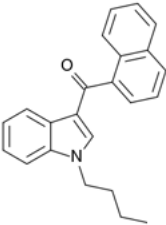
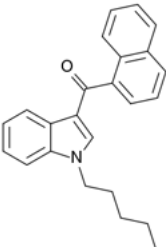
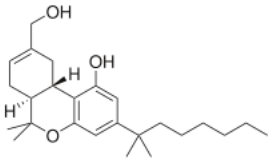
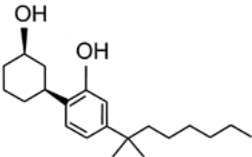


Analysis of Spice and similar herbal smoking mixtures containing cannabinoid receptor agonists by high resolution mass spectrometry.

The following compounds have been detected in "Spice" type "herbal incense" in various European countries or the USA.

JWH-073	JWH-073, 1-butyl-3-(1-naphthoyl) indole is an analgesic drug that acts as a cannabinoid agonist at both the CB1 and CB2 receptors. It probably produces effects very similar to those of THC itself. The JWH prefix stands for John W. Huffman, one of the team that first described these compounds.	
JWH-018	JWH-018, 1-pentyl-3-(1-naphthoyl) indole is an analgesic drug that acts as a cannabinoid agonist at both the CB1 and CB2 receptors. It produces effects in animals very similar to those of THC itself, but with a shorter duration of action. It has been investigated as a potential analgesic..	
HU-210	HU-210 is a synthetic cannabinoid that was synthesised in the late 1980s at the Hebrew University. It is several hundred times more potent than natural THC from cannabis.	
CP47497	CP47-497, 2-[(1R,3S)-3-hydroxycyclohexyl]-5-(2-methyloctan-2-yl)phenol, is a cannabinoid receptor agonist developed by Pfizer with analgesic effects.	

Analytical details

LCMS analysis of methanolic extracts using a ThermoFisher LTQ Orbitrap Discovery interfaced to a ThermoFisher Accela LC system

LC parameters

Column	Phenomenex 100mmx2.0ID 2.5µm HST Luna C18(2)			
Guard Column	Phenomenex Security Guard, C18			
Solvent A	0.1% Acetic acid in water (+ 300µg/litre uradl as a lock mass)			
Solvent C	0.1% Acetic acid in methanol (+ 300µg/litre uracil as a lock mass)			
Solvent D	20mM pH4 acetate buffer in methanol (+ 300µg/litre uracil as a lock mass)			
Injection	10µl, no waste, wash solvent – 50/50 methanol/water			
Autosampler	10°C with a wait time pre run of 1.00 min			
Column Temp.	40°C			
Gradient				
Time (mins)	% Solvent A	% Solvent C	% Solvent D	Flow rate (µl/min)
0	90	10	0	400
1.00	40	60	0	400
3.49	2	98	0	400
3.50	2	23	75	400
4.00	2	23	75	400
4.20	2	23	75	500
4.50	2	23	75	500
4.51	2	98	0	500
4.99	2	98	0	500
5.00	90	10	0	400
5.50	90	10	0	400

Ion Source: Electrospray operating in +ve ion mode. Optimised using m/z 166 ion from ephedrine infusion.

MS conditions – full scan

Duration (minutes)	Scan
0.5-5.5	FTMS Full Scan +ve (m/z 100-550) @ 30,000 resolution, centroid mode. Lock mass enabled – uracil – m/z 113.034550

