

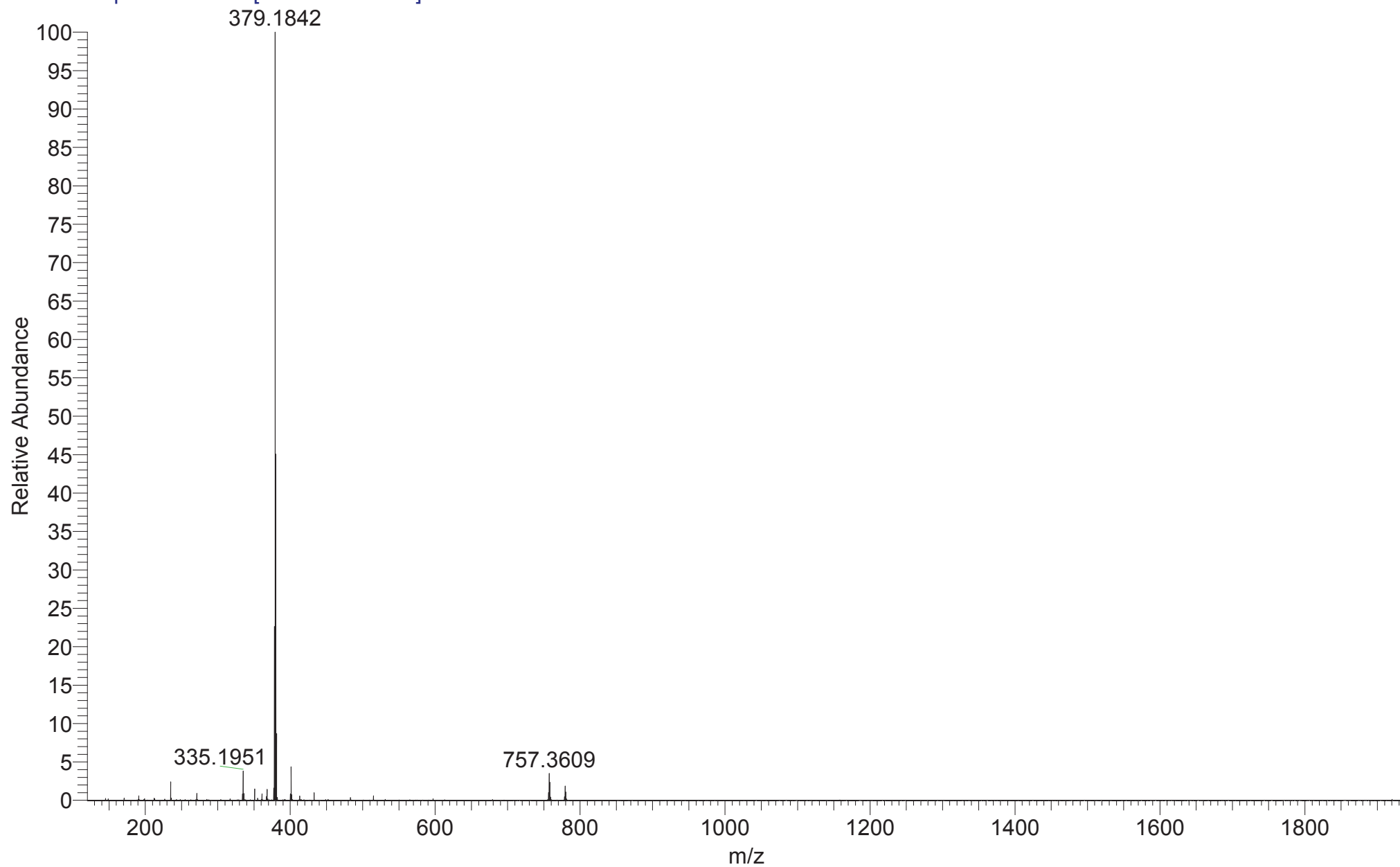
O:\IMPBUL_TWUKA_50443
(DCM)/MeOH + NH₄OAc
DAN3-326

