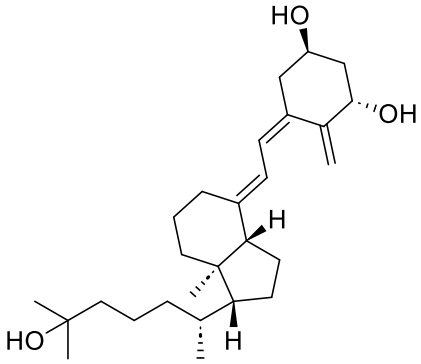
COMPOUND INFORMATION

Calcitriol

CAS Registry No.:	32222-06-3
Formal Name:	(1R,3S,Z)-5-(2-((1R,3aS,7aR,E)-1-((R)-6-hydroxy-6-methylheptan-2-yl)-7a-methyloctahydro-4H-inden-4-ylidene)ethylidene)-4-methylenecyclohexane-1,3-diol
EUBOPEN ID:	EUB0001478a
Molecular Formula:	$C_{27}H_{44}O_3$
Molecular Weight:	416.65 g/mol
Smiles:	O[C@H](C/C1=C/C=C2[C@@]([H])([C@@]3(CCC/2)C)CC[C@]3([H])[C@@H](CCCC(O)(C)C)C[C@@H](C1=C)O
Recommended concentration:	1 µM



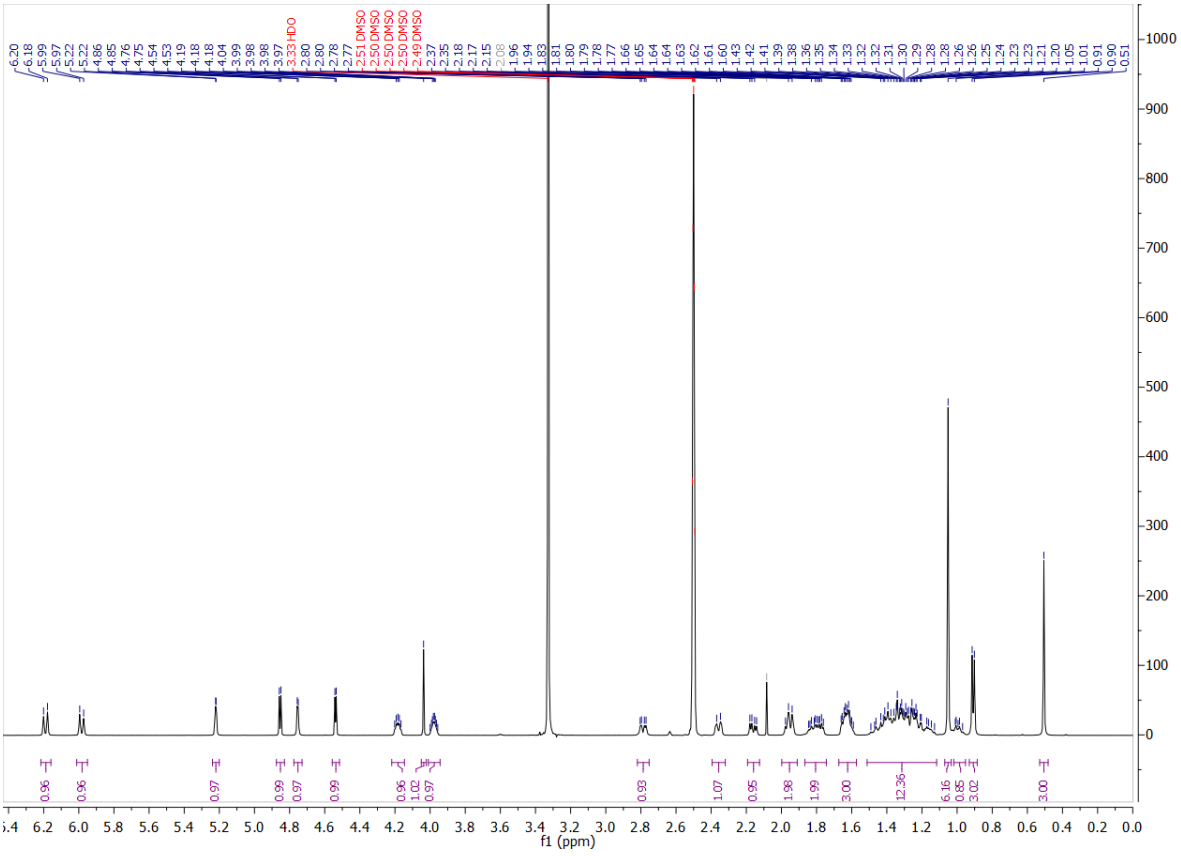
Biological activity

		Type	IC_{50}/EC_{50} [µM]	Reference
Main NR target:	NR1I1 (VDR)	Agonist	0.10	inhouse
NR off-target:				

