

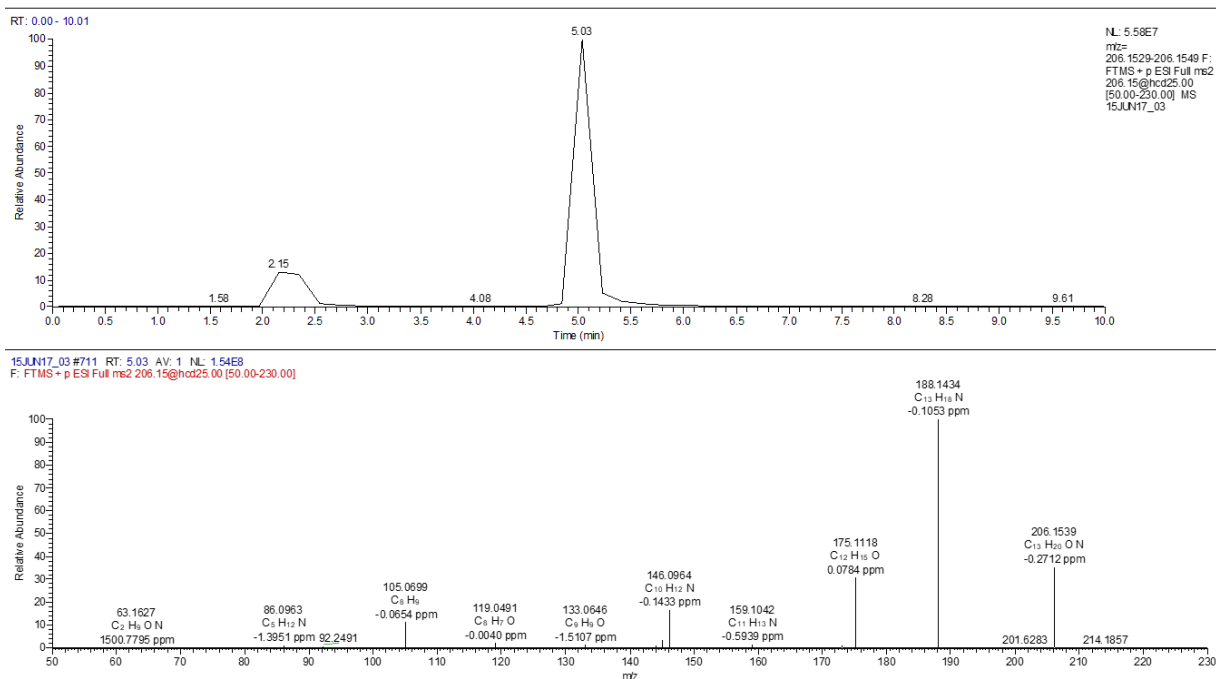
# In Vitro Metabolic Study of Four Synthetic Cathinones: 4-MPD, 2-NMC, 4F-PHP and bk-EPDP

Ivana Gavrilović<sup>1</sup>, Yunita Gelu<sup>2</sup> and Vincenzo Abbate<sup>2,\*</sup>

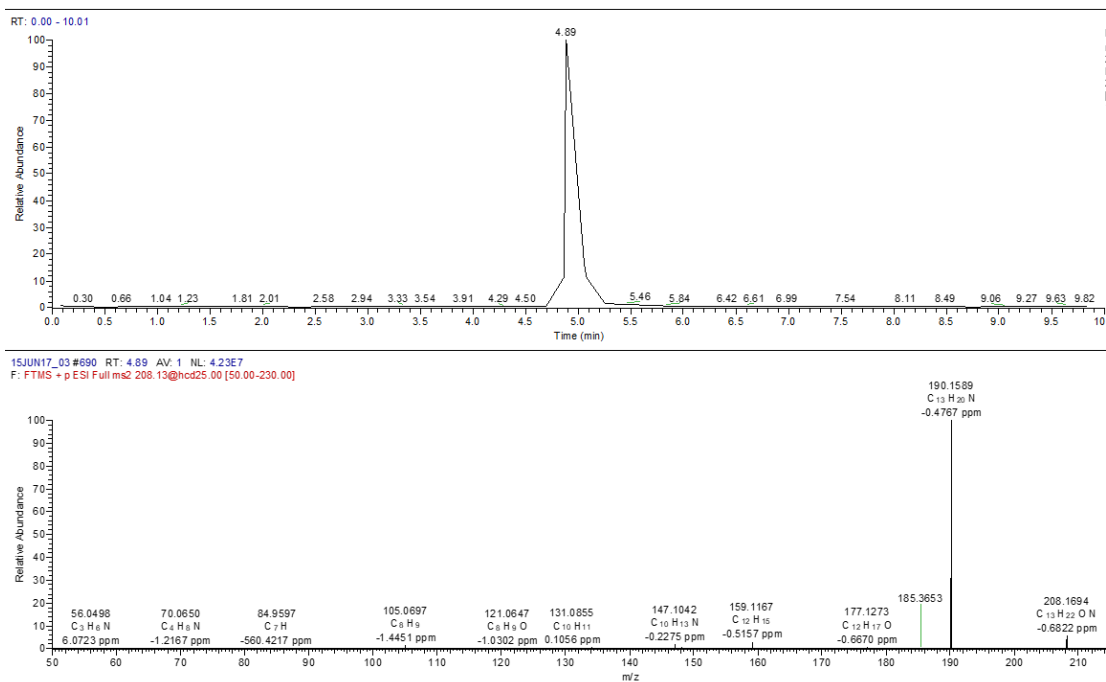
<sup>1</sup> Drug Control Centre, King's College London, Franklin Wilkins Building, 150 Stamford Street, London SE1 9NH, UK; ivana.gavrilovic@kcl.ac.uk

