

Supplementary Material

Exploiting polycyclic aromatic isonitriles in GBB strategy for the design of functional scaffolds

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^b*Laboratory of Medicinal Chemistry, Universitat de Barcelona, Faculty of Pharmacy and Food Sciences, Barcelona, Spain*

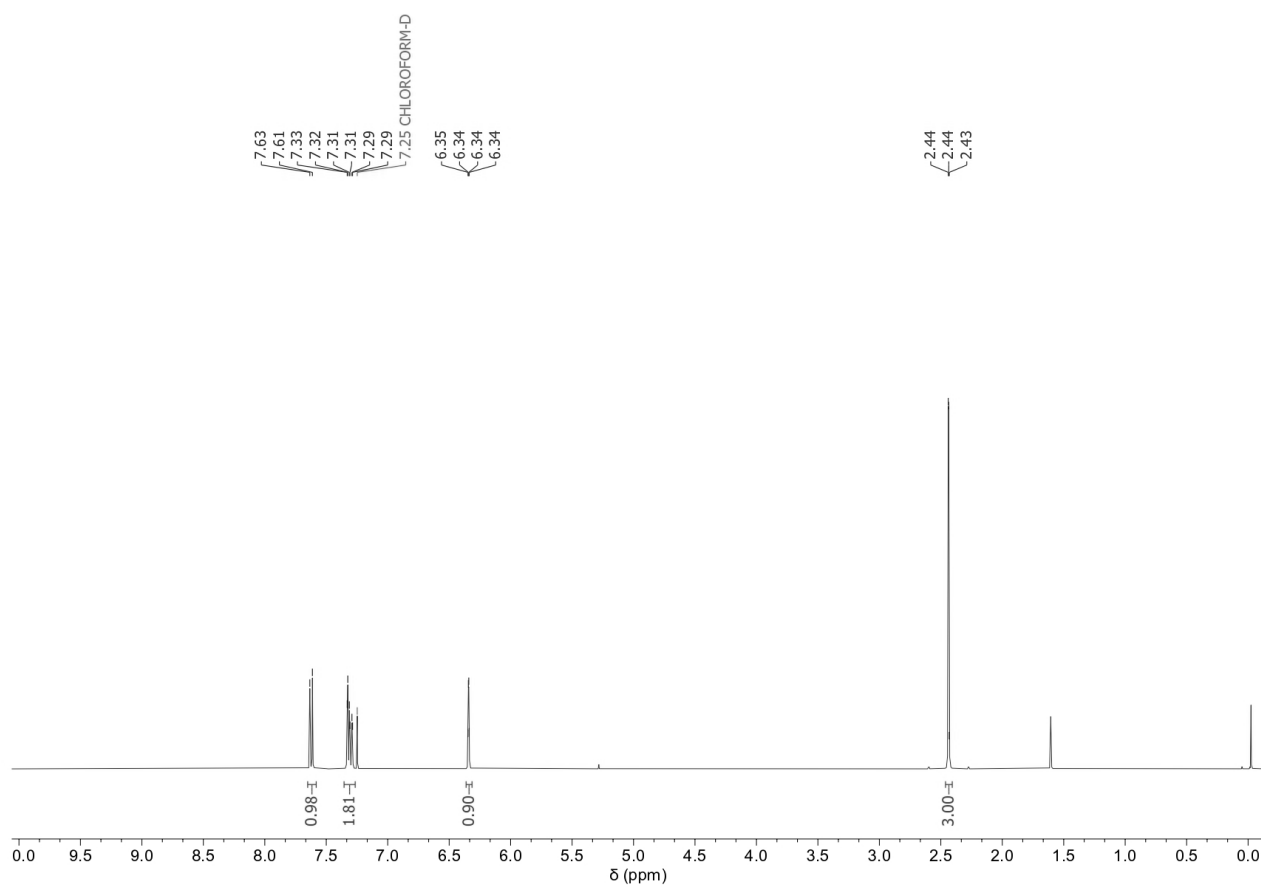
^c*Immunity, Inflammation and Cancer Group, Oncobell Program, Institut d'Investigació Biomèdica de Bellvitge, Gran Via de l'Hospitalet, 199, 08908 Hospitalet de Llobregat, Spain*

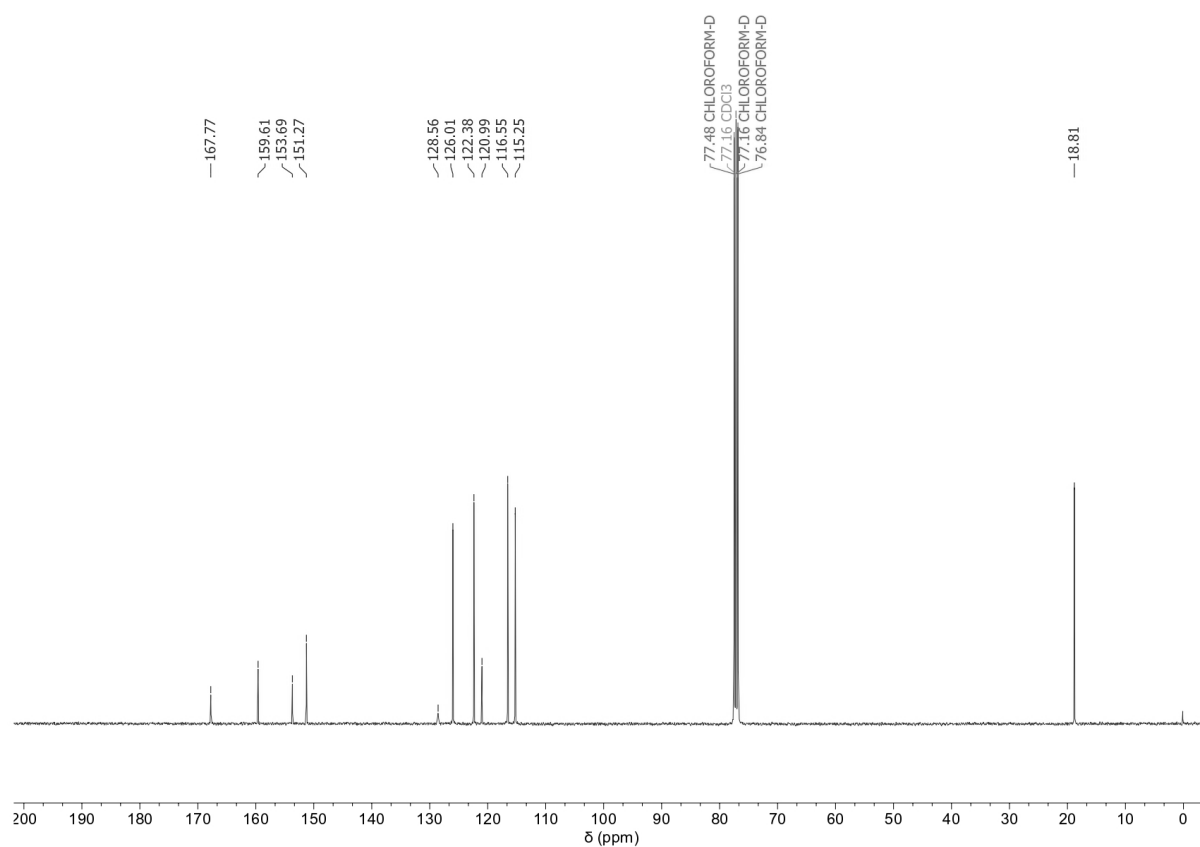
^d*Leibniz-Institut für Pflanzenbiochemie, Halle, Germany*

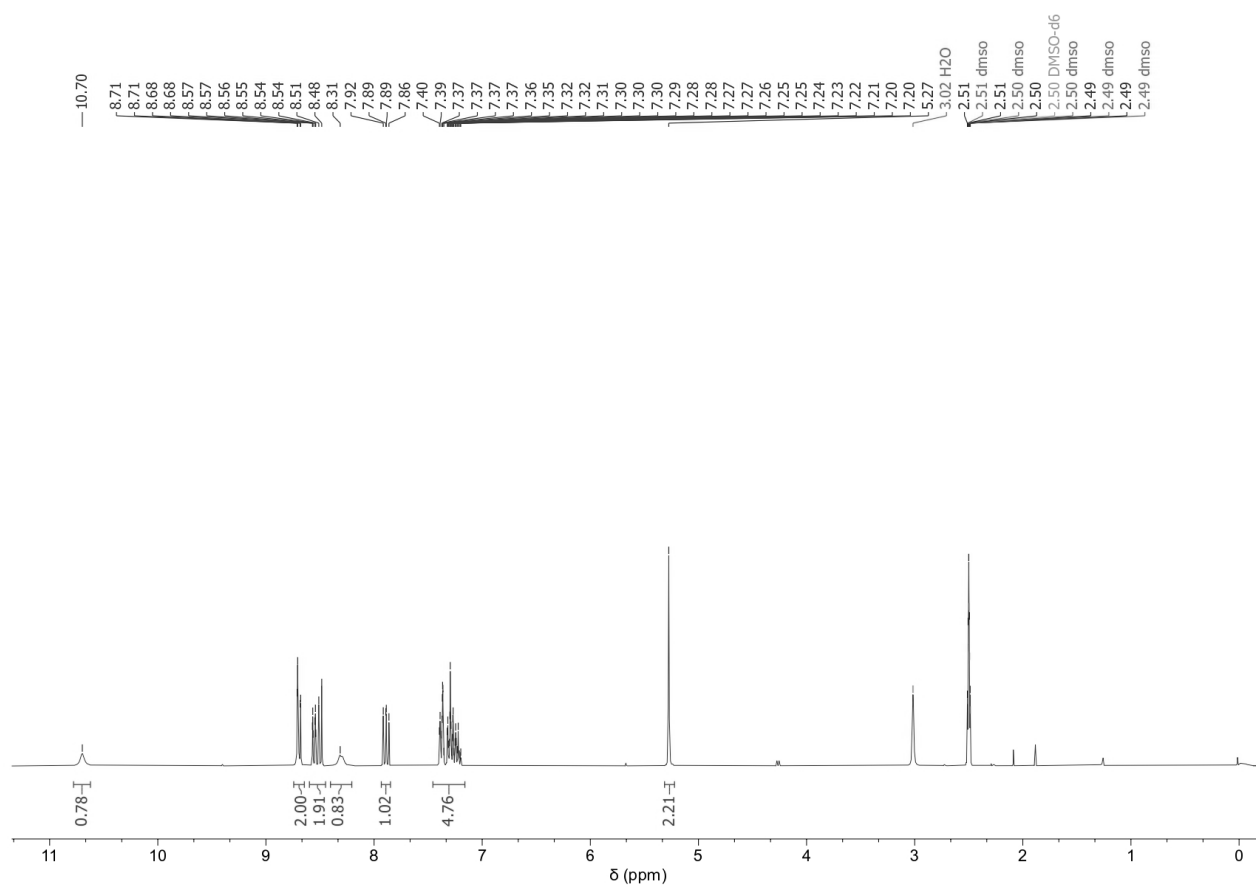
Email: rlavilla@ub.edu; fabio.demoliner@ipb-halle.de ; andrea.basso@unige.it

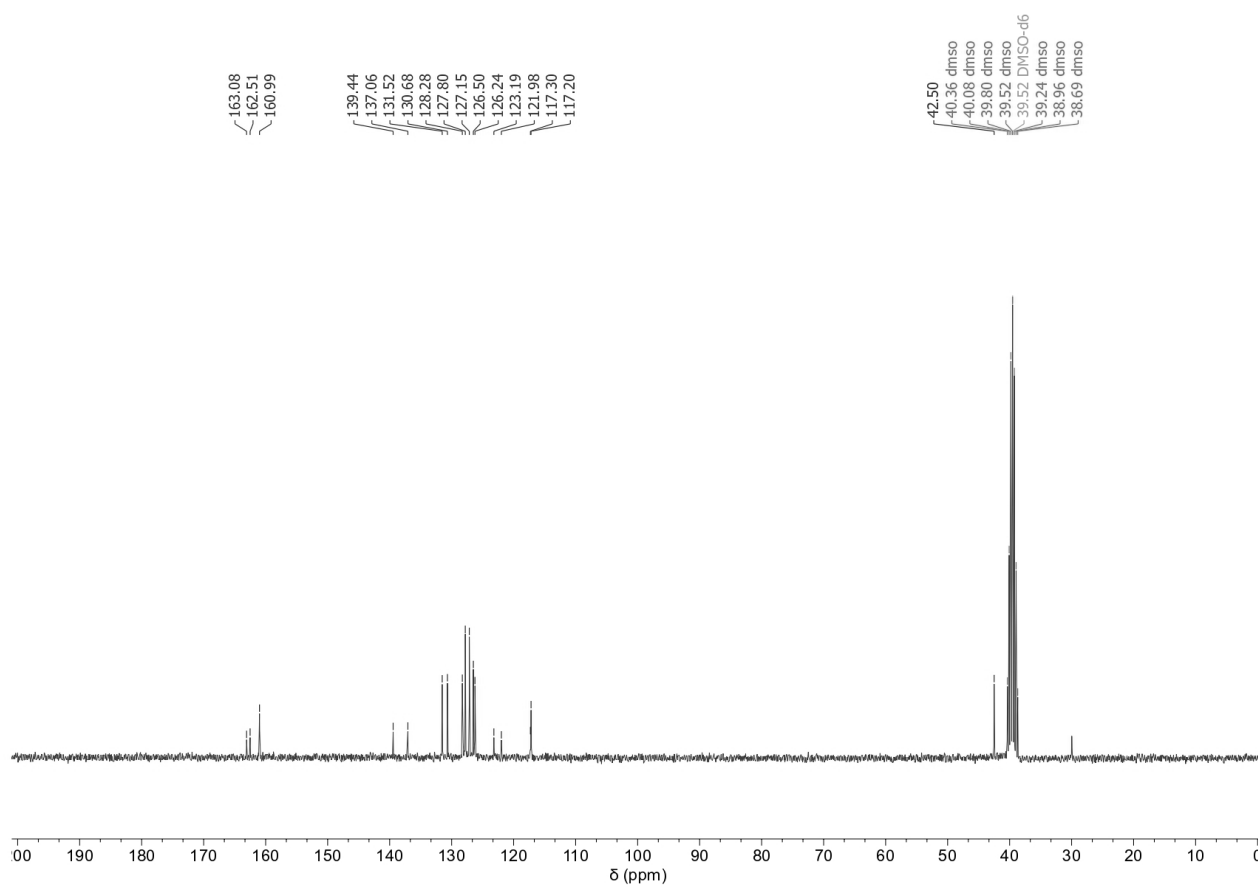
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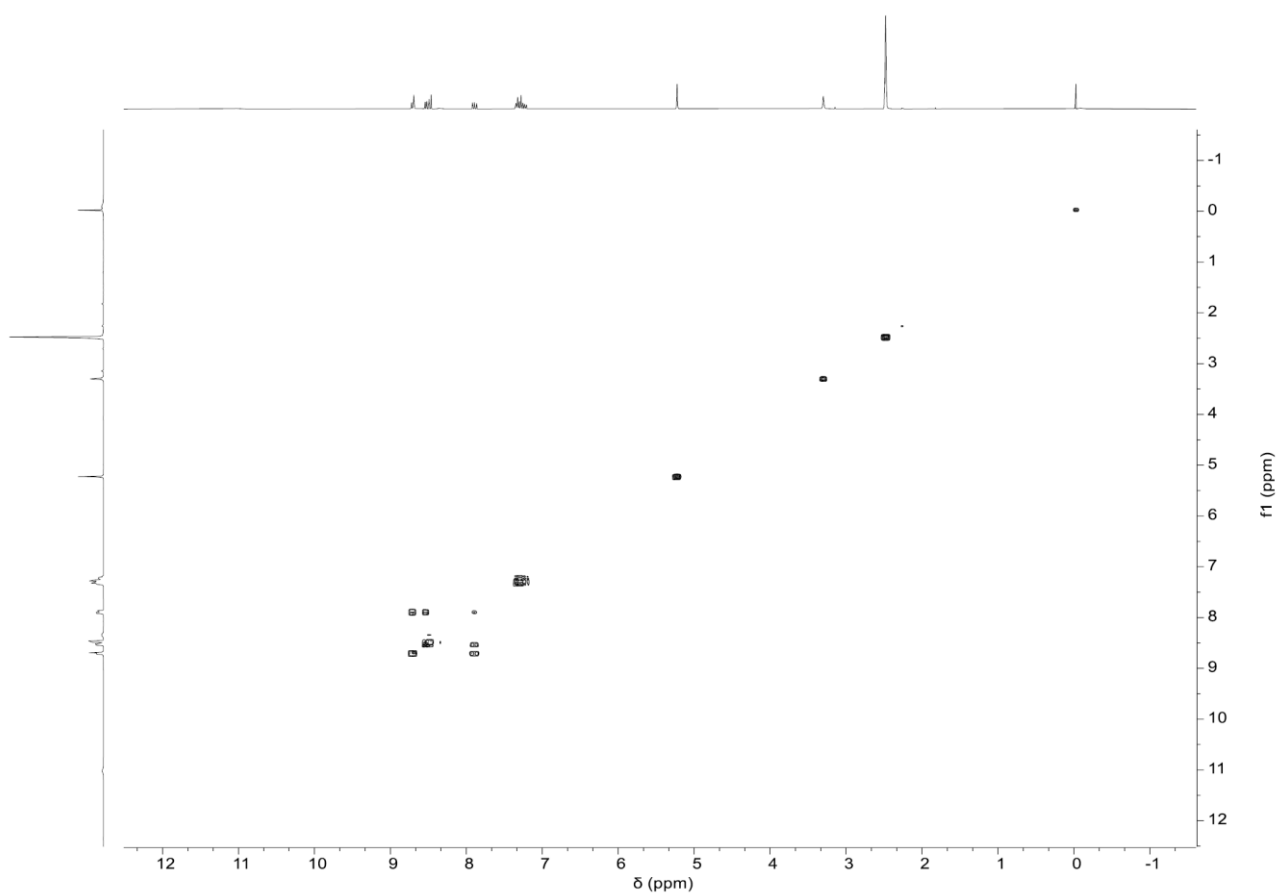
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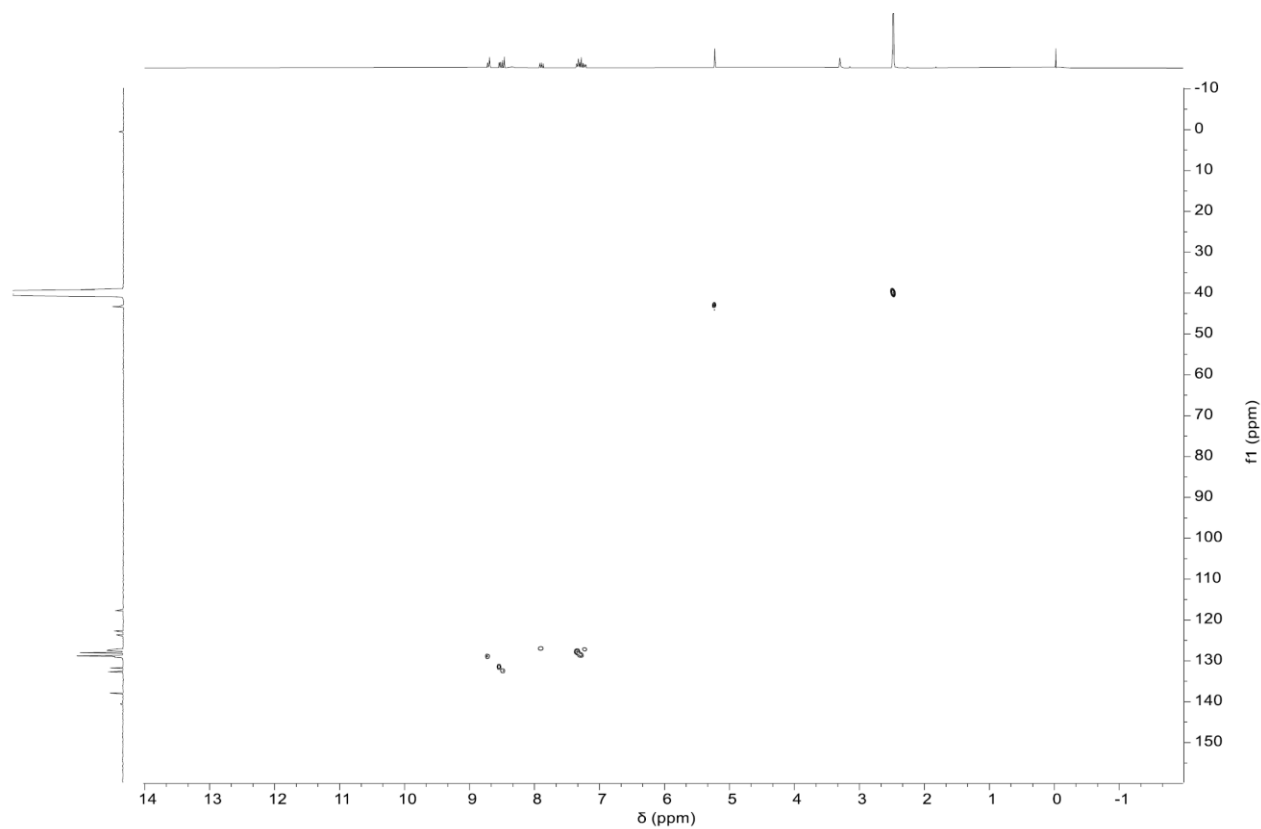
7-isocyano-4-methylcoumarin (3). ^1H NMR (400 MHz, CDCl_3)

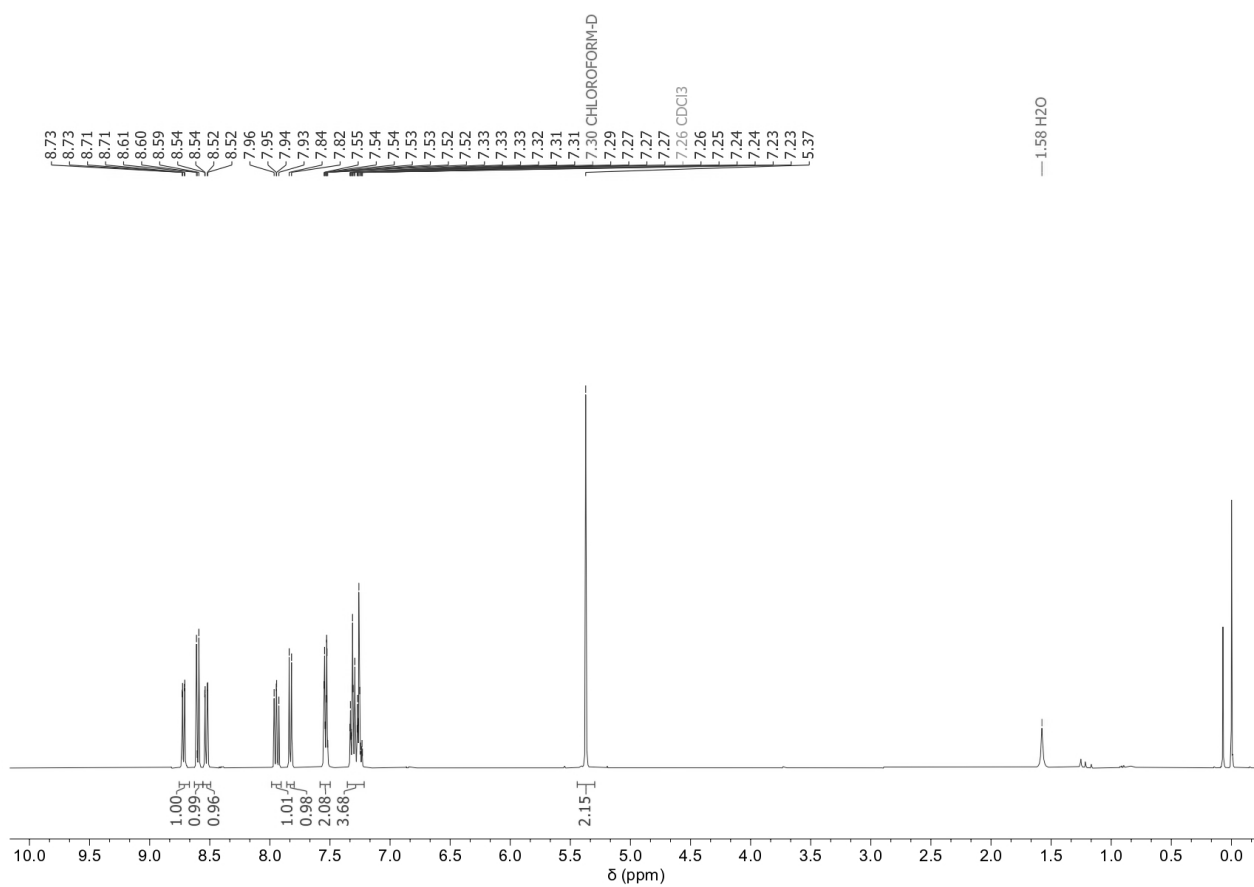
7-isocyano-4-methylcoumarin (3). ^{13}C NMR (101 MHz, CDCl_3)

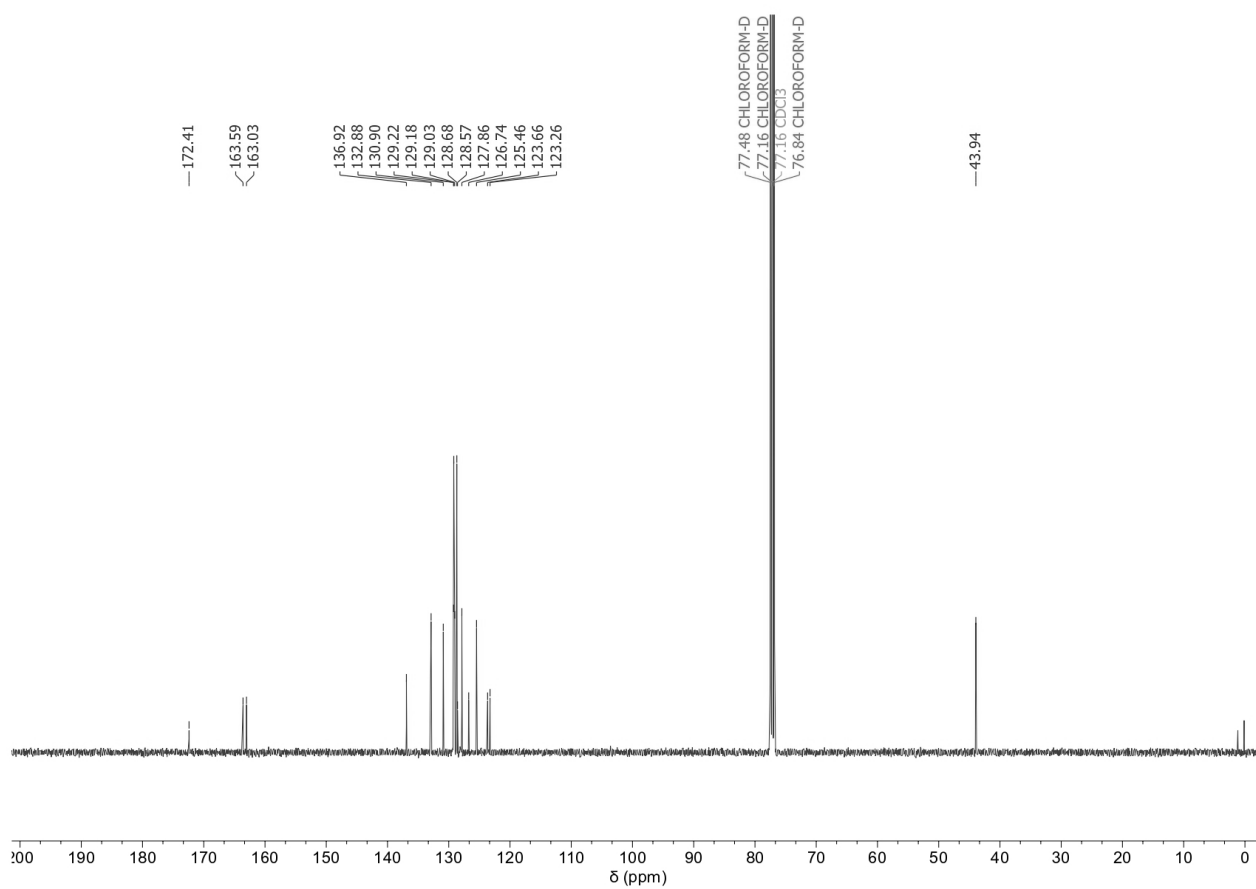
4-formamido-N-benzyl-1,8-naphthalimide (7). ^1H NMR (300 MHz, $\text{DMSO}-d_6$)

