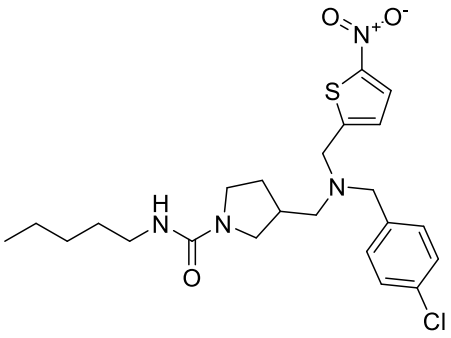
COMPOUND INFORMATION

SR9011

CAS Registry No.:	1379686-29-9
Formal Name:	3-(((4-chlorobenzyl)((5-nitrothiophen-2-yl)methyl)amino)methyl)-N-pentylpyrrolidine-1-carboxamide
EUBOPEN ID:	EUB0001155a
Molecular Formula:	$C_{23}H_{31}ClN_4O_3S$
Molecular Weight:	479.04 g/mol
Smiles:	ClC1=CC=C(CN(CC2=CC=C(S2)[N+]([O])=O)CC3CCN(C3)C(NCCCCC)=O)C=C1
Recommended concentration:	10 µM



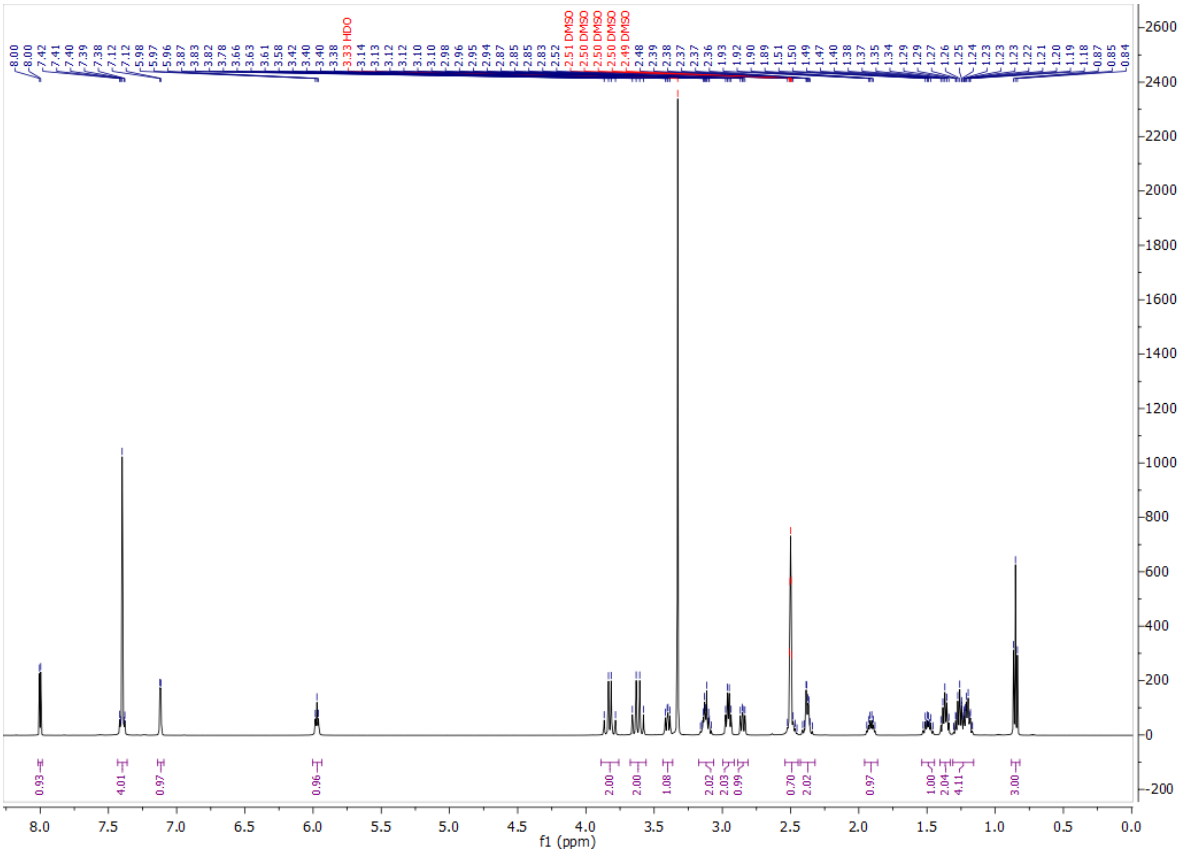
Biological activity

		Type	IC_{50}/EC_{50} [µM]	Reference
Main NR target:	NR1D1 (revERBα)	Agonist	2	inhouse
	NR1D2 (revERBβ)	Agonist	3.1	inhouse
NR off-target:				

