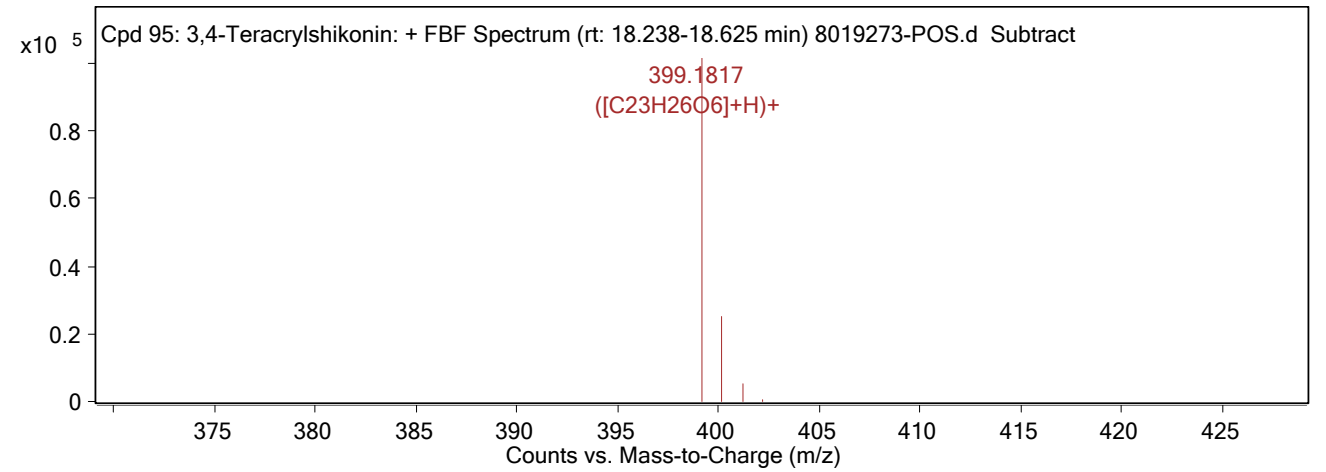
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 373.1296 | 1 | 15307.04 | C20H20O7 | (M+H)+ |
| 374.1334 | 1 | 3236.85 | C20H20O7 | (M+H)+ |
| 375.1363 | 1 | 564.31 | C20H20O7 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 95: 3,4-Teracrylshikonin | **3,4-Teracrylshikonin** | 399.1817 | 18.367 | Find By Formula | 398.1744 |

**Compound Chromatograms**




MS Zoomed Spectrum

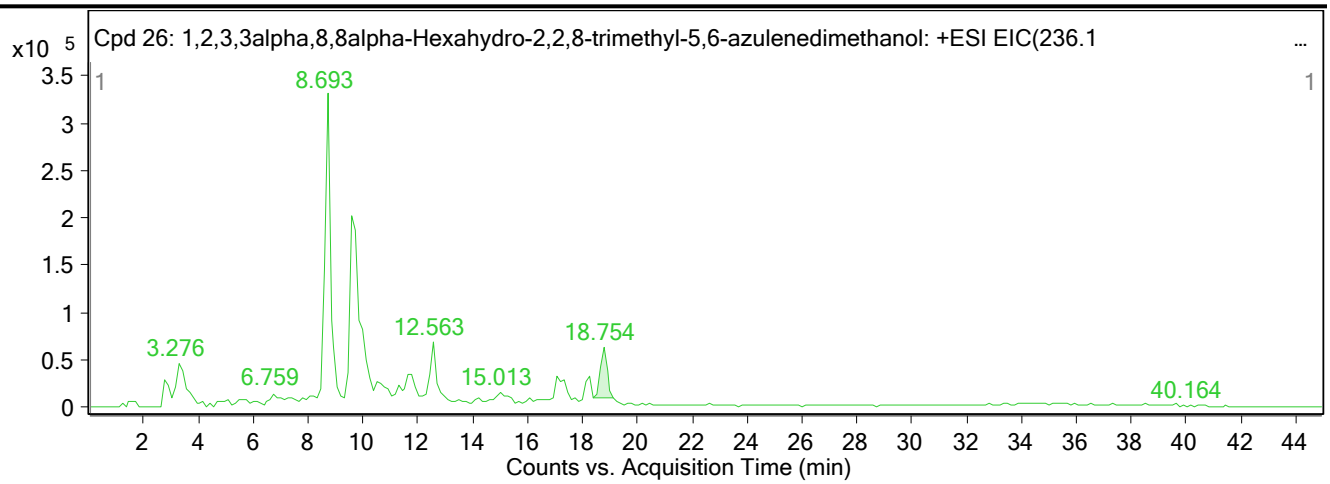



**MS Spectrum Peak List**

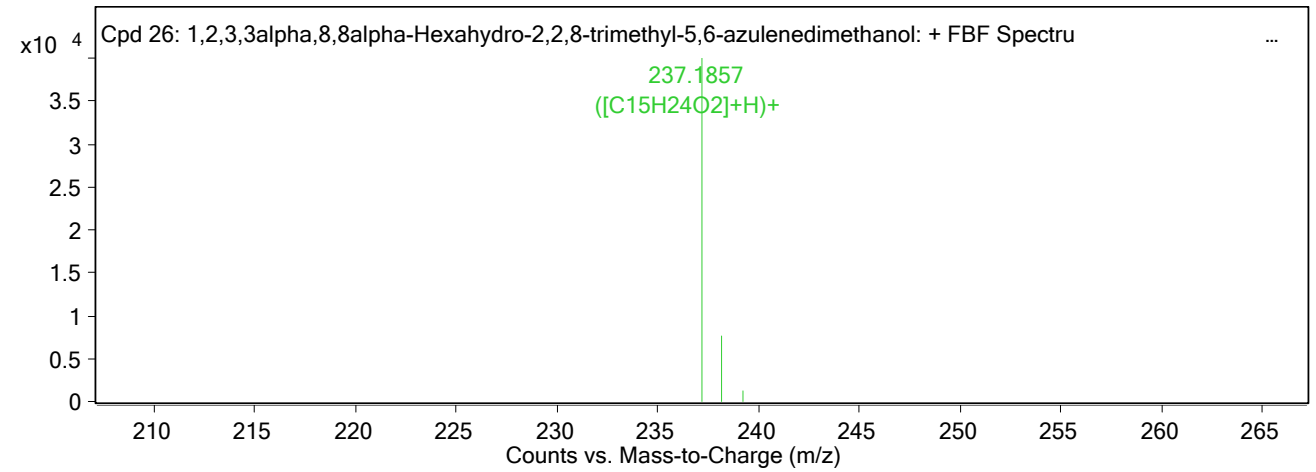
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 399.1817 | 1 | 101518.63 | C23H26O6 | (M+H)+ |
| 400.1848 | 1 | 25163.98 | C23H26O6 | (M+H)+ |
| 401.188 | 1 | 5362.9 | C23H26O6 | (M+H)+ |
| 402.2052 | 1 | 382.17 | C23H26O6 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 26: 1,2,3,3alpha,8,8alpha-Hexahydro-2,2,8-trimethyl-5,6-azulenedimethanol | **1,2,3,3alpha,8,8alpha-Hexahydro-2,2,8-trimethyl-5,6-azulenedimethanol** | 237.1857 | 18.754 | Find By Formula | 236.1785 |

**Compound Chromatograms**




MS Zoomed Spectrum

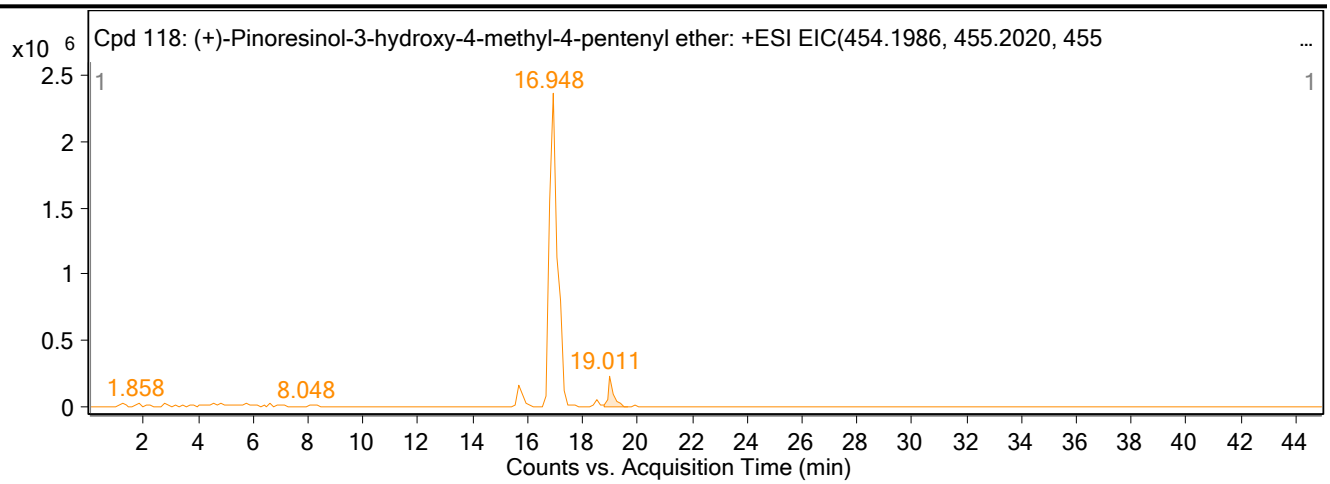



**MS Spectrum Peak List**

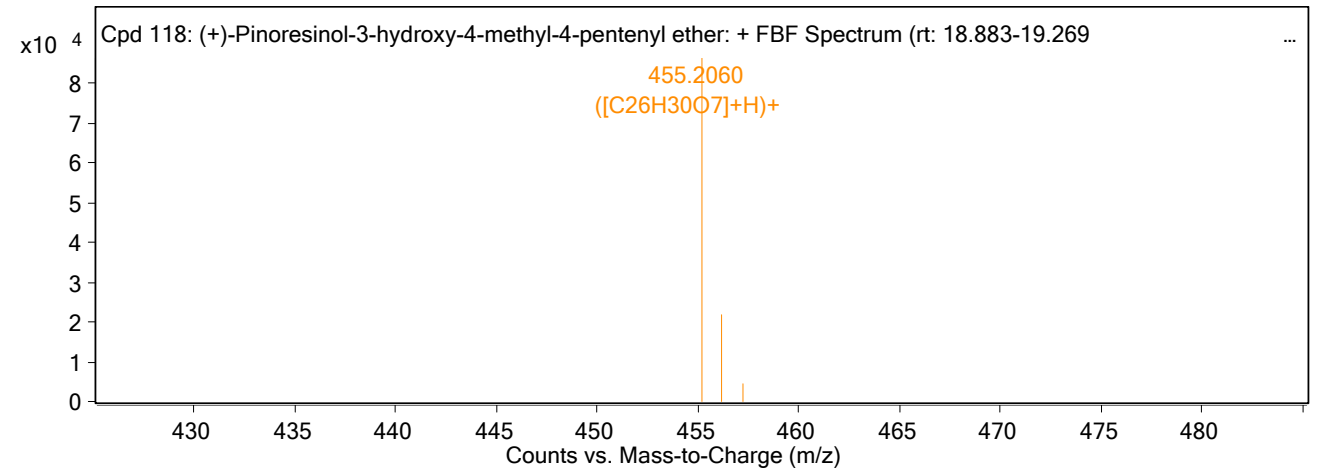
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 237.1857 | 1 | 40039.75 | C15H24O2 | (M+H)+ |
| 238.1891 | 1 | 7702.27 | C15H24O2 | (M+H)+ |
| 239.1972 | 1 | 1177.66 | C15H24O2 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 118: (+)-Pinoresinol-3-hydroxy-4-methyl-4-pentenyl ether | **(+)-Pinoresinol-3-hydroxy-4-methyl-4-pentenyl ether** | 455.206 | 19.011 | Find By Formula | 454.1987 |

**Compound Chromatograms**




MS Zoomed Spectrum

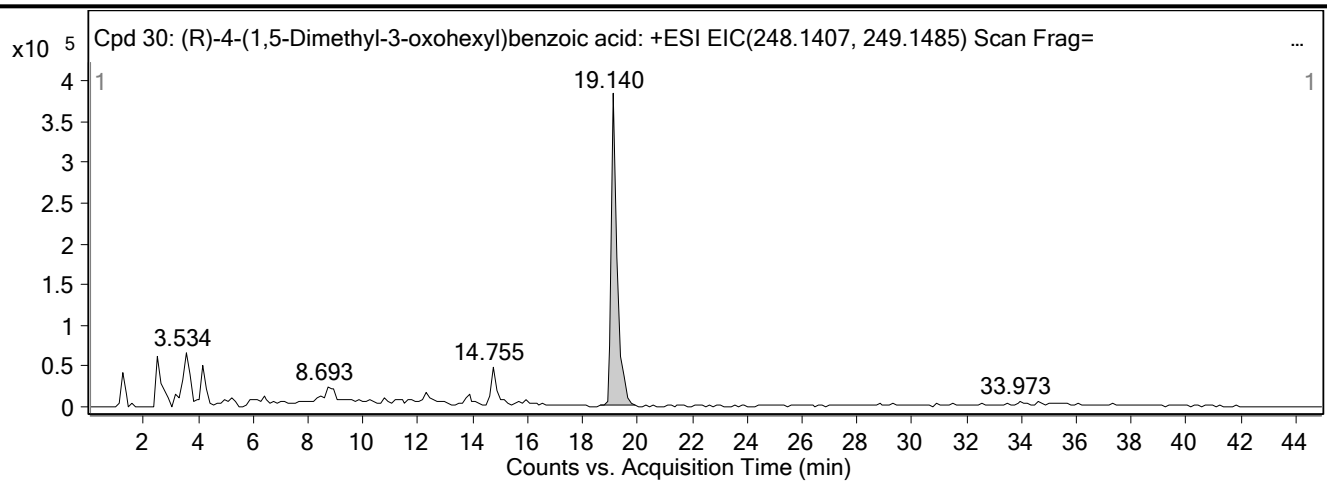



**MS Spectrum Peak List**

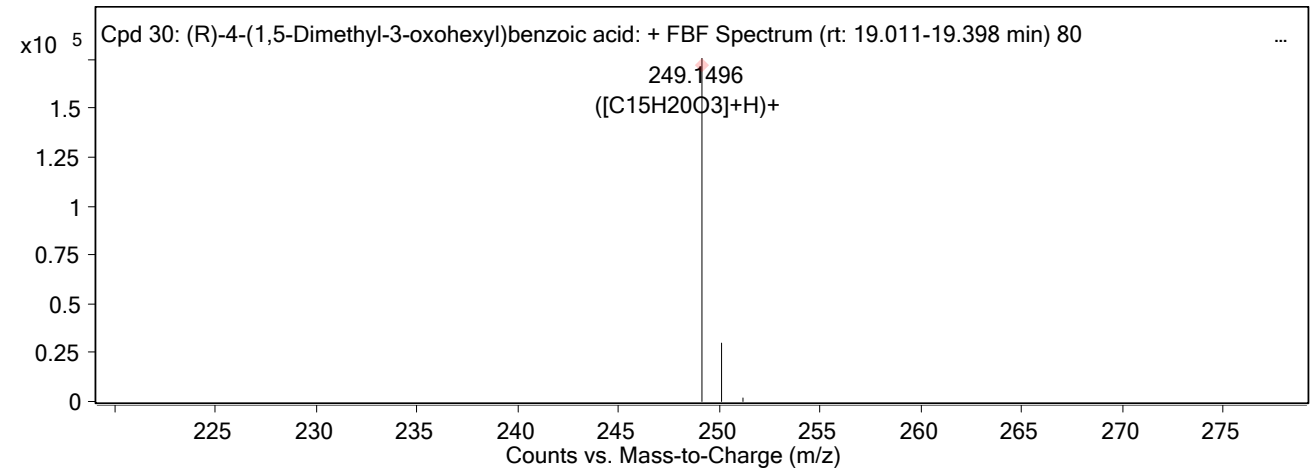
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 455.206 | 1 | 86256.23 | C26H30O7 | (M+H)+ |
| 456.2093 | 1 | 21850.13 | C26H30O7 | (M+H)+ |
| 457.2122 | 1 | 4330.15 | C26H30O7 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 30: (R)-4-(1,5-Dimethyl-3-oxohexyl)benzoic acid | **(R)-4-(1,5-Dimethyl-3-oxohexyl)benzoic acid** | 249.1496 | 19.14 | Find By Formula | 248.1423 |

**Compound Chromatograms**




MS Zoomed Spectrum

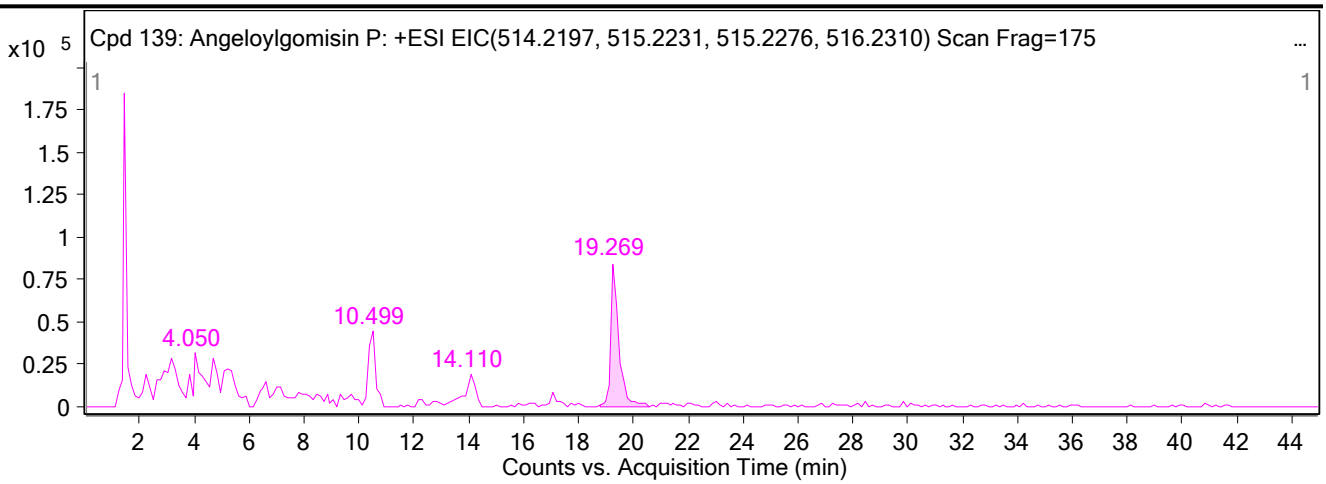



**MS Spectrum Peak List**

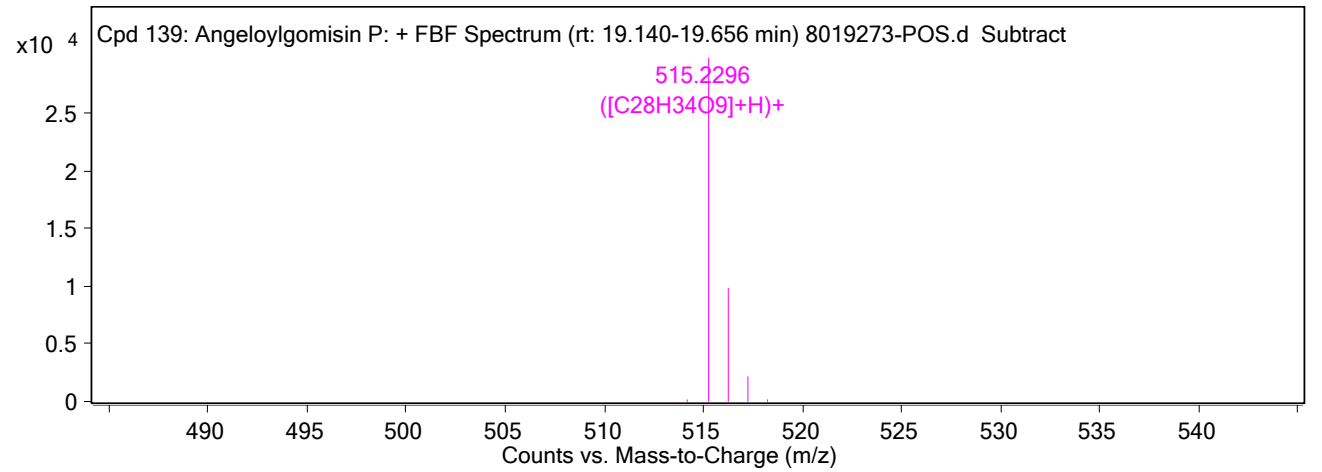
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 249.1496 | 1 | 175780.7 | C15H20O3 | (M+H)+ |
| 250.1523 | 1 | 30184.13 | C15H20O3 | (M+H)+ |
| 251.1583 | 1 | 2027.37 | C15H20O3 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 139: Angeloylgomisin P | **Angeloylgomisin P** | 515.2296 | 19.269 | Find By Formula | 514.2224 |

**Compound Chromatograms**




MS Zoomed Spectrum

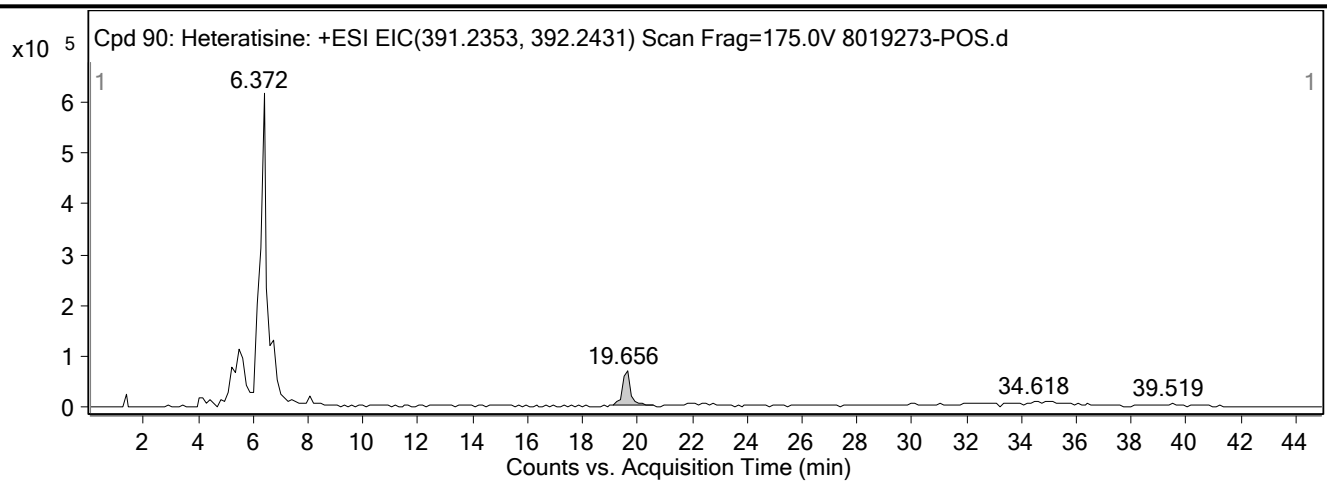



**MS Spectrum Peak List**

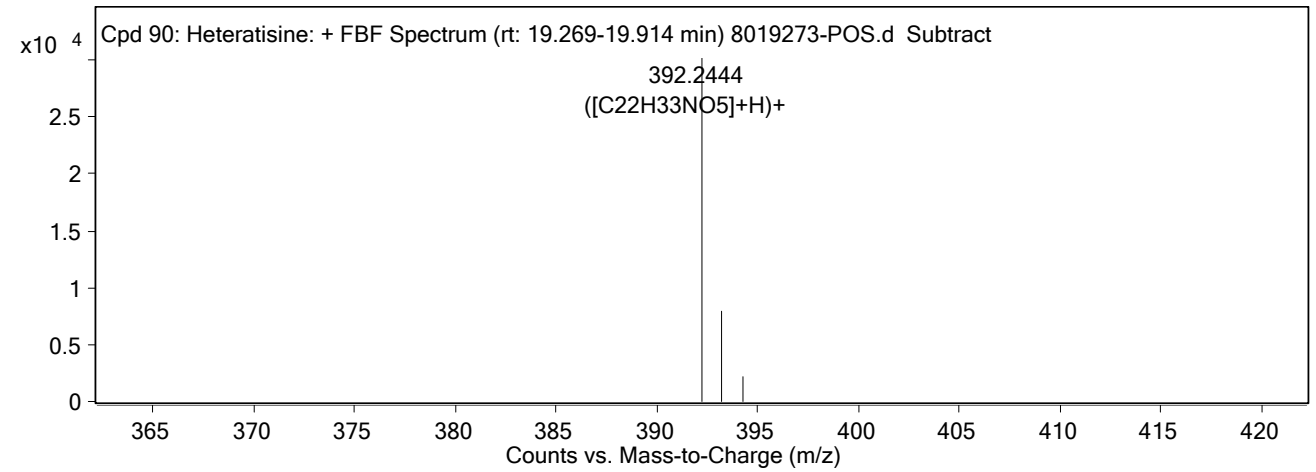
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 514.2099 | 1 | 117.14 | C28H34O9 | M+ |
| 515.2296 | 1 | 29806.95 | C28H34O9 | (M+H)+ |
| 516.2328 | 1 | 9805.28 | C28H34O9 | (M+H)+ |
| 517.2373 | 1 | 2233.2 | C28H34O9 | (M+H)+ |
| 518.2393 | 1 | 237.87 | C28H34O9 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 90: Heteratisine | **Heteratisine** | 392.2444 | 19.656 | Find By Formula | 391.237 |