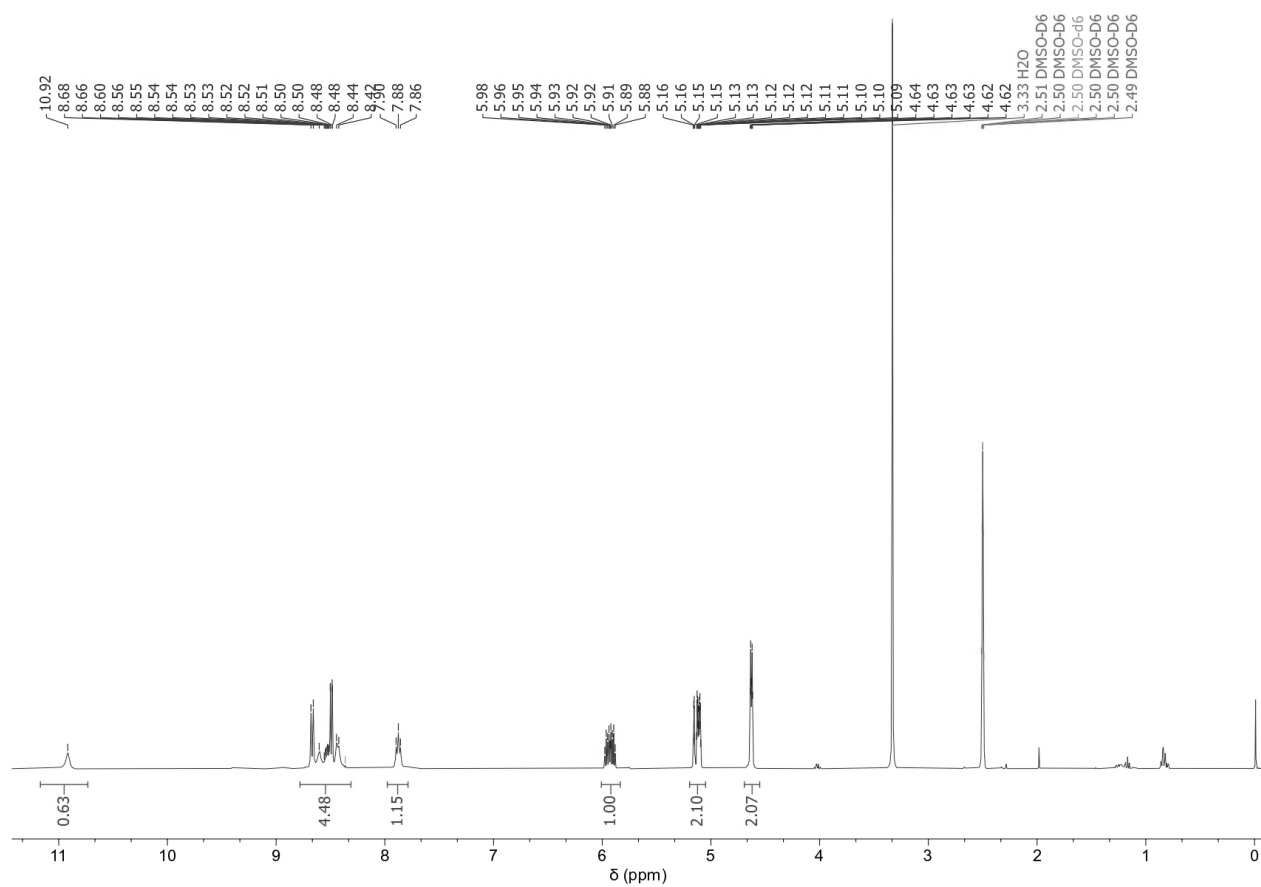
4-formamido-N-benzyl-1,8-naphthalimide (7). ^{13}C NMR (75 MHz, $\text{DMSO}-d_6$)

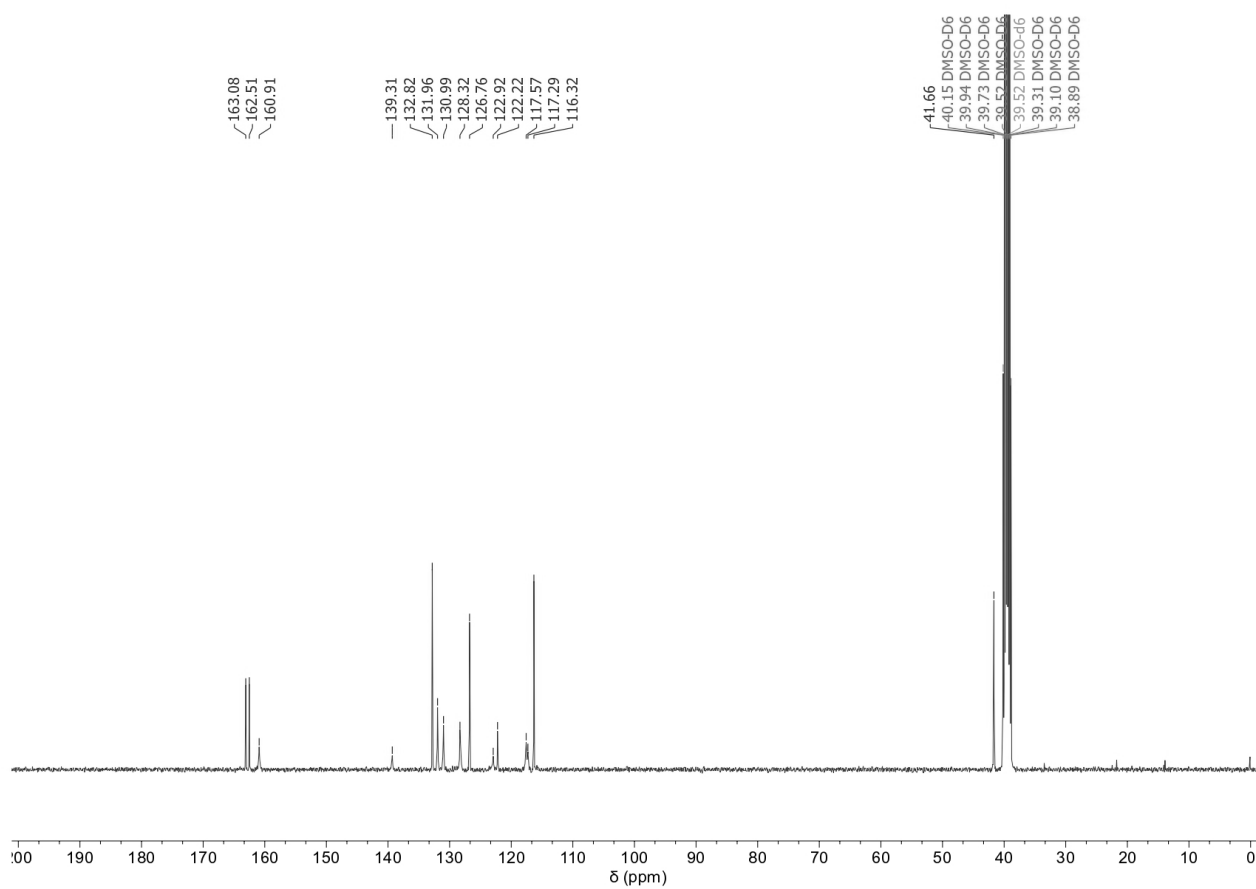
4-formamido-N-benzyl-1,8-naphthalimide (7). ^1H - ^1H COSY NMR (300 MHz for ^1H , CDCl_3)

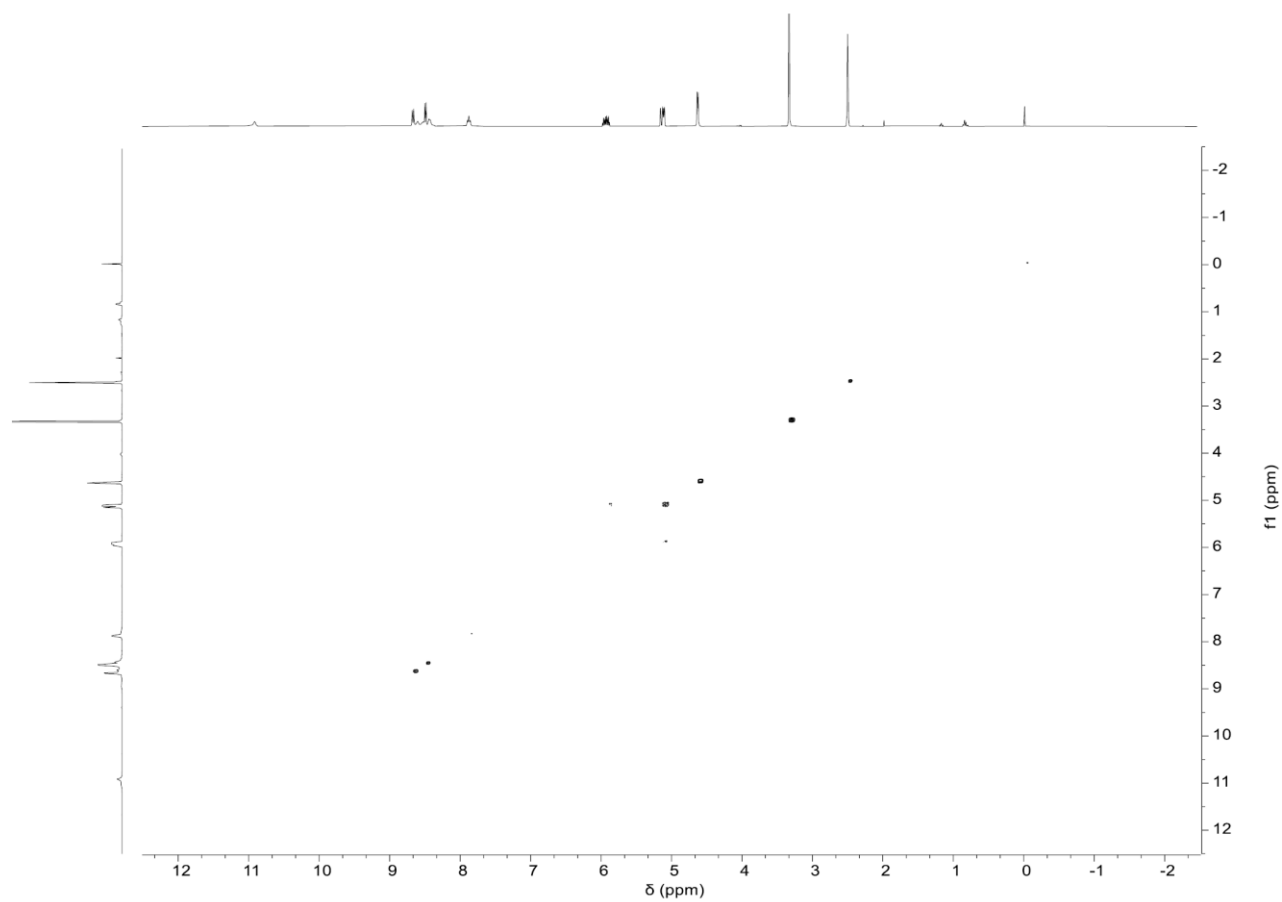
4-formamido-N-benzyl-1,8-naphthalimide (7). ^1H - ^{13}C HSQC NMR (300 MHz for ^1H , CDCl_3)

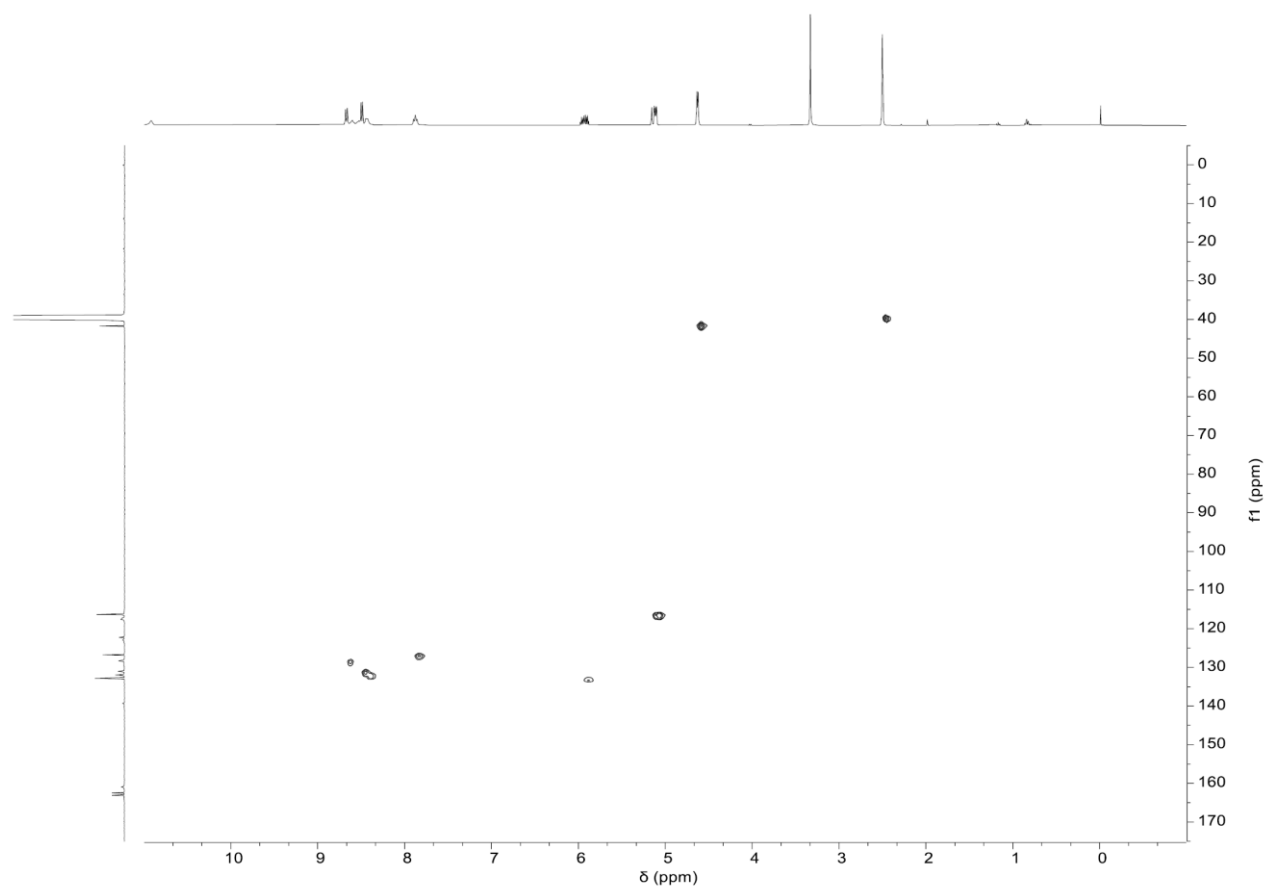
4-isocyano-N-benzyl-1,8-naphthalimide (8). ^1H NMR (400 MHz, CDCl_3)

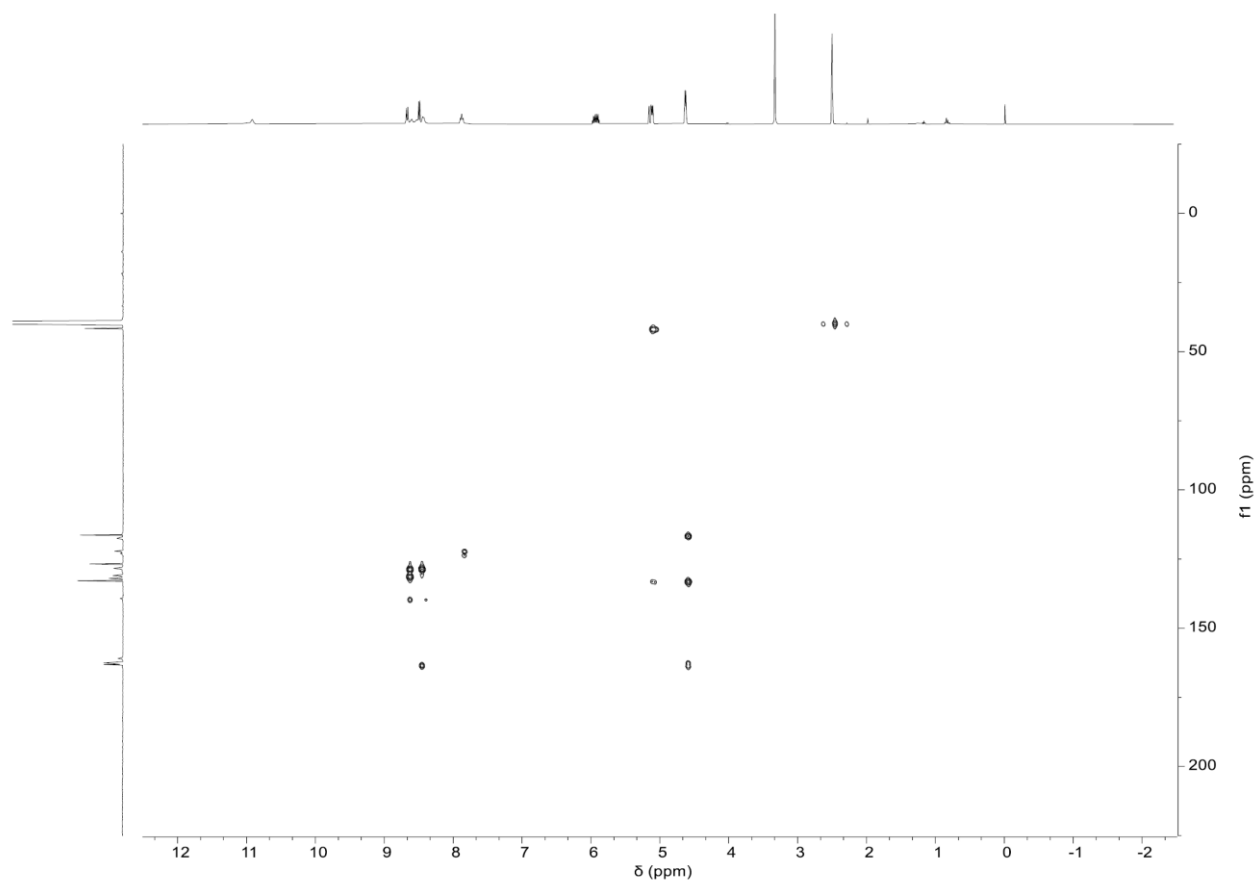
4-isocyano-N-benzyl-1,8-naphthalimide (8). ^{13}C NMR (101 MHz, CDCl_3)

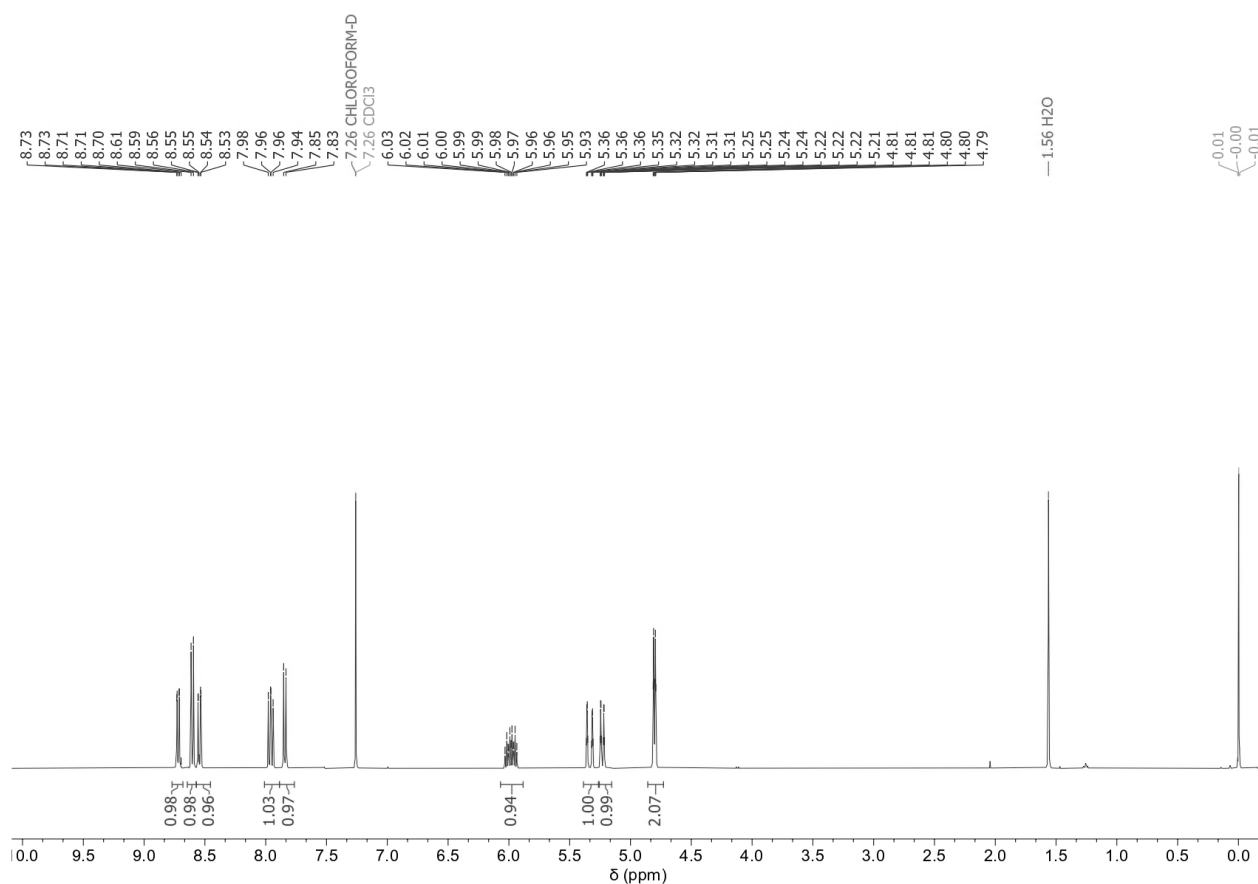
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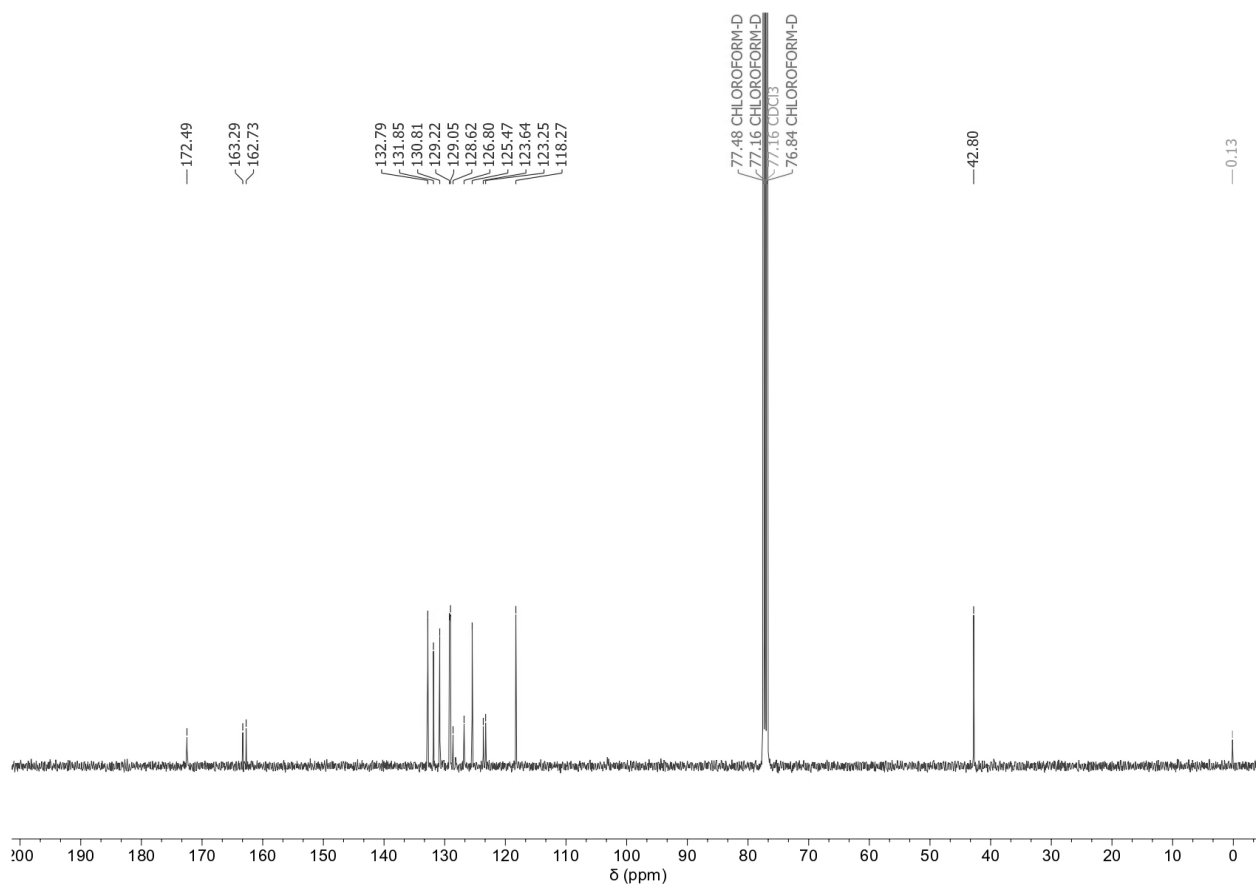
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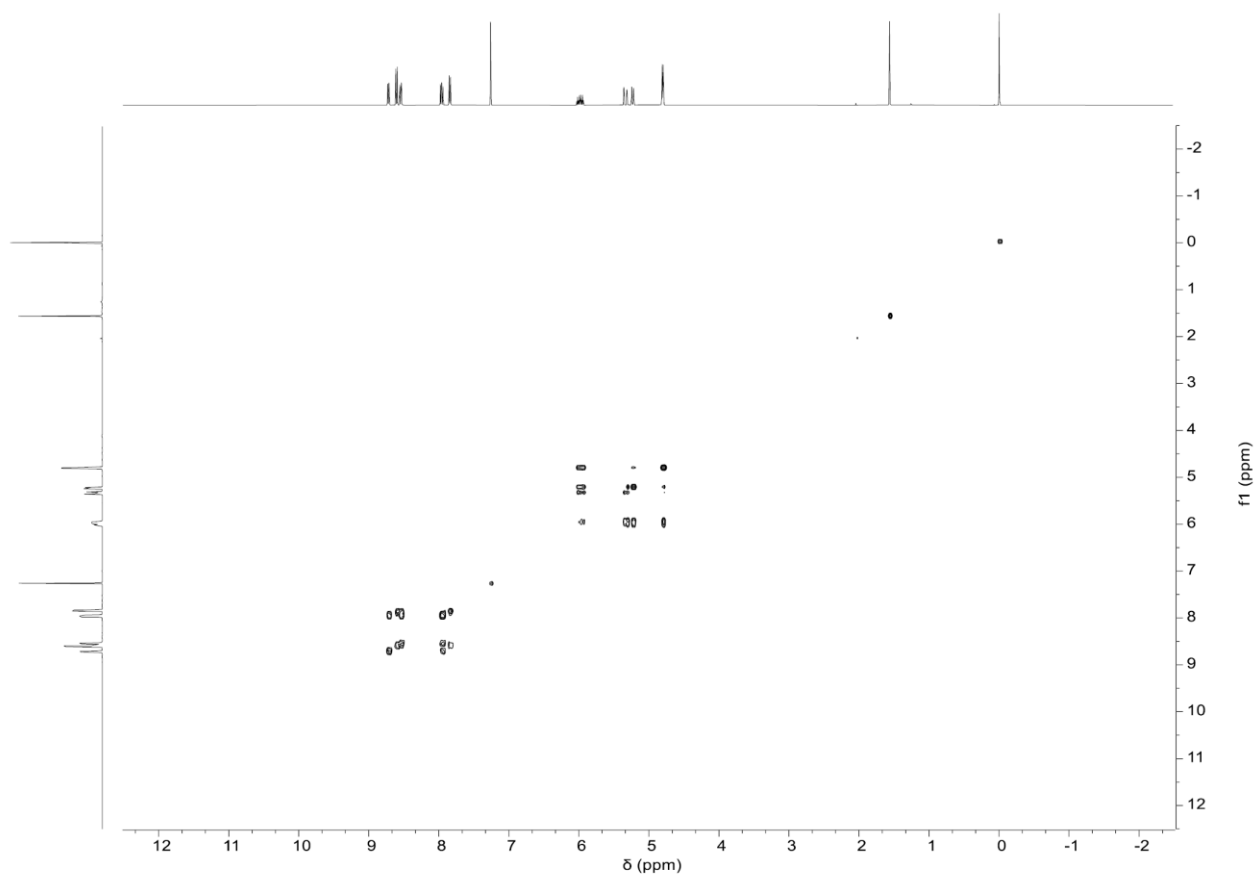
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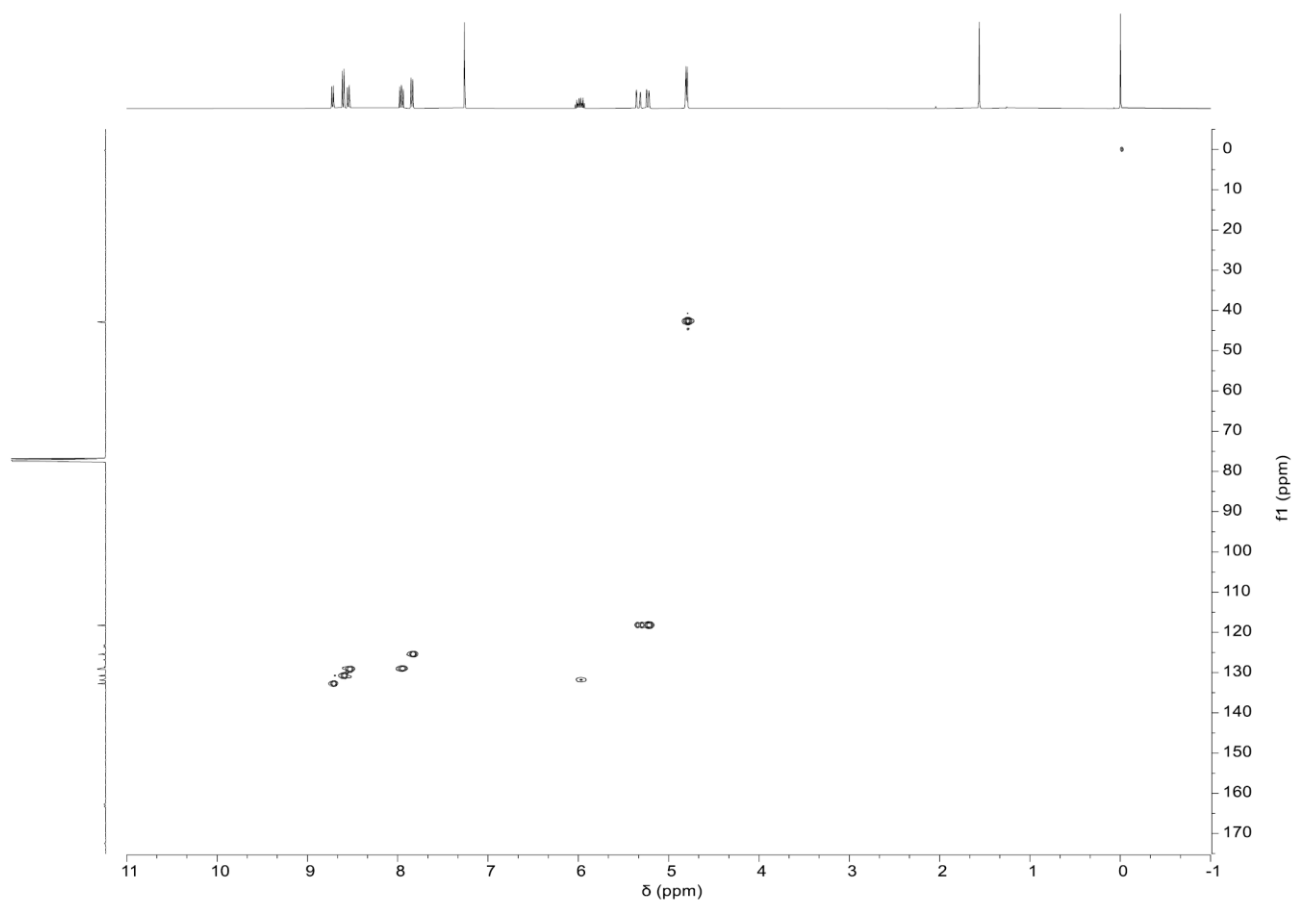
4-formamido-N-allyl-1,8-naphthalimide (11). ^1H - ^{13}C HSQC NMR (400 MHz for ^1H , CDCl_3)

