





Design and Synthesis of AMPK Activators and GDF15 Inducers

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† These authors contributed equally to this work.

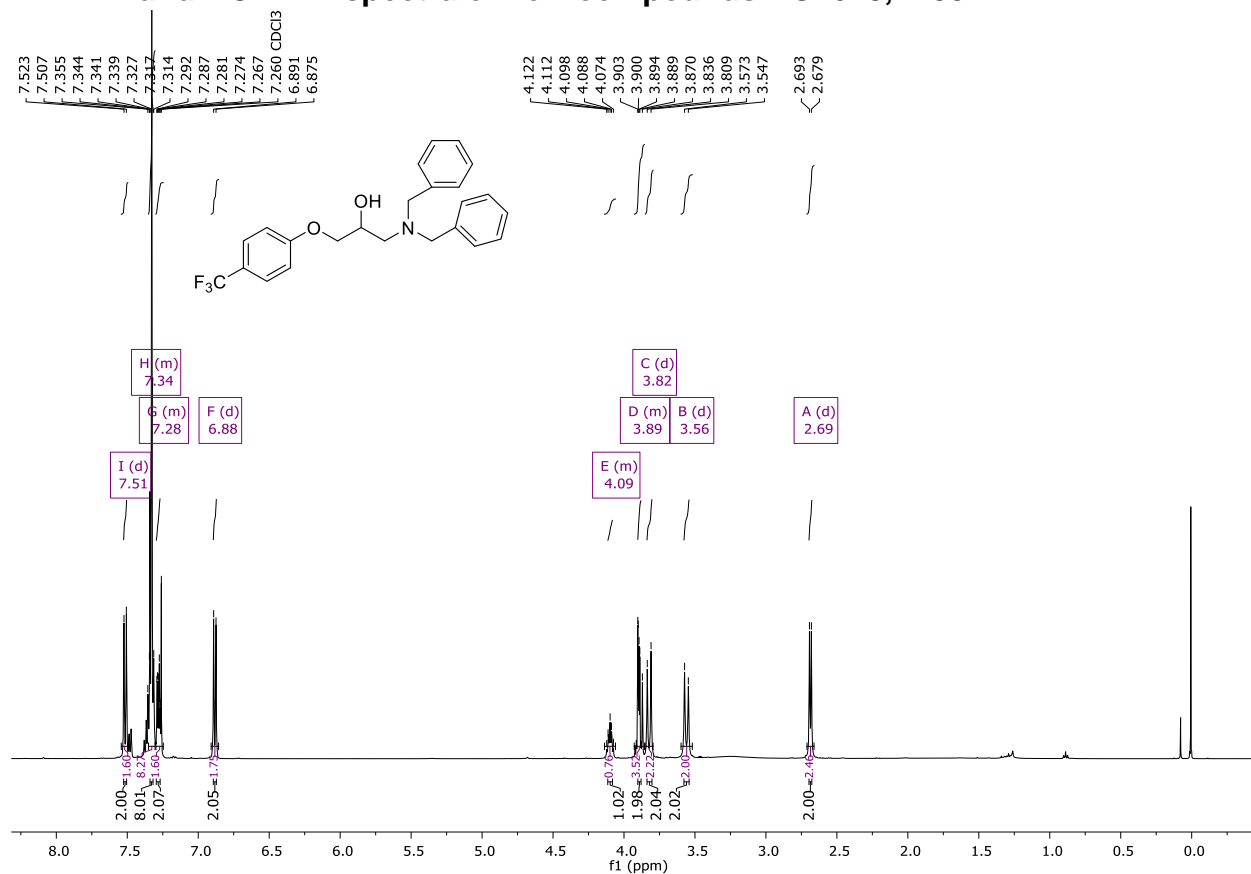
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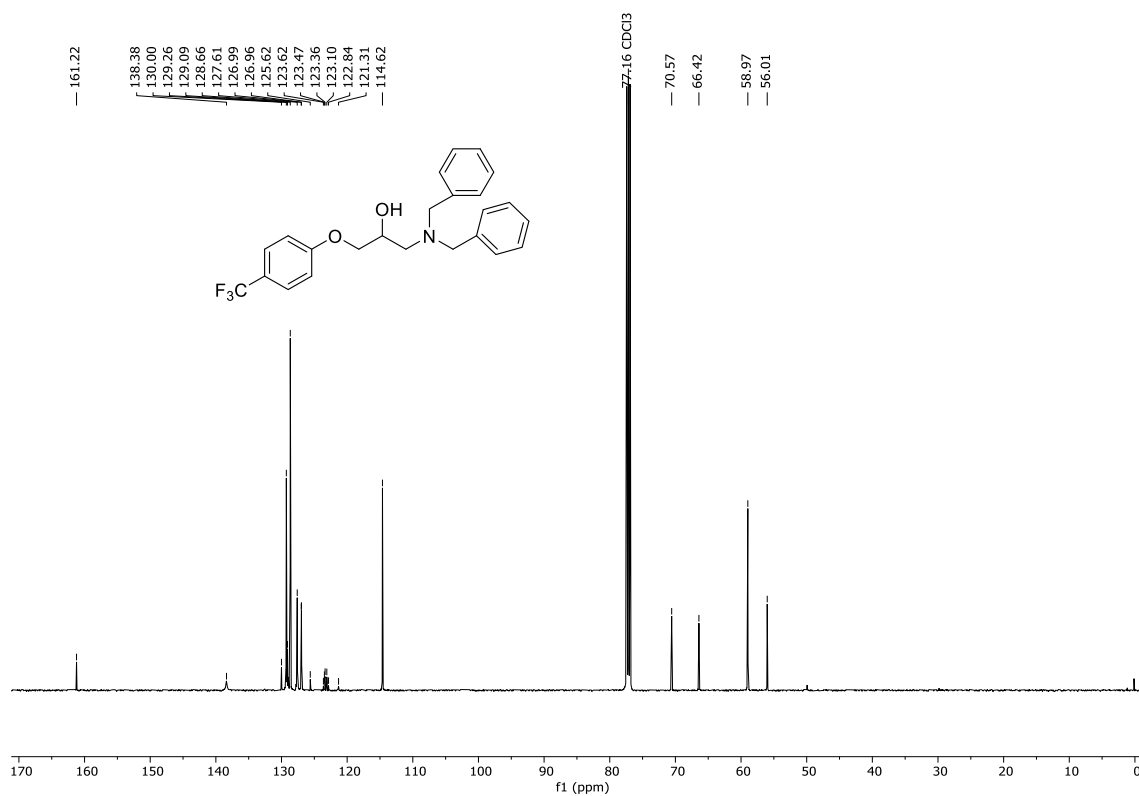
1.1.1. General Procedure for the synthesis of phenoxymethyloxirane derivatives.

A mixture of the corresponding phenol derivative (1 equiv) [4-(trifluoromethyl)phenol, phenol, 4-chlorophenol, 4-methylphenol, 4-isopropylphenol, 4-*tert*-butylphenol, 4-cyclohexylphenol, 4-cyclopentylphenol, 4-benzyloxyphenol, 3,4-dimethylphenol, 4-methoxyphenol, 4-propoxyphenol, 3,4-dichlorophenol, 4-chloro-3-(trifluoromethyl)phenol, 4-nitro-3-(trifluoromethyl)phenol, 2,4-dichlorophenol], (\pm)-epichlorohydrin (10 equiv) and K₂CO₃ (1.2 equiv) was stirred in methanol at 120 °C for 4 h. The mixture was evaporated to yield a residue, which was purified by column chromatography (hexane/AcOEt) to afford pure products; 2-[[4-(trifluoromethyl)phenoxy]methyl]oxirane; 2-(phenoxymethyl)oxirane; 2-[(4-chlorophenoxy)methyl]oxirane; 2-[(*p*-tolyl)oxy)methyl]oxirane; 2-[(4-isopropylphenoxy)methyl]oxirane, 2-[[4-(*tert*-butyl)phenoxy]methyl]oxirane, 2-[(4-cyclohexylphenoxy)methyl]oxirane, 2-[(4-cyclopentylphenoxy)methyl]oxirane, 2-[(4-benzyloxy)phenoxy]methyl]oxirane, 2-[(3,4-dimethylphenoxy)methyl]oxirane, 2-[(4-methoxyphenoxy)methyl]oxirane, 2-[(4-propoxyphenoxy)methyl]oxirane, 2-[(3,4-dichlorophenoxy)methyl]oxirane, 2-[[4-chloro-3-(trifluoromethyl)phenoxy]methyl]oxirane, 2-[[4-nitro-3-(trifluoromethyl)phenoxy]methyl]oxirane, 2-[(2,4-dichlorophenoxy)methyl]oxirane.

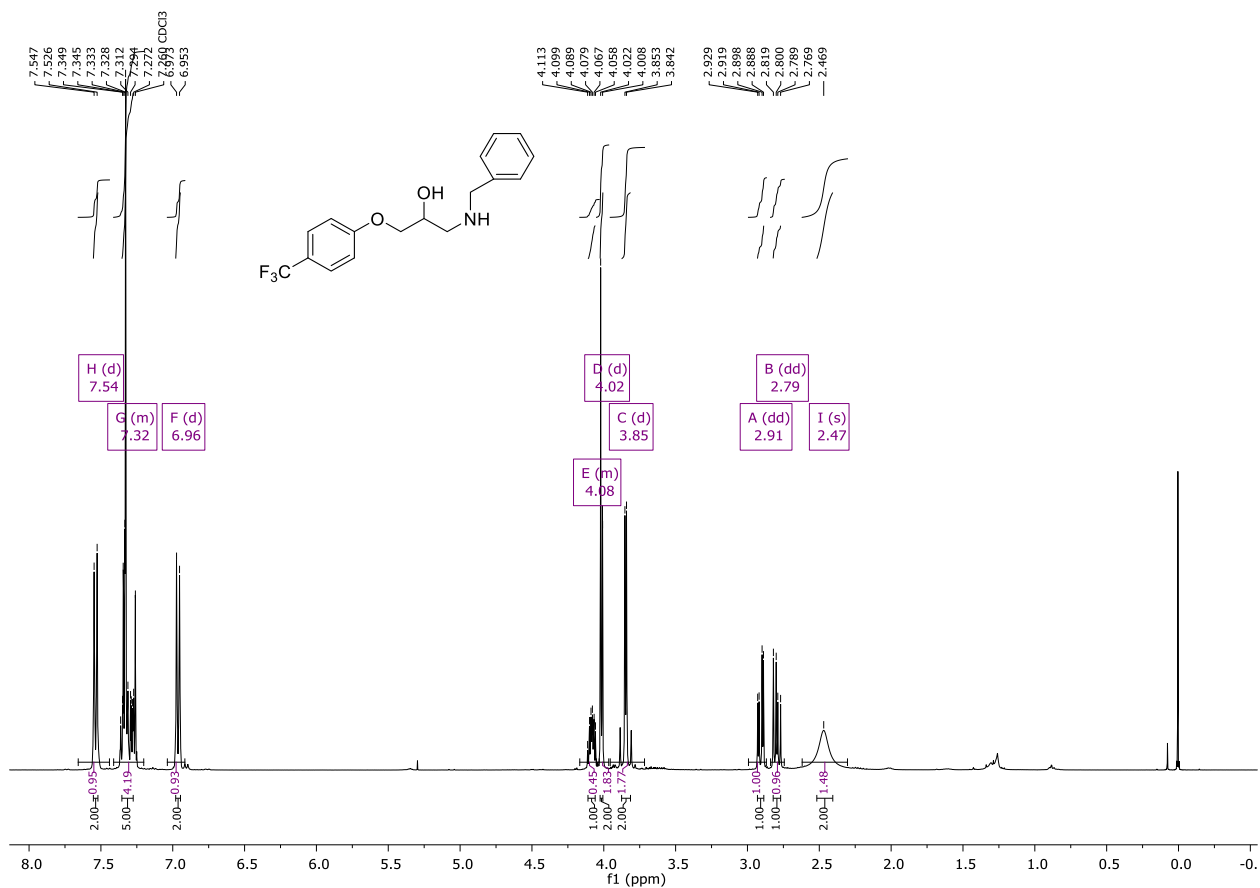
¹H-NMR and ¹³C-NMR spectra of new compounds BC1618, 1-35



