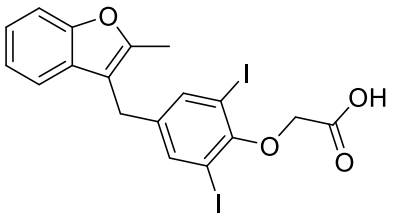
COMPOUND INFORMATION

KB-130015

CAS Registry No.:	147030-48-6
Formal Name:	2-[2,6-diiodo-4-[(2-methyl-1-benzofuran-3-yl)methyl]phenoxy]acetic acid
EUbOPEN ID:	EUB0002355a
Molecular Formula:	$C_{18}H_{14}I_2O_4$
Molecular Weight:	548.1 g/mol
Smiles:	CC1=C(C2=CC=CC=C2O1)CC3=CC(=C(C(=C3)I)OCC(=O)O)I
Recommended concentration:	3 µM



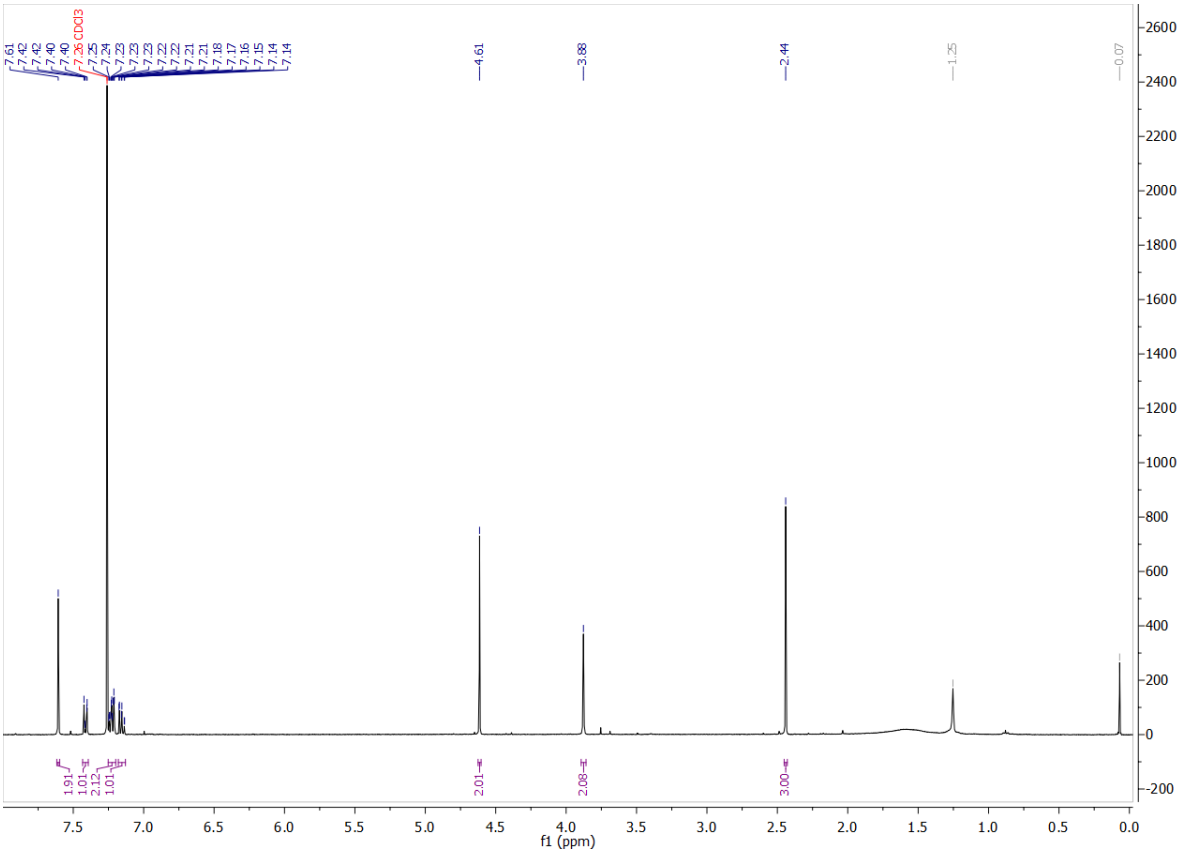
Biological activity

		Type	IC_{50}/EC_{50} [µM]	Reference
Main NR target:	NR1A2 (THRβ)	Antagonist	2.0	inhouse
NR off-target:				

