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Identification of the novel synthetic cannabimimetic 8-quinolinyl 4-methyl-3-(1-piperidinylsulfonyl)benzoate (QMPSB) and other designer drugs in herbal incense

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ABSTRACT

The identification and structural elucidation of the novel synthetic cannabimimetic 8-quinolinyl 4-methyl-3-(1-piperidinylsulfonyl)benzoate (QMPSB) by GC-MS, LC-MS and NMR is reported. QMPSB was identified in Queensland, Australia on plant material packaged as herbal incense. The identification of QMPSB was initially hampered due to trans-esterification occurring in the extraction solvent. An investigation of the trans-esterification of QMPSB in methanol and ethanol was conducted and analytical data for the respective methyl and ethyl esters are reported. Analytical data is presented for two other compounds detected on seized plant material packaged as herbal incense: the synthetic cannabimimetic 1-[(N-methylpiperidin-2-yl)methyl]-3-(4-methyl-1-naphthoyl)indole (MAM-1220) and the JWH-081 analogue 1-(cyclohexylmethyl)-3-(4-methoxy-1-naphthoyl)indole (CHM-081).

1. Introduction

The detection of synthetic cannabimimetics, also referred to as synthetic cannabinoid receptor agonists or "synthetic cannabinoids", within the recreational drug market was first reported in Germany in 2008, and has since spread to become a world-wide phenomenon [1,2]. These compounds are commonly distributed on plant material branded as herbal incense. While the herbal incense brand name "Spice" was prevalent in early reported detections across Europe [1–6], in Australia the brand name "Kronic" became synonymous with herbal incense products [7–9]. In June 2013, a national interim ban on consumer products branded under names including "Kronic" and "Herbal Incense" was enacted under the Australian Competition and Consumer Act 2010 [10] in an attempt to stem the sale of products containing synthetic cannabinoids. Since that time, branding has changed to include products such as potpourri, herbal tea, wine essence and pheromones.

Drug seizures containing synthetic cannabimimetics were first encountered in Queensland, Australia in 2010, with JWH-018 the first compound of this class detected. Initially, JWH-018 was encountered in powders and capsules, but this was soon followed by branded packets of plant material. JWH-018 was one of the first cannabinoid receptor agonists subjected to legislative control in Queensland, being added to drug legislation in September 2011. Subsequent to this the 5-fluoropentyl analogue of JWH-018, AM-2201 emerged as the predominant compound encountered in products marketed as herbal incense. The legislative listing in Queensland of AM-2201, along with eighteen other synthetic cannabinoids, in November 2011, was soon followed by the emergence of a new generation of compounds not specifically listed in the legislation; including the N-methyl piperidinyl indoles such as AM-2233 and AM-1220, first reported by Makriyannis [11]. Seized plant material packaged as herbal incense under the brand names "Shhhh" and "X" were found to contain varying ratios of four compounds: MAM-2201, AM-2233, AM-1220 and an unknown compound **1** (Fig. 1).

