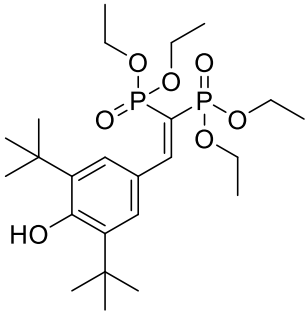
# COMPOUND INFORMATION

## SR12813

| | |
|---|---|
| **CAS Registry No.:** | 126411-39-0 |
| **Formal Name:** | Tetraethyl (2-(3,5-di-tert-butyl-4-hydroxyphenyl)ethene-1,1-diyl)bis(phosphonate) |
| **EUBOPEN ID:** | EUB0000576a |
| **Molecular Formula:** | $C_{24}H_{42}O_7P_2$ |
| **Molecular Weight:** | 504.54 g/mol |
| **Smiles:** | CCOP(/C(P(OCC)(OCC)=O)=C/C1=CC(C(C)(C)C)=C(O)C(C(C)(C)C)=C1)(OCC)=O |
| **Recommended concentration:** | 1 µM |



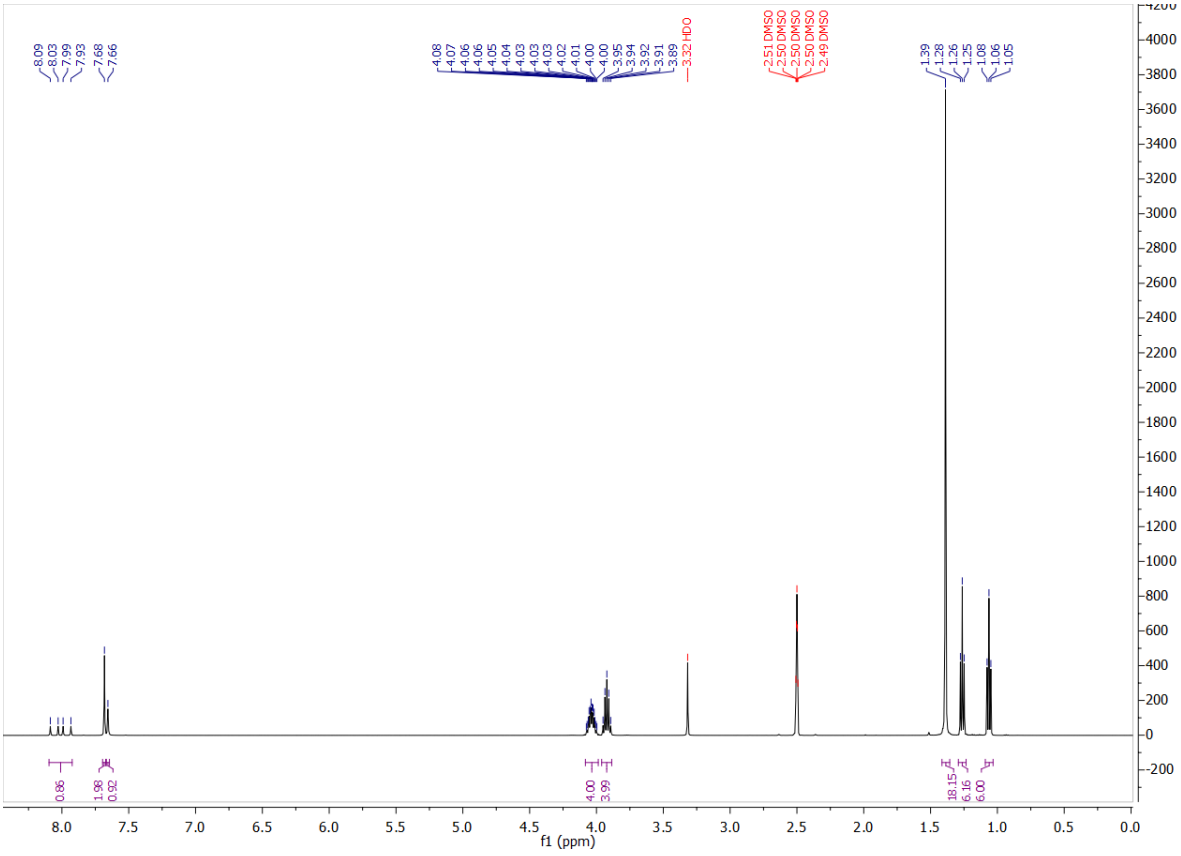

**Biological activity**

| | | Type | $IC_{50}/EC_{50}$ [µM] | Reference |
|---|---|---|---|---|
| Main NR target: | NR1I2 (PXR) | Agonist | 0.14 | https://doi.org/10.1124/mol.106.033415 |
| NR off-target: | | | | |