**Compound Chromatograms**




MS Zoomed Spectrum

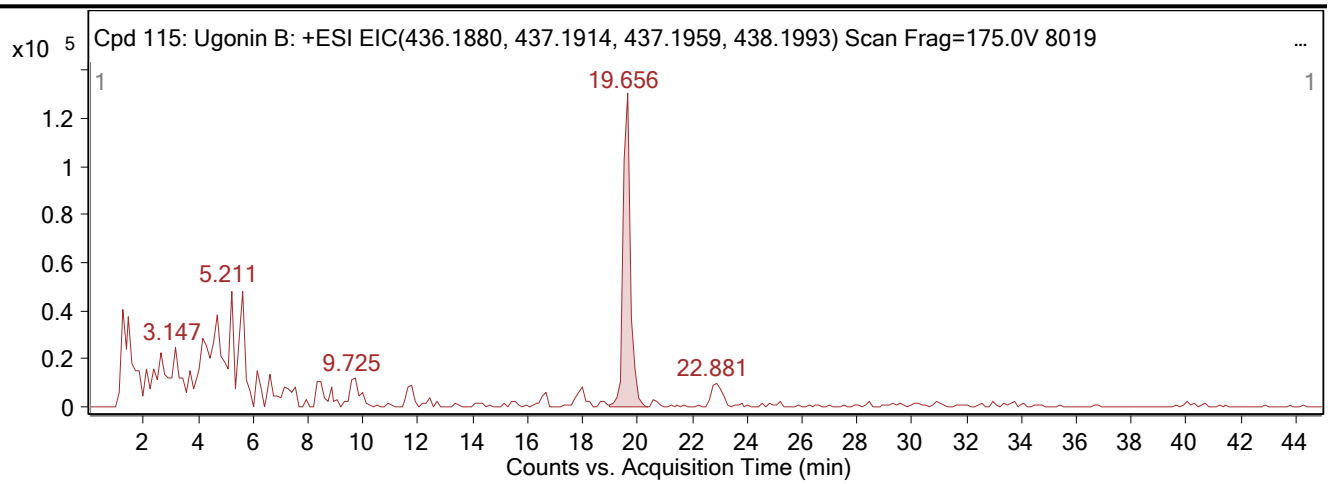



**MS Spectrum Peak List**

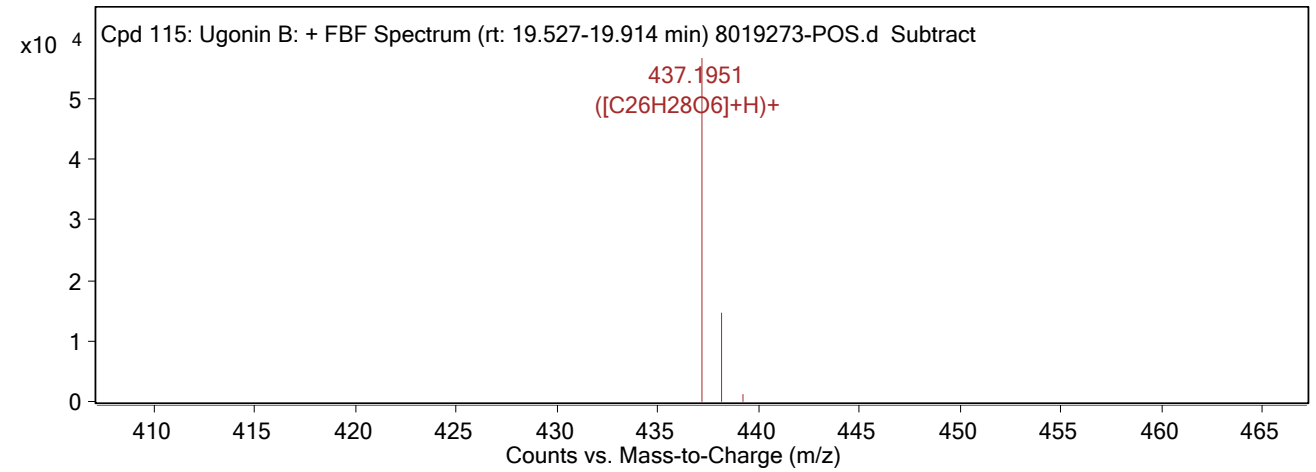
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 392.2444 | 1 | 30188.99 | C22H33NO5 | (M+H)+ |
| 393.2467 | 1 | 7876.78 | C22H33NO5 | (M+H)+ |
| 394.2509 | 1 | 2124.01 | C22H33NO5 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 115: Ugonin B | **Ugonin B** | 437.1951 | 19.656 | Find By Formula | 436.1878 |

**Compound Chromatograms**




MS Zoomed Spectrum

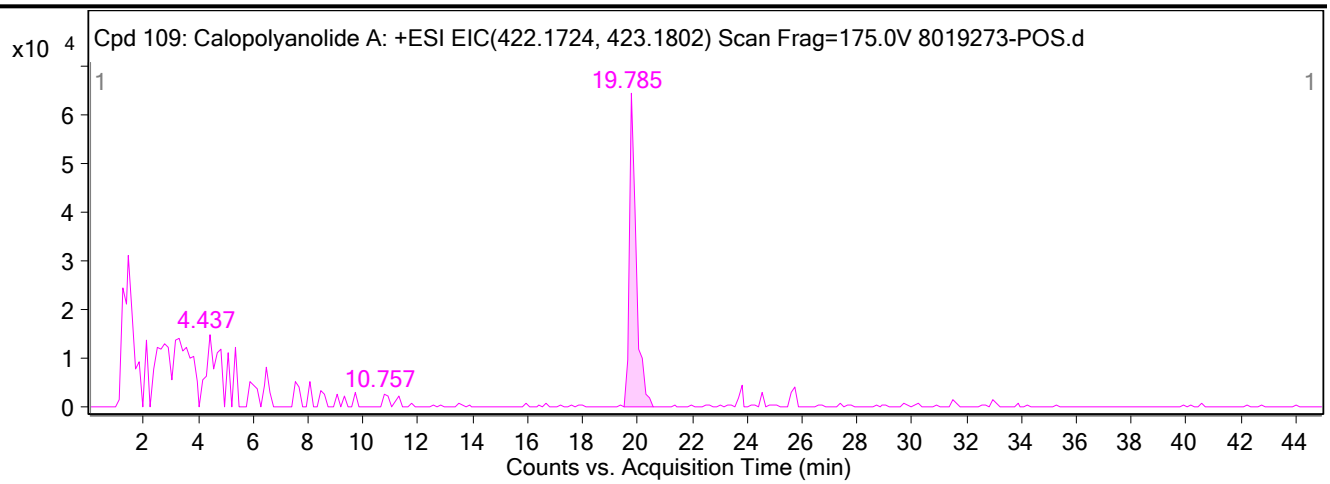



**MS Spectrum Peak List**

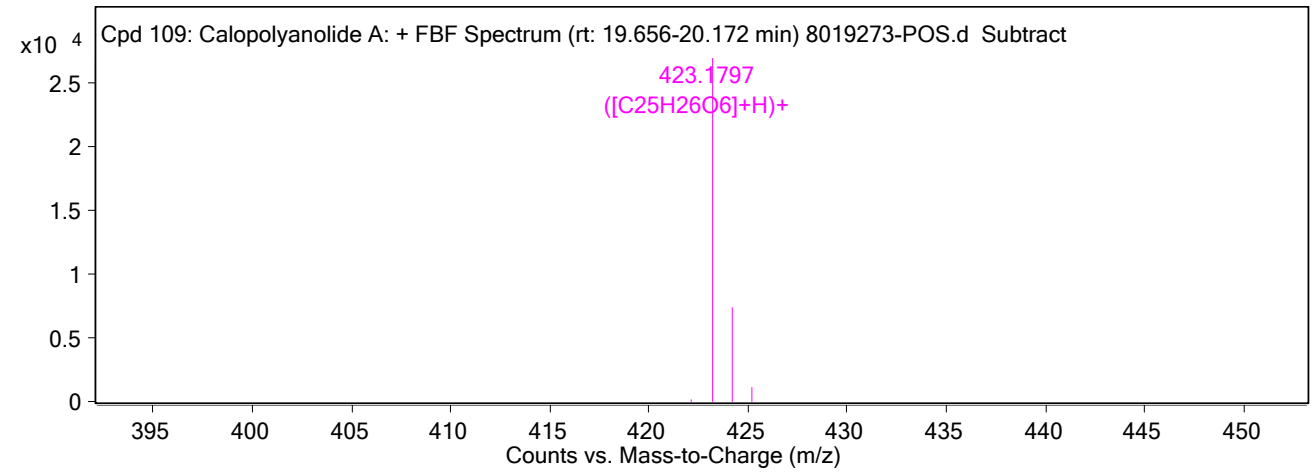
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 437.1951 | 1 | 56734.92 | C26H28O6 | (M+H)+ |
| 438.1984 | 1 | 14716.15 | C26H28O6 | (M+H)+ |
| 439.1975 | 1 | 1201.85 | C26H28O6 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 109: Calopolyanolide A | **Calopolyanolide A** | 423.1797 | 19.785 | Find By Formula | 422.1725 |

**Compound Chromatograms**




MS Zoomed Spectrum

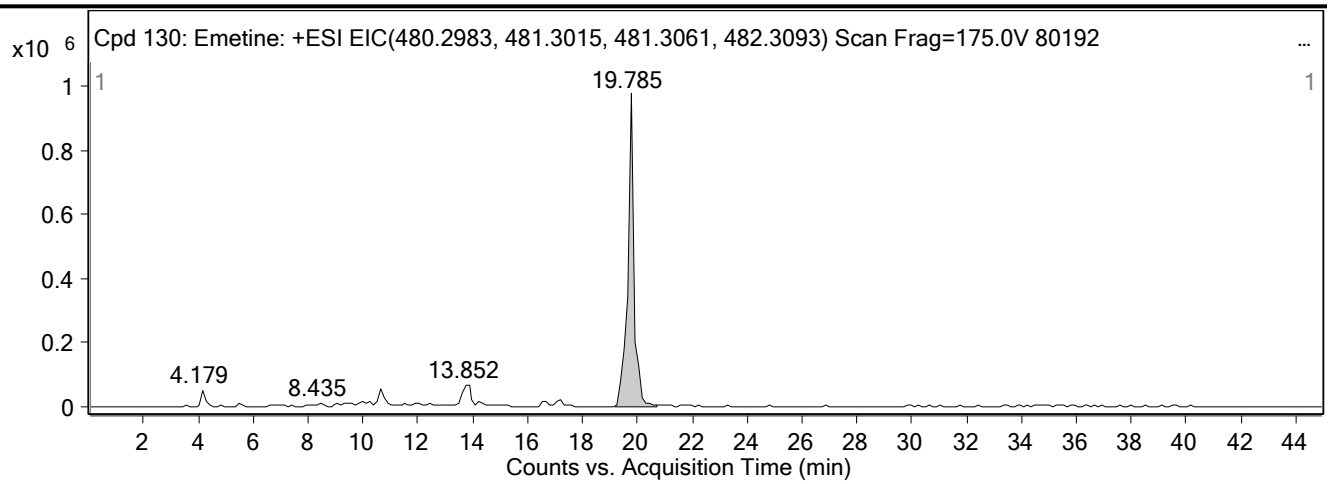



**MS Spectrum Peak List**

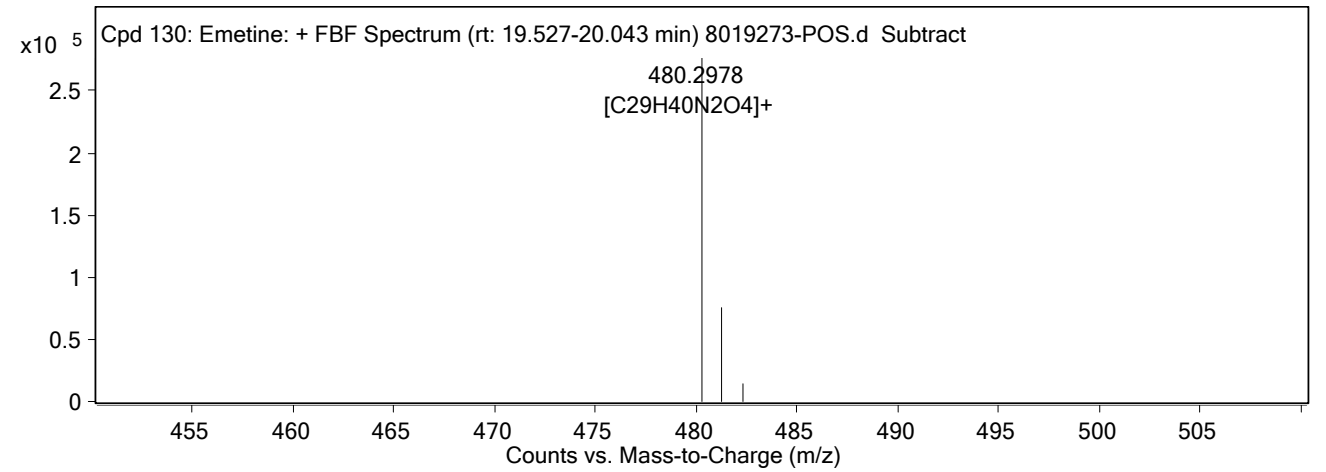
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 422.178 | 1 | 194.51 | C25H26O6 | M+ |
| 423.1797 | 1 | 26978.31 | C25H26O6 | (M+H)+ |
| 424.1833 | 1 | 7313.22 | C25H26O6 | (M+H)+ |
| 425.1854 | 1 | 1110.54 | C25H26O6 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 130: Emetine | **Emetine** | 480.2978 | 19.785 | Find By Formula | 480.2982 |

**Compound Chromatograms**




MS Zoomed Spectrum

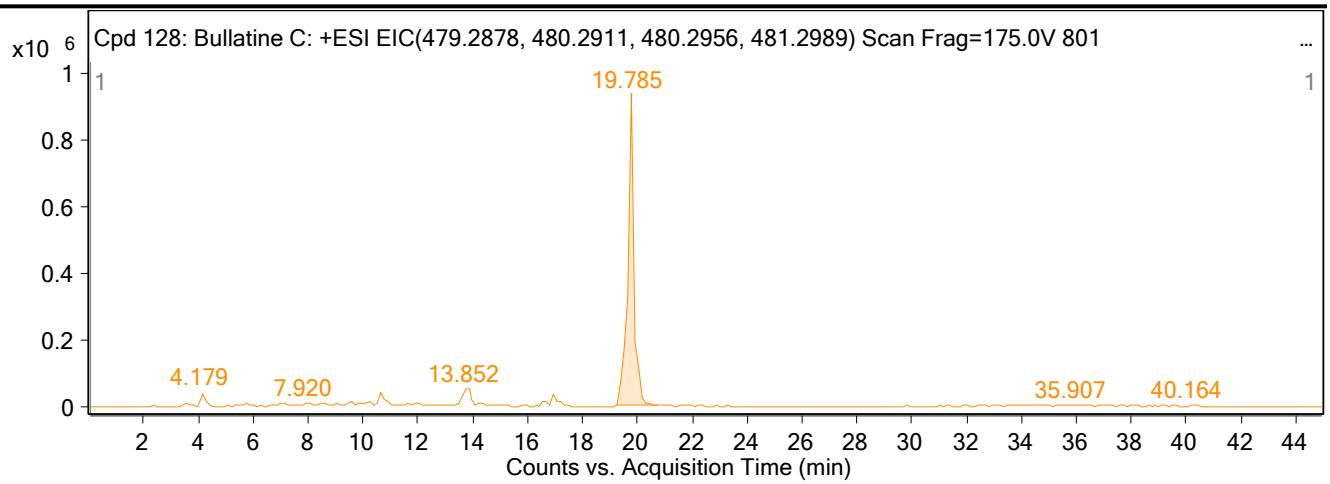



**MS Spectrum Peak List**

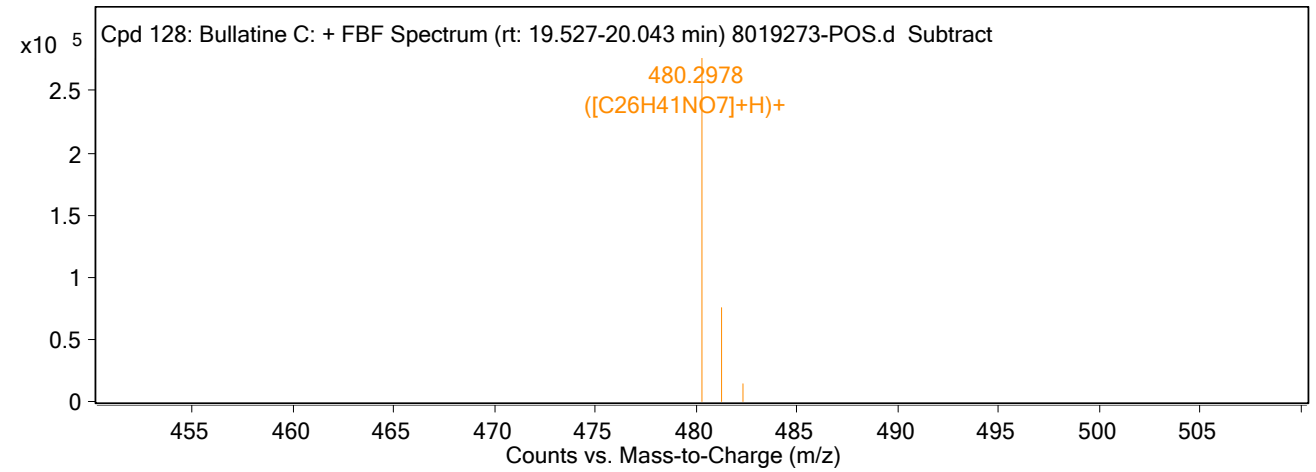
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 480.2978 | 1 | 276286.44 | C29H40N2O4 | M+ |
| 481.3007 | 1 | 75688.23 | C29H40N2O4 | M+ |
| 482.3032 | 1 | 14939.6 | C29H40N2O4 | M+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 128: Bullatine C | **Bullatine C** | 480.2978 | 19.785 | Find By Formula | 479.2904 |

**Compound Chromatograms**




MS Zoomed Spectrum

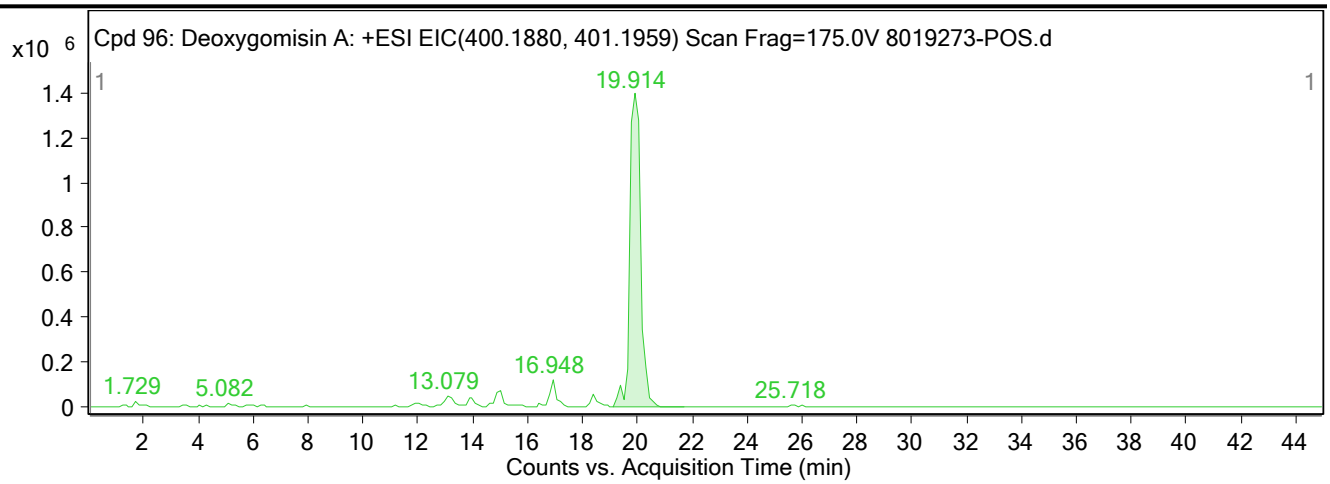



**MS Spectrum Peak List**

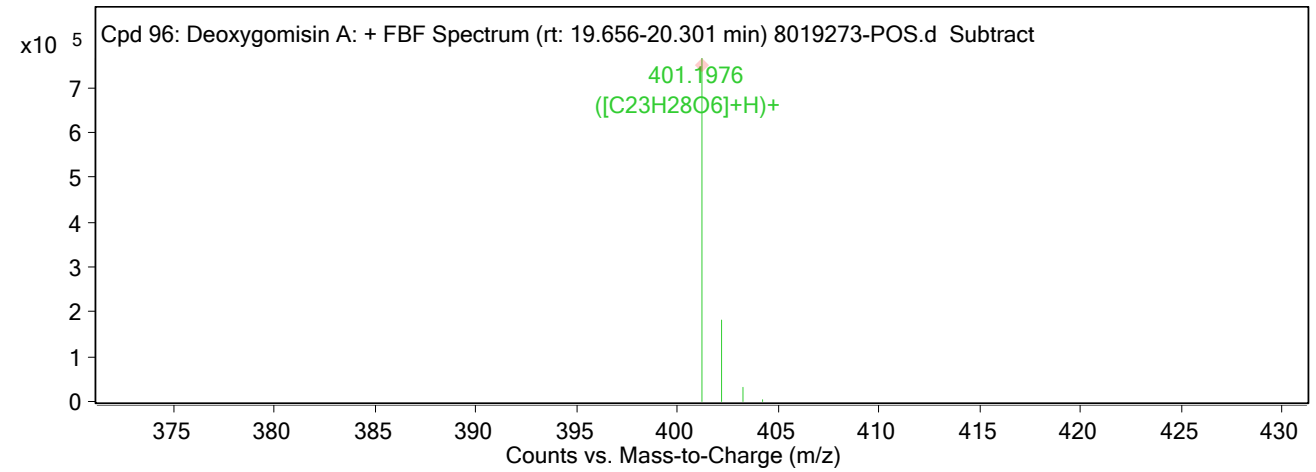
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 480.2978 | 1 | 276286.44 | C26H41NO7 | (M+H)+ |
| 481.3007 | 1 | 75688.23 | C26H41NO7 | (M+H)+ |
| 482.3032 | 1 | 14939.6 | C26H41NO7 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 96: Deoxygomisin A | **Deoxygomisin A** | 401.1976 | 19.914 | Find By Formula | 400.1903 |

**Compound Chromatograms**




MS Zoomed Spectrum

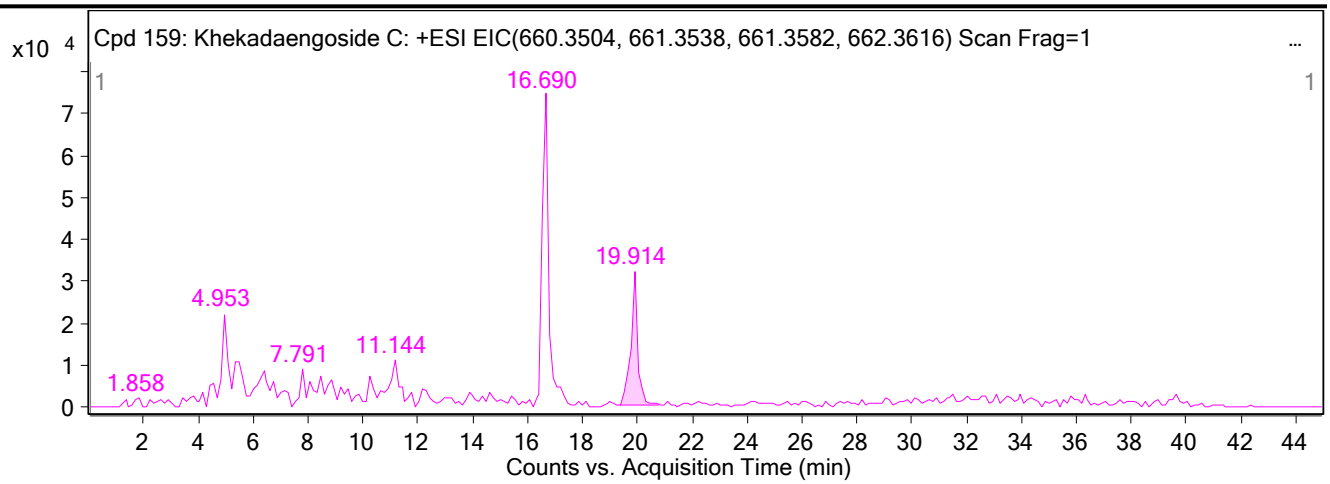



**MS Spectrum Peak List**

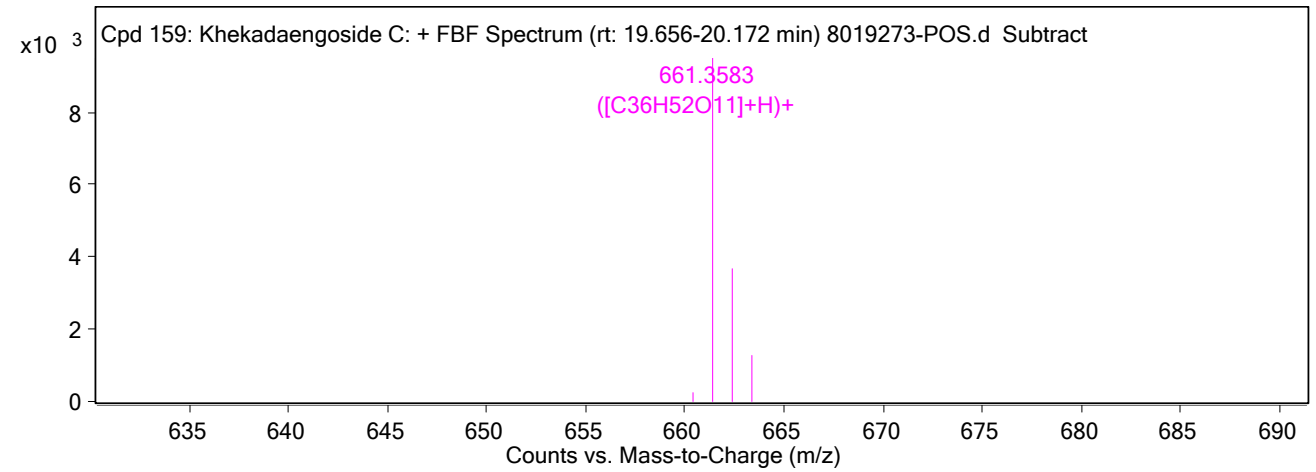
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 401.1976 | 1 | 765089 | C23H28O6 | (M+H)+ |
| 402.201 | 1 | 181489.13 | C23H28O6 | (M+H)+ |
| 403.2034 | 1 | 29929.22 | C23H28O6 | (M+H)+ |
| 404.2104 | 1 | 4773.13 | C23H28O6 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 159: Khekadaengoside C | **Khekadaengoside C** | 661.3583 | 19.914 | Find By Formula | 660.3511 |

