

Adapalene

CAS Registry No.: 106685-40-9

Formal Name: 6-(3-(adamantan-1-yl)-4-methoxyphenyl)-2-naphthoic acid

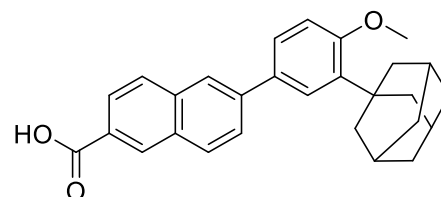
EUBOPEN ID: EUB0000564a

Molecular Formula: C₂₈H₂₈O₃

Molecular Weight: 412.53 g/mol

Smiles:
COC1=CC=C(C=C1C2=CC3=C(C=C2)C=C(C=C3)C(=O)O)C45CC6CC(C4)CC(C6)C5

Recommended concentration: 1 μM



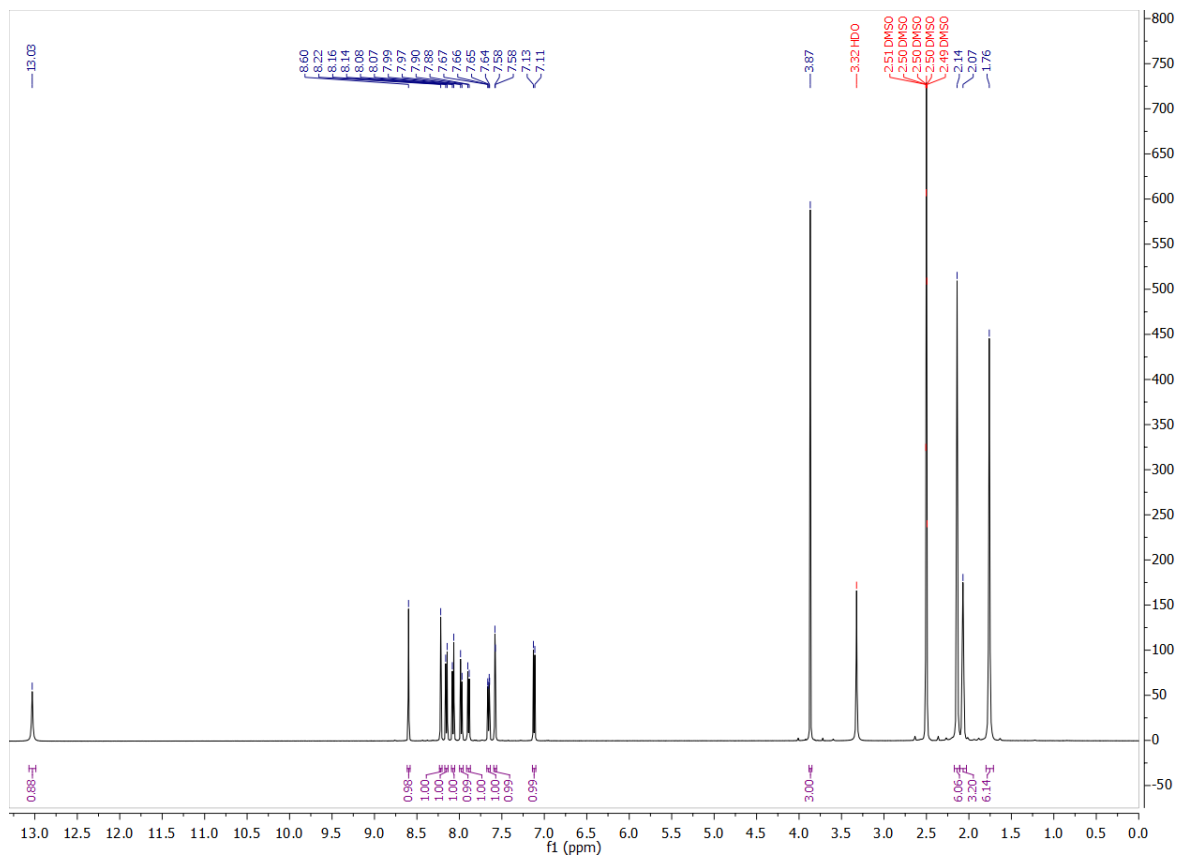
Biological activity

	Type	IC ₅₀ /EC ₅₀ [μM]	Reference
Main NR target:	NR1B1 (RARα)	Agonist	0.02
	NR1B2 (RARβ)	Agonist	0.002
	NR1B3 (RARγ)	Agonist	0.003
NR off-target:			https://doi.org/10.1016/j.bmcl.2018.04.036

