

Doxercalciferol

CAS Registry No.: 54573-75-0

Formal Name: (1R,3S,Z)-5-(2-((1R,3aS,7aR,E)-1-((2R,5R,E)-5,6-dimethylhept-3-en-2-yl)-7a-methyloctahydro-4H-inden-4-ylidene)ethylidene)-4-methylenecyclohexane-1,3-diol

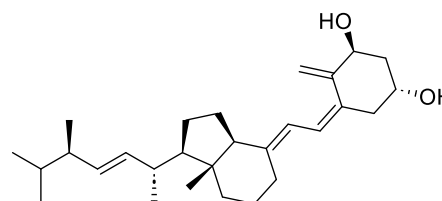
EUBOPEN ID: EUB0000583a

Molecular Formula: C₂₈H₄₄O₂

Molecular Weight: 412.66 g/mol

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

Recommended concentration: 1 μM



Biological activity

		Type	IC ₅₀ /EC ₅₀ [μM]	Reference
Main NR target:	NR111 (VDR)	Agonist	0.96	inhouse
NR off-target:				

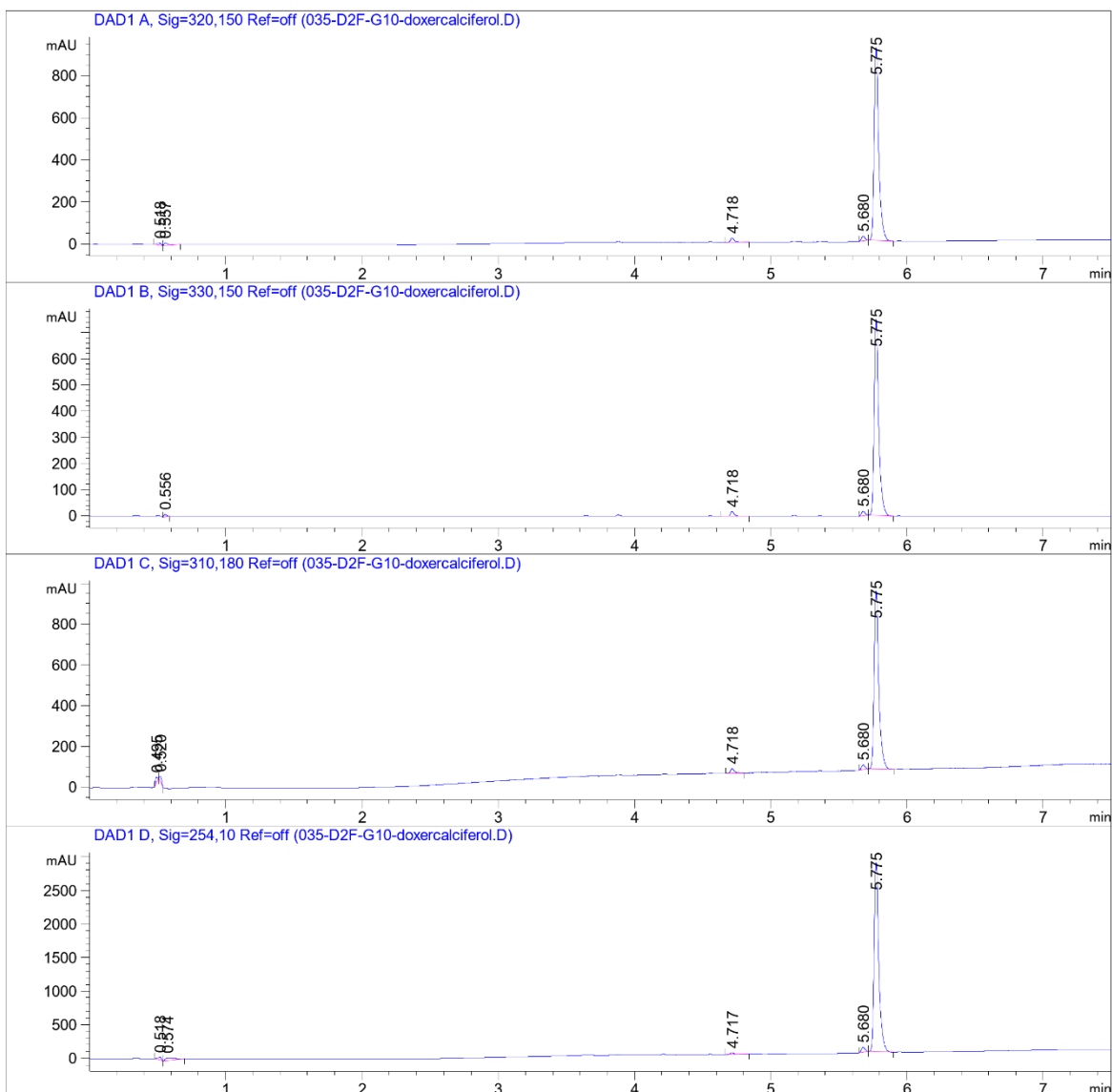
COMPOUND INFORMATION

Purity

Data File W:\analyti...CH01-3_SecondPass 2021-03-25 18-09-21\035-D2F-G10-doxercalciferol.D