**Compound Chromatograms**




MS Zoomed Spectrum

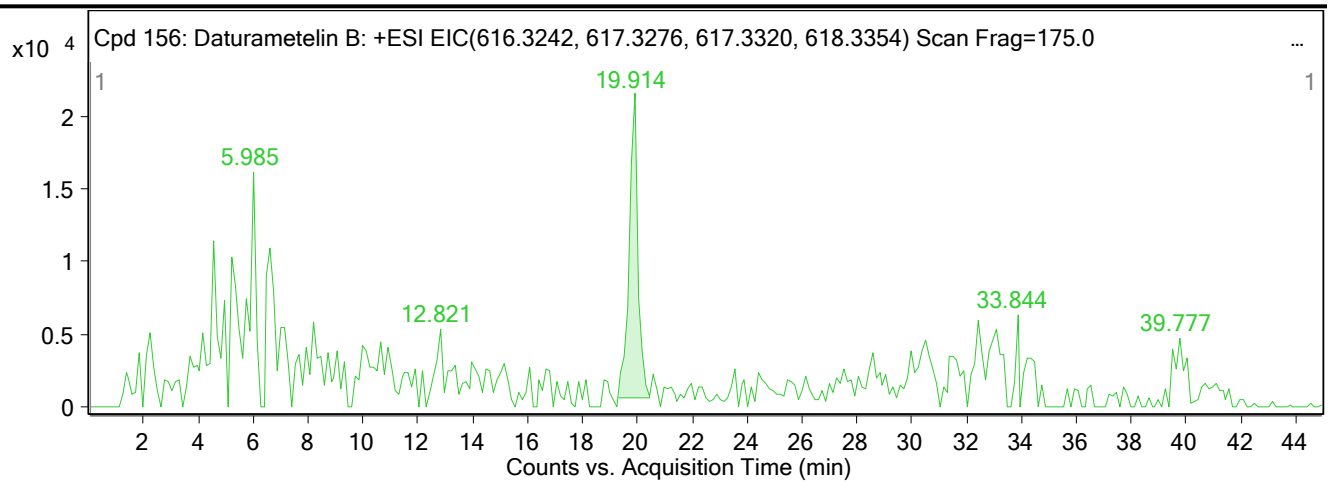



**MS Spectrum Peak List**

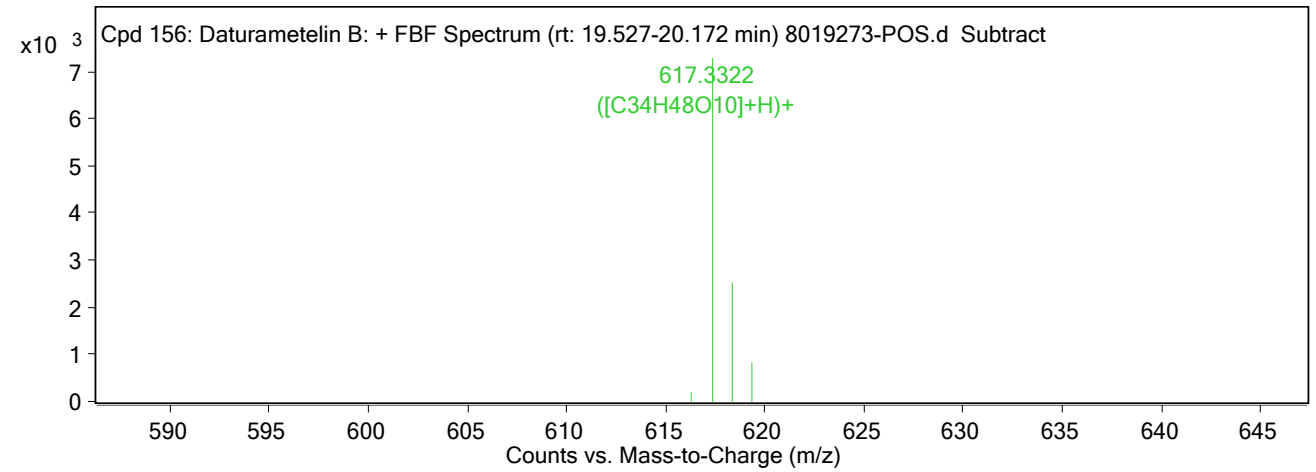
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 660.3631 | 1 | 228.87 | C36H52O11 | M+ |
| 661.3583 | 1 | 9496.53 | C36H52O11 | (M+H)+ |
| 662.3617 | 1 | 3668.79 | C36H52O11 | (M+H)+ |
| 663.3635 | 1 | 1289.19 | C36H52O11 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 156: Daturametelin B | **Daturametelin B** | 617.3322 | 19.914 | Find By Formula | 616.3253 |

**Compound Chromatograms**




MS Zoomed Spectrum

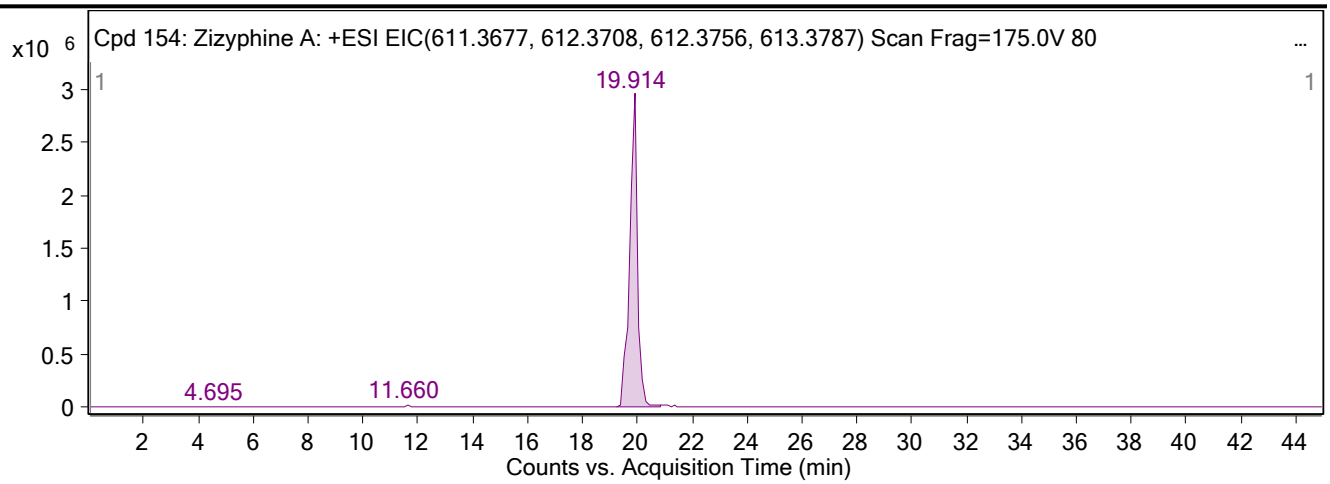



**MS Spectrum Peak List**

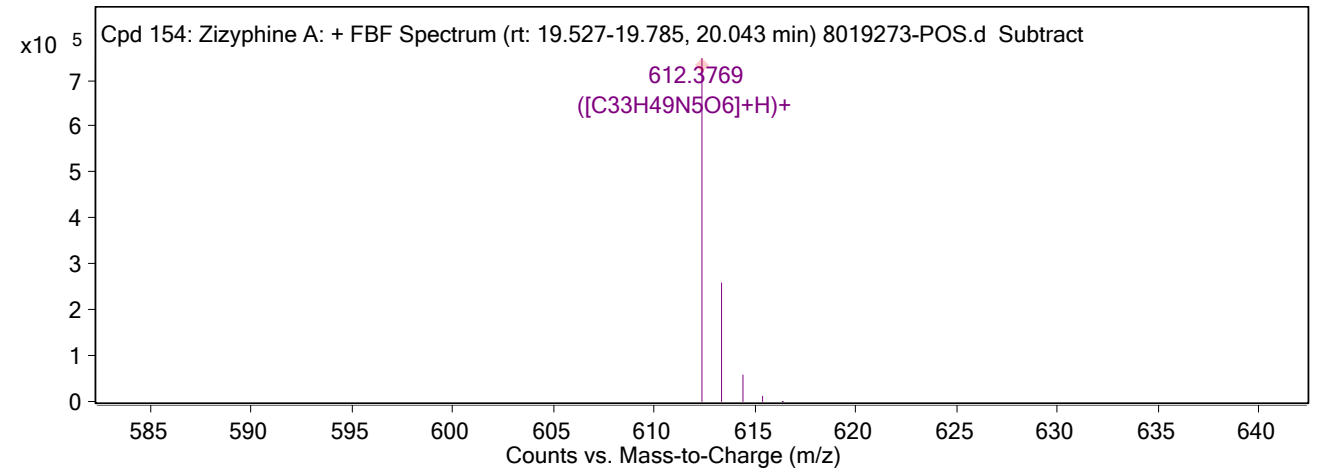
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 616.3255 | 1 | 198.6 | C34H48O10 | M+ |
| 617.3322 | 1 | 7283.35 | C34H48O10 | (M+H)+ |
| 618.3373 | 1 | 2509.39 | C34H48O10 | (M+H)+ |
| 619.3384 | 1 | 830.8 | C34H48O10 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 154: Zizyphine A | **Zizyphine A** | 612.3769 | 19.914 | Find By Formula | 611.3696 |

**Compound Chromatograms**




MS Zoomed Spectrum

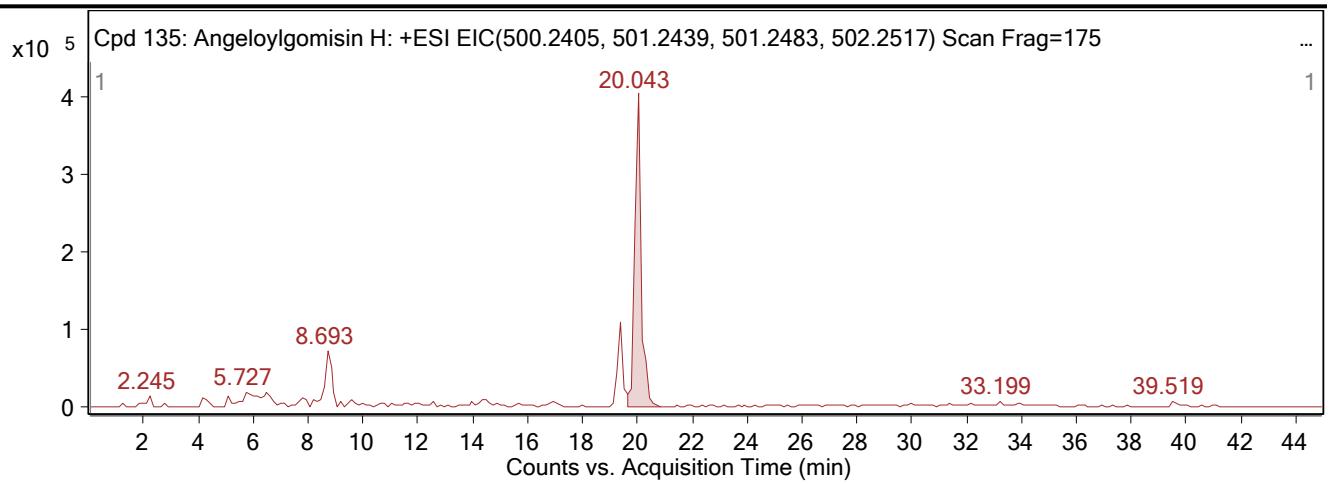



**MS Spectrum Peak List**

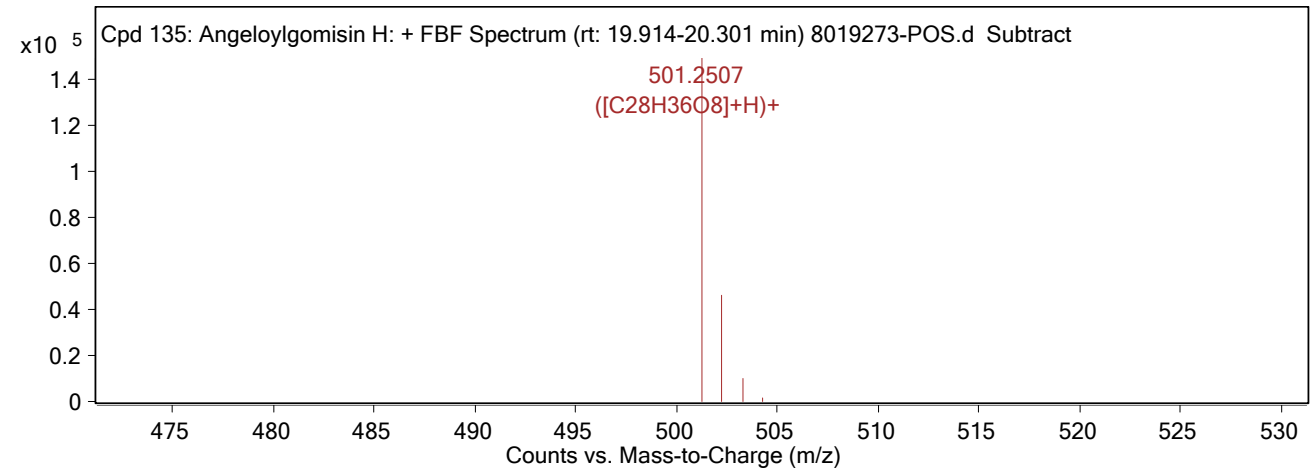
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 612.3769 | 1 | 748331.13 | C33H49N5O6 | (M+H)+ |
| 613.3803 | 1 | 260490.69 | C33H49N5O6 | (M+H)+ |
| 614.3826 | 1 | 56470.95 | C33H49N5O6 | (M+H)+ |
| 615.3843 | 1 | 10299.12 | C33H49N5O6 | (M+H)+ |
| 616.3823 | 1 | 1668.37 | C33H49N5O6 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 135: Angeloylgomisin H | **Angeloylgomisin H** | 501.2507 | 20.043 | Find By Formula | 500.2433 |

**Compound Chromatograms**




MS Zoomed Spectrum

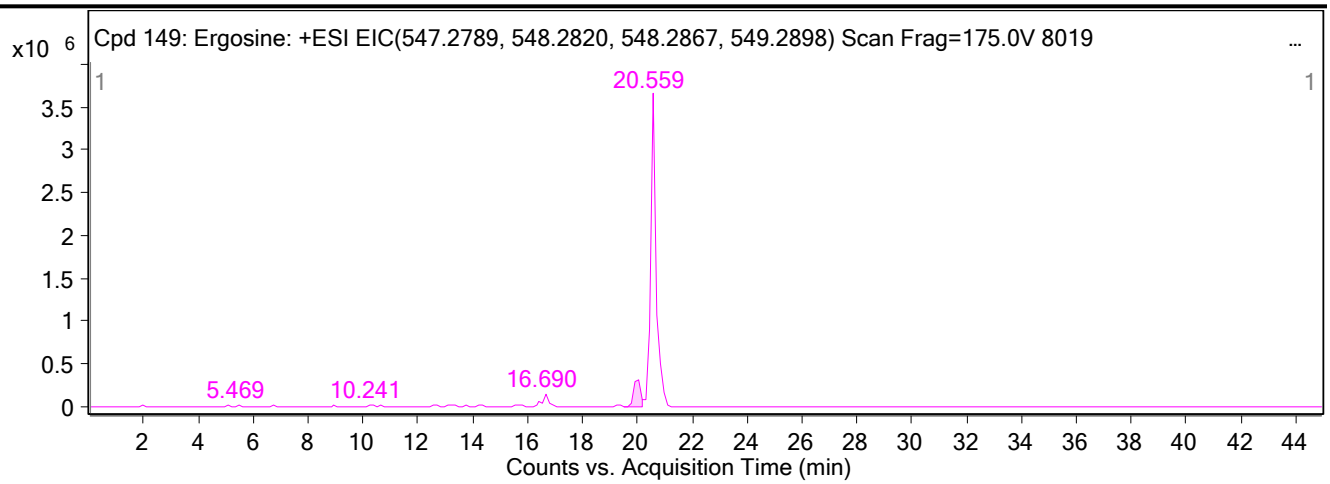



**MS Spectrum Peak List**

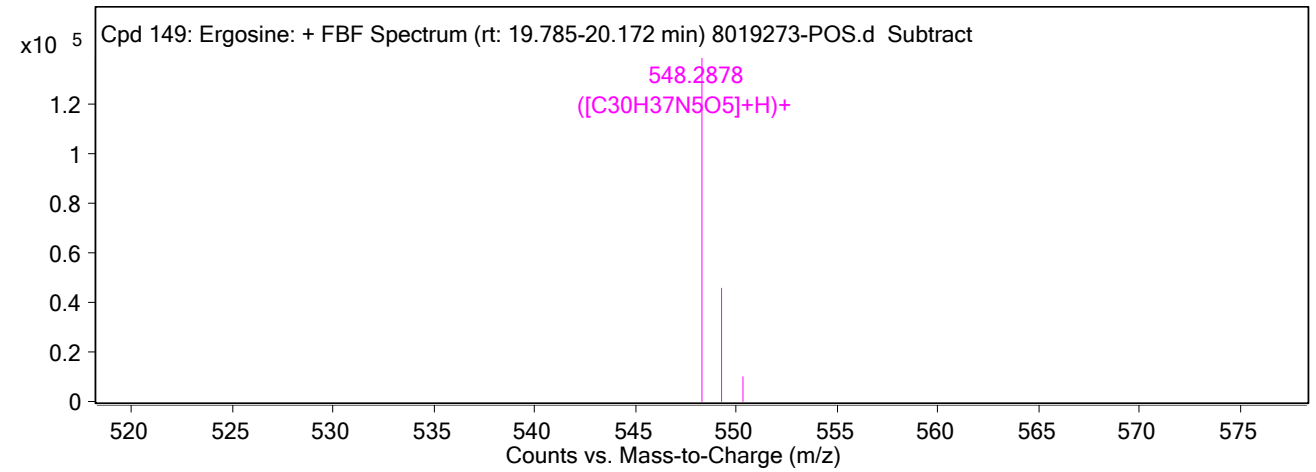
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 501.2507 | 1 | 149594.72 | C28H36O8 | (M+H)+ |
| 502.2537 | 1 | 46034.13 | C28H36O8 | (M+H)+ |
| 503.257 | 1 | 9930.25 | C28H36O8 | (M+H)+ |
| 504.2595 | 1 | 1580.7 | C28H36O8 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 149: Ergosine | **Ergosine** | 548.2878 | 20.043 | Find By Formula | 547.2805 |

**Compound Chromatograms**




MS Zoomed Spectrum

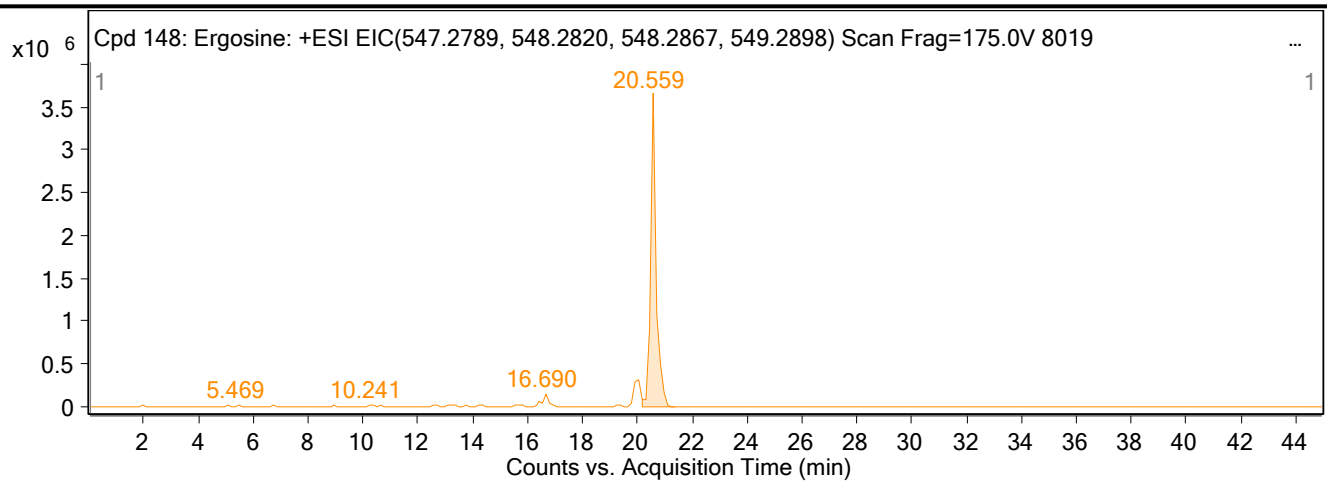



**MS Spectrum Peak List**

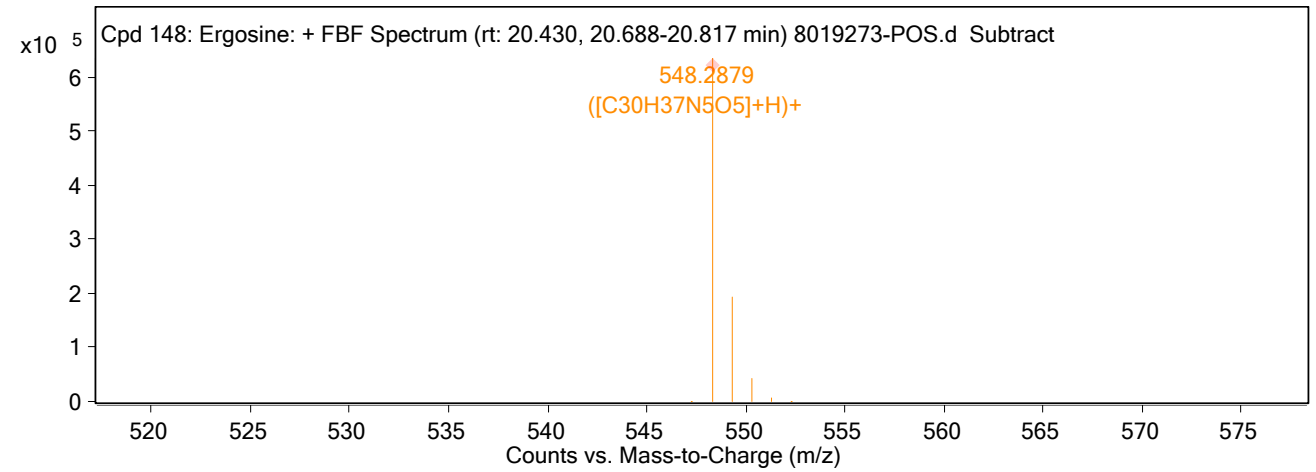
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 548.2878 | 1 | 138343.36 | C30H37N5O5 | (M+H)+ |
| 549.2908 | 1 | 45391.89 | C30H37N5O5 | (M+H)+ |
| 550.2928 | 1 | 9964.2 | C30H37N5O5 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 148: Ergosine | **Ergosine** | 548.2879 | 20.559 | Find By Formula | 547.2806 |