<sup>2</sup> Department of Analytical, Environmental and Forensic Sciences, King's College London, 150 Stamford Street, London SE1 9NH, UK; yunita.gelu@kcl.ac.uk

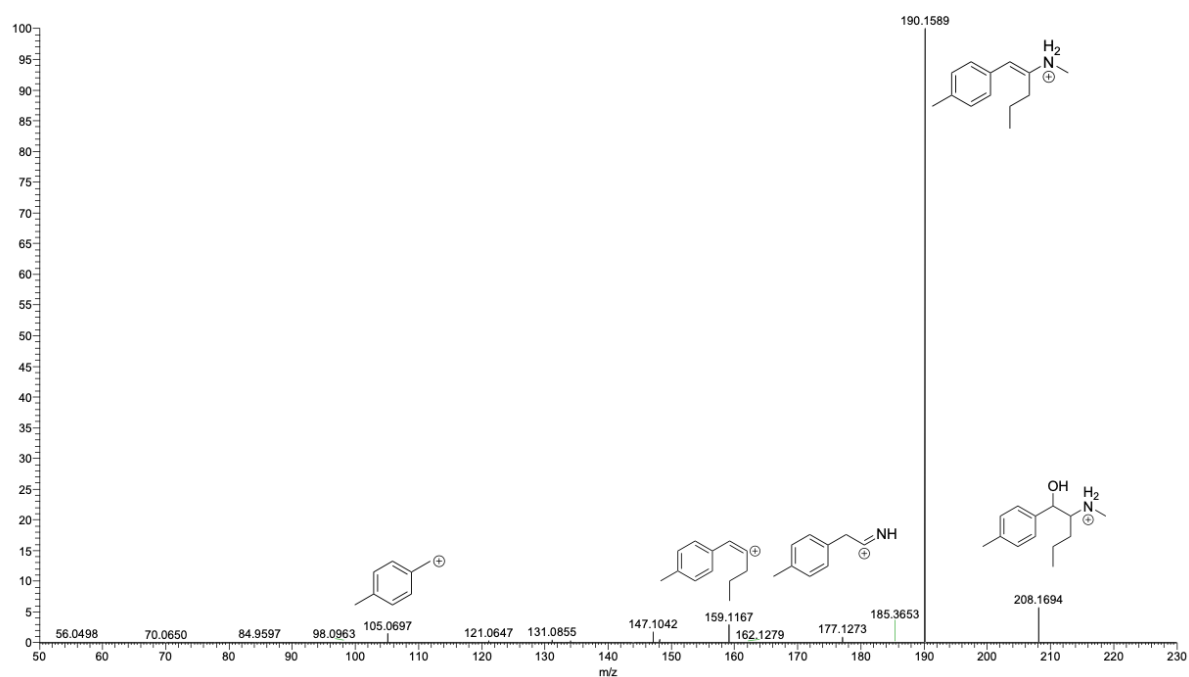
\* Correspondence: vincenzo.abbate@kcl.ac.uk; Tel.: +44-(0)207-83895



**Figure S1:** Extracted ion chromatogram and MS<sup>2</sup> spectra of unmetabolized 4-MPD (proposed fragment ion structures were reported by Apirakkan et al doi:10.1002/dta.2218).