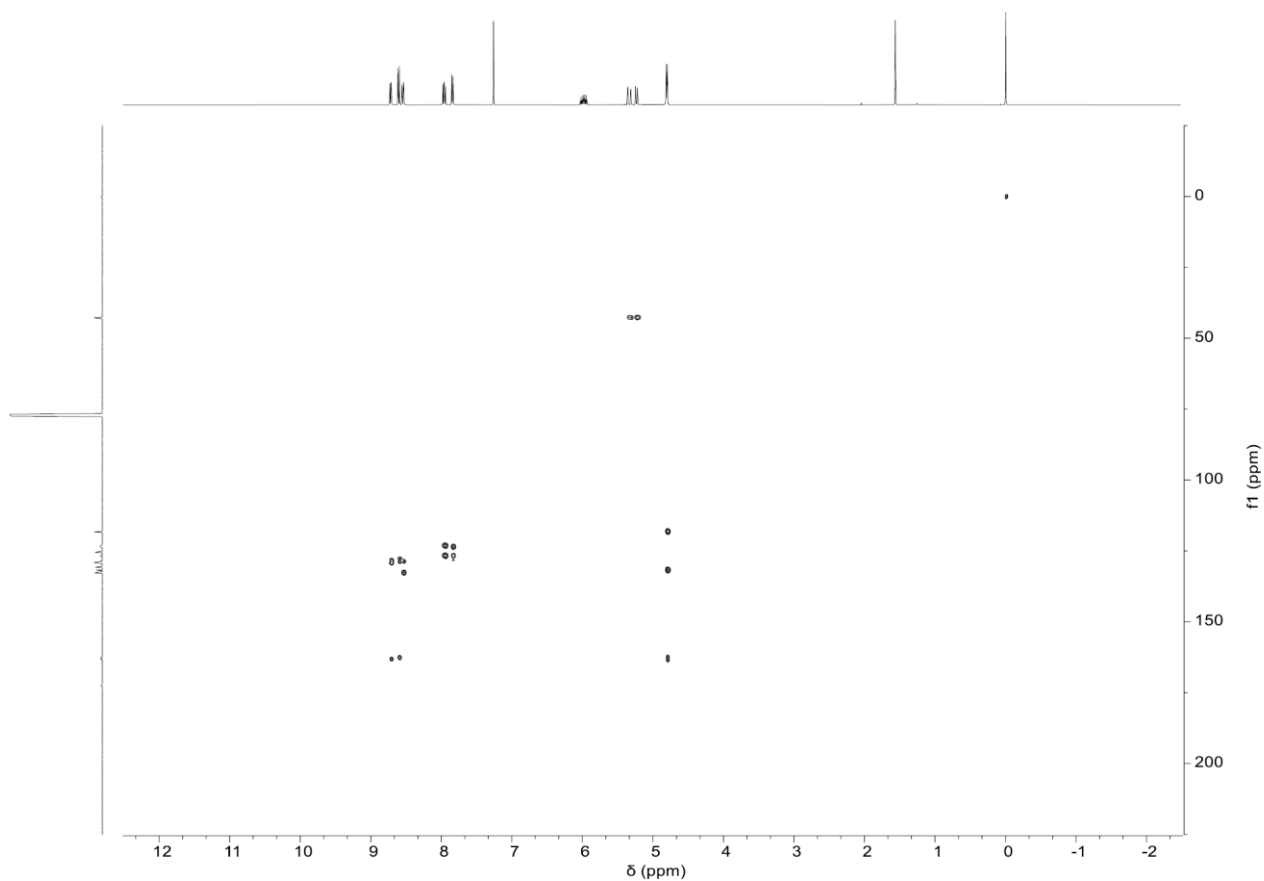
4-formamido-N-allyl-1,8-naphthalimide (11). ^1H - ^{13}C HMBC NMR (400 MHz for ^1H , CDCl_3)

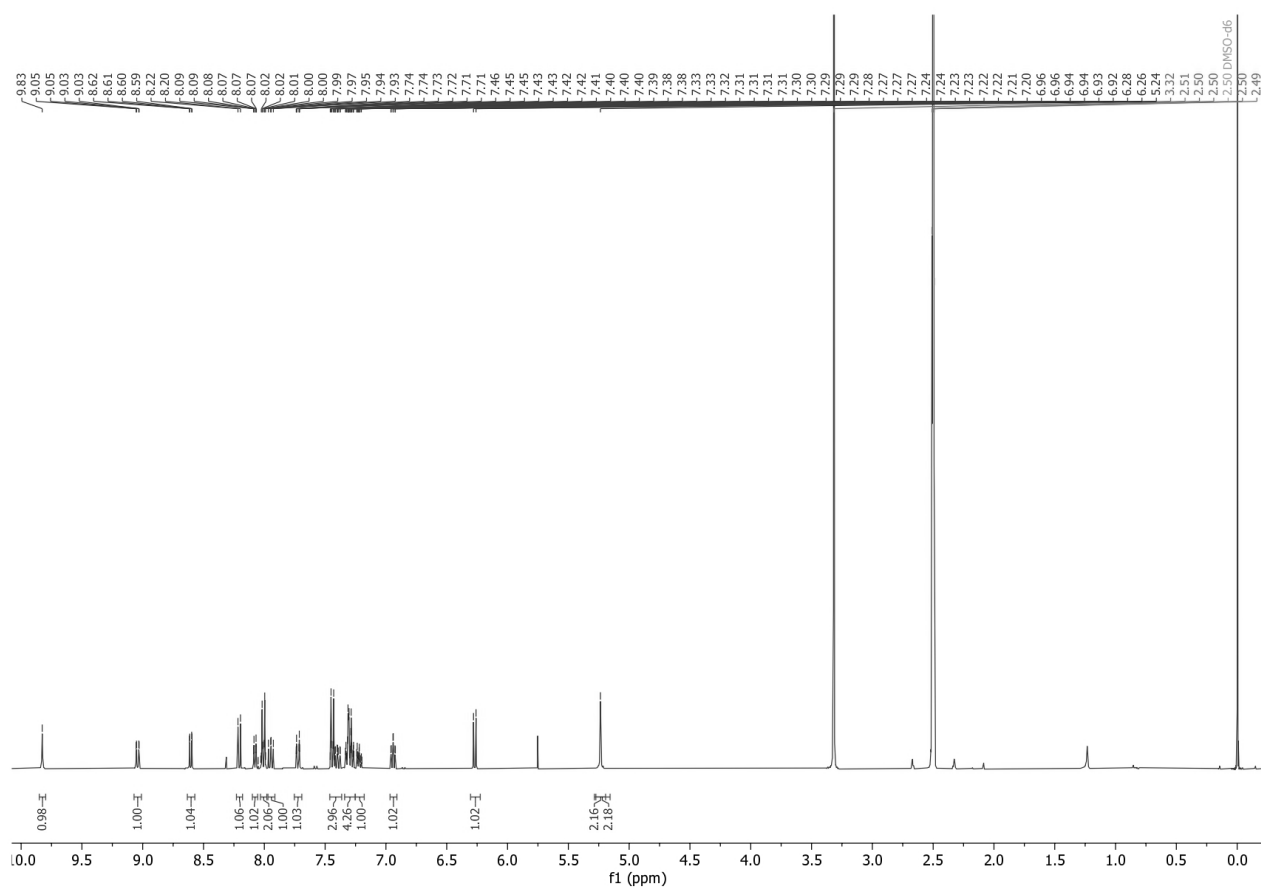
4-isocyano-N-allyl-1,8-naphthalimide (12). ^1H NMR (400 MHz, CDCl_3)

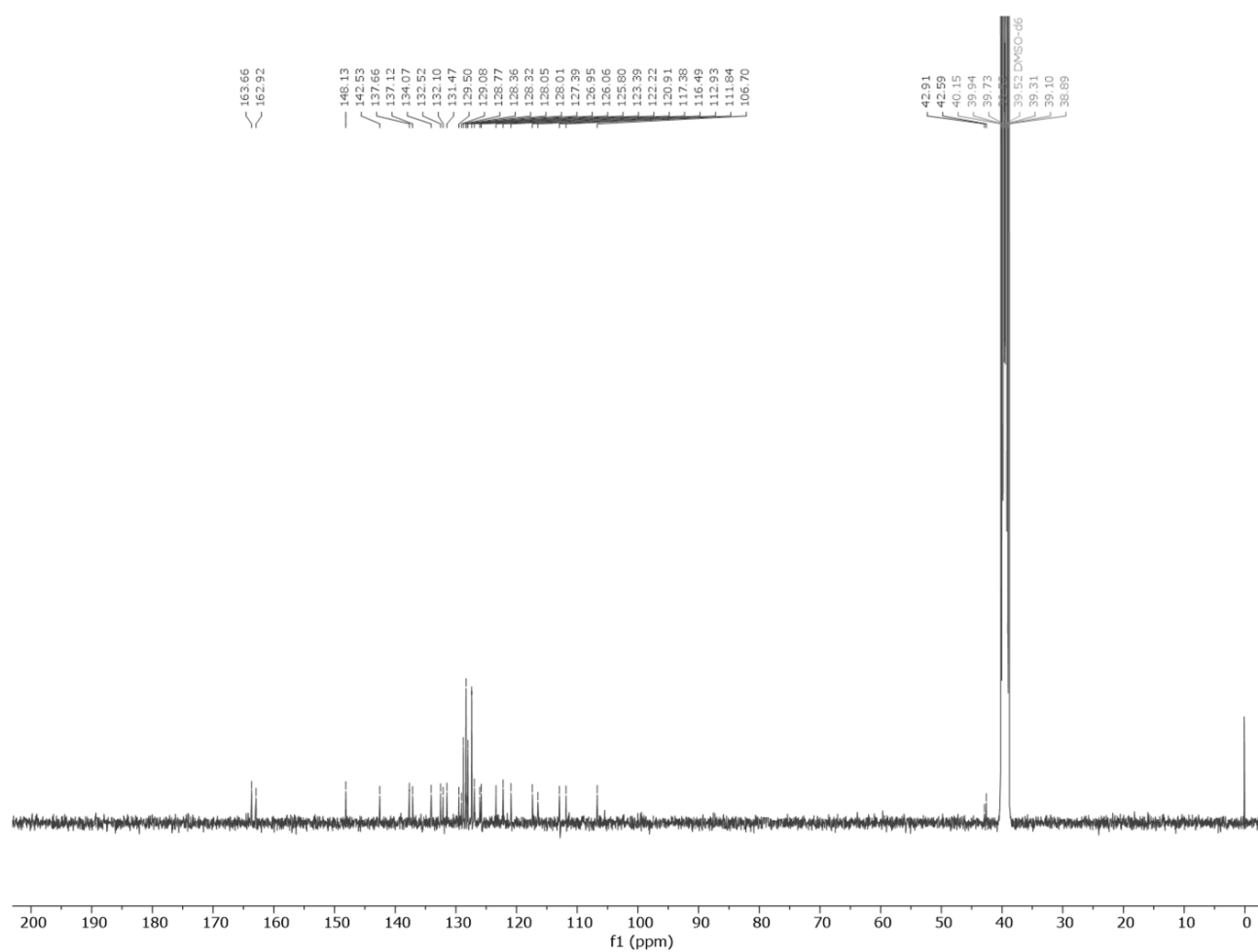
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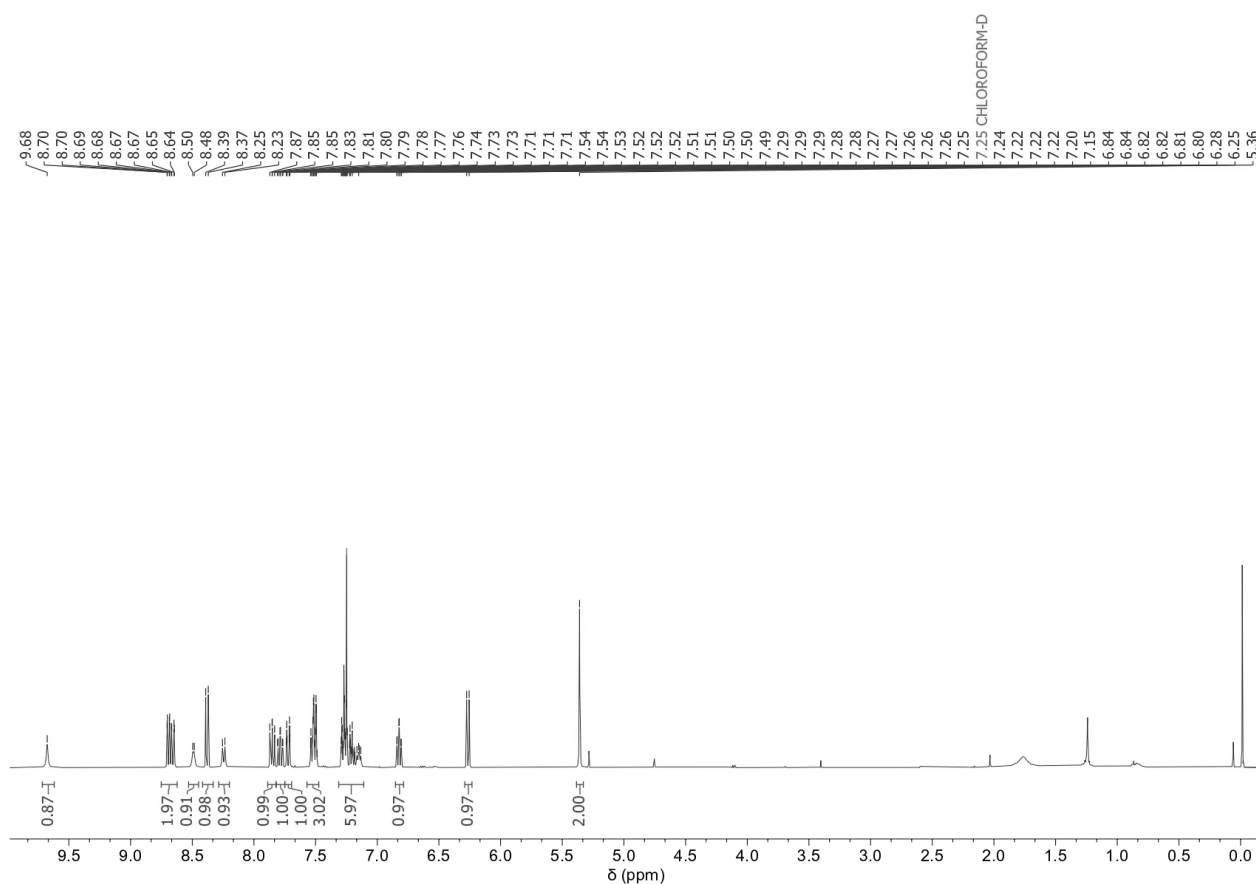
4-isocyano-N-allyl-1,8-naphthalimide (12). ^1H - ^1H COSY NMR (400 MHz for ^1H , CDCl_3)

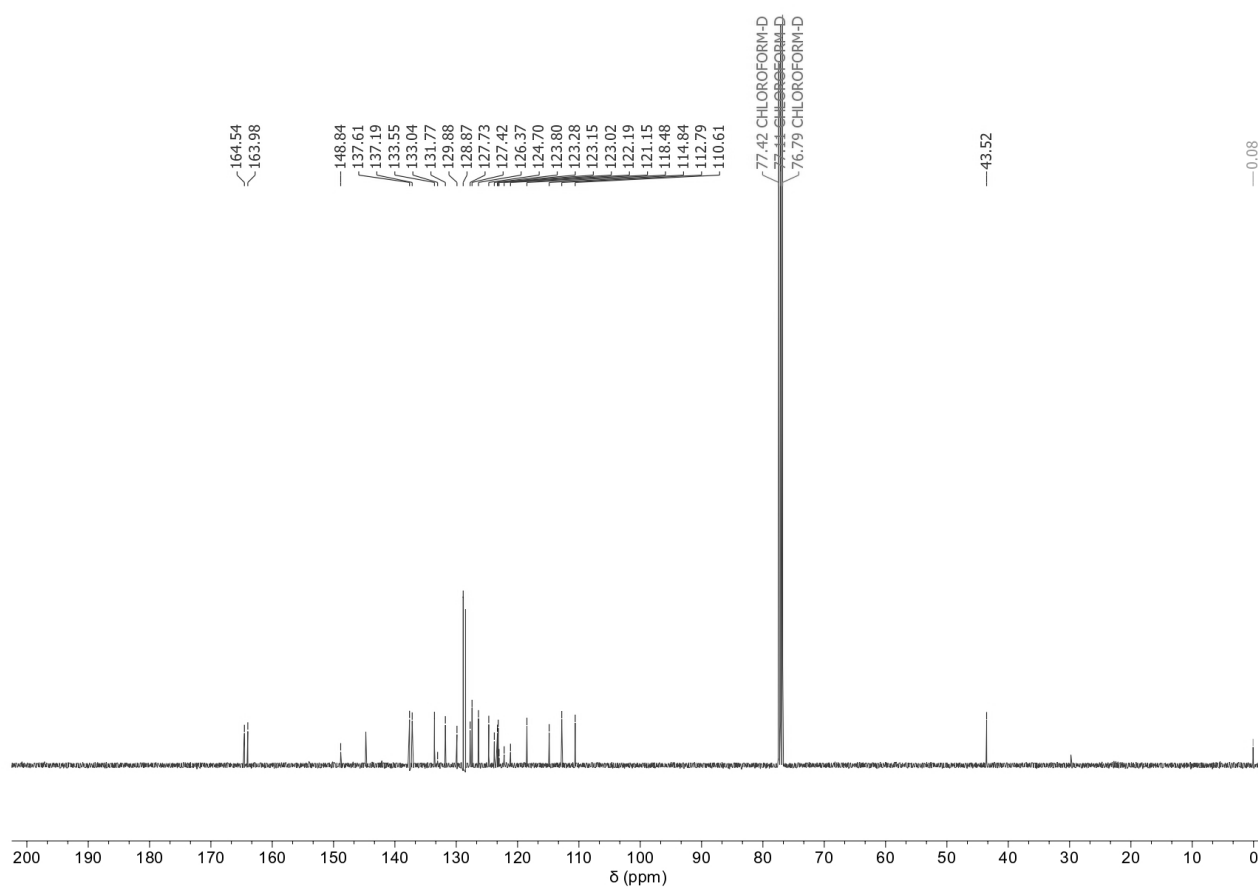
4-isocyano-N-allyl-1,8-naphthalimide (12) ^1H - ^{13}C HSQC NMR (400 MHz for ^1H , CDCl_3)

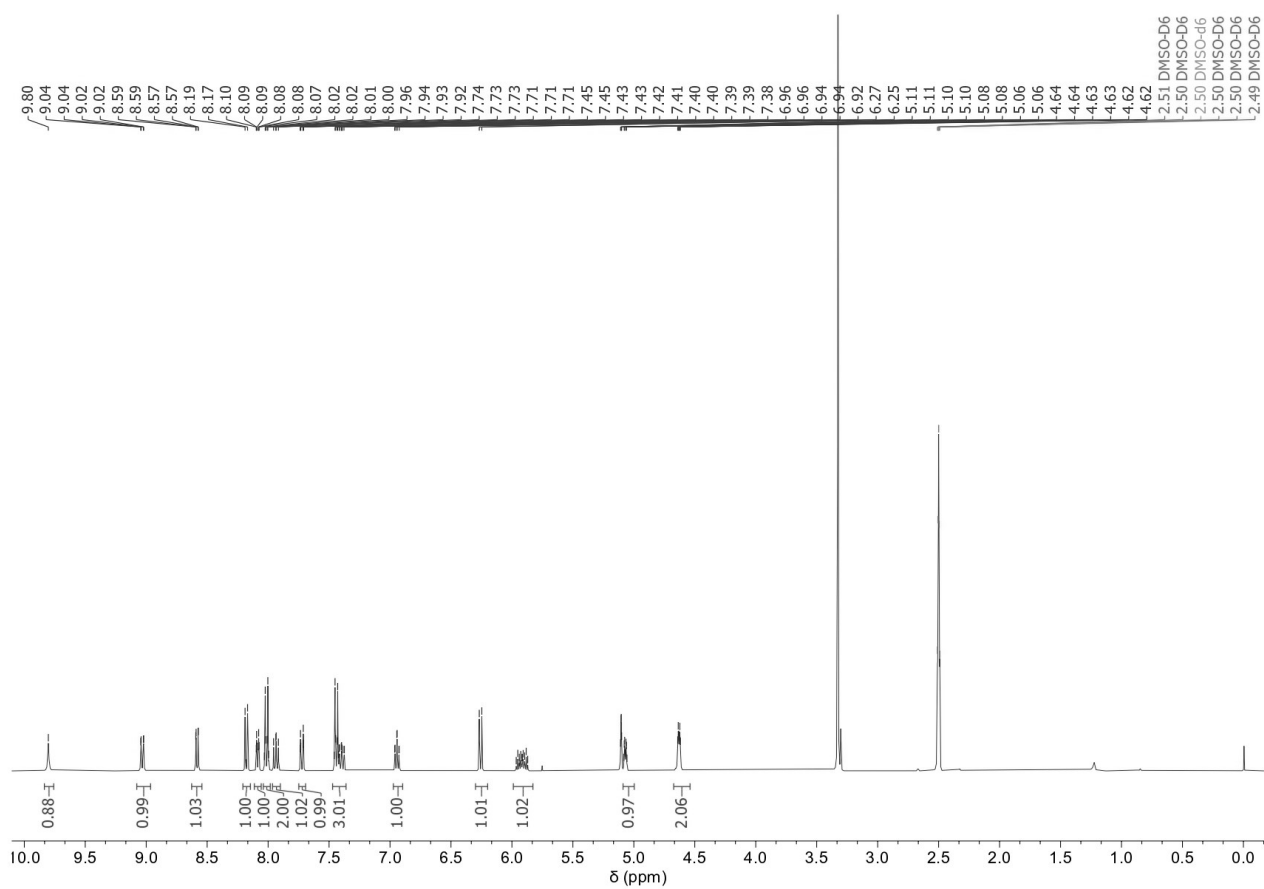
4-isocyano-N-allyl-1,8-naphthalimide (12) ^1H - ^{13}C HMBC NMR (400 MHz for ^1H , CDCl_3)

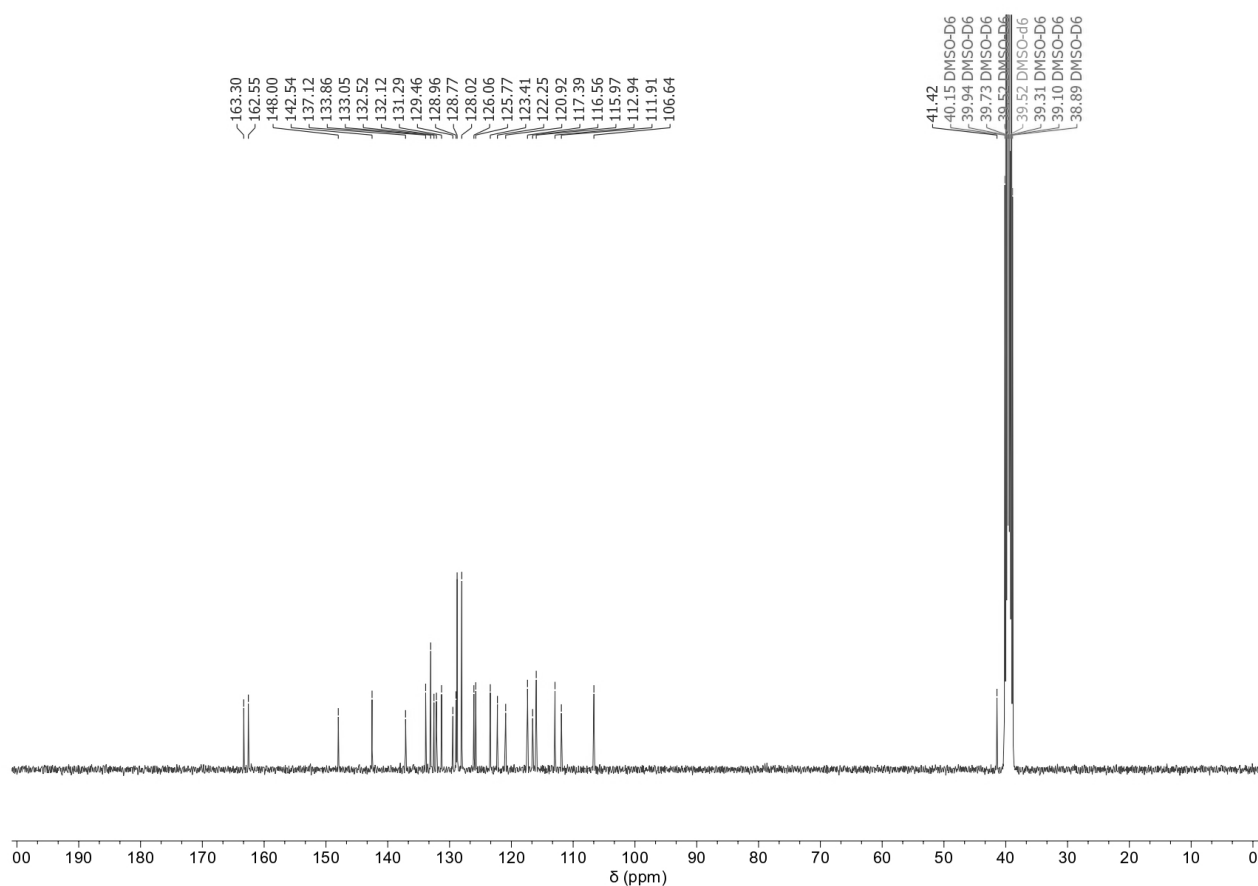
N-benzyl-1,8-naphthalimide-based GBB adduct (15). ^1H NMR (300 MHz, $\text{DMSO}-d_6$)

