

Head Shop 'Legal Highs' Active Constituents Identification Chart (July - August 2010, '714' – '823')

(The Criminal Justice (Psychoactive Substances) Act 2010 came into force on August 23rd)

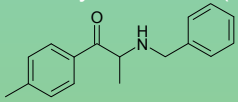


•3',4'-Methylenedioxy- α -pyrrolidinobutiophenone (MDPBP)
(identified using a characterized sample of MDPBP extracted from Vanilla Sky as a reference standard)

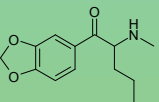
•Caffeine

•4-Methylethcathinone (4-MEC) †

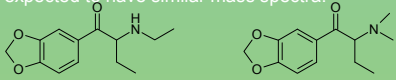
•4-Methyl-N-benzylcathinone ('Benedrone') †



•Pentylone*



Note: We also considered the isomers below which would be expected to have similar mass spectra.



However, based on first principles, the preparation of derivatives and comparison with the mass spectra analogous molecules, the mass spectral data most closely fits pentylone. In this case the mass spectrum displays a significant m/z 44 ion which may arise by loss of propylene from m/z 86 iminium ion.



•Glucine*
•Caffeine (trace)

Note: GCMS analysis also revealed several unidentified peaks. Could be compounds related to glucine?



•Glucine*
•Caffeine
•Synephrine
•Dimethylamylamine (DMAA)

Note: GCMS analysis also revealed an unidentified peak. Could be a compound related to glucine?



•Dimethylamylamine (DMAA)
•Caffeine



•Dimethylamylamine (DMAA)
•2-Phenylethylamine (2-PEA)
•Caffeine



•3',4'-Methylenedioxy- α -pyrrolidinobutiophenone (MDPBP) †
Note: This product contained MDPV and lignocaine before the '511' ban.



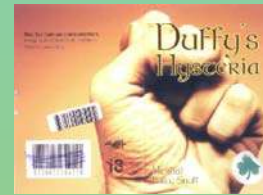
•Naphyrone†



•Naphyrone†
•Caffeine



•AM-694 *



•Naphyrone†
•Caffeine



•AM-694 *



•Benzocaine
•Caffeine

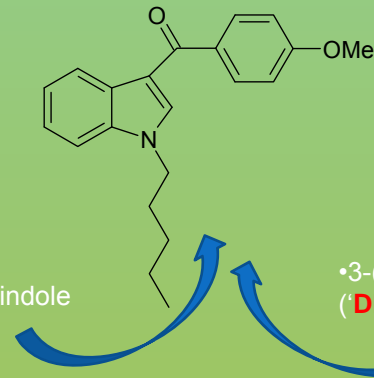
Note: This product contained mephedrone before the '511' ban.



•Oleamide
•3-(4-Methoxybenzoyl)-1-pentylindole ('DD-001') †



•Oleamide
•3-(4-Methoxybenzoyl)-1-pentylindole ('DD-001') † ‡



•3-(4-Methoxybenzoyl)-1-pentylindole ('DD-001') †



•AM-694*

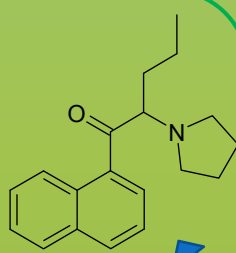


•AM-694*



•Caffeine
•Naphyrone†

Based on mass spectrometric data we also suspect the presence of '1-naphyrone'
Note: Purchased on July 31, 2010.



•Dimethocaine*

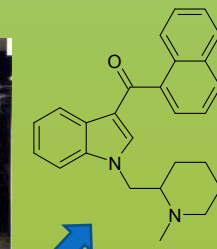
Note: Also contains desethyl dimethocaine. Manufacturing by-product?

This product contained butylone and lignocaine before the '511' ban. At the time of purchase the sales assistant said that this was the same as "Amplified"

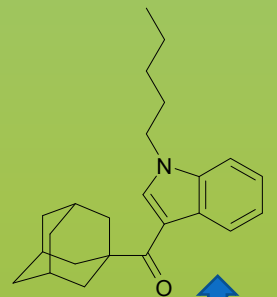


NMR analysis indicates that this product contains 1-[(N-methyl-2-piperidinyl)methyl]-3-(1-naphthoyl)indole. MS data is consistent with this. Investigations are continuing.

In Patent no. WO 01/28557 (University of Connecticut, Makriyannis and Deng) this compound is referred to as both AM1296 and AM1220.



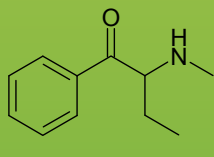
Based on NMR and MS data we suspect the presence of 3-[(adamantan-1-yl)carbonyl]-1-pentylindole ('AB-001'). Investigations are continuing.



•Buphedrone †

Note: Previously this contained ethcathinone and ethcathinone /iso-ethcathinone.

Note: Purchased to check if these products still contained the same ingredients as reported previously



•Dimethocaine*

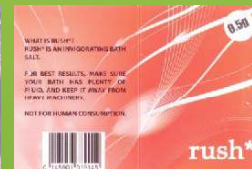
Note: Also contains desethyl dimethocaine. Manufacturing by-product?



•Octopamine
•Caffeine
•Synephrine
•Dimethylamylamine (DMAA)
•Hordenine



•AM-694*



•Fluorotropacocaine*

Note: GCMS analysis also revealed an unidentified peak. Could be a compound related to fluorotropacocaine?



•AM-694*



•AM-694*

● Powder

● Capsule

● Tablet

● 'Herbal mix'

● Resin

* Tentatively identified from its mass spectrum as no standard was available

† Reference standard synthesized in our laboratory

‡ Extracted, purified by column chromatography and characterized NMR/HRMS.

Red text – This compound does not have a common name so we've given it one.

These are the active constituents identified to date. Analysis is on-going. If you have any questions please contact us - id.lab.team@gmail.com

We wish to thank Dr. István Ujváry for his immense help with this work

Pierce Kavanagh¹, Paul Spiers¹, John O'Brien², Sinead McNamara³, Daniel Angelov¹, Daniel Mullan¹, Brian Talbot⁴ and Sheila Ryder⁴

¹ Department of Pharmacology and Therapeutics, School of Medicine, Trinity Centre for Health Sciences, St. James's Hospital, Dublin 8.

² School of Chemistry, Trinity College, Dublin 2

³ Drug Treatment Centre Board, Trinity Court, Pearse Street, Dublin 2.

⁴ School of Pharmacy and Pharmaceutical Sciences, Trinity College, Dublin 2.