Supporting information: Synthetic Cannabinoid Receptor Agonist Detecting Using Fluorescence Spectral Fingerprinting

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Tables

Table S1. A range of species comprising different SCRAs.

Core	Core substituent	Tail	Linker	Ring	Ring substituent
indole	2-methyl	2-morpholin-4-yl ether	methanone	carbamoyl	Isopropyl tert-butyl
indazole		tetrahydropyran-4-yl methyl	ethanone	methoxycarbonyl	tert-butyl
Pyrrole	5-phenyl, 5-(2-methyl)phenyl, 5-(2-fluoro)phenyl, 5-(3-bromo)phenyl	methylazepan-3-yl	carboxamide	CUMYL	
naphthalene		methylpiperidin-2-yl methyl	Carboxylate	naphthyl	4-methoxy, 2-chloro, 4-methyl, 4-ethyl, 4-propyl, 4-fluoro, 4-bromo
γ-carboline		fluorobenzyl		adamantly	
γ-carboline		fluorobenzyl cyclohexylmethyl		cyclopropyl	2,2,3,3-tetramethyl
		heptyl		Q quinolinyl	
		hexyl		phenyl	2-methyl (ring-substituent), 2-ethyl, 2-methoxy, 4-methoxy, 2-iodo, 2-chloro
		5-bromopentyl			
		5-chloropentyl			
		5-fluoropentyl			
		4-cyanobutyl			
		pentoxy			
		pent-4-enyl			
		pentyl			
		butyl			
		propyl			
		methyl			

Data as found at http://www.emcdda.europa.eu/topics/pods/synthetic-cannabinoids_en, with the exception of γ-carboline.

Table S2. Results of fitting Eq 1 to saliva FSFs.

|	Ave.	M1	M2	M3	F1	F2	F3
F_0	0.012	0.013	0.005	0.107	0.009	0.009	0.012
A_1 (AU)	1.797	1.976	1.160	3.638	1.253	2.518	1.797
λ_{Em1} (nm)	352.146	352.732	353.048	371.002	350.911	352.073	352.146
λ_{Ex1} (nm)	263.836	263.604	263.972	275.479	260.692	265.731	263.836
$w_{1(1)}$ (nm)	71.315	68.118	68.534	82.087	68.867	74.293	71.315
$w_{2(1)}$ (nm)	25.849	21.389	25.895	38.369	22.653	30.467	25.849
$b_{1(1)}$	0.275	0.324	0.288	-0.260	0.292	0.293	0.275
$b_{2(1)}$	0.494	0.724	0.635	-0.167	0.577	0.576	0.494
A_2 (AU)	0.209	0.191	0.233	0.001	0.140	0.161	0.209
λ_{Em2} (nm)	412.113	413.650	451.631	410.252	398.879	411.140	412.113
λ_{Ex2} (nm)	343.837	346.963	352.793	335.353	339.752	342.702	343.837
$w_{1(2)}$ (nm)	167.839	83.089	124.690	114.249	132.471	128.922	167.839
$w_{2(2)}$ (nm)	91.948	92.466	110.934	101.011	88.429	77.344	91.948
$b_{1(2)}$	0.120	0.203	0.061	-0.361	0.147	-0.031	0.120
$b_{2(2)}$	0.548	0.382	0.598	-0.022	0.634	0.468	0.548

