

## Supporting Information

### A High-resolution MS, MS/MS, and UV Database of Fungal Secondary Metabolites as a Dereplication Protocol for Bioactive Natural Products

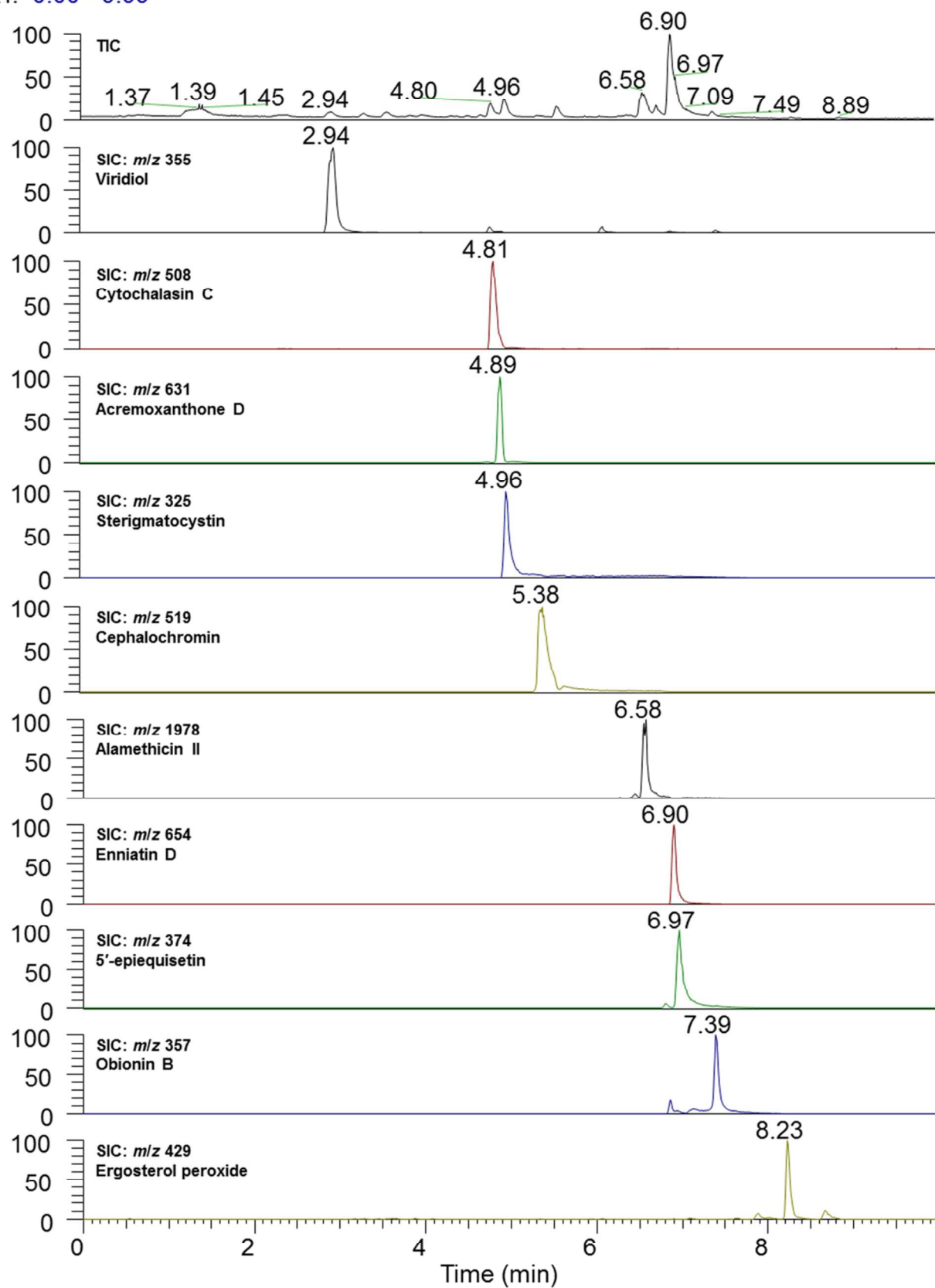
Tamam El-Elimat, Mario Figueroa, Brandie M. Ehrmann, Nadja B. Cech, Cedric J. Pearce, and Nicholas H. Oberlies

**Figure S1.** (+)-ESI TIC and SIC ( $m/z$ : 355, 508, 631, 325, 519, 1978, 654, 374, 357, and 429) of a mixture of ten standard compounds

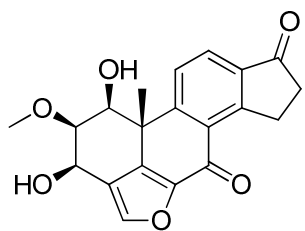
**Figure S2.** Structures of the ten compounds analyzed in figure S1

**Table S1.** Chemical structures, chemical formulas, retention times, UV absorption maxima, (+)/(-)-ESI HRMS, and (+)/(-)-ESI CID MS/MS of 172 fungal secondary metabolites

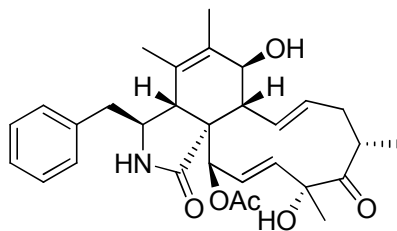
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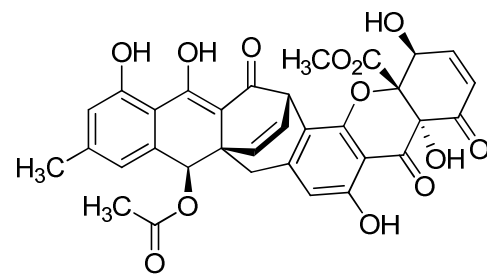
**Figure S1.** (+)-ESI TIC and SIC ( $m/z$ : 355, 508, 631, 325, 519, 1978, 654, 374, 357, and 429) of a mixture of ten standard compounds



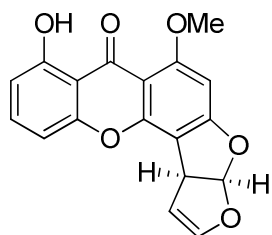
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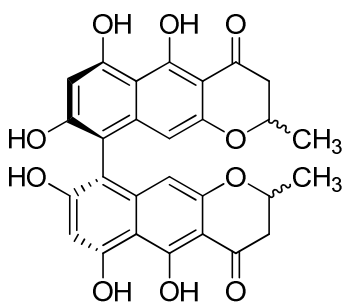
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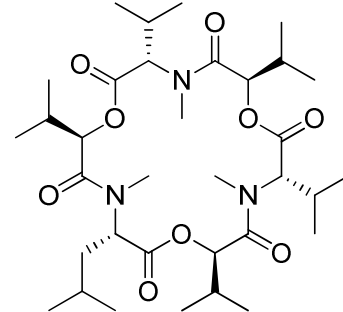
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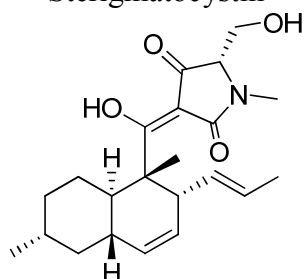
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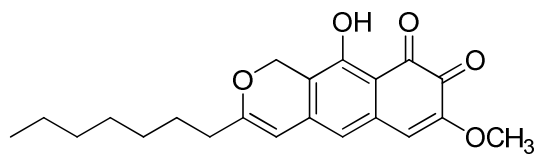
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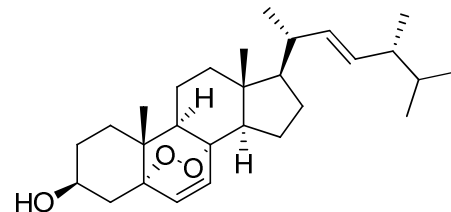
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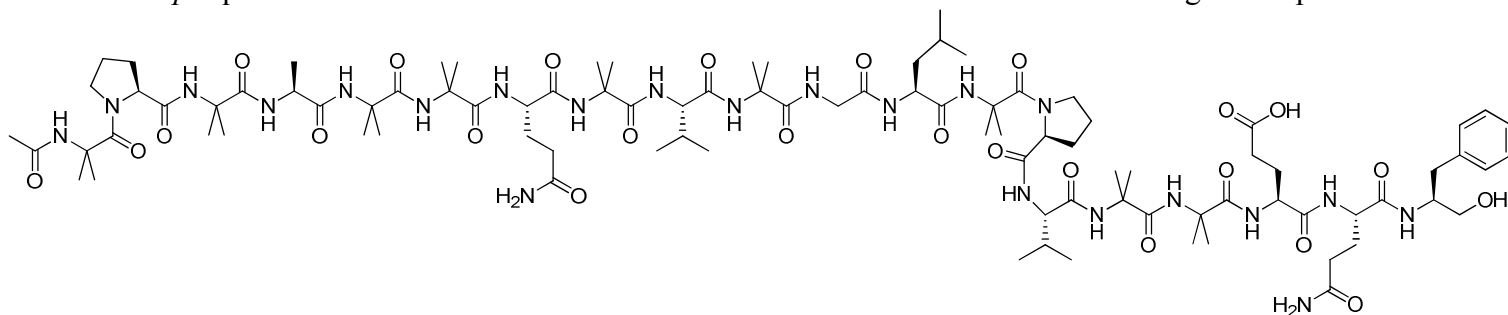
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Obionin B



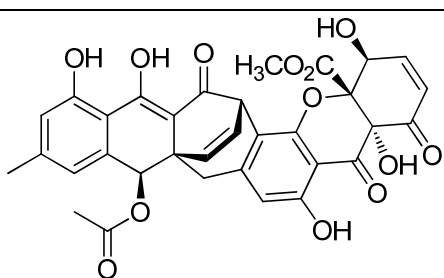
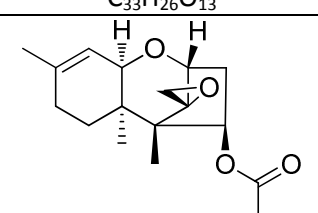
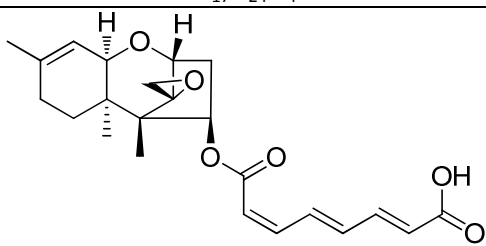
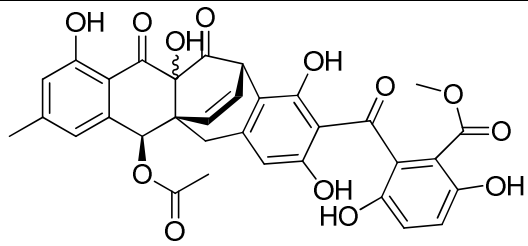
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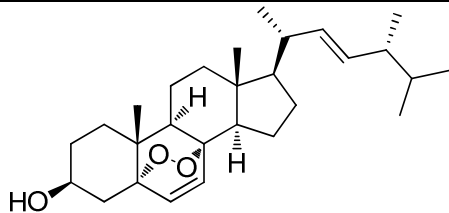
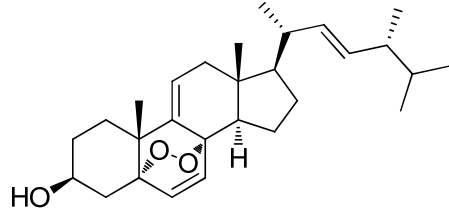
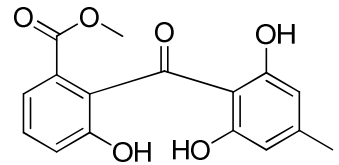
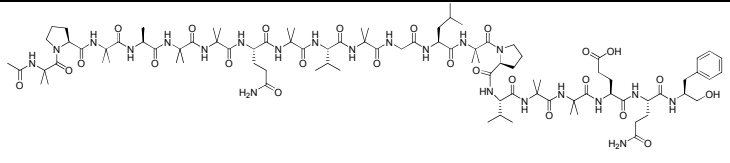
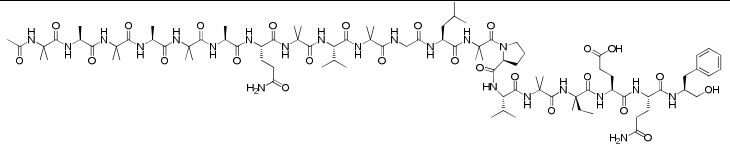


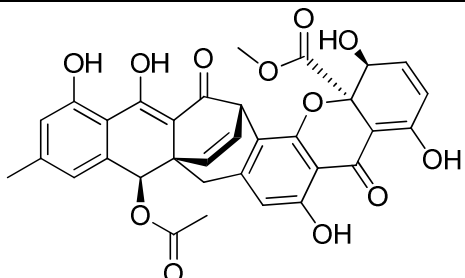
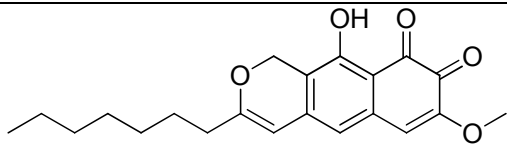
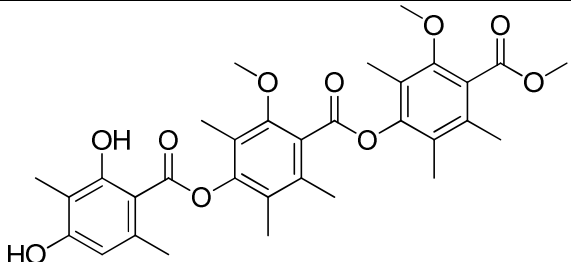
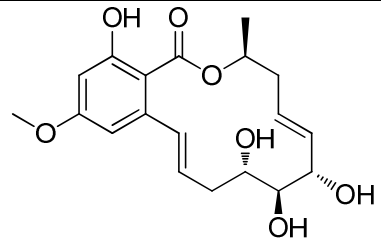
Alamethicin II

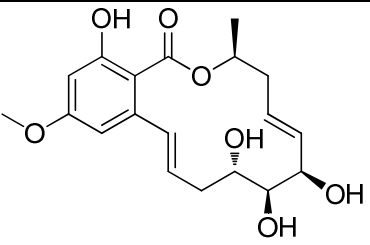
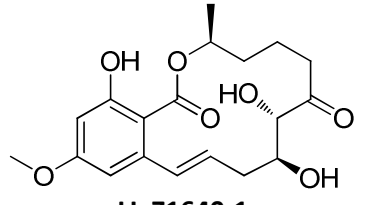
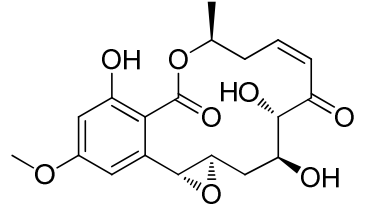
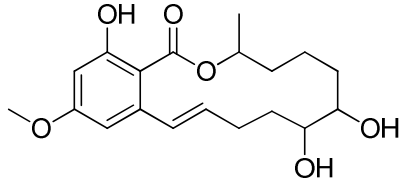
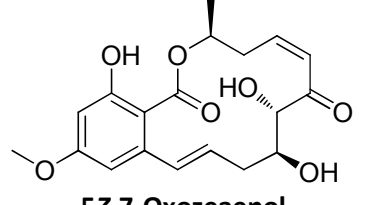
**Figure S2.** Structures of the ten compounds analyzed in figure S1

