Supplementary information

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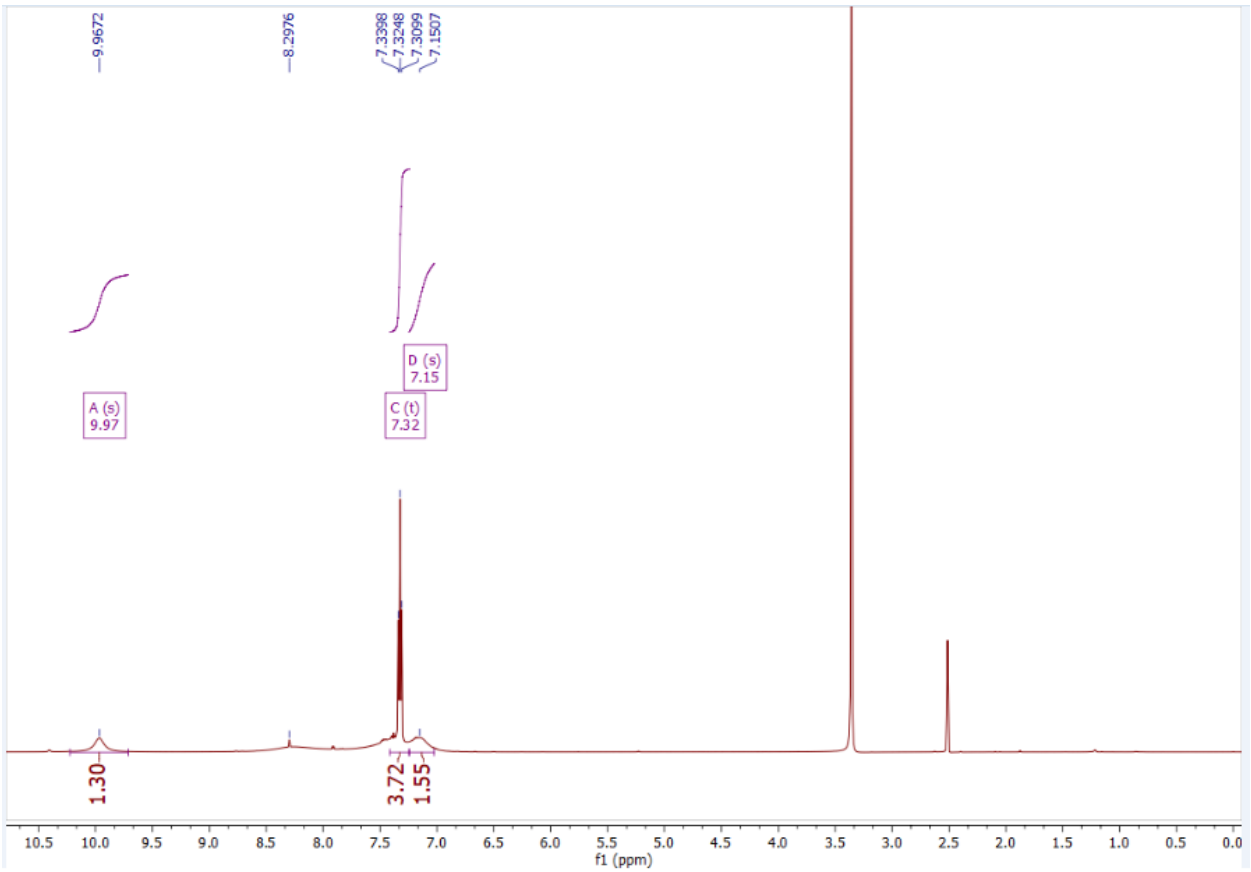