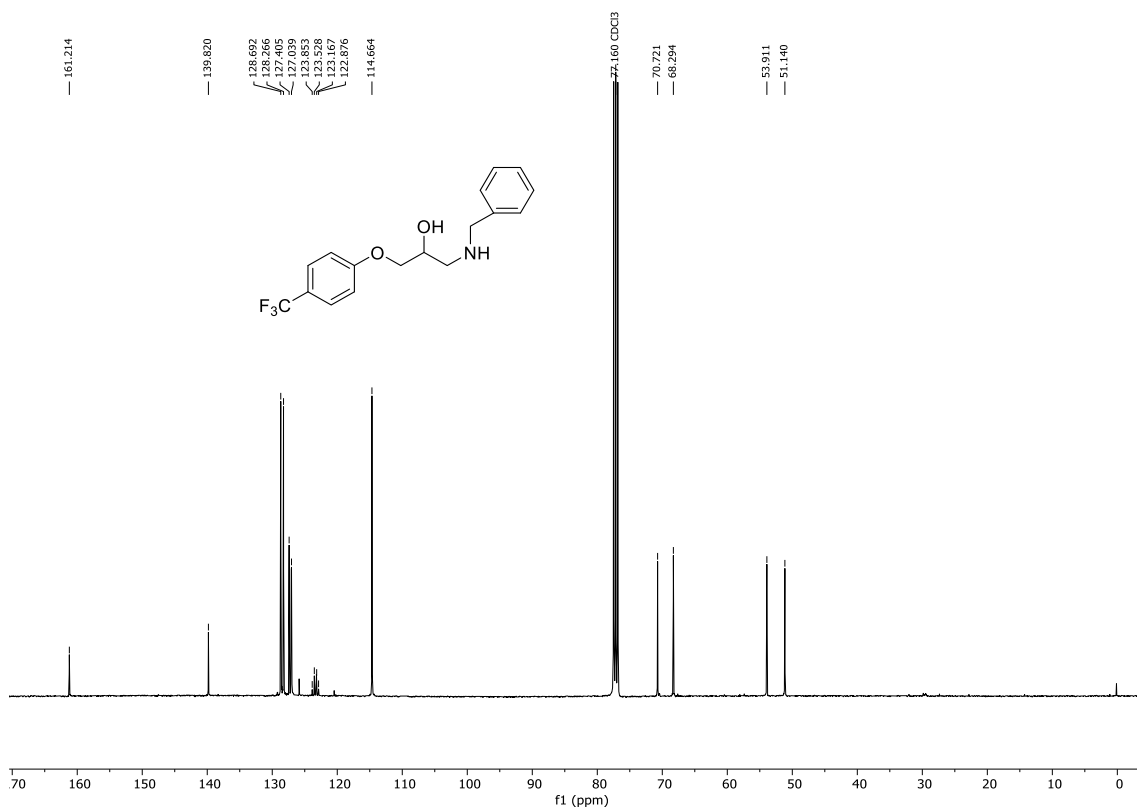
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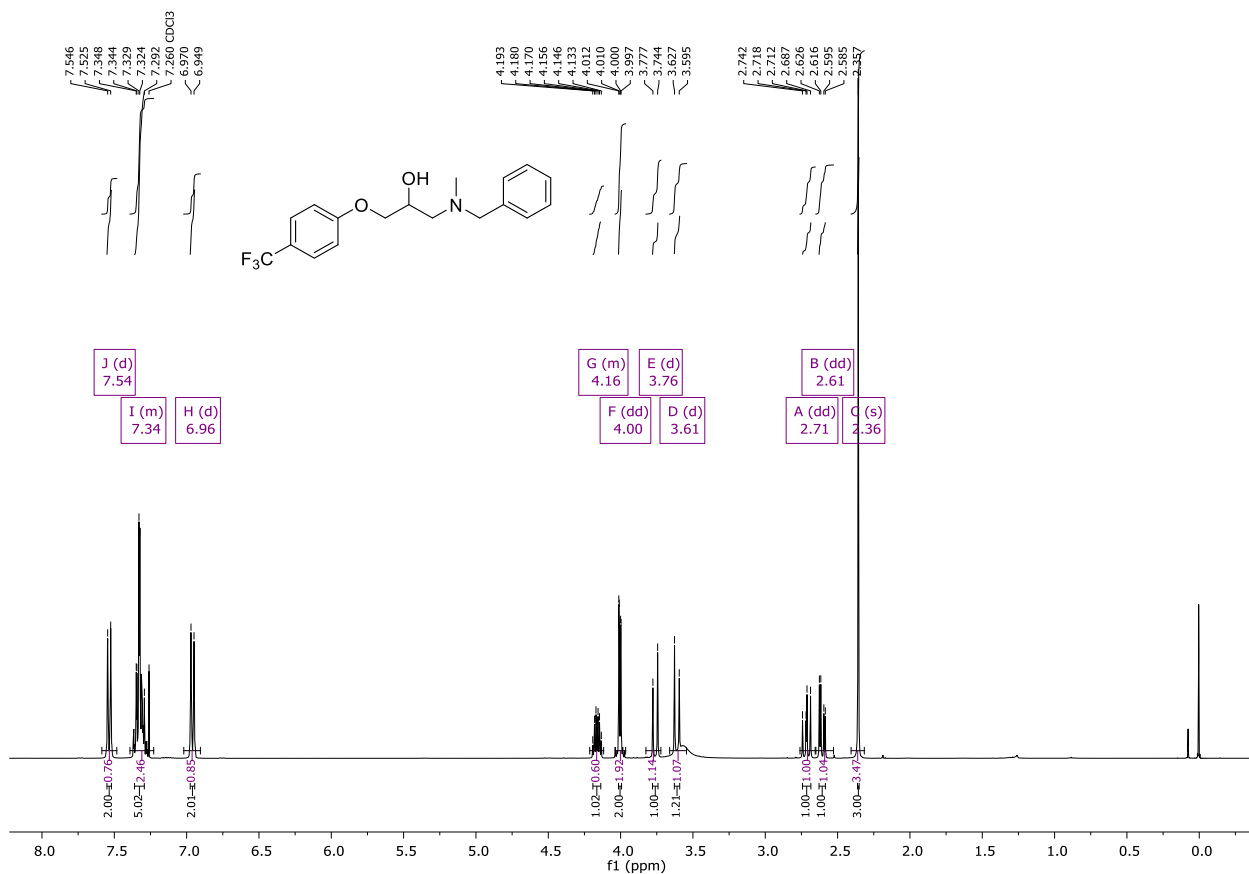
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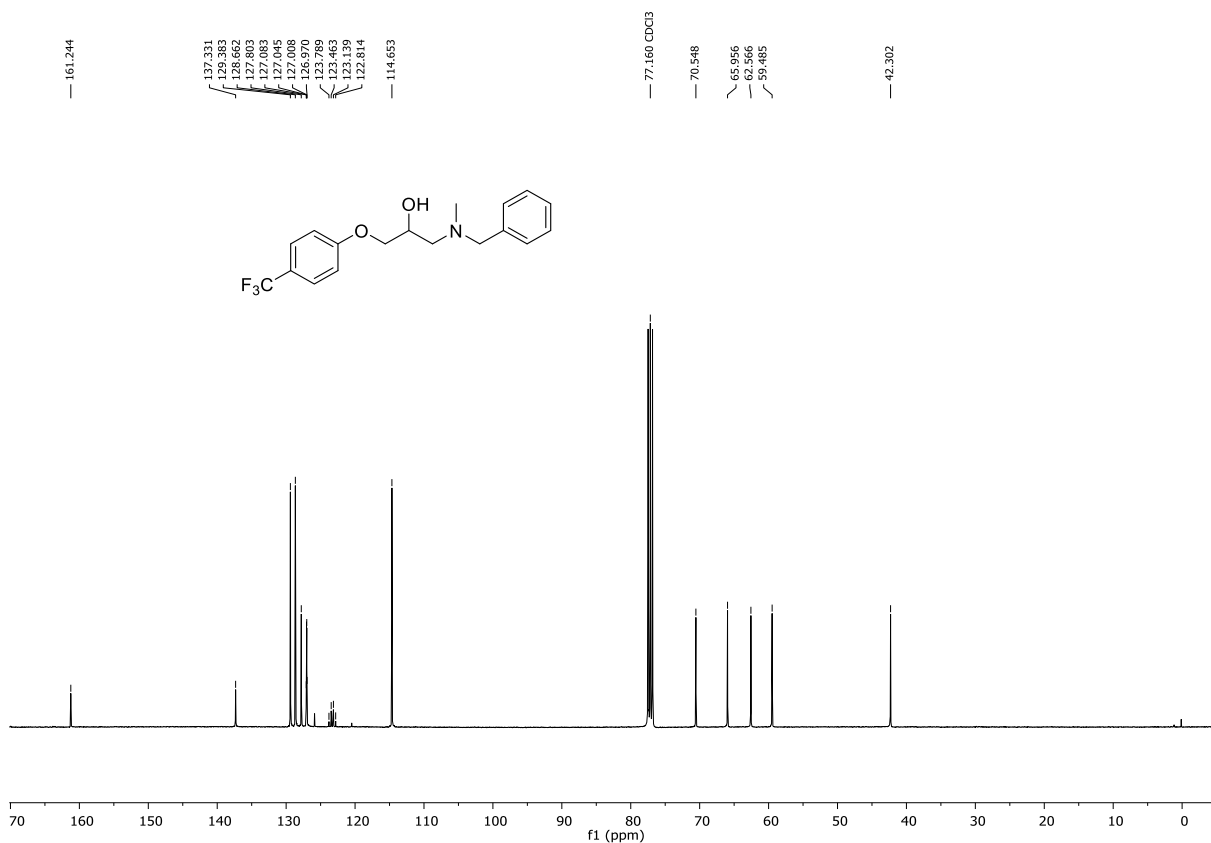
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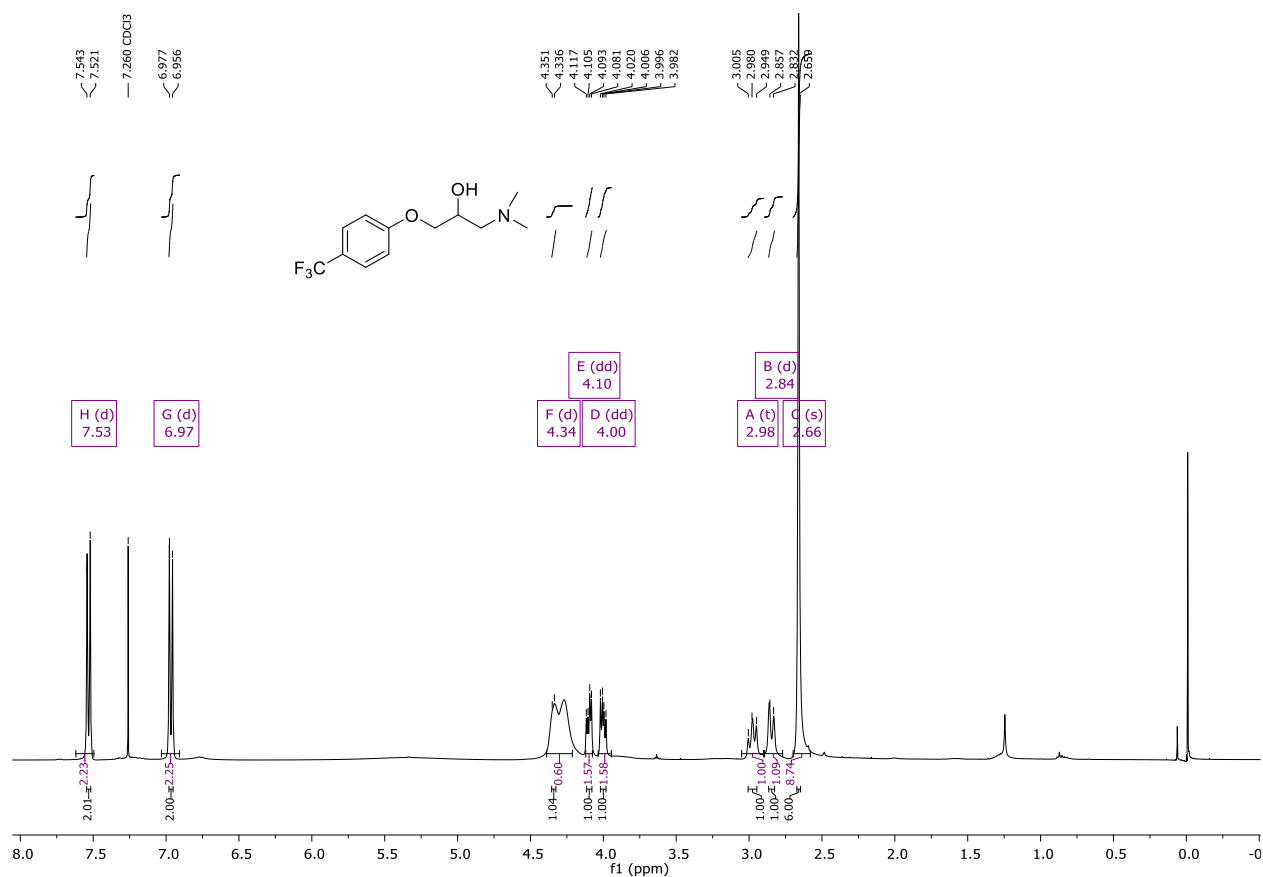
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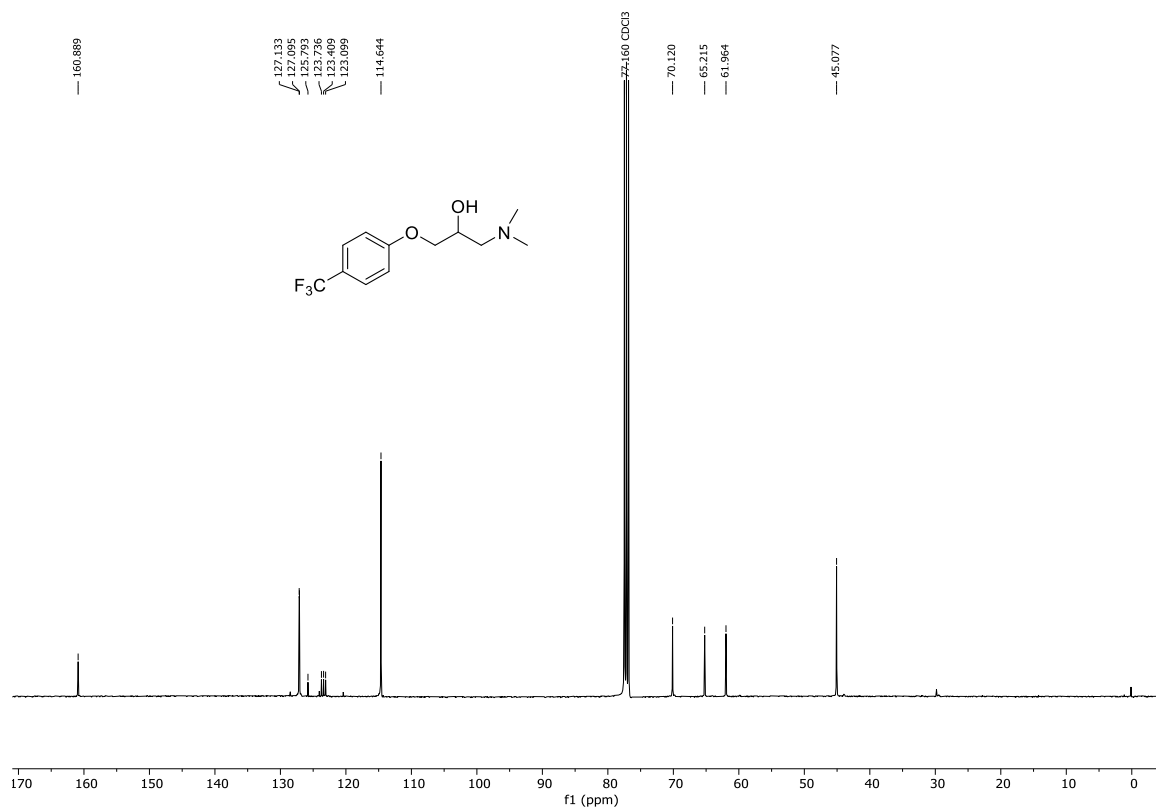
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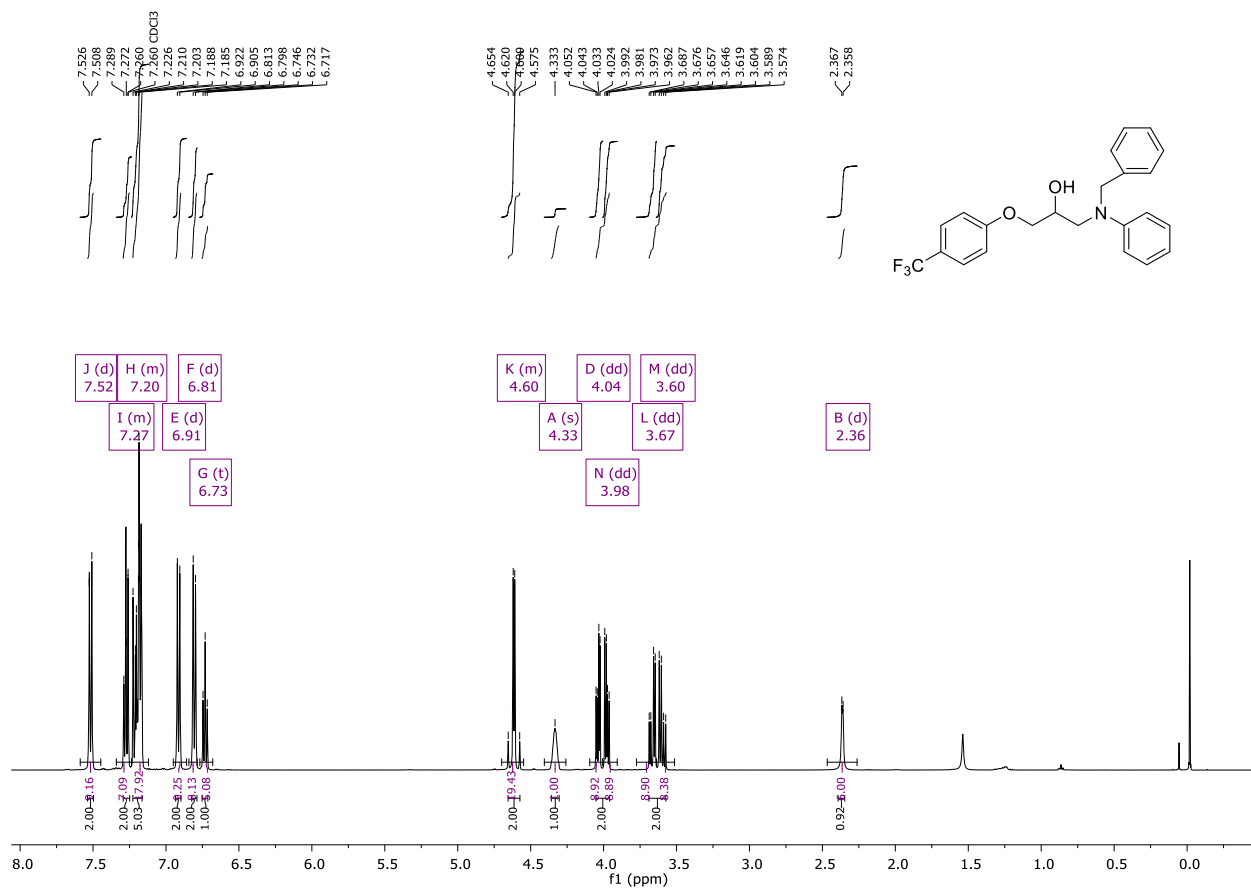
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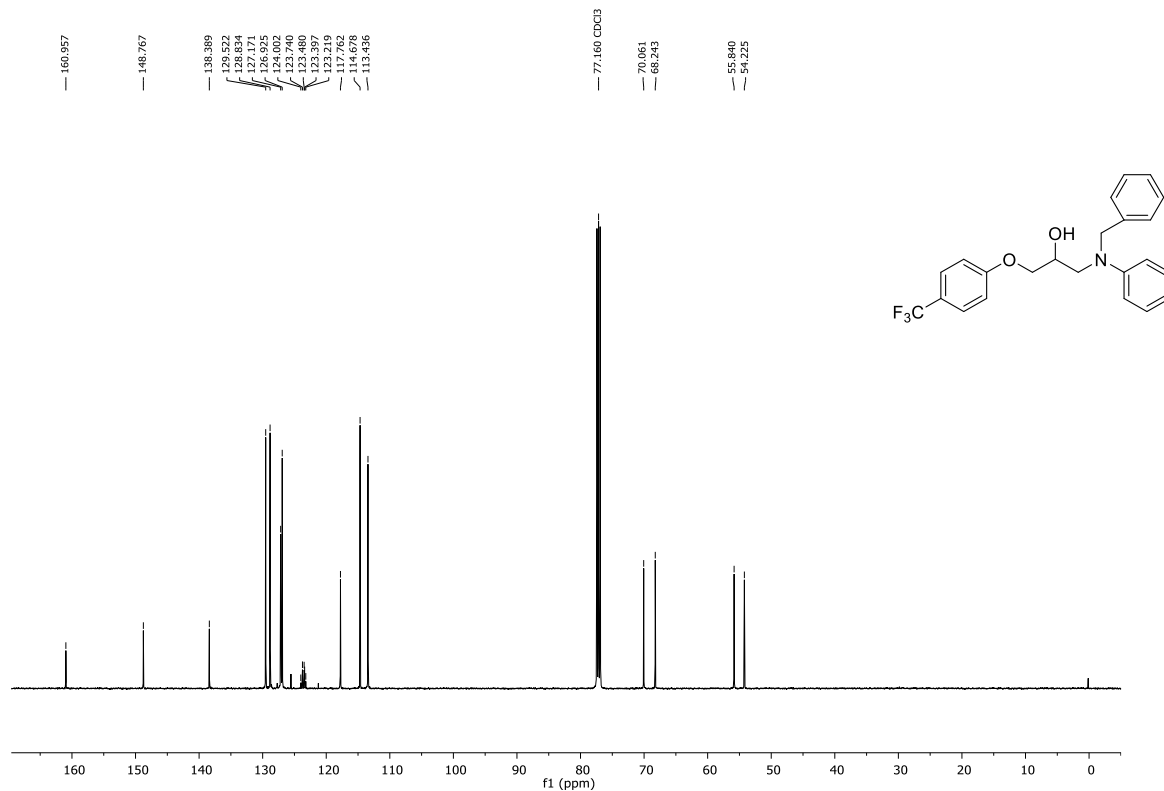
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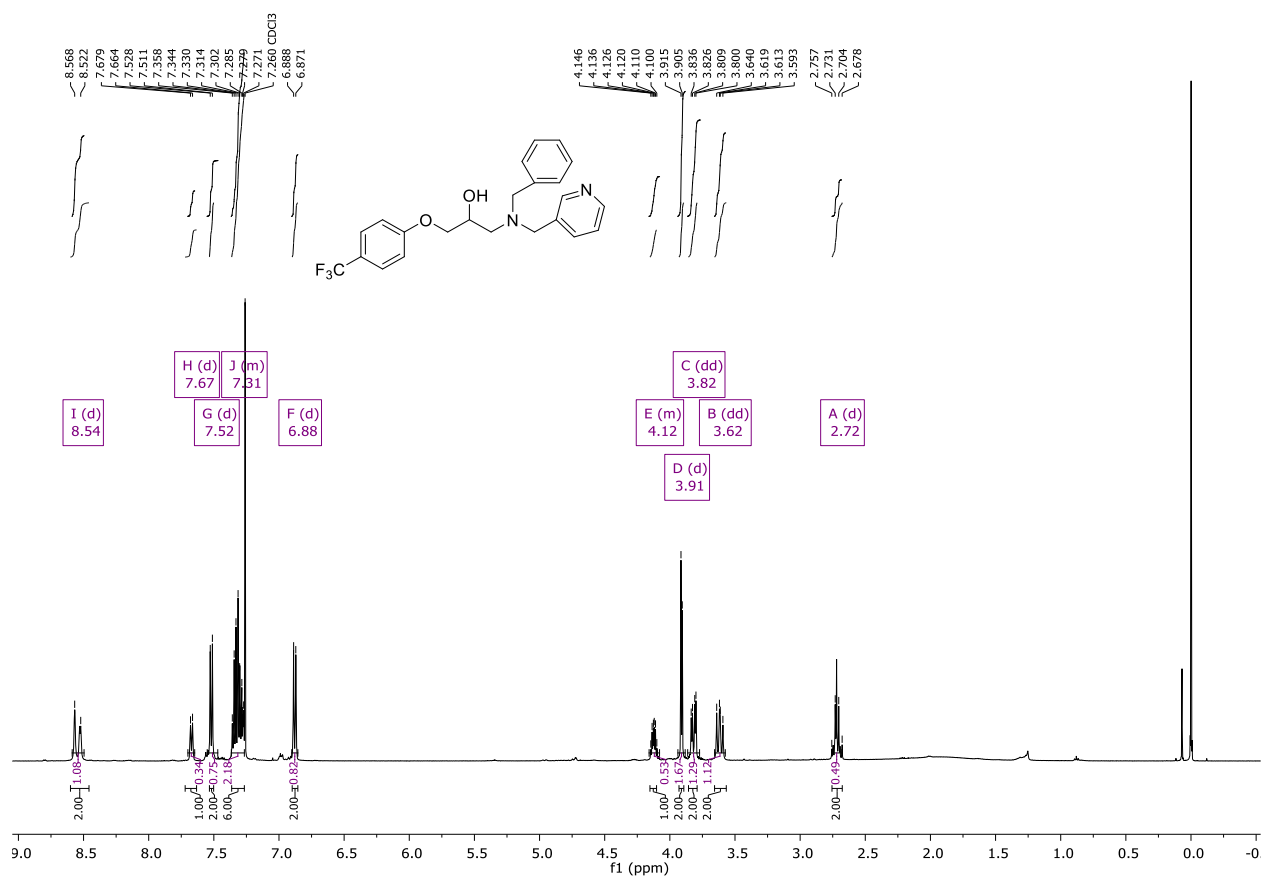
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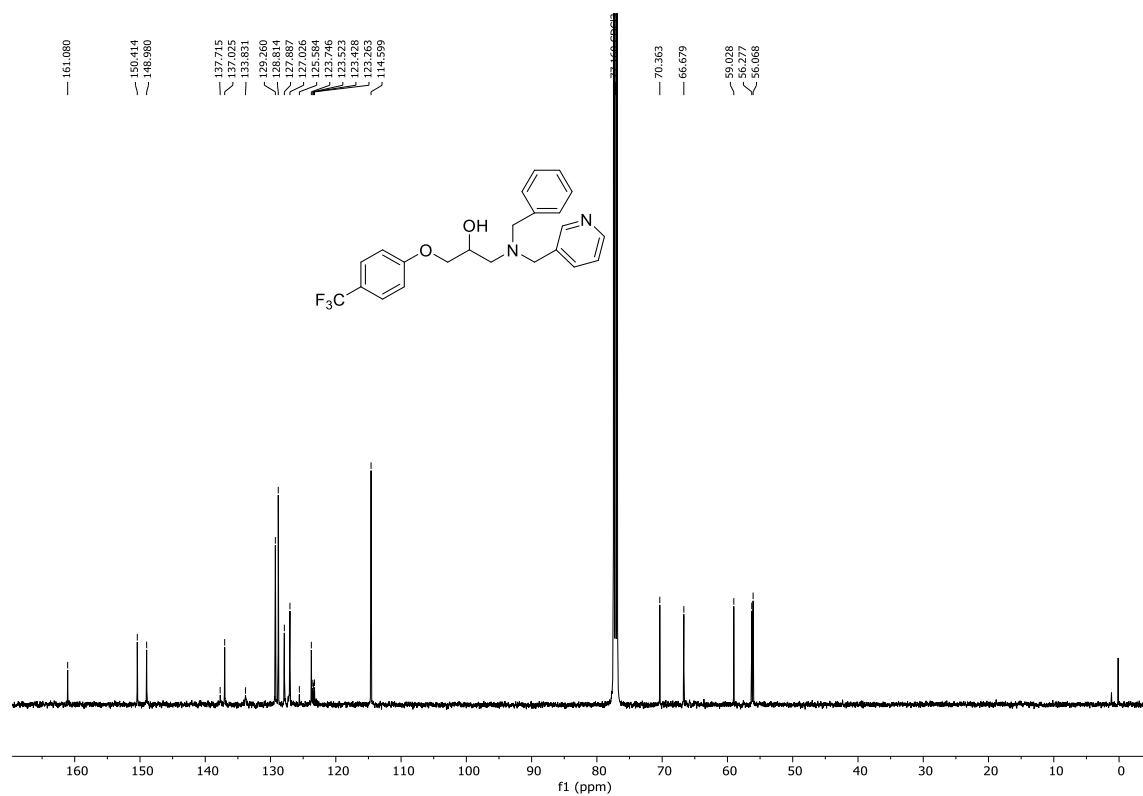
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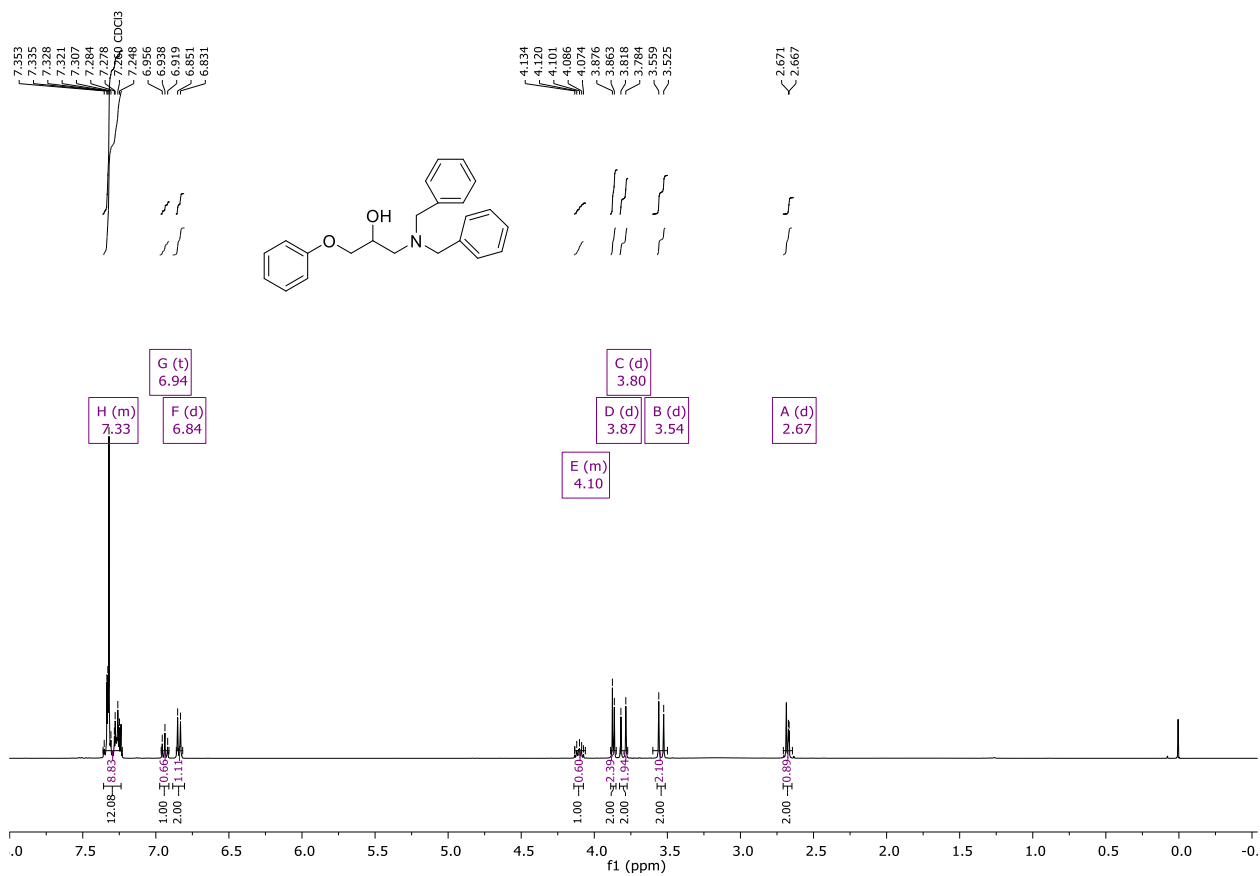
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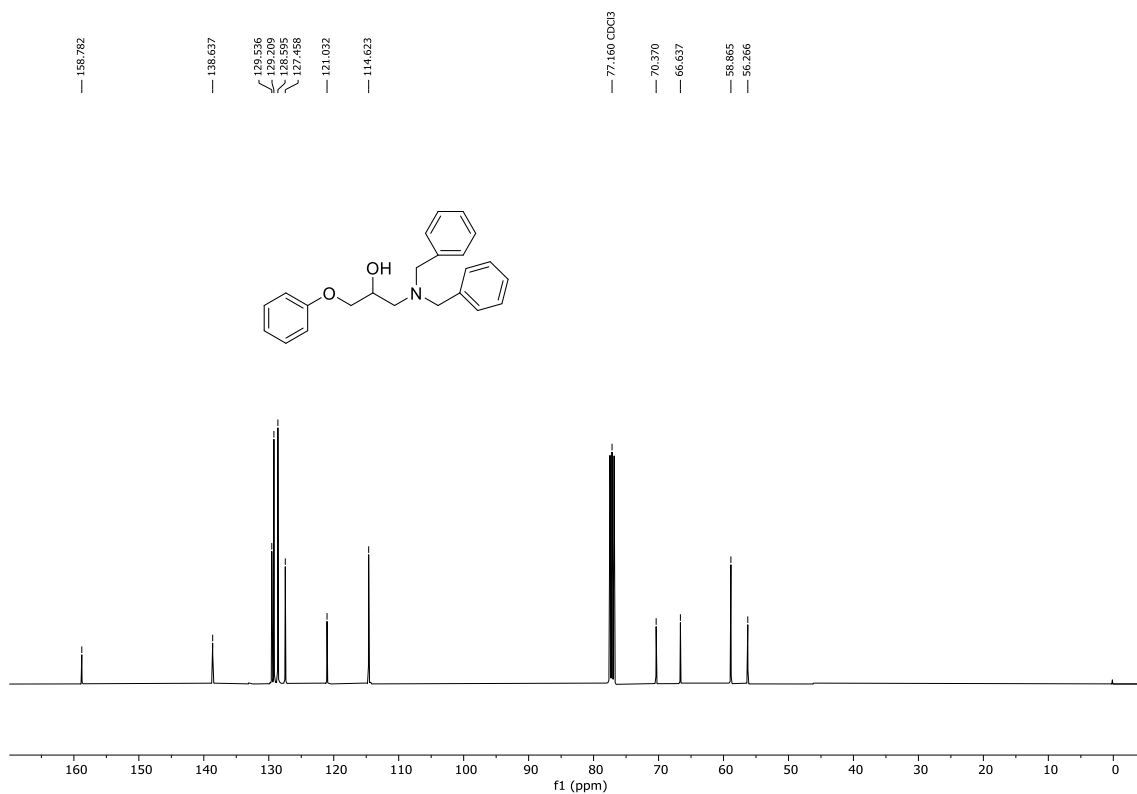
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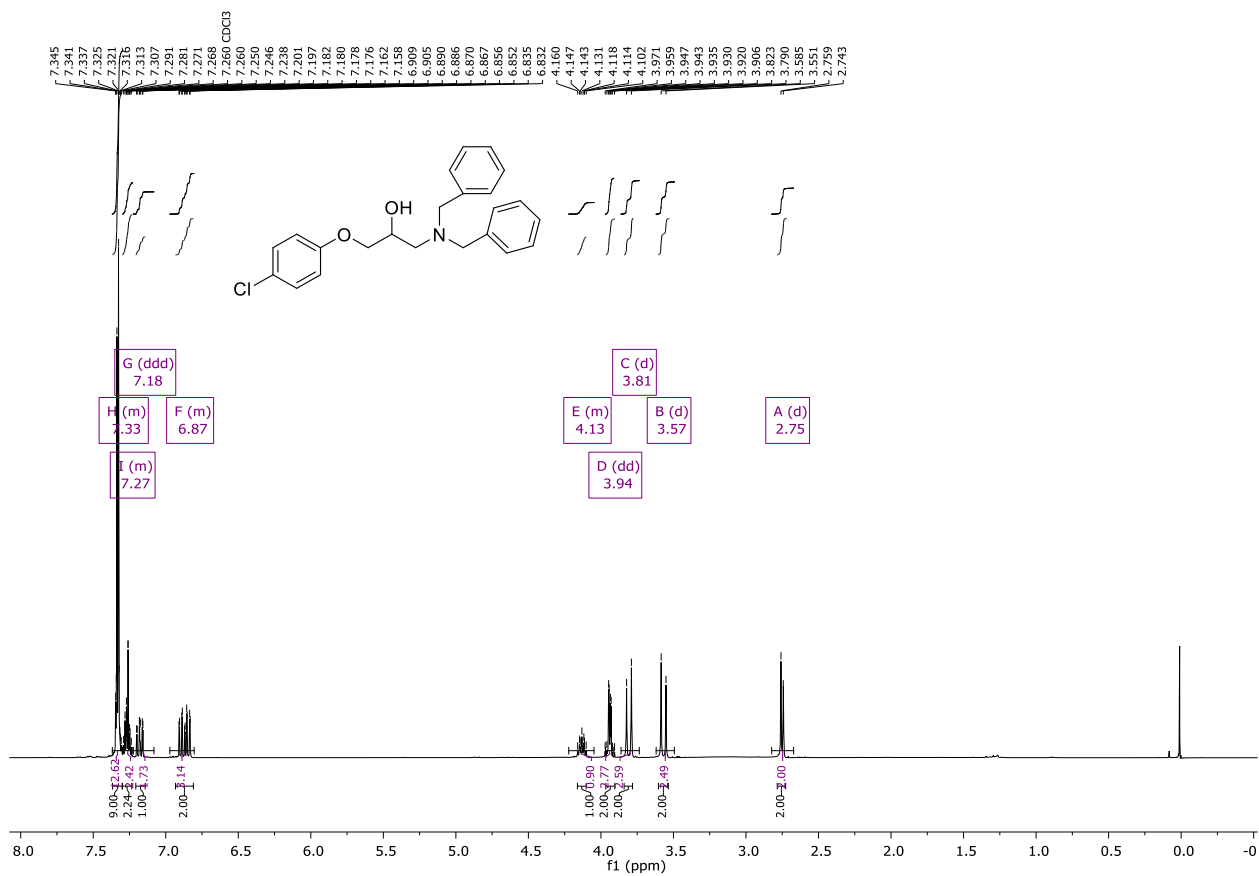
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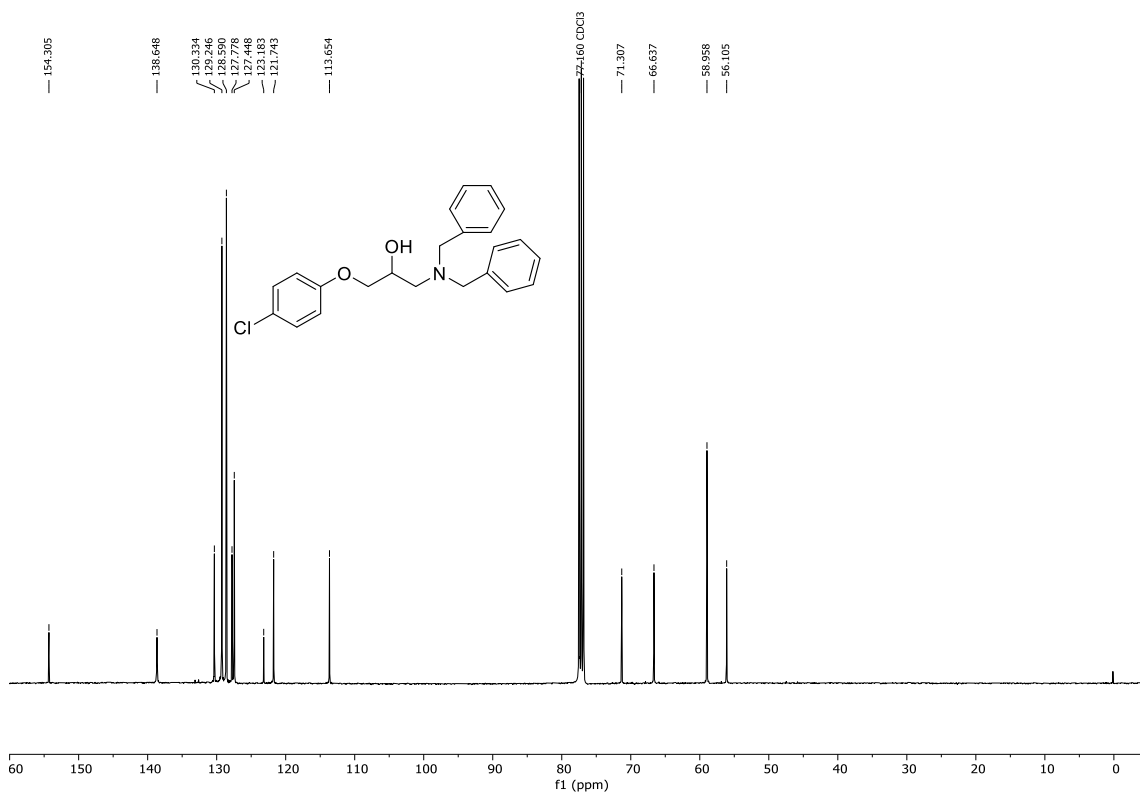
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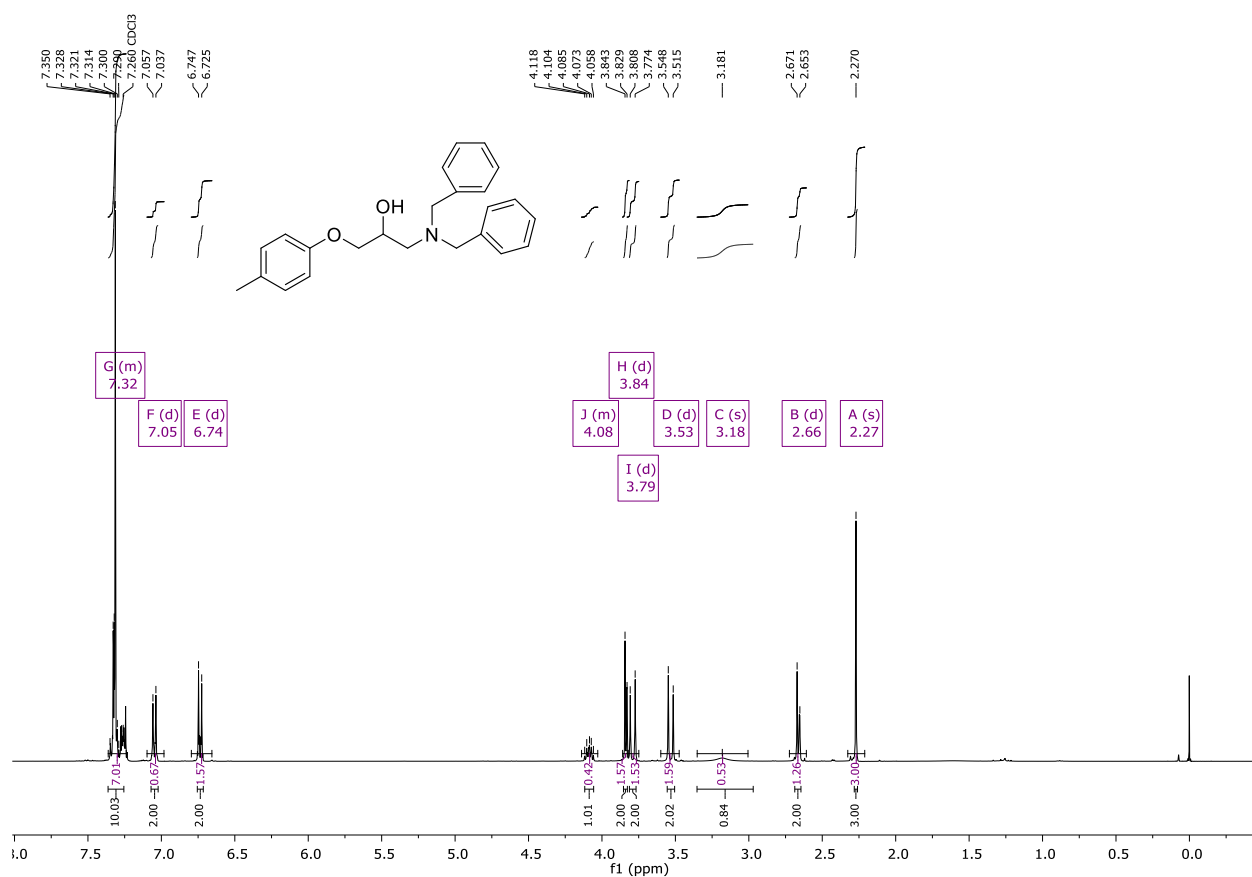
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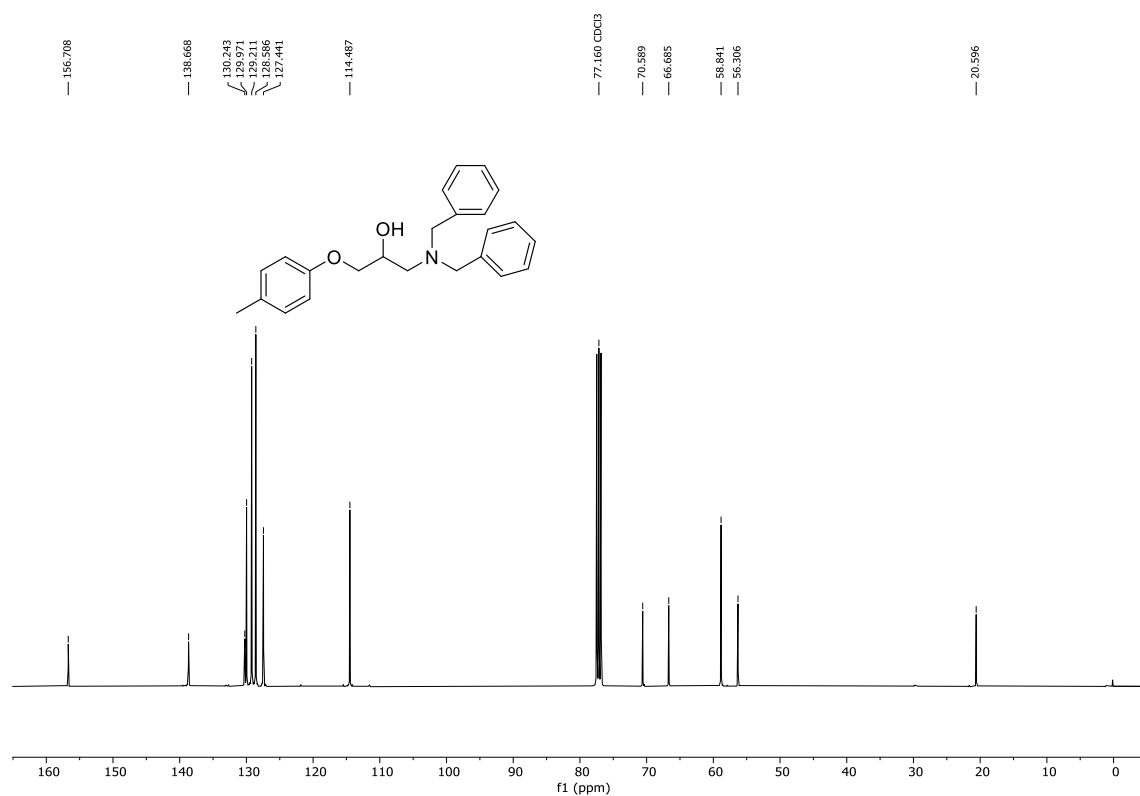
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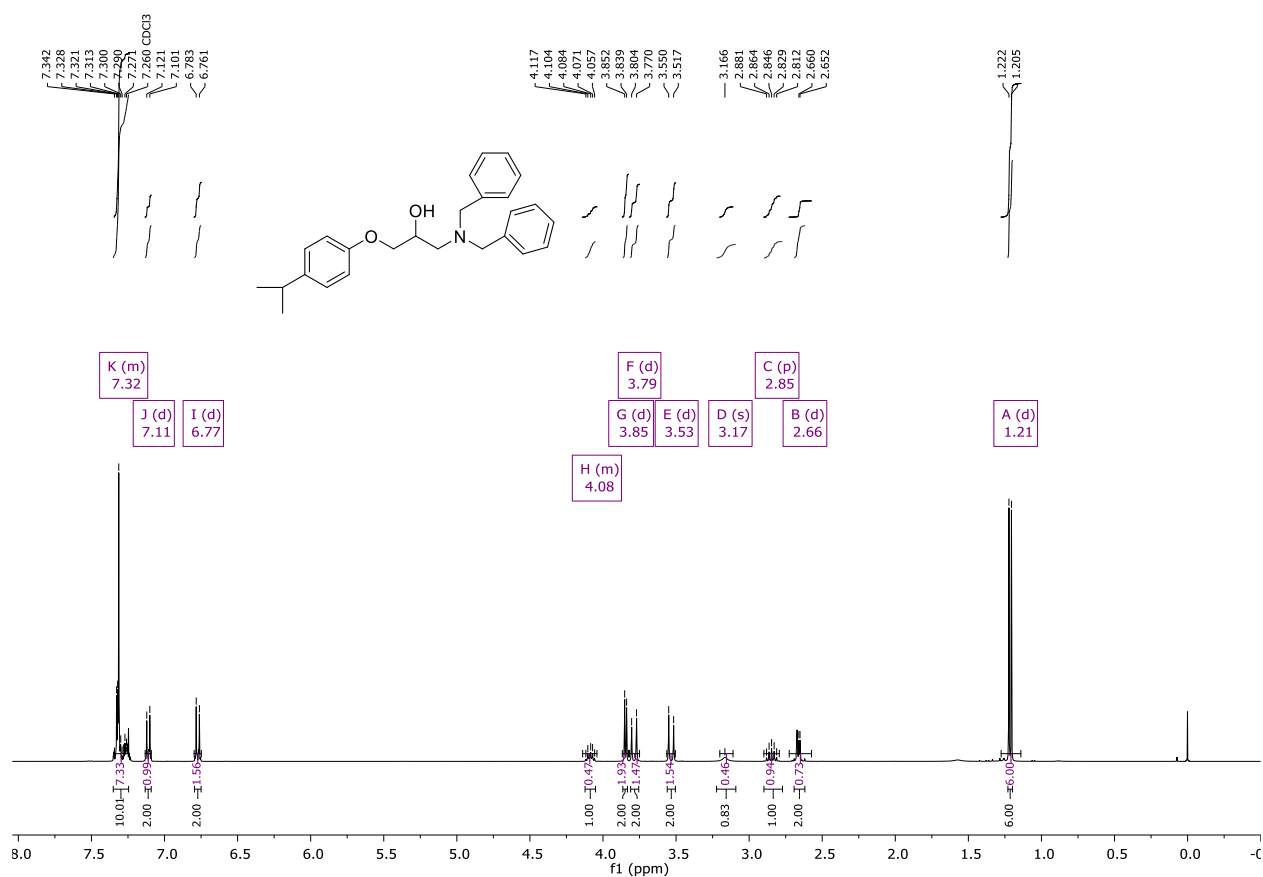
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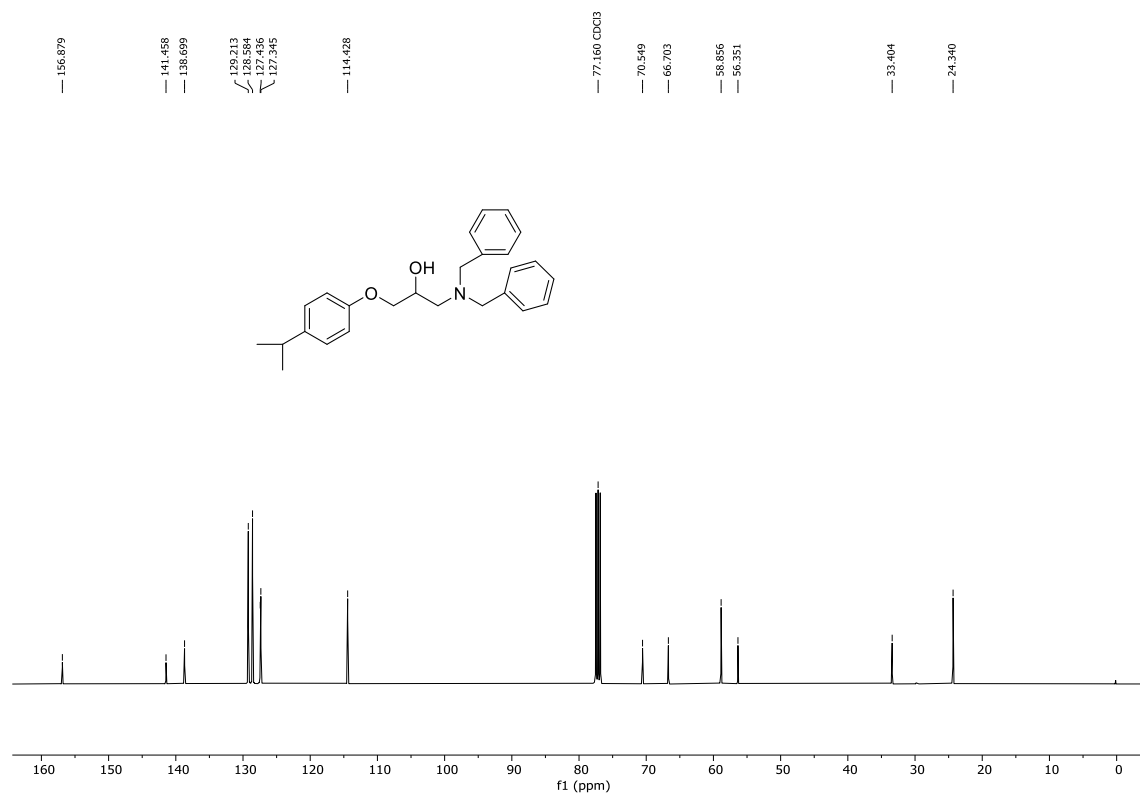
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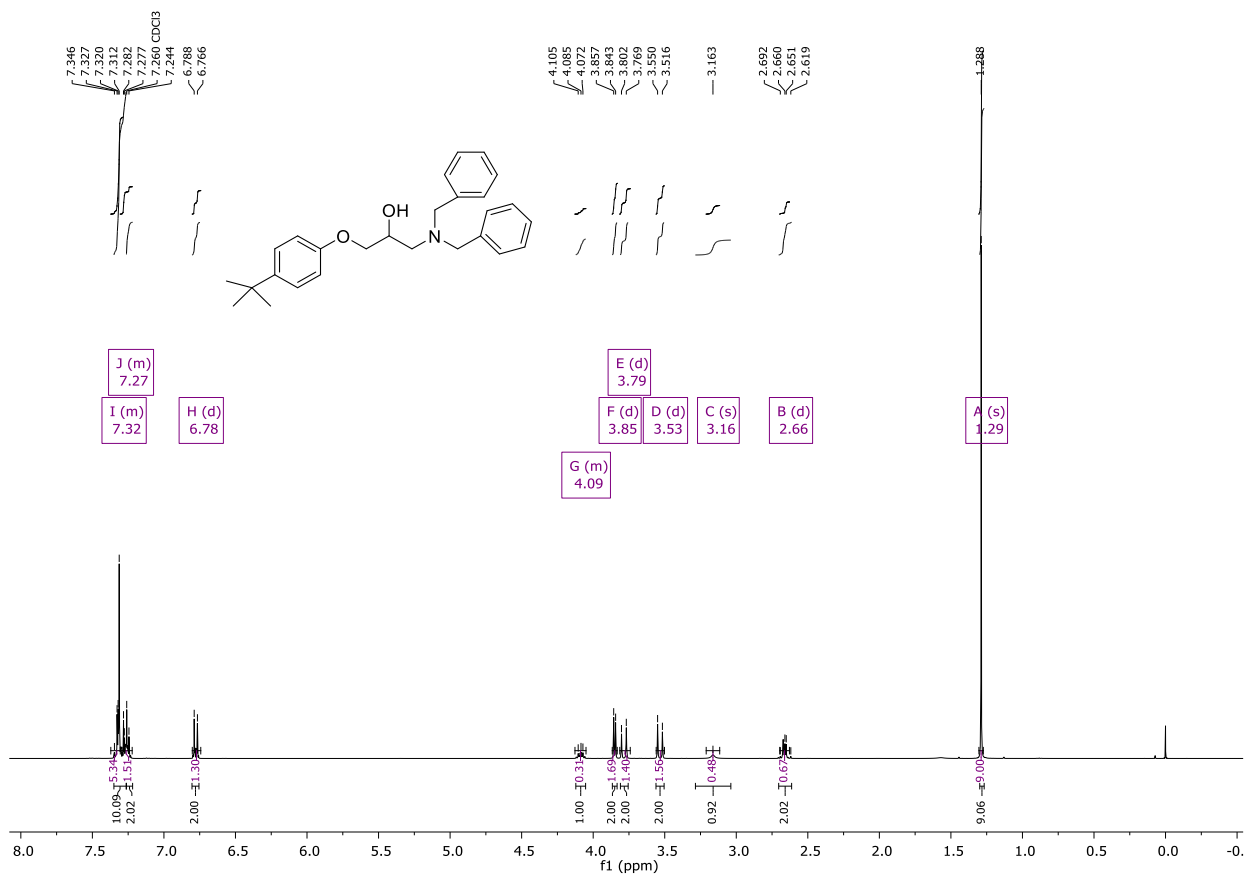
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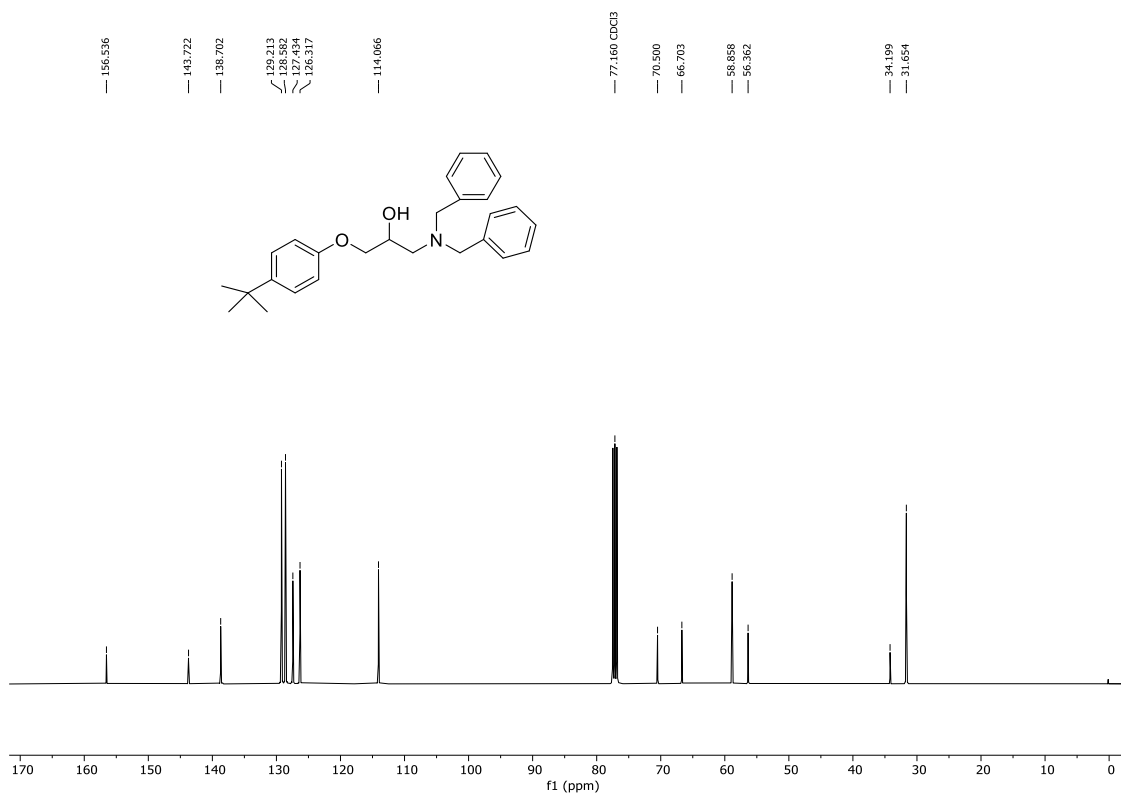
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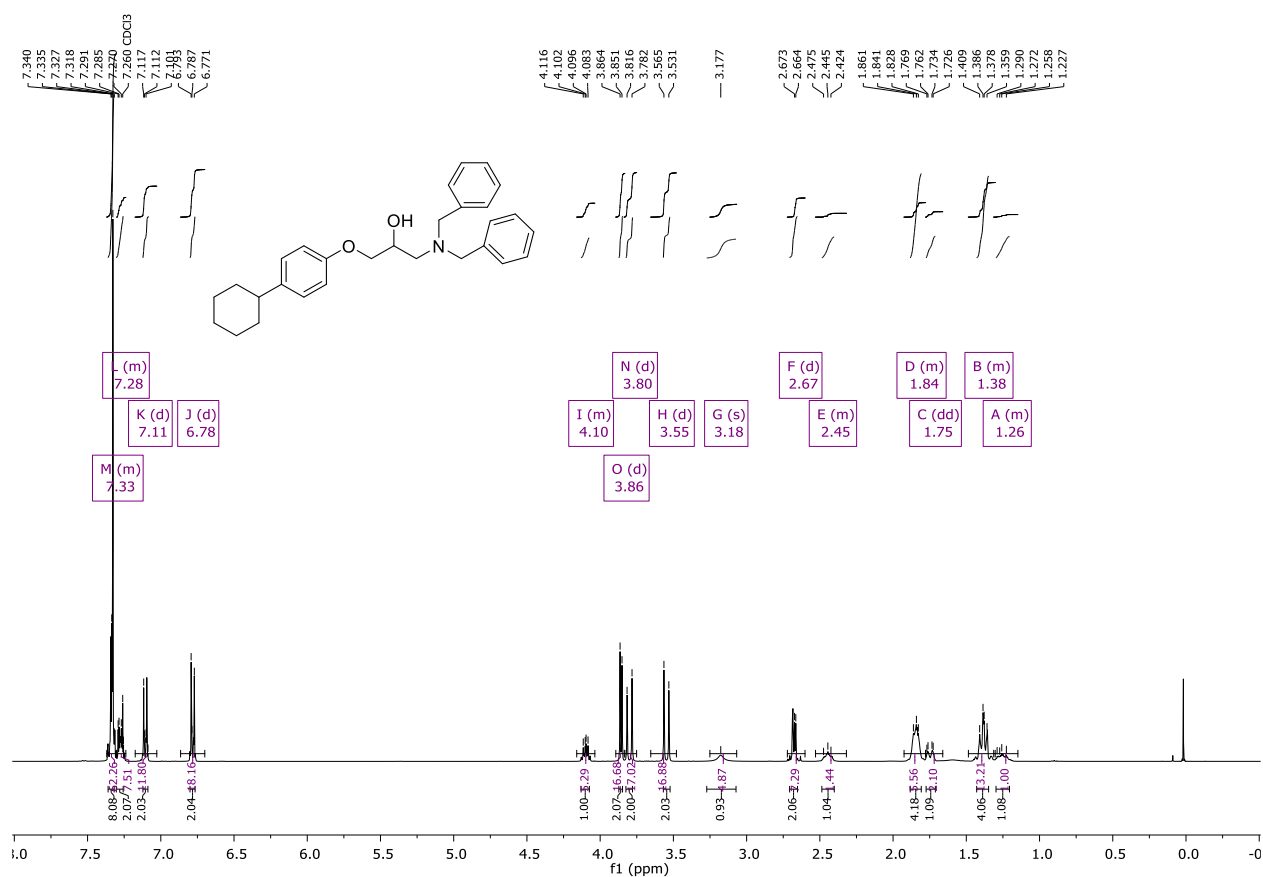
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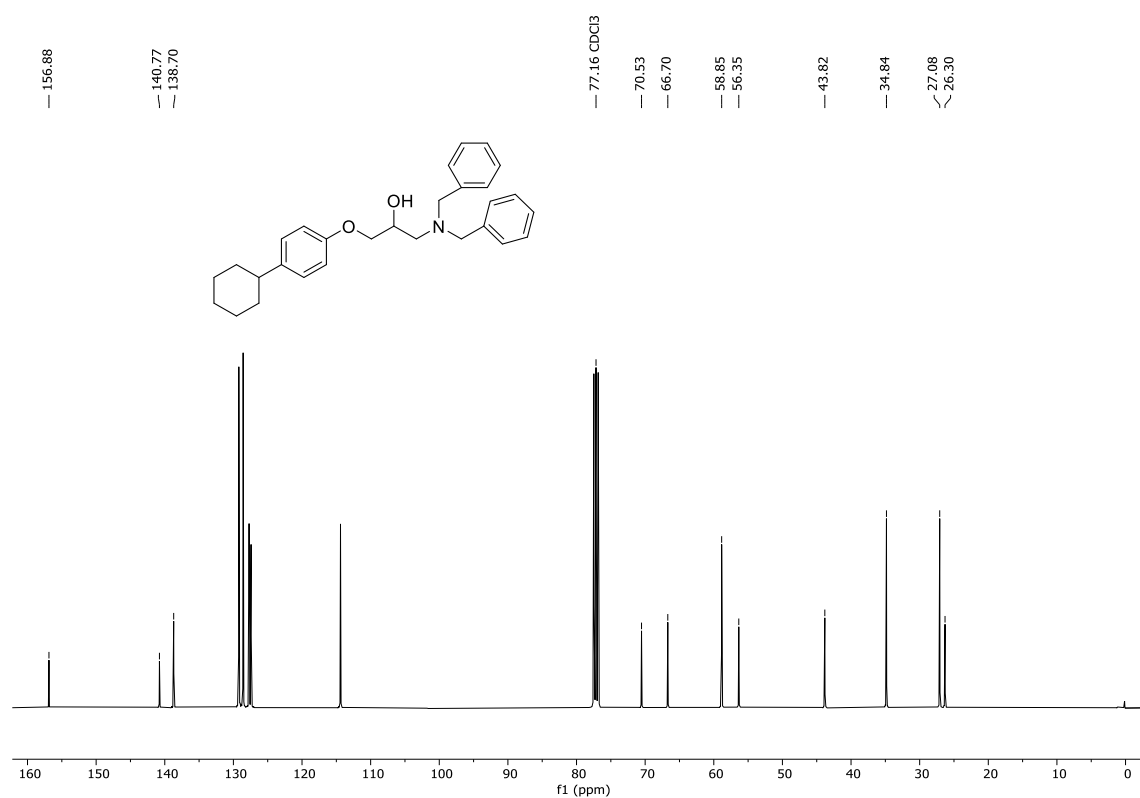
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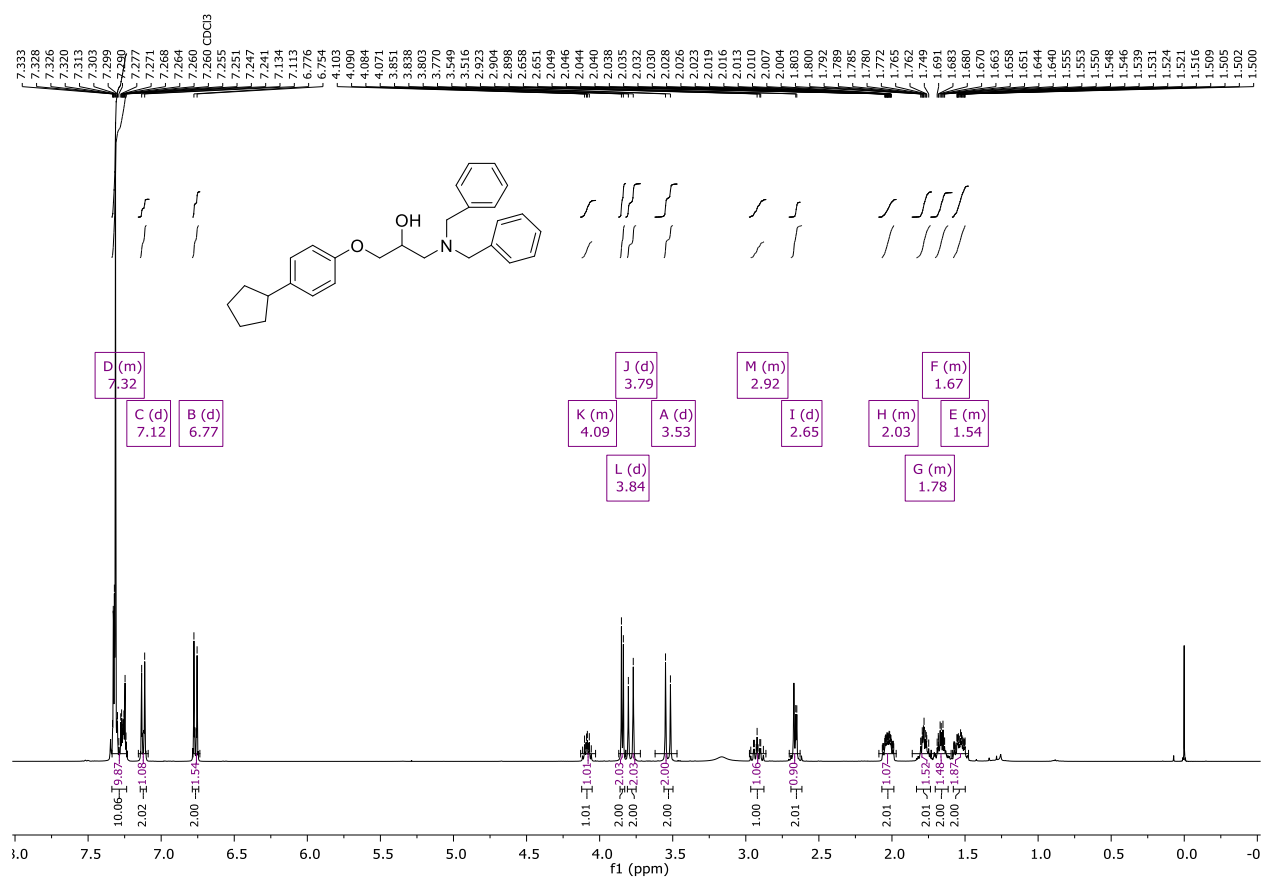
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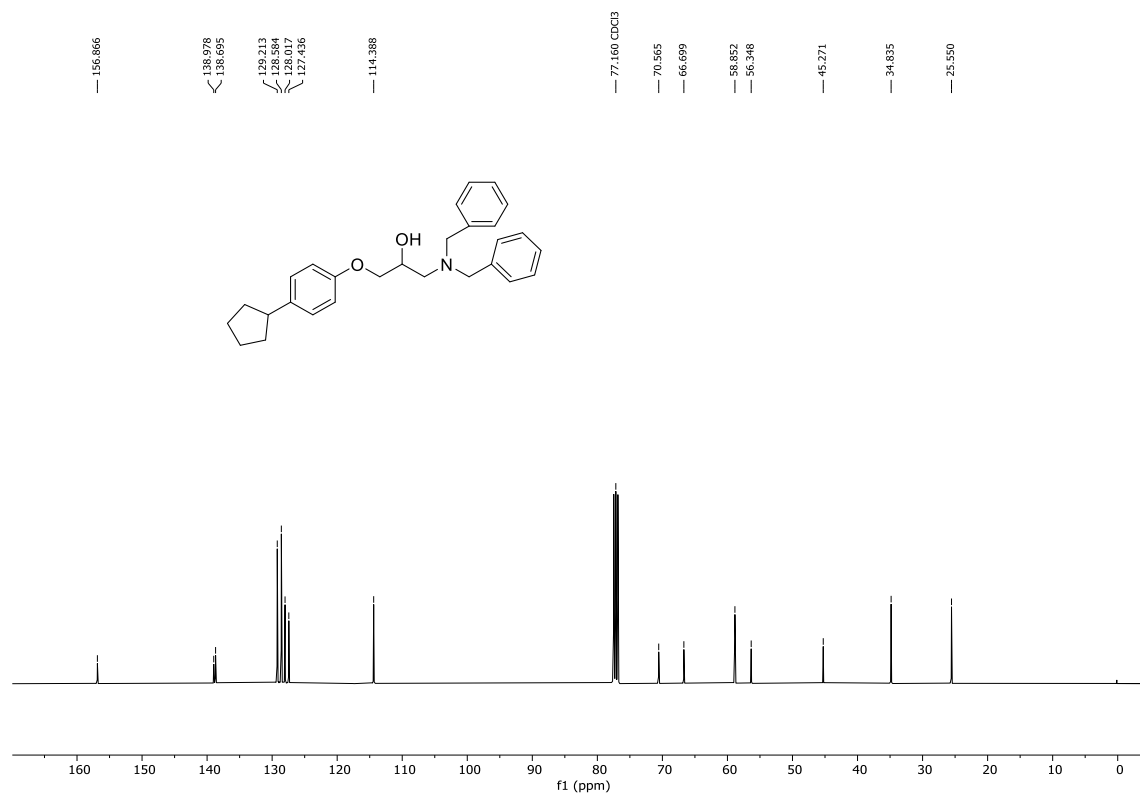
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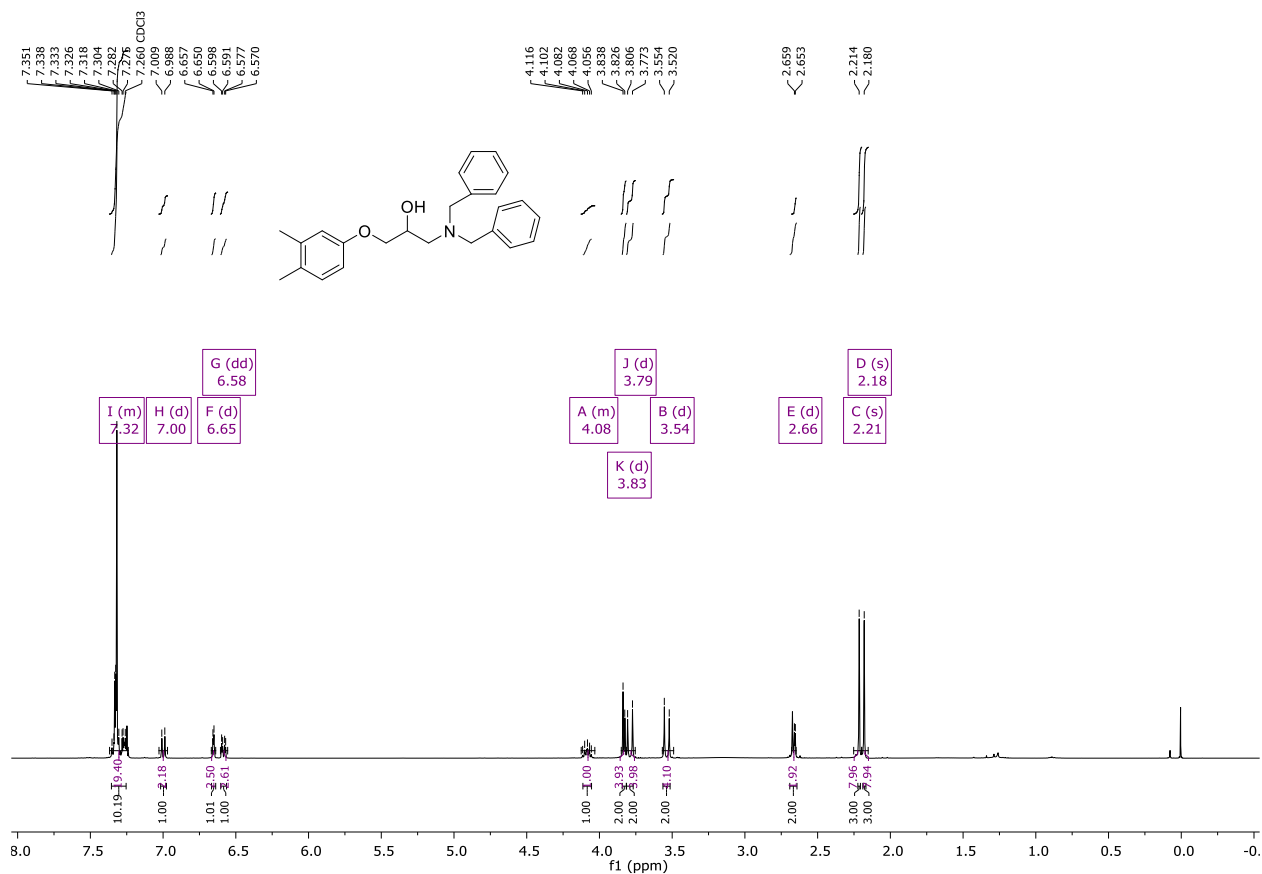
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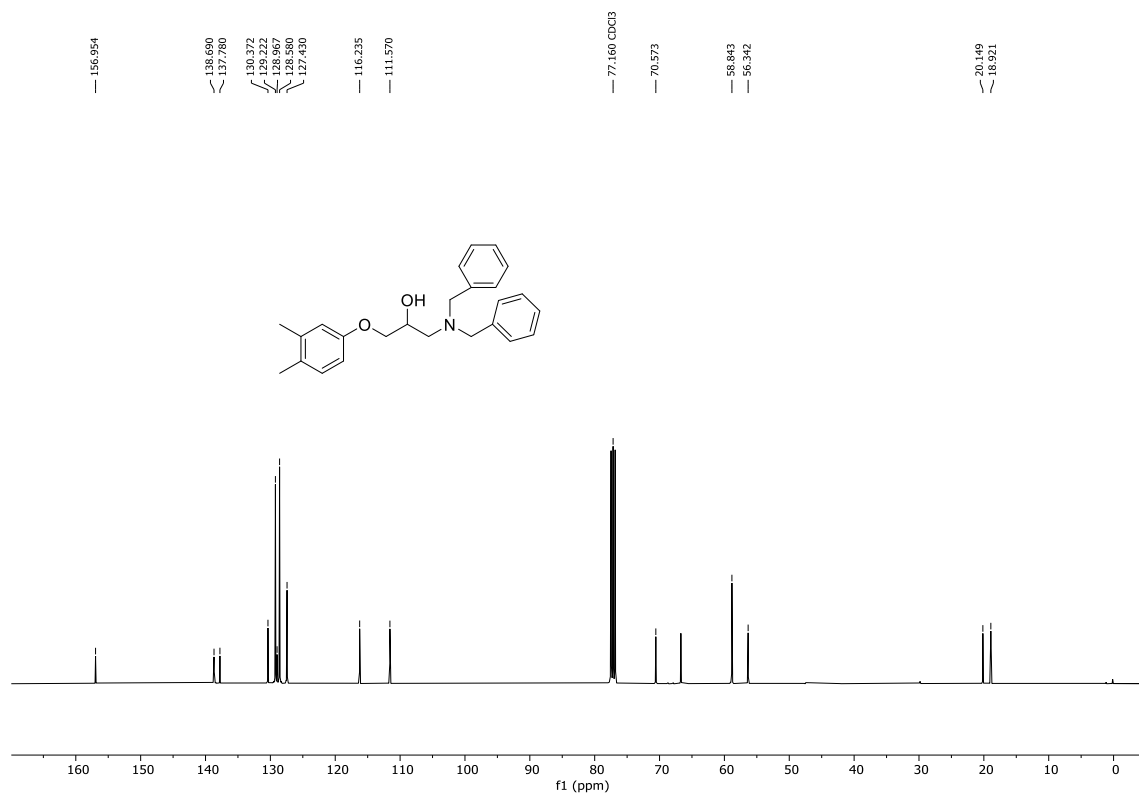
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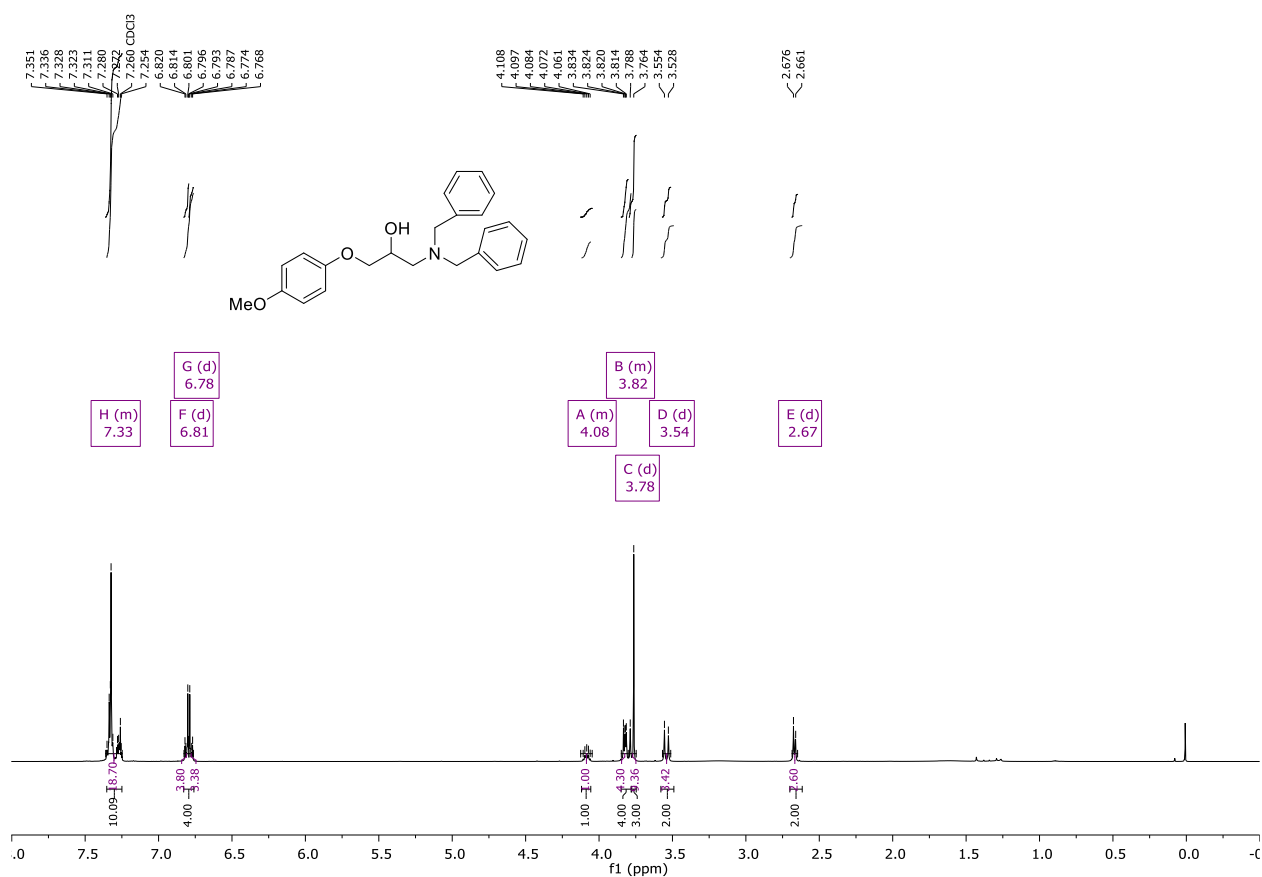
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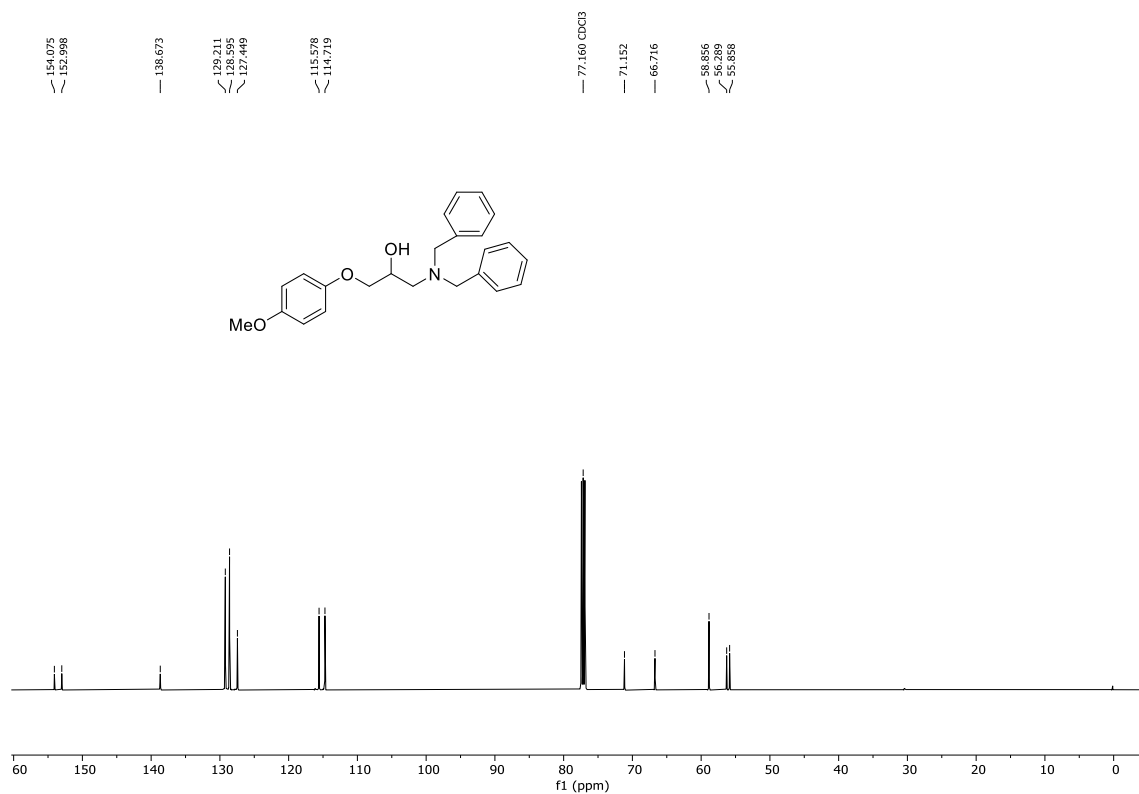
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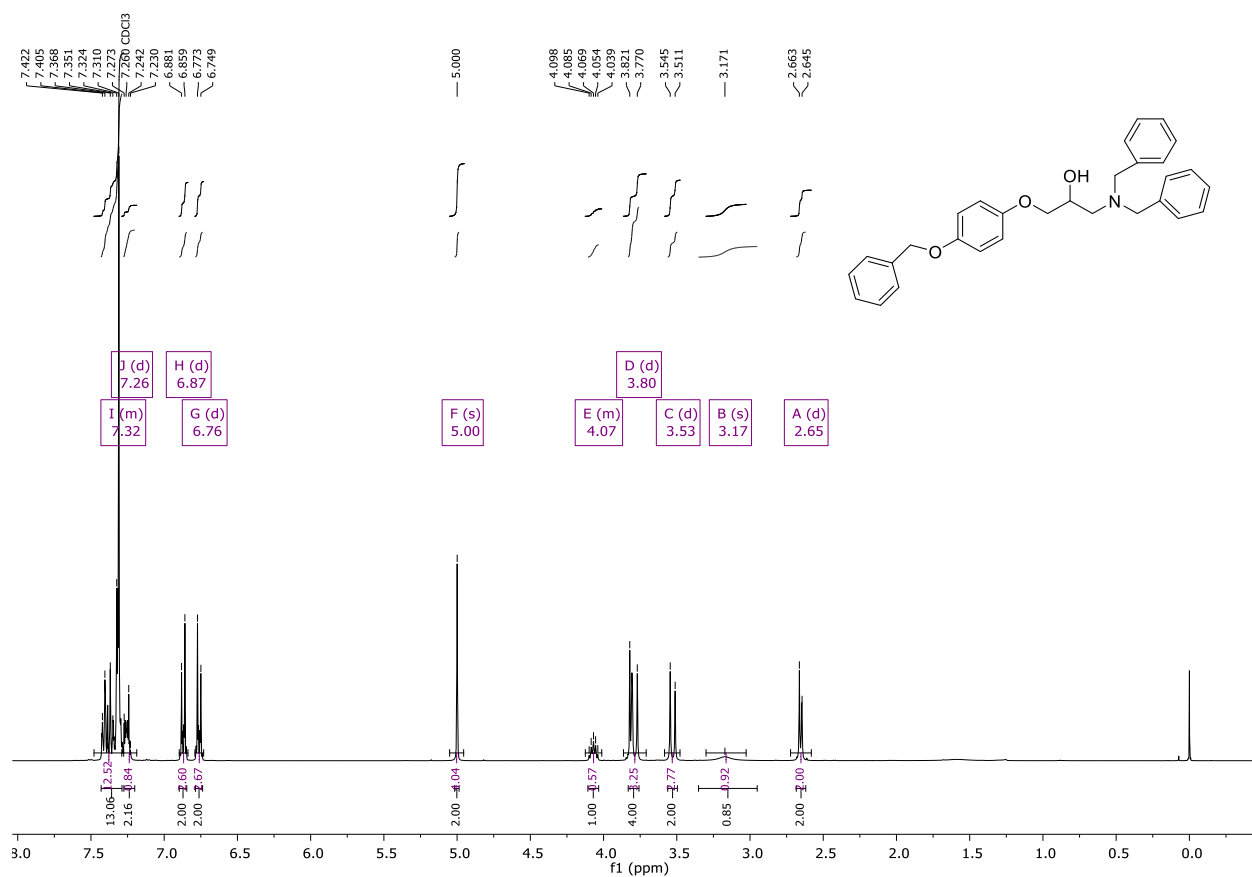
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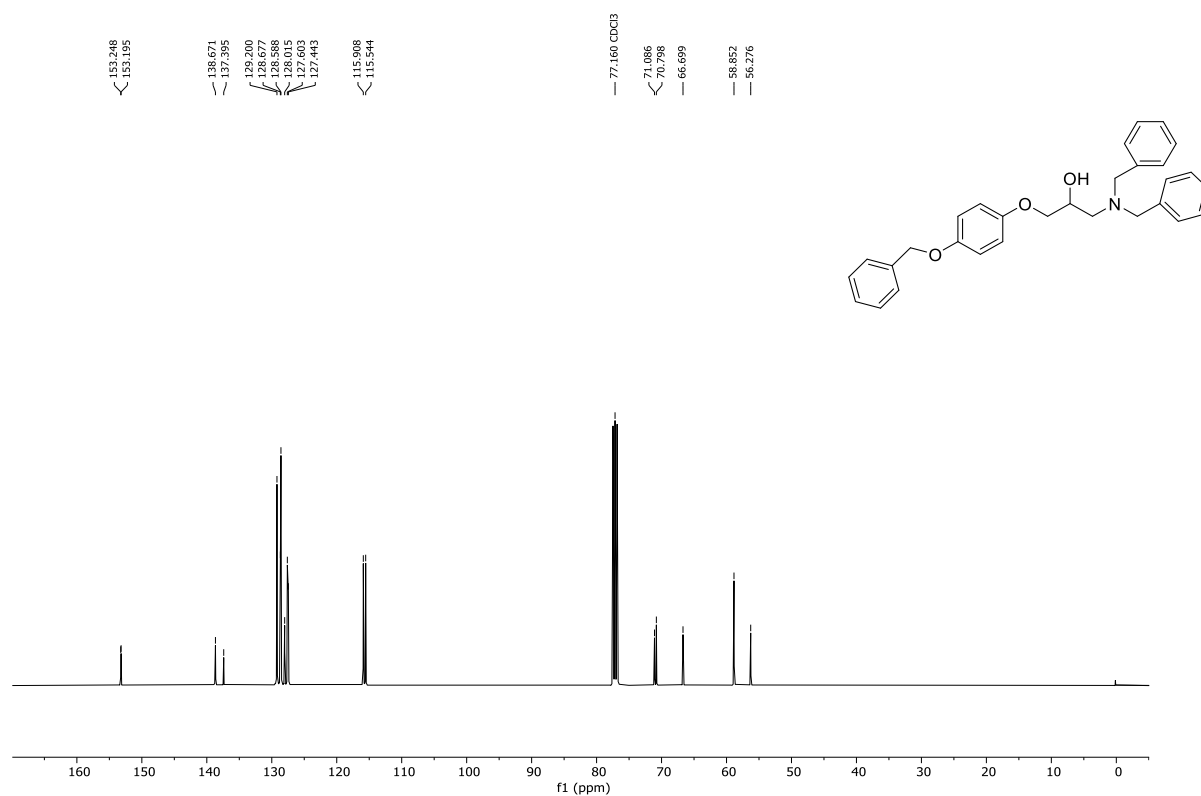
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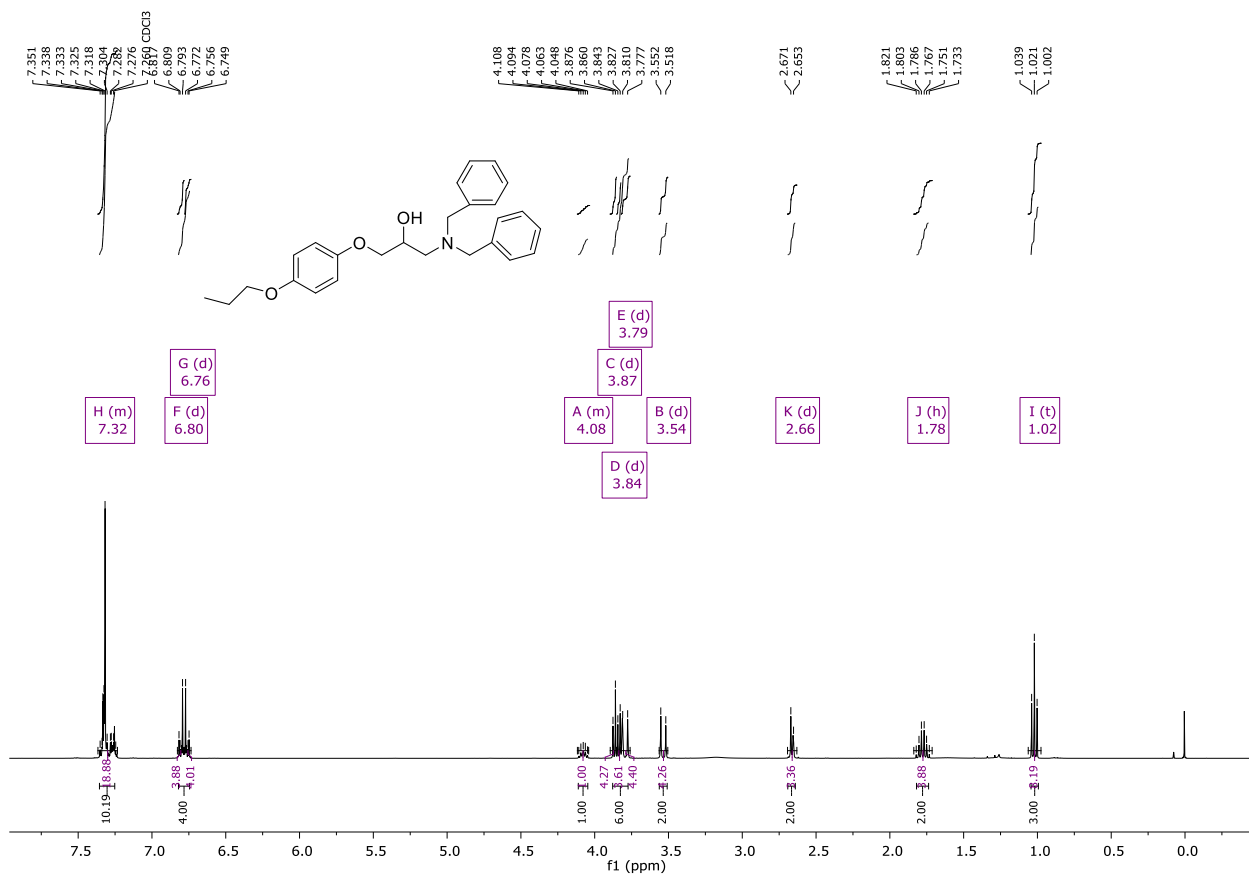
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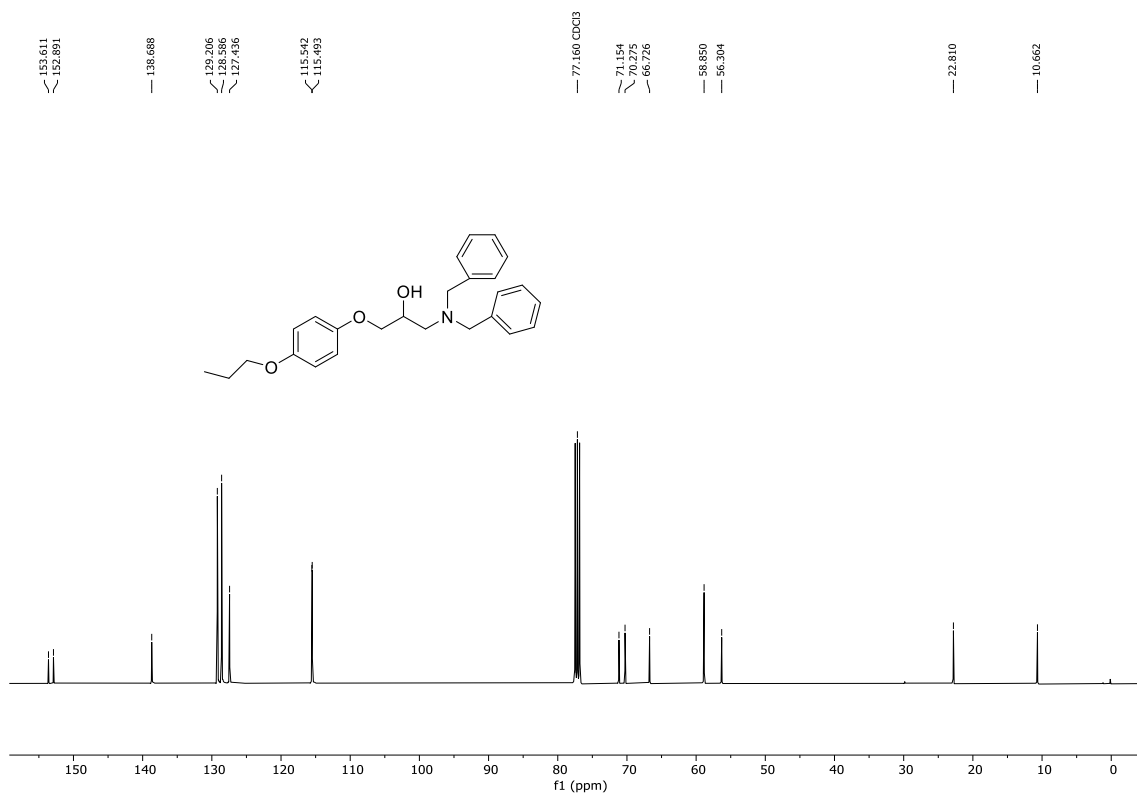
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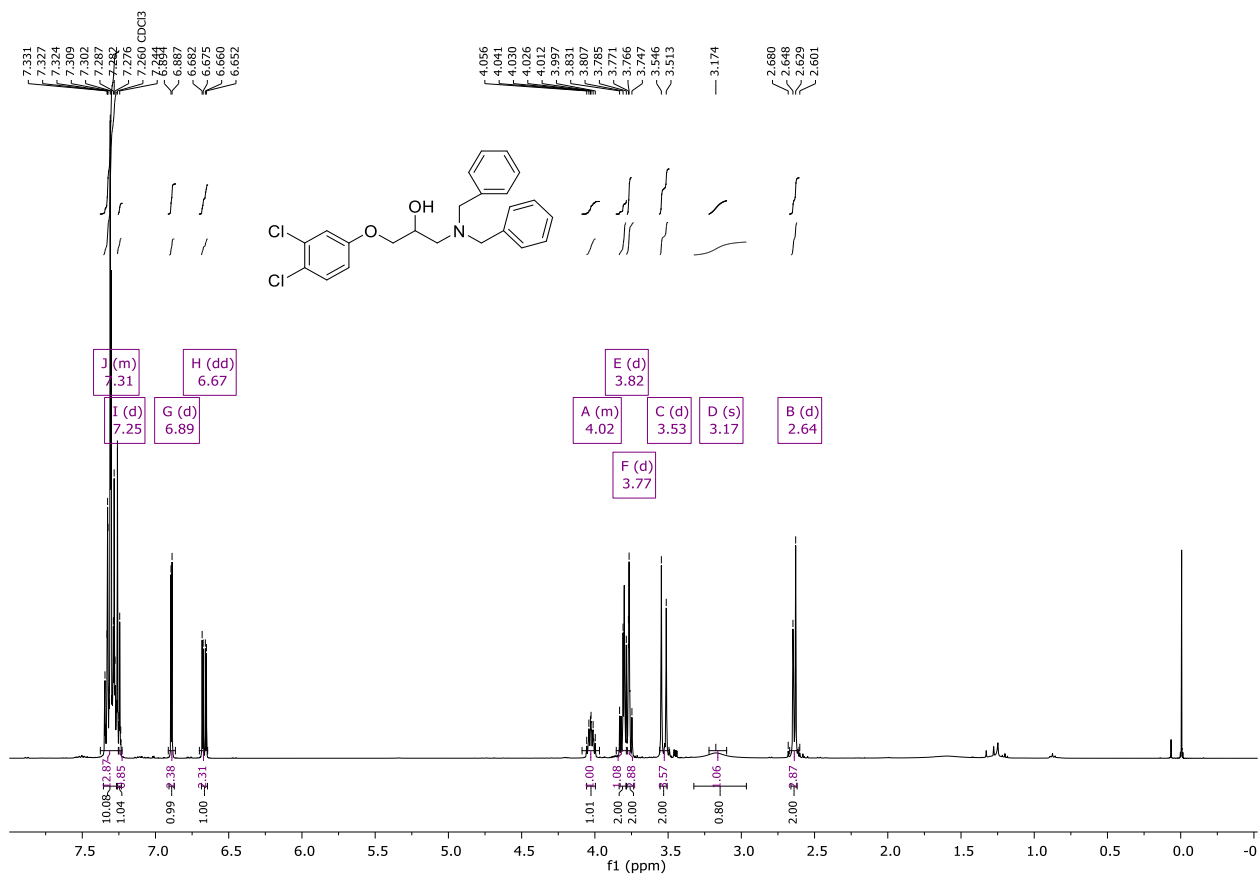
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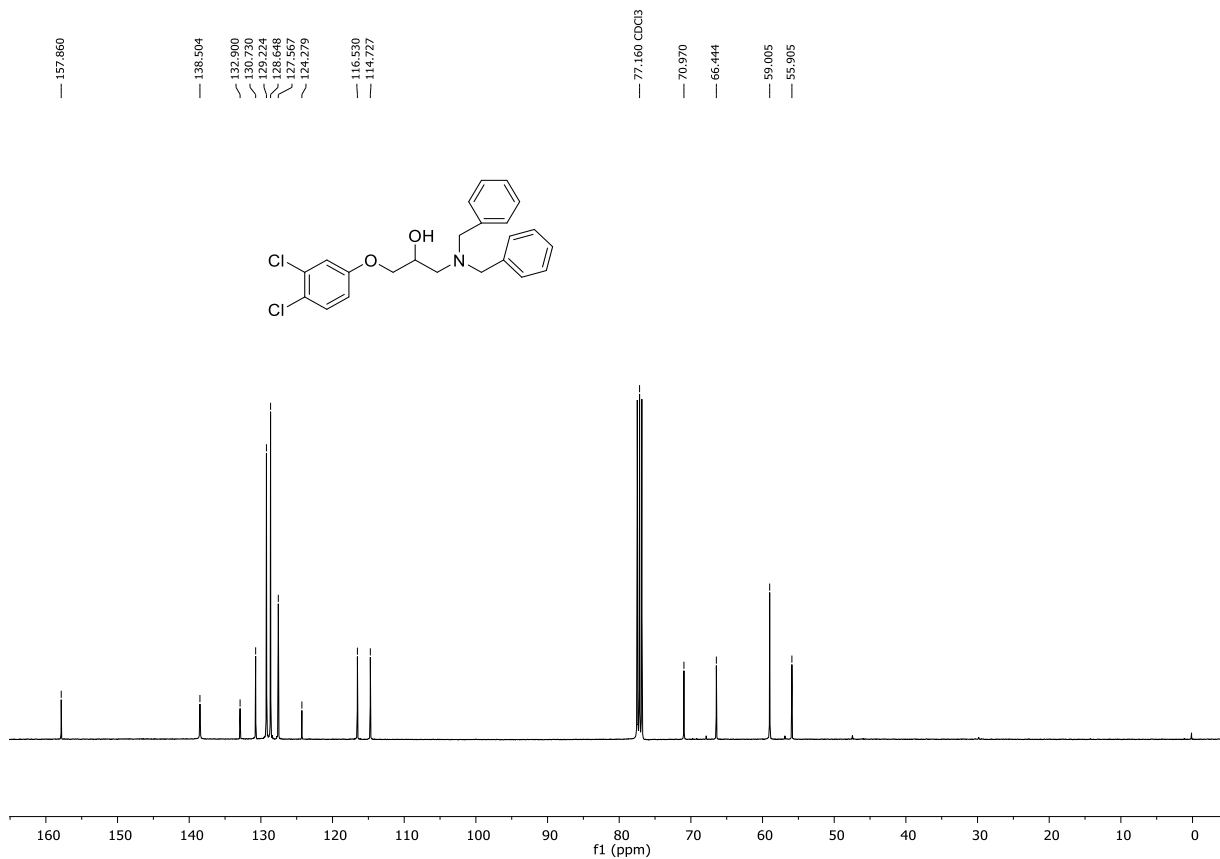
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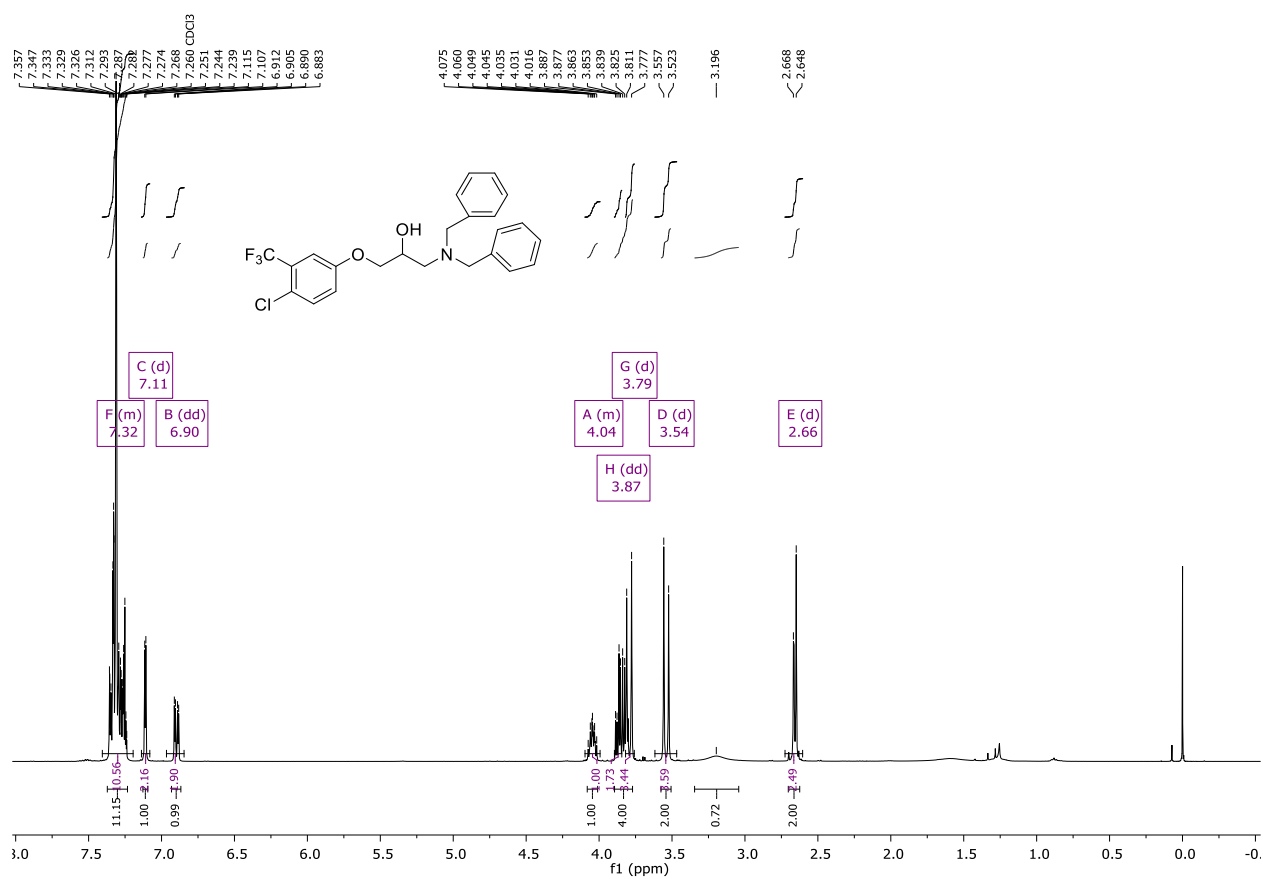
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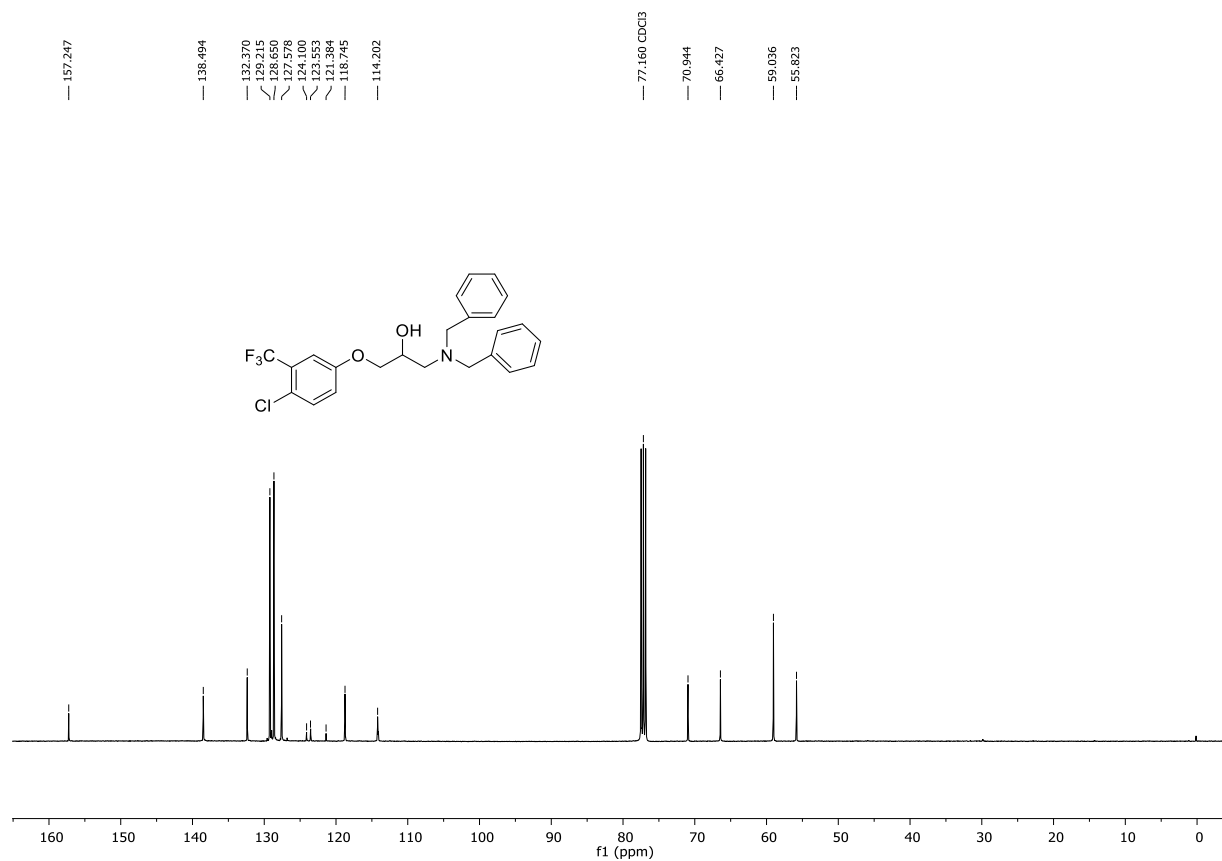
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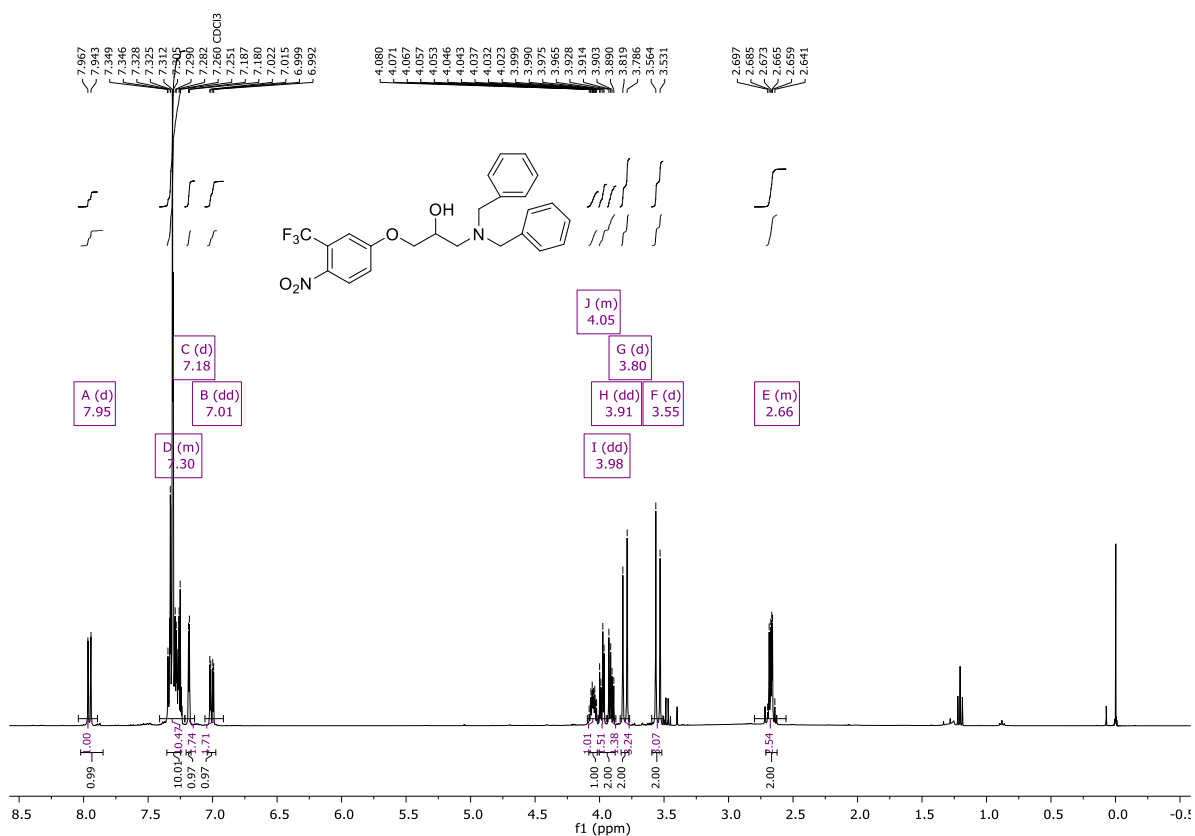
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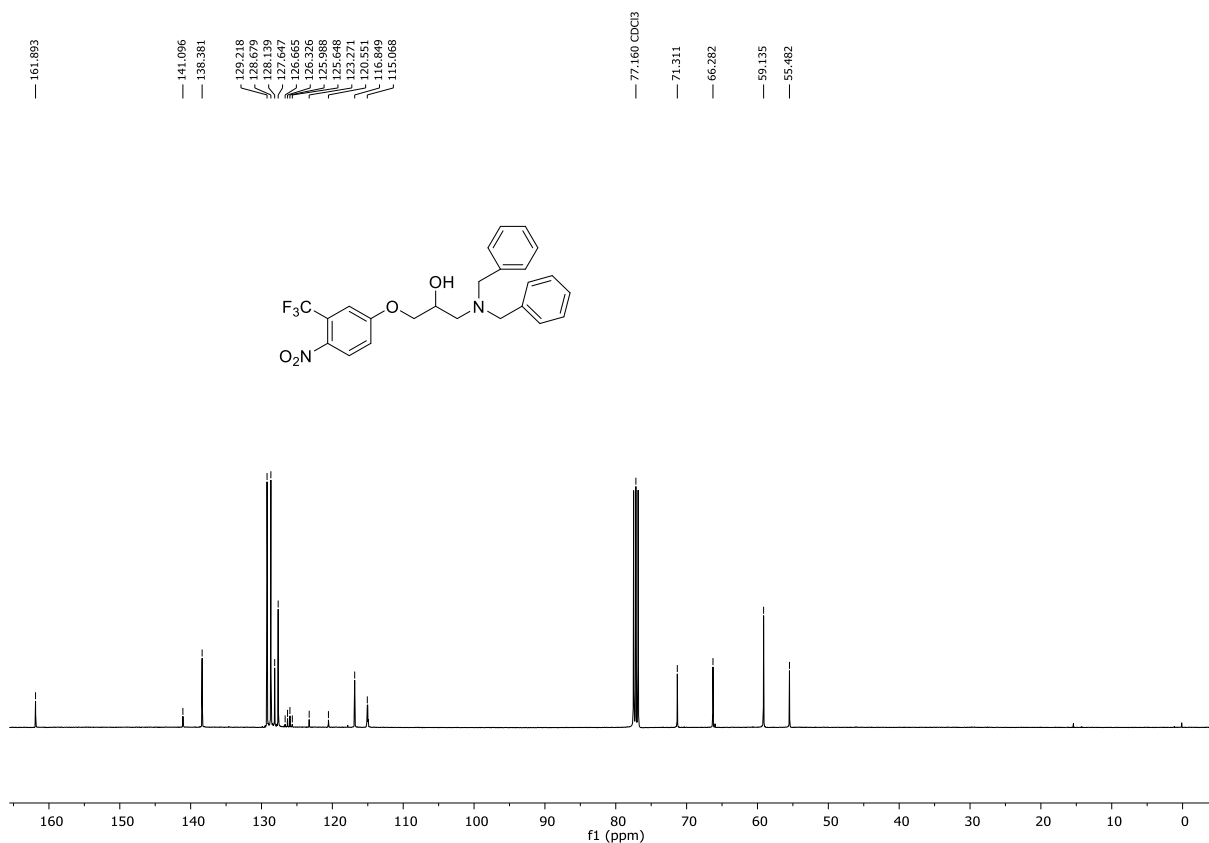
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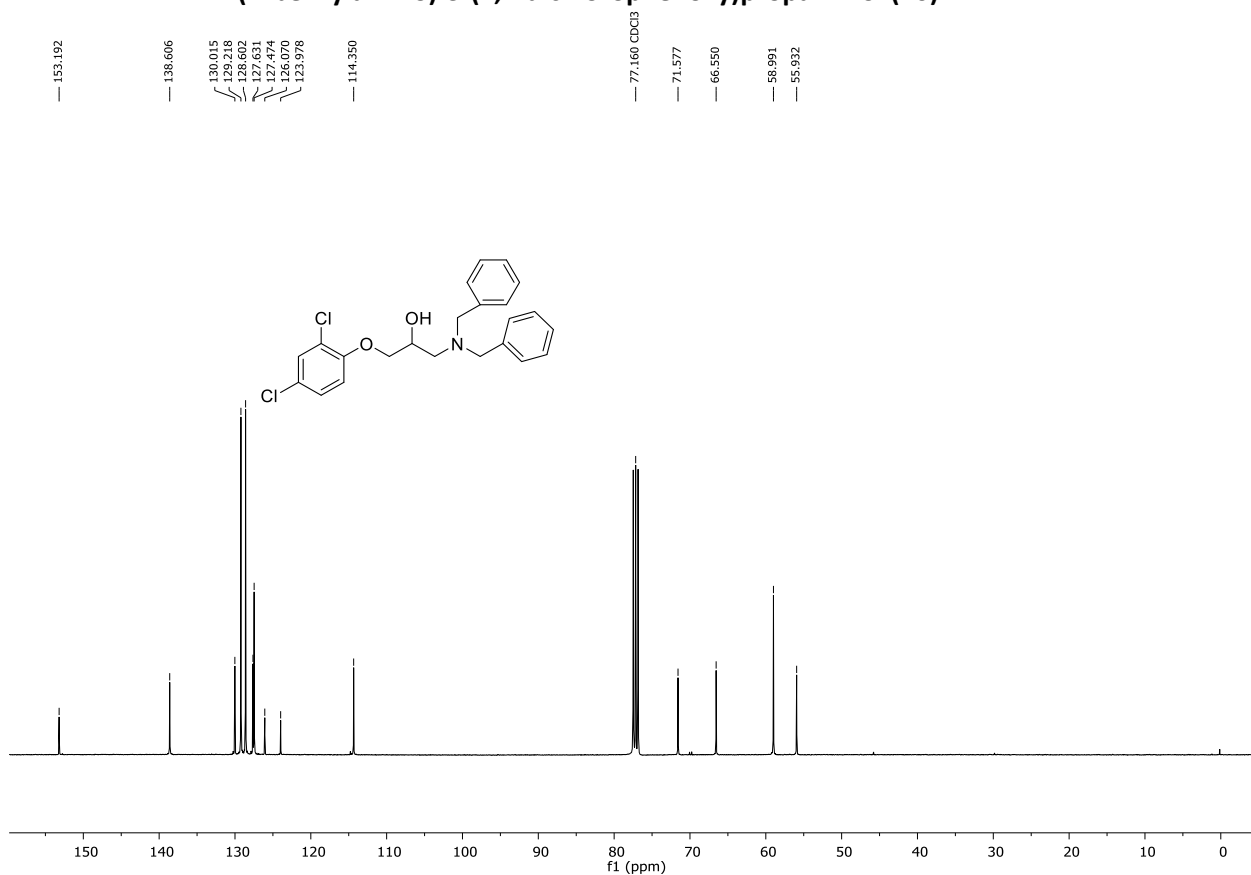
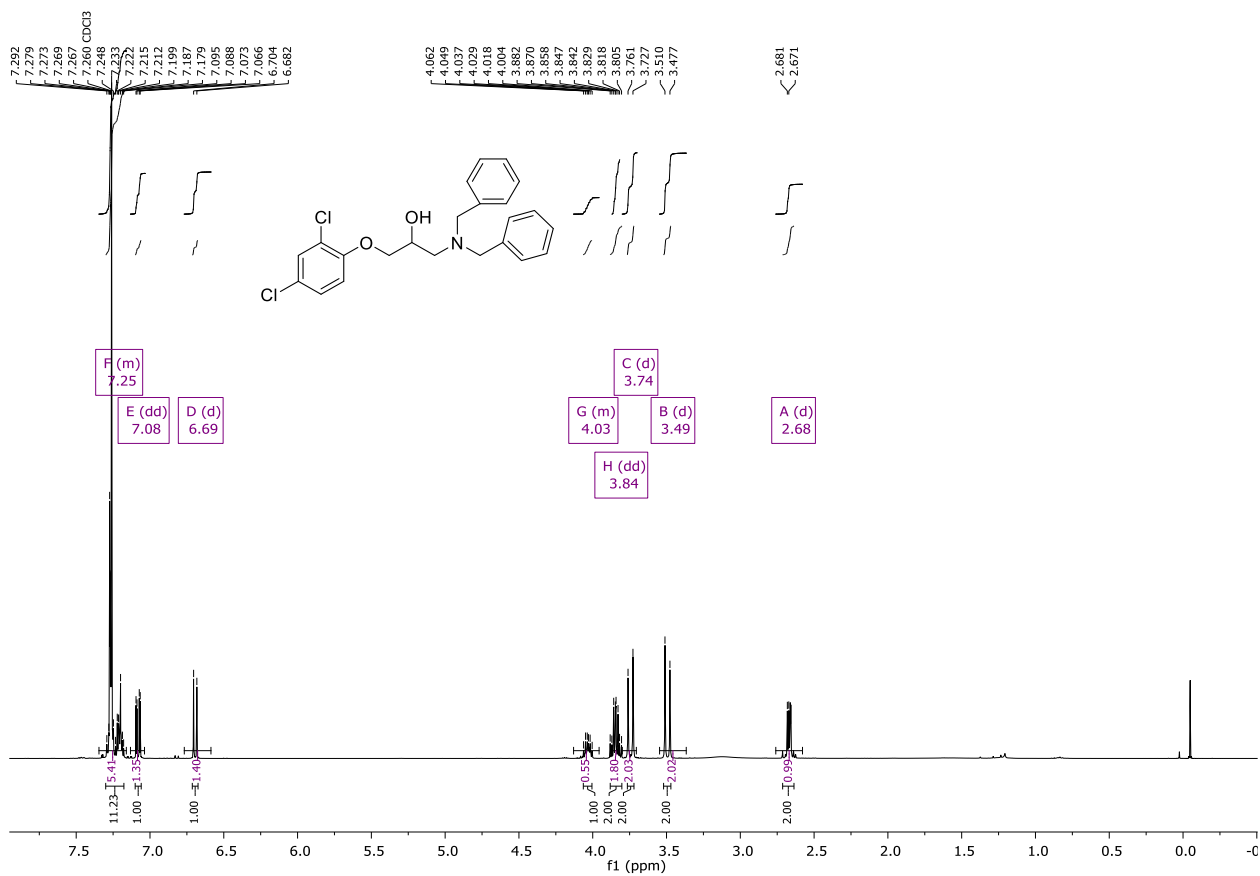
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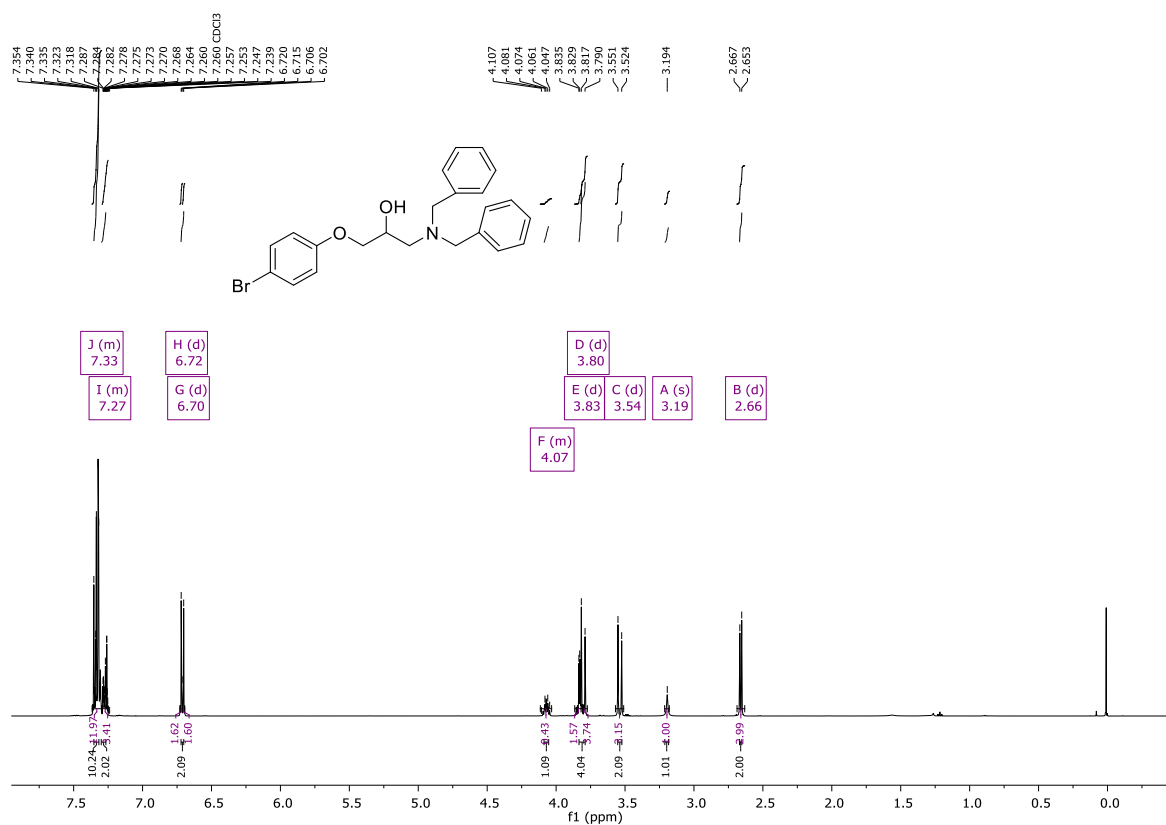


