

## Supplemental Figures

**Figure S1: Representative LC-MS chromatograms (BPC) from fruits samples from all accessions. Representative chromatograms are showing in (A) negative and (B) positive mode.**

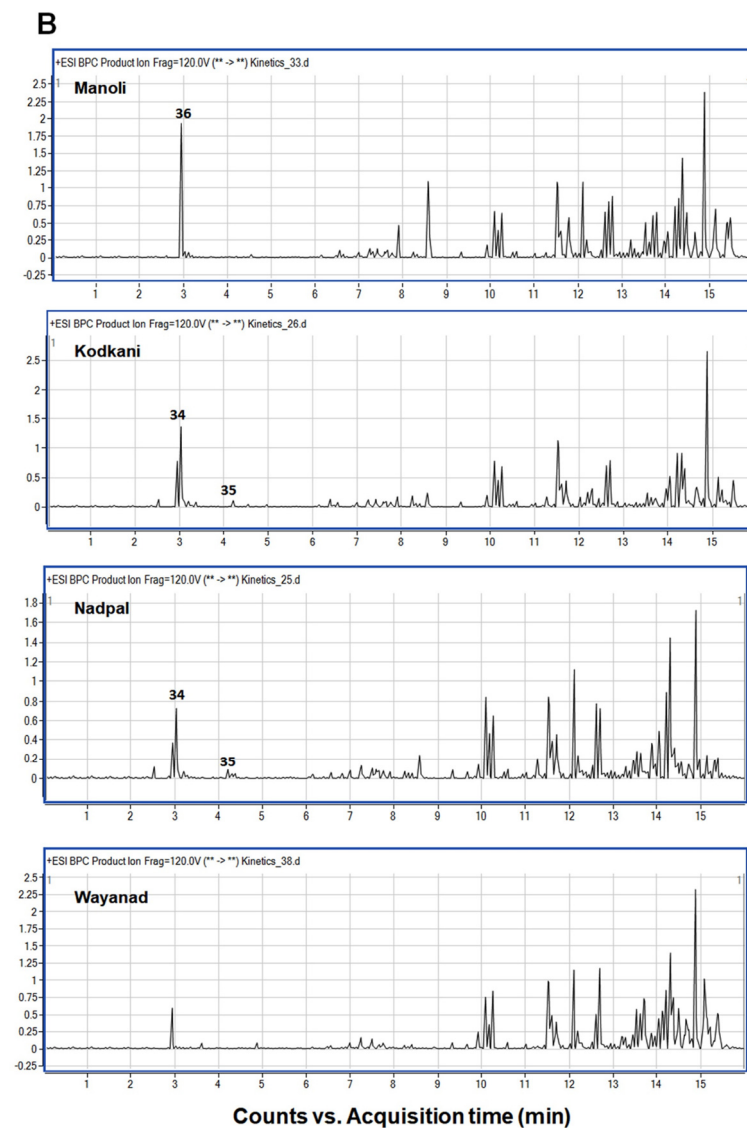
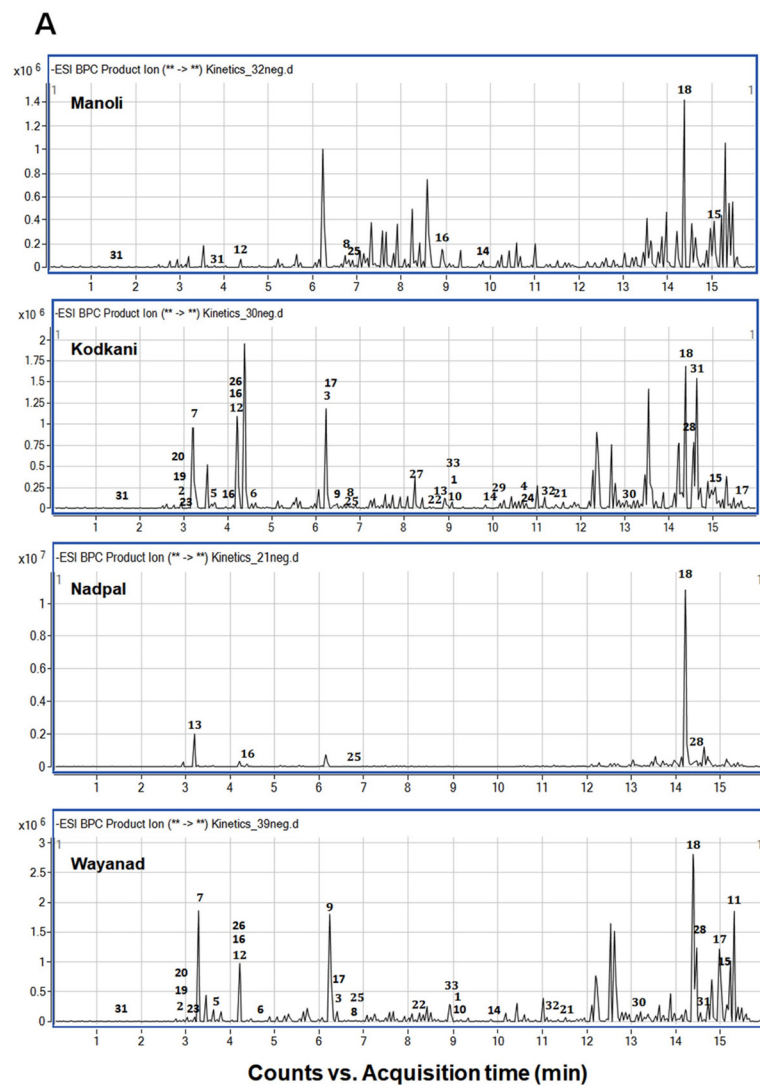
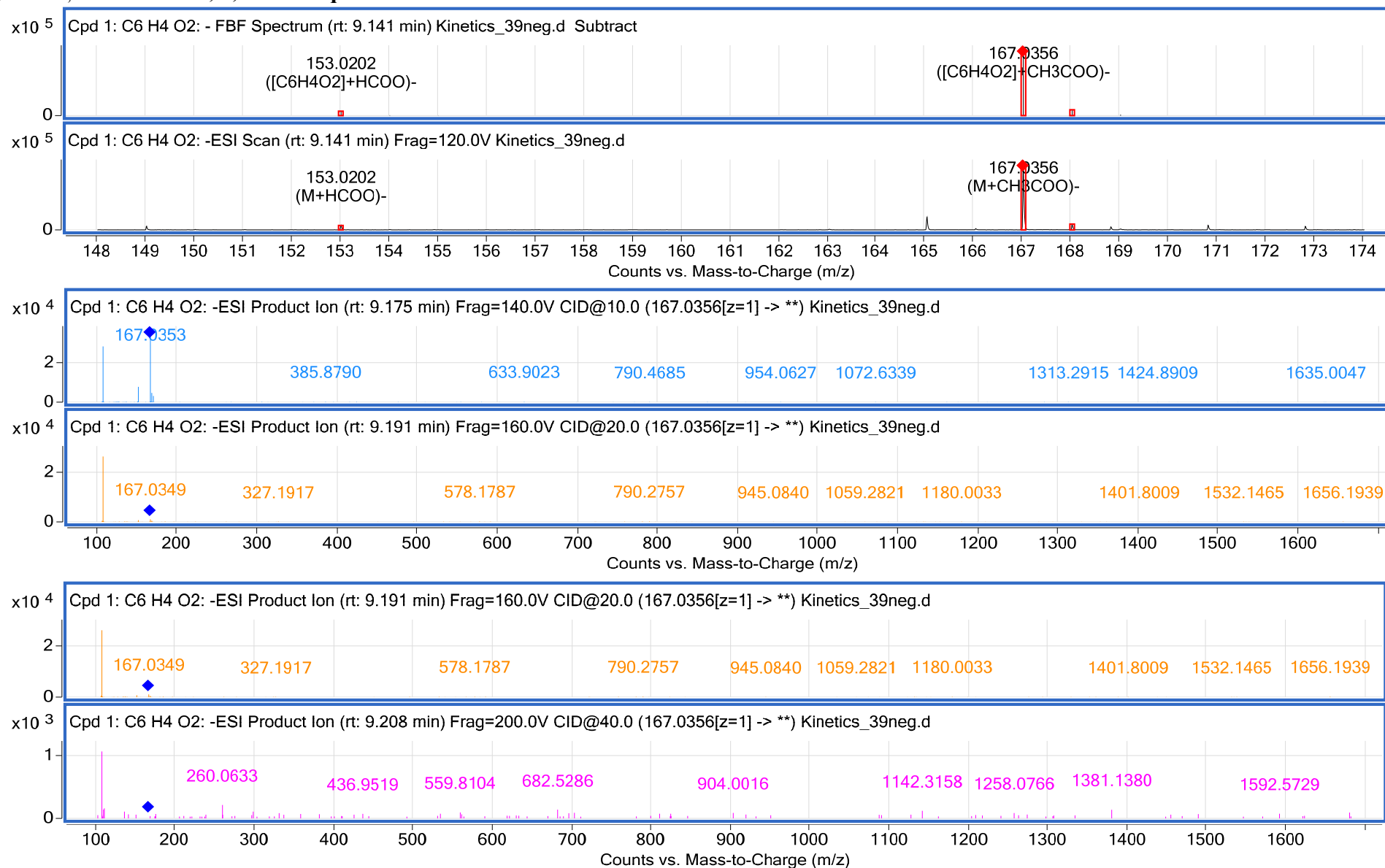
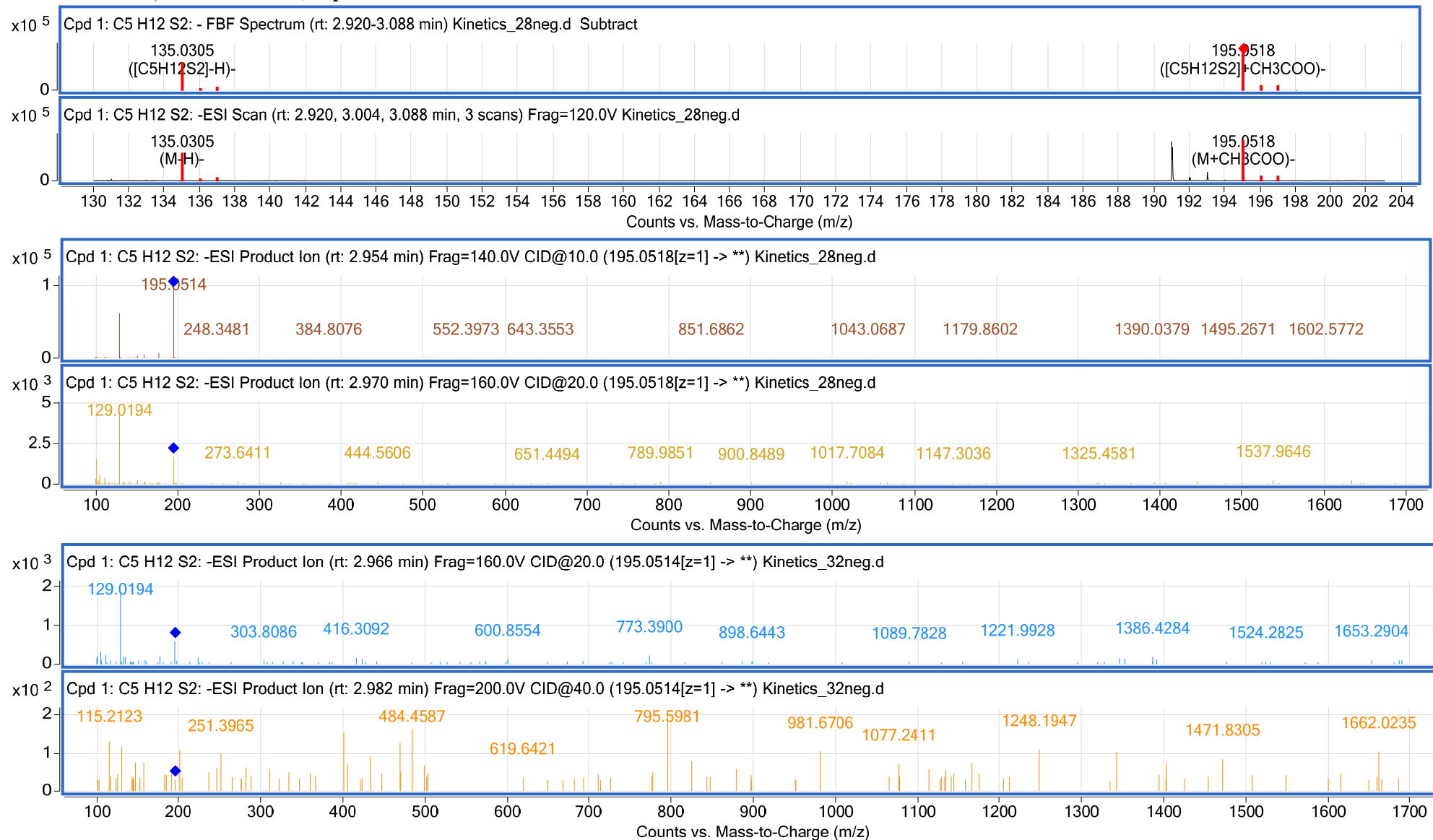


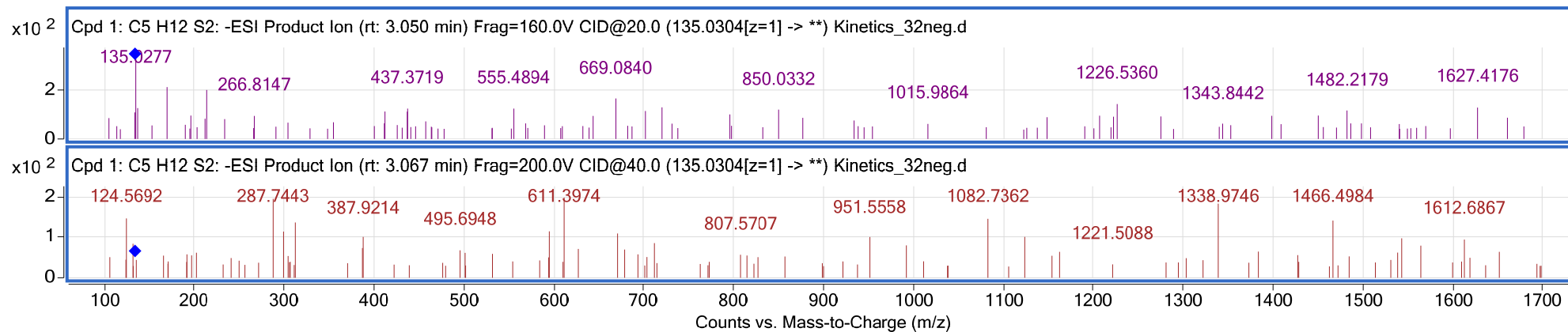
Figure S2: MS and MS-MS spectra for 36 identified compounds from different accessions of Embelia fruits.

1.  $C_6H_4O_2$ ,  $m/z$ -153.0197, 1, 2-Benzoquinone

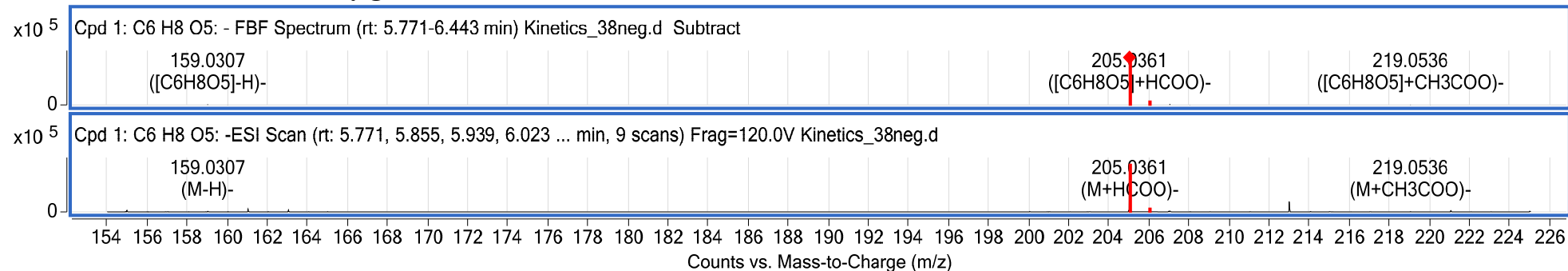


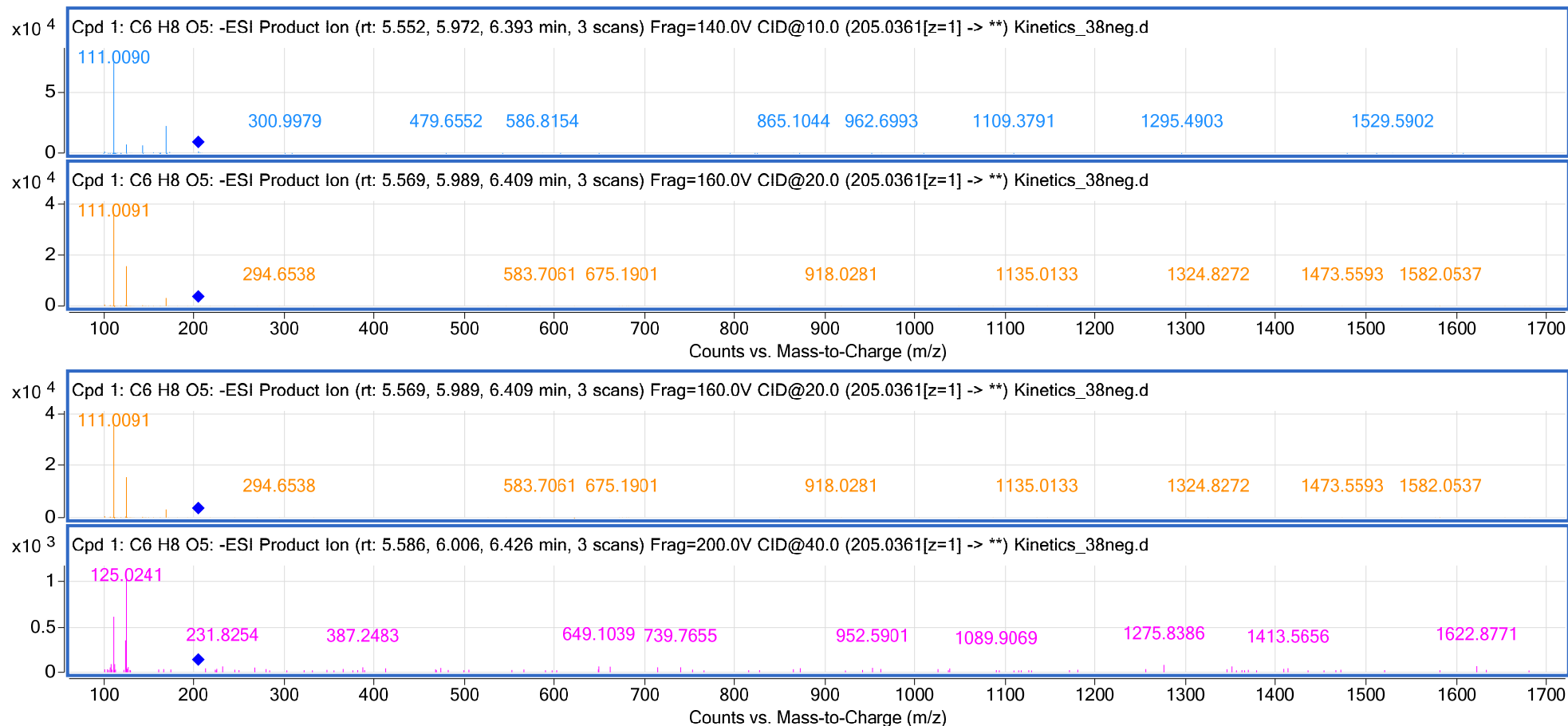
## 2. $C_5H_{12}S_2$ , m/z - 135.0307, 1-pentanesulfenothoic acid



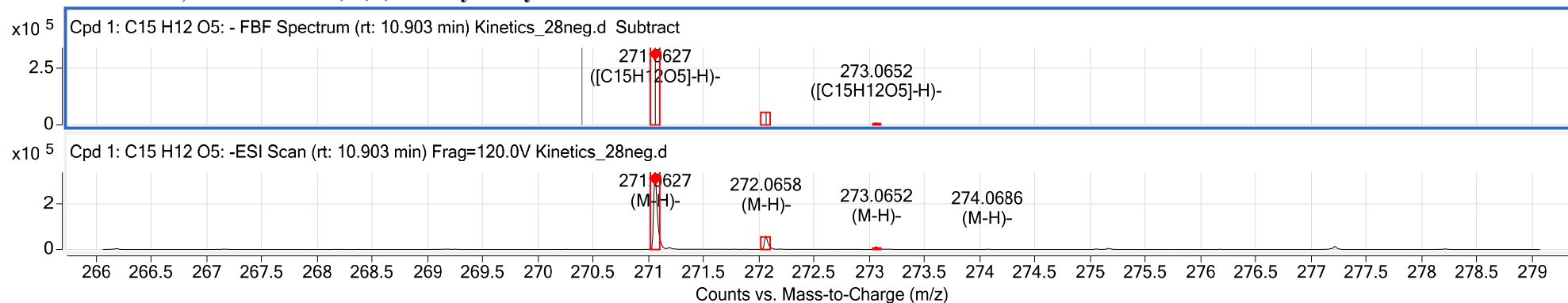


### 3. C<sub>6</sub> H<sub>8</sub> O<sub>5</sub>, m/z- 205.0361, 2-Formylglutarate



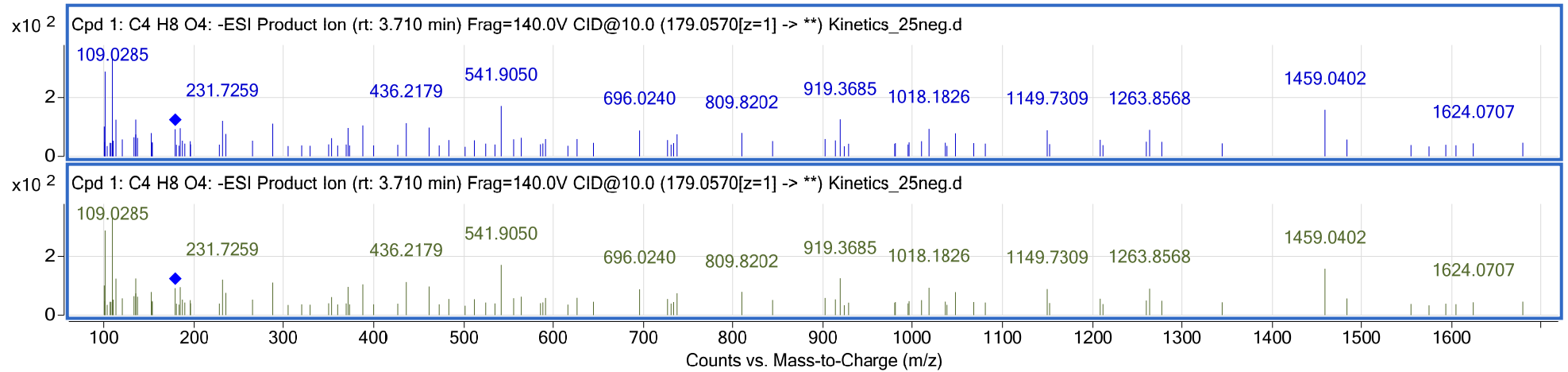
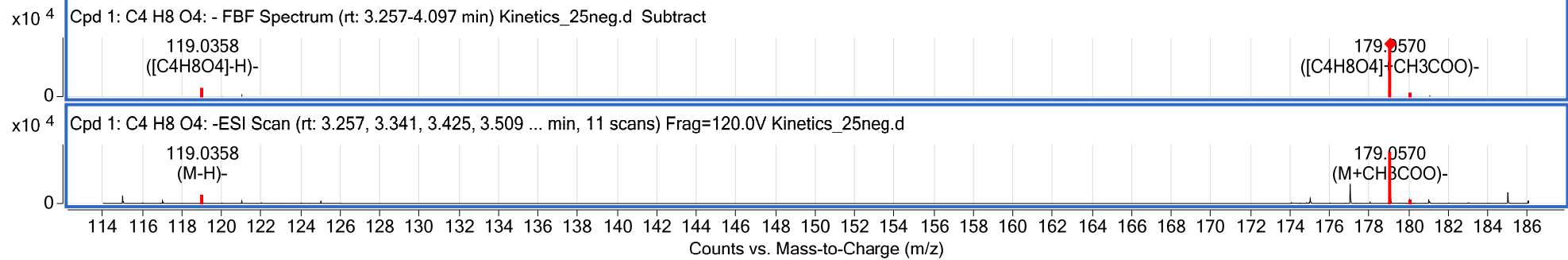


