

Ro40-6055 (AM580)

CAS Registry No.: 102121-60-8

Formal Name: 4-(5,5,8,8-tetramethyl-5,6,7,8-tetrahydronaphthalene-2-carboxamido)benzoic acid

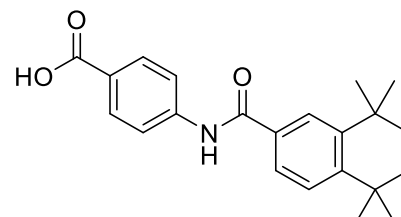
EUBOPEN ID: EUB0000567a

Molecular Formula: C₂₂H₂₅NO₃

Molecular Weight: 351.45 g/mol

Smiles: CC1(CCC(C2=C1C=CC(=C2)C(=O)NC3=CC=C(C=C3)C(=O)O)(C)C)C

Recommended concentration: 1 μM



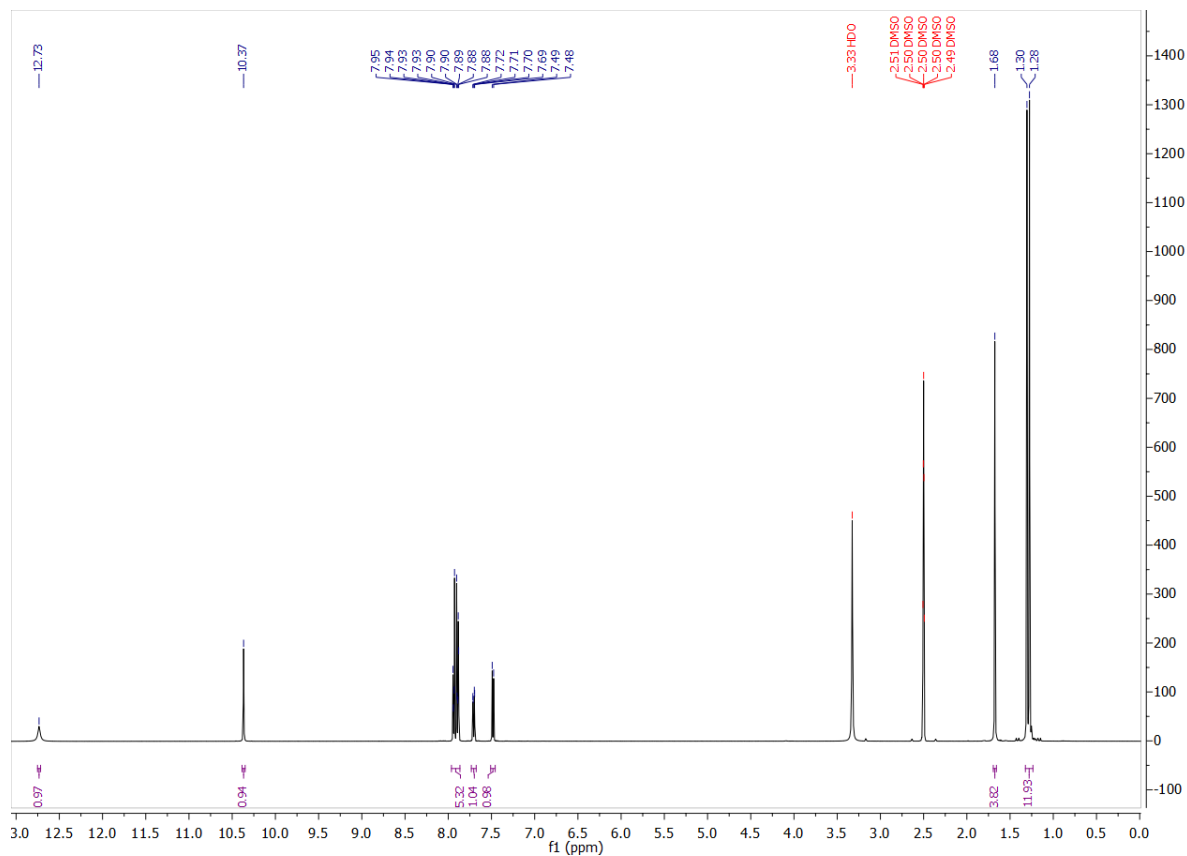
Biological activity

| | | Type | IC ₅₀ /EC ₅₀ [μM] | Reference |
|-----------------|--------------|---------|--|---|
| Main NR target: | NR1B1 (RARα) | Agonist | 0.0003 | https://doi.org/10.1016/j.bmcl.2008.11.040 |
| | NR1B2 (RARβ) | Agonist | 0.009 | |
| | NR1B3 (RARγ) | Agonist | 0.01 | |
| NR off-target: | | | | |