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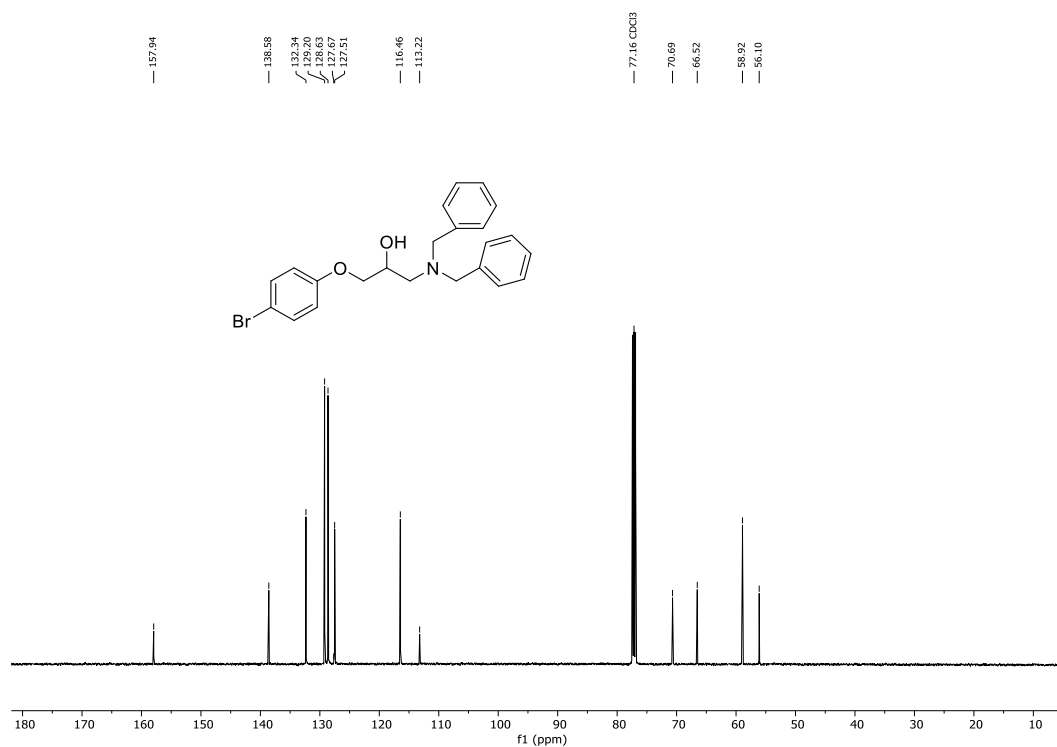


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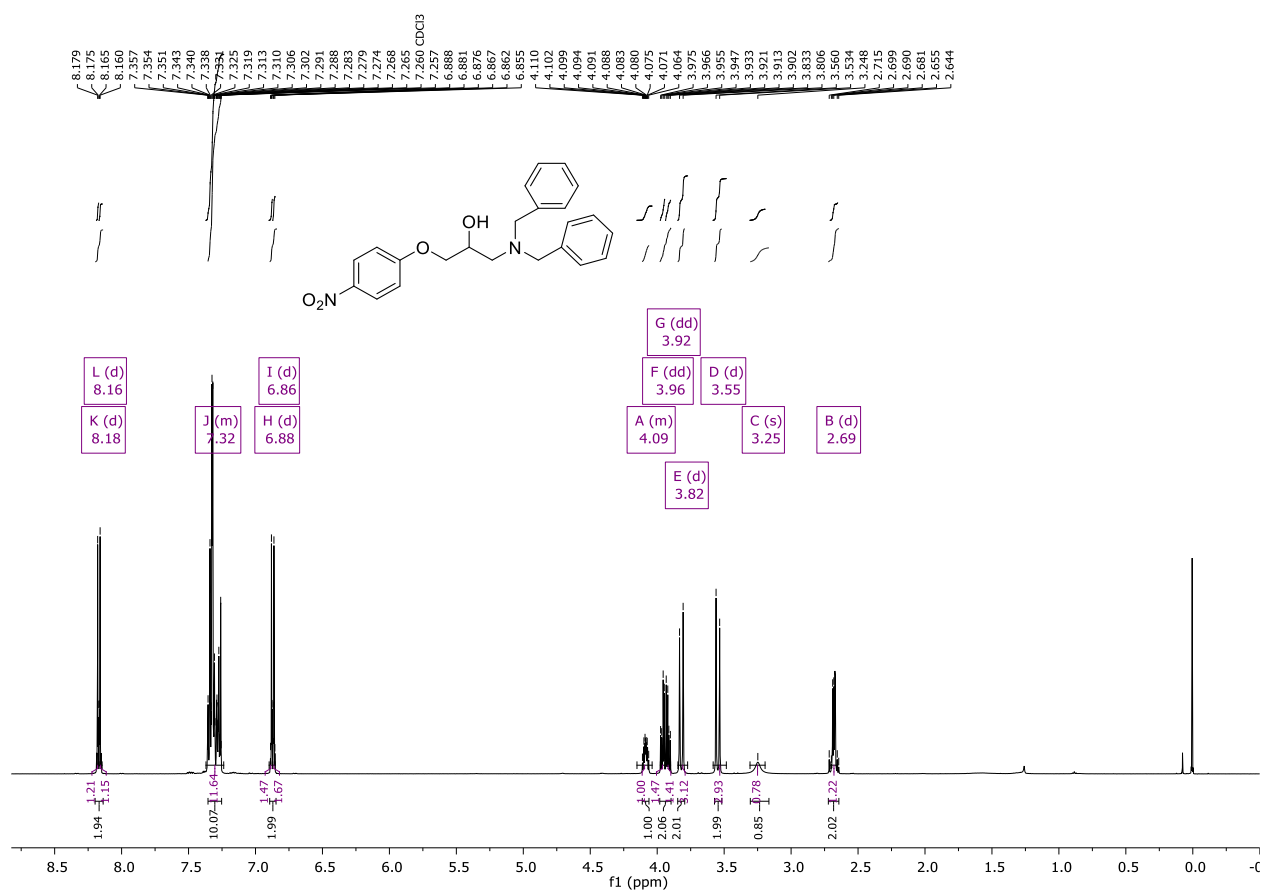