**Figure S2:** Extracted ion chromatogram and MS<sup>2</sup> spectra of 4-MPD M1.



**Figure S3:** 4-MPD M1 proposed fragmentation pattern.

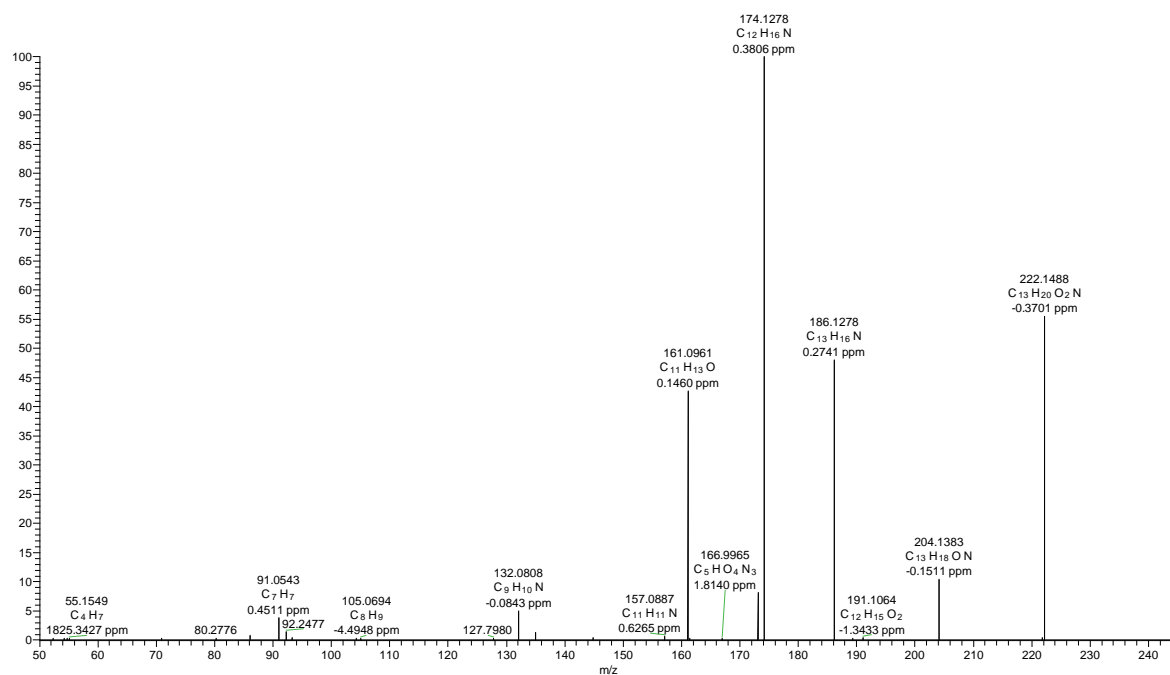


Figure S4: 4-MPD M2 MS<sup>2</sup> spectra.