MS conditions – MS²

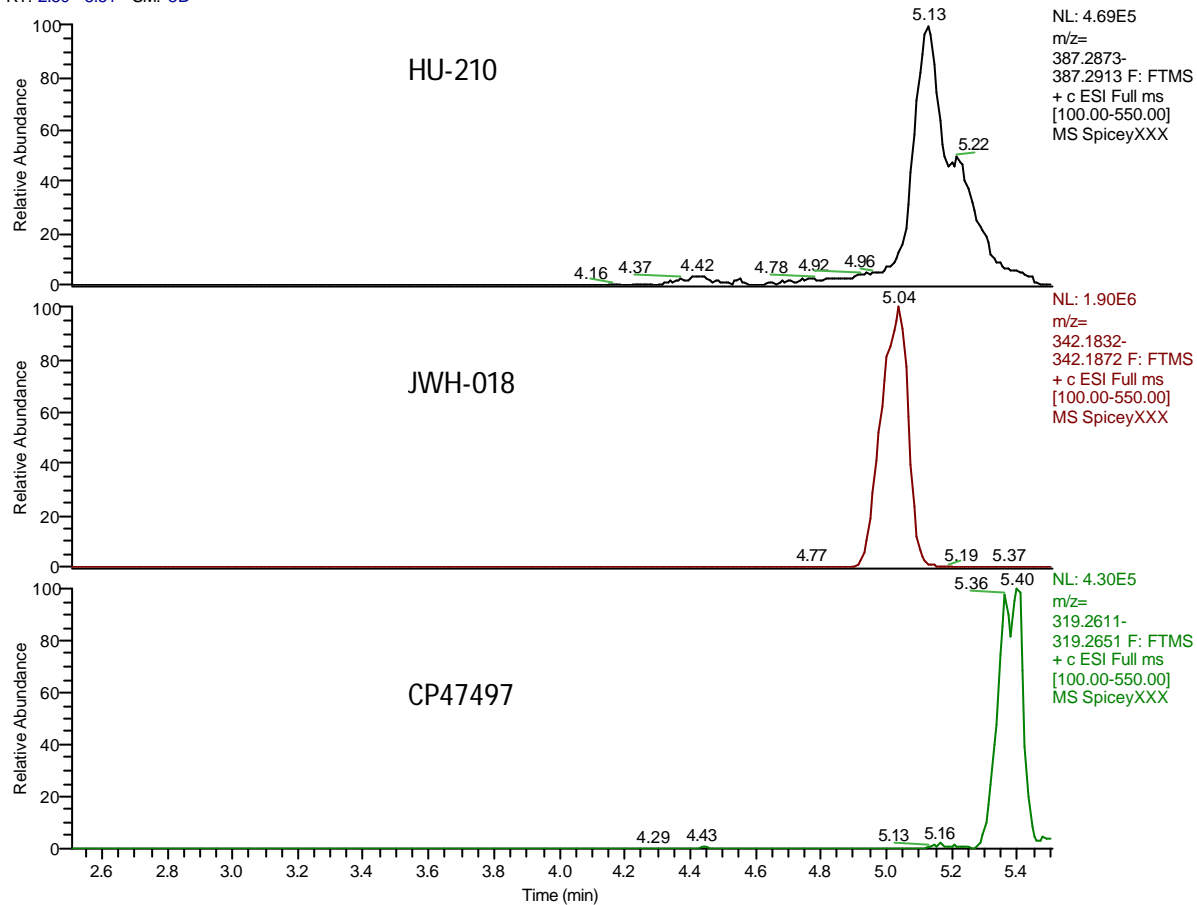
Duration (minutes)	Scan
0.5-5.5	MS ² 387.28, 342.18 and 319.26 all with CID of 35.0 using a 1amu isolation window. Product ions measured using orbitrap operating at 30,000 resolution in centroid mode Lock mass enabled – uracil – m/z 113.034550

Monoisotopic masses of detected compounds

HU-210	C ₂₅ H ₃₈ O ₃	protonated monoisotopic mass:	387.2893
JWH-018	C ₂₄ H ₂₃ NO	protonated monoisotopic mass:	342.1852
CP47497	C ₂₁ H ₃₄ O ₂	protonated monoisotopic mass:	319.2631

Full scan accurate mass ion chromatograms ($\pm 2\text{mmu}$)

