SUPPLEMENTAL MATERIAL TO:

Bioinspired Honokiol Analogs and Their Evaluation for Activity on the Norepinephrine Transporter

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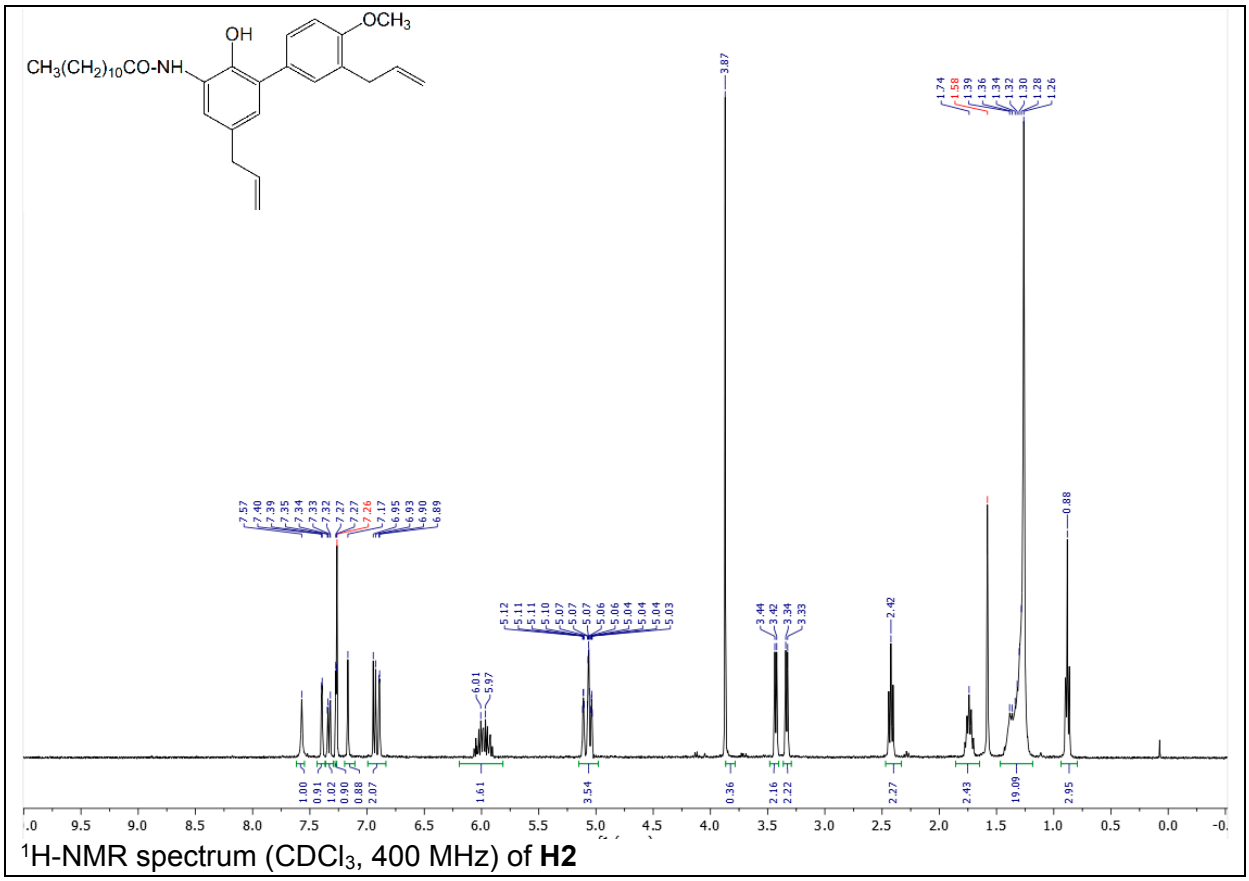
Content of supporting information file:

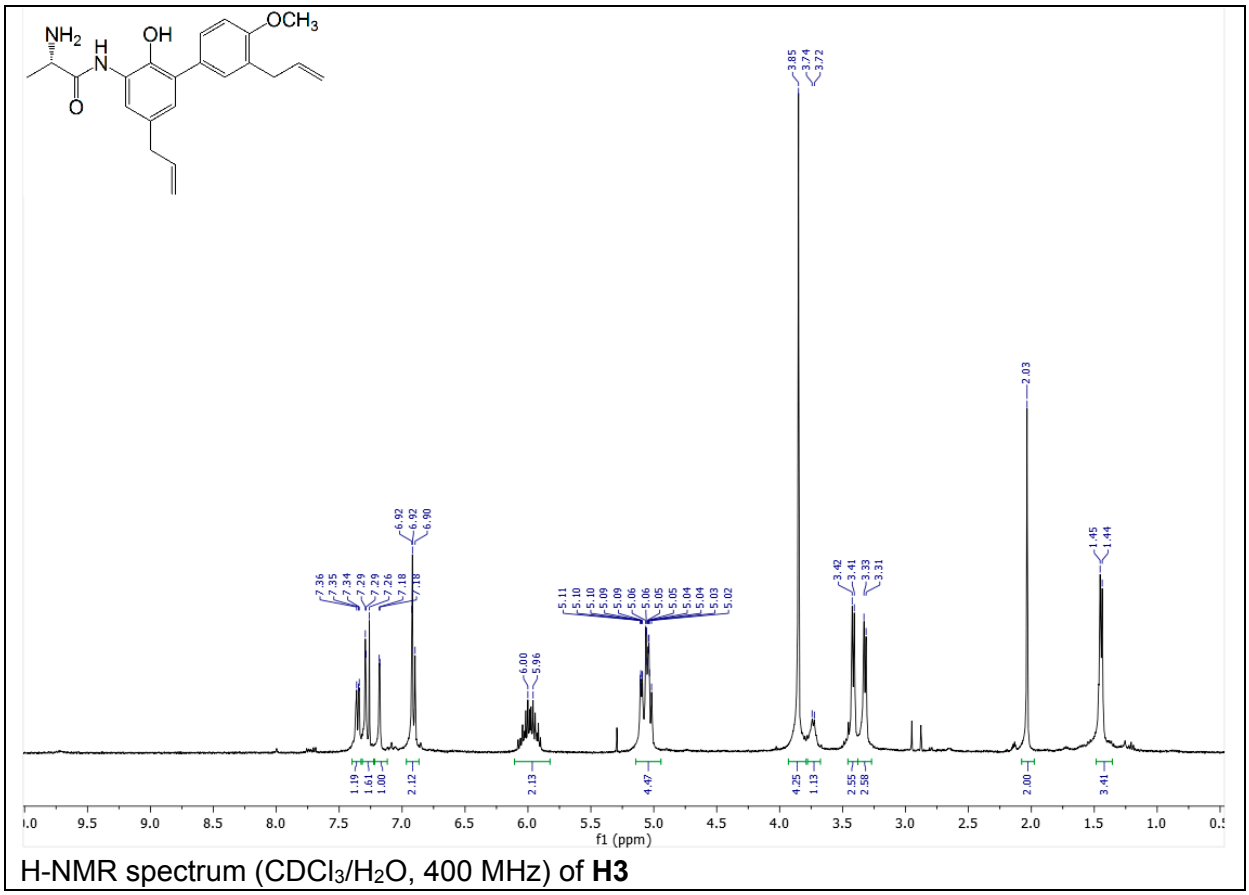
1. ^{1}H-NMR spectra ($CDCl_3$, 400 MHz) of the new compounds (page 3-12)

2. Dose-Response (measured as fluorescence) curves for tested compounds (page 13-23)

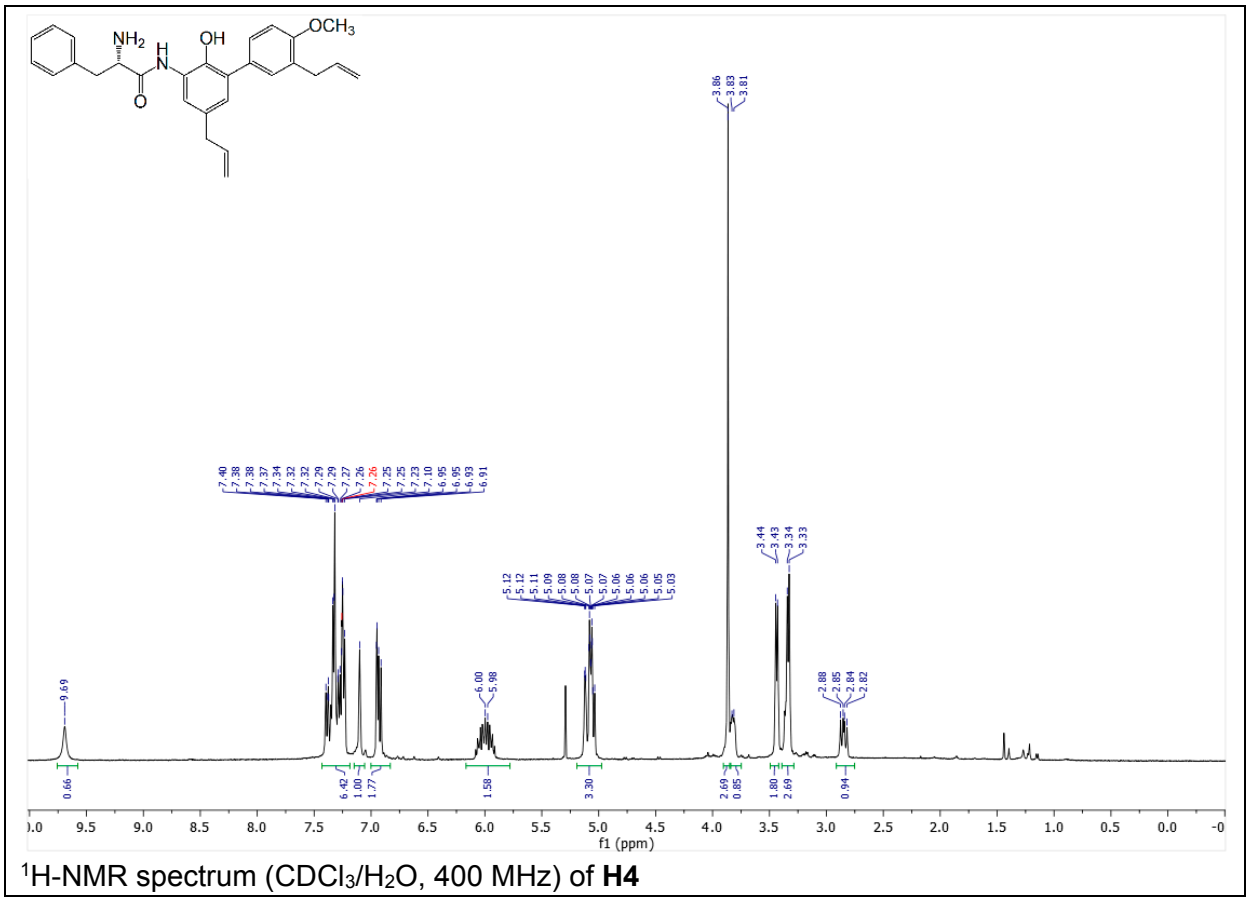
1. ^{1}H-NMR spectra of the new compounds



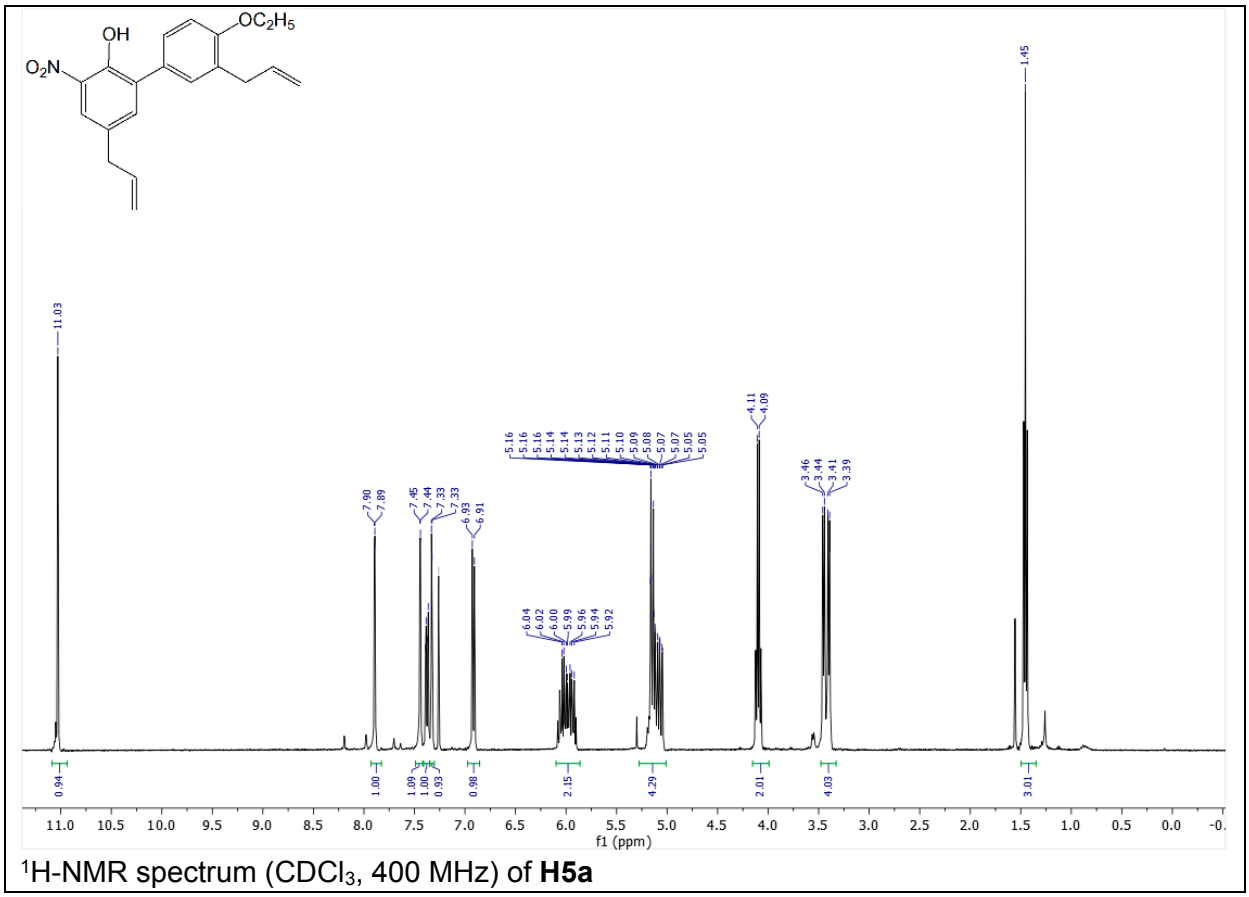
^{1}H-NMR spectrum ($CDCl_3$, 400 MHz) of **H2**