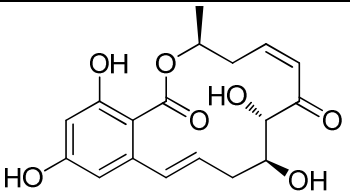
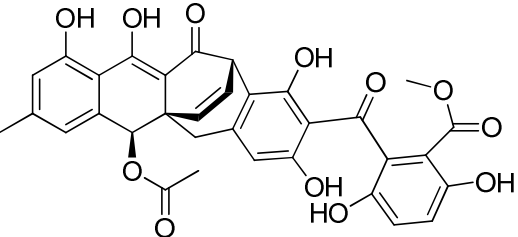
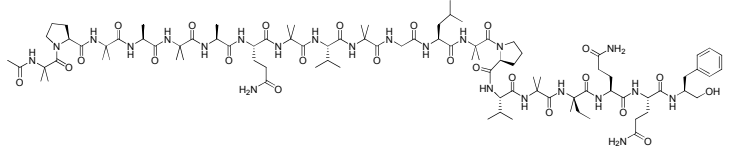
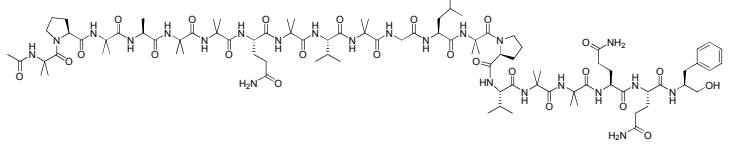
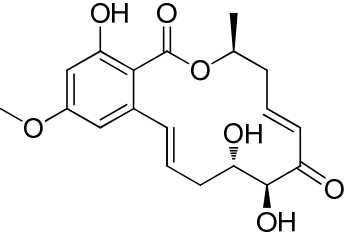
**Table S1.** Chemical structures, chemical formulas, retention times, UV absorption maxima, (+)/(-)-ESI HRMS, and (+)/(-)-ESI CID MS/MS of 172 fungal secondary metabolites

#	Chemical Structure and Chemical formula	Rt (min)	UV (nm)	Positive Ionization Mode		Negative Ionization Mode	
				[M+H] <sup>+</sup>	MS/MS	[M-H] <sup>-</sup>	MS/MS
1.	 <p><b>Acremoxanthone D</b> C<sub>33</sub>H<sub>26</sub>O<sub>13</sub></p>	4.91	228, 278, 289 363	631.14288 (-2.8)	543.18, 571.13 554.20, 525.21 553.16, 497.21 493.12, 509.20 477.12, 387.19	629.12921 (-1.4)	567.16, 507.17 445.15, 569.13 385.15, 492.13 493.18, 357.10 611.20, 463.10
2.	 <p><b>Trichodermin</b> C<sub>17</sub>H<sub>24</sub>O<sub>4</sub></p>	4.57	213	293.17474 (0.0)	233.13, 215.12 187.04, 168.96 108.91, 275.05 197.08, 124.98 189.12, 205.09	ND	ND
3.	 <p><b>Harzianum A</b> C<sub>23</sub>H<sub>28</sub>O<sub>6</sub></p>	4.25	306	401.19519 (-1.7)	215.18, 233.16 383.14, 187.06 151.00, 159.11 197.12, 132.97 145.06, 171.10	399.18127 (-0.1)	231.07, 248.76 213.25, 149.07 123.73, 337.35 249.58, 265.41 194.85, 369.14
4.	 <p><b>Acremonidin C</b> C<sub>33</sub>H<sub>26</sub>O<sub>13</sub></p>	5.20	226, 280, 345, 434	631.14264 (-3.1)	547.16, 459.14 487.15, 571.19 543.14, 447.17 387.13, 359.16 599.16, 553.21	629.12860 (-2.3)	597.18, 461.16 401.09, 383.09 357.18, 435.23 373.17, 553.26 493.17, 331.16

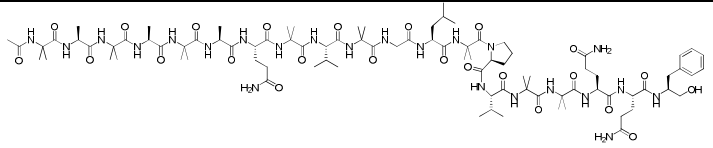
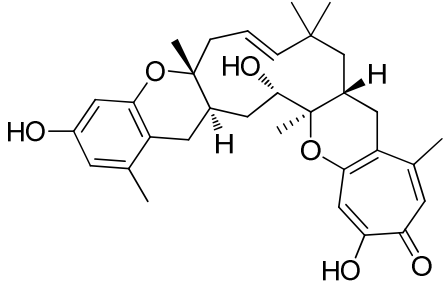
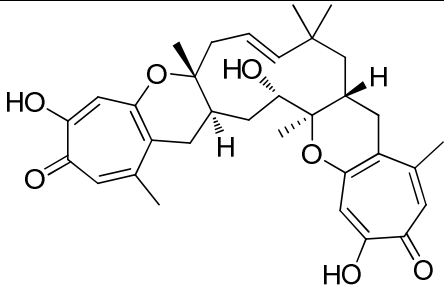
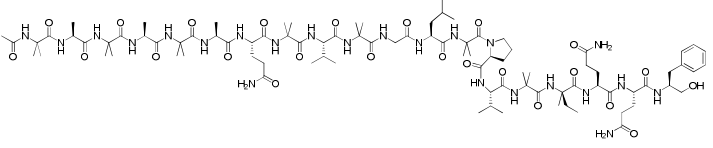
5.	 <p><b>Ergosterol peroxide</b> C<sub>28</sub>H<sub>44</sub>O<sub>3</sub></p>	8.73	226	429.33652 (+0.5)	411.36, 393.33 287.17, 269.26 305.14, 191.09 267.17, 177.10 375.32, 341.39	ND	ND
6.	 <p><b>5,8-Epidioxyergosta-6,9(11),22-trien-3-ol</b> C<sub>28</sub>H<sub>42</sub>O<sub>3</sub></p>	7.90	244	427.31998 (-1.6)	409.31, 285.15 303.19, 391.39 339.23, 381.39 267.18, 175.12 363.32, 147.09	ND	ND
7.	 <p><b>Moniliphenone</b> C<sub>16</sub>H<sub>14</sub>O<sub>6</sub></p>	3.62	215, 283	303.08652 (+0.7)	179.00, 271.08 150.97, 146.89 179.98, 284.16 259.84, 285.15 302.19, 183.24	301.07196 (+0.7)	269.04, 283.19 148.96, 225.03 256.87, 150.76 122.96, 104.82 241.03, 211.02
8.	 <p><b>Alamethicin II</b> C<sub>93</sub>H<sub>152</sub>N<sub>22</sub>O<sub>25</sub></p>	6.58	210	1978.13318 (-2.0)	934.81, 764.93 950.41, 948.92 1203.09, 1959.34, 752.58, 1205.46 1206.28, 949.75	1976.11743 (-2.6)	1849.16, 1440.77 773.41, 1568.03 1412.95, 1327.86 1958.19, 1667.01 1848.52, 1425.92
9.	 <p><b>Longibranchin III</b> C<sub>91</sub>H<sub>150</sub>N<sub>22</sub>O<sub>25</sub></p>	6.16	209	1952.11621 (-2.7)	1932.67, 922.42 1177.72, 919.79 823.55, 1933.51 836.82, 924.43 738.34, 774.65	1950.10376 (-1.6)	1932.22, 787.52 1541.78, 1513.92 1422.84, 1667.16 1414.89, 1523.87 1931.44, 1511.01

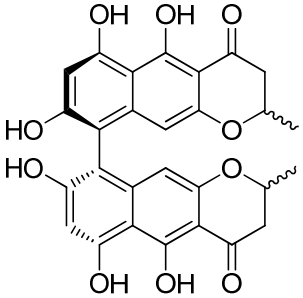
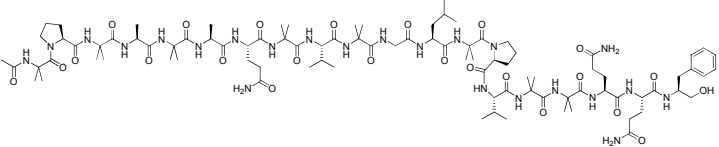
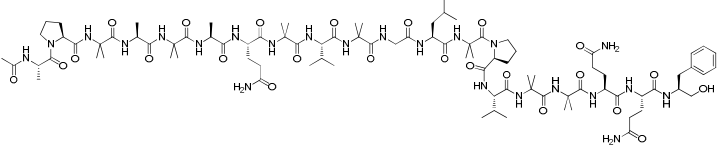
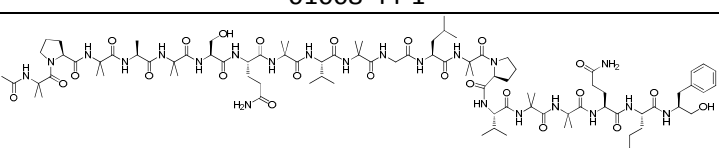
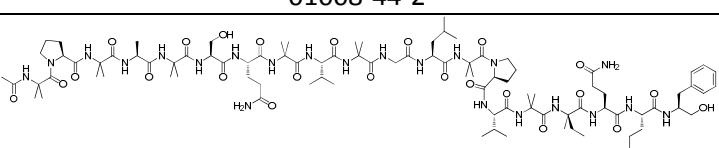
10.	 <p><b>Acremoxanthone C</b> C<sub>33</sub>H<sub>26</sub>O<sub>12</sub></p>	6.22	222, 272, 365	615.14807 (-2.7)	555.21, 495.18 467.20, 523.15 387.12, 195.05 527.18, 583.19 477.17, 505.21	613.13428 (-1.4)	581.13, 477.28 385.10, 551.17 445.07, 553.20 521.06, 491.09 537.21, 359.17
11.	 <p><b>Obionin B</b> C<sub>21</sub>H<sub>24</sub>O<sub>5</sub></p>	7.47	241, 298, 465	357.16922 (-1.2)	339.25, 259.03 357.28, 311.18 329.20, 273.14 245.04, 342.19 258.09, 231.13	355.15579 (+2.0)	341.15, 340.38 355.17, 256.00 270.21, 257.10 327.22, 312.04 313.17, 354.50
12.	 <p><b>Thielavin Q (or Thielavin B methyl ester)</b> C<sub>32</sub>H<sub>36</sub>O<sub>10</sub></p>	6.87	222, 274	581.23682 (-2.2)	548.65, 165.05 417.27, 357.02 193.01, 547.61 563.31, 562.36 581.57, 549.61	579.22321 (-0.6)	223.07, 414.86 162.98, 414.21 207.93, 176.05 165.05, 491.30 178.01, 535.83
13.	 <p><b>Zeaenol</b> C<sub>19</sub>H<sub>24</sub>O<sub>7</sub></p>	3.72	237, 270, 311	365.15948 (0.0)	285.09, 311.28 329.25, 267.18 219.09, 293.15 237.06, 175.08 347.16, 243.17	363.14493 (0.0)	188.95, 207.04 162.92, 173.94 249.15, 191.02 235.07, 161.04 205.11, 187.08

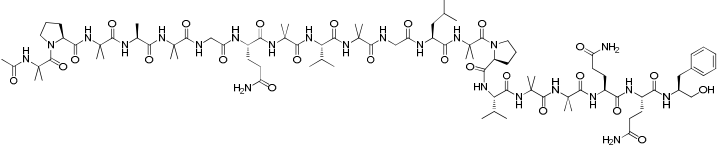
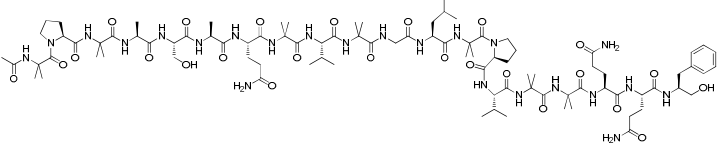
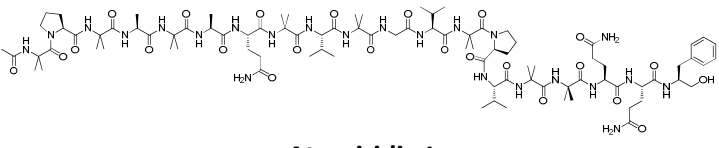
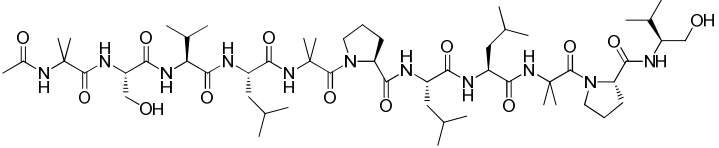
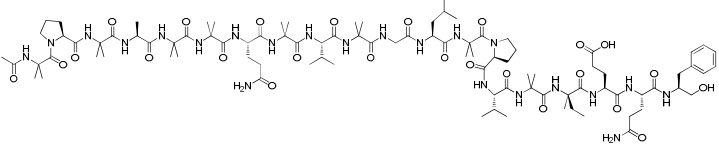
14.	 <p><b>7-epi-Zeaenol</b> 01003-58-2 C<sub>19</sub>H<sub>24</sub>O<sub>7</sub></p>	3.97	237, 270, 311	ND	ND	363.14423 (-1.9)	206.98, 189.07 163.04, 148.01 249.09, 173.98 191.15, 235.09 230.96, 204.98
15.	 <p><b>LL-Z1640-1</b> C<sub>19</sub>H<sub>24</sub>O<sub>7</sub></p>	4.26	232, 270, 311	365.15900 (-1.3)	347.18, 329.27 311.27, 237.00 219.00, 128.99 285.18, 175.00 251.11, 301.19	363.14499 (+0.2)	189.01, 345.07 235.02, 206.93 217.06, 174.00 261.05, 205.09 319.14, 301.29
16.	 <p><b>Hypothemycin</b> C<sub>19</sub>H<sub>22</sub>O<sub>8</sub></p>	3.93	230, 265, 306	379.13797 (-2.0)	253.04, 235.08 217.14, 329.13 347.13, 207.08 249.07, 303.07 311.17, 191.10	377.12473 (+1.4)	251.05, 359.05 207.06, 178.99 305.13, 341.19 205.06, 232.90 315.12, 193.00
17.	 <p><b>5,6-Dihydro-9-deoxyzeaenol</b> C<sub>19</sub>H<sub>26</sub>O<sub>6</sub></p>	4.71	228, 269, 309	351.18033 (+0.3)	333.16, 315.12 297.11, 289.22 271.16, 263.14 279.13, 245.22 231.19, 249.08	349.16568 (+0.1)	303.21, 285.20 302.24, 301.16 259.13, 332.16 329.15, 269.30 347.27, 235.12
18.	 <p><b>5Z-7-Oxozeaenol</b> C<sub>19</sub>H<sub>22</sub>O<sub>7</sub></p>	4.20	228, 272, 313	363.14349 (-0.9)	345.05, 327.19 237.01, 219.13 309.22, 283.17 319.12, 301.20 299.25, 281.09	361.12903 (-0.7)	235.01, 191.08 343.15, 189.04 217.06, 124.88 299.16, 317.14 273.13, 207.18

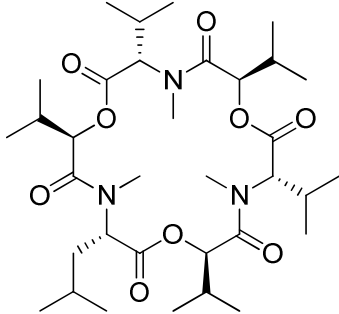
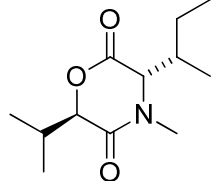
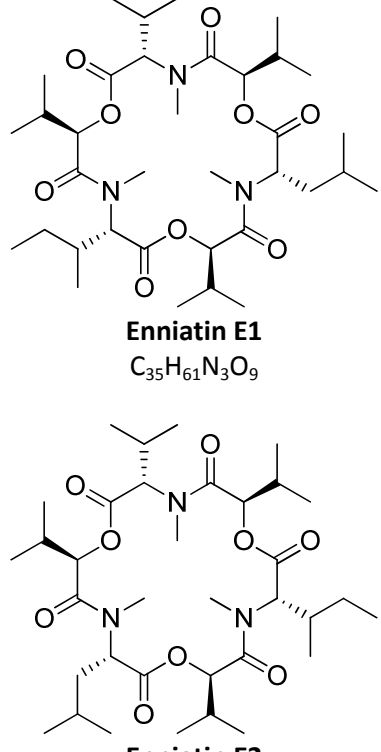
19.	 <p><b>15-O-Desmethyl-5Z-7-oxozeaenol</b> C<sub>18</sub>H<sub>20</sub>O<sub>7</sub></p>	3.42	233, 274, 313	ND	ND	347.11292 (+1.1)	220.93, 202.99 176.98, 174.98 329.07, 284.99 303.18, 227.01 311.17, 243.03
20.	 <p><b>Acremonidin A</b> C<sub>33</sub>H<sub>26</sub>O<sub>12</sub></p>	5.59	217, 278, 287, 359	615.14734 (-3.8)	421.19, 195.00 583.19, 333.16 361.23, 523.23 447.18, 555.24 387.23, 495.24	613.13367 (-2.4)	581.18, 445.17 595.27, 521.19 385.16, 477.24 537.13, 419.15 503.19, 563.37
21.	 <p><b>Atroviridin B</b> C<sub>93</sub>H<sub>153</sub>N<sub>23</sub>O<sub>24</sub></p>	6.31	211	1977.14978 (-1.7)	1008.80, 949.36 1009.60, 1205.57 1747.43, 1006.63 1332.12, 771.44 812.59, 1120.45	1975.13513 (-1.8)	1848.16, 1847.55 786.59, 1509.94 1665.82, 1830.44 1421.91, 998.63 1310.65, 1801.09
22.	 <p><b>Polysporin B</b> C<sub>93</sub>H<sub>153</sub>N<sub>23</sub>O<sub>24</sub></p>	6.46	210	1977.15137 (-0.9)	949.10, 949.91 750.45, 823.92 765.90, 1204.52 752.50, 935.66 1848.75, 773.11	1975.13428 (-2.2)	1848.06, 772.50 1848.80, 1666.00 1830.22, 1046.68 1212.17, 1649.47 1956.35, 1424.98
23.	 <p><b>5E-7-Oxozeaenol</b> C<sub>19</sub>H<sub>22</sub>O<sub>7</sub></p>	4.02	228, 270, 311	363.14325 (-1.6)	345.18, 327.18 237.10, 219.09 309.12, 301.16 265.15, 283.19 233.11, 275.12	361.12933 (+0.1)	234.99, 191.09 189.04, 343.19 217.09, 125.03 317.24, 299.12 261.15, 273.08