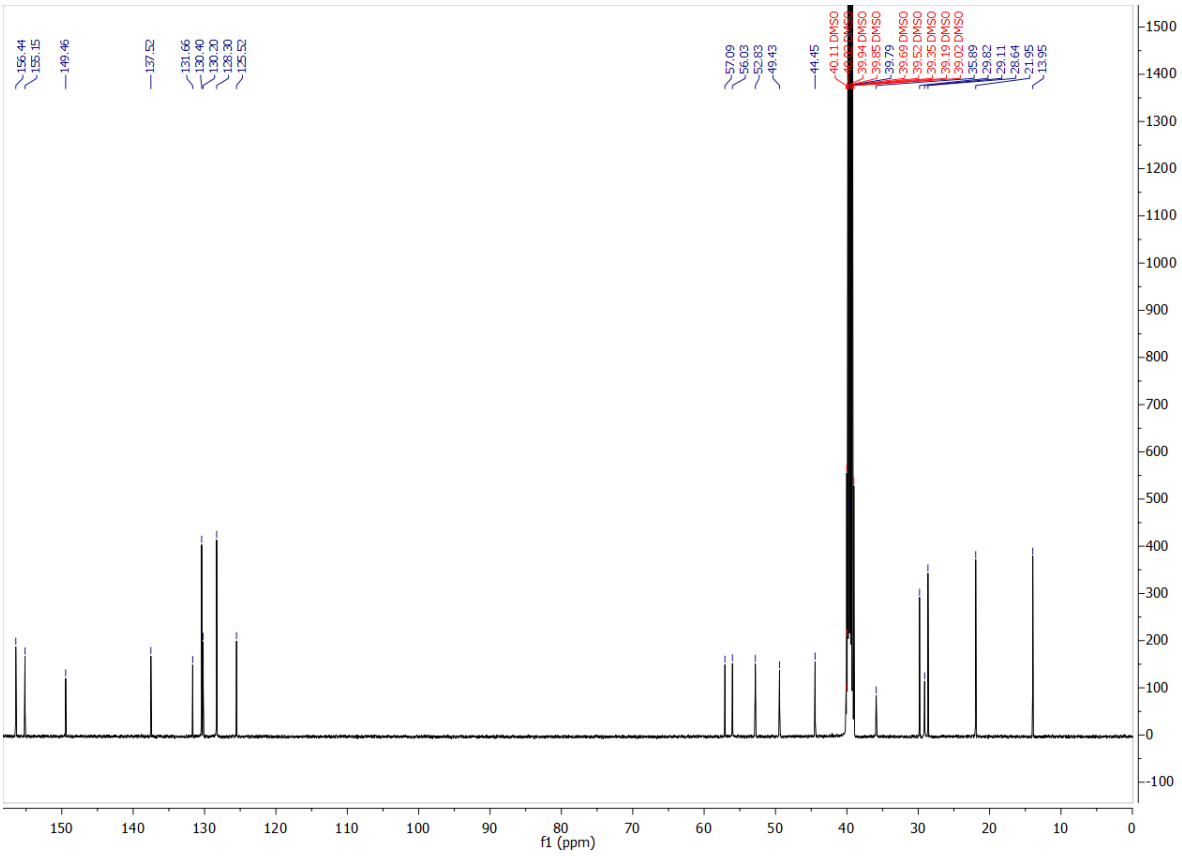
COMPOUND INFORMATION

Identity

^{1}H NMR



^{13}C NMR



COMPOUND INFORMATION

Purity

Data File W:\analyti...OPEN\CGC_wave3_1_FirstPassB 2023-01-04 18-28-02\073-D2F-G1-SR9011.D
Sample Name: SR9011

```
======================================================================
Acq. Operator   : SYSTEM                        Seq. Line :  73
Sample Operator : SYSTEM
Acq. Instrument : LCMS test                      Location :  D2F-G1
Injection Date  : 1/5/2023 7:46:59 AM                Inj :  1
                                                Inj Volume : Inj prog