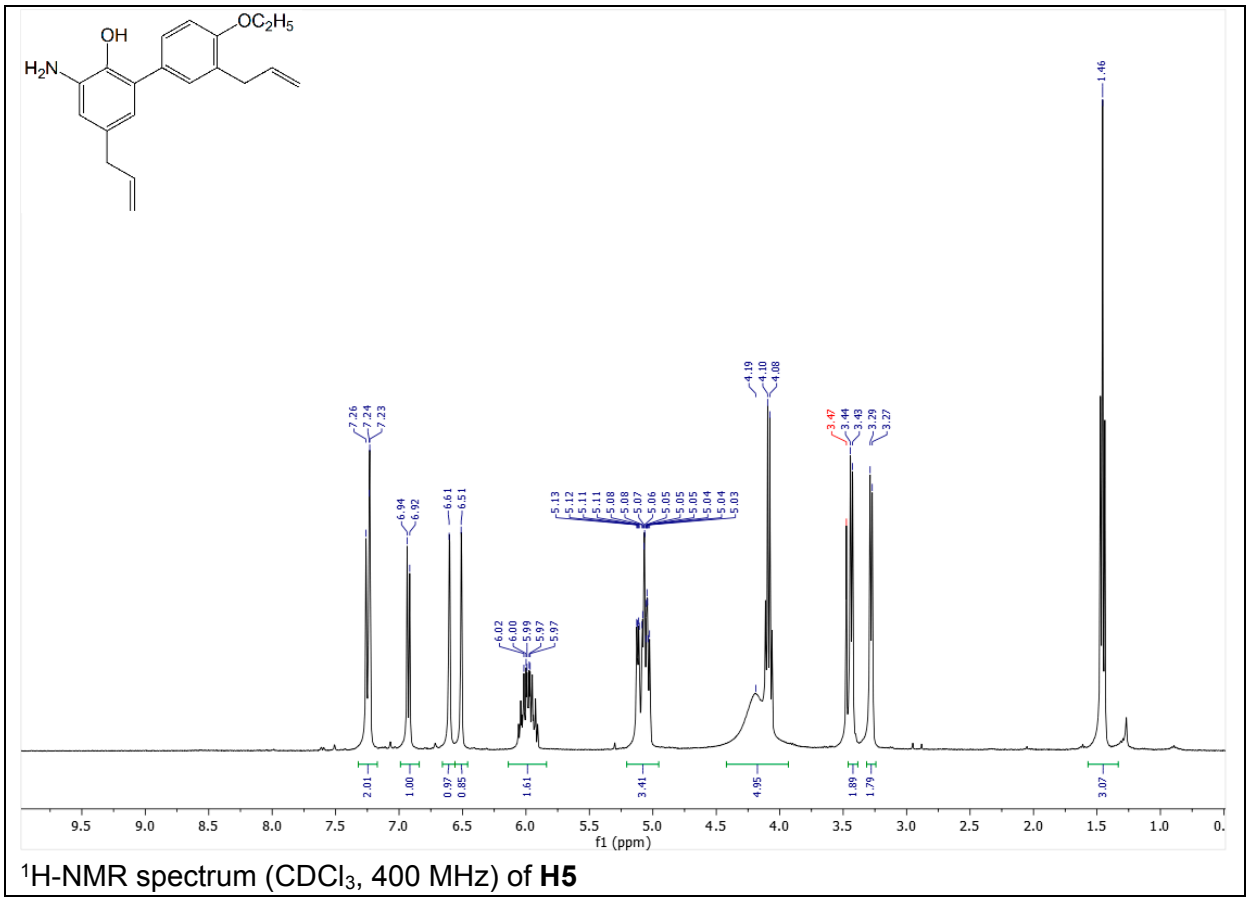
H-NMR spectrum ($CDCl_3/H_2O$, 400 MHz) of **H3**



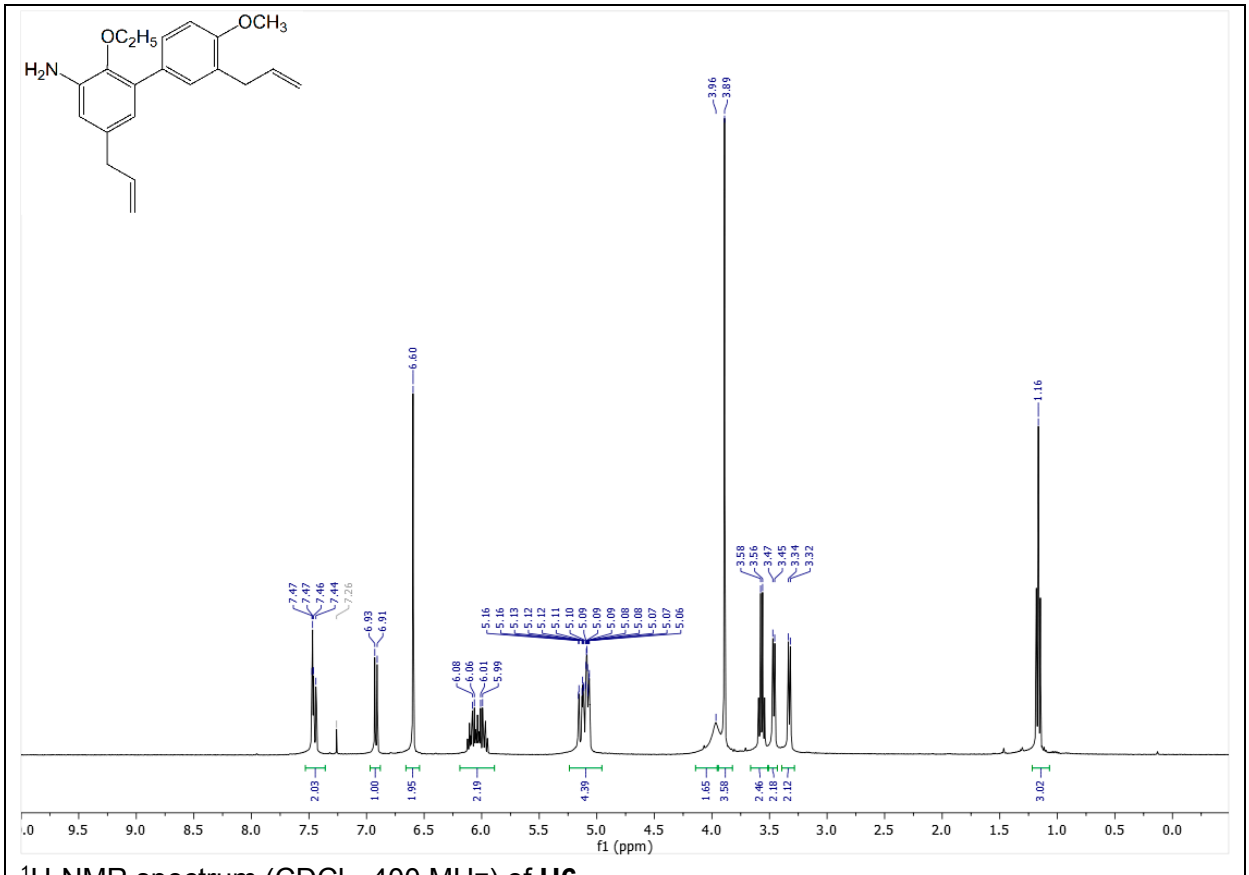
^{1}H-NMR spectrum ($CDCl_3/H_2O$, 400 MHz) of **H4**



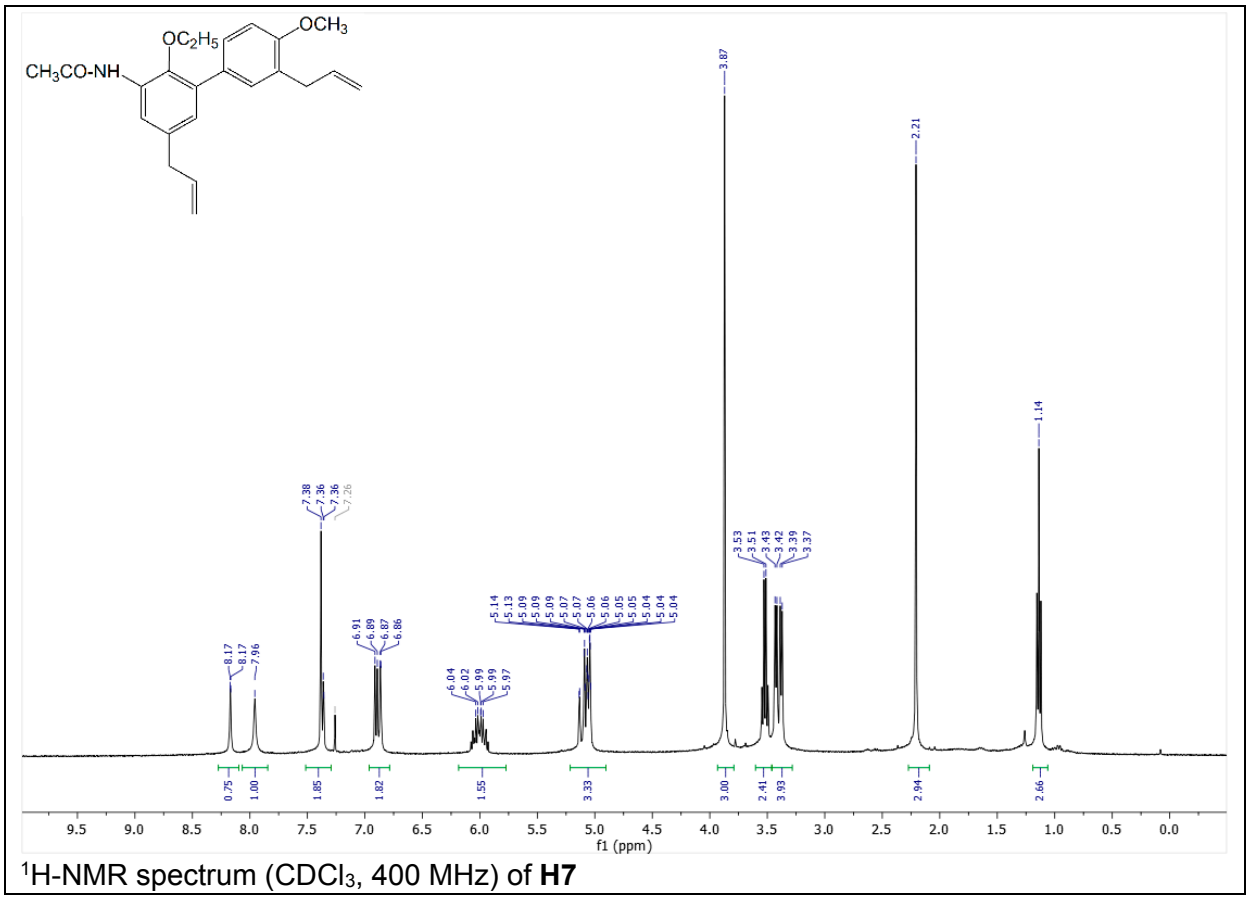
^{1}H-NMR spectrum ($CDCl_3$, 400 MHz) of **H5a**