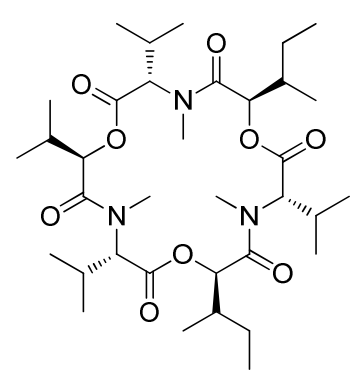
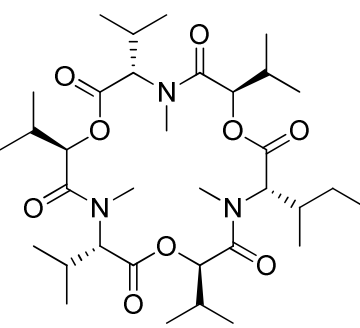
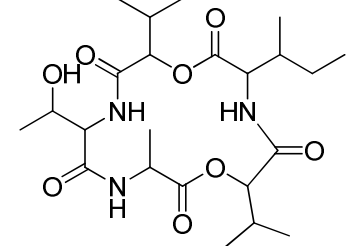


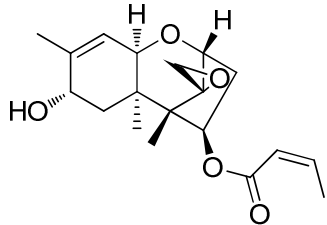
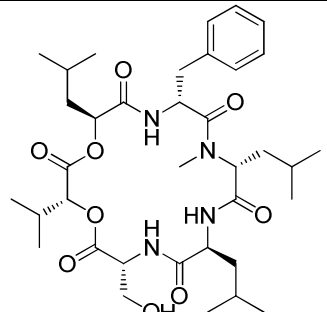
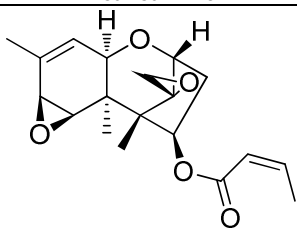
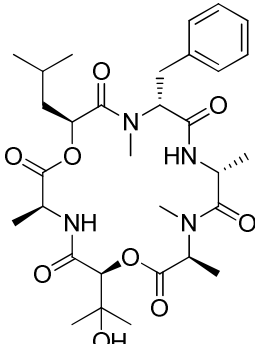
24.	 <p><b>Trichokonin VI</b> C<sub>90</sub>H<sub>149</sub>N<sub>23</sub>O<sub>24</sub></p>	5.87	210	1937.11853 (-1.7)	1657.07, 726.46 922.29, 756.39 1180.44, 1178.94 1298.93, 923.33 1586.79, 1564.66	1935.10242 (-2.5)	772.43, 1917.19 1651.98, 1495.80 1296.80, 1808.14 1737.05, 1407.86 1581.23, 1161.67
25.	 <p><b>Epolone A</b> C<sub>32</sub>H<sub>40</sub>O<sub>6</sub></p>	6.42	206, 220, 254, 363	521.28815 (-3.1)	367.26, 503.39 385.29, 201.19 337.26, 164.93 177.11, 245.16 203.07, 189.00	519.27509 (-0.2)	477.25, 383.31 478.36, 459.46 501.27, 164.01 479.56, 419.06 182.00, 351.47
26.	 <p><b>Pycnidione</b> C<sub>33</sub>H<sub>40</sub>O<sub>7</sub></p>	5.95	220, 254, 363	549.28290 (-3.2)	531.39, 485.31 385.26, 513.41 367.20, 365.31 383.26, 201.02 397.42, 503.40	547.26941 (-1.2)	162.99, 505.35 383.28, 487.39 503.36, 529.28 463.32, 461.41 519.35, 469.32
27.	 <p><b>Trichokonin VII</b> C<sub>91</sub>H<sub>151</sub>N<sub>23</sub>O<sub>24</sub></p>	6.01	210	1951.13403 (-1.8)	724.56, 908.17 1461.13, 1092.90 687.73, 823.14 1844.45, 1933.36 772.75, 1906.27	1949.11682 (-3.1)	786.56, 1931.13 1665.97, 1509.98 1822.11, 1310.83 1751.15, 1913.04 1161.58, 1906.97

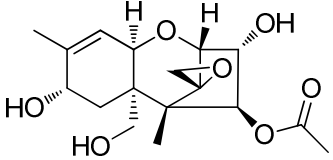
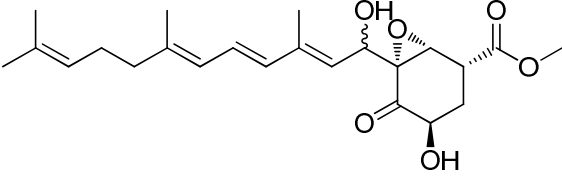
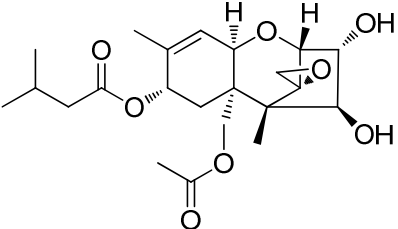
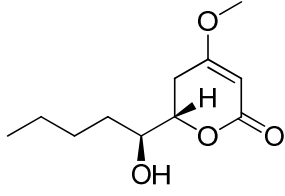
28.	 <p><b>Cephalochromin</b> C<sub>28</sub>H<sub>22</sub>O<sub>10</sub></p>	5.45	230, 270, 293, 328, 417	519.12671 (-3.6)	260.09, 501.21 477.23, 459.17 519.24, 473.13 245.02, 476.34 218.04, 219.01	517.11383 (-0.4)	499.12, 517.14 473.29, 258.04 475.15, 457.23 449.17, 500.23 474.17, 431.27
29.	 <p><b>Alamethicin F50</b> C<sub>92</sub>H<sub>151</sub>N<sub>23</sub>O<sub>24</sub></p>	6.15	217	1963.13428 (-1.6)	949.25, 1120.19 752.50, 751.32 950.26, 772.65 950.87, 849.58 1012.56, 1006.82	1961.11914 (-1.9)	1834.13, 772.55 1651.85, 1943.13 1424.79, 1495.89 1816.28, 1900.07 1832.65, 1835.08
30.	 <p><b>Atroviridin D</b> C<sub>91</sub>H<sub>149</sub>N<sub>23</sub>O<sub>24</sub> 01008-44-1</p>	5.27	217	1949.11841 (-1.8)	720.23, 1016.80 1090.70, 1192.25 1551.42, 580.30 739.55	1947.10364 (-1.9)	772.49, 1834.02 1929.20, 1496.03 1652.13, 1296.88 1173.65, 1407.82 1581.10, 651.41
31.	 <p><b>Atroviridin E</b> C<sub>92</sub>H<sub>151</sub>N<sub>23</sub>O<sub>25</sub> 01008-44-2</p>	5.35	215	1979.12988 (-1.3)	987.49, 988.14 988.93, 1009.45 1010.91, 1010.27 1011.88, 623.04 1001.74, 1000.73	1977.11316 (-2.4)	1032.40, 1849.36 1685.33, 1496.26 1903.04, 1061.79 1800.68, 1820.18 1795.63, 1737.30
32.	 <p><b>Atroviridin F</b> C<sub>93</sub>H<sub>153</sub>N<sub>23</sub>O<sub>25</sub> 01008-44-3</p>	5.51	210	1993.14758 (-0.2)	1002.30, 1010.24 665.31, 928.88 1710.32, 1483.93 933.94, 1174.82 1104.70, 1276.67	1991.13818 (+2.3)	1535.84, 1919.80 1187.93, 1115.79

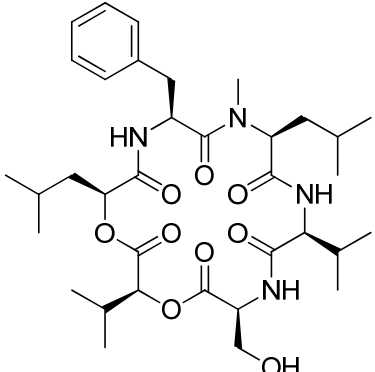
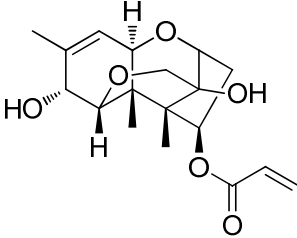
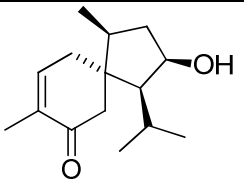
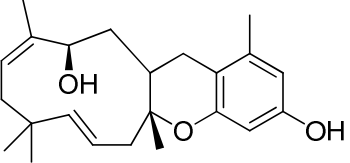
33.	 <p><b>Atroviridin G</b>  <math>C_{91}H_{149}N_{23}O_{24}</math>  01008-44-4</p>	5.55	217	1949.11914 (-1.4)	920.33, 1175.79 1018.75, 1334.09 1635.51, 1611.10 921.22, 1573.14 795.61, 972.47	1947.10217 (-2.6)	1820.12, 1819.52 1802.04, 772.46 1482.02, 1911.05 1322.50, 1567.10 1296.50, 1480.89
34.	 <p><b>Atroviridin H</b>  <math>C_{91}H_{149}N_{23}O_{25}</math>  01008-44-5</p>	6.25	217	1965.12109 (+2.2)	951.65, 767.41 952.69, 766.55 1207.64, 866.30 867.39, 1206.61 950.37, 865.36	1963.10486 (+1.3)	1835.18, 773.56 1427.01, 1944.18 1836.29, 1399.03 1313.84, 1408.86 1553.87, 1834.49
35.	 <p><b>Atroviridin I</b>  <math>C_{91}H_{149}N_{23}O_{24}</math>  01008-44-6</p>	5.98	217	1949.12170 (-0.1)	923.37, 921.46 751.22, 754.46 948.45, 1559.24 1009.45, 936.56 752.66, 1175.47	1947.10352 (-1.9)	1820.18, 772.63 1637.75, 1393.90 637.41, 754.55 1801.87, 933.88 1802.49, 1929.50
36.	 <p><b>Trichobrachin D-I</b>  <math>C_{55}H_{97}N_{11}O_{13}</math>  01008-44-7</p>	6.04	220	1120.72974 (-3.8)	920.58, 512.31 609.43, 921.58 1120.73, 610.43 513.31, 1121.73 922.58, 201.16	1118.71753 (-1.7)	1088.78, 1100.73 1089.53, 1046.47 1109.49, 1047.08 1058.74, 1071.04 1076.45, 1101.51
37.	 <p><b>Atroviridin J</b>  <math>C_{94}H_{154}N_{22}O_{25}</math>  01008-44-12</p>	6.75	219	1992.15002 (-1.4)	948.23, 1203.45 764.30, 863.19 770.48, 1968.08 1972.89, 877.11 962.47, 756.66	1990.13391 (-2.2)	1863.14, 1454.96 787.52, 1426.88 1582.04, 1327.88 1862.52, 1972.16 1681.03, 1422.89

38.	 <p><b>Enniatin D</b> C<sub>34</sub>H<sub>59</sub>N<sub>3</sub>O<sub>9</sub></p>	6.95	211	654.42932 (-4.7)	196.06, 541.26 210.09, 214.04 441.23, 228.07 626.34, 427.29 328.30, 527.48	652.41669 (-1.8)	229.99, 457.46 439.15, 212.15 425.28, 244.21 226.20, 421.19 339.28, 407.34
39.	 <p><b>1,4-Perhydrooxazine-2,5-dione II</b> 10700-97-13 C<sub>12</sub>H<sub>21</sub>NO<sub>3</sub></p>	7.44	211	228.16049 (4.7)	200.09, 99.99 114.03, 156.23 146.07, 210.27 175.29, 228.27 153.99, 159.93	226.14508 (+0.9)	182.10, 183.00 144.13, 184.05 164.03, 208.13 112.09, 154.11 128.03, 197.32
40.	 <p><b>Enniatin E1</b> C<sub>35</sub>H<sub>61</sub>N<sub>3</sub>O<sub>9</sub></p> <p><b>Enniatin E2</b></p>	7.17	206	668.44592 (-3.2)	210.12, 228.10 541.36, 196.09 555.34, 214.04 441.25, 640.35 455.36, 328.22	666.43359 (+0.1)	226.18, 439.34 244.13, 230.13 212.03, 453.22 421.40, 435.44 333.04, 236.16

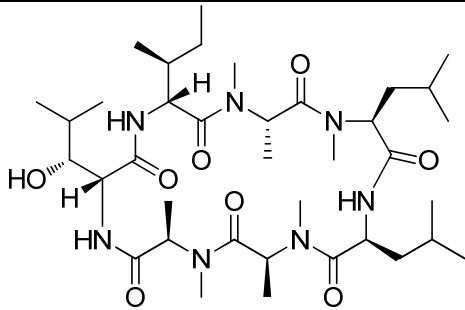
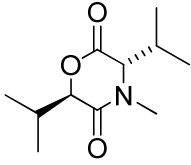
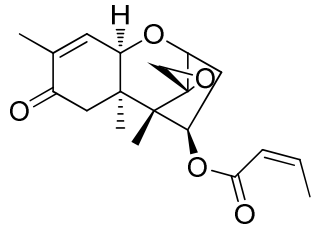
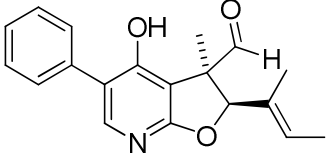
41.	<p style="text-align: center;"><math>C_{35}H_{61}N_3O_9</math></p>  <p style="text-align: center;"><b>Enniatin I</b> <math>C_{35}H_{61}N_3O_9</math></p>	7.22	211	668.44495 (-4.6)	210.13, 541.35 228.14, 196.12 214.11, 441.28 555.35, 640.41 455.29, 328.21	666.43353 (0.0)	226.18, 439.38 244.19, 453.45 212.18, 230.08 421.37, 435.23 339.44, 223.84
42.	 <p style="text-align: center;"><b>Enniatin B1</b> <math>C_{34}H_{59}N_3O_9</math></p>	7.01	211	654.43042 (-3.0)	210.08, 196.09 214.13, 541.45 527.39, 228.09 441.23, 626.45 427.28, 314.16	652.41779 (-0.1)	439.37, 212.01 230.03, 425.27 226.20, 244.12 421.39, 438.61 339.43, 407.27
43.	 <p style="text-align: center;"><b>Roseotoxin S</b> <math>C_{23}H_{39}N_3O_8</math></p>	4.12	220	486.27963 (-2.8)	468.34, 458.30 440.35, 385.19 287.18, 414.32 273.18, 357.16 333.26, 314.15	484.26636 (-0.2)	440.12, 245.06 289.21, 227.21 440.77, 270.86 466.34, 287.38 301.38, 269.18

