

Retinoic acid (Tretinoin)

CAS Registry No.: 302-79-4

Formal Name: (2E,4E,6E,8E)-3,7-dimethyl-9-(2,6,6-trimethylcyclohex-1-en-1-yl)nona-2,4,6,8-tetraenoic acid

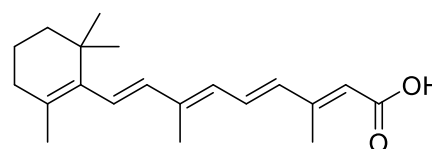
EUBOPEN ID: EUB0001136a

Molecular Formula: C₂₀H₂₈O₂

Molecular Weight: 300.44 g/mol

Smiles: CC1=C(C(CCC1)(C)C)/C=C/C(=C/C=C/C(=C/C(=O)O)/C)/C

Recommended concentration: 1 μM

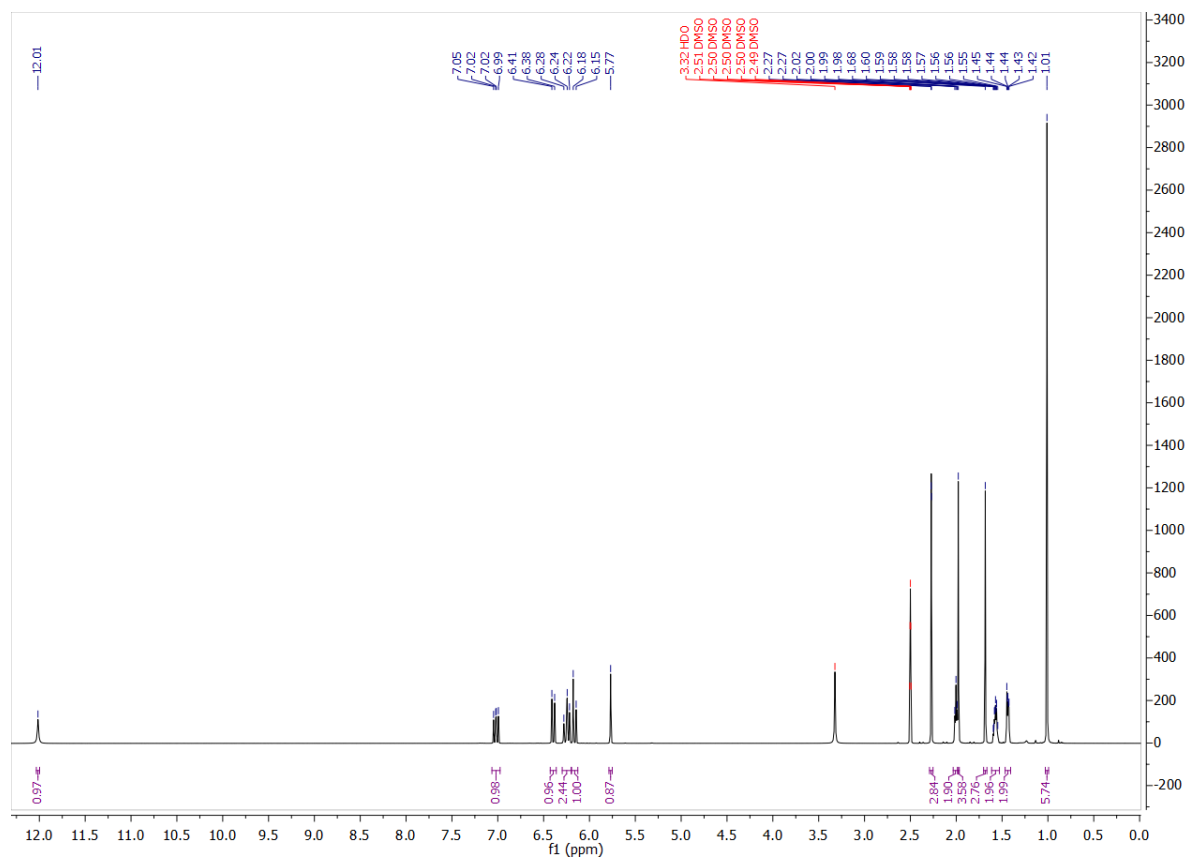


Biological activity

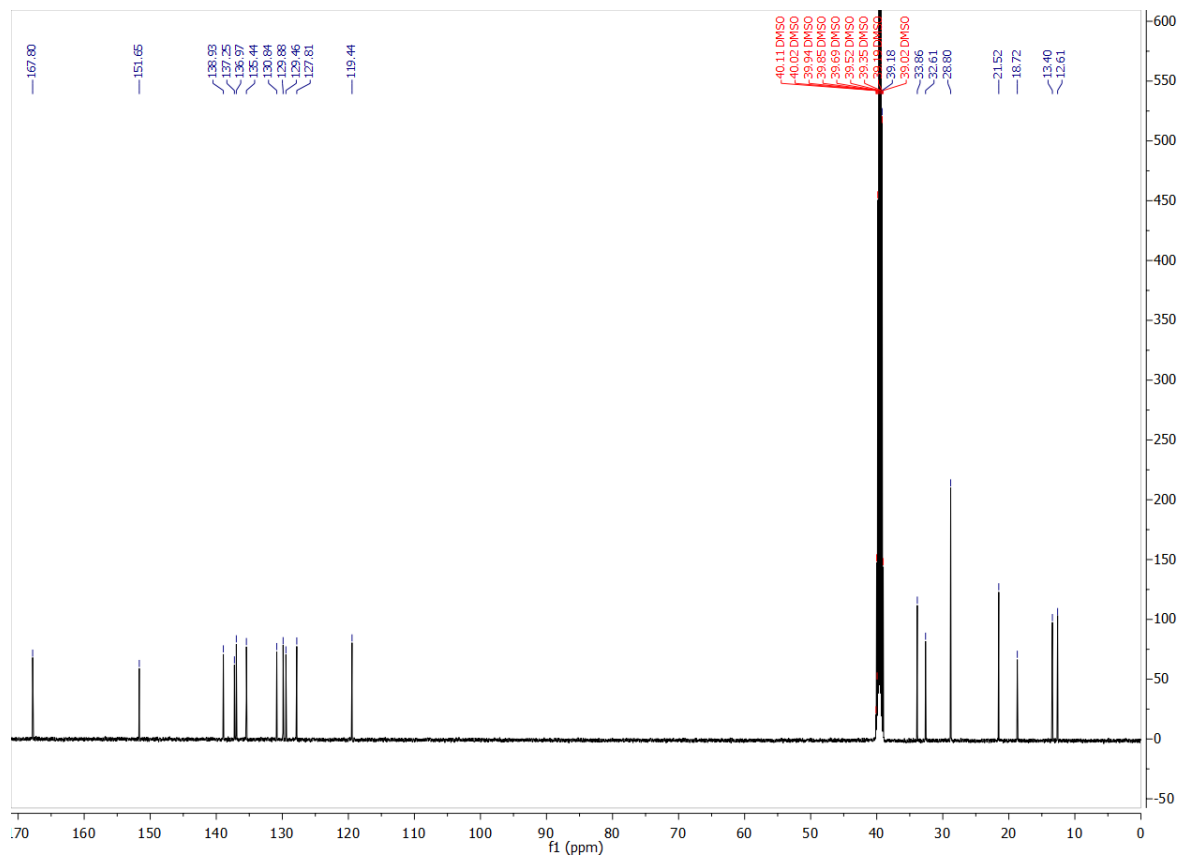
| | | Type | IC ₅₀ /EC ₅₀ [μM] | Reference |
|-----------------|--------------|-----------------|--|---|
| Main NR target: | NR1B1 (RARα) | Agonist | 0.4 | |
| | NR1B2 (RARβ) | Agonist | 0.36 | inhouse |
| | NR1B3 (RARγ) | Agonist | 0.34 | |
| NR off-target: | NR1F1 (RORα) | Inverse agonist | 0.2 | |
| | NR1F2 (RORβ) | Inverse agonist | 0.1 | https://doi.org/10.1016/j.bmcl.2014.09.053 |
| | NR1F3 (RORγ) | Inverse agonist | 0.2 | |
| | NR2B1 (RXRα) | Agonist | 41-fold act. | inhouse |