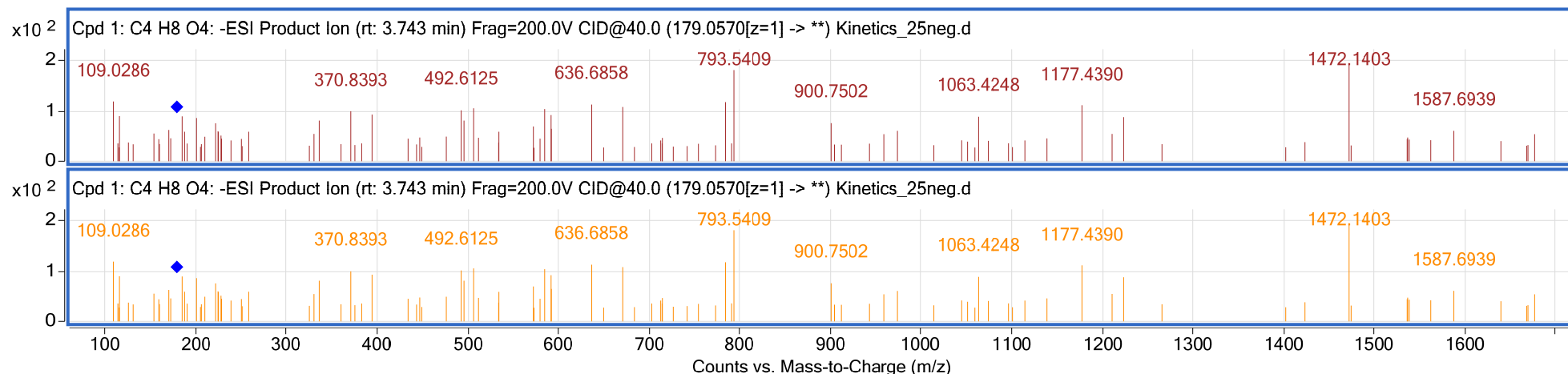
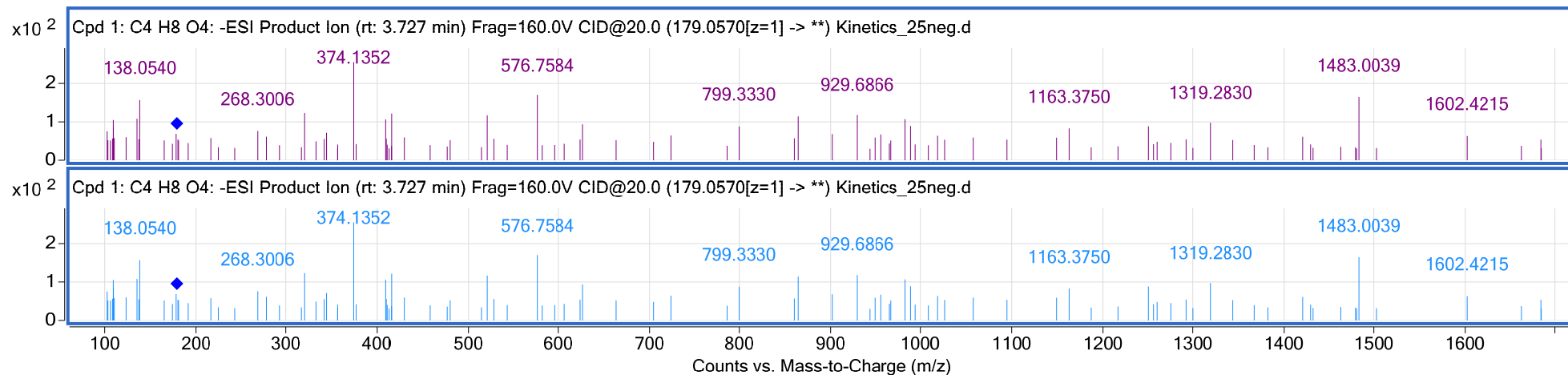
#### 4. **C<sub>15</sub> H<sub>12</sub> O<sub>5</sub>, m/z- 271.0626, 3,4,5-Trihydroxyflavanone**



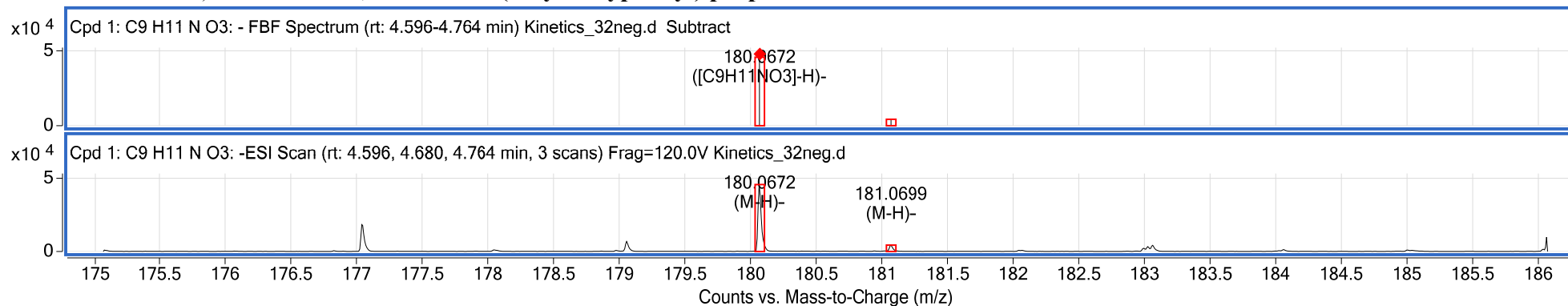


5. **C<sub>4</sub> H<sub>8</sub> O<sub>4</sub>, m/z- 179.0566, mass-120.0432, 3, 4-Dihydroxybutyric acid**

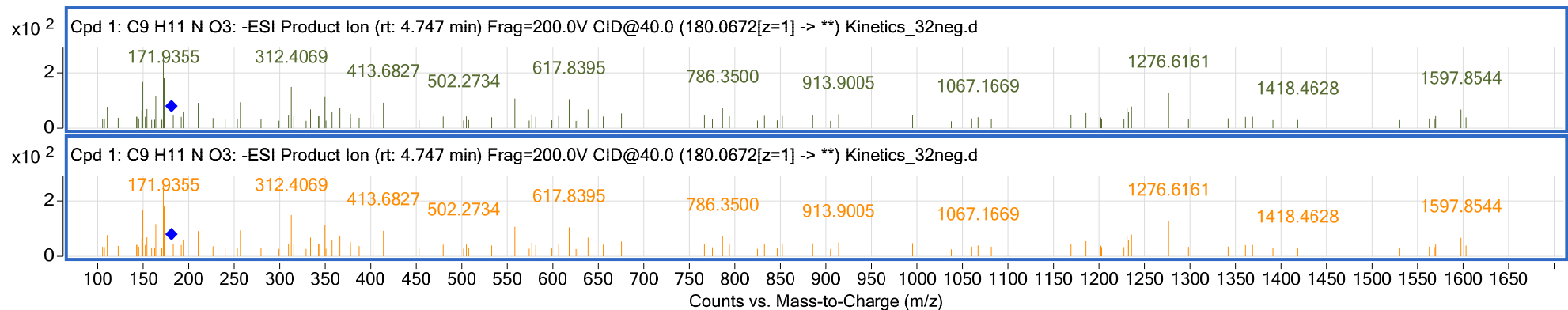
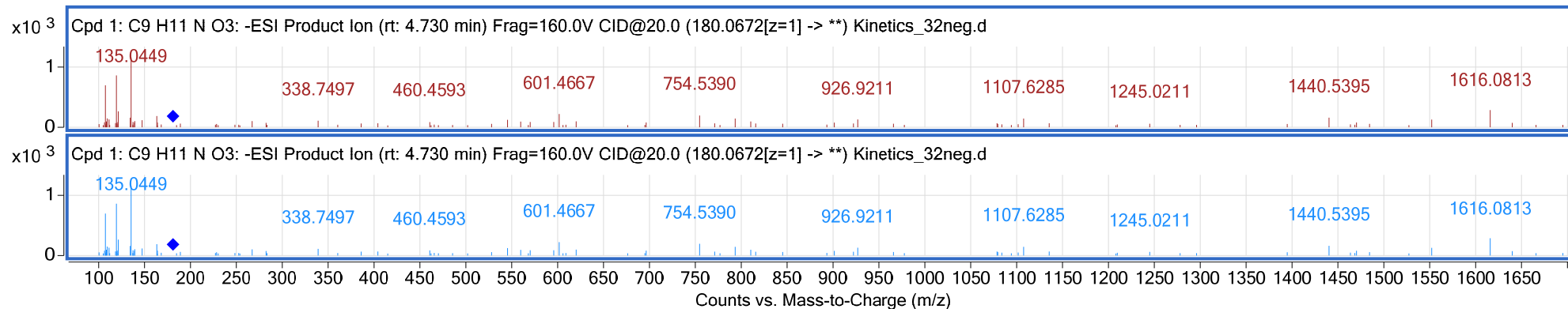
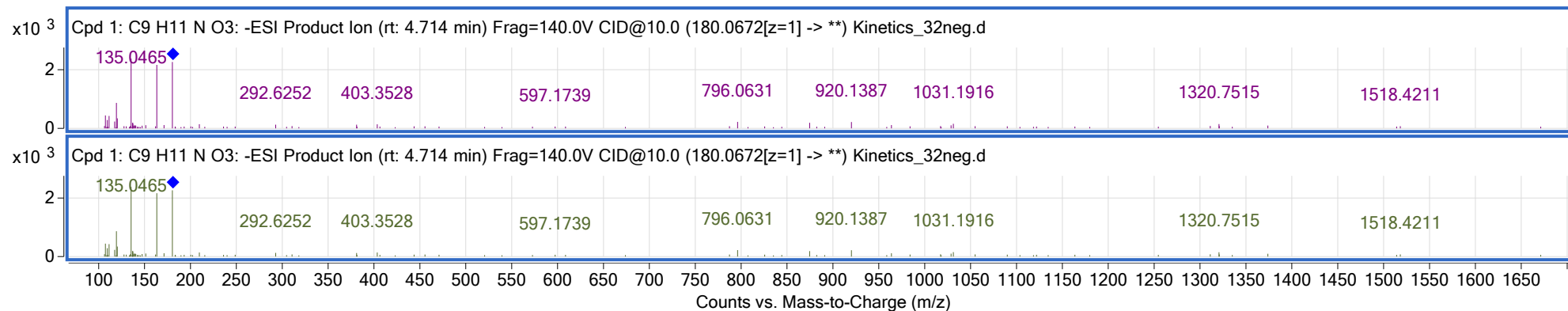




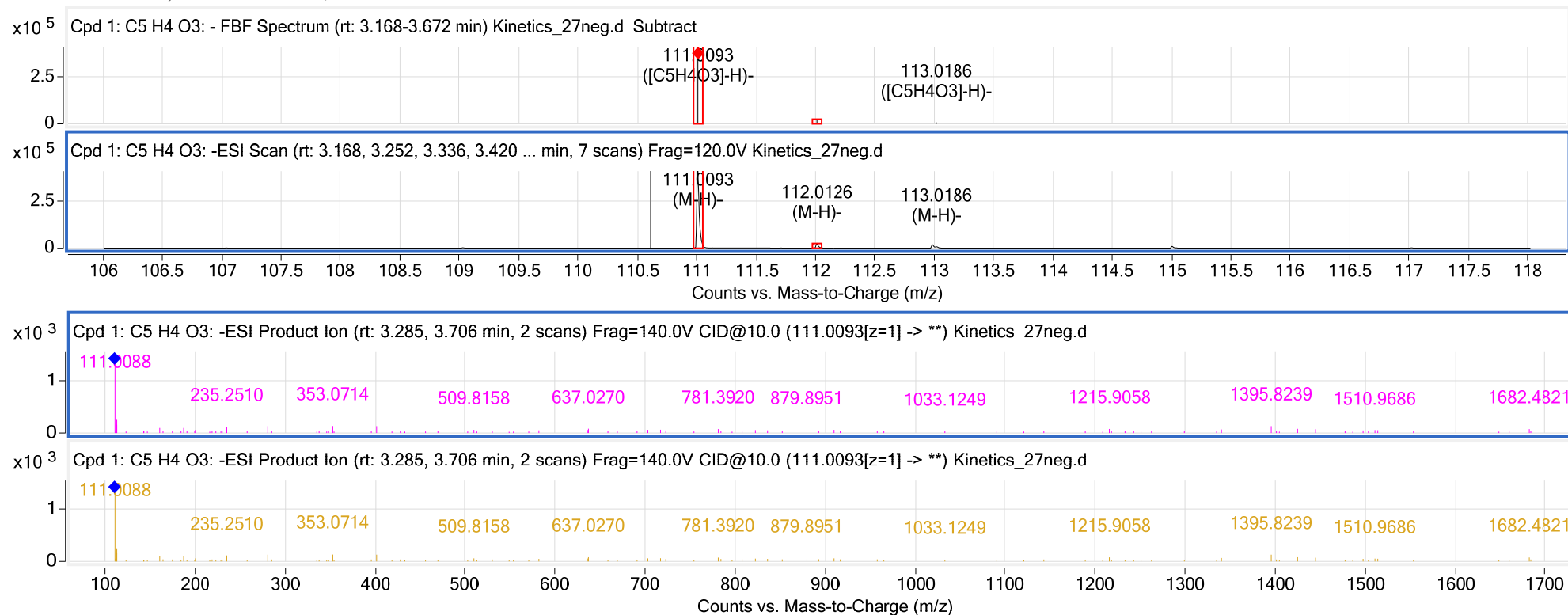
## 6. C<sub>9</sub> H<sub>11</sub> N O<sub>3</sub>, m/z- 180.0672, 3-Amino-3-(4-hydroxyphenyl) propanoate

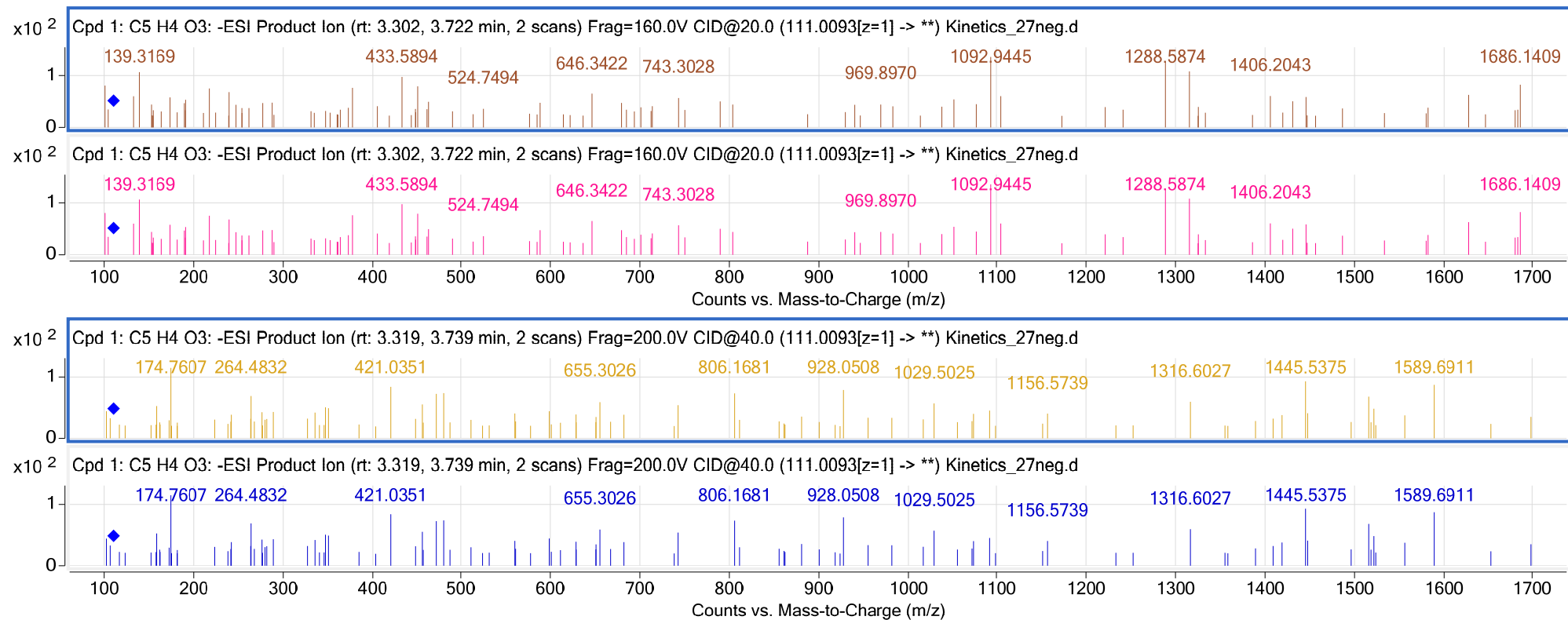




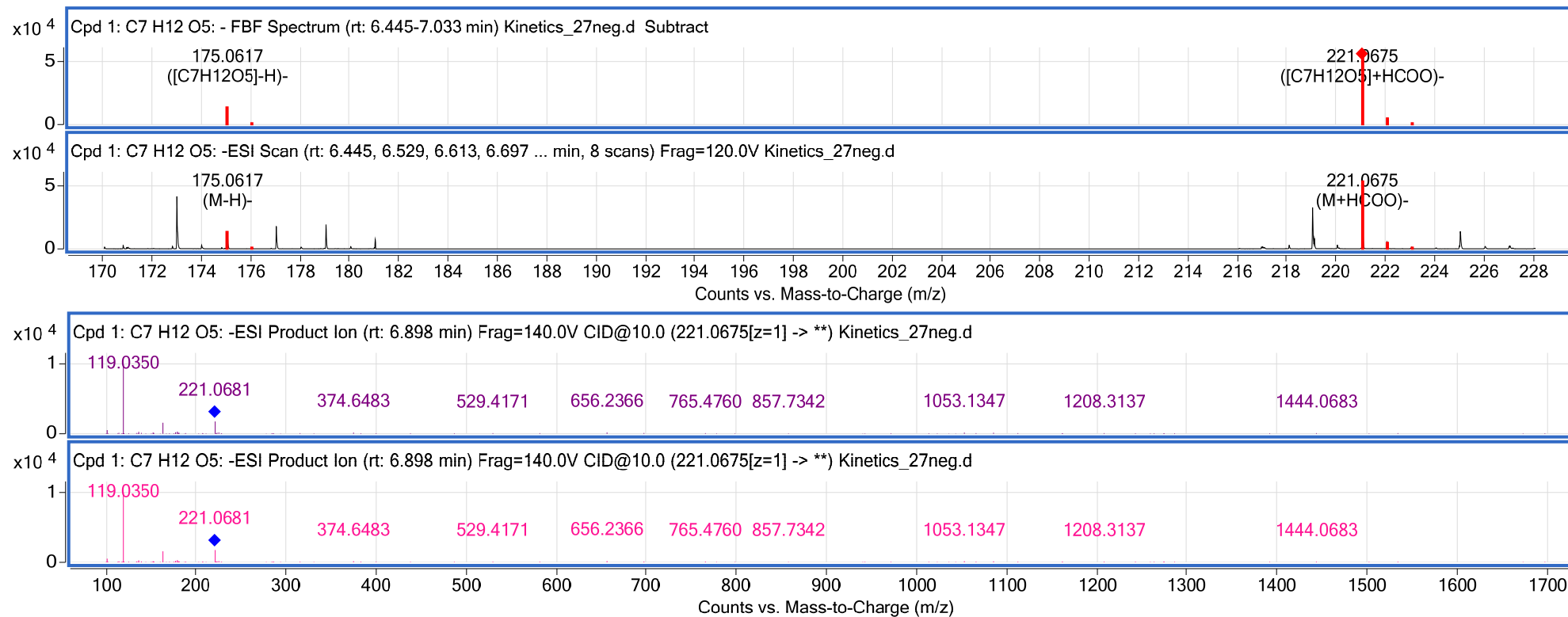


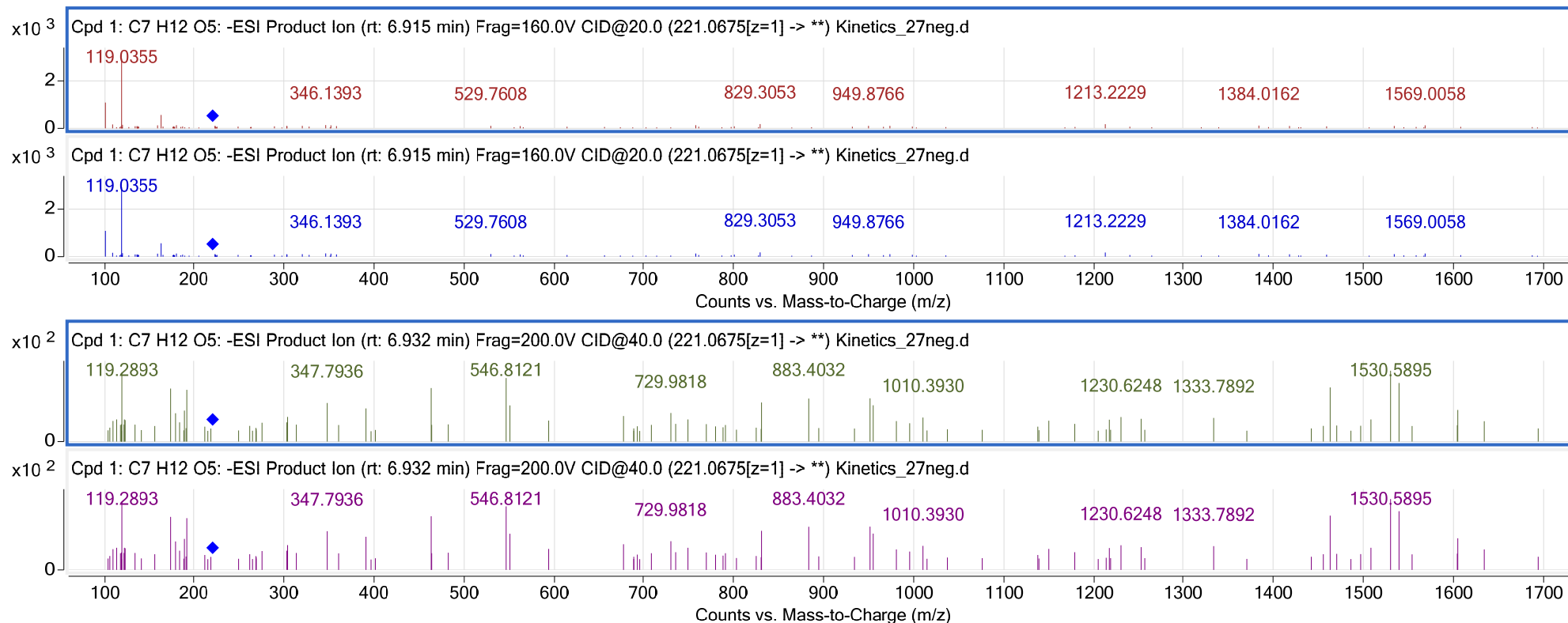
7. **C<sub>5</sub> H<sub>4</sub> O<sub>3</sub>, m/s- 111.0093, 3-Furoic acid**



