使用 Agilent 6495 三重四极杆质谱仪实现水中药物和个人护理用品 (PPCP) 的高灵敏度检测

应用简报

作者
Dan-Hui Dorothy Yang、Mark A. Murphy 和 Sue Zhang

安捷伦科技公司，5301 Stevens Creek Blvd, Santa Clara, CA 95051, USA

美国环保署第 8 区实验室，16194 West 45th Drive, Golden, CO 80403, USA

摘要
本应用简报介绍了使用 Agilent 6495 三重四极杆质谱仪检测水中 ppt 级别药物和个人护理用品的两种方法。根据所需流动相的不同分为正离子模式方法和负离子模式方法。动态多反应监测 (DMRM) 可对正离子模式下具有 316 种 MRM 离子对的 118 种化合物，以及负离子模式下具有 62 种 MRM 离子对的 22 种化合物实现精密、准确的定量分析。利用高灵敏度 6495 三重四极杆质联用系统简化分析流程，仅可直接进样 40 μL 水而无需采用固相萃取 (SPE) 进行繁琐的分析物富集流程。
实验部分
试剂与化学品
所有试剂和溶剂均为 HPLC MS 级。乙腈购自 Honeywell (015-4)。超纯水产自配备 LC-Pak Polisher 和 0.22 μm 膜式终端过滤器 (Millipak) 的 Milli-Q Integral 水纯化系统。5 M 乙酸铵溶液购自 Fluka (09691-250ML)。乙酸购自 Aldrich (338828-25ML)。PPCP 标准品和一些内标由外部合作方提供。正离子模式方法和负离子模式方法下分析物及其内标以及 MRM 离子对分别列于表 1 和表 2 中。
<table>
<thead>
<tr>
<th>化合物名称</th>
<th>母离子</th>
<th>子离子</th>
<th>CE (eV)</th>
<th>ISTD</th>
<th>母离子</th>
<th>子离子</th>
<th>CE (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>利卡西平</td>
<td>255.12</td>
<td>237</td>
<td>4</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>利卡西平</td>
<td>255.12</td>
<td>194.1</td>
<td>20</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>6-乙酰吗啡</td>
<td>328.16</td>
<td>211.1</td>
<td>24</td>
<td>D6</td>
<td>6-乙酰吗啡</td>
<td>334.19</td>
<td>211.1</td>
</tr>
<tr>
<td>6-乙酰吗啡</td>
<td>328.16</td>
<td>165.1</td>
<td>44</td>
<td>D6</td>
<td>6-乙酰吗啡</td>
<td>334.19</td>
<td>165.1</td>
</tr>
<tr>
<td>阿替洛尔</td>
<td>337.21</td>
<td>116</td>
<td>16</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>阿替洛尔</td>
<td>337.21</td>
<td>56</td>
<td>40</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>对乙氨基酚</td>
<td>152.07</td>
<td>110</td>
<td>12</td>
<td>D4</td>
<td>对乙氨基酚</td>
<td>156.1</td>
<td>114.1</td>
</tr>
<tr>
<td>对乙氨基酚</td>
<td>152.07</td>
<td>65.1</td>
<td>32</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>沙丁胺醇</td>
<td>240.16</td>
<td>222.2</td>
<td>0</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>沙丁胺醇</td>
<td>240.16</td>
<td>148</td>
<td>12</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>阿米替林</td>
<td>278.19</td>
<td>202.2</td>
<td>68</td>
<td>D3</td>
<td>阿米替林</td>
<td>281.21</td>
<td>91.1</td>
</tr>
<tr>
<td>阿米替林</td>
<td>278.19</td>
<td>91</td>
<td>24</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>阿米替林代谢物</td>
<td>294.19</td>
<td>276.2</td>
<td>8</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>阿米替林代谢物</td>
<td>294.19</td>
<td>214.9</td>
<td>48</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>安非他明</td>
<td>136.11</td>
<td>119.1</td>
<td>4</td>
<td>D5</td>
<td>安非他明</td>
<td>141.1</td>
<td>96.1</td>
</tr>
<tr>
<td>安非他明</td>
<td>136.11</td>
<td>91.1</td>
<td>12</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>阿立哌唑</td>
<td>448.16</td>
<td>285.1</td>
<td>24</td>
<td>D8</td>
<td>阿立哌唑</td>
<td>456.21</td>
<td>283.1</td>
</tr>
<tr>
<td>阿立哌唑</td>
<td>448.16</td>
<td>98.2</td>
<td>40</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>阿替洛尔</td>
<td>267.17</td>
<td>145.1</td>
<td>24</td>
<td>D7</td>
<td>阿替洛尔</td>
<td>274.22</td>
<td>145.1</td>
</tr>
<tr>
<td>阿替洛尔</td>
<td>267.17</td>
<td>74</td>
<td>20</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>阿托伐他汀</td>
<td>559.26</td>
<td>440.2</td>
<td>20</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>阿托伐他汀</td>
<td>559.26</td>
<td>250.2</td>
<td>40</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>阿拉任津</td>
<td>216.1</td>
<td>174.1</td>
<td>8</td>
<td>D6</td>
<td>阿拉任津</td>
<td>221.14</td>
<td>179.2</td>
</tr>
<tr>
<td>阿拉任津</td>
<td>216.1</td>
<td>68.2</td>
<td>36</td>
<td>D6</td>
<td>阿拉任津</td>
<td>221.14</td>
<td>69.1</td>
</tr>
<tr>
<td>苯甲酰爱康宁</td>
<td>290.14</td>
<td>168.2</td>
<td>16</td>
<td>D3</td>
<td>苯甲酰爱康宁</td>
<td>293.16</td>
<td>171.2</td>
</tr>
<tr>
<td>苯甲酰爱康宁</td>
<td>290.14</td>
<td>77</td>
<td>64</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>丁丙诺嗪</td>
<td>468.31</td>
<td>84.2</td>
<td>48</td>
<td>D4</td>
<td>丁丙诺嗪</td>
<td>472.34</td>
<td>59.2</td>
</tr>
<tr>
<td>丁丙诺嗪</td>
<td>468.31</td>
<td>55.1</td>
<td>52</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>安非他酮</td>
<td>240.12</td>
<td>184</td>
<td>4</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>安非他酮</td>
<td>240.12</td>
<td>131</td>
<td>20</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>咖啡因</td>
<td>195.09</td>
<td>138.1</td>
<td>20</td>
<td>13C3咖啡因</td>
<td>198.1</td>
<td>140.1</td>
<td>20</td>
</tr>
<tr>
<td>咖啡因</td>
<td>195.09</td>
<td>110.3</td>
<td>20</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>卡马西平</td>
<td>237.1</td>
<td>194.1</td>
<td>12</td>
<td>D10</td>
<td>卡马西平</td>
<td>247.17</td>
<td>204.2</td>
</tr>
<tr>
<td>卡马西平</td>
<td>237.1</td>
<td>193.1</td>
<td>28</td>
<td>D10</td>
<td>卡马西平</td>
<td>247.17</td>
<td>202.1</td>
</tr>
<tr>
<td>卡马西平 10,11-环氧化物</td>
<td>253.1</td>
<td>210.2</td>
<td>8</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>卡马西平 10,11-环氧化物</td>
<td>253.1</td>
<td>180.1</td>
<td>24</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>卡立普多</td>
<td>261.18</td>
<td>176.2</td>
<td>0</td>
<td>D7</td>
<td>卡立普多</td>
<td>268.23</td>
<td>183.1</td>
</tr>
<tr>
<td>卡立普多</td>
<td>261.18</td>
<td>55.1</td>
<td>24</td>
<td>D7</td>
<td>卡立普多</td>
<td>268.23</td>
<td>62.2</td>
</tr>
<tr>
<td>扑尔敏</td>
<td>275.13</td>
<td>230</td>
<td>8</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>扑尔敏</td>
<td>275.13</td>
<td>167.1</td>
<td>44</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>可卡因</td>
<td>304.16</td>
<td>182.2</td>
<td>16</td>
<td>D3</td>
<td>可卡因</td>
<td>307.18</td>
<td>185.1</td>
</tr>
</tbody>
</table>