EPSRC UK National MS Facility
LTQ Orbitrap XL

C22H18D3N3O3
28/11/2018 07:27:22

IMPBUL_TWUKA_50443 #38-54 RT: 0.66-1.04 AV: 16 SM: 7G NL: 4.75E7

T: FTMS + p NSI Full ms [120.00-1935.00]

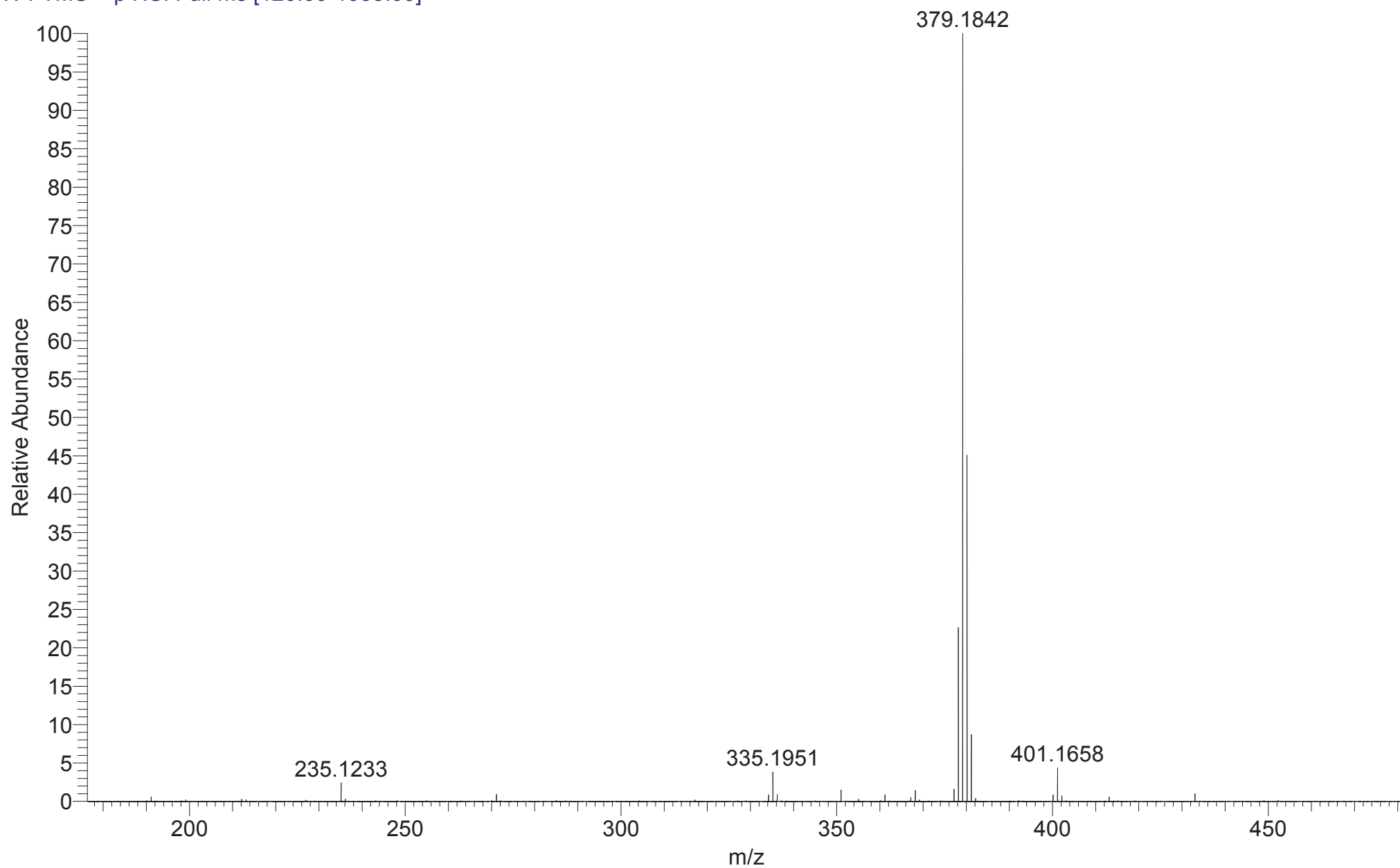


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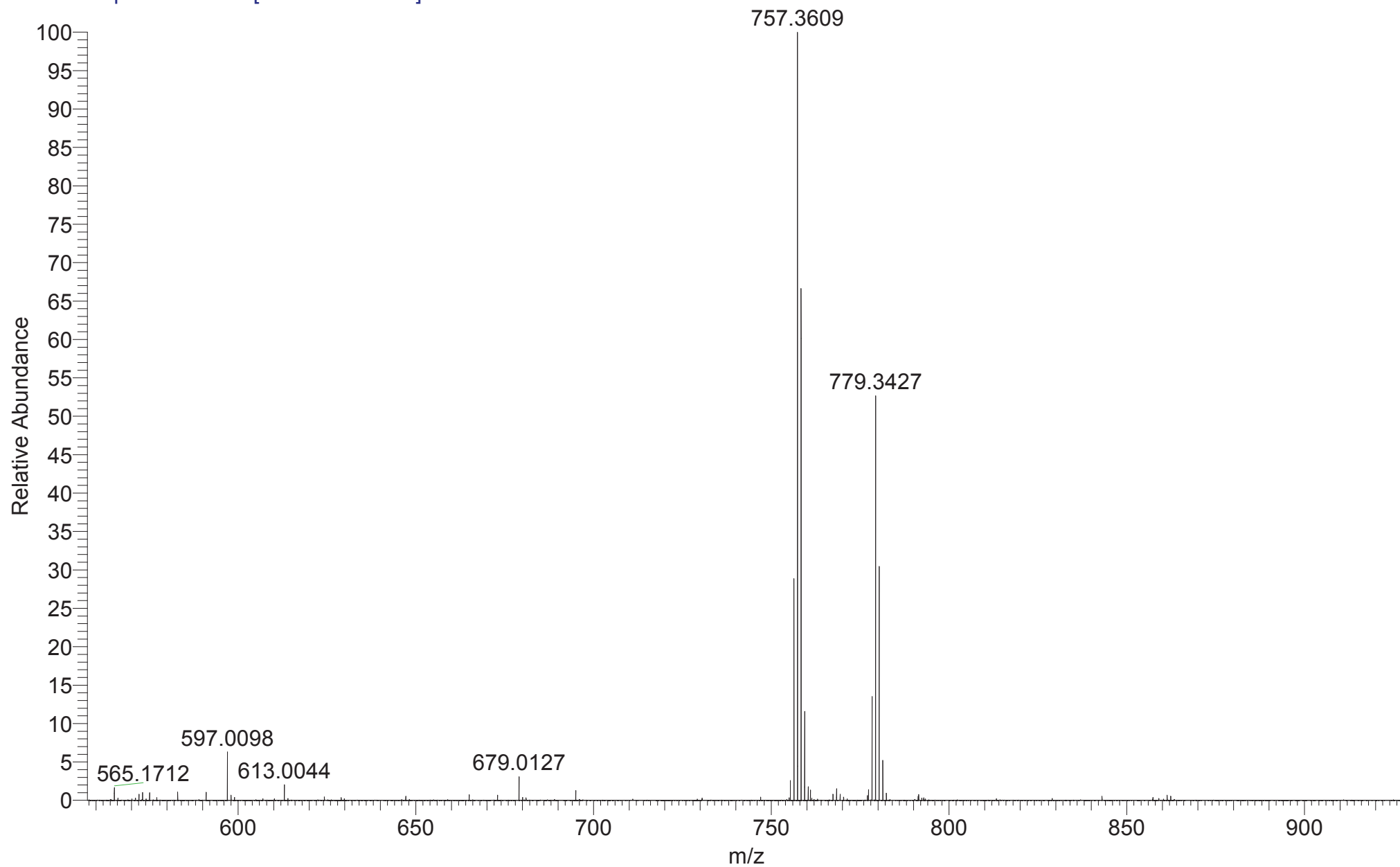
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DAN3-326