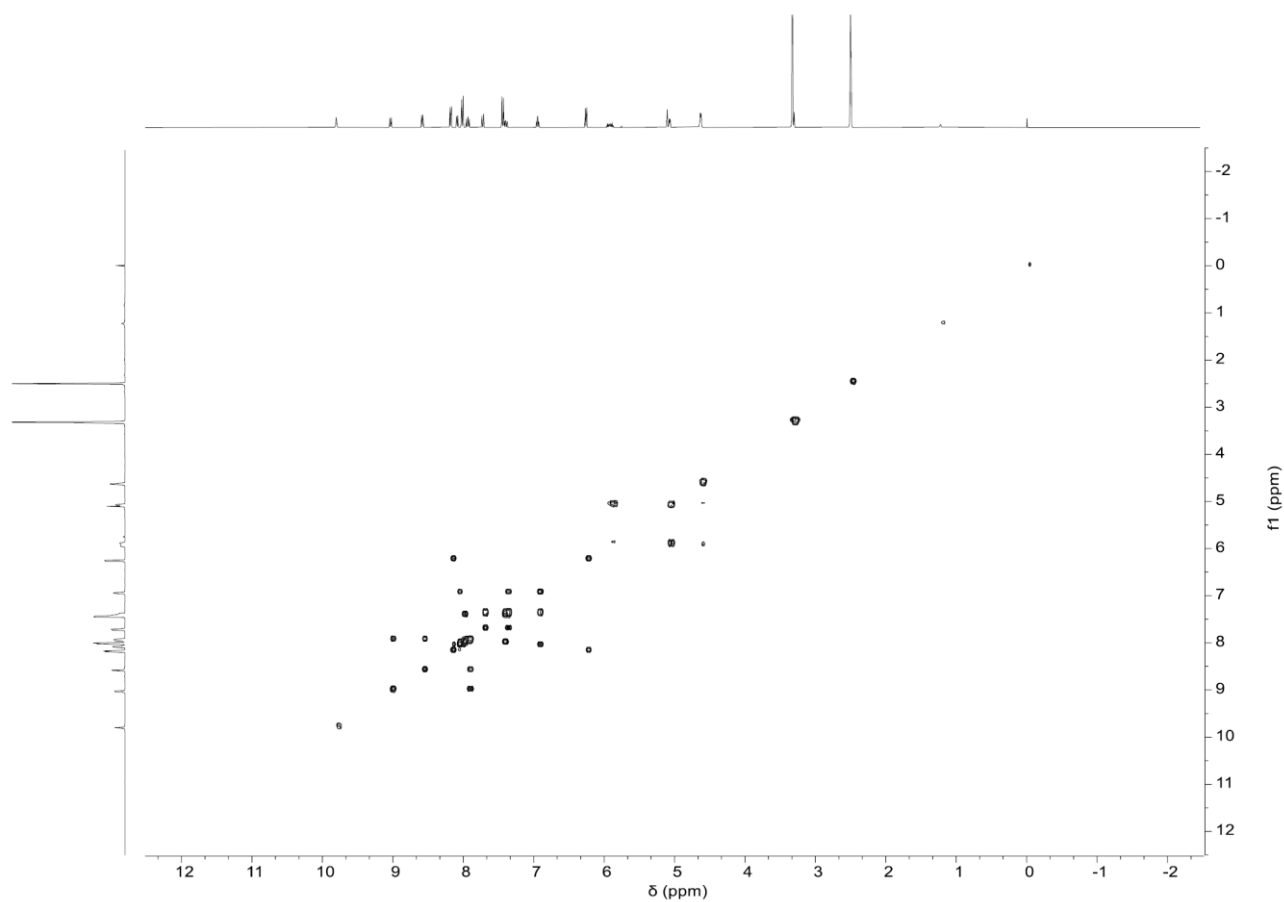
N-benzyl-1,8-naphthalimide-based GBB adduct (15). ^{13}C NMR (75 MHz, $\text{DMSO}-d_6$)

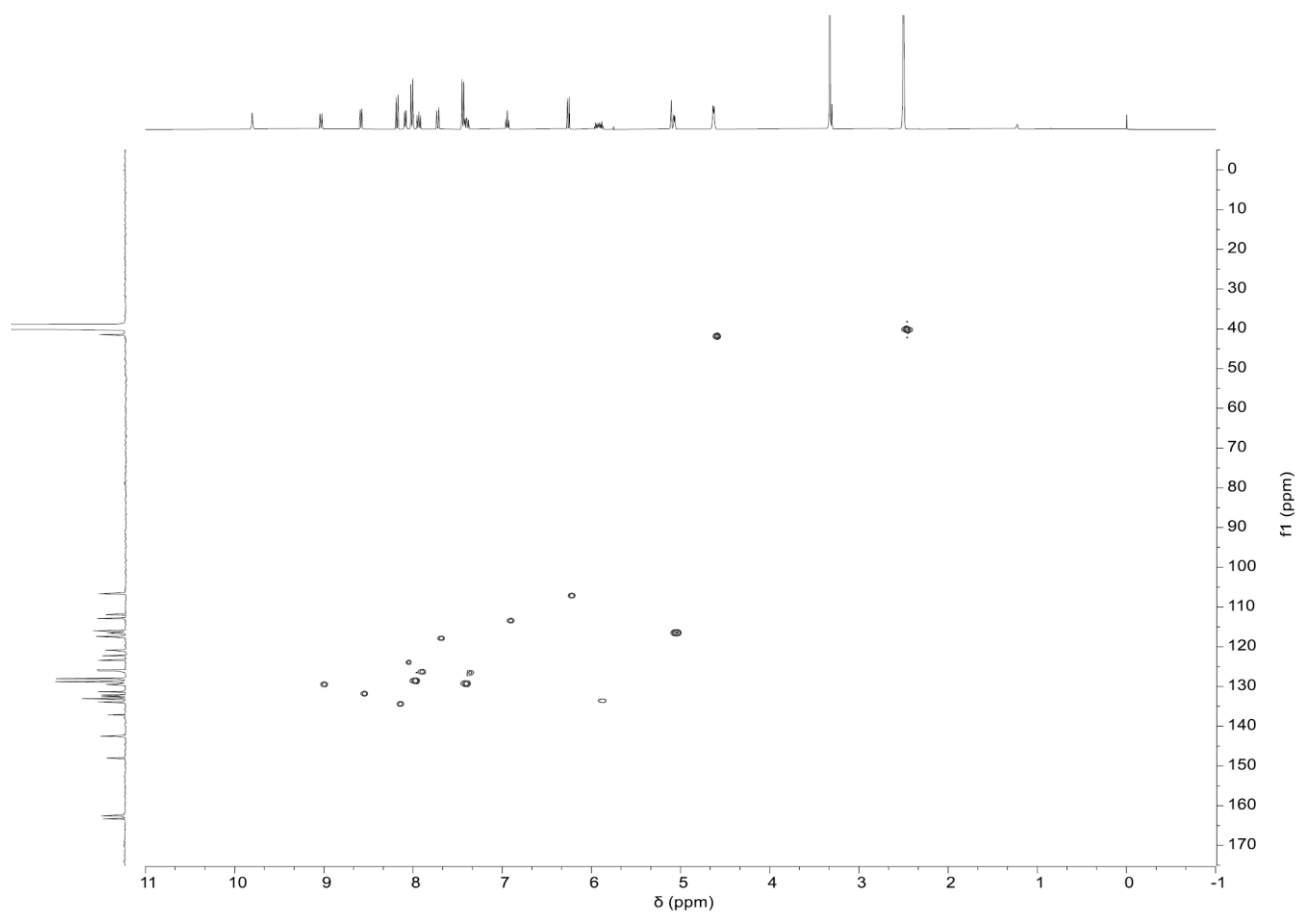
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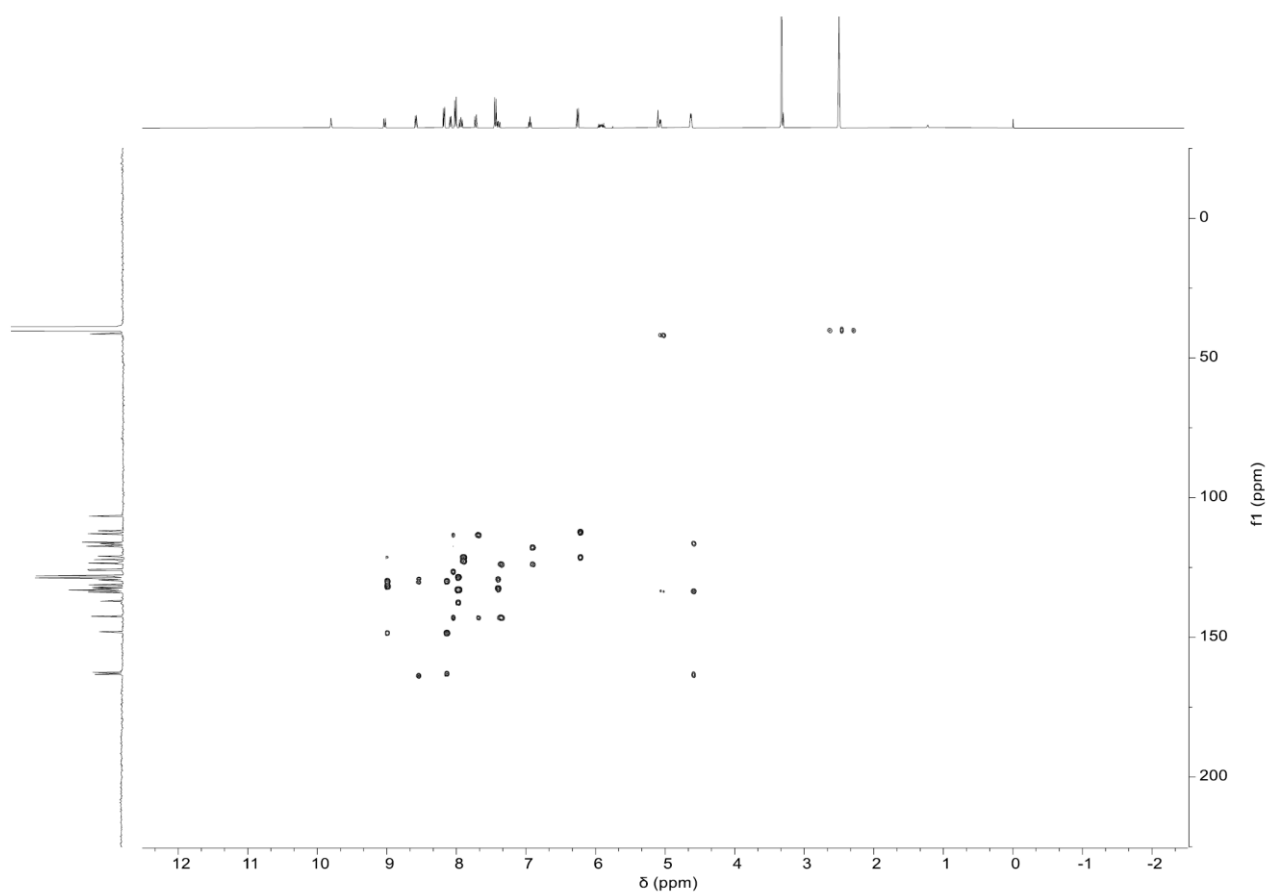
N-benzyl-1,8-naphthalimide-based GBB adduct (16). ^{13}C NMR (101 MHz, CDCl_3)

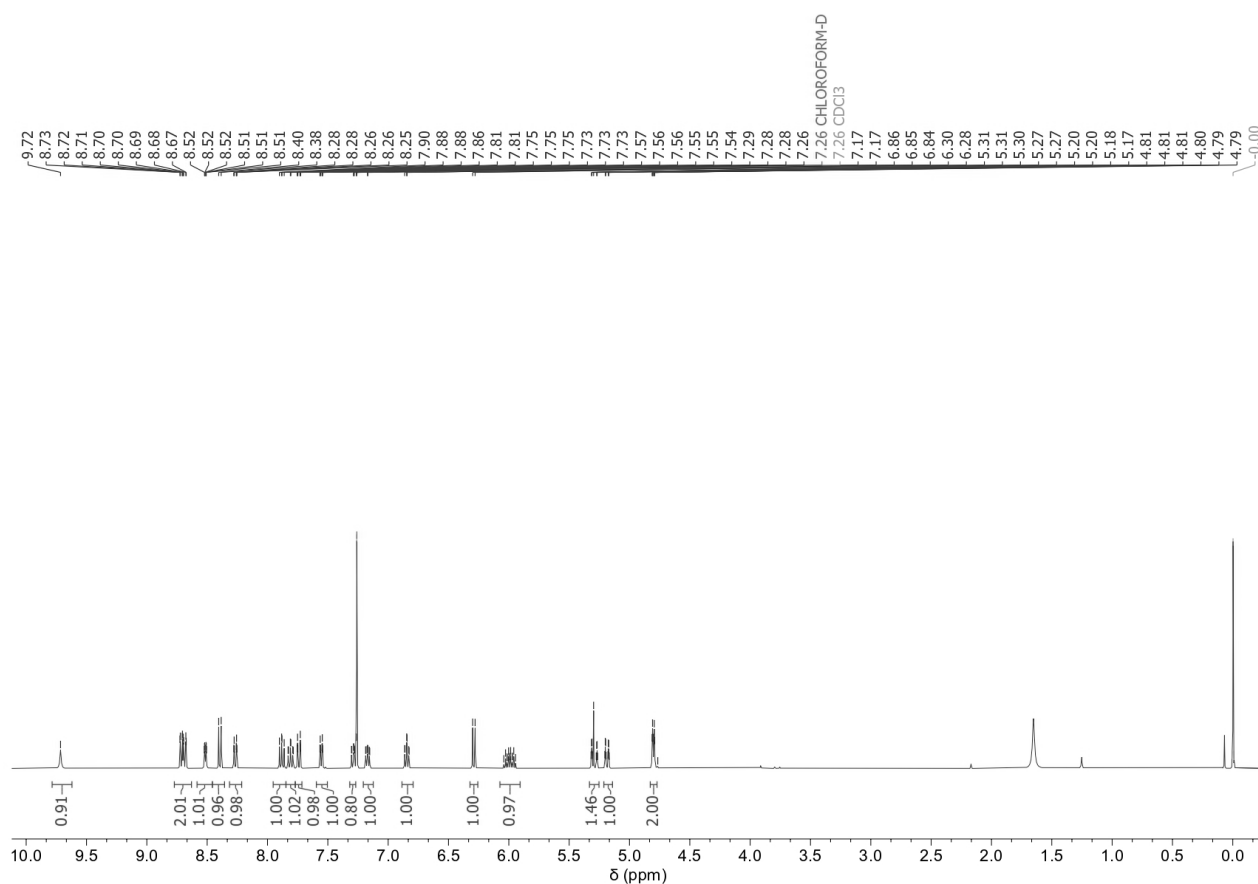
N-allyl-1,8-naphthalimide-based GBB adduct (17). ^1H NMR (400 MHz, $\text{DMSO}-d_6$)

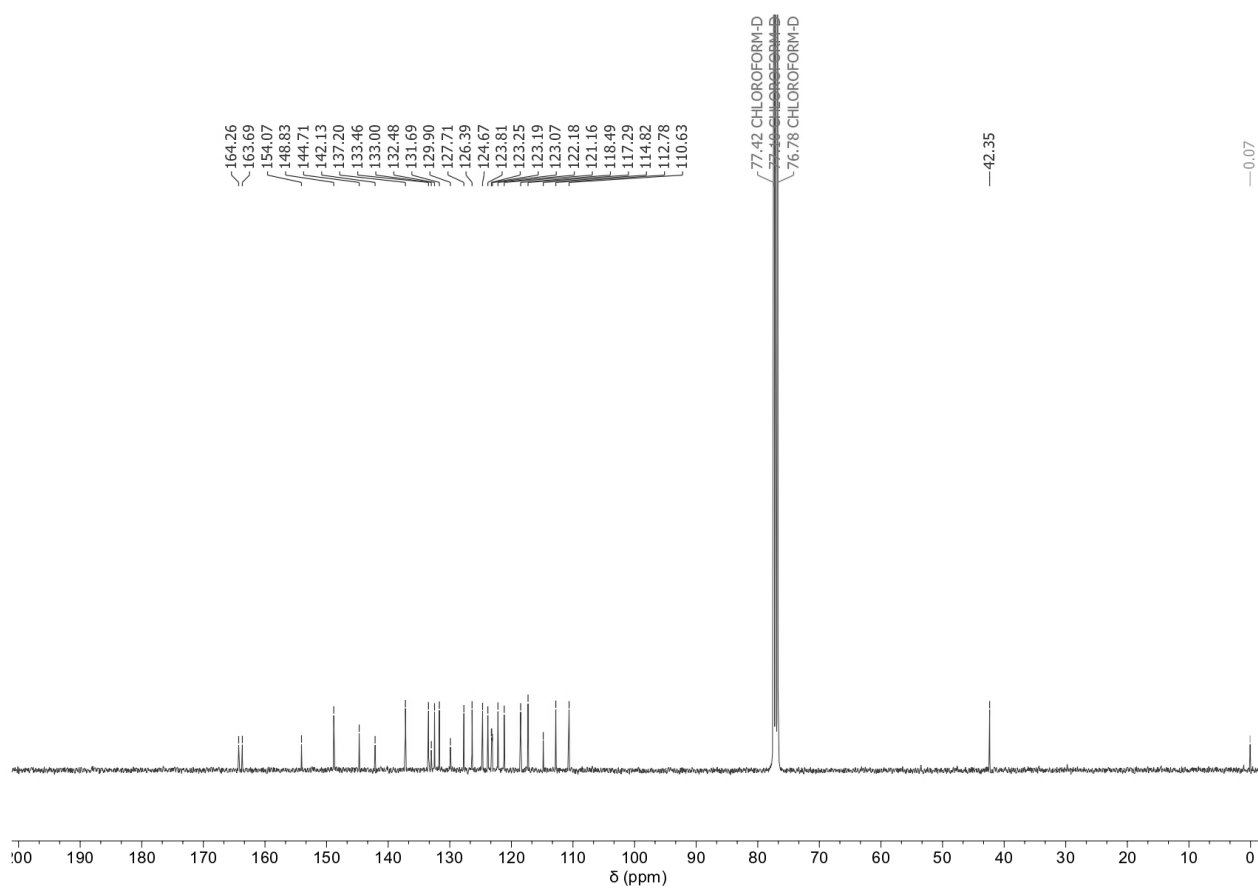
N-allyl-1,8-naphthalimide-based GBB adduct (17). ^{13}C NMR (101 MHz, $\text{DMSO-}d_6$)

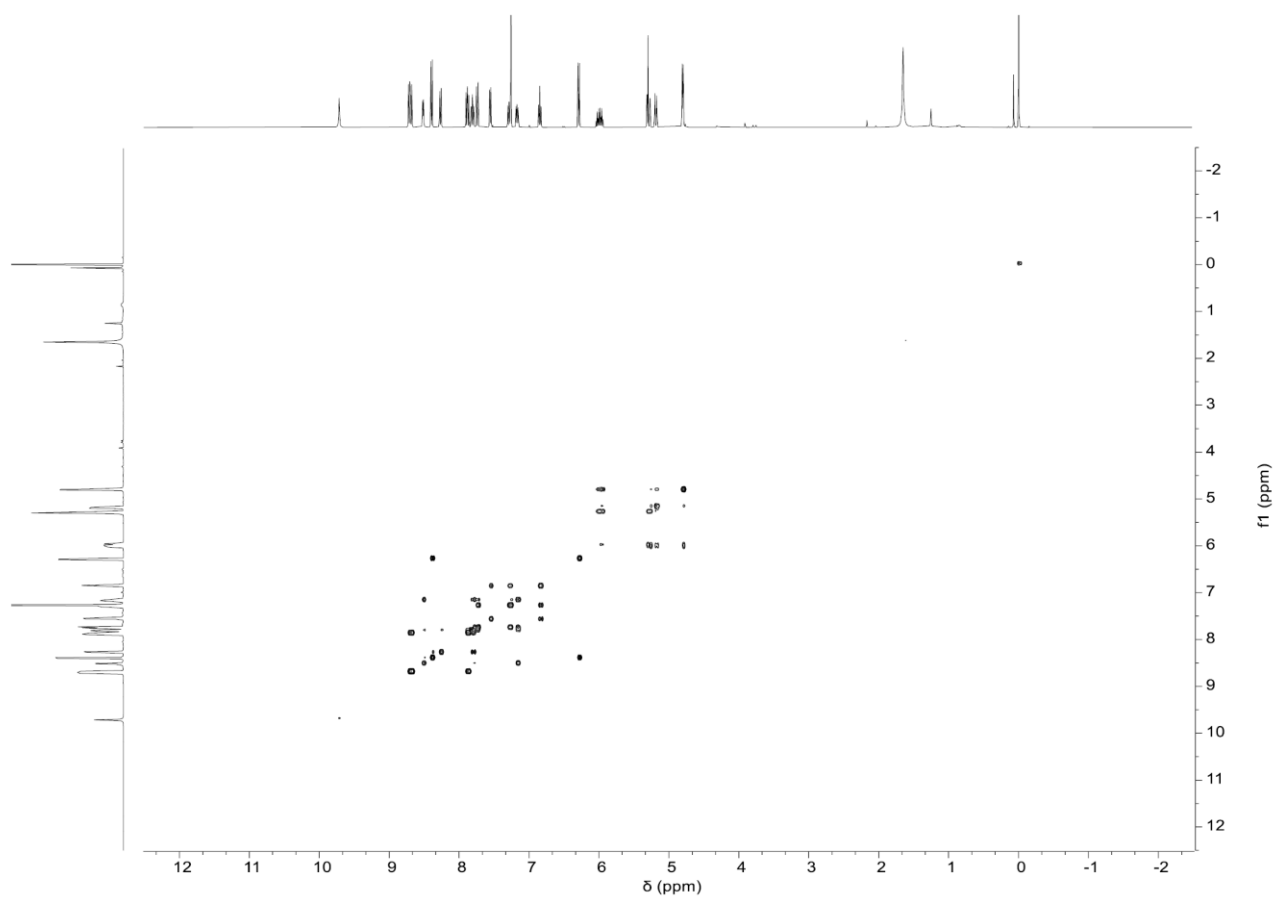
N-allyl-1,8-naphthalimide-based GBB adduct (17) ^1H - ^1H COSY NMR (400 MHz for ^1H , CDCl_3)

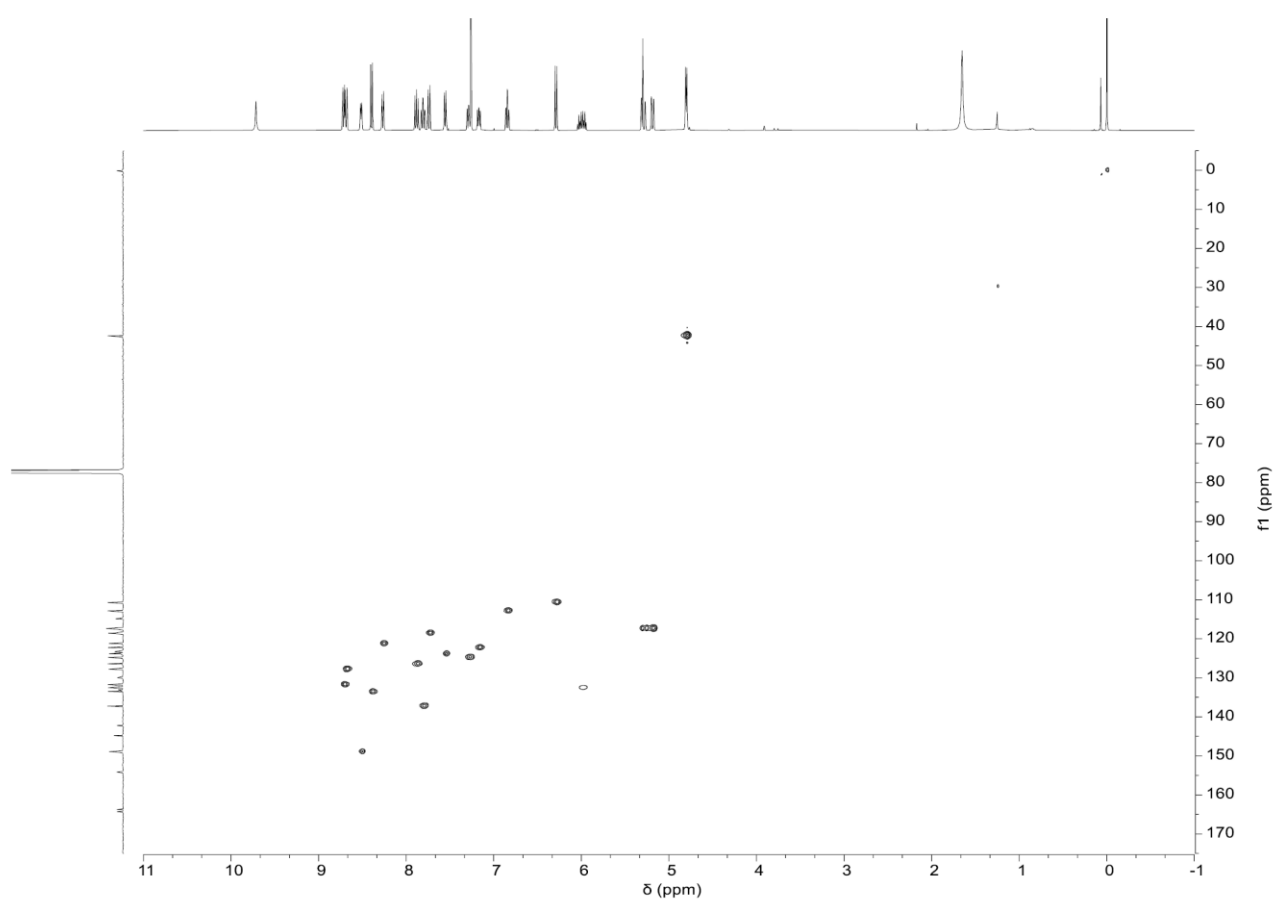
N-allyl-1,8-naphthalimide-based GBB adduct (17) ^1H - ^{13}C HSQC NMR (400 MHz for ^1H , CDCl_3)

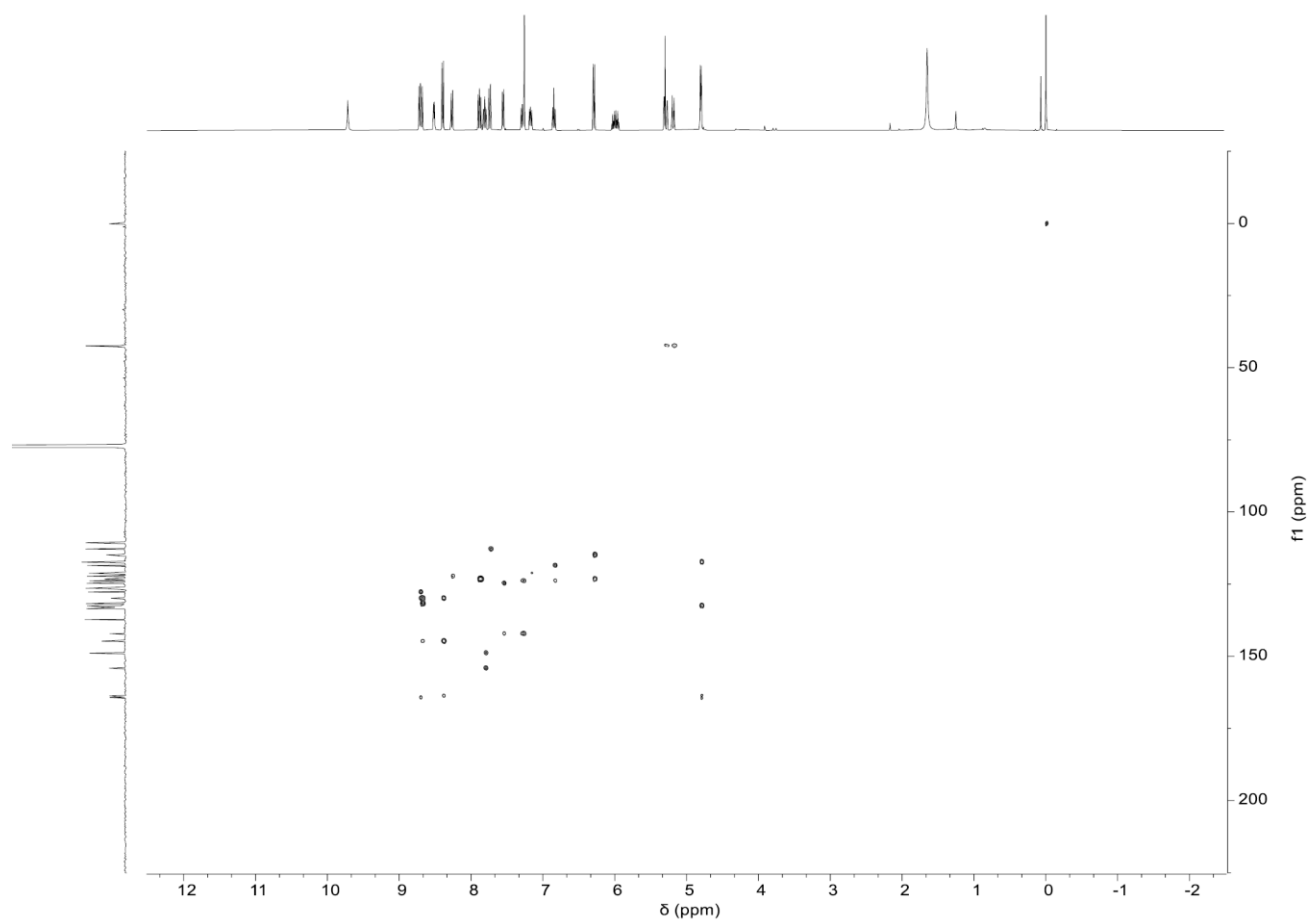
N-allyl-1,8-naphthalimide-based GBB adduct (17) ^1H - ^{13}C HMBC NMR (400 MHz for ^1H , CDCl_3)