表 1. 正离子模式方法中分析物和内标的 MRM 离子对
<table>
<thead>
<tr>
<th>化合物名称</th>
<th>母离子</th>
<th>子离子</th>
<th>CE (eV)</th>
<th>ISTD</th>
<th>母离子</th>
<th>子离子</th>
<th>CE (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>可卡因</td>
<td>304.16</td>
<td>77</td>
<td>64</td>
<td></td>
<td>306.2</td>
<td>202</td>
<td>52</td>
</tr>
<tr>
<td>可待因</td>
<td>300.16</td>
<td>198.1</td>
<td>76 D6</td>
<td>可待因</td>
<td>306.2</td>
<td>153</td>
<td>52</td>
</tr>
<tr>
<td>可待因</td>
<td>300.16</td>
<td>152</td>
<td>72 D6</td>
<td>可待因</td>
<td>306.2</td>
<td></td>
<td></td>
</tr>
<tr>
<td>可待因</td>
<td>300.16</td>
<td>115.2</td>
<td>76</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>可铁宁</td>
<td>177.1</td>
<td>88</td>
<td>24 D3</td>
<td>可铁宁</td>
<td>180.12</td>
<td>101</td>
<td>24</td>
</tr>
<tr>
<td>可铁宁</td>
<td>177.1</td>
<td>80.1</td>
<td>36 D3</td>
<td>可铁宁</td>
<td>180.12</td>
<td>79.8</td>
<td>28</td>
</tr>
<tr>
<td>DEET</td>
<td>192.14</td>
<td>119.3</td>
<td>16 D6</td>
<td>DEET</td>
<td>198.18</td>
<td>118.9</td>
<td>16</td>
</tr>
<tr>
<td>DEET</td>
<td>192.14</td>
<td>91</td>
<td>32 D6</td>
<td>DEET</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>诺氟沙星</td>
<td>446.14</td>
<td>285.1</td>
<td>24</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>诺氟沙星</td>
<td>446.14</td>
<td>98.1</td>
<td>44</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>去甲西酞普兰</td>
<td>311.16</td>
<td>262.2</td>
<td>8 D3</td>
<td>去甲西酞普兰</td>
<td>314.18</td>
<td>109.1</td>
<td>20</td>
</tr>
<tr>
<td>去甲西酞普兰</td>
<td>311.16</td>
<td>109.1</td>
<td>20</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>去甲文拉法辛</td>
<td>264.2</td>
<td>246.2</td>
<td>4 D6</td>
<td>去甲文拉法辛</td>
<td>270.24</td>
<td>64</td>
<td>12</td>
</tr>
<tr>
<td>去甲文拉法辛</td>
<td>264.2</td>
<td>58.1</td>
<td>16</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>右美沙芬</td>
<td>272.2</td>
<td>171.1</td>
<td>36 D3</td>
<td>右美沙芬</td>
<td>275.22</td>
<td>171.2</td>
<td>36</td>
</tr>
<tr>
<td>右美沙芬</td>
<td>272.2</td>
<td>128.1</td>
<td>64</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>地尔硫卓</td>
<td>415.17</td>
<td>178.1</td>
<td>20</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>地尔硫卓</td>
<td>415.17</td>
<td>109.1</td>
<td>76</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>苯海拉明</td>
<td>256.17</td>
<td>165.1</td>
<td>48 D3</td>
<td>苯海拉明</td>
<td>259.19</td>
<td>167.2</td>
<td>8</td>
</tr>
<tr>
<td>苯海拉明</td>
<td>256.17</td>
<td>152.1</td>
<td>44</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>丙吡胺</td>
<td>340.24</td>
<td>239.1</td>
<td>8</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>丙吡胺</td>
<td>340.24</td>
<td>194.2</td>
<td>48</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>多奈哌齐</td>
<td>380.22</td>
<td>91.1</td>
<td>40</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>多奈哌齐</td>
<td>380.22</td>
<td>65.2</td>
<td>76</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>丁洛西汀</td>
<td>298.13</td>
<td>153.9</td>
<td>0 D3</td>
<td>丁洛西汀</td>
<td>301.15</td>
<td>157.1</td>
<td>0</td>
</tr>
<tr>
<td>丁洛西汀</td>
<td>298.13</td>
<td>44</td>
<td>12 D3</td>
<td>丁洛西汀</td>
<td>301.15</td>
<td>46.9</td>
<td>16</td>
</tr>
<tr>
<td>素子碱甲酯</td>
<td>200.13</td>
<td>182</td>
<td>12 D3</td>
<td>素子碱甲酯</td>
<td>203.15</td>
<td>185.2</td>
<td>12</td>
</tr>
<tr>
<td>素子碱甲酯</td>
<td>200.13</td>
<td>82.1</td>
<td>24</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>EDDP</td>
<td>278.19</td>
<td>249</td>
<td>20 D3</td>
<td>EDDP</td>
<td>281.21</td>
<td>234</td>
<td>24</td>
</tr>
<tr>
<td>EDDP</td>
<td>278.19</td>
<td>234.1</td>
<td>24</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>红霉素</td>
<td>734.47</td>
<td>158.1</td>
<td>24</td>
<td>^13C2 红霉素</td>
<td>736.48</td>
<td>160</td>
<td>24</td>
</tr>
<tr>
<td>红霉素</td>
<td>734.47</td>
<td>83.1</td>
<td>68</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>无水红霉素</td>
<td>716.46</td>
<td>158</td>
<td>24</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>无水红霉素</td>
<td>716.46</td>
<td>83.2</td>
<td>76</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>艾司西酞普兰</td>
<td>325.17</td>
<td>262.2</td>
<td>16</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>艾司西酞普兰</td>
<td>325.17</td>
<td>109.1</td>
<td>20</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>法莫替丁</td>
<td>338.05</td>
<td>189.1</td>
<td>12</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>法莫替丁</td>
<td>338.05</td>
<td>155</td>
<td>28</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>辛伐他汀</td>
<td>337.23</td>
<td>188.3</td>
<td>20 D5</td>
<td>辛伐他汀</td>
<td>342.2</td>
<td>105.1</td>
<td>36</td>
</tr>
<tr>
<td>辛伐他汀</td>
<td>337.23</td>
<td>105.1</td>
<td>36</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>枚西汀</td>
<td>310.14</td>
<td>148.2</td>
<td>4 D6</td>
<td>枚西汀</td>
<td>316.18</td>
<td>44</td>
<td>16</td>
</tr>
<tr>
<td>枚西汀</td>
<td>310.14</td>
<td>76</td>
<td>16</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>丙酸酰替卡松</td>
<td>501.19</td>
<td>313</td>
<td>8</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>丙酸酰替卡松</td>
<td>501.19</td>
<td>293.2</td>
<td>12</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>阿普唑丁</td>
<td>172.14</td>
<td>154.1</td>
<td>8 D10</td>
<td>阿普唑丁</td>
<td>182.2</td>
<td>164.1</td>
<td>12</td>
</tr>
<tr>
<td>阿普唑丁</td>
<td>172.14</td>
<td>55</td>
<td>24</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>芳基苯胺</td>
<td>494.15</td>
<td>369</td>
<td>12</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>化合物名称</td>