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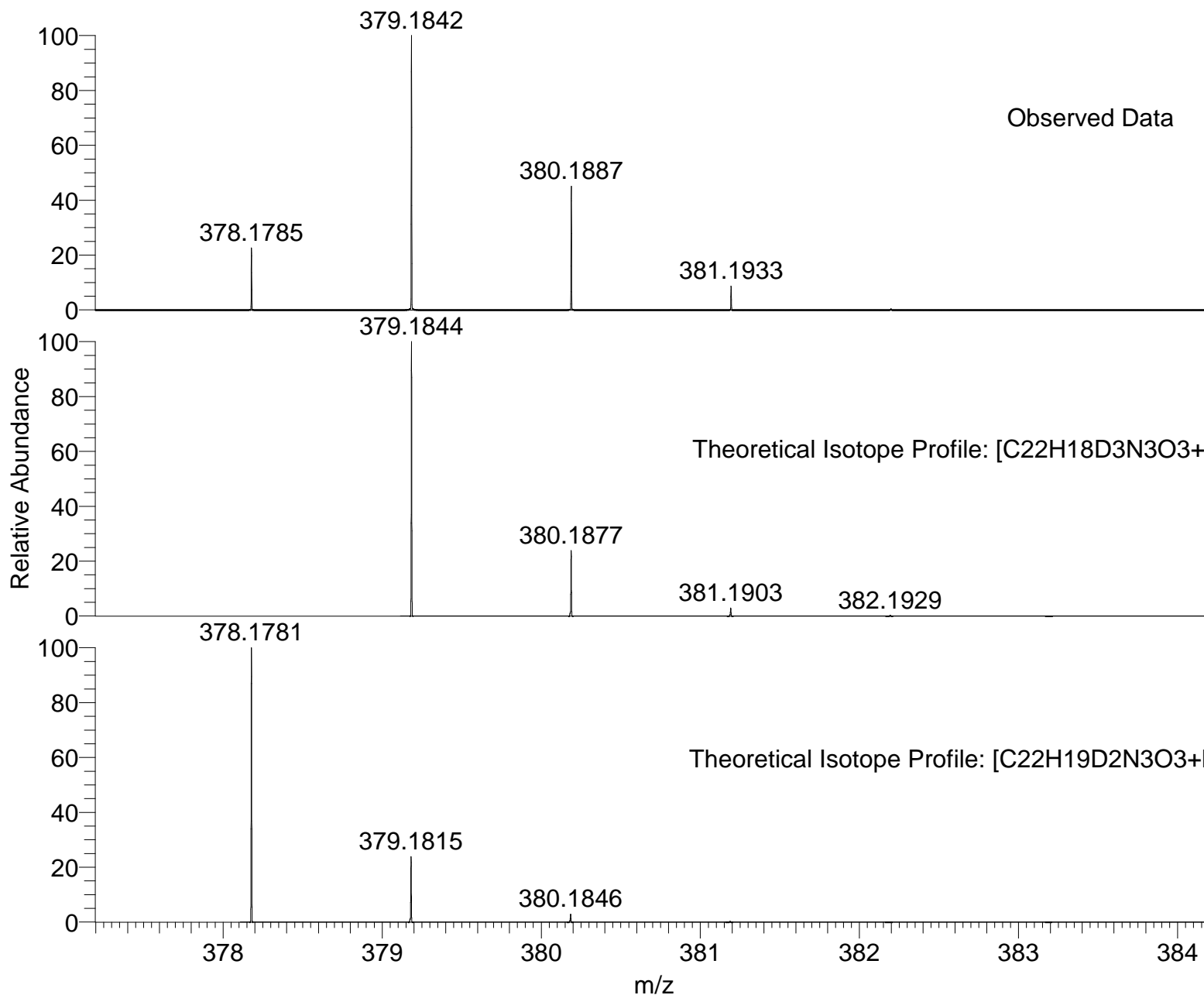
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28/11/2018 07:27:22

IMPBUL_TWUKA_50443 #38-54 RT: 0.66-1.04 AV: 16 SM: 7G NL: 1.67E6

T: FTMS + p NSI Full ms [120.00-1935.00]



SM: 7G



NL:
4.75E7
IMPBUL_TWUKA_50443#38-
54 RT: 0.66-1.04 AV: 16 T:
FTMS + p NSI Full ms
[120.00-1935.00]