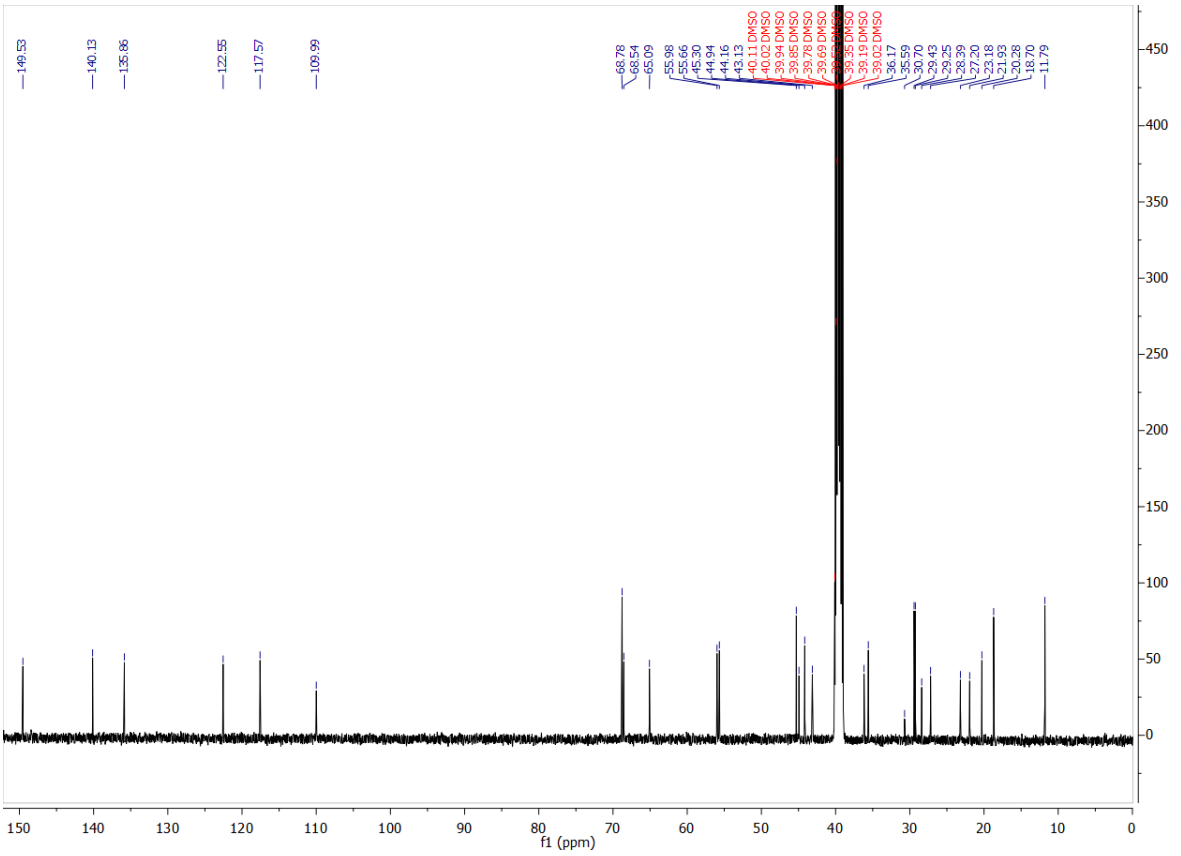
COMPOUND INFORMATION

Identity

^{1}H NMR



^{13}C NMR



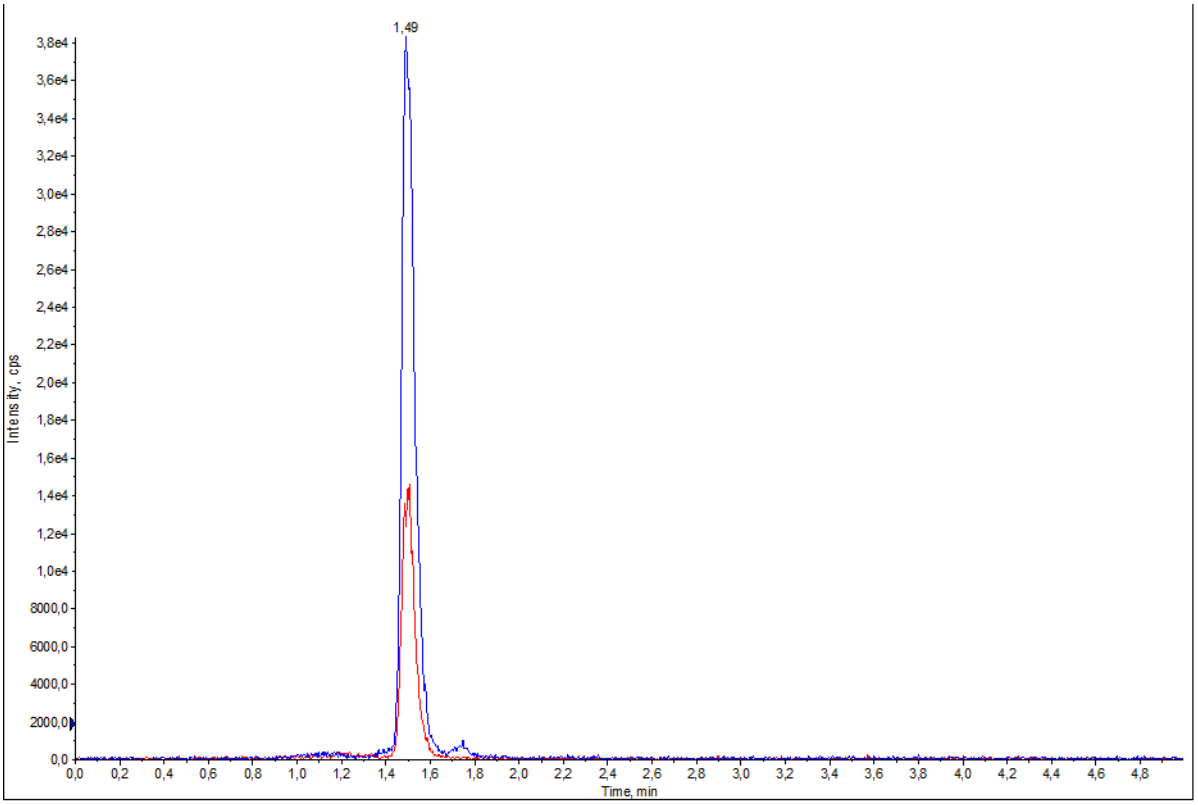
COMPOUND INFORMATION

Purity

LC-MS

MS: ESI-positive, m/z 399/133 (blue), m/z 399/151 (red), loss of H2O under these conditions (see e.g. D.A. Vollmer et al., Mass Spectrom. Rev. 2-23, 34, 2015 and C.J. Hedman et al., J. Chromatogr. B. Analyt. Technol. Biomed. Life Sci. 62–67,2014)