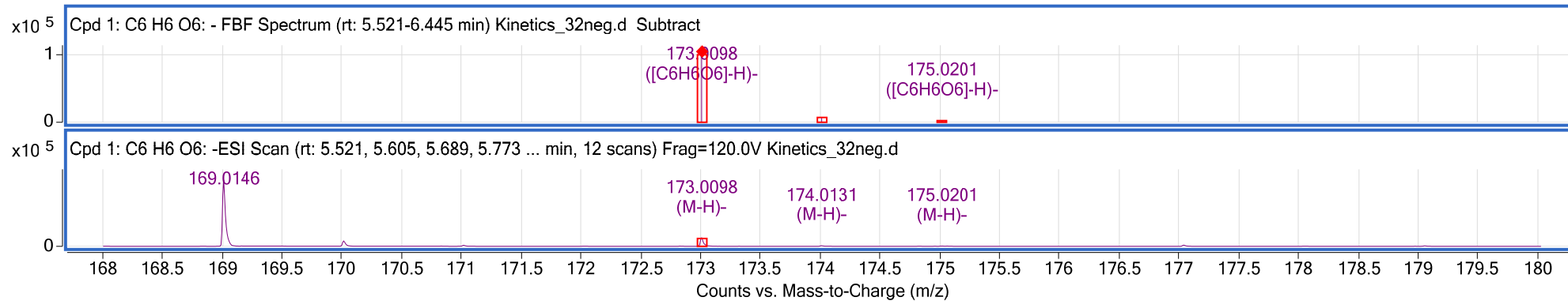


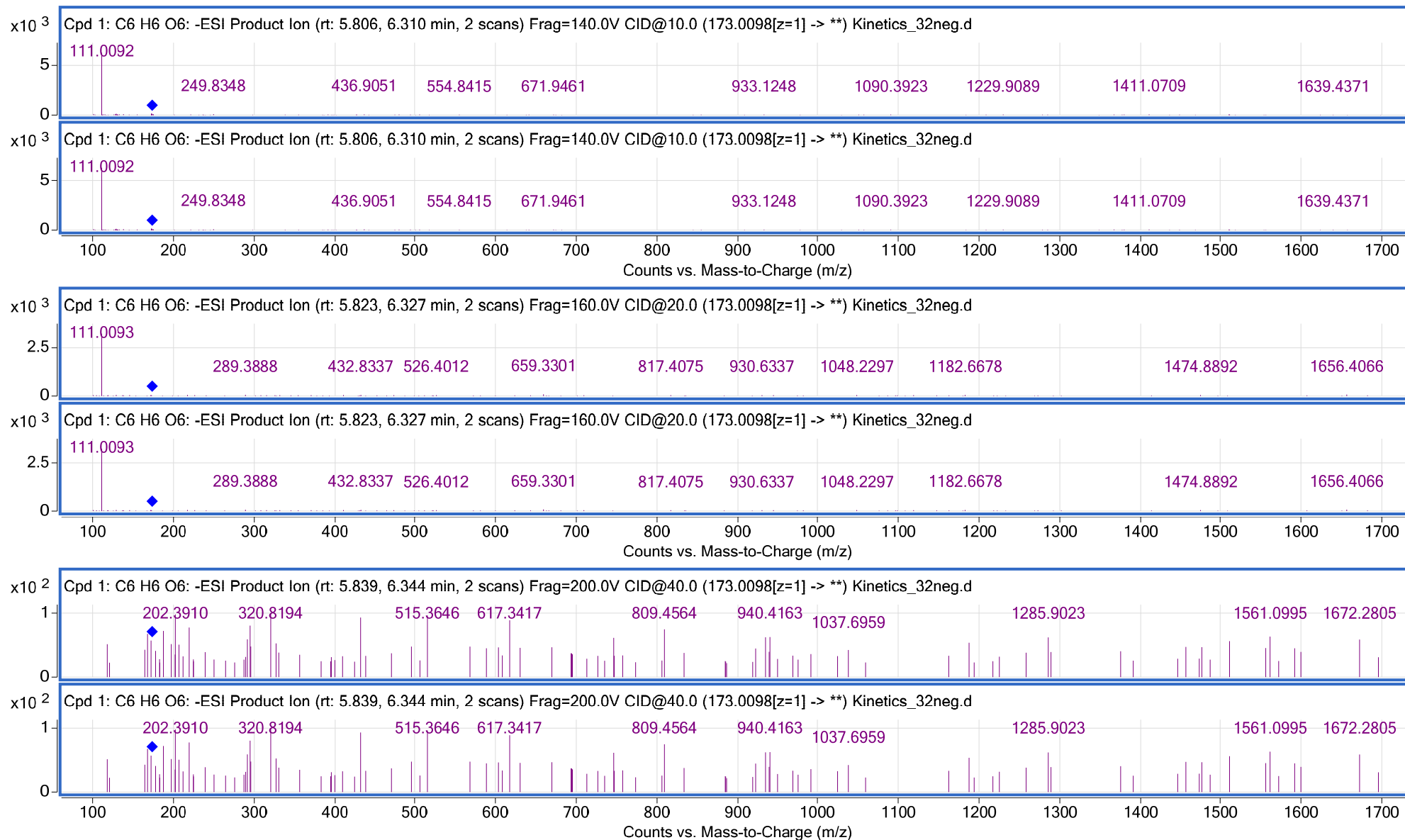
8.  $C_7H_{12}O_5$ , m/z-221.0675, 3-Isopropylmalic acid



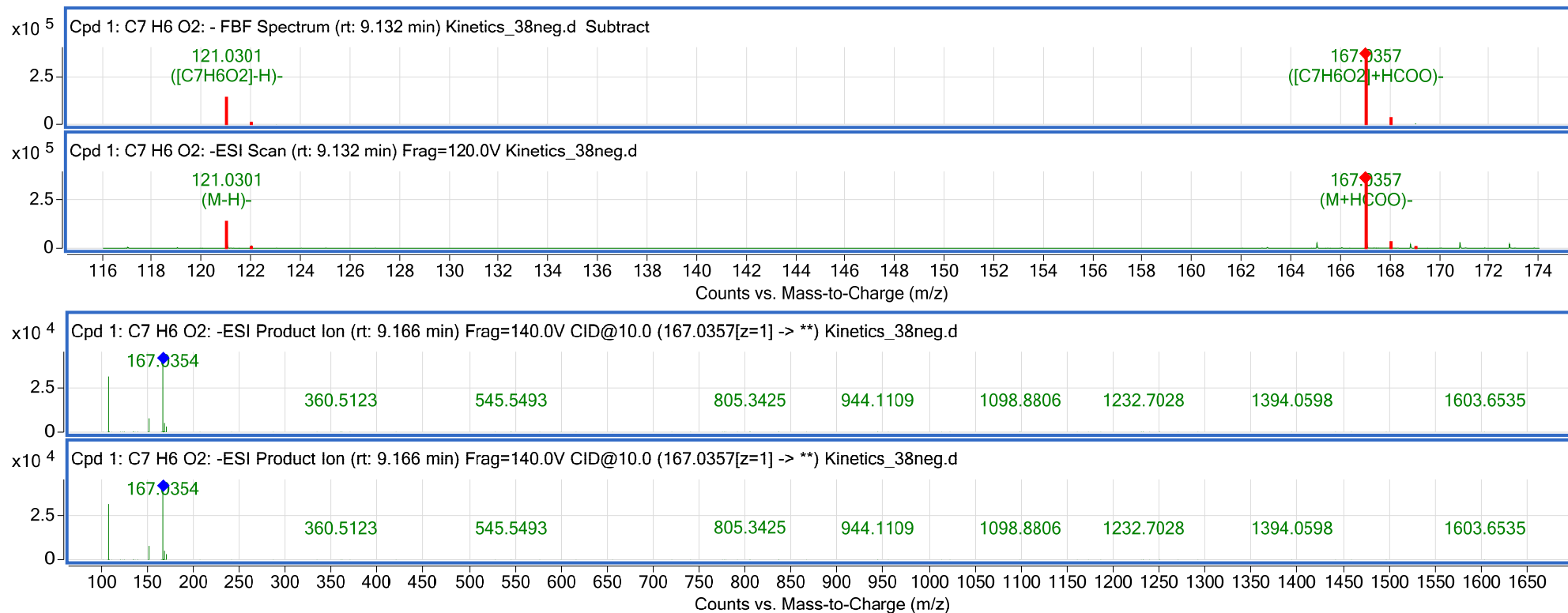


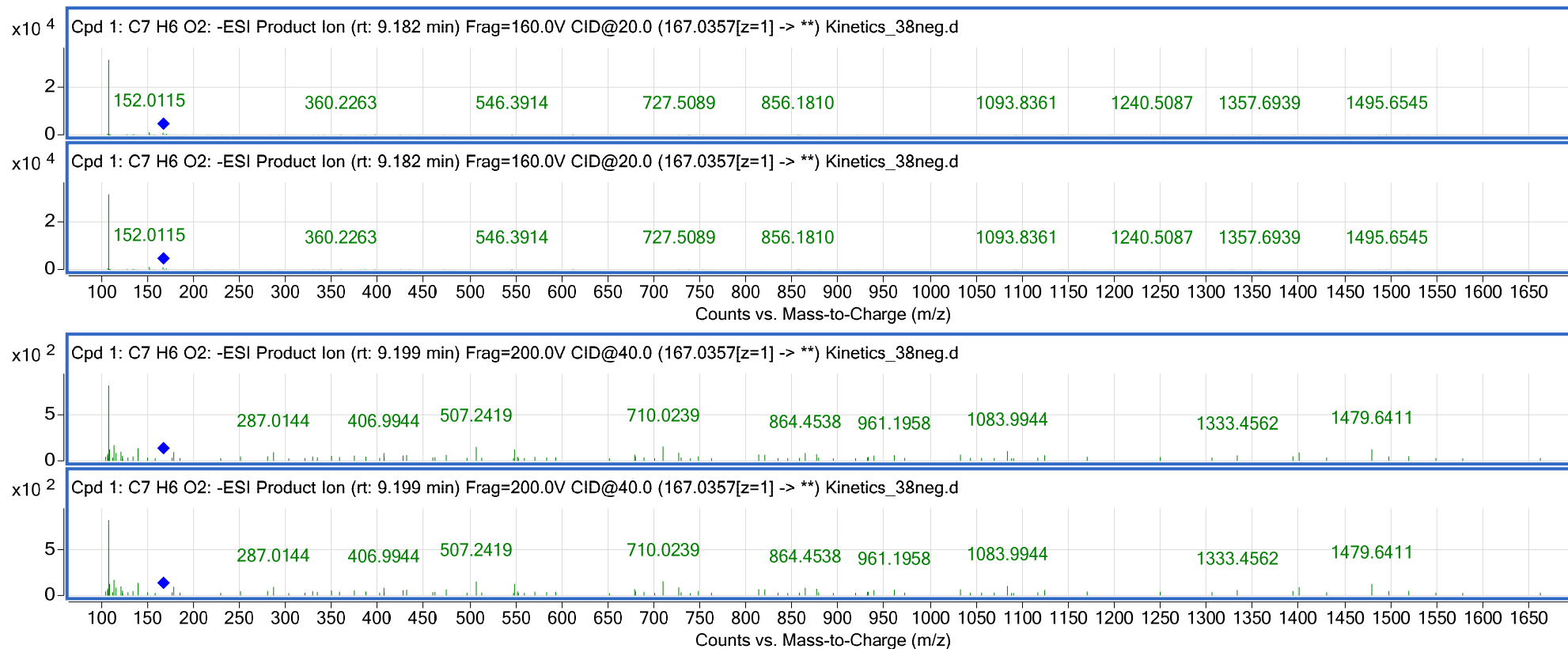
## 9. C<sub>6</sub>H<sub>6</sub>O<sub>6</sub>, m/z- 173.0097, Aconitic acid



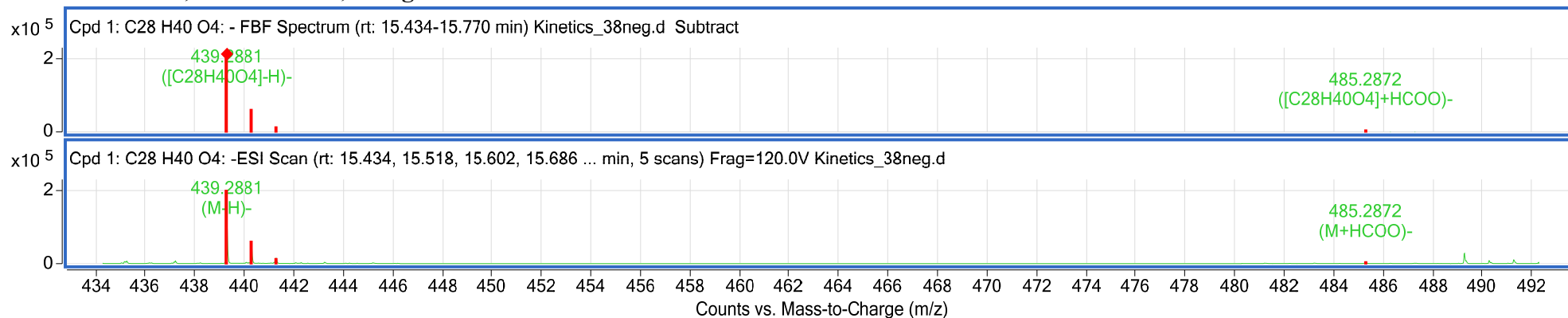


10. C<sub>7</sub>H<sub>6</sub>O<sub>2</sub>, m/z-121.03, Benzoic acid

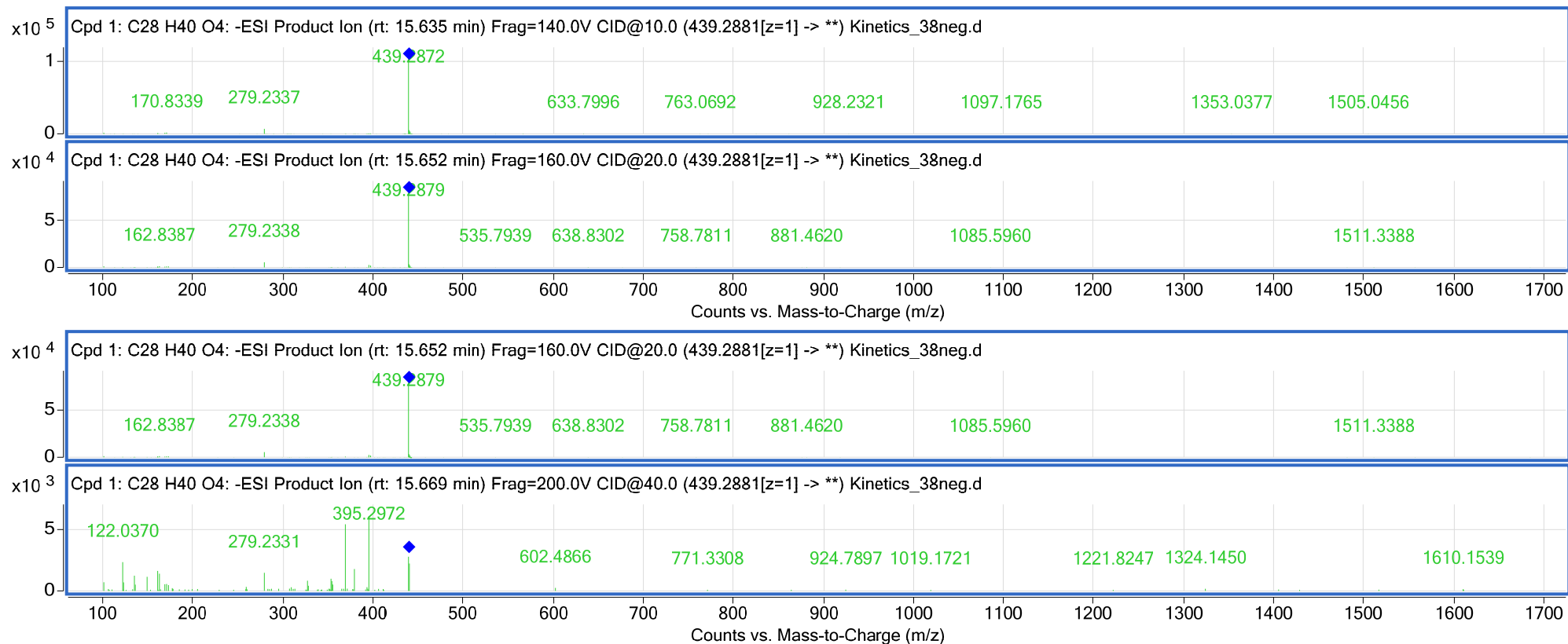




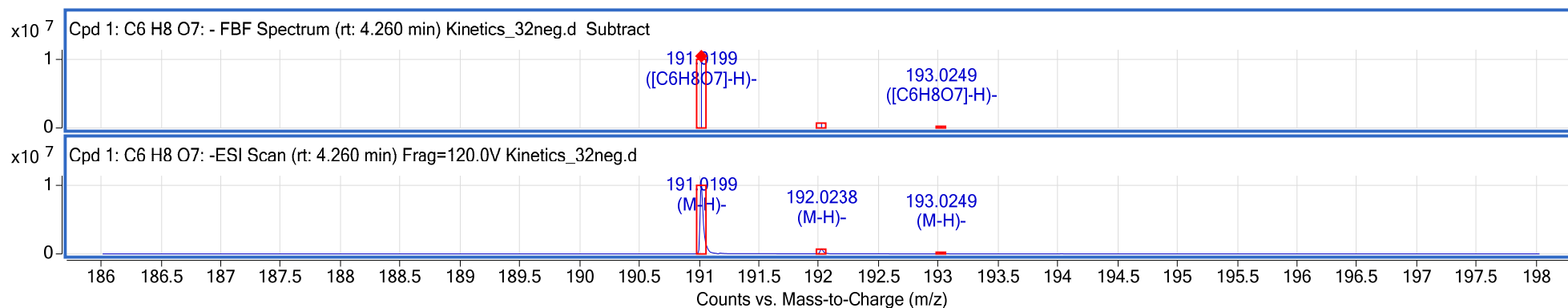
# 11. C<sub>28</sub> H<sub>40</sub> O<sub>4</sub>, m/z-439.2854, Bolegrevilol

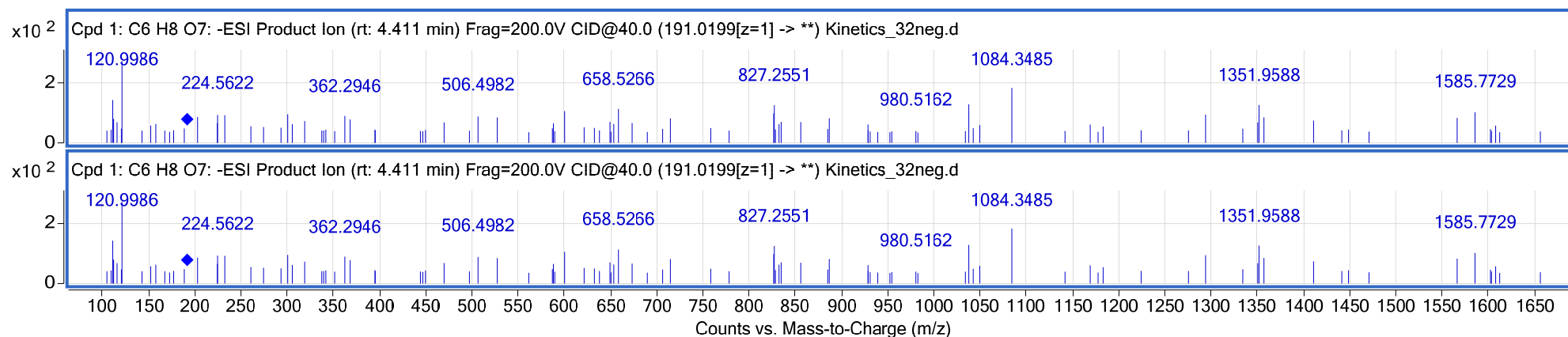
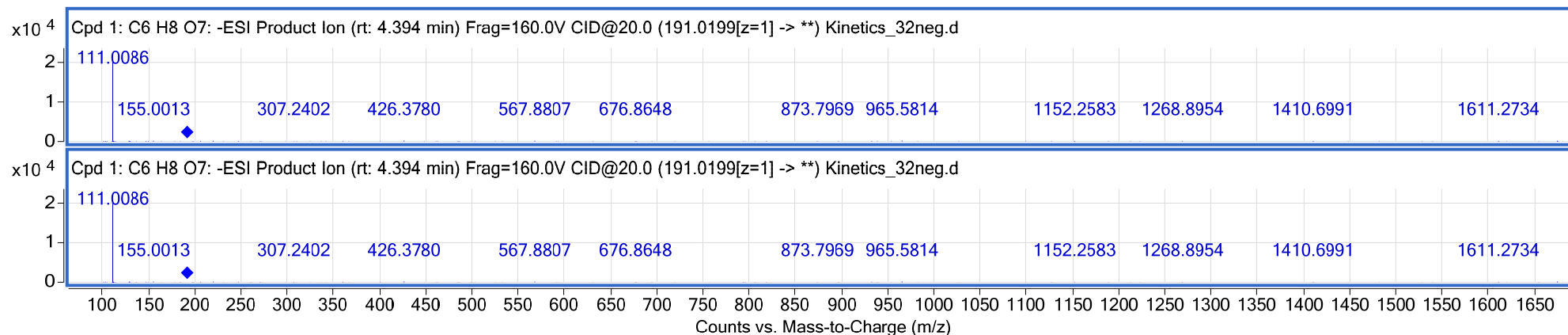
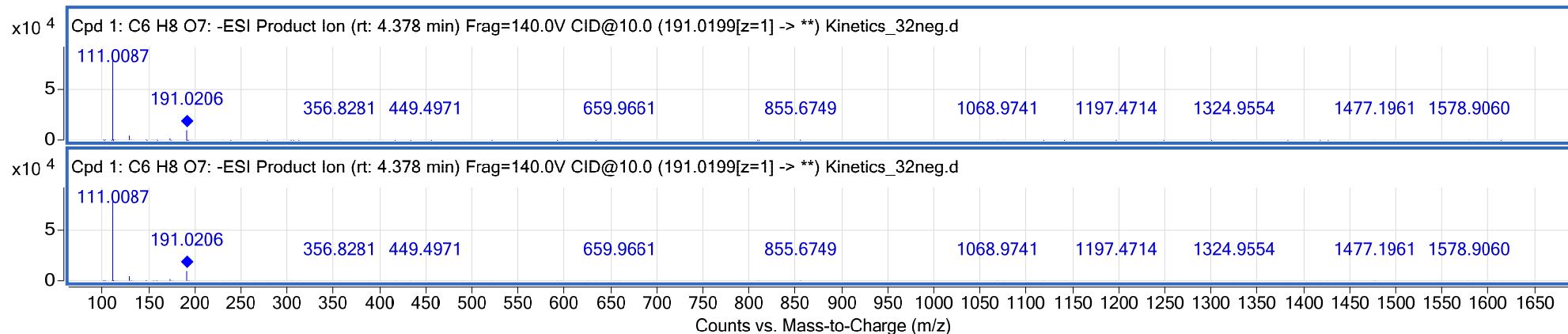




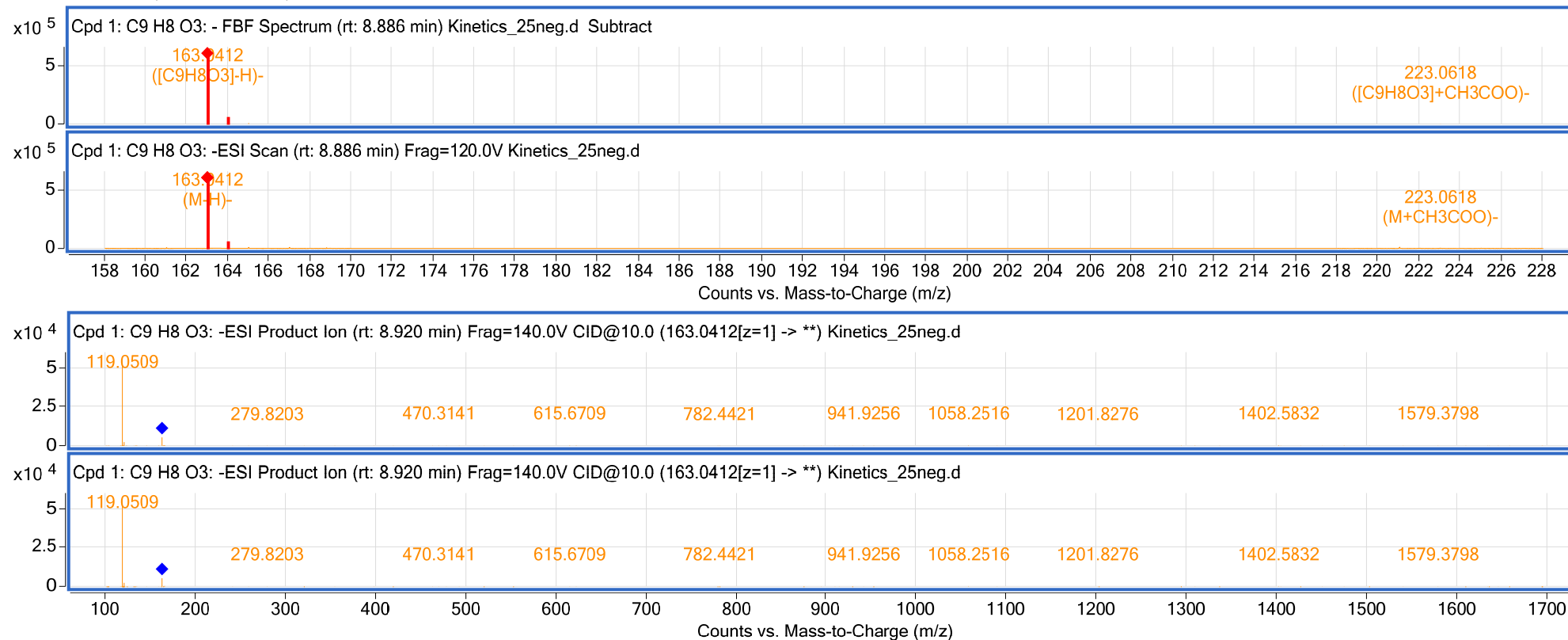


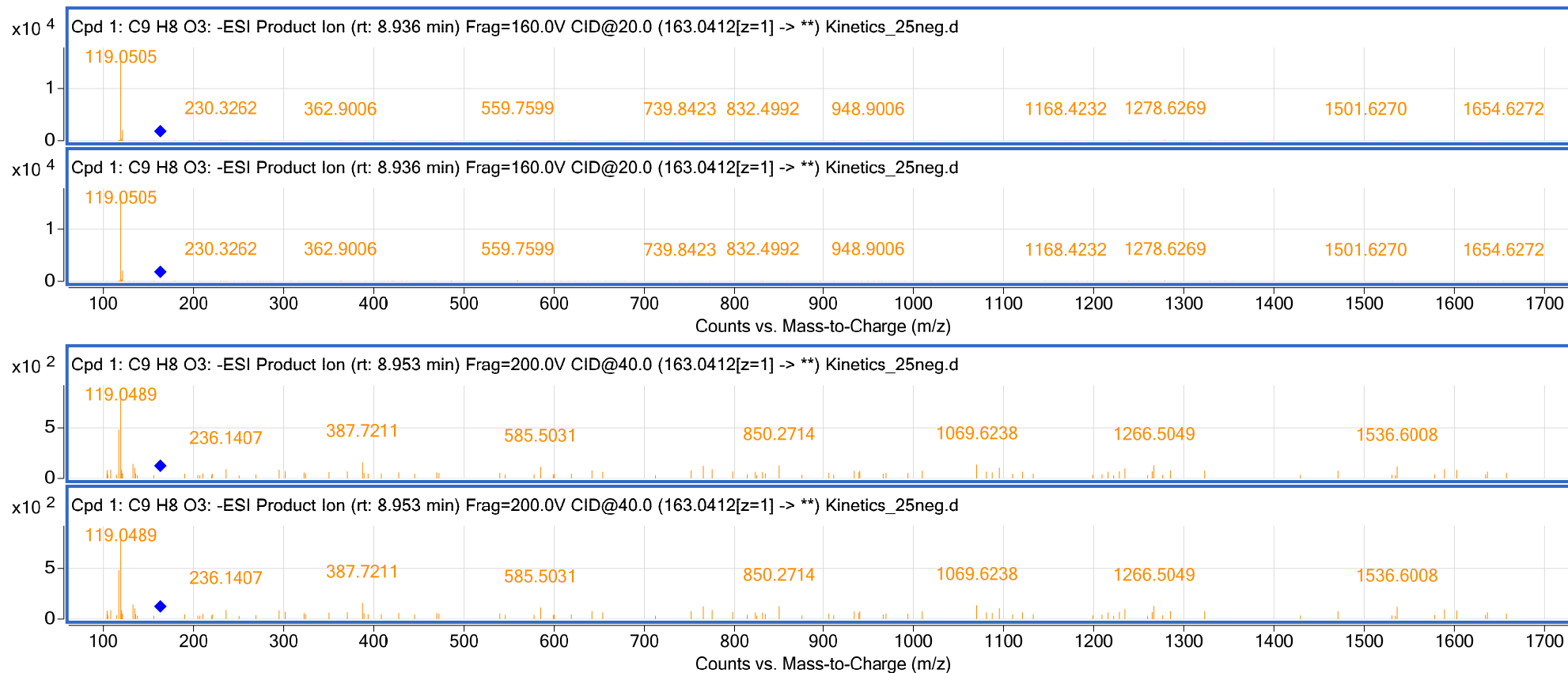
## 12. C<sub>6</sub> H<sub>8</sub> O<sub>7</sub>, m/z-191.0201, Citric acid