NL:
1.81E4
C₂₂H₁₈D₃N₃O₃H:
C₂₂H₁₉D₃N₃O₃
p (gss, s /p:40) Chrg 1
R: 100000 Res .Pwr . @FWHM

NL:
1.81E4
C₂₂H₁₉D₂N₃O₃H:
C₂₂H₂₀D₂N₃O₃
p (gss, s /p:40) Chrg 1
R: 100000 Res .Pwr . @FWHM

Isotope: Min. .. Max.
 14 N 0....15
 16 O 0....20
 12 C 0....80
 1 H 0....100
 23 Na 0....0
 2 H 0....6
 Tolerance Window: +- 5.00 ppm
 Db/Ring Equiv: -10.. 500
 Fits: 300

N-Rule: Do not use
 Charge: 1

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
378.1785	378.1785	-0.1	13.5	C ₁₈ H ₂₀ O ₁ N ₉
	378.1785	-0.1	8.0	C ₁₉ H ₂₆ O ₆ N ₂
	378.1784	0.2	1.0	C ₁₀ H ₂₂ ² H ₃ O ₁₀ N ₅
	378.1784	0.2	6.5	C ₉ H ₁₆ ² H ₃ O ₅ N ₁₂
	378.1786	-0.3	6.5	C ₇ H ₁₆ ² H ₂ O ₄ N ₁₅
	378.1786	-0.3	1.0	C ₈ H ₂₂ ² H ₂ O ₉ N ₈
	378.1786	-0.4	-4.5	C ₉ H ₂₈ ² H ₂ O ₁₄ N ₁
	378.1783	0.5	13.5	C ₂₀ H ₂₀ ² H ₁ O ₂ N ₆
	378.1783	0.5	-6.0	C ₁ H ₁₈ ² H ₆ O ₁₄ N ₈
	378.1783	0.5	-0.5	H ₁₂ ² H ₆ O ₉ N ₁₅
	378.1782	0.7	1.0	C ₁₂ H ₂₂ ² H ₄ O ₁₁ N ₂
	378.1782	0.8	6.5	C ₁₁ H ₁₆ ² H ₄ O ₆ N ₉
	378.1788	-0.9	1.0	C ₆ H ₂₂ ² H ₁ O ₈ N ₁₁
	378.1788	-0.9	-4.5	C ₇ H ₂₈ ² H ₁ O ₁₃ N ₄
	378.1781	1.0	13.5	C ₂₂ H ₂₀ ² H ₂ O ₃ N ₃
	378.1780	1.3	6.5	C ₁₃ H ₁₆ ² H ₅ O ₇ N ₆
	378.1780	1.3	12.0	C ₁₂ H ₁₀ ² H ₅ O ₂ N ₁₃
	378.1790	-1.4	1.0	C ₄ H ₂₂ O ₇ N ₁₄
	378.1790	-1.4	-4.5	C ₅ H ₂₈ O ₁₂ N ₇
	378.1790	-1.4	18.5	C ₂₇ H ₁₆ ² H ₄ O ₁ N ₁
	378.1791	-1.5	-10.0	C ₆ H ₃₄ O ₁₇
	378.1779	1.5	13.5	C ₂₄ H ₂₀ ² H ₃ O ₄
	378.1791	-1.7	11.5	C ₁₆ H ₁₂ ² H ₆ O ₄ N ₇
	378.1791	-1.7	6.0	C ₁₇ H ₁₈ ² H ₆ O ₉
	378.1778	1.8	6.5	C ₁₅ H ₁₆ ² H ₆ O ₈ N ₃
	378.1778	1.9	12.0	C ₁₄ H ₁₀ ² H ₆ O ₃ N ₁₀
	378.1793	-2.0	18.5	C ₂₅ H ₁₆ ² H ₃ N ₄
	378.1777	2.1	-9.5	C ₄ H ₃₂ O ₁₆ N ₃
	378.1777	2.1	19.0	C ₂₅ H ₁₄ ² H ₄ N ₄
	378.1777	2.1	-4.0	C ₃ H ₂₆ O ₁₁ N ₁₀
	378.1793	-2.2	11.5	C ₁₄ H ₁₂ ² H ₅ O ₃ N ₁₀