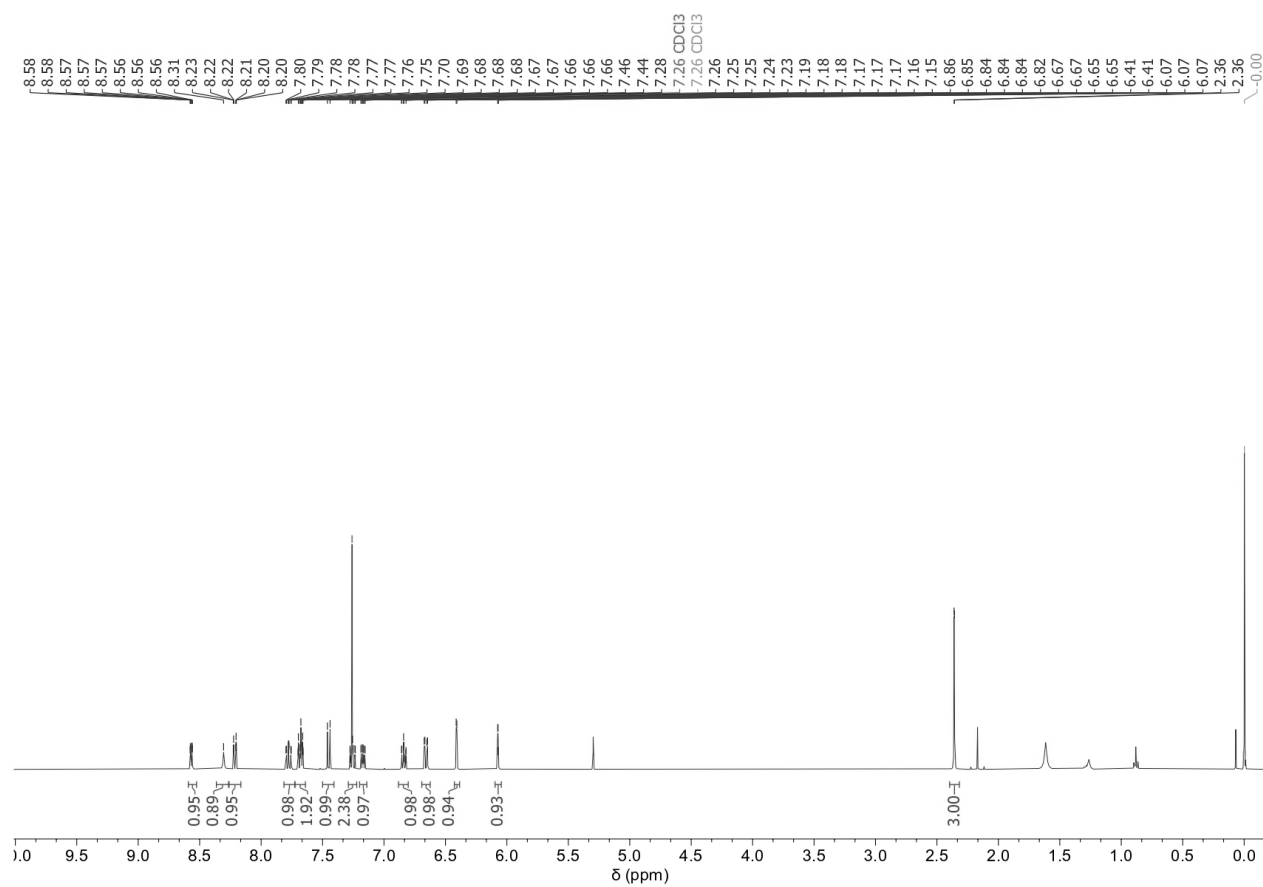
N-allyl-1,8-naphthalimide-based GBB adduct (18). ^1H NMR (400 MHz, CDCl_3)

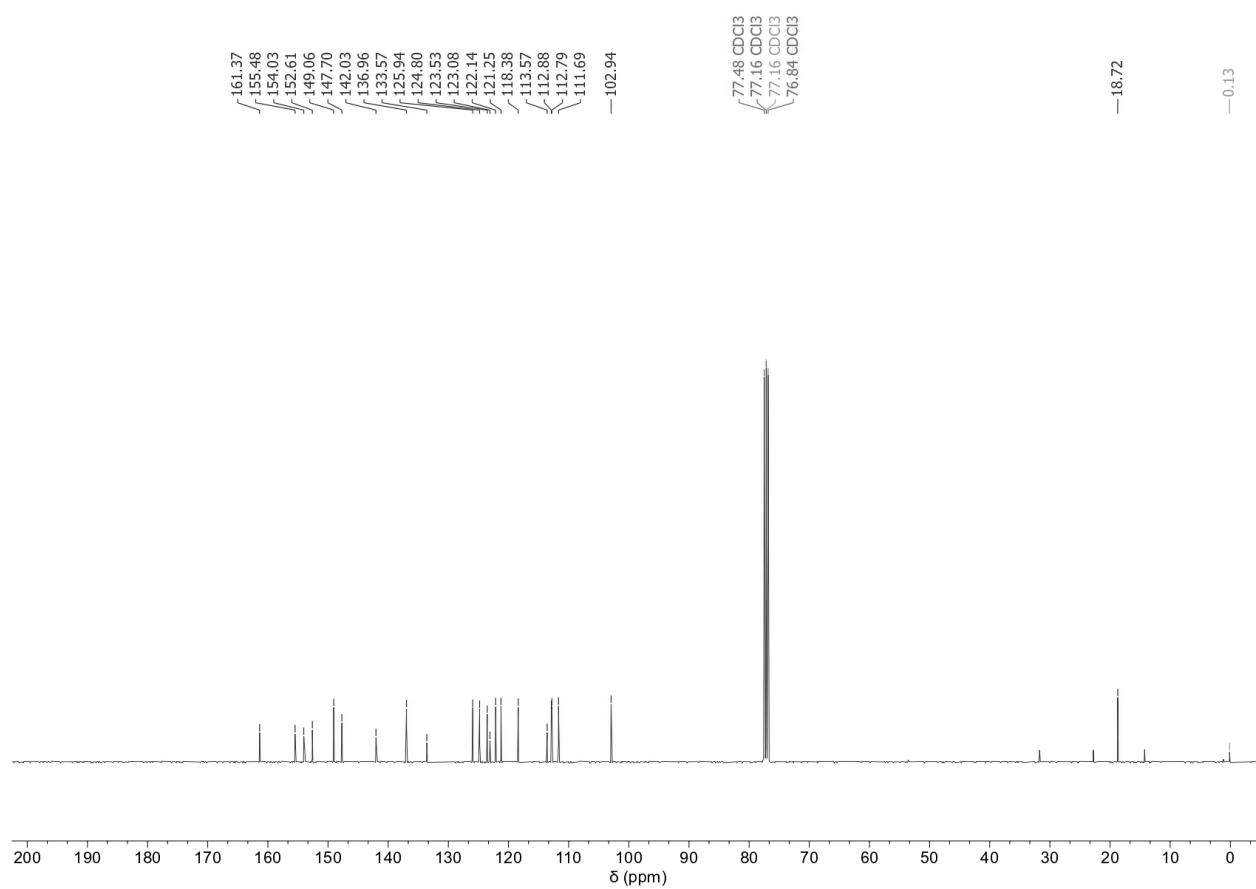
N-allyl-1,8-naphthalimide-based GBB adduct (18). ^{13}C NMR (101 MHz, CDCl_3)

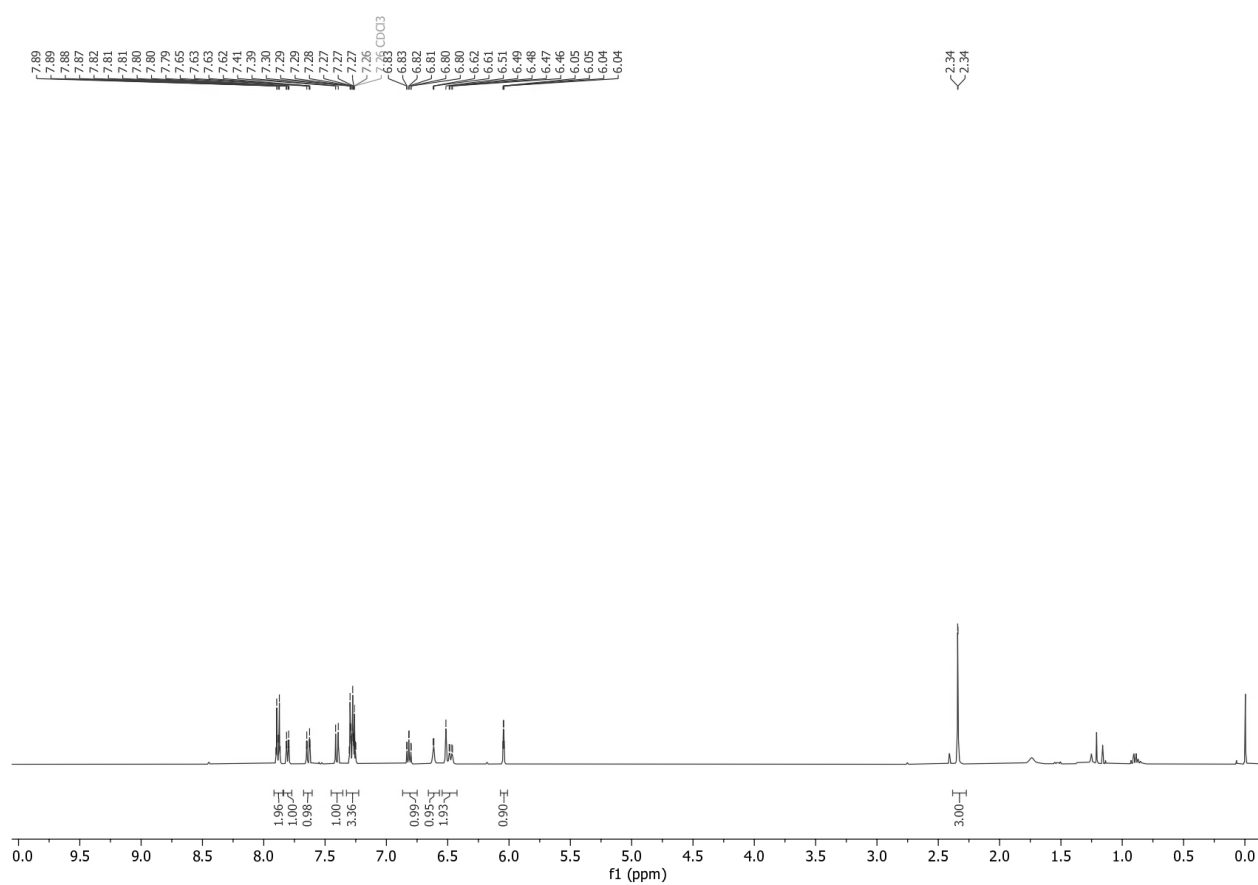
N-allyl-1,8-naphthalimide-based GBB adduct (18) ^1H - ^1H COSY NMR (400 MHz for ^1H , CDCl_3)

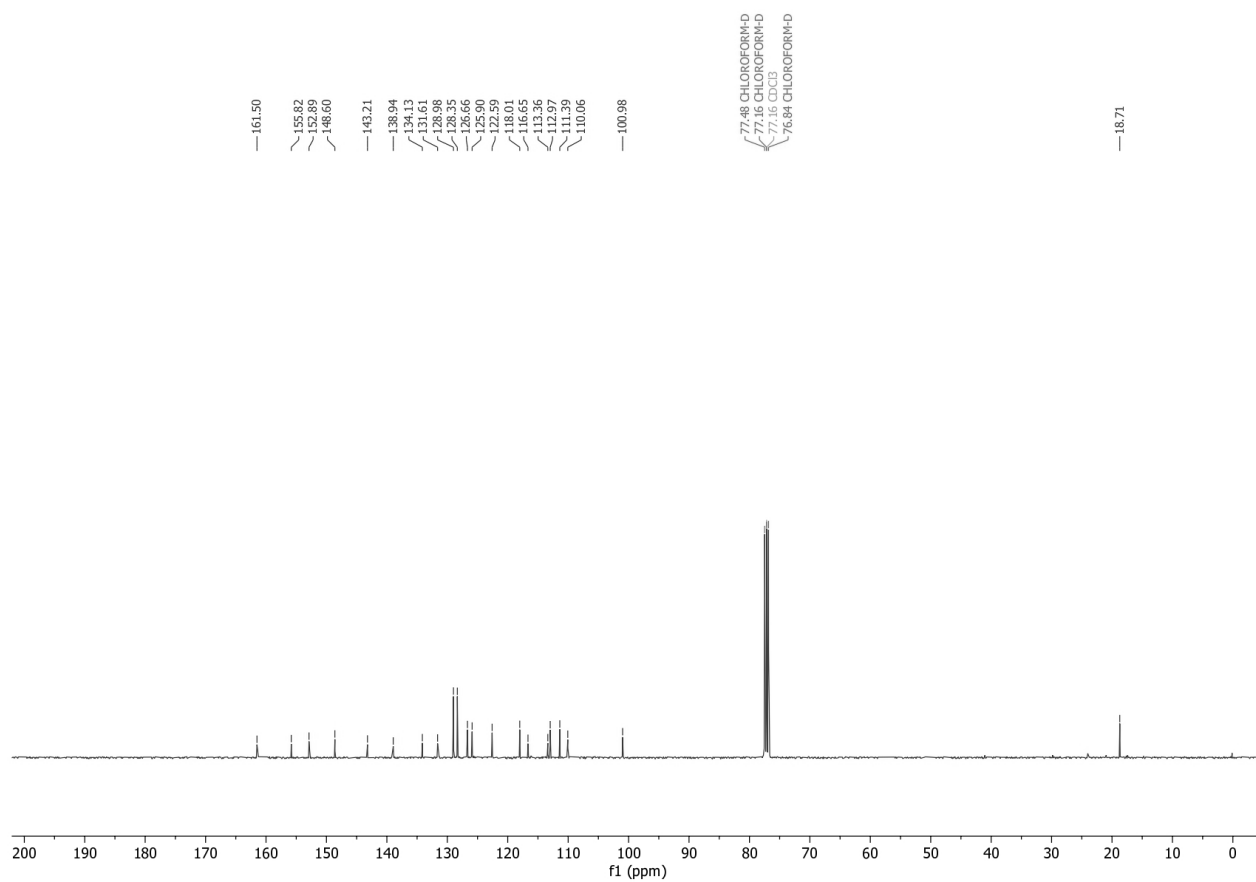
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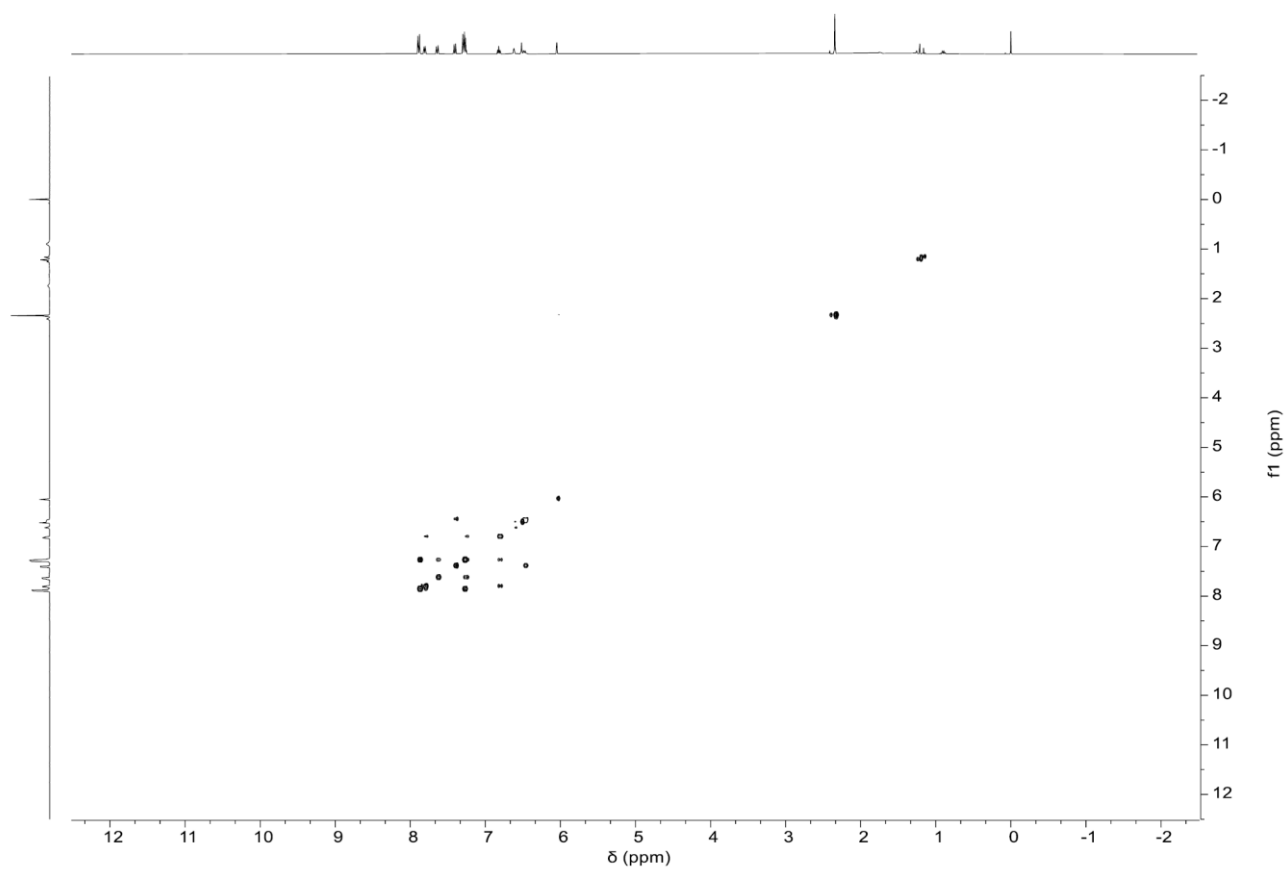
N-allyl-1,8-naphthalimide-based GBB adduct (18) ^1H - ^{13}C HMBC NMR (400 MHz for ^1H , CDCl_3)

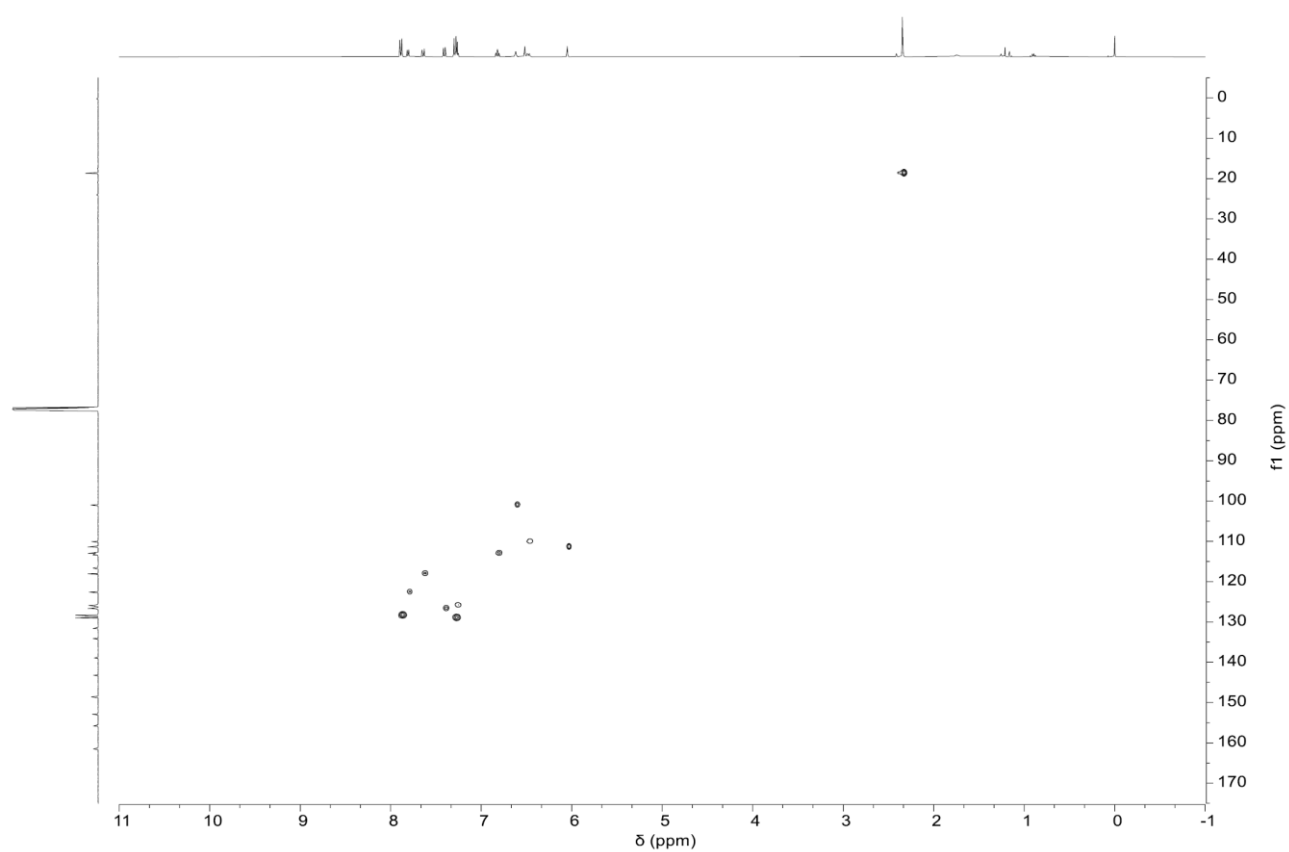
Coumarin-based GBB adduct (19). ^1H NMR (400 MHz, CDCl_3)

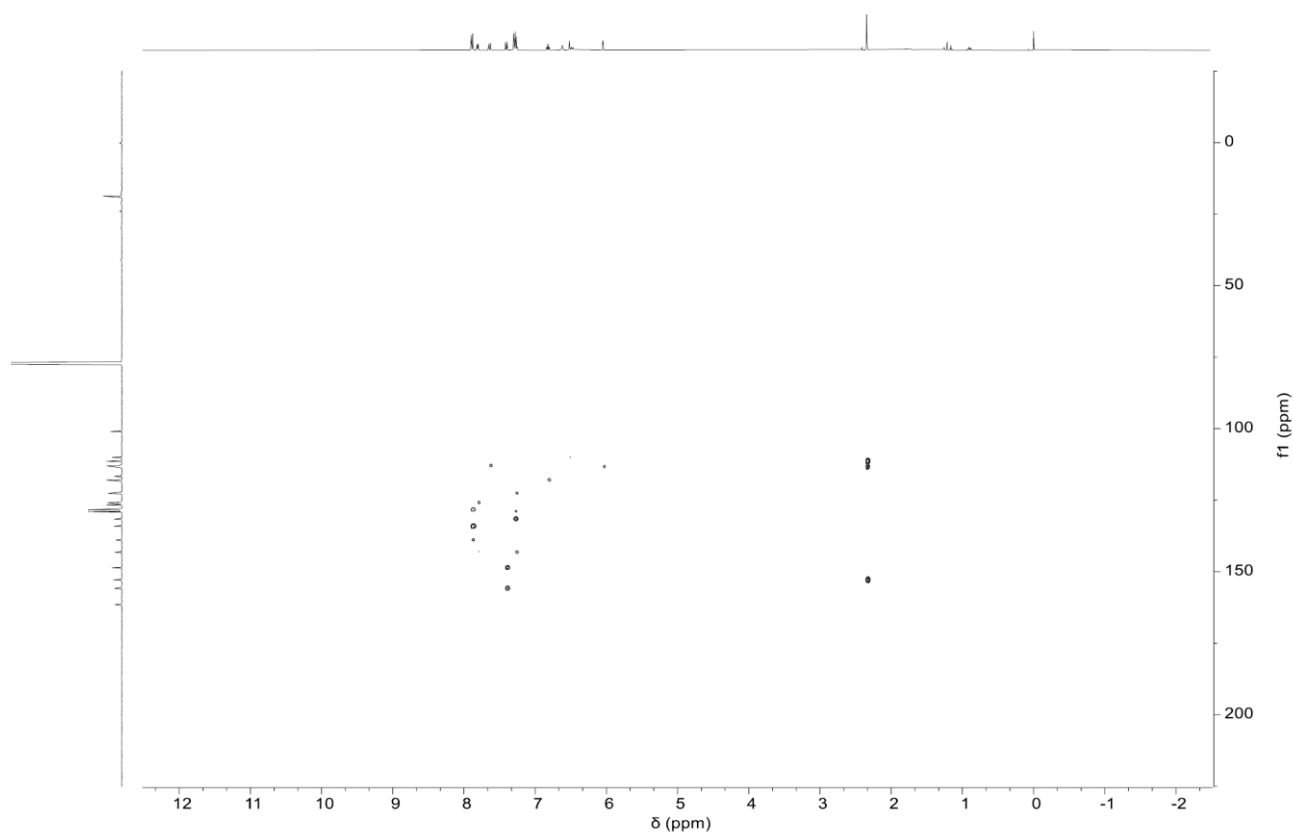
Coumarin-based GBB adduct (19). ^{13}C NMR (101 MHz, CDCl_3)

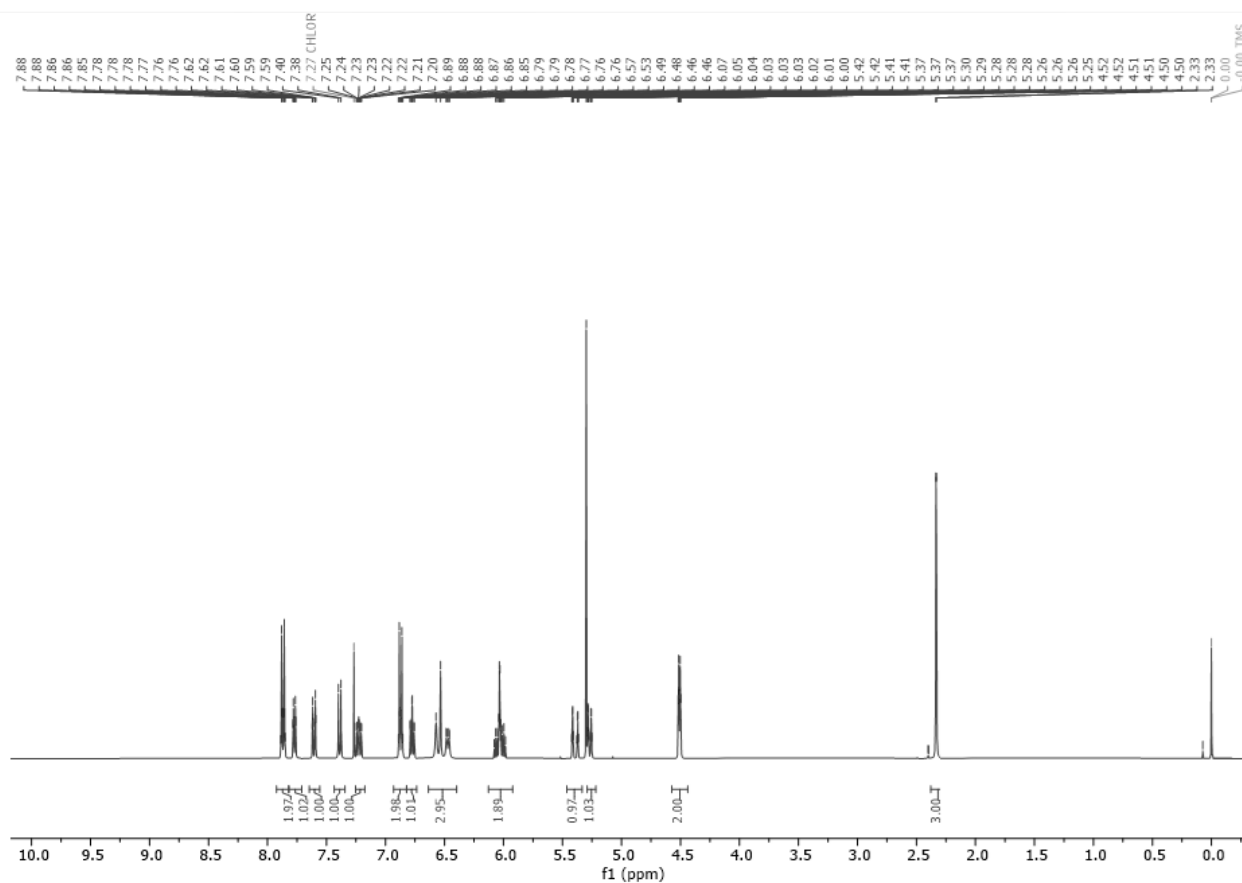
Coumarin-based GBB adduct (20). ^1H NMR (300 MHz, CDCl_3)

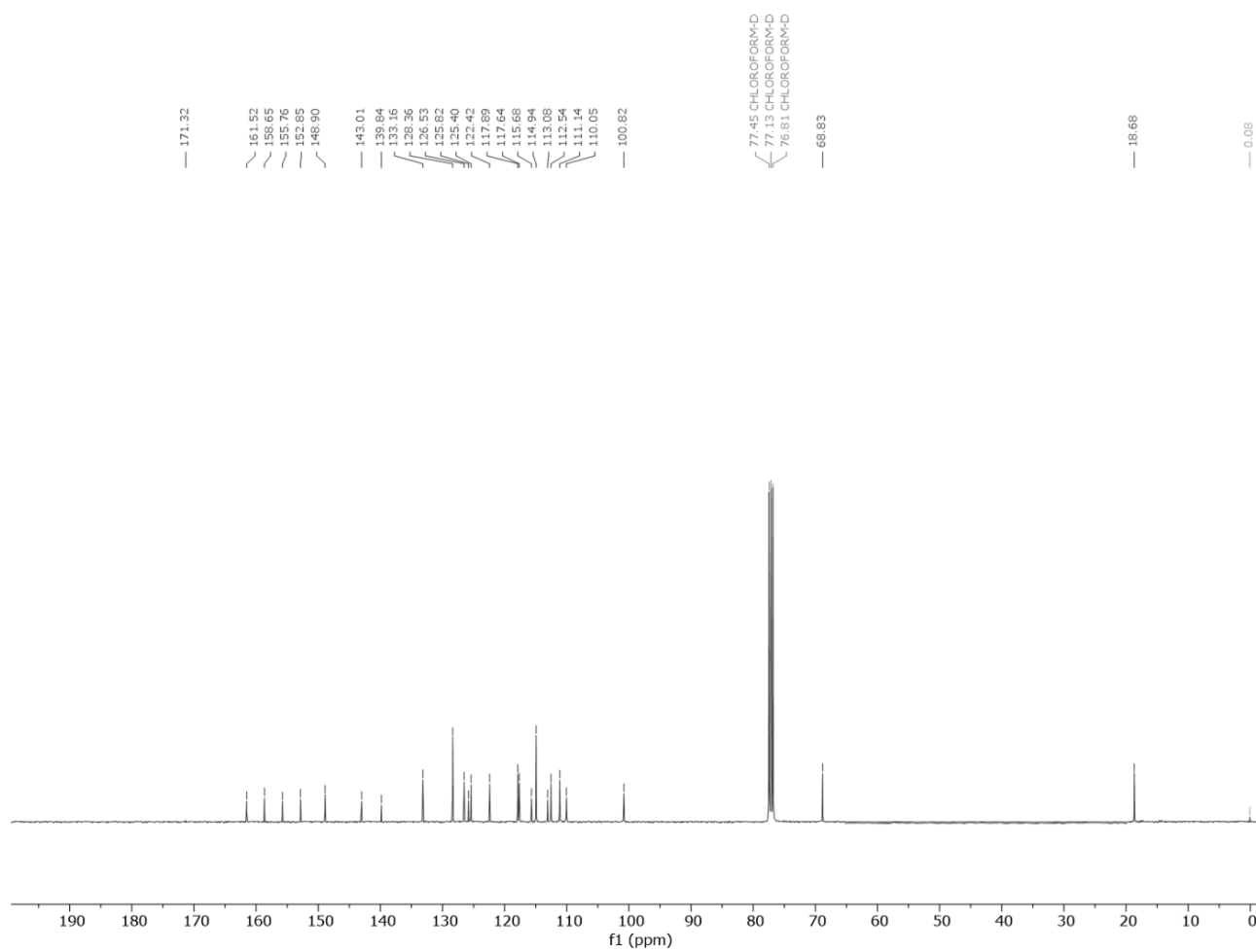
Coumarin-based GBB adduct (20). ^{13}C NMR (75 MHz, CDCl_3)