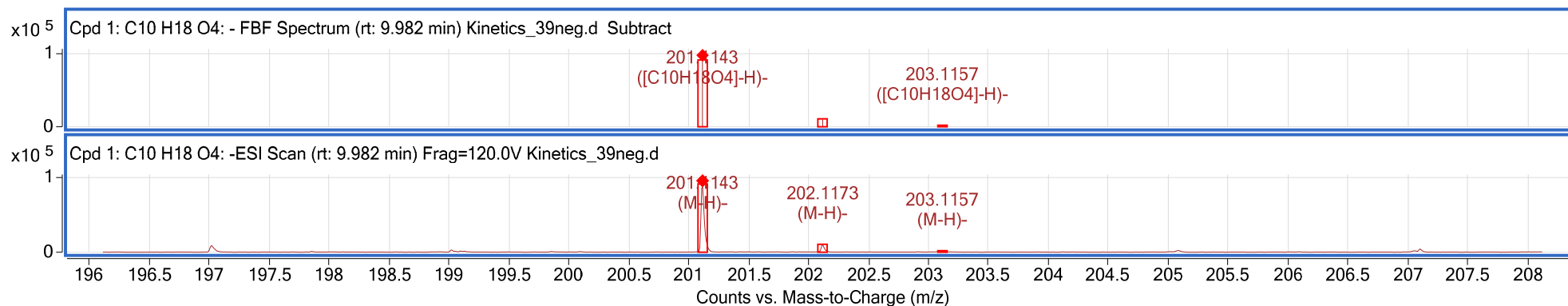


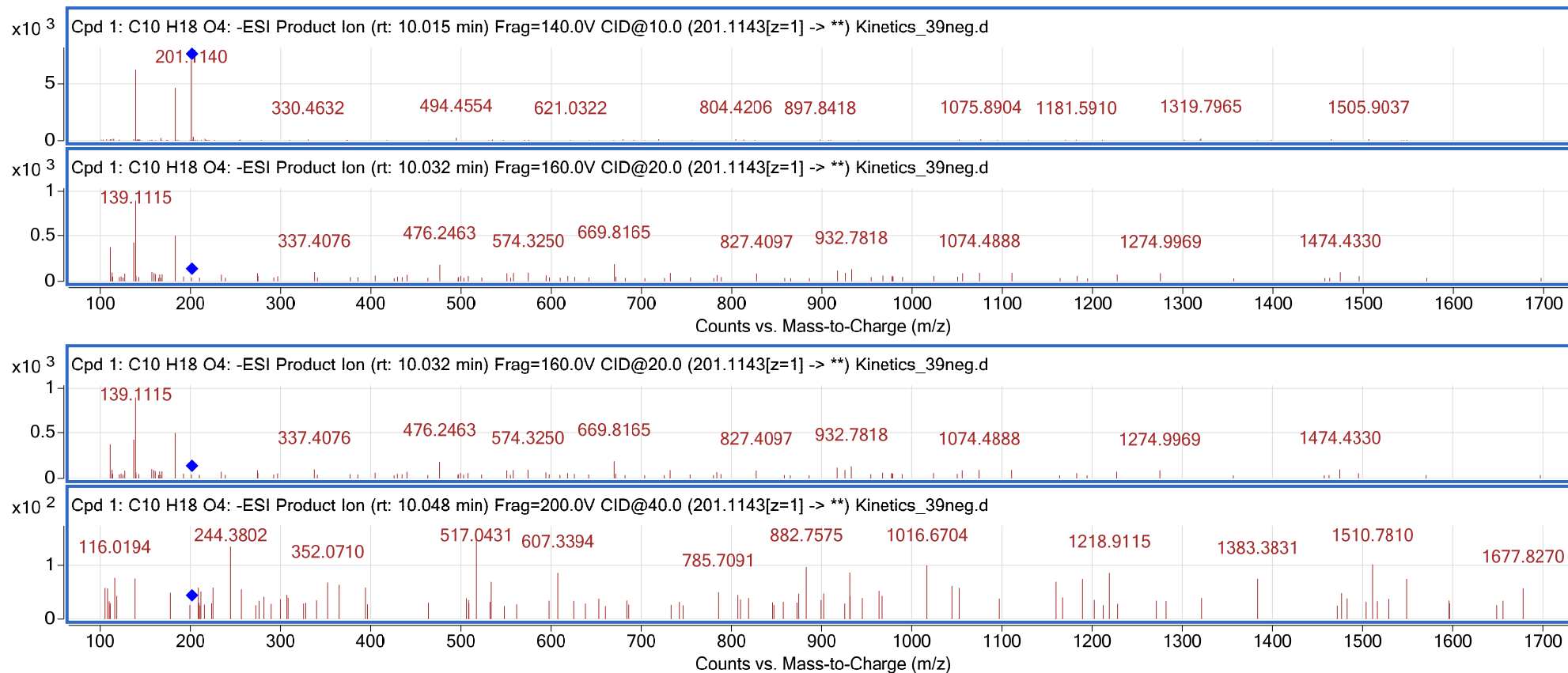
### 13. $\text{C}_9\text{H}_8\text{O}_3$ , m/z-163.04, Coumaric acid



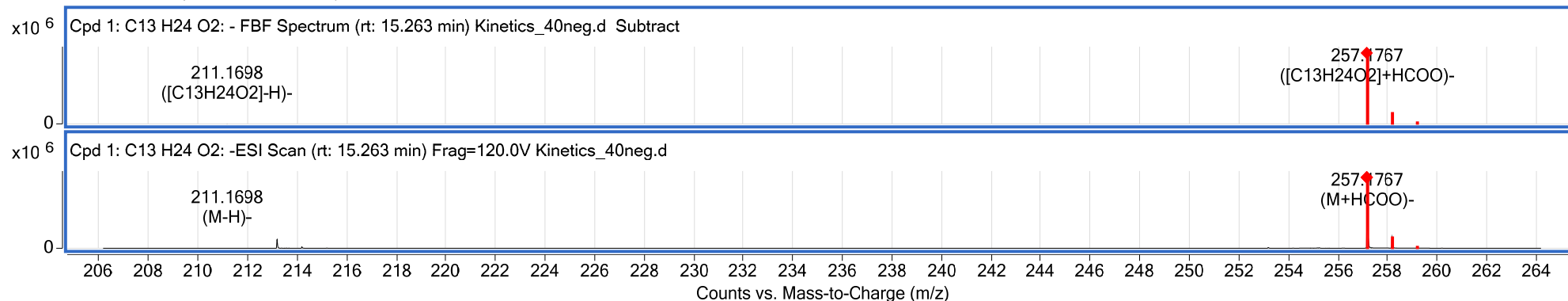


#### 14. C<sub>10</sub> H<sub>18</sub> O<sub>4</sub>, m/z-201.1143, Decanedioic acid



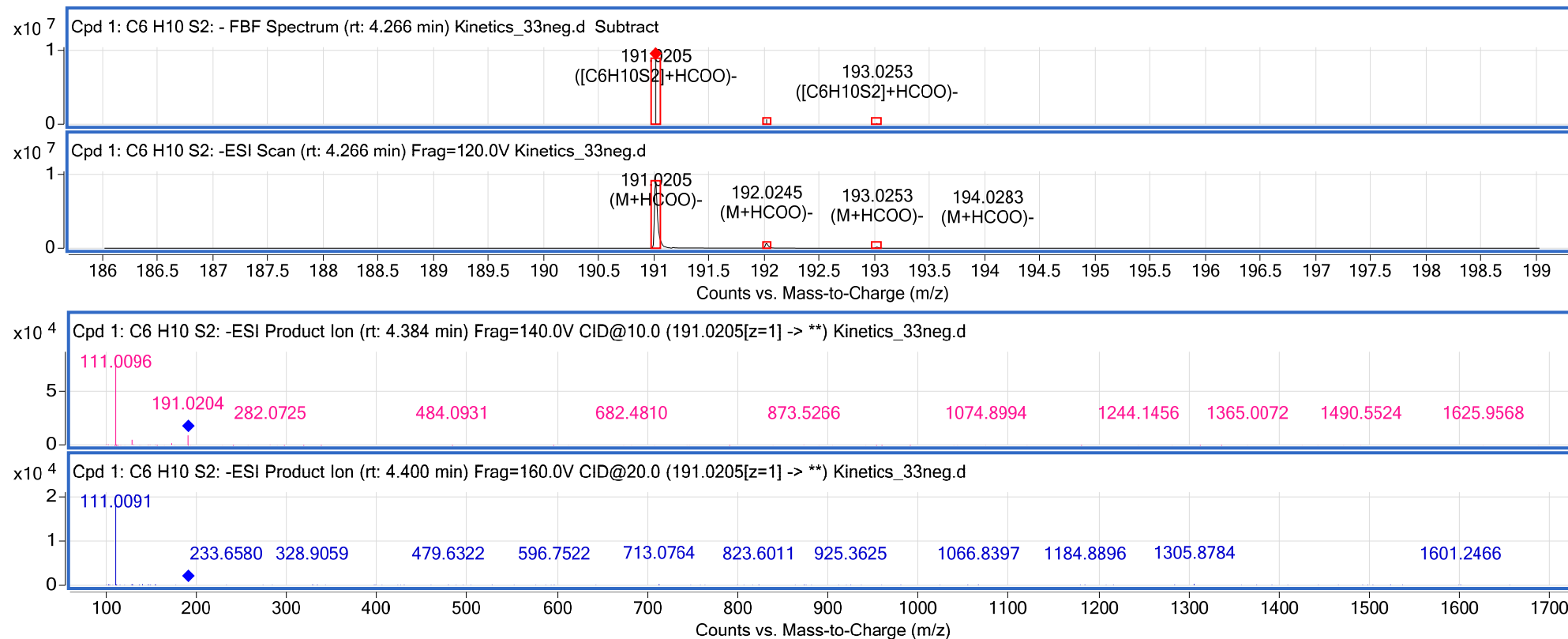


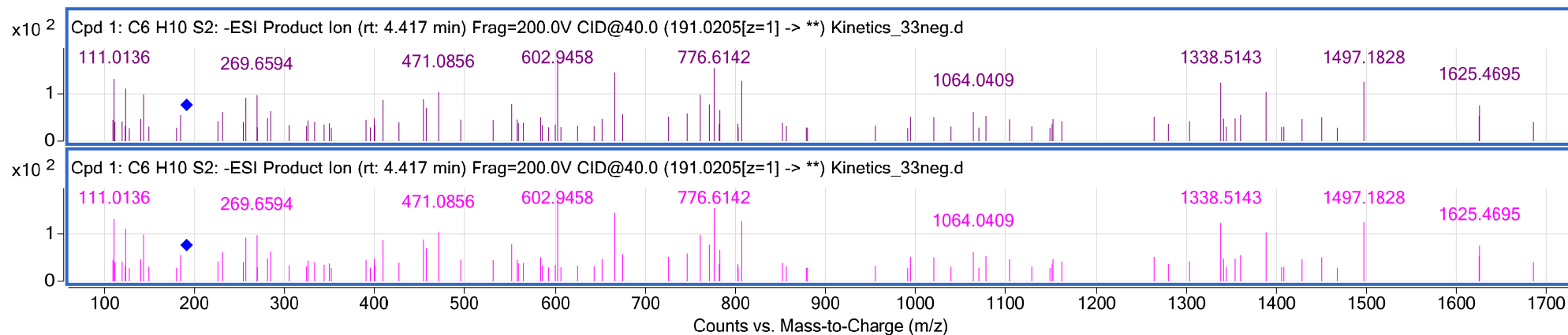
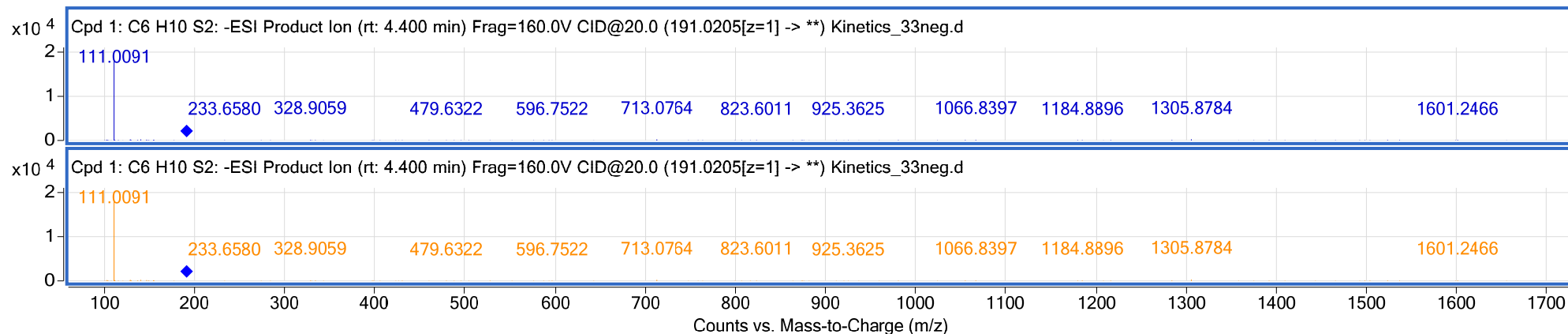
**15. C<sub>13</sub> H<sub>24</sub> O<sub>2</sub>, m/z-271.1918, Delta-tridecalactone**



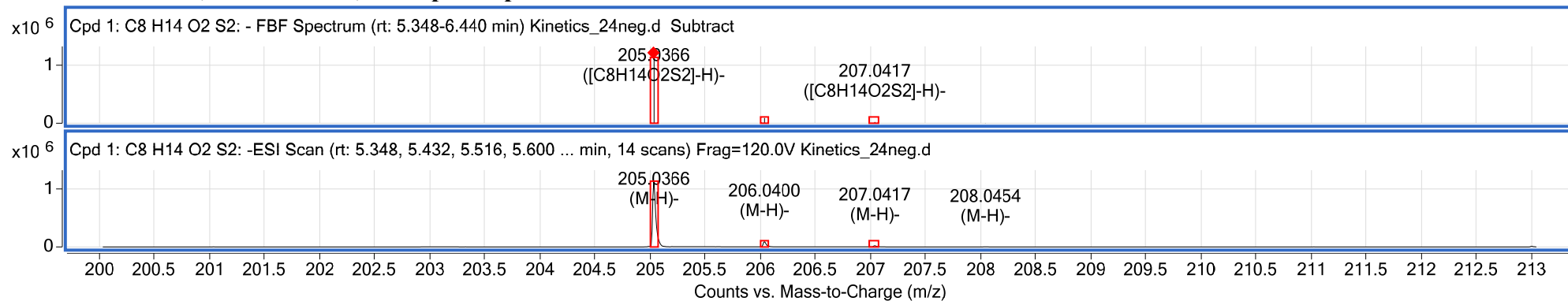


16.  $C_6H_{10}S_2$ , m/z-191.0199, Di-2-propenyl disulfide





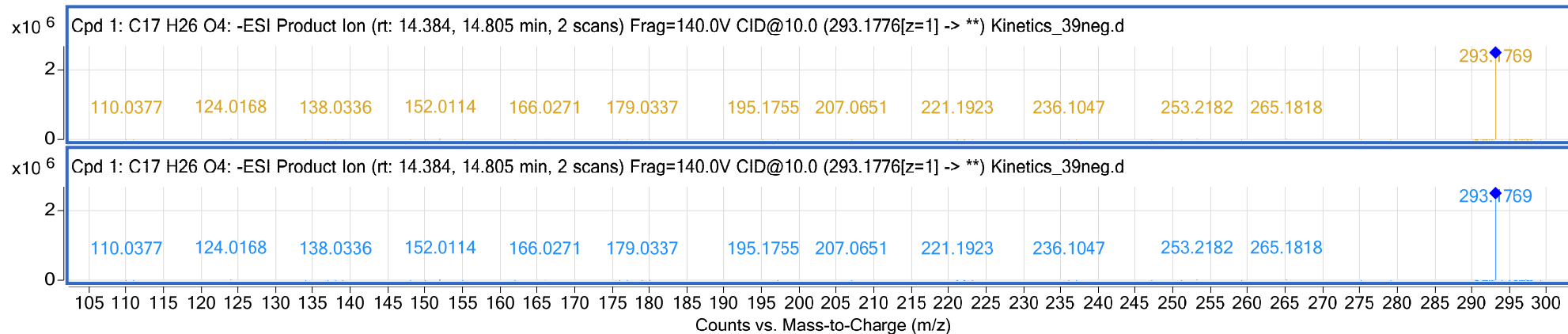
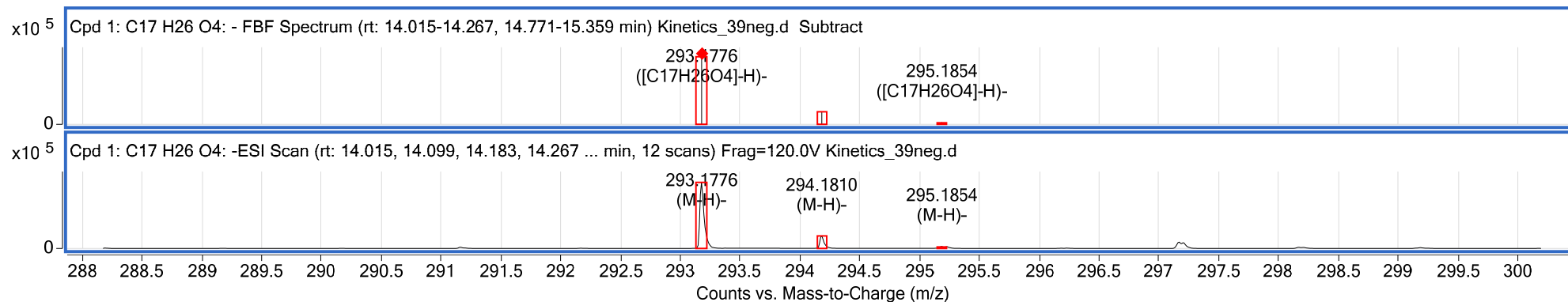
**17. C<sub>8</sub> H<sub>14</sub> O<sub>2</sub> S<sub>2</sub>, m/z-205.0365, DL- $\alpha$ -Lipoic acid**