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
	378.1793	-2.2	6.0	C ₁₅ H ₁₈ ² H ₅ O ₈ N ₃
	378.1795	-2.5	13.0	C ₂₄ H ₂₂ ² H ₂ O ₄
	378.1775	2.6	-9.5	C ₆ H ₃₂ ² H ₁ O ₁₇
	378.1775	2.6	19.0	C ₂₇ H ₁₄ ² H ₅ O ₁ N ₁
	378.1775	2.7	-4.0	C ₅ H ₂₆ ² H ₁ O ₁₂ N ₇
	378.1775	2.7	1.5	C ₄ H ₂₀ ² H ₁ O ₇ N ₁₄
	378.1796	-2.8	11.5	C ₁₂ H ₁₂ ² H ₄ O ₂ N ₁₃
	378.1796	-2.8	6.0	C ₁₃ H ₁₈ ² H ₄ O ₇ N ₆
	378.1796	-3.0	-1.0	C ₂ H ₁₄ ² H ₆ O ₁₀ N ₁₂
	378.1797	-3.0	-6.5	C ₃ H ₂₀ ² H ₆ O ₁₅ N ₅
	378.1797	-3.1	13.0	C ₂₂ H ₂₂ ² H ₁ O ₃ N ₃
	378.1773	3.2	-4.0	C ₇ H ₂₆ ² H ₂ O ₁₃ N ₄
	378.1773	3.2	1.5	C ₆ H ₂₀ ² H ₂ O ₈ N ₁₁
	378.1798	-3.3	6.0	C ₁₁ H ₁₈ ² H ₃ O ₆ N ₉
	378.1798	-3.3	0.5	C ₁₂ H ₂₄ ² H ₃ O ₁₁ N ₂
	378.1772	3.4	8.5	C ₁₇ H ₂₄ O ₅ N ₅
	378.1772	3.5	14.0	C ₁₆ H ₁₈ N ₁₂
	378.1799	-3.6	-1.0	H ₁₄ ² H ₅ O ₉ N ₁₅
	378.1799	-3.6	-6.5	C ₁ H ₂₀ ² H ₅ O ₁₄ N ₈
	378.1799	-3.6	13.0	C ₂₀ H ₂₂ O ₂ N ₆
	378.1771	3.7	-4.0	C ₉ H ₂₆ ² H ₃ O ₁₄ N ₁
	378.1771	3.8	1.5	C ₈ H ₂₀ ² H ₃ O ₉ N ₈
	378.1771	3.8	7.0	C ₇ H ₁₄ ² H ₃ O ₄ N ₁₅
	378.1800	-3.9	6.0	C ₉ H ₁₈ ² H ₂ O ₅ N ₁₂
	378.1800	-3.9	0.5	C ₁₀ H ₂₄ ² H ₂ O ₁₀ N ₅
	378.1770	4.0	8.5	C ₁₉ H ₂₄ ² H ₁ O ₆ N ₂
	378.1770	4.0	14.0	C ₁₈ H ₁₈ ² H ₁ O ₁ N ₉
	378.1769	4.3	1.5	C ₁₀ H ₂₀ ² H ₄ O ₁₀ N ₅
	378.1769	4.3	7.0	C ₉ H ₁₄ ² H ₄ O ₅ N ₁₂
	378.1802	-4.4	6.0	C ₇ H ₁₈ ² H ₁ O ₄ N ₁₅
	378.1802	-4.4	0.5	C ₈ H ₂₄ ² H ₁ O ₉ N ₈
	378.1802	-4.4	-5.0	C ₉ H ₃₀ ² H ₁ O ₁₄ N ₁
	378.1768	4.6	14.0	C ₂₀ H ₁₈ ² H ₂ O ₂ N ₆
	378.1767	4.8	1.5	C ₁₂ H ₂₀ ² H ₅ O ₁₁ N ₂
	378.1767	4.9	7.0	C ₁₁ H ₁₄ ² H ₅ O ₆ N ₉
	378.1804	-5.0	0.5	C ₆ H ₂₄ O ₈ N ₁₁
	378.1804	-5.0	-5.0	C ₇ H ₃₀ O ₁₃ N ₄
379.1842	379.1842	0.0	13.5	C ₂₄ H ₁₉ ² H ₄ O ₄
	379.1842	0.0	-9.5	C ₂ H ₃₁ O ₁₅ N ₆
	379.1842	0.0	-4.0	C ₁ H ₂₅ O ₁₀ N ₁₃
	379.1843	-0.2	12.0	C ₁₂ H ₉ ² H ₆ O ₂ N ₁₃
	379.1843	-0.2	6.5	C ₁₃ H ₁₅ ² H ₆ O ₇ N ₆
	379.1844	-0.5	13.5	C ₂₂ H ₁₉ ² H ₃ O ₃ N ₃