RT: 2.50 - 5.51 SM: 3B

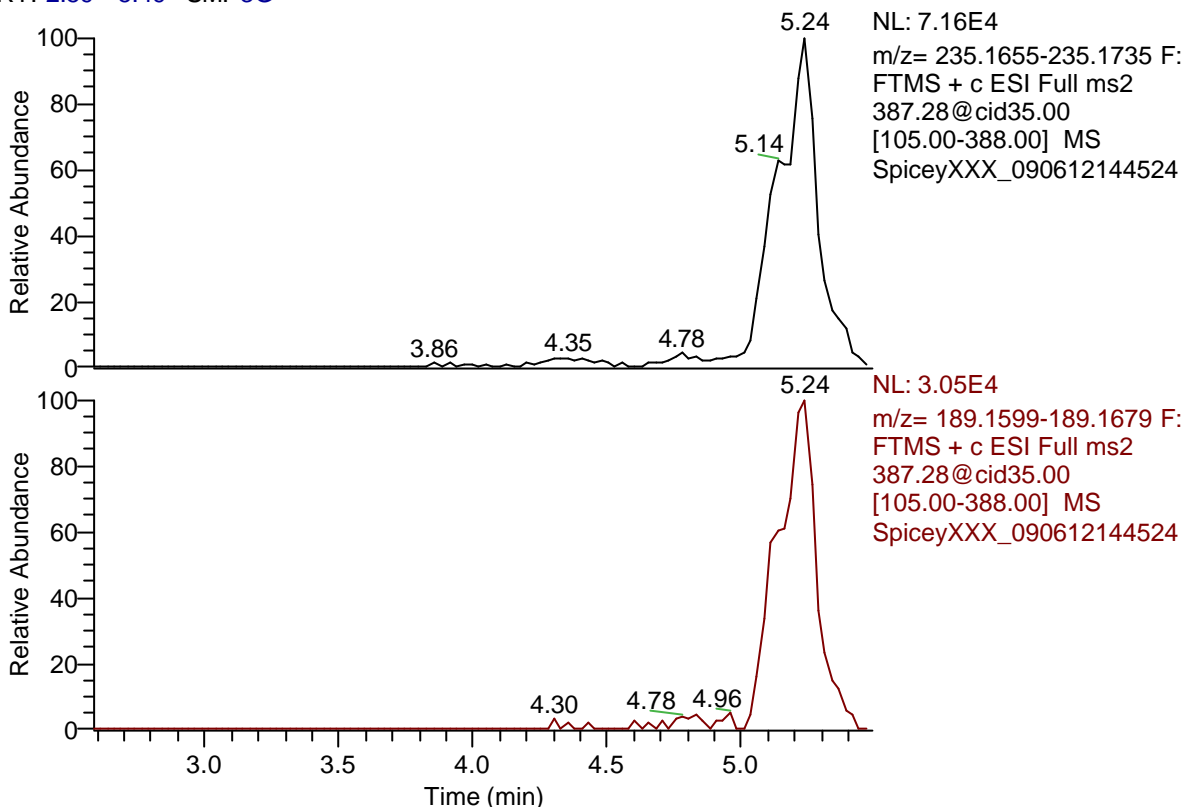


Full scan MS² of HU-210

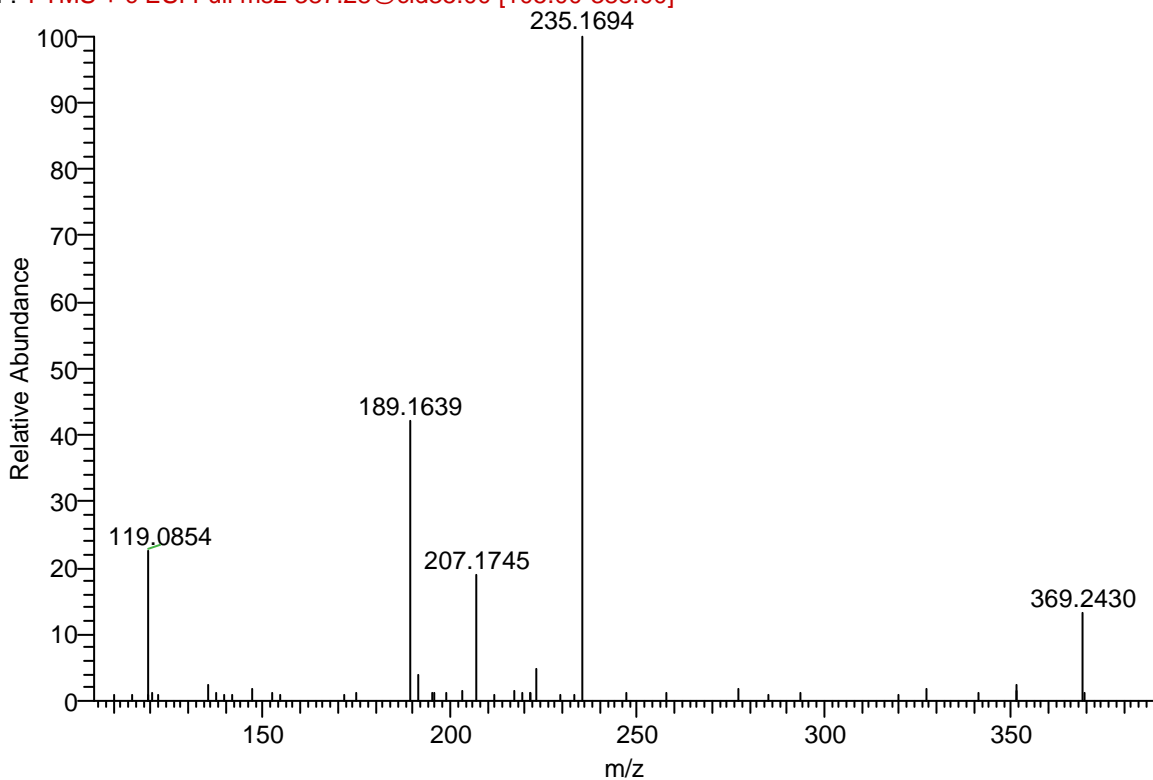
SpiceyXXX_090612144524

12/06/2009 14:45:24

RT: 2.59 - 5.49 SM: 3G



SpiceyXXX_090612144524 #370 RT: 5.24 AV: 1 SB: 2 5.49 , 5.49 NL: 7.18E4
F: FTMS + c ESI Full ms2 387.28@cid35.00 [105.00-388.00]