<td>母离子</td>
<td>子离子</td>
<td>CE (eV)</td>
<td>ISTD</td>
<td>母离子</td>
<td>子离子</td>
<td>CE (eV)</td>
</tr>
<tr>
<td>-----------</td>
<td>--------</td>
<td>--------</td>
<td>---------</td>
<td>------</td>
<td>--------</td>
<td>--------</td>
<td>---------</td>
</tr>
<tr>
<td>格列本脲</td>
<td>494.15</td>
<td>169.1</td>
<td>36</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>格列本脲</td>
<td>300.16</td>
<td>199.1</td>
<td>28</td>
<td>D6</td>
<td>氢可酮</td>
<td>306.2</td>
<td>202</td>
</tr>
<tr>
<td>氢可酮</td>
<td>300.16</td>
<td>171.1</td>
<td>40</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>氢可酮</td>
<td>286.15</td>
<td>185.1</td>
<td>24</td>
<td>D3</td>
<td>氢吗啡酮</td>
<td>289.17</td>
<td>185</td>
</tr>
<tr>
<td>氢吗啡酮</td>
<td>286.15</td>
<td>157.1</td>
<td>48</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>氢基安非他酮</td>
<td>256.11</td>
<td>238.1</td>
<td>4</td>
<td>D6</td>
<td>氢基安非他酮</td>
<td>262.15</td>
<td>244.1</td>
</tr>
<tr>
<td>氢基安非他酮</td>
<td>256.11</td>
<td>130.1</td>
<td>48</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>氢吗啡酮</td>
<td>255.1</td>
<td>209.2</td>
<td>4</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>氢吗啡酮</td>
<td>255.1</td>
<td>77.1</td>
<td>52</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>拉莫三嗪</td>
<td>256.02</td>
<td>108.2</td>
<td>52</td>
<td></td>
<td>C13</td>
<td>C14 N4</td>
<td>拉莫三嗪</td>
</tr>
<tr>
<td>拉莫三嗪</td>
<td>256.02</td>
<td>74.2</td>
<td>76</td>
<td></td>
<td>C13</td>
<td>C14 N4</td>
<td>拉莫三嗪</td>
</tr>
<tr>
<td>左啡诺</td>
<td>258.19</td>
<td>199.1</td>
<td>20</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>左啡诺</td>
<td>258.19</td>
<td>157.2</td>
<td>32</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>利多卡因</td>
<td>235.18</td>
<td>86.2</td>
<td>8</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>利多卡因</td>
<td>235.18</td>
<td>58.1</td>
<td>32</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>氯苯他定</td>
<td>383.15</td>
<td>337.2</td>
<td>20</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>氯苯他定</td>
<td>383.15</td>
<td>266.9</td>
<td>32</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>劳拉西泮</td>
<td>321.02</td>
<td>275.1</td>
<td>12</td>
<td>D4</td>
<td>劳拉西泮</td>
<td>325.05</td>
<td>279</td>
</tr>
<tr>
<td>劳拉西泮</td>
<td>321.02</td>
<td>229.2</td>
<td>28</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>MDA</td>
<td>180.1</td>
<td>163.2</td>
<td>4</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>MDA</td>
<td>180.1</td>
<td>105.2</td>
<td>20</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>MDEA</td>
<td>208.14</td>
<td>163.1</td>
<td>4</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>MDEA</td>
<td>208.14</td>
<td>77.1</td>
<td>44</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>MDMA</td>
<td>194.12</td>
<td>163.1</td>
<td>8</td>
<td>D5</td>
<td>MDMA</td>
<td>199.15</td>
<td>165.1</td>
</tr>
<tr>
<td>MDMA</td>
<td>194.12</td>
<td>77.1</td>
<td>40</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>甲苯那酸</td>
<td>242.12</td>
<td>224.2</td>
<td>16</td>
<td>D3</td>
<td>甲苯那酸</td>
<td>245.14</td>
<td>227</td>
</tr>
<tr>
<td>甲苯那酸</td>
<td>242.12</td>
<td>208.2</td>
<td>36</td>
<td>D3</td>
<td>甲苯那酸</td>
<td>245.14</td>
<td>212</td>
</tr>
<tr>
<td>哌替啶</td>
<td>248.17</td>
<td>220.2</td>
<td>16</td>
<td>D4</td>
<td>哌替啶</td>
<td>252.19</td>
<td>224.2</td>
</tr>
<tr>
<td>哌替啶</td>
<td>248.17</td>
<td>174.1</td>
<td>16</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>眠尔通</td>
<td>219.14</td>
<td>158.1</td>
<td>0</td>
<td>D7</td>
<td>眠尔通</td>
<td>226.18</td>
<td>165</td>
</tr>
<tr>
<td>眠尔通</td>
<td>219.14</td>
<td>97.1</td>
<td>12</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>二甲双氫</td>
<td>130.1</td>
<td>71.1</td>
<td>24</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>二甲双氫</td>
<td>130.1</td>
<td>60.1</td>
<td>12</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>美沙酮</td>
<td>310.22</td>
<td>265.2</td>
<td>8</td>
<td>D9</td>
<td>美沙酮</td>
<td>319.28</td>
<td>267.9</td>
</tr>
<tr>
<td>美沙酮</td>
<td>310.22</td>
<td>104.9</td>
<td>28</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>甲基苯丙胺</td>
<td>150.13</td>
<td>119.1</td>
<td>8</td>
<td>D11</td>
<td>甲基苯丙胺</td>
<td>161.2</td>
<td>127.2</td>
</tr>
<tr>
<td>甲氨蝶呤</td>
<td>455.18</td>
<td>308.2</td>
<td>16</td>
<td>D3</td>
<td>甲氨蝶呤</td>
<td>458.2</td>
<td>311.2</td>
</tr>
<tr>
<td>甲氨蝶呤</td>
<td>455.18</td>
<td>175.1</td>
<td>36</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>哌甲酯</td>
<td>234.15</td>
<td>84.2</td>
<td>20</td>
<td>D9</td>
<td>哌甲酯</td>
<td>243.21</td>
<td>93.2</td>
</tr>
<tr>
<td>哌甲酯</td>
<td>234.15</td>
<td>56.2</td>
<td>52</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>美托洛尔</td>
<td>268.19</td>
<td>76.9</td>
<td>56</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>美托洛尔</td>
<td>268.19</td>
<td>56.2</td>
<td>24</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>美伐他汀</td>
<td>391.25</td>
<td>185.1</td>
<td>8</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>美伐他汀</td>
<td>391.25</td>
<td>159.1</td>
<td>24</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>间羟基苯甲酰苯甲酸</td>
<td>306.14</td>
<td>168.1</td>
<td>12</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>间羟基苯甲酰苯甲酸</td>
<td>306.14</td>
<td>65.2</td>
<td>72</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>莫达非尼</td>
<td>296.1</td>
<td>129.2</td>
<td>8</td>
<td>D10</td>
<td>莫达非尼</td>
<td>306.14</td>
<td>129</td>
</tr>
<tr>
<td>化合物名称</td>
<td>母离子</td>
<td>子离子</td>