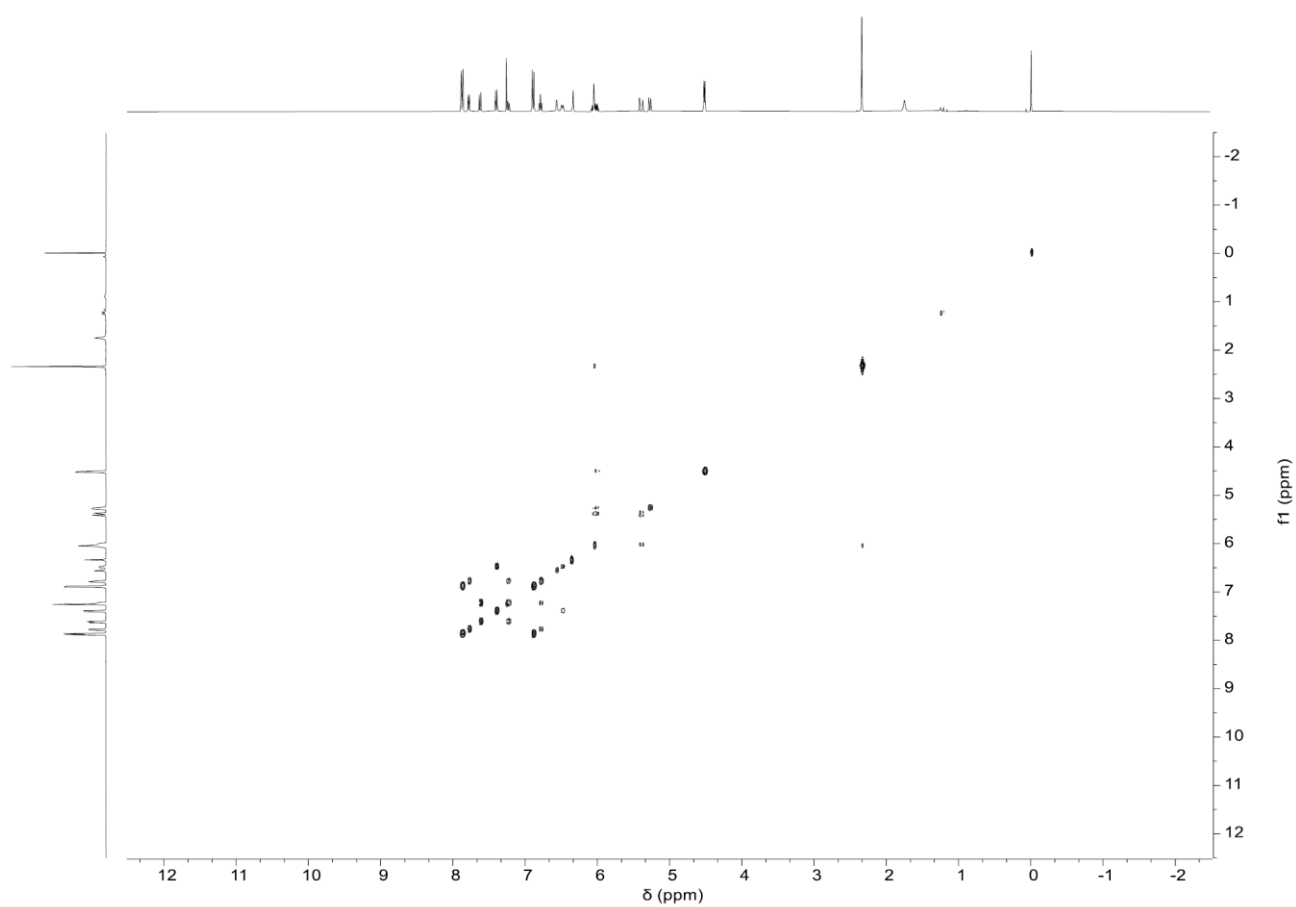
Coumarin-based GBB adduct (20). ^1H - ^1H COSY NMR (400 MHz for ^1H , CDCl_3)

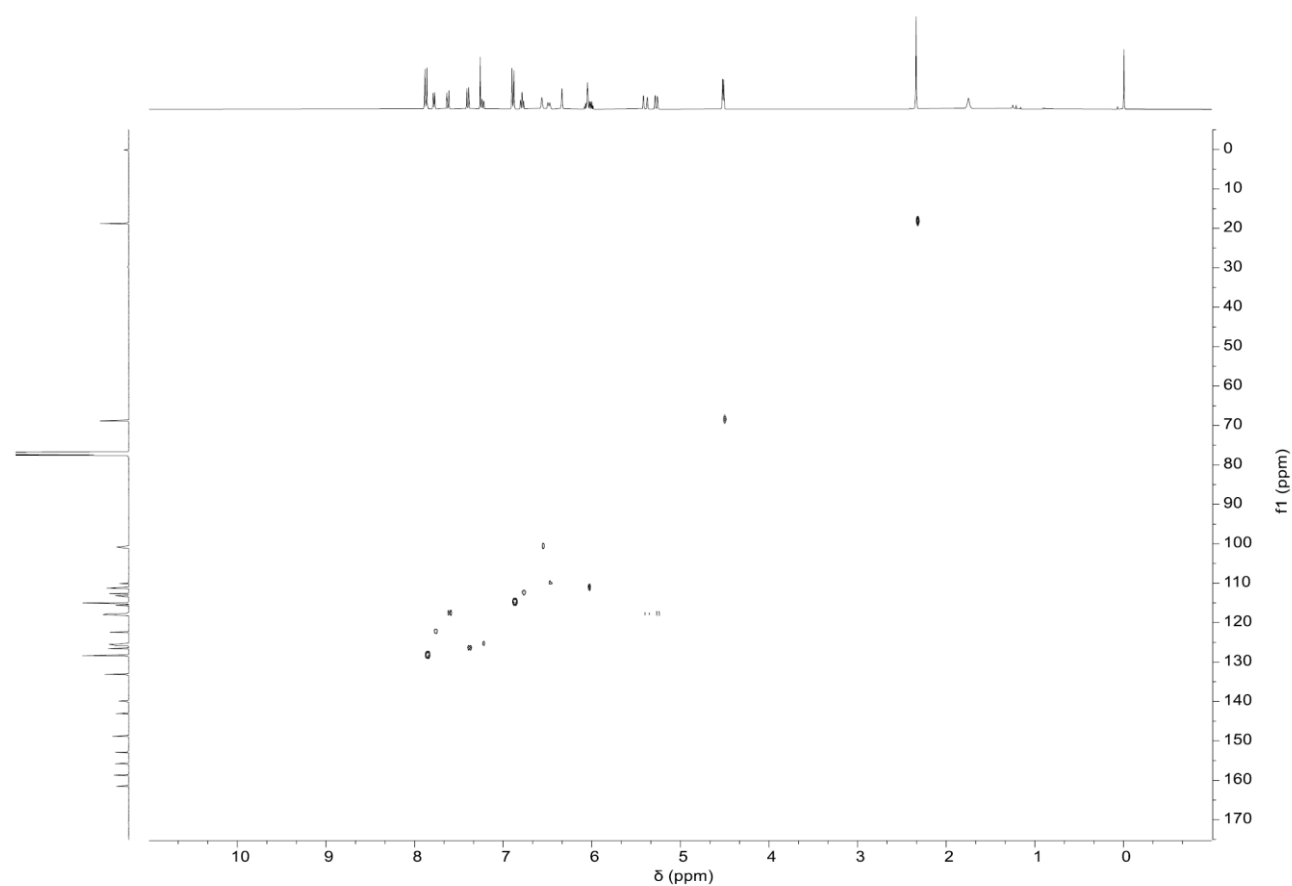
Coumarin-based GBB adduct (20). ^1H - ^{13}C HSQC NMR (400 MHz for ^1H , CDCl_3)

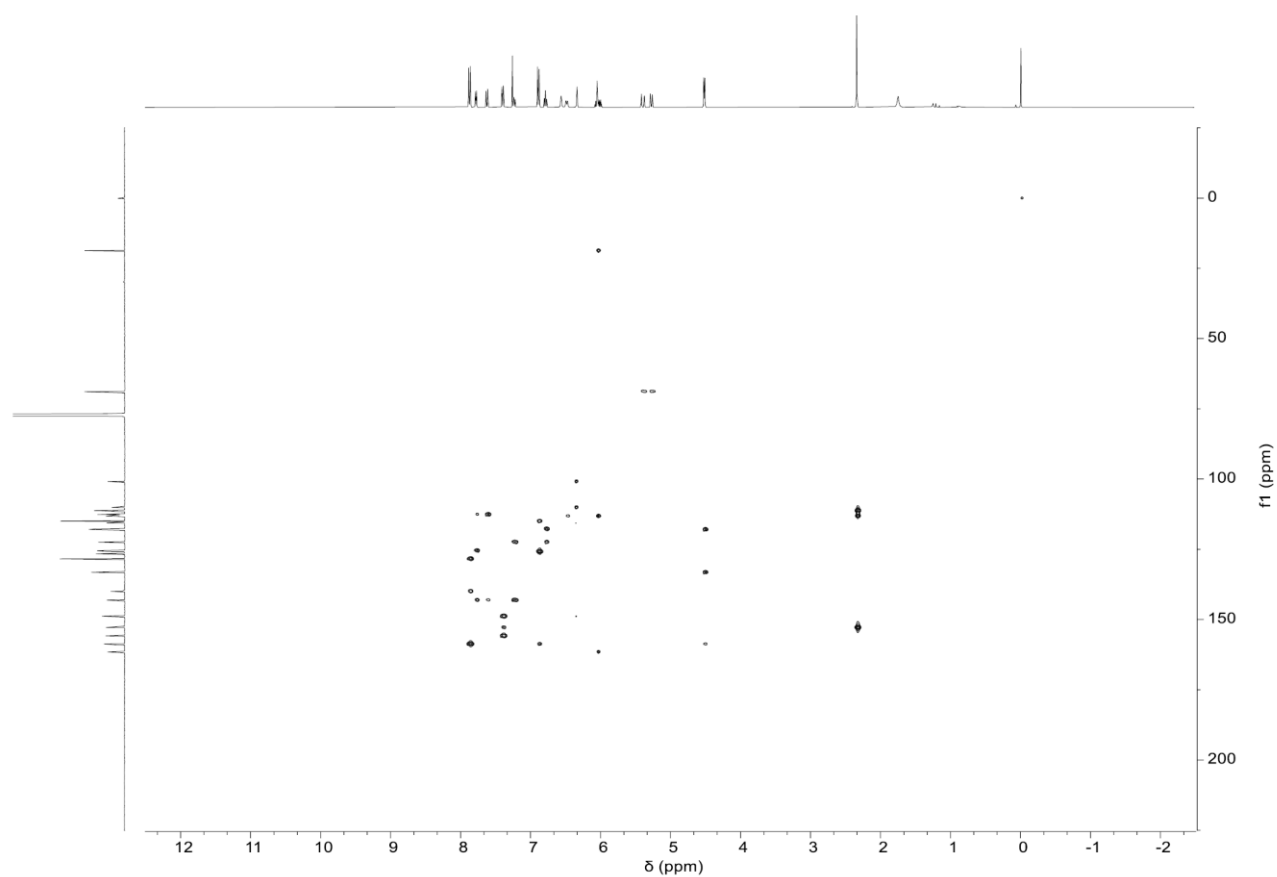
Coumarin-based GBB adduct (20). ^1H - ^{13}C HMBC NMR (400 MHz for ^1H , CDCl_3)

Coumarin-based GBB adduct (21). ^1H NMR (400 MHz, CDCl_3)

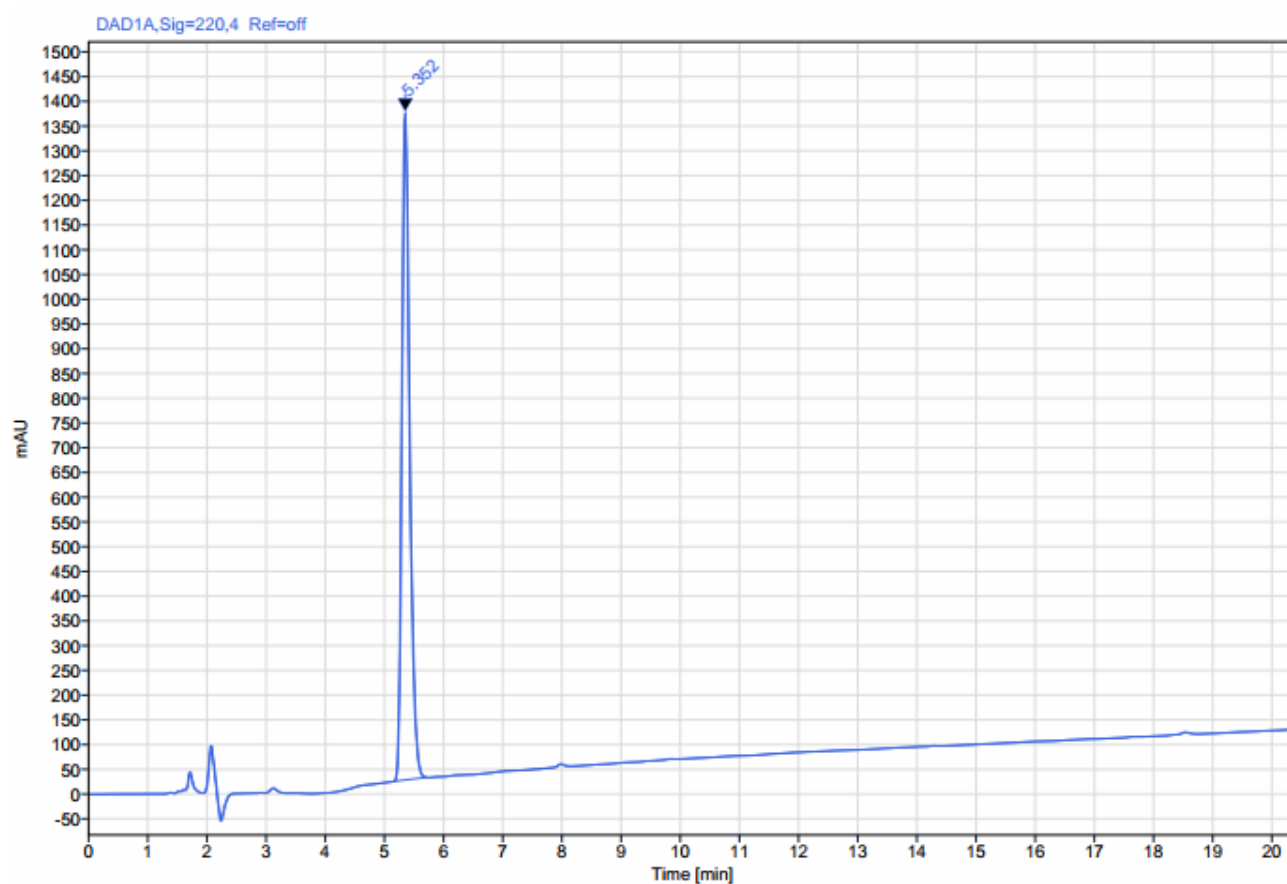
Coumarin-based GBB adduct (21). ^{13}C NMR (101 MHz, CDCl_3)

Coumarin-based GBB adduct (21). ^1H - ^1H COSY NMR (400 MHz for ^1H , CDCl_3)

Coumarin-based GBB adduct (21). ^1H - ^{13}C HSQC NMR (400 MHz for ^1H , CDCl_3)

Coumarin-based GBB adduct (21). ^1H - ^{13}C HMBC NMR (400 MHz for ^1H , CDCl_3)

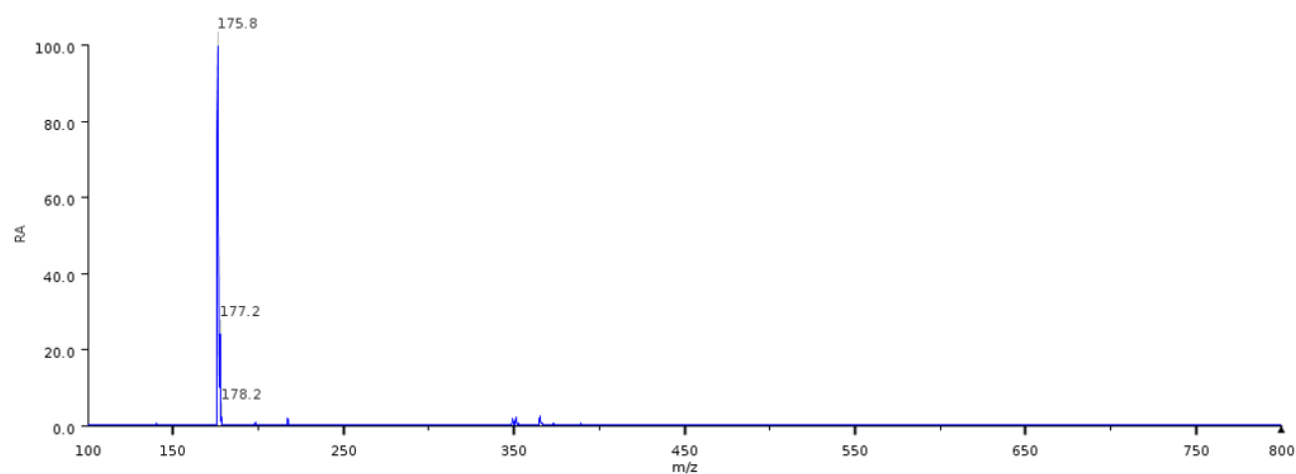
7-amino-4-methylcoumarin (1) HPLC-MS analysis



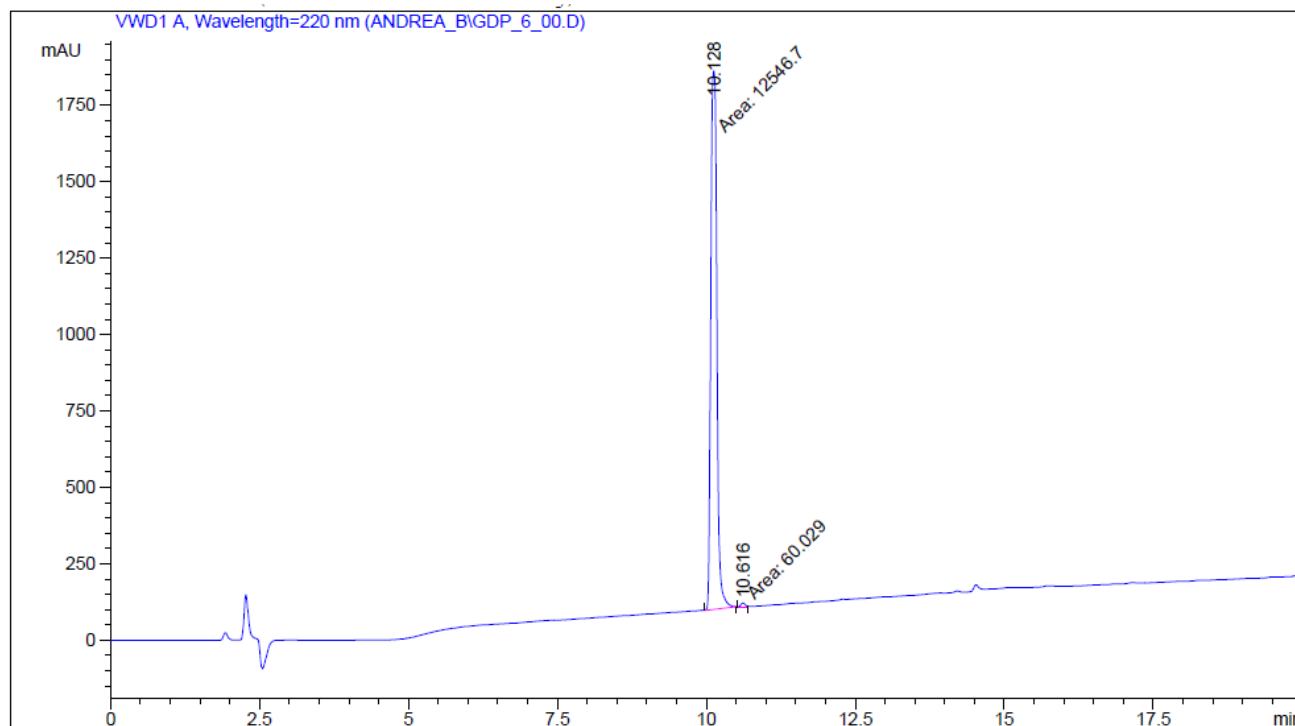
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Sum 12439.1716



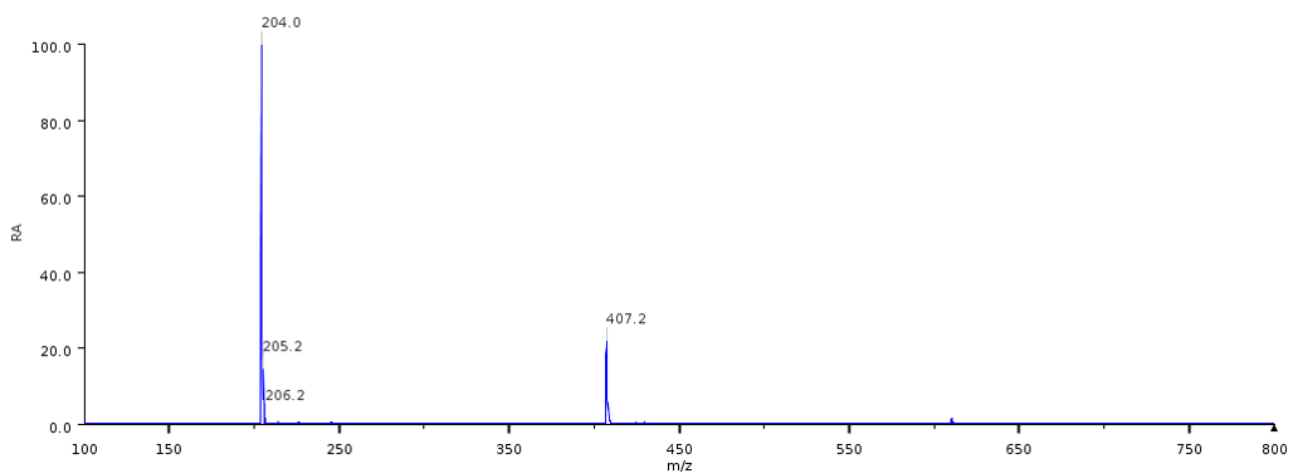
7-formamido-4-methylcoumarin (2) HPLC-MS analysis



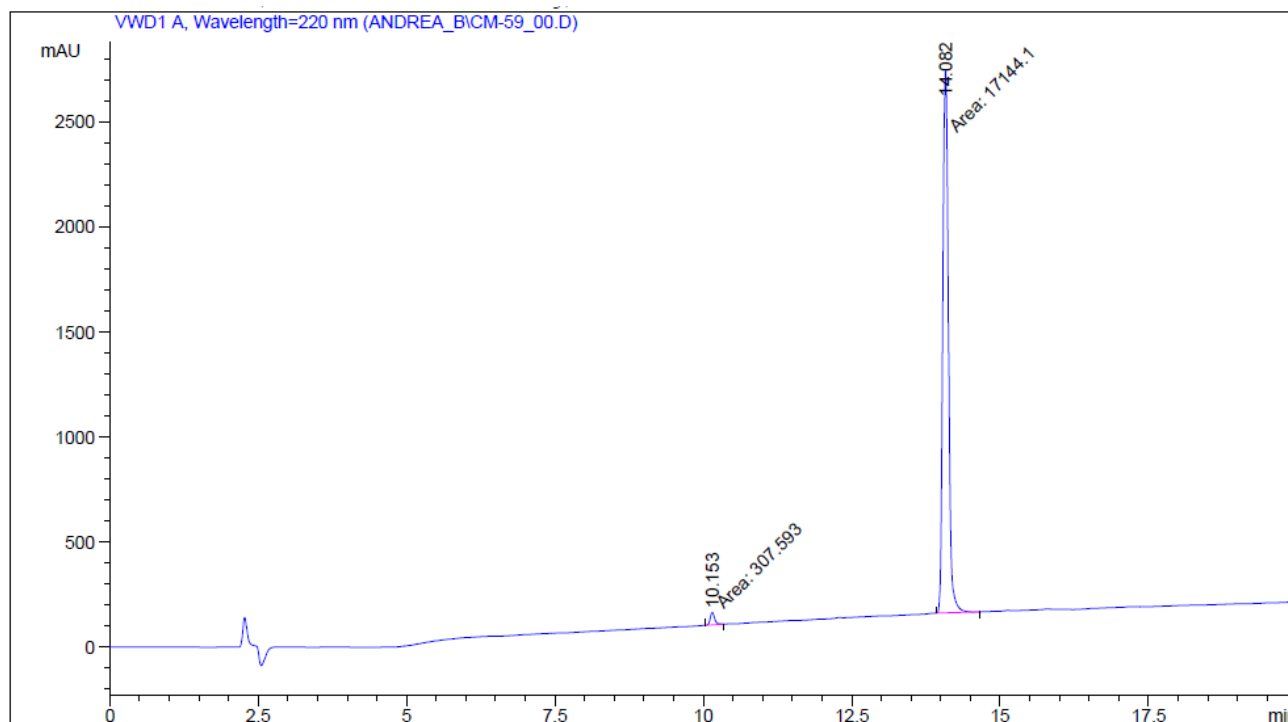
Signal 1: VWD1 A, Wavelength=220 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU * s	Height [mAU]	Area %
1	10.128	MM	0.1186	1.25467e4	1762.91650	99.5238
2	10.616	MM	0.0801	60.02896	12.49684	0.4762

Totals : 1.26068e4 1775.41334



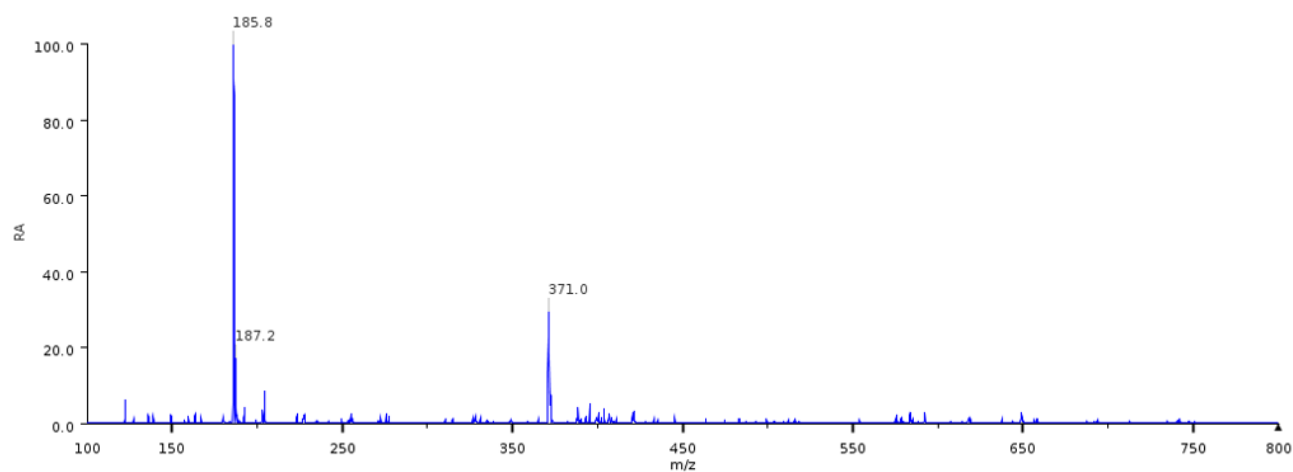
7-isocyano-4-methylcoumarin (3) HPLC-MS analysis