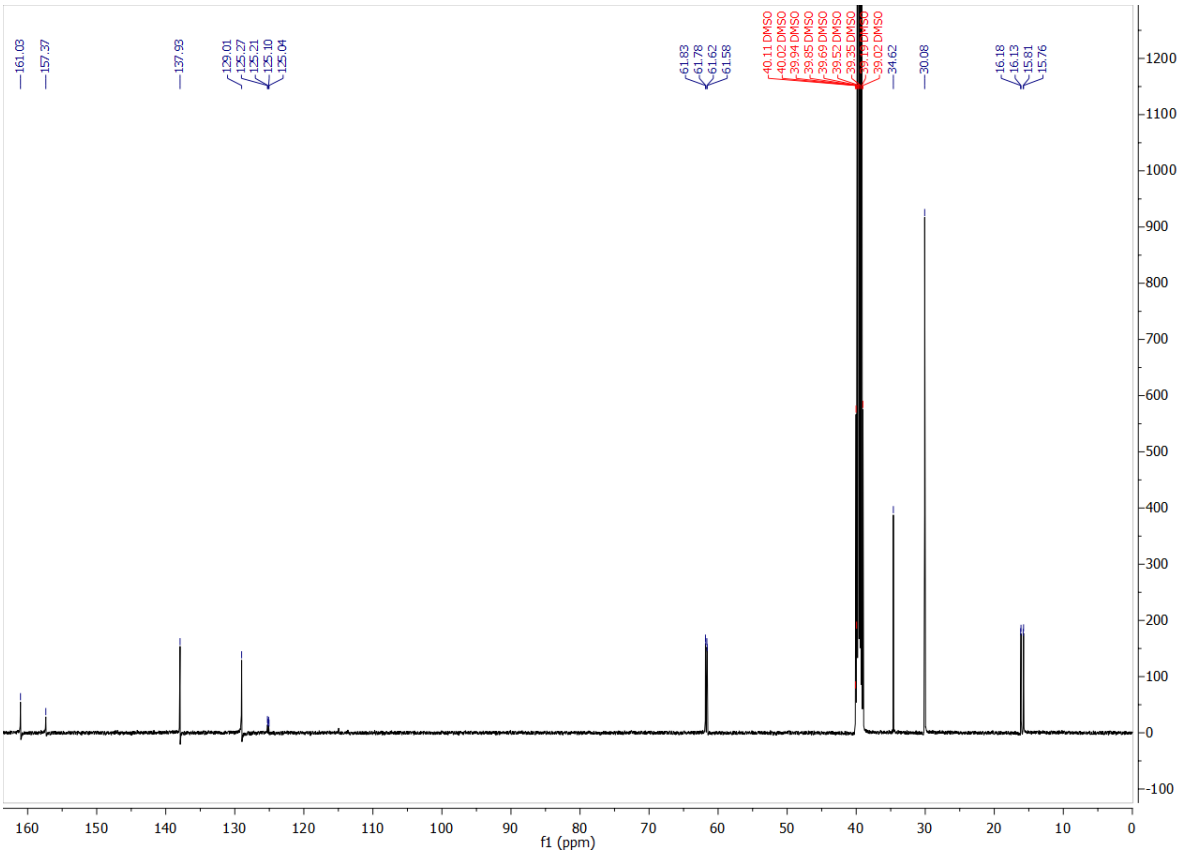
# **COMPOUND** INFORMATION

## Identity

### $^{1}$H NMR




### $^{13}$C NMR

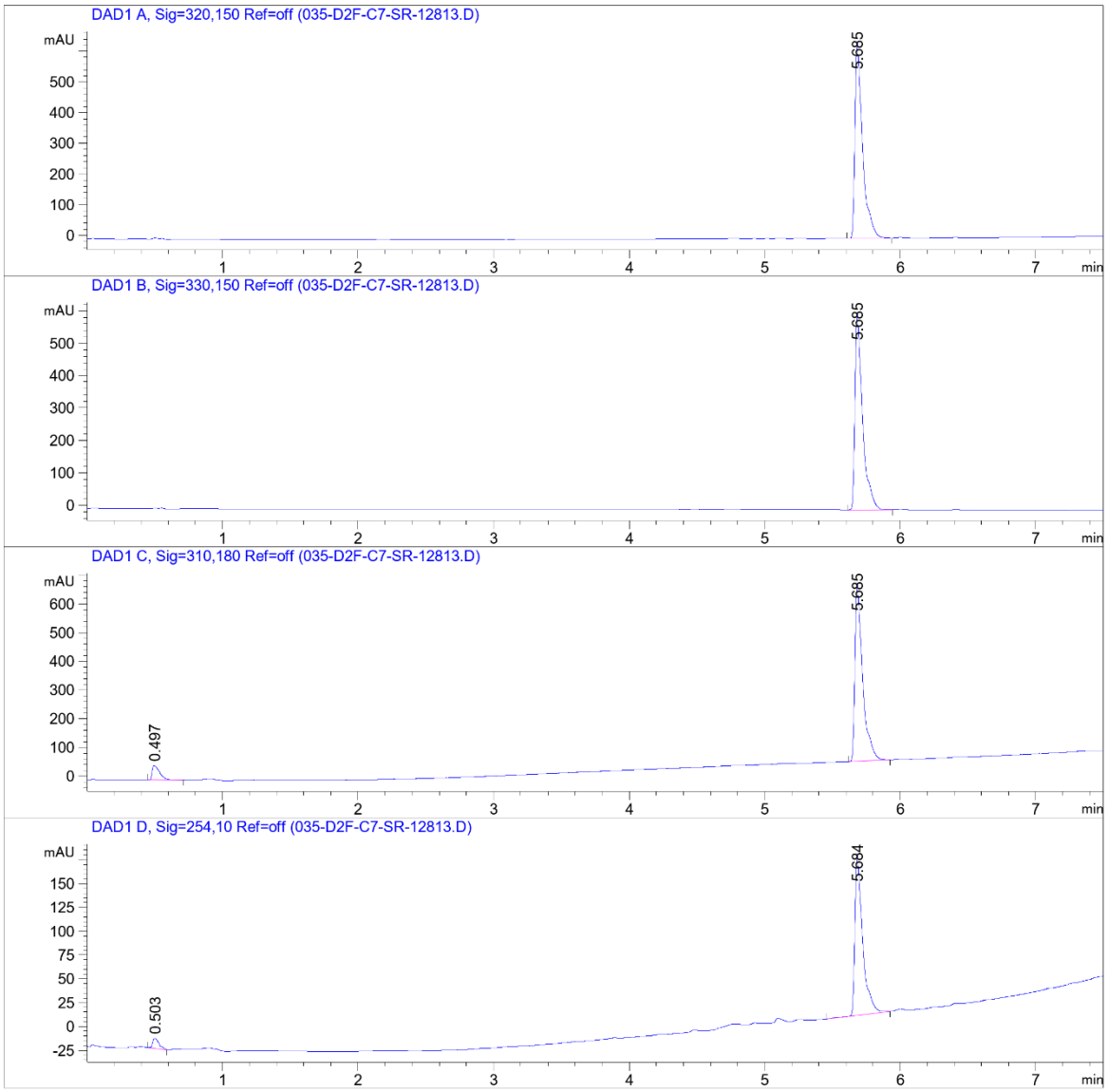


# COMPOUND INFORMATION

## Purity

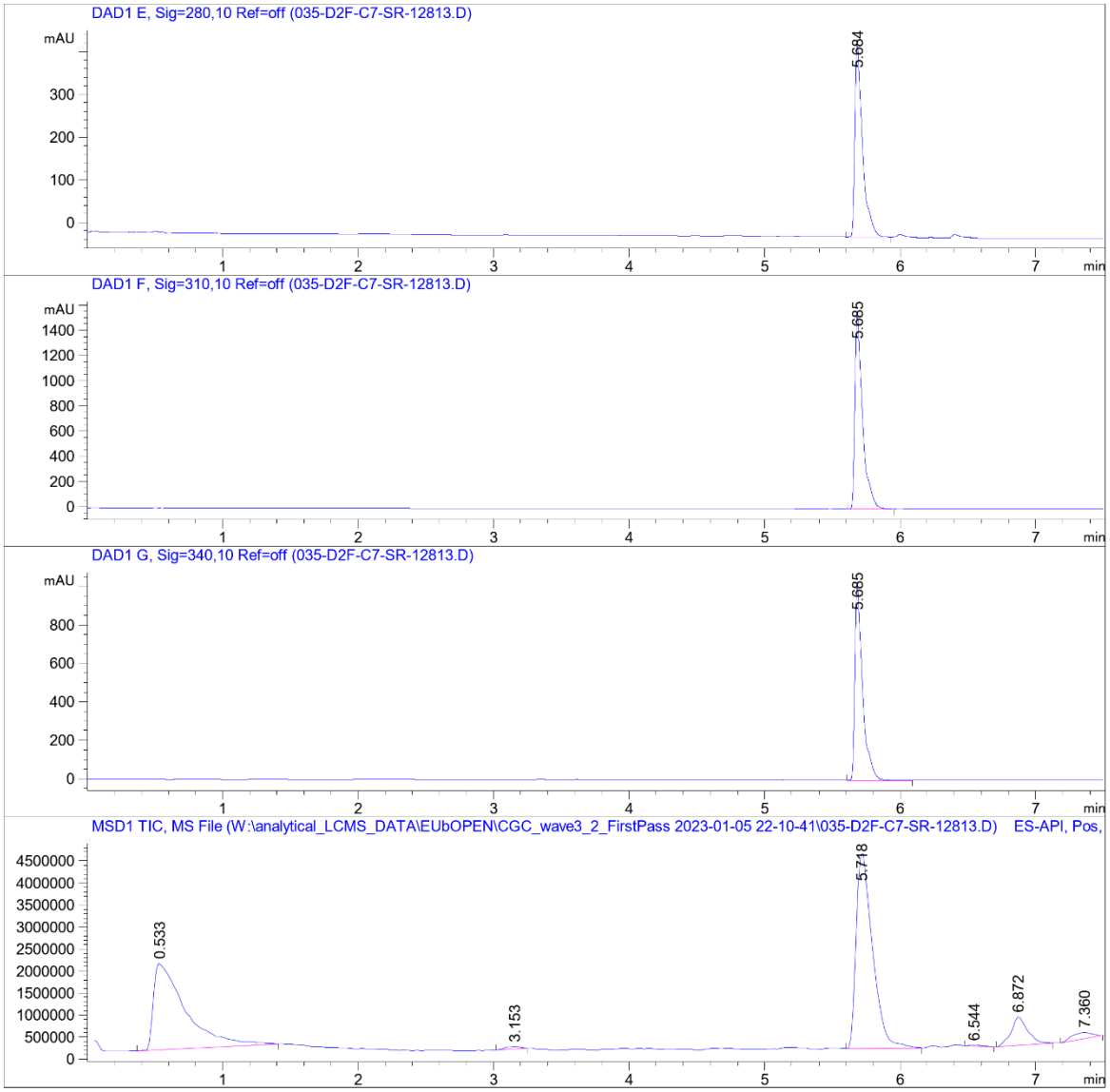
Data File W:\analyti...PEN\CGC_wave3_2_FirstPass 2023-01-05 22-10-41\035-D2F-C7-SR-12813.D
Sample Name: SR-12813

```
======================================================================
Acq. Operator   : SYSTEM                        Seq. Line :  35
Sample Operator : SYSTEM
Acq. Instrument : LCMS test                      Location :   D2F-C7