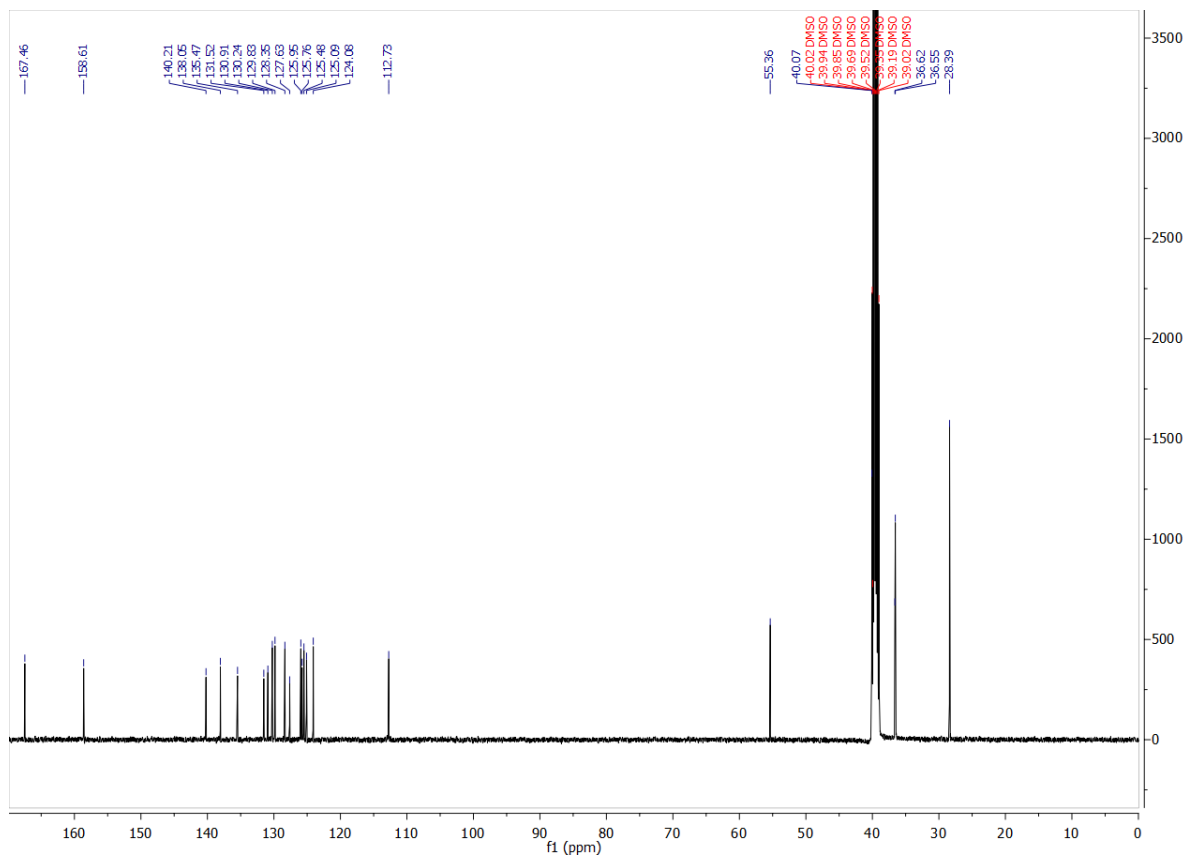
COMPOUND INFORMATION

Identity

¹H NMR



¹³C NMR



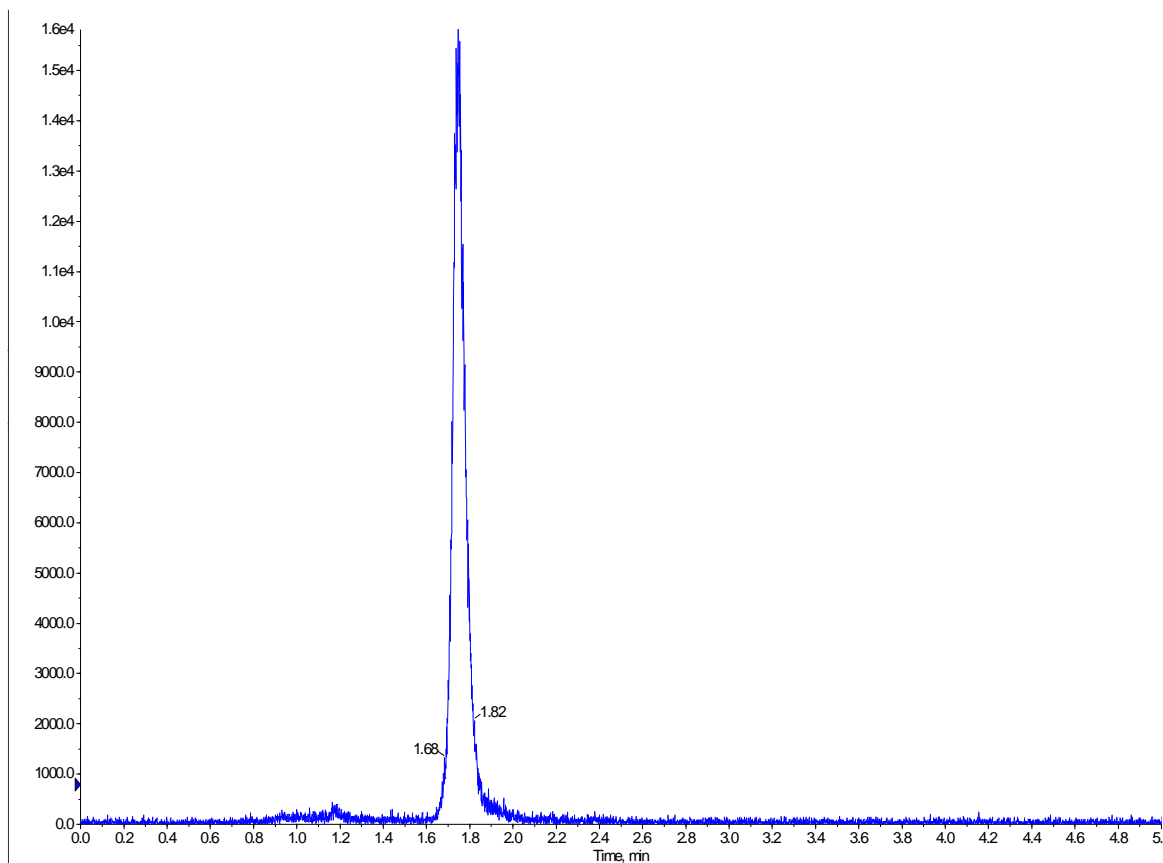
COMPOUND INFORMATION

Purity

M_r 412.53

MS: ESI-negative, m/z 411/367

LC: 0.1% HCOOH/ACN (20/80)



COMPOUND INFORMATION

LC-UV

LC: 0.1% HCOOH/ACN (30/70)

DAD: 210, 230, 240, 254 (XWC), 280 nm