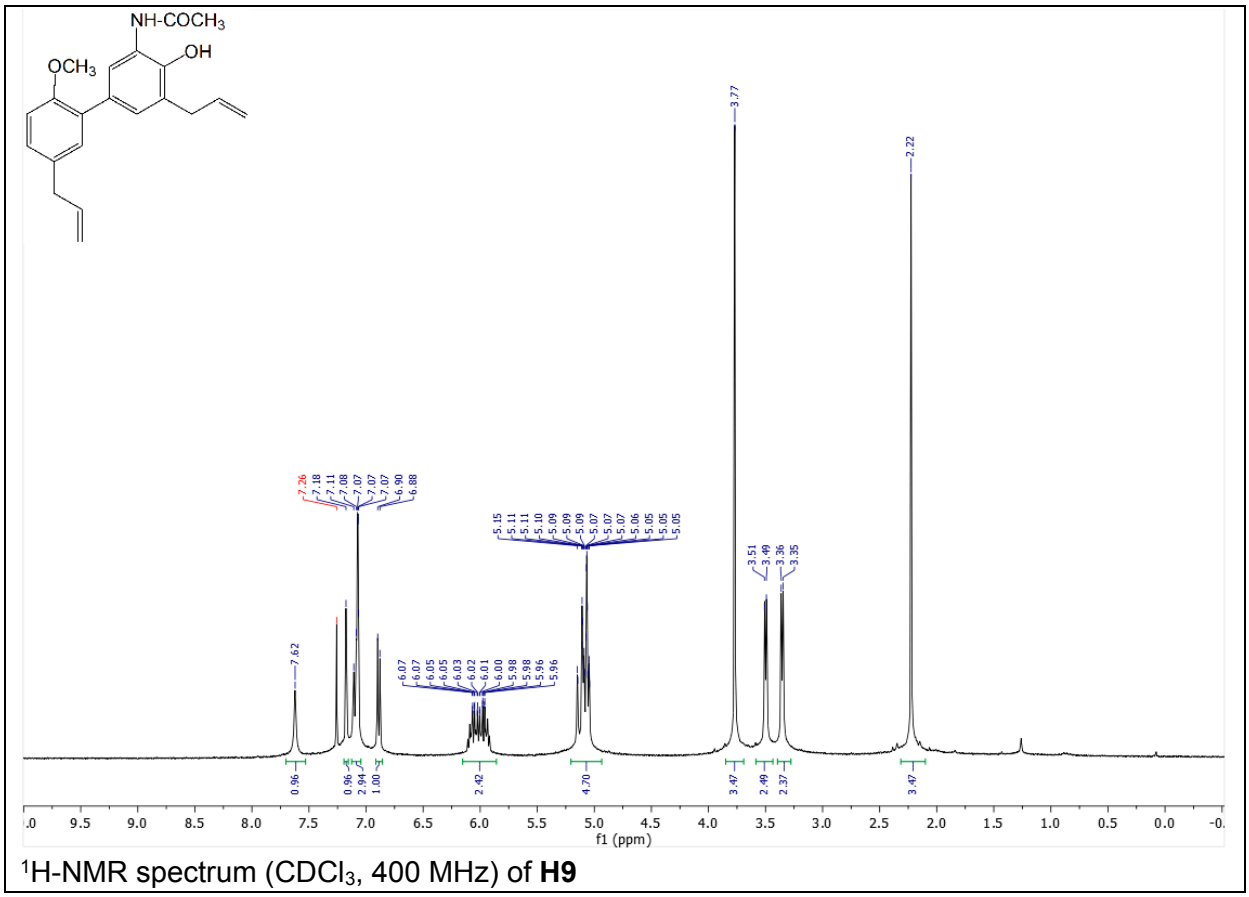
^{1}H-NMR spectrum ($CDCl_3$, 400 MHz) of **H5**



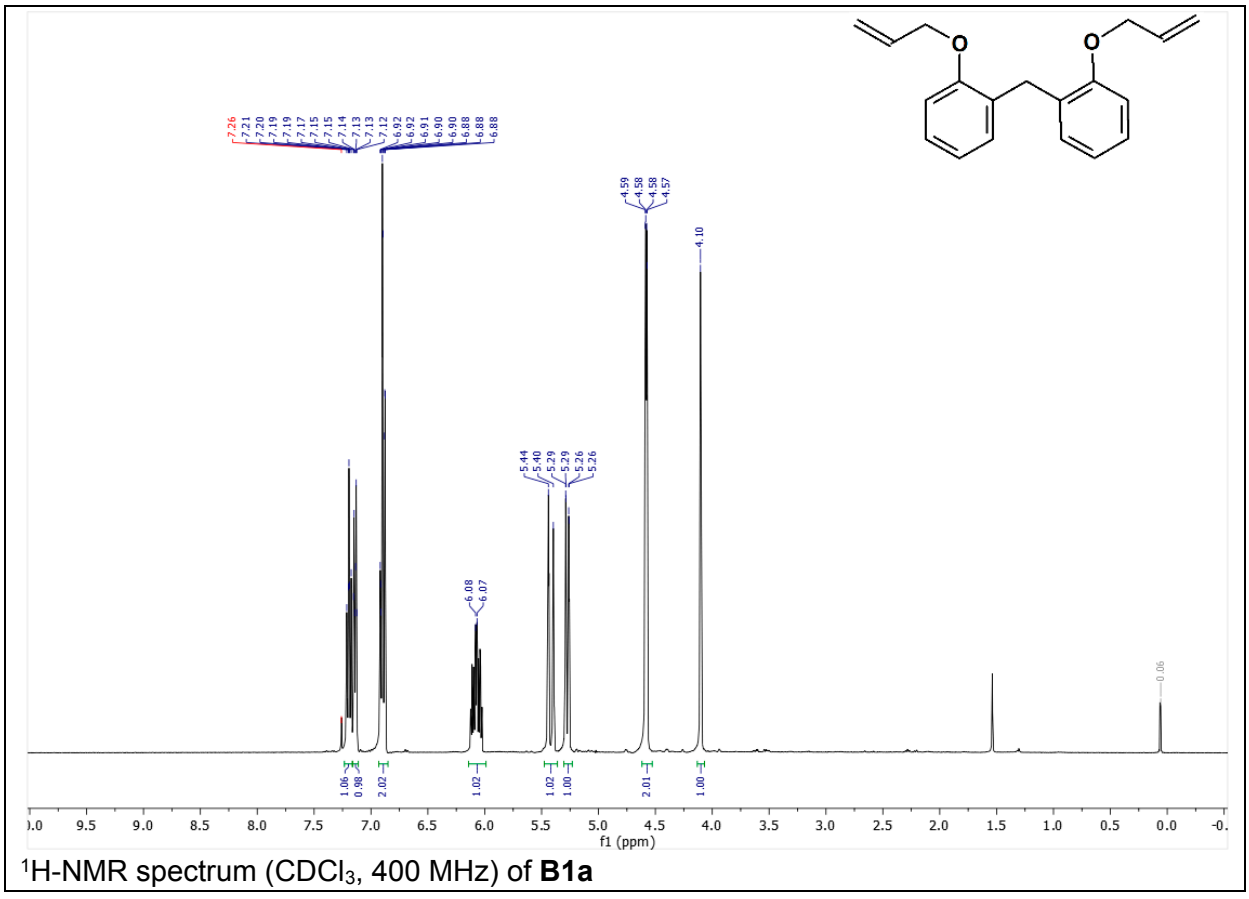
^{1}H-NMR spectrum ($CDCl_3$, 400 MHz) of **H6**



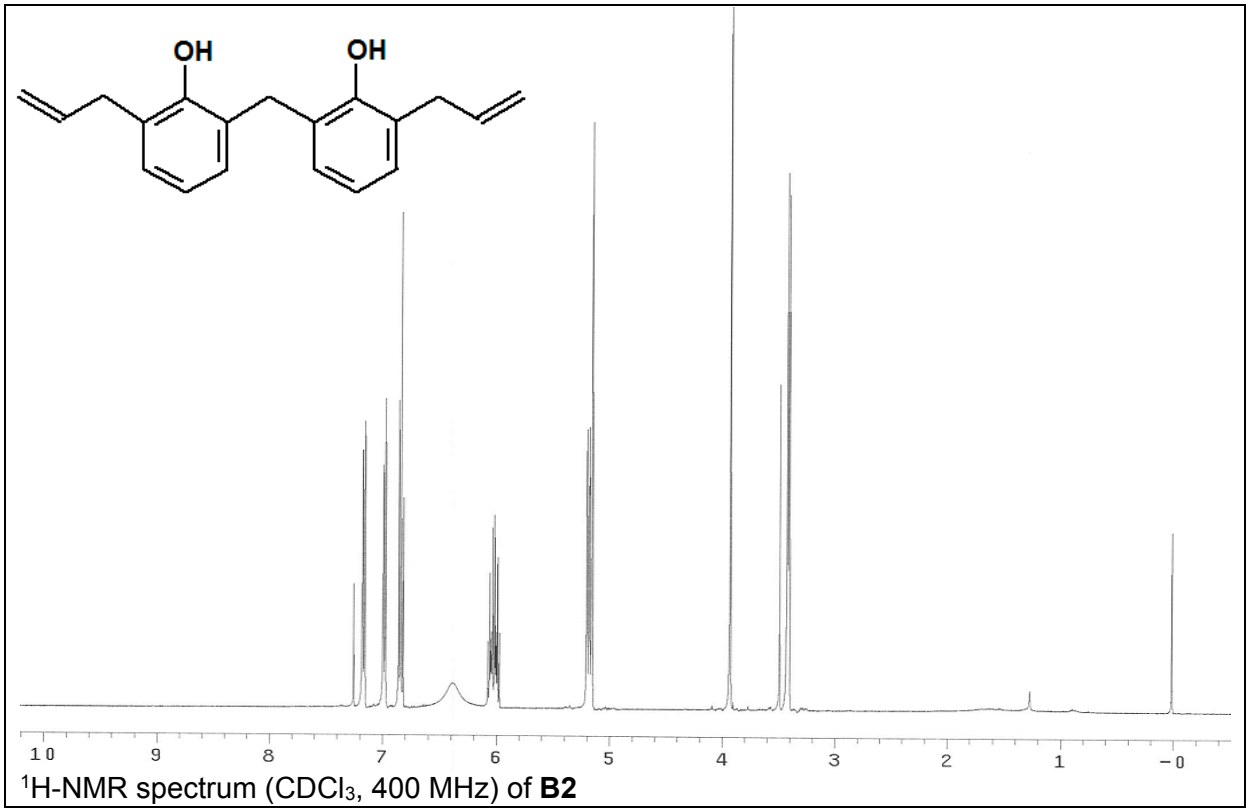
^{1}H-NMR spectrum ($CDCl_3$, 400 MHz) of **H7**



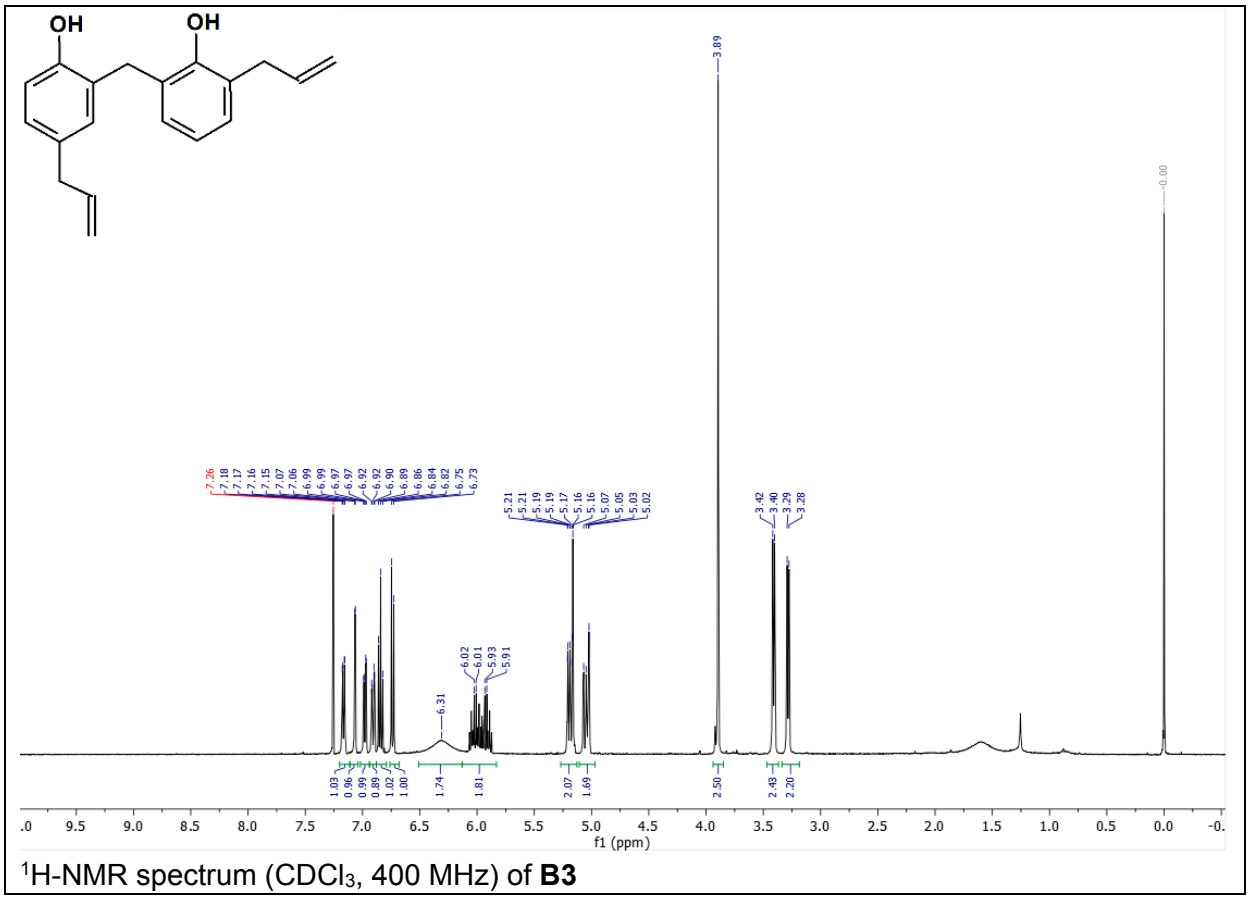
^{1}H-NMR spectrum ($CDCl_3$, 400 MHz) of **H9**