Identity

¹H NMR



¹³C NMR



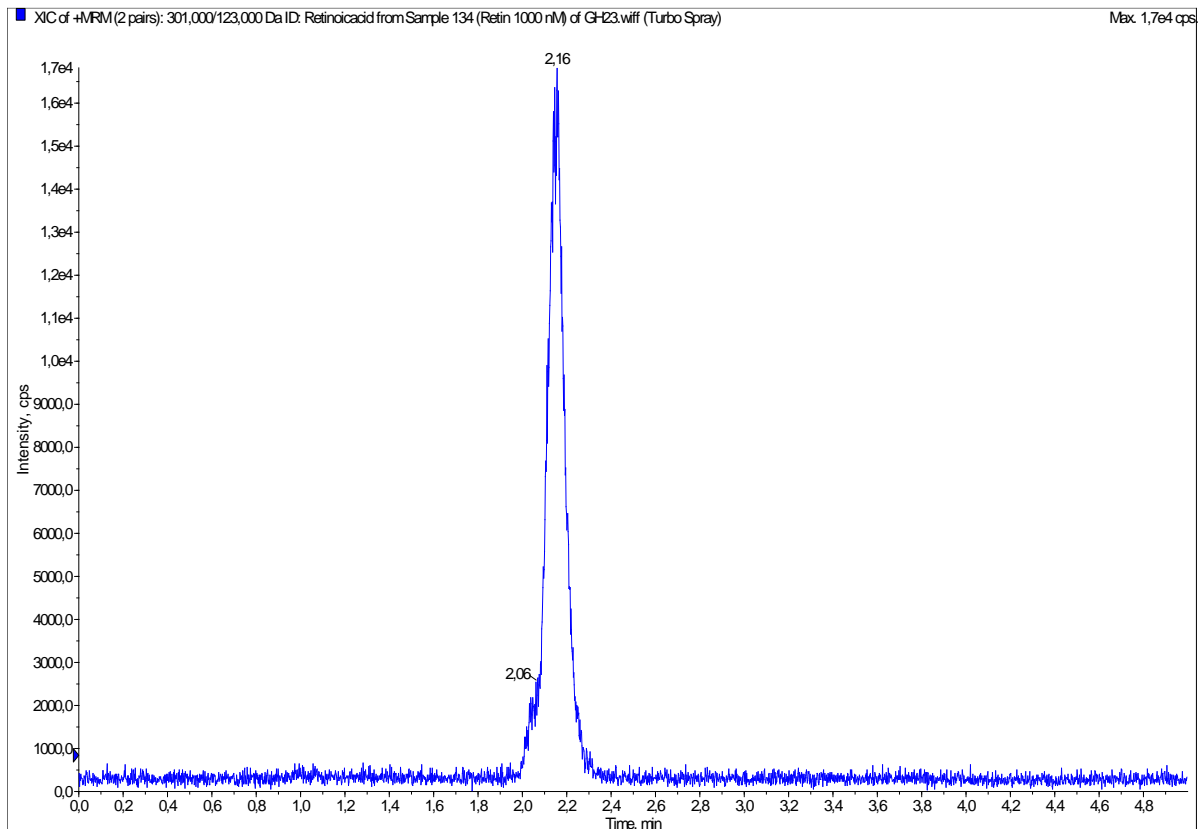
COMPOUND INFORMATION

Purity

M_r 300.44

MS: ESI-positive, m/z 301/123

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

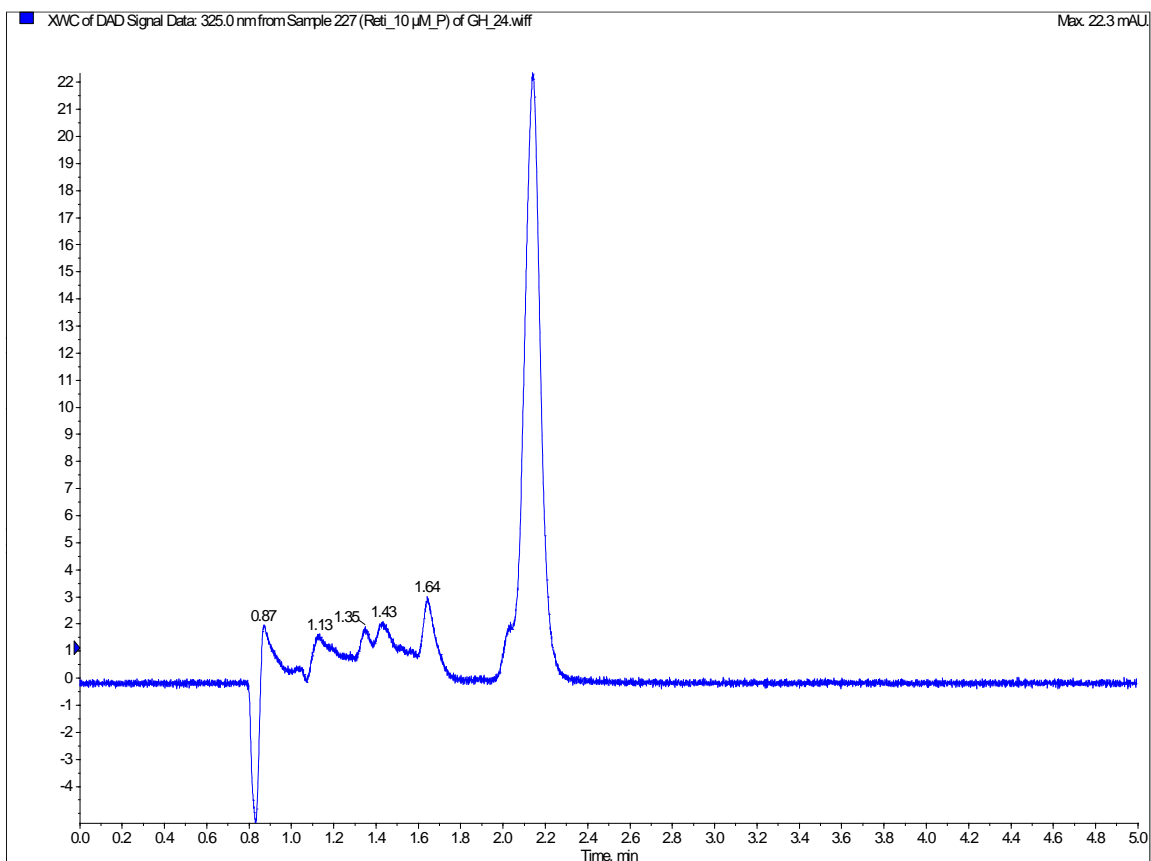