Figures
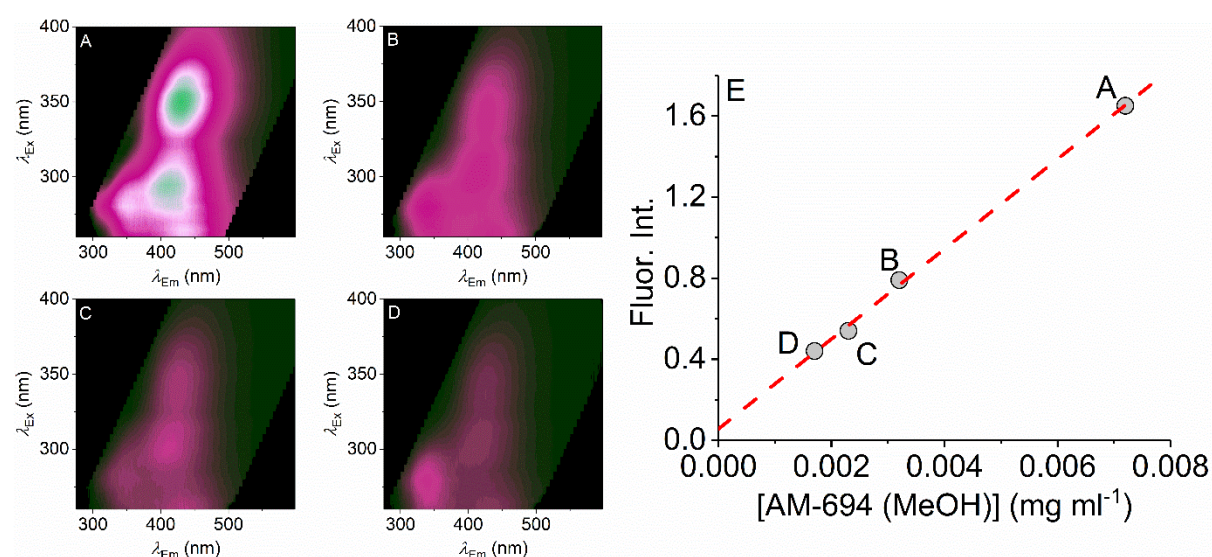
Figure S1. Concentration dependence of AM-694 (MeOH) FSFs. **A-D,** FSFs for different concentration of AB FUBINACA with the decreasing concentration shown in panels A → D. **E,** Plot of concentration *versus* peak emission intensity. The red dashed line shows the linear range of the SCRA concentrations with respect to intensity. Colour levels as Figure 2 (relative emission).
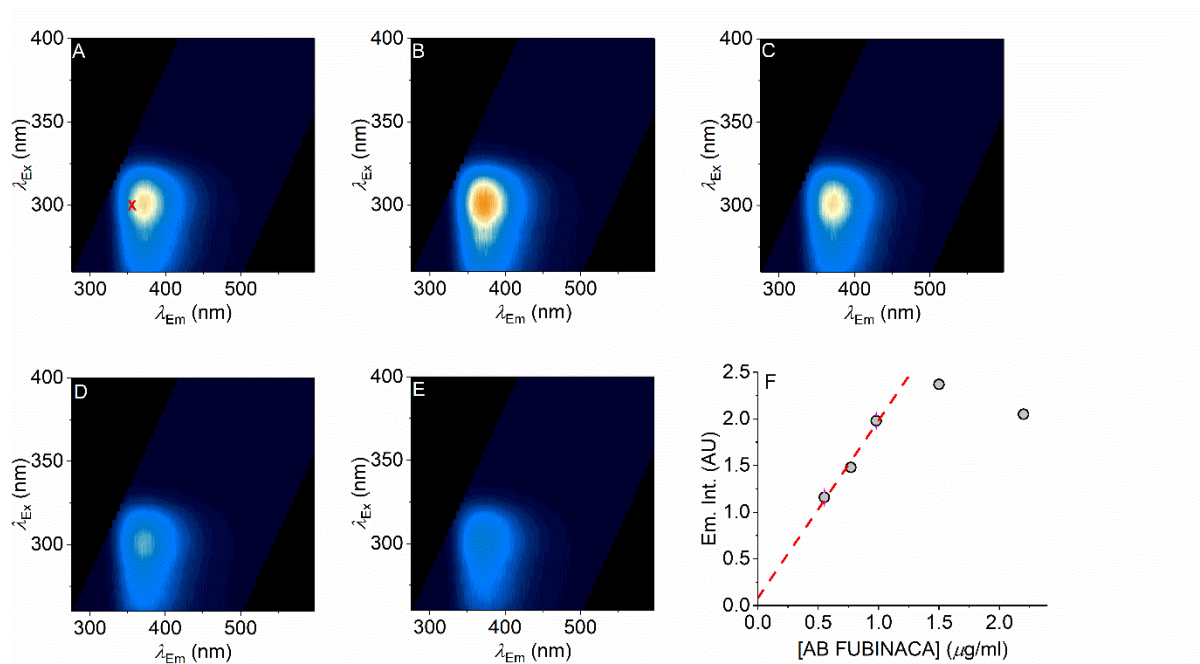
Figure S2. Concentration dependence of AB-FUBINACA (H_2O) FSFs. **A-D,** FSFs for different concentration of AB FUBINACA with the decreasing concentration shown in panels