

## Rifampicin

**CAS Registry No.:** 13292-46-1

**Formal Name:**

[2,15,17,27,29-pentahydroxy-11-methoxy-3,7,12,14,16,18,22-heptamethyl-26-[(E)-(4-methylpiperazin-1-yl)iminomethyl]-6,23-dioxo-8,30-dioxa-24-azatetracyclo[23.3.1.14,7.05,28]trianta-1(29),2,4,9,19,21,25,27-octaen-13-yl] acetate

**EUBOPEN ID:** EUB0000574a

**Molecular Formula:** C<sub>43</sub>H<sub>58</sub>N<sub>4</sub>O<sub>12</sub>

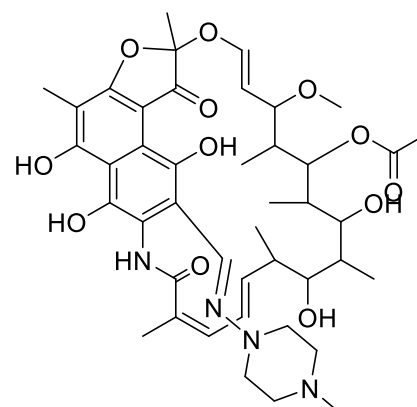
**Molecular Weight:** 822.95 g/mol

**Smiles:**

CC1/C=C/C=C(C)C(NC2=C(/C=N/N3CCN(C)CC3)C(O)=C4C(C(O)=C(C)C5=C4C(C(O/C=C/C(OC)C(C)C(OC(C)=O)C(C)C(O)C(C)C1O)(C)O5)=O)=C2O)=O