Sequence File   : W:\analytical_LCMS_DATA\EUbOPEN\CGC_wave3_1_FirstPassB 2023-01-04 18-28-02
                  \CGC_wave3_1_FirstPassB.S
Method          : W:\analytical_LCMS_DATA\EUbOPEN\CGC_wave3_1_FirstPassB 2023-01-04 18-28-02
                  \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
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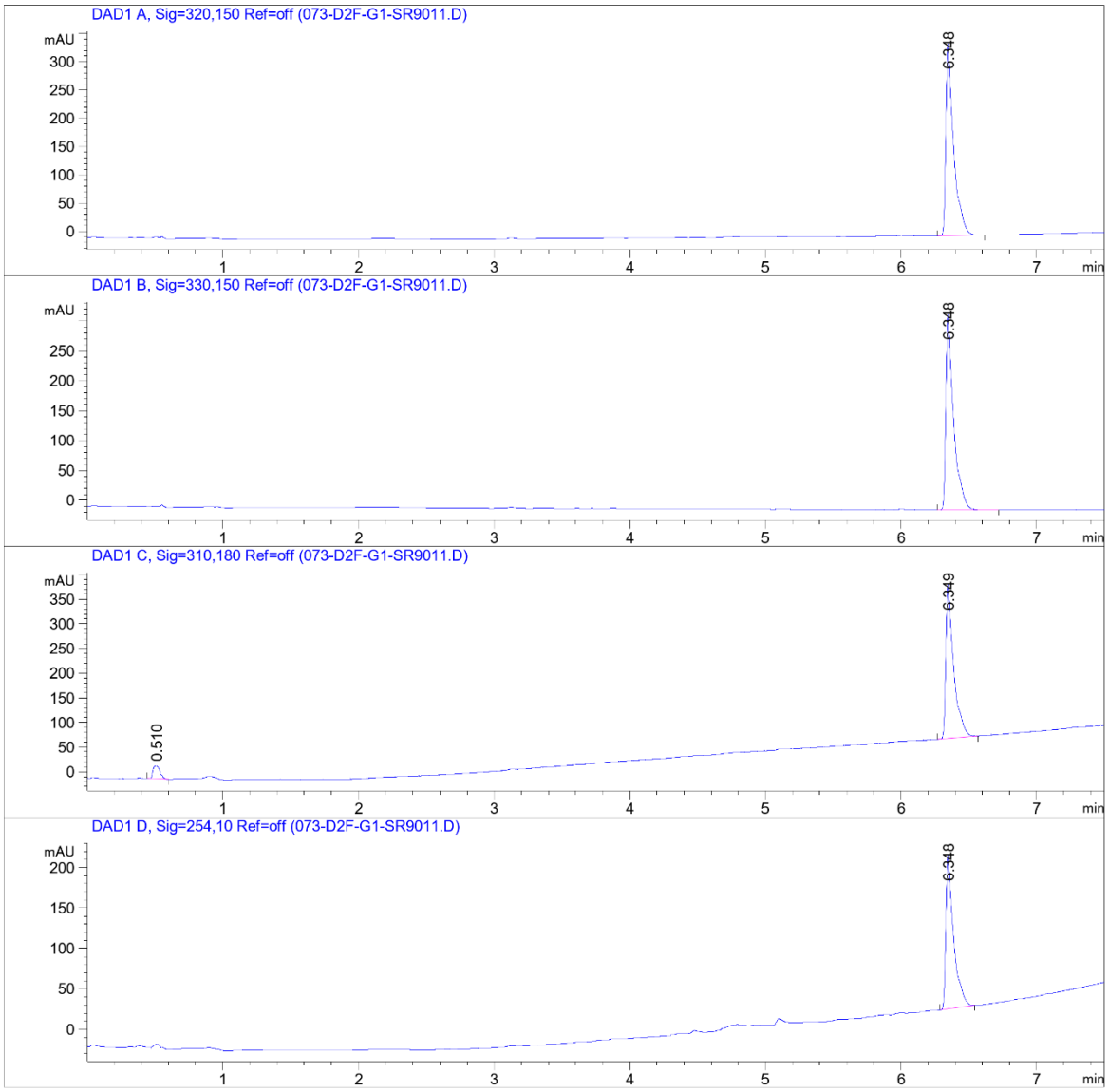
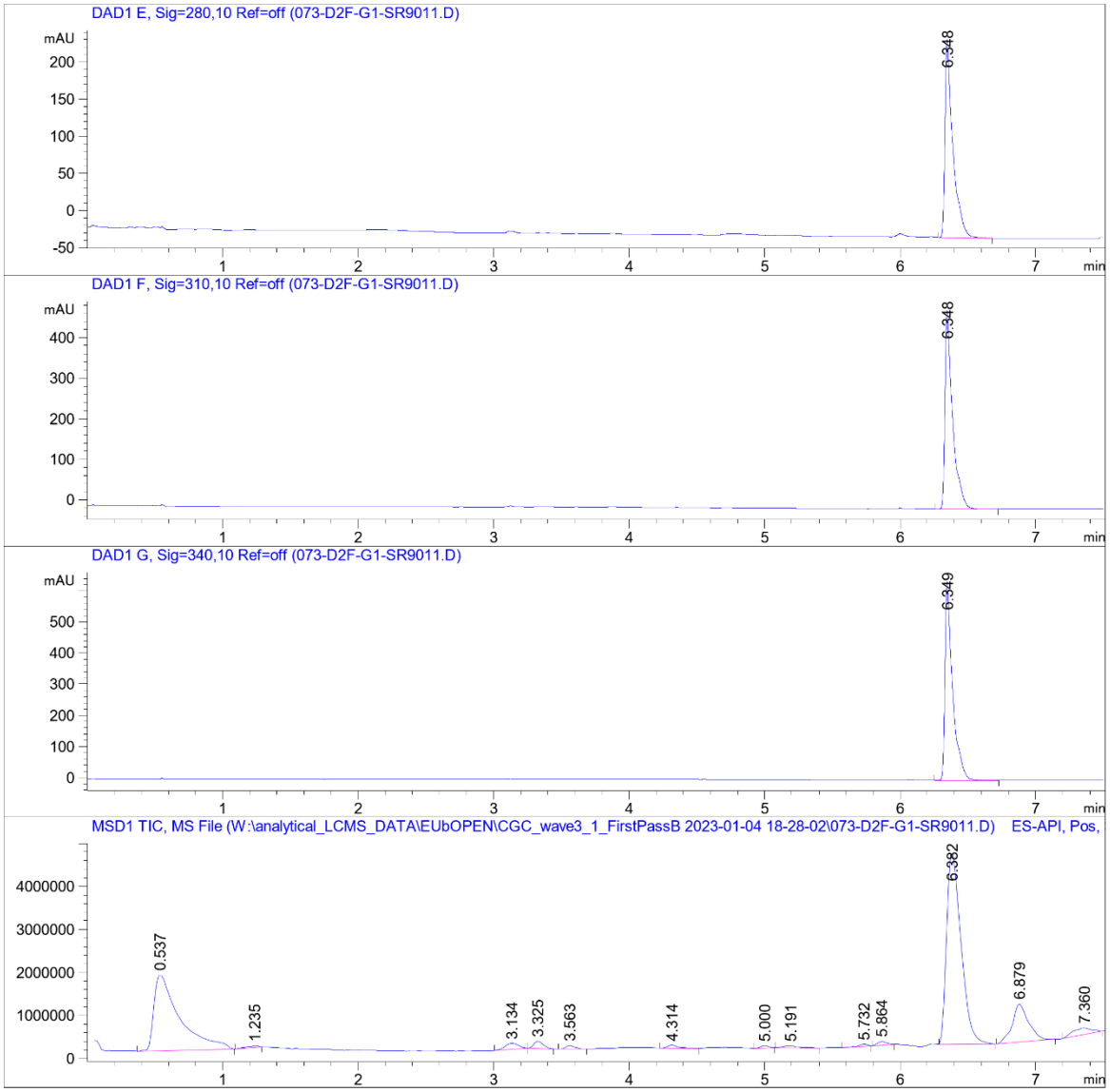


COMPOUND INFORMATION

Data File W:\analyti...OPEN\CGC_wave3_1_FirstPassB 2023-01-04 18-28-02\073-D2F-G1-SR9011.D
Sample Name: SR9011

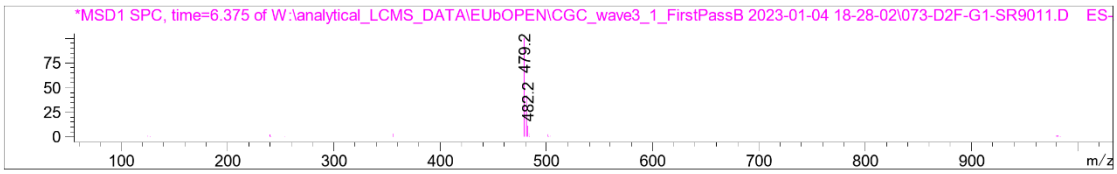


COMPOUND INFORMATION

Data File W:\analyti...OPEN\CGC_wave3_1_FirstPassB 2023-01-04 18-28-02\073-D2F-G1-SR9011.D
Sample Name: SR9011

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
-	-	0.537	23147890	157.00 I
-	-	1.235	239192	157.00 I
-	-	3.134	963696	239.10 I
				217.10 I
				188.10 I
-	-	3.325	810373	338.20 I
-	-	3.563	437907	215.10 I
-	-	4.314	405057	257.10 I
-	-	5.000	242234	271.20 I
-	-	5.191	471579	510.40 I
				170.90 I
				137.10 I
-	-	5.732	190906	280.20 I
-	-	5.864	390894	318.20 I
				296.20 I
6.348	1346	6.382	32871608	479.20 I
-	-	6.879	7439279	282.20 I
-	-	7.360	1563593	400.30 I
				282.20 I



COMPOUND INFORMATION

Biological activity