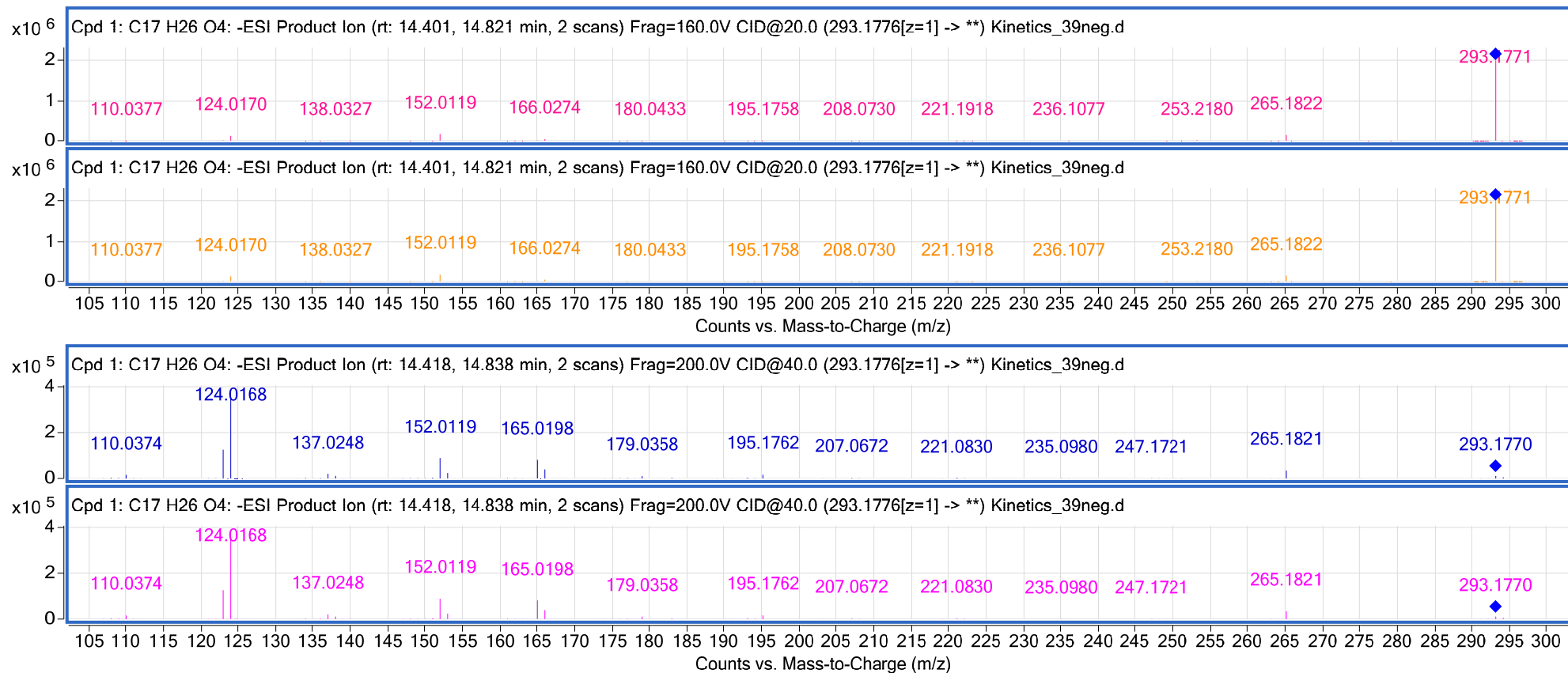




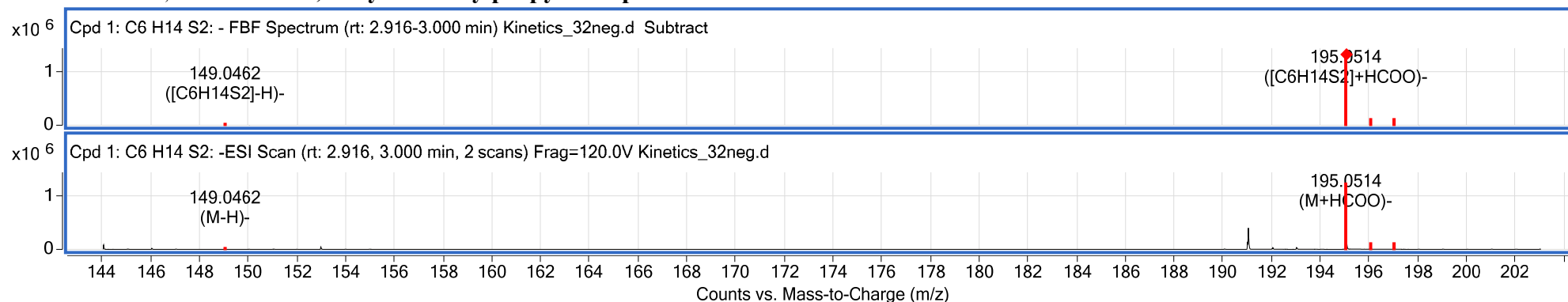


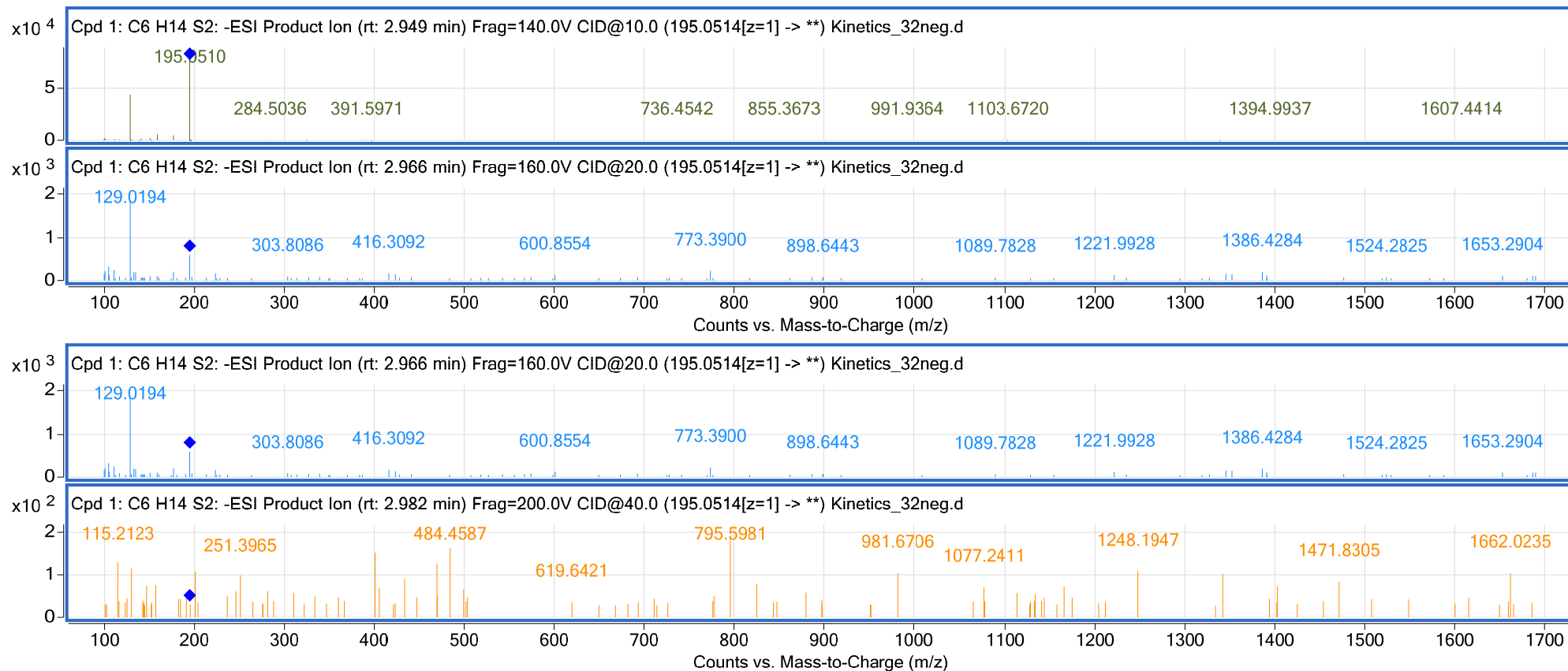
18. C<sub>17</sub> H<sub>26</sub> O<sub>4</sub>, m/z-293.1771, Embelin



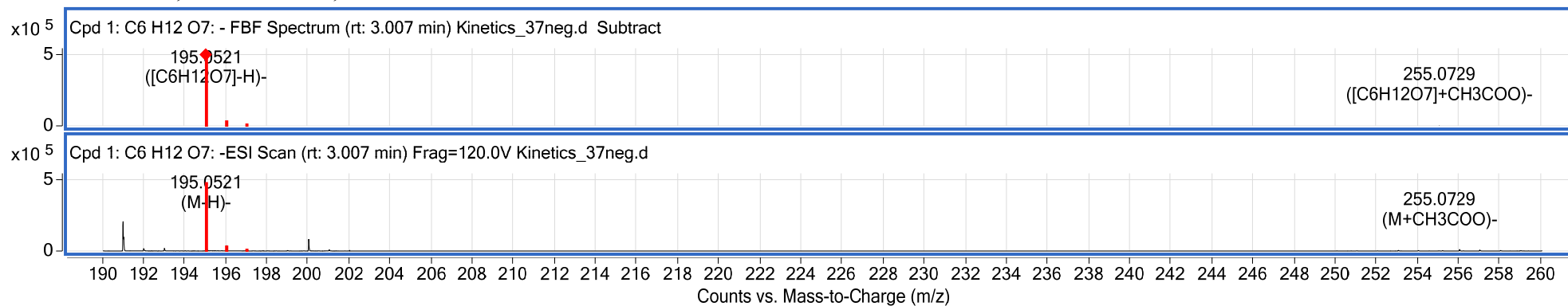


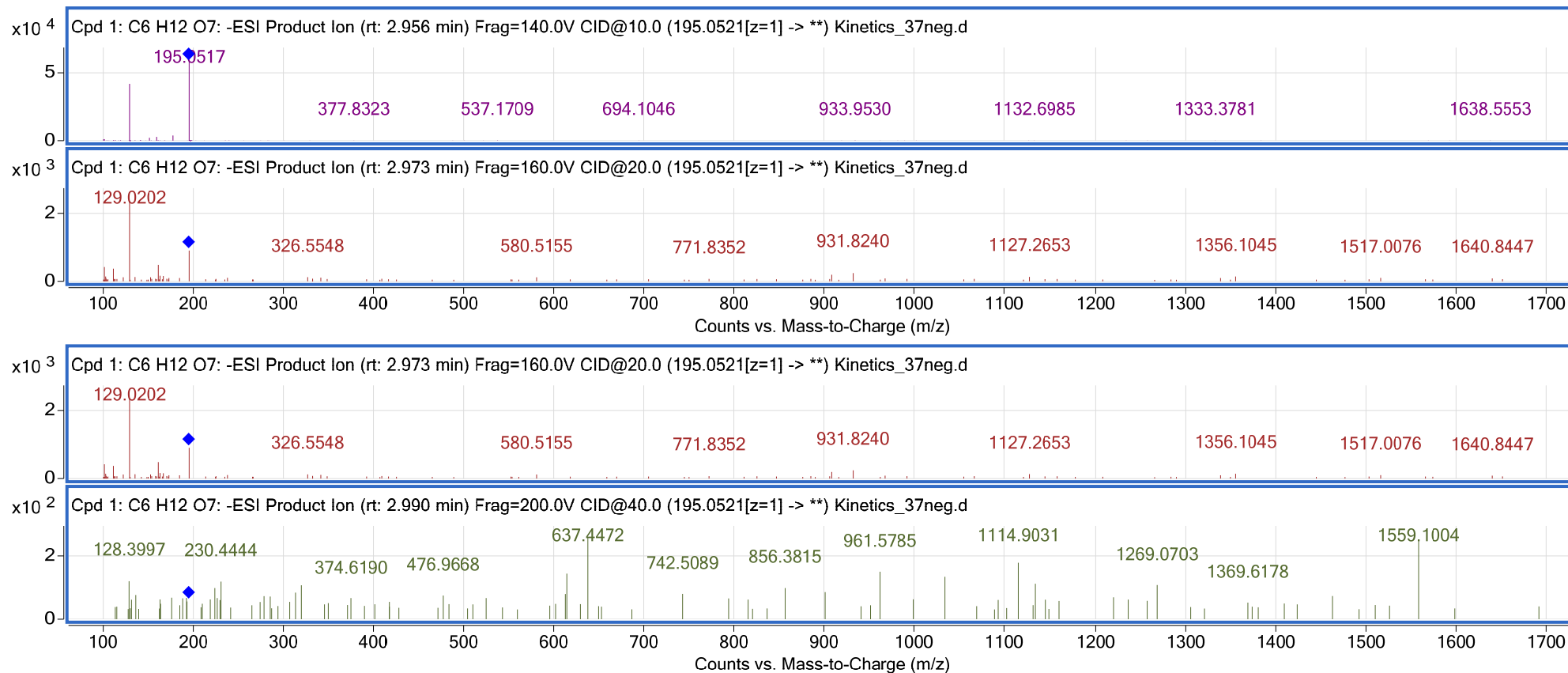
**19. C<sub>6</sub>H<sub>14</sub>S<sub>2</sub>, m/z-195.0514, Ethyl-1-methylpropyl disulphide**



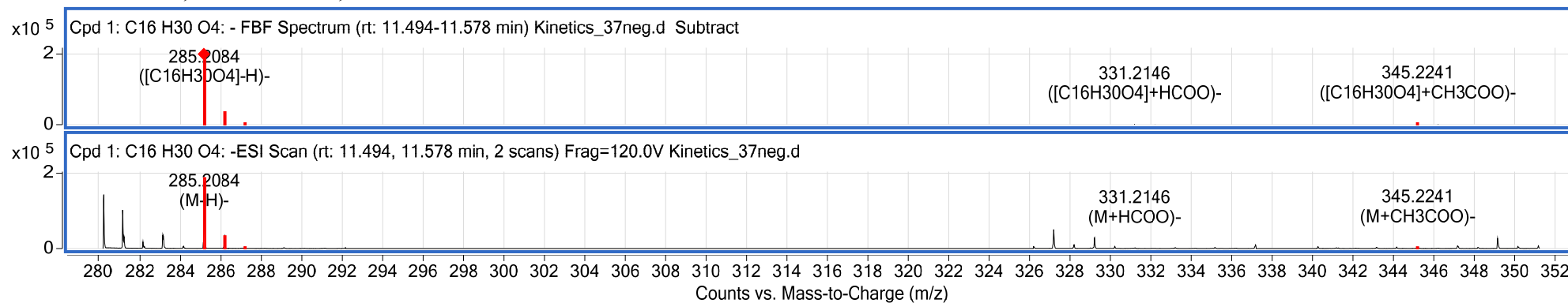


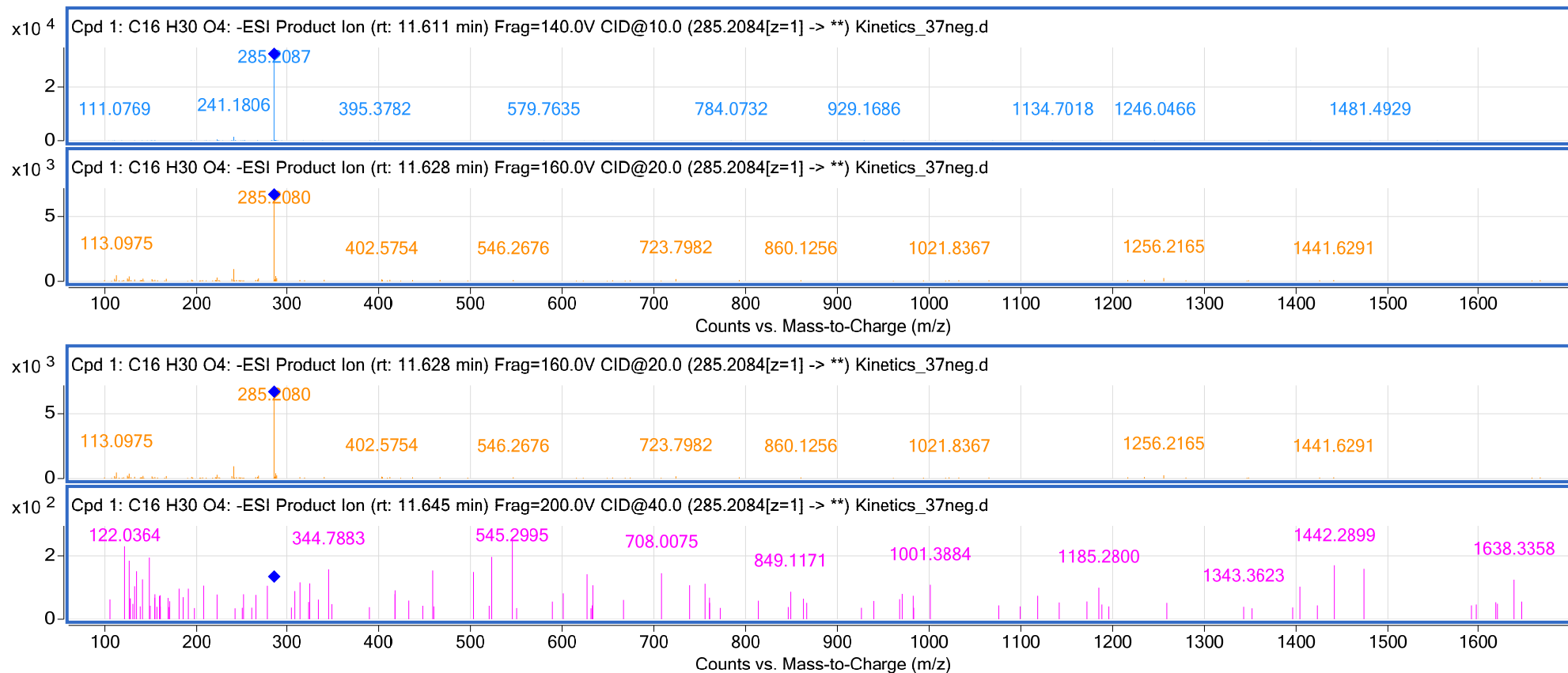
## 20. $C_6 H_{12} O_7$ , m/z-195.0514, Galactonic acid



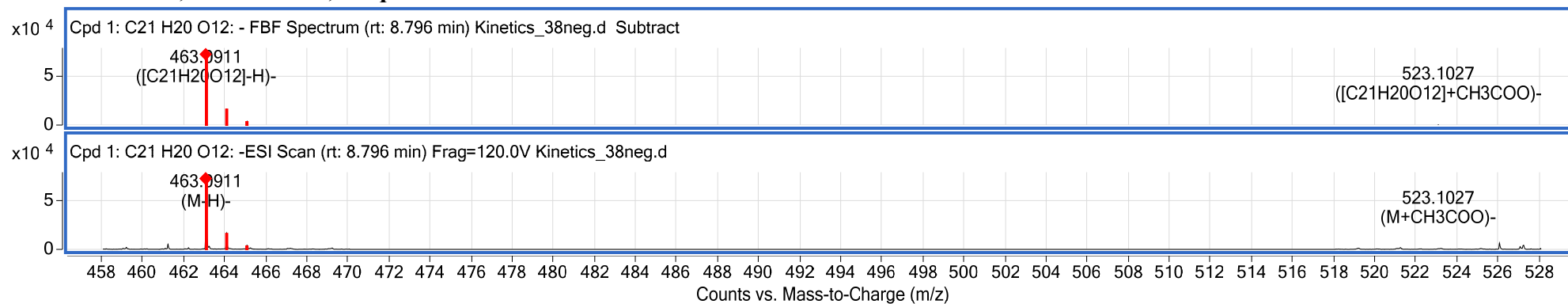


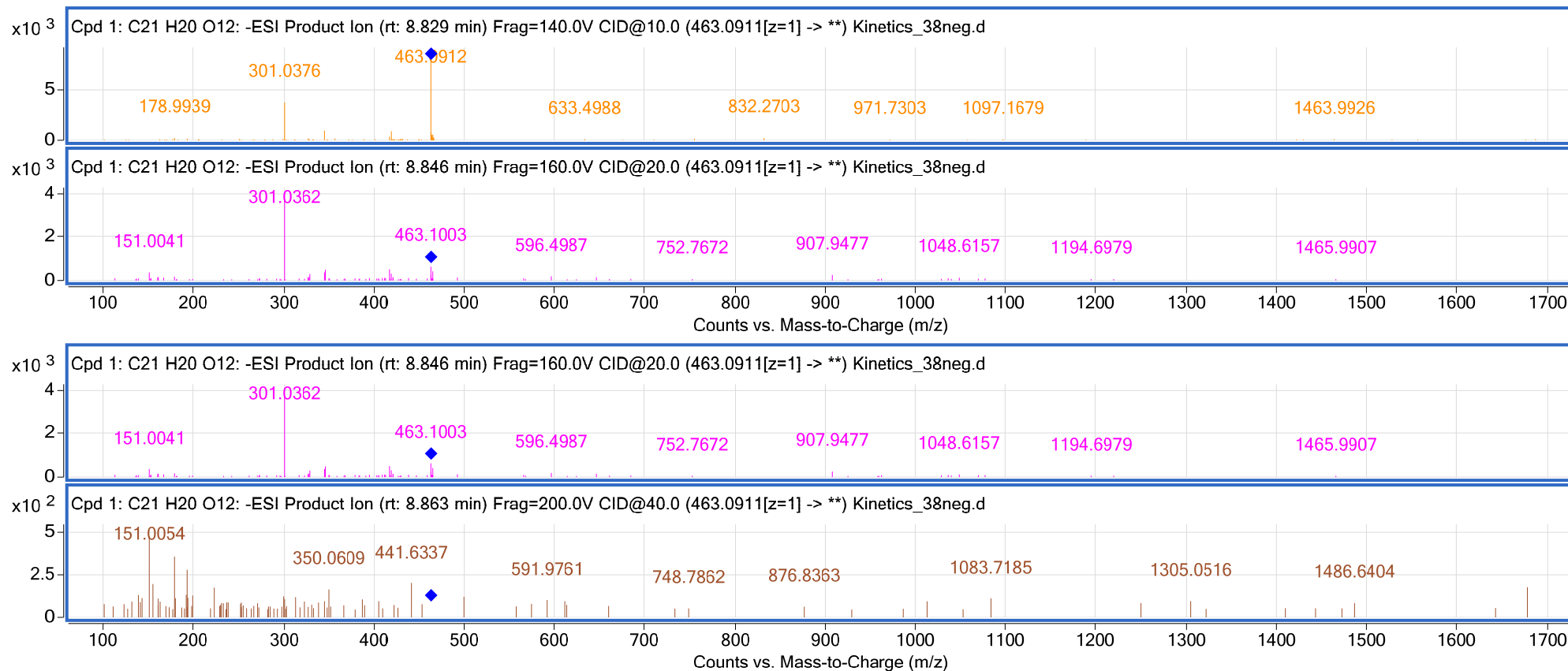
## 21. C<sub>16</sub>H<sub>30</sub>O<sub>4</sub>, m/z-285.2083, Hexadecanedioic acid



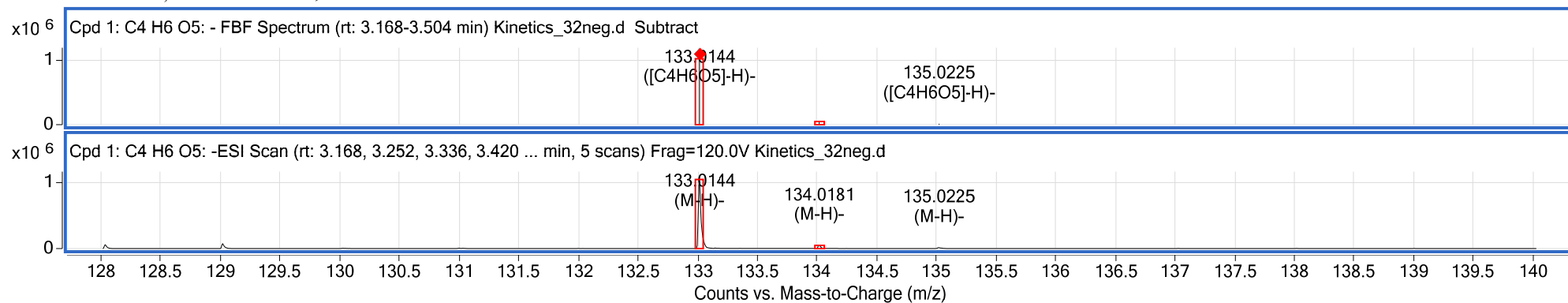


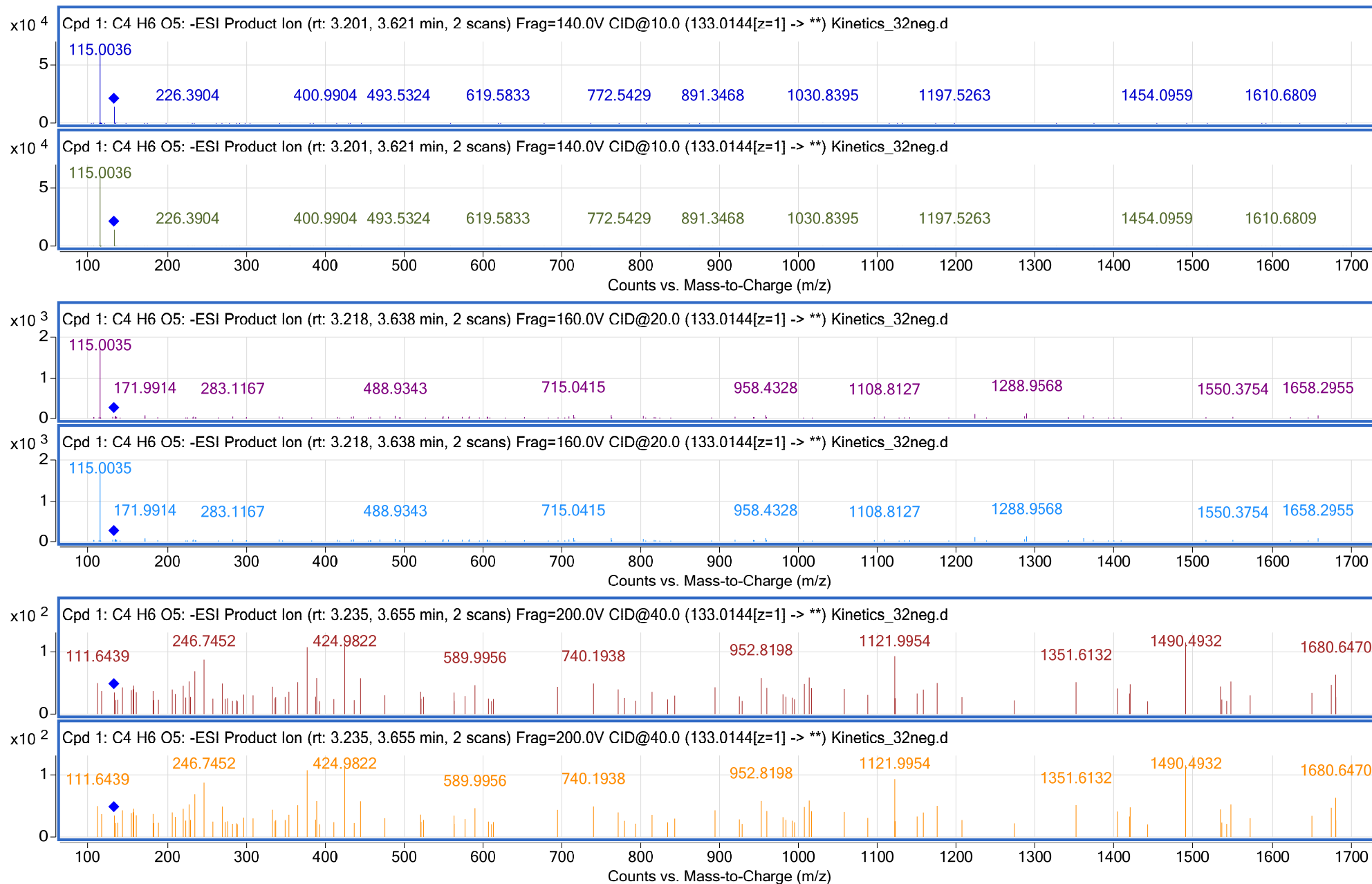
22. **C<sub>21</sub>H<sub>20</sub>O<sub>12</sub>, m/z-219.135, Isoquercitrin**