**Recommended concentration:**

10 μM

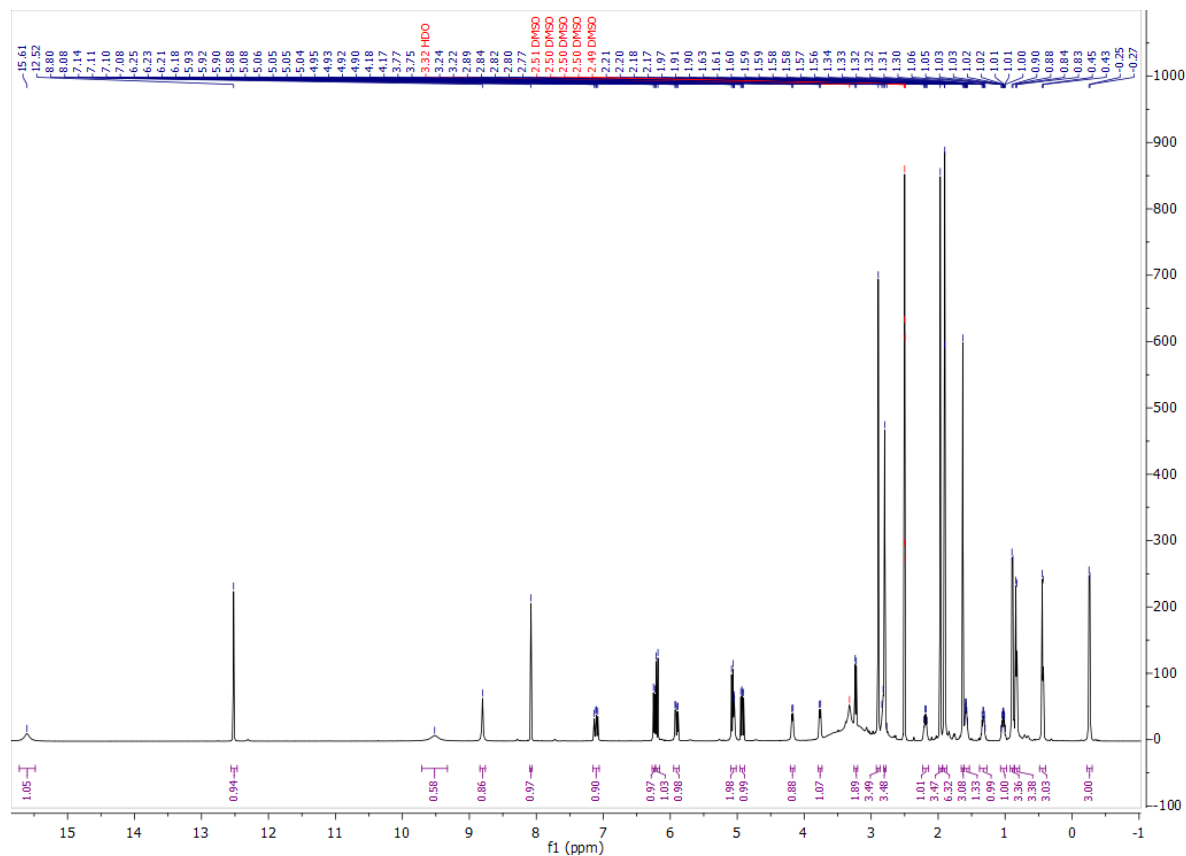


### Biological activity

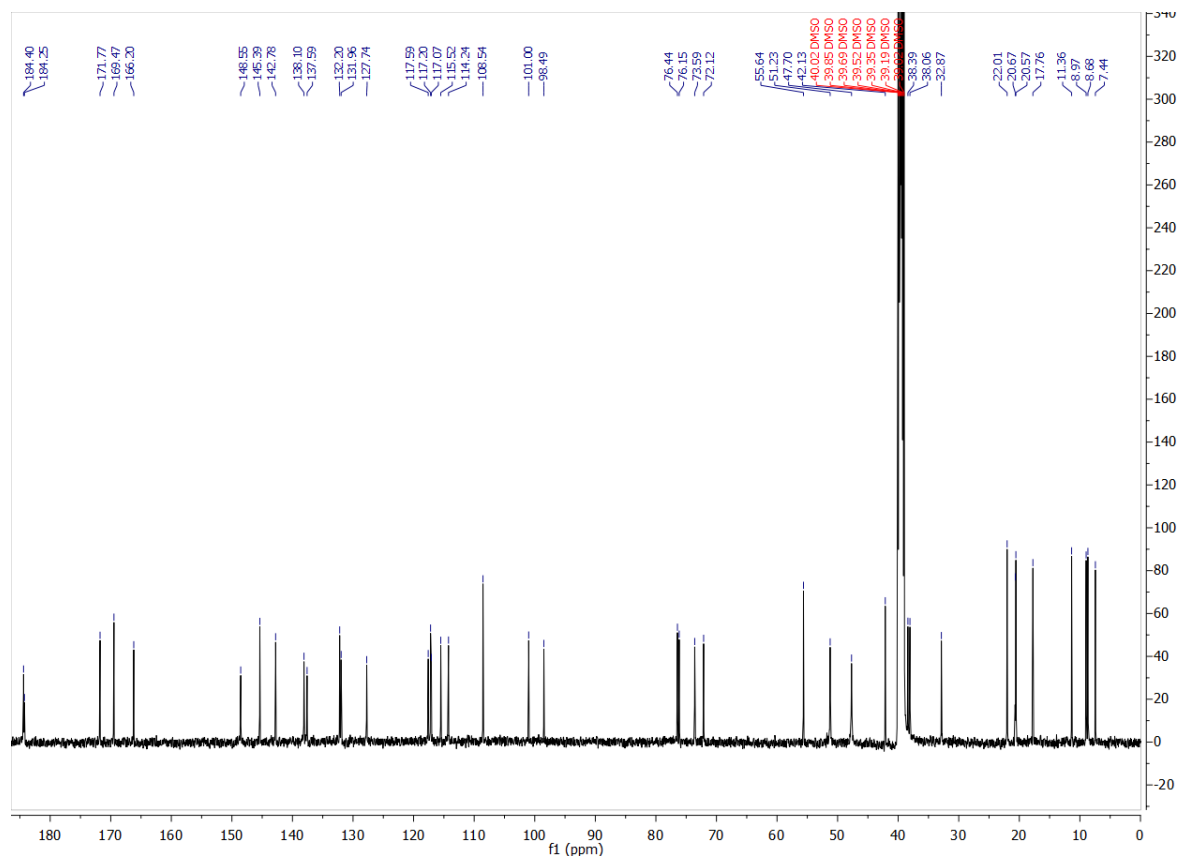
	Type	IC <sub>50</sub> /EC <sub>50</sub> [μM]	Reference
Main NR target:	NR112 (PXR) Agonist	1	<a href="https://doi.org/10.1016/j.bmcl.2016.02.031">https://doi.org/10.1016/j.bmcl.2016.02.031</a>
NR off-target:			