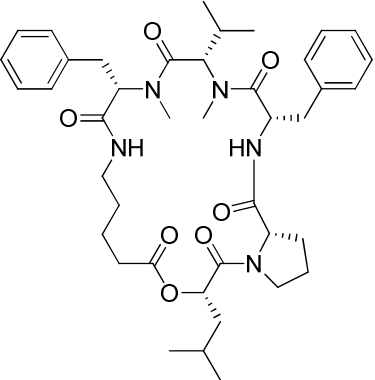
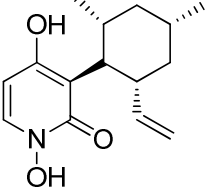
44.	 <p><b>Trichothecinol B</b> C<sub>19</sub>H<sub>26</sub>O<sub>5</sub></p>	4.03	206	335.18533 (+0.1)	231.06, 195.09 213.06, 249.08 185.05, 125.05 123.06, 201.17 317.21, 171.08	333.17102 (+1.0)	289.19, 286.96 303.30, 318.13 331.33, 226.95 253.36, 248.81 297.38, 265.09
45.	 <p><b>Trichodepsipeptide A</b> C<sub>36</sub>H<sub>56</sub>N<sub>4</sub>O<sub>9</sub></p>	6.41	224	689.41101 (-1.4)	671.41, 661.44 446.29, 576.35 489.44, 428.35 544.36, 421.38 449.20, 371.29	687.39838 (+1.3)	657.39, 518.22 656.73, 291.21 619.46, 611.42 601.38, 643.31 587.48, 307.35
46.	 <p><b>Crotoicin</b> C<sub>19</sub>H<sub>24</sub>O<sub>5</sub></p>	4.24	215	333.16998 (1.0)	247.10, 229.09 201.09, 173.09 211.06, 123.04 187.04, 183.12 159.01, 124.98	ND	ND
47.	 <p><b>Guangomide A</b> C<sub>31</sub>H<sub>46</sub>N<sub>4</sub>O<sub>9</sub></p>	5.49	217	619.33246 (-2.1)	362.18, 258.11 445.20, 601.30 344.19, 544.28 276.18, 516.27 473.38, 206.05	617.31836 (-1.4)	461.21, 448.27 274.17, 292.30 185.93, 430.24 204.10, 256.19 217.04, 403.07

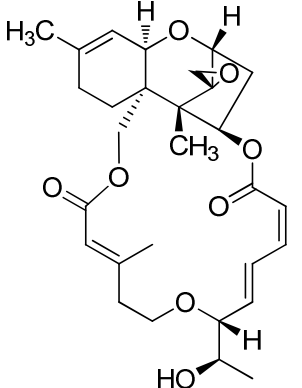
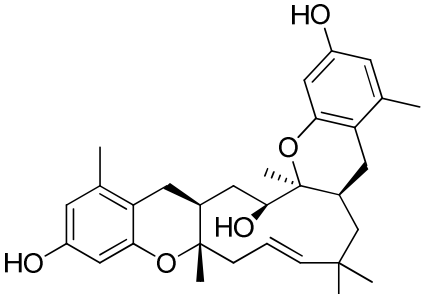
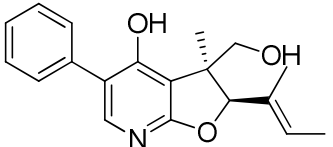
48.	 <p><b>Neosolaniol</b> C<sub>19</sub>H<sub>26</sub>O<sub>8</sub></p>	1.71	200	383.17029 (+0.6)	365.33, 355.37 382.51, 245.18 340.74, 335.32 305.14, 323.00 215.34, 383.33	ND	ND
49.	 <p><b>Trichothosporon A</b> C<sub>22</sub>H<sub>30</sub>O<sub>7</sub></p>	3.24	226	407.20605 (-0.9)	389.17, 371.24 375.05, 353.20 233.21, 303.18 347.20, 247.22 357.14, 379.22	405.19235 (+1.2)	361.30, 373.03 387.01, 390.26 377.26, 262.47 346.04, 241.19 347.37, 316.90
50.	 <p><b>HT-2 Toxin</b> C<sub>22</sub>H<sub>32</sub>O<sub>8</sub></p>	3.90	222	425.21704 (+0.1)	263.05, 245.08 407.35, 408.29 325.29, 227.10 323.19, 199.17 305.19, 215.06	423.20224 (-0.5)	291.24, 355.16 387.15, 393.04 377.22, 278.55 267.20, 404.90 305.90, 395.79
51.	 <p><b>Pestalotin</b> C<sub>11</sub>H<sub>18</sub>O<sub>4</sub></p>	3.20	237	215.12779 (0.0)	197.05, 153.11 183.13, 137.08 141.06, 171.06 165.13, 151.10 169.02, 139.09	213.11349 (+1.2)	169.08, 112.88 151.10, 197.79 181.05, 172.09 139.04, 153.00 185.97, 148.84
52.	01008-35-5*	3.65	254, 359	293.13907 (2.5)	275.14, 229.23 257.18, 261.22 191.13, 135.00 215.02, 247.22 233.27, 263.25	291.12457 (+2.7)	249.00, 205.06 163.00, 176.99 175.06, 204.03 231.97, 164.96 243.18, 273.11
53.	01008-34-4*	3.26	254, 359	293.13794 (-1.4)	275.22, 229.23 191.12, 135.04 257.16, 215.14 107.07, 175.10 177.15, 201.22	291.12411 (+1.1)	249.14, 205.08 162.97, 243.09 263.20, 151.01 135.03, 204.07 175.01, 176.87

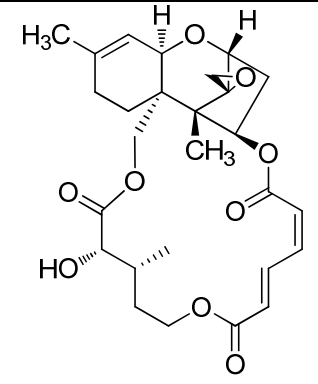
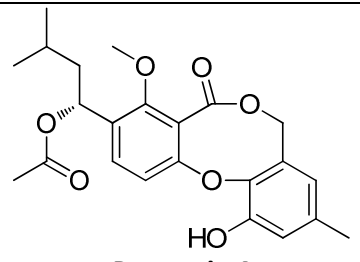
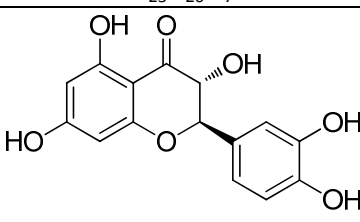
54.	 <p><b>Trichodepsipeptide B</b> C<sub>35</sub>H<sub>54</sub>N<sub>4</sub>O<sub>9</sub></p>	5.00	219	675.39630 (-0.1)	657.39, 647.44 432.29, 576.42 421.35, 414.29 449.29, 489.40 530.29, 674.45	673.38123 (-0.9)	643.36, 645.42 504.37, 291.09 655.23, 641.47 485.66, 486.27 559.42, 629.47
55.	 <p><b>Synthetic intermediate</b> C<sub>19</sub>H<sub>26</sub>O<sub>6</sub></p>	2.87	211	351.17999 (-0.6)	247.10, 229.07 217.11, 211.08 201.16, 187.05 333.15, 265.09 173.08, 199.10	ND	ND
56.	 <p><b>2-Hydroxyacoronene</b> C<sub>15</sub>H<sub>24</sub>O<sub>2</sub></p>	4.02	244	237.18456 (-1.5)	219.09, 201.06 147.04, 161.06 151.02, 191.04 163.05, 177.21 165.05, 135.04	235.17094 (+2.5)	217.18, 191.06 235.04, 207.30 192.00, 189.08 149.00, 150.86 175.01, 166.82
57.	 <p><b>Pughinin A</b> C<sub>23</sub>H<sub>32</sub>O<sub>3</sub></p>	5.15	226, 282	357.24219 (-0.6)	136.93, 215.13 339.28, 203.14 173.05, 159.12 297.19, 145.03 146.98, 191.10	355.22855 (+1.9)	355.20, 313.08 311.19, 134.90 341.18, 244.98 337.22, 327.19 285.84, 269.04

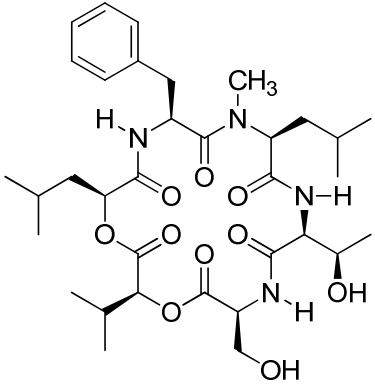
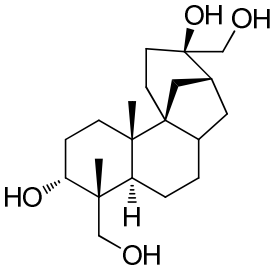
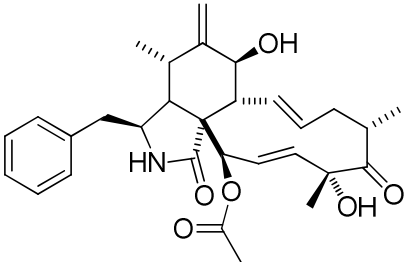
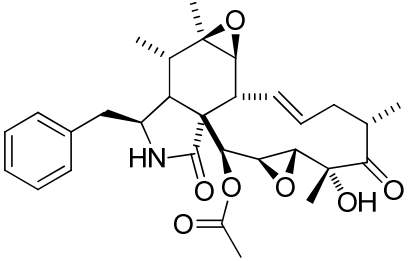


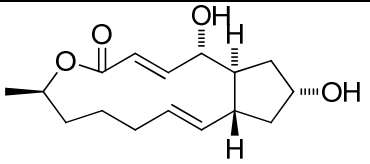
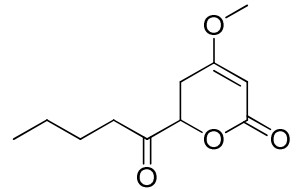
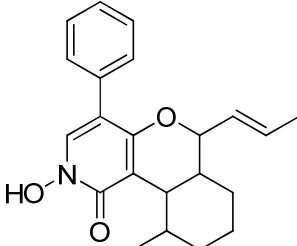
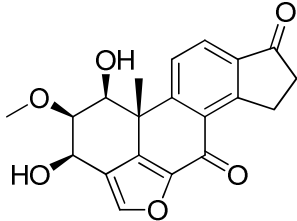
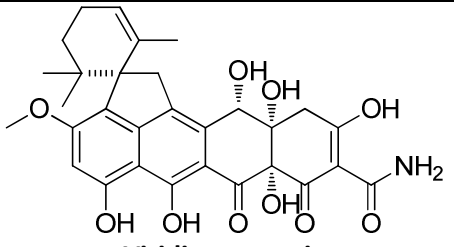
58.	 <p><b>Ternatin</b> C<sub>37</sub>H<sub>67</sub>N<sub>7</sub>O<sub>8</sub></p>	5.72	215	738.51019 (-3.0)	411.34, 720.51 666.41, 326.20 295.23, 395.30 681.51, 635.46 413.20, 710.54	736.49689 (-1.3)	664.49, 511.46 455.35, 665.23 466.11, 493.43 355.50, 357.34 448.55, 466.71
59.	 <p><b>1,4-Perhydrooxazine-2,5-dione I</b> 10700-97-3 C<sub>11</sub>H<sub>19</sub>NO<sub>3</sub></p>	6.75	217	214.14348 (-1.4)	186.06, 85.96 157.97, 140.94 168.14, 172.04 179.17	212.12924 (+0.1)	167.98, 129.88 169.18, 194.16 111.79, 170.12 170.96, 197.96 150.12, 128.07
60.	 <p><b>Trichothecin</b> C<sub>19</sub>H<sub>24</sub>O<sub>5</sub></p>	4.60	226	333.16989 (+0.7)	211.08, 229.09 247.13, 201.08 186.98, 203.09 173.13, 175.10 158.95, 125.03	331.15533 (+0.7)	287.25, 263.06 269.34, 313.13 299.11, 271.15 285.14, 277.34 303.75, 258.90
61.	 <p><b>CJ-15,696</b> C<sub>19</sub>H<sub>19</sub>NO<sub>3</sub></p>	3.91	204, 233	310.14337 (-1.3)	292.17, 268.18 282.15, 200.07 238.11, 214.07 188.03, 254.11 242.15, 240.17	308.12881 (-1.3)	280.11, 308.18 293.12, 236.21 266.16, 262.17 250.12, 198.06 251.05, 281.17

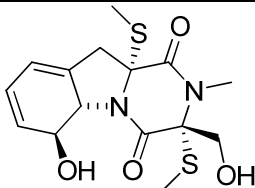
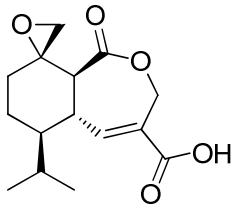
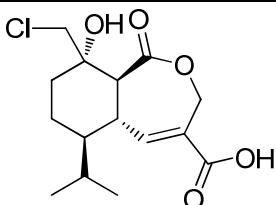
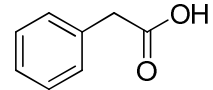
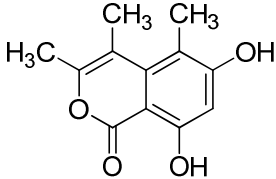
62.	 <p><b>T987A</b> C<sub>41</sub>H<sub>57</sub>N<sub>5</sub>O<sub>7</sub></p>	5.84	224	732.43097 (-2.7)	619.36, 591.43 704.43, 688.54 520.33, 581.48 458.29, 472.42 633.46, 575.54	730.41754 (-1.3)	631.41, 420.32 501.38, 520.38 402.20, 545.44 273.08, 259.14 547.39, 519.38
63.	01009-22-3P*	3.22	237	215.12820 (+1.9)	197.07, 153.09 183.10, 137.07 169.09, 151.06 165.14, 141.06 179.16, 119.11	213.11360 (+1.7)	169.06, 198.08 112.92, 150.93 180.97, 141.40 136.78, 82.97 212.89, 170.04
64.	 <p><b>Pyridoxatin</b> C<sub>15</sub>H<sub>21</sub>NO<sub>3</sub></p>	4.55	213, 289	264.15979 (+1.4)	139.93, 153.92 167.97, 182.03 180.03, 194.07 208.03, 196.07 166.04, 127.98	262.14429 (-2.2)	234.09, 218.10 243.98, 262.17 242.20, 200.19 124.98, 245.14 216.18, 175.14
65.	01007-114-3*	6.01	219	338.21103 (-1.3)	216.04, 230.09 202.15, 189.95 258.17, 256.13 244.08, 282.14 268.25, 242.14	ND	ND

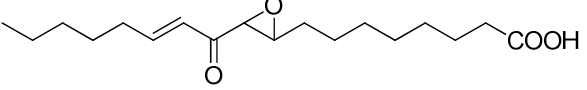
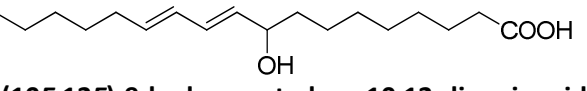
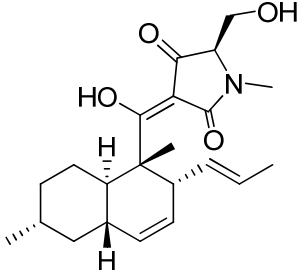
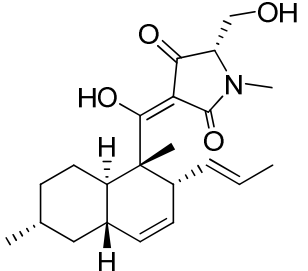
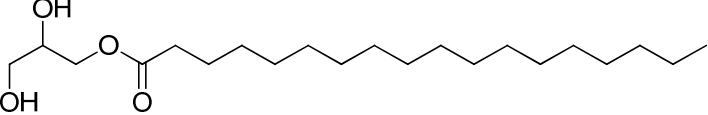
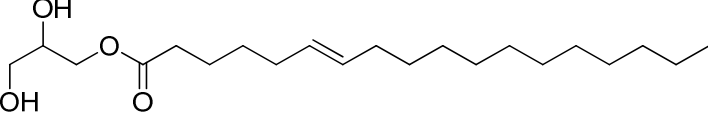
66.	 <p><b>Roridin E</b> C<sub>29</sub>H<sub>38</sub>O<sub>8</sub></p>	5.32	222, 263	515.26343 (-1.0)	361.21, 231.11 249.13, 497.35 331.25, 213.08 343.23, 185.02 203.11, 159.11	513.24957 (+0.3)	359.23, 402.67 469.45, 385.42 483.30, 451.41 201.13, 265.11 433.69, 429.01
67.	 <p><b>Ramiferin</b> C<sub>31</sub>H<sub>40</sub>O<sub>5</sub></p>	6.09	224, 282	493.29407 (-1.6)	339.19, 475.31 351.38, 369.33 215.24, 189.03 175.10, 203.20 227.13, 357.35	491.27982 (-1.0)	473.43, 445.27 447.38, 474.30 344.18, 491.15 326.24, 455.41 227.03, 421.59
68.	 <p><b>CJ-16,169</b> C<sub>19</sub>H<sub>21</sub>NO<sub>3</sub></p>	4.19	206, 232	312.15927 (-0.5)	294.19, 282.25 200.07, 254.11 214.11, 188.05 240.15, 228.08 270.19, 268.17	310.14450 (-1.2)	280.15, 310.20 308.13, 281.23 252.11, 209.13 236.18, 198.05 262.07, 309.21