Sample Name: doxercalciferol

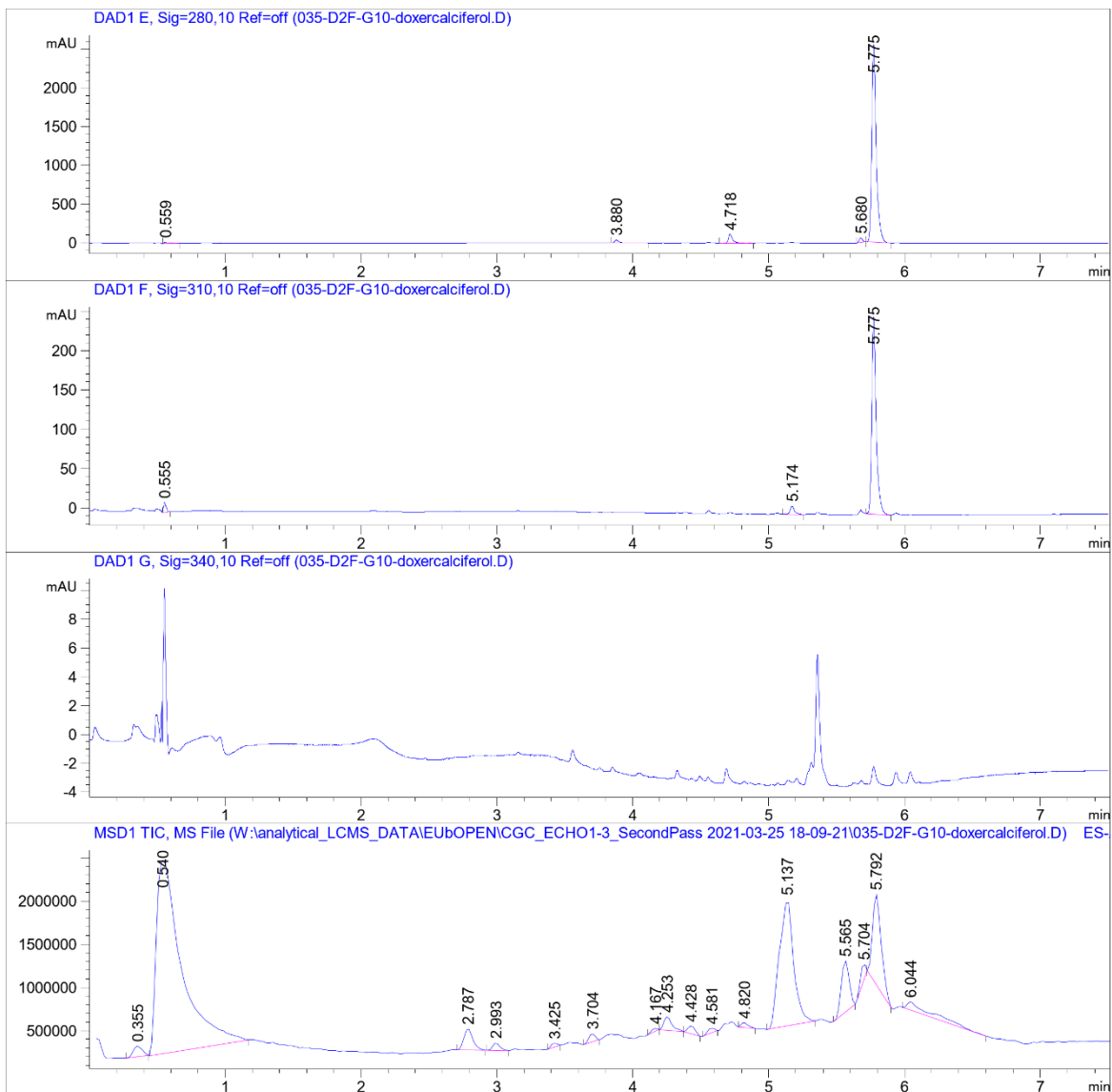
```
=====
Acq. Operator   : SYSTEM                      Seq. Line :   35
Sample Operator : SYSTEM
Acq. Instrument : LCMS test                   Location  : D2F-G10
Injection Date  : 3/26/2021 12:27:14 AM      Inj       :    1
                                           Inj Volume: Inj prog
Sequence File   : W:\analytical_LCMS_DATA\EUBOPEN\CGC_ECH01-3_SecondPass 2021-03-25 18-09-21
                                           \CGC_ECH01-3_SecondPass.S
Method          : W:\analytical_LCMS_DATA\EUBOPEN\CGC_ECH01-3_SecondPass 2021-03-25 18-09-21
                                           \CGL_SECONDPASS_NONPOLCOMP_VIAL2+4_20210323.M (Sequence Method)
Last changed    : 3/25/2021 4:32:02 PM by SYSTEM
Method Info     : CGL wellplate, 0.5 uL of 10 mM DMSO. Dilution with MeCN only (9+9 uL)
=====
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COMPOUND INFORMATION

Data File W:\analyti...CH01-3_SecondPass 2021-03-25 18-09-21\035-D2F-G10-doxercalciferol.D

Sample Name: doxercalciferol



COMPOUND INFORMATION

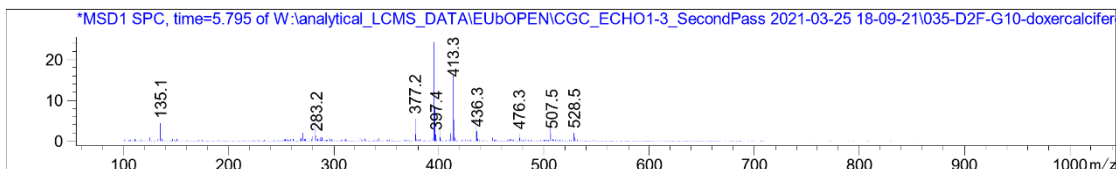