<td>CE (eV)</td>
<td>ISTD</td>
<td>母离子</td>
<td>子离子</td>
<td>CE (eV)</td>
</tr>
<tr>
<td>-------------------</td>
<td>--------</td>
<td>--------</td>
<td>---------</td>
<td>------</td>
<td>--------</td>
<td>--------</td>
<td>---------</td>
</tr>
<tr>
<td>单乙基甘氨酰二甲苯胺</td>
<td>207.15</td>
<td>122.2</td>
<td>8</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>单乙基甘氨酰二甲苯胺</td>
<td>207.15</td>
<td>58.2</td>
<td>4</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>孟鲁司特</td>
<td>586.22</td>
<td>422.1</td>
<td>20</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>孟鲁司特</td>
<td>586.22</td>
<td>278.1</td>
<td>28</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>吗啡</td>
<td>286.15</td>
<td>152.2</td>
<td>64</td>
<td>D3 吗啡</td>
<td>289.17</td>
<td>152.1</td>
<td>64</td>
</tr>
<tr>
<td>吗啡</td>
<td>286.15</td>
<td>128.1</td>
<td>68</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>硝苯地平</td>
<td>347.13</td>
<td>315.2</td>
<td>0</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>硝苯地平</td>
<td>347.13</td>
<td>195.1</td>
<td>36</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>氧化硝苯地平</td>
<td>345.11</td>
<td>284.1</td>
<td>24</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>氧化硝苯地平</td>
<td>345.11</td>
<td>268.1</td>
<td>24</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>去甲芬太尼</td>
<td>233.17</td>
<td>84.2</td>
<td>12</td>
<td>D6 去甲芬太尼</td>
<td>238.2</td>
<td>83.9</td>
<td>16</td>
</tr>
<tr>
<td>去甲芬太尼</td>
<td>233.17</td>
<td>55.2</td>
<td>40</td>
<td>D6 去甲芬太尼</td>
<td>238.2</td>
<td>55.2</td>
<td>40</td>
</tr>
<tr>
<td>诺氟西汀</td>
<td>296.13</td>
<td>134.1</td>
<td>0</td>
<td>D6 诺氟西汀</td>
<td>302.17</td>
<td>140.2</td>
<td>0</td>
</tr>
<tr>
<td>诺氟西汀</td>
<td>296.13</td>
<td>30.1</td>
<td>8</td>
<td>D6 诺氟西汀</td>
<td>302.17</td>
<td>30.1</td>
<td>8</td>
</tr>
<tr>
<td>去甲哌替啶</td>
<td>234.15</td>
<td>160.3</td>
<td>8</td>
<td>D4 去甲哌替啶</td>
<td>238.18</td>
<td>164.3</td>
<td>8</td>
</tr>
<tr>
<td>去甲哌替啶</td>
<td>234.15</td>
<td>91.2</td>
<td>48</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>去甲哌替啶</td>
<td>234.15</td>
<td>56.1</td>
<td>20</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>去甲酸硫平</td>
<td>296.12</td>
<td>210.1</td>
<td>24</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>去甲酸硫平</td>
<td>296.12</td>
<td>139.1</td>
<td>60</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>吗啡</td>
<td>275.15</td>
<td>159.1</td>
<td>16</td>
<td>13C6 吗啡</td>
<td>281.15</td>
<td>158.9</td>
<td>16</td>
</tr>
<tr>
<td>吗啡</td>
<td>275.15</td>
<td>89.1</td>
<td>72</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>芬水拉帕米</td>
<td>441.28</td>
<td>165.1</td>
<td>20</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>芬水拉帕米</td>
<td>441.28</td>
<td>150.3</td>
<td>36</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>氧可酮</td>
<td>346.12</td>
<td>198.1</td>
<td>4</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>氧可酮</td>
<td>346.12</td>
<td>136.2</td>
<td>28</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>奥美拉唑</td>
<td>287.06</td>
<td>268.9</td>
<td>8</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>奥美拉唑</td>
<td>287.06</td>
<td>240.9</td>
<td>16</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>奥卡西平</td>
<td>253.1</td>
<td>208.1</td>
<td>16</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>奥卡西平</td>
<td>253.1</td>
<td>180.1</td>
<td>24</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>氧可酮</td>
<td>316.16</td>
<td>298.2</td>
<td>8</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>氧可酮</td>
<td>316.16</td>
<td>241.1</td>
<td>24</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>芳香酸</td>
<td>302.14</td>
<td>284.1</td>
<td>12</td>
<td>D3 芳香酸</td>
<td>305.16</td>
<td>287.1</td>
<td>12</td>
</tr>
<tr>
<td>芳香酸</td>
<td>302.14</td>
<td>227.1</td>
<td>20</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>芳香酸葡萄糖苷酸</td>
<td>478.17</td>
<td>284.1</td>
<td>28</td>
<td>D3 芳香酸葡萄糖苷酸</td>
<td>481.19</td>
<td>287.2</td>
<td>32</td>
</tr>
<tr>
<td>芳香酸葡萄糖苷酸</td>
<td>478.17</td>
<td>227.1</td>
<td>48</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>帕罗西汀</td>
<td>330.15</td>
<td>192.1</td>
<td>16</td>
<td>D6 帕罗西汀</td>
<td>336.19</td>
<td>76.1</td>
<td>32</td>
</tr>
<tr>
<td>帕罗西汀</td>
<td>330.15</td>
<td>70.1</td>
<td>32</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>芬苯拉嗪</td>
<td>178.13</td>
<td>115.1</td>
<td>32</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>芬苯拉嗪</td>
<td>178.13</td>
<td>91.1</td>
<td>36</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>芬特明</td>
<td>150.13</td>
<td>133.1</td>
<td>4</td>
<td>D6 芬特明</td>
<td>155.16</td>
<td>96.2</td>
<td>20</td>
</tr>
<tr>
<td>去甲基黄曲霉素</td>
<td>152.11</td>
<td>134.1</td>
<td>4</td>
<td>D3 去甲基黄曲霉素</td>
<td>155.13</td>
<td>136.9</td>
<td>8</td>
</tr>
<tr>
<td>去甲基黄曲霉素</td>
<td>152.11</td>
<td>117.1</td>
<td>12</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>呋格列酮</td>
<td>357.13</td>
<td>133.9</td>
<td>24</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>呋格列酮</td>
<td>357.13</td>
<td>119.1</td>
<td>48</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>奥瑞巴林</td>
<td>160.14</td>
<td>142.2</td>
<td>8</td>
<td>D6 奥瑞巴林</td>
<td>166.17</td>
<td>148.1</td>
<td>8</td>
</tr>
<tr>
<td>奥瑞巴林</td>
<td>160.14</td>
<td>55.2</td>
<td>20</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>咪未拉嗪</td>
<td>219.12</td>
<td>162.1</td>
<td>4</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
表 1. 正离子模式方法中分析物和内标的 MRM 离子对（续）

