

6-ECDCA (Obeticholic acid)

CAS Registry No.: 459789-99-2

Formal Name: (R)-4-((3R,5S,6R,7R,8S,9S,10S,13R,14S,17R)-6-ethyl-3,7-dihydroxy-10,13-dimethylhexadecahydro-1H-cyclopenta[a]phenanthren-17-yl)pentanoic acid

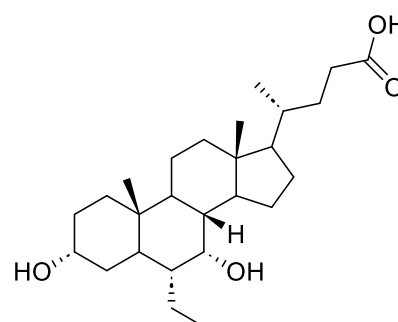
EUBOPEN ID: EUB0000081c

Molecular Formula: C₂₆H₄₄O₄

Molecular Weight: 420.63 g/mol

Smiles: O[C@@H]1CC[C@]2([C@@]([H])(C1)[C@H]([C@H]([C@@]3([C@@]2(CC[C@]4([C@]3(CC[C@@]4([C@H](C)CCC(O)=O)[H])[H]C)[H])[H])O)CC)C

Recommended concentration: 1 μM



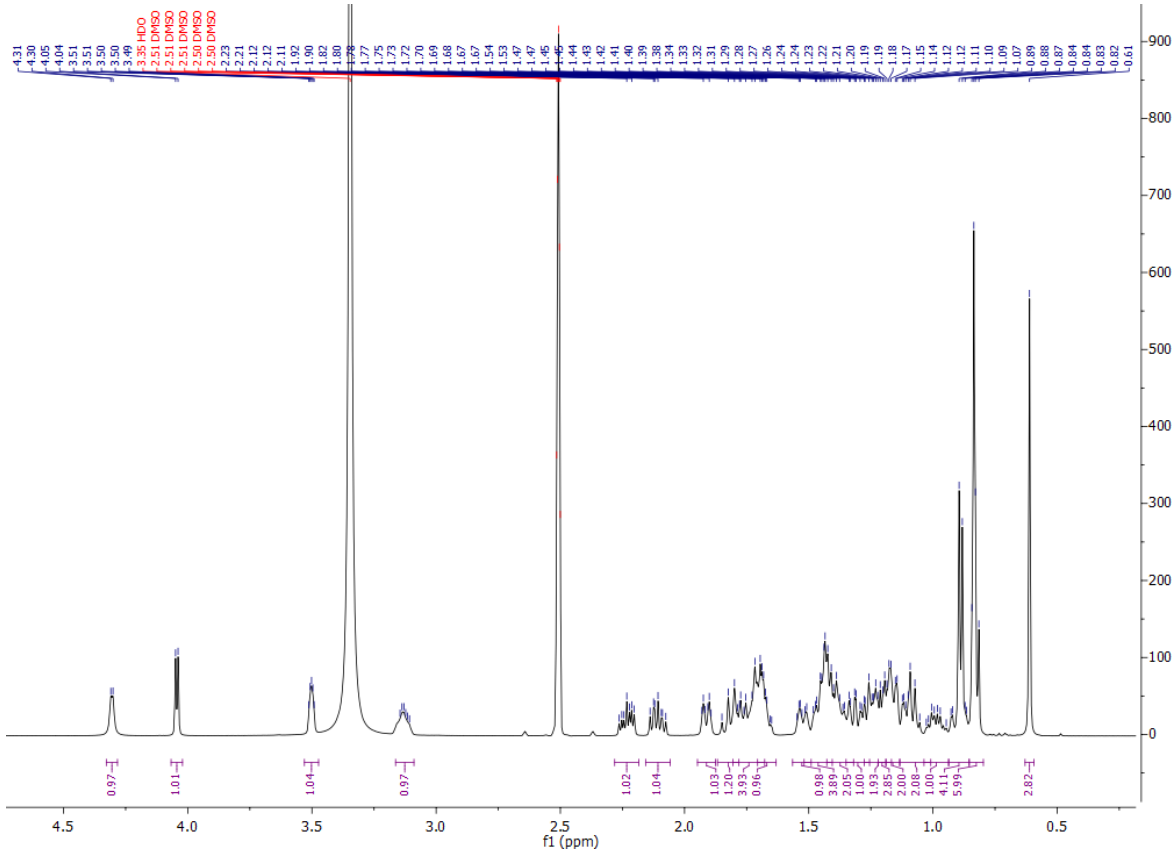
Biological activity

		Type	IC ₅₀ /EC ₅₀ [μM]	Reference
Main NR target:	NR1H4 (FXR)	Agonist	0.30	inhouse
NR off-target:				