69.	 <p><b>Verrucarin A</b> C<sub>27</sub>H<sub>34</sub>O<sub>9</sub></p>	4.49	226, 259	503.22672 (-1.7)	457.12, 373.16 249.10, 231.18 333.29, 390.90 213.09, 439.25 185.12, 195.14	501.21329 (+0.6)	253.17, 457.35 473.30, 371.34 225.08, 483.25 209.16, 353.19 335.13, 191.13
70.	 <p><b>Purpactin A</b> C<sub>23</sub>H<sub>26</sub>O<sub>7</sub></p>	5.85	230, 282	415.17535 (+0.5)	NF	413.16061 (+0.1)	309.07, 353.15 294.28, 323.17 321.14, 134.88 278.15, 191.12 279.14, 293.21
71.	 <p><b>Dihydroquercetin</b> C<sub>15</sub>H<sub>12</sub>O<sub>7</sub></p>	2.12	228, 289	305.06595 (+1.2)	258.99, 287.01 152.93, 194.94 148.99, 231.02 179.07, 122.88 166.92, 161.07	303.05081 (-0.7)	285.08, 176.90 124.80, 275.06 258.99, 179.00 274.30, 241.09 217.05, 214.83

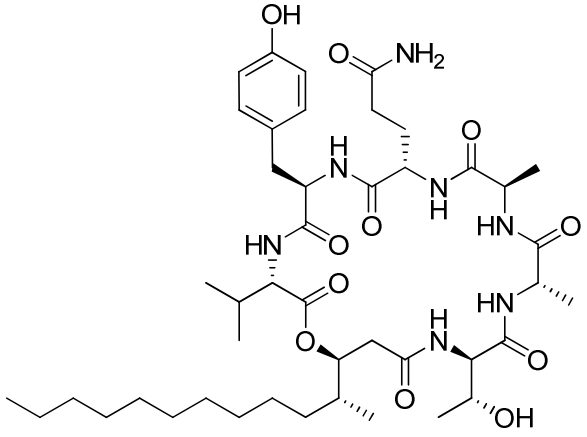
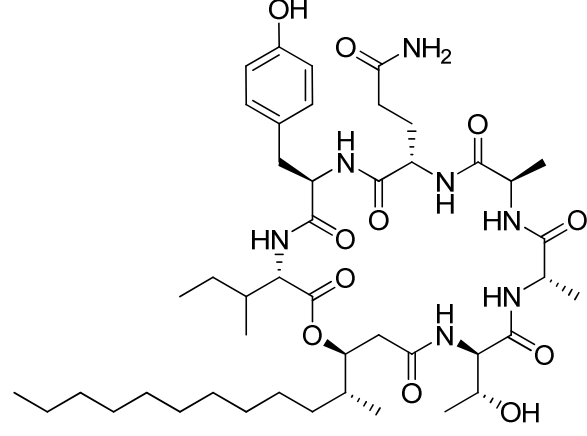
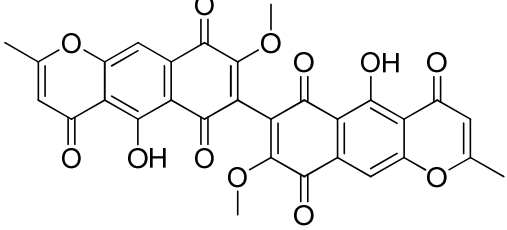
72.	 <p><b>Hirsutatin A</b> C<sub>34</sub>H<sub>52</sub>N<sub>4</sub>O<sub>10</sub></p>	5.50	217	677.37390 (-2.5)	659.37, 641.42 434.27, 649.49 514.28, 532.28 489.22, 416.30 421.33, 398.30	675.36121 (+0.2)	645.31, 506.34 505.25, 488.00 444.11, 470.23 291.25, 631.48 613.37, 601.44
73.	 <p><b>Aphidicolin</b> C<sub>20</sub>H<sub>34</sub>O<sub>4</sub></p>	3.62	ND	321.24268 (+0.8) (M+H-H <sub>2</sub> O)	222.08, 321.27 295.29, 169.08 339.37, 178.20 322.40, 120.98 269.28, 216.17	ND	ND
74.	 <p><b>Cytochalasin D; Zygosporin A</b> C<sub>30</sub>H<sub>37</sub>NO<sub>6</sub></p>	4.33	220, 285	508.26886 (-1.0)	430.24, 490.15 448.25, 412.34 388.44, 406.32 370.27, 472.29 384.42, 402.38	506.25522 (+0.8)	348.33, 446.28 366.27, 488.15 428.23, 402.99 385.26, 464.40 462.34, 287.10
75.	 <p><b>19,20-epoxycytochalasin Q</b> C<sub>30</sub>H<sub>37</sub>NO<sub>7</sub></p>	4.71	212	524.26288 (-2.7)	404.26, 428.29 446.28, 390.27 386.22, 464.39 368.17, 376.30 418.26, 358.34	522.25012 (+0.8)	462.37, 422.23 480.36, 504.20 444.28, 284.23 401.30, 266.10 404.21, 419.45

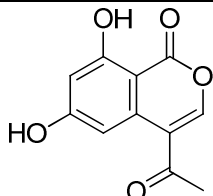
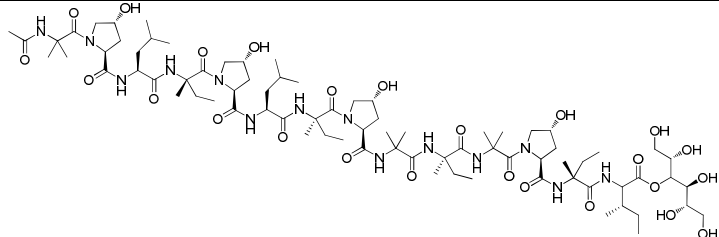
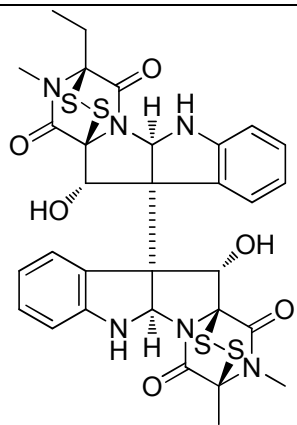
76.	 <p><b>Brefeldin A</b> C<sub>16</sub>H<sub>24</sub>O<sub>4</sub></p>	3.71	228	281.17532 (+2.1)	245.08, 263.11 199.08, 217.16 227.13, 163.04 185.03, 132.98 189.04, 235.12	279.16049 (+1.1)	235.13, 261.12 161.23, 251.17 280.00, 252.07 96.85, 190.99 173.20, 138.84
77.	 <p><b>PC<sub>3</sub></b> C<sub>11</sub>H<sub>16</sub>O<sub>4</sub></p>	3.34 3.67	230	213.11263 (+2.3)	213.09, 110.88 167.04, 195.10 84.89, 138.93 152.98, 124.99 108.94, 106.94	211.09760 (+0.1)	167.13, 183.93 181.02, 211.08 137.13, 178.84 183.12, 96.85 112.93, 192.84
78.	 <p><b>Leporin B</b> C<sub>22</sub>H<sub>25</sub>NO<sub>3</sub></p>	6.10	220, 241	352.19003 (-2.0)	216.01, 230.09 244.08, 296.17 270.11, 335.20 258.14, 282.13 272.11, 278.11	350.17621 (+0.1)	350.12, 115.88 306.22, 197.97 228.03, 332.30 201.00, 214.01 185.98, 322.16
79.	 <p><b>Viridiol</b> C<sub>20</sub>H<sub>18</sub>O<sub>6</sub></p>	2.95	244, 319	355.11725 (-1.0)	281.05, 309.14 337.12, 249.08 277.13, 308.39 279.21, 305.17 253.15, 291.08	353.10342 (+1.0)	278.96, 325.17 335.16, 297.15 338.10, 279.87 294.41, 321.26 277.25, 309.15
80.	 <p><b>Viridicatumtoxin</b> C<sub>30</sub>H<sub>31</sub>NO<sub>10</sub></p>	5.74	235, 383, 432	548.19080 (-1.3) M+H-H <sub>2</sub> O	509.19, 548.23 510.21, 549.23 492.20, 380.23 493.22, 523.23 522.12, 530.21	564.18689 (-1.1)	502.31, 547.22 546.17, 520.27 529.22, 485.19 405.23, 459.32 503.27, 379.25

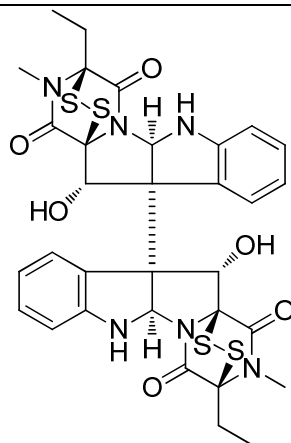
81.	 <p><b>Bisdethiobis(methylthio) gliotoxin</b> C<sub>15</sub>H<sub>20</sub>N<sub>2</sub>O<sub>4</sub>S<sub>2</sub></p>	3.33	215, 267	357.09399 (+0.7)	309.04, 243.12 291.01, 215.17 192.11, 233.19 261.20, 143.95 281.22, 278.11	355.07996 (+2.2)	277.11, 340.12 325.09, 307.04 327.11, 337.12 309.09, 354.96 278.08, 283.19
82.	 <p><b>Heptelidic acid</b> C<sub>15</sub>H<sub>20</sub>O<sub>5</sub></p>	3.80	226	281.13898 (+2.2)	263.02, 245.02 217.05, 221.06 235.06, 203.06 189.04, 199.06 227.05, 171.10	279.12384 (+0.2)	205.23, 173.17 235.10, 191.11 217.03, 149.12 207.11, 189.16 176.94, 248.97
83.	 <p><b>Heptelidic acid chlorhydrin</b> C<sub>15</sub>H<sub>21</sub>ClO<sub>5</sub></p>	3.88	232	317.11490 (-2.1) neutral	298.98, 253.10 281.02, 245.06 217.11, 263.07 239.10, 203.13 227.17, 235.20	315.10062 (+2.2)	279.14, 271.02 261.06, 234.92 191.16, 204.95 243.35, 217.04
84.	 <p><b>Phenylacetic acid</b> C<sub>8</sub>H<sub>8</sub>O<sub>2</sub></p>	1.41	211	137.05965 (-0.4)	91.92, 136.93 90.86, 119.97 119.34, 115.92 118.29, 124.57	135.04526 (+0.8)	90.88, 134.93 107.99, 119.71 81.79, 92.88
85.	 <p><b>Decarboxy-citrinone</b> C<sub>12</sub>H<sub>12</sub>O<sub>4</sub></p>	4.37	246, 267, 339	221.08017 (-3.0)	174.99, 203.01 192.99, 220.98 164.99, 151.09 146.99, 122.99 137.01, 179.06	219.06602 (-1.2)	219.04, 204.02 174.97, 191.01 177.02, 201.05 148.94, 151.04 217.13, 189.02

86.	 <p><b>(E)-8-(3-(oct-2-enoyl)oxiran-2-yl)octanoic acid</b> C<sub>18</sub>H<sub>30</sub>O<sub>4</sub></p>	5.52	232	311.22174 (+0.2)	293.25, 275.16 257.17, 265.17 110.93, 139.05 247.20, 163.05 177.02, 197.09	309.20663 (-1.6)	291.16, 281.22 273.12, 267.18 265.30, 263.25 247.29, 211.14 209.08, 193.03
87.	 <p><b>(10E,12E)-9-hydroxyoctadeca-10,12-dienoic acid</b> C<sub>18</sub>H<sub>32</sub>O<sub>3</sub></p>	6.10	220	297.24216 (-0.9)	282.04, 279.19 283.06, 269.36 297.29, 280.24 251.18, 241.19 237.14, 261.21	295.22803 (+0.5)	182.98, 277.22 155.06, 251.27 138.92, 295.22 267.21, 233.17 137.05, 195.14
88.	 <p><b>Equisetin</b> C<sub>22</sub>H<sub>31</sub>NO<sub>4</sub></p>	6.87	230, 295	374.23221 (-1.0)	356.22, 346.27 175.10, 170.04 200.03, 177.15 205.12, 184.02 143.98, 231.14	372.21686 (-0.2)	342.28, 298.18 324.22, 343.37 111.87, 123.85 314.20, 281.97 256.09, 371.94
89.	 <p><b>5'-epiequisetin</b> C<sub>22</sub>H<sub>31</sub>NO<sub>4</sub></p>	7.01	231, 296	374.23230 (-0.8)	356.24, 346.27 175.13, 170.01 200.02, 177.11 205.13, 184.02 143.96, 231.13	372.21729 (+1.0)	342.25, 298.29 324.29, 343.26 112.07, 124.01 241.15, 135.95 314.30, 230.14
90.	 <p><b>2,3-dihydroxypropyl stearate</b> C<sub>21</sub>H<sub>42</sub>O<sub>4</sub></p>	8.55	ND	359.31537 (-0.6)	341.36, 267.16 313.39, 359.35 285.29, 342.06 274.89, 331.37 303.32, 255.14	ND	
91.	 <p><b>(E)-2,3-dihydroxypropyl octadec-6-enoate</b> C<sub>21</sub>H<sub>40</sub>O<sub>4</sub></p>	7.98	226	357.29962 (-0.9)	339.32, 265.26 247.24, 283.17 135.08, 149.09 120.96, 163.08 151.09, 177.07	ND	

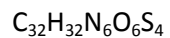


92.	 <p><b>Acuminatum C</b> C<sub>44</sub>H<sub>71</sub>N<sub>7</sub>O<sub>11</sub></p>	6.13	224, 276	874.52637 (-2.4)	856.60, 551.29 857.52, 775.52 534.39, 839.51 768.23, 434.17 757.46, 838.57	872.51196 (-2.2)	828.49, 854.69 588.47, 549.41 674.57, 606.53 632.45, 437.49 630.24, 829.34
93.	 <p><b>Acuminatum B</b> C<sub>45</sub>H<sub>73</sub>N<sub>7</sub>O<sub>11</sub></p>	6.42	224, 276	888.54095 (-3.5)	870.54, 565.30 871.56, 775.48 548.33, 853.61 434.17, 782.39 852.78, 757.65	886.52802 (-1.7)	842.49, 868.60 563.48, 602.36 646.45, 620.51 688.46, 664.48 437.28, 644.22
94.	 <p><b>Aurofusarin</b> C<sub>30</sub>H<sub>18</sub>O<sub>12</sub></p>	4.84	243, 269, 380	571.08600 (-1.9)	556.12, 511.15 539.15, 557.18 541.19, 512.17 540.13, 497.18 528.18, 524.11	569.07257 (0.0)	523.16, 538.08 537.29, 539.13 524.01, 554.02 509.19, 525.06 540.12, 569.14

95.	 <p><b>AGI-7</b> C<sub>11</sub>H<sub>8</sub>O<sub>5</sub></p>	3.04	230, 263, 326	221.04536 (+4.1)	178.98, 221.02 160.96, 203.04 136.92, 150.99 175.11, 165.08 193.06, 133.06	219.02966 (-1.1)	218.85, 216.95 177.01, 174.97 191.05, 130.95 146.90, 132.97 148.87, 172.92
96.	 <p><b>Clonostachin</b> C<sub>78</sub>H<sub>134</sub>N<sub>14</sub>O<sub>25</sub></p>	5.38	220	1667.97253 (+0.5)	1612.73, 763.39 1650.04, 1583.62 1616.32, 1671.57	1665.95349 (-2.2)	1501.97, 1538.92 1374.79, 1483.88 1501.33, 1049.60 1288.72, 1356.65 1161.68, 1502.62
97.	01009-91-5*	5.41	219	1681.98291 (-2.7)	847.22, 846.48 854.06, 848.06 845.84, 1403.76 1077.69, 1516.99 855.21, 1419.15	1679.96924 (-2.1)	1516.01, 1515.00 1552.42, 1370.88 1063.34, 1553.23 1372.96, 850.95 1388.48, 1374.97
98.	 <p><b>Sch 52901</b> C<sub>31</sub>H<sub>30</sub>N<sub>6</sub>O<sub>6</sub>S<sub>4</sub></p>	5.75	209, 300	711.11609 (-3.0)	629.17, 647.13 646.52, 383.22 397.25, 465.13 233.16, 479.12 565.21, 232.11	709.10400 (+0.4)	645.00, 610.97 579.24, 613.26 643.15, 554.17 508.90, 577.26 461.20, 463.31



**Verticillin H**



99.