**Compound Chromatograms**




MS Zoomed Spectrum

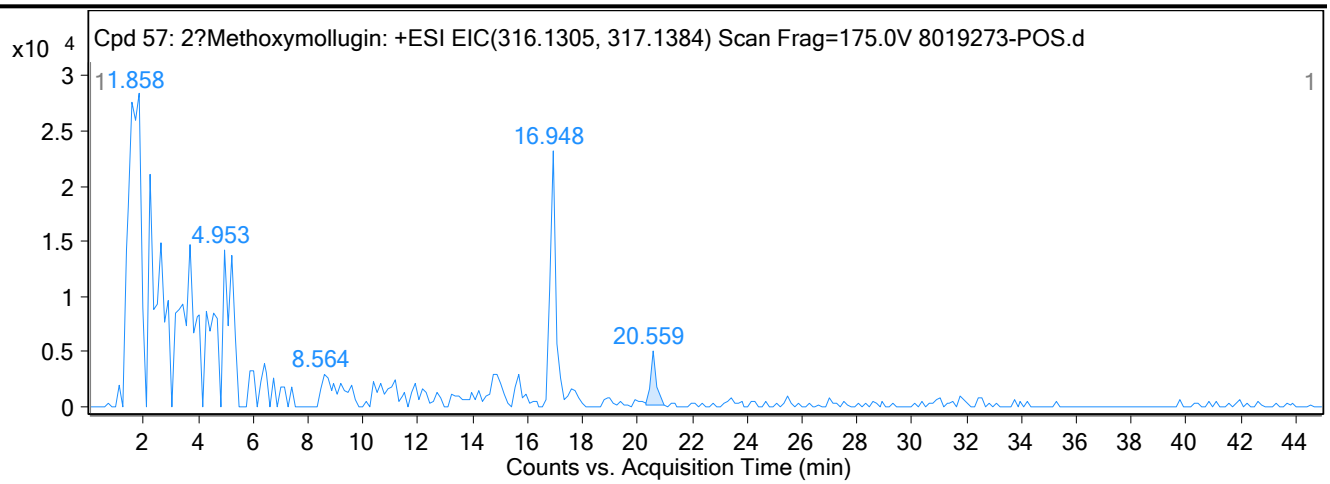



**MS Spectrum Peak List**

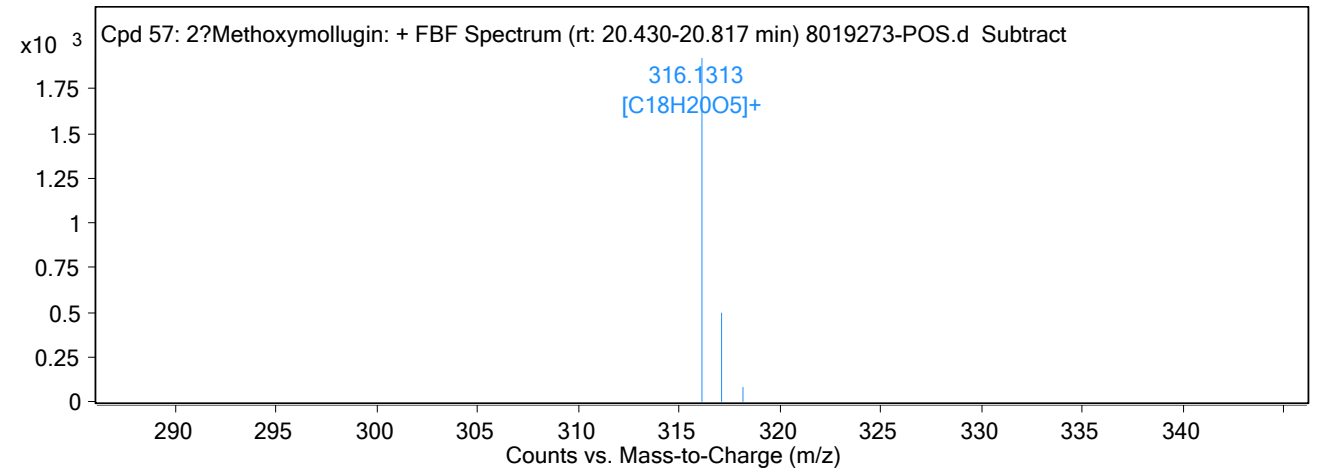
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 547.2749 | 1 | 220.01 | C30H37N5O5 | M+ |
| 548.2879 | 1 | 635076.56 | C30H37N5O5 | (M+H)+ |
| 549.2912 | 1 | 194628.19 | C30H37N5O5 | (M+H)+ |
| 550.2938 | 1 | 41192.07 | C30H37N5O5 | (M+H)+ |
| 551.2958 | 1 | 6602.94 | C30H37N5O5 | (M+H)+ |
| 552.2961 | 1 | 1072.49 | C30H37N5O5 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 57: 2?Methoxymollugin | **2?Methoxymollugin** | 316.1313 | 20.559 | Find By Formula | 316.1316 |

**Compound Chromatograms**




MS Zoomed Spectrum

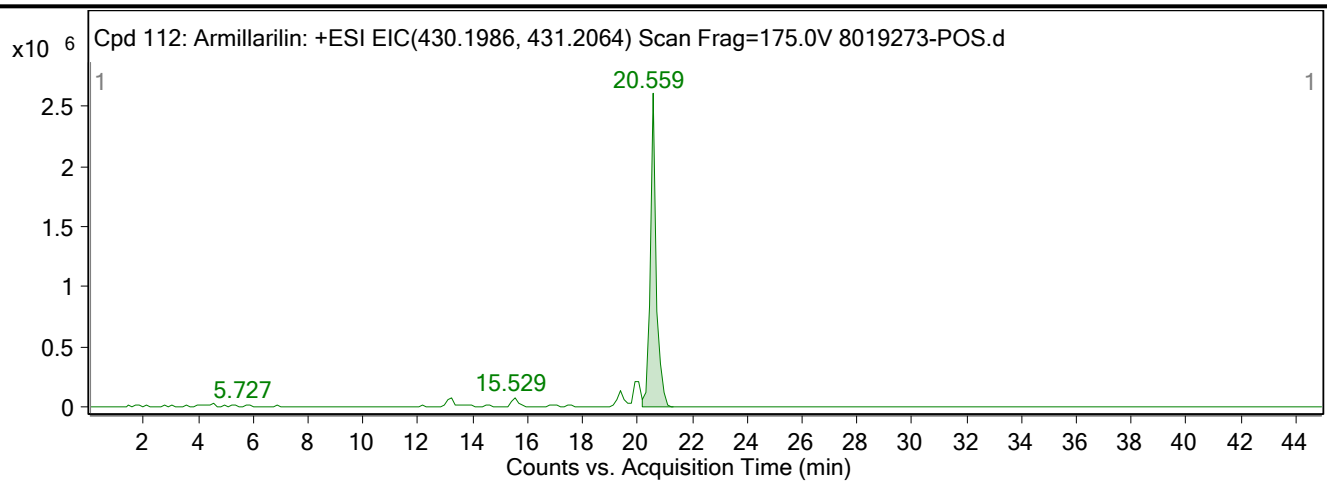



**MS Spectrum Peak List**

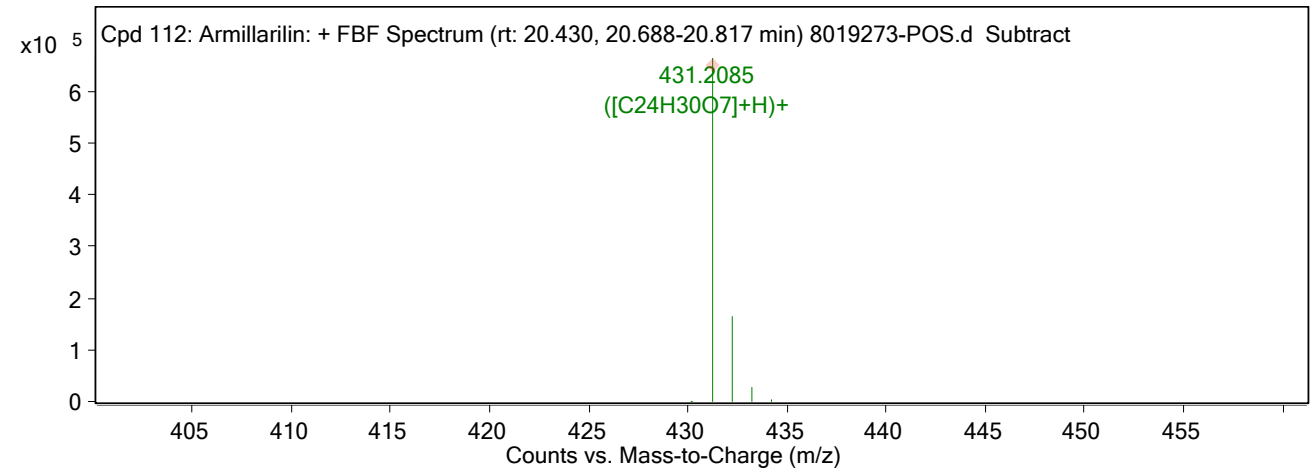
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 316.1313 | 1 | 1922.58 | C18H20O5 | M+ |
| 317.1334 | 1 | 492.42 | C18H20O5 | M+ |
| 318.1357 | 1 | 81.1 | C18H20O5 | M+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 112: Armillarilin | **Armillarilin** | 431.2085 | 20.559 | Find By Formula | 430.2011 |

**Compound Chromatograms**




MS Zoomed Spectrum

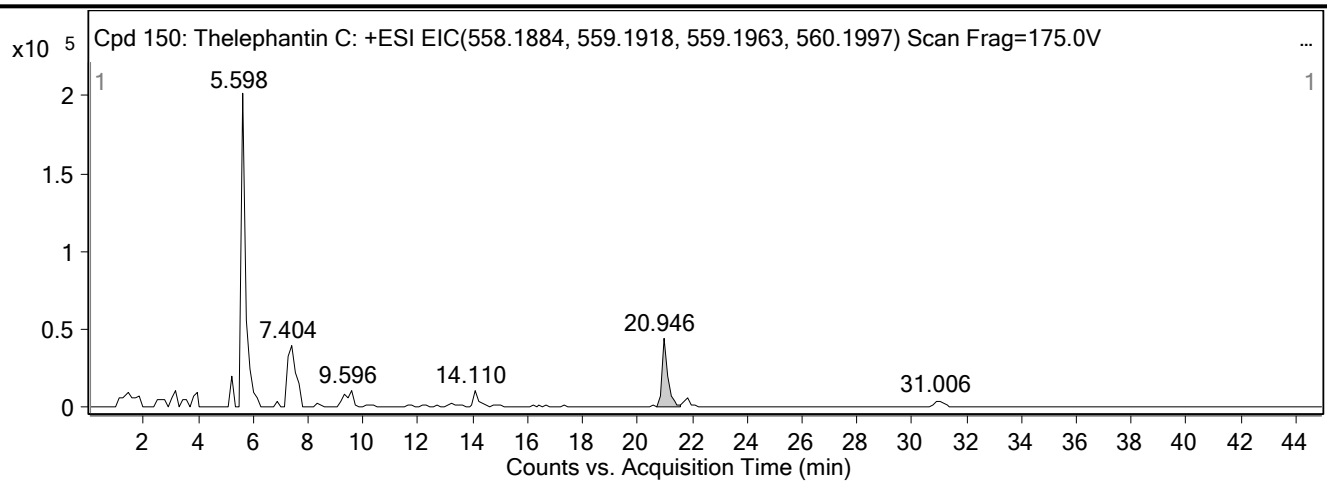



**MS Spectrum Peak List**

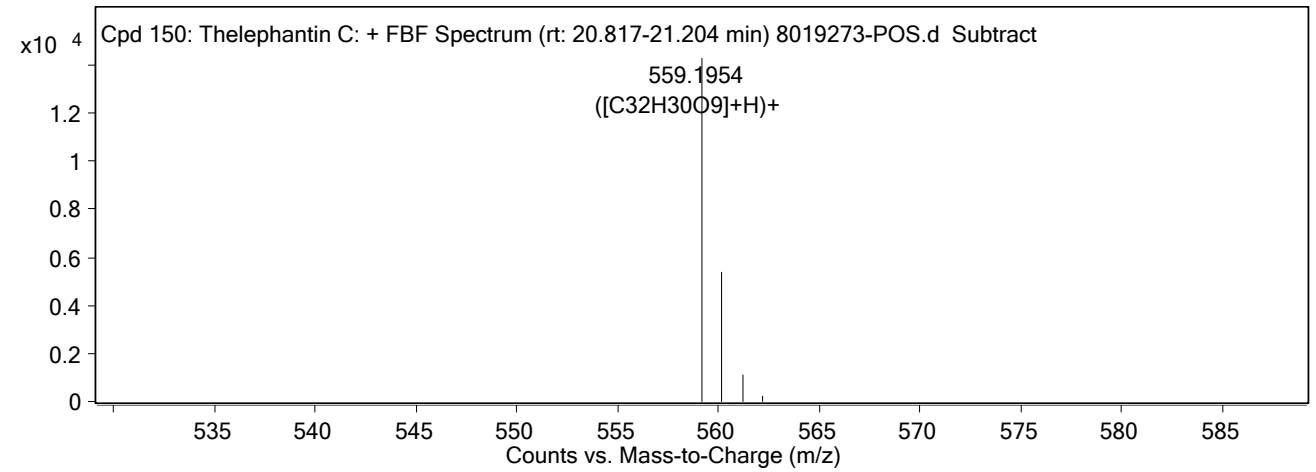
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 430.1972 | 1 | 261.05 | C24H30O7 | M+ |
| 431.2085 | 1 | 664452 | C24H30O7 | (M+H)+ |
| 432.2117 | 1 | 164041.8 | C24H30O7 | (M+H)+ |
| 433.2141 | 1 | 26836.26 | C24H30O7 | (M+H)+ |
| 434.2192 | 1 | 4300.02 | C24H30O7 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 150: Thelephantin C | **Thelephantin C** | 559.1954 | 20.946 | Find By Formula | 558.1879 |

**Compound Chromatograms**




MS Zoomed Spectrum

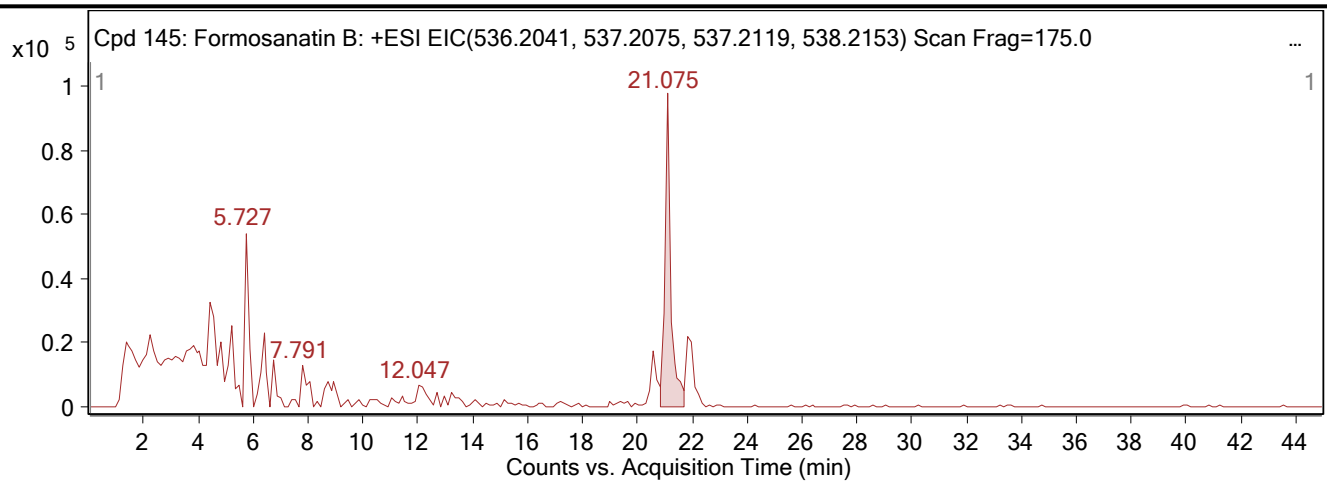



**MS Spectrum Peak List**

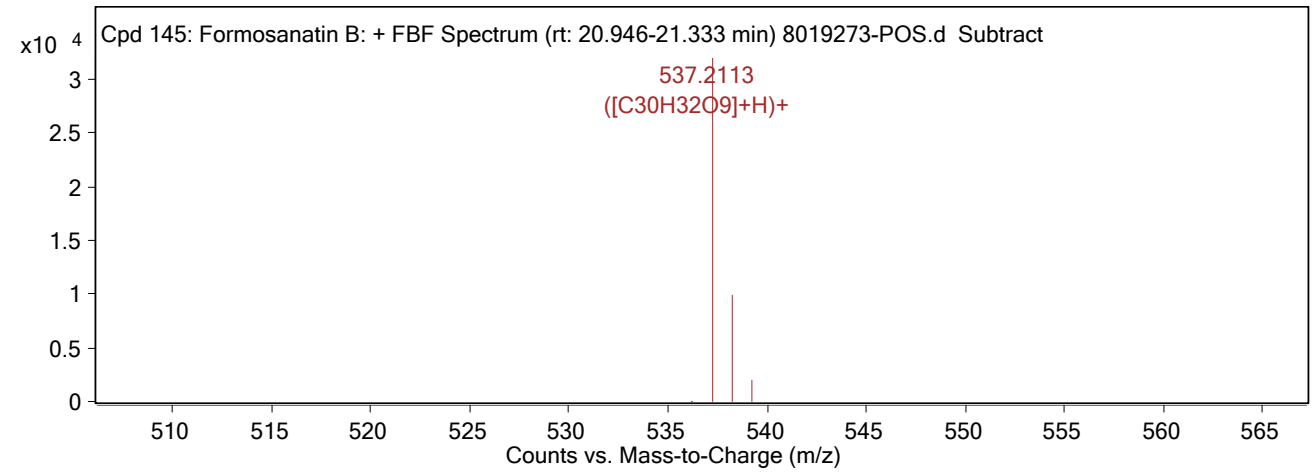
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 559.1954 | 1 | 14303.4 | C32H30O9 | (M+H)+ |
| 560.1984 | 1 | 5374.61 | C32H30O9 | (M+H)+ |
| 561.2014 | 1 | 1140.48 | C32H30O9 | (M+H)+ |
| 562.2003 | 1 | 236.98 | C32H30O9 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 145: Formosanatin B | **Formosanatin B** | 537.2113 | 21.075 | Find By Formula | 536.2041 |

**Compound Chromatograms**




MS Zoomed Spectrum

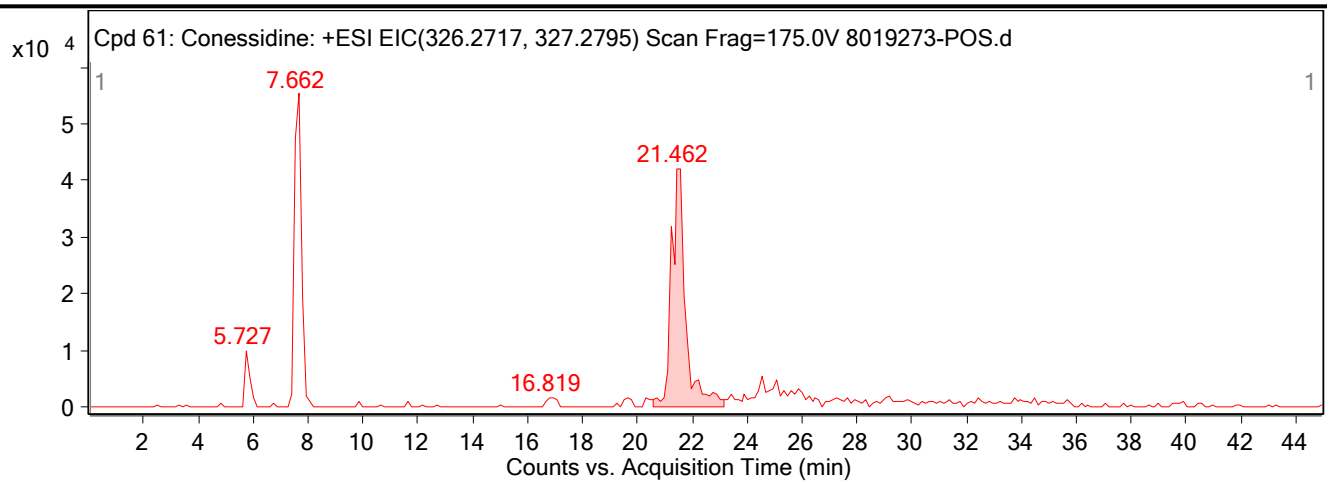



**MS Spectrum Peak List**

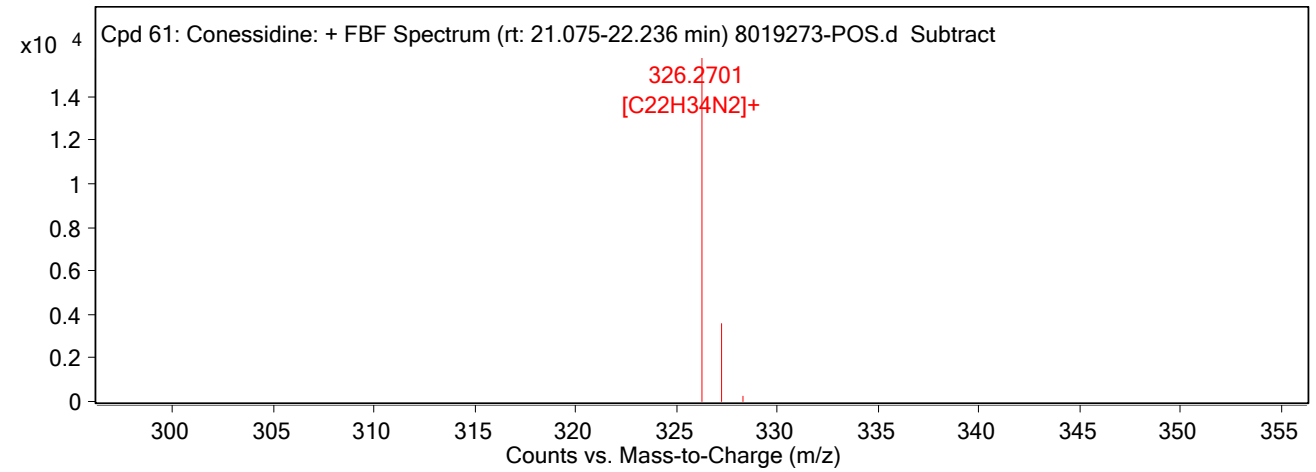
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 536.2083 | 1 | 67.18 | C30H32O9 | M+ |
| 537.2113 | 1 | 31940.29 | C30H32O9 | (M+H)+ |
| 538.2145 | 1 | 9930.76 | C30H32O9 | (M+H)+ |
| 539.219 | 1 | 2006.9 | C30H32O9 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 61: Conessidine | **Conessidine** | 326.2701 | 21.462 | Find By Formula | 326.2707 |

**Compound Chromatograms**




MS Zoomed Spectrum

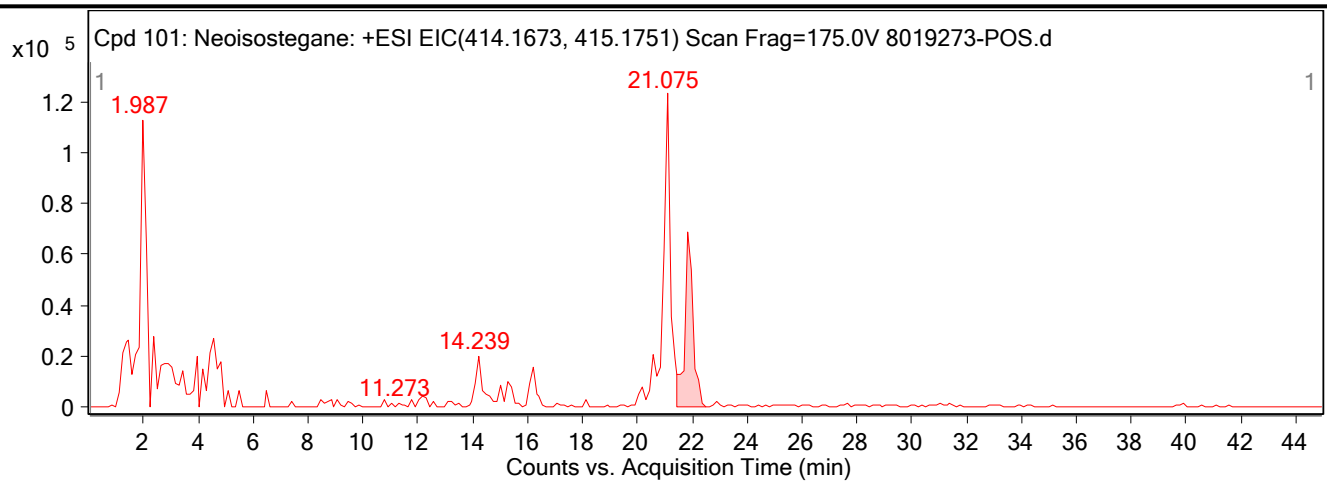



**MS Spectrum Peak List**

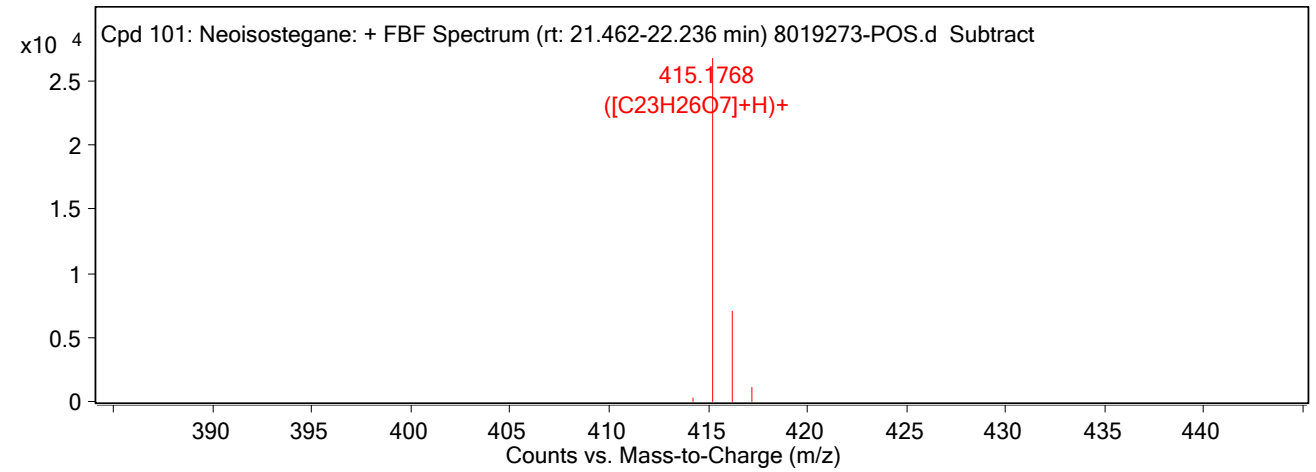
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 326.2701 | 1 | 15782.29 | C22H34N2 | M+ |
| 327.2731 | 1 | 3587.06 | C22H34N2 | M+ |
| 328.279 | 1 | 255.91 | C22H34N2 | M+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 101: Neoisostegane | **Neoisostegane** | 415.1768 | 21.849 | Find By Formula | 414.1696 |