<table>
<thead>
<tr>
<th>化合物名称</th>
<th>母离子</th>
<th>子离子</th>
<th>CE (eV)</th>
<th>ISTD</th>
<th>母离子</th>
<th>子离子</th>
<th>CE (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>扑米酮</td>
<td>219.12</td>
<td>91.2</td>
<td>24</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>心得安</td>
<td>260.17</td>
<td>116.1</td>
<td>12</td>
<td>D7</td>
<td>心得安</td>
<td>267.21</td>
<td>56</td>
</tr>
<tr>
<td>心得安</td>
<td>260.17</td>
<td>56.1</td>
<td>24</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>伪麻黄碱</td>
<td>166.13</td>
<td>115.1</td>
<td>24</td>
<td>D3</td>
<td>伪麻黄碱</td>
<td>169.14</td>
<td>151.1</td>
</tr>
<tr>
<td>伪麻黄碱</td>
<td>166.13</td>
<td>91</td>
<td>32</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>舍曲林</td>
<td>306.08</td>
<td>275</td>
<td>4</td>
<td>D3</td>
<td>舍曲林</td>
<td>309.1</td>
<td>275</td>
</tr>
<tr>
<td>舍曲林</td>
<td>306.08</td>
<td>159.1</td>
<td>20</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>西地那非</td>
<td>475.21</td>
<td>100</td>
<td>24</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>西地那非</td>
<td>475.21</td>
<td>58.1</td>
<td>40</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>碘化剂</td>
<td>419.28</td>
<td>198.9</td>
<td>12</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>碘化剂</td>
<td>419.28</td>
<td>173</td>
<td>28</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>索他洛尔</td>
<td>273.13</td>
<td>255.1</td>
<td>4</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>索他洛尔</td>
<td>273.13</td>
<td>133.1</td>
<td>20</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>硝酸二甲氨基</td>
<td>279.09</td>
<td>186</td>
<td>8</td>
<td>13C6</td>
<td>硝酸二甲氨基</td>
<td>285.11</td>
<td>98</td>
</tr>
<tr>
<td>硝酸二甲氨基</td>
<td>279.09</td>
<td>92.1</td>
<td>28</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>舒马曲坦</td>
<td>296.15</td>
<td>155.9</td>
<td>52</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>舒马曲坦</td>
<td>296.15</td>
<td>58.1</td>
<td>12</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>他达拉非</td>
<td>390.15</td>
<td>268</td>
<td>0</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>他达拉非</td>
<td>390.15</td>
<td>204</td>
<td>80</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>替硝西泮</td>
<td>301.08</td>
<td>283</td>
<td>4</td>
<td>D6</td>
<td>替硝西泮</td>
<td>306.11</td>
<td>288</td>
</tr>
<tr>
<td>替硝西泮</td>
<td>301.08</td>
<td>255</td>
<td>16</td>
<td>D5</td>
<td>替硝西泮</td>
<td>306.11</td>
<td>260</td>
</tr>
<tr>
<td>嘌呤灵</td>
<td>202.05</td>
<td>175</td>
<td>24</td>
<td>13C6</td>
<td>嘌呤灵</td>
<td>208.07</td>
<td>181</td>
</tr>
<tr>
<td>嘌呤灵</td>
<td>202.05</td>
<td>131.1</td>
<td>32</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>曲马多</td>
<td>264.2</td>
<td>58.1</td>
<td>12</td>
<td>13C-D3</td>
<td>曲马多</td>
<td>268.22</td>
<td>58.1</td>
</tr>
<tr>
<td>曲马多</td>
<td>264.2</td>
<td>56.1</td>
<td>68</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>曲唑酮</td>
<td>372.16</td>
<td>176.1</td>
<td>20</td>
<td>D6</td>
<td>曲唑酮</td>
<td>378.2</td>
<td>182.1</td>
</tr>
<tr>
<td>曲唑酮</td>
<td>372.16</td>
<td>148.1</td>
<td>36</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>氨苯蝶啶</td>
<td>254.12</td>
<td>237.1</td>
<td>24</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>氨苯蝶啶</td>
<td>254.12</td>
<td>104.1</td>
<td>32</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>甲氧苄啶</td>
<td>291.15</td>
<td>230.2</td>
<td>20</td>
<td>13C3</td>
<td>甲氧苄啶</td>
<td>294.16</td>
<td>233</td>
</tr>
<tr>
<td>甲氧苄啶</td>
<td>291.15</td>
<td>123.2</td>
<td>24</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>曲马多</td>
<td>436.24</td>
<td>235.1</td>
<td>12</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>曲马多</td>
<td>436.24</td>
<td>207.2</td>
<td>20</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>曲唑酮</td>
<td>308.18</td>
<td>235.2</td>
<td>32</td>
<td>D7</td>
<td>曲唑酮</td>
<td>315.22</td>
<td>242</td>
</tr>
<tr>
<td>曲唑酮</td>
<td>308.18</td>
<td>65.2</td>
<td>72</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>曲唑酮苯基-4-羧酸</td>
<td>338.15</td>
<td>265</td>
<td>36</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>曲唑酮苯基-4-羧酸</td>
<td>338.15</td>
<td>65.1</td>
<td>76</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>名称</td>
<td>母离子</td>
<td>子离子</td>
<td>CE (eV)</td>
<td>ISTD</td>
<td>母离子</td>
<td>子离子</td>
<td>CE (eV)</td>
</tr>
<tr>
<td>--------------------</td>
<td>--------</td>
<td>--------</td>
<td>---------</td>
<td>--------</td>
<td>--------</td>
<td>--------</td>
<td>---------</td>
</tr>
<tr>
<td>(±)-11-nor-9-羟基-\Delta-THC</td>
<td>343.19</td>
<td>299.3</td>
<td>20</td>
<td>D9</td>
<td>(±)-11-nor-9-羟基-\Delta-THC</td>
<td>352.25</td>
<td>308.1</td>
</tr>
<tr>
<td>(±)-11-nor-9-羟基-\Delta-THC</td>
<td>343.19</td>
<td>245.1</td>
<td>24</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>苯扎贝特</td>
<td>360.1</td>
<td>274.1</td>
<td>12</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>苯扎贝特</td>
<td>360.1</td>
<td>154.1</td>
<td>28</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>雷米普普</td>
<td>380.1</td>
<td>316.1</td>
<td>20</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>雷米普普</td>
<td>380.1</td>
<td>276.1</td>
<td>28</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>氯霉素</td>
<td>321.1</td>
<td>152.1</td>
<td>12</td>
<td>D5</td>
<td>氯霉素</td>
<td>326.03</td>
<td>157.1</td>
</tr>
<tr>
<td>氯霉素</td>
<td>321.1</td>
<td>46.1</td>
<td>80</td>
<td>D5</td>
<td>氯霉素</td>
<td>326.03</td>
<td>45.9</td>
</tr>
<tr>
<td>双氯芬酸</td>
<td>294.01</td>
<td>250.1</td>
<td>8</td>
<td>D4</td>
<td>双氯芬酸</td>
<td>298.1</td>
<td>254.1</td>
</tr>
<tr>
<td>双氯芬酸</td>
<td>294.01</td>
<td>35.1</td>
<td>32</td>
<td>D4</td>
<td>双氯芬酸</td>
<td>298.1</td>
<td>34.9</td>
</tr>
<tr>
<td>(±)-羟基双氯芬酸</td>
<td>310.1</td>
<td>265.1</td>
<td>8</td>
<td>(±)C6</td>
<td>(±)-羟基双氯芬酸</td>
<td>316.1</td>
<td>272.1</td>
</tr>
<tr>
<td>(±)-羟基双氯芬酸</td>
<td>310.1</td>
<td>34.7</td>
<td>32</td>
<td>(±)C6</td>
<td>(±)-羟基双氯芬酸</td>
<td>316.1</td>
<td>34.8</td>
</tr>
<tr>
<td>芬布芬</td>
<td>253.08</td>
<td>153.1</td>
<td>20</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>芬布芬</td>
<td>253.08</td>
<td>55.1</td>
<td>24</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>呋塞米</td>
<td>329.1</td>
<td>285.1</td>
<td>8</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>呋塞米</td>
<td>329.1</td>
<td>204.9</td>
<td>16</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>吉非罗齐</td>
<td>249.15</td>
<td>127.1</td>
<td>4</td>
<td>D6</td>
<td>吉非罗齐</td>
<td>255.18</td>
<td>121.1</td>
</tr>
<tr>
<td>吉非罗齐</td>
<td>249.15</td>
<td>121.1</td>
<td>4</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>氮苯那嗪</td>
<td>295.95</td>
<td>265.8</td>
<td>12</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>氮苯那嗪</td>
<td>295.95</td>
<td>205.2</td>
<td>20</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>布洛芬</td>
<td>205.12</td>
<td>161.2</td>
<td>2</td>
<td>(±)C3</td>
<td>布洛芬</td>
<td>208.13</td>
<td>163.1</td>
</tr>
<tr>
<td>尼泊金甲酯</td>
<td>151.04</td>
<td>135.9</td>
<td>8</td>
<td>(±)C6</td>
<td>尼泊金甲酯</td>
<td>157.1</td>
<td>141.8</td>
</tr>
<tr>
<td>尼泊金甲酯</td>
<td>151.04</td>
<td>92.1</td>
<td>16</td>
<td>(±)C6</td>
<td>尼泊金甲酯</td>
<td>157.1</td>
<td>97.9</td>
</tr>
<tr>
<td>莫达非尼酸</td>
<td>273.06</td>
<td>161.1</td>
<td>8</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>莫达非尼酸</td>
<td>273.06</td>
<td>165.1</td>
<td>36</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>奥昔泊宁</td>
<td>229.08</td>
<td>170.1</td>
<td>4</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>奥昔泊宁</td>
<td>229.08</td>
<td>168.9</td>
<td>28</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>尼泊金丁酯</td>
<td>193.08</td>
<td>136.1</td>
<td>12</td>
<td>(±)C6</td>
<td>尼泊金丁酯</td>
<td>199.1</td>
<td>141.9</td>
</tr>
<tr>
<td>尼泊金丁酯</td>
<td>193.08</td>
<td>92.1</td>
<td>20</td>
<td>(±)C6</td>
<td>尼泊金丁酯</td>
<td>199.1</td>
<td>98.1</td>
</tr>
<tr>
<td>苯巴比妥</td>
<td>231.07</td>
<td>188.1</td>
<td>0</td>
<td>D5</td>
<td>苯巴比妥</td>
<td>236.11</td>
<td>42.1</td>
</tr>
<tr>
<td>苯巴比妥</td>
<td>231.07</td>
<td>42.1</td>
<td>12</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>苯妥英</td>
<td>251.1</td>
<td>102.1</td>
<td>20</td>
<td>D10</td>
<td>苯妥英</td>
<td>261.1</td>
<td>106.1</td>
</tr>
<tr>
<td>苯妥英</td>
<td>251.1</td>
<td>41.7</td>
<td>60</td>
<td>D10</td>
<td>苯妥英</td>
<td>261.1</td>
<td>41.9</td>
</tr>
<tr>
<td>普伐他汀</td>
<td>423.2</td>
<td>320.9</td>
<td>12</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>普伐他汀</td>
<td>423.2</td>
<td>302.2</td>
<td>12</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>硫酸甲恶唑</td>
<td>252.04</td>
<td>156.1</td>
<td>8</td>
<td>(±)C6</td>
<td>硫酸甲恶唑</td>
<td>258.06</td>
<td>162.1</td>
</tr>
<tr>
<td>硫酸甲恶唑</td>
<td>252.04</td>
<td>63.8</td>
<td>36</td>
<td>(±)C6</td>
<td>硫酸甲恶唑</td>
<td>258.06</td>
<td>63.9</td>
</tr>
<tr>
<td>三氯卡班</td>
<td>312.97</td>
<td>160.1</td>
<td>8</td>
<td>(±)C6</td>
<td>三氯卡班</td>
<td>319.1</td>
<td>159.9</td>
</tr>
<tr>
<td>三氯卡班</td>
<td>312.97</td>
<td>35.4</td>
<td>44</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>三氯生</td>
<td>286.94</td>
<td>35.4</td>
<td>4</td>
<td>(±)C12</td>
<td>三氯生</td>
<td>299.1</td>
<td>34.8</td>
</tr>
<tr>
<td>华法令</td>
<td>307.09</td>
<td>250.9</td>
<td>16</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>华法令</td>
<td>307.09</td>
<td>161.2</td>
<td>16</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
仪器