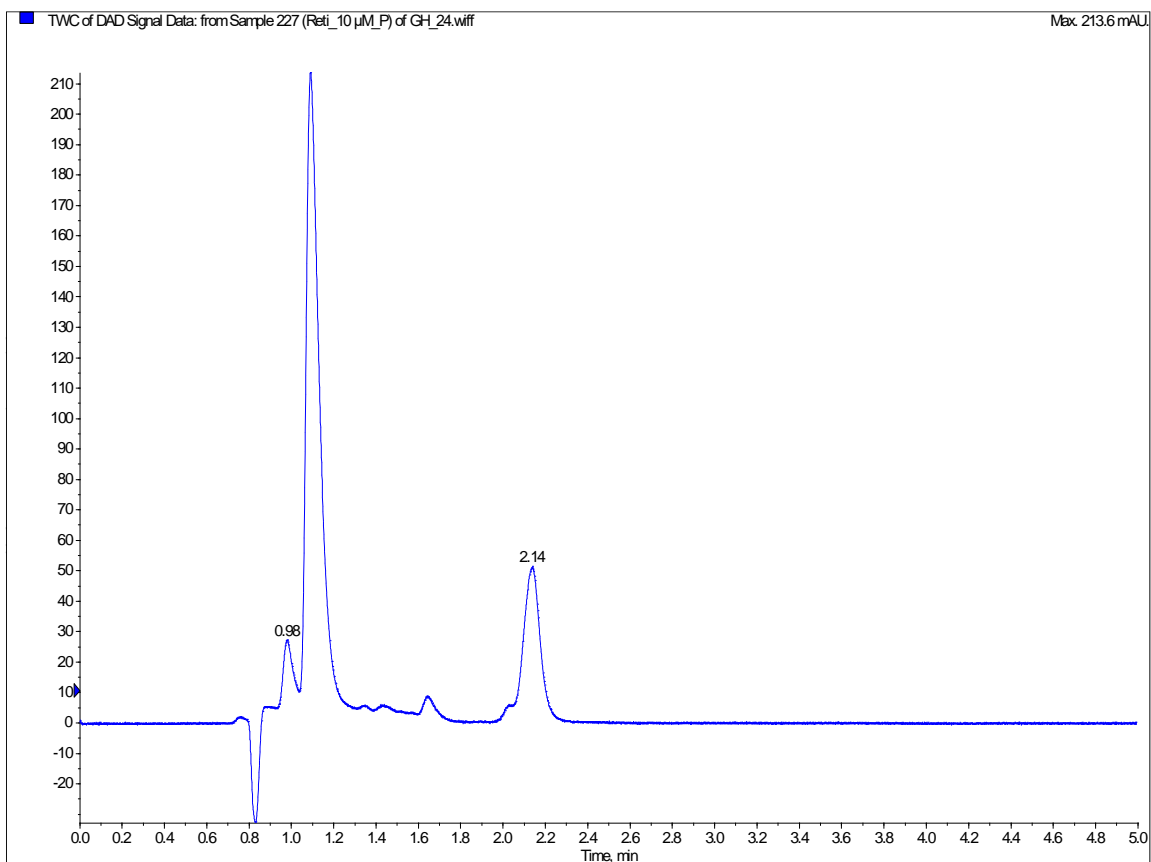


COMPOUND INFORMATION

LC-UV

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

DAD: 230, 250, 238, 270, 325 (XWC) nm



COMPOUND INFORMATION

Biological activity