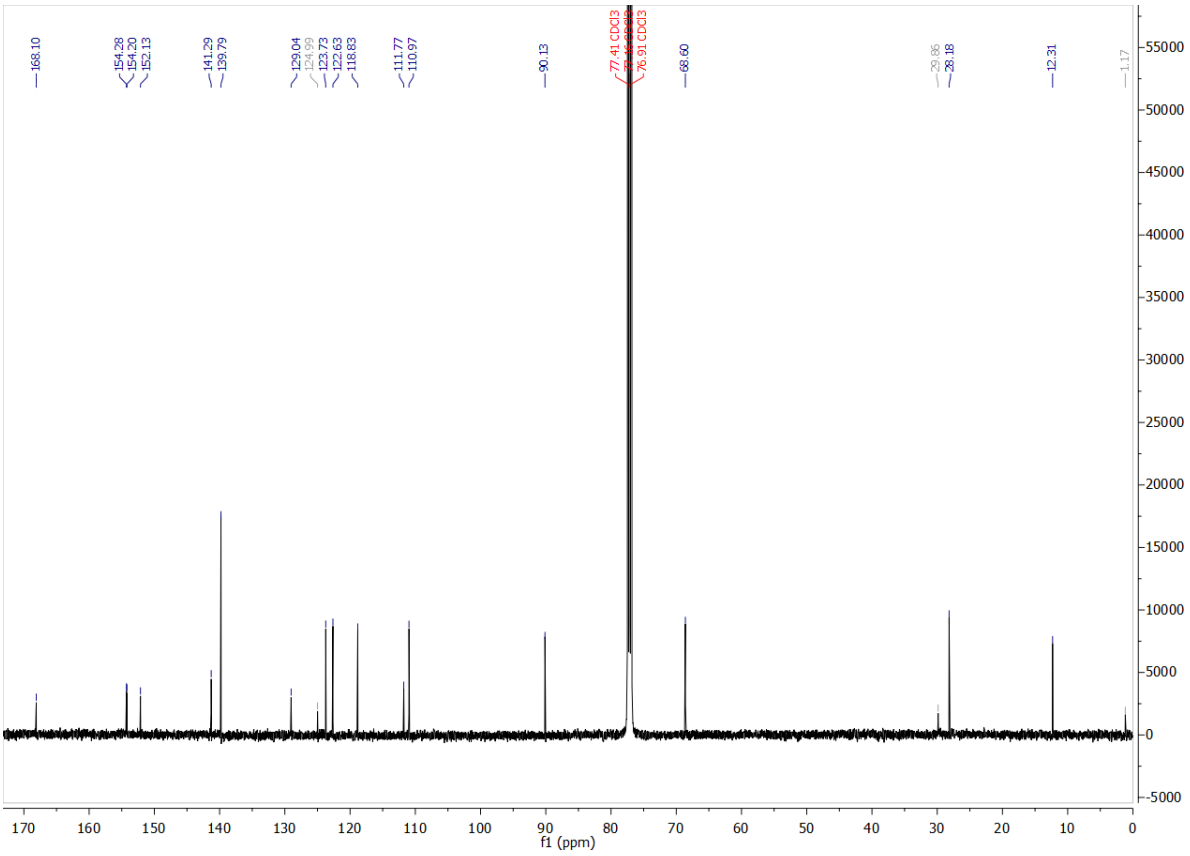
COMPOUND INFORMATION

Identity

^{1}H NMR



^{13}C NMR



COMPOUND INFORMATION