- Agilent 1290 Infinity 二元泵 (G4220A)
- Agilent 1290 Infinity 标准自动进样器 (G4226A) 和样品冷却装置 (G1330B)
- Agilent 1290 Infinity 柱温箱 (G1316C)

正离子模式方法和负离子模式方法所用的 UHPLC 条件分别列于表 3 和表 4 中。

表 3. 用于正离子模式方法的 Agilent 1290 UHPLC 条件

<table>
<thead>
<tr>
<th>参数</th>
<th>值</th>
</tr>
</thead>
<tbody>
<tr>
<td>色谱柱</td>
<td>安捷伦 ZORBAX Eclipse Plus C18 柱, 2.1 × 100 mm, 1.8 μm（部件号 959758-902）</td>
</tr>
<tr>
<td>柱温</td>
<td>40 °C</td>
</tr>
<tr>
<td>进样量</td>
<td>40 μL</td>
</tr>
<tr>
<td>速度</td>
<td>抽取 100 μL/min；推出 100 μL/min</td>
</tr>
<tr>
<td>自动进样器温度</td>
<td>6 °C</td>
</tr>
<tr>
<td>注射针清洗</td>
<td>5 s（80% 甲醇/20% 水）</td>
</tr>
<tr>
<td>流动相 A)</td>
<td>5 mM 乙酸铵 + 0.02% 乙酸的水溶液</td>
</tr>
<tr>
<td>流动相 B)</td>
<td>乙腈</td>
</tr>
<tr>
<td>流速</td>
<td>0.3 mL/min</td>
</tr>
<tr>
<td>梯度程序</td>
<td>时间 B %</td>
</tr>
<tr>
<td>0</td>
<td>5</td>
</tr>
<tr>
<td>0.5</td>
<td>5</td>
</tr>
<tr>
<td>11</td>
<td>100</td>
</tr>
<tr>
<td>13</td>
<td>100</td>
</tr>
<tr>
<td>13.1</td>
<td>5</td>
</tr>
<tr>
<td>停止时间</td>
<td>15 min</td>
</tr>
<tr>
<td>后运行时间</td>
<td>1 min</td>
</tr>
</tbody>
</table>

表 4. 用于负离子模式方法的 Agilent 1290 UHPLC 条件

<table>
<thead>
<tr>
<th>参数</th>
<th>值</th>
</tr>
</thead>
<tbody>
<tr>
<td>色谱柱</td>
<td>安捷伦 ZORBAX Eclipse Plus C18 柱, 2.1 × 100 mm, 1.8 μm（部件号 959758-902）</td>
</tr>
<tr>
<td>柱温</td>
<td>40 °C</td>
</tr>
<tr>
<td>进样量</td>
<td>40 μL</td>
</tr>
<tr>
<td>速度</td>
<td>抽取 100 μL/min；推出 100 μL/min</td>
</tr>
<tr>
<td>自动进样器温度</td>
<td>6 °C</td>
</tr>
<tr>
<td>注射针清洗</td>
<td>5 s（80% 甲醇/20% 水）</td>
</tr>
<tr>
<td>流动相 A)</td>
<td>0.005% 乙酸水溶液</td>
</tr>
<tr>
<td>流动相 B)</td>
<td>乙腈</td>
</tr>
<tr>
<td>流速</td>
<td>0.3 mL/min</td>
</tr>
<tr>
<td>梯度程序</td>
<td>时间 B %</td>
</tr>
<tr>
<td>0</td>
<td>5</td>
</tr>
<tr>
<td>0.5</td>
<td>5</td>
</tr>
<tr>
<td>6</td>
<td>100</td>
</tr>
<tr>
<td>8</td>
<td>100</td>
</tr>
<tr>
<td>8.1</td>
<td>5</td>
</tr>
<tr>
<td>停止时间</td>
<td>10 min</td>
</tr>
<tr>
<td>后运行时间</td>
<td>1 min</td>
</tr>
</tbody>
</table>
质谱检测

配备安捷伦喷射流电喷雾离子源的 Agilent 6495 三重四极杆质谱仪

安捷伦喷射流离子源参数和漏斗 RF 电压对分析物的高灵敏度检测非常关键。安捷伦 MassHunter B.07 采集软件包括 MassHunter Source 和 iFunnel Optimizer 软件，可帮助用户以自动连续方式获得分析物的最佳条件。采用低压和高压离子漏斗 RF 电压等由 Optimizer 软件获得的所有最佳参数可显著提高分析物的响应[i]。在多种分析物应用中，参数设置通常侧重于难以检测的分析物。正离子模式方法和负离子模式方法下由 Optimizer 软件优化的质谱离子源条件分别列于表 5 和表 6 中。

软件

- 安捷伦三重四极杆质谱仪
  MassHunter 数据采集软件，版本 B.07.00
- 安捷伦 MassHunter 定性分析软件，版本 B.06.0.633.10 SP1
- 安捷伦 MassHunter 定量分析软件，版本 B.07.00/Build 7.0.457.0

稀释方法

分析物标准品和内标的储备溶液以乙腈配制，其中各化合物的浓度均为 25 ppb。所有样品中均添加了 250 ppt 恒定浓度的内标，而校准标样中则分别加入了 10 ppt、25 ppt、50 ppt、100 ppt、250 ppt、500 ppt 和 1000 ppt（7 个浓度水平）的内标，并以 MilliQ 纯水配制。

三种未知样品中的两种由外部合作方提供，一种样品取自远离主要人为水源的偏远地区，另一种则取自城市地表水源。第三种样品为当地的饮用自来水（美国圣克拉拉市）。所有未知样品经过滤后均加入了浓度为 250 ppt 的内标。

表 5. 用于正离子模式方法的 Agilent 6495 三重四极杆质谱仪离子源参数

<table>
<thead>
<tr>
<th>参数</th>
<th>值</th>
</tr>
</thead>
<tbody>
<tr>
<td>离子模式</td>
<td>正</td>
</tr>
<tr>
<td>干燥气温度</td>
<td>250</td>
</tr>
<tr>
<td>干燥气流速</td>
<td>16</td>
</tr>
<tr>
<td>鞘气温度</td>
<td>400</td>
</tr>
<tr>
<td>鞘气流速</td>
<td>12</td>
</tr>
<tr>
<td>雾化器压力</td>
<td>40</td>
</tr>
<tr>
<td>毛细管电压</td>
<td>3000</td>
</tr>
<tr>
<td>喷嘴电压</td>
<td>0</td>
</tr>
<tr>
<td>Delta EMV</td>
<td>200</td>
</tr>
<tr>
<td>LPF RF</td>
<td>60</td>
</tr>
<tr>
<td>HPF RF</td>
<td>160</td>
</tr>
<tr>
<td>MS1 和 MS2 分辨率</td>
<td>单位</td>
</tr>
</tbody>
</table>

表 6. 用于负离子模式方法的 Agilent 6495 三重四极杆质谱仪离子源参数

<table>
<thead>
<tr>
<th>参数</th>
<th>值</th>
</tr>
</thead>
<tbody>
<tr>
<td>离子模式</td>
<td>负</td>
</tr>
<tr>
<td>干燥气温度</td>
<td>200</td>
</tr>
<tr>
<td>干燥气流速</td>
<td>12</td>
</tr>
<tr>
<td>鞘气温度</td>
<td>400</td>
</tr>
<tr>
<td>鞘气流速</td>
<td>12</td>
</tr>
<tr>
<td>雾化器压力</td>
<td>40</td>
</tr>
<tr>
<td>毛细管电压</td>
<td>3000</td>
</tr>
<tr>
<td>喷嘴电压</td>
<td>2000</td>
</tr>
<tr>
<td>Delta EMV</td>
<td>200</td>
</tr>
<tr>
<td>LPF RF</td>
<td>40</td>
</tr>
<tr>
<td>HPF RF</td>
<td>90</td>
</tr>
<tr>
<td>MS1 和 MS2 分辨率</td>
<td>单位</td>
</tr>
</tbody>
</table>
结果与讨论

提高的方法性能

6495 三重四极杆液质联用系统的设计改进可实现高效离子传输。图 1 和图 2 分别显示了正离子模式下 118 种分析物的响应以及负离子模式下 22 种分析物的响应，分析物浓度均为 10 ppt。