6.02

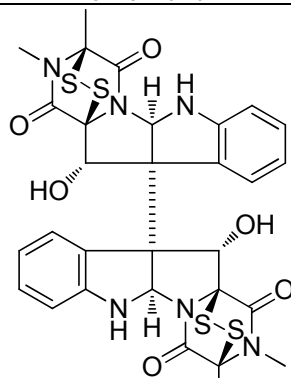
211,  
302

725.13208  
(-2.5)

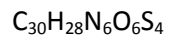
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397.26, 415.10  
479.22, 579.36  
233.05, 232.12  
298.20, 478.50

723.11993  
(+0.8)

659.17, 658.53  
657.04, 625.13  
477.09, 411.16  
593.07, 595.43  
526.08, 568.45



**Verticillin A**



100.

5.45

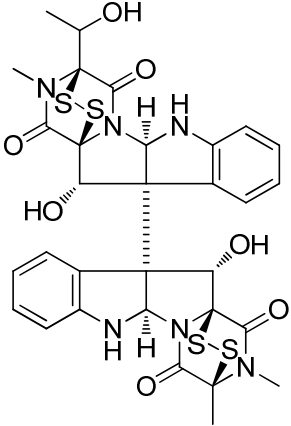
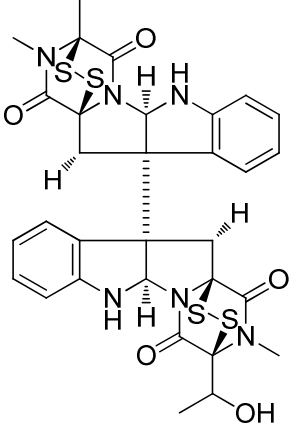
217,  
298

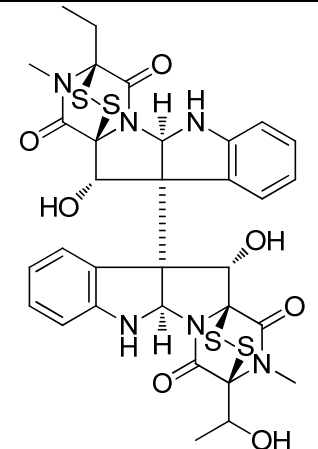
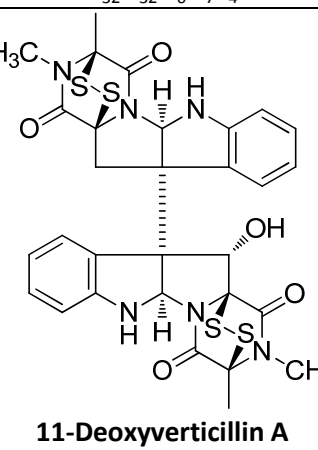
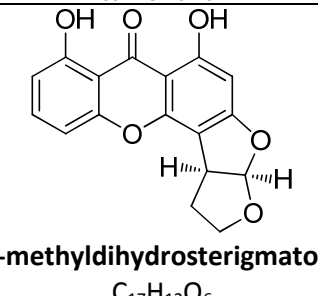
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(-1.5)

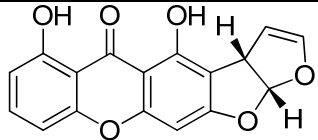
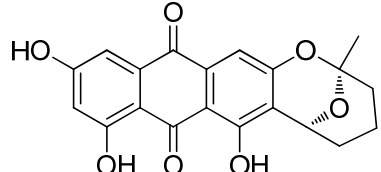
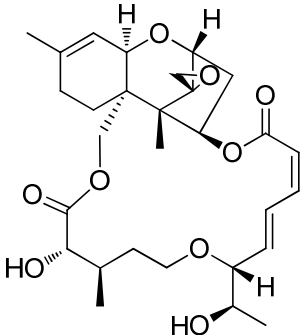
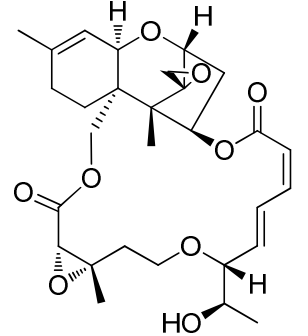
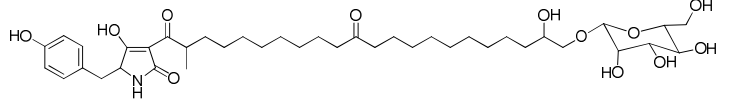
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233.09, 401.22  
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284.13, 232.11

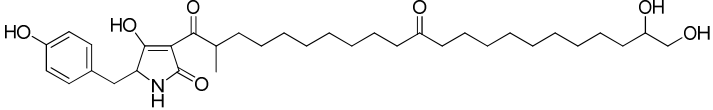
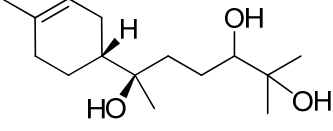
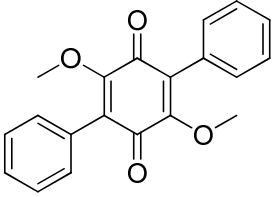
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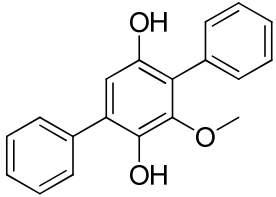
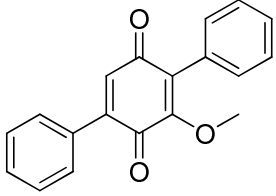
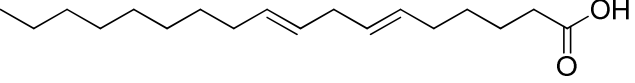
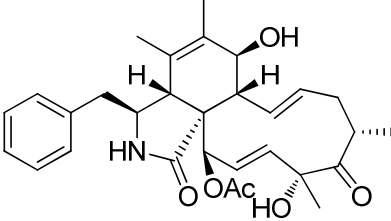
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565.19, 599.19  
660.91, 495.01  
463.07, 598.58  
629.20, 446.96

101.	 <p><b>Sch 52900</b> C<sub>31</sub>H<sub>30</sub>N<sub>6</sub>O<sub>7</sub>S<sub>4</sub></p>	5.19	213, 300	727.11115 (-2.3)	645.10, 663.10 413.23, 266.14 383.22, 495.16 662.42, 465.08 296.16, 233.14	725.09814 (-0.6)	661.01, 583.16 597.09, 647.07 661.98, 627.14 643.08, 595.24 617.16, 659.21
102.	 <p><b>Gliocladicillin A</b> C<sub>31</sub>H<sub>30</sub>N<sub>6</sub>O<sub>5</sub>S<sub>4</sub></p>	5.41	206, 298	695.12158 (-2.5)	629.09, 631.15 479.00, 630.31 397.18, 280.08 268.17, 233.13 613.17, 384.25	693.10822 (-0.8)	629.06, 595.23 627.06, 563.30 461.24, 446.95 561.35, 381.23 597.05, 395.14

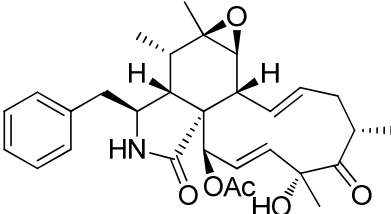
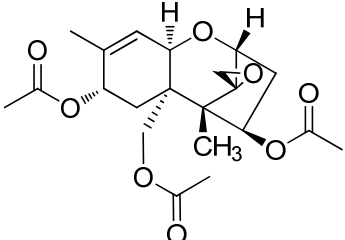
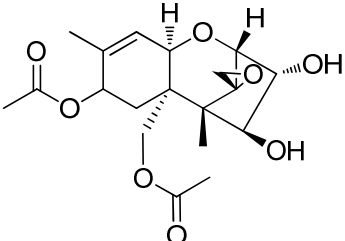
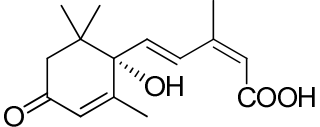
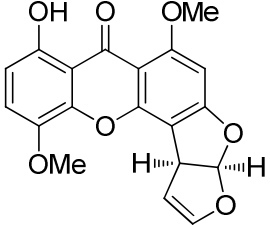
103.	 <p><b>Gliocladicillin C</b> C<sub>32</sub>H<sub>32</sub>N<sub>6</sub>O<sub>7</sub>S<sub>4</sub></p>	5.54	207 298	741.12683 (-2.7)	659.16, 677.04 413.26, 280.16 495.12, 676.40 397.31, 296.16 479.00, 233.06	739.11279 (-2.0)	675.09, 597.19 611.07, 643.21 657.26, 660.95 567.21, 631.23 675.94, 565.26
104.	 <p><b>11-Deoxyverticillin A</b> C<sub>30</sub>H<sub>28</sub>N<sub>6</sub>O<sub>5</sub>S<sub>4</sub></p>	5.12	215, 298	681.10596 (-2.5)	615.11, 465.02 617.22, 383.22 616.30, 233.12 268.15, 266.10 384.23, 385.23	679.09326 (+0.2)	615.00, 581.10 613.06, 547.10 446.93, 381.31 549.33, 583.11 644.81, 587.84
105.	 <p><b>De-O-methyldihydrosterigmatocystin</b> C<sub>17</sub>H<sub>12</sub>O<sub>6</sub></p>	5.92	230, 248, 333	313.06998 (-2.2)	285.11, 313.09 257.04, 286.19 295.12, 243.11 284.25, 202.99 269.09, 258.10	311.05634 (+0.7)	311.04, 282.99 312.16, 283.99 255.04, 242.89 281.13, 182.99 293.00, 255.99

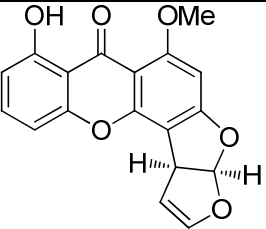
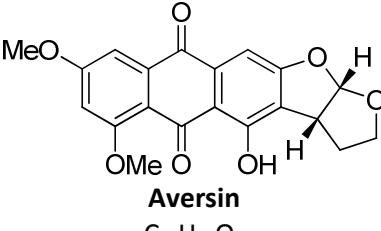
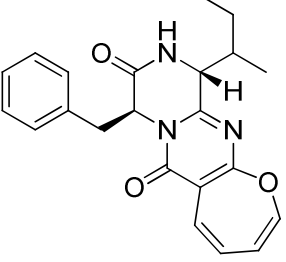
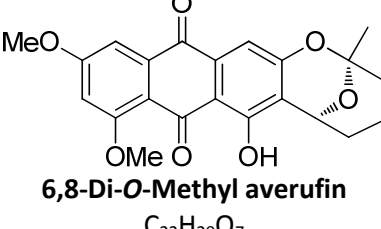
106.	 <p><b>Sterigmatin</b> C<sub>17</sub>H<sub>10</sub>O<sub>6</sub></p>	6.22	224, 250, 322	311.05511 (+0.3)	283.10, 255.19 269.07, 284.12 293.25, 265.07 311.18, 241.14 267.13, 292.57	309.03961 (-2.8)	309.19, 264.94 281.12, 282.02 240.83, 96.92 248.11, 280.47 266.22, 262.77
107.	 <p><b>Averufin</b> C<sub>20</sub>H<sub>16</sub>O<sub>7</sub></p>	6.35	222, 267, 293, 321, 450	369.09604 (-2.3)	351.11, 311.09 299.12, 327.09 285.09, 309.11 333.12, 273.03 323.12, 369.12	367.08197 (-1.0)	367.05, 284.08 295.14, 285.15 368.25, 297.13 282.98, 310.08 296.05, 308.97
108.	 <p><b>Roridin A</b> C<sub>29</sub>H<sub>40</sub>O<sub>9</sub></p>	4.46	224, 263	533.27319 (-2.5)	249.09, 231.12 333.22, 403.01 385.10, 213.17 185.06, 195.03 203.15, 247.10	531.26093 (+1.8)	401.39, 513.39 487.27, 371.34 469.34, 365.20 357.21, 501.45 237.16, 265.19
109.	 <p><b>Roridin D</b> C<sub>29</sub>H<sub>38</sub>O<sub>9</sub></p>	4.81	224, 259	531.25763 (-2.3)	249.10, 231.21 485.27, 403.03 185.11, 213.12 347.20, 203.13 195.18, 331.22	529.24548 (+2.2)	263.12, 485.19 511.27, 501.29 235.14, 441.26 374.94 163.04 237.13, 219.17
110.	 <p><b>Virgineone</b> C<sub>40</sub>H<sub>63</sub>NO<sub>12</sub></p>	5.41	222, 280	750.44183 (-0.6)	588.47, 570.44 732.39, 552.64 678.38, 612.61 714.36, 552.04 540.43, 696.54	748.42511 (-3.5)	642.41, 686.41 643.53, 480.41 586.45, 687.58 524.39, 436.45 654.46, 506.58

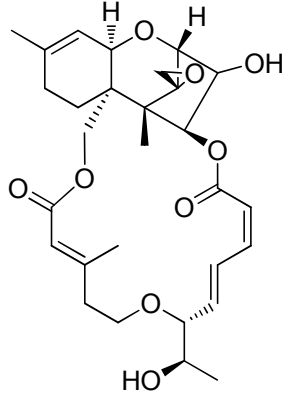
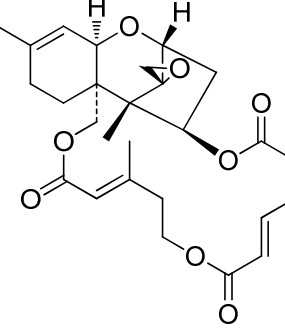
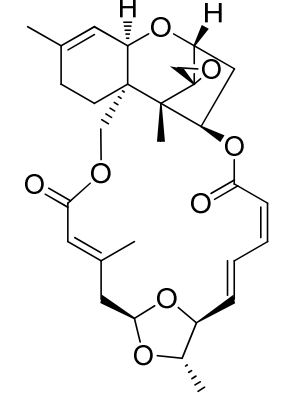
111.	 <b>Virgineone aglycone</b> $C_{34}H_{53}NO_7$	6.10	224, 280	588.38794 (-2.6)	570.49, 552.40 206.11, 534.43 540.50, 337.39 464.45, 400.34 440.50, 365.43	586.37305 (-3.2)	480.44, 481.53 524.51, 436.42 492.60, 542.61 204.02, 406.33 418.22, 525.65
112.	01009-74-3*	5.91	226, 293, 374		586.43, 568.38 730.27, 550.52 676.40, 694.46 587.13, 365.34 538.43, 712.76		584.35, 585.45 746.57, 540.39 566.52, 626.47 522.53, 702.54 703.57, 541.48
113.	 <b>5,6-dihydroxybisabolol</b> $C_{15}H_{28}O_3$	3.73	220, 281	257.21182 (+2.7)	221.12, 239.09 203.11, 127.02 118.97, 133.05 108.98, 147.03 149.07, 240.04	255.19684 (+1.1)	211.18, 237.25 159.01, 136.96 227.97, 81.03 212.60, 201.22 219.13, 208.92
114.	01007-150-1*	5.24	232, 257, 293, 372	287.09180 (+1.4)	269.12, 272.07 254.07, 259.15 287.16, 257.09 258.13, 226.08 267.11, 270.00	285.07736 (+1.8)	255.15, 284.98 270.11, 240.97 257.04, 225.02 239.92, 270.98 196.83, 242.03
115.	01007-150-3 (01008-93-2)*	6.39	228, 259, 287, 380	257.08112 (+1.1)	257.09, 242.02 214.11, 243.05 258.11, 225.04 226.14, 227.13 213.25, 215.06	ND	ND
116.	01007-150-4*	6.77	232, 254, 289, 369	271.09628 (-0.8)	256.08, 271.10 239.04, 228.10 257.10, 241.11 240.07, 272.22 227.25, 212.95	ND	ND
117.	 <b>Betulinan A</b> $C_{20}H_{16}O_4$	5.52	224, 265, 324	321.11212 (0.0)	289.26, 306.11 293.15, 274.21 258.08, 271.11 290.17, 261.22 259.18, 233.11	319.09845 (+2.7)	304.00, 291.10 276.01, 319.20 287.20, 289.18 247.08, 292.07 277.13, 231.27

