

# Environmental Method

## Illicit drugs analysis in water

*Elevate your environmental testing with the X500R QTOF System*

Method details and access to HR-MS/MS libraries to detect, quantify, and confirm illicit drugs in water samples using HPLC coupled with the X500R QTOF system, powered by SCIEX OS Software.

### Sample Prep

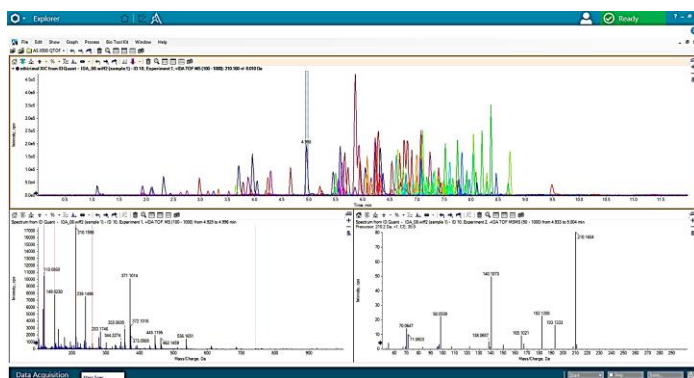
- Step 1**
  - Samples acidified to pH 2 using HCL and stored in the dark at 4°C until required
- Step 2**
  - Transfer 1mL of sample into an analytical vial



SCIEX OS can deliver faster method set-up

### LC Method

Column	Phenomenex Kinetex C18, 100 x 4.6 mm, 5 um column	
Mobile Phase A	0.1% formic acid in water + 2mM ammonium formate	
Mobile Phase B	Acetonitrile	
Flow rate	0.9 mL/min	
Column temperature	30°C	
Injection volume	100 uL	
Gradient profile	<b>Time (min)</b>	<b>% B</b>
	0	2
	1	2
	7	65
	7.1	100
	9	100
	9.1	2
	12	2



SCIEX OS delivers enhanced data exploration of your acquired TOF MS and TOF MS/MS data

# MS Method

Suggested IDA (Information Dependent Acquisition) conditions for routine environmental testing as displayed in SCIEX OS.

## Data Processing

Review your results with utmost efficiency using SCIEX OS for simultaneous quantitation and MS/MS library confirmation.