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
379.1840	379.1840	0.6	-9.5	C ₄ H ₃₁ ² H ₁ O ₁₆ N ₃
379.1840	379.1840	0.6	19.0	C ₂₅ H ₁₃ ² H ₅ N ₄
379.1840	379.1840	0.6	-4.0	C ₃ H ₂₅ ² H ₁ O ₁₁ N ₁₀
379.1845	379.1845	-0.8	6.5	C ₁₁ H ₁₅ ² H ₅ O ₆ N ₉
379.1845	379.1845	-0.8	1.0	C ₁₂ H ₂₁ ² H ₅ O ₁₁ N ₂
379.1846	379.1846	-1.1	13.5	C ₂₀ H ₁₉ ² H ₂ O ₂ N ₆
379.1838	379.1838	1.1	-9.5	C ₆ H ₃₁ ² H ₂ O ₁₇
379.1838	379.1838	1.1	19.0	C ₂₇ H ₁₃ ² H ₆ O ₁ N ₁
379.1838	379.1838	1.1	-4.0	C ₅ H ₂₅ ² H ₂ O ₁₂ N ₇
379.1838	379.1838	1.1	1.5	C ₄ H ₁₉ ² H ₂ O ₇ N ₁₄
379.1847	379.1847	-1.3	6.5	C ₉ H ₁₅ ² H ₄ O ₅ N ₁₂
379.1847	379.1847	-1.3	1.0	C ₁₀ H ₂₁ ² H ₄ O ₁₀ N ₅
379.1837	379.1837	1.4	3.0	C ₁₆ H ₂₉ O ₉ N ₁
379.1837	379.1837	1.4	8.5	C ₁₅ H ₂₃ O ₄ N ₈
379.1848	379.1848	-1.6	13.5	C ₁₈ H ₁₉ ² H ₁ O ₁ N ₉
379.1848	379.1848	-1.6	8.0	C ₁₉ H ₂₅ ² H ₁ O ₆ N ₂
379.1836	379.1836	1.7	-4.0	C ₇ H ₂₅ ² H ₃ O ₁₃ N ₄
379.1836	379.1836	1.7	1.5	C ₆ H ₁₉ ² H ₃ O ₈ N ₁₁
379.1849	379.1849	-1.8	6.5	C ₇ H ₁₅ ² H ₃ O ₄ N ₁₅
379.1849	379.1849	-1.9	1.0	C ₈ H ₂₁ ² H ₃ O ₉ N ₈
379.1849	379.1849	-1.9	-4.5	C ₉ H ₂₇ ² H ₃ O ₁₄ N ₁
379.1835	379.1835	1.9	8.5	C ₁₇ H ₂₃ ² H ₁ O ₅ N ₅
379.1835	379.1835	1.9	14.0	C ₁₆ H ₁₇ ² H ₁ N ₁₂
379.1850	379.1850	-2.1	13.5	C ₁₆ H ₁₉ N ₁₂
379.1850	379.1850	-2.2	8.0	C ₁₇ H ₂₅ O ₅ N ₅
379.1834	379.1834	2.2	-4.0	C ₉ H ₂₅ ² H ₄ O ₁₄ N ₁
379.1834	379.1834	2.2	1.5	C ₈ H ₁₉ ² H ₄ O ₉ N ₈
379.1834	379.1834	2.2	7.0	C ₇ H ₁₃ ² H ₄ O ₄ N ₁₅
379.1851	379.1851	-2.4	1.0	C ₆ H ₂₁ ² H ₂ O ₈ N ₁₁
379.1851	379.1851	-2.4	-4.5	C ₇ H ₂₇ ² H ₂ O ₁₃ N ₄
379.1833	379.1833	2.5	8.5	C ₁₉ H ₂₃ ² H ₂ O ₆ N ₂
379.1833	379.1833	2.5	14.0	C ₁₈ H ₁₇ ² H ₂ O ₁ N ₉
379.1832	379.1832	2.8	1.5	C ₁₀ H ₁₉ ² H ₅ O ₁₀ N ₅
379.1831	379.1831	2.8	7.0	C ₉ H ₁₃ ² H ₅ O ₅ N ₁₂
379.1853	379.1853	-2.9	1.0	C ₄ H ₂₁ ² H ₁ O ₇ N ₁₄
379.1853	379.1853	-3.0	-4.5	C ₅ H ₂₇ ² H ₁ O ₁₂ N ₇
379.1853	379.1853	-3.0	18.5	C ₂₇ H ₁₅ ² H ₅ O ₁ N ₁
379.1853	379.1853	-3.0	-10.0	C ₆ H ₃₃ ² H ₁ O ₁₇
379.1831	379.1831	3.0	14.0	C ₂₀ H ₁₇ ² H ₃ O ₂ N ₆
379.1829	379.1829	3.3	1.5	C ₁₂ H ₁₉ ² H ₆ O ₁₁ N ₂
379.1829	379.1829	3.3	7.0	C ₁₁ H ₁₃ ² H ₆ O ₆ N ₉
379.1855	379.1855	-3.5	-4.5	C ₃ H ₂₇ O ₁₁ N ₁₀
379.1855	379.1855	-3.5	18.5	C ₂₅ H ₁₅ ² H ₄ N ₄