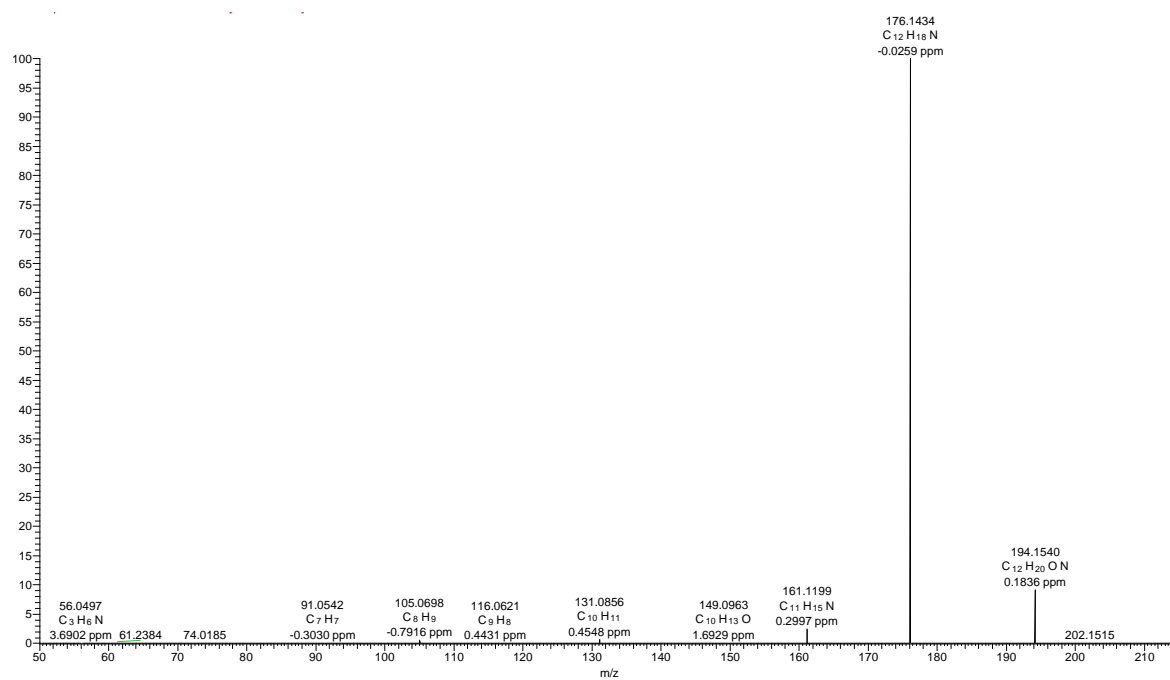
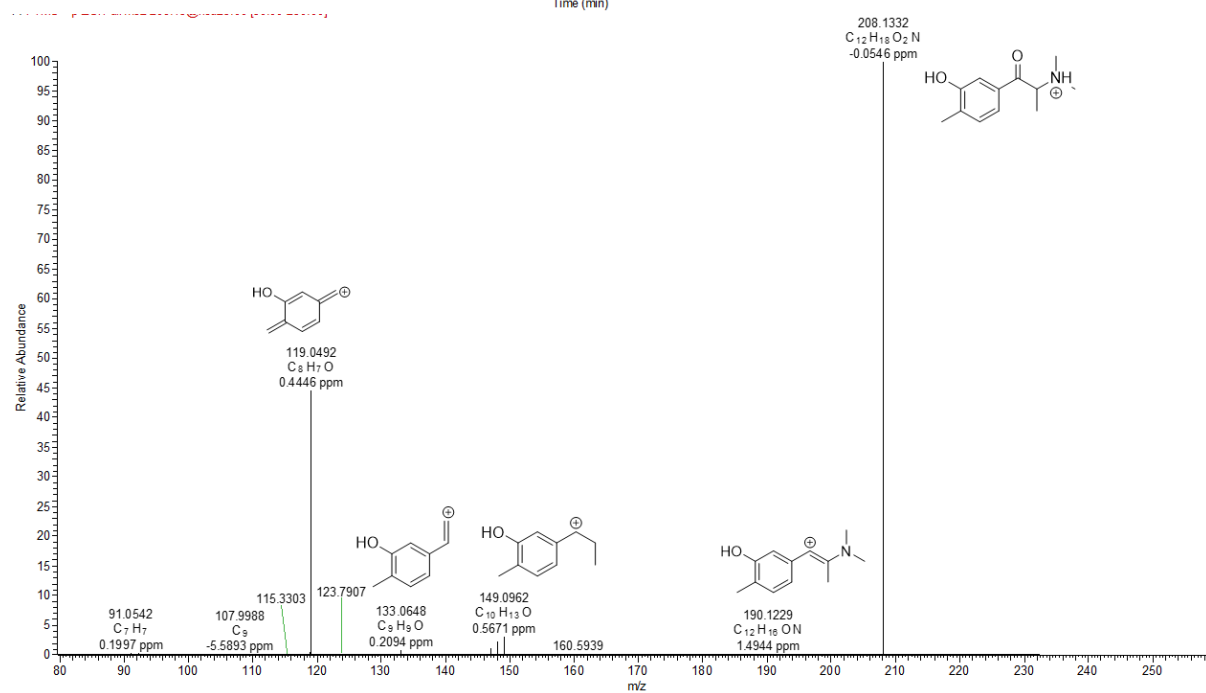