**Compound Chromatograms**




MS Zoomed Spectrum

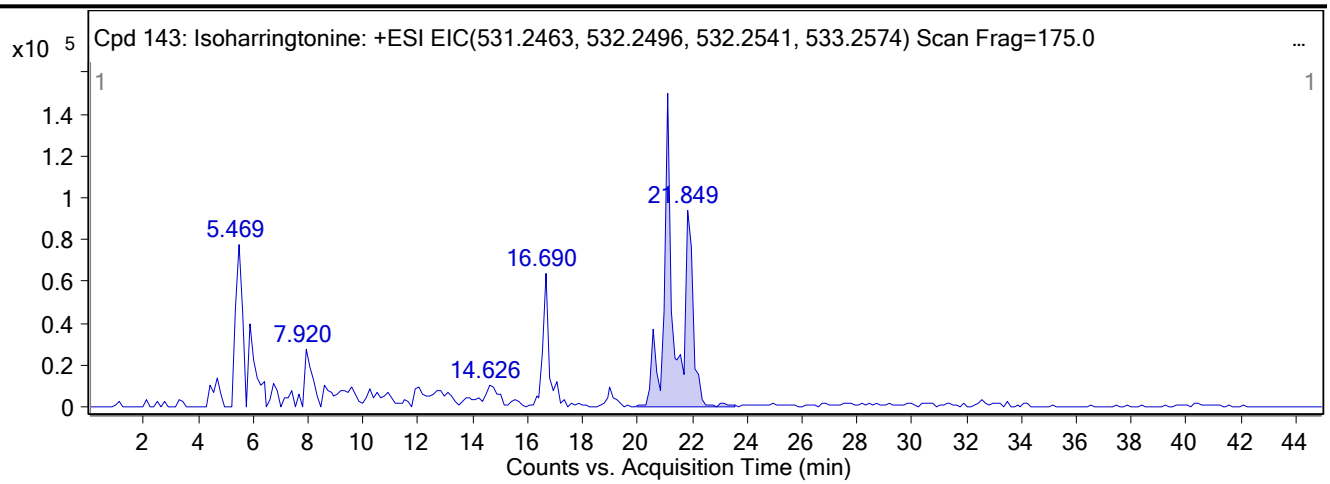



**MS Spectrum Peak List**

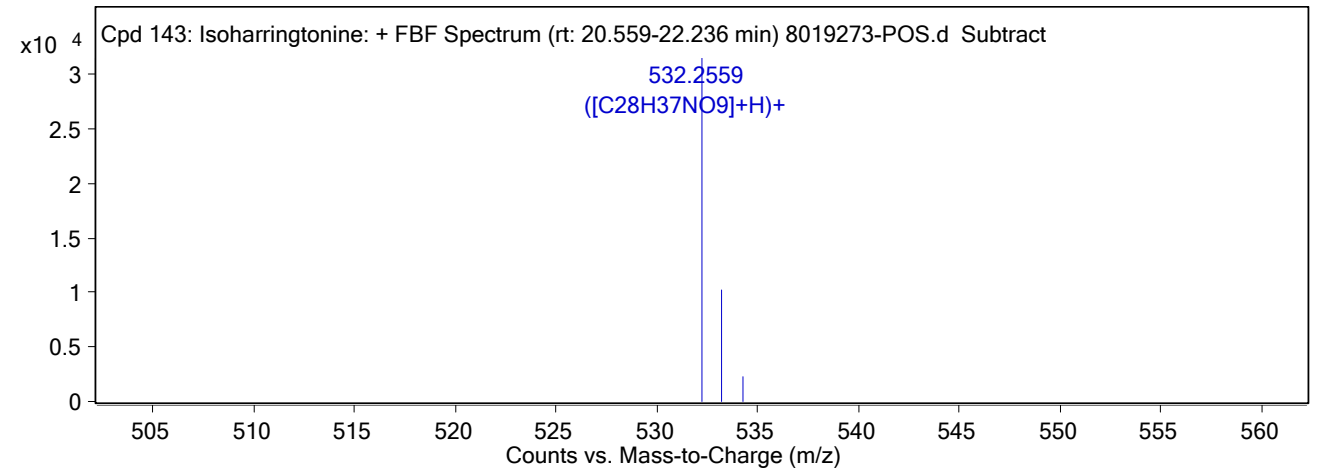
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 414.1787 | 1 | 317.49 | C23H26O7 | M+ |
| 415.1768 | 1 | 26778.09 | C23H26O7 | (M+H)+ |
| 416.18 | 1 | 7010.06 | C23H26O7 | (M+H)+ |
| 417.1833 | 1 | 1057.72 | C23H26O7 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 143: Isoharringtonine | **Isoharringtonine** | 532.2559 | 21.849 | Find By Formula | 531.2486 |

**Compound Chromatograms**




MS Zoomed Spectrum

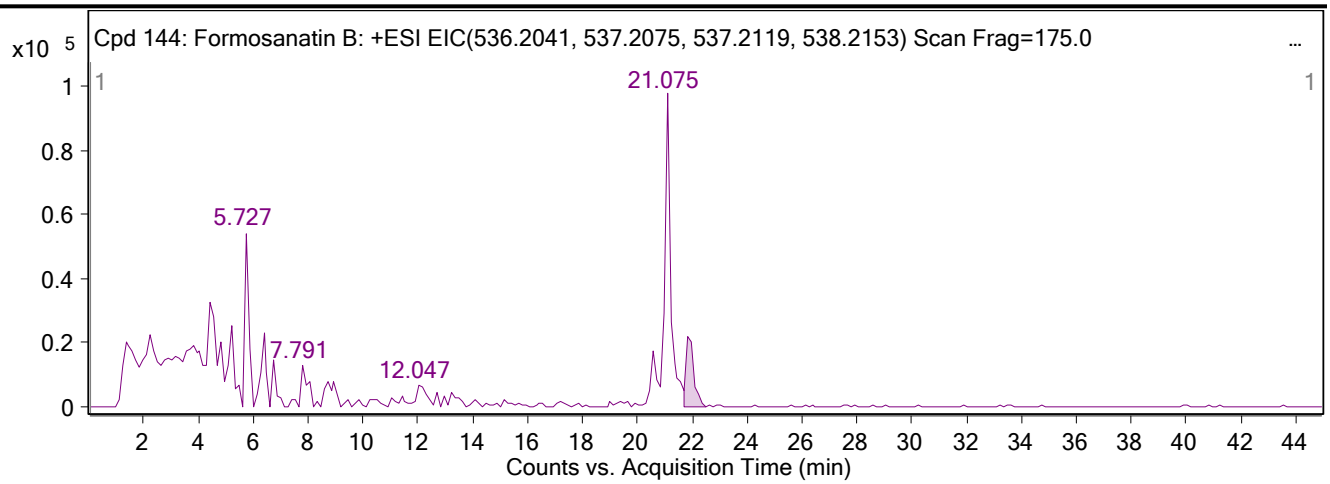



**MS Spectrum Peak List**

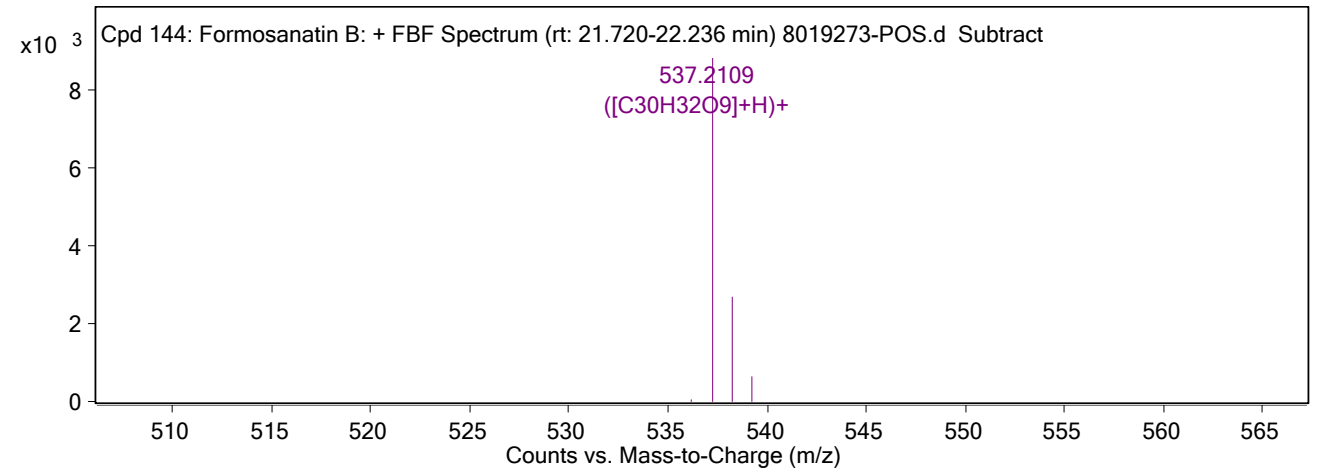
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 532.2559 | 1 | 31487.16 | C28H37NO9 | (M+H)+ |
| 533.2592 | 1 | 10235.5 | C28H37NO9 | (M+H)+ |
| 534.2624 | 1 | 2219.17 | C28H37NO9 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 144: Formosanatin B | **Formosanatin B** | 537.2109 | 21.849 | Find By Formula | 536.2035 |

**Compound Chromatograms**




MS Zoomed Spectrum

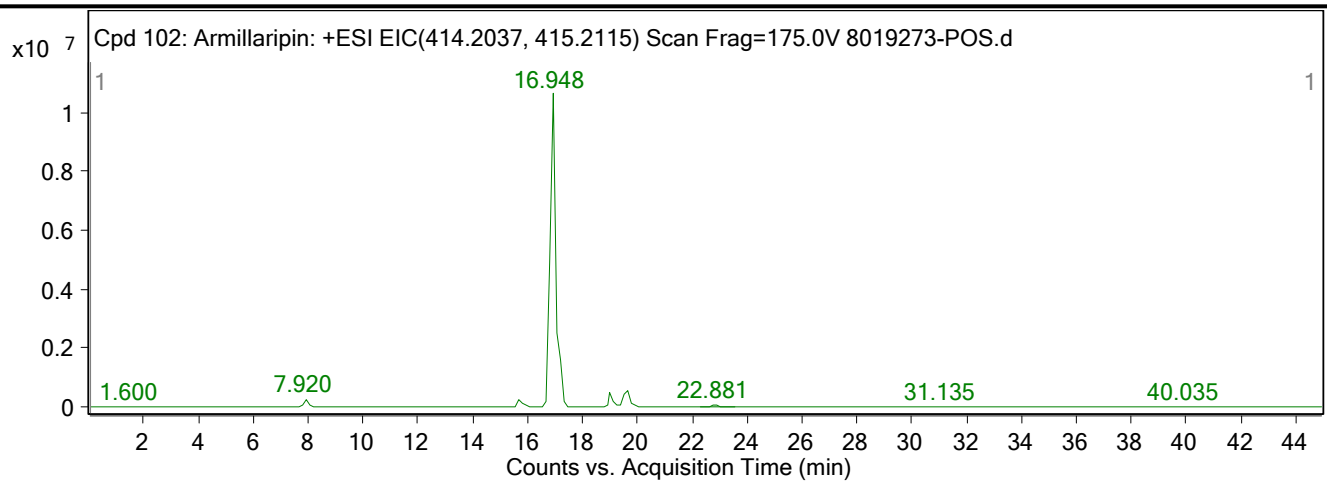



**MS Spectrum Peak List**

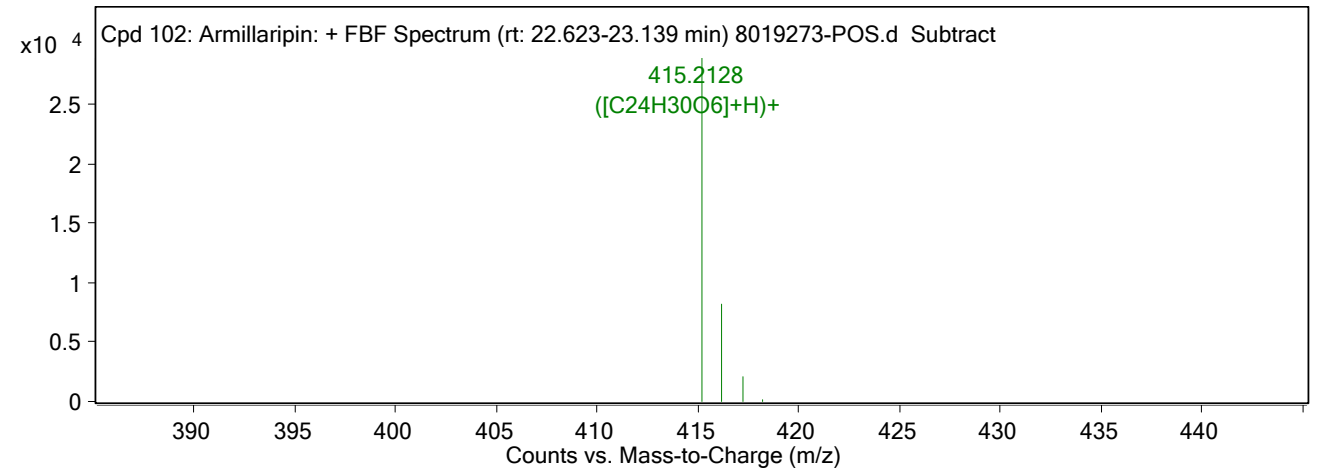
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 536.203 | 1 | 67.44 | C30H32O9 | M+ |
| 537.2109 | 1 | 8823.75 | C30H32O9 | (M+H)+ |
| 538.2142 | 1 | 2664.28 | C30H32O9 | (M+H)+ |
| 539.2161 | 1 | 659.18 | C30H32O9 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 102: Armillaripin | **Armillaripin** | 415.2128 | 22.881 | Find By Formula | 414.2057 |

**Compound Chromatograms**




MS Zoomed Spectrum

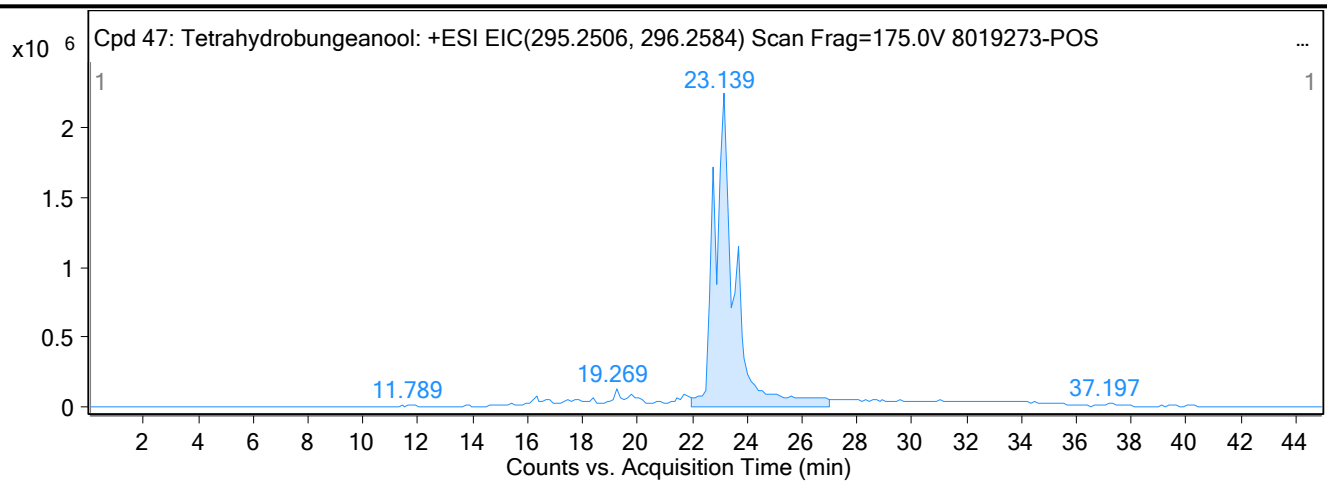



**MS Spectrum Peak List**

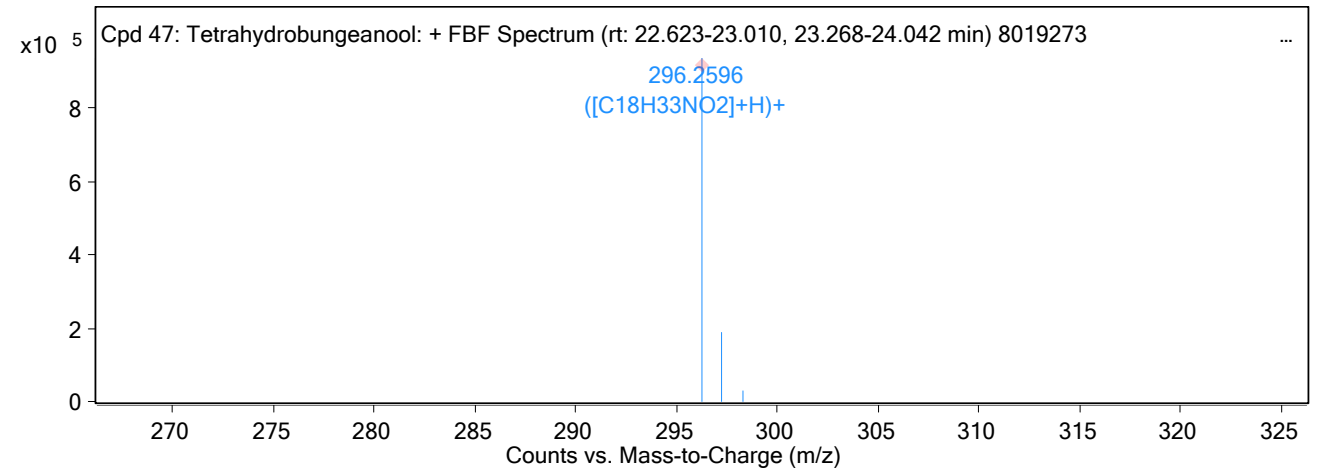
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 415.2128 | 1 | 28870.68 | C24H30O6 | (M+H)+ |
| 416.2175 | 1 | 8162.89 | C24H30O6 | (M+H)+ |
| 417.2179 | 1 | 2053.72 | C24H30O6 | (M+H)+ |
| 418.2158 | 1 | 83.58 | C24H30O6 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 47: Tetrahydrobungeanool | Tetrahydrobungeanool | 296.2596 | 23.139 | Find By Formula | 295.2524 |

**Compound Chromatograms**




MS Zoomed Spectrum

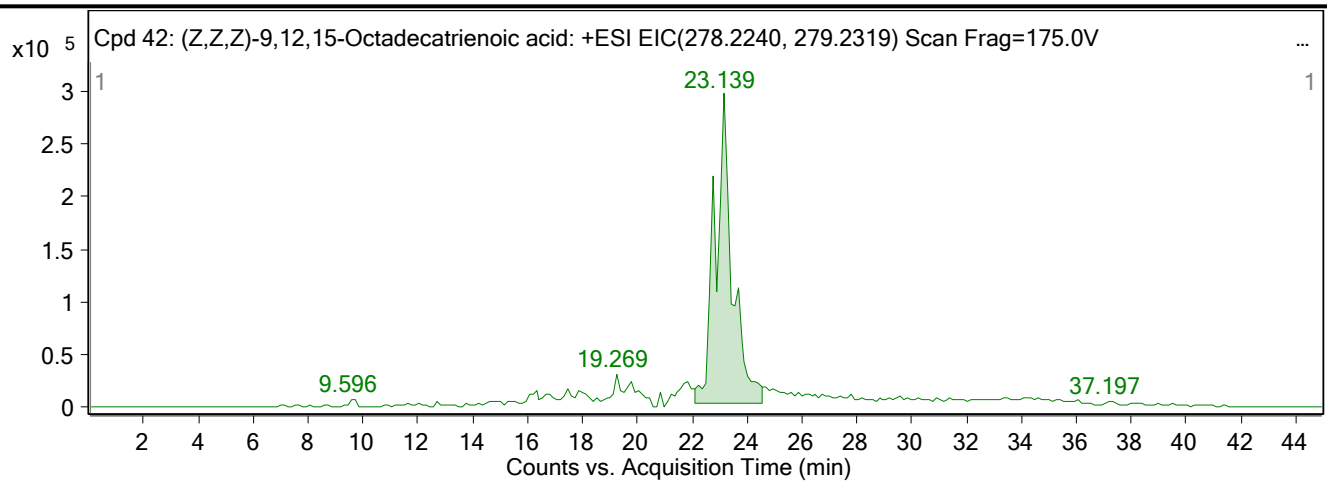



**MS Spectrum Peak List**

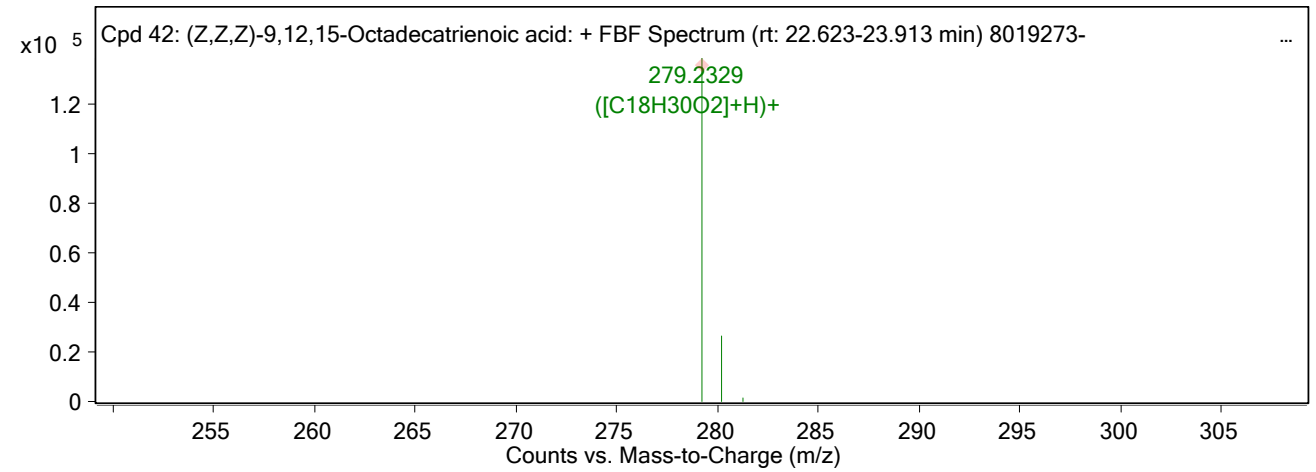
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 296.2596 | 1 | 936041.44 | C18H33NO2 | (M+H)+ |
| 297.2629 | 1 | 190536.64 | C18H33NO2 | (M+H)+ |
| 298.2698 | 1 | 27101.05 | C18H33NO2 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 42: (Z,Z,Z)-9,12,15-Octadecatrienoic acid | **(Z,Z,Z)-9,12,15-Octadecatrienoic acid** | 279.2329 | 23.139 | Find By Formula | 278.2256 |