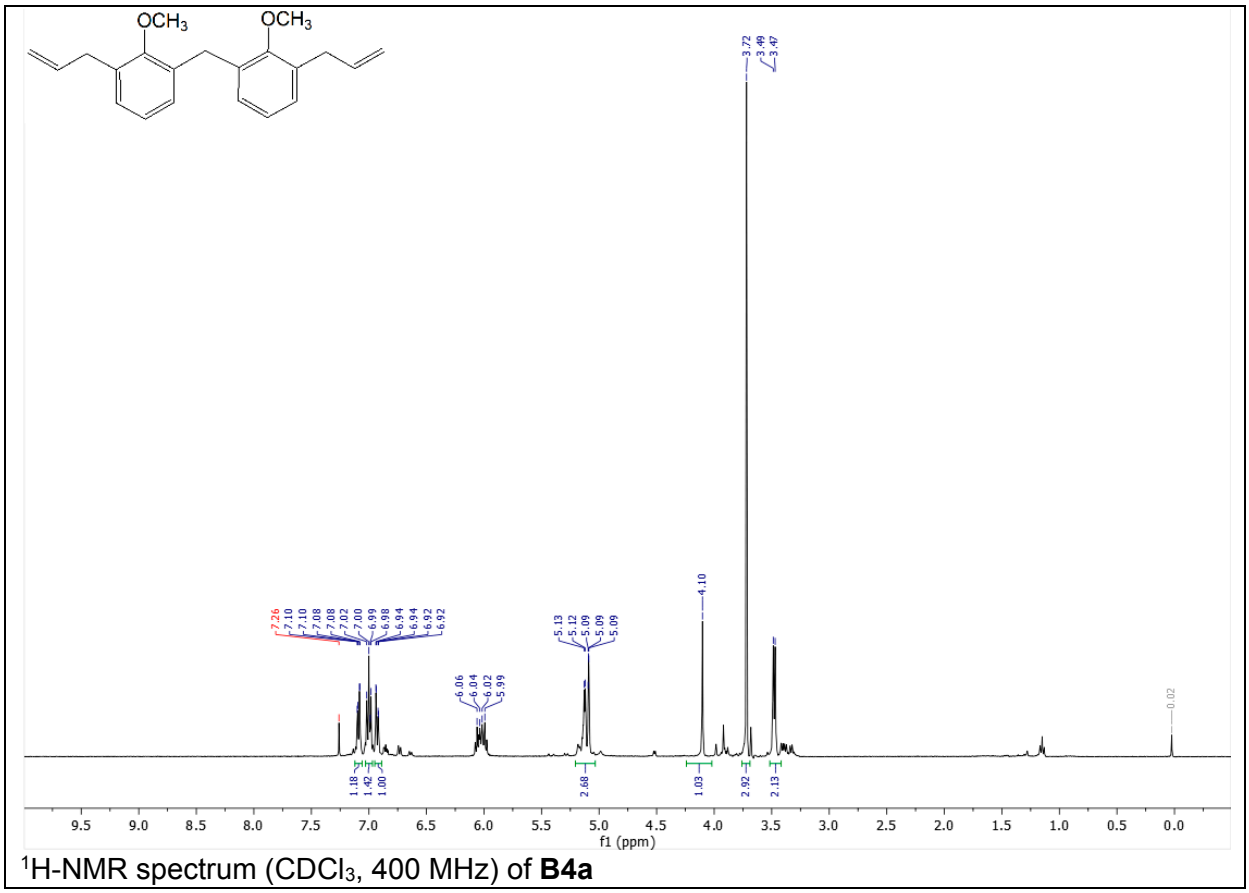
^{1}H-NMR spectrum ($CDCl_3$, 400 MHz) of **B1a**



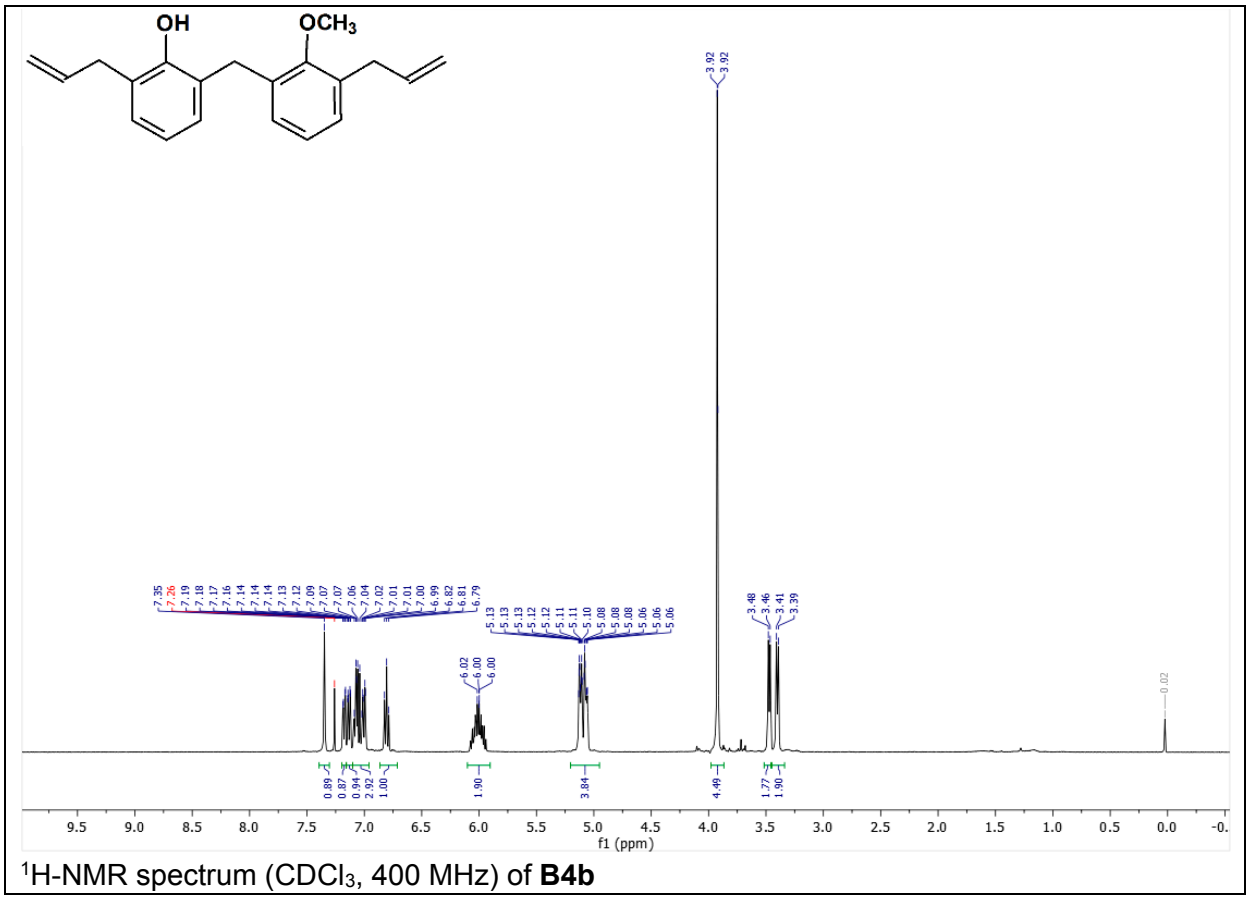
^{1}H-NMR spectrum ($CDCl_3$, 400 MHz) of **B2**



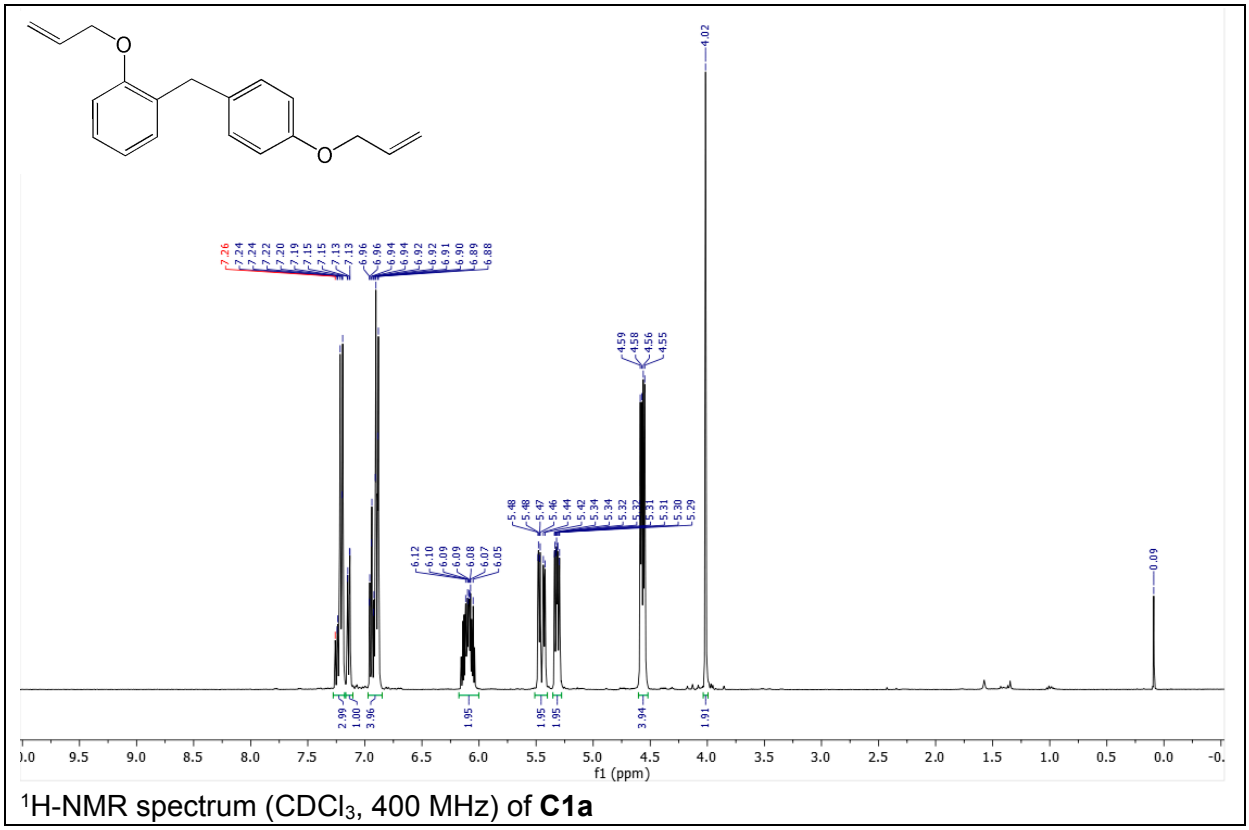
^{1}H-NMR spectrum ($CDCl_3$, 400 MHz) of **B3**



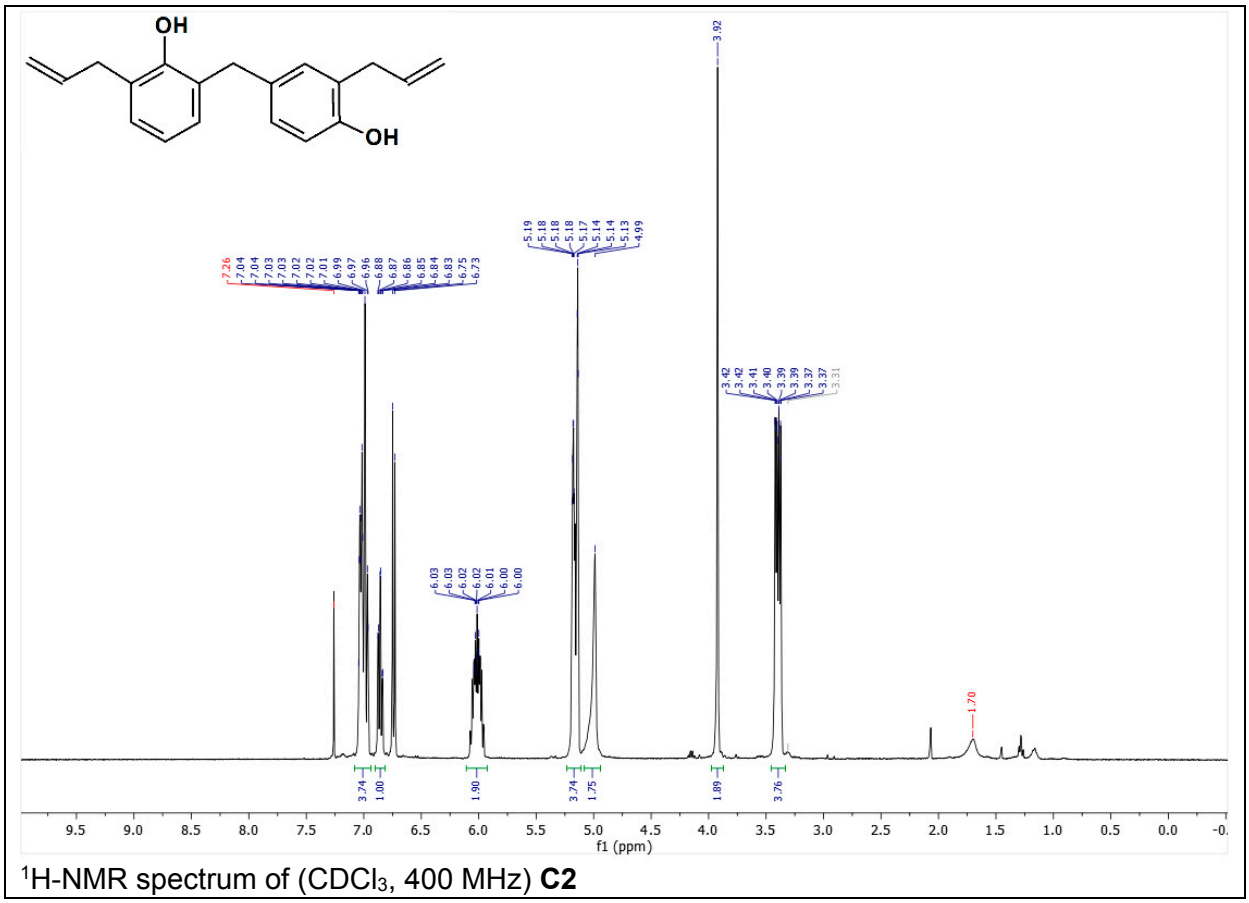
^{1}H-NMR spectrum ($CDCl_3$, 400 MHz) of **B4a**