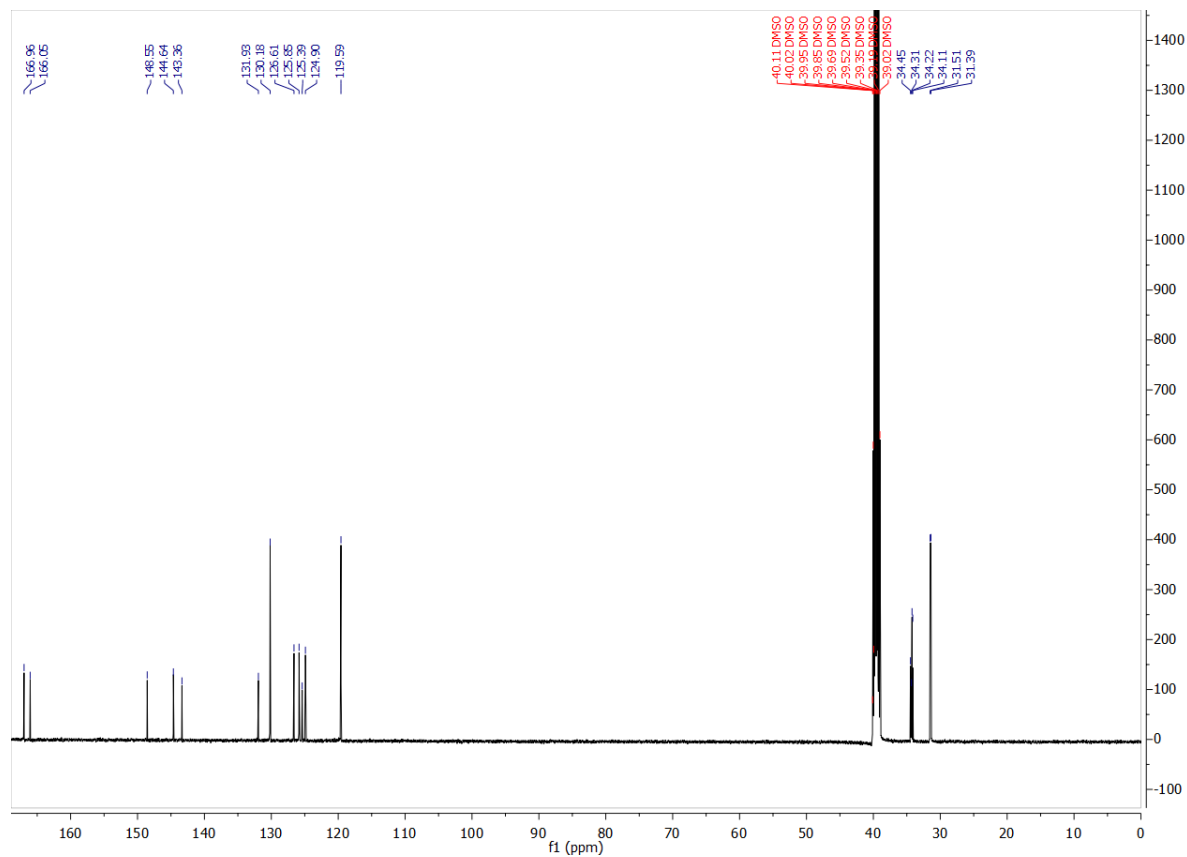
COMPOUND INFORMATION

Identity

¹H NMR



¹³C NMR



COMPOUND INFORMATION