**Compound Chromatograms**




MS Zoomed Spectrum

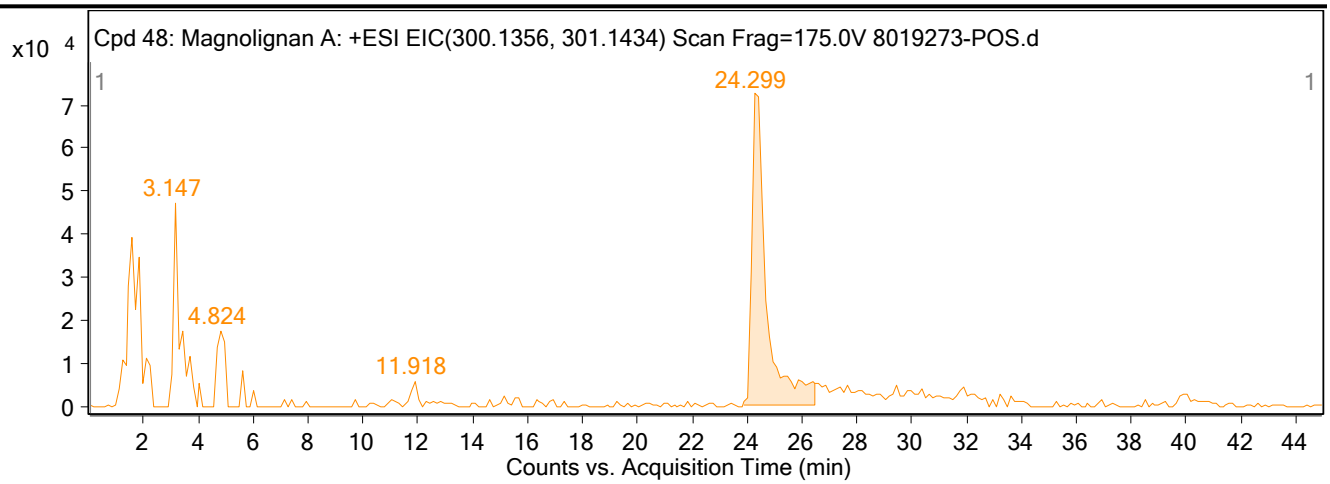



**MS Spectrum Peak List**

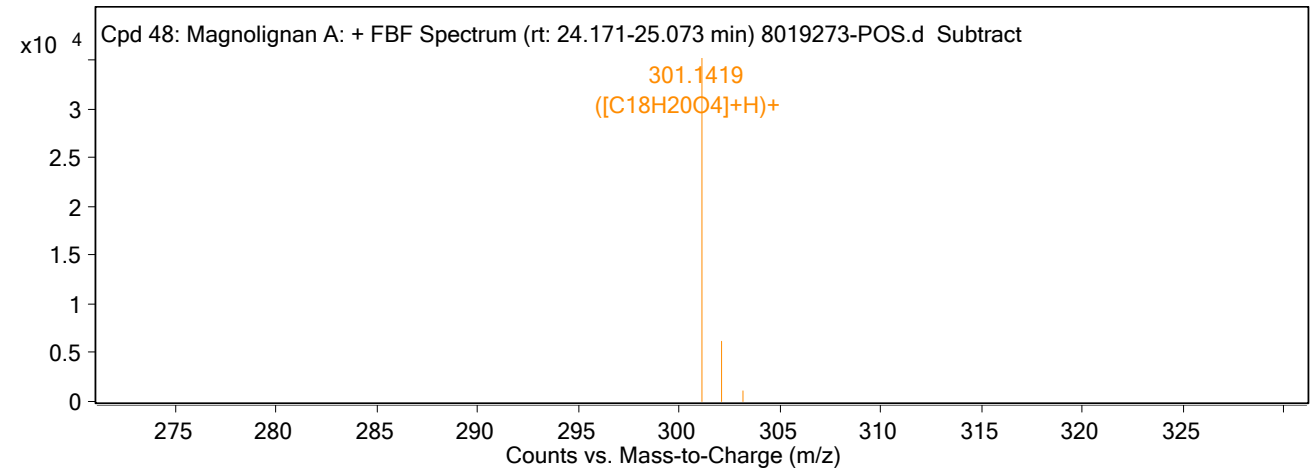
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 279.2329 | 1 | 138489.63 | C18H30O2 | (M+H)+ |
| 280.2361 | 1 | 26640.17 | C18H30O2 | (M+H)+ |
| 281.24 | 1 | 1183.23 | C18H30O2 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 48: Magnolignan A | **Magnolignan A** | 301.1419 | 24.299 | Find By Formula | 300.1348 |

**Compound Chromatograms**




MS Zoomed Spectrum

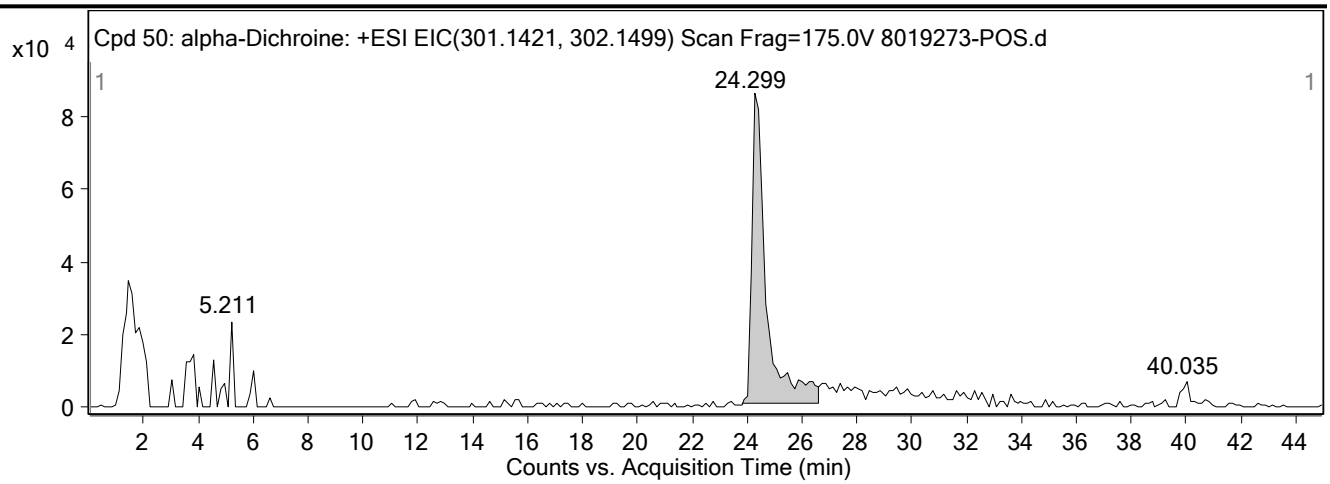



**MS Spectrum Peak List**

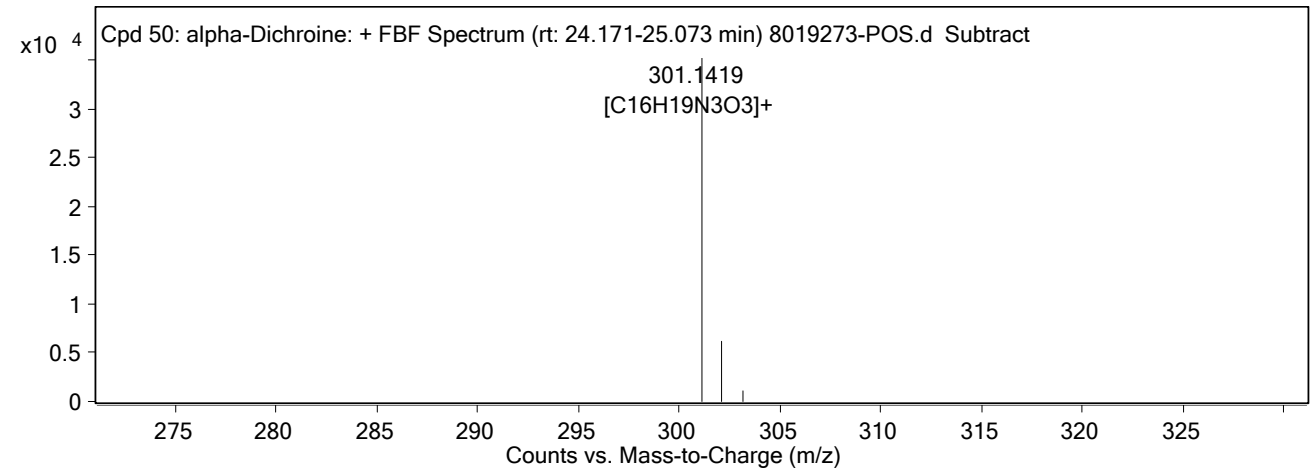
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 301.1419 | 1 | 35271.2 | C18H20O4 | (M+H)+ |
| 302.1462 | 1 | 6279.06 | C18H20O4 | (M+H)+ |
| 303.1509 | 1 | 1105.14 | C18H20O4 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 50: alpha-Dichroine | **alpha-Dichroine** | 301.1419 | 24.299 | Find By Formula | 301.1427 |

**Compound Chromatograms**




MS Zoomed Spectrum

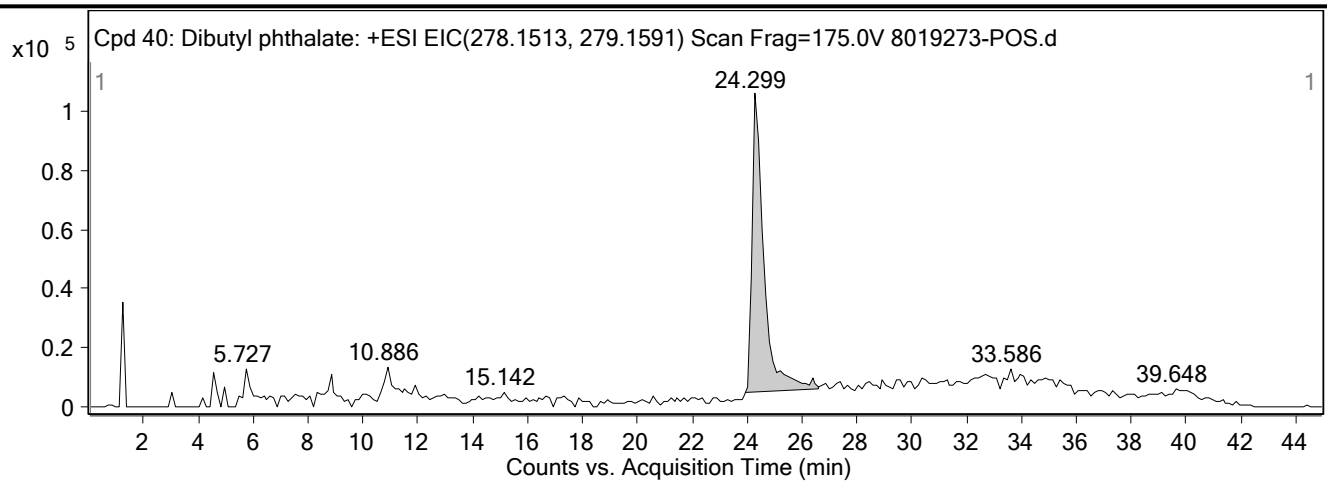



**MS Spectrum Peak List**

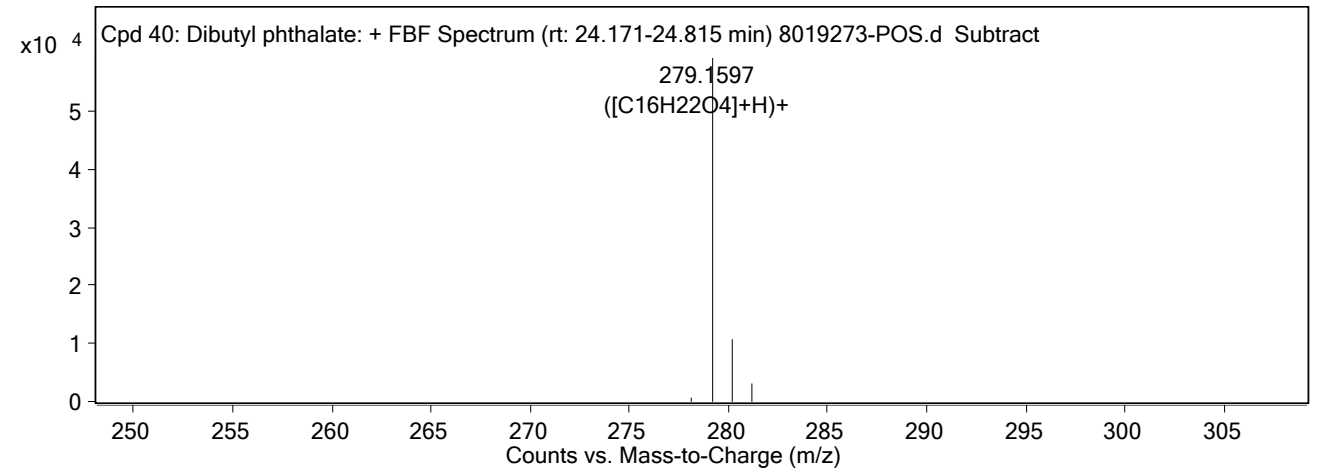
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 301.1419 | 1 | 35271.2 | C16H19N3O3 | M+ |
| 302.1462 | 1 | 6279.06 | C16H19N3O3 | M+ |
| 303.1509 | 1 | 1105.14 | C16H19N3O3 | M+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 40: Dibutyl phthalate | **Dibutyl phthalate** | 279.1597 | 24.299 | Find By Formula | 278.1527 |

**Compound Chromatograms**




MS Zoomed Spectrum

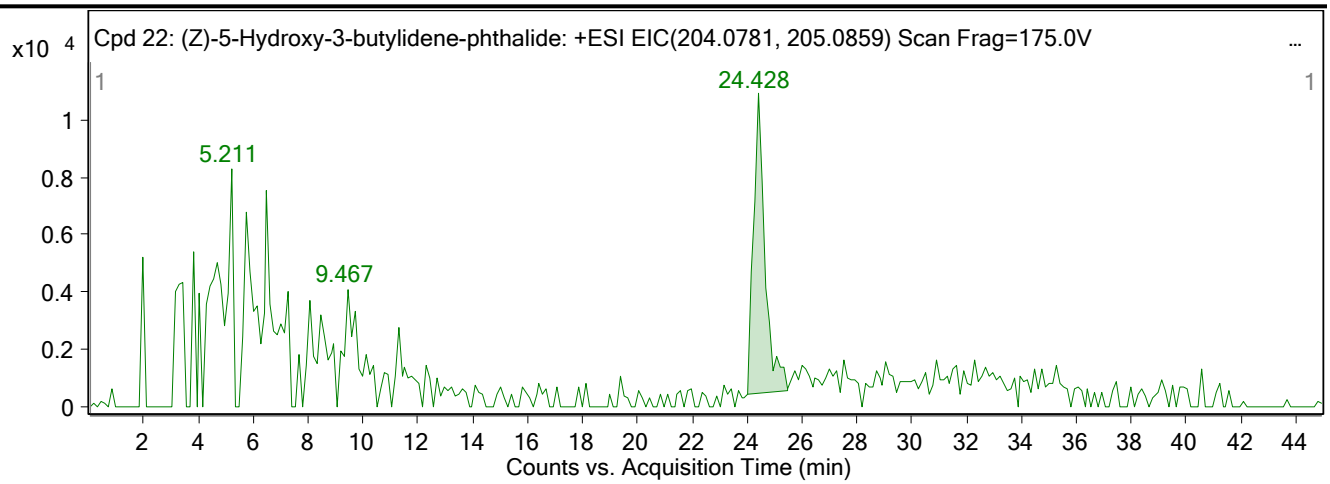



**MS Spectrum Peak List**

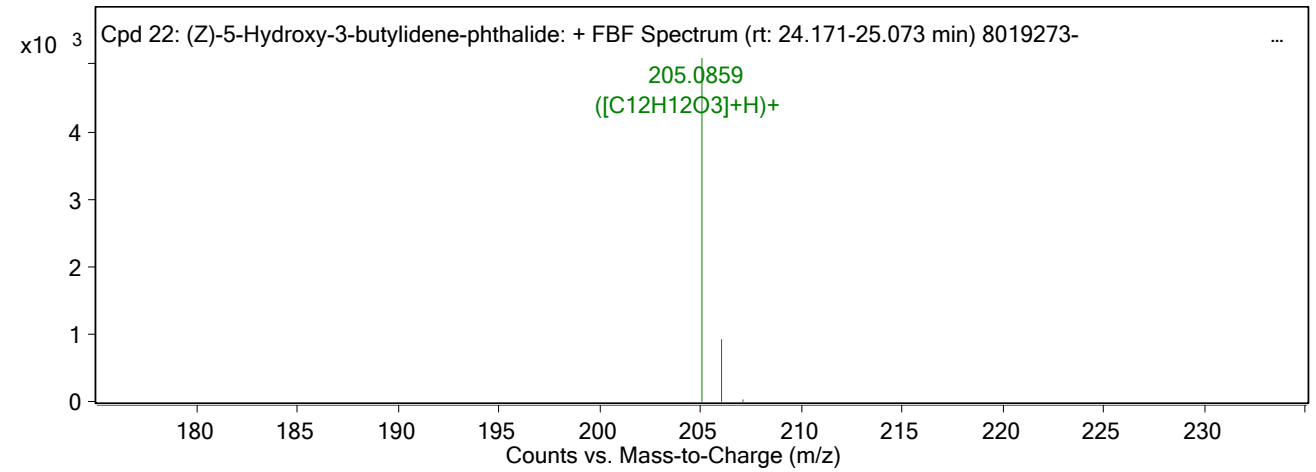
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 278.1563 | 1 | 510.5 | C16H22O4 | M+ |
| 279.1597 | 1 | 59235.58 | C16H22O4 | (M+H)+ |
| 280.1631 | 1 | 10586.59 | C16H22O4 | (M+H)+ |
| 281.1708 | 1 | 3160.51 | C16H22O4 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 22: (Z)-5-Hydroxy-3-butylidene-phthalide | **(Z)-5-Hydroxy-3-butylidene-phthalide** | 205.0859 | 24.428 | Find By Formula | 204.0785 |

**Compound Chromatograms**




MS Zoomed Spectrum

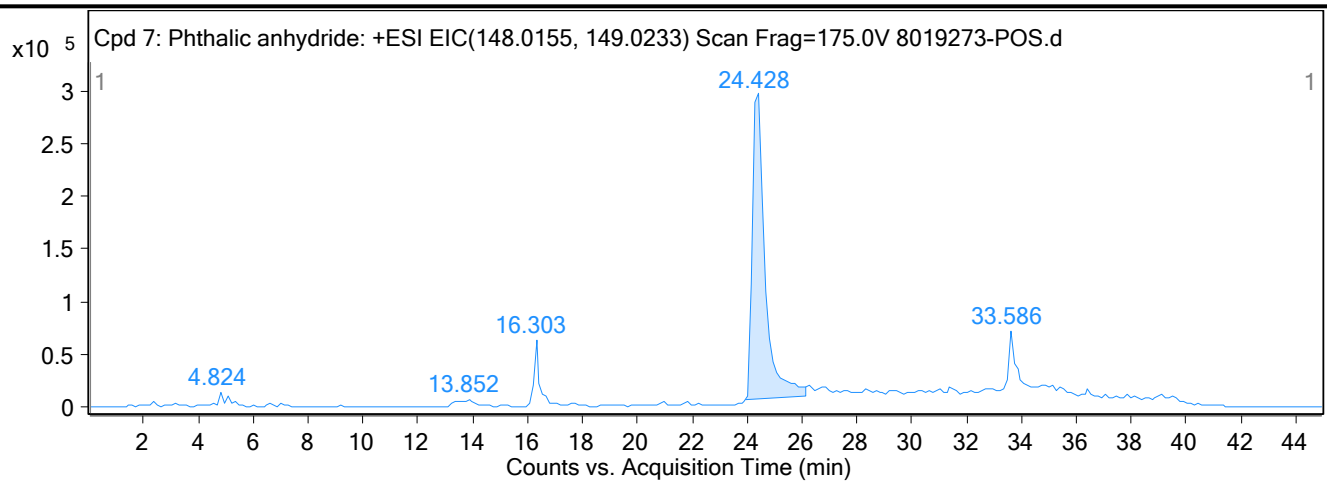



**MS Spectrum Peak List**

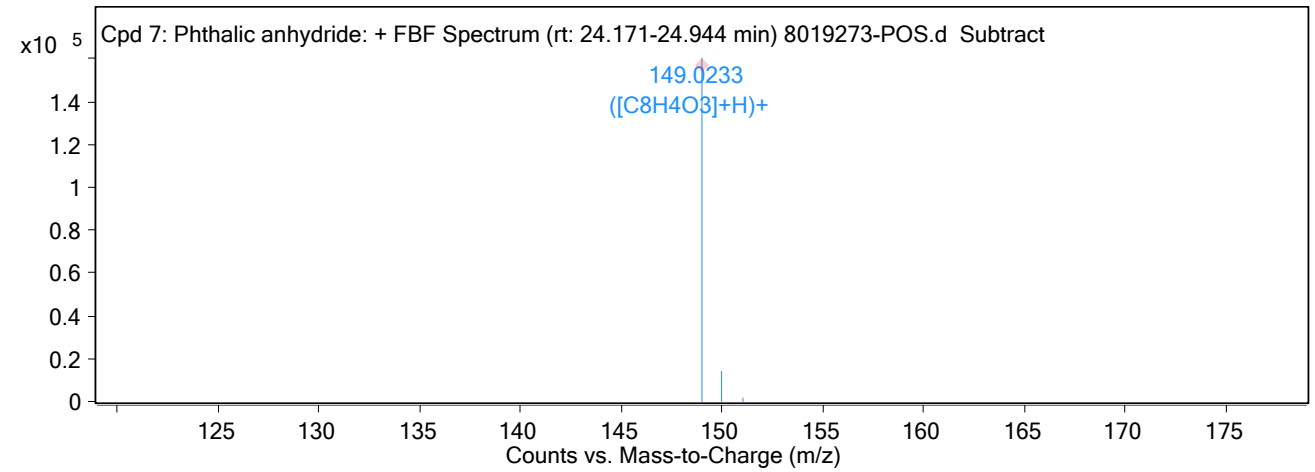
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 205.0859 | 1 | 5090.17 | C12H12O3 | (M+H)+ |
| 206.0889 | 1 | 928.46 | C12H12O3 | (M+H)+ |
| 207.0818 | 1 | 33.96 | C12H12O3 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 7: Phthalic anhydride | **Phthalic anhydride** | 149.0233 | 24.428 | Find By Formula | 148.016 |

**Compound Chromatograms**




MS Zoomed Spectrum

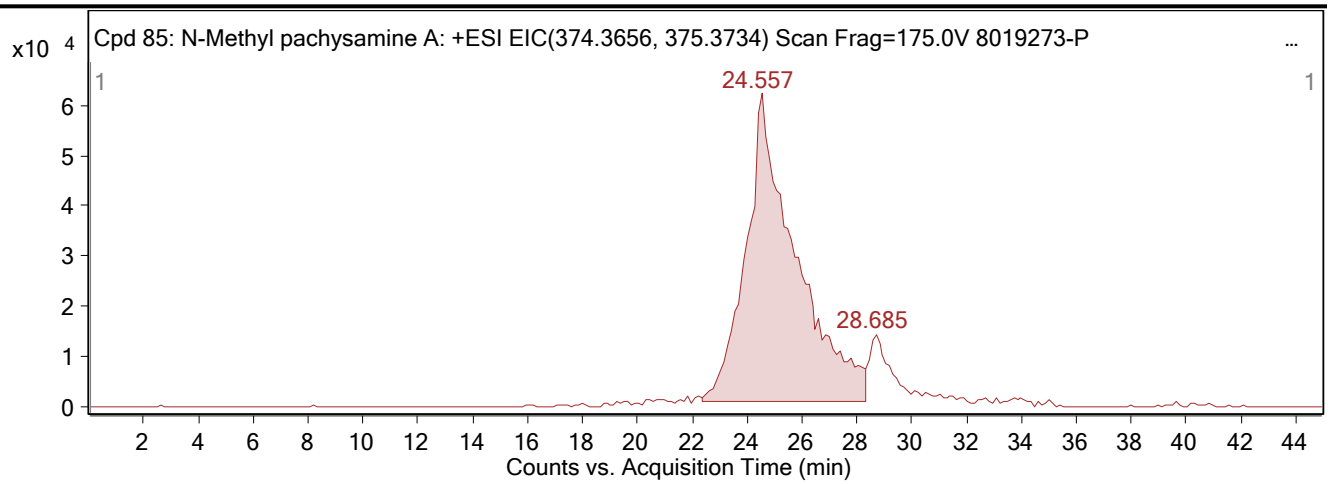



**MS Spectrum Peak List**

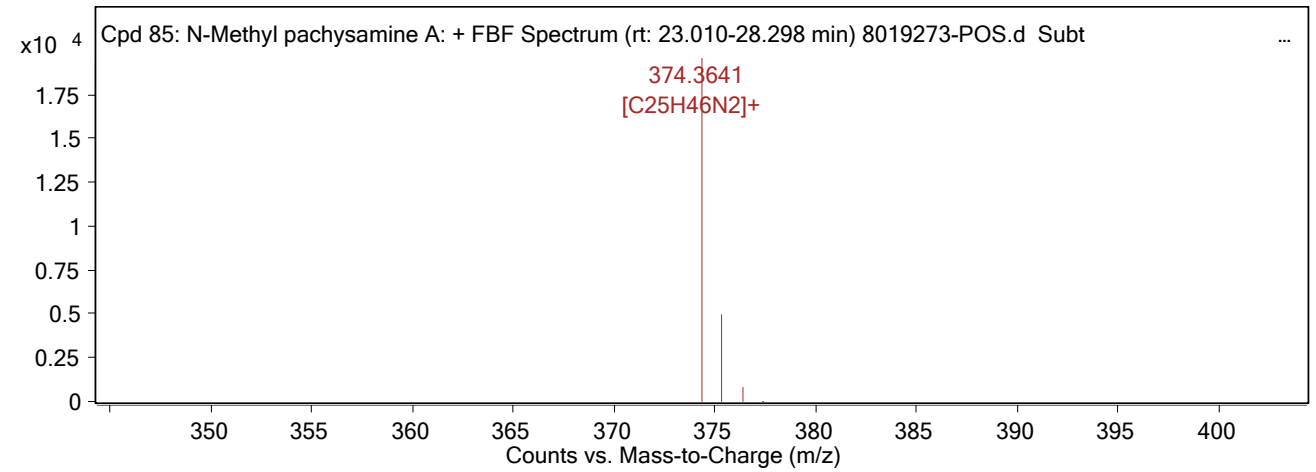
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 149.0233 | 1 | 160328.08 | C8H4O3 | (M+H)+ |
| 150.0266 | 1 | 14032.21 | C8H4O3 | (M+H)+ |
| 151.0283 | 1 | 1557.77 | C8H4O3 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 85: N-Methyl pachysamine A | **N-Methyl pachysamine A** | 374.3641 | 24.557 | Find By Formula | 374.3646 |