## X500R High Resolution Libraries

Compound	CAS Number	Formula	Elemental Weight
2,2-Dimethylbutane	2880-08-4	C <sub>6</sub> H <sub>14</sub>	86.1708
2,2-Dimethylpropane	68-122-6	C <sub>5</sub> H <sub>12</sub>	72.1508
2,2,4,4-Tetramethylpentane	68-176-2	C <sub>8</sub> H <sub>18</sub>	114.2308
2,2,4,6-Tetramethylheptane	68-182-0	C <sub>10</sub> H <sub>22</sub>	142.2908
2,2,4,6,6-Pentamethylheptane	68-183-8	C <sub>11</sub> H <sub>24</sub>	156.2708
2,2,4,6,6-Pentamethyloctane	68-184-6	C <sub>12</sub> H <sub>26</sub>	170.2508
2,2,4,6,6-Pentamethylnonane	68-185-4	C <sub>13</sub> H <sub>28</sub>	184.2308
2,2,4,6,6-Pentamethyldecane	68-186-2	C <sub>14</sub> H <sub>30</sub>	198.2108
2,2,4,6,6-Pentamethylundecane	68-187-0	C <sub>15</sub> H <sub>32</sub>	212.1908
2,2,4,6,6-Pentamethyltridecane	68-188-8	C <sub>17</sub> H <sub>36</sub>	238.3408
2,2,4,6,6-Pentamethylpentadecane	68-189-6	C <sub>19</sub> H <sub>40</sub>	264.4908
2,2,4,6,6-Pentamethylheptadecane	68-190-4	C <sub>21</sub> H <sub>44</sub>	290.6408
2,2,4,6,6-Pentamethylnonadecane	68-191-2	C <sub>23</sub> H <sub>48</sub>	316.7908
2,2,4,6,6-Pentamethylheneicosane	68-192-0	C <sub>25</sub> H <sub>52</sub>	342.9408
2,2,4,6,6-Pentamethyltricosane	68-192-8	C <sub>27</sub> H <sub>56</sub>	369.0908
2,2,4,6,6-Pentamethyltriacontane	68-193-6	C <sub>30</sub> H <sub>62</sub>	416.7408
2,2,4,6,6-Pentamethyltriacontane	68-194-4	C <sub>32</sub> H <sub>66</sub>	442.8908
2,2,4,6,6-Pentamethyltriacontane	68-195-2	C <sub>34</sub> H <sub>70</sub>	469.0408
2,2,4,6,6-Pentamethyltriacontane	68-196-0	C <sub>36</sub> H <sub>74</sub>	495.1908
2,2,4,6,6-Pentamethyltriacontane	68-196-8	C <sub>38</sub> H <sub>78</sub>	521.3408
2,2,4,6,6-Pentamethyltriacontane	68-197-6	C <sub>40</sub> H <sub>82</sub>	547.4908
2,2,4,6,6-Pentamethyltriacontane	68-198-4	C <sub>42</sub> H <sub>86</sub>	573.6408
2,2,4,6,6-Pentamethyltriacontane	68-199-2	C <sub>44</sub> H <sub>90</sub>	599.7908
2,2,4,6,6-Pentamethyltriacontane	68-200-0	C <sub>46</sub> H <sub>94</sub>	625.9408
2,2,4,6,6-Pentamethyltriacontane	68-200-8	C <sub>48</sub> H <sub>98</sub>	652.0908
2,2,4,6,6-Pentamethyltriacontane	68-201-6	C <sub>50</sub> H <sub>102</sub>	678.2408
2,2,4,6,6-Pentamethyltriacontane	68-202-4	C <sub>52</sub> H <sub>106</sub>	704.3908
2,2,4,6,6-Pentamethyltriacontane	68-203-2	C <sub>54</sub> H <sub>110</sub>	730.5408
2,2,4,6,6-Pentamethyltriacontane	68-204-0	C <sub>56</sub> H <sub>114</sub>	756.6908
2,2,4,6,6-Pentamethyltriacontane	68-204-8	C <sub>58</sub> H <sub>118</sub>	782.8408
2,2,4,6,6-Pentamethyltriacontane	68-205-6	C <sub>60</sub> H <sub>122</sub>	808.9908
2,2,4,6,6-Pentamethyltriacontane	68-206-4	C <sub>62</sub> H <sub>126</sub>	835.1408
2,2,4,6,6-Pentamethyltriacontane	68-207-2	C <sub>64</sub> H <sub>130</sub>	861.2908
2,2,4,6,6-Pentamethyltriacontane	68-208-0	C <sub>66</sub> H <sub>134</sub>	887.4408
2,2,4,6,6-Pentamethyltriacontane	68-208-8	C <sub>68</sub> H <sub>138</sub>	913.5908
2,2,4,6,6-Pentamethyltriacontane	68-209-6	C <sub>70</sub> H <sub>142</sub>	939.7408
2,2,4,6,6-Pentamethyltriacontane	68-210-4	C <sub>72</sub> H <sub>146</sub>	965.8908