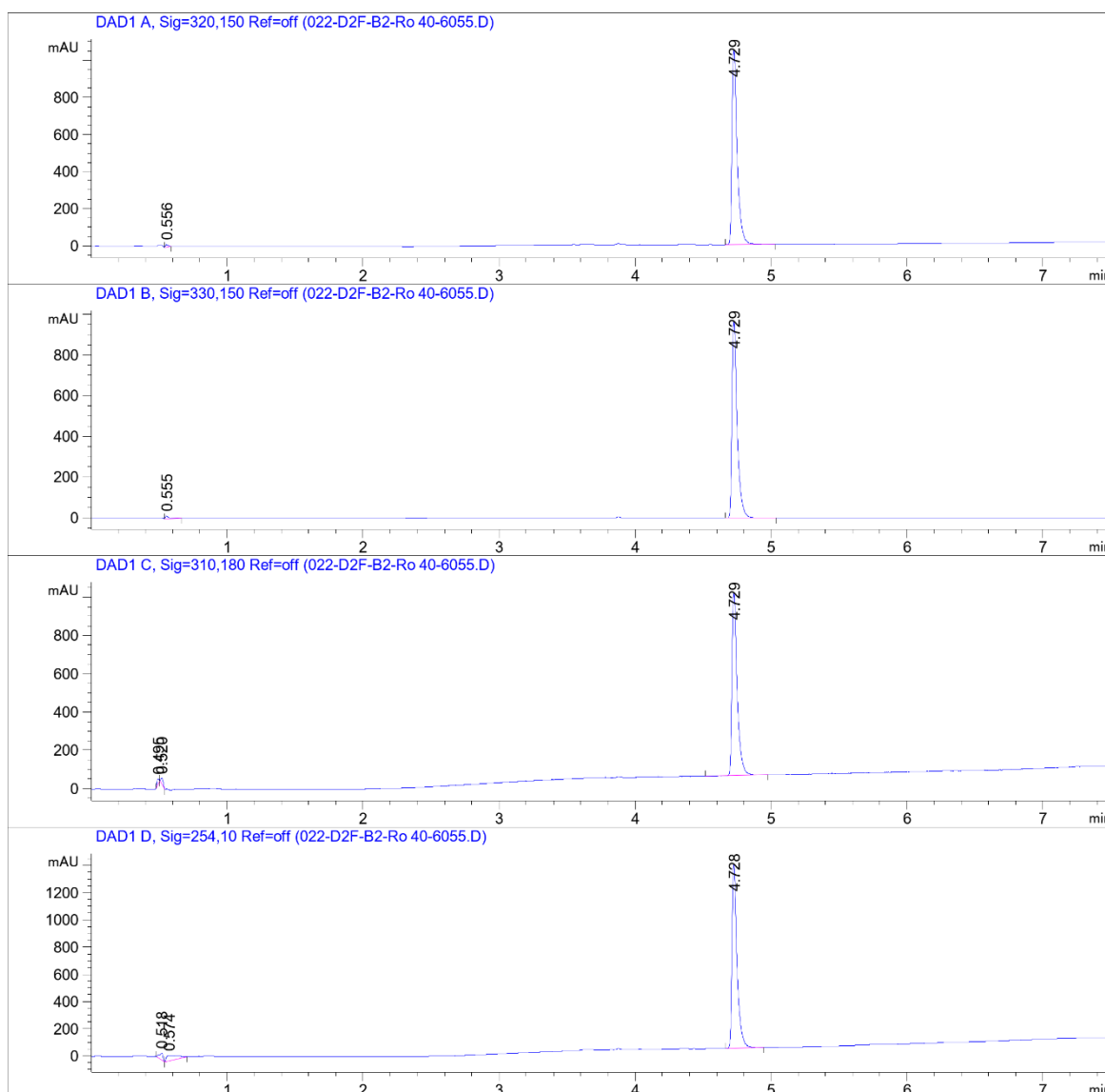
Purity

Data File W:\analyti...\CGC_ECH01-3_SecondPass 2021-03-25 18-09-21\022-D2F-B2-Ro 40-6055.D