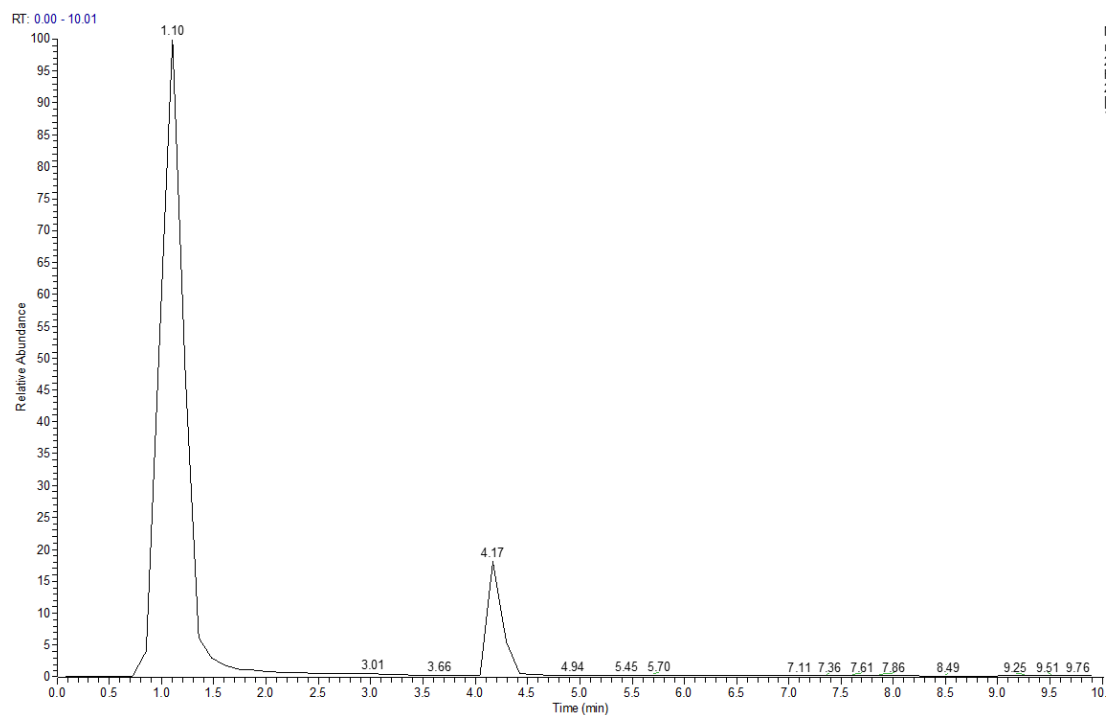
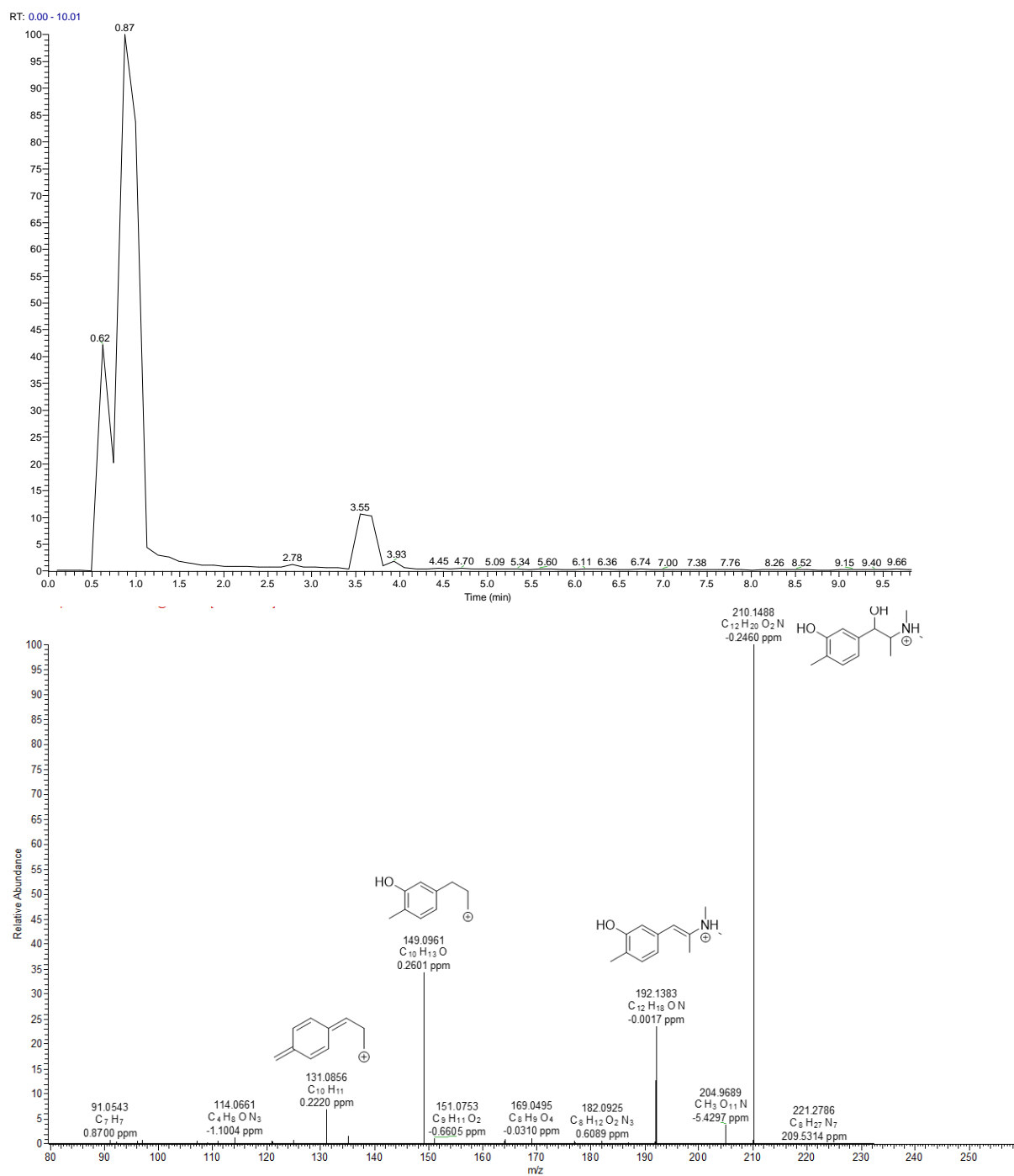