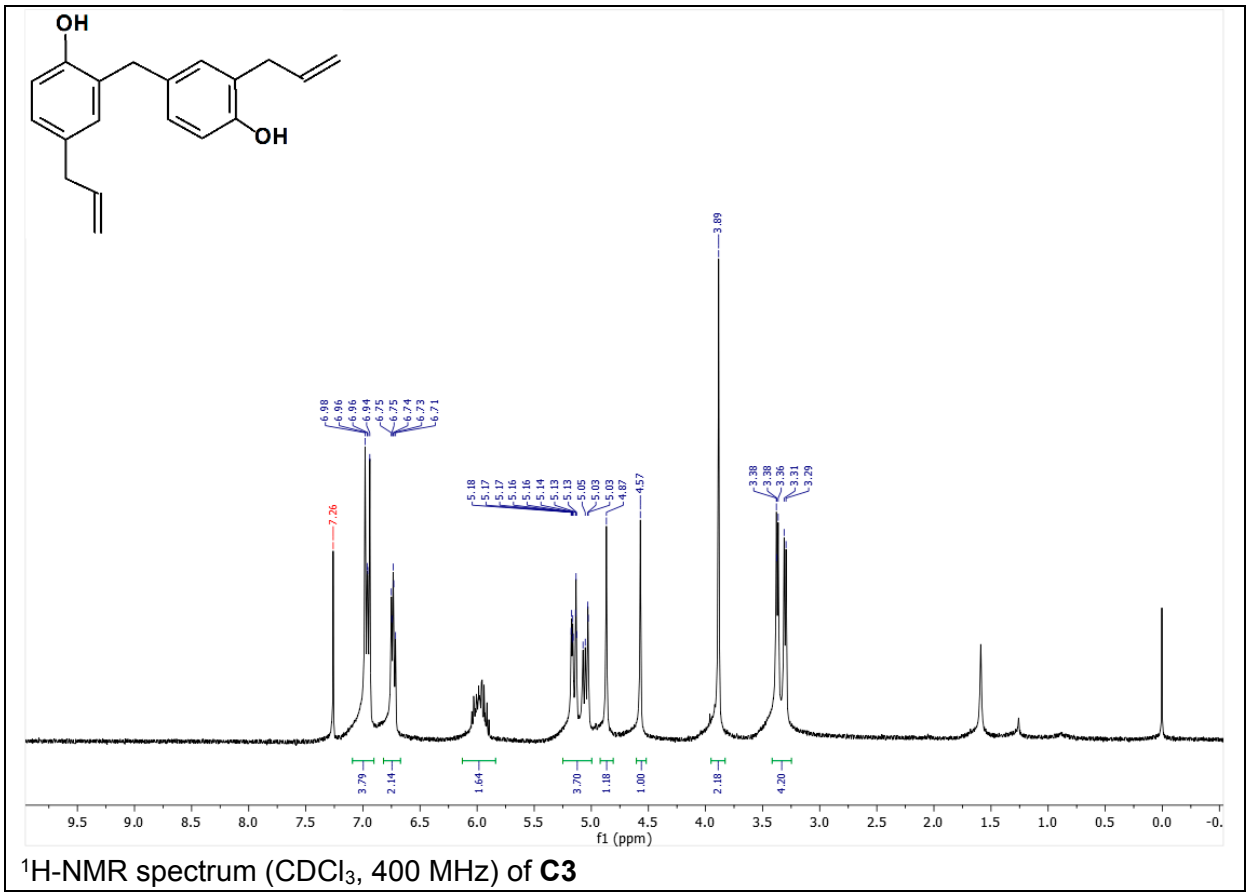
^{1}H-NMR spectrum ($CDCl_3$, 400 MHz) of **B4b**



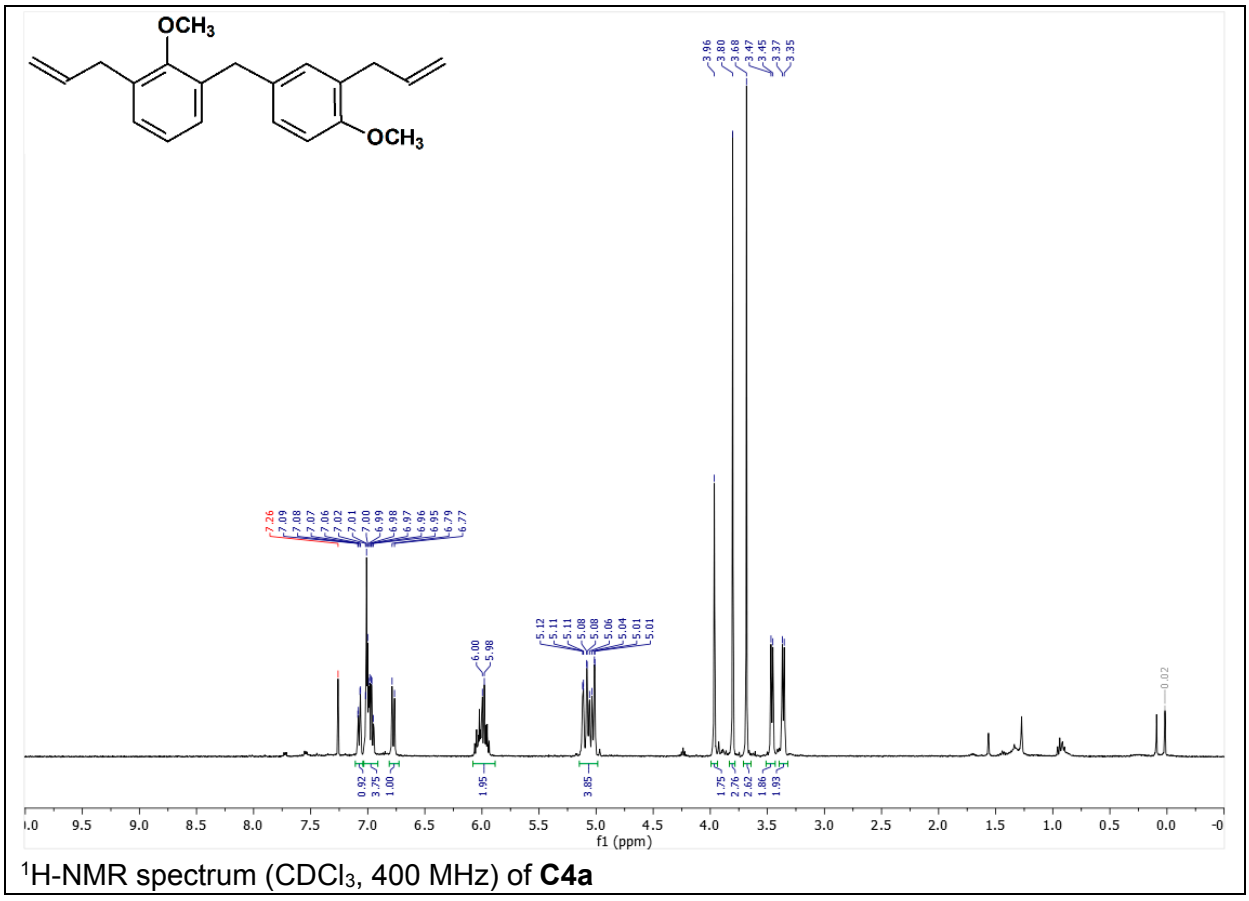
^{1}H-NMR spectrum ($CDCl_3$, 400 MHz) of **C1a**



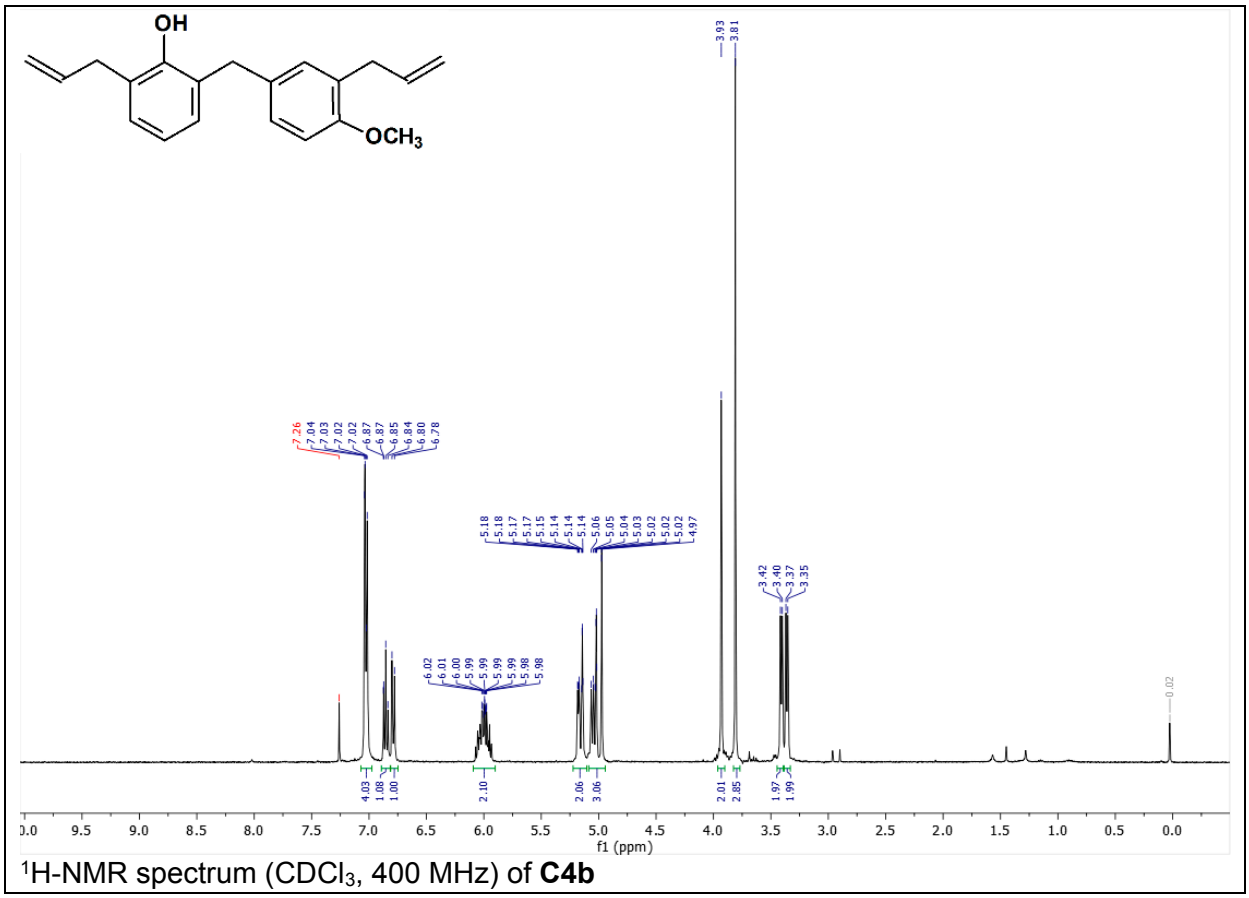
^{1}H-NMR spectrum of ($CDCl_3$, 400 MHz) **C2**



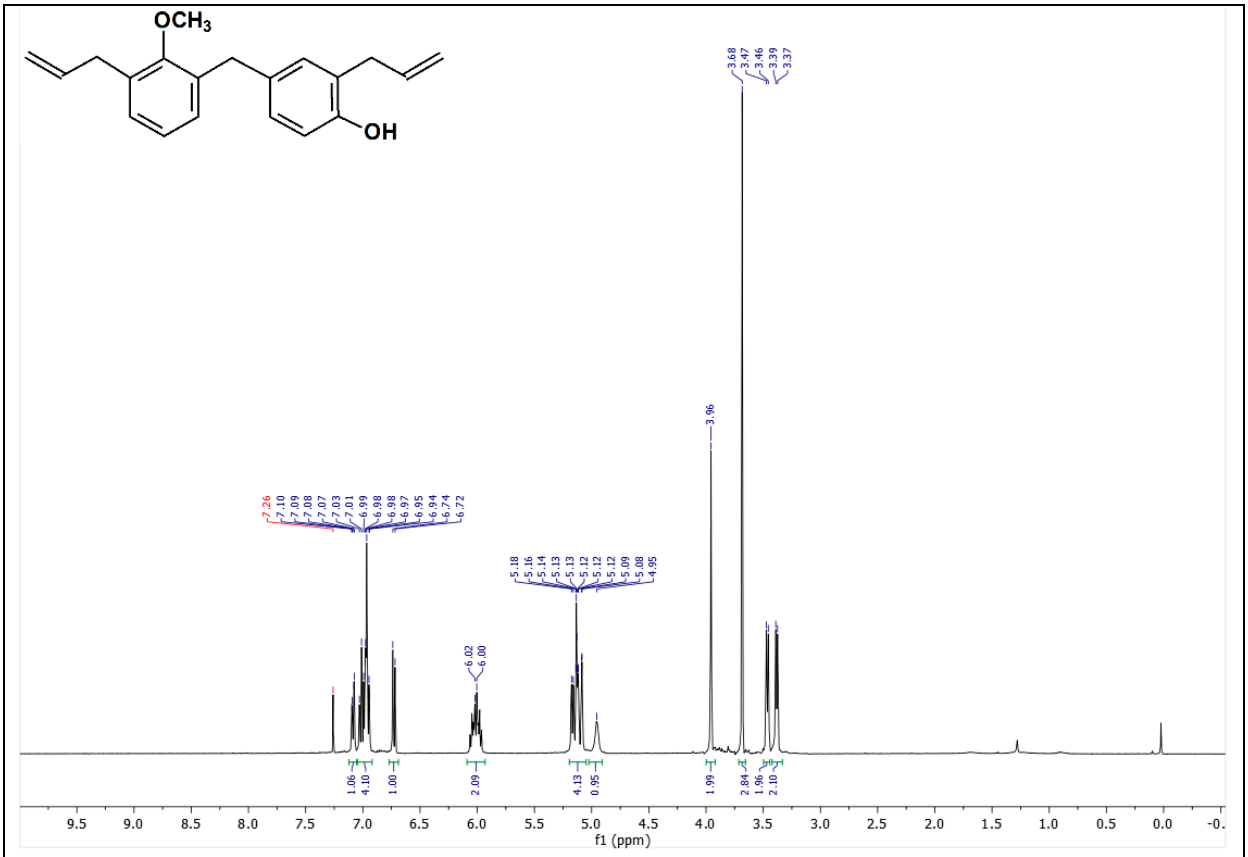
^{1}H-NMR spectrum ($CDCl_3$, 400 MHz) of **C3**