**Compound Chromatograms**




MS Zoomed Spectrum

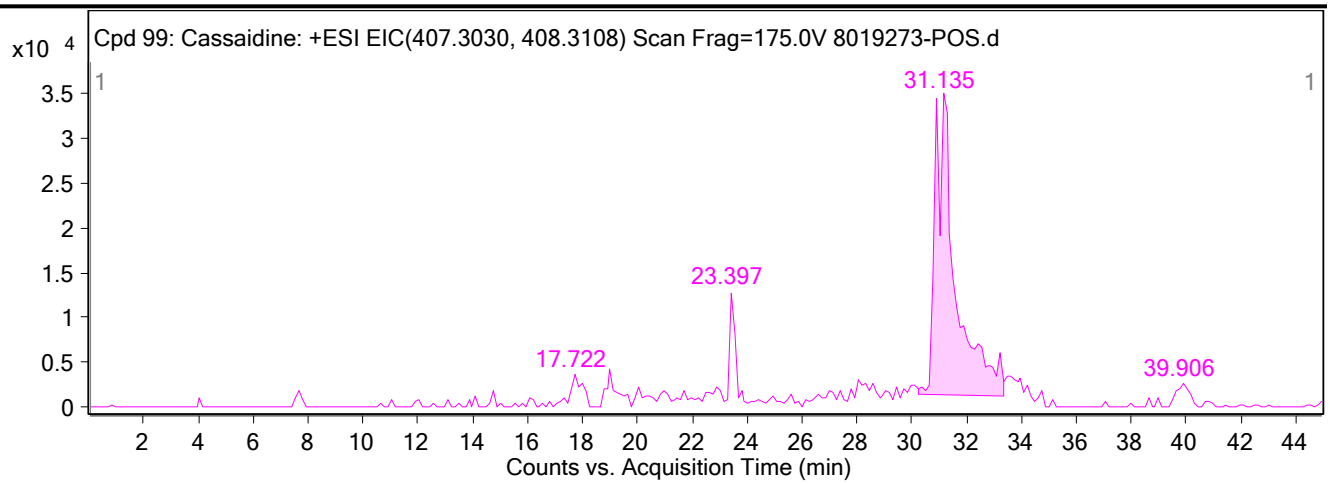



**MS Spectrum Peak List**

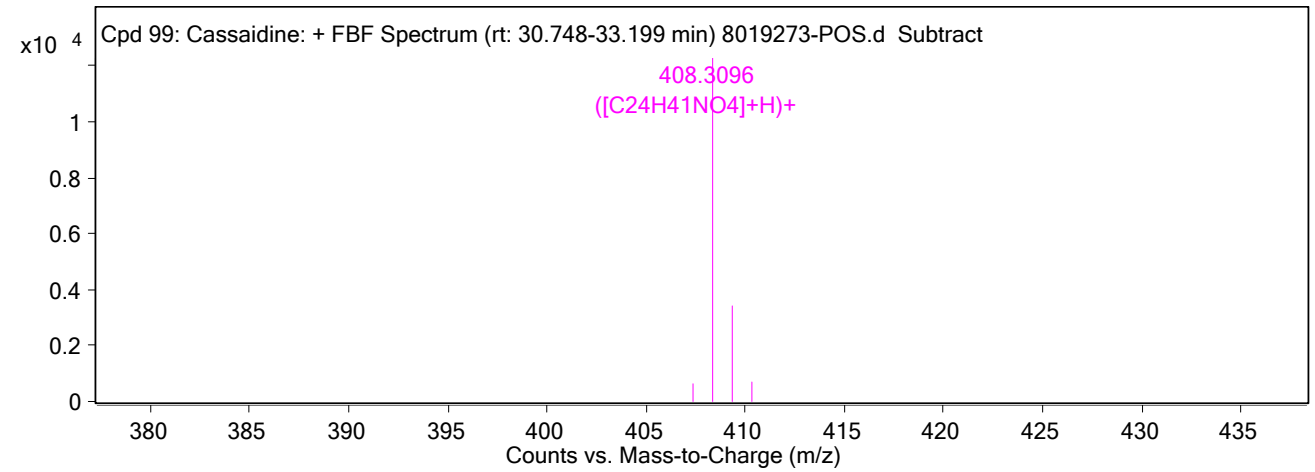
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 374.3641 | 1 | 19591.81 | C25H46N2 | M+ |
| 375.3674 | 1 | 4934.22 | C25H46N2 | M+ |
| 376.3694 | 1 | 773.69 | C25H46N2 | M+ |
| 377.3718 | 1 | 53.71 | C25H46N2 | M+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 99: Cassaidine | **Cassaidine** | 408.3096 | 31.135 | Find By Formula | 407.3029 |

**Compound Chromatograms**




MS Zoomed Spectrum

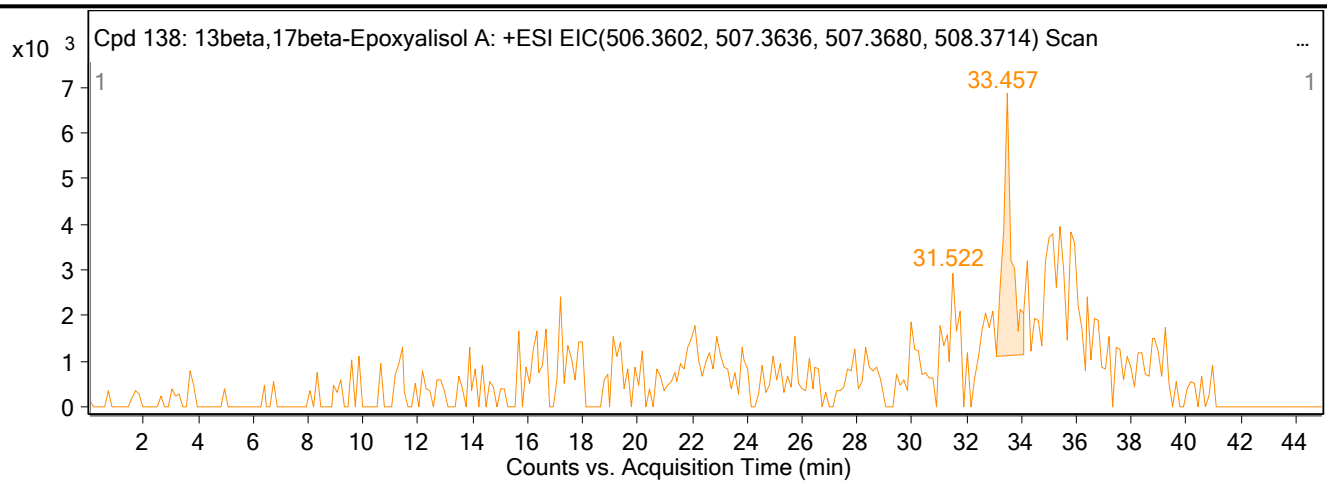



**MS Spectrum Peak List**

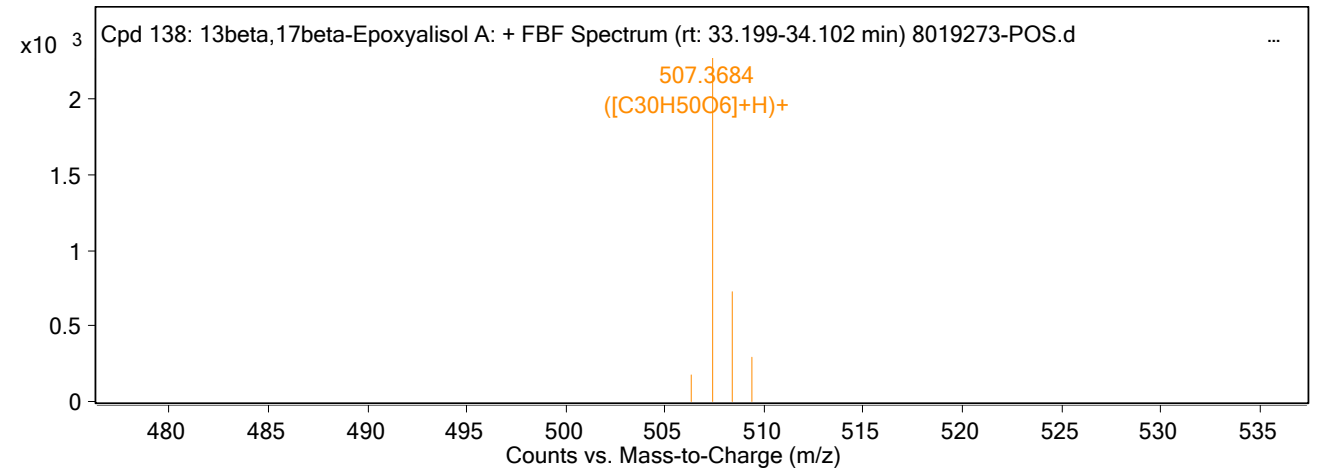
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 407.3136 | 1 | 614.65 | C24H41NO4 | M+ |
| 408.3096 | 1 | 12272.72 | C24H41NO4 | (M+H)+ |
| 409.3134 | 1 | 3393.66 | C24H41NO4 | (M+H)+ |
| 410.3155 | 1 | 729.18 | C24H41NO4 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 138: 13beta,17beta-Epoxyalisol A | **13beta,17beta-Epoxyalisol A** | 507.3684 | 33.457 | Find By Formula | 506.3615 |

**Compound Chromatograms**




MS Zoomed Spectrum

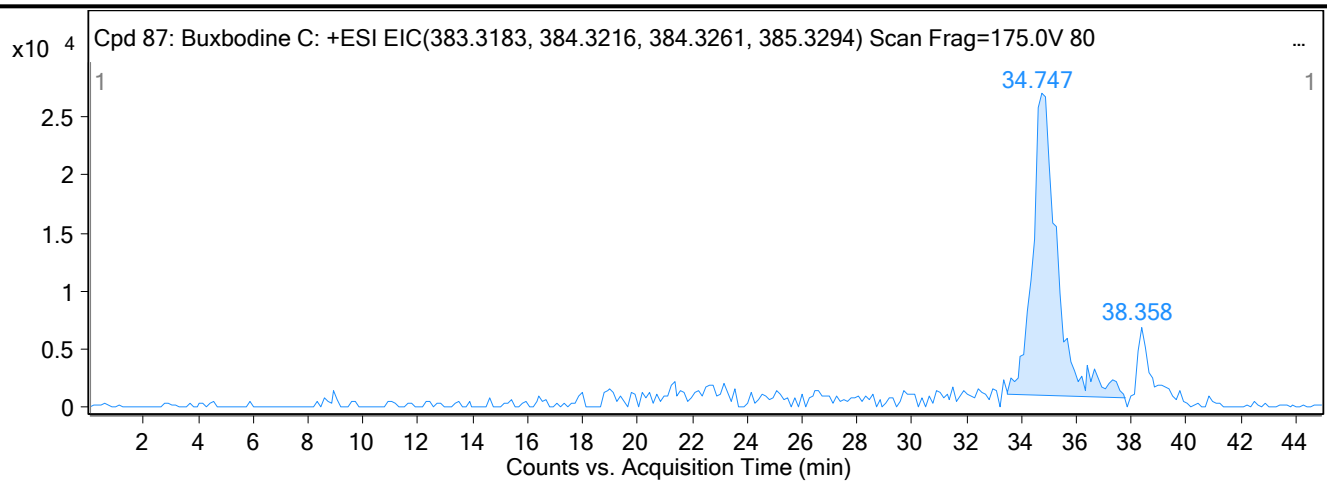



**MS Spectrum Peak List**

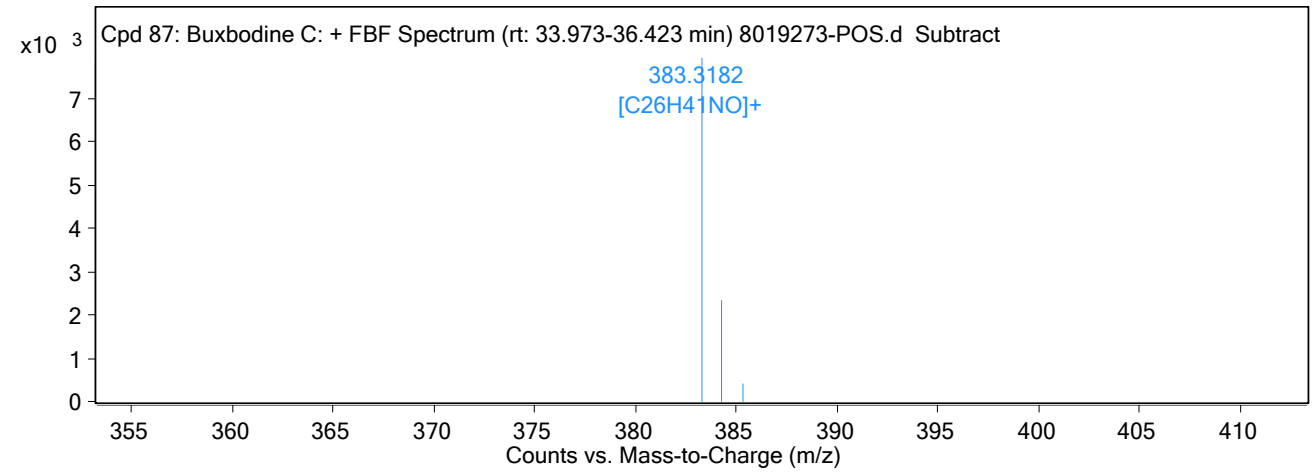
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 506.3664 | 1 | 181.99 | C30H50O6 | M+ |
| 507.3684 | 1 | 2273.78 | C30H50O6 | (M+H)+ |
| 508.3714 | 1 | 725.88 | C30H50O6 | (M+H)+ |
| 509.3764 | 1 | 288.67 | C30H50O6 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 87: Buxbodine C | **Buxbodine C** | 383.3182 | 34.747 | Find By Formula | 383.3187 |

**Compound Chromatograms**




MS Zoomed Spectrum

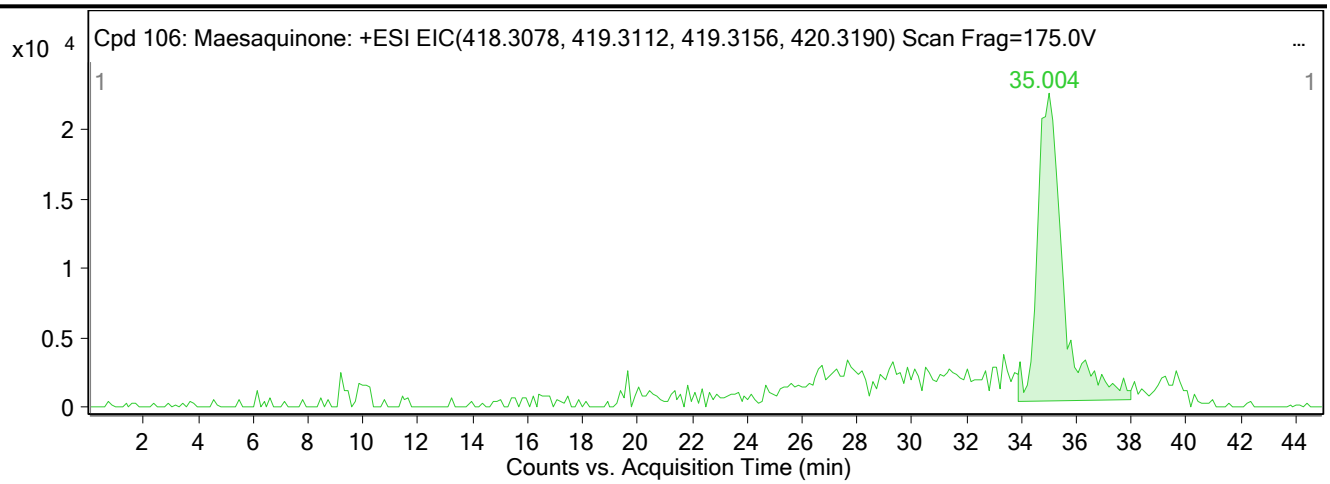



**MS Spectrum Peak List**

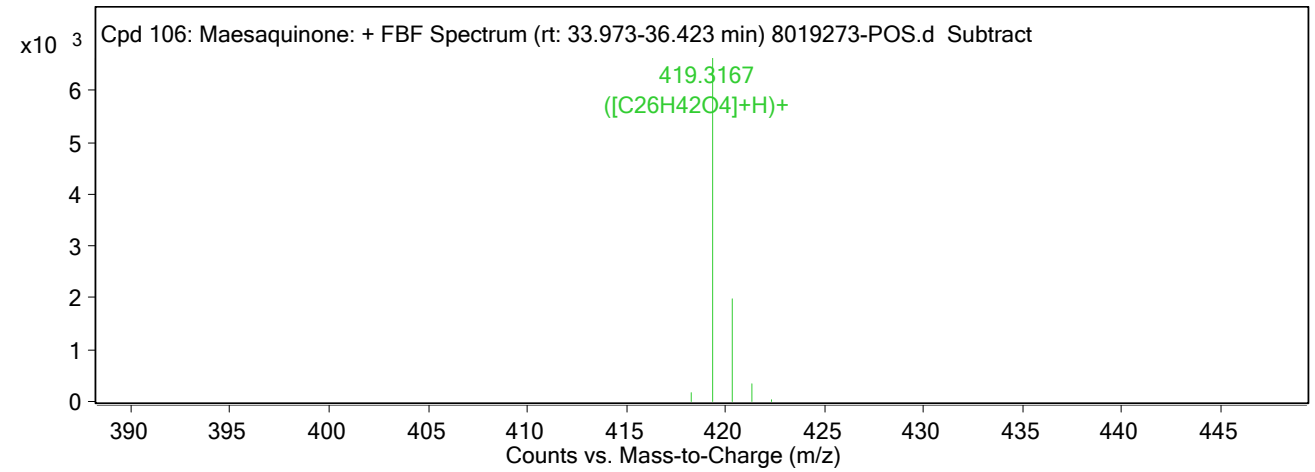
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 383.3182 | 1 | 7918.9 | C26H41NO | M+ |
| 384.3217 | 1 | 2315.22 | C26H41NO | M+ |
| 385.3213 | 1 | 426.75 | C26H41NO | M+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 106: Maesaquinone | **Maesaquinone** | 419.3167 | 35.004 | Find By Formula | 418.3096 |

**Compound Chromatograms**




MS Zoomed Spectrum

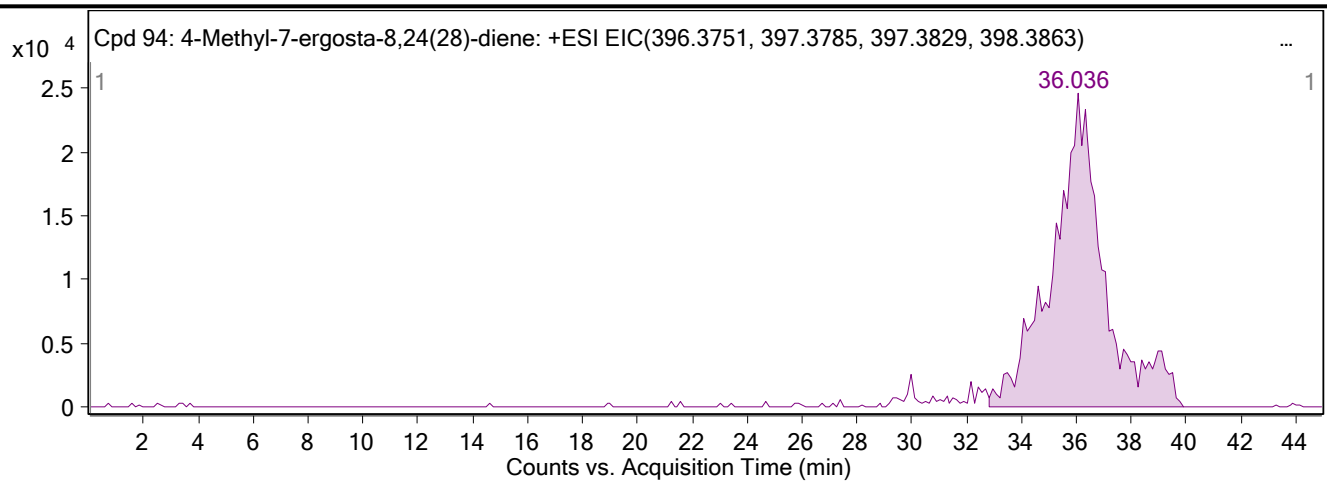



**MS Spectrum Peak List**

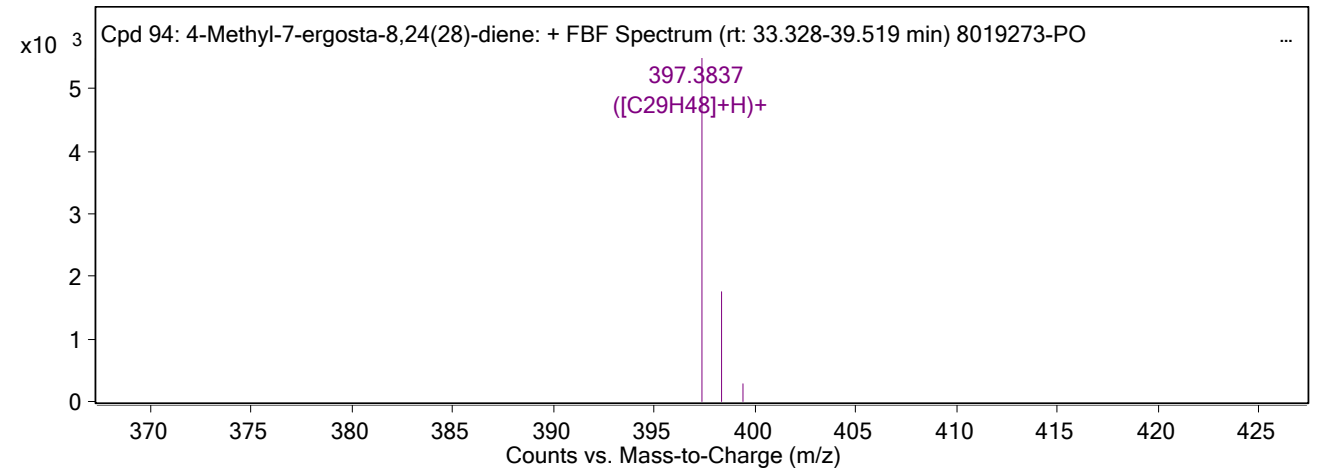
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 418.3073 | 1 | 186.76 | C26H42O4 | M+ |
| 419.3167 | 1 | 6629.26 | C26H42O4 | (M+H)+ |
| 420.3208 | 1 | 1995.39 | C26H42O4 | (M+H)+ |
| 421.3262 | 1 | 340.58 | C26H42O4 | (M+H)+ |
| 422.3196 | 1 | 41.57 | C26H42O4 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 94: 4-Methyl-7-ergosta-8,24(28)-diene | **4-Methyl-7-ergosta-8,24(28)-diene** | 397.3837 | 36.036 | Find By Formula | 396.3765 |