Sample Name: Ro 40-6055

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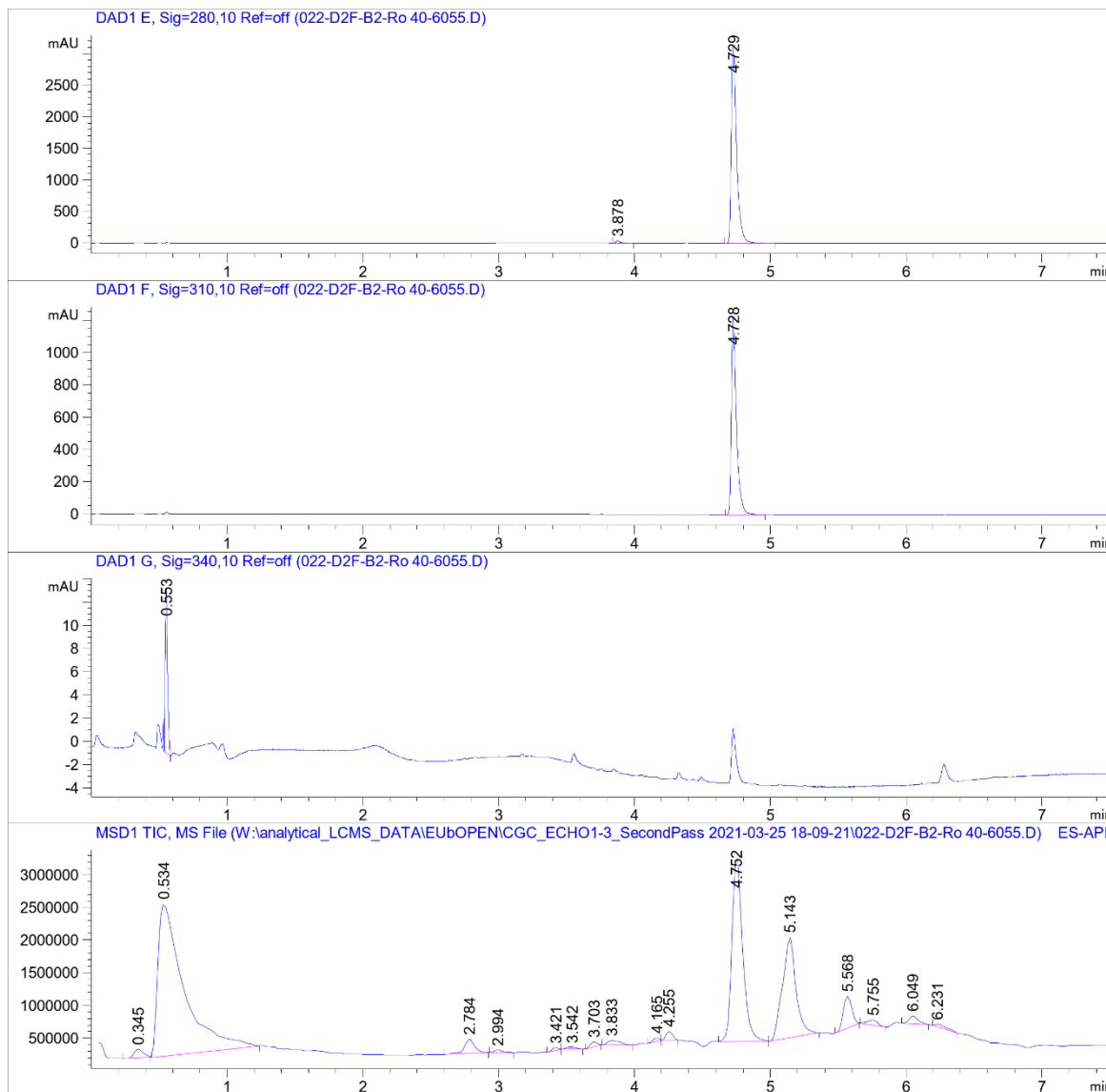
| | | | |
|-----------------|---|------------|------------|
| Acq. Operator | : SYSTEM | Seq. Line | : 22 |
| Sample Operator | : SYSTEM | | |
| Acq. Instrument | : LCMS test | Location | : D2F-B2 |
| Injection Date | : 3/25/2021 10:03:50 PM | Inj | : 1 |
| | | Inj Volume | : Inj prog |
| Sequence File | : 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) | | |



COMPOUND INFORMATION

Data File W:\analyti...\CGC_ECH01-3_SecondPass 2021-03-25 18-09-21\022-D2F-B2-Ro 40-6055.D

Sample Name: Ro 40-6055



COMPOUND INFORMATION



Data File W:\analyti...\CGC_ECH01-3_SecondPass 2021-03-25 18-09-21\022-D2F-B2-Ro 40-6055.D

Sample Name: Ro 40-6055

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 |
|---------------------|---------|---------------------|----------|--|
| - | - | 0.345 | 598066 | 200.00 I 183.00 I 159.00 I 142.00 I 110.10 I |
| 0.556 | 20 | 0.534 | 30935600 | 157.00 I |
| - | - | 2.784 | 1077283 | 217.10 I |
| - | - | 2.994 | 160001 | 274.30 I |
| - | - | 3.421 | 138476 | 326.40 I |
| - | - | 3.542 | 163486 | 332.30 I 326.30 I 296.30 I 282.30 I 200.00 I 159.00 I 158.20 I 151.20 I 111.10 I 110.10 I 102.20 I |
| - | - | 3.703 | 279175 | 214.10 I |
| - | - | 3.833 | 447341 | 316.20 I 298.30 I |
| - | - | 4.165 | 160749 | 280.30 I |
| - | - | 4.255 | 460486 | 296.30 I |
| 4.729 | 2788 | 4.752 | 15417600 | 352.20 I |
| - | - | 5.143 | 10493235 | 282.30 I |
| - | - | 5.568 | 2079847 | 381.30 I 359.30 I 341.30 I 284.30 I 282.30 I |
| - | - | 5.755 | 410310 | 400.40 I 282.30 I |
| - | - | 6.049 | 580429 | 338.30 I 282.30 I |
| - | - | 6.231 | 248440 | 282.20 I |