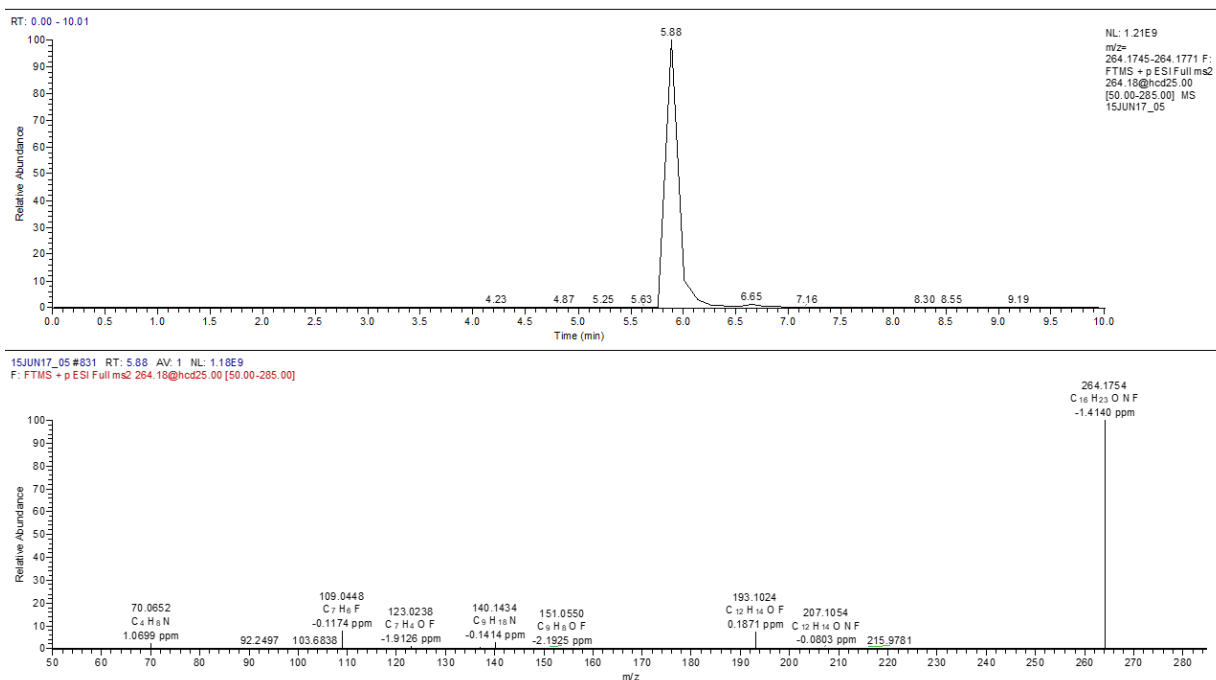
Figure S5: 2-NMC M6 MS<sup>2</sup> spectra.