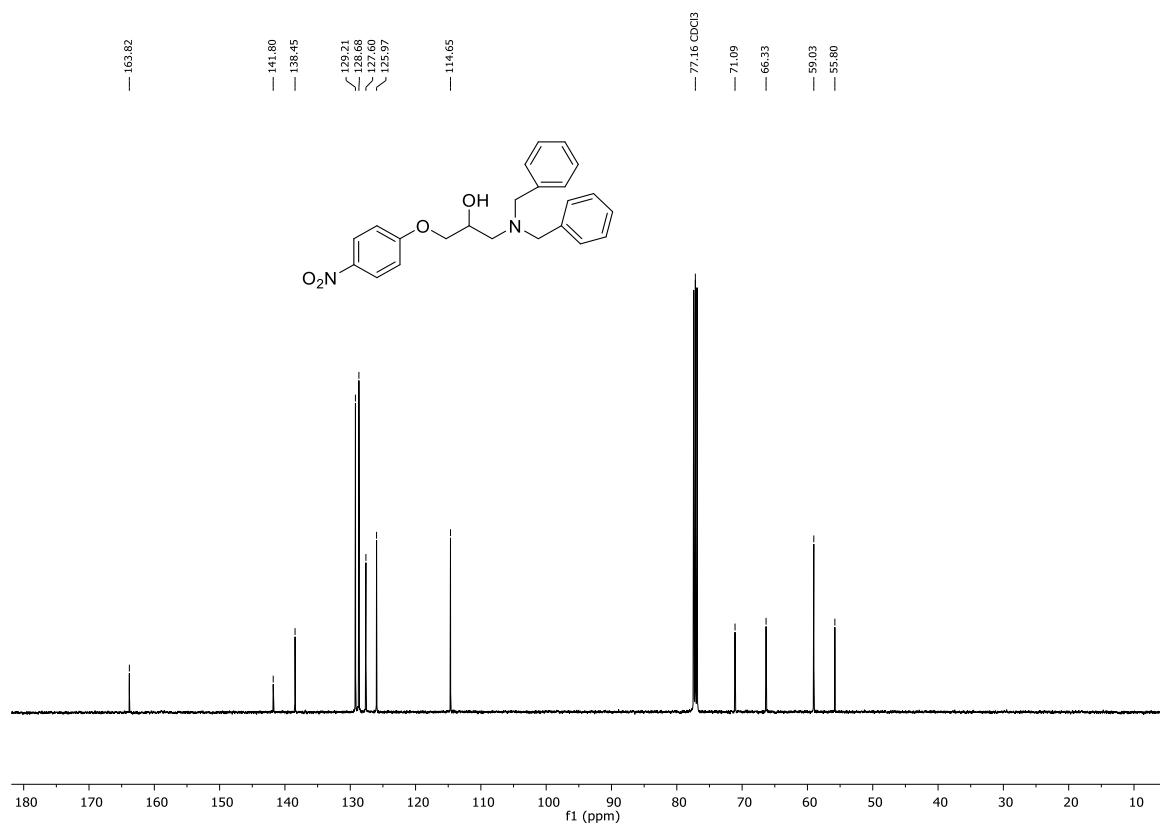
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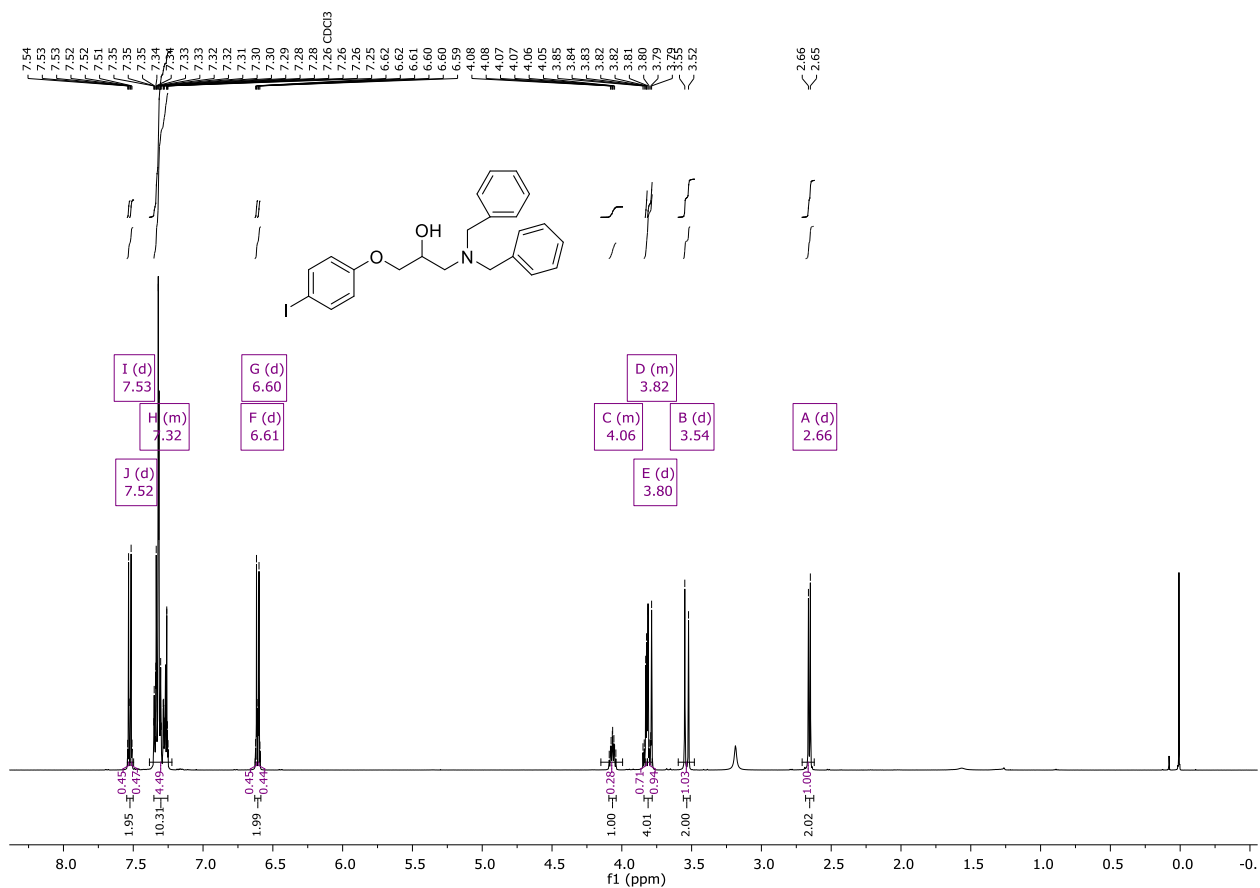
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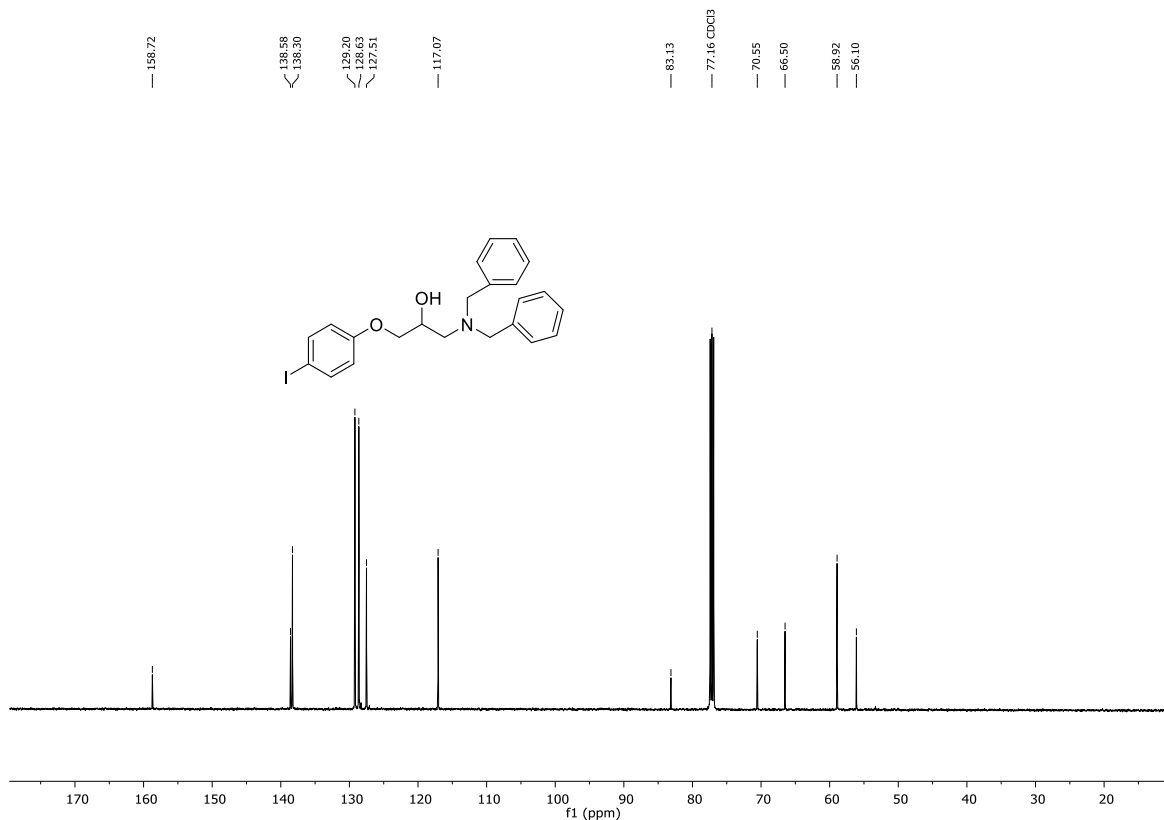
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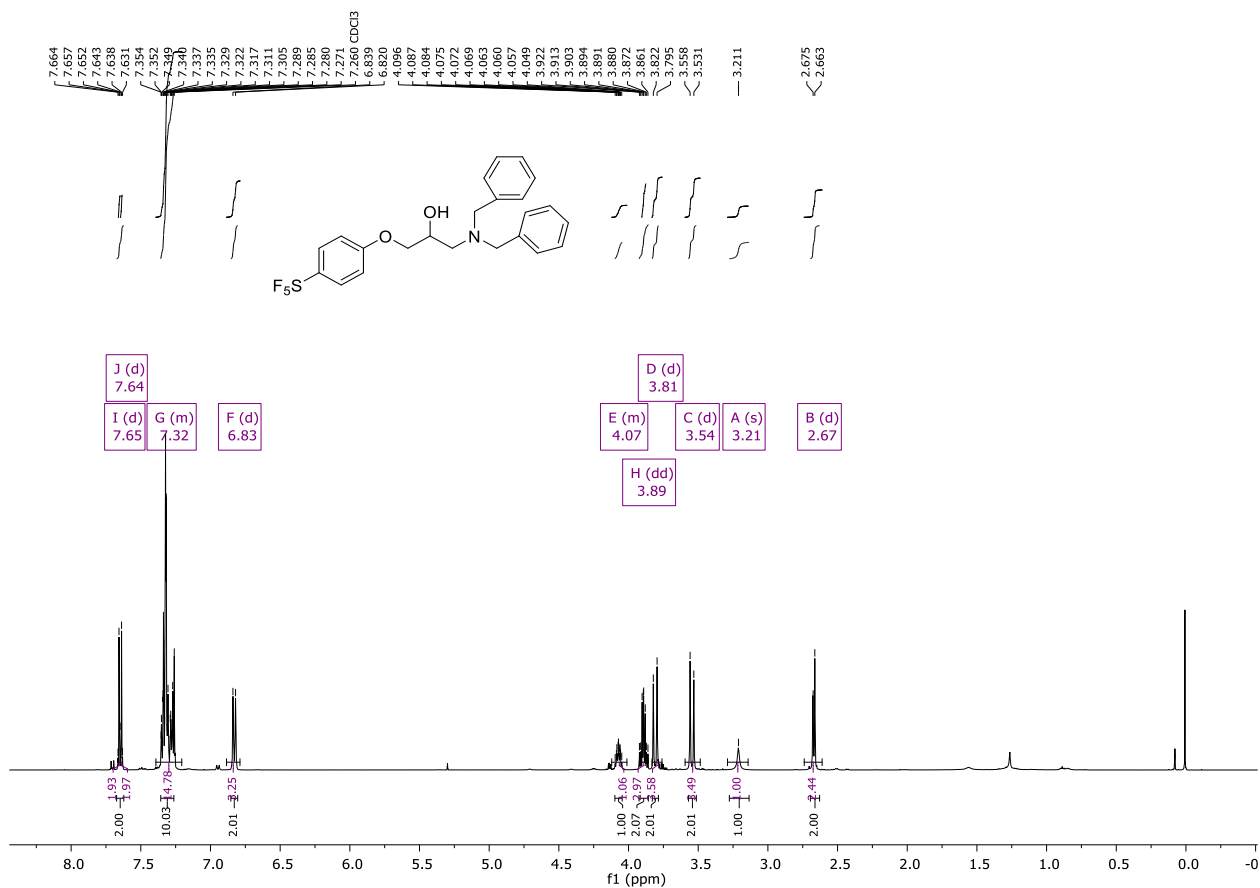
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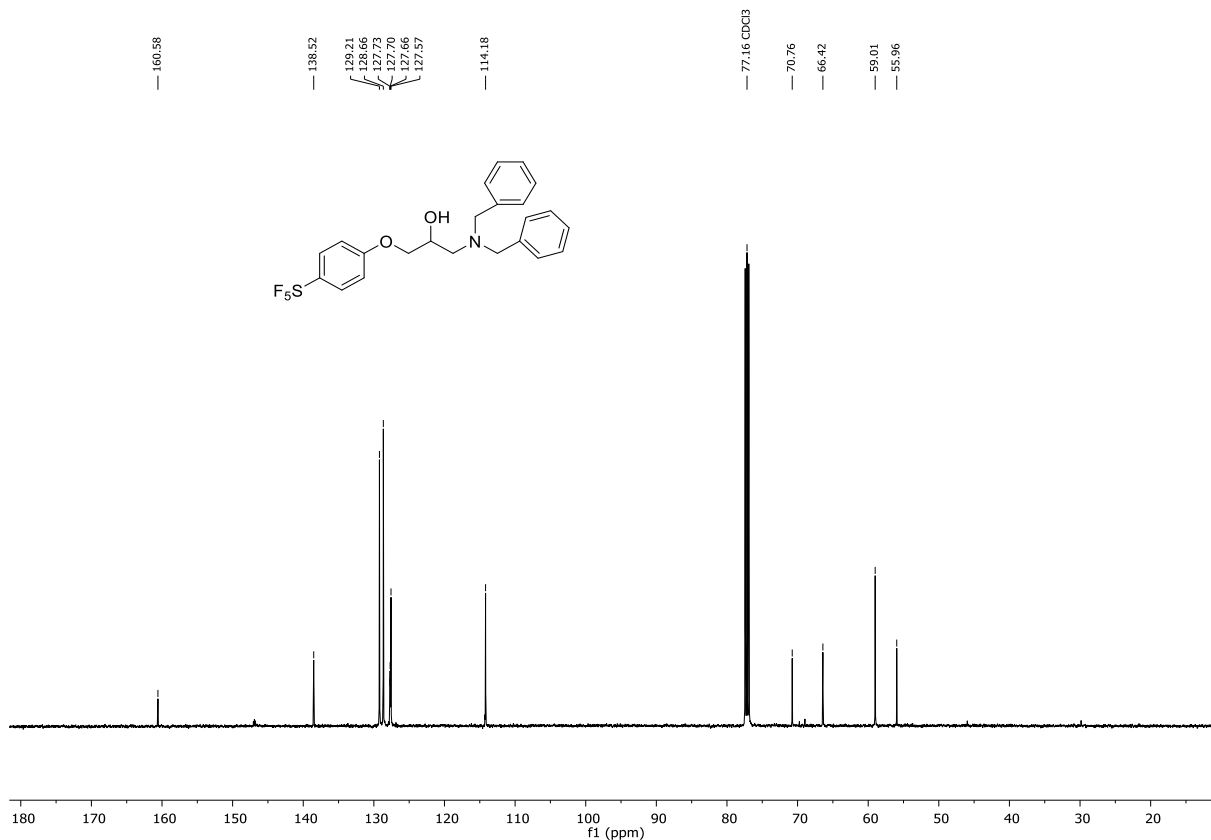
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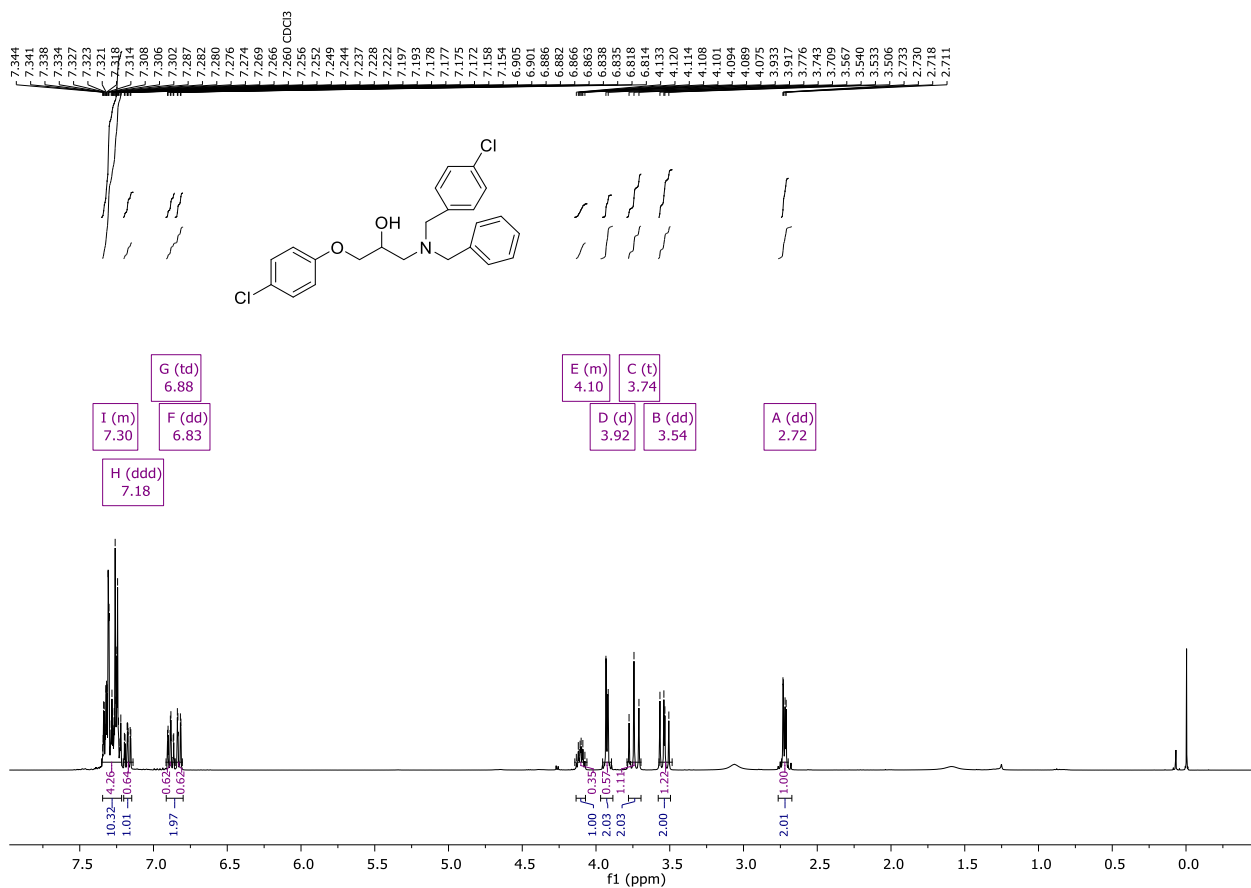
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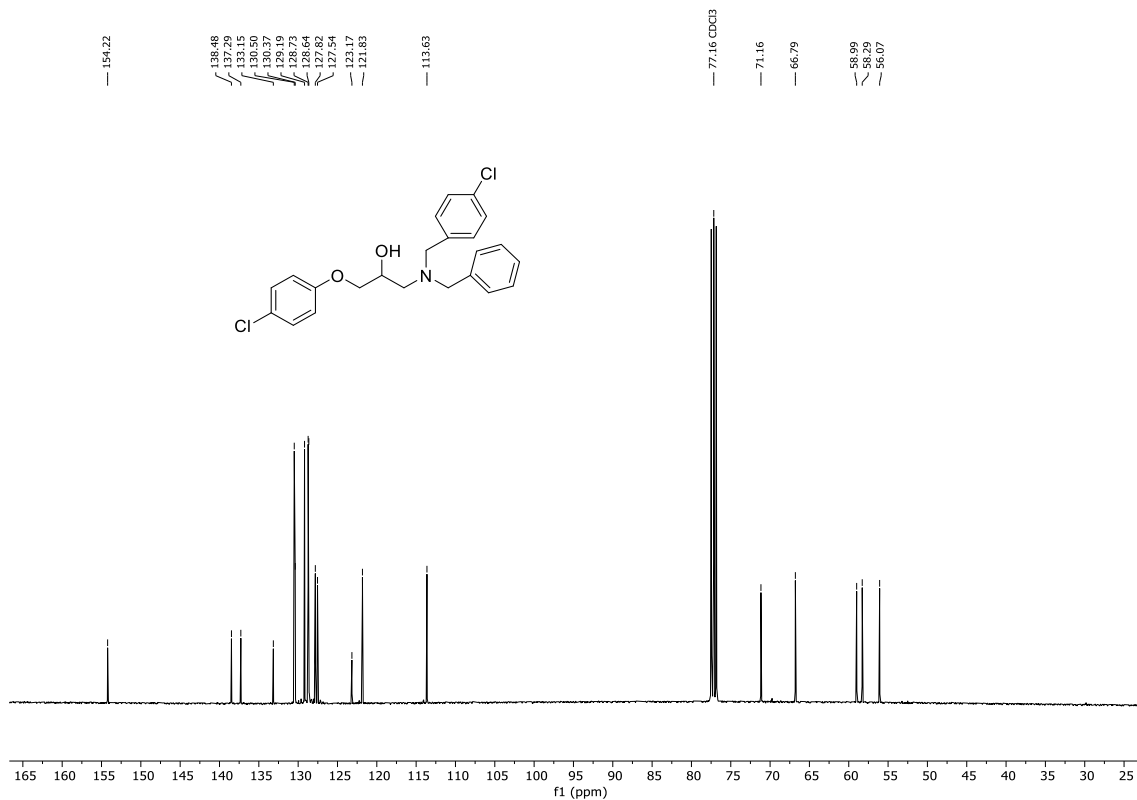
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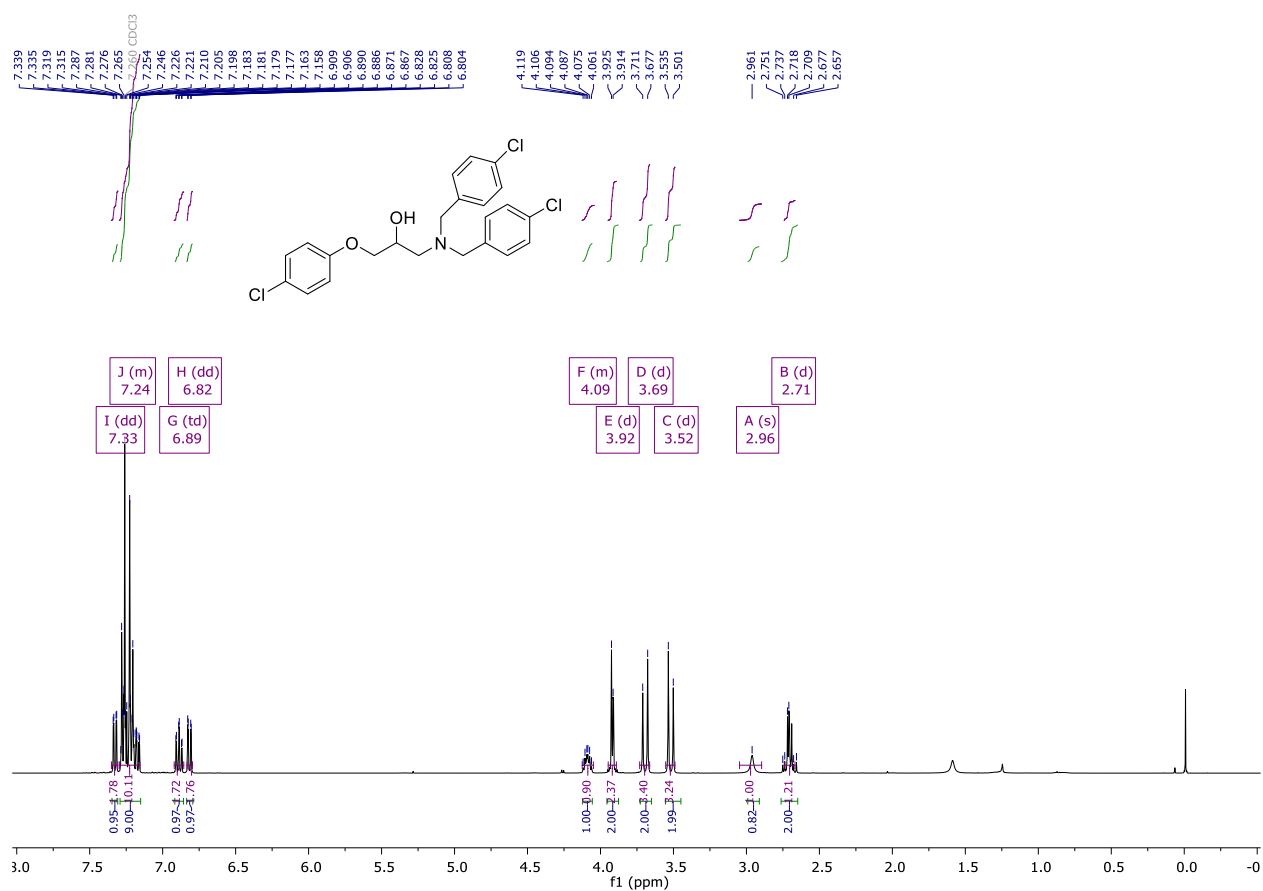
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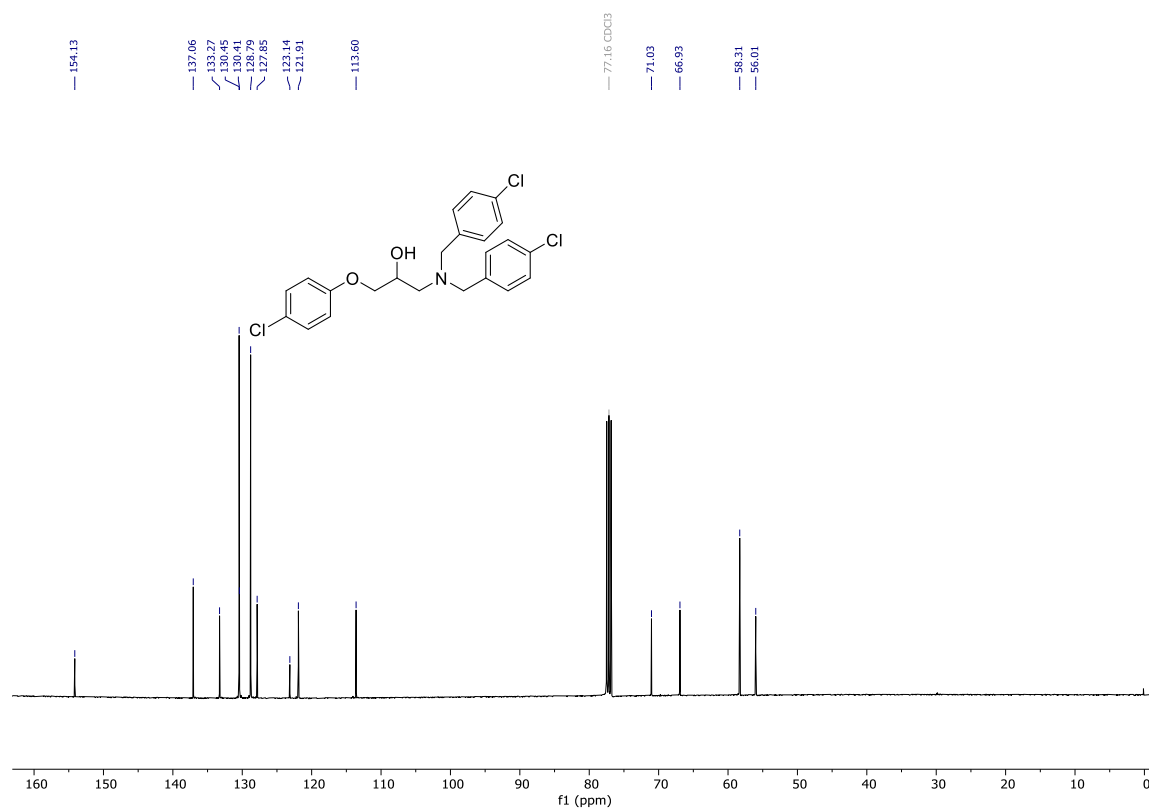
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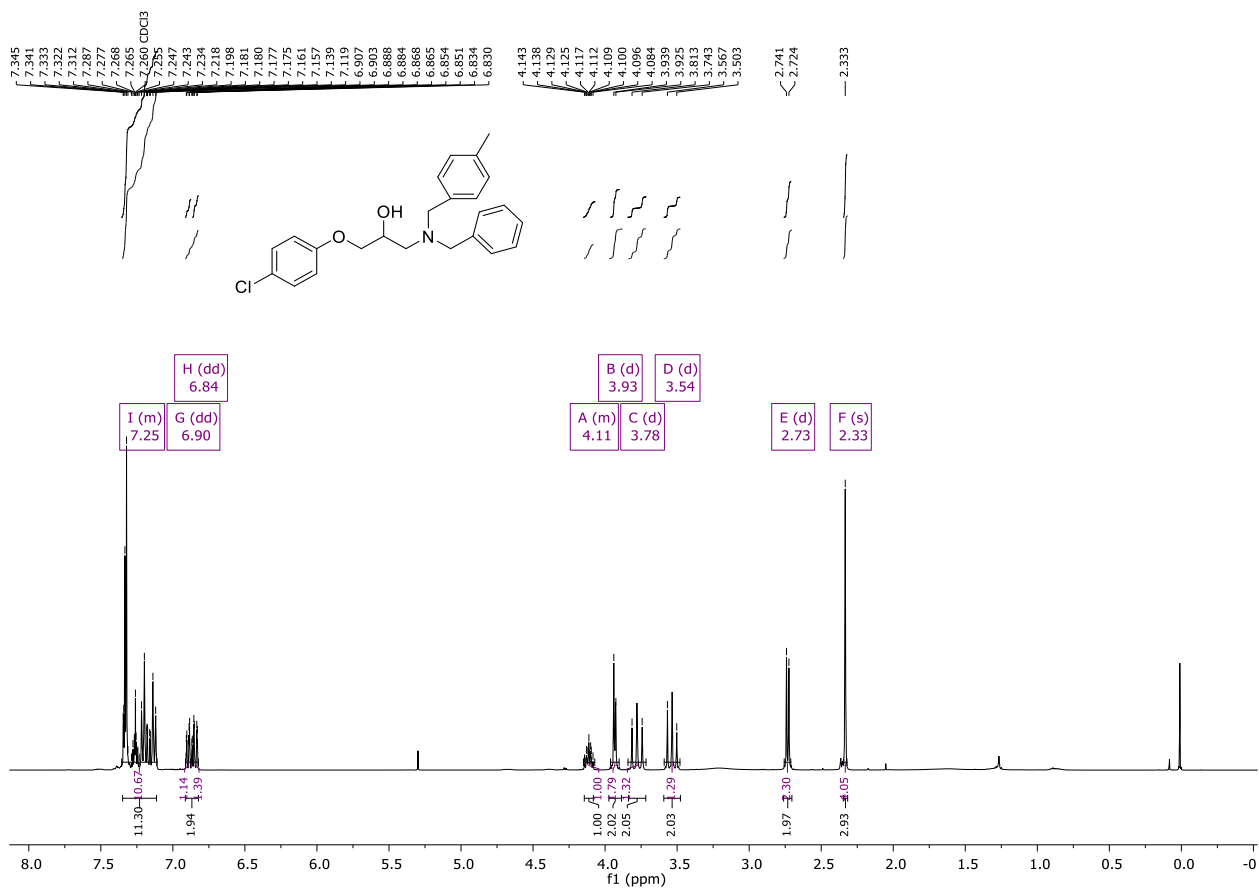
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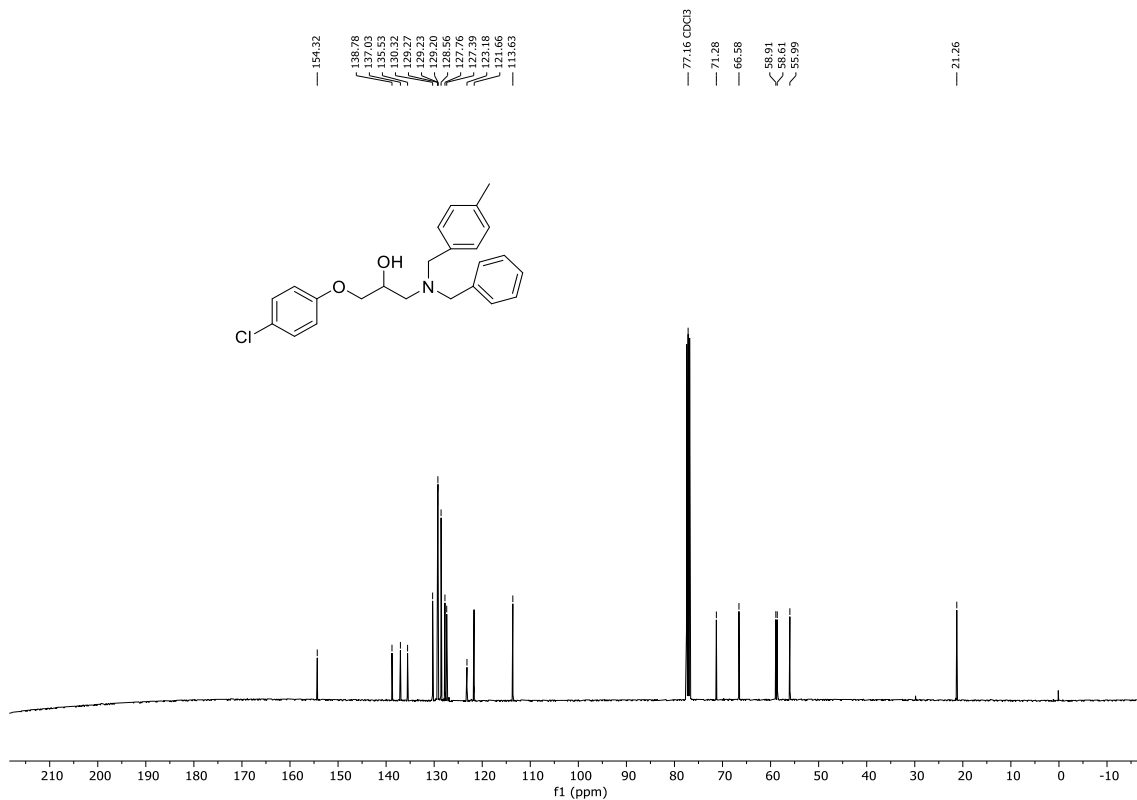
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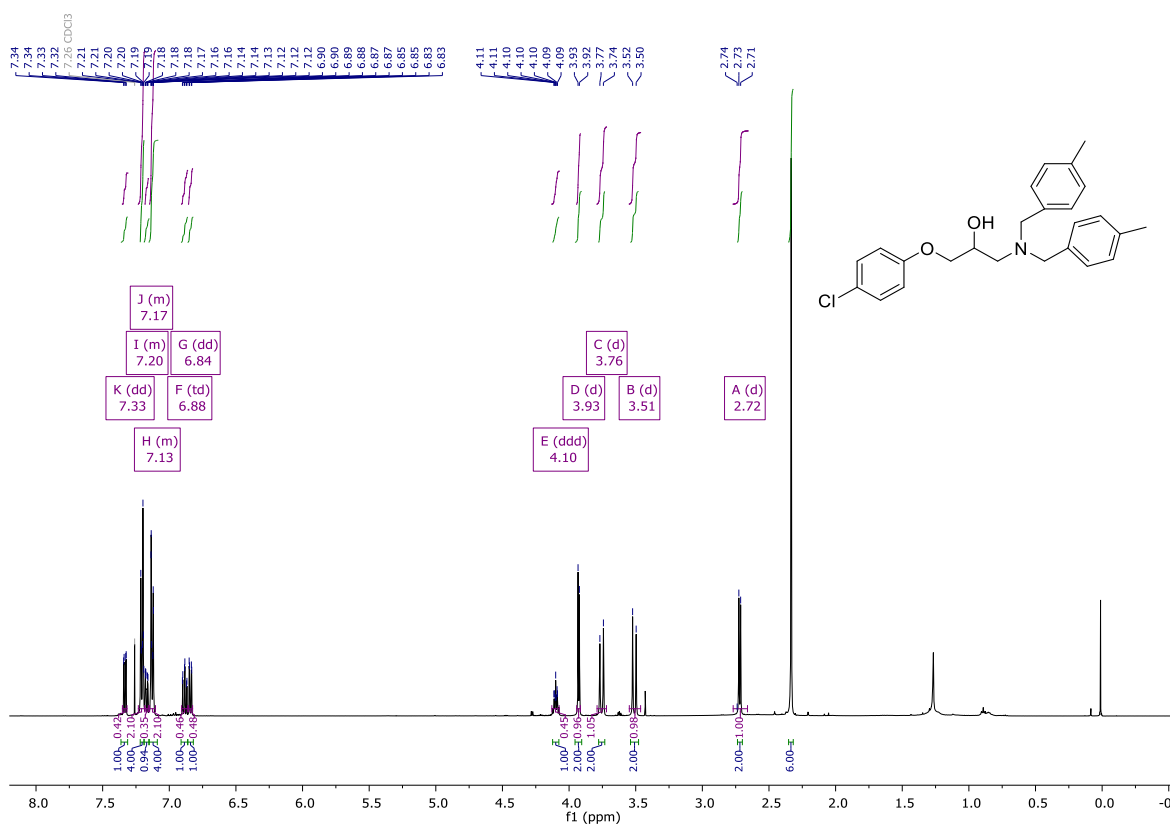
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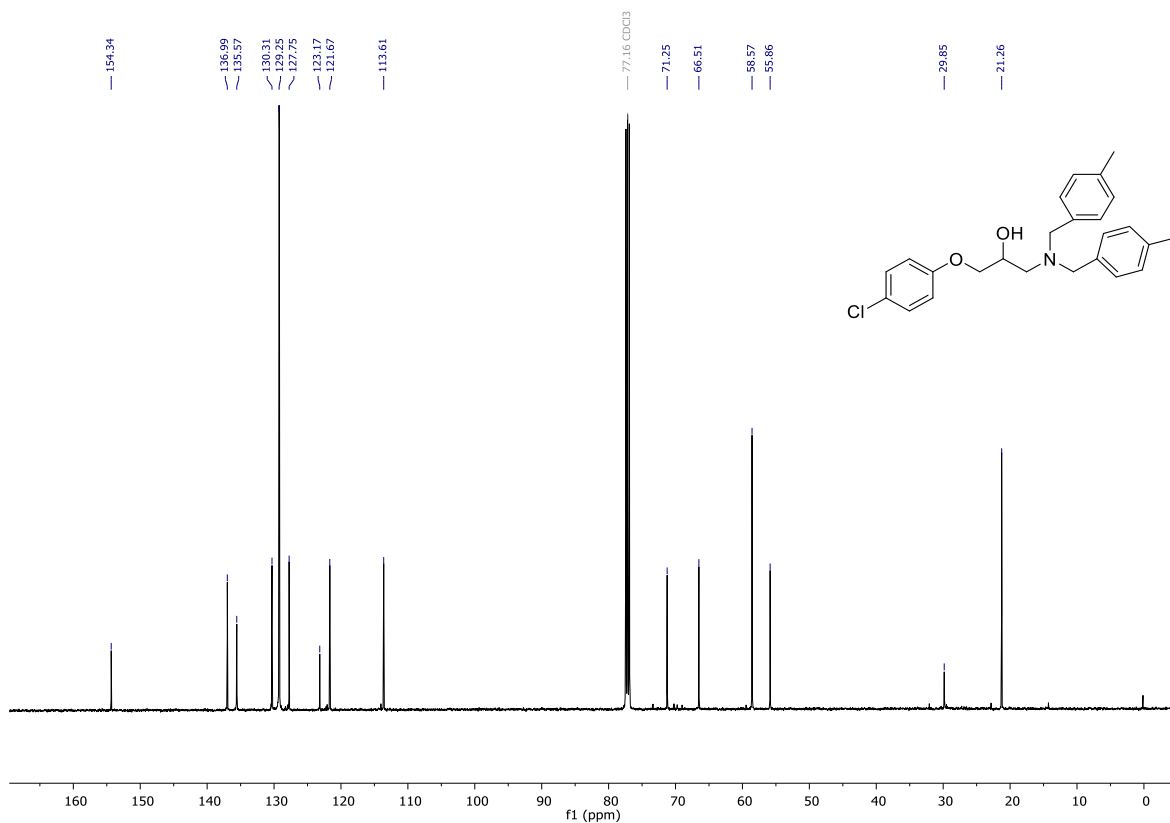
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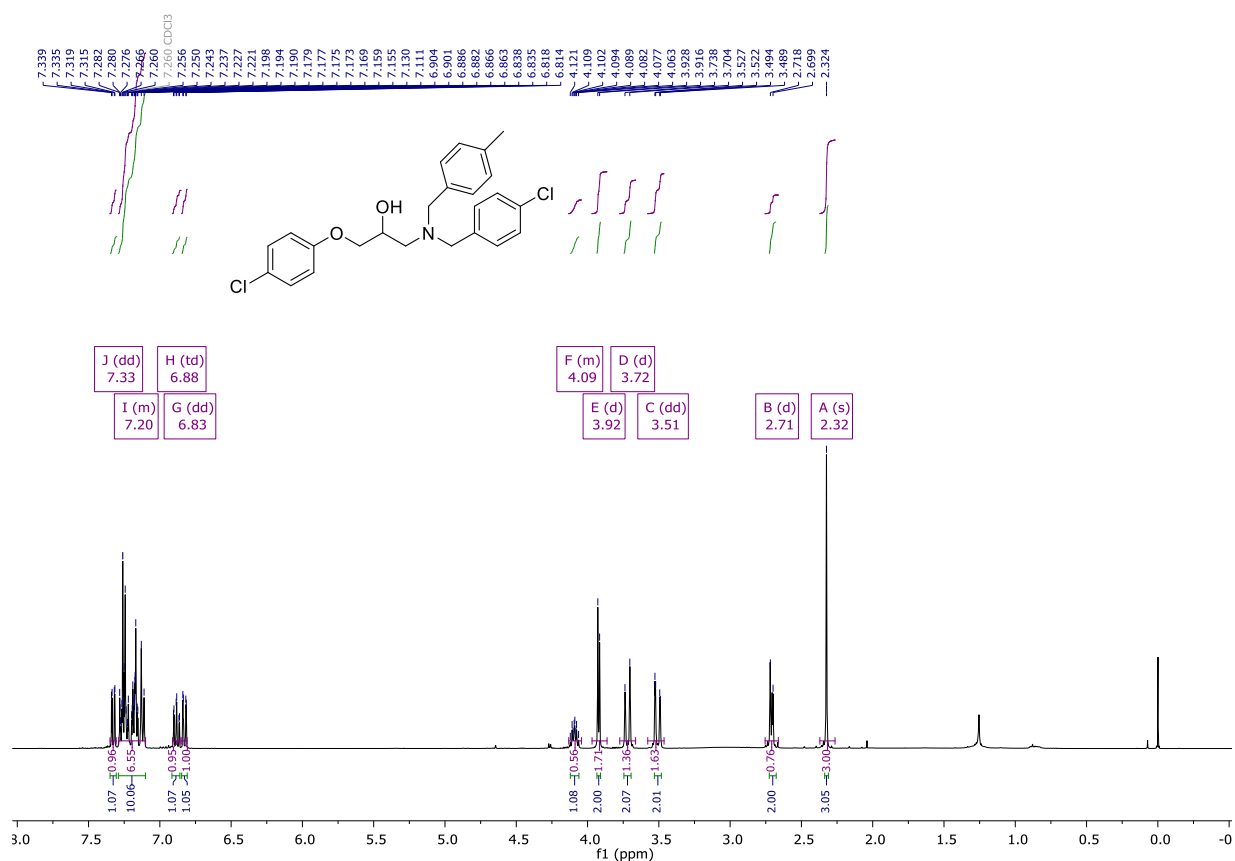
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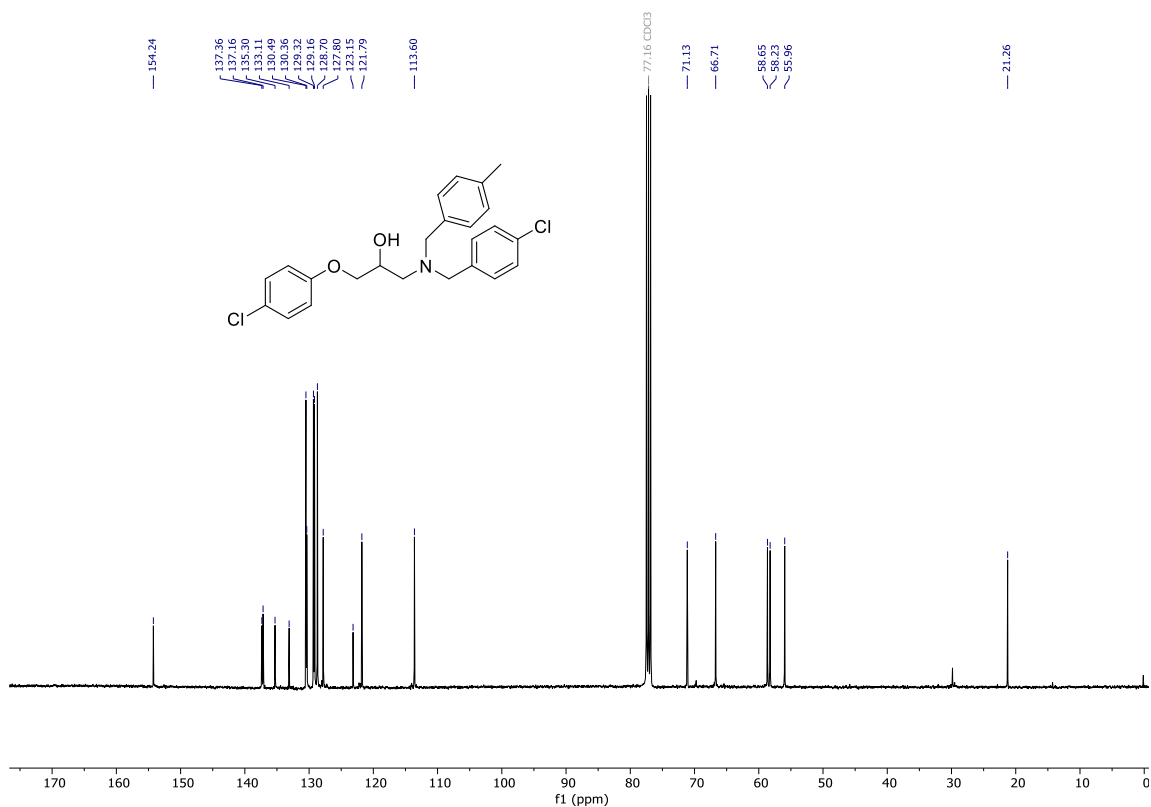
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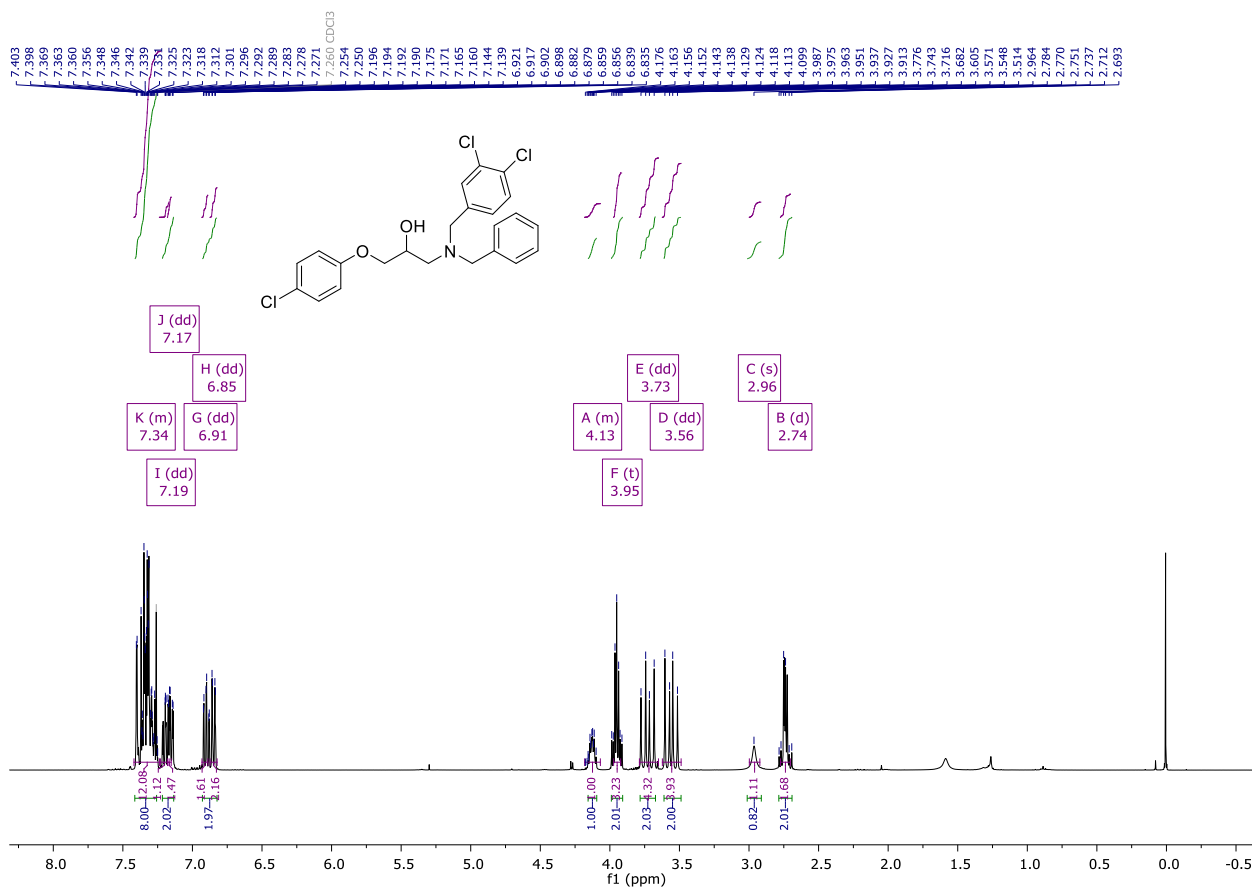
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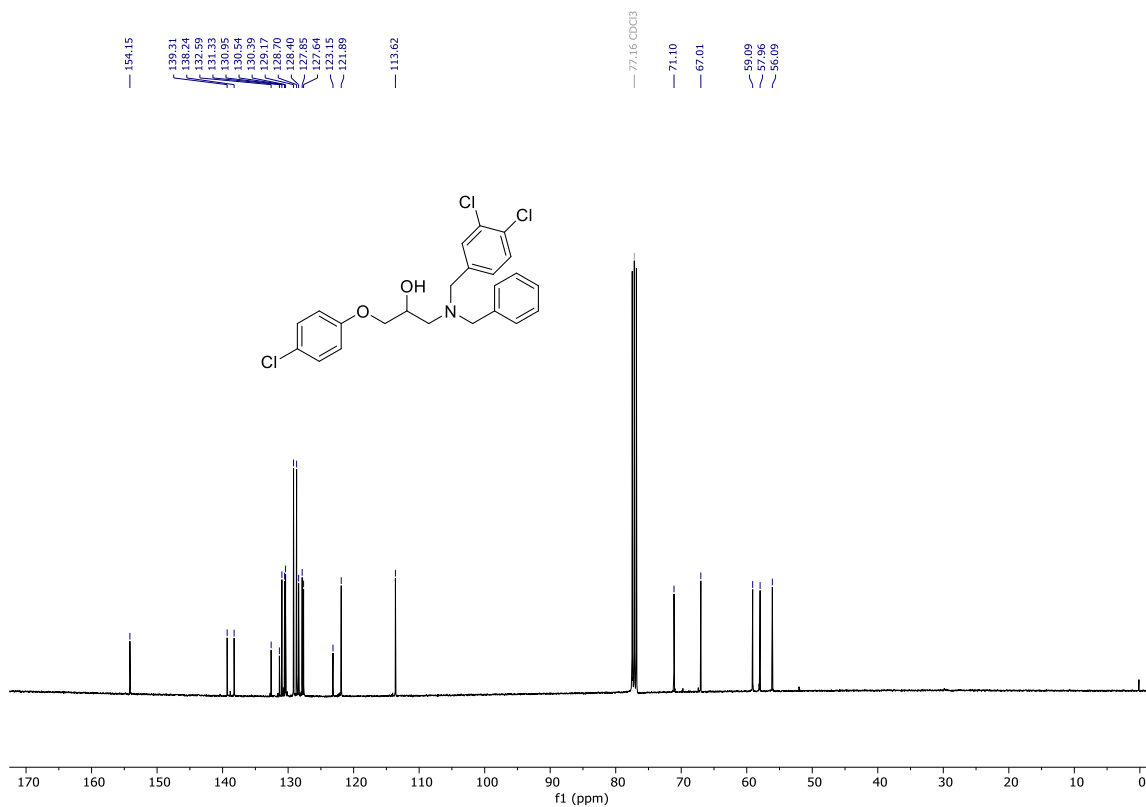
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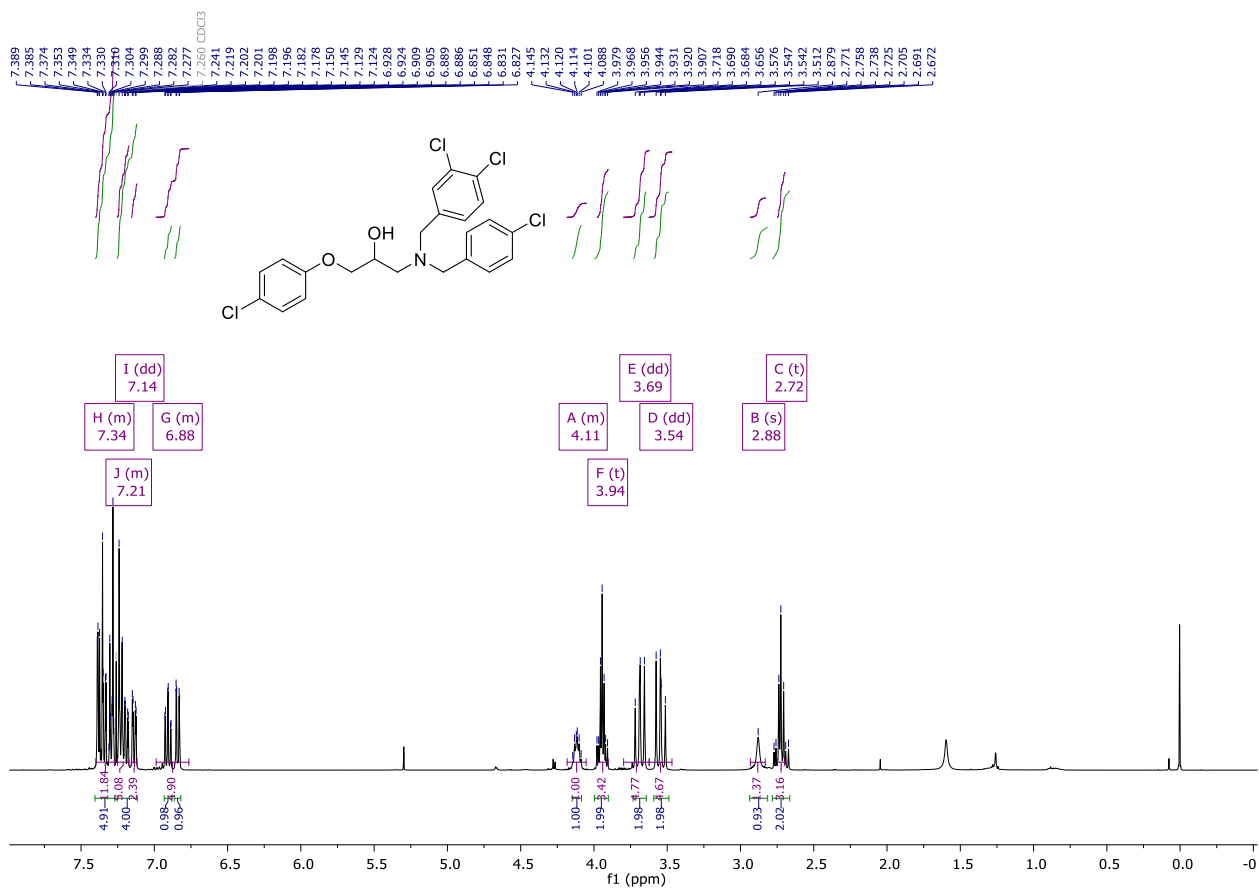
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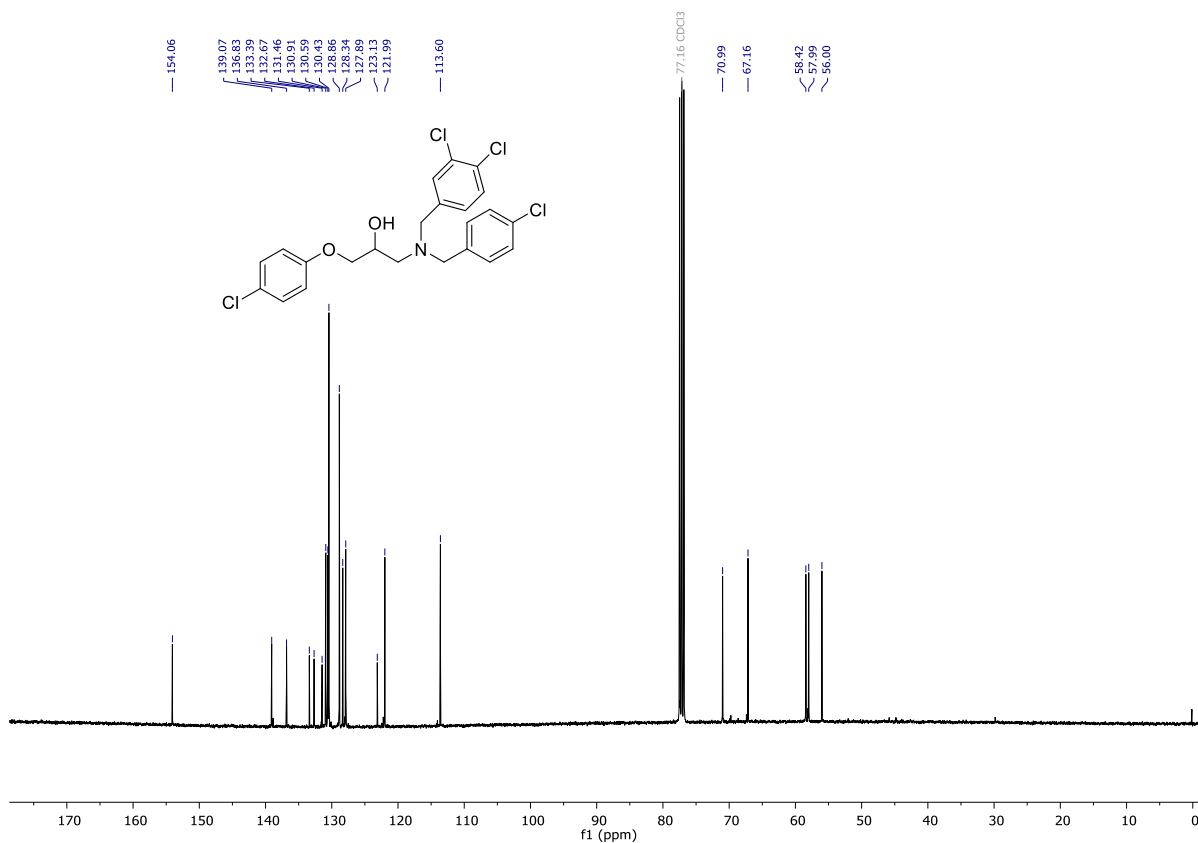
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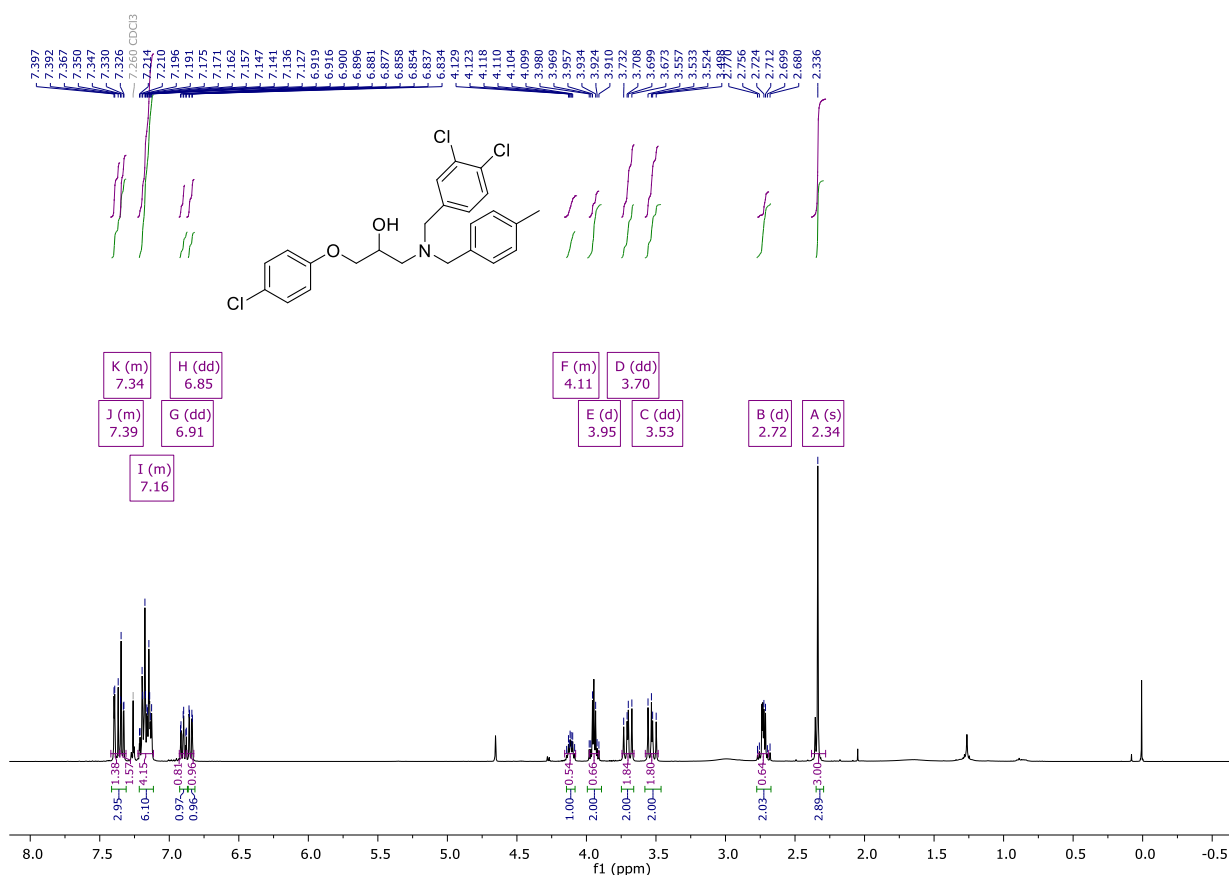
1-[Benzyl(3,4-dichlorobenzyl)amino]-3-(4-chlorophenoxy)propan-2-ol (30)



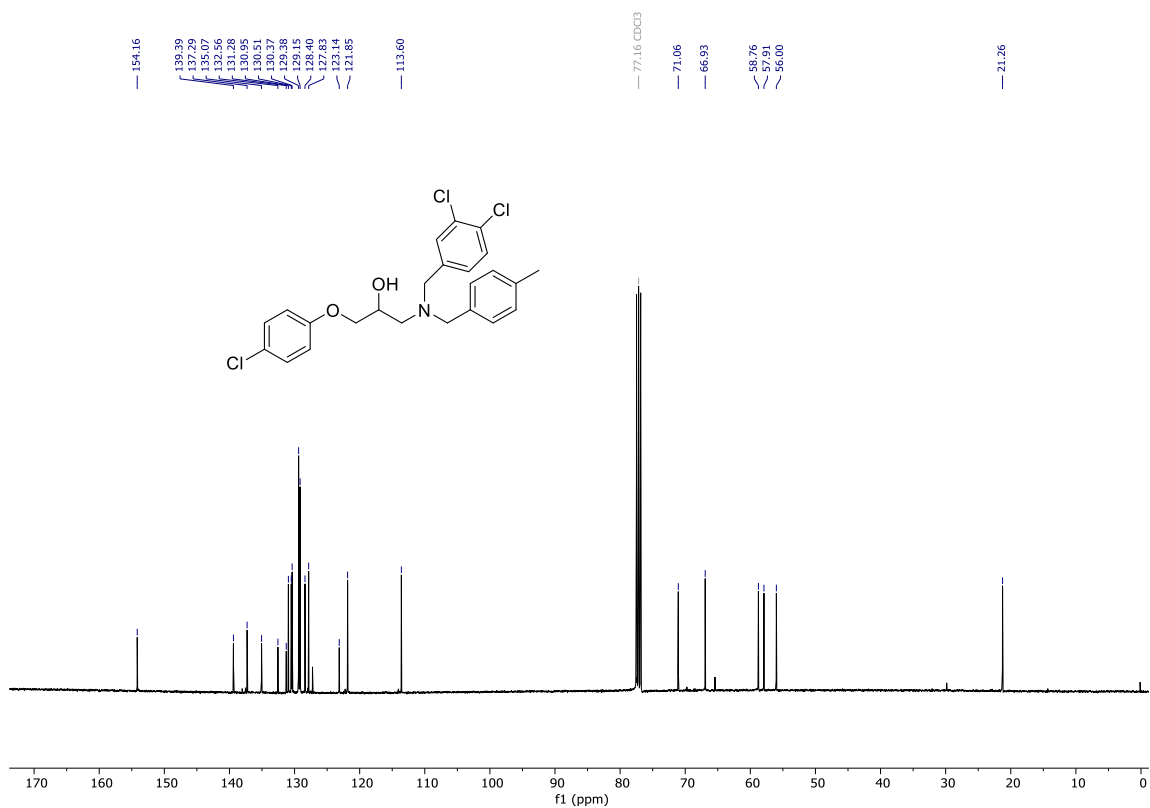
1-[(4-Chlorobenzyl)(3,4-dichlorobenzyl)amino]-3-(4-chlorophenoxy)propan-2-ol (31)



