Supplementary Information File: ***Investigation of John W. Huffman cannabinoid dataset***

As described in the manuscript the curation and mapping of the JWH cannabinoid dataset identified multiple ambiguous and conflicted pages and manual curation was required to evaluate and make corrections. Details of the identified conflicts and corrections applied are provided below.

1. *JWH-210.* The Wikipedia page for JWH-210 included CASRNs for both JWH-210 (824959-81-1) and JWH-182 (824960-02-3). DSSTox contained no mappings for the former CASRN; the mapping for the latter CASRN correctly used JWH-182 as a name, but incorrectly used the structure for JWH-210, and additionally incorrectly accepted JWH-210 as a synonym. The existing record (DTXSID301010019) was corrected to use the appropriate name (JWH-210) and CASRN (824959-81-1) for the structure, and the mapping to the JWH-210 Wikipedia page left in place; an additional record for JWH-182 (DTXSID401337155), with CASRN 824960-02-3 and the 4-n-propyl derivative structure, was created with no Wikipedia page mapping. The decision to not link back to Wikipedia was retained since, while JWH-182 is discussed in the article, the article lede shown on the Dashboard would reference JWH-210, potentially leading to confusion.
2. *JWH-203.* The Wikipedia page entitled JWH-203 included CASRNs for both JWH-203 (864445-54-5) and JWH-204 (864445-55-6). DSSTox contains mappings for both CASRNs: the mapping for the former uses the appropriate name and structure and links back to Wikipedia, while the mapping for the latter uses a correct structure but does not include the name JWH-204 and does not link back to Wikipedia. JWH-204 was added as a synonym for the latter mapping, but the record was left without a Wikipedia mapping as described in (1).
3. *JWH-359.* The Wikipedia SMILES was corrected to match the curated structure and ensure consistency between the IUPAC Name and the InChIKey.
4. *JWH-176.* The Wikipedia SMILES, InChI string, and InChIKey were edited to match the E-orientation around the double bond after confirming consistency with the publicly available data on Common Chemistry (https://commonchemistry.cas.org/results?q=619294-62-1). Based on the information in the Wikipedia article, a DSSTox record for JWH-171, the E-/Z-isomer mixture, was also created; this record was again left without a Wikipedia mapping, as in (1) and (2).