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

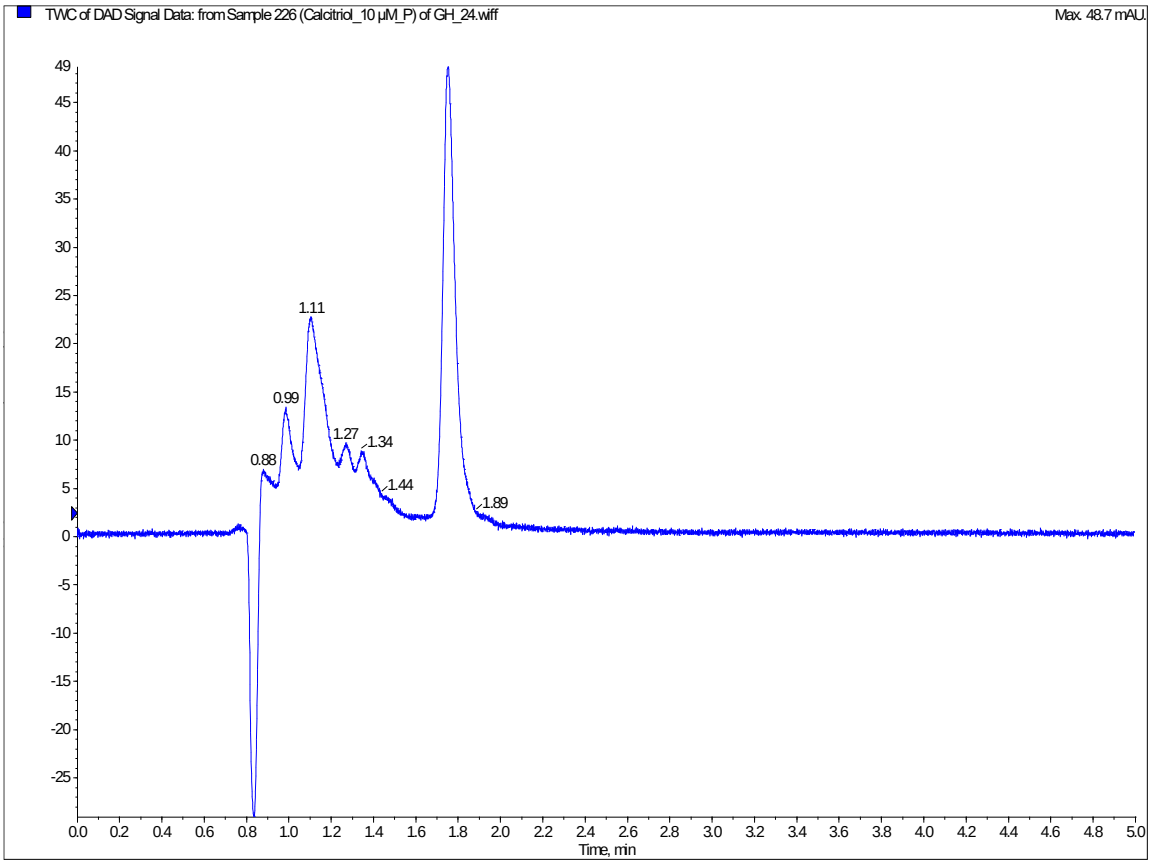


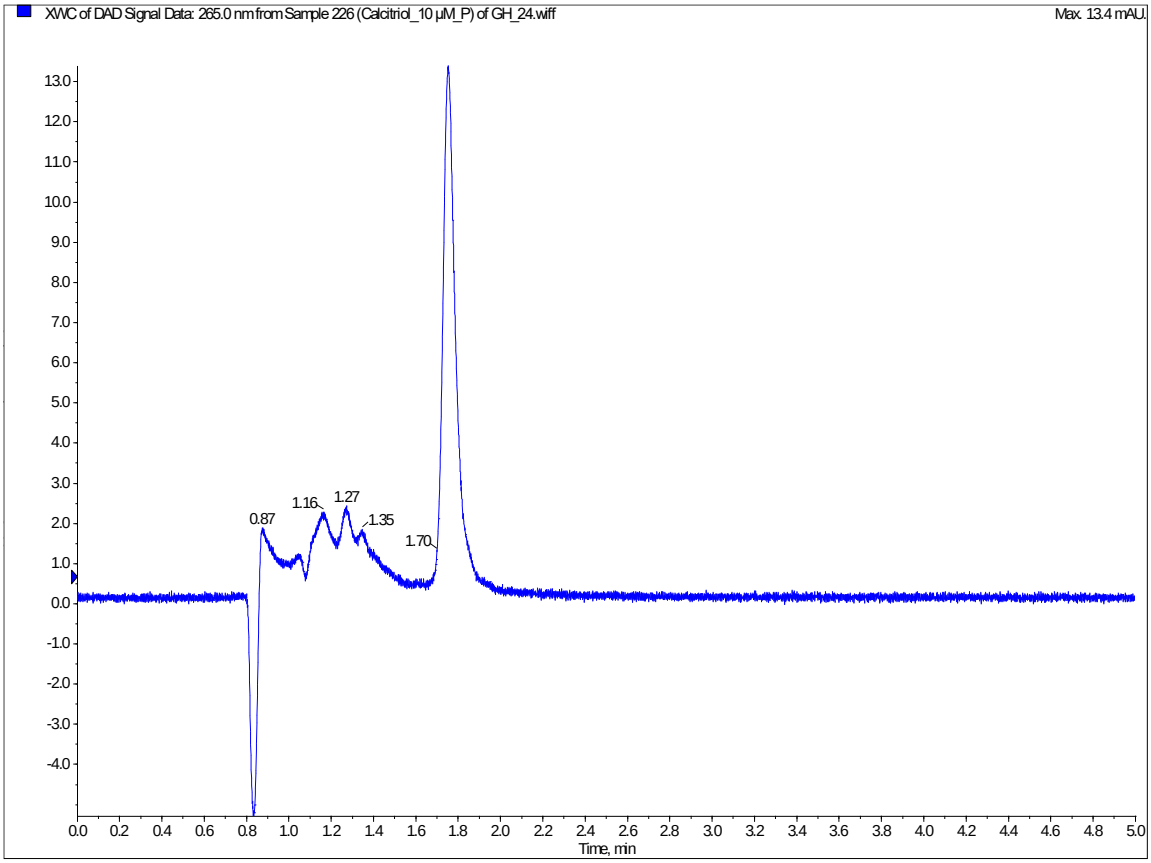
COMPOUND INFORMATION

LC-UV

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

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





COMPOUND INFORMATION

Biological activity