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
	379.1855	-3.5	-10.0	C ₄ H ₃₃ O ₁₆ N ₃
	379.1829	3.6	14.0	C ₂₂ H ₁₇ ² H ₄ O ₃ N ₃
	379.1828	3.6	-9.0	H ₂₉ O ₁₄ N ₉
	379.1856	-3.7	11.5	C ₁₄ H ₁₁ ² H ₆ O ₃ N ₁₀
	379.1856	-3.8	6.0	C ₁₅ H ₁₇ ² H ₆ O ₈ N ₃
	379.1857	-4.1	13.0	C ₂₄ H ₂₁ ² H ₃ O ₄
	379.1826	4.1	14.0	C ₂₄ H ₁₇ ² H ₅ O ₄
	379.1826	4.1	-9.0	C ₂ H ₂₉ ² H ₁ O ₁₅ N ₆
	379.1826	4.1	-3.5	C ₁ H ₂₃ ² H ₁ O ₁₀ N ₁₃
	379.1858	-4.3	11.5	C ₁₂ H ₁₁ ² H ₅ O ₂ N ₁₃
	379.1858	-4.3	6.0	C ₁₃ H ₁₇ ² H ₅ O ₇ N ₆
	379.1859	-4.6	13.0	C ₂₂ H ₂₁ ² H ₂ O ₃ N ₃
	379.1824	4.7	-9.0	C ₄ H ₂₉ ² H ₂ O ₁₆ N ₃
	379.1824	4.7	19.5	C ₂₅ H ₁₁ ² H ₆ N ₄
	379.1824	4.7	-3.5	C ₃ H ₂₃ ² H ₂ O ₁₁ N ₁₀
	379.1860	-4.8	6.0	C ₁₁ H ₁₇ ² H ₄ O ₆ N ₉
	379.1860	-4.9	0.5	C ₁₂ H ₂₃ ² H ₄ O ₁₁ N ₂
	379.1823	4.9	3.5	C ₁₄ H ₂₇ O ₈ N ₄
	379.1823	4.9	9.0	C ₁₃ H ₂₁ O ₃ N ₁₁