

Seocalcitol

CAS Registry No.: 134404-52-7

Formal Name: (1R,3S,Z)-5-(2-((1R,3aS,7aR,E)-1-((R,3E,5E)-7-ethyl-7-hydroxynona-3,5-dien-2-yl)-7a-methyloctahydro-4H-inden-4-ylidene)ethylidene)-4-methylenecyclohexane-1,3-diol

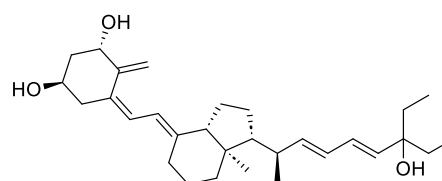
EUBOPEN ID: EUB0000582a

Molecular Formula: C₃₀H₄₆O₃

Molecular Weight: 454.70 g/mol

Smiles:
CCC/C=C/C=C/[C@H]([C@H]1CC[C@@H]2[C@]1(C)CCC/C2=C\C=C3C[C@@H](O)C[C@H](O)C\3=C)C(O)CC

Recommended concentration: 1 μM



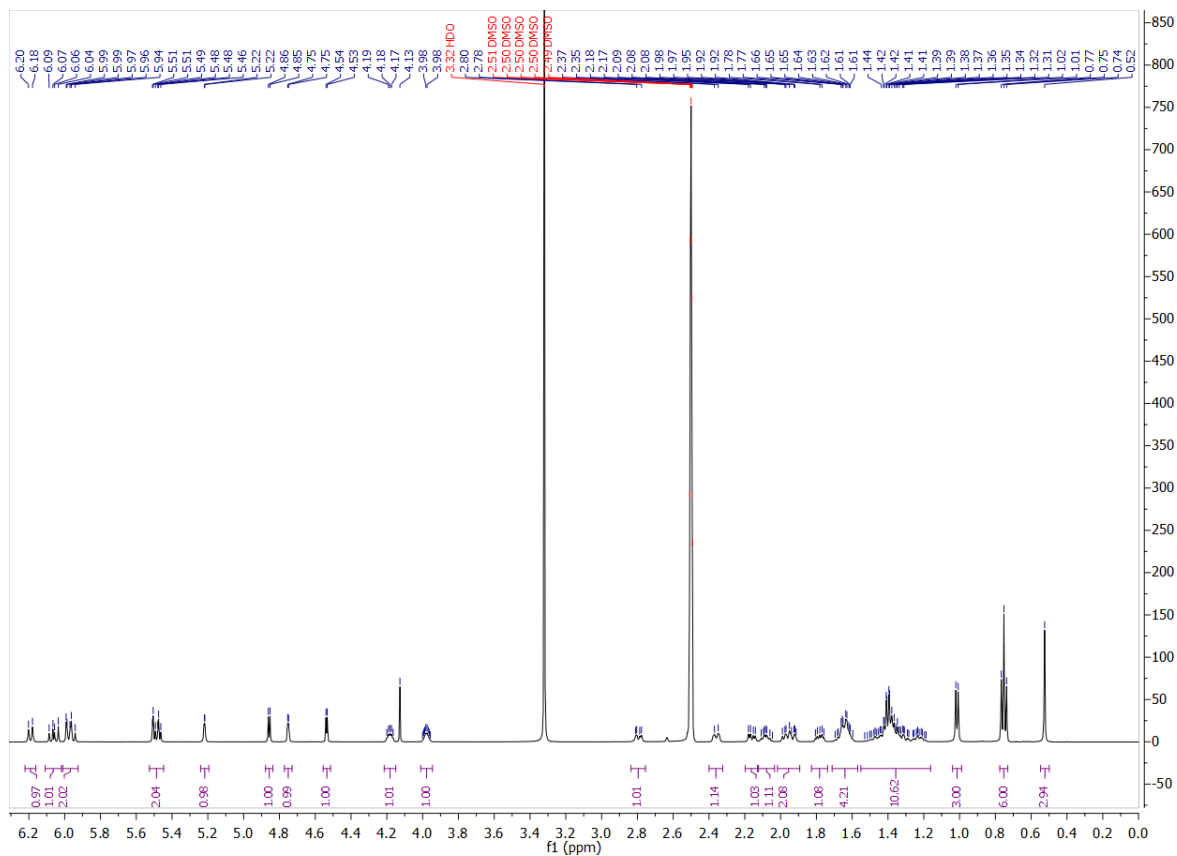
Biological activity

		Type	IC ₅₀ /EC ₅₀ [μM]	Reference
Main NR target:	NR111 (VDR)	Agonist	0.11	inhouse
NR off-target:				