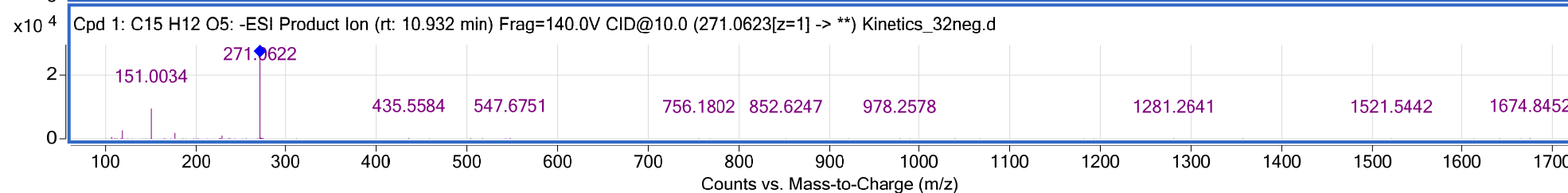
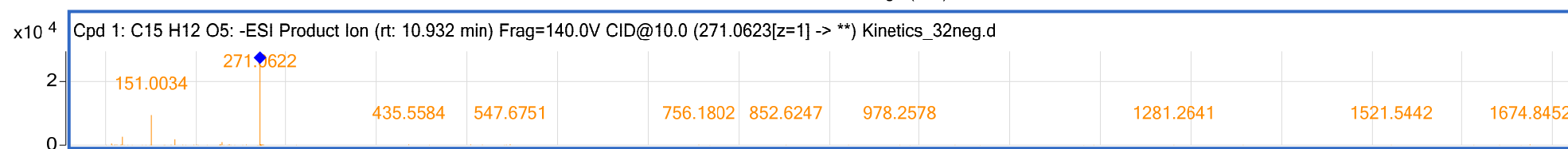
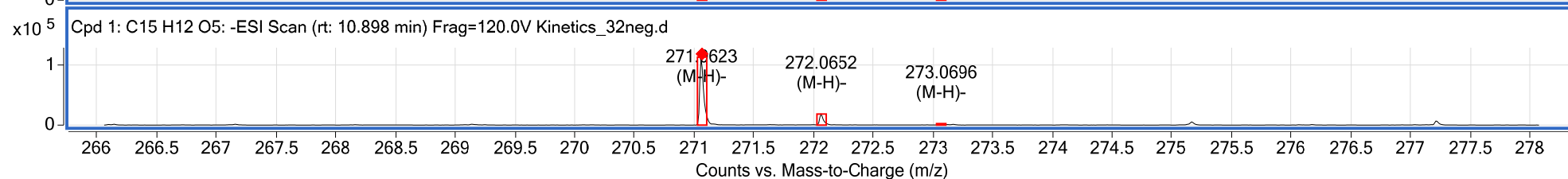
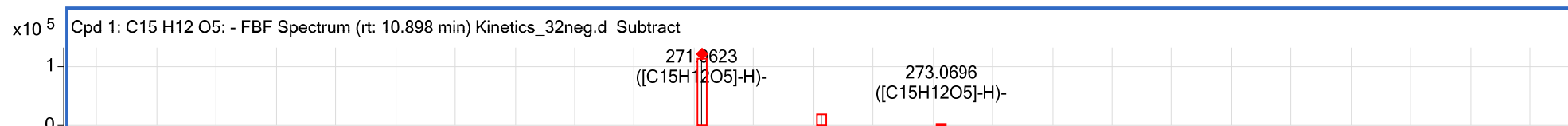
23. C<sub>4</sub> H<sub>6</sub> O<sub>5</sub>, m/z-133.0148, Malic acid

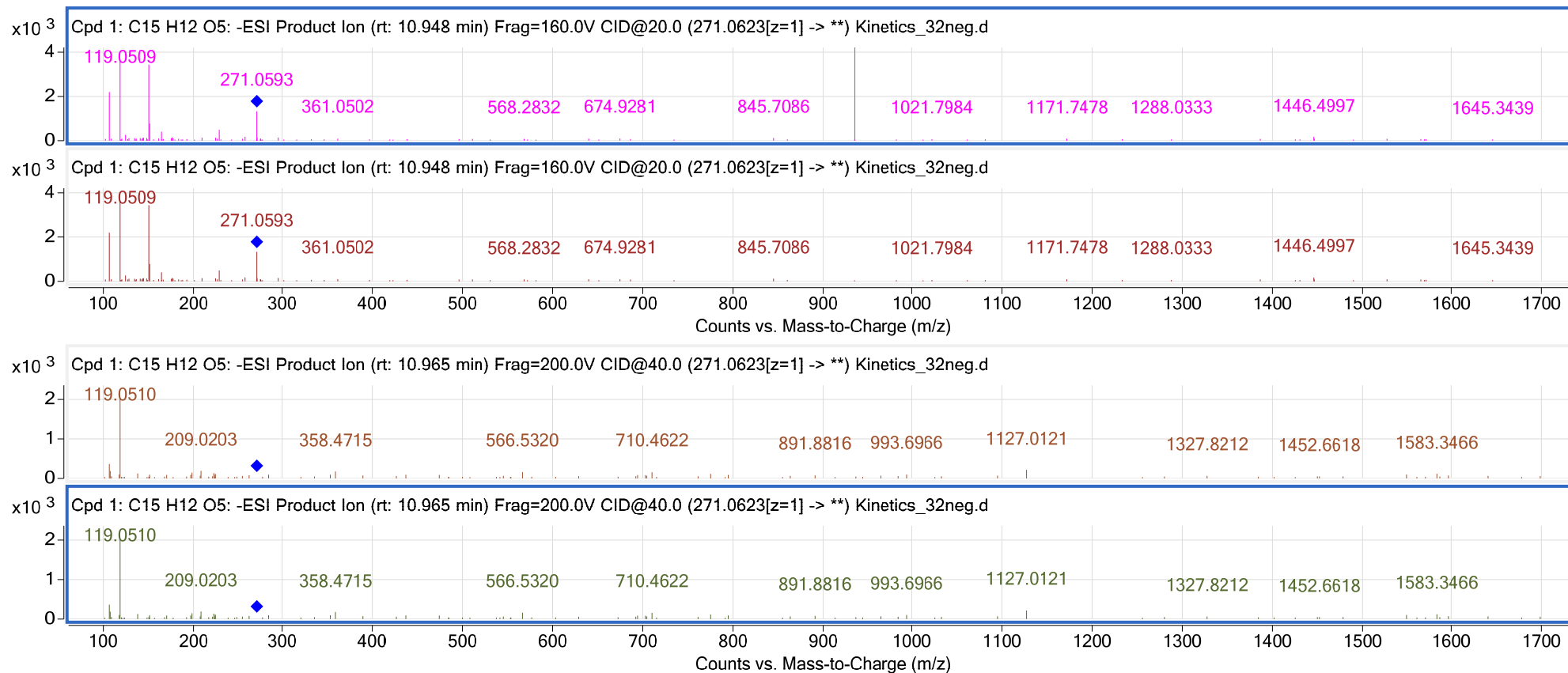




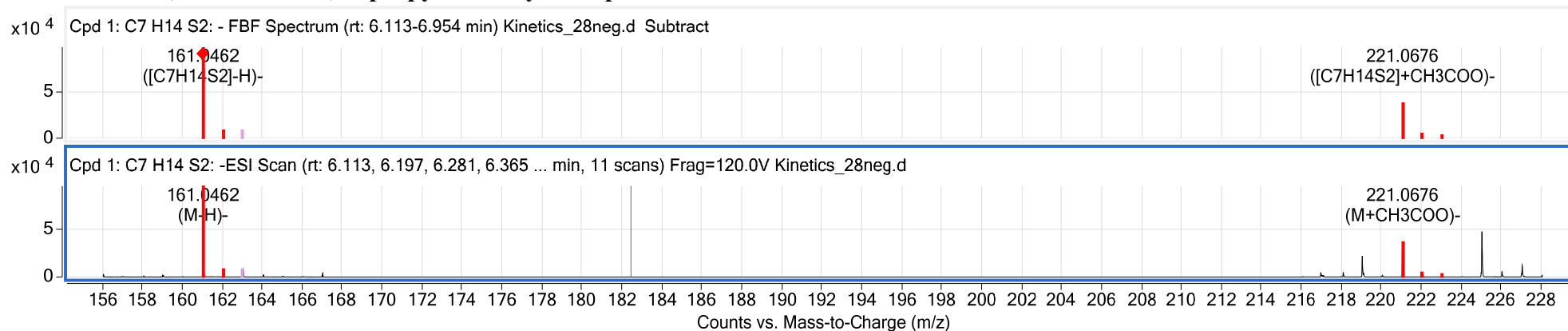
24.  $C_{15}H_{12}O_5$ , m/z-271.0623, Naringenin

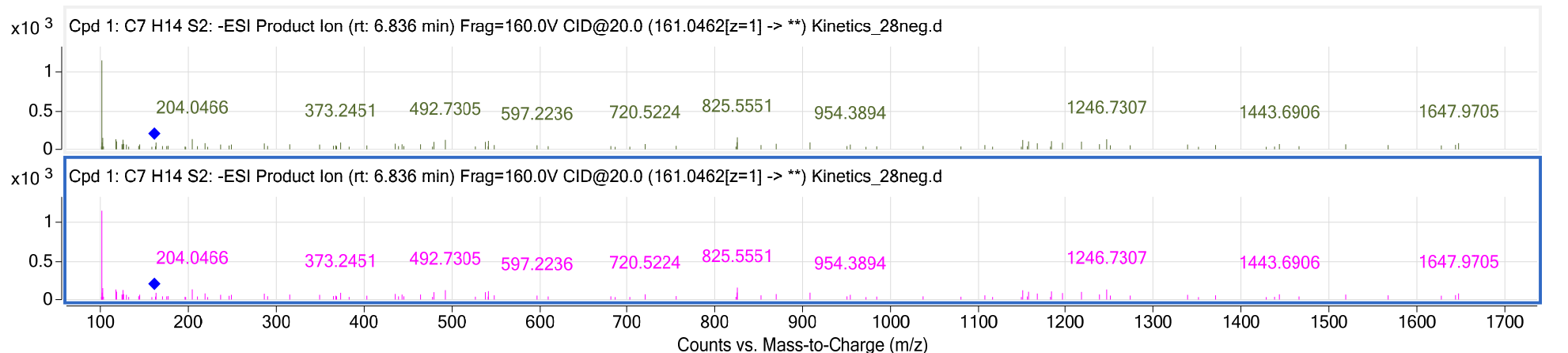
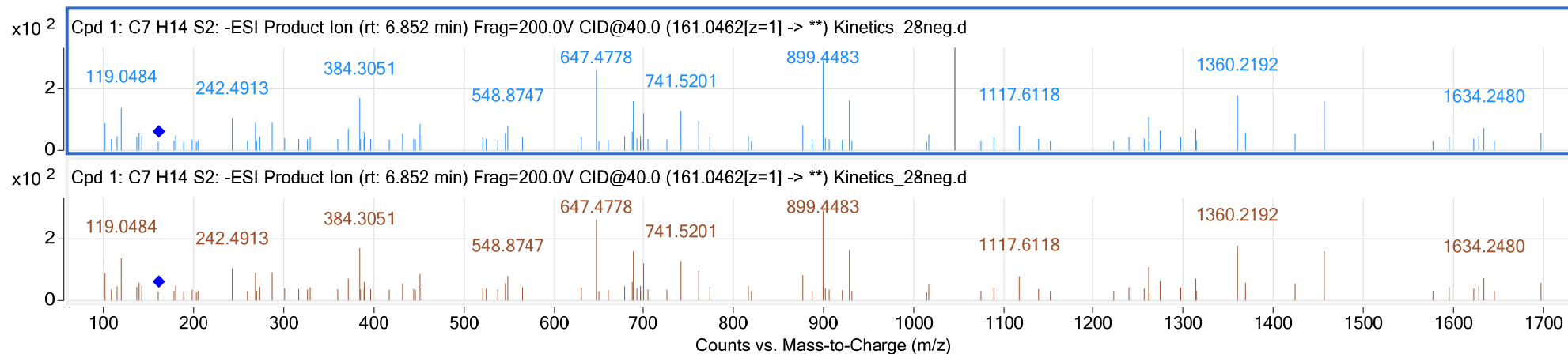
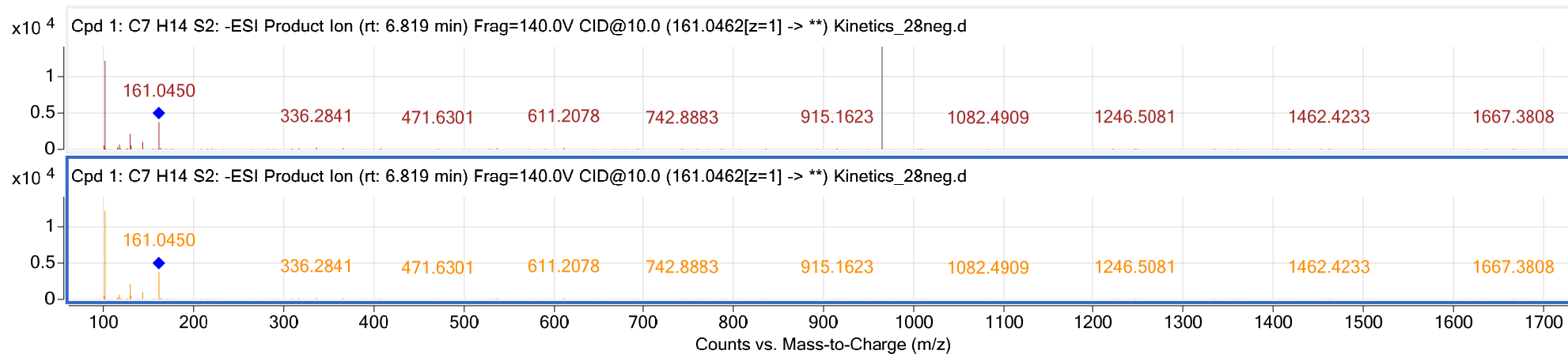






## 25. C<sub>7</sub> H<sub>14</sub> S<sub>2</sub>, m/z- 221.0675, N-propyl sec-butyl disulphide

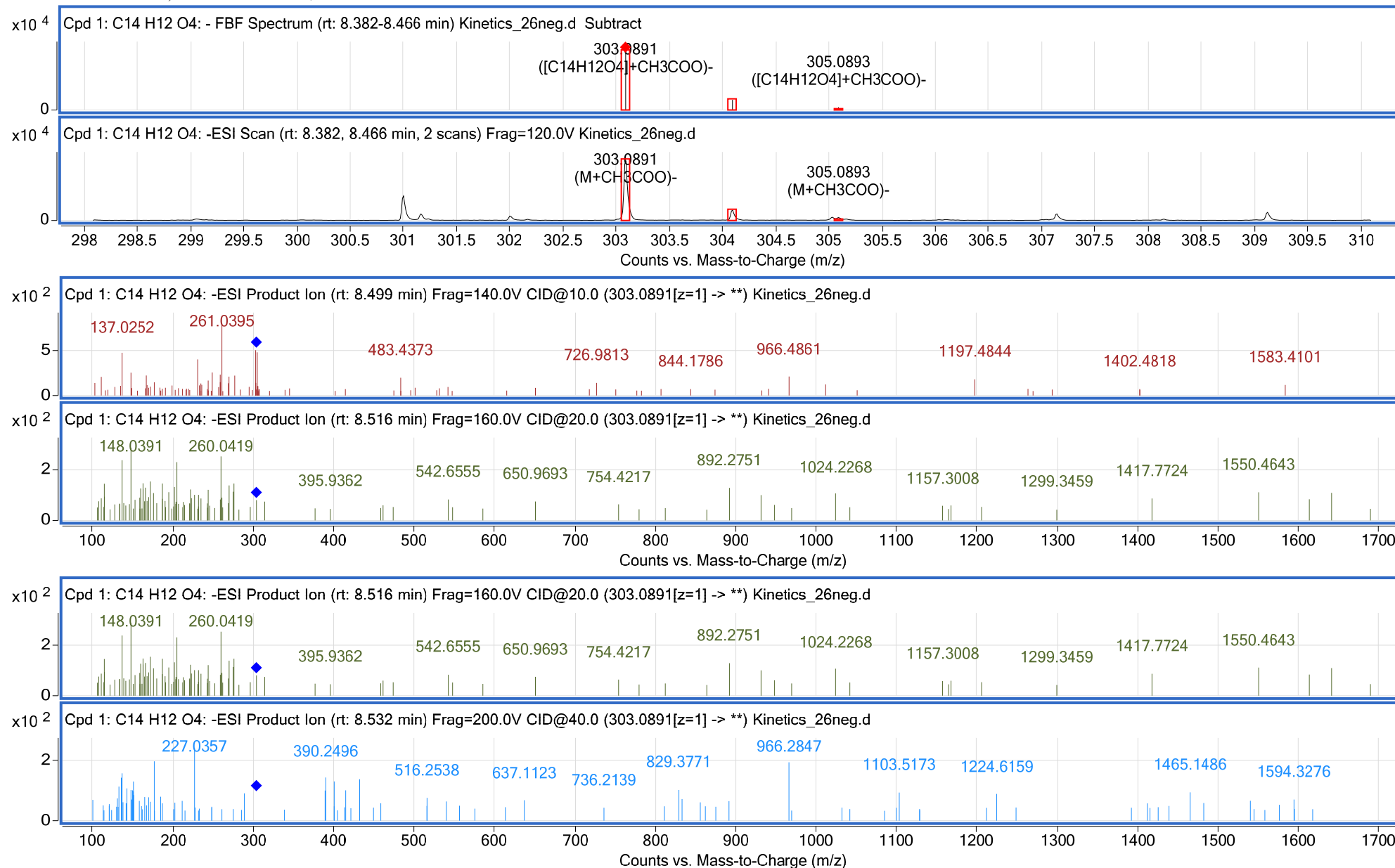




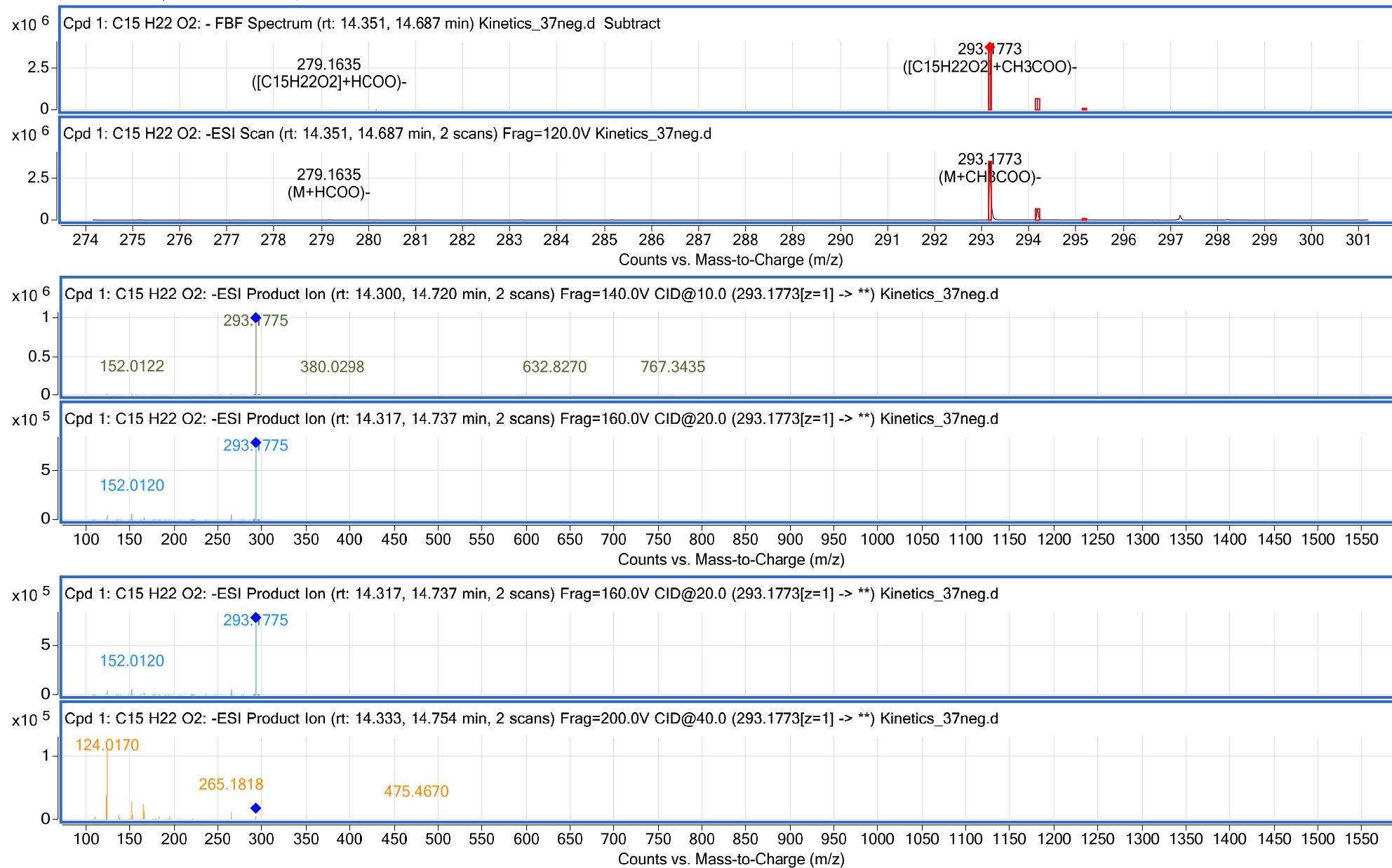
## 26. C<sub>4</sub>H<sub>4</sub>O<sub>5</sub>, m/z-191.0201, Oxaloacetate



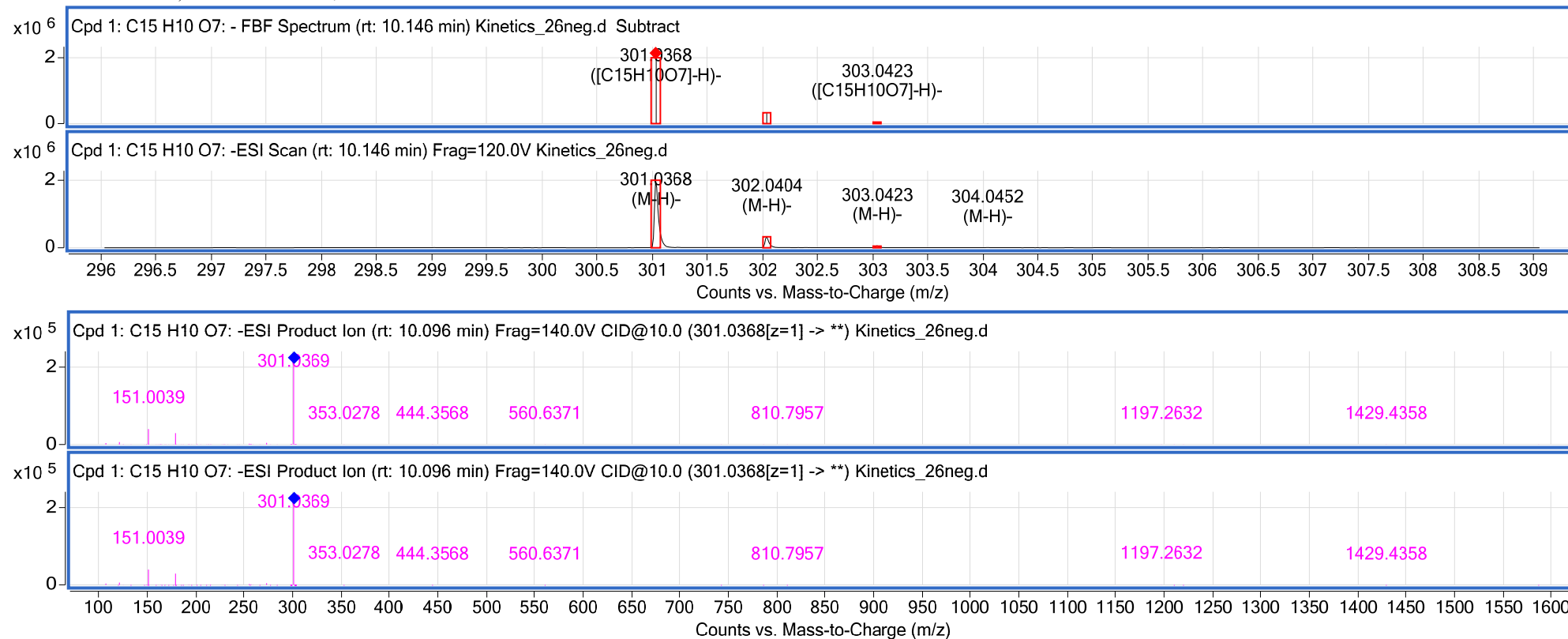
27. **C<sub>14</sub>H<sub>12</sub>O<sub>4</sub>, m/z- 303.0885, Picetannol**