**Figure S6:** 2-NMC M7 extracted ion chromatogram (Rt = 4.17 min) and MS<sup>2</sup> spectra with proposed fragmentation pattern.



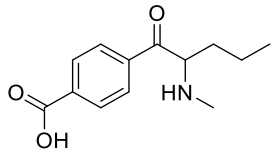
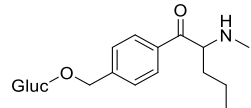
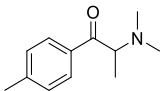
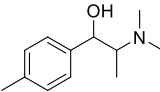
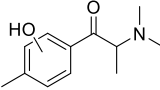
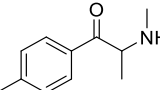
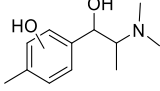
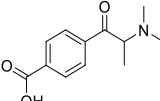
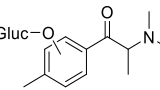
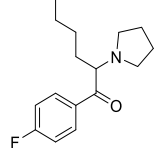
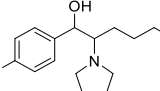
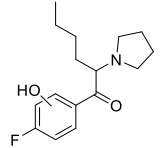
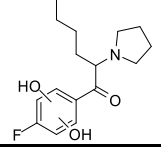
**Figure S7:** 2-NMC M9 extracted ion chromatogram ( $R_t = 3.55$  min) and  $MS^2$  spectra with proposed fragmentation pattern.

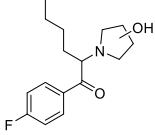
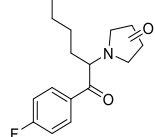
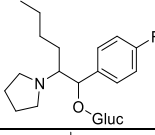
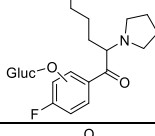
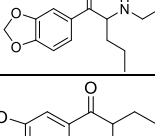
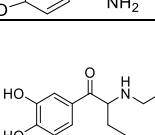
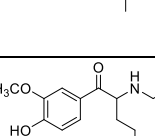
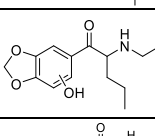
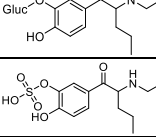




**Figure S8:** Extracted ion chromatogram and MS<sup>2</sup> spectra of unmetabolized 4F-PHP (proposed fragment ion structures were reported by Apirakkan et al doi:10.1002/dta.2218).

**Table S1:** Detected phase I and phase II metabolites for 4-MPD, 2-NMC, 4F-PHP and bk-EPDP including summarised diagnostic product ions as discussed in the paper.

Compound	Proposed structure	Chemical formula	Exact mass [M+H] <sup>+</sup>	Diagnostic product ions (m/z) with proposed chemical formula	Rt (min)
4-MPD		C <sub>13</sub> H <sub>19</sub> NO	206.1539	206.1539, C <sub>13</sub> H <sub>20</sub> NO, 188.1434, C <sub>13</sub> H <sub>18</sub> N 175.1118, C <sub>12</sub> H <sub>15</sub> O 146.0964, C <sub>10</sub> H <sub>12</sub> N 133.0646, C <sub>9</sub> H <sub>9</sub> O 105.0699, C <sub>8</sub> H <sub>9</sub>	5.03
M1		C <sub>13</sub> H <sub>21</sub> NO	208.1696	208.1694, C <sub>13</sub> H <sub>22</sub> NO 190.1589, C <sub>13</sub> H <sub>20</sub> N 177.1273, C <sub>12</sub> H <sub>17</sub> O 105.0697, C <sub>8</sub> H <sub>9</sub>	4.89
M2 (a)		C <sub>13</sub> H <sub>19</sub> NO <sub>2</sub>	222.1489	222.1488, C <sub>13</sub> H <sub>20</sub> NO <sub>2</sub> 204.1383, C <sub>13</sub> H <sub>18</sub> NO 186.1278, C <sub>13</sub> H <sub>16</sub> N 174.1278, C <sub>12</sub> H <sub>13</sub> N	2.62
M3		C <sub>12</sub> H <sub>17</sub> NO	192.1383	192.1383, C <sub>12</sub> H <sub>18</sub> NO 174.1278, C <sub>12</sub> H <sub>16</sub> N 119.0492, C <sub>8</sub> H <sub>7</sub> O 105.0699, C <sub>8</sub> H <sub>9</sub>	4.80