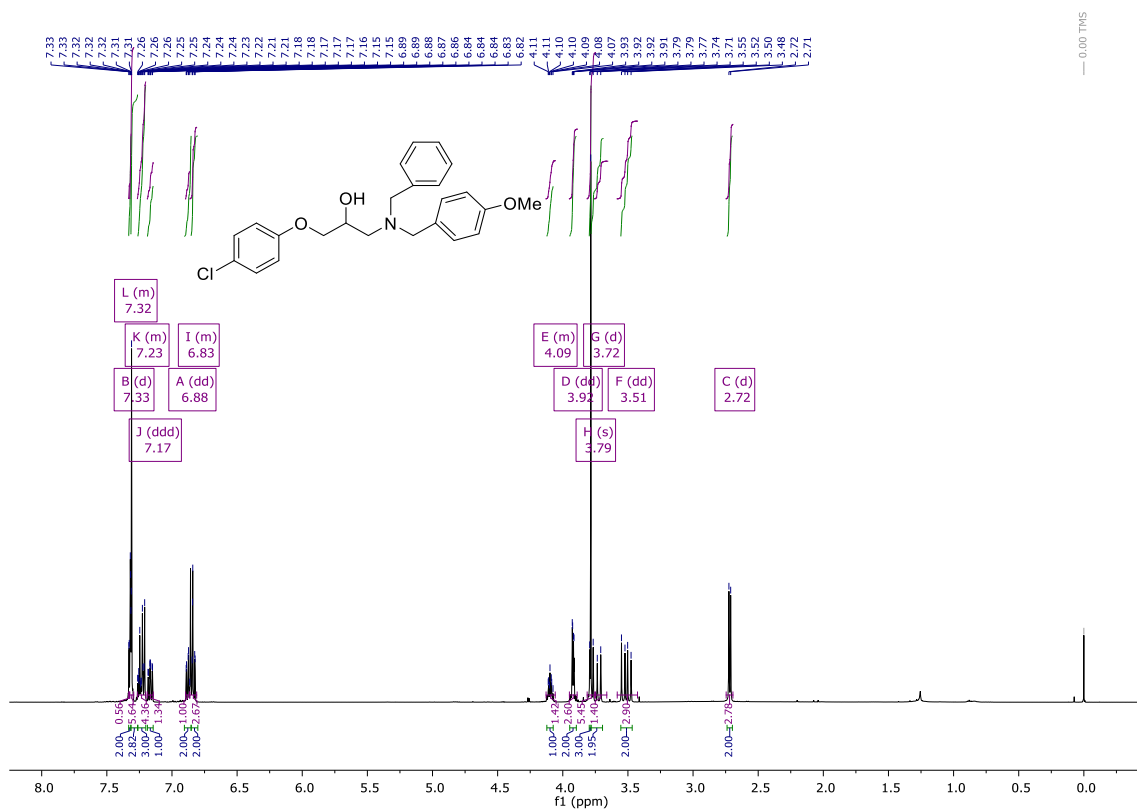
1-[(4-Chlorobenzyl)(3,4-dichlorobenzyl)amino]-3-(4-chlorophenoxy)propan-2-ol (31)



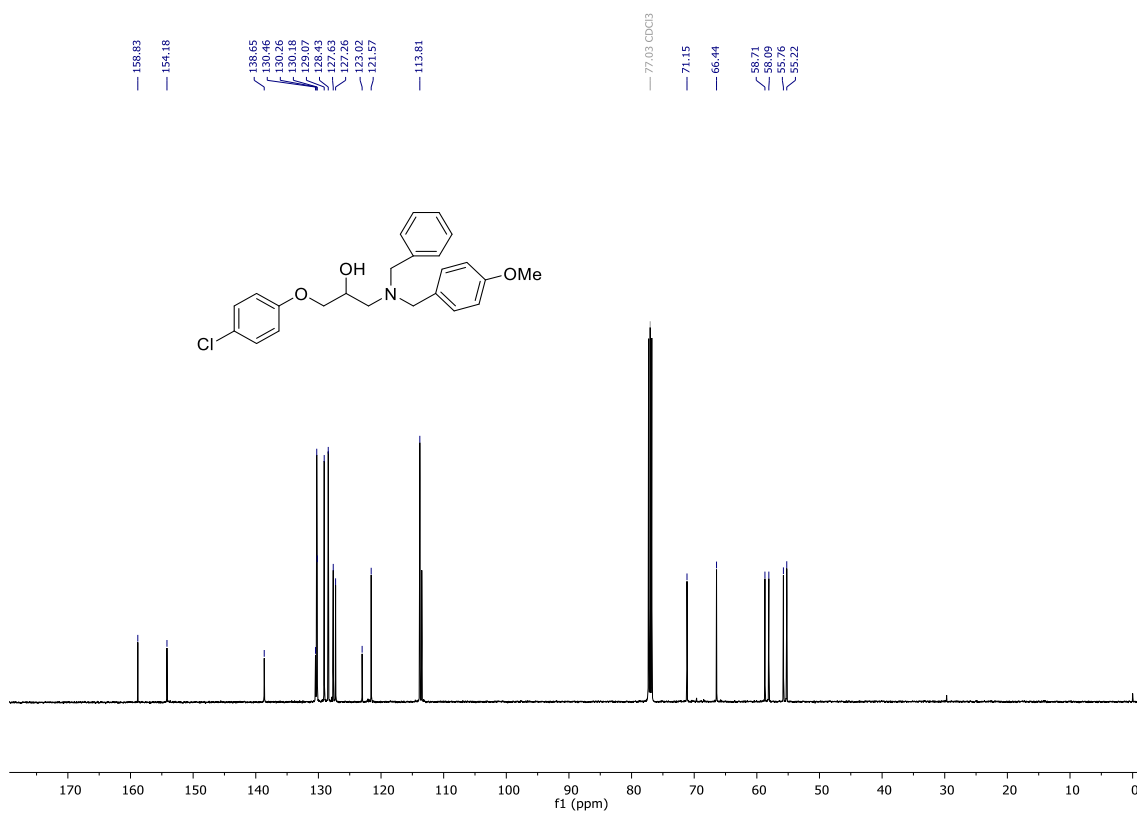
1-(4-Chlorophenoxy)-3-[(3,4-dichlorobenzyl)(4-methylbenzyl)amino]propan-2-ol (32)



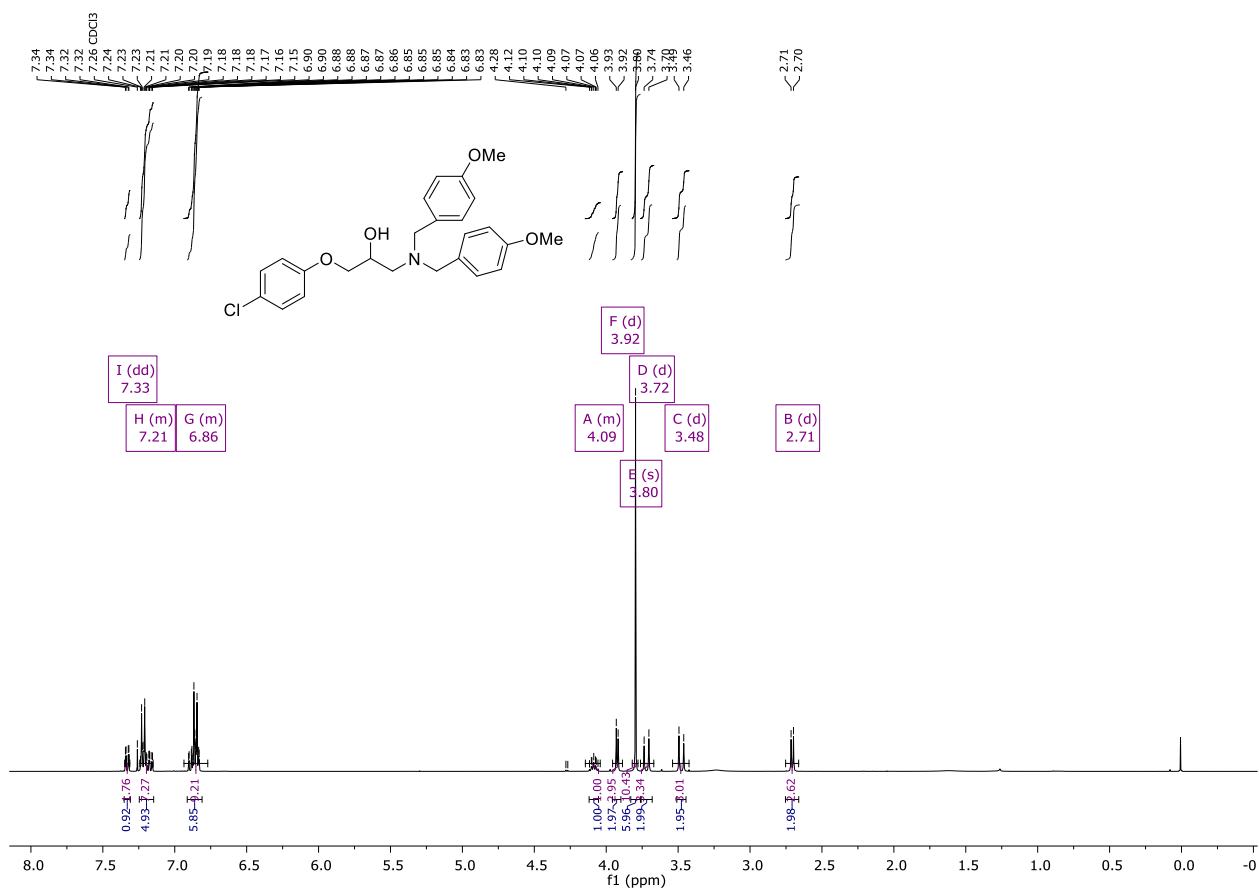
1-(4-Chlorophenoxy)-3-[(3,4-dichlorobenzyl)(4-methylbenzyl)amino]propan-2-ol (32)



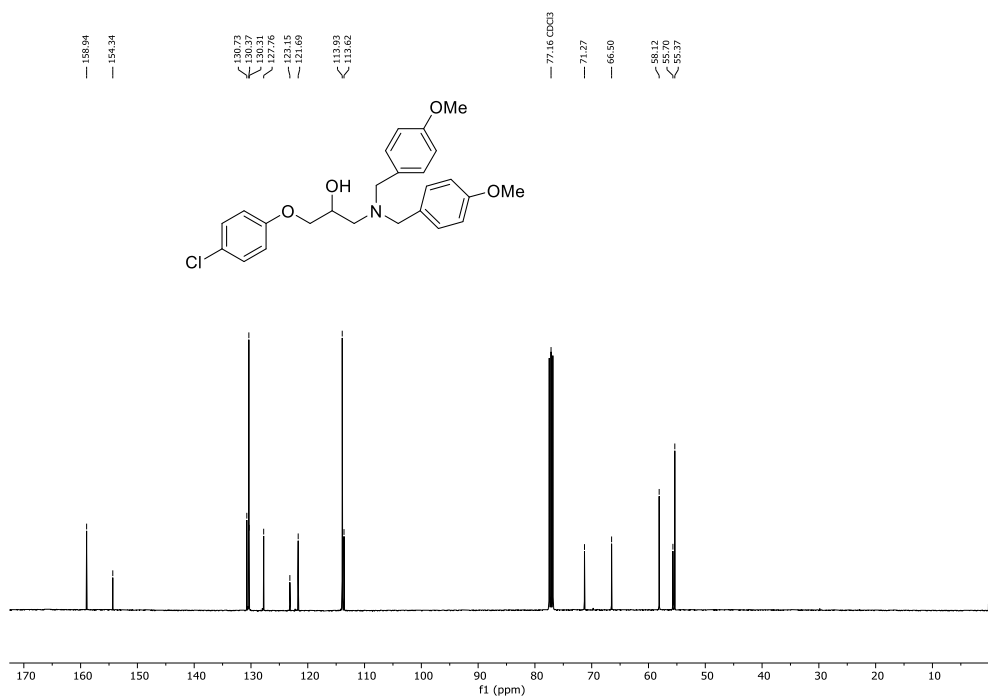
1-[Benzyl(4-methoxybenzyl)amino]-3-(4-chlorophenoxy)propan-2-ol (33)



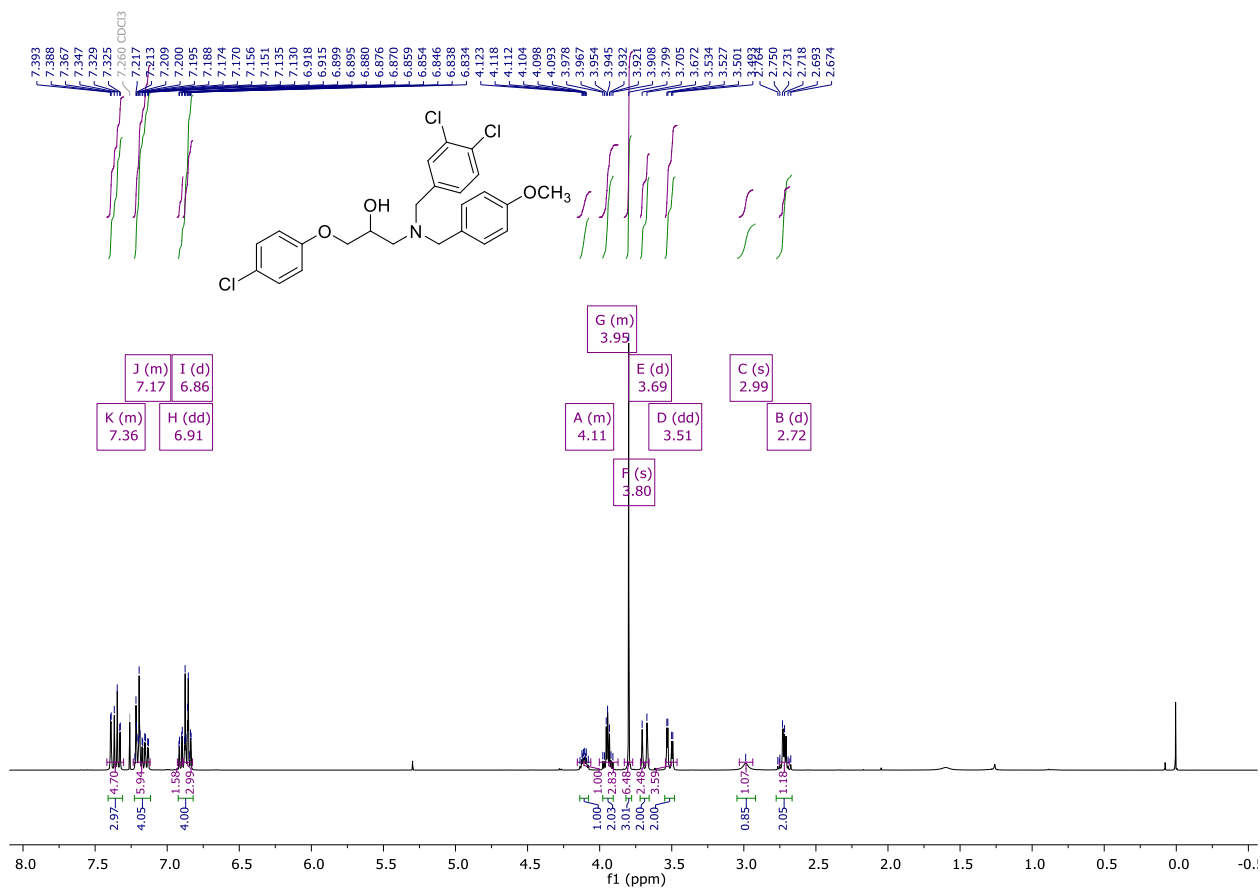
1-[Benzyl(4-methoxybenzyl)amino]-3-(4-chlorophenoxy)propan-2-ol (33)



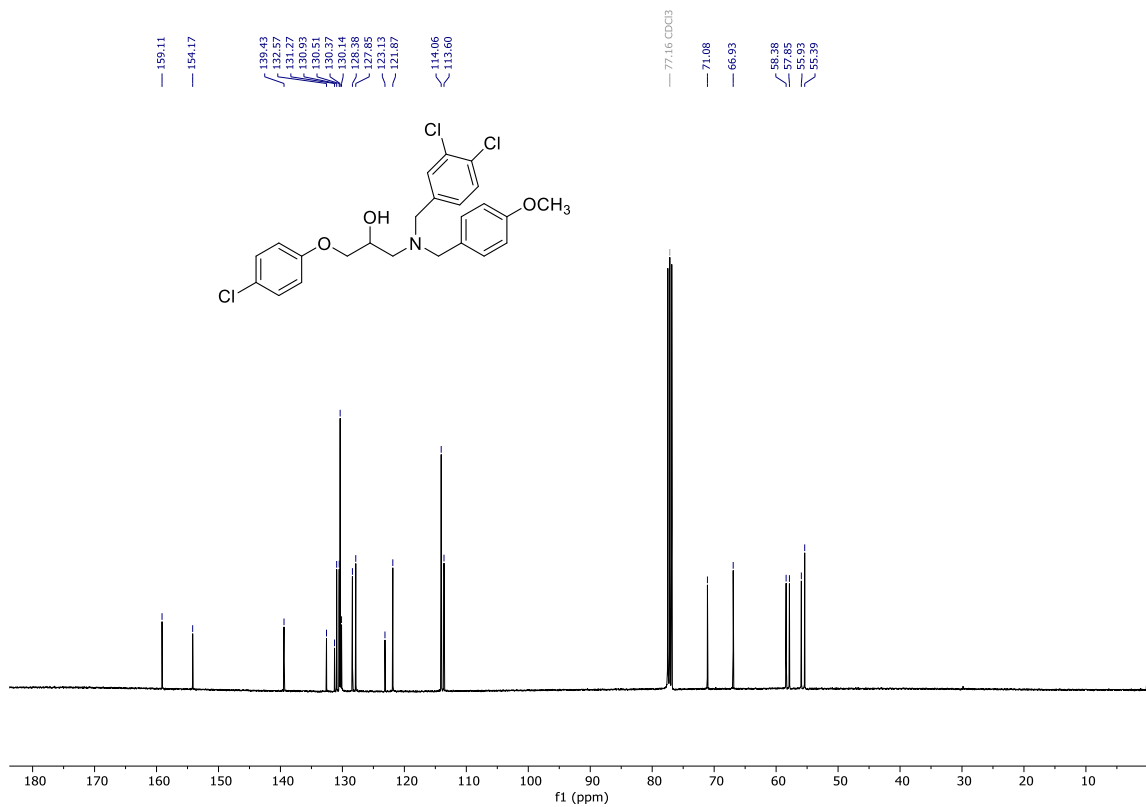
1-[Bis(4-methoxybenzyl)amino]-3-(4-chlorophenoxy)propan-2-ol (34)



1-[Bis(4-methoxybenzyl)amino]-3-(4-chlorophenoxy)propan-2-ol (34)



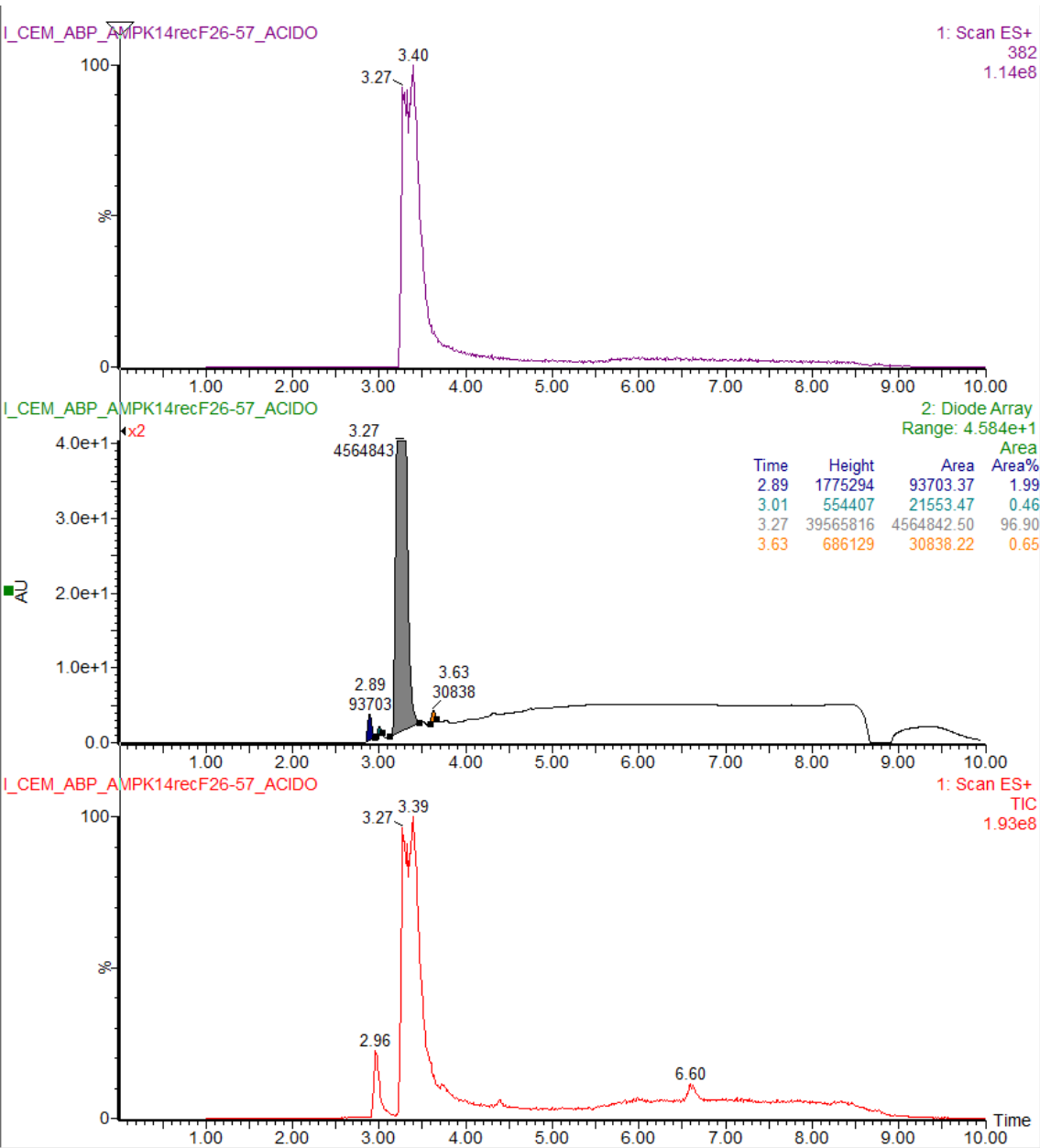
1-(4-Chlorophenoxy)-3-[(3,4-dichlorobenzyl)(4-methoxybenzyl)amino]propan-2-ol (35)



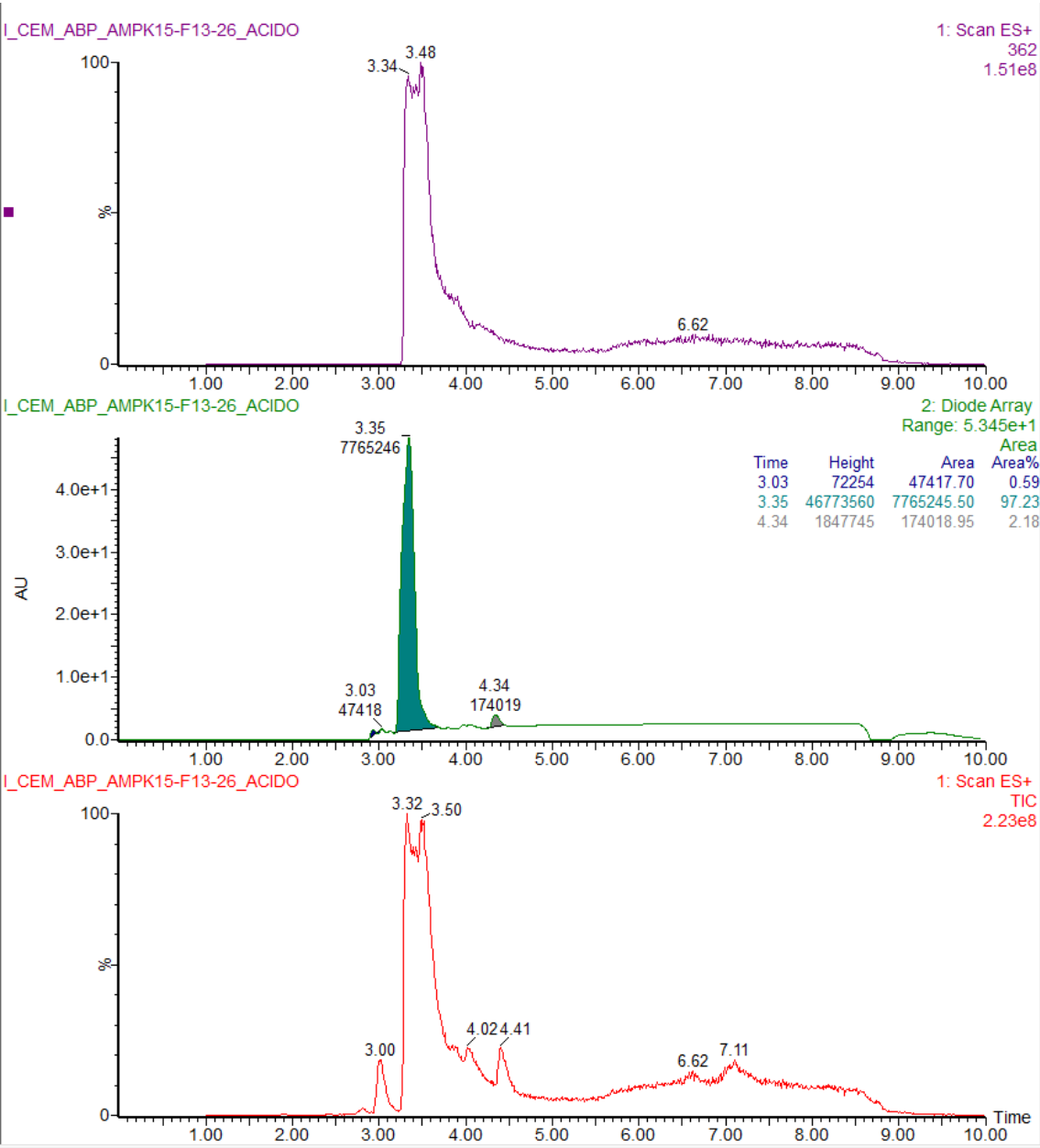
1-(4-Chlorophenoxy)-3-[(3,4-dichlorobenzyl)(4-methoxybenzyl)amino]propan-2-ol (35)

HPLC/MS analysis of BC1618, 1-35

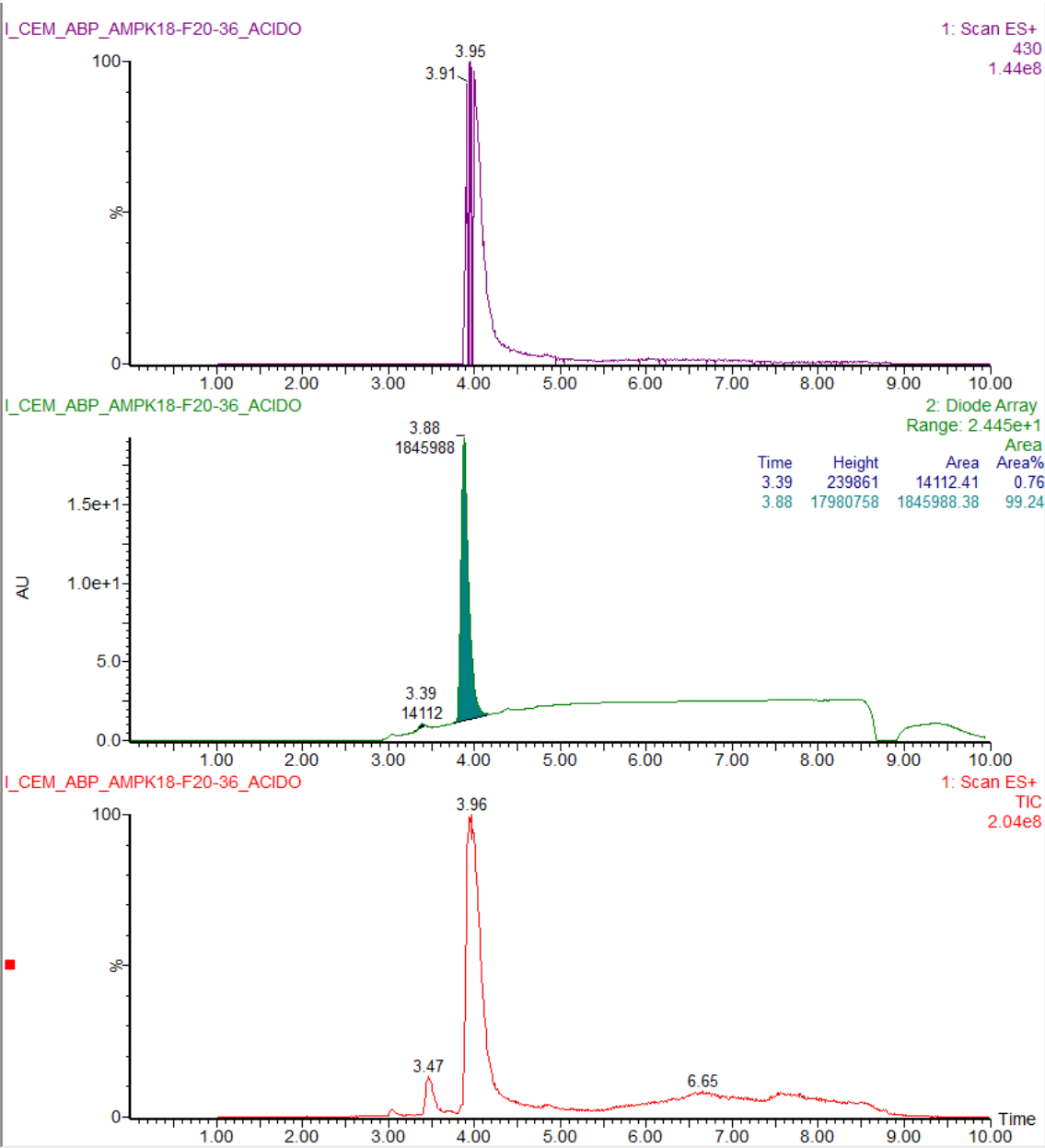
1-(4-Chlorophenoxy)-3-(dibenzylamino)propan-2-ol



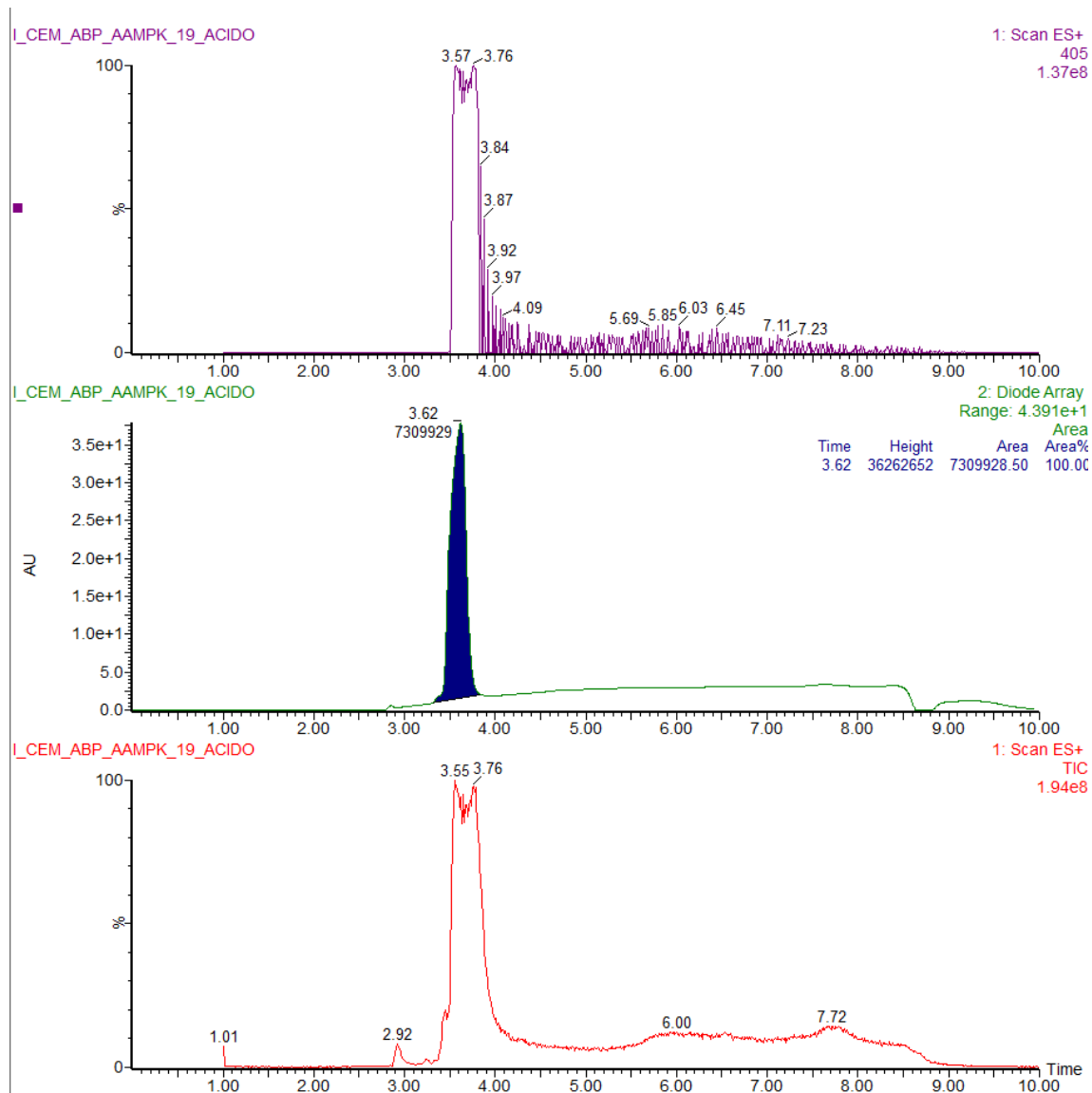
1-(Dibenzylamino)-3-(*p*-tolylloxy)propan-2-ol



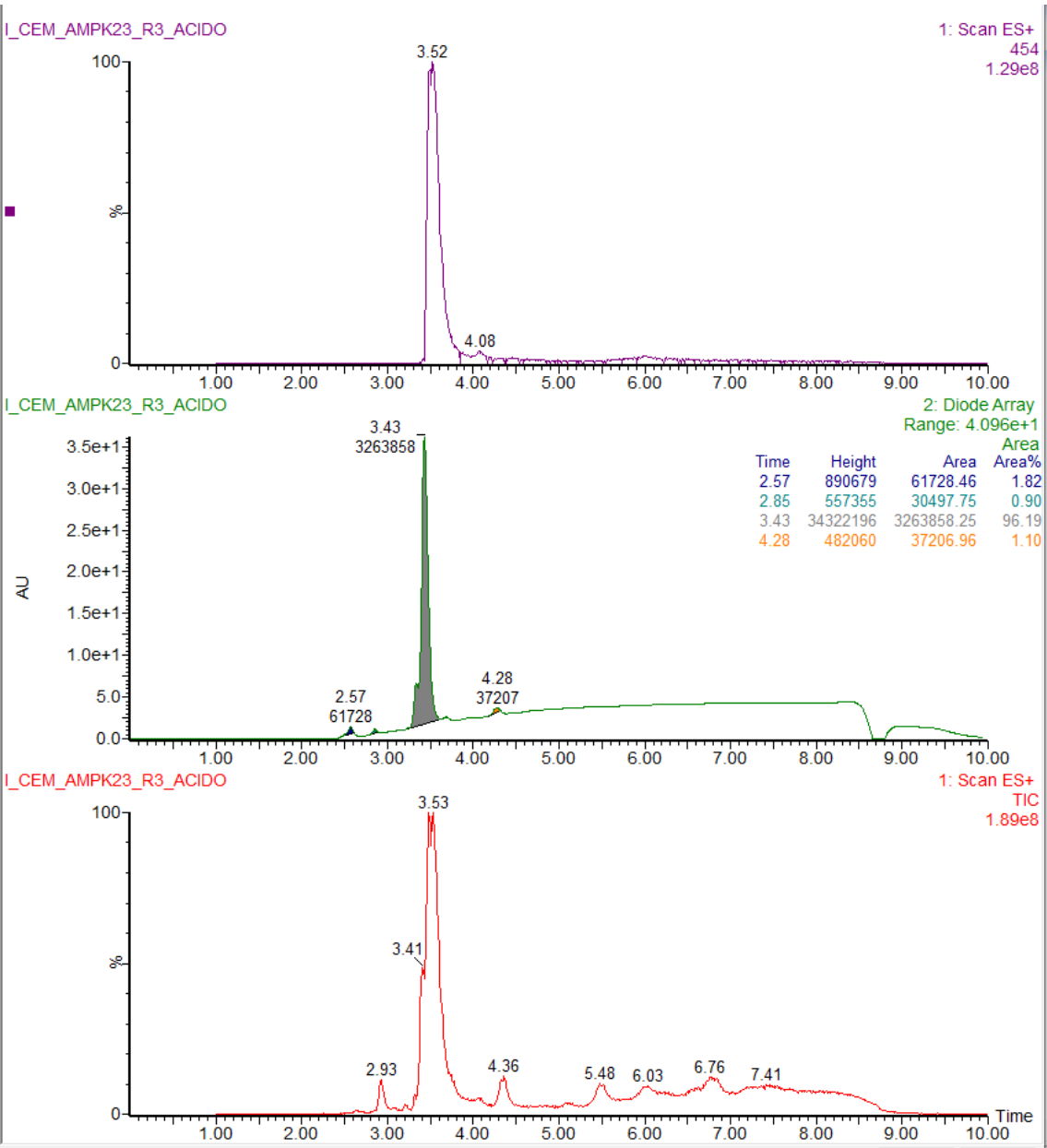
1-(4-Cyclohexylphenoxy)-3-(dibenzylamino)propan-2-ol



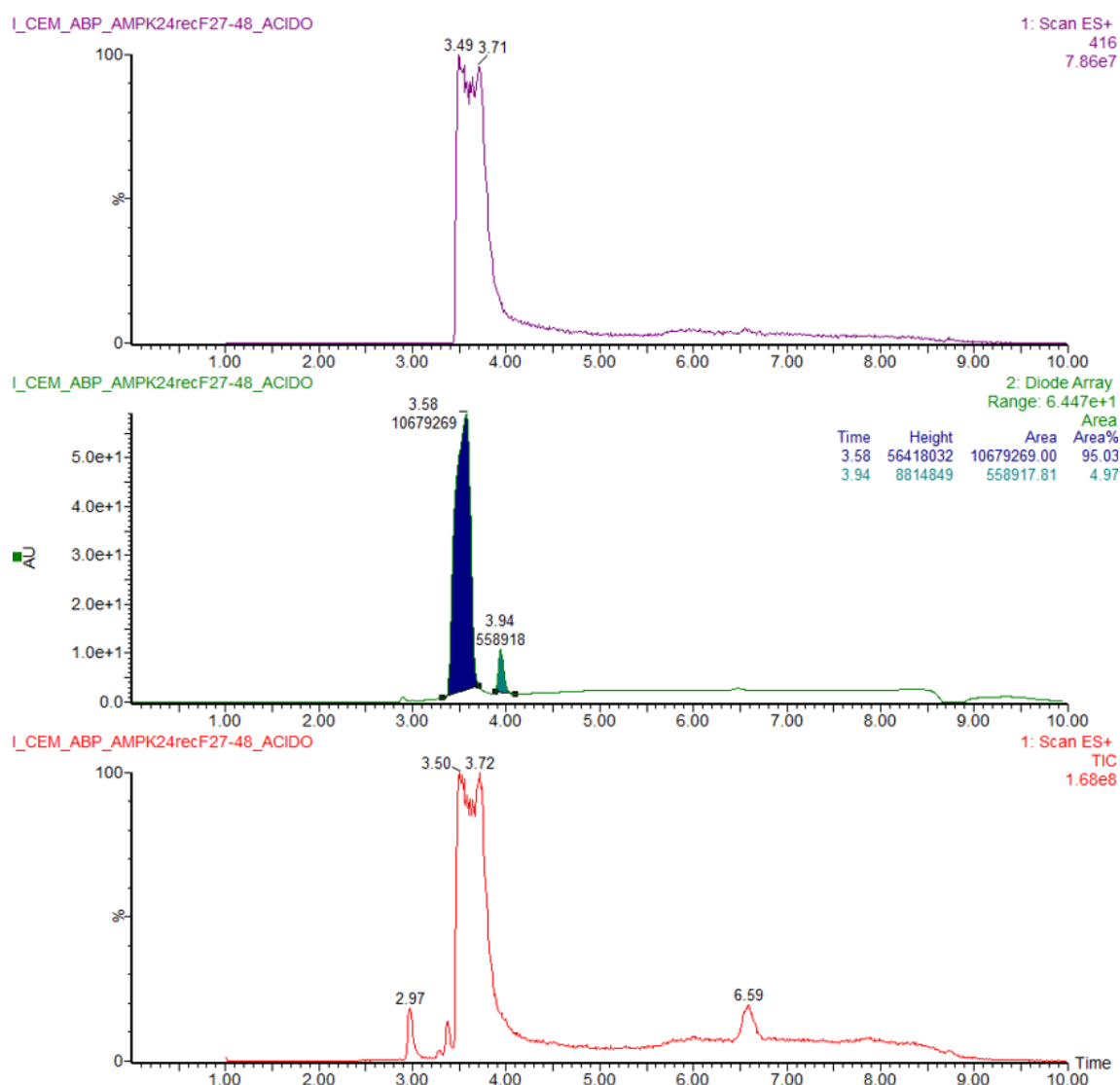
1-[4-(*Tert*-butyl)phenoxy]-3-(dibenzylamino)propan-2-ol



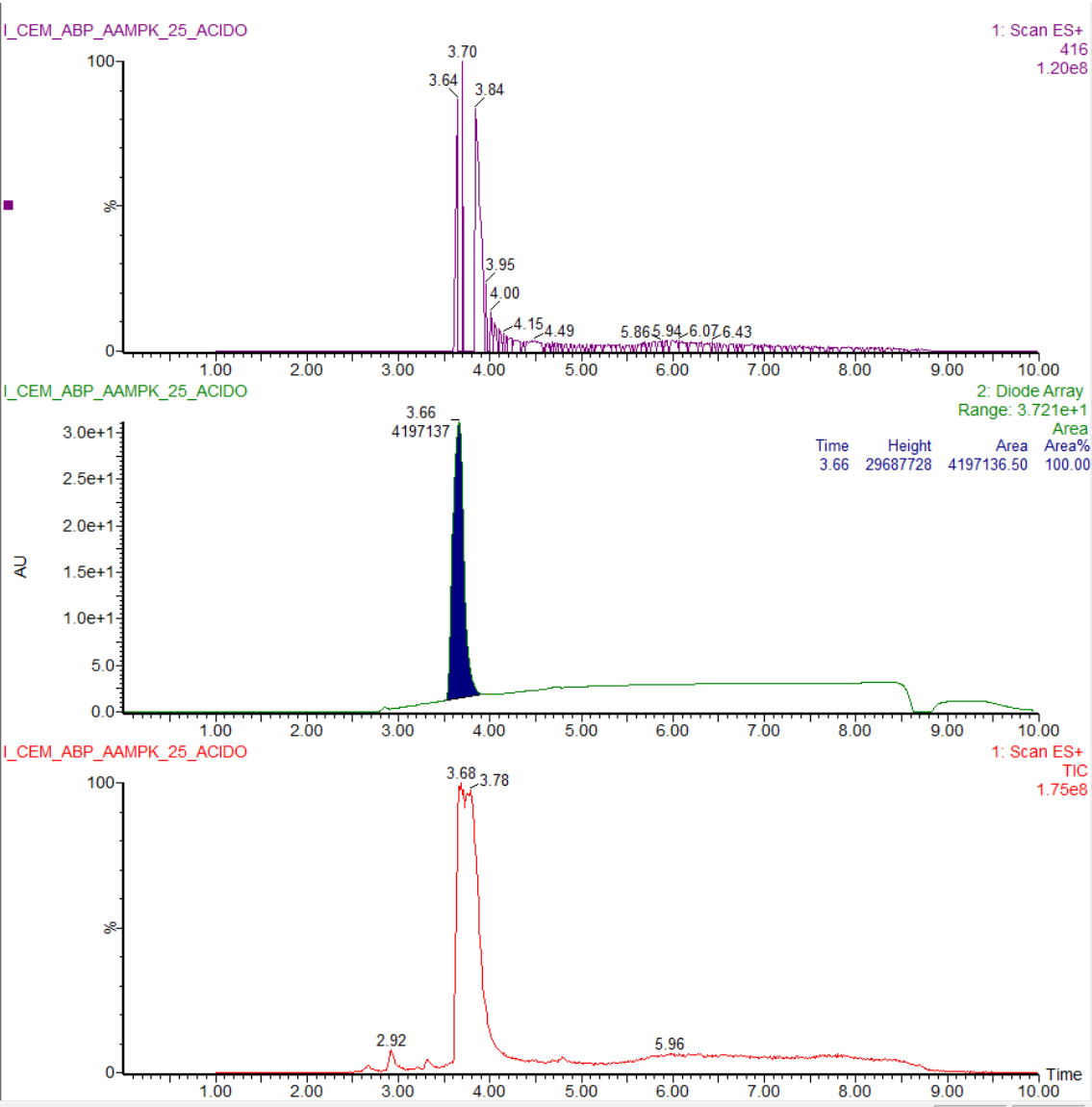
1-[4-(Benzyloxy)phenoxy]-3-(dibenzylamino)propan-2-ol



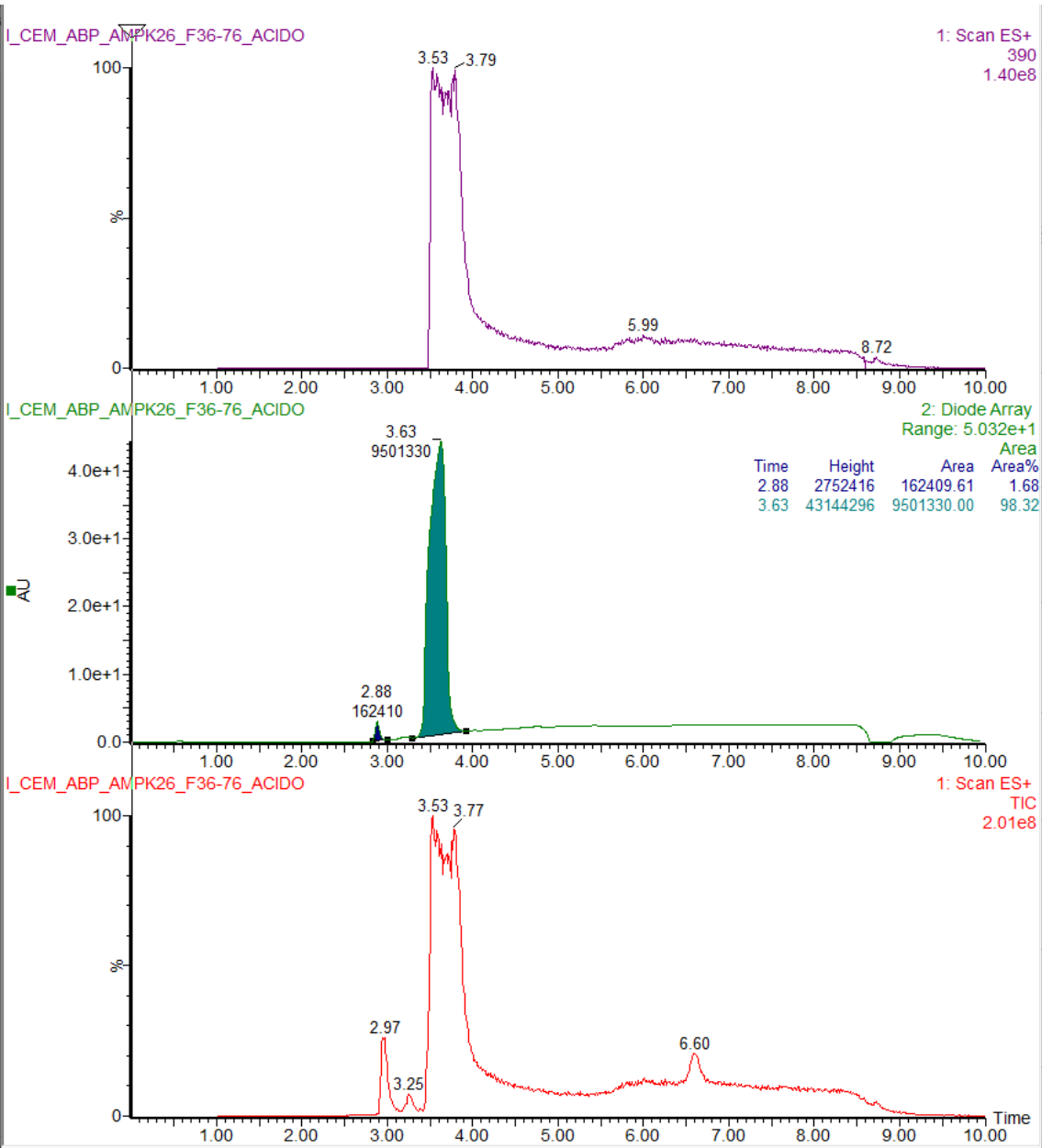
1-(Dibenzylamino)-3-(2,4-dichlorophenoxy)propan-2-ol



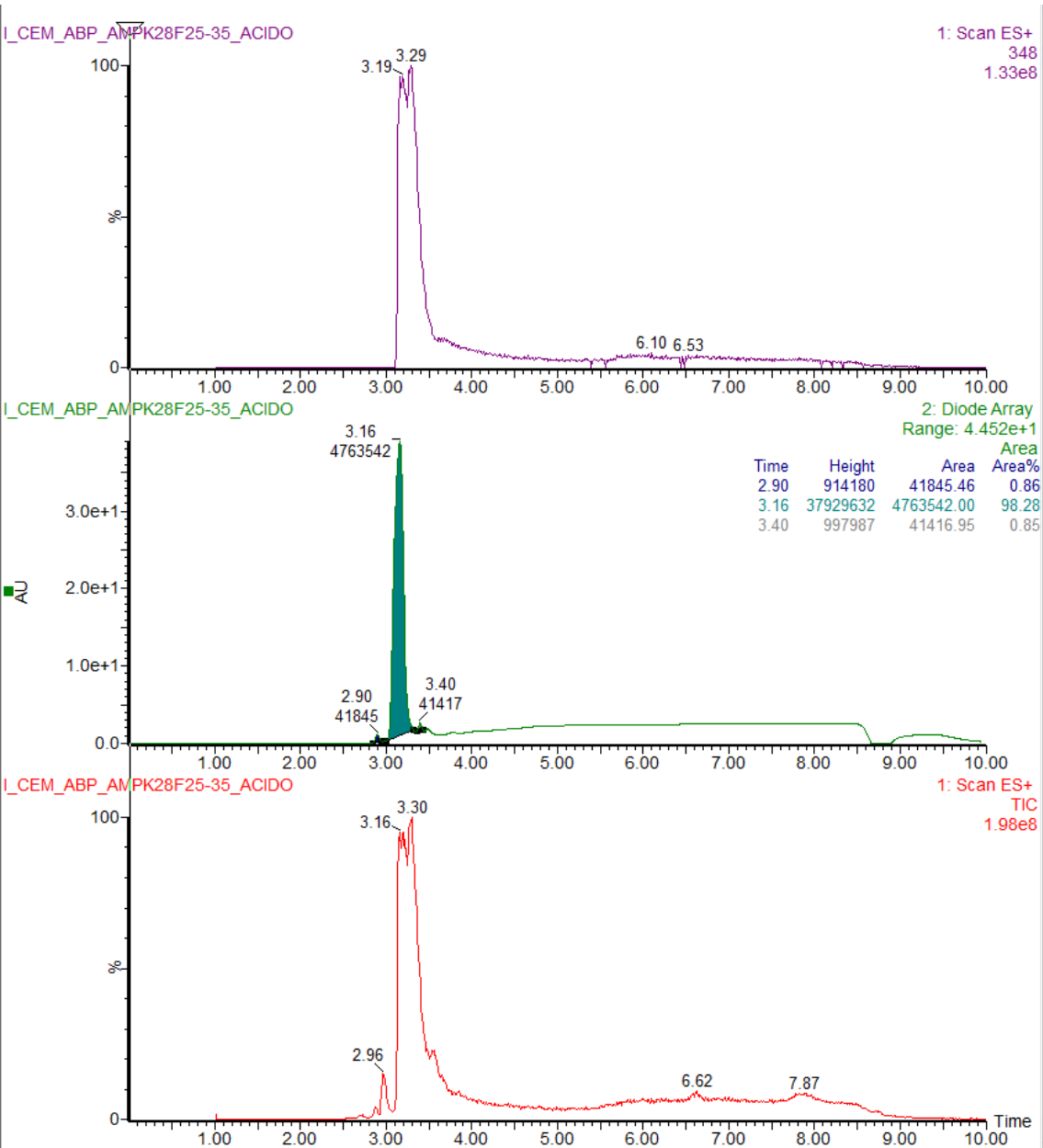
1-(4-Cyclopentylphenoxy)-3-(dibenzylamino)propan-2-ol