图 1. Agilent 6495 系统在正离子模式下的信号响应（浓度 10 ppt，直接进样 40 μL）

图 2. Agilent 6495 系统在负离子模式下的信号响应（浓度 10 ppt，直接进样 40 μL）
校准曲线
以 MilliQ 水样中加标，从 10 ppt 到 1000 ppt 的 PPCP 标样做校准曲线。正离子模式下二甲双胍的校准曲线以及负离子模式下布洛芬的校准曲线示例如图 3 所示。校准方程采用 1/x 的加权因子以及包含原点的二次拟合生成。两种极性模式下所有目标分析物的相关系数 (R^2) 均大于 0.99，且多数大于 0.995。正离子模式下的喹硫平除外 (R^2 = 0.982)，因为该化合物附近存在系统干扰峰。

精密度和准确度
绘制校准曲线时，各浓度水平的标样均重复进样三次。多数情况下，精密度非常理想。少数情况下，准确度会超出 80% – 120% 的范围。他汀类药物、丁丙诺啡和孟鲁司特等五到六种强疏水性化合物在低浓度下的准确度将超出正常范围。这可能是由于在较低的加标浓度下，化合物在 HPLC 样品瓶表面发生了吸附。总体而言，如果在正离子模式下考察准确度时剔除五种异常化合物，则仅有 2.3% 的测定结果准确度超出 80% – 120% 的范围（在每种化合物测定 21 次的情况下，每两种化合物的准确度异常情况 < 1 次）。在负离子模式下，除塞来昔布外的所有化合物均表现出优异的准确度。塞来昔布的准确度问题可能是由于在缺少相应内标的情况下，低浓度化合物在不平的 HPLC 样品瓶表面上发生了吸附。

实际样品
实验测试了三种样品。第一种样品取自当地的自来水（美国圣克拉拉市）。其他两种样品由外部合作方提供：一种取自远离主要人为水源的偏远地区，另一种则取自城市地表水源。每种样品均重复进样。如果两次运行得到的某种化合物的平均浓度高于 10 ppt，则认为该化合物的检测结果呈阳性。这些样品的阳性检测结果列于表 7 - 10。图 4 和图 5 分别显示了圣克拉拉市自来水和偏远地区水样的色谱图。检出每种样品中三种化合物的浓度均高于 10 ppt。
### 表 7. 利用正离子模式方法在饮用水中检出的化合物

<table>
<thead>
<tr>
<th>名称</th>
<th>进样 1 (ppt)</th>
<th>进样 2 (ppt)</th>
<th>平均浓度 (ppt)</th>
</tr>
</thead>
<tbody>
<tr>
<td>加巴喷丁</td>
<td>21</td>
<td>20</td>
<td>20</td>
</tr>
<tr>
<td>二甲双胍</td>
<td>31</td>
<td>30</td>
<td>31</td>
</tr>
<tr>
<td>孟鲁司特</td>
<td>13</td>
<td>12</td>
<td>13</td>
</tr>
</tbody>
</table>

### 图 4. 利用正离子模式方法在当地饮用水（加利福尼亚州圣克拉拉市）中检出的 PPCP 的色谱图

### 表 8. 利用正离子模式方法在偏远地区水样中检出的化合物

<table>
<thead>
<tr>
<th>名称</th>
<th>进样 1 (ppt)</th>
<th>进样 2 (ppt)</th>
<th>平均浓度 (ppt)</th>
</tr>
</thead>
<tbody>
<tr>
<td>孟鲁司特</td>
<td>12</td>
<td>12</td>
<td>12</td>
</tr>
<tr>
<td>咖啡因</td>
<td>27</td>
<td>15</td>
<td>21</td>
</tr>
<tr>
<td>DEET</td>
<td>107</td>
<td>119</td>
<td>113</td>
</tr>
</tbody>
</table>

### 表 5. 利用正离子模式方法在偏远地区水样中检出的 PPCP 的色谱图
表 9. 利用正离子模式方法在城市地表水样中检出的化合物

<table>
<thead>
<tr>
<th>名称</th>
<th>进样 1 (ppt)</th>
<th>进样 2 (ppt)</th>
<th>平均浓度 (ppt)</th>
</tr>
</thead>
<tbody>
<tr>
<td>利卡西平</td>
<td>903</td>
<td>861</td>
<td>882</td>
</tr>
<tr>
<td>阿米替林代谢物</td>
<td>30</td>
<td>30</td>
<td>30</td>
</tr>
<tr>
<td>阿米替林</td>
<td>29</td>
<td>29</td>
<td>29</td>
</tr>
<tr>
<td>阿普洛尔</td>
<td>2,599</td>
<td>2,212</td>
<td>2,405</td>
</tr>
<tr>
<td>阿托伐他汀</td>
<td>40</td>
<td>37</td>
<td>39</td>
</tr>
<tr>
<td>阿替拉津</td>
<td>43</td>
<td>41</td>
<td>42</td>
</tr>
<tr>
<td>苯甲酰爱康宁</td>
<td>221</td>
<td>206</td>
<td>214</td>
</tr>
<tr>
<td>安非他酮</td>
<td>169</td>
<td>154</td>
<td>162</td>
</tr>
<tr>
<td>咖啡因</td>
<td>1,473</td>
<td>1,241</td>
<td>1,357</td>
</tr>
<tr>
<td>卡马西平 10,11-环氧化物</td>
<td>38</td>
<td>36</td>
<td>37</td>
</tr>
<tr>
<td>卡马西平</td>
<td>214</td>
<td>229</td>
<td>221</td>
</tr>
<tr>
<td>卡立普多</td>
<td>27</td>
<td>28</td>
<td>28</td>
</tr>
<tr>
<td>氯吡格雷按酸</td>
<td>223</td>
<td>204</td>
<td>214</td>
</tr>
<tr>
<td>吨卡因</td>
<td>37</td>
<td>35</td>
<td>36</td>
</tr>
<tr>
<td>可待因</td>
<td>67</td>
<td>67</td>
<td>67</td>
</tr>
<tr>
<td>可体松</td>
<td>98</td>
<td>90</td>
<td>94</td>
</tr>
<tr>
<td>DEET</td>
<td>503</td>
<td>570</td>
<td>536</td>
</tr>
<tr>
<td>去甲替普兰</td>
<td>107</td>
<td>88</td>
<td>97</td>
</tr>
<tr>
<td>去甲文拉法辛</td>
<td>744</td>
<td>827</td>
<td>786</td>
</tr>
<tr>
<td>右美沙芬</td>
<td>31</td>
<td>42</td>
<td>36</td>
</tr>
<tr>
<td>地尔硫卓</td>
<td>55</td>
<td>61</td>
<td>58</td>
</tr>
<tr>
<td>苯海拉明</td>
<td>205</td>
<td>205</td>
<td>205</td>
</tr>
<tr>
<td>美他醇甲酯</td>
<td>39</td>
<td>39</td>
<td>39</td>
</tr>
<tr>
<td>EDDP</td>
<td>102</td>
<td>100</td>
<td>101</td>
</tr>
<tr>
<td>红霉素</td>
<td>44</td>
<td>44</td>
<td>44</td>
</tr>
<tr>
<td>无水红霉素</td>
<td>38</td>
<td>31</td>
<td>34</td>
</tr>
<tr>
<td>艾司西酞普兰</td>
<td>192</td>
<td>179</td>
<td>186</td>
</tr>
<tr>
<td>氟西汀</td>
<td>30</td>
<td>28</td>
<td>29</td>
</tr>
<tr>
<td>加巴敏丁</td>
<td>&gt;&gt;1,000</td>
<td>&gt;&gt;1,000</td>
<td>&gt;&gt;1,000</td>
</tr>
<tr>
<td>氯丙嗪</td>
<td>28</td>
<td>24</td>
<td>26</td>
</tr>
<tr>
<td>硝基非尼非他酮</td>
<td>260</td>
<td>253</td>
<td>257</td>
</tr>
<tr>
<td>塞洛芬</td>
<td>17</td>
<td>15</td>
<td>16</td>
</tr>
<tr>
<td>拉莫三嗪</td>
<td>868</td>
<td>1,013</td>
<td>940</td>
</tr>
<tr>
<td>左啡洛</td>
<td>213</td>
<td>205</td>
<td>209</td>
</tr>
<tr>
<td>利多卡因</td>
<td>360</td>
<td>325</td>
<td>343</td>
</tr>
<tr>
<td>氯雷他定</td>
<td>10</td>
<td>10</td>
<td>10</td>
</tr>
</tbody>
</table>
采用负离子模式方法时，未检出当地自来水或偏远地区水样中具有 PPCP 化合物。在负离子模式下检出的城市地表水样中的化合物列于表 10 中。