**Compound Chromatograms**




MS Zoomed Spectrum

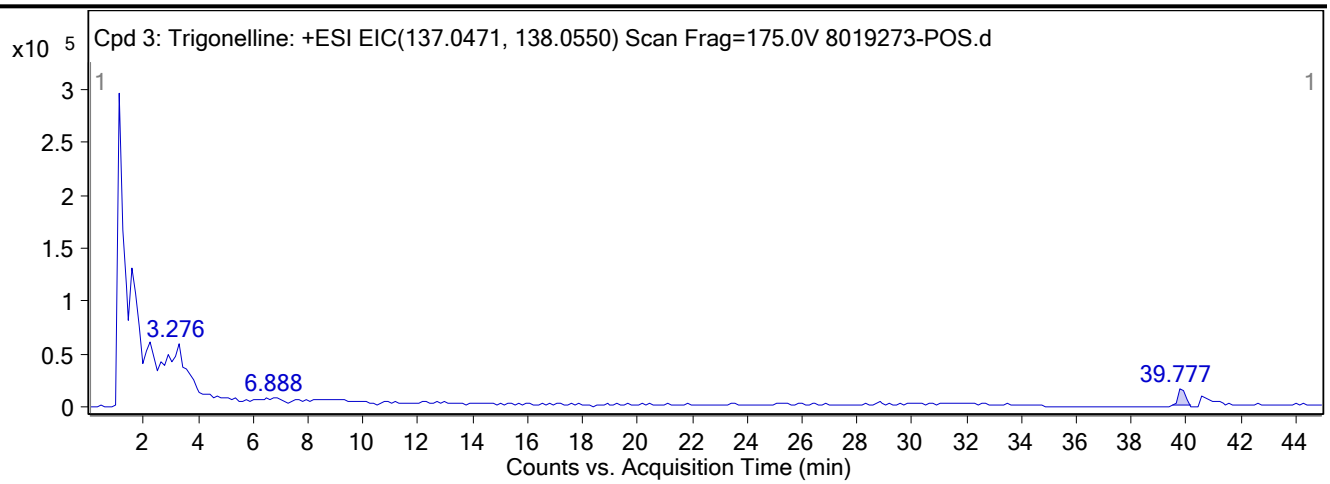



**MS Spectrum Peak List**

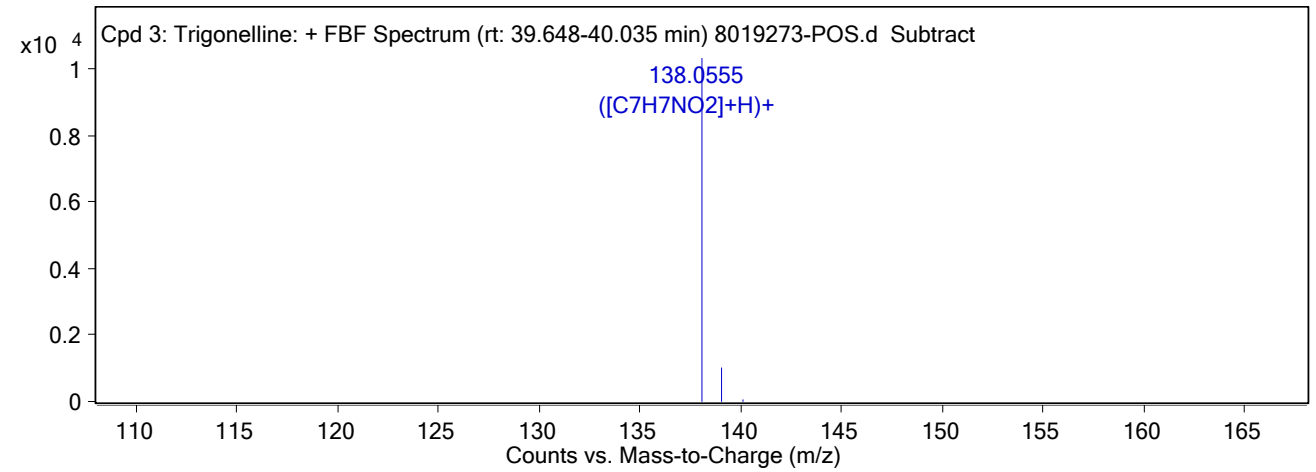
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 397.3837 | 1 | 5486.37 | C29H48 | (M+H)+ |
| 398.3871 | 1 | 1761.76 | C29H48 | (M+H)+ |
| 399.3905 | 1 | 274.4 | C29H48 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 3: Trigonelline | **Trigonelline** | 138.0555 | 39.777 | Find By Formula | 137.0481 |

**Compound Chromatograms**




MS Zoomed Spectrum

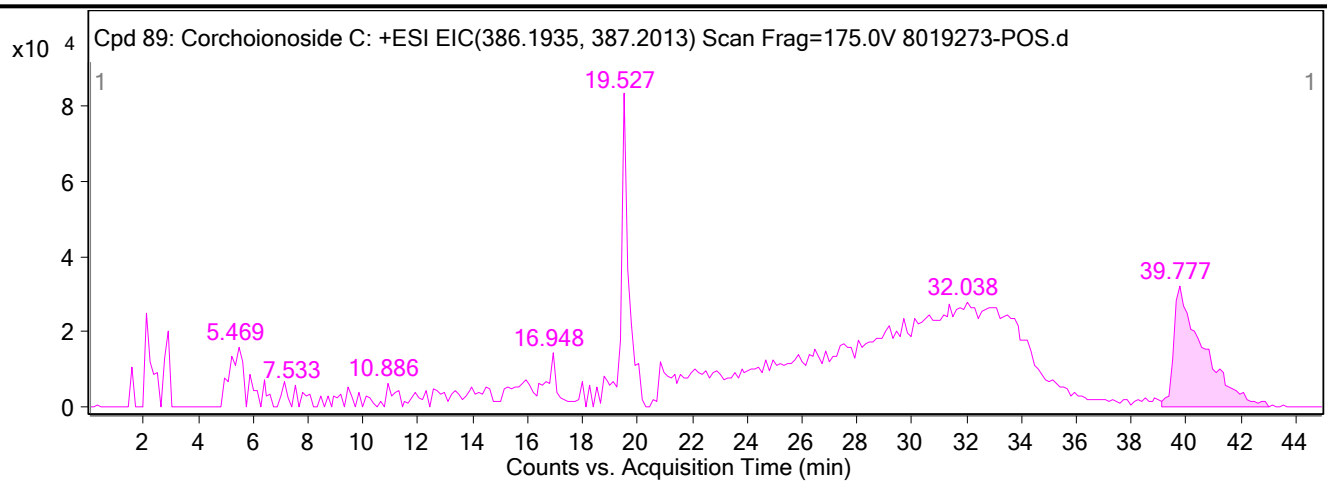



**MS Spectrum Peak List**

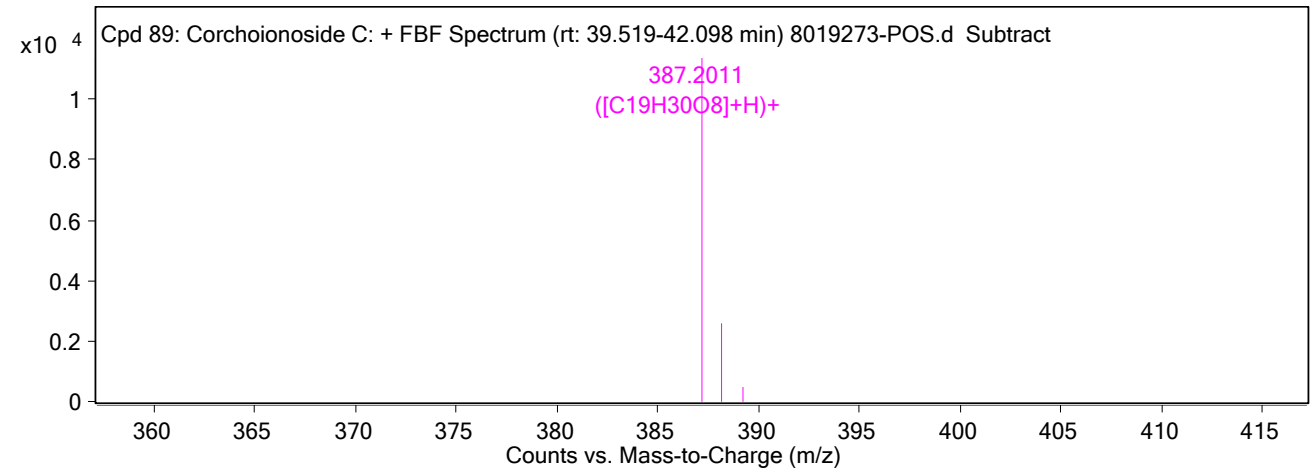
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 138.0555 | 1 | 10339.73 | C7H7NO2 | (M+H)+ |
| 139.0574 | 1 | 1038.92 | C7H7NO2 | (M+H)+ |
| 140.0557 | 1 | 69.24 | C7H7NO2 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 89: Corchoionoside C | **Corchoionoside C** | 387.2011 | 39.777 | Find By Formula | 386.1938 |

**Compound Chromatograms**




MS Zoomed Spectrum

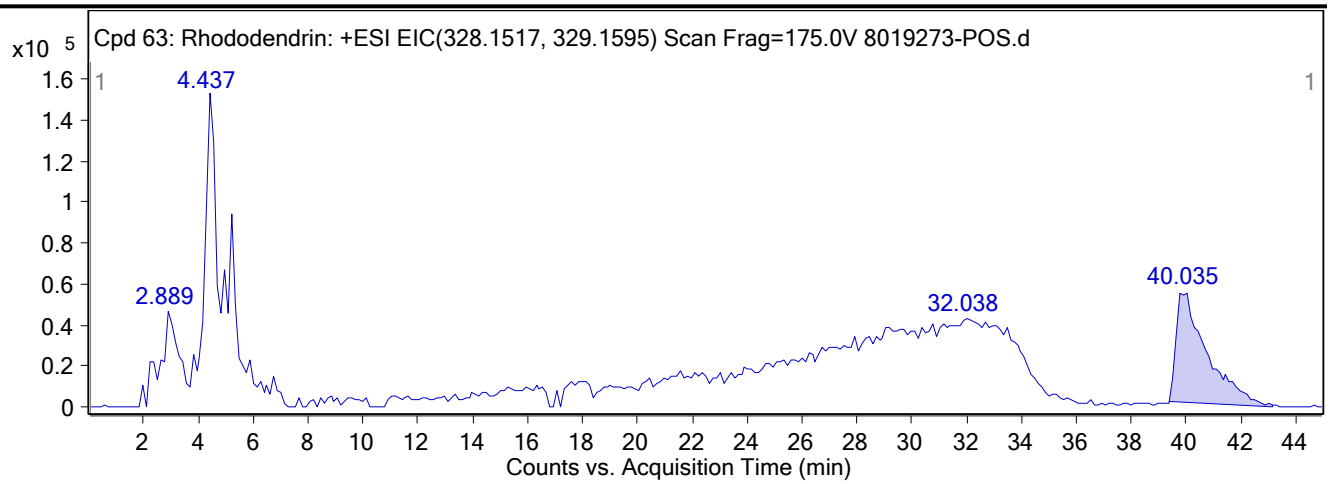



**MS Spectrum Peak List**

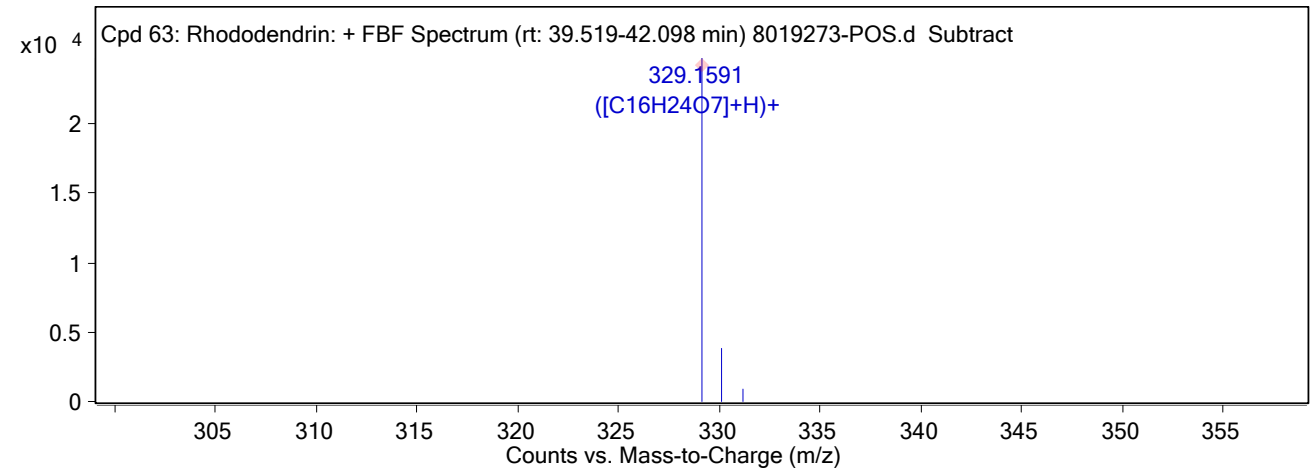
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 387.2011 | 1 | 11357.34 | C19H30O8 | (M+H)+ |
| 388.2048 | 1 | 2593.24 | C19H30O8 | (M+H)+ |
| 389.2046 | 1 | 486.55 | C19H30O8 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 63: Rhododendrin | **Rhododendrin** | 329.1591 | 40.035 | Find By Formula | 328.1519 |

**Compound Chromatograms**




MS Zoomed Spectrum

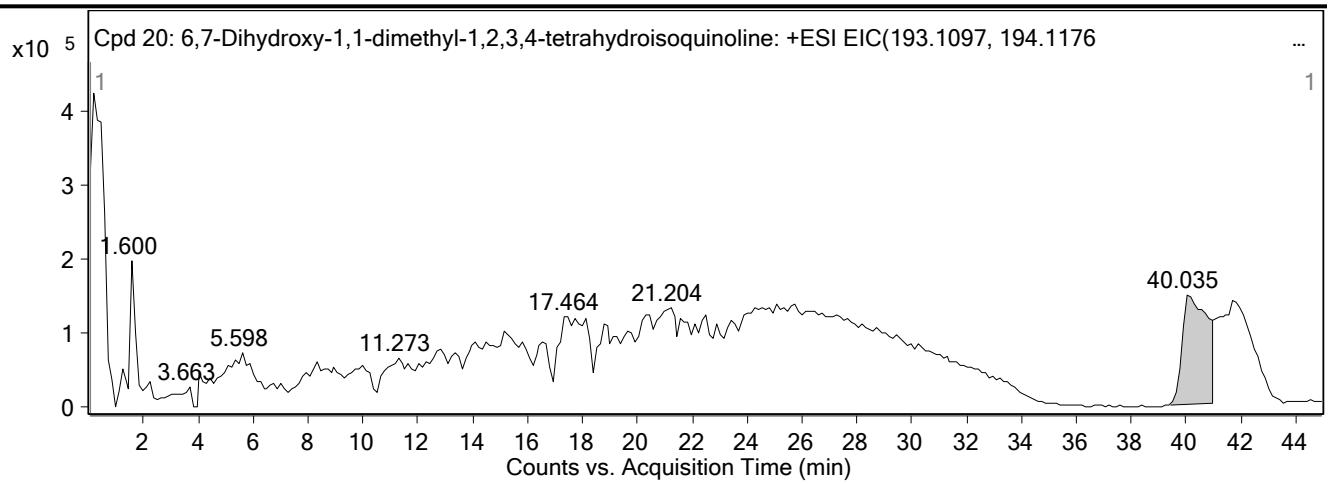



**MS Spectrum Peak List**

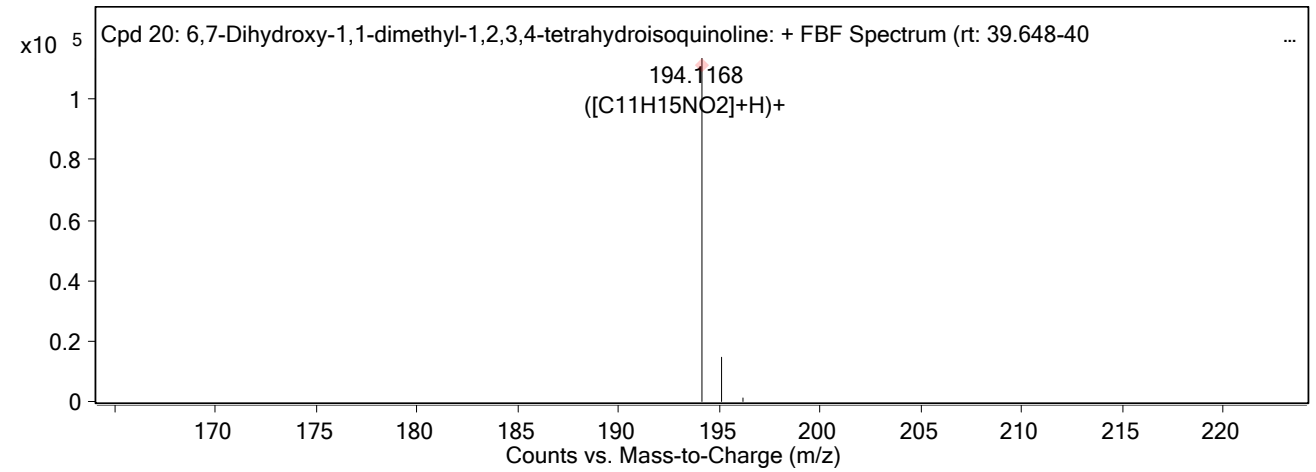
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 329.1591 | 1 | 24716.75 | C16H24O7 | (M+H)+ |
| 330.163 | 1 | 3794.79 | C16H24O7 | (M+H)+ |
| 331.1666 | 1 | 889.09 | C16H24O7 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 20: 6,7-Dihydroxy-1,1-dimethyl-1,2,3,4-tetrahydroisoquinoline | **6,7-Dihydroxy-1,1-dimethyl-1,2,3,4-tetrahydroisoquinoline** | 194.1168 | 40.035 | Find By Formula | 193.1097 |

**Compound Chromatograms**




MS Zoomed Spectrum

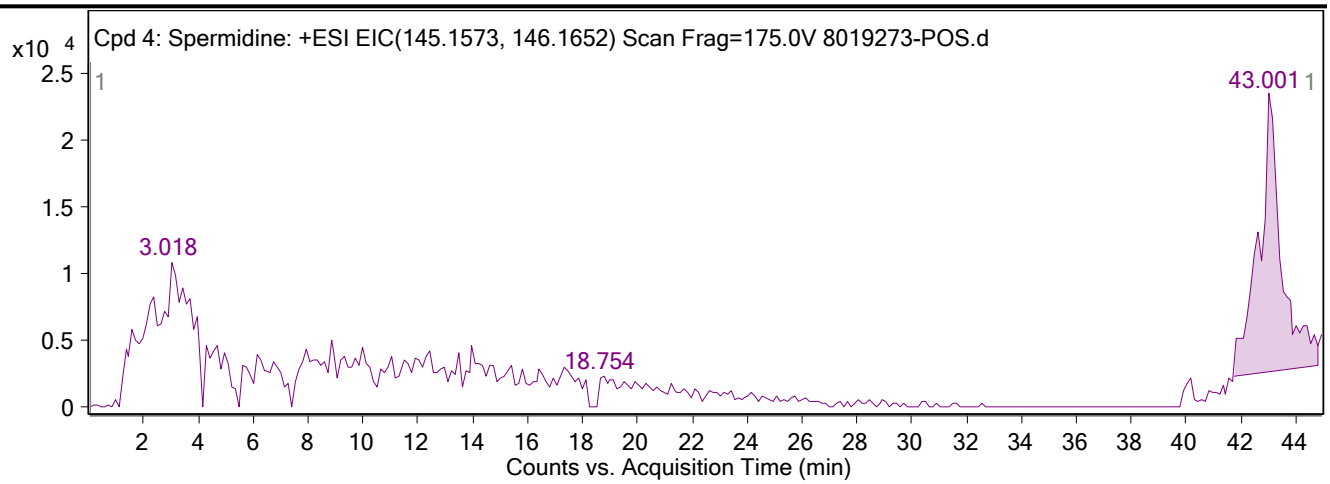



**MS Spectrum Peak List**

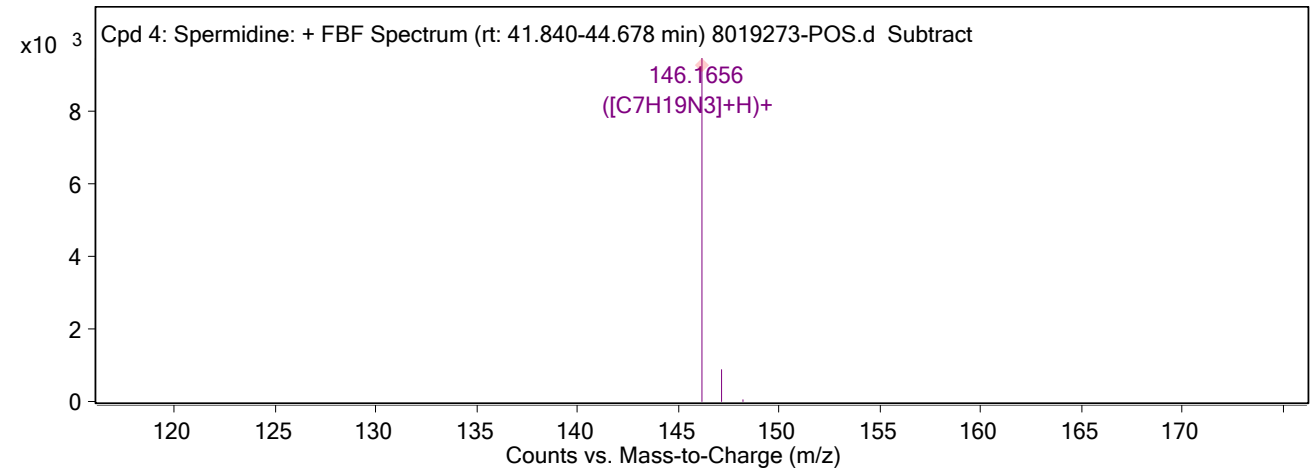
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 194.1168 | 1 | 113610.05 | C11H15NO2 | (M+H)+ |
| 195.121 | 1 | 14813.92 | C11H15NO2 | (M+H)+ |
| 196.1202 | 1 | 1222.41 | C11H15NO2 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 4: Spermidine | **Spermidine** | 146.1656 | 43.001 | Find By Formula | 145.1583 |

**Compound Chromatograms**




MS Zoomed Spectrum

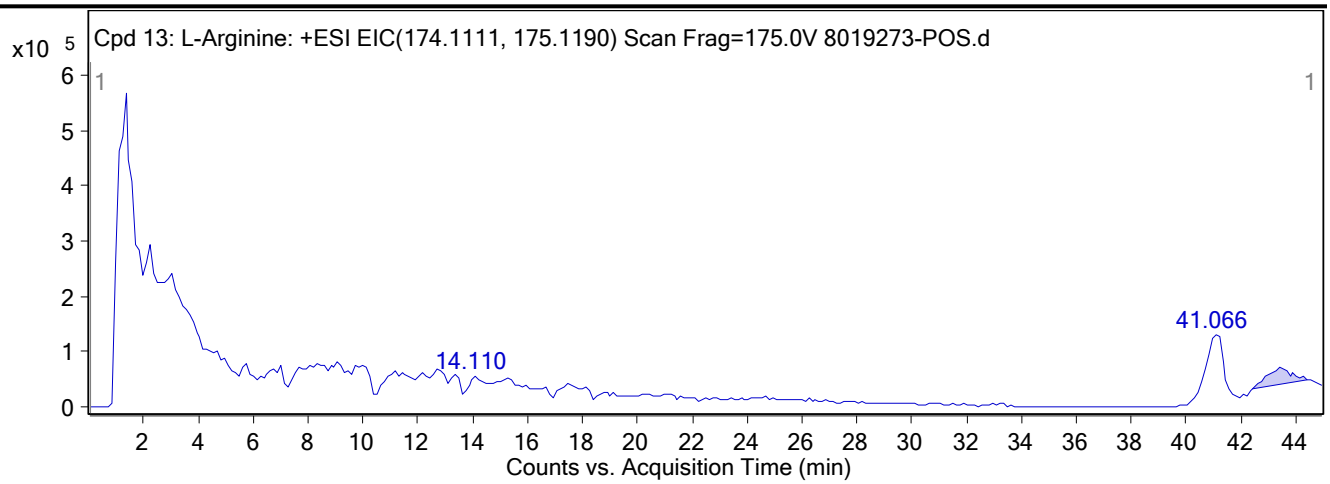



**MS Spectrum Peak List**

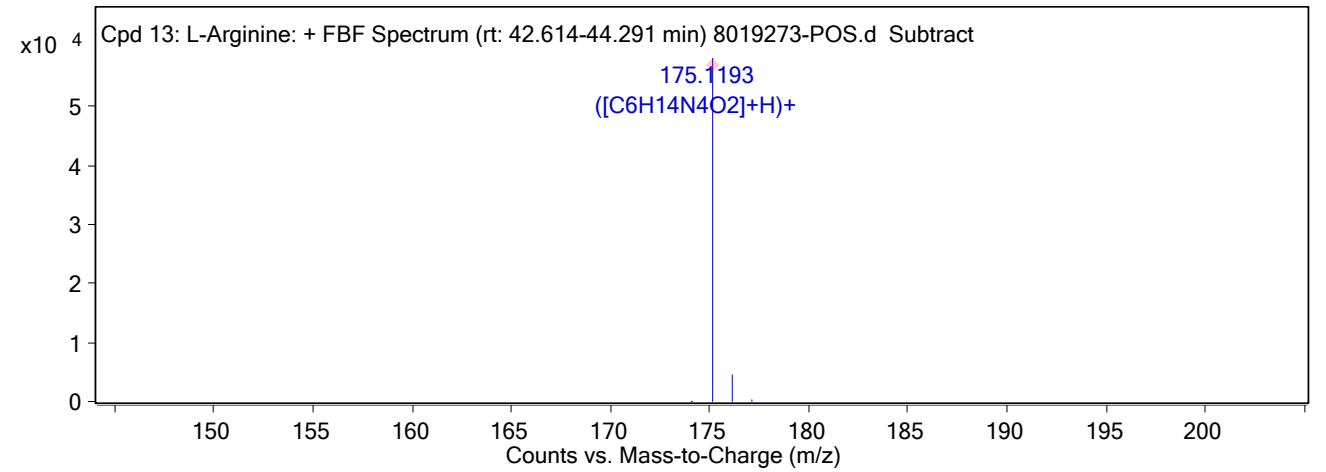
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 146.1656 | 1 | 9473.63 | C7H19N3 | (M+H)+ |
| 147.1685 | 1 | 904.53 | C7H19N3 | (M+H)+ |
| 148.1634 | 1 | 33.7 | C7H19N3 | (M+H)+ |

| Compound Label | Name | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|---|
| Cpd 13: L-Arginine | **L-Arginine** | 175.1193 | 43.388 | Find By Formula | 174.1121 |

**Compound Chromatograms**




MS Zoomed Spectrum




**MS Spectrum Peak List**

| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 174.1123 | 1 | 73.79 | C6H14N4O2 | M+ |
| 175.1193 | 1 | 58162.5 | C6H14N4O2 | (M+H)+ |
| 176.1222 | 1 | 4606.51 | C6H14N4O2 | (M+H)+ |
| 177.1256 | 1 | 309.55 | C6H14N4O2 | (M+H)+ |

--- End Of Report ---