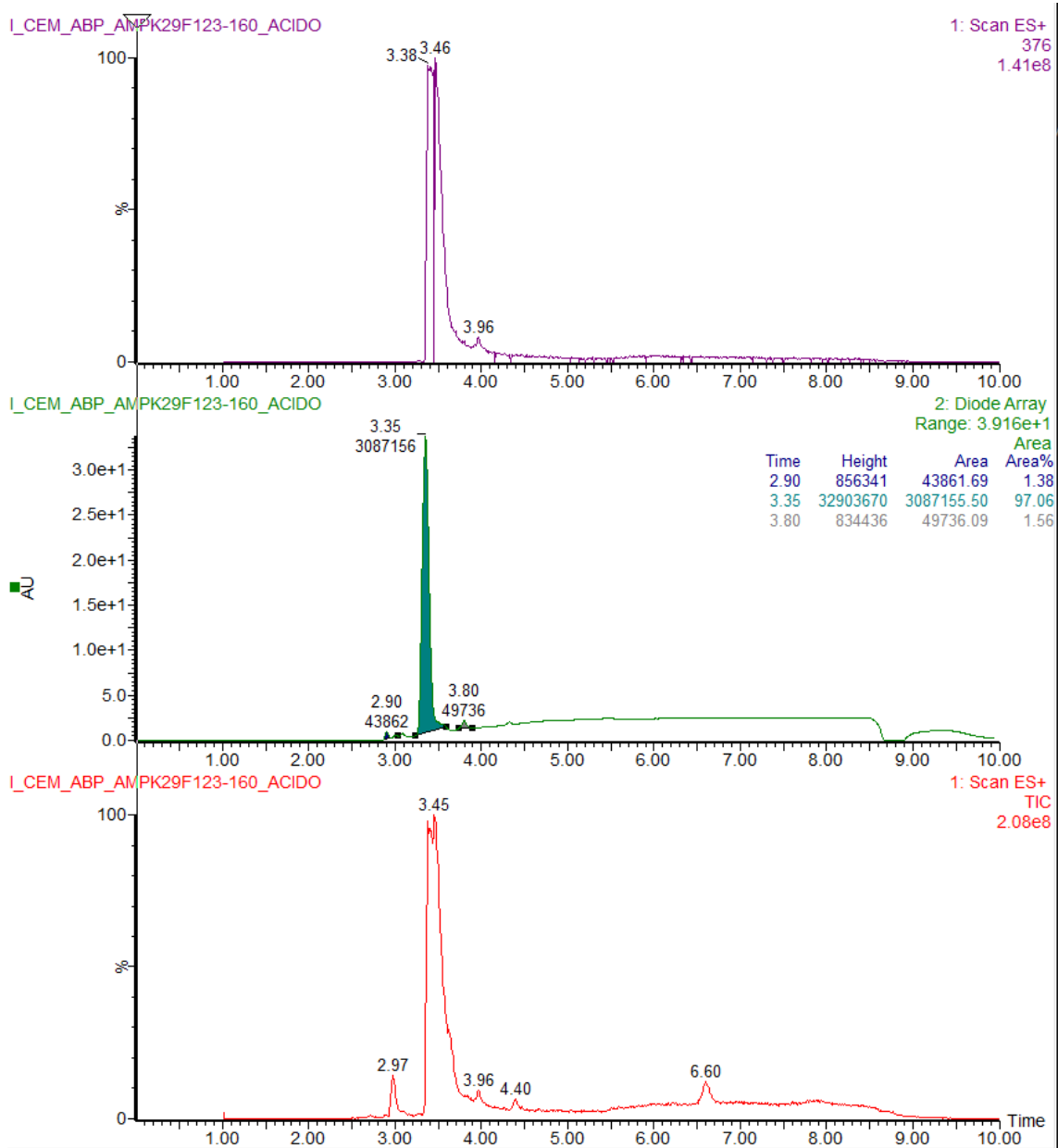
1-(Dibenzylamino)-3-(4-isopropylphenoxy)propan-2-ol



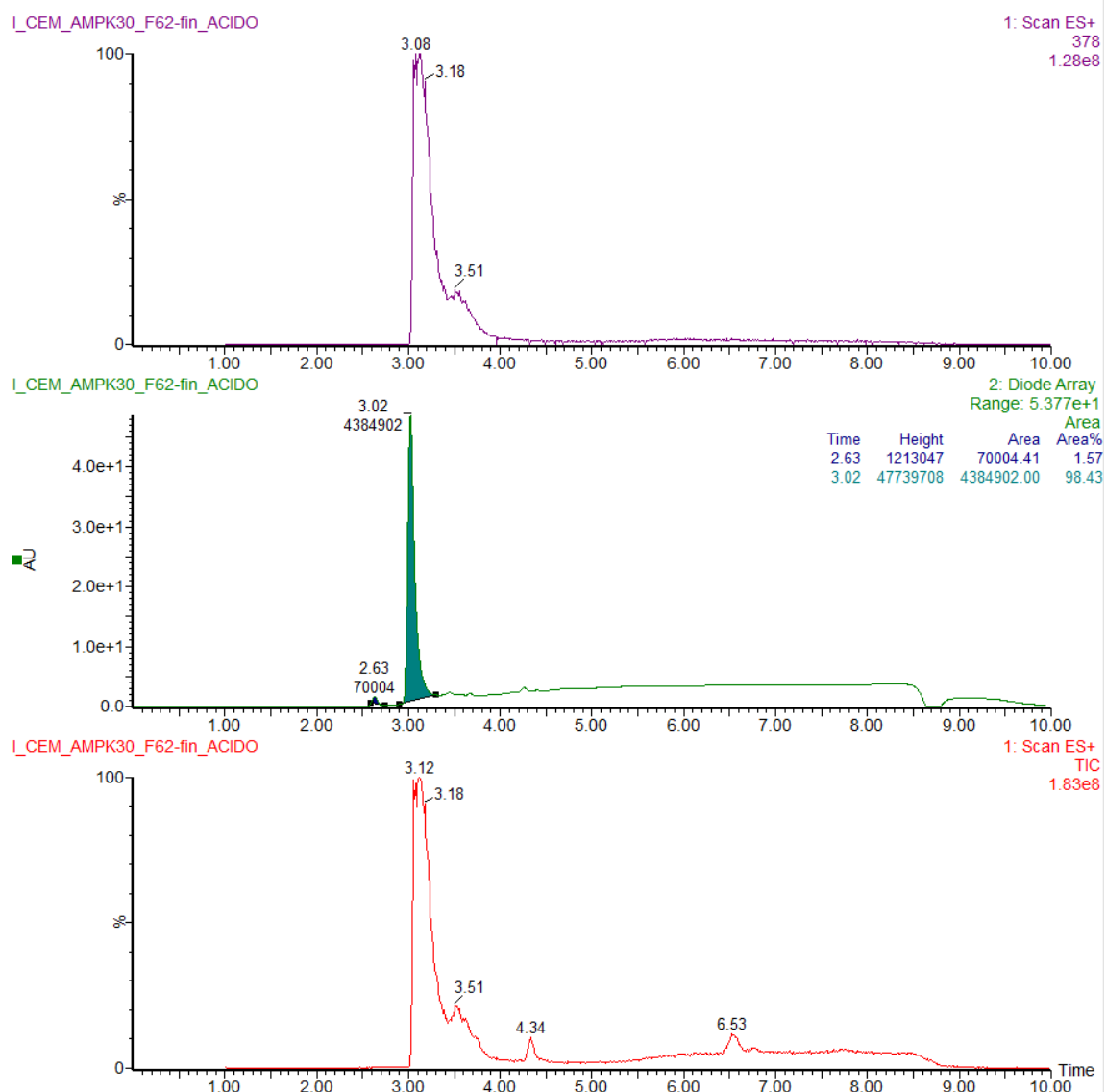
1-(Dibenzylamino)-3-phenoxypropan-2-ol



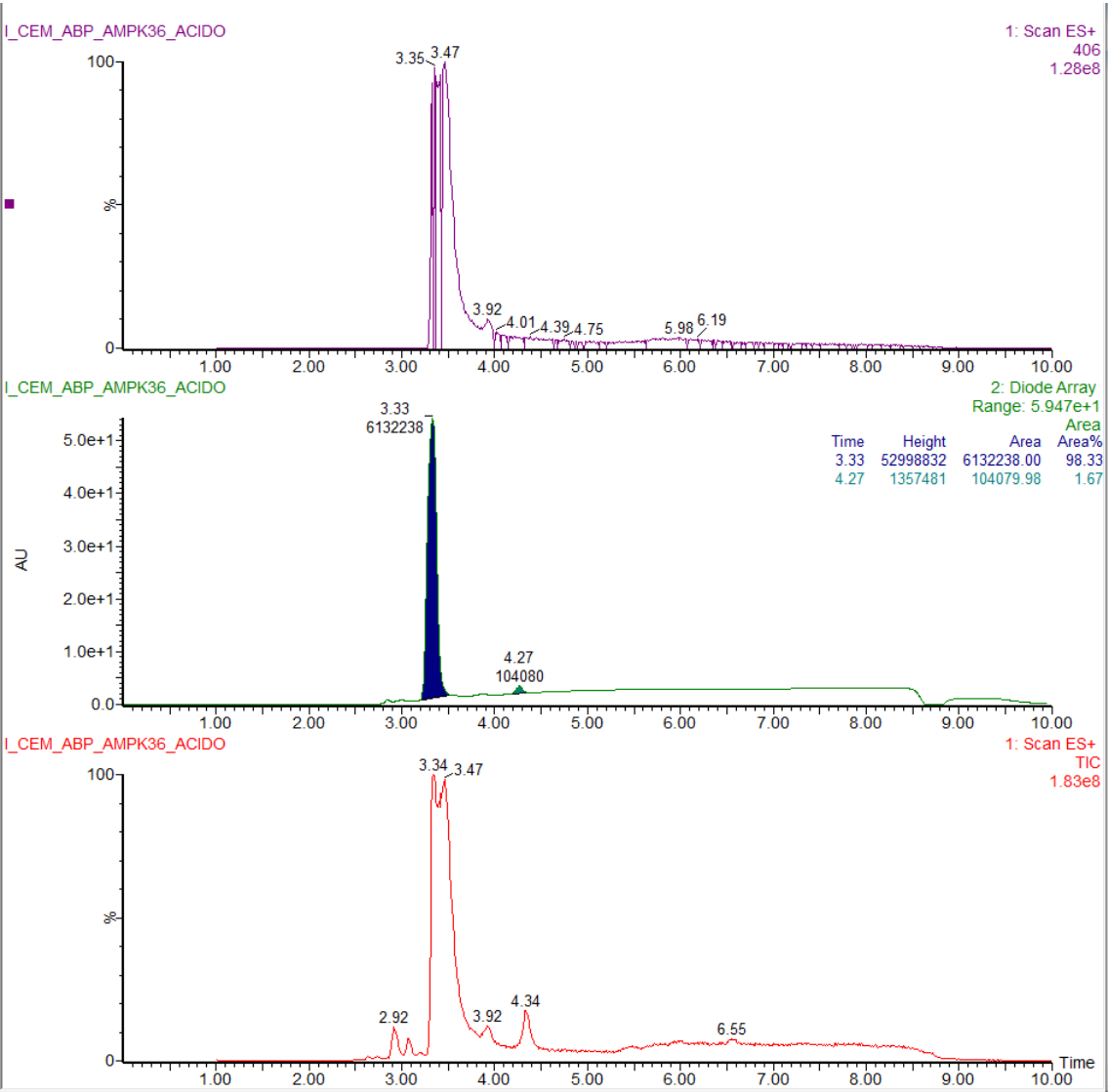
1-(Dibenzylamino)-3-(3,4-dimethylphenoxy)propan-2-ol



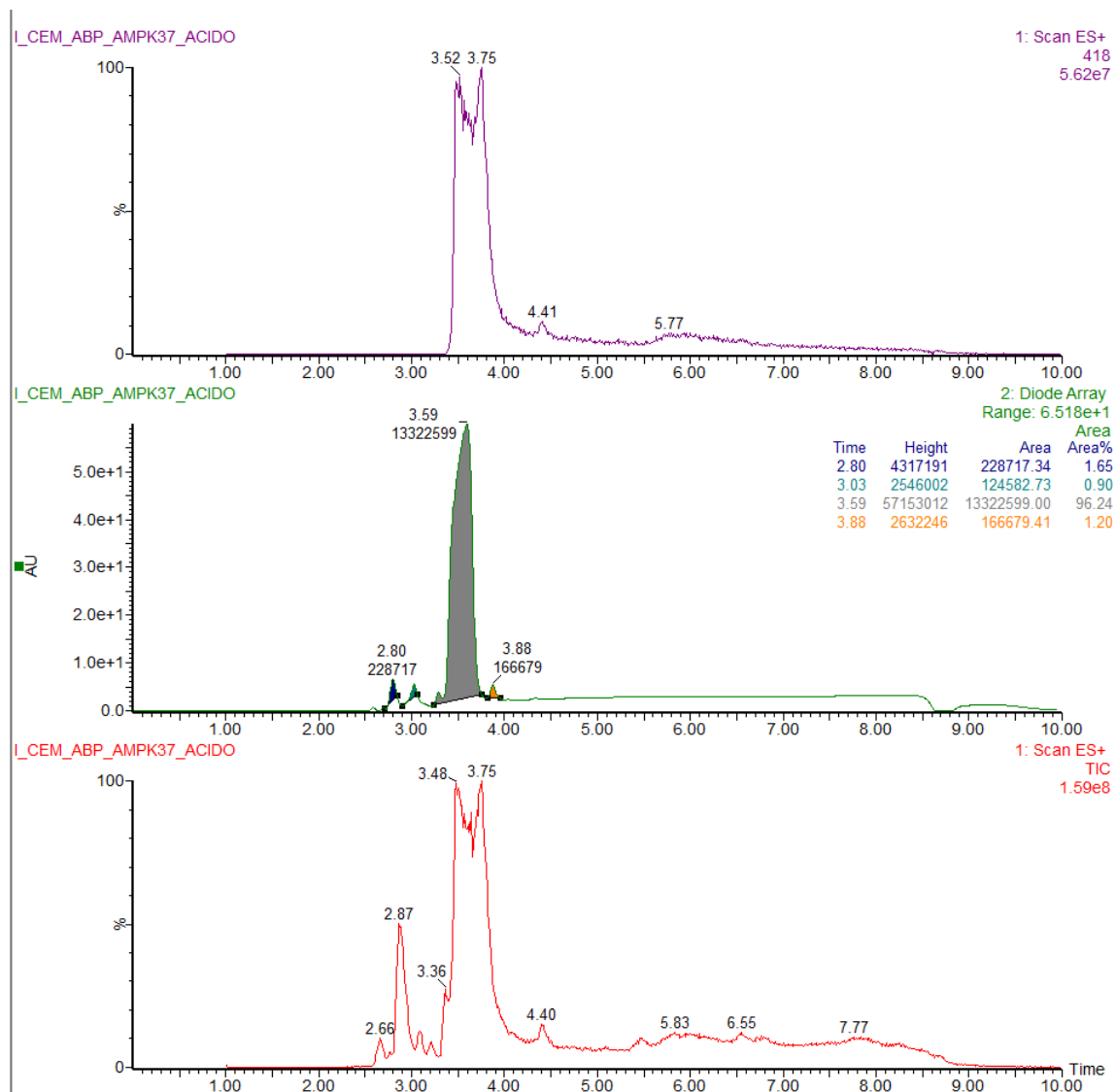
1-(Dibenzylamino)-3-(4-methoxyphenoxy)propan-2-ol



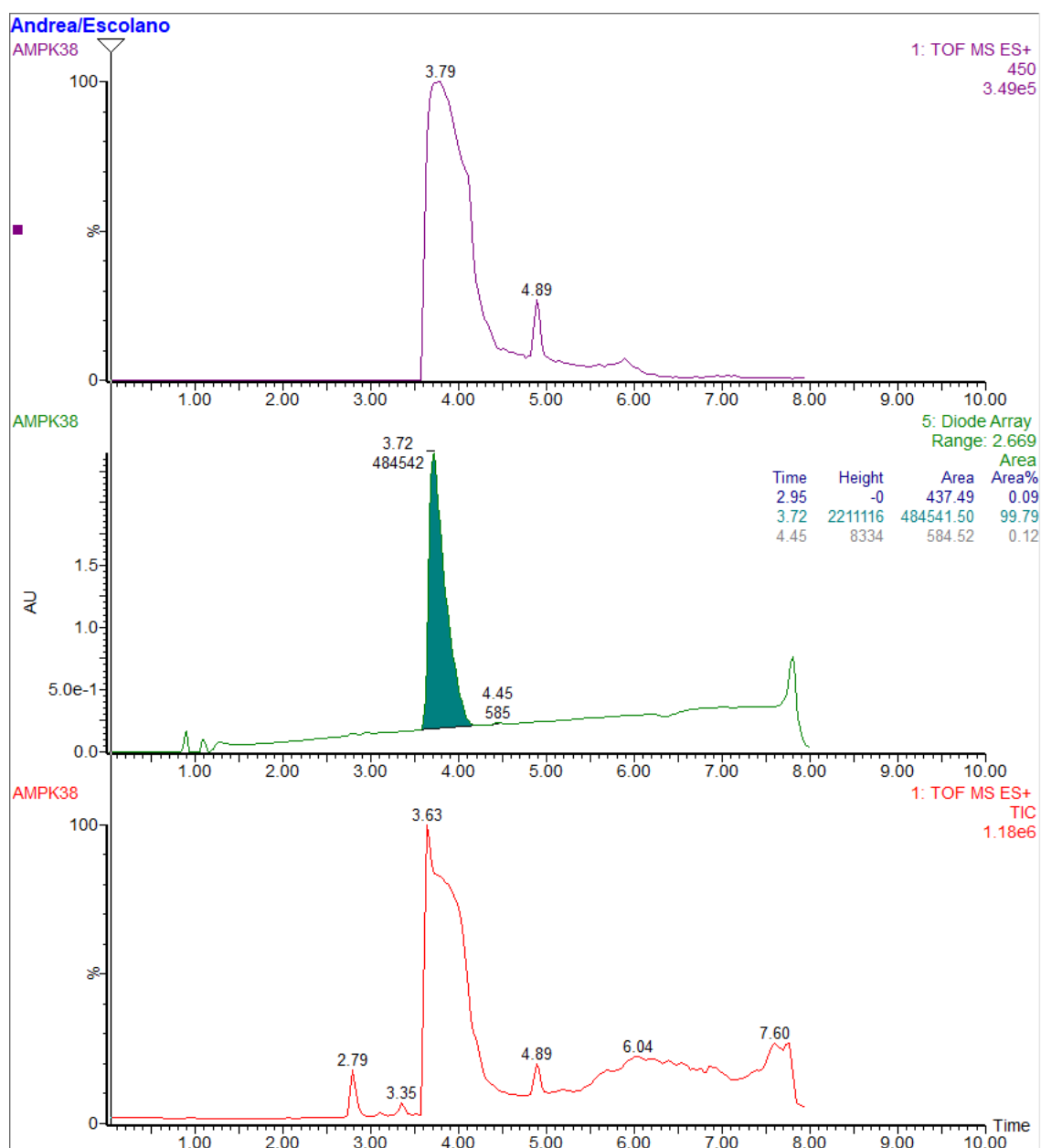
1-(Dibenzylamino)-3-(4-propoxyphenoxy)propan-2-ol



1-(Dibenzylamino)-3-(3,4-dichlorophenoxy)propan-2-ol



1-[4-Chloro-3-(trifluoromethyl)phenoxy]-3-(dibenzylamino)propan-2-ol

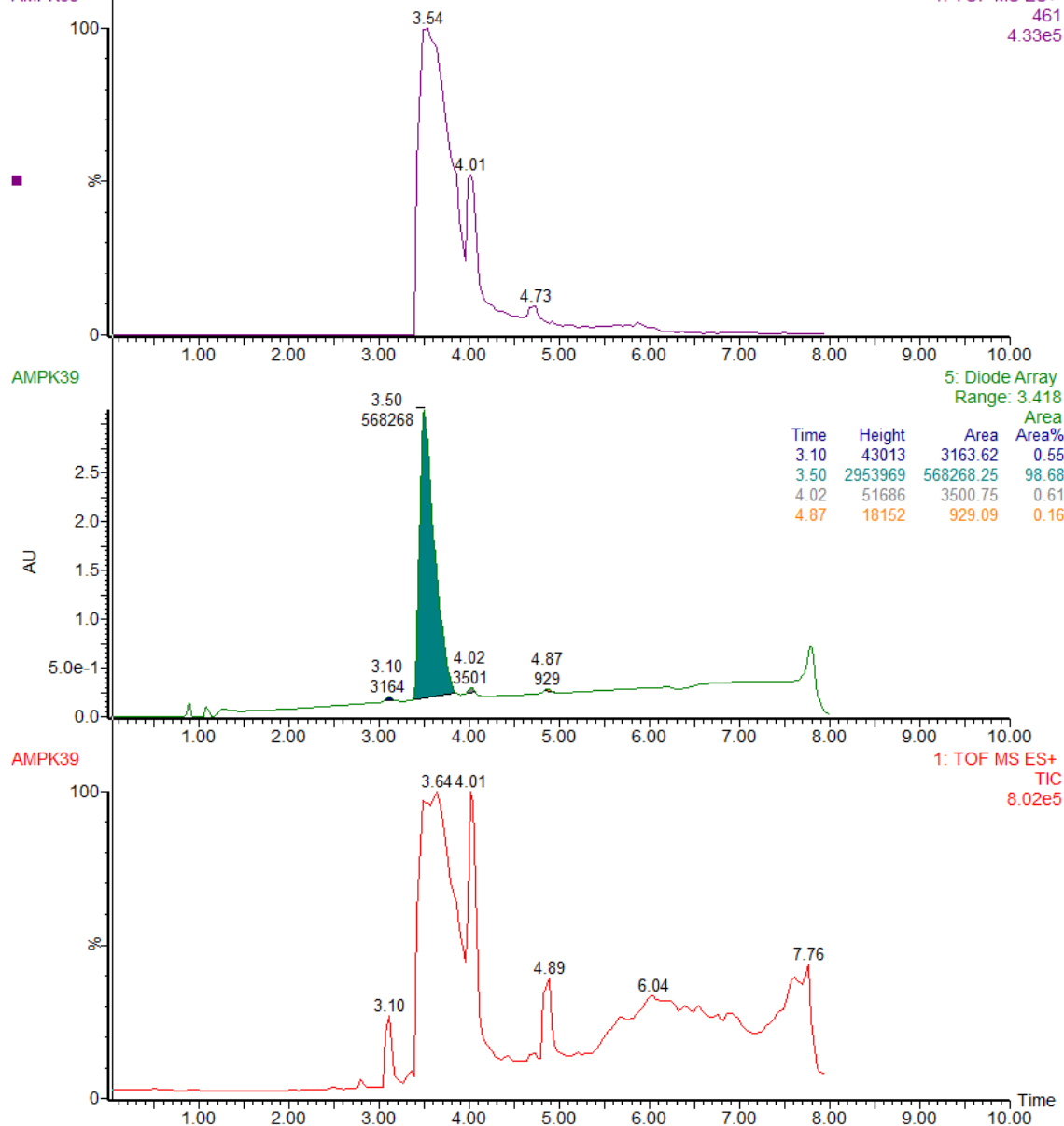


1-(Dibenzylamino)-3-[4-nitro-3-(trifluoromethyl)phenoxy]propan-2-ol

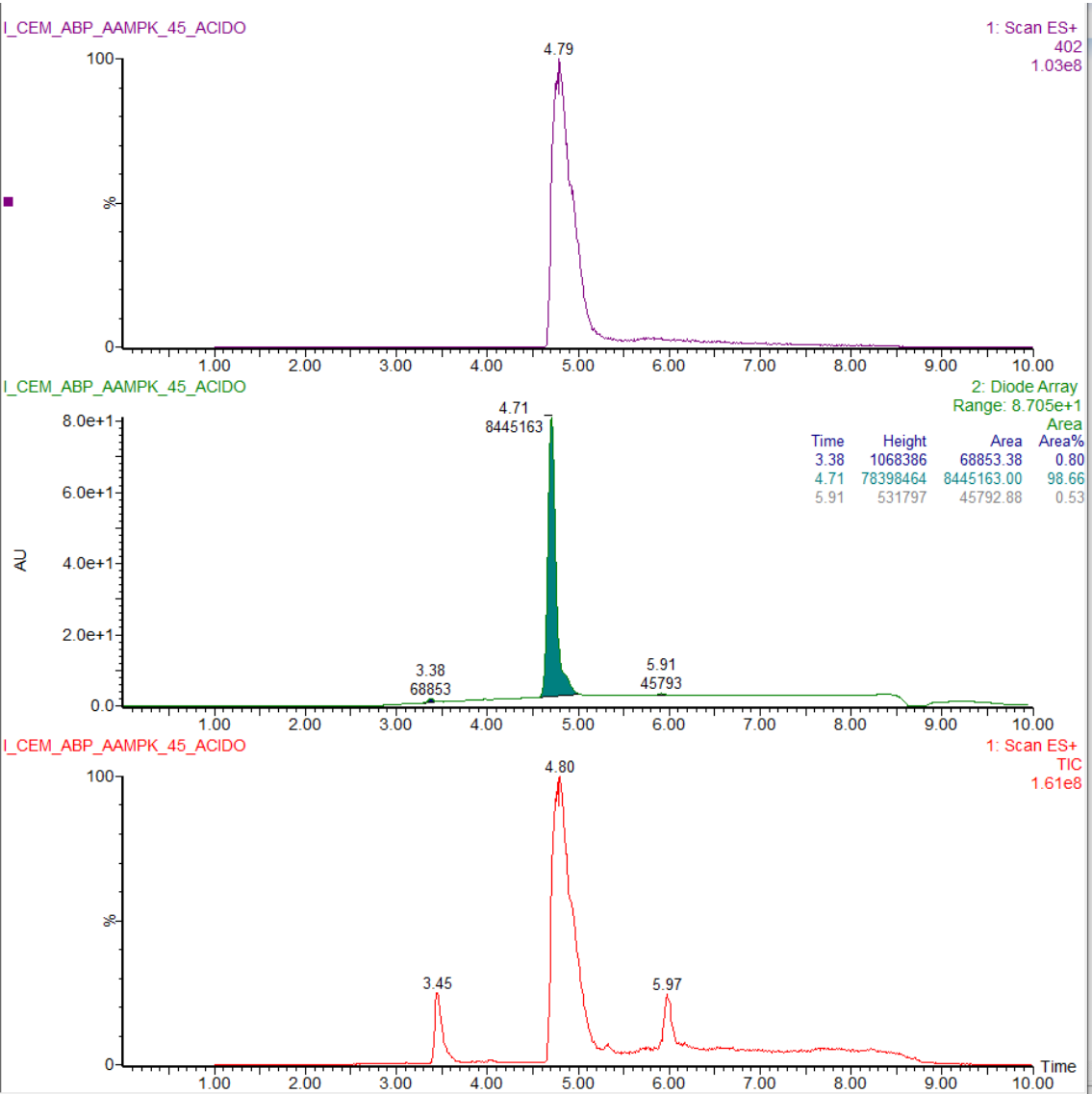
Andrea/Escolano

AMPK39

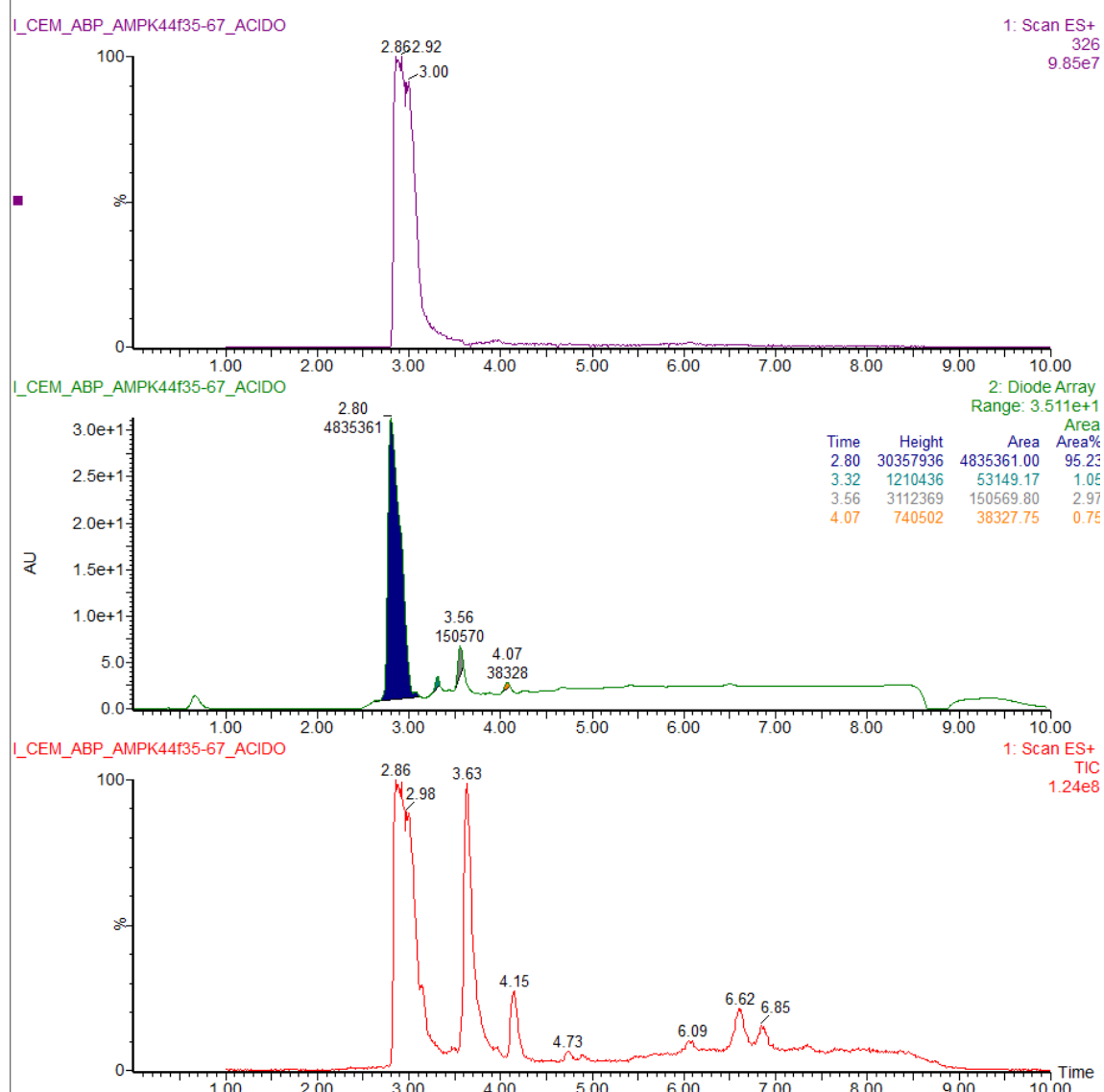
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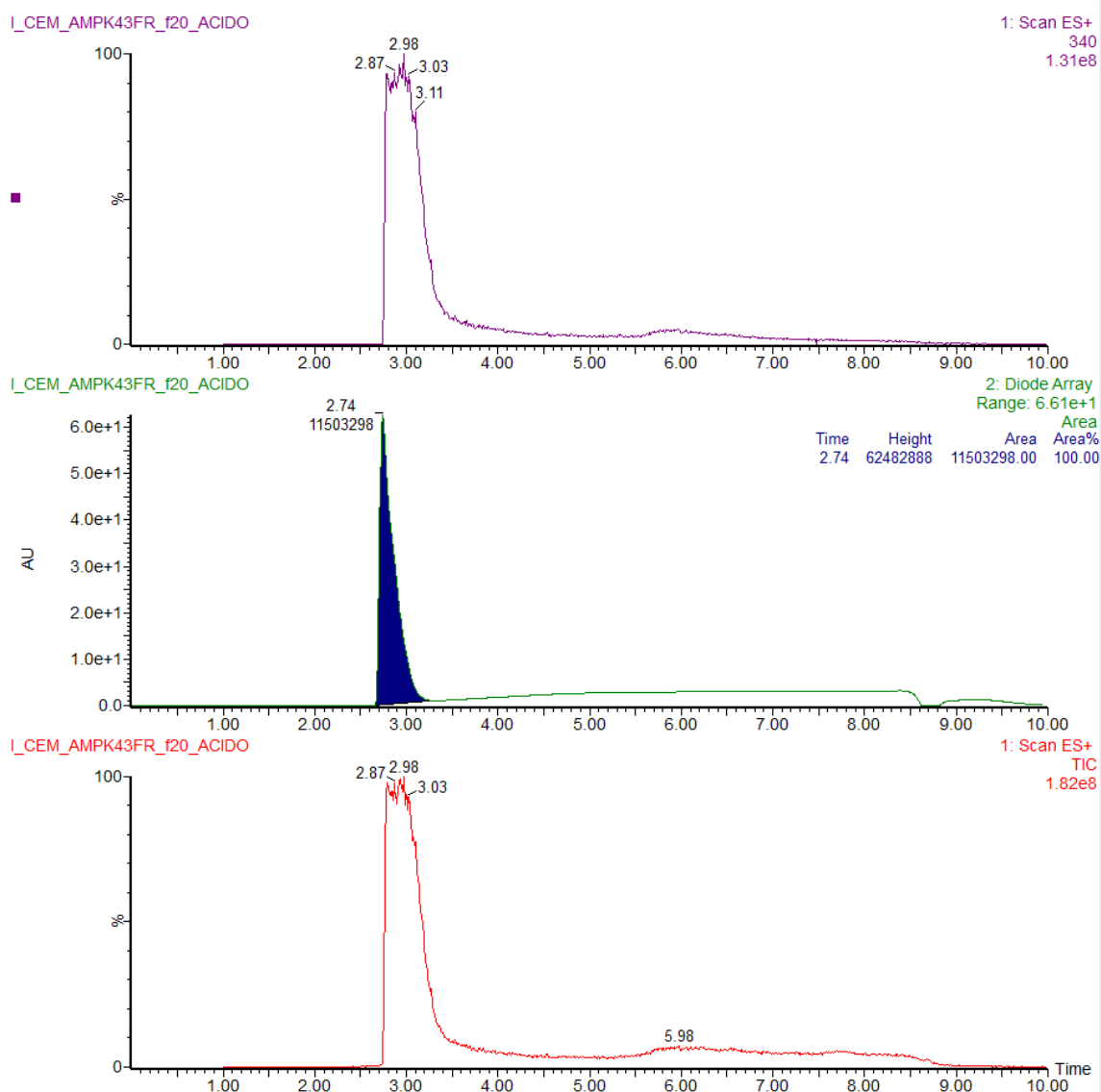
1-[Benzyl(phenyl)amino]-3-[4-(trifluoromethyl)phenoxy]propan-2-ol



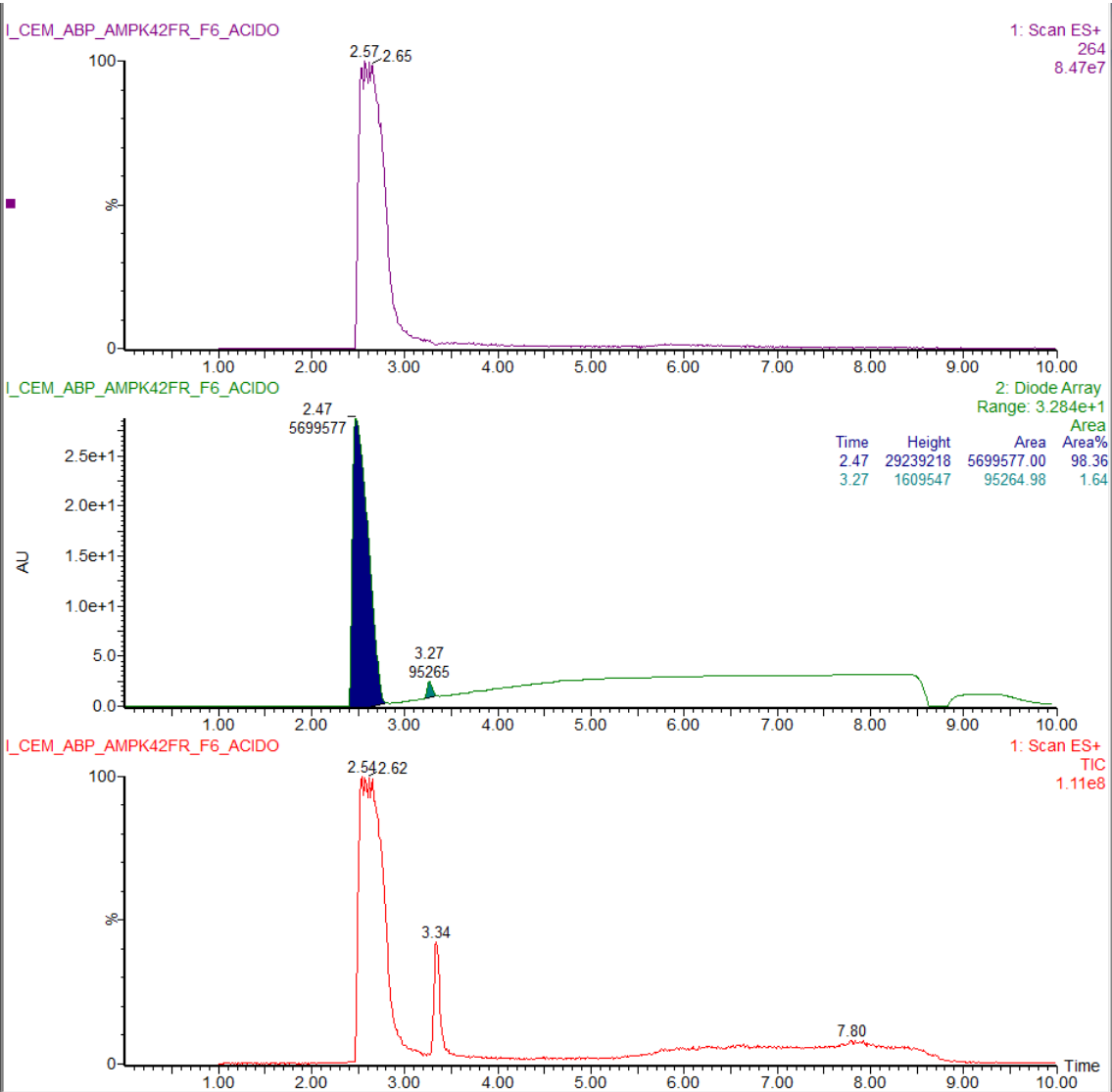
1-(Benzylamino)-3-[4-(trifluoromethyl)phenoxy]propan-2-ol



1-[Methyl(phenyl)amino]-3-[4-(trifluoromethyl)phenoxy]propan-2-ol



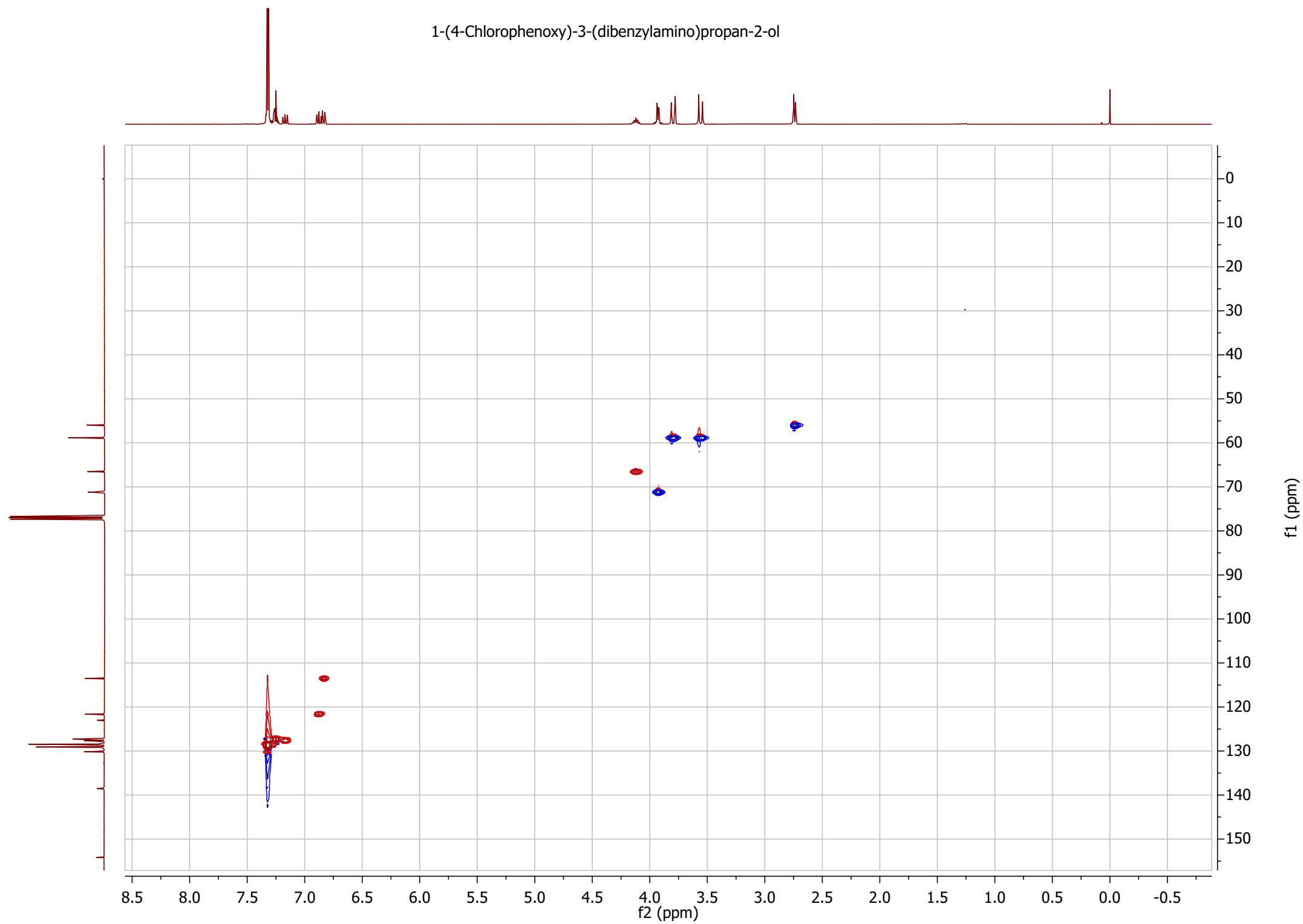
1-(Dimethylamino)-3-[4-(trifluoromethyl)phenoxy]propan-2-ol



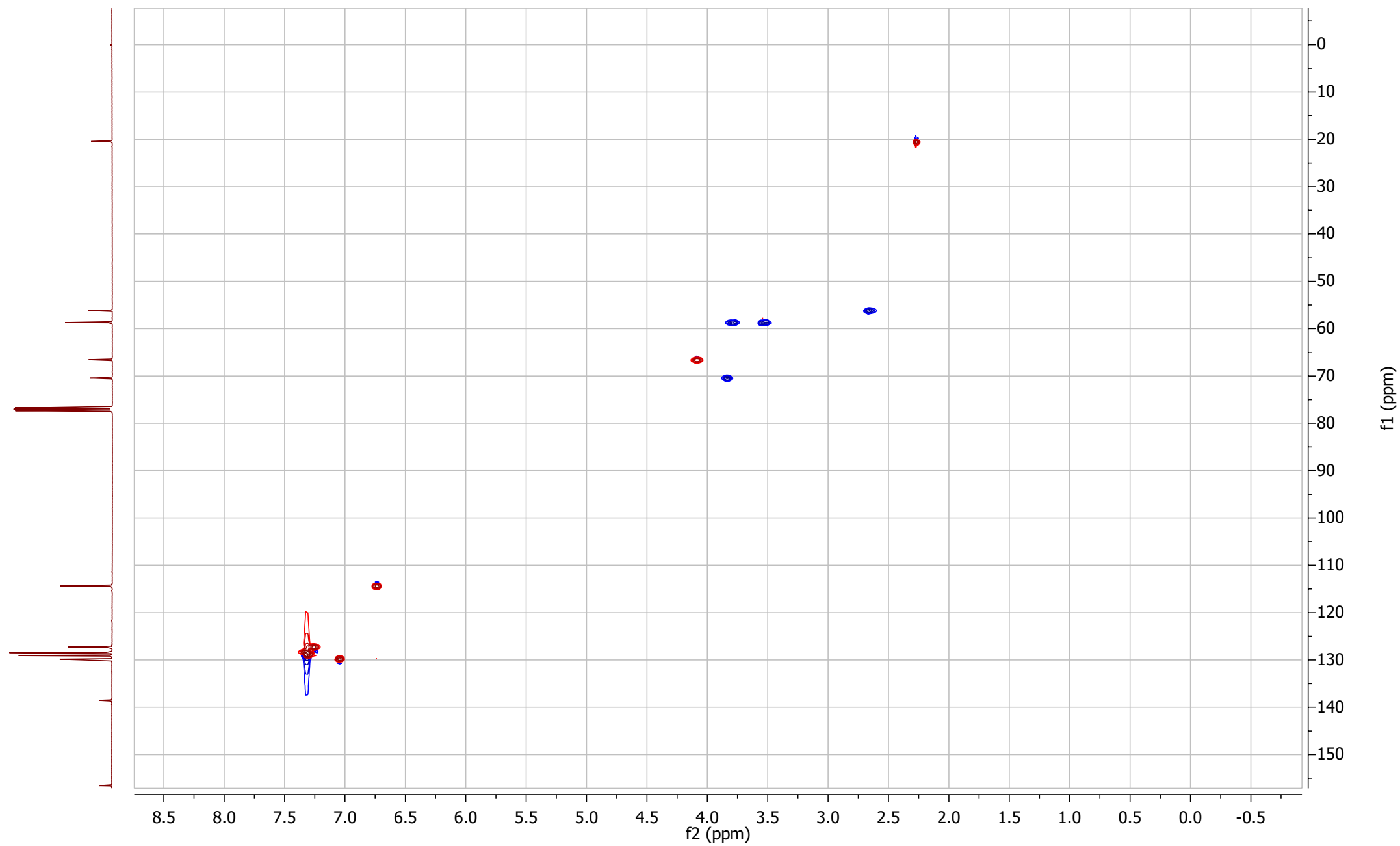
Molecular Formula Strings (Smiles)

Compound	SMILE
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1	<chem>OC(COC1=CC=C(C(F)(F)F)C=C1)CNCC2=CC=CC=C2</chem>
2	<chem>OC(COC1=CC=C(C(F)(F)F)C=C1)CN(C)CC2=CC=CC=C2</chem>
3	<chem>CN(C)CC(O)COC1=CC=C(C(F)(F)F)C=C1</chem>
4	<chem>OC(COC1=CC=C(C(F)(F)F)C=C1)CN(CC2=CC=CC=C2)C3=CC=CC=C3</chem>
5	<chem>OC(COC1=CC=C(C(F)(F)F)C=C1)CN(CC2=CC=CC=C2)CC3=CC=CN=C3</chem>
6	<chem>OC(COC1=CC=CC=C1)CN(CC2=CC=CC=C2)CC3=CC=CC=C3</chem>
7	<chem>ClC1=CC=C(OCC(O)CN(CC2=CC=CC=C2)CC3=CC=CC=C3)C=C1</chem>
8	<chem>CC1=CC=C(OCC(O)CN(CC2=CC=CC=C2)CC3=CC=CC=C3)C=C1</chem>
9	<chem>OC(COC1=CC=C(C(C)C)C=C1)CN(CC2=CC=CC=C2)CC3=CC=CC=C3</chem>
10	<chem>OC(COC1=CC=C(C(C)(C)C)C=C1)CN(CC2=CC=CC=C2)CC3=CC=CC=C3</chem>
11	<chem>OC(COC1=CC=C(C2CCCC2)C=C1)CN(CC3=CC=CC=C3)CC4=CC=CC=C4</chem>
12	<chem>OC(COC1=CC=C(C2CCCC2)C=C1)CN(CC3=CC=CC=C3)CC4=CC=CC=C4</chem>
13	<chem>CC1=C(C)C=C(OCC(O)CN(CC2=CC=CC=C2)CC3=CC=CC=C3)C=C1</chem>
14	<chem>OC(COC1=CC=C(OC)C=C1)CN(CC2=CC=CC=C2)CC3=CC=CC=C3</chem>
15	<chem>OC(COC1=CC=C(OCC2=CC=CC=C2)C=C1)CN(CC3=CC=CC=C3)CC4=CC=CC=C4</chem>
16	<chem>OC(COC1=CC=C(OCCC)C=C1)CN(CC2=CC=CC=C2)CC3=CC=CC=C3</chem>
17	<chem>ClC1=C(Cl)C=C(OCC(O)CN(CC2=CC=CC=C2)CC3=CC=CC=C3)C=C1</chem>
18	<chem>ClC1=C(C(F)(F)F)C=C(OCC(O)CN(CC2=CC=CC=C2)CC3=CC=CC=C3)C=C1</chem>
19	<chem>OC(COC1=CC(C(F)(F)F)=C([N+])([O-])=O)C=C1)CN(CC2=CC=CC=C2)CC3=CC=CC=C3</chem>
20	<chem>ClC1=CC(Cl)=C(OCC(O)CN(CC2=CC=CC=C2)CC3=CC=CC=C3)C=C1</chem>
21	<chem>BrC1=CC=C(OCC(O)CN(CC2=CC=CC=C2)CC3=CC=CC=C3)C=C1</chem>
22	<chem>OC(COC1=CC=C([N+])([O-])=O)C=C1)CN(CC2=CC=CC=C2)CC3=CC=CC=C3</chem>
23	<chem>IC1=CC=C(OCC(O)CN(CC2=CC=CC=C2)CC3=CC=CC=C3)C=C1</chem>
24	<chem>OC(COC1=CC=C(S(F)(F)F)C=C1)CN(CC2=CC=CC=C2)CC3=CC=CC=C3</chem>
25	<chem>ClC1=CC=C(OCC(O)CN(CC2=CC=C(Cl)C=C2)CC3=CC=CC=C3)C=C1</chem>
26	<chem>OC(COC1=CC=C(Cl)C=C1)CN(CC2=CC=C(Cl)C=C2)CC3=CC=C(Cl)C=C3</chem>
27	<chem>ClC1=CC=C(OCC(O)CN(CC2=CC=C(C)C=C2)CC3=CC=CC=C3)C=C1</chem>
28	<chem>ClC1=CC=C(OCC(O)CN(CC2=CC=C(C)C=C2)CC3=CC=C(C)C=C3)C=C1</chem>
29	<chem>ClC1=CC=C(OCC(O)CN(CC2=CC=C(C)C=C2)CC3=CC=CC=C3)C=C1</chem>
30	<chem>OC(COC1=CC=C(Cl)C=C1)CN(CC2=CC=C(Cl)C(Cl)=C2)CC3=CC=CC=C3</chem>
31	<chem>OC(COC1=CC=C(Cl)C=C1)CN(CC2=CC=C(Cl)C(Cl)=C2)CC3=CC=C(Cl)C=C3</chem>
32	<chem>OC(COC1=CC=C(Cl)C=C1)CN(CC2=CC=C(Cl)C(Cl)=C2)CC3=CC=C(C)C=C3</chem>
33	<chem>ClC1=CC=C(OCC(O)CN(CC2=CC=CC=C2)CC3=CC=C(OC)C=C3)C=C1</chem>
34	<chem>ClC1=CC=C(OCC(O)CN(CC2=CC=C(OC)C=C2)CC3=CC=C(OC)C=C3)C=C1</chem>
35	<chem>OC(COC1=CC=C(Cl)C=C1)CN(CC2=CC=C(Cl)C(Cl)=C2)CC3=CC=C(OC)C=C3</chem>