2,2,4,6,6-Pentamethyltriacontane	68-211-2	C <sub>74</sub> H <sub>150</sub>	992.0408
2,2,4,6,6-Pentamethyltriacontane	68-212-0	C <sub>76</sub> H <sub>154</sub>	1018.1908
2,2,4,6,6-Pentamethyltriacontane	68-212-8	C <sub>78</sub> H <sub>158</sub>	1044.3408
2,2,4,6,6-Pentamethyltriacontane	68-213-6	C <sub>80</sub> H <sub>162</sub>	1070.4908
2,2,4,6,6-Pentamethyltriacontane	68-214-4	C <sub>82</sub> H <sub>166</sub>	1096.6408
2,2,4,6,6-Pentamethyltriacontane	68-215-2	C <sub>84</sub> H <sub>170</sub>	1122.7908
2,2,4,6,6-Pentamethyltriacontane	68-216-0	C <sub>86</sub> H <sub>174</sub>	1148.9408
2,2,4,6,6-Pentamethyltriacontane	68-216-8	C <sub>88</sub> H <sub>178</sub>	1175.0908
2,2,4,6,6-Pentamethyltriacontane	68-217-6	C <sub>90</sub> H <sub>182</sub>	1201.2408
2,2,4,6,6-Pentamethyltriacontane	68-218-4	C <sub>92</sub> H <sub>186</sub>	1227.3908
2,2,4,6,6-Pentamethyltriacontane	68-219-2	C <sub>94</sub> H <sub>190</sub>	1253.5408
2,2,4,6,6-Pentamethyltriacontane	68-220-0	C <sub>96</sub> H <sub>194</sub>	1279.6908
2,2,4,6,6-Pentamethyltriacontane	68-220-8	C <sub>98</sub> H <sub>198</sub>	1305.8408
2,2,4,6,6-Pentamethyltriacontane	68-221-6	C <sub>100</sub> H <sub>202</sub>	1331.9908
2,2,4,6,6-Pentamethyltriacontane	68-222-4	C <sub>102</sub> H <sub>206</sub>	1358.1408
2,2,4,6,6-Pentamethyltriacontane	68-223-2	C <sub>104</sub> H <sub>210</sub>	1384.2908
2,2,4,6,6-Pentamethyltriacontane	68-224-0	C <sub>106</sub> H <sub>214</sub>	1410.4408
2,2,4,6,6-Pentamethyltriacontane	68-224-8	C <sub>108</sub> H <sub>218</sub>	1436.5908
2,2,4,6,6-Pentamethyltriacontane	68-225-6	C <sub>110</sub> H <sub>222</sub>	1462.7408
2,2,4,6,6-Pentamethyltriacontane	68-226-4	C <sub>112</sub> H <sub>226</sub>	1488.8908
2,2,4,6,6-Pentamethyltriacontane	68-227-2	C <sub>114</sub> H <sub>230</sub>	1515.0408
2,2,4,6,6-Pentamethyltriacontane	68-228-0	C <sub>116</sub> H <sub>234</sub>	1541.1908
2,2,4,6,6-Pentamethyltriacontane	68-228-8	C <sub>118</sub> H <sub>238</sub>	1567.3408
2,2,4,6,6-Pentamethyltriacontane	68-229-6	C <sub>120</sub> H <sub>242</sub>	1593.4908
2,2,4,6,6-Pentamethyltriacontane	68-230-4	C <sub>122</sub> H <sub>246</sub>	1619.6408
2,2,4,6,6-Pentamethyltriacontane	68-231-2	C <sub>124</sub> H <sub>250</sub>	1645.7908
2,2,4,6,6-Pentamethyltriacontane	68-232-0	C <sub>126</sub> H <sub>254</sub>	1671.9408
2,2,4,6,6-Pentamethyltriacontane	68-232-8	C <sub>128</sub> H <sub>258</sub>	1698.0908
2,2,4,6,6-Pentamethyltriacontane	68-233-6	C <sub>130</sub> H <sub>262</sub>	1724.2408
2,2,4,6,6-Pentamethyltriacontane	68-234-4	C <sub>132</sub> H <sub>266</sub>	1750.3908
2,2,4,6,6-Pentamethyltriacontane	68-235-2	C <sub>134</sub> H <sub>270</sub>	1776.5408
2,2,4,6,6-Pentamethyltriacontane	68-236-0	C <sub>136</sub> H <sub>274</sub>	1802.6908
2,2,4,6,6-Pentamethyltriacontane	68-236-8	C <sub>138</sub> H <sub>278</sub>	1828.8408
2,2,4,6,6-Pentamethyltriacontane	68-237-6	C <sub>140</sub> H <sub>282</sub>	1854.9908
2,2,4,6,6-Pentamethyltriacontane	68-238-4	C <sub>142</sub> H <sub>286</sub>	1881.1408
2,2,4,6,6-Pentamethyltriacontane	68-239-2	C <sub>144</sub> H <sub>290</sub>	1907.2908