## Identity

### <sup>1</sup>H NMR



### <sup>13</sup>C NMR



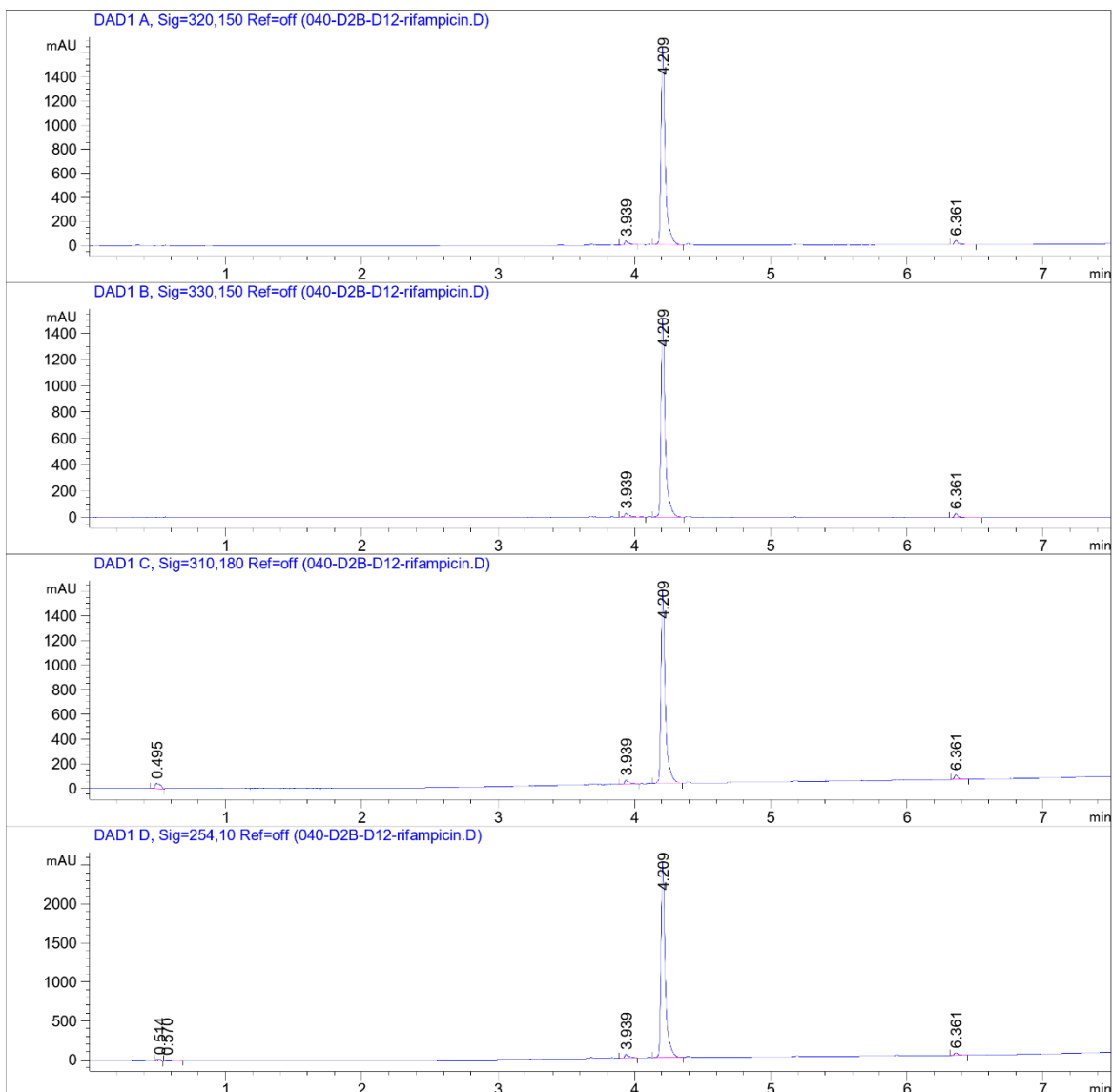
# COMPOUND INFORMATION

## Purity

Data File W:\analyti...\CGC\_ECH01-3\_FirstPass 2021-03-20 13-21-54\040-D2B-D12-rifampicin.D