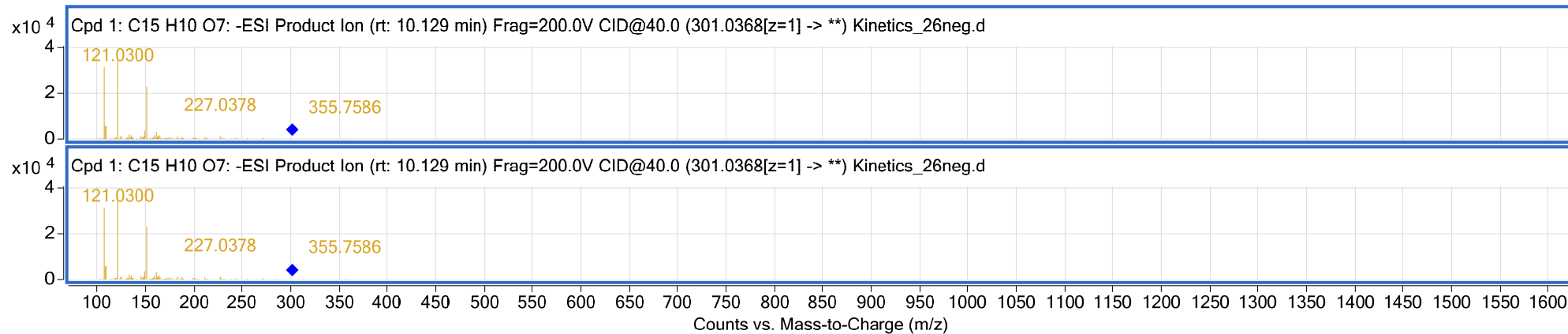
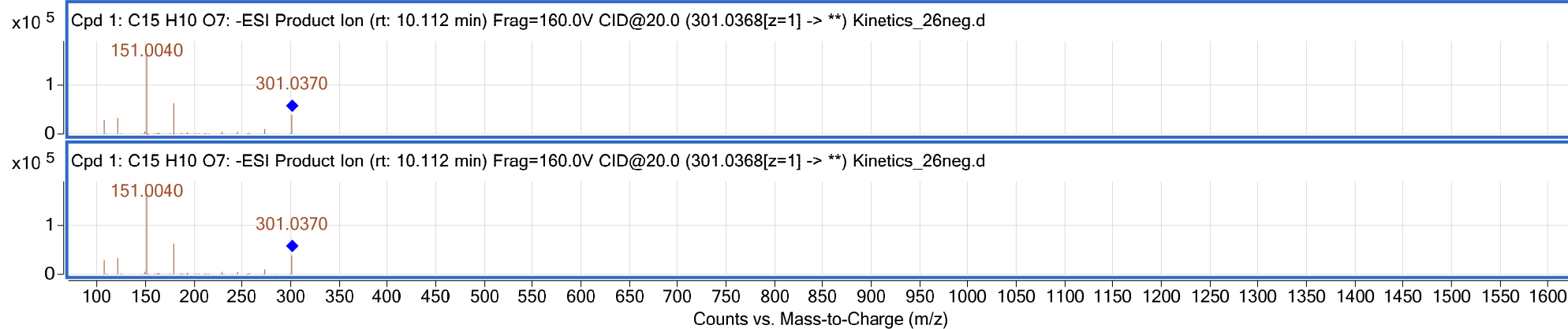


## 28. C<sub>15</sub>H<sub>22</sub>O<sub>2</sub>, m/z-293.1776, Procurcumenol



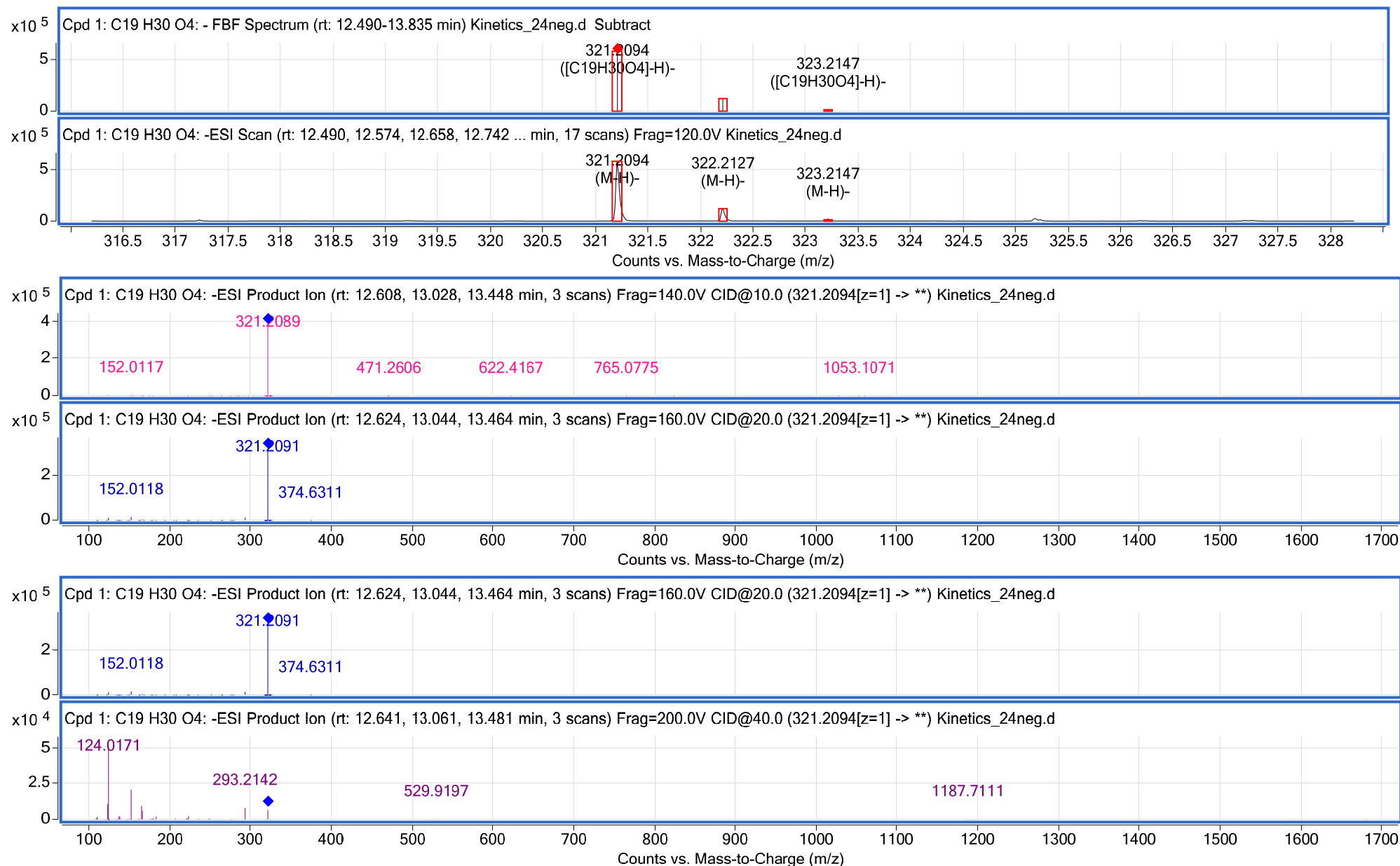
29. **C<sub>15</sub> H<sub>10</sub> O<sub>7</sub>, m/z-301.0367, Quercetin**



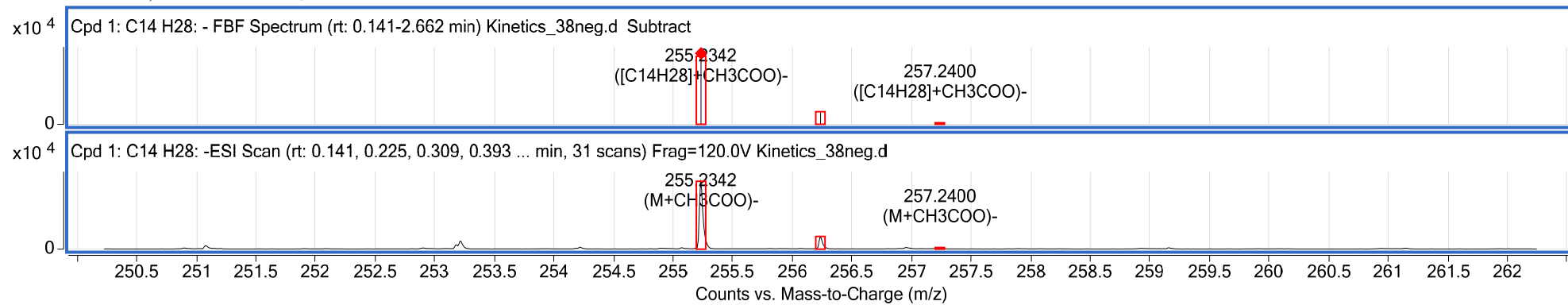


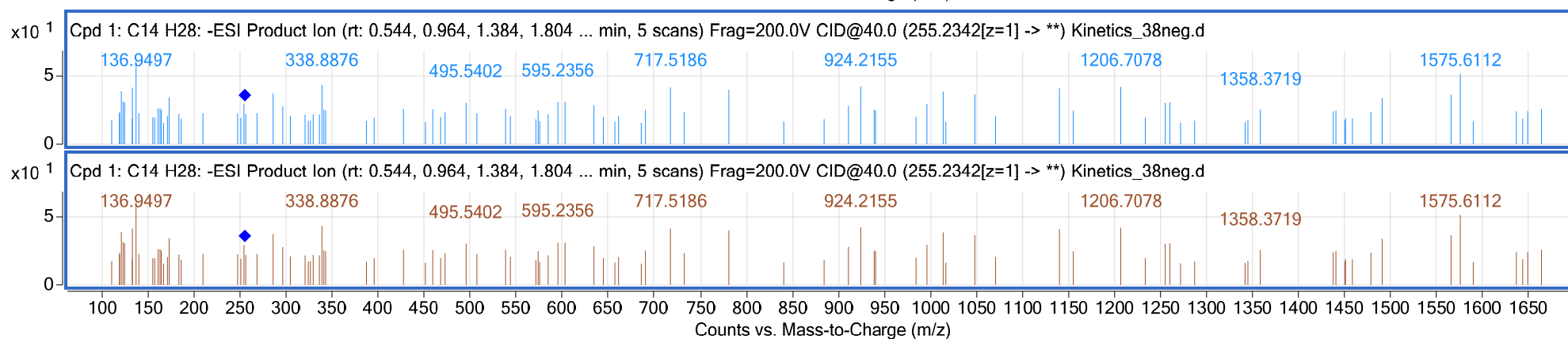
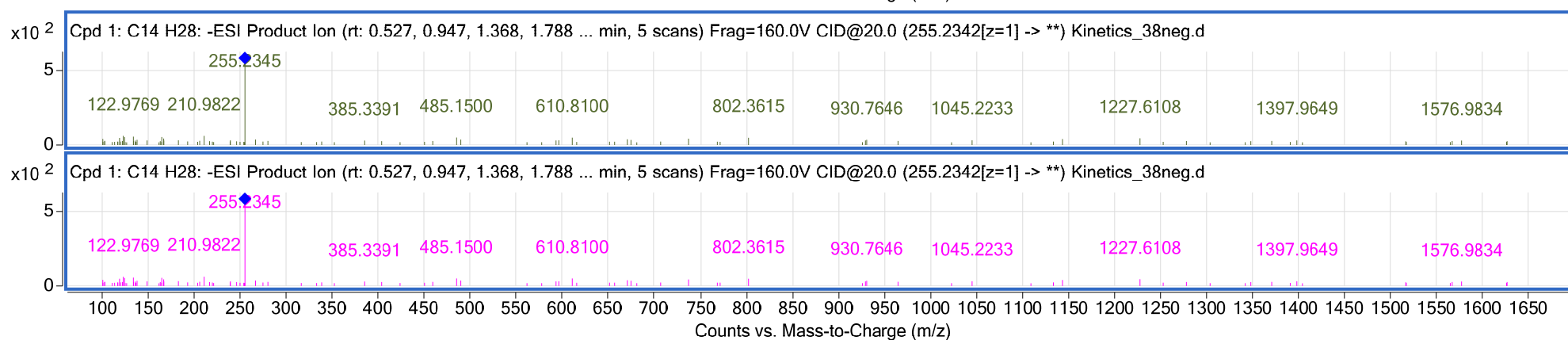
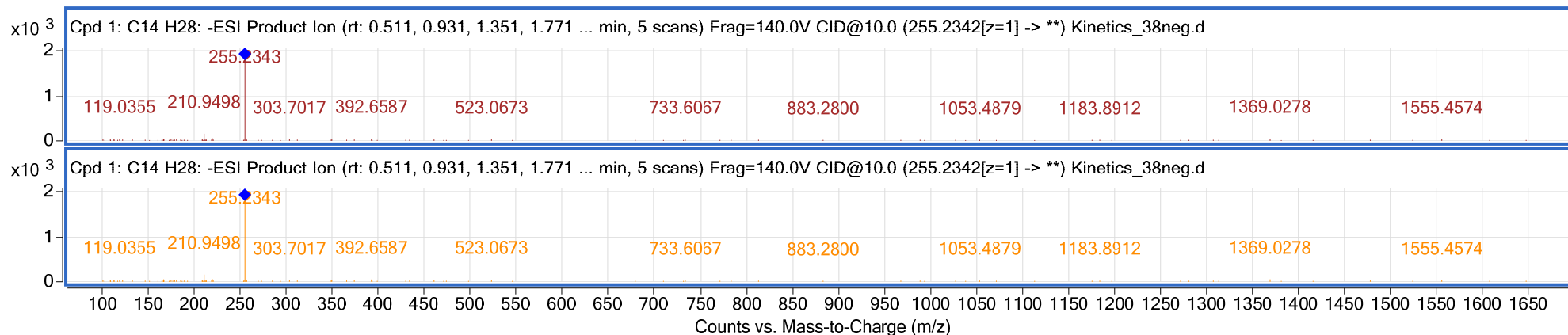


### 30. C<sub>19</sub> H<sub>30</sub> O<sub>4</sub>, m/z-321.2093, Rapanone

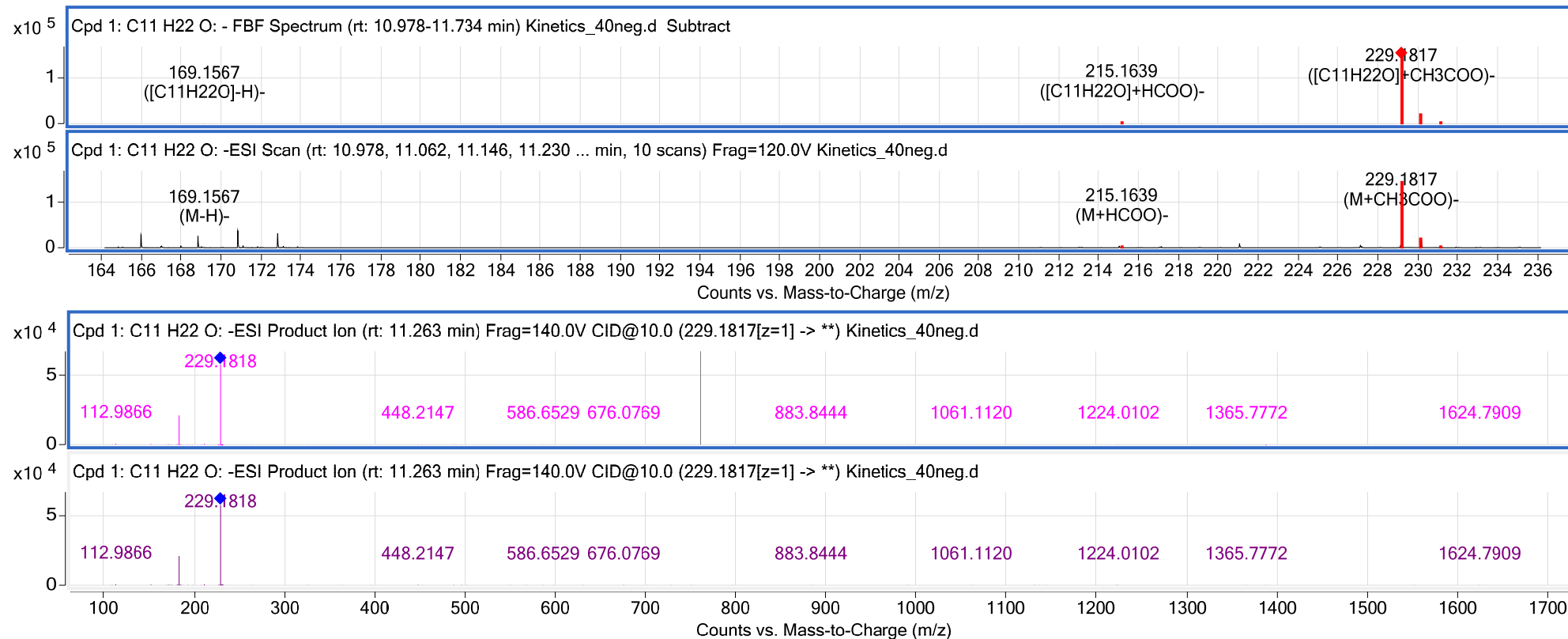


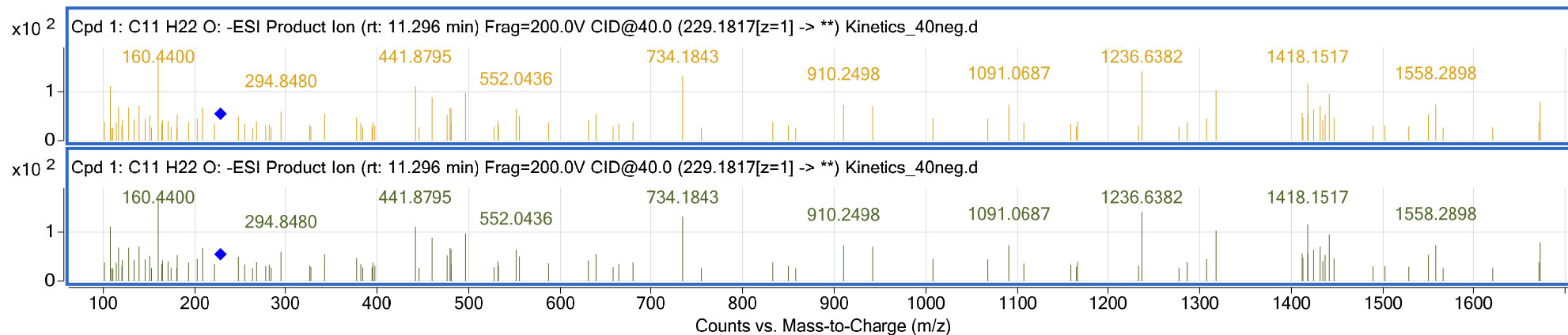
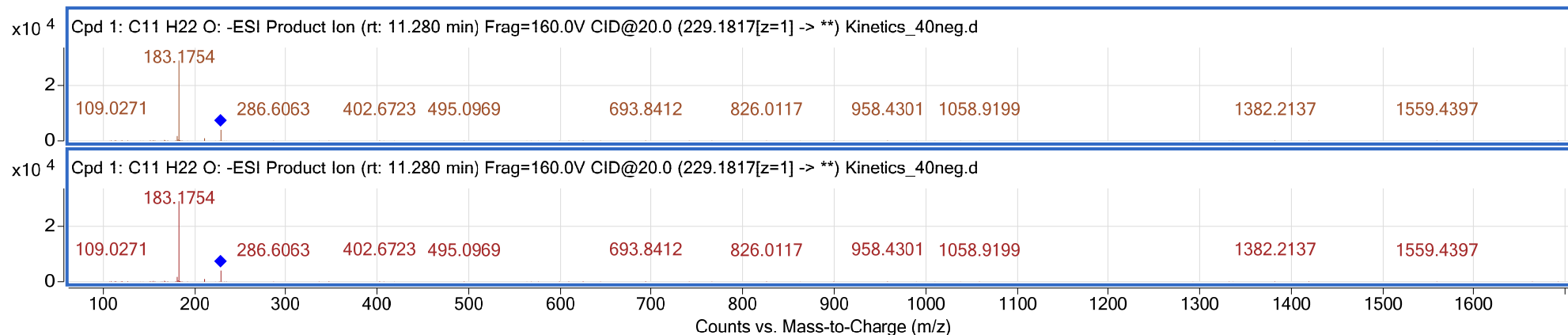
31. **C<sub>14</sub>H<sub>28</sub>, m/z-255.2338, Tetradecene**



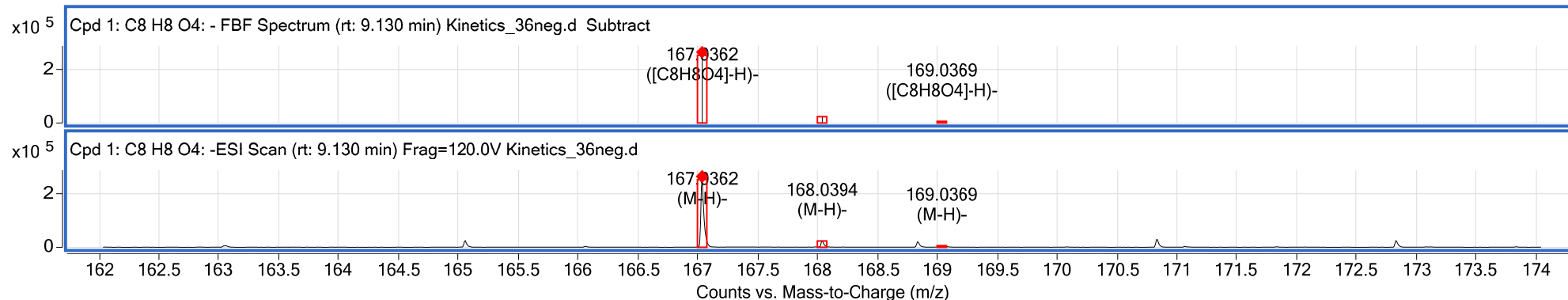


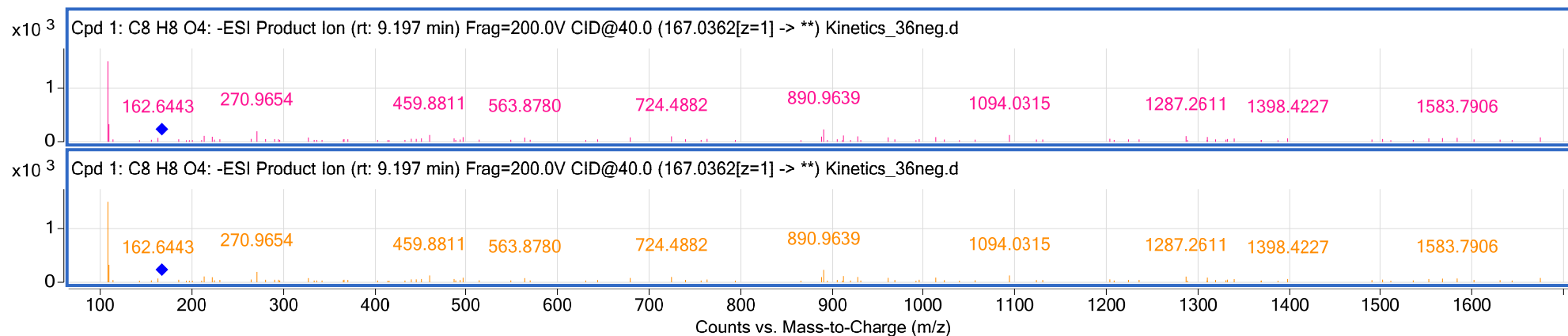
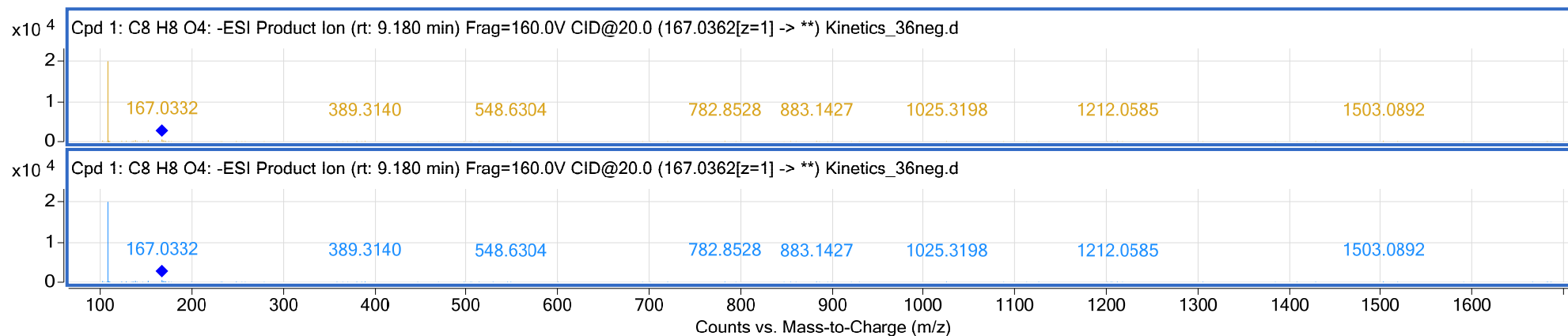
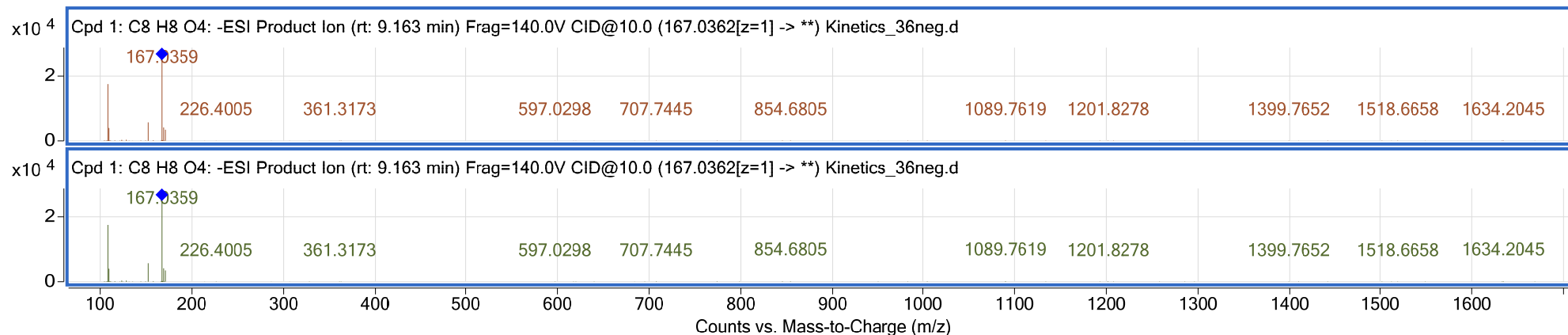
# 32. **C<sub>11</sub> H<sub>22</sub> O, m/z-229.1817, Undecan-2-one**