^{1}H-NMR spectrum ($CDCl_3$, 400 MHz) of **C4a**



^{1}H-NMR spectrum ($CDCl_3$, 400 MHz) of **C4b**

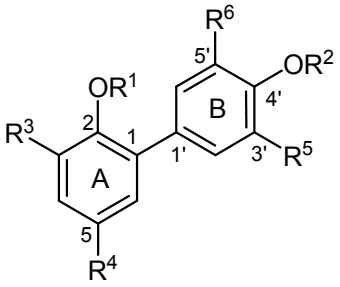


^{1}H-NMR spectrum ($CDCl_3$, 400 MHz) of **C4c**

2. Dose-Response (measured as fluorescence) curves for tested compounds

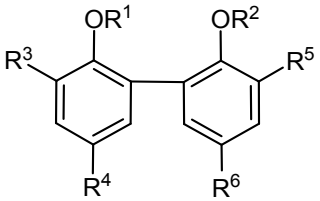
Legend to compound test codes (tables S1 to S5):

Table S1. Structures of Compounds Based on Honokiol



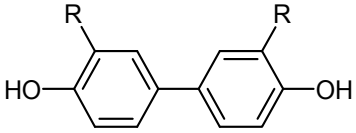
Cpd.	test code	R^1	R^2	R^3	R^4	R^5	R^6
H	A4	H	H	H	allyl	allyl	H
H1	F1	H	Me	NH_2	allyl	allyl	H
H2	G5	H	Me	NH-$COC_{11}H_{23}$	allyl	allyl	H
H3	G6	H	Me	NH-Ala	allyl	allyl	H
H4	G7	H	Me	NH-Phe	allyl	allyl	H
H5	F4	H	Et	NH_2	allyl	allyl	H
H6	F5	Et	Me	NH_2	allyl	allyl	H
H7	F6	Et	Me	NH-Ac	allyl	allyl	H
H8	G1	H	Me	NH-Ac	allyl	allyl	H
H9	G2	Me	H	H	allyl	allyl	NH-Ac
H10	E2	H	Et	H	allyl	allyl	H
H11	F7	Me	H	H	allyl	allyl	NH_2
H12	B5	H	H	H	allyl	1-propenyl	H
H13	C1	H	H	H	*n*-propyl	*n*-propyl	H
H14	B2	Me	H	H	allyl	allyl	H
H15	B1	H	Me	H	allyl	allyl	H
H16	B7	Me	Me	H	allyl	allyl	H
H17	B4	H	Me	H	allyl	1-propenyl	H
H18	B6	H	Me	H	2,3-dihydroxy-propyl	2,3-dihydroxy-propyl	H
H19	B3	H	Me	H	*n*-propyl	*n*-propyl	H
H20	B8	Me	Me	H	*n*-propyl	*n*-propyl	H
H21	E1	Et	-	H	allyl	allyl	H
H22	E3	H	Et	H	allyl	allyl	H
H23	E4	Et	H	H	*n*-propyl	*n*-propyl	H
H24	E5	Et	Et	H	*n*-propyl	*n*-propyl	H
H25	C2	H	Me	H	2-bromo-propyl	allyl	H
H26	E6	Me	H	H	allyl	allyl	NO_2
H27	E7	Me	H	H	*n*-propyl	*n*-propyl	NO_2
H28	E8	H	Me	NO_2	allyl	allyl	H
H29	F2	Me	H	H	*n*-propyl	*n*-propyl	NH_2
H30	F3	H	Me	NH_2	*n*-propyl	*n*-propyl	H
H31	G3	Me	H	H	*n*-propyl	*n*-propyl	NH-Ac
H32	G4	H	Me	NH-Ac	*n*-propyl	*n*-propyl	H

Table S2. Structures of Compounds Based on Biphenyl-2,2'-diol



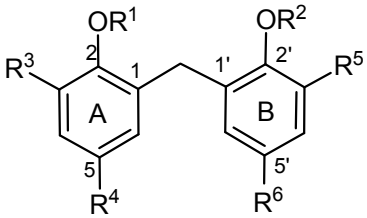
Cpd.	test code	R^1	R^2	R^3	R^4	R^5	R^6
M	A3	H	H	H	allyl	H	allyl
M1	A1	H	H	H	H	H	H
M2	A6	H	H	H	*n*-propyl	H	*n*-propyl
M3	A7	Me	H	H	allyl	H	allyl
M4	A8	Me	Me	H	allyl	H	allyl
M5	C5	H	H	H	Me	H	Me
M6	C6	H	H	H	*t*-butyl	H	*t*-butyl
M7	C4	H	H	allyl	H	allyl	H

Table S3. Structures of Compounds Based on Biphenyl-4,4'-diol



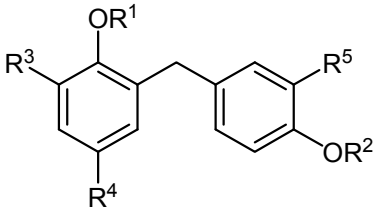
Cpd.	test code	R
A1	A2	H
A2	C5	allyl

Table S4. Structures of Compounds Based on bis(2-hydroxyphenyl)methane

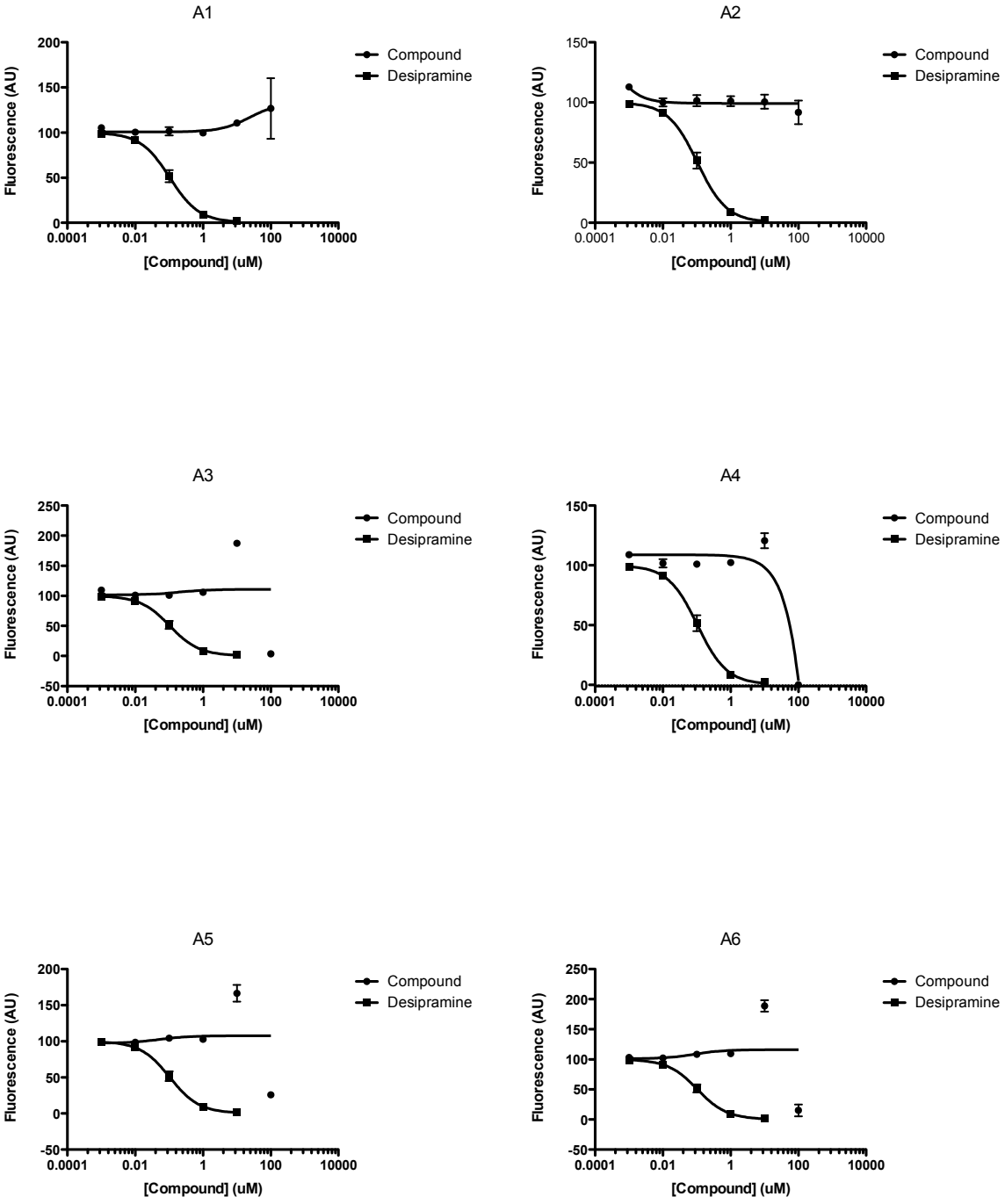


Cpd.	test code	R^1	R^2	R^3	R^4	R^5	R^6
B1	D1	H	H	H	H	H	H
B2	D4	H	H	allyl	H	allyl	H
B4b	D5	Me	H	allyl	H	allyl	H
B4a	D6	Me	Me	allyl	H	allyl	H

Table S5. Structures of Compounds Based on 2,4'-dihydroxydiphenylmethane

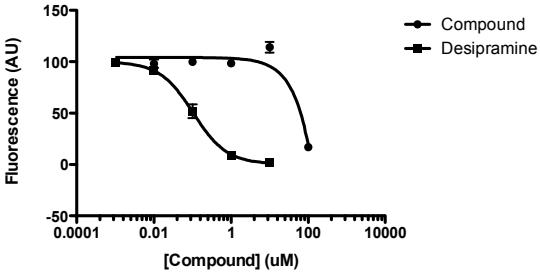


Cpd.	test code	R^1	R^2	R^3	R^4	R^5
C1	D2	H	H	H	H	H
C2	D3	H	H	allyl	H	allyl
C4c	D8	Me	H	allyl	H	allyl
C4b	D7	H	Me	allyl	H	allyl
C4a	D9	Me	Me	allyl	H	allyl



A5 does not belong to the compounds of this article

A7



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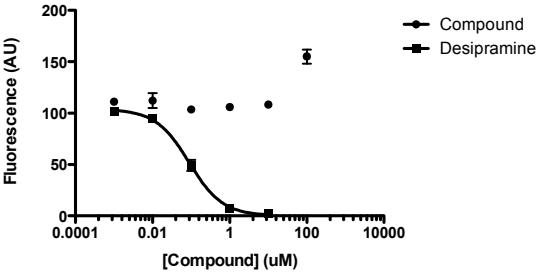

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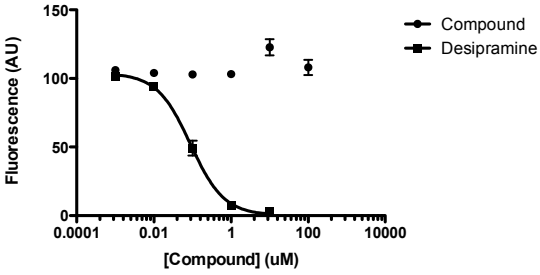

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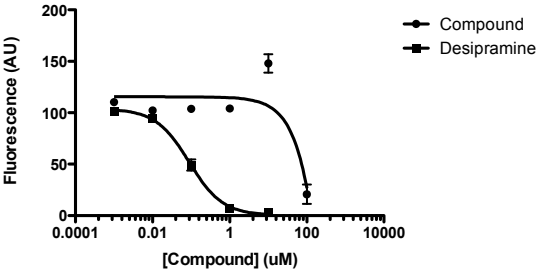

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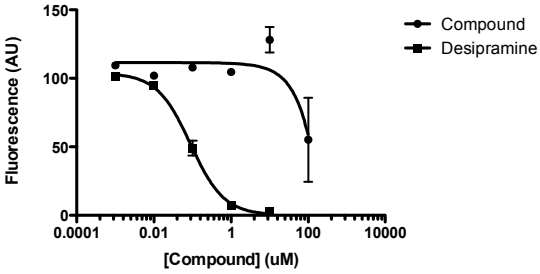

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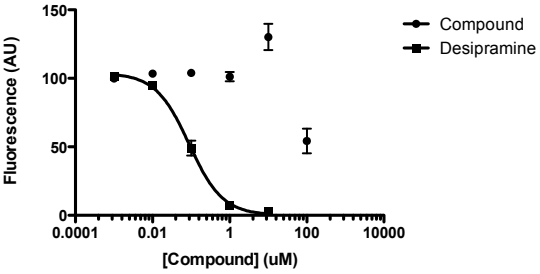