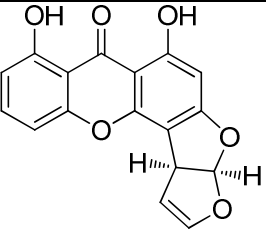
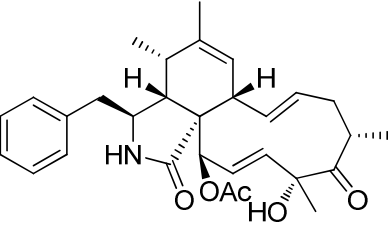
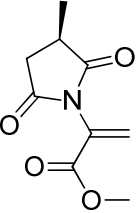
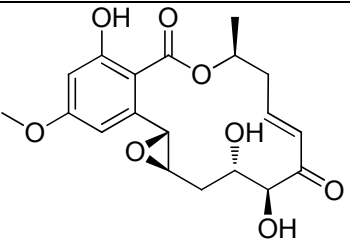
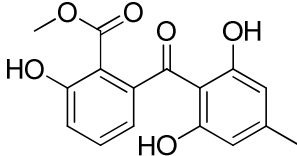
118.	 <p><b>BTH-II0204-207:A</b> C<sub>19</sub>H<sub>16</sub>O<sub>3</sub></p>	4.87	224, 259, 311	293.11716 (-0.2)	261.16, 278.08 277.13, 275.16 292.20, 233.18 262.12, 243.12 259.20, 232.11	291.10327 (+2.1)	276.05, 263.00 291.00, 173.00 275.09, 219.09 247.18, 273.11 264.07, 249.12
119.	 <p><b>Betulinan C</b> C<sub>19</sub>H<sub>14</sub>O<sub>3</sub></p>	5.64	226, 259, 337	291.10175 (+0.6)	276.06, 259.08 260.10, 231.11 273.09, 213.08 263.08, 258.09 245.16, 291.16	289.08813 (+3.8)	289.07, 261.03 275.06, 260.11 288.20, 245.03 271.15, 287.09 262.00, 259.09
120.	01008-147-2*	3.56	220	239.12782 (+0.1)	221.04, 195.16 154.93, 183.07 203.06, 132.98 137.01, 193.14 164.96, 177.12	237.11336 (+0.5)	181.06, 237.22 219.15, 123.06 174.97, 152.93 146.84, 146.04 137.01, 192.98
121.	 <p><b>6,9-Octadecadienoic acid</b> C<sub>18</sub>H<sub>32</sub>O<sub>2</sub></p>	7.25		281.24756 (+0.2)	263.21, 264.23 246.28, 245.18 148.84, 151.06 120.97, 135.15 221.24, 163.15	ND	ND
122.	 <p><b>Cytochalasin C</b> C<sub>30</sub>H<sub>37</sub>NO<sub>6</sub></p>	4.83	219, 283	508.26840 (-1.9)	430.32, 490.16 448.38, 412.30 388.37, 406.40 472.20, 402.26 466.27, 370.55	506.25427 (-1.1)	446.26, 488.23 241.16, 428.18 460.29, 464.51 418.24, 436.11 403.32, 291.21

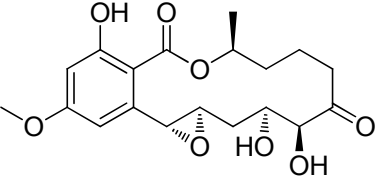
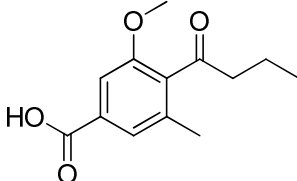
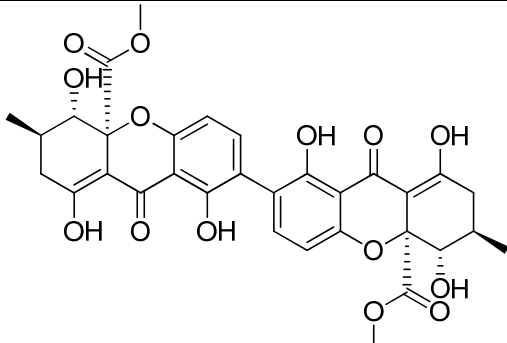


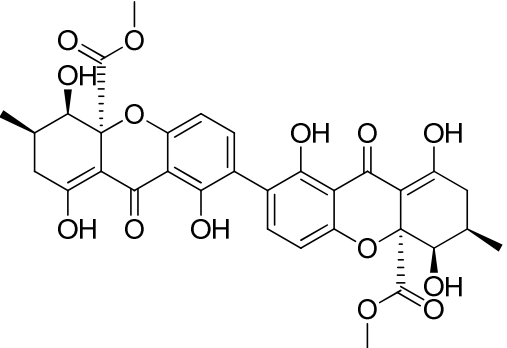
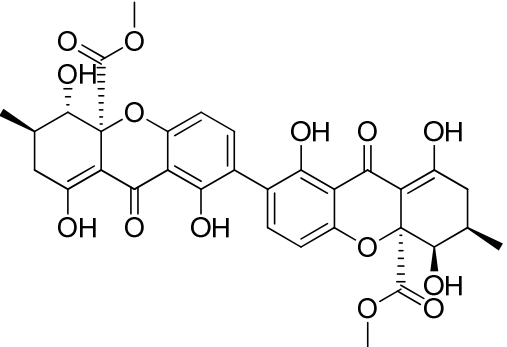
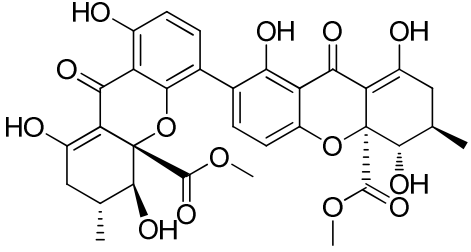
123.	 <p><b>Cytochalasin Q<sub>HYP</sub></b> C<sub>30</sub>H<sub>37</sub>NO<sub>6</sub></p>	5.00	213, 285	508.26831 (-2.1)	490.20, 430.31 448.26, 412.26 402.36, 388.40 406.31, 394.32 384.27, 374.42	506.25439 (-0.8)	446.28, 464.46 488.25, 428.27 463.70, 385.33 388.33, 436.35 354.36, 418.37
124.	 <p><b>8-Acetoxyneosolaniol</b> C<sub>21</sub>H<sub>28</sub>O<sub>9</sub></p>	3.28	226	425.18039 (-0.5)	305.18, 215.13 245.03, 263.05 173.12, 365.33 199.07, 191.08 227.17, 169.12	ND	ND
125.	 <p><b>Isonesosolaniol</b> C<sub>19</sub>H<sub>26</sub>O<sub>8</sub></p>	2.42	219	383.16956 (-1.3)	263.11, 323.10 245.14, 305.09 365.11, 227.08 199.07, 287.15 215.07, 217.11	ND	ND
126.	 <p><b>Abscisic acid</b> C<sub>15</sub>H<sub>20</sub>O<sub>4</sub></p>	3.16	222, 263	265.14374 (+1.1)	247.07, 229.09 219.14, 209.10 201.16, 205.09 187.18, 163.07 203.11, 185.15	263.12872 (-0.6)	152.92, 219.08 204.05, 201.09 110.91, 161.04 245.06, 186.10 138.14, 137.38
127.	 <p><b>5-Methoxysterigmatocystin</b> C<sub>19</sub>H<sub>14</sub>O<sub>7</sub></p>	4.84	230, 244, 274, 330	355.08124 (0.0)	340.09, 327.16 325.07, 341.19 355.17, 312.12 311.19, 326.09 328.18, 297.10	353.06625 (-1.2)	338.04, 325.12 257.01, 307.33 308.88, 353.36 285.03, 339.18 262.81, 269.23

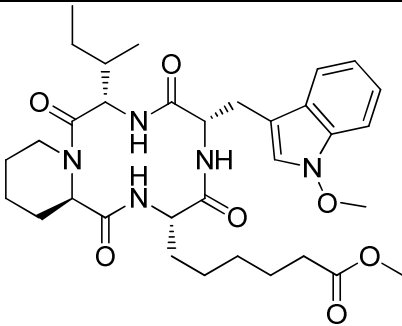
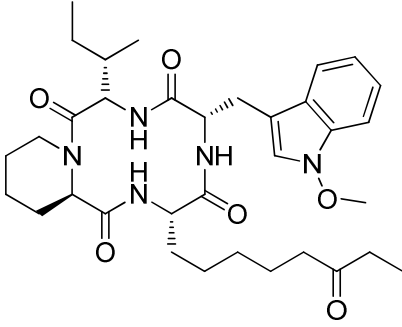
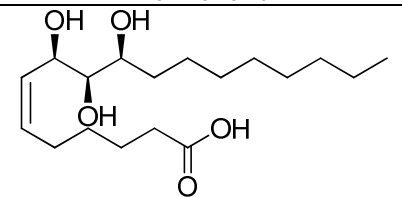
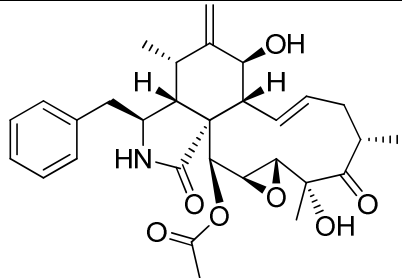
128.	 <p><b>Sterigmatocystin</b> C<sub>18</sub>H<sub>12</sub>O<sub>6</sub></p>	5.03	232, 244, 326	325.07071 (+0.1)	310.11, 297.13 325.10, 311.13 282.12, 281.08 293.10, 296.09 298.15, 283.12	323.05594 (-0.5)	323.18, 308.18 294.99, 323.96 276.69, 305.33 280.00, 252.45 309.09, 278.90
129.	 <p><b>Aversin</b> C<sub>20</sub>H<sub>16</sub>O<sub>7</sub></p>	5.21	222, 285, 315, 441	369.09662 (-0.7)	351.16, 341.13 339.15, 340.17 313.13, 352.18 323.19, 369.13 327.14, 354.13	367.08228 (-0.1)	337.10, 339.15 338.08, 352.05 353.22, 349.14 292.85, 323.30 367.09, 329.15
130.	 <p><b>Brevianamide P</b> C<sub>22</sub>H<sub>23</sub>N<sub>3</sub>O<sub>3</sub></p>	4.92	224, 287, 443	378.18057 (-1.7)	231.11, 361.21 322.18, 321.15 360.22, 287.19 350.28, 243.16 248.11, 230.11	376.16626 (-1.1)	285.07, 284.07 319.09, 229.11 256.19, 188.01 160.86, 227.98 244.21, 333.16
131.	 <p><b>6,8-Di-O-Methyl averufin</b> C<sub>22</sub>H<sub>20</sub>O<sub>7</sub></p>	6.55	224, 287, 443	397.12772 (-1.2)	339.17, 379.18 313.13, 327.14 355.17, 337.07 361.25, 301.22 351.22, 380.22	395.11386 (+0.6)	311.92, 297.02 395.27, 377.22 313.05, 327.12 323.12, 309.09 337.02, 291.47

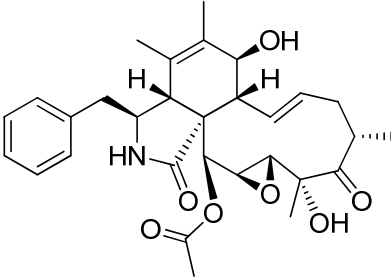
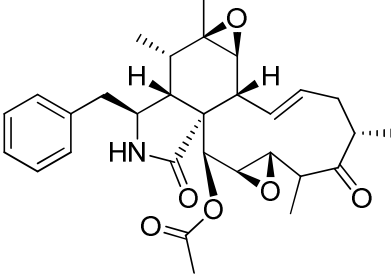
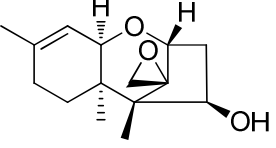
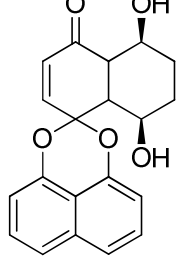
132.	 <p><b>Roridin L</b> C<sub>29</sub>H<sub>38</sub>O<sub>9</sub></p>	4.37	222, 259	531.25781 (-2.0)	377.25, 513.22 359.34, 401.21 247.10, 229.15 265.19, 383.30 395.21, 495.36	529.24420 (-0.2)	375.26, 485.37 401.04, 247.14 417.35, 511.32 451.09, 265.12 499.05, 233.32
133.	 <p><b>Verrucarins J, Muconomycin B</b> C<sub>27</sub>H<sub>32</sub>O<sub>8</sub></p>	5.53	222, 261	485.21613 (-1.8)	343.25, 231.12 373.25, 213.20 249.17, 185.05 201.07, 187.11 203.13, 159.01	483.20267 (+0.5)	389.21, 439.15 173.09, 465.21 235.05, 395.32 160.81, 373.07 211.28, 254.99
134.	 <p><b>Roridin H; Verrucarins H</b> C<sub>29</sub>H<sub>36</sub>O<sub>8</sub></p>	6.07	224, 259	513.24719 (-2.2)	231.12, 359.22 249.15, 213.20 201.12, 495.19 182.76, 203.18 185.10, 331.23	ND	ND

135.	 <p><b>De-O-methylsterigmatocystin</b> C<sub>17</sub>H<sub>10</sub>O<sub>6</sub></p>	6.03	228, 248, 333	311.05505 (+0.1)	283.07, 311.11 282.10, 284.20 269.01, 255.03 241.04, 200.97 264.02, 312.15	309.04068 (+0.7)	309.14, 265.07 281.18, 240.94 266.10, 263.12 96.88, 290.17 156.71, 172.94
136.	 <p><b>Zygosporin G</b> C<sub>30</sub>H<sub>37</sub>NO<sub>5</sub></p>	5.93	217, 276	492.27356 (-1.8)	474.18, 414.34 396.30, 432.33 267.19, 249.30 372.32, 386.41 322.32, 390.41	490.26102 (+2.3)	444.37, 472.40 462.36, 446.30 315.53, 307.06 428.46, 460.32 399.45, 193.24
137.	 <p><b>Versimide</b> C<sub>9</sub>H<sub>11</sub>NO<sub>4</sub></p>	1.65	214	198.07603 (-0.3)	165.95, 198.10 96.98, 82.96 80.90, 95.01 68.91, 92.98 106.95, 121.02	ND	ND
138.	 <p><b>Aigialomycin A</b> C<sub>19</sub>H<sub>22</sub>O<sub>8</sub></p>	3.77	232, 263, 304	379.13791 (-2.2)	253.00, 235.00 343.25, 361.09 325.15, 231.00 265.00, 206.98 249.05, 126.98	377.12354 (-1.7)	251.01, 359.09 207.03, 305.07 341.21, 178.98 233.12, 315.16 205.06, 263.06
139.	 <p><b>Nidulalin B</b> C<sub>16</sub>H<sub>14</sub>O<sub>6</sub></p>	3.60	222, 276	303.08591 (-1.3)	192.95, 271.13 178.99, 136.86 167.09, 179.59 193.75, 286.30 88.99, 109.03	301.07086 (-3.0)	268.99, 283.08 134.84, 225.04 257.20, 241.05 91.00, 108.87 165.03, 269.74