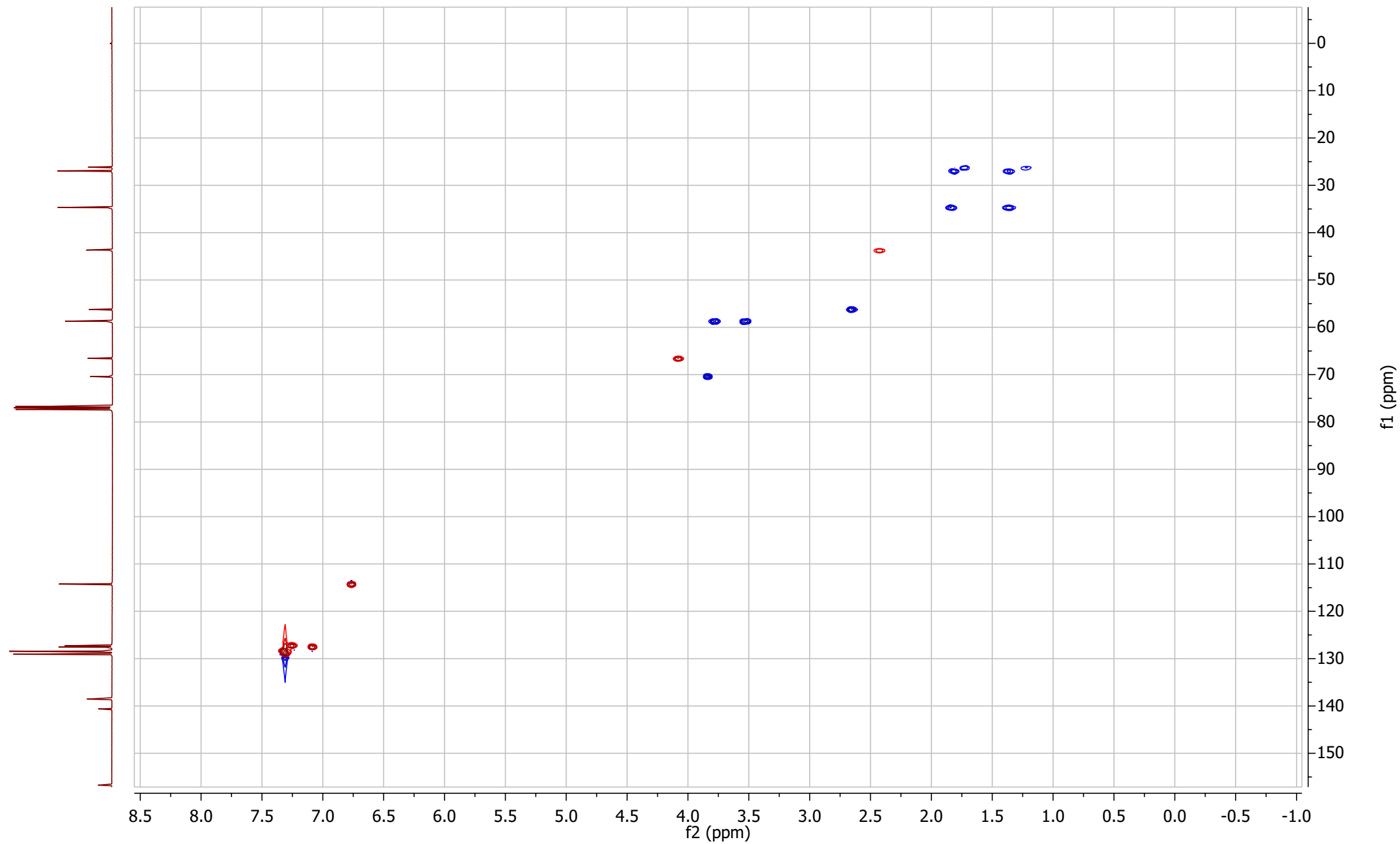
1-(4-Chlorophenoxy)-3-(dibenzylamino)propan-2-ol



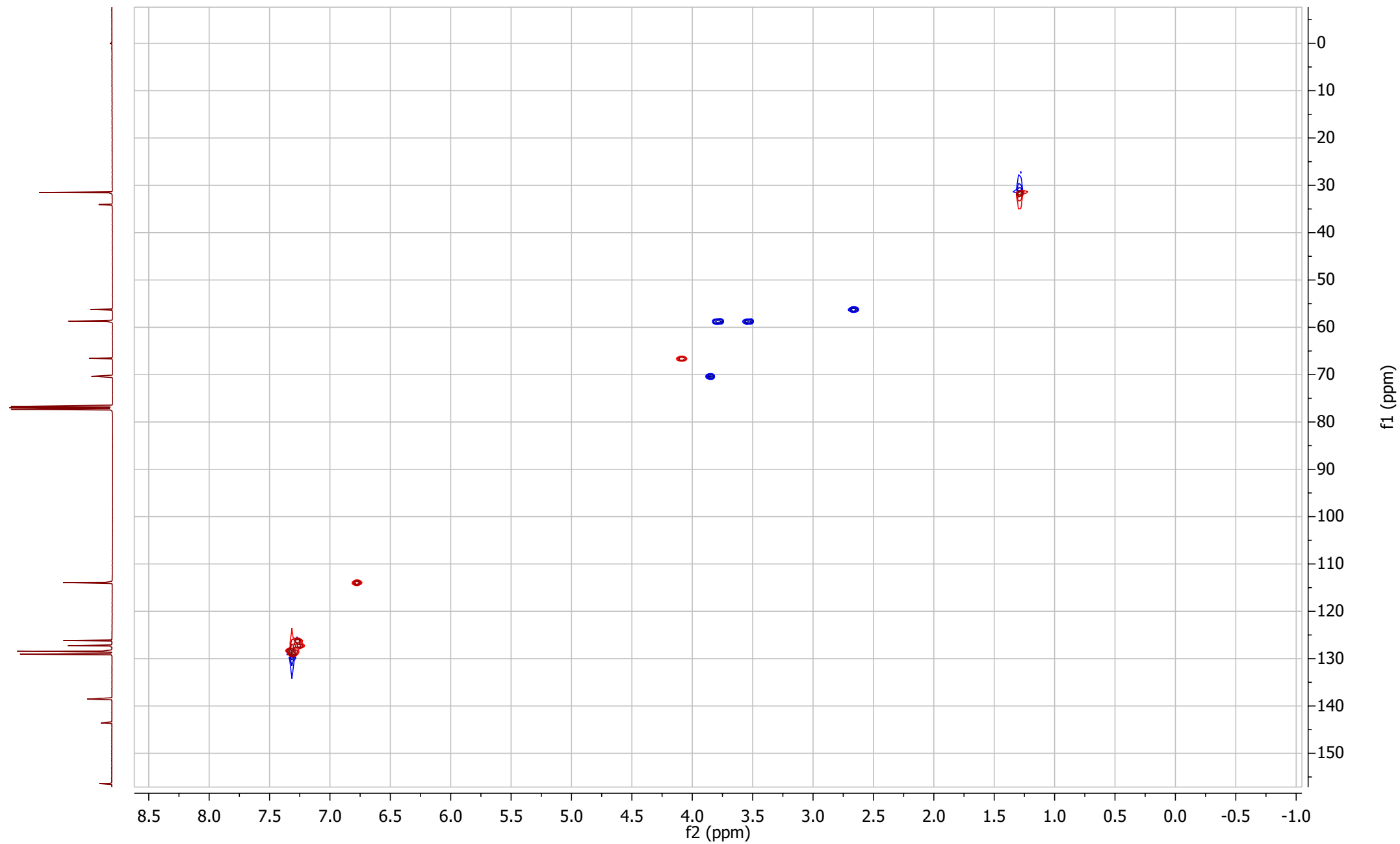
1-(Dibenzylamino)-3-(p-tolyloxy)propan-2-ol



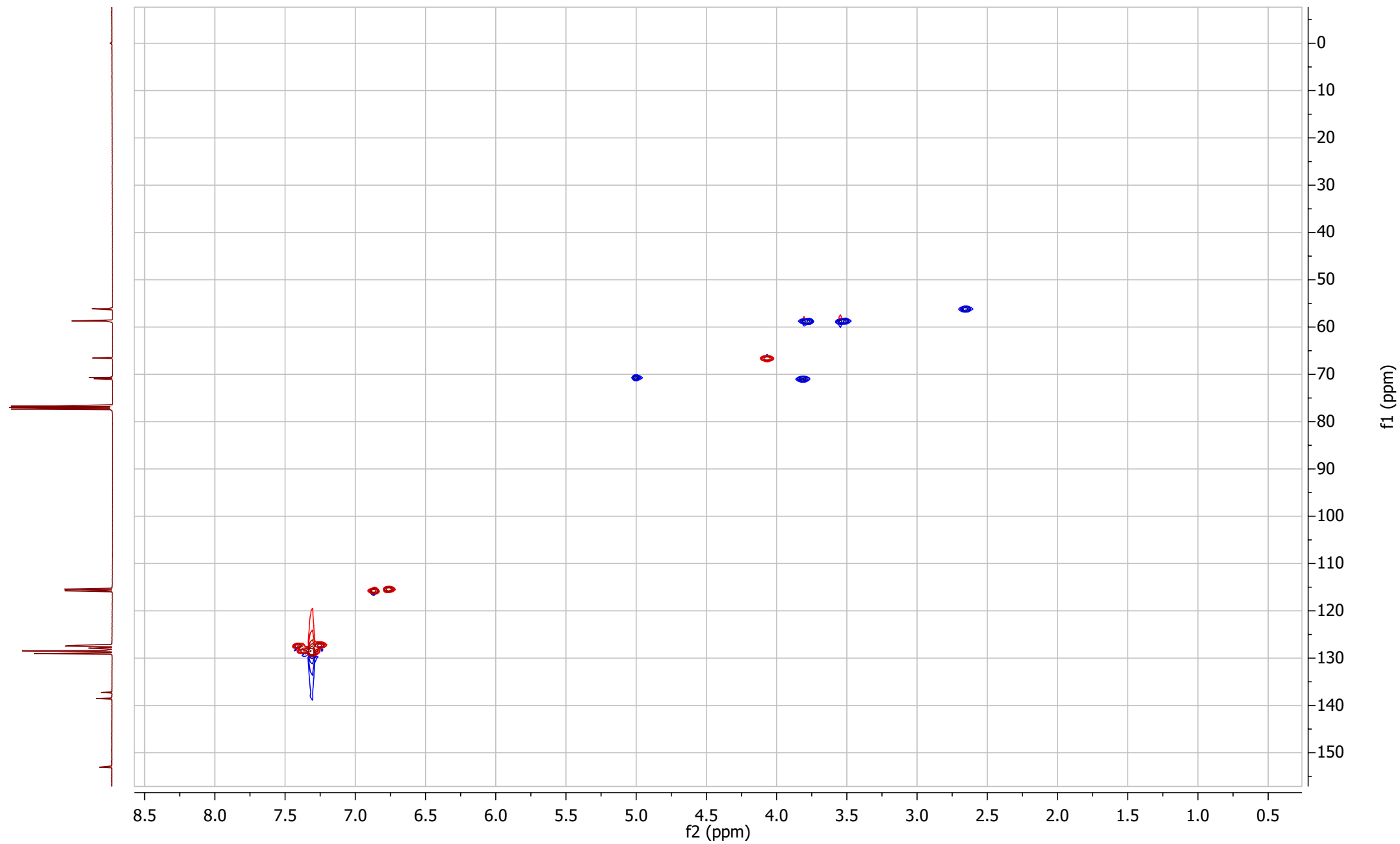
1-(4-Cyclohexylphenoxy)-3-(dibenzylamino)propan-2-ol



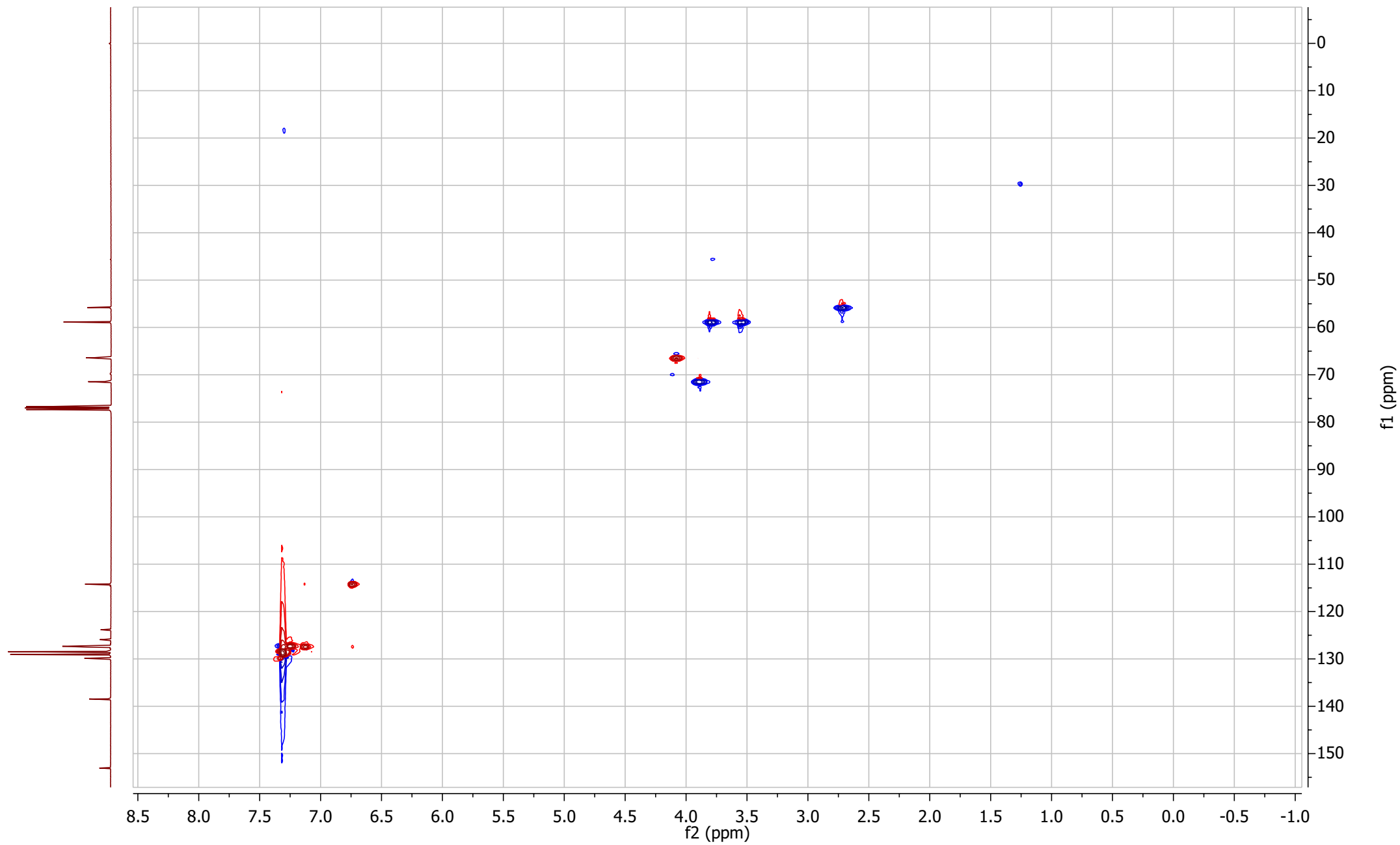
1-[4-(Tert-butyl)phenoxy]-3-(dibenzylamino)propan-2-ol



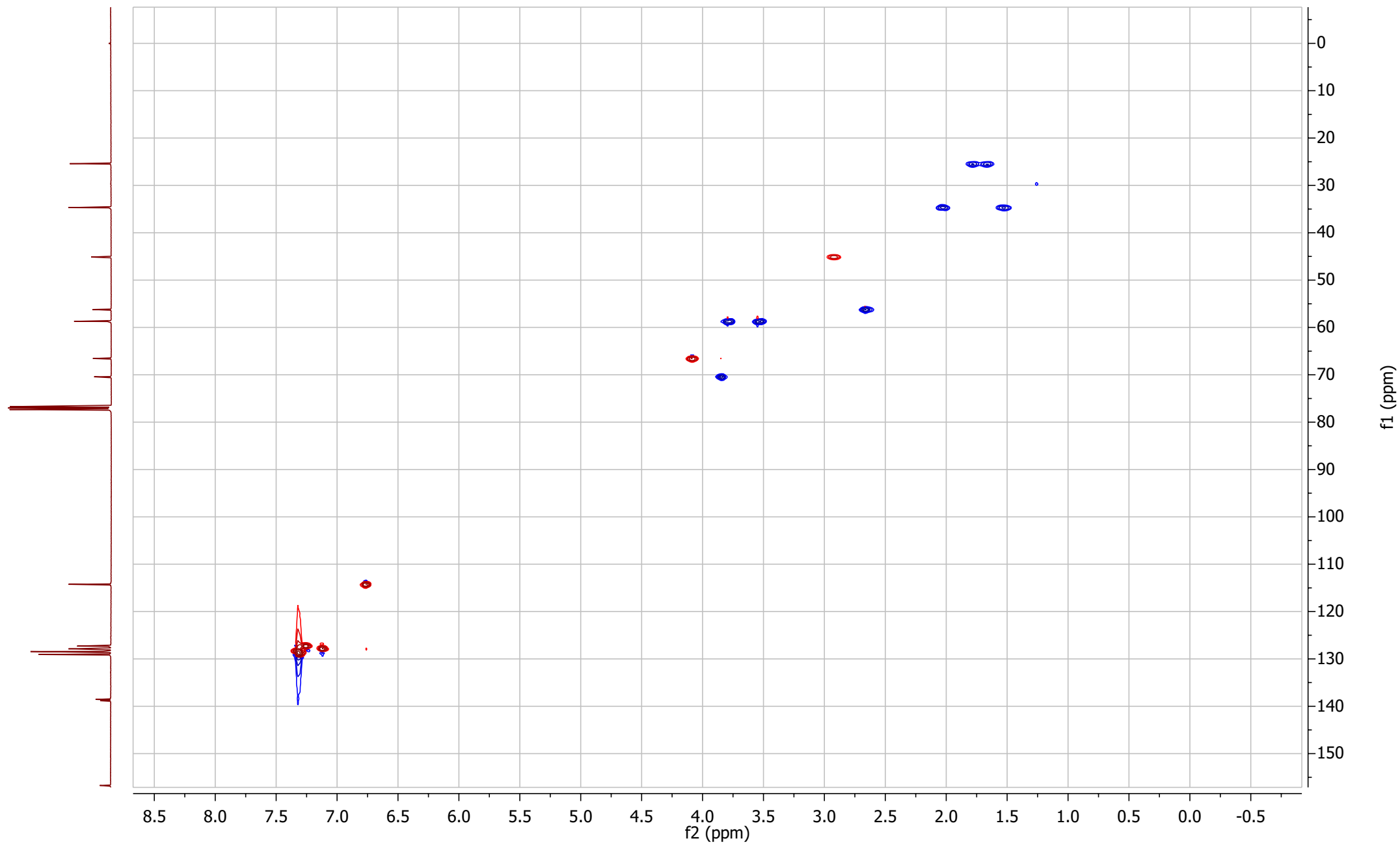
1-[4-(Benzyloxy)phenoxy]-3-(dibenzylamino)propan-2-ol



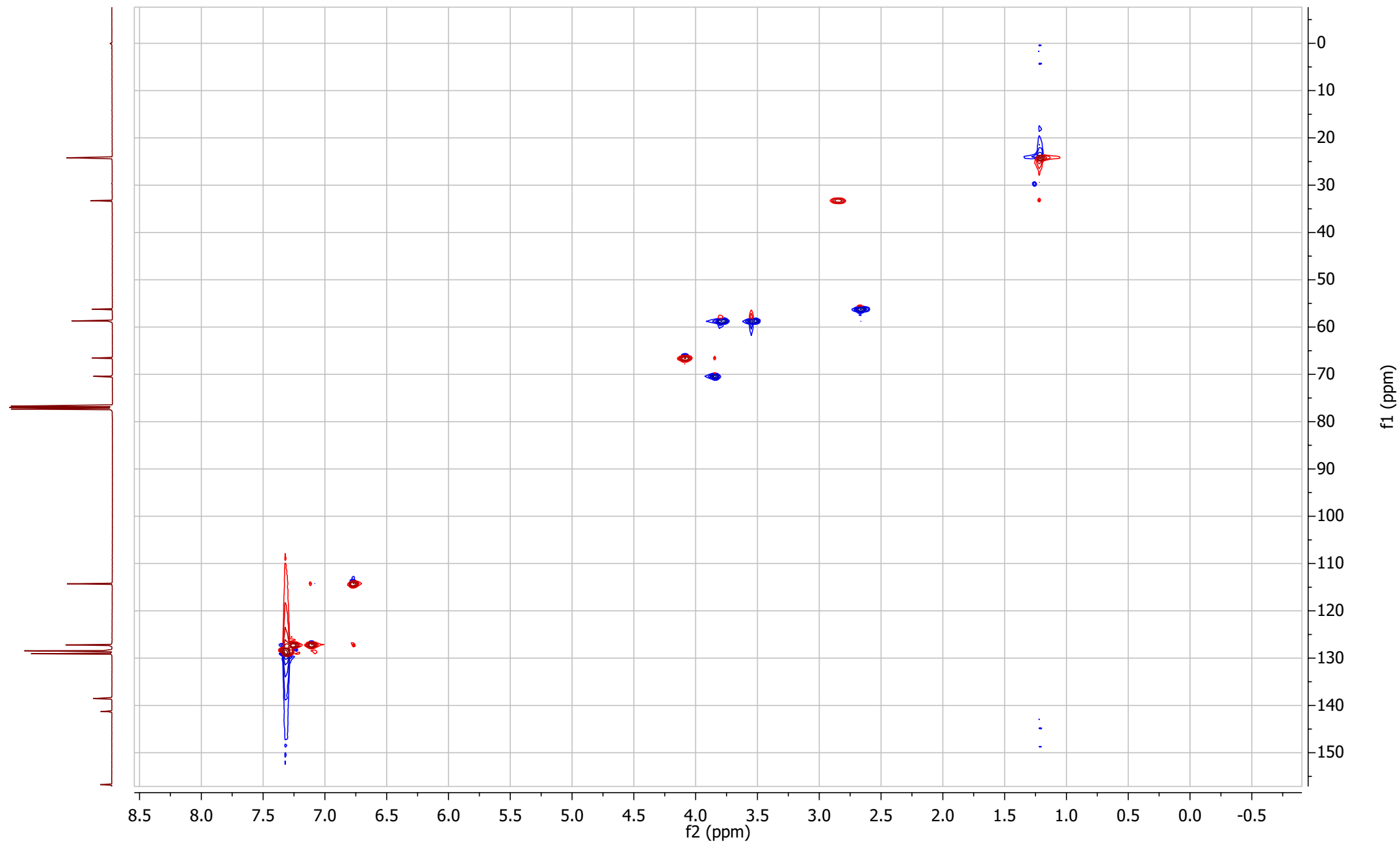
1-(Dibenzylamino)-3-(2,4-dichlorophenoxy)propan-2-ol



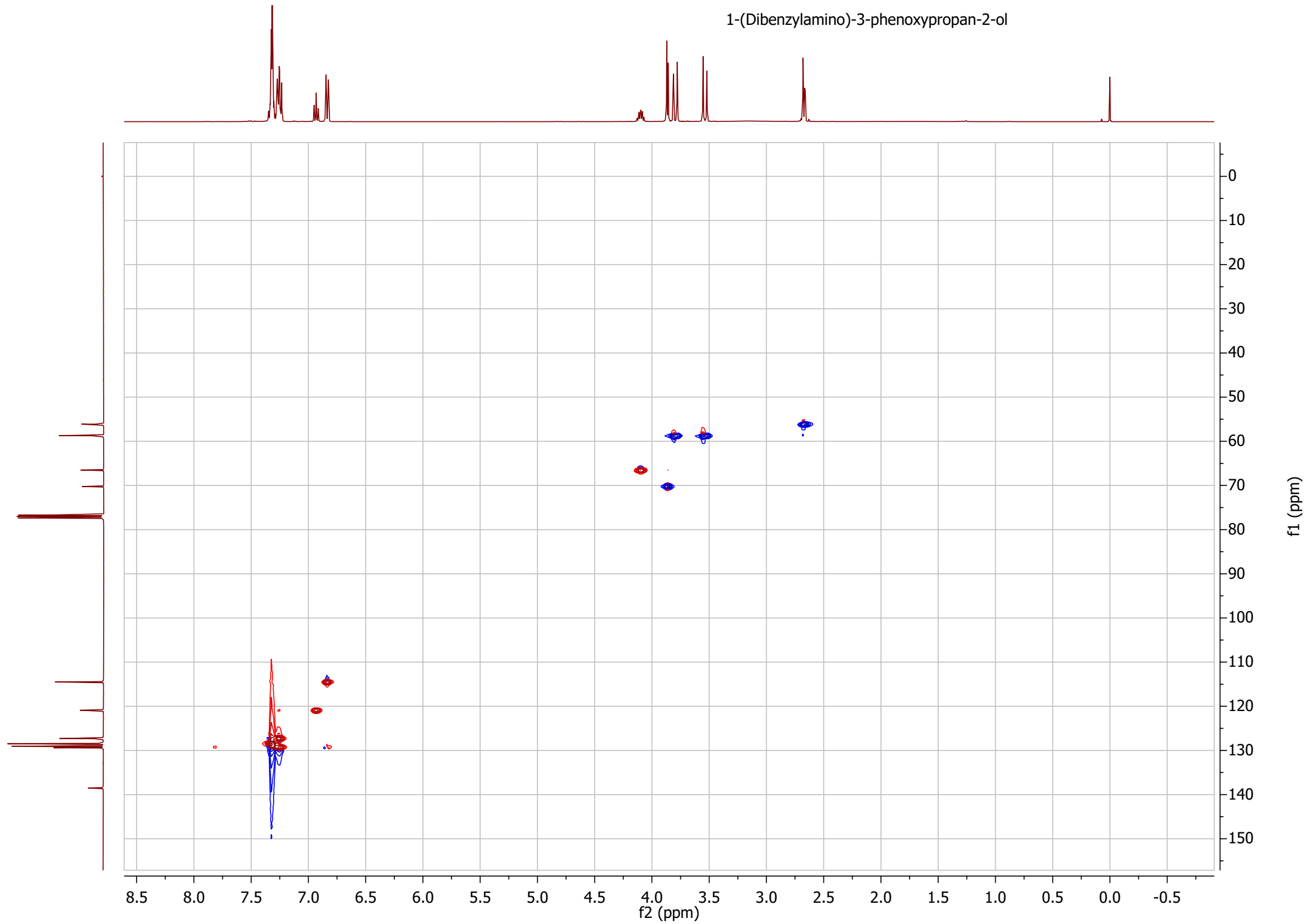
1-(4-Cyclopentylphenoxy)-3-(dibenzylamino)propan-2-ol



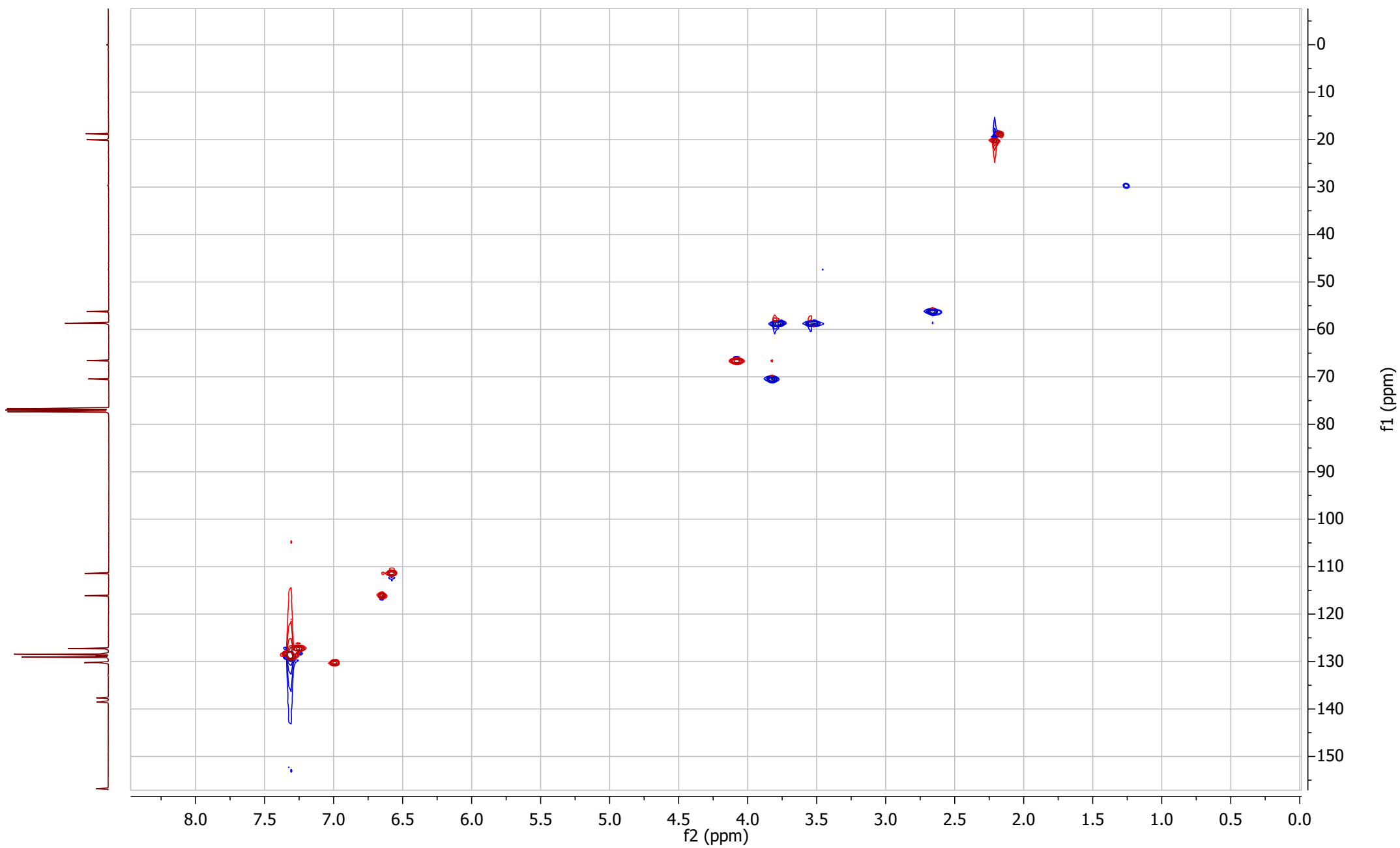
1-(Dibenzylamino)-3-(4-isopropylphenoxy)propan-2-ol



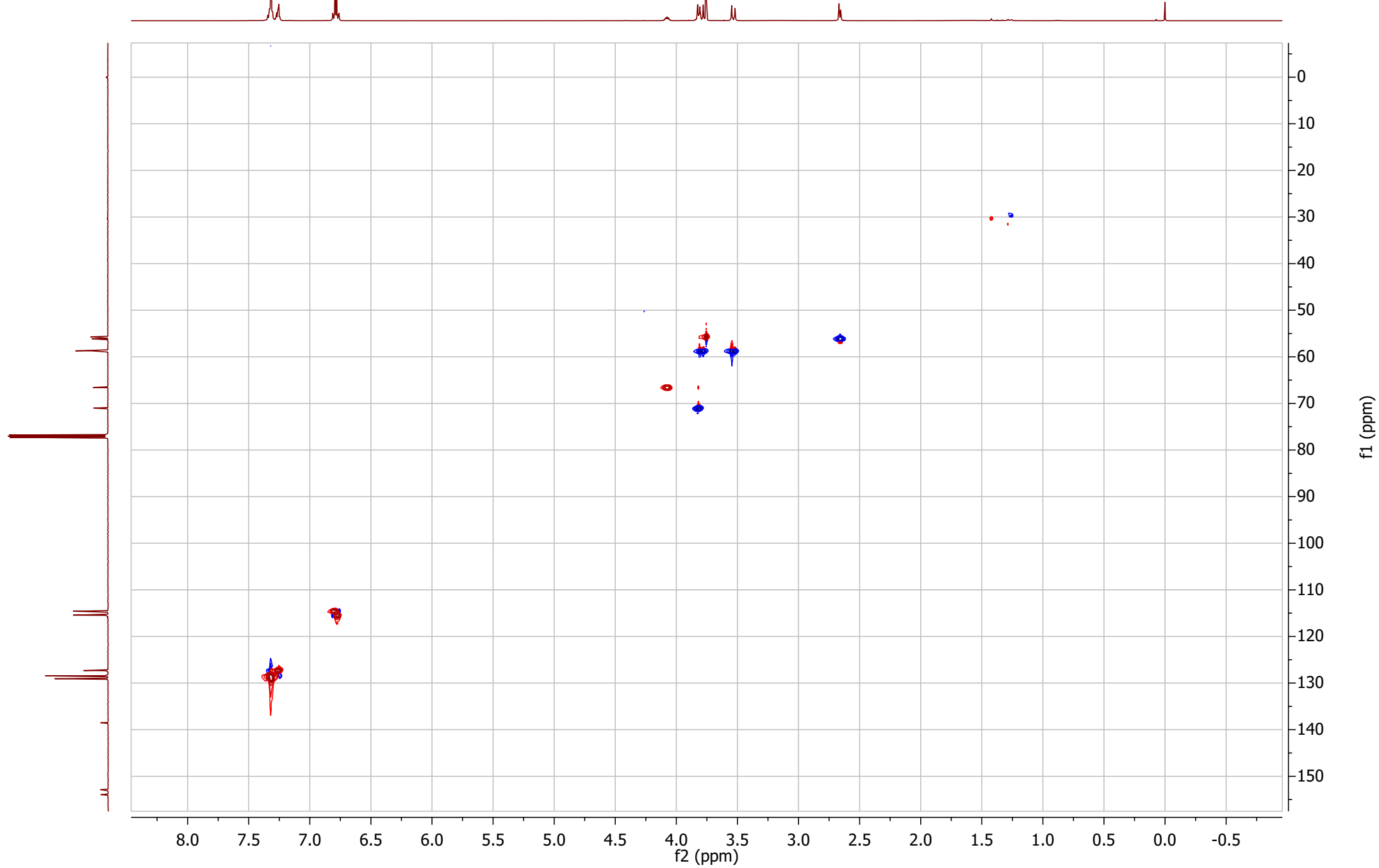
1-(Dibenzylamino)-3-phenoxypropan-2-ol



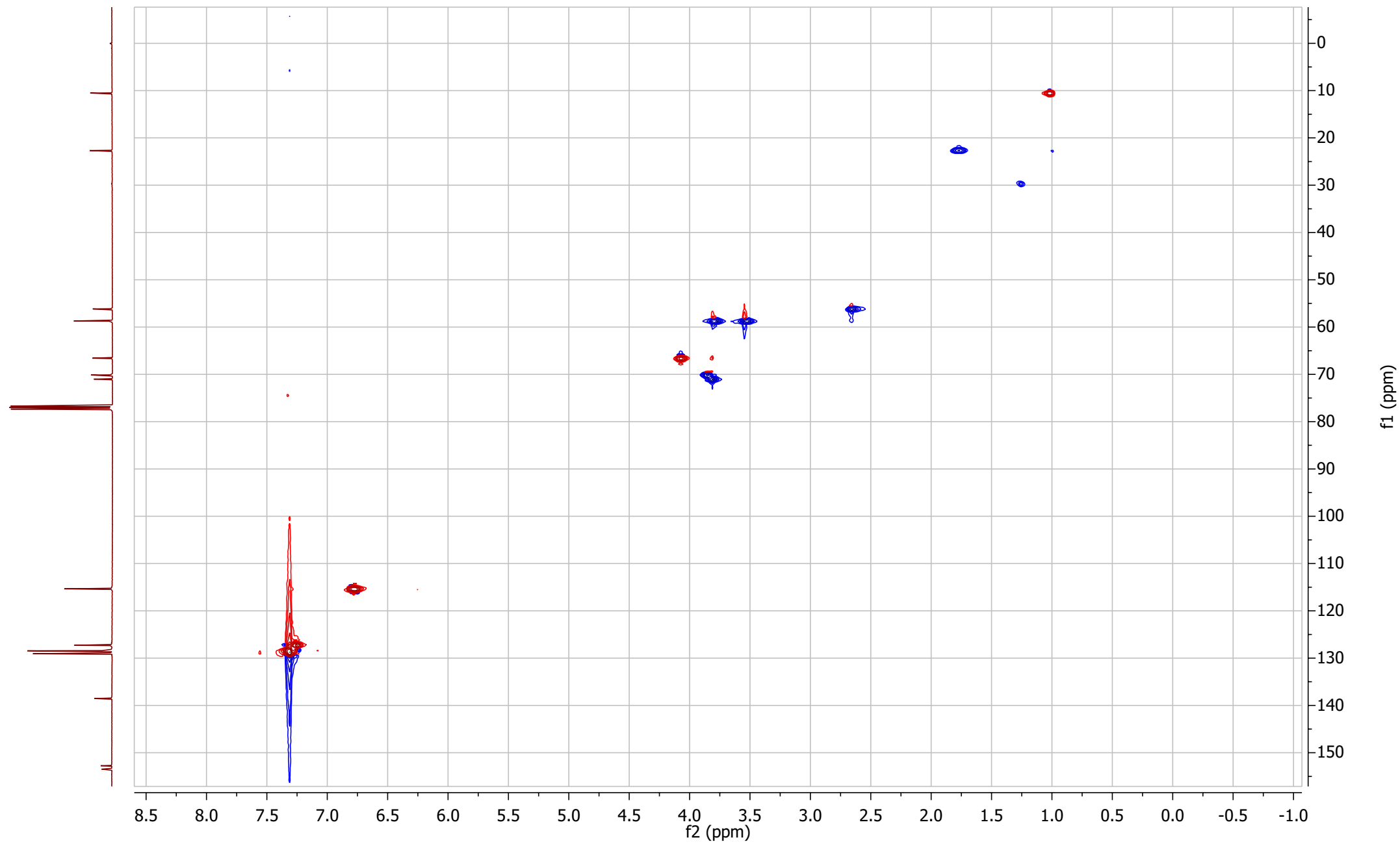
1-(Dibenzylamino)-3-(3,4-dimethylphenoxy)propan-2-ol



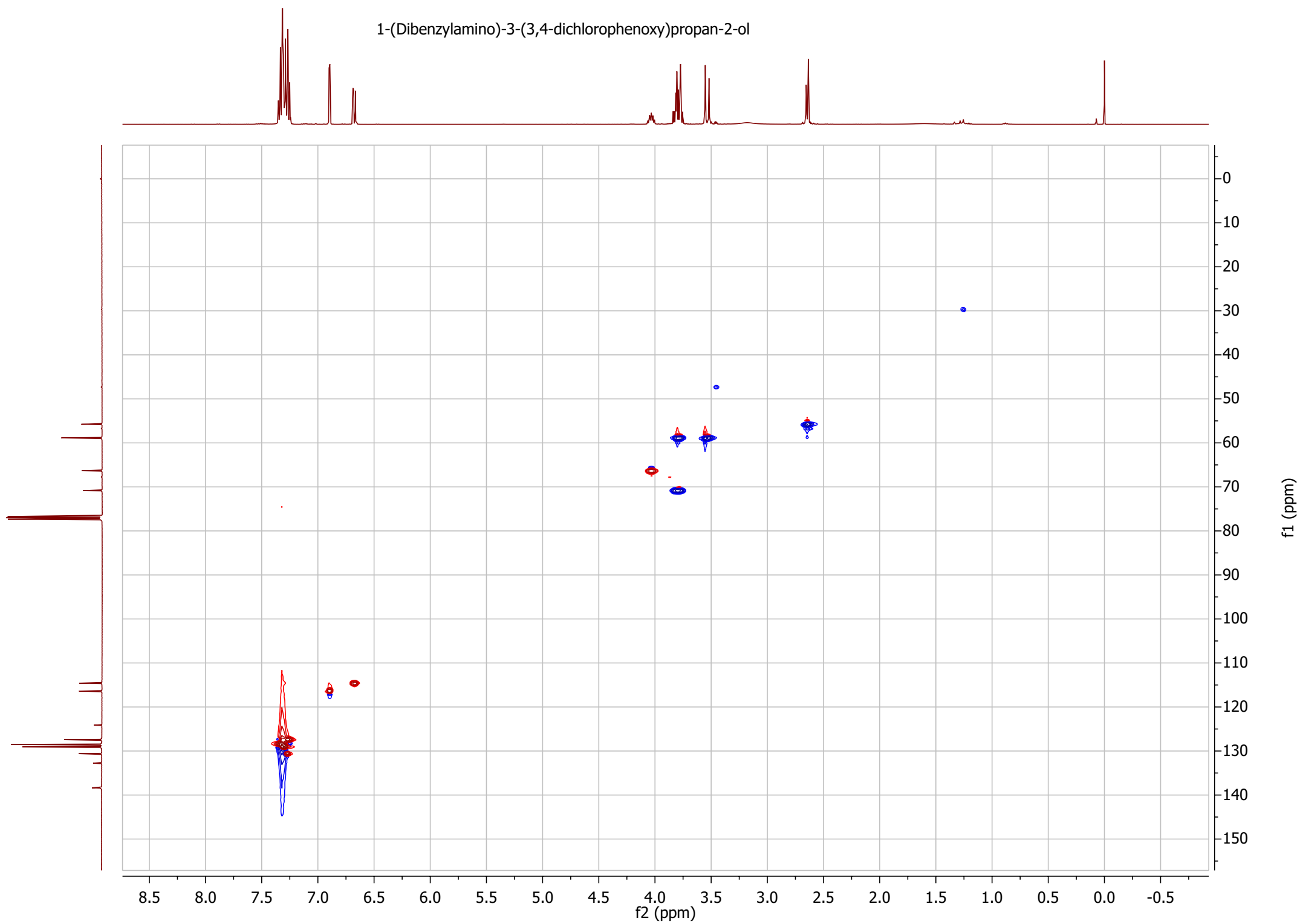
1-(Dibenzylamino)-3-(4-methoxyphenoxy)propan-2-ol



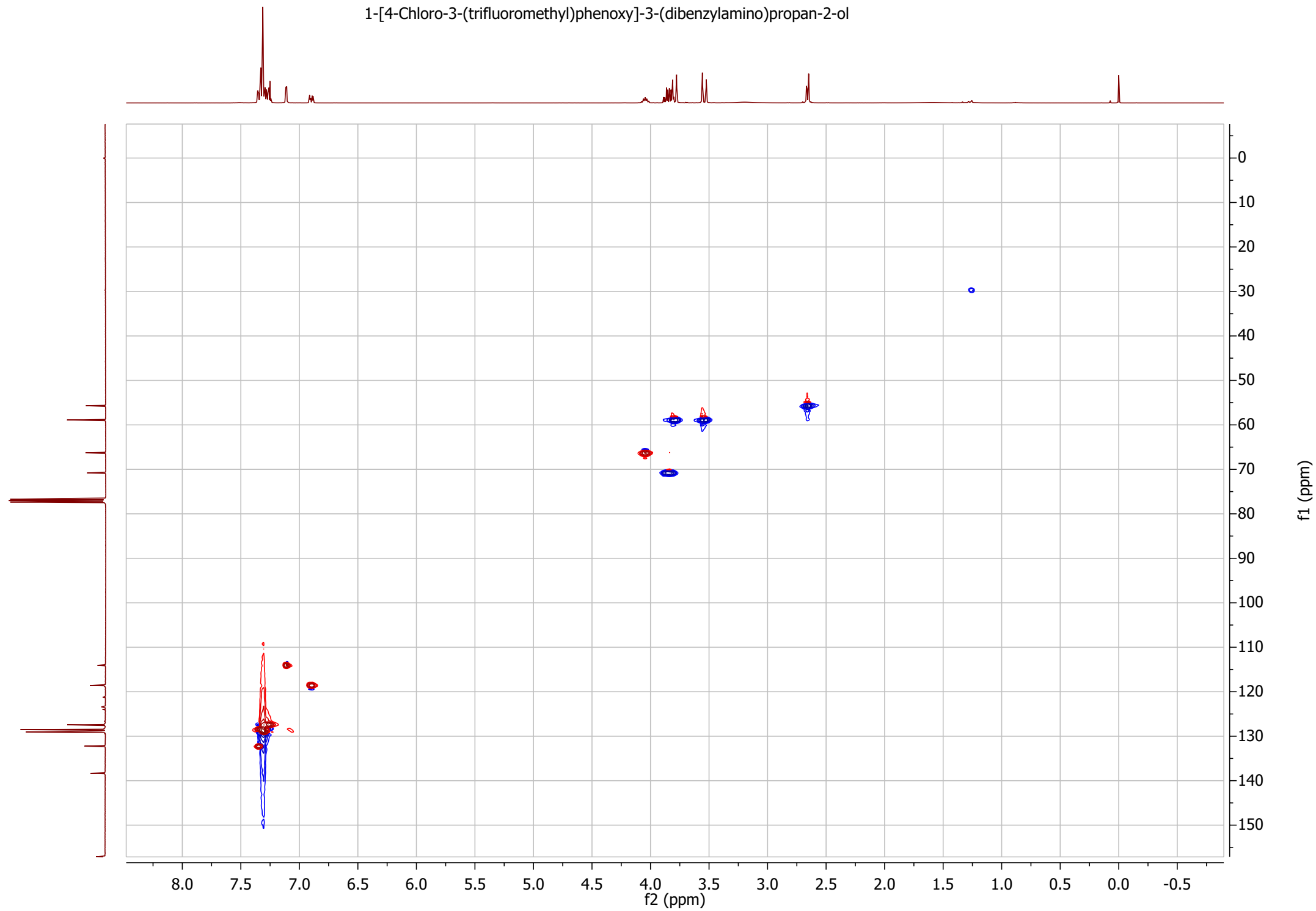
1-(Dibenzylamino)-3-(4-propoxyphenoxy)propan-2-ol



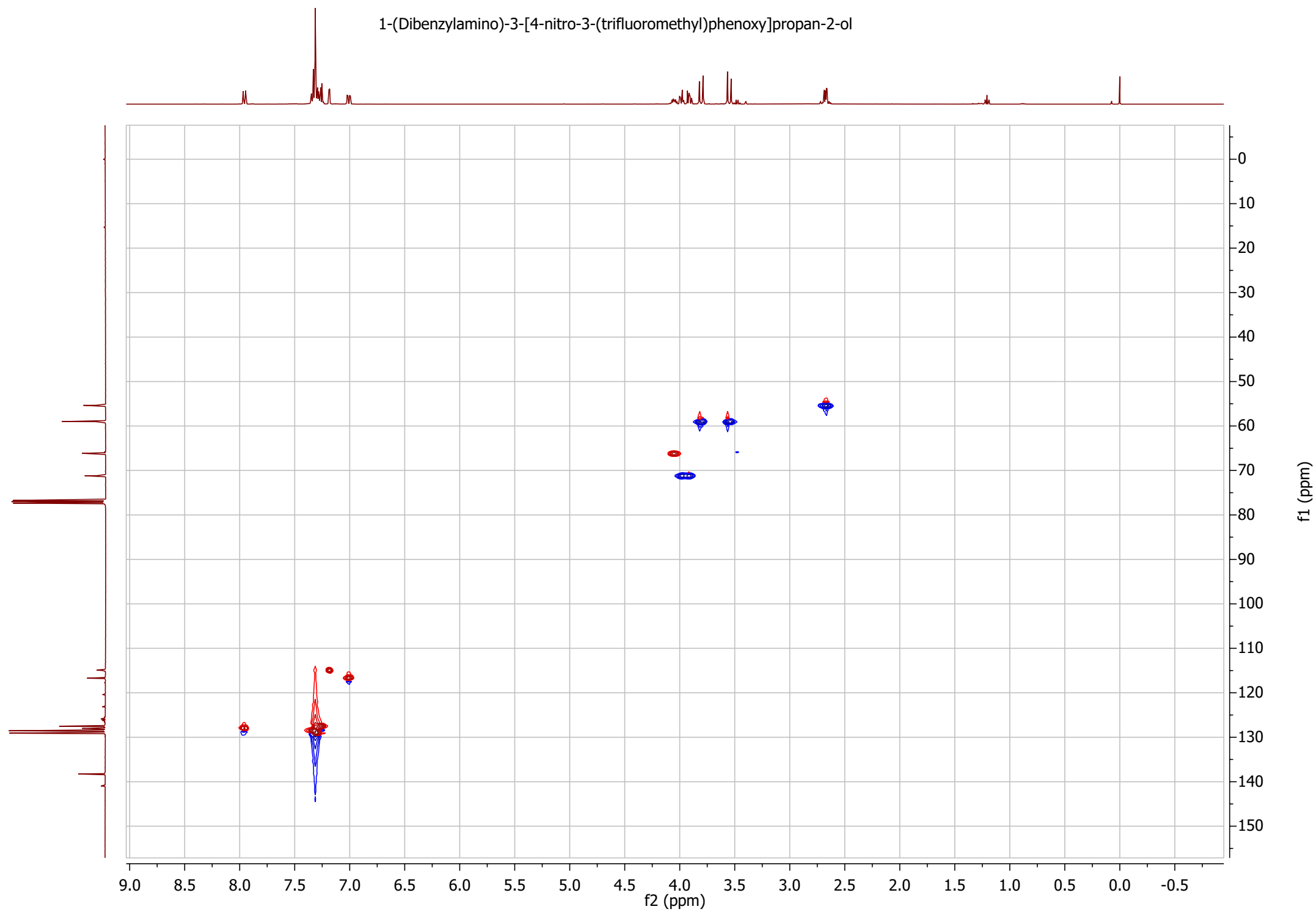
1-(Dibenzylamino)-3-(3,4-dichlorophenoxy)propan-2-ol



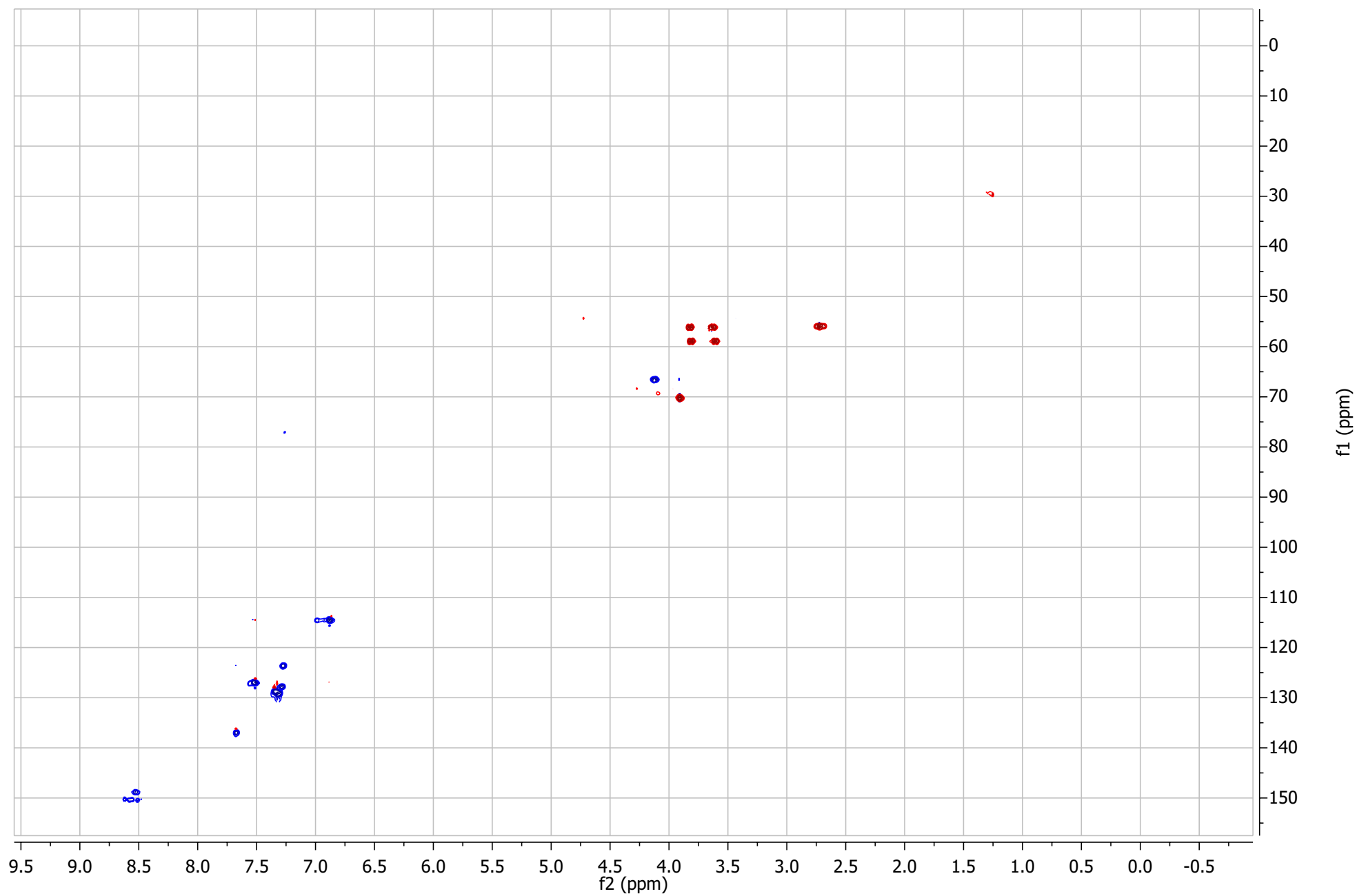
1-[4-Chloro-3-(trifluoromethyl)phenoxy]-3-(dibenzylamino)propan-2-ol



