The pharmacology of indole and indazole synthetic cannabinoid designer drugs AB-FUBINACA, ADB-FUBINACA, AB-PINACA, ADB-PINACA, 5F-AB-PINACA, 5F-ADB-PINACA, ADBICA and 5F-ADBICA


Contents:

Names, CAS numbers, and references for selected compounds: S2–S4.

$^1$H and $^{13}$C NMR spectra for selected compounds: S5–S16.

AUC for AB-PINACA and AB-FUBINACA hypothermia following pretreatment with CB$_1$ and CB$_2$ antagonists: S17.
Table S1. IUPAC names, CAS numbers, and literature references for valinamide- and tert-leucinamide-derived indole and indazole synthetic cannabinoids.

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<th>CAS</th>
<th>CAS</th>
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<td>N-(1-amino-3-methyl-1-oxobutyl-2-y1)-1-(4-fluorobenzyl)-1H-indazole-3-carboxamide</td>
<td>1629062-56-1 (racemate)</td>
<td>4 July 2013, Belgium 1–5</td>
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<td>1445583-51-6 (racemate)</td>
<td>28 November 2013, Turkey and Germany 1, 4, 6–8</td>
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<td>21 May 2013, Sweden 2, 4, 5, 7</td>
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*aAn advisory was issued in September 2013 after information provided by law enforcement agencies in the United States, supplemented by information from the EMCDDA’s monitoring of open source information, identified a series of non-fatal
intoxications in the United States associated with ADB-PINACA and 5F-ADBICA. These substances are known to be present on the EU drug market and have been reported by several Member States.

References


Figure S1. $^1$H NMR spectrum (500 MHz, CDCl$_3$, 300 K) of AB-FUBINACA (7).
Figure S2. $^{13}$C NMR spectrum (125 MHz, CDCl$_3$, 300 K) of AB-FUBINACA (7).
Figure S3. $^1$H NMR spectrum (500 MHz, CDCl$_3$, 300 K) of AB-PINACA (9).
Figure S4. $^{13}$C NMR spectrum (125 MHz, CDCl$_3$, 300 K) of AB-PINACA (9).
Figure S5. $^1$H NMR spectrum (400 MHz, CDCl$_3$, 300 K) of ADB-PINACA (10).
Figure S6. $^{13}$C NMR spectrum (100 MHz, CDCl$_3$, 300 K) of ADB-PINACA (10).
Figure S7. $^1$H NMR spectrum (400 MHz, DMSO-$d_6$, 300 K) of AB-PICA (15).
Figure S8. $^{13}$C NMR spectrum (100 MHz, DMSO-d$_6$, 300 K) of AB-PICA (15).
Figure S9. $^1$H NMR spectrum (400 MHz, DMSO-d$_6$, 300 K) of 5F-AB-PICA (17).
Figure S10. $^{13}$C NMR spectrum (100 MHz, DMSO-d$_6$, 300 K) of 5F-AB-PICA (17).
Figure S11. $^1$H NMR spectrum (400 MHz, CDCl$_3$, 300 K) of 5F-ADBICA (18).
Figure S12. $^{13}\text{C}$ NMR spectrum (100 MHz, CDCl$_3$, 300 K) of 5F-ADBICA (18).
Figure S13. Mean area under the vehicle-vehicle baseline curve (AUC ± SEM) for body temperature for (A) AB-PINACA and (B) AB-FUBINACA (3 mg/kg), following pretreatment with vehicle, rimonabant (CB₁ antagonist, 3 mg/kg), or SR144528 (CB₂ antagonist, 3 mg/kg). The area was significantly reduced for both AB-PINACA and AB-FUBINACA by rimonabant but not SR144528. * p < .05 compared to vehicle.