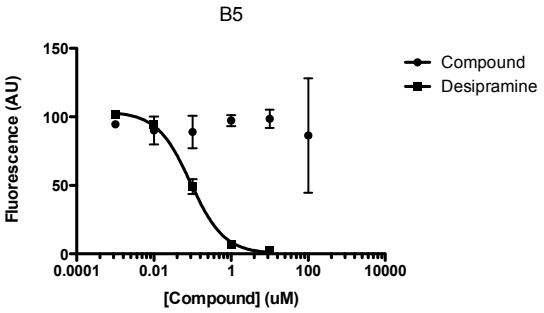
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Compound
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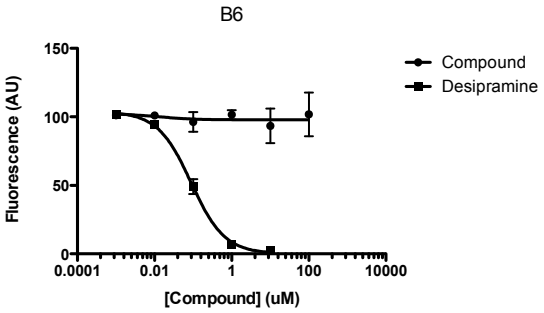
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Compound
Desipramine
Fluorescence (AU)
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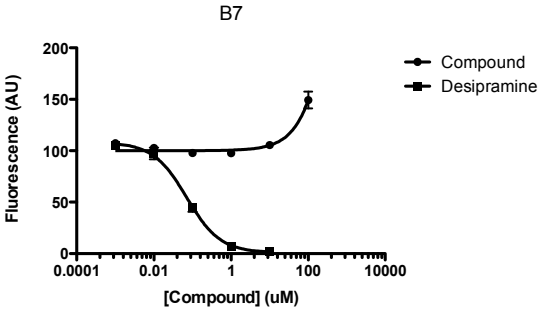
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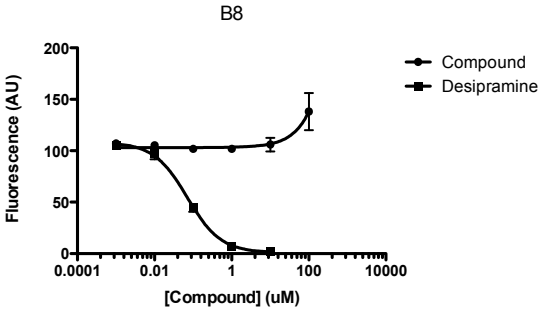
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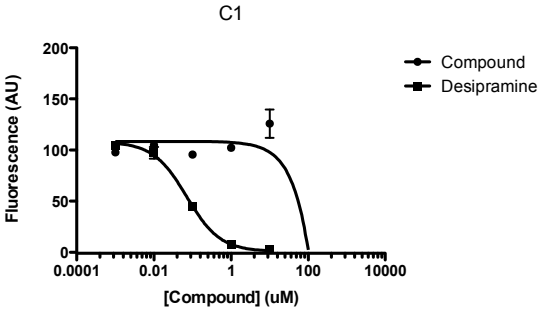
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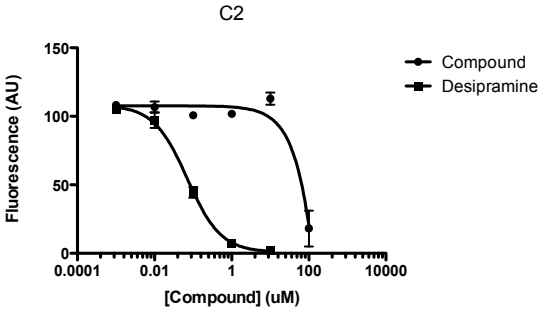
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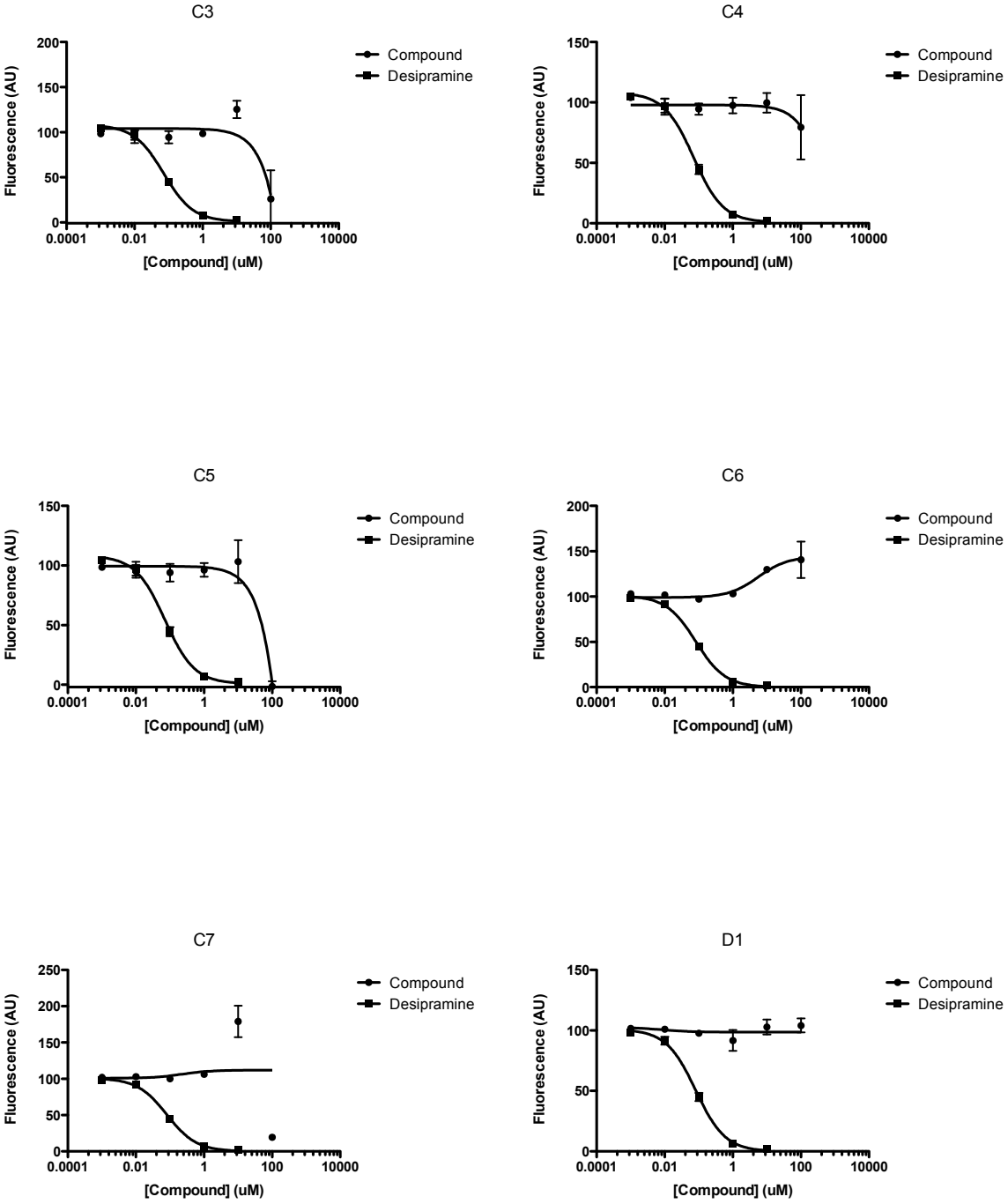
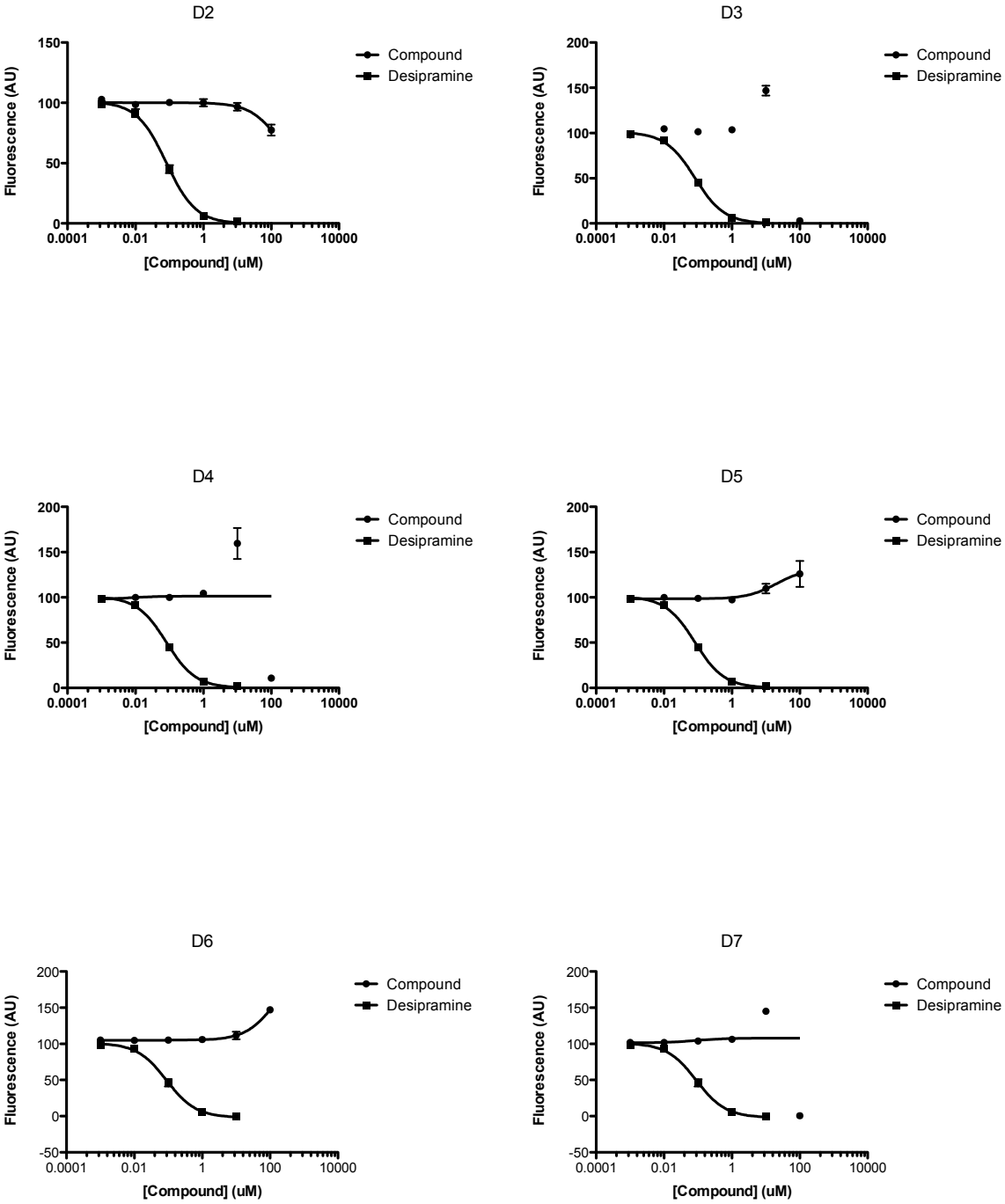


C3 does not belong to the compounds of this article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Desipramine
D4
Fluorescence (AU)
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D5
Fluorescence (AU)
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D6
Fluorescence (AU)
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D7
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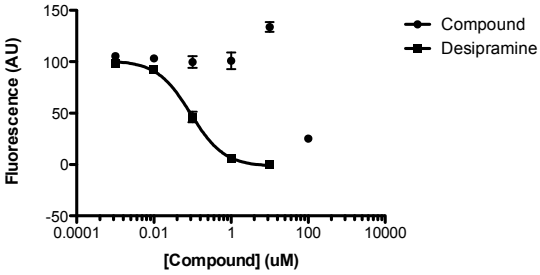
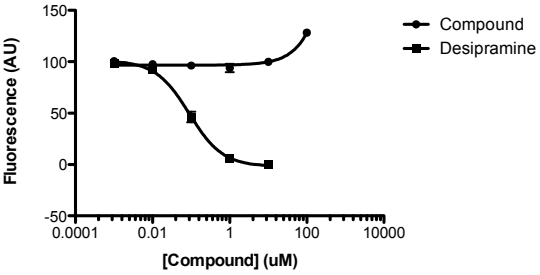
Compound
Desipramine