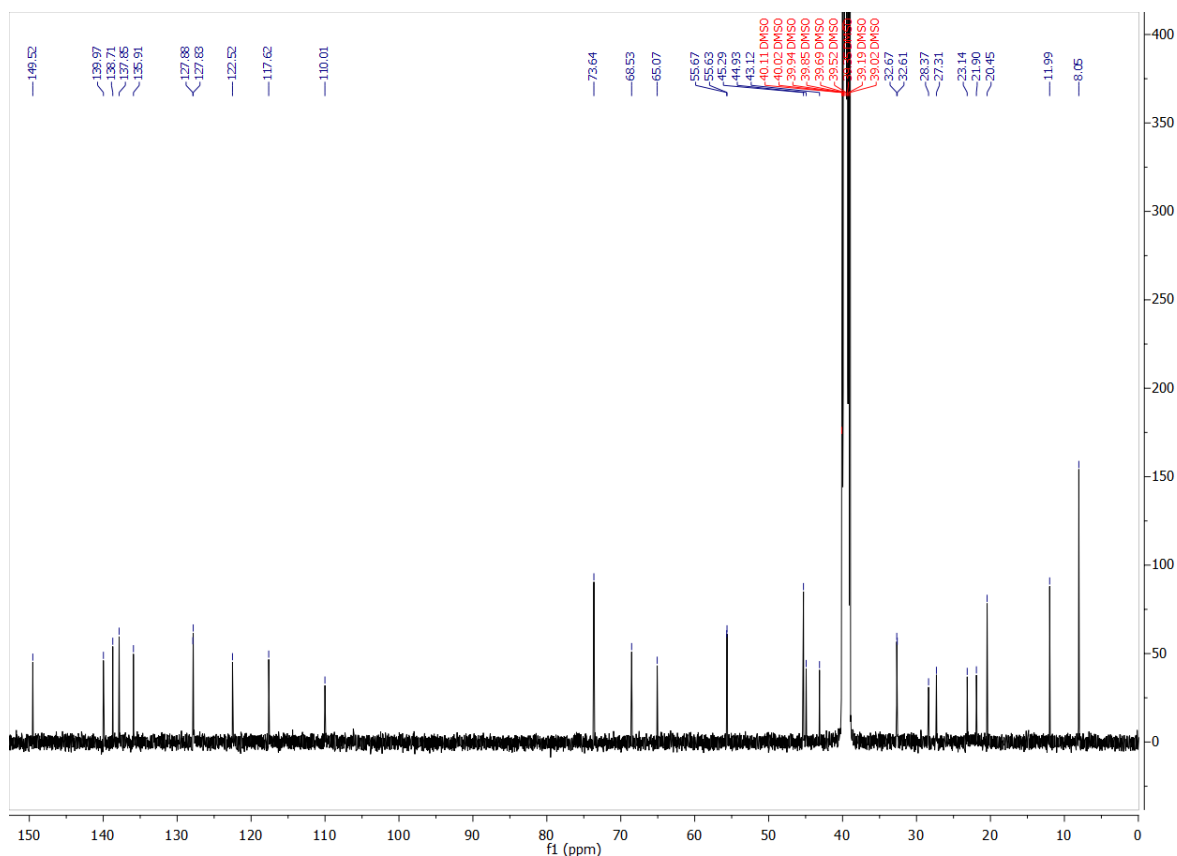
COMPOUND INFORMATION

Identity

¹H NMR



¹³C NMR



COMPOUND INFORMATION

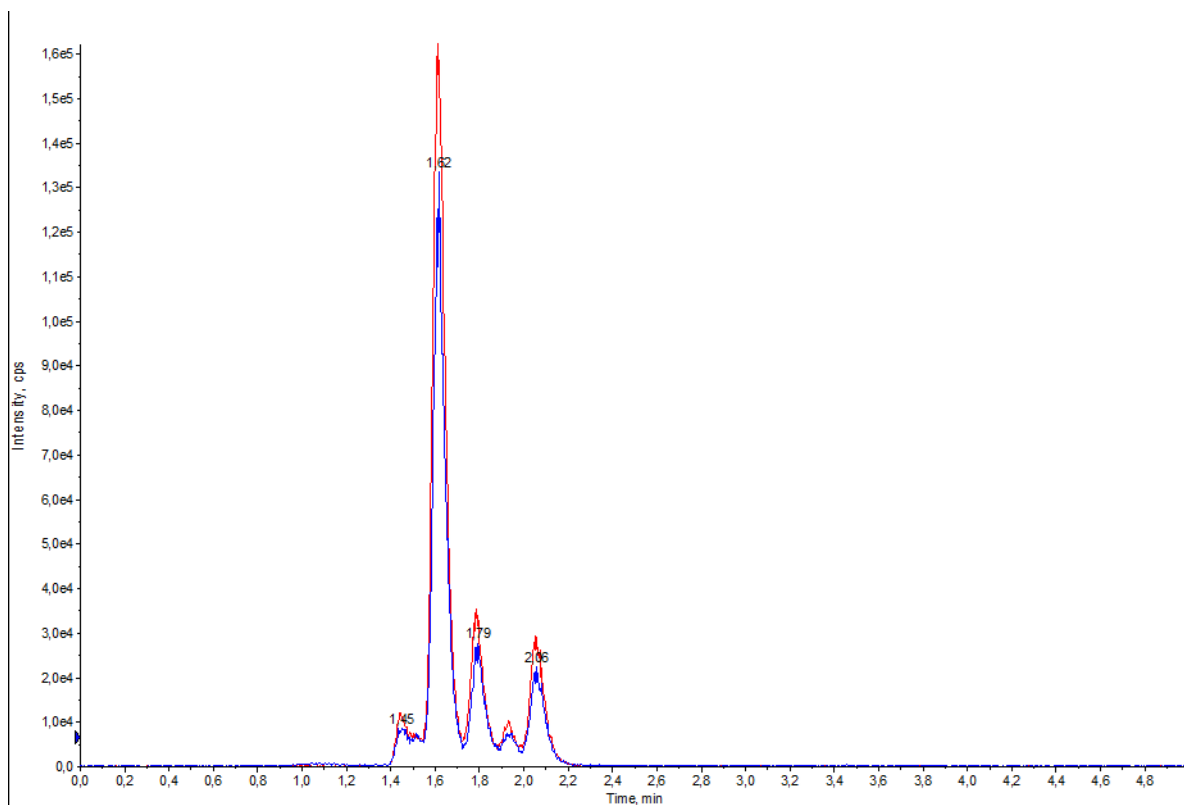
Purity

LC-MS

M_r 454.70

MS: ESI-positive, m/z 437/419 (blue), m/z 437/133 (red), loss of H₂O under these conditions (see e.g. D.A. Vollmer et al., Mass Spectrom. Rev. 2-23, 34, 2015)