Injection Date  : 1/6/2023 4:29:43 AM                 Inj :   1
                                                Inj Volume : Inj prog
Sequence File   : W:\analytical_LCMS_DATA\EUbOPEN\CGC_wave3_2_FirstPass 2023-01-05 22-10-41
                  \CGC_wave3_2_FirstPass.S
Method          : W:\analytical_LCMS_DATA\EUbOPEN\CGC_wave3_2_FirstPass 2023-01-05 22-10-41
                  \CGL_FIRSTPASS_GENERALMETHOD_VIAL1+2_20210319.M (Sequence Method)
Last changed    : 1/25/2022 4:36:18 PM by SYSTEM
Method Info     : CGL wellplate, 0.5 uL of 10 mM DMSO, general method
```



# **COMPOUND** INFORMATION

Data File W:\analyti...PEN\CGC_wave3_2_FirstPass 2023-01-05 22-10-41\035-D2F-C7-SR-12813.D
Sample Name: SR-12813



# **COMPOUND** INFORMATION

Data File W:\analyti...PEN\CGC_wave3_2_FirstPass 2023-01-05 22-10-41\035-D2F-C7-SR-12813.D
Sample Name: SR-12813

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 |
|---|---|---|---|---|
| - | - | 0.533 | 32099910 | 157.00 I |
| - | - | 3.153 | 457253 | 188.10 I |
| | | | | 170.10 I |
| 5.685 | 2483 | 5.718 | 37039984 | 505.30 I |
| - | - | 6.544 | 209209 | 507.30 I |
| | | | | 280.20 I |
| - | - | 6.872 | 5459114 | 282.20 I |
| - | - | 7.360 | 1514067 | 400.30 I |
| | | | | 282.20 I |