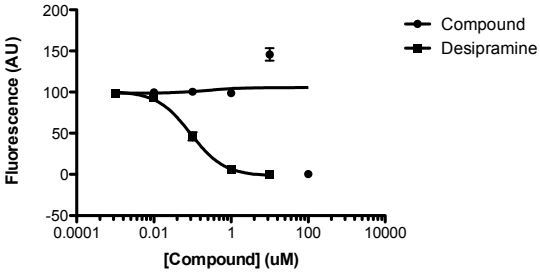
D8



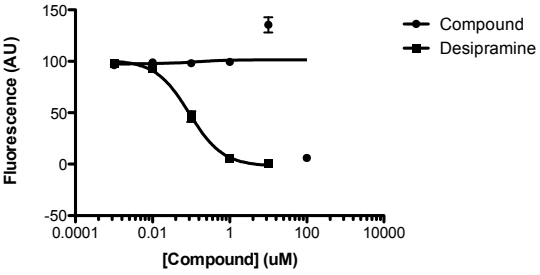
D9



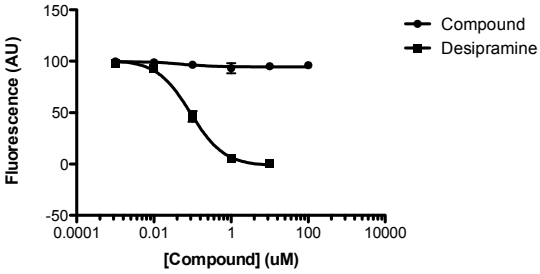
E1



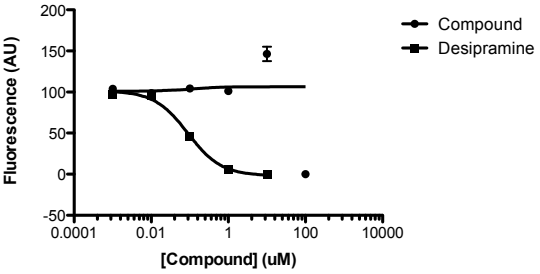
E2

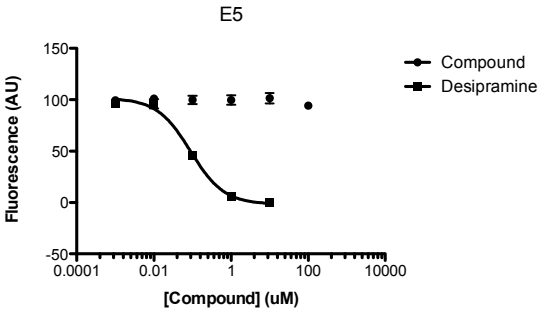


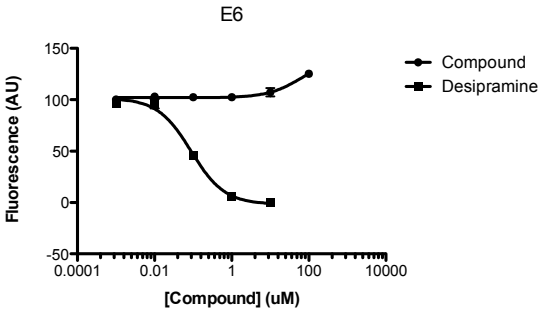
E3



E4




E5
Compound
Desipramine
Fluorescence (AU)
150
100
50
0
-50
0.0001
0.01
1
100
10000
[Compound] (uM)


E6
Compound
Desipramine
Fluorescence (AU)
150
100
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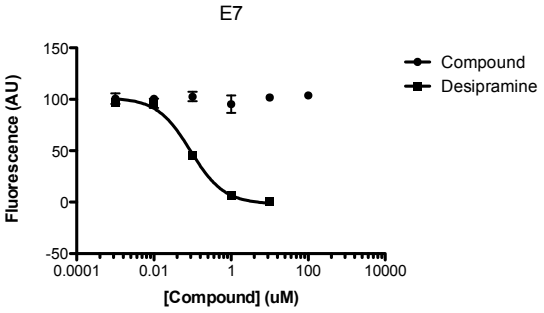
-50
0.0001
0.01
1
100
10000
[Compound] (uM)


E7
Compound
Desipramine
Fluorescence (AU)
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100
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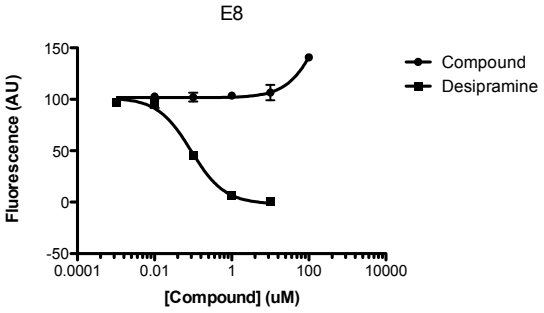
-50
0.0001
0.01
1
100
10000
[Compound] (uM)


E8
Compound
Desipramine
Fluorescence (AU)
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-50
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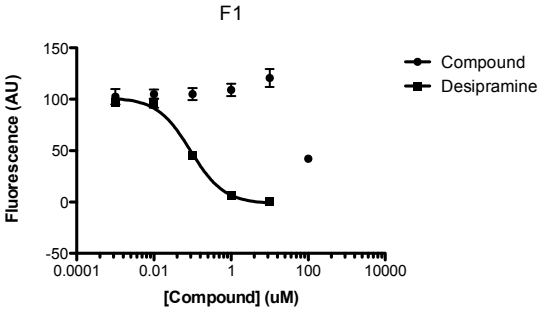
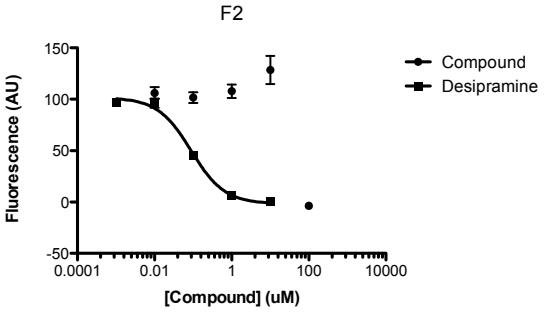
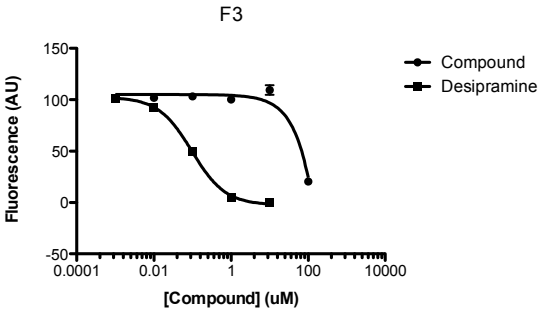
0.01
1
100
10000
[Compound] (uM)


F1
Compound
Desipramine
Fluorescence (AU)
150
100
50
0
-50
0.0001
0.01
1
100
10000
[Compound] (uM)


F2
Compound
Desipramine
Fluorescence (AU)
150
100
50
0
-50
0.0001
0.01
1
100
10000
[Compound] (uM)


F3
Fluorescence (AU)
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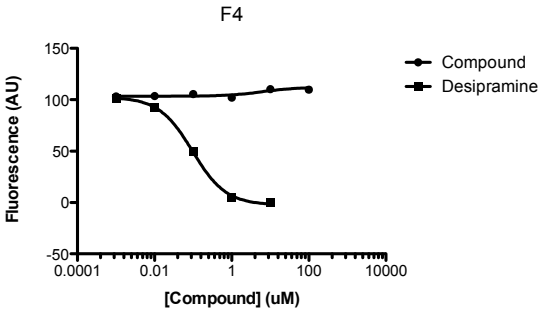
50
0
-50
0.0001
0.01
1
100
10000
[Compound] (uM)
Compound
Desipramine


F4
Fluorescence (AU)
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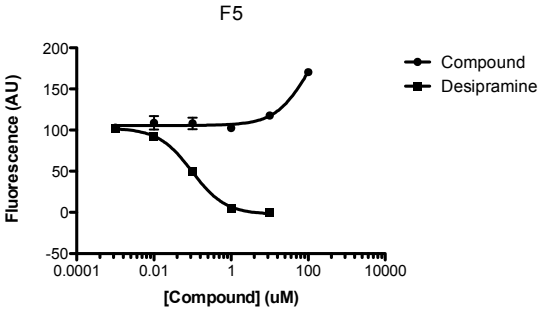
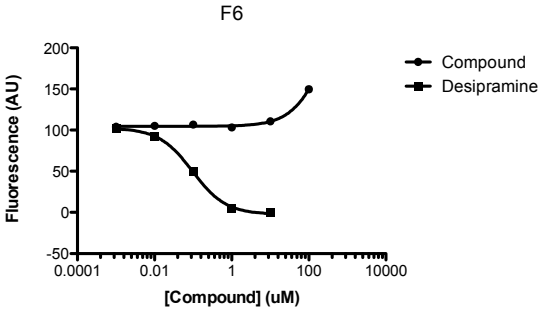
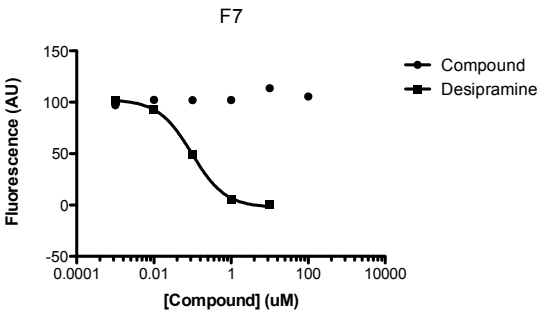
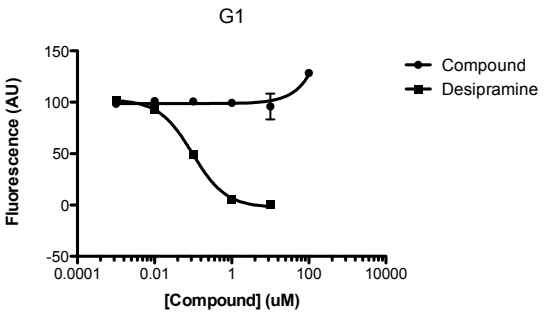
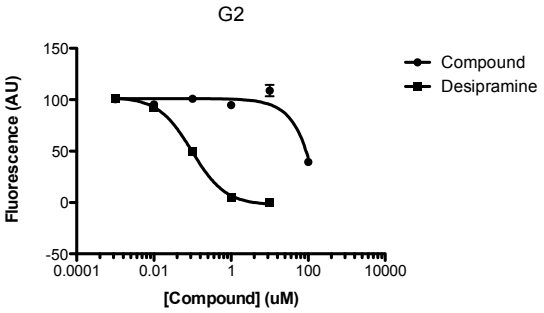
50
0
-50
0.0001
0.01
1
100
10000
[Compound] (uM)
Compound
Desipramine

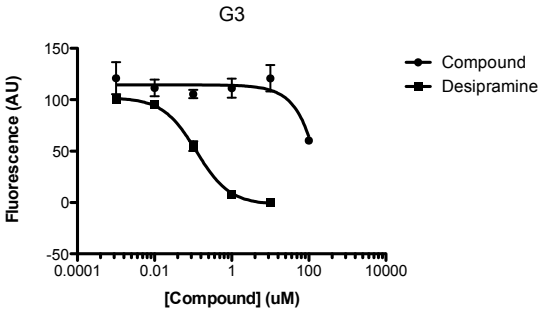

F5
Fluorescence (AU)
200
150
100
50
0
-50
0.0001
0.01
1
100
10000
[Compound] (uM)
Compound
Desipramine

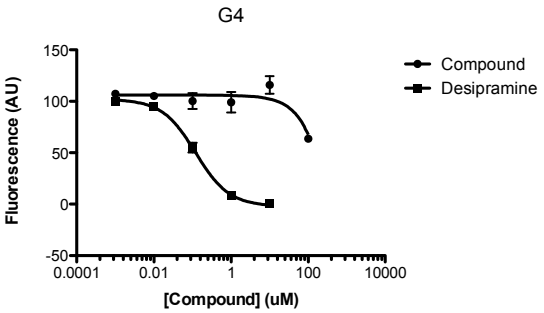

F6
Fluorescence (AU)
200
150
100
50
0
-50
0.0001
0.01
1
100
10000
[Compound] (uM)
Compound
Desipramine

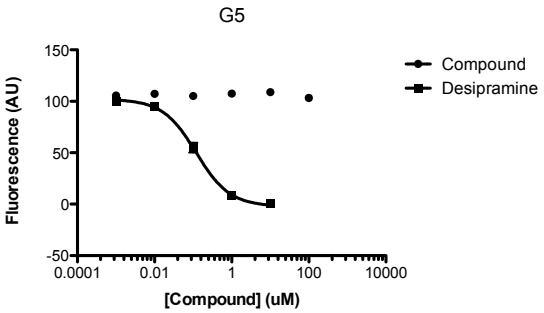

F7
Fluorescence (AU)
150
100
50
0
-50
0.0001
0.01
1
100
10000
[Compound] (uM)
Compound
Desipramine

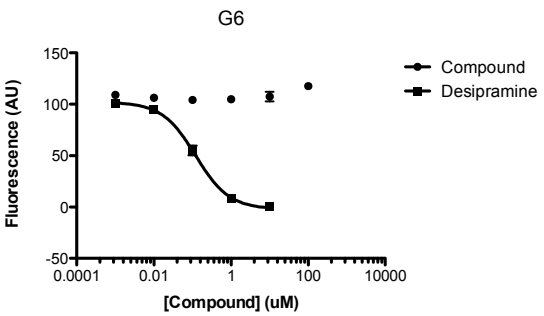

G1
Fluorescence (AU)
150
100
50
0
-50
0.0001
0.01
1
100
10000
[Compound] (uM)
Compound
Desipramine

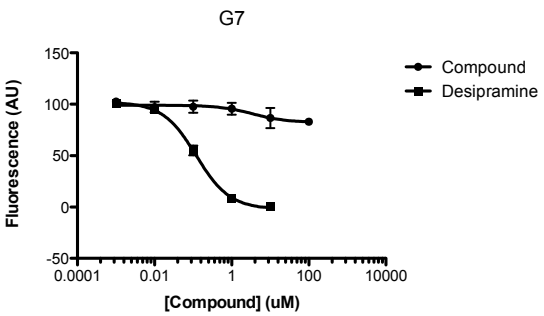

G2
Compound
Desipramine
Fluorescence (AU)
150
100
50
0
-50
0.0001
0.01
1
100
10000
[Compound] (uM)


G3
Compound
Desipramine
Fluorescence (AU)
150
100
50
0
-50
0.0001
0.01
1
100
10000
[Compound] (uM)


G4
Compound
Desipramine
Fluorescence (AU)
150
100
50
0
-50
0.0001
0.01
1
100
10000
[Compound] (uM)


G5
Compound
Desipramine
Fluorescence (AU)
150
100
50
0
-50
0.0001
0.01
1
100
10000
[Compound] (uM)


G6
Compound
Desipramine
Fluorescence (AU)
150
100
50
0
-50
0.0001
0.01
1
100
10000
[Compound] (uM)


G7
Compound
Desipramine
Fluorescence (AU)
150
100
50
0
-50
0.0001
0.01
1
100
10000
[Compound] (uM)