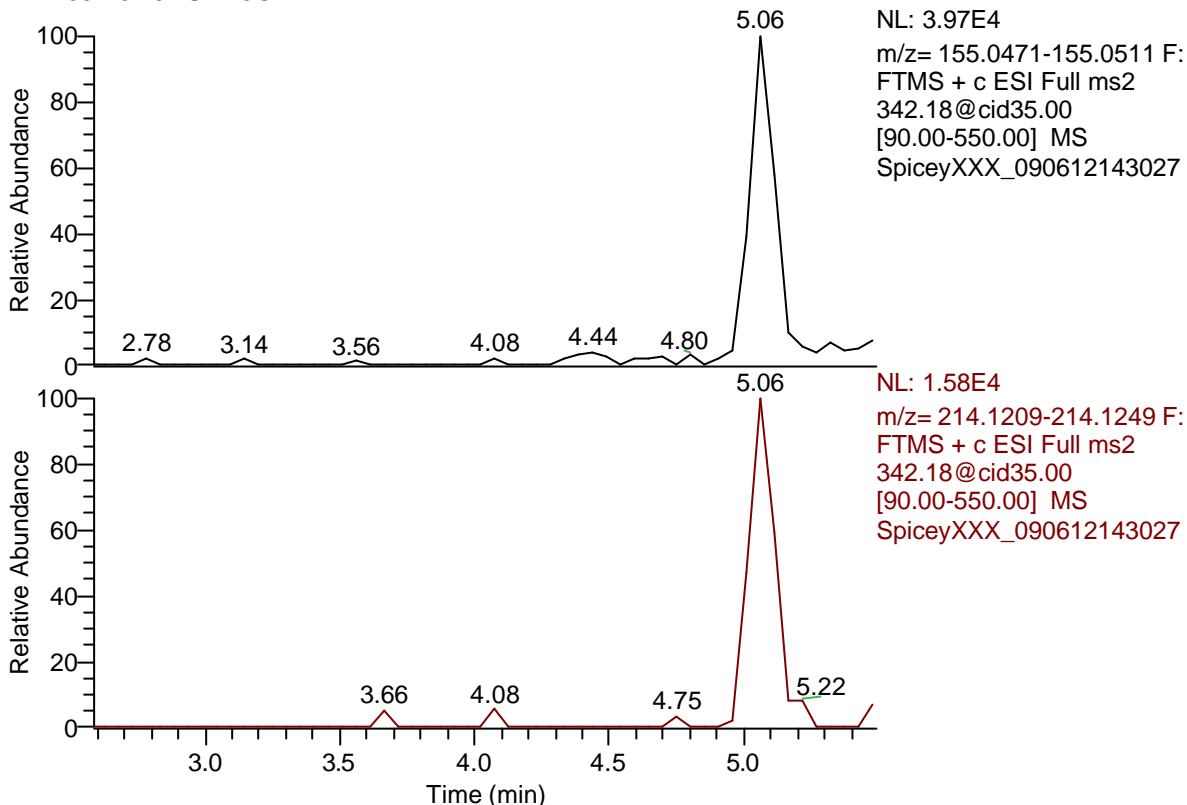


Full scan MS² of JWH-018

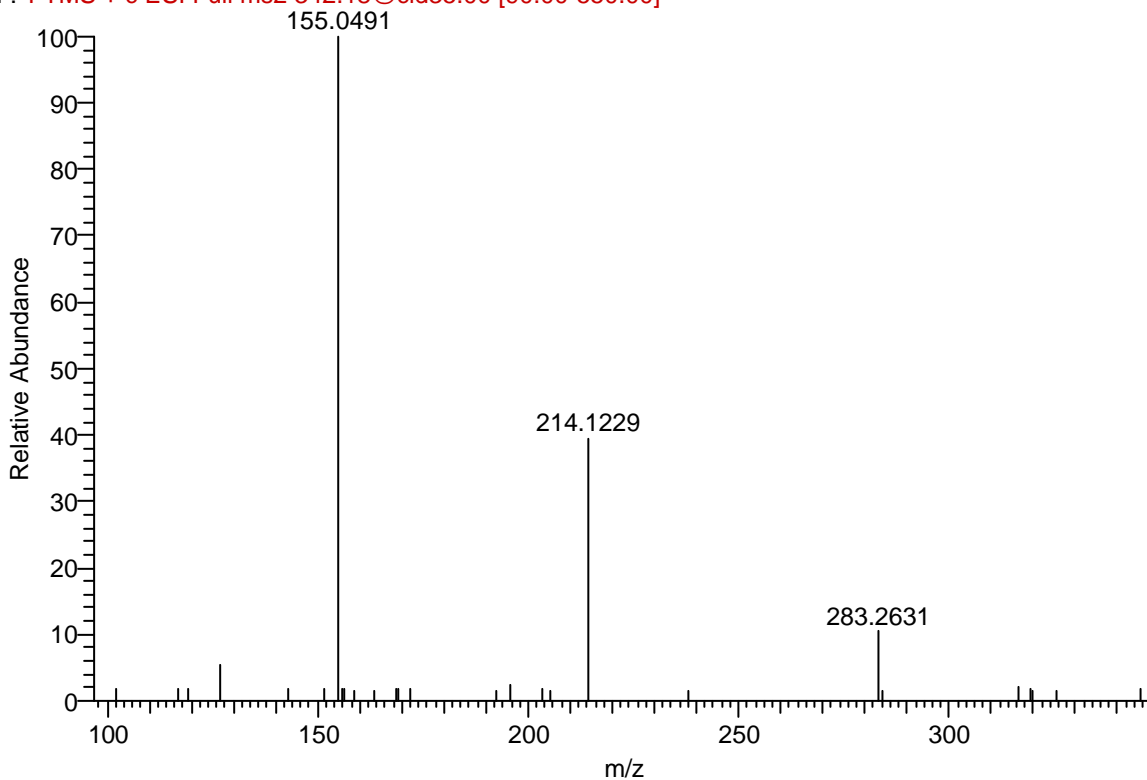
SpiceyXXX_090612143027

12/06/2009 14:30:27

RT: 2.59 - 5.49 SM: 3G



SpiceyXXX_090612143027 #265 RT: 5.06 AV: 1 NL: 4.18E4
F: FTMS + c ESI Full ms2 342.18@cid35.00 [90.00-550.00]