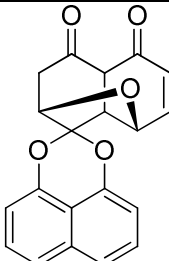
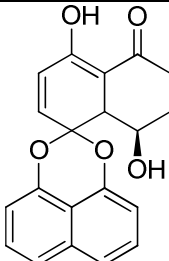
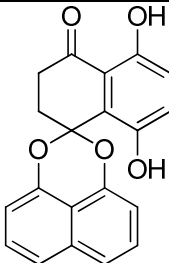
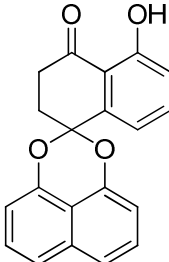
140.	 <p><b>Dihydrohypothemycin</b> C<sub>19</sub>H<sub>24</sub>O<sub>8</sub></p>	4.01	219, 265, 304	381.15338 (-2.7)	363.12, 345.18 327.12, 303.13 253.00, 265.09 309.24, 249.15 285.11, 235.02	379.13925 (-1.6)	178.94, 307.11 233.05, 361.05 277.12, 163.98 180.96, 343.13 205.03, 335.13
141.	01020-76-1*	4.16	222, 272, 350	321.09613 (-2.3)	261.04, 303.11 289.09, 219.00 247.06, 271.11 192.95, 149.02 275.17, 136.98	319.08191 (-1.3)	275.18, 243.22 287.23, 257.09 205.13, 300.92 162.74, 219.88 215.03, 220.99
142.	 <p><b>Pyrenochaetic acid C</b> C<sub>13</sub>H<sub>16</sub>O<sub>4</sub></p>	4.40	217, 250, 304	237.1185 (-1.2)	219.08, 175.09 194.05, 195.10 236.06, 200.99 192.95, 161.95 160.01, 177.05	235.09740 (-0.8)	191.00, 176.06 235.09, 163.18 120.96, 191.60 177.23, 207.15 179.11, 68.98
143.	 <p><b>Secalonic acid A</b> C<sub>32</sub>H<sub>30</sub>O<sub>14</sub></p>	5.26	222, 263, 337	639.16882 (-2.8)	561.27, 589.16 579.27, 621.25 501.27, 571.27 455.21, 543.17 603.28, 511.28	637.15448 (-2.8)	577.30, 619.24 543.19, 417.23 605.23, 559.11 587.15, 541.34 593.29, 499.24

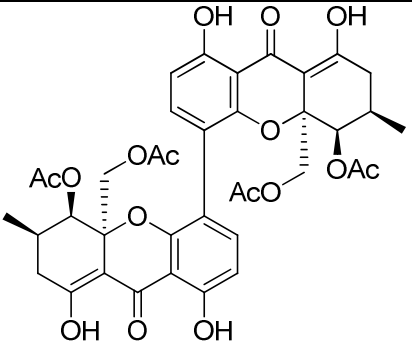
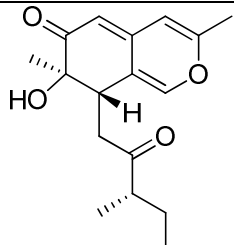
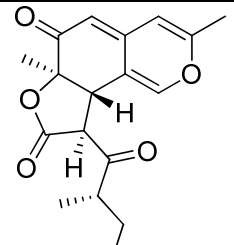
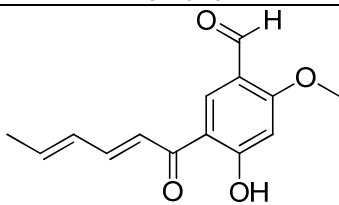
144.	 <p><b>Secalonic acid E</b> C<sub>32</sub>H<sub>30</sub>O<sub>14</sub></p>	5.50	220, 265, 337	639.16913 (-2.7)	561.24, 589.26 579.26, 621.20 455.31, 571.26 501.19, 603.25 543.35, 607.30	637.15381 (-3.1)	593.25, 543.30 605.30, 619.19 549.29, 577.20 561.22, 499.29 575.37, 587.15
145.	 <p><b>Secalonic acid G</b> C<sub>32</sub>H<sub>30</sub>O<sub>14</sub></p>	5.39	220, 259, 337	639.16925 (-2.5)	561.28, 589.23 579.24, 621.23 571.22, 455.32 501.28, 543.20 603.35, 511.28	637.15417 (-3.3)	577.20, 593.13 543.19, 619.21 605.25, 561.31 499.29, 587.18 533.24, 525.23
146.	 <p><b>Penicillixanthone A</b> C<sub>32</sub>H<sub>30</sub>O<sub>14</sub></p>	5.90	220, 262, 335	639.16943 (-2.2)	621.23, 589.24 579.26, 561.24 571.32, 603.37 501.40, 543.14 589.94, 455.33	637.15424 (-3.2)	605.18, 577.26 619.12, 593.22 543.15, 561.36 587.20, 557.20 551.21, 525.24
147.	01020-138-1*	5.29	220, 259, 335	639.16907 (-2.8)	561.23, 589.24 579.27, 571.24 501.21, 455.22 621.23, 565.29 547.35, 193.01	637.15411 (-3.4)	593.19, 561.21 543.33, 549.29 517.20, 365.25 577.19, 605.35 533.21, 575.22

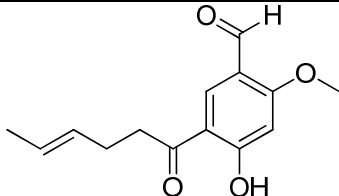
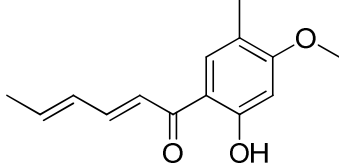
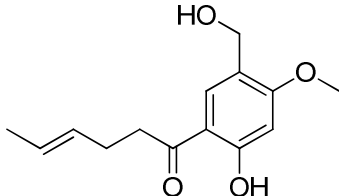
148.	 <p><b>New Natural Product, reported by synthesis</b> 01020-71-4/ 01009-145-5 C<sub>33</sub>H<sub>47</sub>N<sub>5</sub>O<sub>7</sub></p>	5.29	222, 289	626.35333 (-2.4)	466.26, 594.46 595.36, 513.32 598.38, 422.31 483.37, 296.13 596.38, 297.22	624.33868 (-2.6)	464.24, 594.42 465.41, 592.44 477.23, 254.21 562.46, 225.21 595.04, 340.21
149.	 <p><b>Apicidin</b> C<sub>34</sub>H<sub>49</sub>N<sub>5</sub>O<sub>6</sub></p>	5.44	222, 287	624.37372 (-2.9)	464.24, 592.44 593.37, 511.36 294.20, 596.46 420.28, 481.33 467.17, 594.47	622.35925 (-2.8)	462.32, 592.46 463.44, 475.22 590.57, 223.01 252.07, 336.32 310.22, 183.04
150.	 <p><b>(8R*,9R*,10S*,6Z)-trihydroxyoctadec-6-enoic acid (Oxylipin)</b> C<sub>18</sub>H<sub>34</sub>O<sub>5</sub></p>	4.32	220	331.24762 (-0.8)	313.39, 285.40 289.27, 331.25 316.26, 302.98 295.33, 281.01 275.39, 206.99	329.23221 (-3.5)	311.34, 211.15 199.04, 293.17 168.92, 181.11 275.24, 192.98 227.16, 197.11
151.	 <p><b>19,20-Epoxycytochalasin D</b> C<sub>30</sub>H<sub>37</sub>NO<sub>7</sub></p>	4.03	217	524.26367 (-1.2)	428.30, 446.23 464.30, 404.28 386.33, 390.29 410.32, 400.32 368.28, 239.12	522.24884 (-1.7)	480.38, 504.22 462.32, 444.23 268.27, 422.25 324.37, 404.32 348.24, 266.16

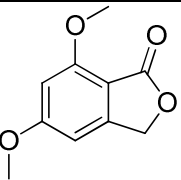
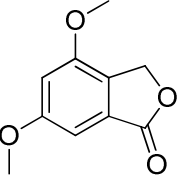
152.	 <p><b>19,20-Epoxychoylochalasin C</b> C<sub>30</sub>H<sub>37</sub>NO<sub>7</sub></p>	4.54	215	524.26343 (-1.6)	428.30, 446.30 386.29, 464.25 404.26, 390.32 400.34, 418.30 410.25, 281.14	522.24902 (-1.4)	404.24, 462.32 480.42, 362.32 504.24, 402.28 401.22, 444.17 464.29, 360.29
153.	 <p><b>18-Deoxy-19,20-epoxychoylochalasin Q</b> C<sub>30</sub>H<sub>37</sub>NO<sub>6</sub></p>	5.18	211	508.26831 (-2.1)	430.29, 412.35 402.31, 448.33 265.17, 267.14 384.31, 346.18 374.38, 372.29	506.25424 (-1.1)	460.19, 446.19 428.34, 464.37 478.00, 308.28 307.25, 318.08 423.13, 436.18
154.	 <p><b>Trichodermol</b> C<sub>15</sub>H<sub>22</sub>O<sub>3</sub></p>	3.22	230	251.16420 (+0.1)	233.12, 215.07 187.20, 205.14 197.13, 108.95 136.92, 158.98 95.03, 173.13	ND	ND
155.	 <p><b>Decaspirone C</b> C<sub>20</sub>H<sub>18</sub>O<sub>5</sub></p>	4.45	230, 298, 326	339.12225 (-1.3)	321.14, 285.07 303.15, 159.00 143.95, 159.98 144.97, 253.07 130.91, 321.77	337.10757 (-1.7)	319.04, 293.17 159.10, 275.04 291.20, 234.95 251.17, 337.01 263.02, 158.02



156.	 <p><b>Palmarumycin CP3</b> C<sub>20</sub>H<sub>14</sub>O<sub>5</sub></p>	5.07	226, 298, 326	335.09125 (-0.4)	307.14, 289.14 174.98, 161.01 279.15, 158.95 175.99, 317.08 147.05, 160.01	333.07599 (-2.6)	158.94, 289.03 305.06, 315.18 271.08, 303.16 157.92, 261.16 287.08, 146.96
157.	 <p><b>Palmarumycin CP4</b> C<sub>20</sub>H<sub>16</sub>O<sub>5</sub></p>	5.36	224, 298, 326	337.10684 (-0.6)	319.17, 158.98 301.14, 160.00 130.97, 253.11 161.09, 291.12 174.96, 277.25	335.09201 (-1.5)	158.91, 251.16 291.13, 157.87 307.14, 317.08 273.05, 250.06 233.04, 289.05
158.	 <p><b>Palmarumycin CP<sub>17</sub></b> C<sub>20</sub>H<sub>14</sub>O<sub>5</sub></p>	5.80	228, 298, 365	335.09103 (-1.1)	303.15, 158.94 285.10, 174.94 161.03, 176.00 317.07, 143.97 160.05, 275.12	333.07639 (-1.4)	159.06, 265.15 315.24, 289.01 158.42, 333.13 189.95, 312.96 178.00, 286.94
159.	 <p><b>Palmarumycin CP<sub>2</sub></b> C<sub>20</sub>H<sub>14</sub>O<sub>4</sub></p>	5.03	222, 331	319.09598 (-1.6)	159.93, 301.14 158.96, 160.96 174.92, 302.12 130.99, 273.08 145.01, 132.92	317.08142 (-1.6)	158.89, 174.96 299.12, 316.98 298.30, 172.97 159.95, 173.99 273.18, 316.09

160.	 <p><b>Phomoxanthone A</b> C<sub>38</sub>H<sub>38</sub>O<sub>16</sub></p>	6.56	220, 254, 333	751.22235 (-1.2)	673.16, 691.17 631.35, 733.04 613.31, 571.20 511.24, 553.30 732.32, 678.34	749.20679 (-2.6)	689.19, 629.24 569.26, 671.24 509.38, 611.31 647.28, 731.25 629.85, 587.18
161.	 <p><b>Chermesinone A</b> C<sub>17</sub>H<sub>22</sub>O<sub>4</sub></p>	4.15	222, 354	291.15845 (-2.2)	189.22, 245.17 273.20, 231.24 201.20, 145.13 255.17, 161.19 174.20, 175.21	ND	ND
162.	 <p><b>Chermesinone B</b> C<sub>18</sub>H<sub>20</sub>O<sub>5</sub></p>	4.50	222, 354	317.13794 (-1.3)	233.08, 215.08 187.07, 159.08 245.13, 273.12 205.14, 189.11 281.14, 188.12	315.12302 (-2.5)	273.15, 229.01 271.13, 253.06 189.00, 210.98 231.11, 187.08 243.15, 225.08
163.	 <p><b>5'-formyl-2'-hydroxyl-4'-methoxy-(E,E)-sorbophenone</b> C<sub>14</sub>H<sub>14</sub>O<sub>4</sub></p>	5.33	225, 266, 311, 343	247.09599 (-2.0)	178.95, 197.03 190.97, 218.97 229.03, 201.06 150.93, 190.00 164.98, 177.07	245.08153 (-1.6)	227.09, 230.05 211.96, 183.95 150.02, 245.06 163.93, 213.00 202.07, 200.90

164.	 <p><b>5'-Formyl-2'-hydroxy-4'-methoxy-(E)-4-hexenophenone</b> C<sub>14</sub>H<sub>16</sub>O<sub>4</sub></p>	5.48	253, 282, 322	249.11192 (-0.9)	178.88, 231.02 221.11, 152.94 206.95, 164.93 203.07, 193.08 176.97, 175.05	247.09705 (-2.2)	163.81, 247.07 177.88, 217.12 188.97, 231.00 149.94, 177.14 202.98, 232.04
165.	 <p><b>1-(2'-hydroxy-4'-methoxy-5'-methylphenyl)-2,4-E,E-hexadien-1-one</b> C<sub>14</sub>H<sub>16</sub>O<sub>3</sub></p>	6.16	234, 310, 357	233.11711 (-0.5)	214.99, 164.97 205.05, 191.09 151.01, 187.01 176.99, 204.12 201.12, 233.09	231.10251 (-0.7)	215.97, 197.94 213.00, 203.15 231.08, 175.01 150.00, 137.03 201.02, 184.94
166.	01021-11-2*	5.48	243, 277, 314	279.12302 (+1.1)	247.02, 208.94 235.08, 183.06 229.12, 150.91 261.17, 217.01 204.96, 193.11	277.10773 (-1.5)	277.14, 193.92 192.84, 247.06 219.06, 179.85 261.02, 262.21 206.98, 163.95
167.	 <p><b>1-(2'-hydroxy-4'-methoxy-5'-hydroxymethylphenyl)-E-4-hexen-1-one</b> C<sub>14</sub>H<sub>18</sub>O<sub>4</sub></p>	4.64	233, 275, 319	251.12767 (-0.5)	180.97, 233.16 215.09, 221.09 158.96, 186.99 136.99, 205.08 177.06, 203.02	249.11308 (-0.6)	231.05, 216.06 248.95, 135.05 213.04, 176.99 188.11, 217.09 233.03, 201.01
168.	01021-2-7*	4.44	230, 311, 350	249.11215 (+0.1)	231.05, 180.93 219.15, 207.08 203.00, 200.95 204.08, 213.07 191.07, 174.97	247.09738 (-0.8)	163.96, 232.01 247.19, 199.03 229.11, 178.03 214.03, 217.06 200.94, 230.92
169.	01021-12-1*	4.43	223, 250, 314, 335	263.09131 (-0.3)	245.05, 195.04 204.07, 177.02 187.00, 191.12 188.95, 219.11 217.00, 175.99	261.07651 (-1.3)	188.99, 217.02 187.98, 199.06 171.06, 187.31 173.02, 202.11 246.08, 168.89

170.	 <p><b>5,7-dimethoxy-1(3H)-isobenzofuranone</b>  <b>5,7-Dimethoxyphthalide</b>  <math>C_{10}H_{10}O_4</math>  01021-95-1</p>	2.50	217, 258, 291	195.06467 (-2.6)	194.99, 134.90 149.03, 139.02 165.01, 162.99 145.00, 119.01 120.91, 90.90	193.05014 (-2.6)	177.88, 192.84 148.96, 149.89 162.91, 146.91 165.01, 133.78 175.02, 134.88
171.	 <p><b>4,6-Dimethoxy-1(3H)-isobenzofuranone</b>  <b>4,6-Dimethoxyphthalide</b>  <math>C_{10}H_{10}O_4</math>  01021-95-3</p>	3.53	197, 222, 250, 308	195.06468 (-2.6)	194.99, 134.89 148.92, 162.92 144.87, 118.93 177.01, 166.97 150.99, 138.96	193.05008 (-2.9)	148.93, 193.01 146.85, 177.95 167.00, 121.07 133.91, 134.93 165.19, 174.90
172.	01021-127-2*	6.40	193, 219, 232, 276, 326	235.13222 (-2.8)	165.06, 235.04 217.04, 151.01 193.06, 189.03 191.11, 179.09 174.96, 177.03	233.11761 (-3.0)	233.01, 189.14 149.96, 218.20 136.96, 178.03 174.85, 217.47 203.20, 164.07

ND: Not Detected

\*New compound, not published yet