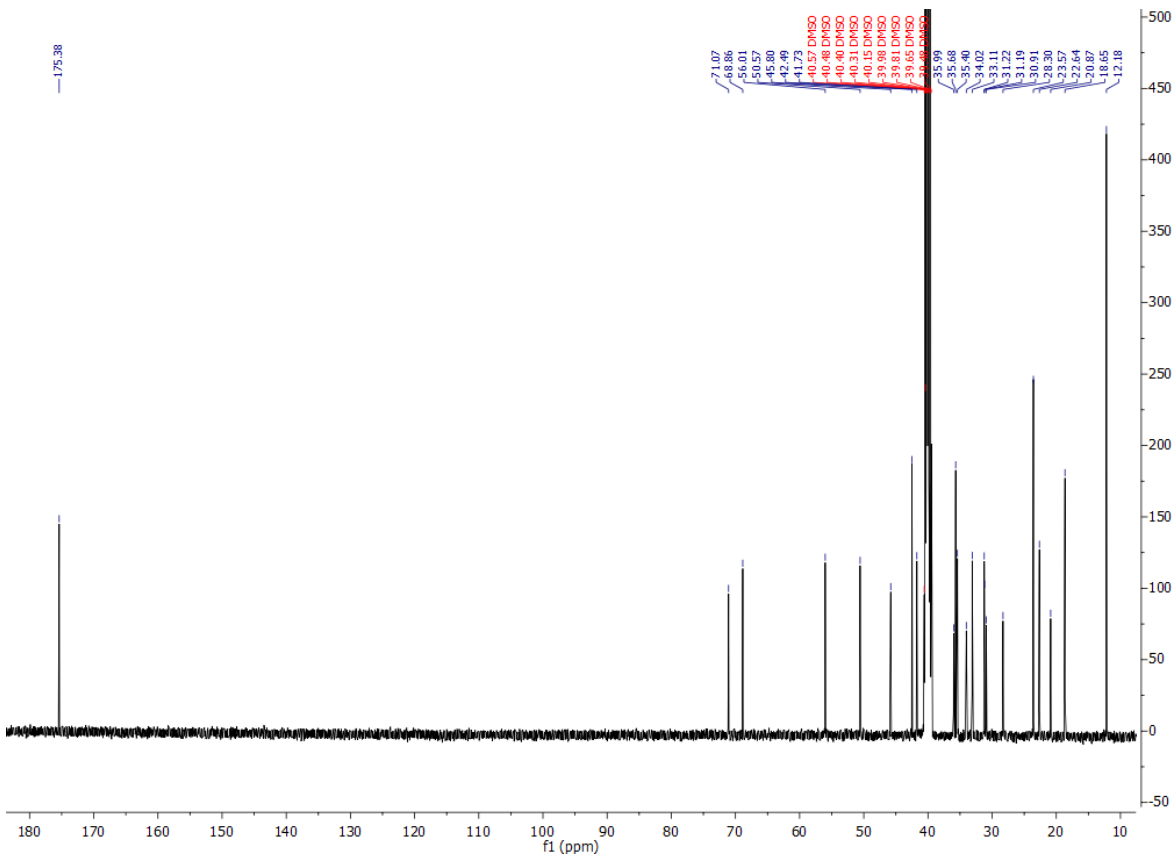
COMPOUND INFORMATION

Identity

¹H NMR



¹³C NMR



COMPOUND INFORMATION

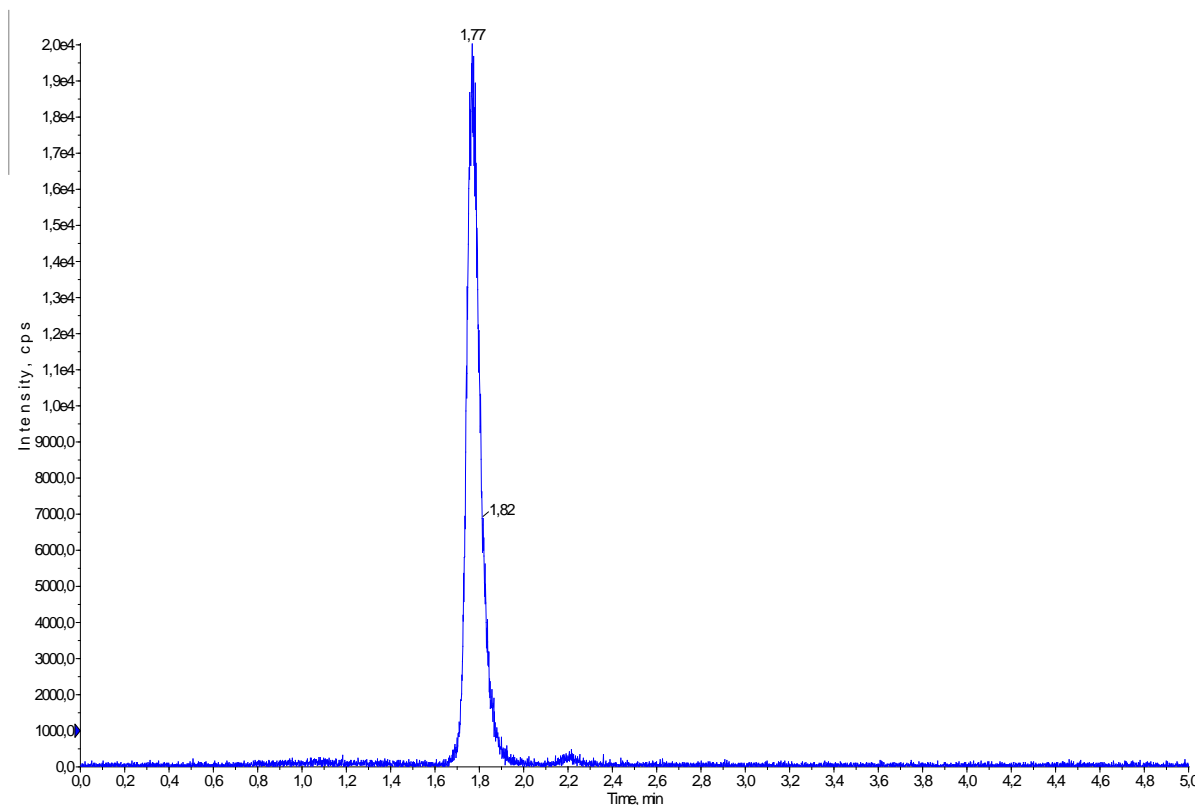
Purity

LC-MS

M_r 420.63

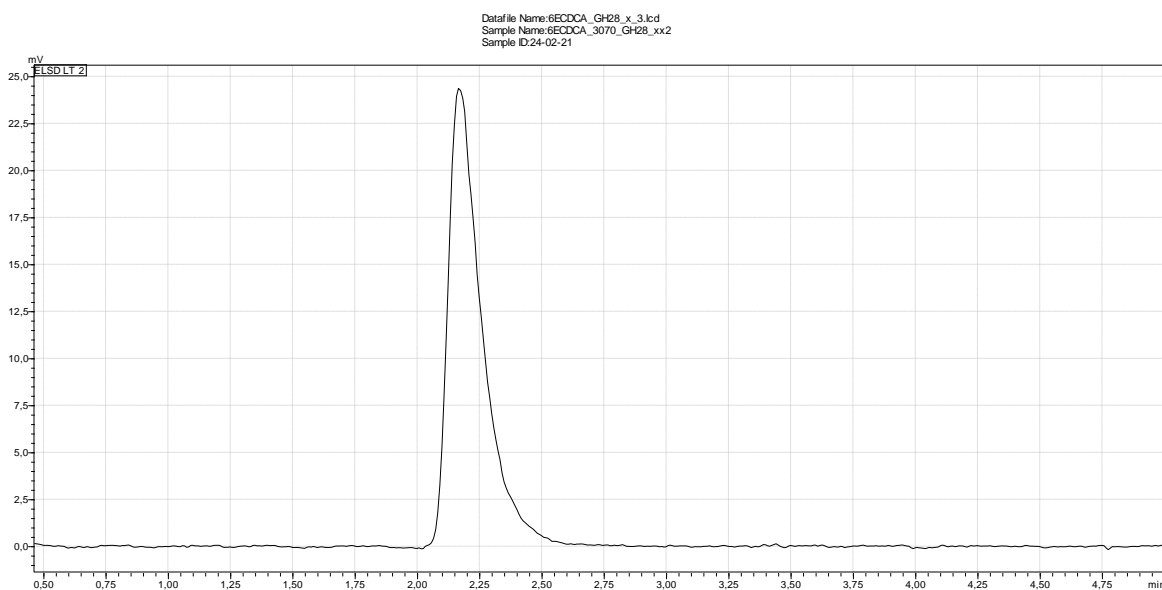
MS: ESI-negative, m/z 419/401

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



LC-ELSD

LC: 0.1% HCOOH/ACN (30/70), sample concentration 100 μ M



COMPOUND INFORMATION

Biological activity

6-ECDCA (Obeticholic acid)
FXR - EC₅₀ 0.30 ± 0.02 μM
432 ± 13 fold activation