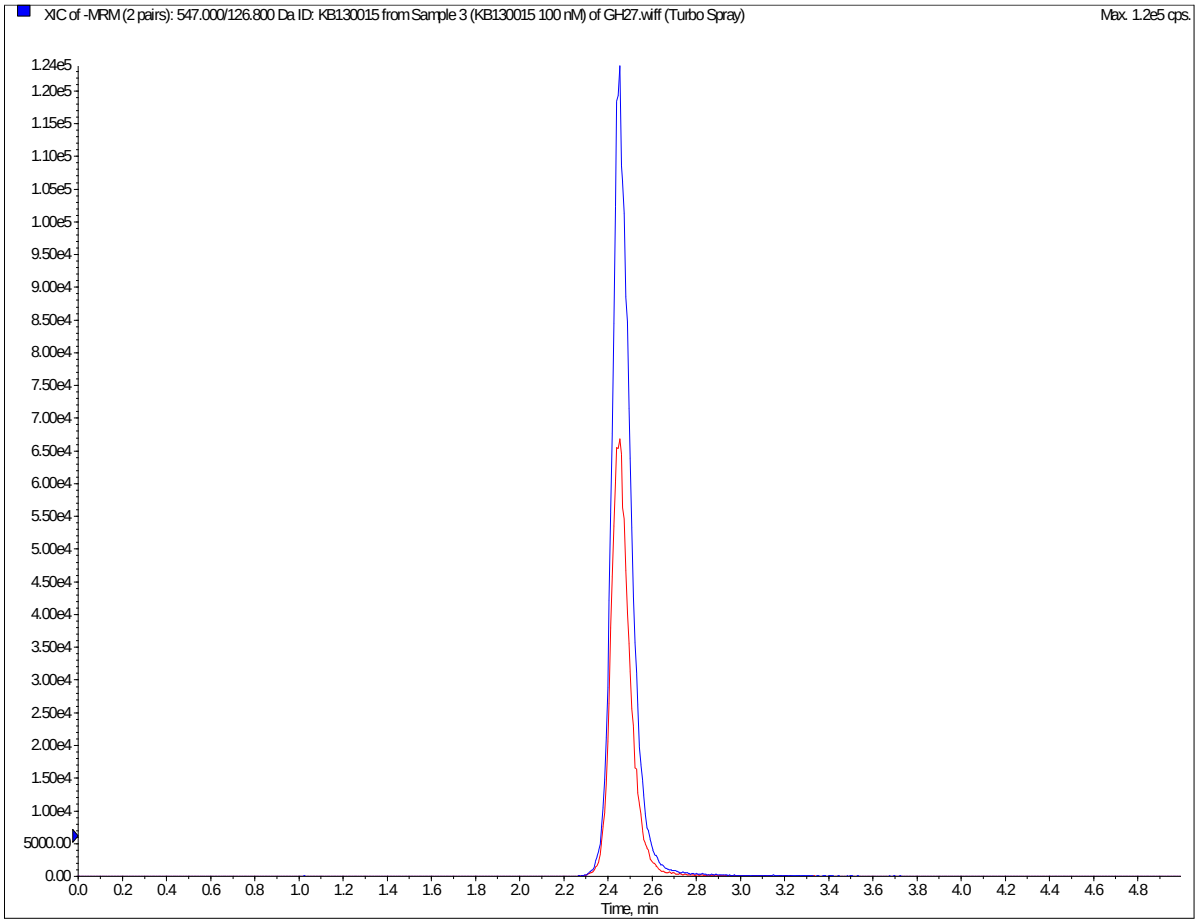
Purity

LC-MS

M_r 548.11

MS: ESI-negative, *m/z* 547/127 (blue), *m/z* 547/489 (red)

LC: 0.1% HCOOH/ACN (40/60)