Sample Name: rifampicin

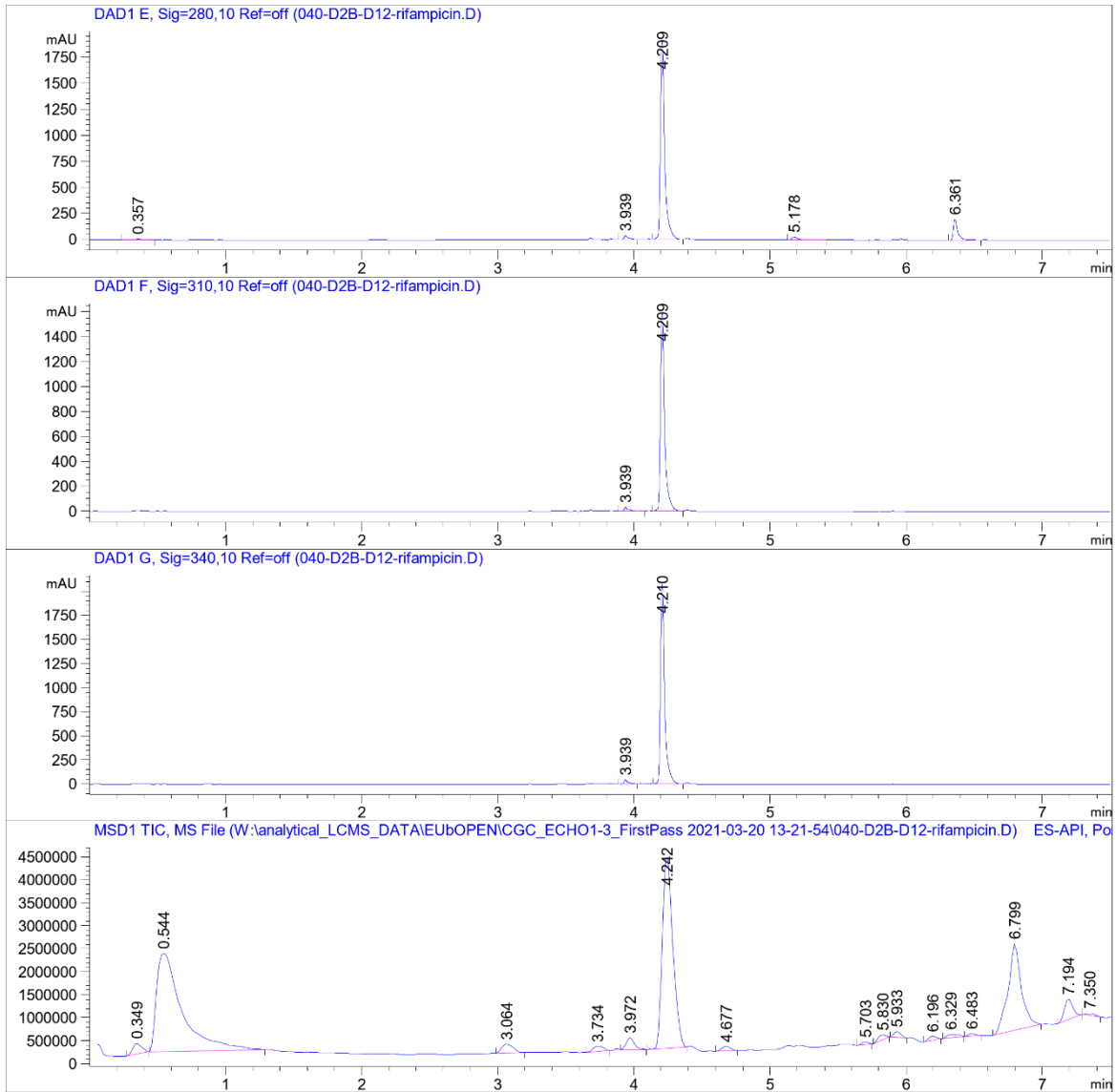
```
=====
Acq. Operator   : SYSTEM                      Seq. Line :   40
Sample Operator : SYSTEM
Acq. Instrument : LCMS test                   Location  : D2B-D12
Injection Date  : 3/20/2021 8:37:50 PM       Inj       :    1
                                           Inj Volume: Inj prog
Sequence File   : W:\analytical_LCMS_DATA\EUBOPEN\CGC_ECH01-3_FirstPass 2021-03-20 13-21-54
                  \CGC_ECH01-3_FirstPass.S
Method          : W:\analytical_LCMS_DATA\EUBOPEN\CGC_ECH01-3_FirstPass 2021-03-20 13-21-54
                  \CGL_FIRSTPASS_GENERALMETHOD_VIAL3+4_20210319.M (Sequence Method)
Last changed    : 3/19/2021 5:35:24 PM by SYSTEM
Method Info     : CGL wellplate, 0.5 uL of 10 mM DMSO, general method
=====
```



# COMPOUND INFORMATION

Data File W:\analyti...\CGC\_ECHO1-3\_FirstPass 2021-03-20 13-21-54\040-D2B-D12-rifampicin.D

Sample Name: rifampicin



# COMPOUND INFORMATION



Data File W:\analyti...\CGC\_ECHO1-3\_FirstPass 2021-03-20 13-21-54\040-D2B-D12-rifampicin.D

Sample Name: rifampicin

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
-	-	0.349	1036918	158.00 I
-	-	0.544	27798364	157.00 I
-	-	3.064	1111412	217.10 I
-	-	3.734	599228	274.20 I
3.939	69	3.972	1075451	808.40 I 807.40 I 749.40 I
4.209	3479	4.242	22688316	824.50 I 823.50 I
-	-	4.677	400338	326.30 I
-	-	5.703	170653	280.20 I
-	-	5.830	416009	296.20 I
-	-	5.933	439643	296.20 I 294.20 I 280.20 I
-	-	6.196	334373	280.20 I 228.20 I
6.361	73	6.329	427603	254.20 I
-	-	6.483	190447	280.20 I
-	-	6.799	12604060	282.20 I
-	-	7.194	1871416	284.20 I 282.20 I
-	-	7.350	228446	400.30 I 282.20 I