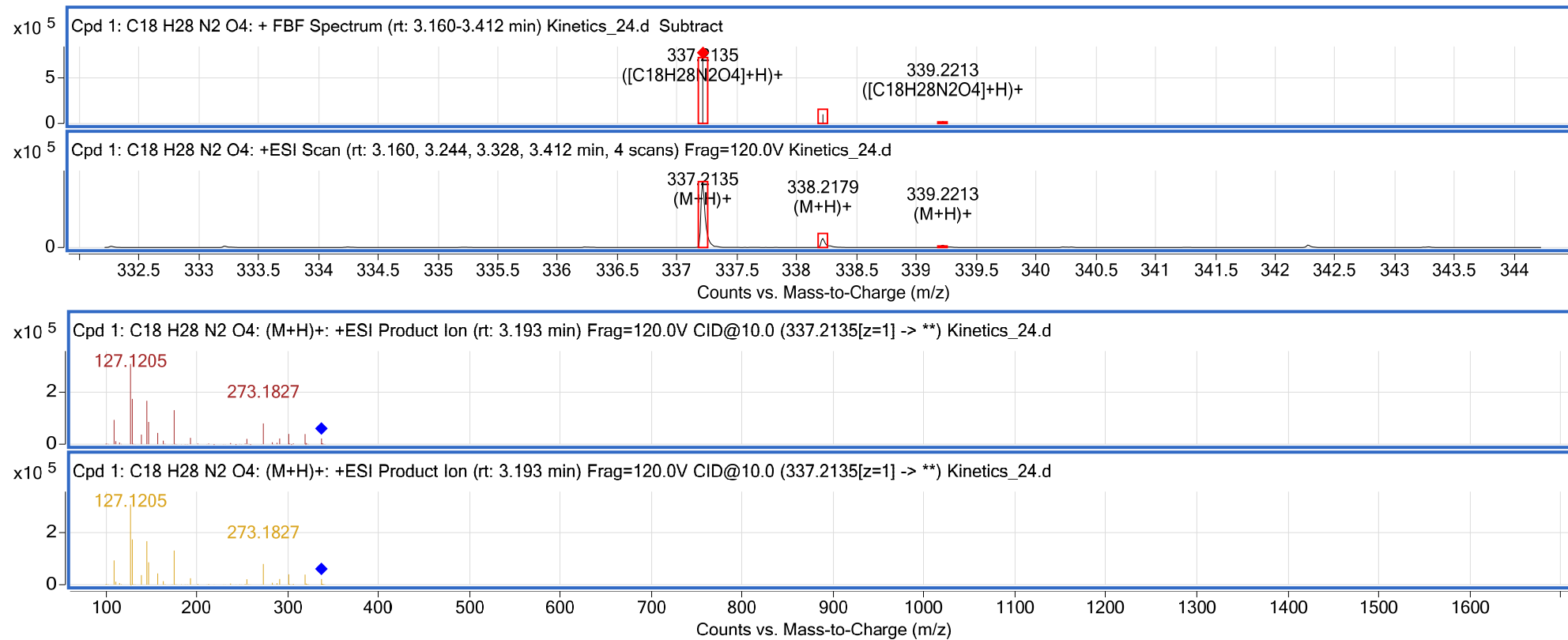


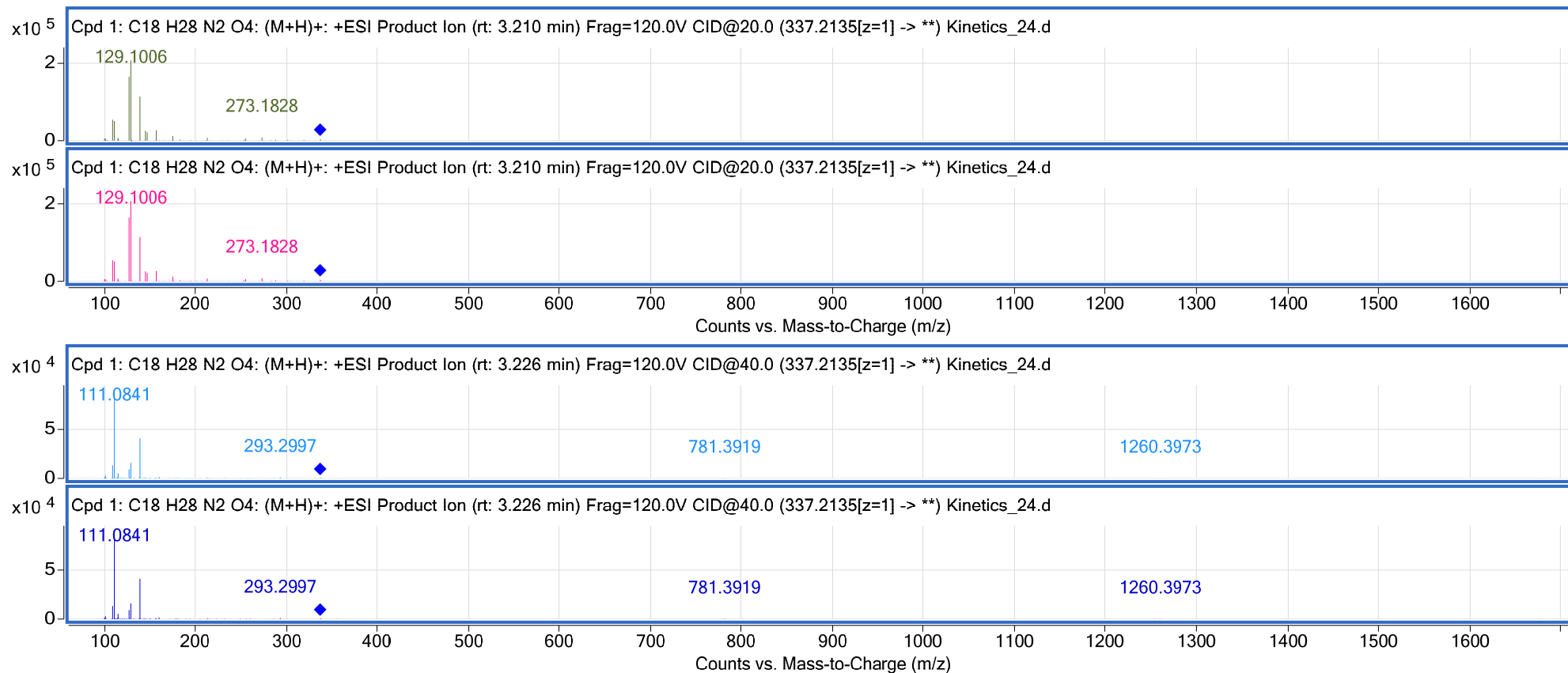
### 33. C<sub>8</sub>H<sub>8</sub>O<sub>4</sub>, m/z-167.0356, Vanillic acid



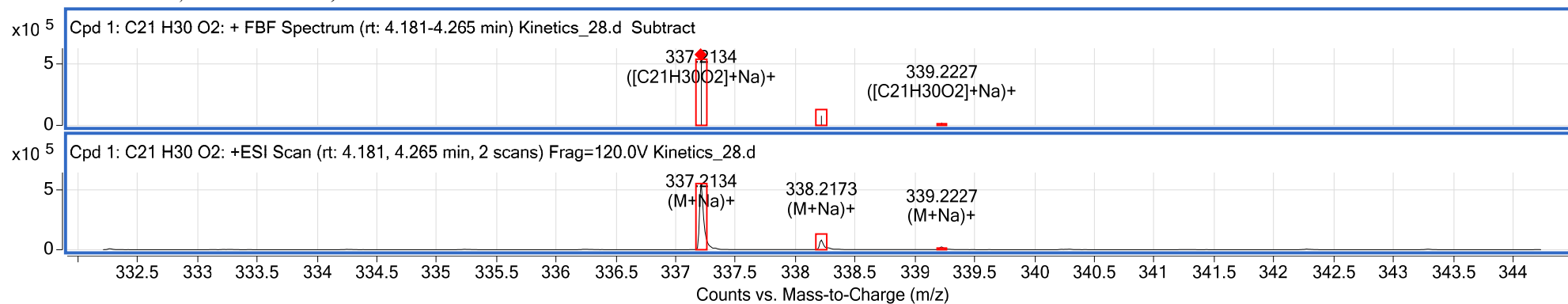


34.  $C_{18}H_{28}N_2O_4$ ,  $m/z$ -337.2135, Acebutolol

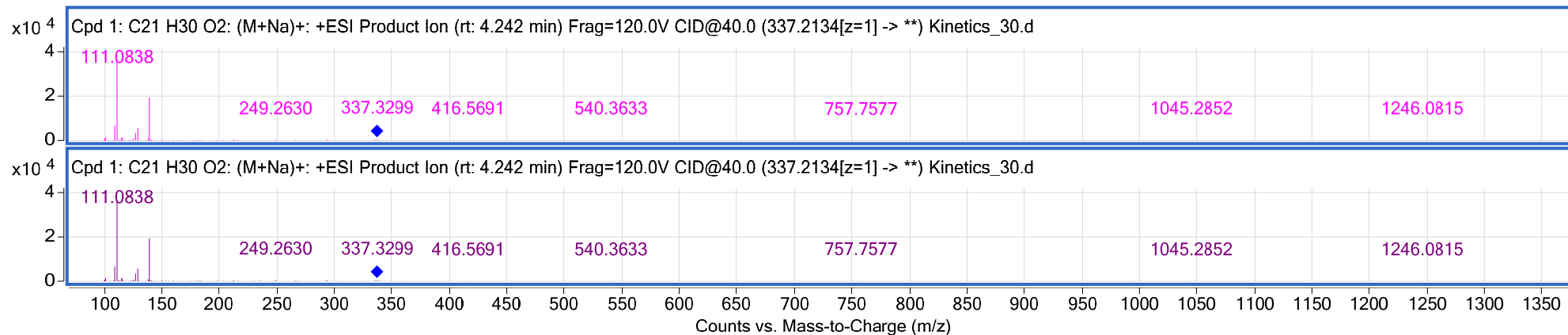
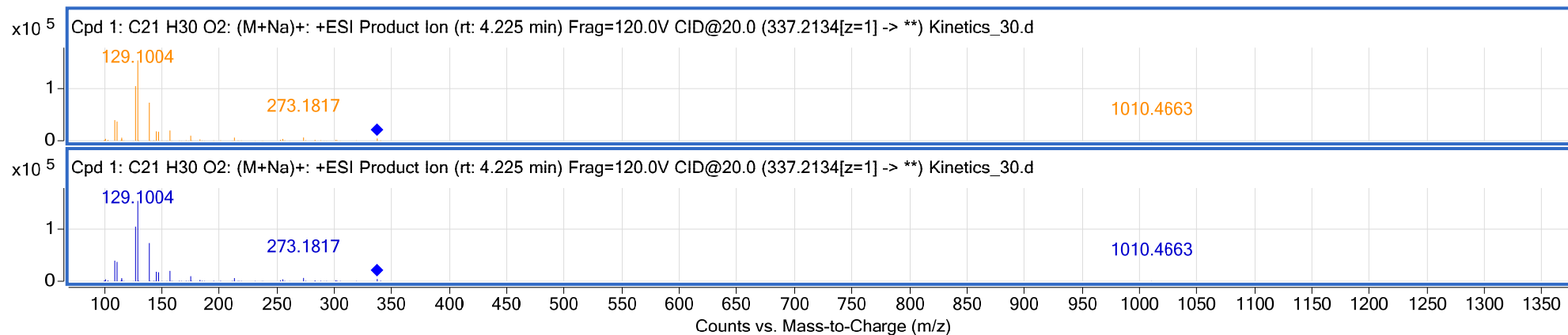
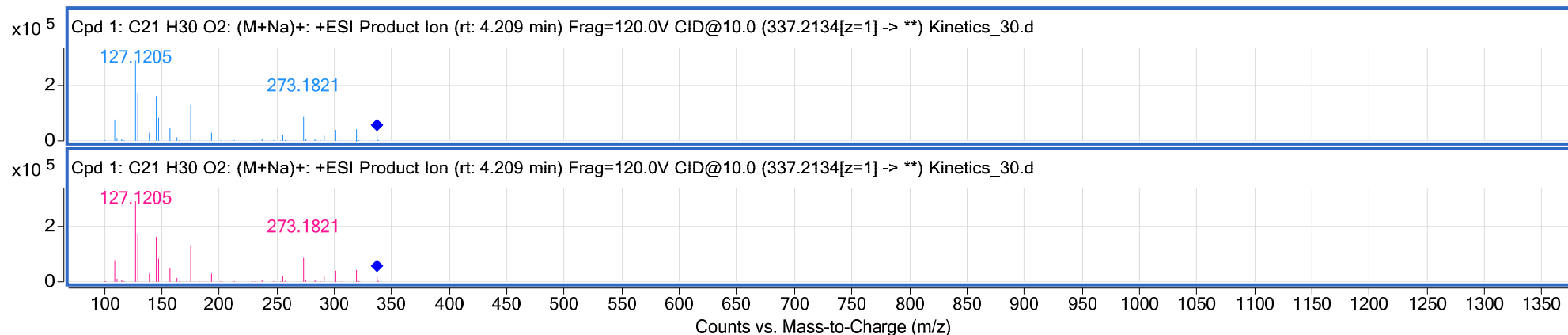




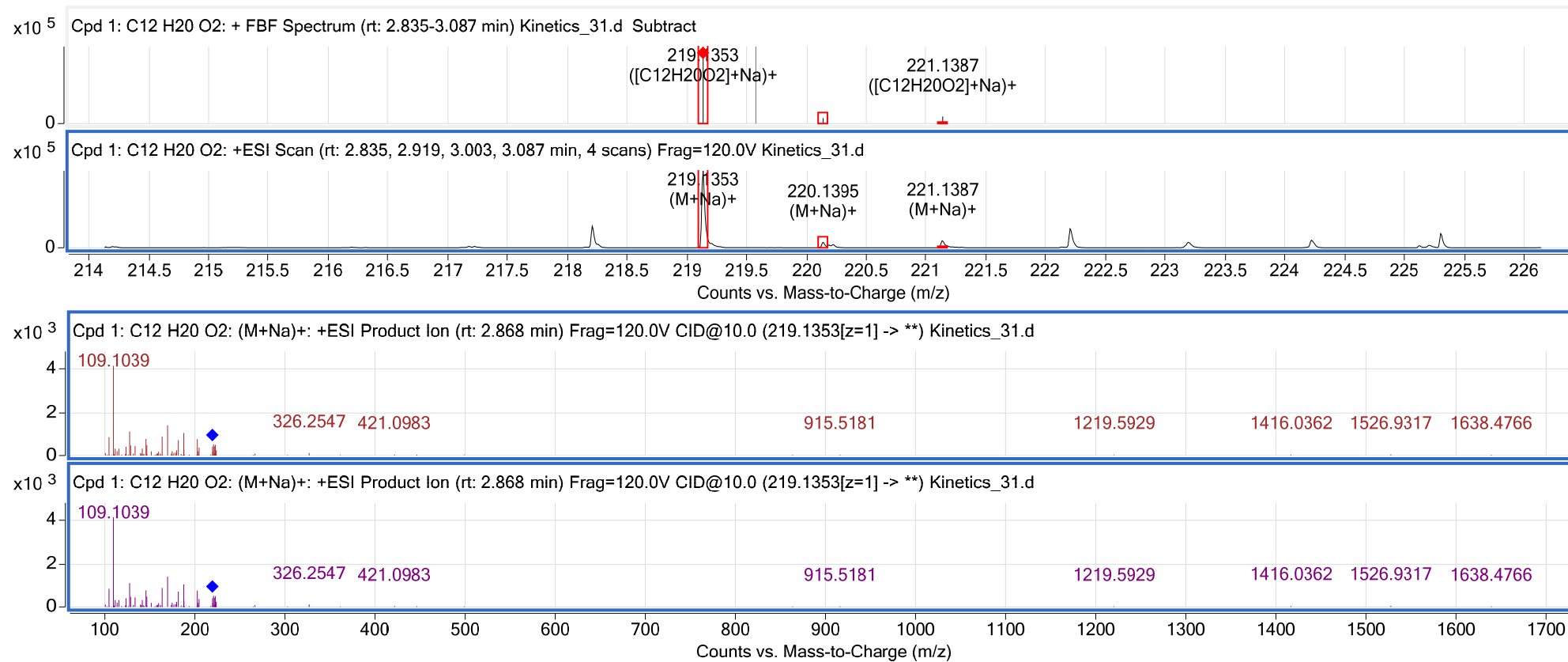
### 35. $C_{21}H_{30}O_2$ , m/z-337.2134, Cannabidiol

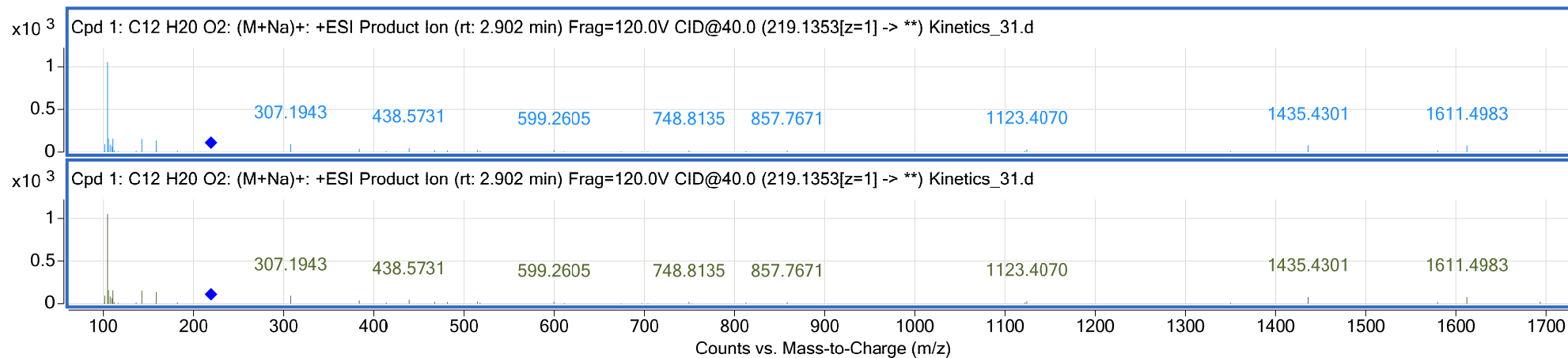
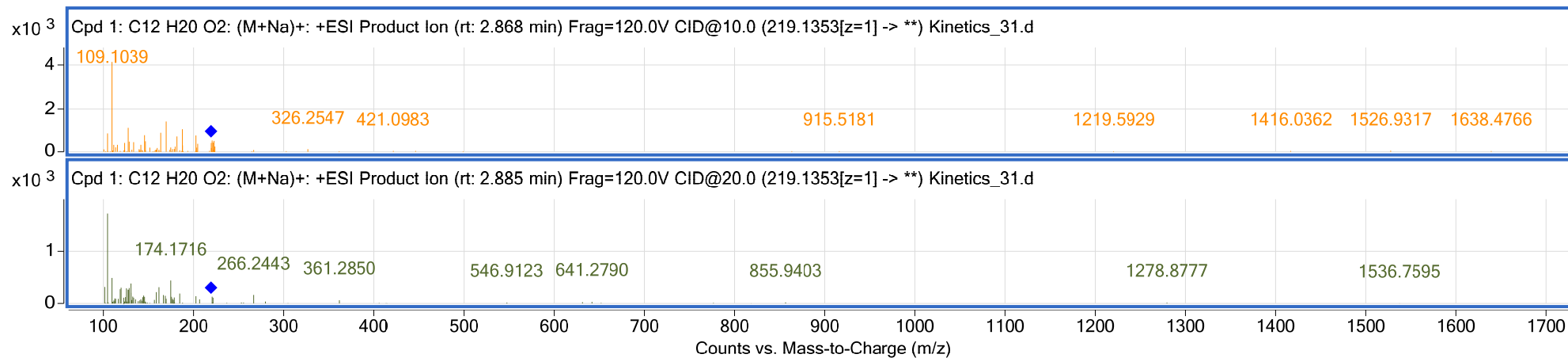






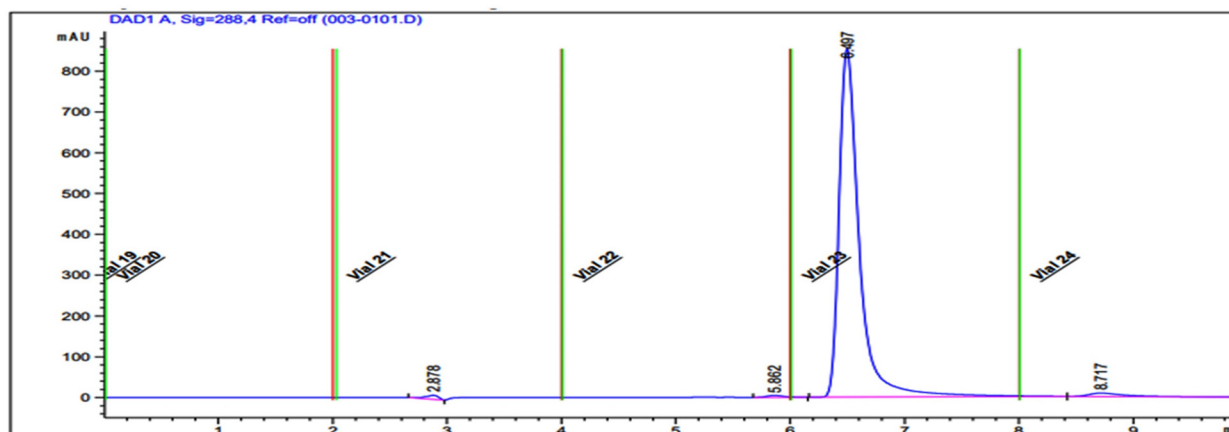
36.  $C_{12}H_{20}O_2$ ,  $m/z$ -219.1353, Hexenyl-(3z)-hexenoate (3z-)



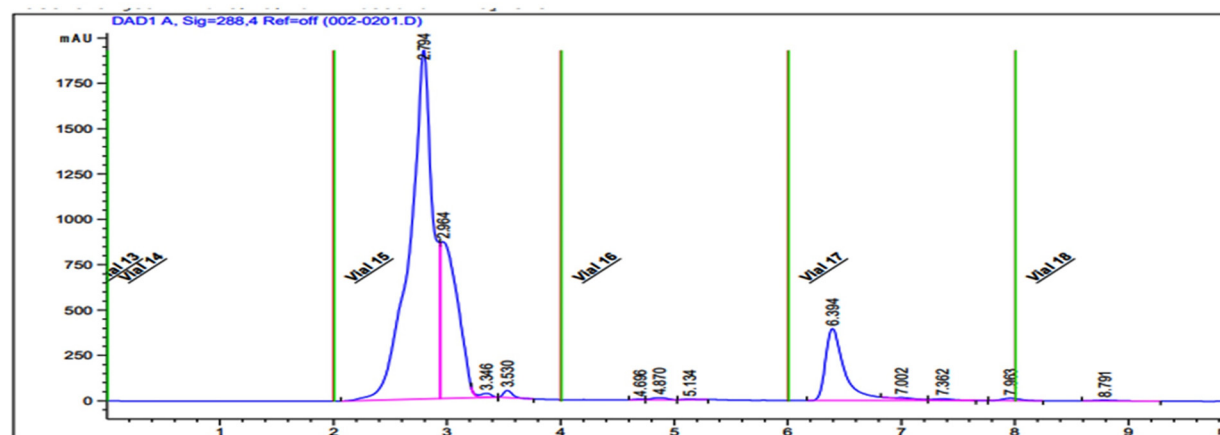


**Figure S3: Confirmation of Embelin from fruit samples.** Embelin standard (Sigma-Aldrich) and fruit extract of Embelia was subjected to HPLC and detected at 288 nm by DAD detector. (A) Peaks eluted from embelin standard and (B) embelia fruit sample are at the same retention time. Concentration of standard embelin was 0.125 ng ml<sup>-1</sup>.

**A**



**B**



Retention time (min)