Data File W:\analyti...CH01-3_SecondPass 2021-03-25 18-09-21\035-D2F-G10-doxercalciferol.D

Sample Name: doxercalciferol

MS Signal: MSD1 TIC, MS File, ES-API, Pos, Scan, Frag: 70, "POS Scan"
 Spectra from peak tops.
 Noise Cutoff: 1000 counts.
 Reportable Ion Abundance: > 50%.
 LC Signal: DAD1 A, Sig=320,150 Ref=off
 Peak matching window: 0.1 min

Retention Time (LC)	LC Area	Retention Time (MS)	MS Area	Mol. Weight or Ion
-	-	0.355	559757	200.00 I 183.00 I 159.00 I 142.00 I 110.10 I
0.518	23	0.540	28999792	157.10 I
0.557	37	-	-	
-	-	2.787	1152758	217.10 I
-	-	2.993	337384	274.30 I
-	-	3.425	149487	326.30 I
-	-	3.704	303418	312.20 I 214.10 I
-	-	4.167	108858	280.20 I
-	-	4.253	658168	296.20 I
-	-	4.428	322461	298.20 I 282.20 I 280.20 I
-	-	4.581	178372	228.10 I
4.718	45	-	-	
-	-	4.820	211631	280.20 I
-	-	5.137	10566713	282.20 I
-	-	5.565	2348025	381.30 I 359.20 I 341.30 I 284.20 I 282.20 I
5.680	40	5.704	482055	400.30 I 395.30 I 282.20 I
5.775	2136	5.792	4661668	413.30 I 395.30 I
-	-	6.044	1293452	338.30 I 282.20 I



COMPOUND INFORMATION

Biological activity

Doxercalciferol
VDR - EC₅₀ 0.96 ± 0.07 μM
87 ± 2 fold activation