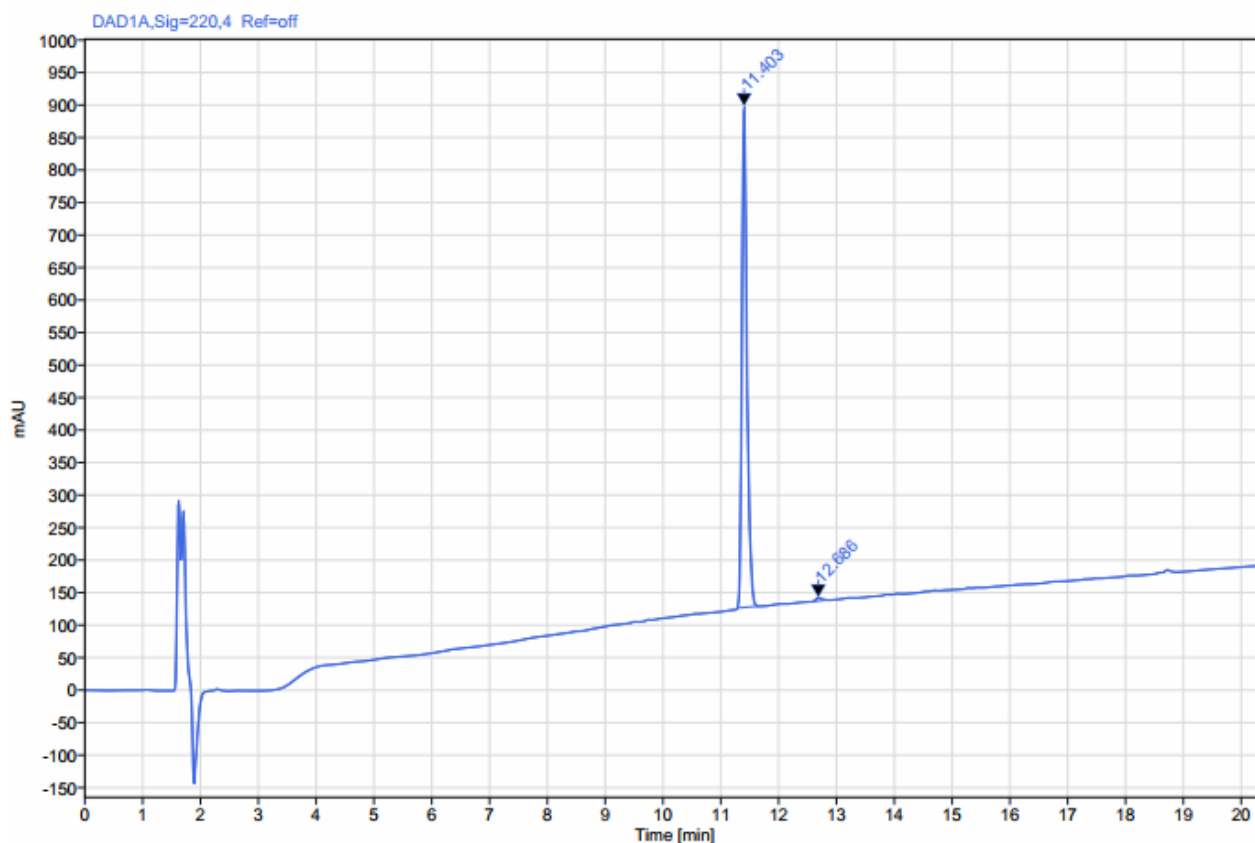
Signal 1: VWD1 A, Wavelength=220 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	10.153	MM	0.0871	307.59326	58.84604	1.7625
2	14.082	MM	0.1105	1.71441e4	2585.14893	98.2375

Totals : 1.74517e4 2643.99496

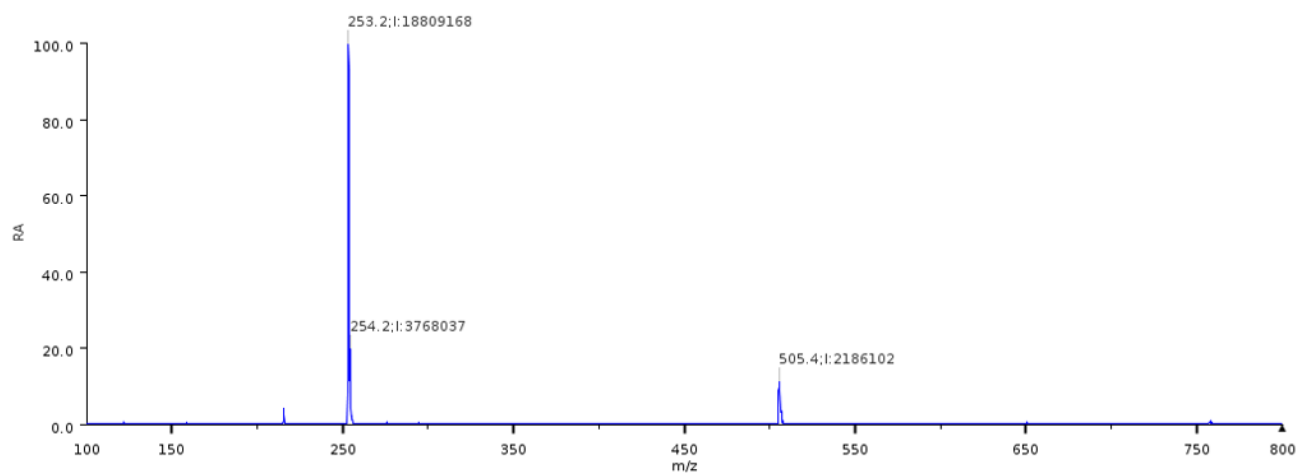


4-amino-N-allyl-1,8-naphthalimide (10)

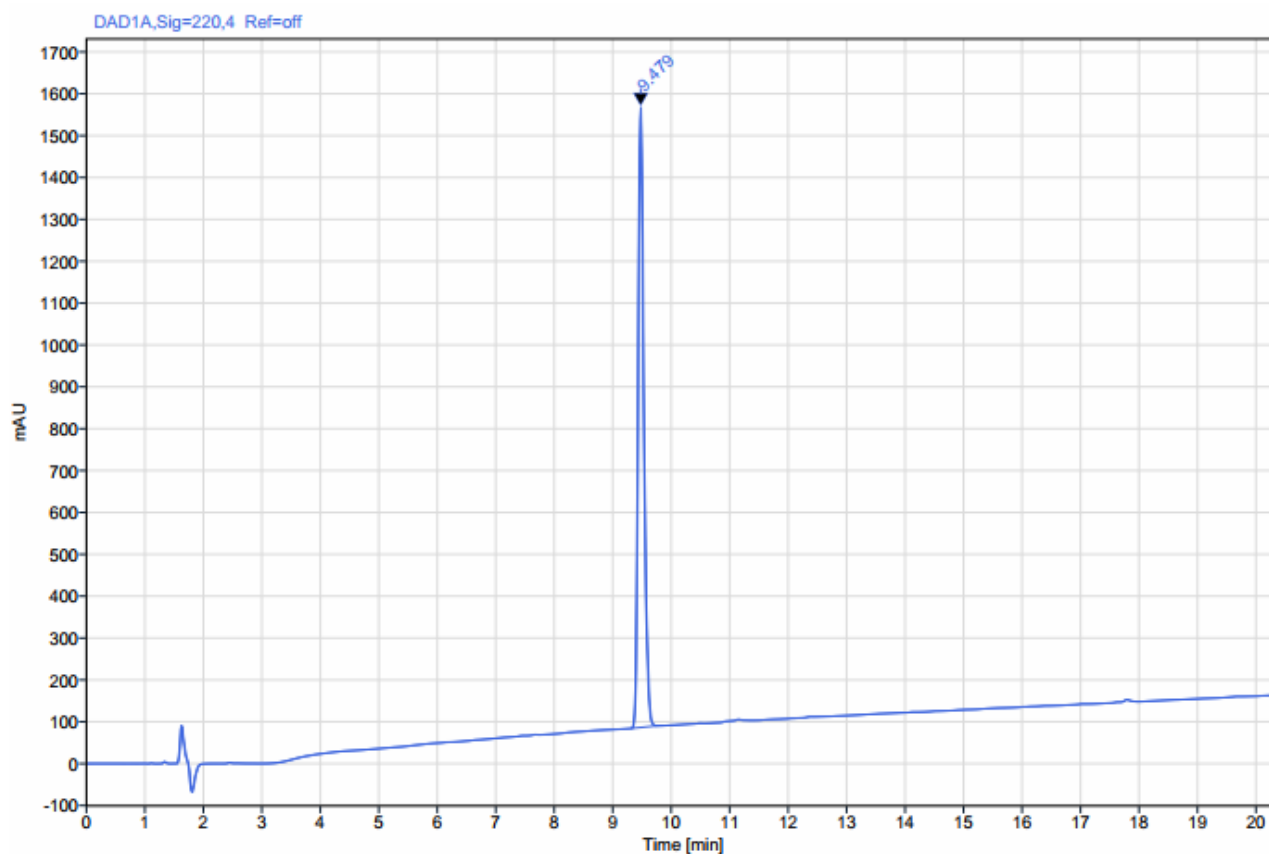


Signal: DAD1A,Sig=220,4 Ref=off

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	11.403	MM m	0.3465	4684.6378	770.4549	99.3098
	12.686	MM m	0.2413	32.5585	5.1815	0.6902
Sum				4717.1964		

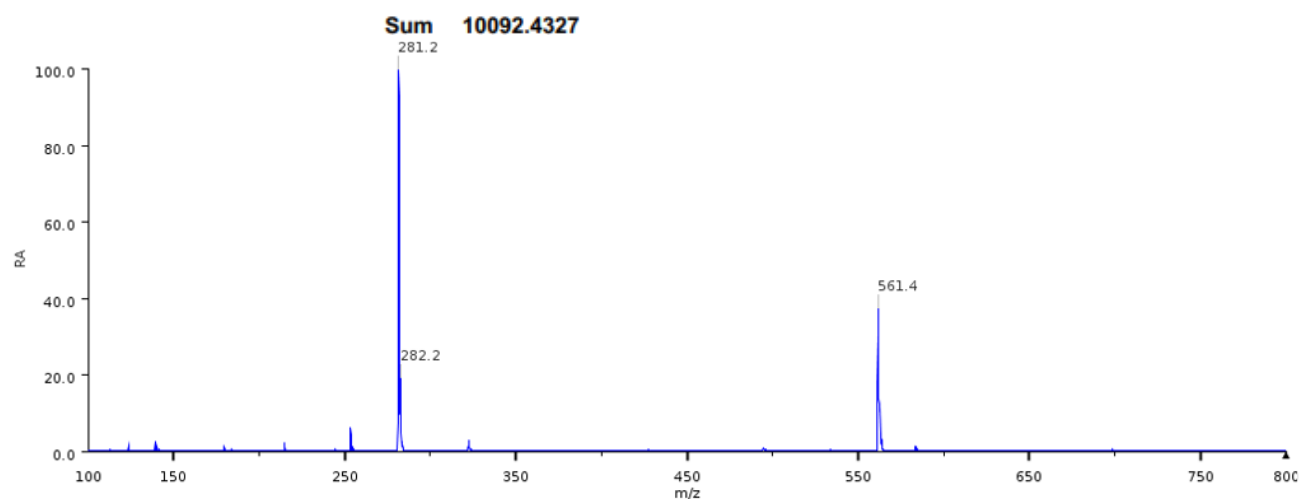


4-formamido-N-allyl-1,8-naphthalimide (11)

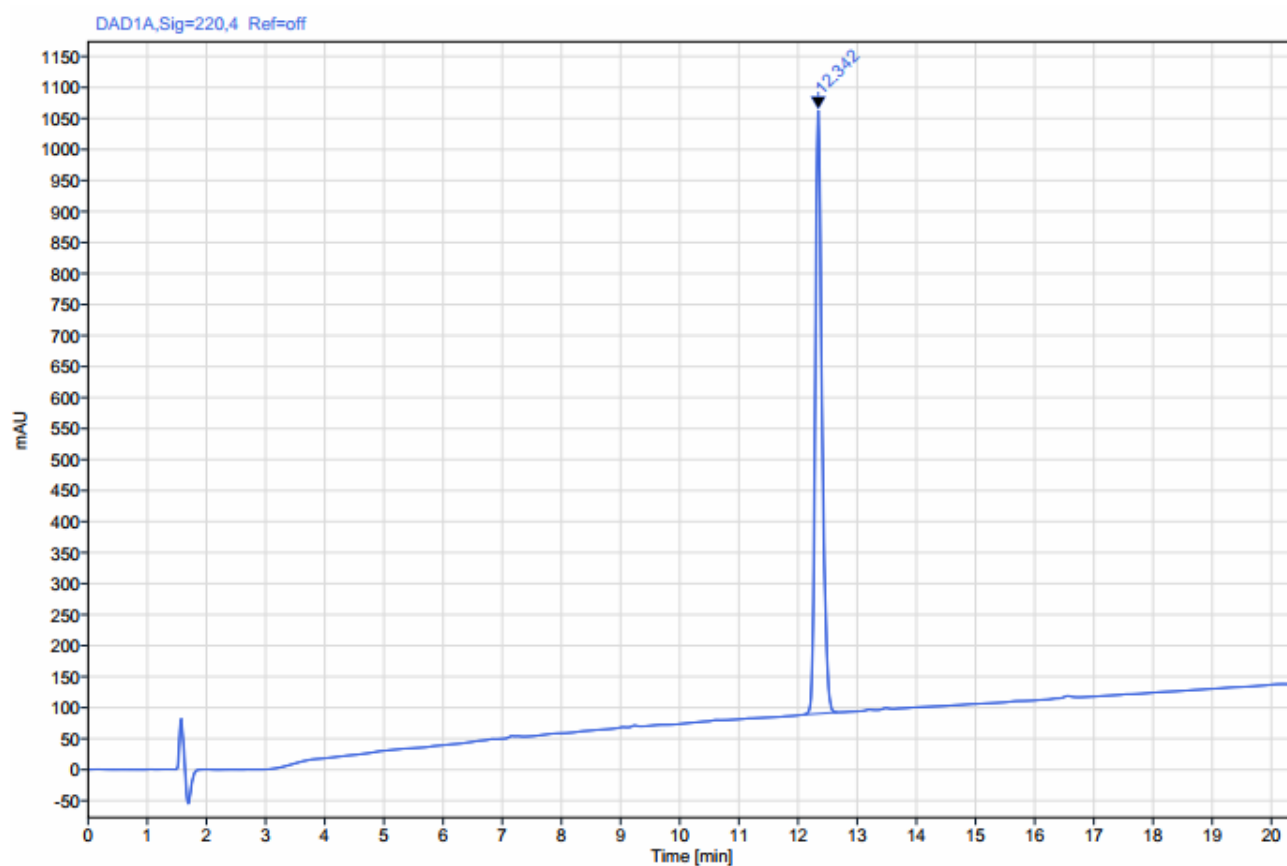


Signal: DAD1A,Sig=220,4 Ref=off

Name	RT [min]	Type	Width [min]	Area	Height	Area%
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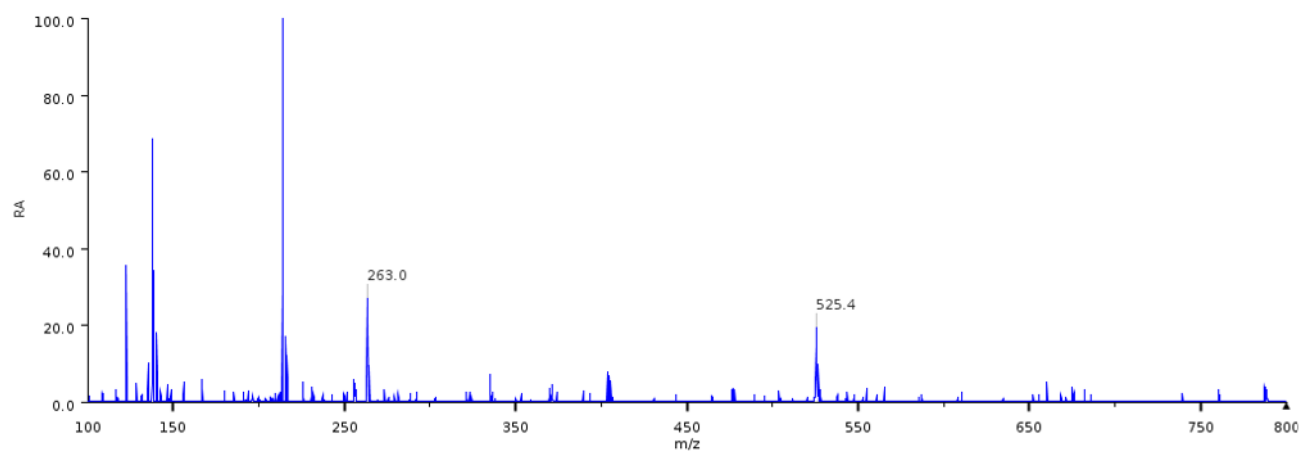
4-isocyano-N-allyl-1,8-naphthalimide (12)



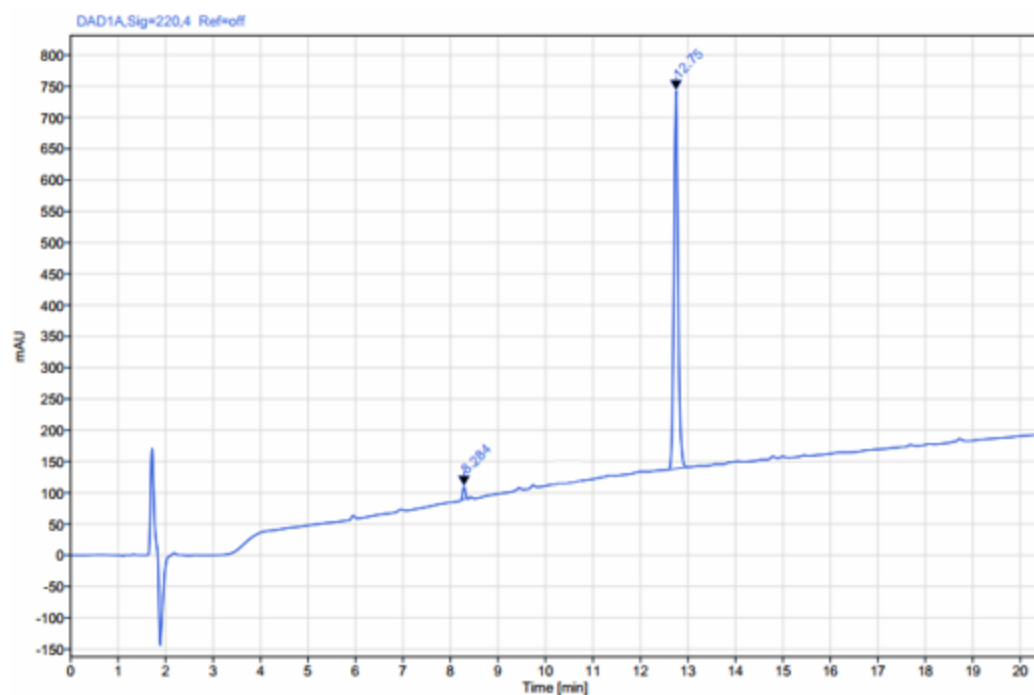
Signal: DAD1A,Sig=220,4 Ref=off

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Sum 7791.5106

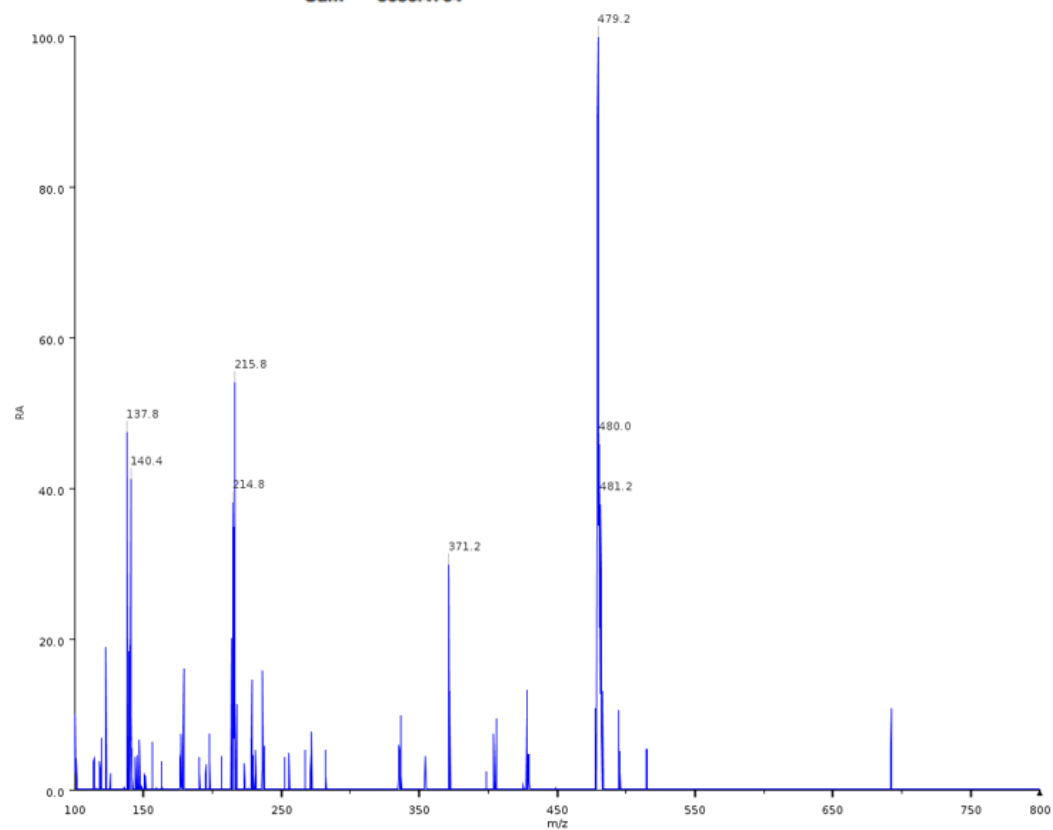


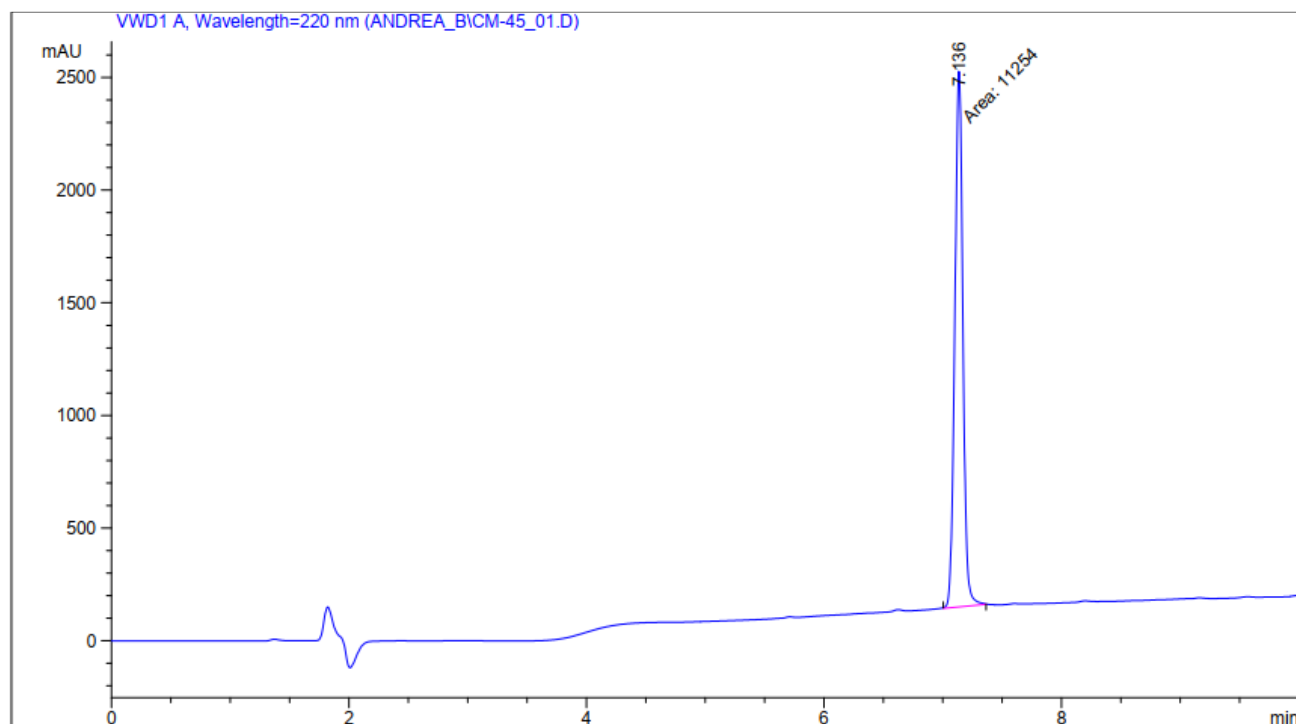
N-allyl-1,8-naphthalimide-based GBB adduct (17)



Signal: DAD1A, Sig=220,4 Ref=off

Time	RT [min]	Type	Width [min]	Area	Height	Area%
8.284	8.284	MM m	0.1187	72.0876	20.2101	1.9555
12.750	12.750	MM m	0.4041	3614.3889	604.2287	98.0445
Sum				3686.4764		

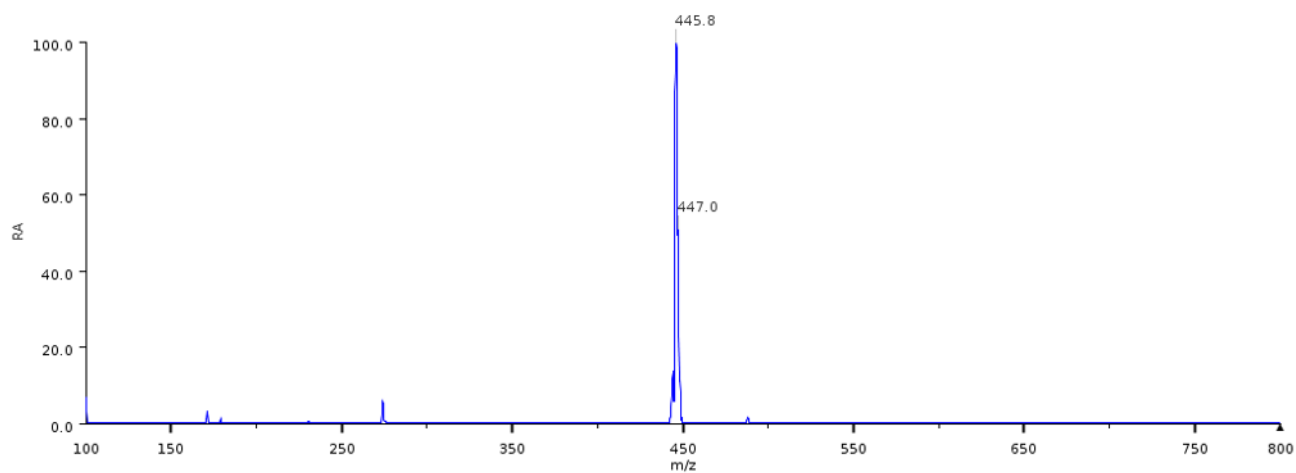


N-allyl-1,8-naphthalimide-based GBB adduct (**18**)

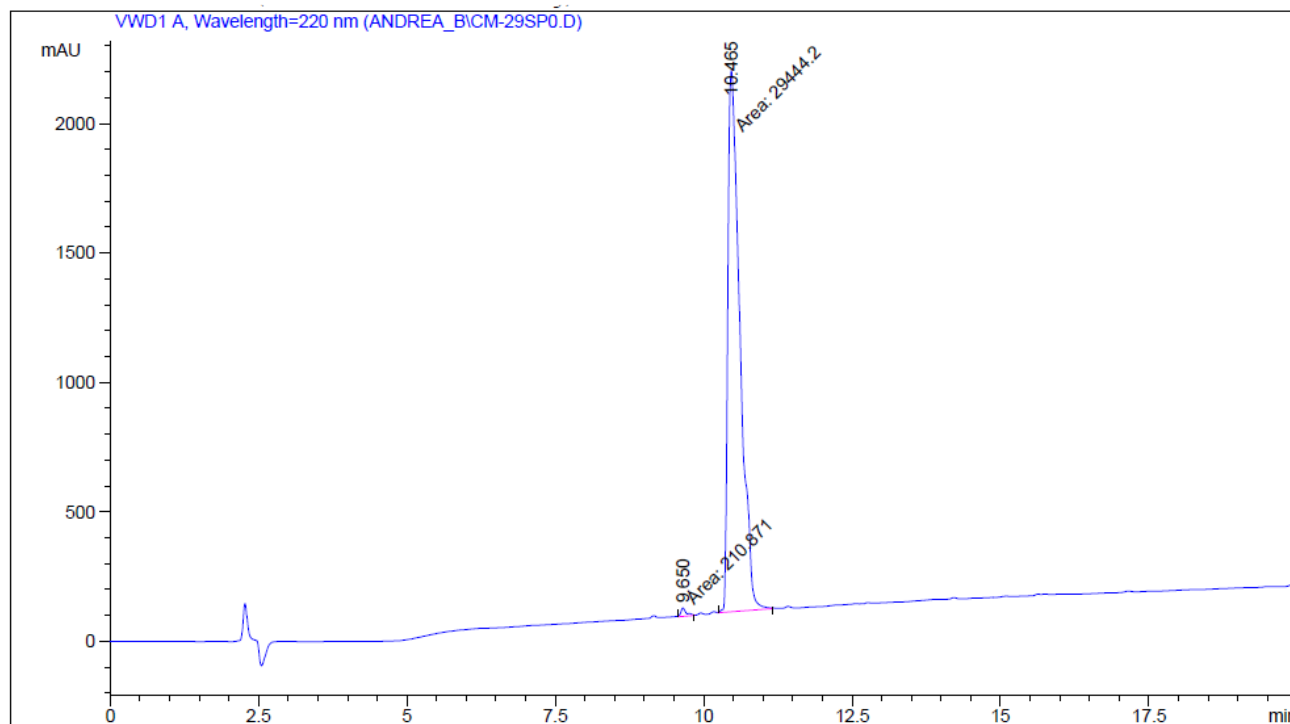
Signal 1: VWD1 A, Wavelength=220 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	7.136	MM	0.0787	1.12540e4	2384.79419	100.0000