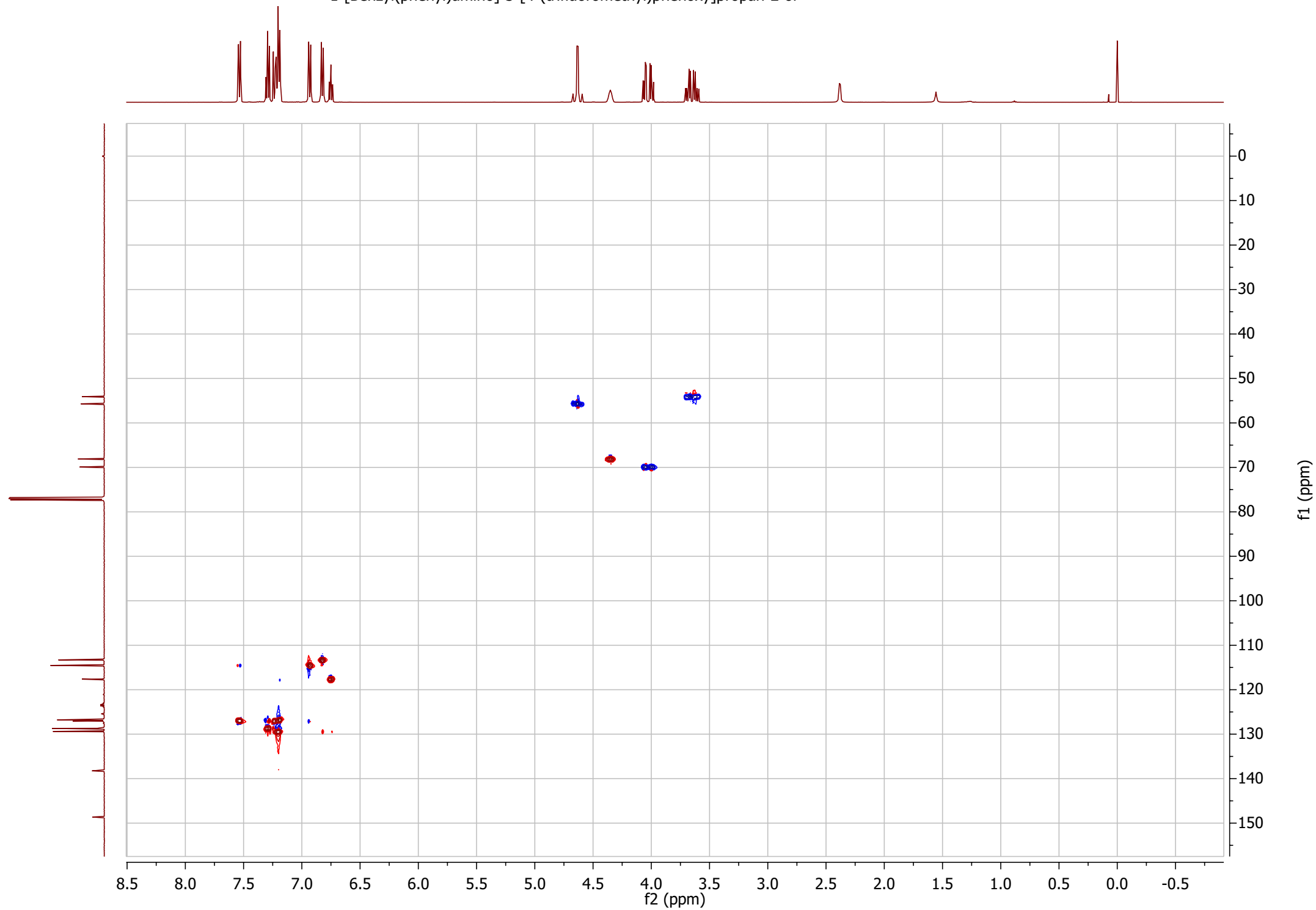
1-(Dibenzylamino)-3-[4-nitro-3-(trifluoromethyl)phenoxy]propan-2-ol



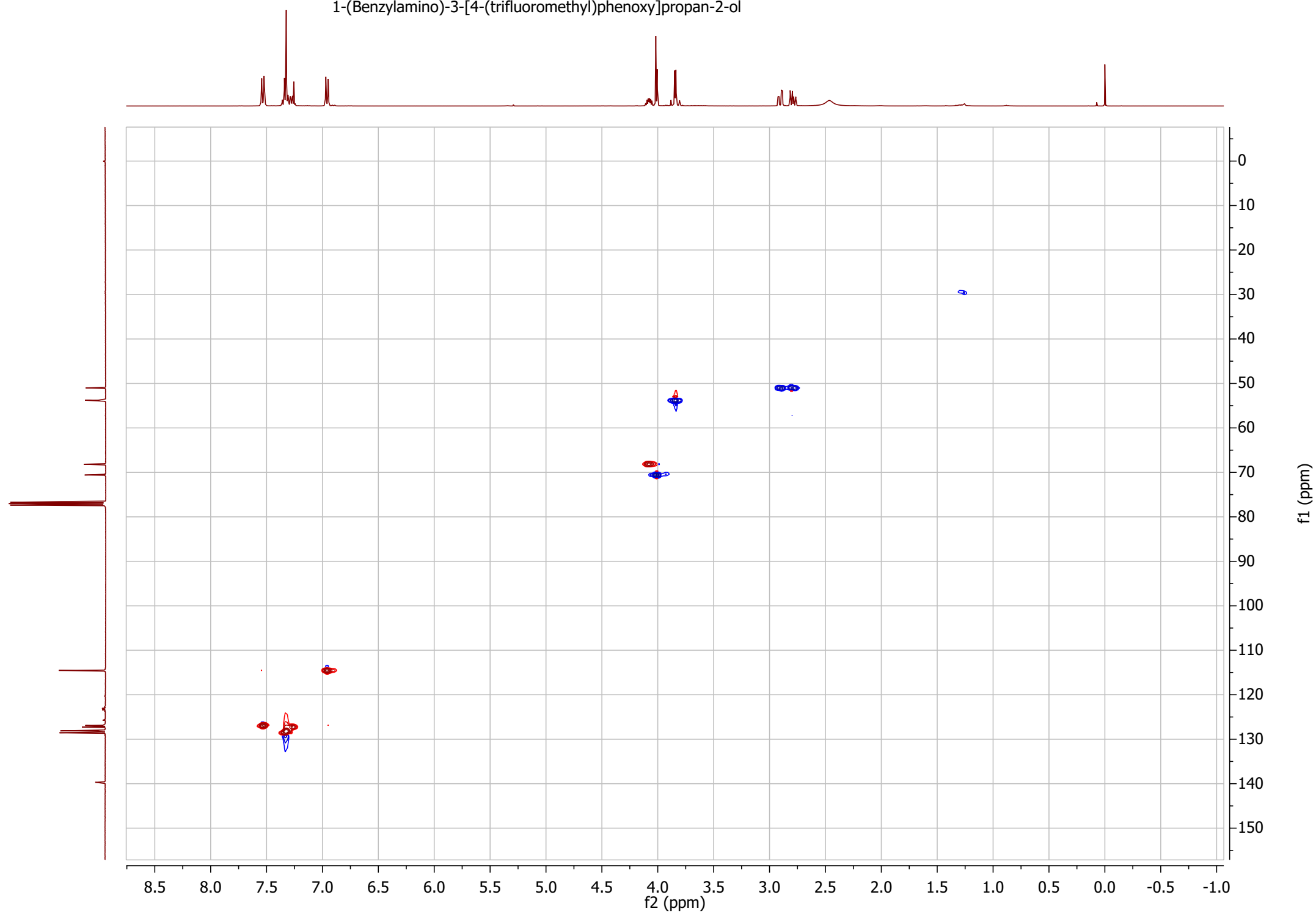
1-[Benzyl(pyridin-3-ylmethyl)amino]-3-[4-(trifluoromethyl)phenoxy]propan-2-ol



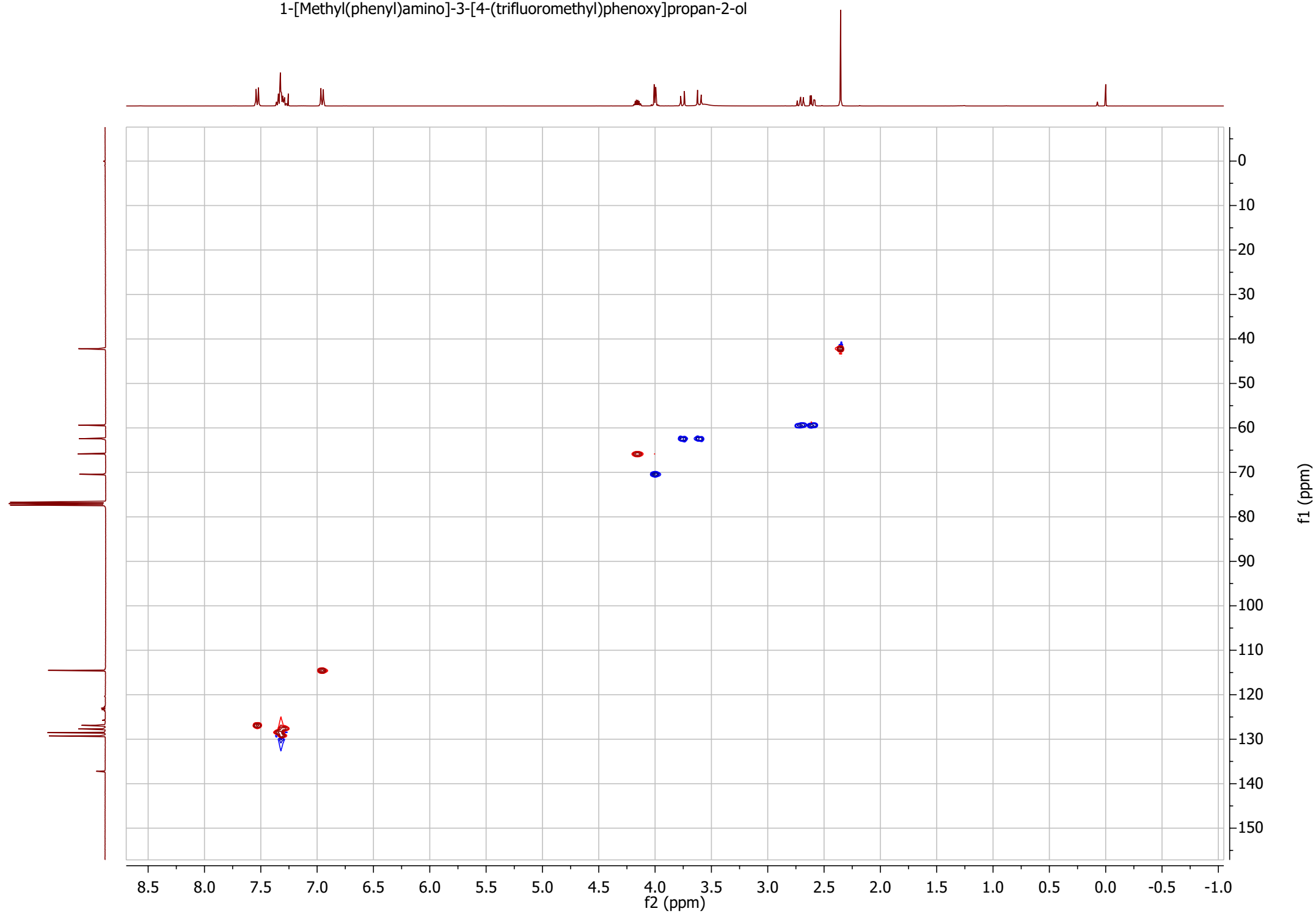
1-[Benzyl(phenyl)amino]-3-[4-(trifluoromethyl)phenoxy]propan-2-ol



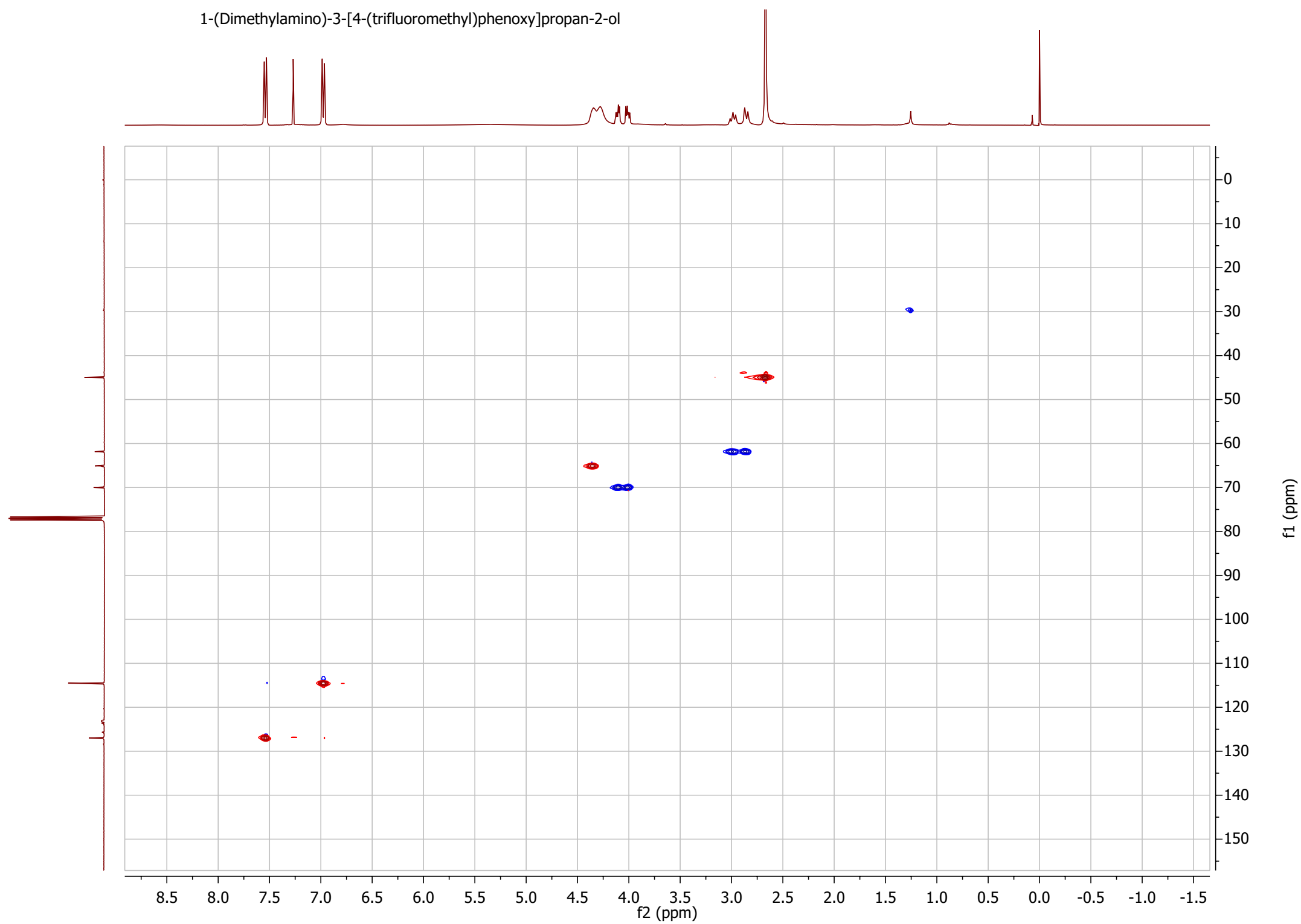
1-(Benzylamino)-3-[4-(trifluoromethyl)phenoxy]propan-2-ol



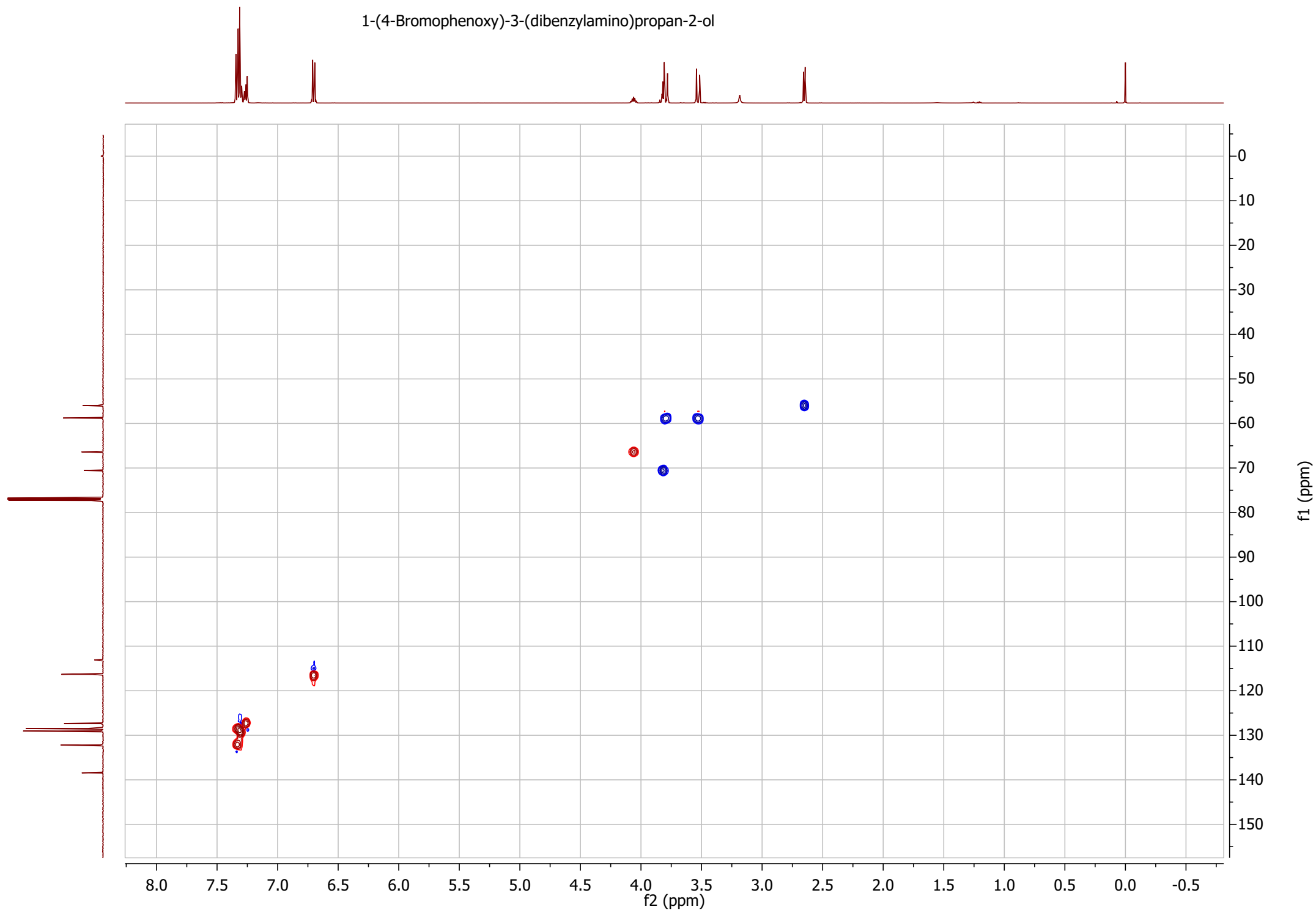
1-[Methyl(phenyl)amino]-3-[4-(trifluoromethyl)phenoxy]propan-2-ol



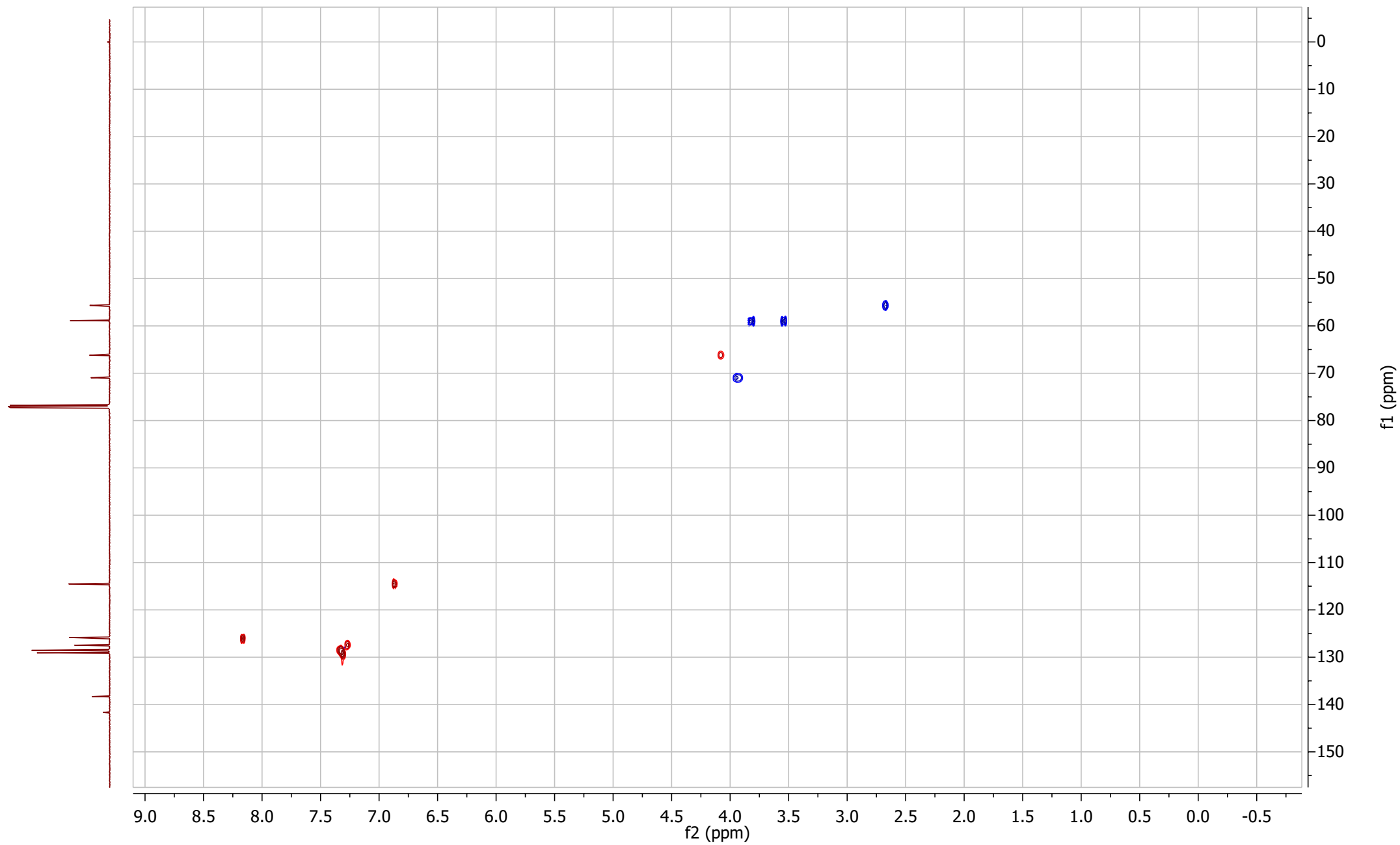
1-(Dimethylamino)-3-[4-(trifluoromethyl)phenoxy]propan-2-ol



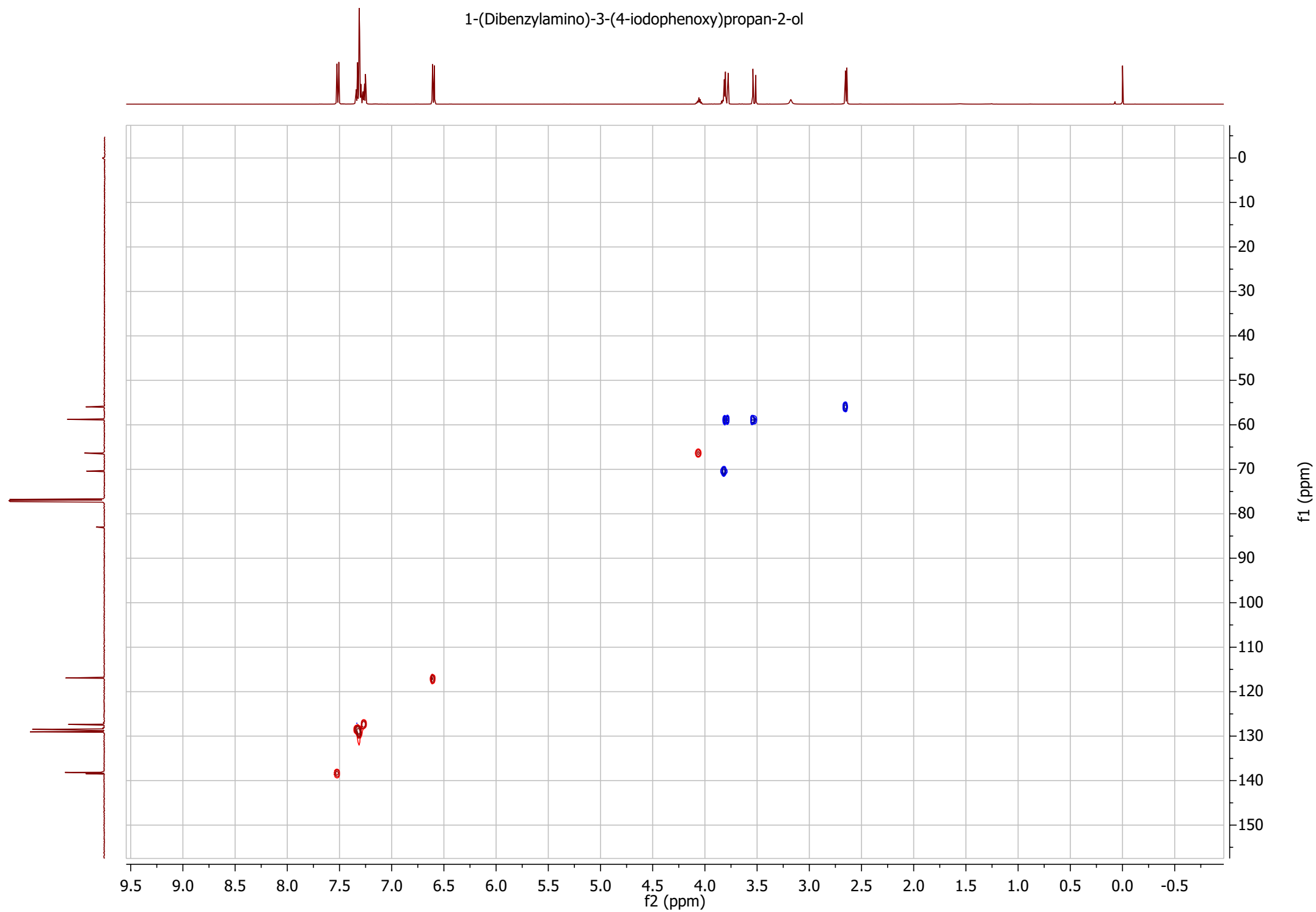
1-(4-Bromophenoxy)-3-(dibenzylamino)propan-2-ol



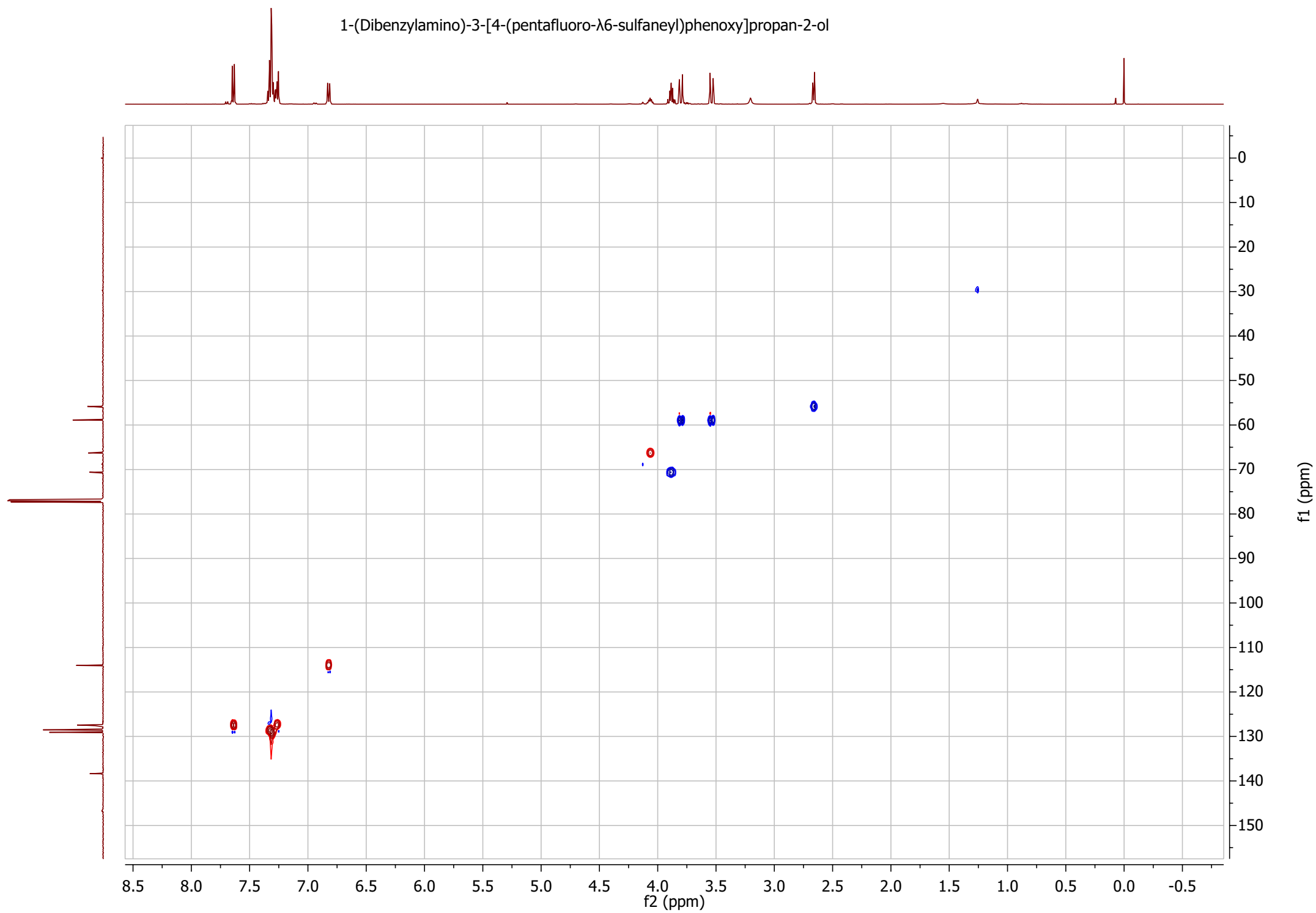
1-(Dibenzylamino)-3-(4-nitrophenoxy)propan-2-ol



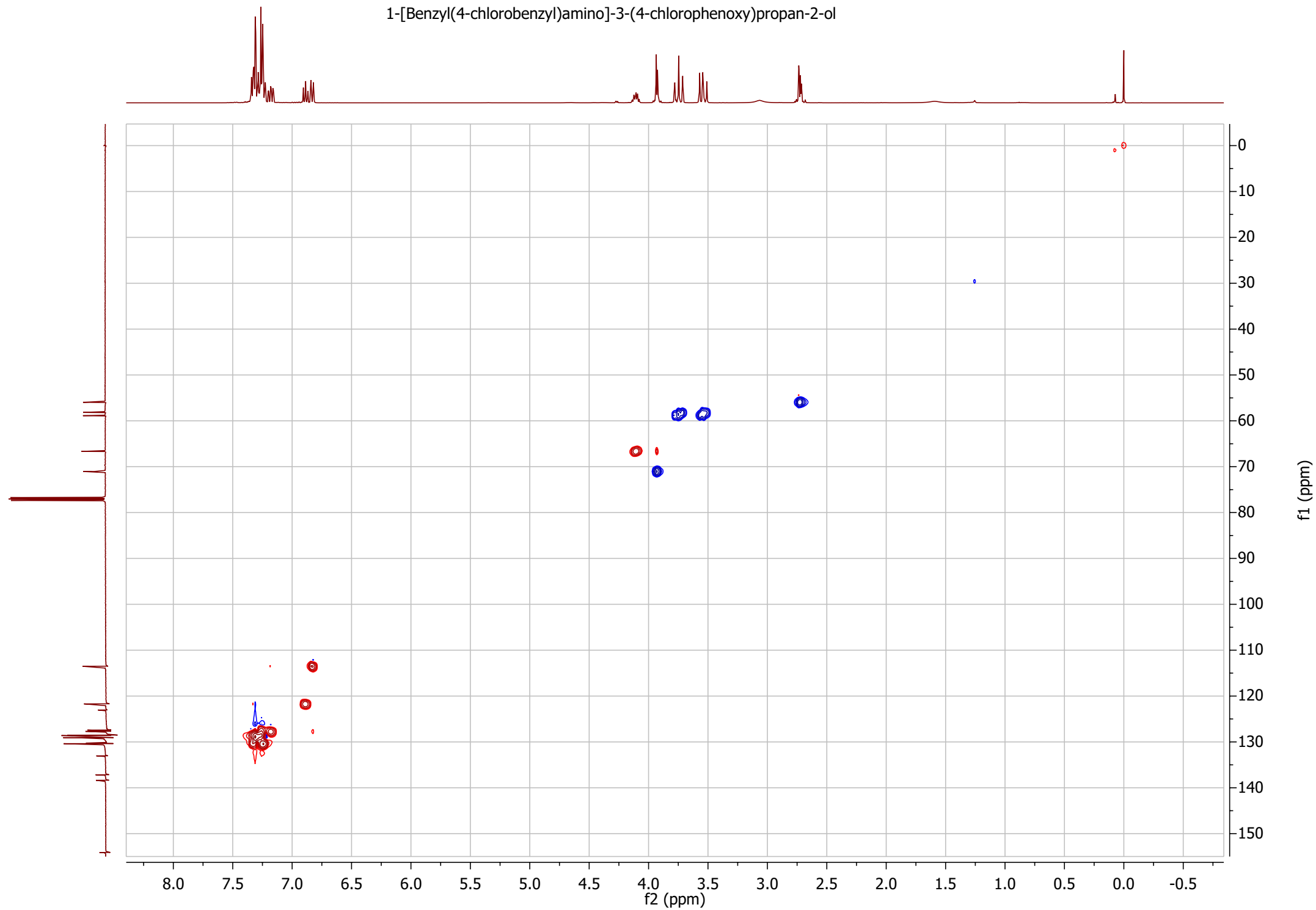
1-(Dibenzylamino)-3-(4-iodophenoxy)propan-2-ol



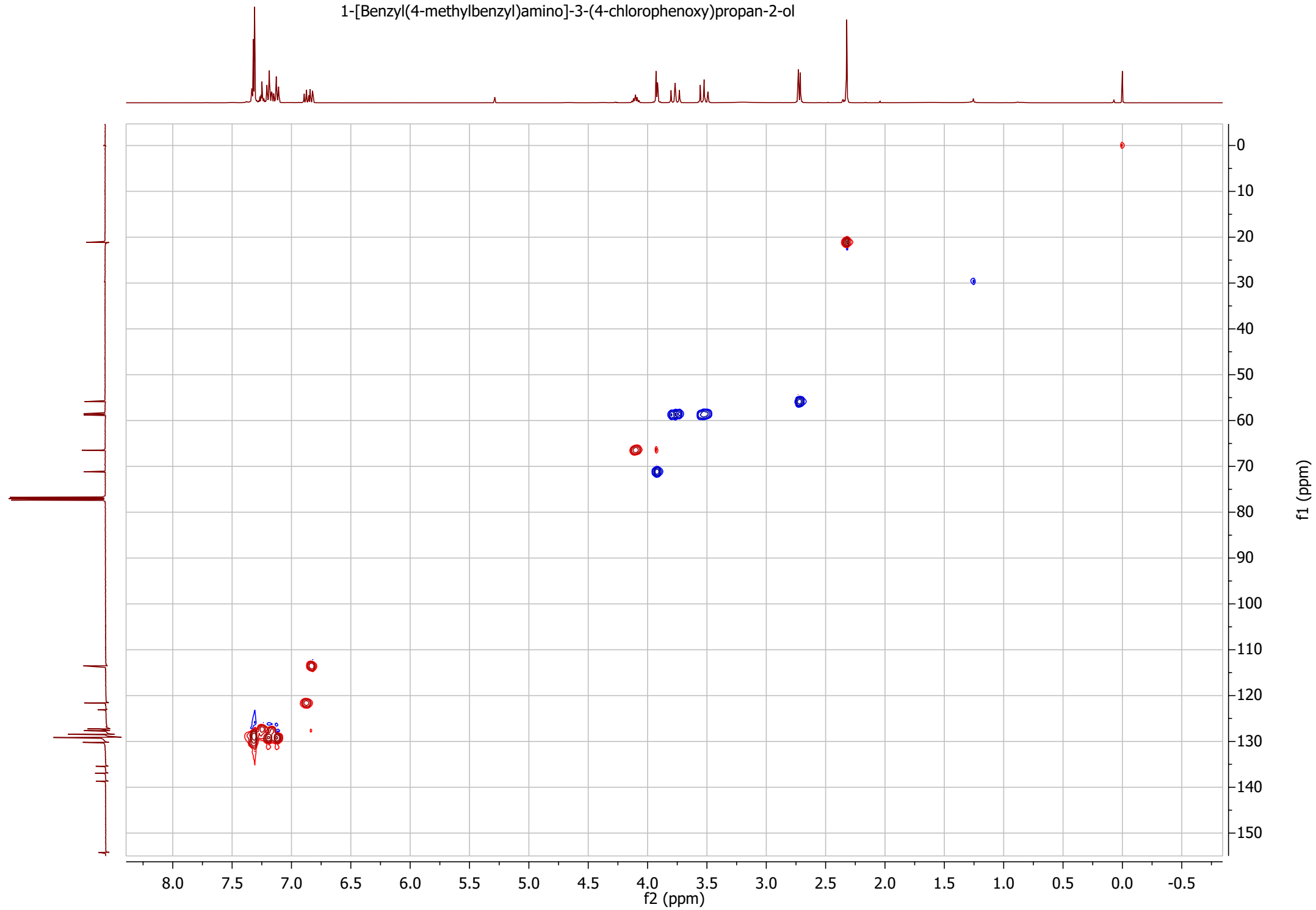
1-(Dibenzylamino)-3-[4-(pentafluoro-λ6-sulfaneyl)phenoxy]propan-2-ol



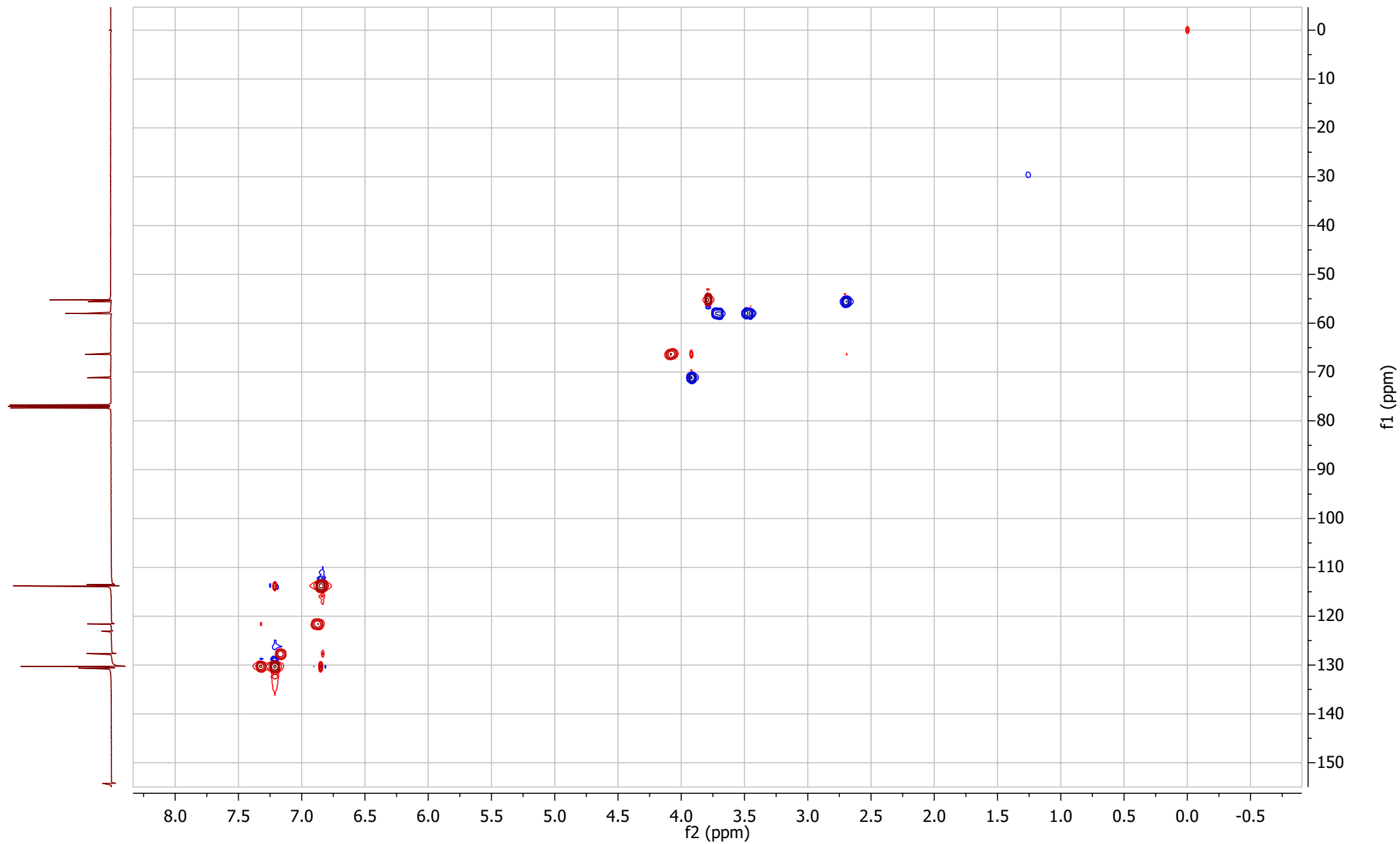
1-[Benzyl(4-chlorobenzyl)amino]-3-(4-chlorophenoxy)propan-2-ol



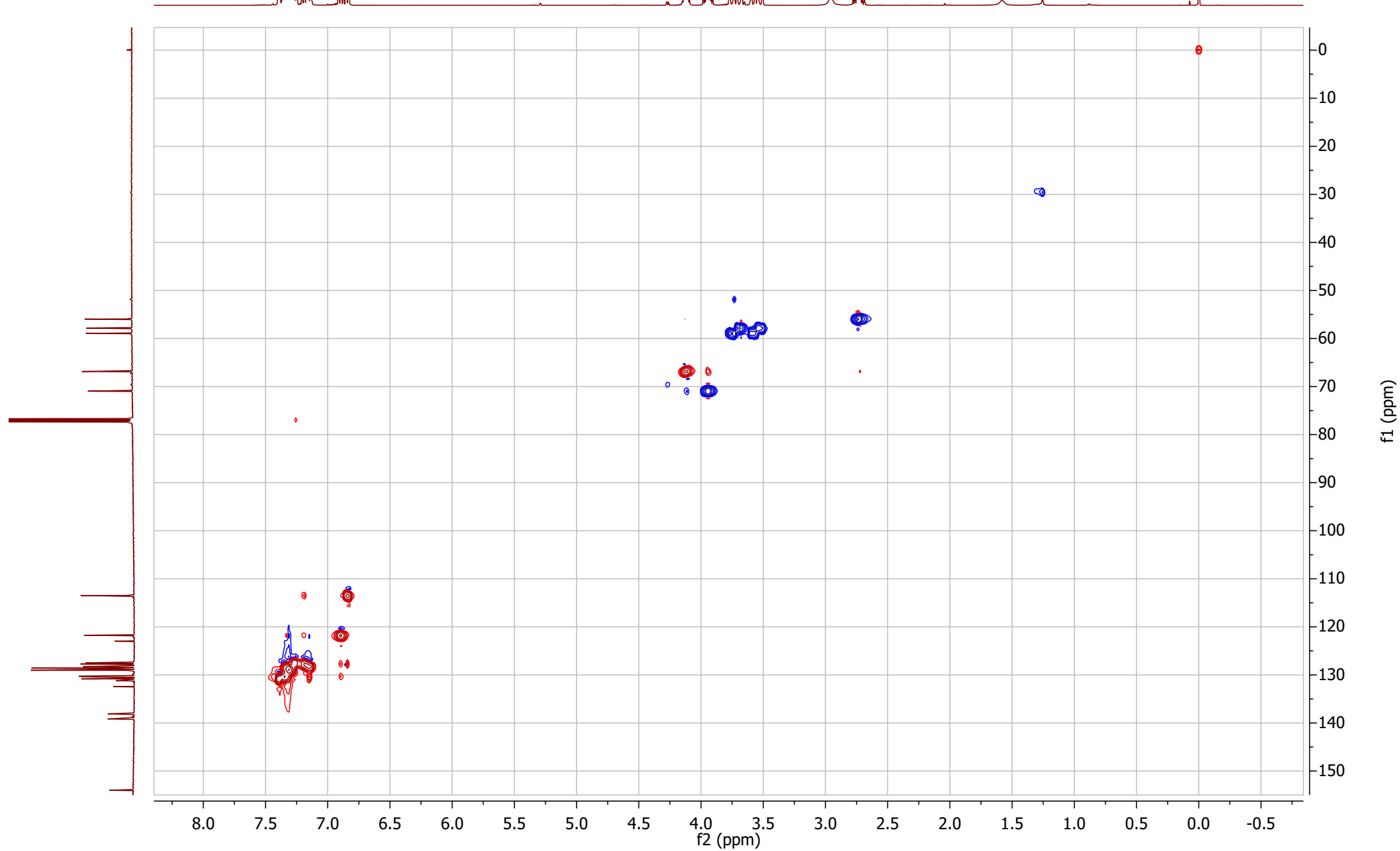
1-[Benzyl(4-methylbenzyl)amino]-3-(4-chlorophenoxy)propan-2-ol



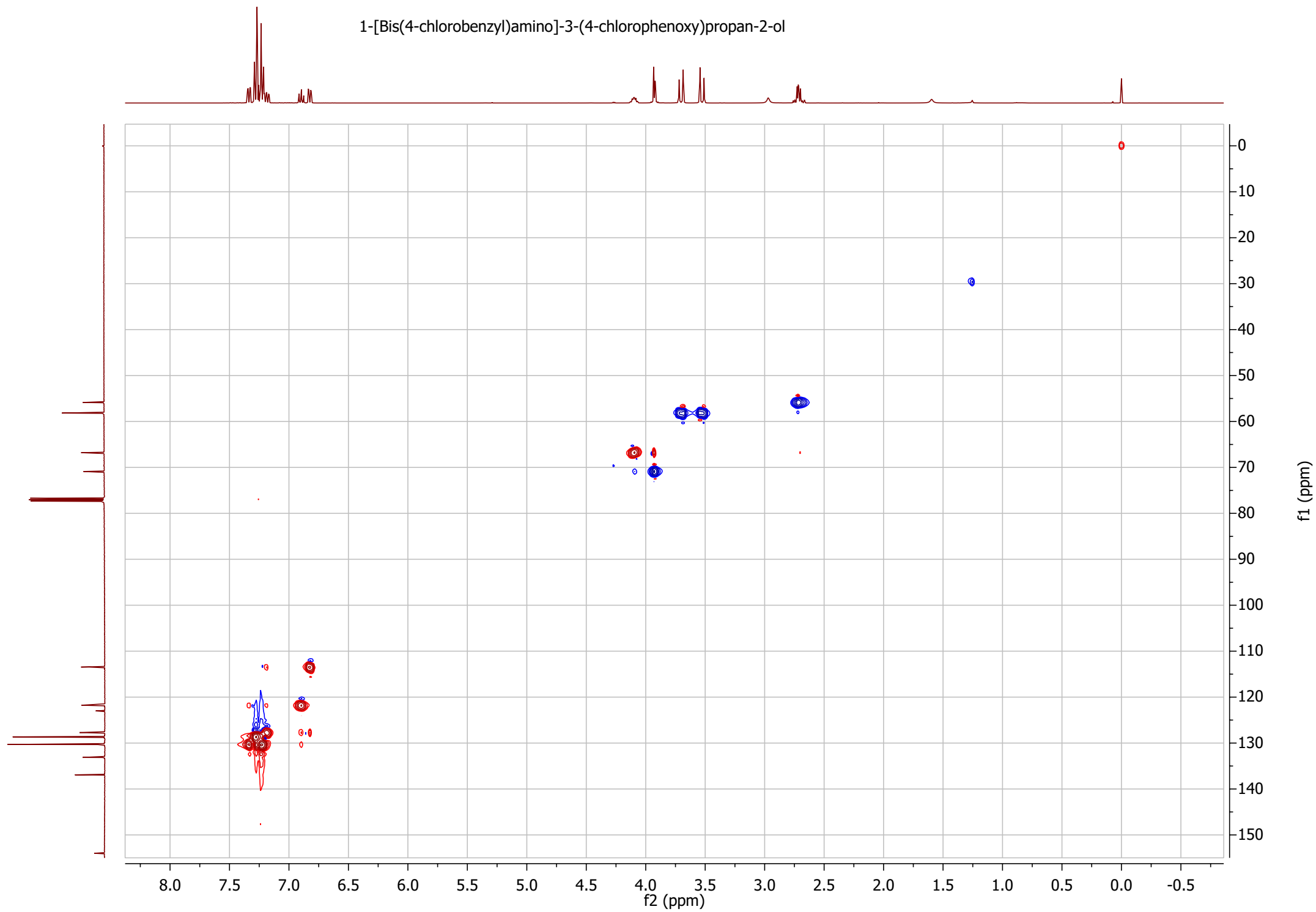
1-[Bis(4-methoxybenzyl)amino]-3-(4-chlorophenoxy)propan-2-ol



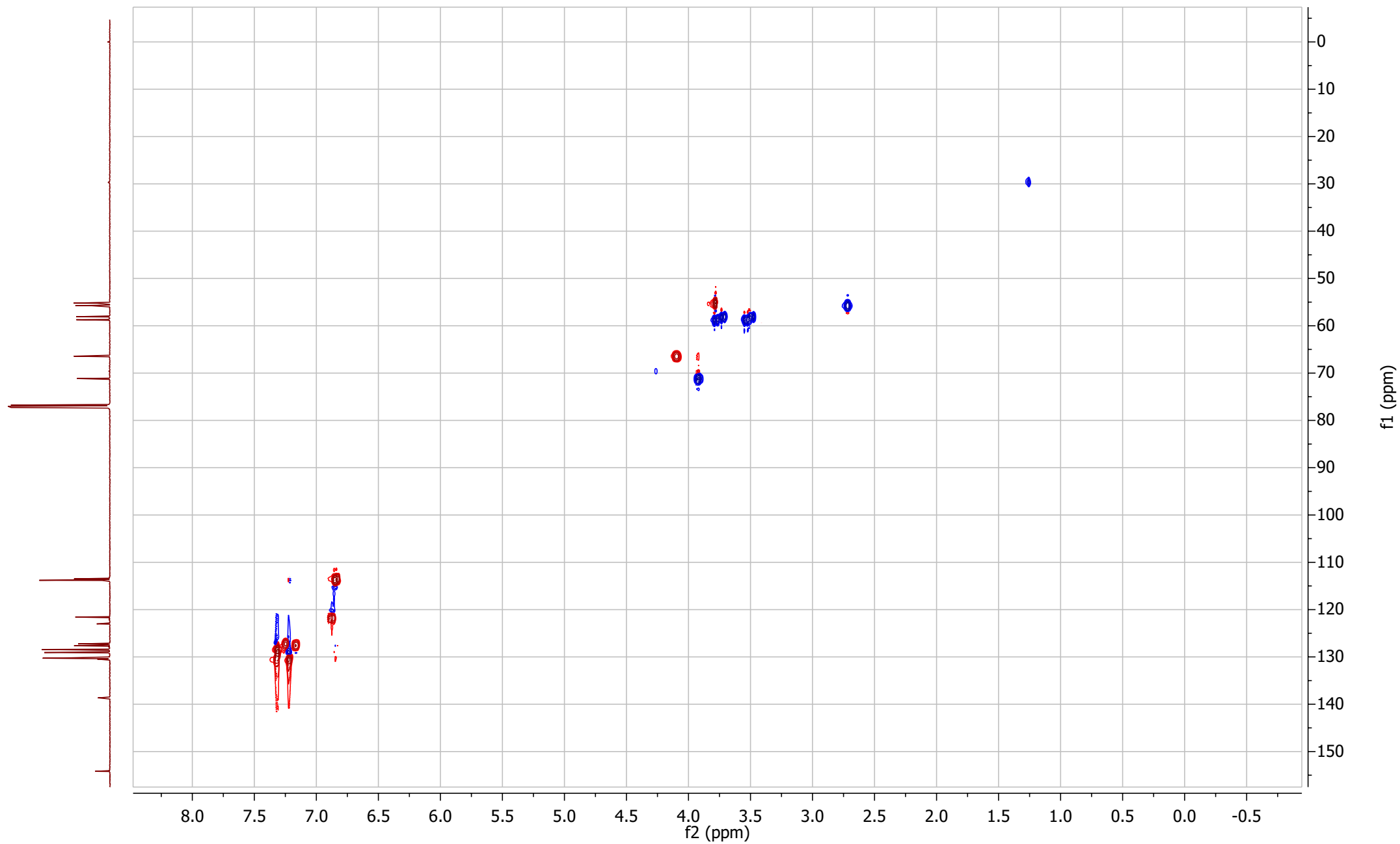
1-[Benzyl(3,4-dichlorobenzyl)amino]-3-(4-chlorophenoxy)propan-2-ol



1-[Bis(4-chlorobenzyl)amino]-3-(4-chlorophenoxy)propan-2-ol



1-[Benzyl(4-methoxybenzyl)amino]-3-(4-chlorophenoxy)propan-2-ol



1-[(4-Chlorobenzyl)(3,4-dichlorobenzyl)amino]-3-(4-chlorophenoxy)propan-2-ol