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

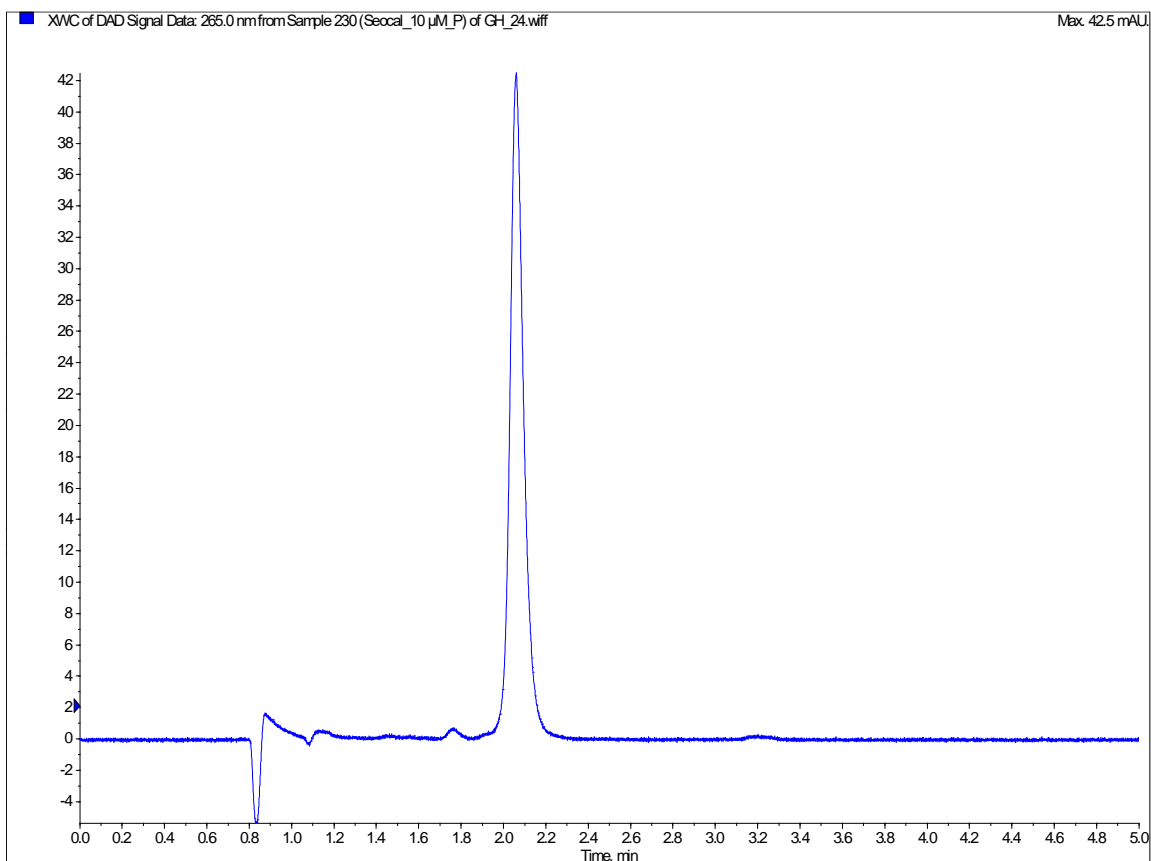
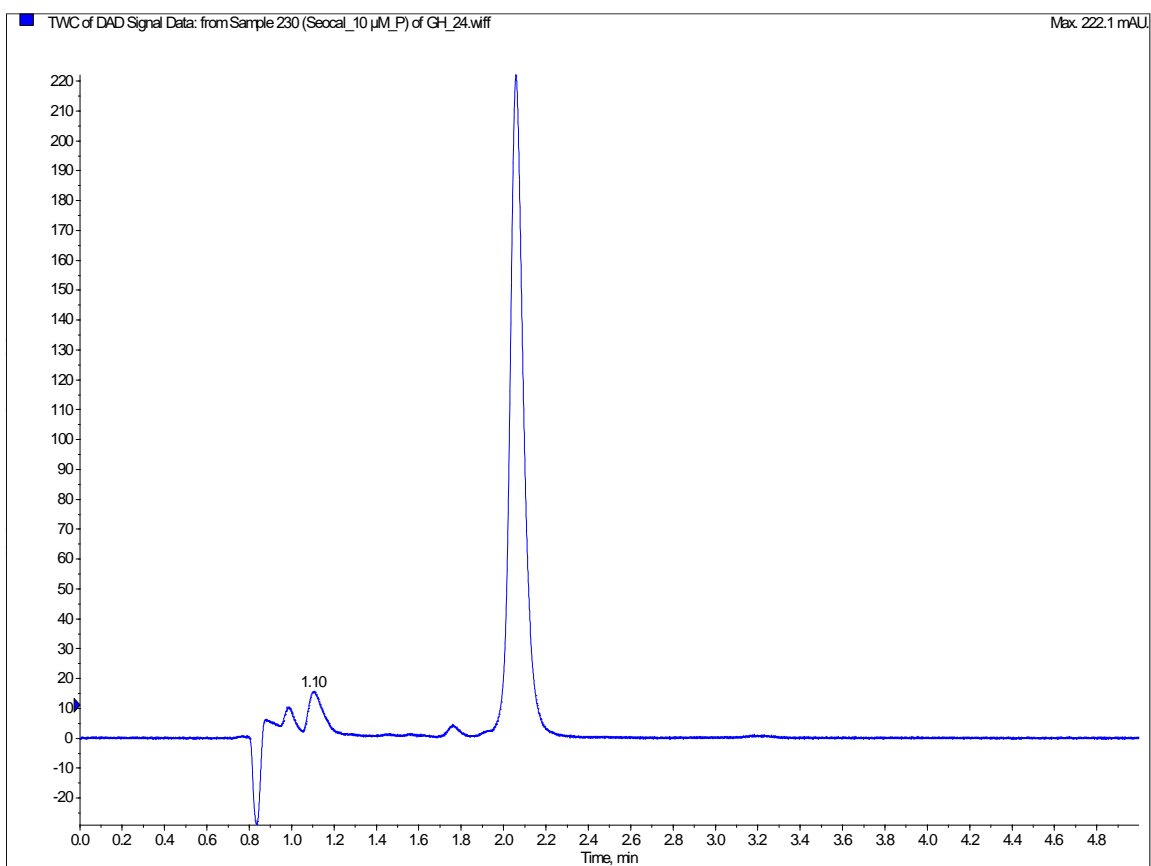


COMPOUND INFORMATION

LC-UV

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

DAD: 240, 250, 265 (XWC), 280, 300 nm



COMPOUND INFORMATION

Biological activity

Seocalcitol
VDR - EC₅₀ 0.11 ± 0.02 μM
70 ± 3 fold activation