MassHunter 定量分析软件 B.07 可提供的灵活报告
用户可利用定量分析软件 B.07 中的快速 PDF 报告系统以所需格式（包括得出重复结果均值、插入偏好徽标和定义样品布局等）生成结果，而无需再将结果导出 Excel 并求得重复结果的均值。可通过在样品组下对重复结果进行分组以获得重复结果均值。

该软件产品中提供不同的 PDF 报告模板供您选择。表 11 列出了定量分析软件 B07 中的所有相关模板。

<table>
<thead>
<tr>
<th>名称</th>
<th>进样 1 (ppt)</th>
<th>进样 2 (ppt)</th>
<th>平均浓度 (ppt)</th>
</tr>
</thead>
<tbody>
<tr>
<td>塞来昔布</td>
<td>45</td>
<td>41</td>
<td>43</td>
</tr>
<tr>
<td>氯霉素</td>
<td>12</td>
<td>12</td>
<td>12</td>
</tr>
<tr>
<td>4-羟基双氯芬酸</td>
<td>41</td>
<td>45</td>
<td>43</td>
</tr>
<tr>
<td>双氯芬酸</td>
<td>237</td>
<td>292</td>
<td>265</td>
</tr>
<tr>
<td>双氯芬酸</td>
<td>400</td>
<td>387</td>
<td>393</td>
</tr>
<tr>
<td>吉非罗齐</td>
<td>309</td>
<td>337</td>
<td>323</td>
</tr>
<tr>
<td>吉非罗齐</td>
<td>503</td>
<td>487</td>
<td>495</td>
</tr>
<tr>
<td>吉非罗齐</td>
<td>140</td>
<td>139</td>
<td>139</td>
</tr>
<tr>
<td>莫达非尼酸</td>
<td>118</td>
<td>114</td>
<td>116</td>
</tr>
<tr>
<td>吉非罗齐</td>
<td>354</td>
<td>347</td>
<td>350</td>
</tr>
<tr>
<td>莫达非尼酸</td>
<td>55</td>
<td>53</td>
<td>54</td>
</tr>
<tr>
<td>丙酮乙醇</td>
<td>126</td>
<td>121</td>
<td>123</td>
</tr>
<tr>
<td>蒽他汀</td>
<td>57</td>
<td>52</td>
<td>54</td>
</tr>
<tr>
<td>磺酸甲恶唑</td>
<td>573</td>
<td>582</td>
<td>577</td>
</tr>
<tr>
<td>双氯芬酸</td>
<td>40</td>
<td>39</td>
<td>39</td>
</tr>
<tr>
<td>布洛芬</td>
<td>242</td>
<td>288</td>
<td>255</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>DIR</th>
<th>SUBDIR</th>
<th>类别</th>
<th>PDF 模板</th>
</tr>
</thead>
<tbody>
<tr>
<td>PDF 报告</td>
<td>法规认证</td>
<td>AuditTrail.report.xml</td>
<td></td>
</tr>
<tr>
<td>PDF 报告</td>
<td>环境</td>
<td>Env_CC_Avg.report.xml</td>
<td></td>
</tr>
<tr>
<td>PDF 报告</td>
<td>环境</td>
<td>Env_CC_MidPoint.report.xml</td>
<td></td>
</tr>
<tr>
<td>PDF 报告</td>
<td>环境</td>
<td>Env_CC_Previous.report.xml</td>
<td></td>
</tr>
<tr>
<td>PDF 报告</td>
<td>环境</td>
<td>Env_DualGCResults.report.xml</td>
<td></td>
</tr>
<tr>
<td>PDF 报告</td>
<td>环境</td>
<td>Env_InitialCal.report.xml</td>
<td></td>
</tr>
<tr>
<td>PDF 报告</td>
<td>环境</td>
<td>Env_LCSSpike.report.xml</td>
<td></td>
</tr>
<tr>
<td>PDF 报告</td>
<td>环境</td>
<td>Env_MSD.report.xml</td>
<td></td>
</tr>
<tr>
<td>PDF 报告</td>
<td>环境</td>
<td>Env_QA_Check.report.xml</td>
<td></td>
</tr>
<tr>
<td>PDF 报告</td>
<td>环境</td>
<td>Env_Results.report.xml</td>
<td></td>
</tr>
<tr>
<td>PDF 报告</td>
<td>环境</td>
<td>Env_Results_withGraphics.report.xml</td>
<td></td>
</tr>
<tr>
<td>PDF 报告</td>
<td>环境</td>
<td>Env_TPH_Validation.report.xml</td>
<td></td>
</tr>
<tr>
<td>PDF 报告</td>
<td>常规</td>
<td>Gen_ByCompound.report.xml</td>
<td></td>
</tr>
<tr>
<td>PDF 报告</td>
<td>常规</td>
<td>Gen_BySample.report.xml</td>
<td></td>
</tr>
<tr>
<td>PDF 报告</td>
<td>常规</td>
<td>Gen_BySample_withSN.report.xml</td>
<td></td>
</tr>
<tr>
<td>PDF 报告</td>
<td>常规</td>
<td>Gen_Calibration.report.xml</td>
<td></td>
</tr>
<tr>
<td>PDF 报告</td>
<td>常规</td>
<td>Gen_Complete.report.xml</td>
<td></td>
</tr>
<tr>
<td>PDF 报告</td>
<td>常规</td>
<td>Gen_ResultsSummary.report.xml</td>
<td></td>
</tr>
<tr>
<td>PDF 报告</td>
<td>常规</td>
<td>Gen_Samples.report.xml</td>
<td></td>
</tr>
<tr>
<td>PDF 报告</td>
<td>专用</td>
<td>Pesticide_Residues.report.xml</td>
<td></td>
</tr>
<tr>
<td>PDF 报告</td>
<td>专用</td>
<td>SIMSscan.report.xml</td>
<td></td>
</tr>
<tr>
<td>PDF 报告</td>
<td>未知物</td>
<td>all-hits.report.xml</td>
<td></td>
</tr>
<tr>
<td>PDF 报告</td>
<td>未知物</td>
<td>best-hits.report.xml</td>
<td></td>
</tr>
</tbody>
</table>
图 6 显示了本研究中采用全新 PDF 报告生成系统生成的某种样品的示例报告。每种样品的结果可排列在单独页面或同一页面中。

结论

我们已经开发出快速、简单的 LC/MS/MS 方法用于对水中的 PPCP 进行准确确证和定量。该方法充分利用了高灵敏度的 Agilent 6495 三重四极杆质谱仪。结果表明，通过直接进样方法定量分析水中的痕量污染物时能够获得低至 ppt 级的定量下限。这些全新的设计改进有助于省掉繁琐的样品富集和净化步骤，从而可以显著提高样品通量。

用户可以利用灵活的 PDF 报告系统生成高质量的报告，同时能够选择多种格式和布局。

参考文献


3. EPA Method 1694, Pharmaceuticals and Personal Care Products in Water, Soil, Sediment, and Biosolids by HPLC/MS/MS; EPA-821-R-08-002, 2007


5. Ferra, I; Thurman, E. M; Zweigenbaum, J, 利用配备喷射流技术的 Agilent 6460 LC/MS/MS 以超灵敏的 EPA 方法 1694 对水中的药物和个人护理用品进行分析，安捷伦科技公司应用简报，出版号 5990-4605CHCN

6. Cullum, N, 利用配备 iFunnel 技术的 Agilent 6490 三重四极杆质谱仪联用系统优化类固醇的检测，安捷伦科技公司应用简报，出版号 5990-9978CHCN

7. Yang, D. D 等, Multi Residue Pesticide Screening and Quantitation in Difficult Food Matrixes Using the Agilent 6495 Triple Quadrupole Mass Spectrometer (利用 Agilent 6495 三重四极杆质谱仪筛查和定量分析复杂食品基质中的多种农药残留)，安捷伦科技公司应用简报，出版号 5991-4687EN

致谢

对各项工作进行了协调。感谢 Ralph Hindle 就方法开发和结果评估提出见解深刻的讨论意见。