Figure S1: ^{1}H-NMR of FCF

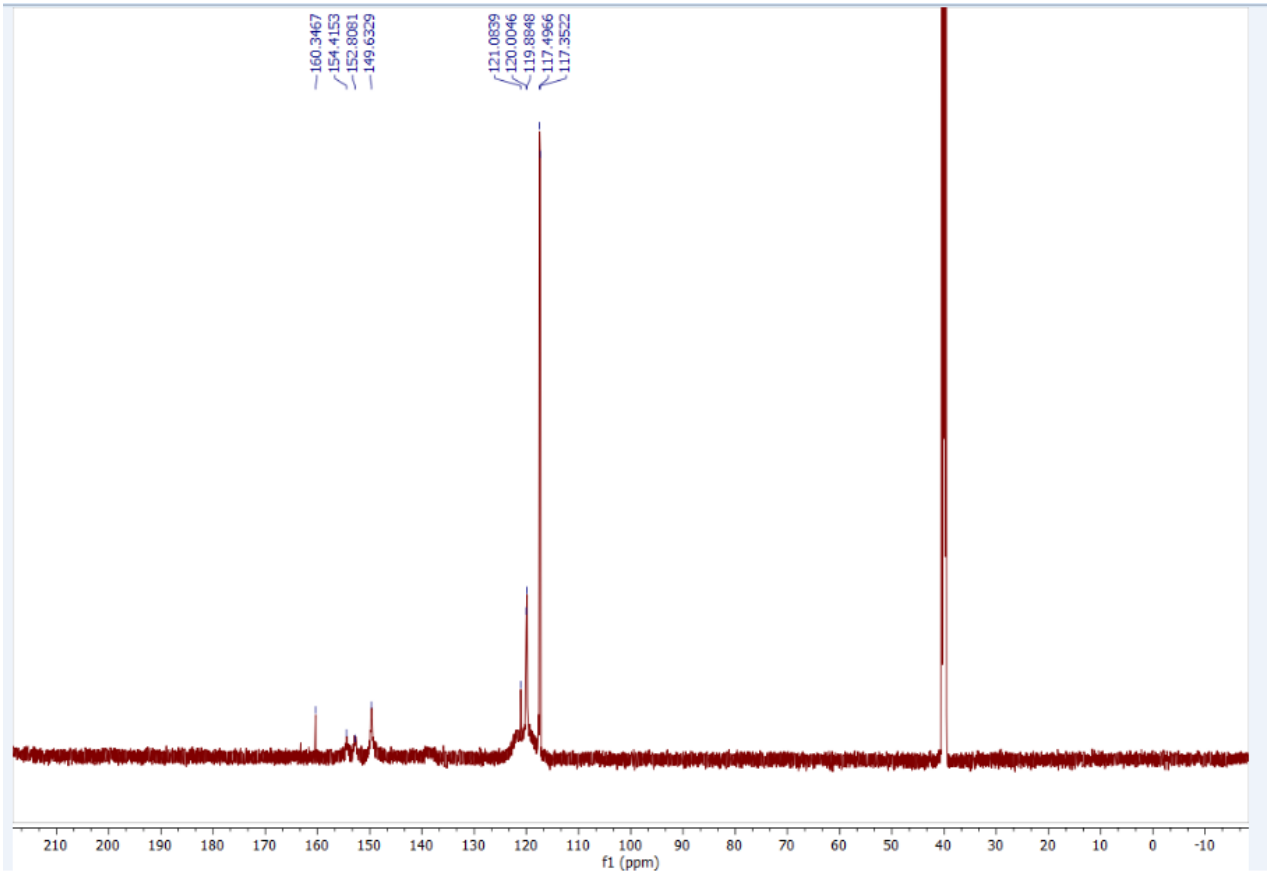

Figure S2: ^{13}C-NMR of FCF

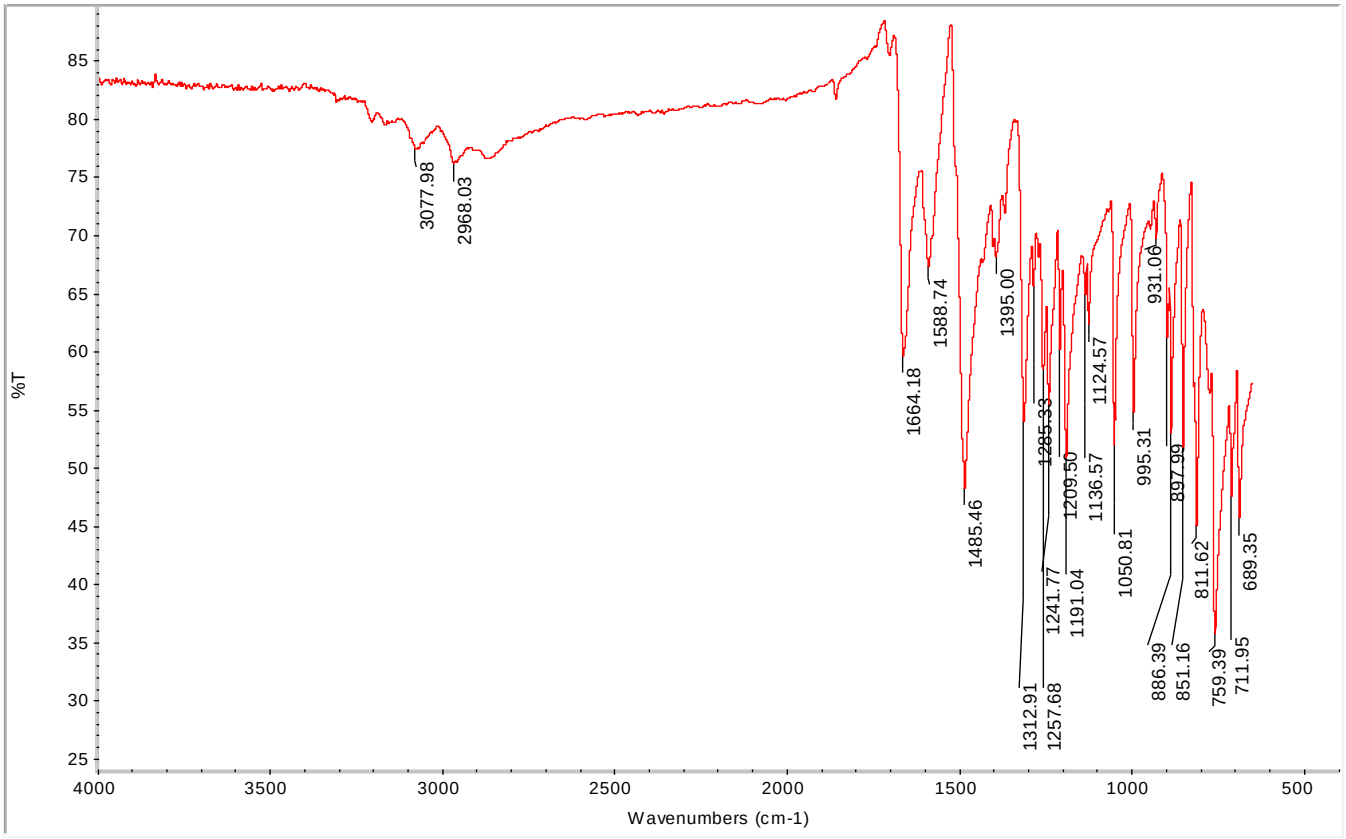

Figure S3: FT-IR of FCF

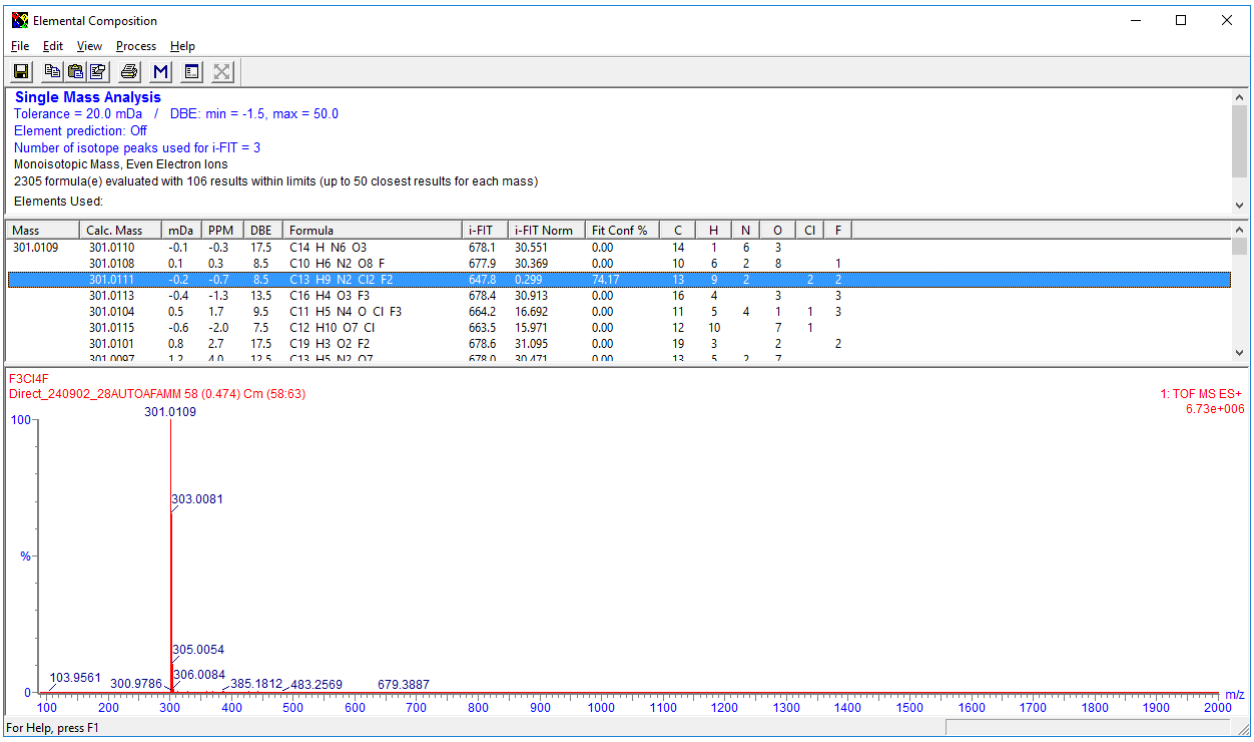

Figure S4: Mass spectrum of FCF

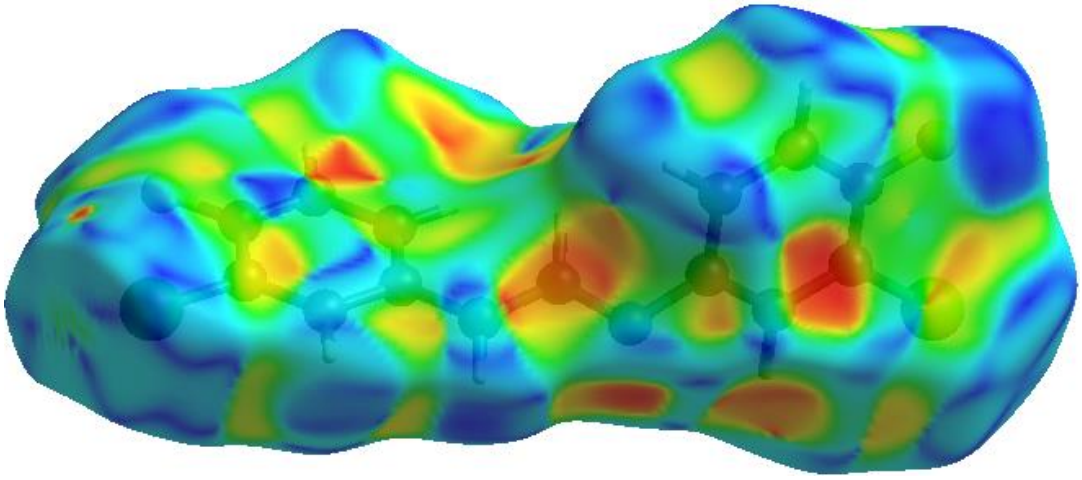

Figure S5: Shape index of **FCF**

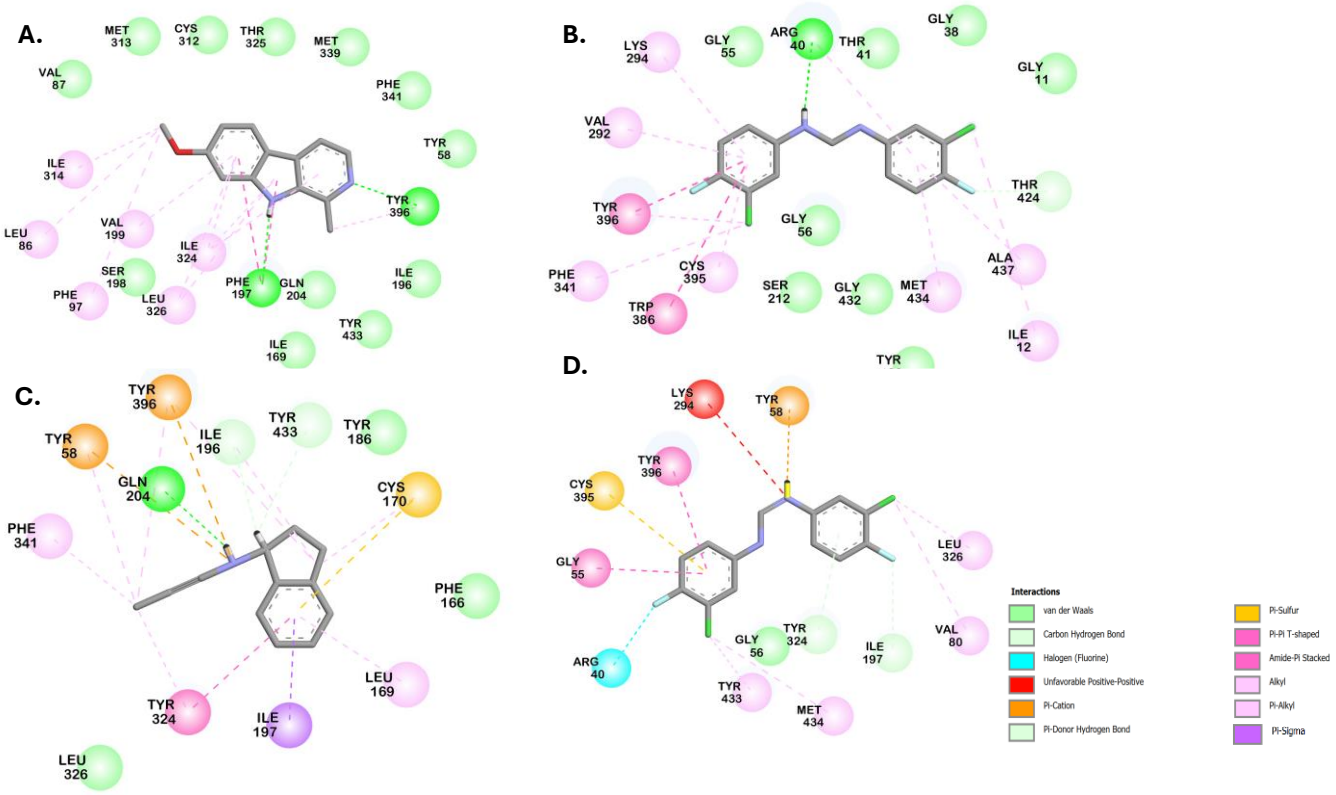

Figure S6: Protein-ligand interaction of **(A)** Harmine-MAO-A (**B**) **FCF**-MAO-A (**C**) Rasagline-MAO-A (**D**) **FCF**-MAO-B