2,2,4,6,6-Pentamethyltriacontane	68-240-0	C <sub>146</sub> H <sub>294</sub>	1933.4408
2,2,4,6,6-Pentamethyltriacontane	68-240-8	C <sub>148</sub> H <sub>298</sub>	1959.5908
2,2,4,6,6-Pentamethyltriacontane	68-241-6	C <sub>150</sub> H <sub>302</sub>	1985.7408
2,2,4,6,6-Pentamethyltriacontane	68-242-4	C <sub>152</sub> H <sub>306</sub>	2011.8908
2,2,4,6,6-Pentamethyltriacontane	68-243-2	C <sub>154</sub> H <sub>310</sub>	2038.0408
2,2,4,6,6-Pentamethyltriacontane	68-244-0	C <sub>156</sub> H <sub>314</sub>	2064.1908
2,2,4,6,6-Pentamethyltriacontane	68-244-8	C <sub>158</sub> H <sub>318</sub>	2090.3408
2,2,4,6,6-Pentamethyltriacontane	68-245-6	C <sub>160</sub> H <sub>322</sub>	2116.4908
2,2,4,6,6-Pentamethyltriacontane	68-246-4	C <sub>162</sub> H <sub>326</sub>	2142.6408
2,2,4,6,6-Pentamethyltriacontane	68-247-2	C <sub>164</sub> H <sub>330</sub>	2168.7908
2,2,4,6,6-Pentamethyltriacontane	68-248-0	C <sub>166</sub> H <sub>334</sub>	2194.9408
2,2,4,6,6-Pentamethyltriacontane	68-248-8	C <sub>168</sub> H <sub>338</sub>	2221.0908
2,2,4,6,6-Pentamethyltriacontane	68-249-6	C <sub>170</sub> H <sub>342</sub>	2247.2408
2,2,4,6,6-Pentamethyltriacontane	68-250-4	C <sub>172</sub> H <sub>346</sub>	2273.3908
2,2,4,6,6-Pentamethyltriacontane	68-251-2	C <sub>174</sub> H <sub>350</sub>	2299.5408
2,2,4,6,6-Pentamethyltriacontane	68-252-0	C <sub>176</sub> H <sub>354</sub>	2325.6908
2,2,4,6,6-Pentamethyltriacontane	68-252-8	C <sub>178</sub> H <sub>358</sub>	2351.8408
2,2,4,6,6-Pentamethyltriacontane	68-253-6	C <sub>180</sub> H <sub>362</sub>	2377.9908
2,2,4,6,6-Pentamethyltriacontane	68-254-4	C <sub>182</sub> H <sub>366</sub>	2404.1408
2,2,4,6,6-Pentamethyltriacontane	68-255-2	C <sub>184</sub> H <sub>370</sub>	2430.2908
2,2,4,6,6-Pentamethyltriacontane	68-256-0	C <sub>186</sub> H <sub>374</sub>	2456.4408
2,2,4,6,6-Pentamethyltriacontane	68-256-8	C <sub>188</sub> H <sub>378</sub>	2482.5908
2,2,4,6,6-Pentamethyltriacontane	68-257-6	C <sub>190</sub> H <sub>382</sub>	2508.7408
2,2,4,6,6-Pentamethyltriacontane	68-258-4	C <sub>192</sub> H <sub>386</sub>	2534.8908
2,2,4,6,6-Pentamethyltriacontane	68-259-2	C <sub>194</sub> H <sub>390</sub>	2561.0408
2,2,4,6,6-Pentamethyltriacontane	68-260-0	C <sub>196</sub> H <sub>394</sub>	2587.1908
2,2,4,6,6-Pentamethyltriacontane	68-260-8	C <sub>198</sub> H <sub>398</sub>	2613.3408
2,2,4,6,6-Pentamethyltriacontane	68-261-6	C <sub>200</sub> H <sub>402</sub>	2639.4908
2,2,4,6,6-Pentamethyltriacontane	68-262-4	C <sub>202</sub> H <sub>406</sub>	2665.6408
2,2,4,6,6-Pentamethyltriacontane	68-263-2	C <sub>204</sub> H <sub>410</sub>	2691.7908
2,2,4,6,6-Pentamethyltriacontane	68-264-0	C <sub>206</sub> H <sub>414</sub>	2717.9408
2,2,4,6,6-Pentamethyltriacontane	68-264-8	C <sub>208</sub> H <sub>418</sub>	2744.0908
2,2,4,6,6-Pentamethyltriacontane	68-265-6	C <sub>210</sub> H <sub>422</sub>	2770.2408
2,2,4,6,6-Pentamethyltriacontane	68-266-4	C <sub>212</sub> H <sub>426</sub>	2796.3908
2,2,4,6,6-Pentamethyltriacontane	68-267-2	C <sub>214</sub> H <sub>430</sub>	2822.5408
2,2,4,6,6-Pentamethyltriacontane	68-268-0	C <sub>216</sub> H <sub>434</sub>	2848.6908