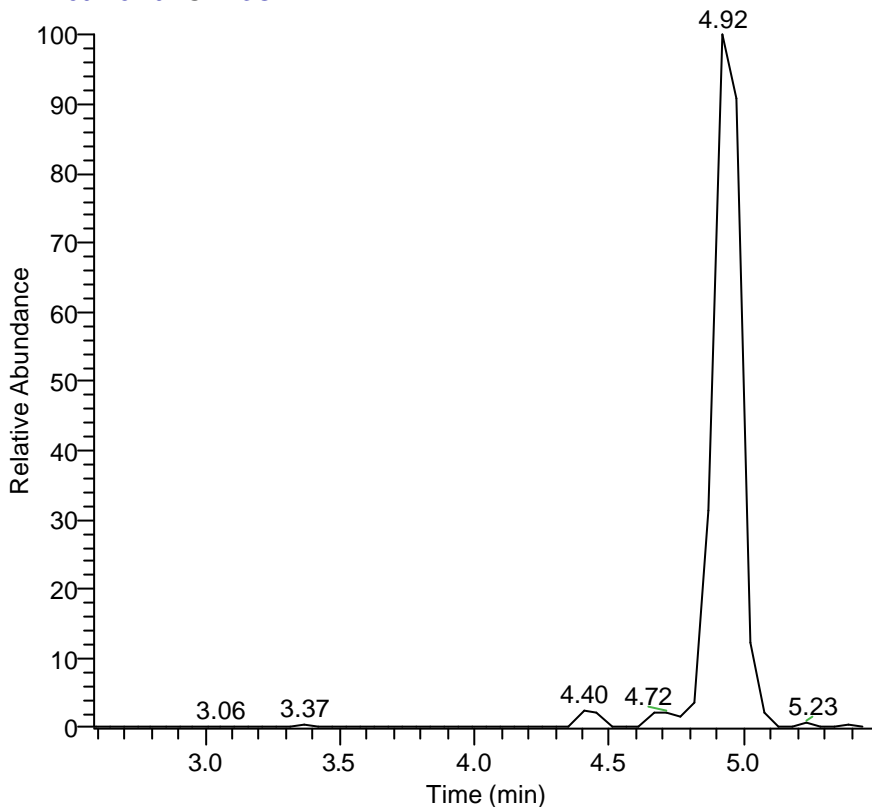


Full scan MS² of CP47497

SpiceyXXX_090612143027

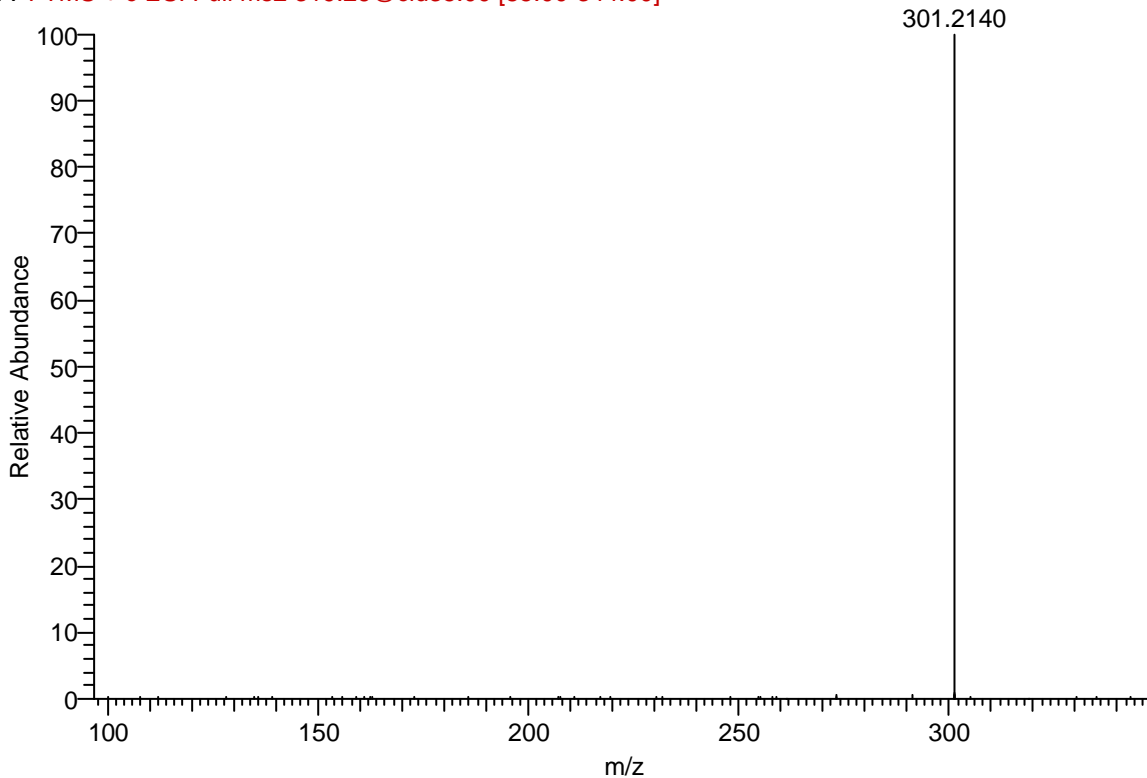
12/06/2009 14:30:27

RT: 2.59 - 5.49 SM: 3G



NL: 6.49E5
m/z= 301.2121-301.2161 F:
FTMS + c ESI Full ms2
319.26@cid35.00
[85.00-344.00] MS
SpiceyXXX_090612143027

SpiceyXXX_090612143027 #257 RT: 4.92 AV: 1 SB: 7 4.56-4.70 , 5.15-5.34 NL: 6.62E5
F: FTMS + c ESI Full ms2 319.26@cid35.00 [85.00-344.00]



The products were purchased from UK websites.

Product		Compounds detected	TICTAC
Spice Gold Graffiti UK http://www.wellcoolstuff.com/ 3g - £20.99		JWH-018 CP47497	24677
Spice Diamond Graffiti UK http://www.wellcoolstuff.com/ 3g - £25.99		JWH-018 CP47497	24674
Ex-ses Platinum aromatic incense blueberry flavour Salvia Dee http://www.salviadee.com/ 1.5g - £9.99		JWH-018 HU-210 CP47497	24726
Spike 99 Ultra Strong blueberry flavour Salvia Dee http://www.salviadee.com/ 1.5g - £11.00		JWH-018 HU-210 CP47497	24729
Spicey XXX Ultra vanilla flavour Salvia Dee http://www.salviadee.com/ 1.5g - £16.99 buy one get one free		JWH-018 HU-210 CP47497	24617



<http://www.tictac.org.uk/>

John Ramsey



<http://www.quotientbioscience.com/>

Simon Hudson
Sarah Timbers
Steve Maynard

June 2009