A $\rightarrow$ E. **F,** Plot of concentration *versus* peak emission intensity. The red dashed line shows the linear range of the SCRA concentrations with respect to intensity. The red cross in panel A shows the peak position of AB FUBINACA in MeOH as in Figure 3D and 4A. Colour levels as Figure 2 (relative emission).
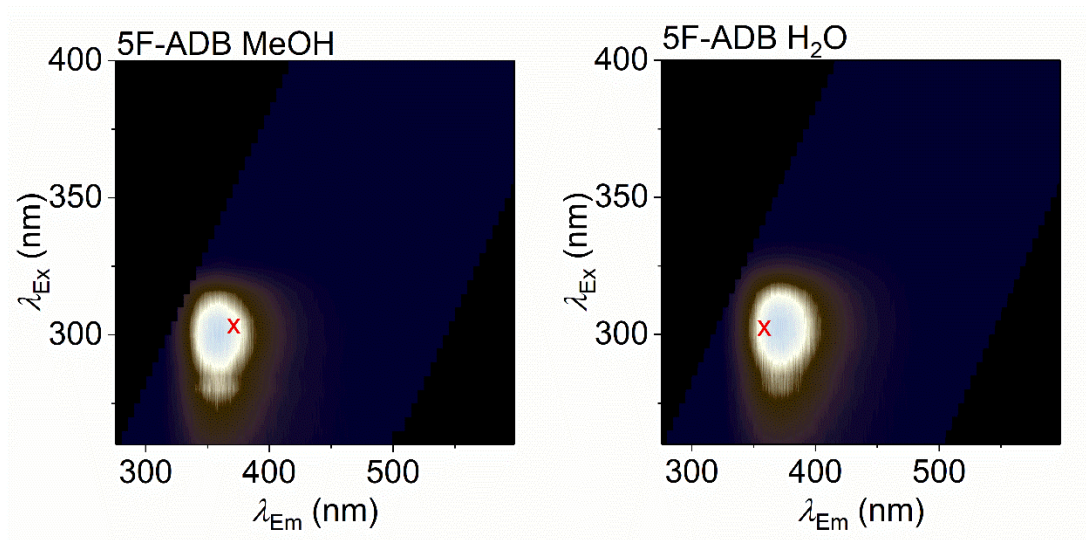
Figure S3. Effect of solvent on 5F-ADB FSF. The red crosses represent the peak intensity of the alternative solvent as assessed from fitting each FSF with Eq 1 as in the main text. Colour levels as Figure 2 (relative emission).
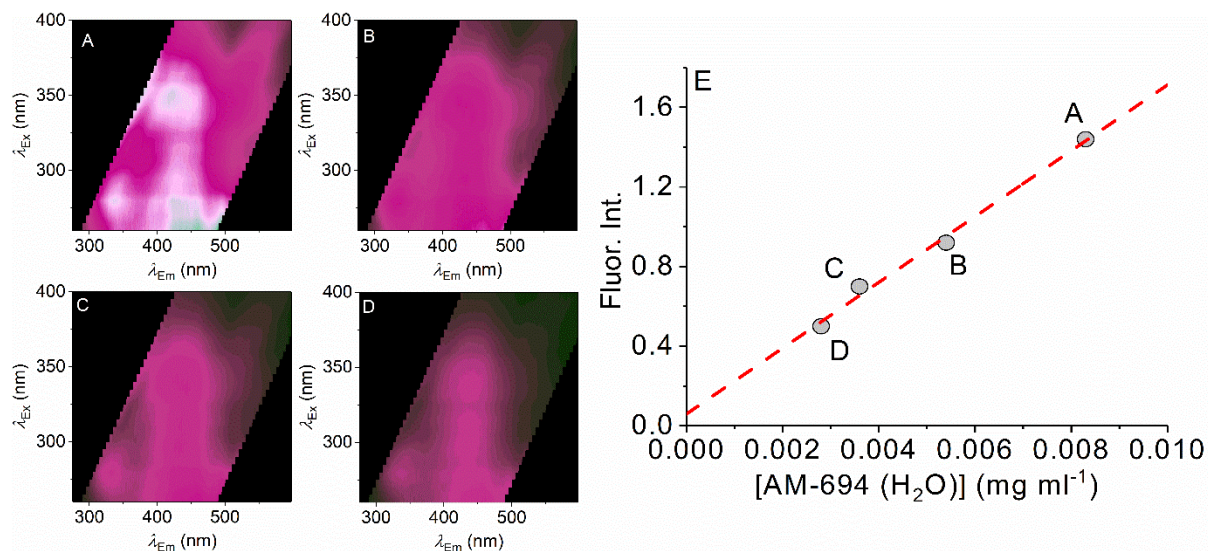