2,2,4,6,6-Pentamethyltriacontane	68-268-8	C <sub>218</sub> H <sub>438</sub>	2874.8408
2,2,4,6,6-Pentamethyltriacontane	68-269-6	C <sub>220</sub> H <sub>442</sub>	2900.9908
2,2,4,6,6-Pentamethyltriacontane	68-270-4	C <sub>222</sub> H <sub>446</sub>	2927.1408
2,2,4,6,6-Pentamethyltriacontane	68-271-2	C <sub>224</sub> H <sub>450</sub>	2953.2908
2,2,4,6,6-Pentamethyltriacontane	68-272-0	C <sub>226</sub> H <sub>454</sub>	2979.4408
2,2,4,6,6-Pentamethyltriacontane	68-272-8	C <sub>228</sub> H <sub>458</sub>	3005.5908
2,2,4,6,6-Pentamethyltriacontane	68-273-6	C <sub>230</sub> H <sub>462</sub>	3031.7408
2,2,4,6,6-Pentamethyltriacontane	68-274-4	C <sub>232</sub> H <sub>466</sub>	3057.8908
2,2,4,6,6-Pentamethyltriacontane	68-275-2	C <sub>234</sub> H <sub>470</sub>	3084.0408
2,2,4,6,6-Pentamethyltriacontane	68-276-0	C <sub>236</sub> H <sub>474</sub>	3110.1908
2,2,4,6,6-Pentamethyltriacontane	68-276-8	C <sub>238</sub> H <sub>478</sub>	3136.3408
2,2,4,6,6-Pentamethyltriacontane	68-277-6	C <sub>240</sub> H <sub>482</sub>	3162.4908
2,2,4,6,6-Pentamethyltriacontane	68-278-4	C <sub>242</sub> H <sub>486</sub>	3188.6408
2,2,4,6,6-Pentamethyltriacontane	68-279-2	C <sub>244</sub> H <sub>490</sub>	3214.7908
2,2,4,6,6-Pentamethyltriacontane	68-280-0	C <sub>246</sub> H <sub>494</sub>	3240.9408
2,2,4,6,6-Pentamethyltriacontane	68-280-8	C <sub>248</sub> H <sub>498</sub>	3267.0908
2,2,4,6,6-Pentamethyltriacontane	68-281-6	C <sub>250</sub> H <sub>502</sub>	3293.2408
2,2,4,6,6-Pentamethyltriacontane	68-282-4	C <sub>252</sub> H <sub>506</sub>	3319.3908
2,2,4,6,6-Pentamethyltriacontane	68-283-2	C <sub>254</sub> H <sub>510</sub>	3345.5408
2,2,4,6,6-Pentamethyltriacontane	68-284-0	C <sub>256</sub> H <sub>514</sub>	3371.6908
2,2,4,6,6-Pentamethyltriacontane	68-284-8	C <sub>258</sub> H <sub>518</sub>	3397.8408
2,2,4,6,6-Pentamethyltriacontane	68-285-6	C <sub>260</sub> H <sub>522</sub>	3423.9908
2,2,4,6,6-Pentamethyltriacontane	68-286-4	C <sub>262</sub> H <sub>526</sub>	3450.1408
2,2,4,6,6-Pentamethyltriacontane	68-287-2	C <sub>264</sub> H <sub>530</sub>	3476.2908
2,2,4,6,6-Pentamethyltriacontane	68-288-0	C <sub>266</sub> H <sub>534</sub>	3502.4408
2,2,4,6,6-Pentamethyltriacontane	68-288-8	C <sub>268</sub> H <sub>538</sub>	3528.5908
2,2,4,6,6-Pentamethyltriacontane	68-289-6	C <sub>270</sub> H <sub>542</sub>	3554.7408
2,2,4,6,6-Pentamethyltriacontane	68-290-4	C <sub>272</sub> H <sub>546</sub>	3580.8908
2,2,4,6,6-Pentamethyltriacontane	68-291-2	C <sub>274</sub> H <sub>550</sub>	3607.0408
2,2,4,6,6-Pentamethyltriacontane	68-292-0	C <sub>276</sub> H <sub>554</sub>	3633.1908
2,2,4,6,6-Pentamethyltriacontane	68-292-8	C <sub>278</sub> H <sub>558</sub>	3659.3408
2,2,4,6,6-Pentamethyltriacontane	68-293-6	C <sub>280</sub> H <sub>562</sub>	3685.4908
2,2,4,6,6-Pentamethyltriacontane	68-294-4	C <sub>282</sub> H <sub>566</sub>	3711.6408
2,2,4,6,6-Pentamethyltriacontane	68-295-2	C <sub>284</sub> H <sub>570</sub>	3737.7908
2,2,4,6,6-Pentamethyltriacontane	68-296-0	C <sub>286</sub> H <sub>574</sub>	3763.9408
2,2,4,6,6-Pentamethyltriacontane	68-296-8	C <sub>288</sub> H <sub>578</sub>	3790.0908
2,2,4,6,6-Pentamethyltriacontane	68-297-6		