Table S1: Structure refinement parameters and data collection of **FCF**

Empirical formula	$C_{13}H_8Cl_2F_2N_2$
Formula weight	301.11
Temperature/K	100(2)
Crystal system	triclinic
Space group	*P*-1
a/Å	6.8673(6)
b/Å	7.9510(7)
c/Å	11.7788(10)
α/°	84.6330(10)
β/°	79.7190(10)
γ/°	88.5530(10)
Volume/Å^3	630.02(9)
Z	2
ρ_{calc}g/cm^3	1.587
μ/mm^{-1}	0.525
F(000)	304
Crystal size/mm^3	0.303 × 0.250 × 0.092
2Θ range for data collection/°	1.764 to 27.560
Index ranges	--8 ≤ *h* ≤ 8, -10 ≤ *k* ≤ 10, -15 ≤ *l* ≤ 15
Reflections collected	27314
Independent reflections	2917 [R_{int} = 0.0251]
Data/restraints/parameters	2917 / 0 / 176
Goodness-of-fit on F^2	1.035
Final R indexes [I>=2σ (I)]	*R*1 = 0.0270, *wR*2 = 0.0688
Final R indexes [all data]	*R*1 = 0.0284, *wR*2 = 0.0698
Largest diff. peak/hole / e Å^{-3}	0.301 and -0.291

Table S2: The binding affinity of (E)-N,N'-bis(3-chloro-4-fluorophenyl)formamidine and reference drugs with MAO-A and MAO-B.

Compound	Binding Score MAO-A	Binding Score MAO-B
Harmine (Reference)	-7.62	
Rasagiline (Reference)		-7.17
FCF	-7.93	-9.49

Table S3: Estimated pharmacokinetics and physicochemical parameters of **FCF**

	FCF	**Acceptable threshold (Ro5)**
Physicochemical properties		
Molecular weight (g/mol)	301.12	<500Da
Log*P*	4.70	<5
LogS	-4.75	0 → -6
TPSA (Å²)	24.39	≤140
HBA	3	≤10
HBD	1	≤5
RotBs	3	<10
Pharmacokinetics properties		
G.I. absorption	High	
B.B.B. Permeant	Yes	
P-gp Substrate	No	
LogKp (skin permeation (cm/s))	-5.01	
AMES Toxicity	No	
Hepatotoxocity	No	
Oral Rat Acute Toxicity (LD50 (mol/kg)	2.704	
T.Pyriformis toxicity ((log ug/L))	2.308	