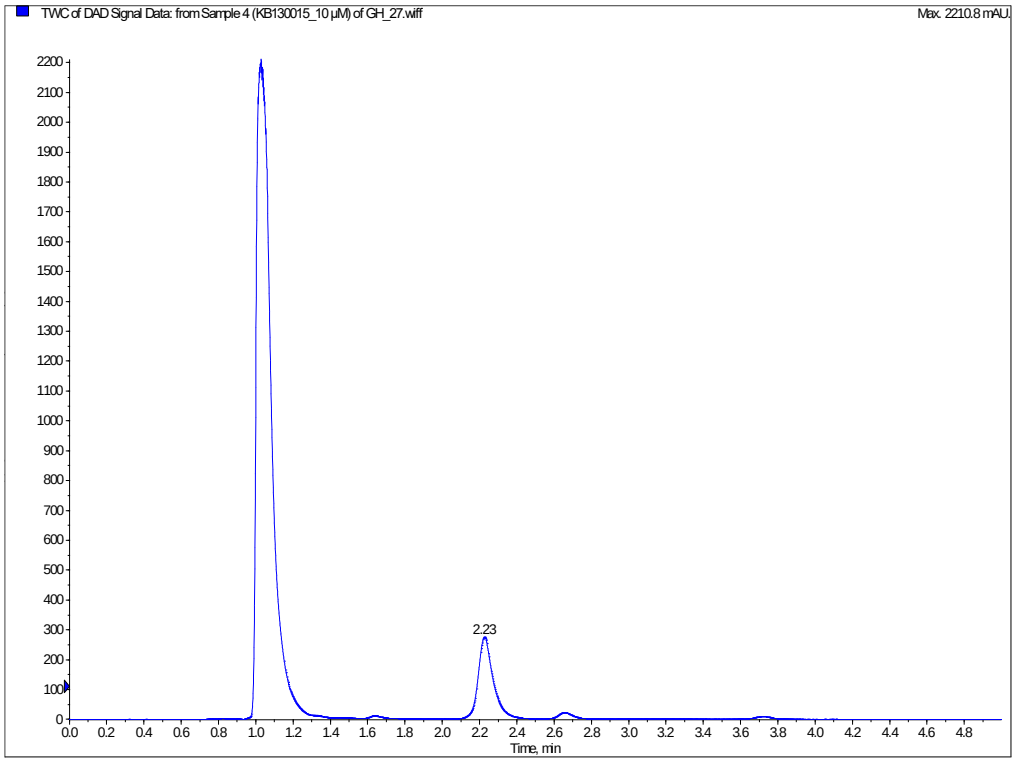


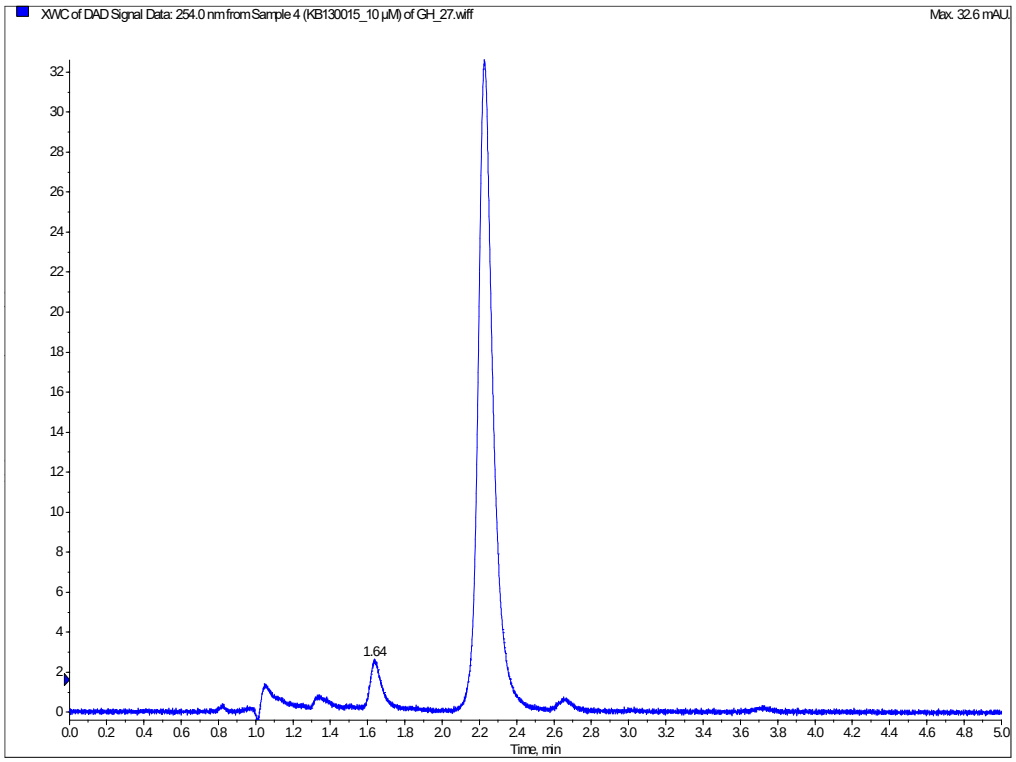
COMPOUND INFORMATION

LC-UV

LC: 0.1% HCOOH/ACN (40/60)

DAD: 215, 230, 240, 254 (XWC), 260 nm





COMPOUND INFORMATION

Biological activity