Figure S4. Concentration dependence of AM-694 (H_2O) FSFs. **A-D,** FSFs for different concentration of AB FUBINACA with the decreasing concentration shown in panels A → D. **E,** Plot of concentration *versus* peak emission intensity. The red dashed line shows the linear range of the SCRA concentrations with respect to intensity. Colour levels as Figure 2 (relative emission).
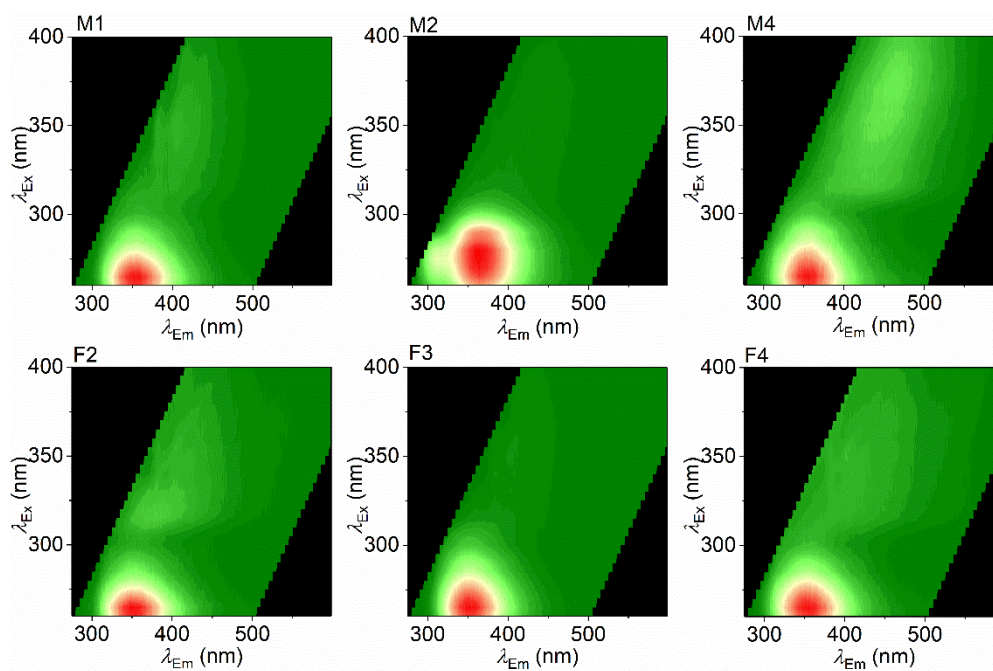
Figure S5. Individual FSFs for saliva participant samples. The averaged sample (Figure 6A) is composed of equal volumes of each of the participant samples (male, A-C; female, D-F). Colour levels as Figure 6 (relative emission).