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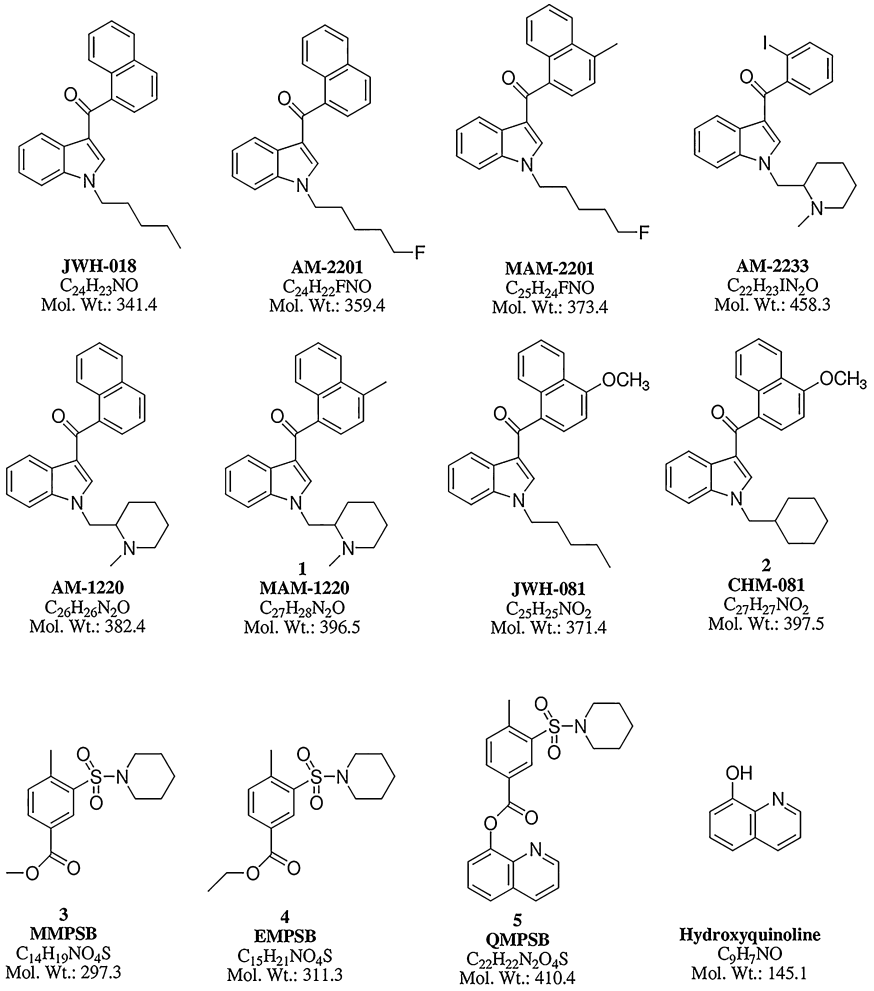

Fig. 1. Structures of detected compounds and associated cannabimimetics.

Compound **1** showed spectral similarities to N-methyl piperidinyl indoles previously detected on herbal incense products [12] and was subsequently identified as 1-[(N-methyl-piperidin-2-yl)methyl]-3-(4-methyl-1-naphthoyl)indole (MAM-1220), a methylated analogue of AM-1220. While MAM-1220 has been reported in the literature as a cannabinoid receptor agonist [13], its detection on herbal incense products has not previously been reported. Both MAM-2201 and MAM-1220 were observed to be advertised for sale as "research chemicals" online [14].

With the addition of MAM-1220 and a number of other compounds to the Queensland controlled substances legislation in April 2013, new compounds continued to be detected on seized plant material. Numerous branded materials were found to contain the unknown compound **2**, which was subsequently identified as a cyclohexylmethyl (CHM) analogue of JWH-081 (Fig. 1). At this time, the CHM group was not commonly encountered amongst compounds reported on seized material, however it had been reported on cannabimimetics such as ORG 28611 and ORG 28312 [15]. More recent reports of compounds such as BB-22 (QUCHIC) and AB-CHMINACA have shown an increasing occurrence of this substituent group in seized materials [16,17].

The vast majority of cannabimimetics and related compounds detected on plant material in Queensland have contained an N-substituted indole or indazole ring. In 2011 and 2012, methanol extracts of numerous seized plant materials showed hydroxyquinoline and the unknown compounds **3** and **4**, occasionally in conjunction with other known synthetic cannabimimetics, such as AKB48 (APINACA) [18]. Compound **3** was purified from methanol extracts and a structure of methyl 4-methyl-3-(1-piperidinylsulfonyl)benzoate (MMPSB) was proposed on the basis of NMR and vapour phase IR data [19]. MMPSB had not previously been reported in the literature and bore no clear structural similarities to previously reported synthetic cannabimimetics detected on seized materials. However, arylsulfonamides had been reported in the literature to be cannabinoid receptor agonists, with the compound 8-quinolinyl 4-methyl-3-(1-piperidinylsulfonyl)-benzoate (QMPSB) identified as having a higher potency than both WIN 55,212-2 and CP 55,490 [20,21]. The presence of hydroxyquinoline in the methanol extracts led to an investigation of the extraction solvent as a potential cause of breakdown of the suspected parent compound. The use of an alternate extraction solvent revealed the presence of compound **5,** which was confirmed through comparison with reference material**.** The analytical results for the parent compound QMPSB **5**, as well as the trans-esterification products MMPSB **3** and ethyl 4-methyl-3-(1-piperidinylsulfonyl)benzoate (EMPSB) **4**, are reported. This is the first report of QMPSB in the recreational drug market.

2. Materials and methods

2.1. General

All reagents and chemicals were purchased from commercial sources and were used without further purification. QMPSB