M4		$C_{13}H_{17}NO_3$	236.1281	236.1279, $C_{13}H_{18}NO_3$ 218.1171, $C_{13}H_{16}NO_2$ 200.1068, $C_{13}H_{14}NO$ 174.1275, $C_{12}H_{16}N$	2.44
M5		$C_{19}H_{27}NO_8$	398.1809	398.1806, $C_{19}H_{28}NO_8$ 222.1488, $C_{13}H_{20}NO_2$	2.24
2-NMC		$C_{12}H_{17}NO$	192.1383	192.1388, $C_{12}H_{18}NO$ 147.0804, $C_{10}H_{11}O$ 119.0855, $C_9H_{11}$	3.49
M6 (a)		$C_{12}H_{19}NO$	194.1539	194.1540, $C_{12}H_{20}NO$ 176.1434, $C_{12}H_{18}N$ 161.1199, $C_{11}H_{15}N$ 131.0856, $C_{10}H_{11}$ 105.0698, $C_8H_9$ 91.0542, $C_7H_7$	3.38
M7		$C_{12}H_{17}NO_2$	208.1332	208.1332, $C_{12}H_{18}NO_2$ 190.1229, $C_{12}H_{16}NO$ 149.0962, $C_{10}H_{13}O$ 133.0648, $C_9H_9O$ 119.0492, $C_8H_7O$	4.17
M8		$C_{11}H_{15}NO$	178.1226	178.1226, $C_{11}H_{16}NO$ 160.1121, $C_{11}H_{14}N$ 145.0886, $C_{10}H_{11}N$	3.34
M9		$C_{12}H_{19}NO_2$	210.1489	210.1488, $C_{12}H_{20}NO_2$ 192.1383, $C_{12}H_{18}NO$ 149.0961, $C_{10}H_{13}O$ 131.0856, $C_{10}H_{11}$	3.55
M10 (b)		$C_{12}H_{15}NO_3$	222.1125	222.1126, $C_{12}H_{16}NO_3$	1.13
M11		$C_{18}H_{25}NO_8$	384.1653	384.1645, $C_{18}H_{26}NO_8$ 208.1330, $C_{12}H_{18}NO_2$	1.03
4F-PHP		$C_{16}H_{22}FNO$	264.1758	264.1754, $C_{16}H_{23}FNO$ 193.1024, $C_{12}H_{14}FO$ 109.0448, $C_7H_6F$	5.88
M12 (a)		$C_{16}H_{24}FNO$	266.1915	266.1911, $C_{16}H_{25}FNO$ 248.1806, $C_{16}H_{23}FN$	6.42
M13		$C_{16}H_{22}FNO_2$	280.1707	280.1703, $C_{16}H_{23}FNO_2$ 123.0239, $C_7H_4FO$	3.39 3.59
M14		$C_{16}H_{22}FNO_3$	296.1656	296.1652, $C_{16}H_{23}FNO_3$	5.94

M15		$C_{16}H_{22}FNO_2$	280.1707	280.1703, $C_{16}H_{23}FNO_2$ 156.1383, $C_9H_{18}NO$	5.31
M16		$C_{16}H_{20}FNO_2$	278.1551	278.1548, $C_{16}H_{21}FNO_2$ 154.1224, $C_9H_{16}NO$	5.77
M17		$C_{22}H_{32}FNO_7$	442.2236	442.2234, $C_{22}H_{33}FNO_7$	5.52
M18		$C_{22}H_{30}FNO_8$	456.2028	456.2025, $C_{22}H_{31}FNO_8$	4.67 4.80
<b>bk-EPDP</b>		$C_{14}H_{19}NO_3$	250.1438	250.1435, $C_{14}H_{20}NO_3$ 232.1330, $C_{14}H_{18}NO_2$	4.38
M19		$C_{12}H_{15}NO_3$	222.1125	222.1124, $C_{12}H_{16}NO_3$ 174.0913, $C_{11}H_{12}NO$	3.95
M20 (a)		$C_{13}H_{19}NO_3$	238.1438	238.1435, $C_{13}H_{20}NO_3$ 220.1330, $C_{13}H_{18}NO_2$ 202.1226, $C_{13}H_{16}NO$ 193.0859, $C_{11}H_{13}O_3$ 123.0440, $C_7H_7O_2$	2.48
M21		$C_{14}H_{21}NO_3$	252.1594	252.1592, $C_{14}H_{22}NO_3$	2.69 4.23
M22		$C_{14}H_{19}NO_4$	266.1387	266.1384, $C_{14}H_{20}NO_4$	3.05 5.27
M23		$C_{19}H_{27}NO_9$	414.1759	414.1754, $C_{19}H_{28}NO_9$	2.06
M24 (b)		$C_{13}H_{19}NO_6S$	318.1006	318.0997, $C_{13}H_{20}NO_6S$	2.48