Totals : 1.12540e4 2384.79419



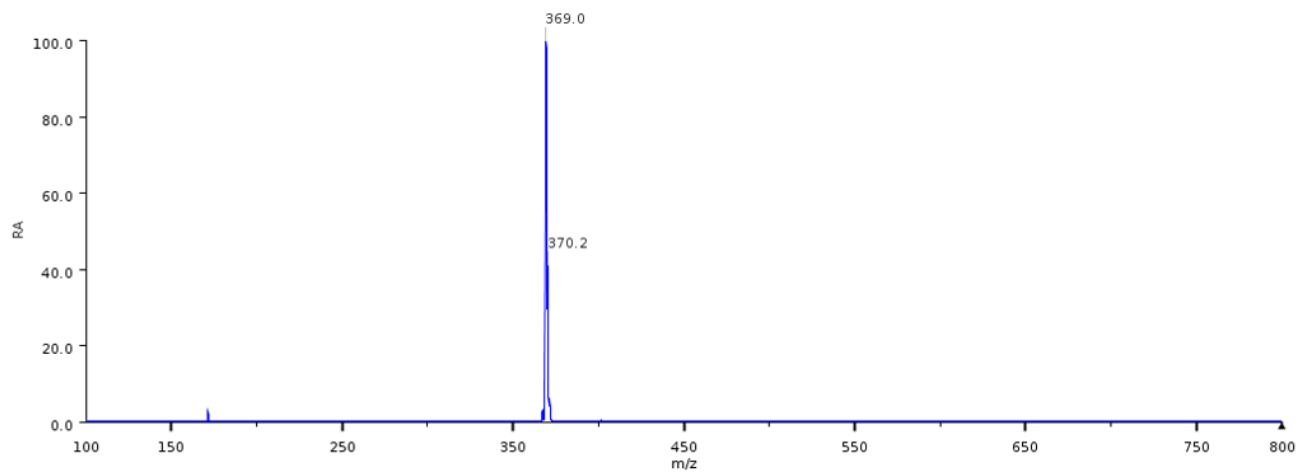
Coumarin-based GBB adduct (19)



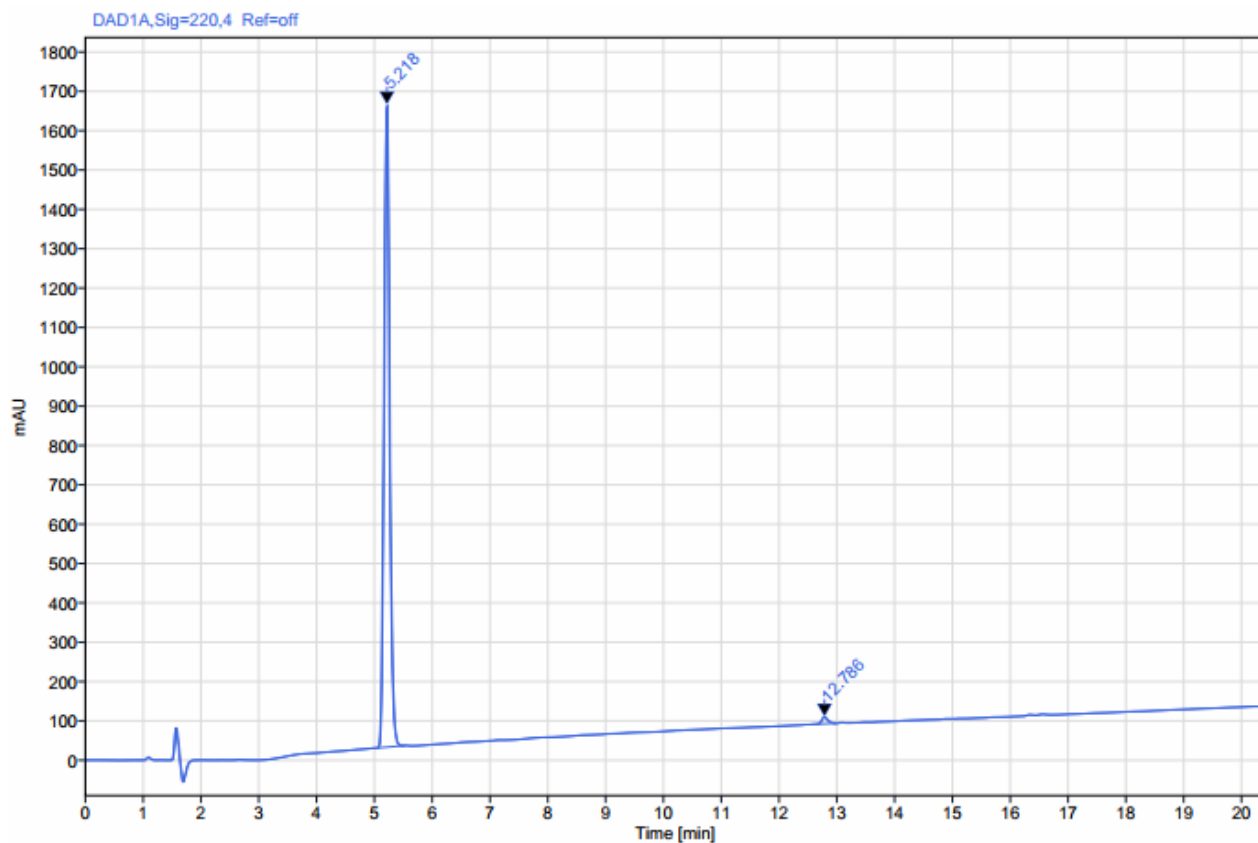
Signal 1: VWD1 A, Wavelength=220 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	9.650	MM	0.1066	210.87082	32.97536	0.7111
2	10.465	MM	0.2346	2.94442e4	2092.09937	99.2889

Totals : 2.96550e4 2125.07472

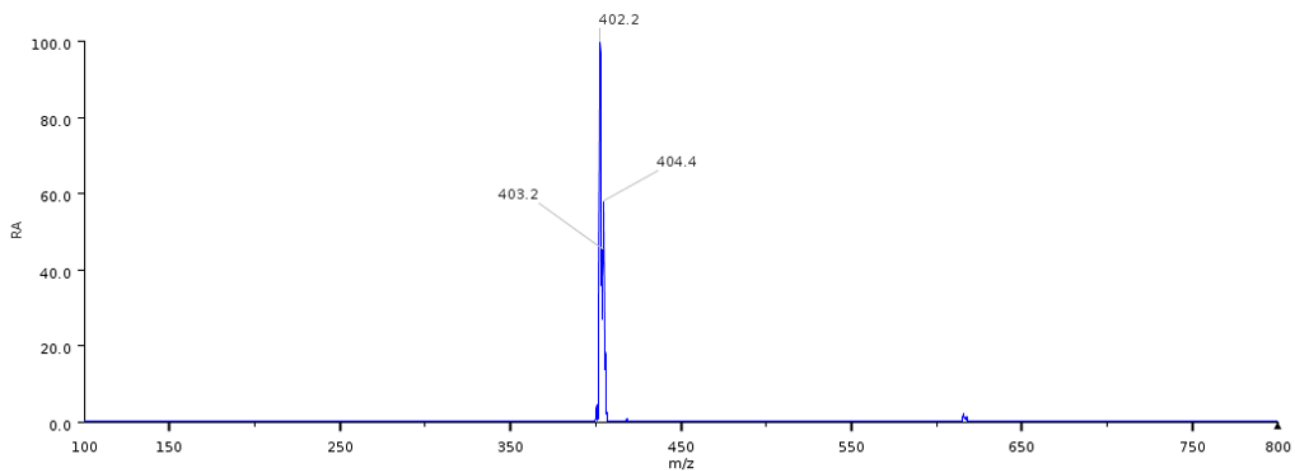


Coumarin-based GBB adduct (20)

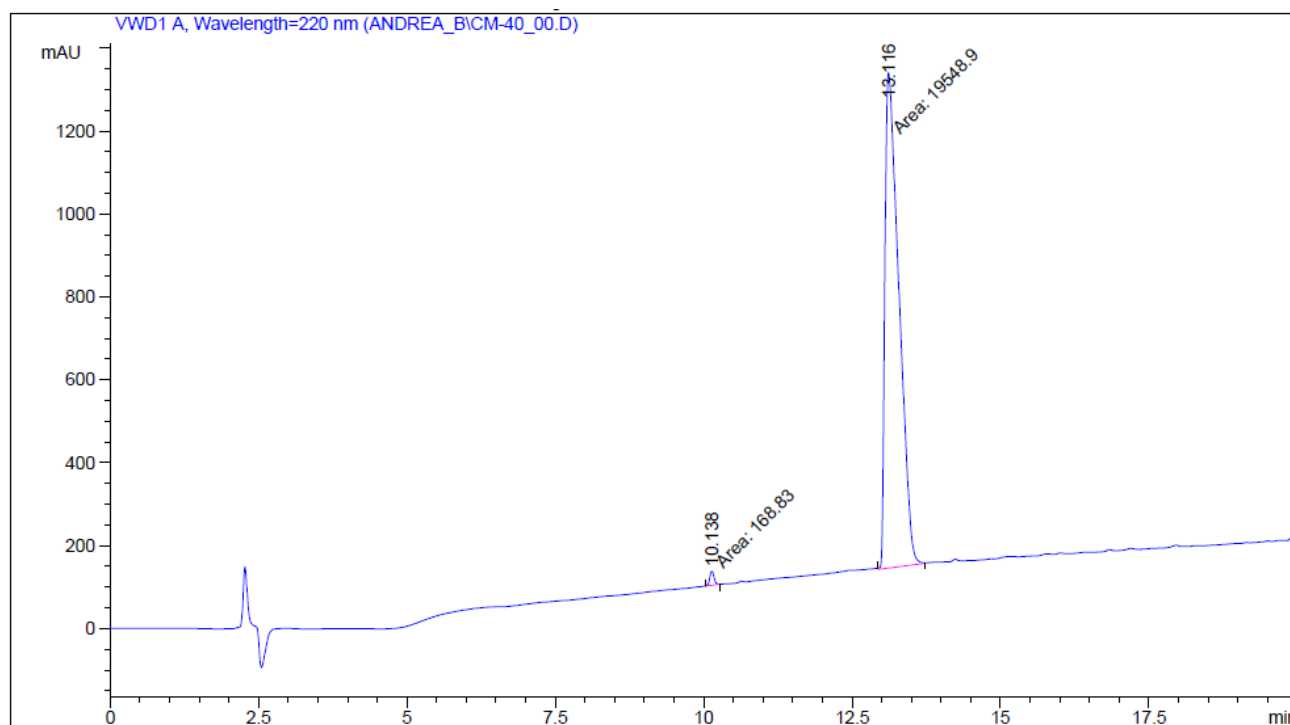


Signal: DAD1A, Sig=220,4 Ref=off

Name	RT [min]	Type	Width [min]	Area	Height	Area%
	5.218	MM m	0.4806	10980.5659	1632.7130	98.8589
	12.786	MM m	0.3304	126.7499	17.5954	1.1411
Sum				11107.3158		



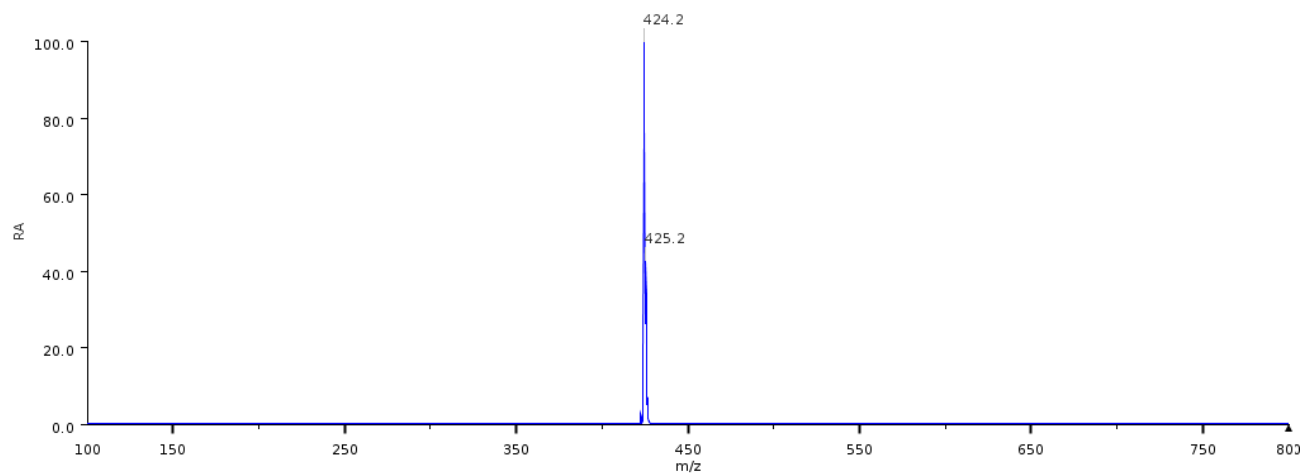
Coumarin-based GBB adduct (21)



Signal 1: VWD1 A, Wavelength=220 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	10.138	MM	0.0832	168.83028	33.82970	0.8562
2	13.116	MM	0.2727	1.95489e4	1194.82629	99.1438

Totals : 1.97178e4 1228.65600



Absorption Spectrum and Fluorescence Emission Spectrum with Excitation at 300 nm of Coumarin-Based Amine 1 (Figure S1)

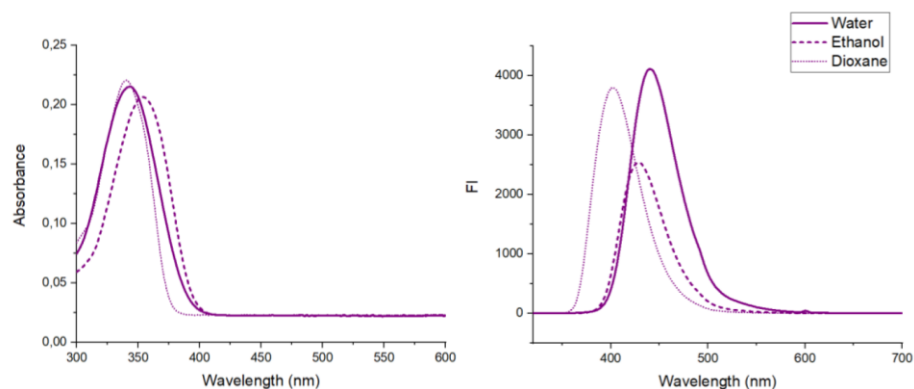


Figure S1

Absorption Spectrum and Fluorescence Emission Spectrum with Excitation at 300 nm of Coumarin-Based Formamide 2 (Figure S2)

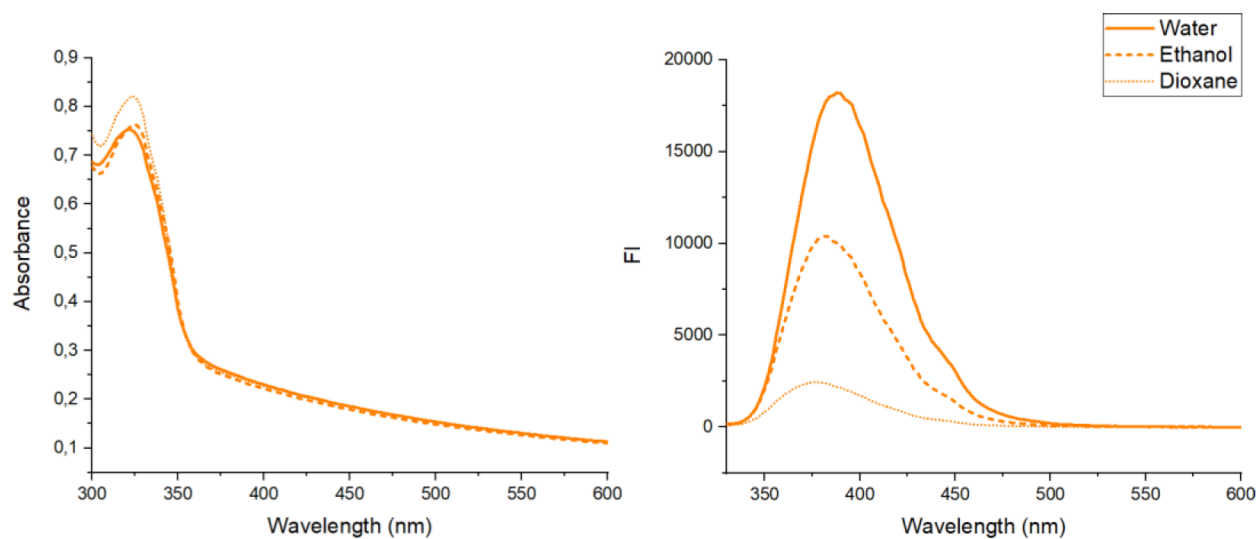


Figure S2

Absorption Spectrum and Fluorescence Emission Spectrum with Excitation at 300 nm of Coumarin-Based Isocyanide 3 (Figure S3)

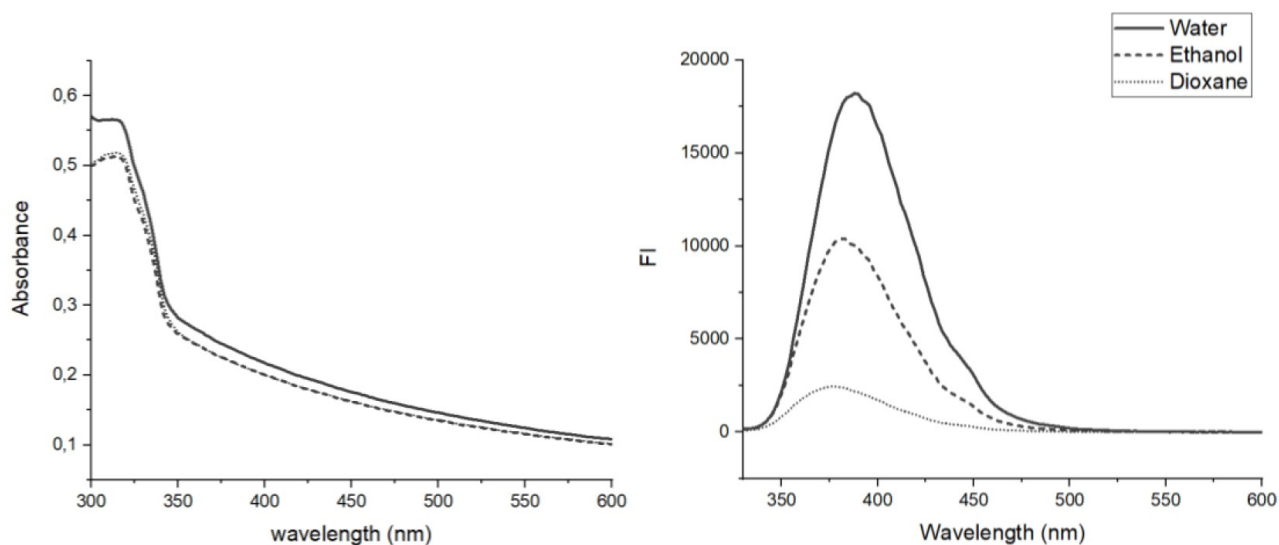


Figure S3

Absorption Spectrum and Fluorescence Emission Spectrum with Excitation at 300 nm of Coumarin-Based GBB adduct 19 (Figure S4)

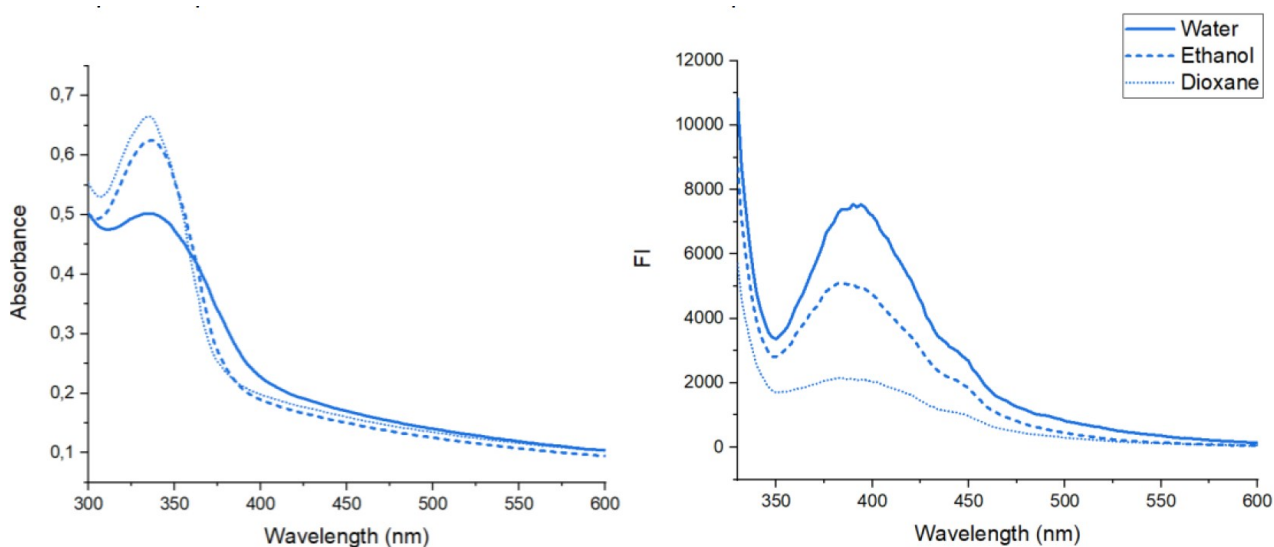


Figure S4

Absorption Spectrum and Fluorescence Emission Spectrum with Excitation at 300 nm of Coumarin-Based GBB adduct 20(Figure S5)

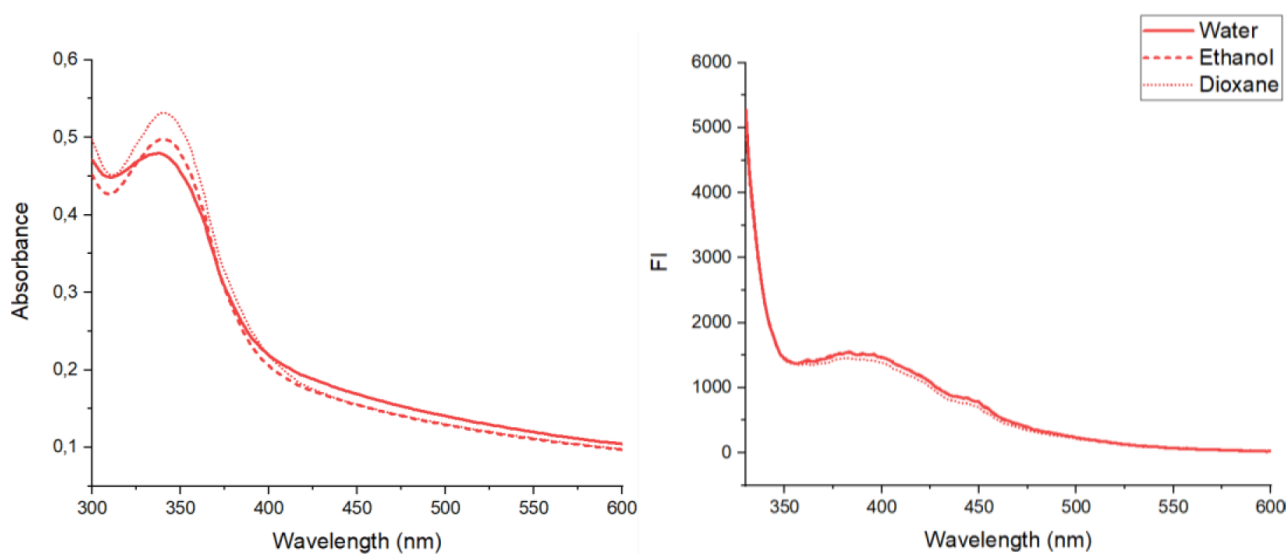


Figure S5

Absorption Spectrum and Fluorescence Emission Spectrum with Excitation at 300 nm of Coumarin-Based GBB adduct 21(Figure S6)

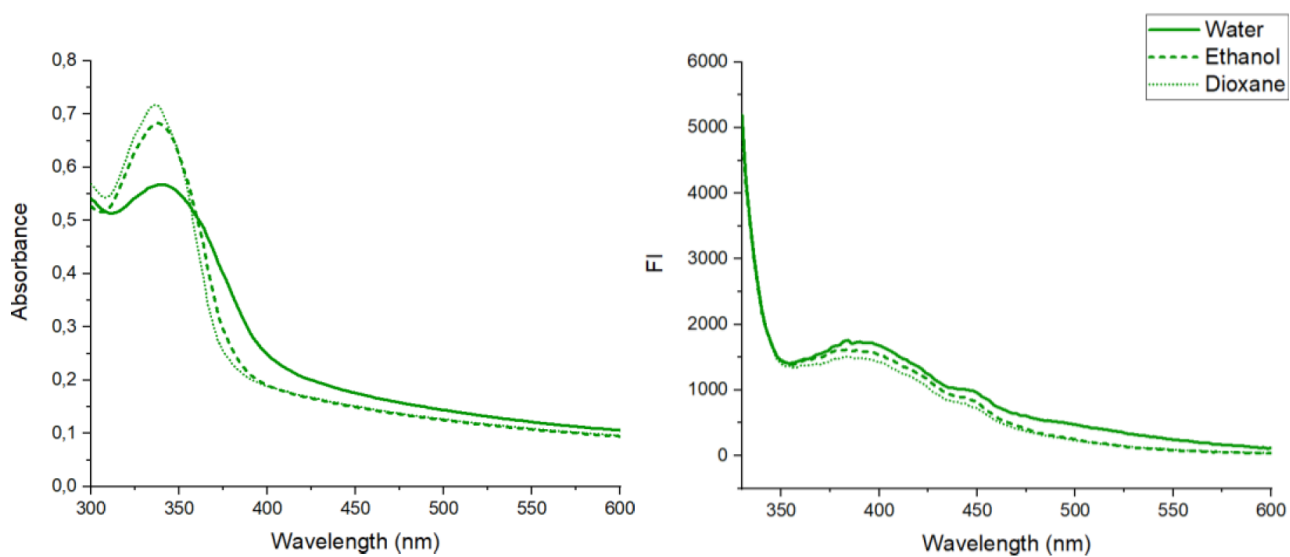


Figure S6

Absorption Spectrum and Fluorescence Emission Spectrum with Excitation at 400 nm of Naphthalimide-Based Amine 10(Figure S7)

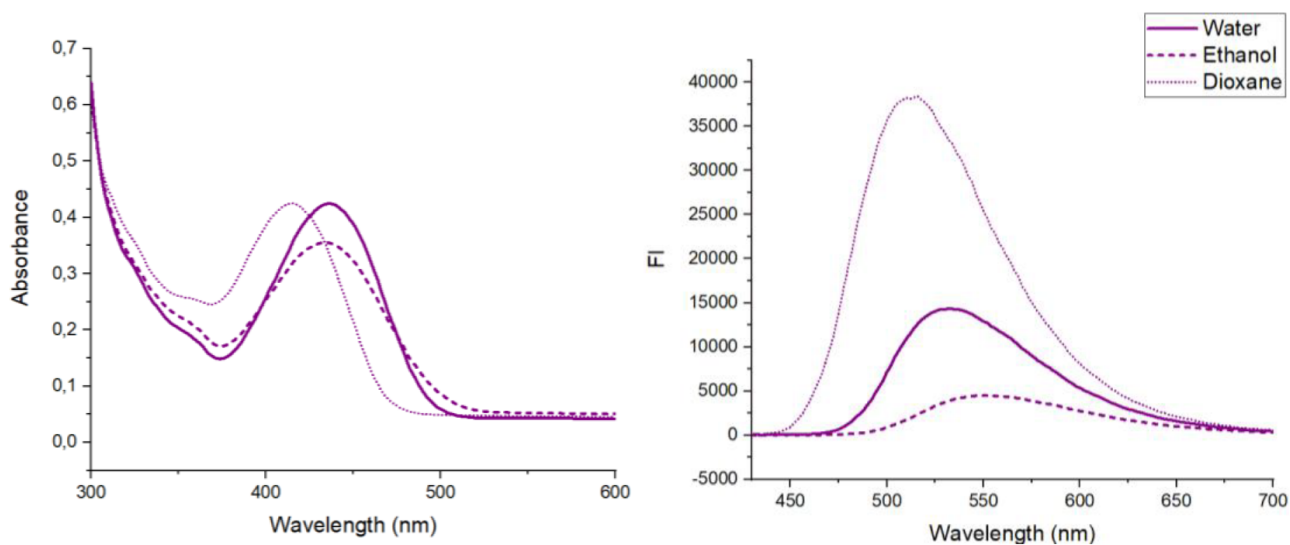


Figure S7

Absorption Spectrum and Fluorescence Emission Spectrum with Excitation at 300 nm of Naphthalimide-Based Formamide 11(Figure S8)

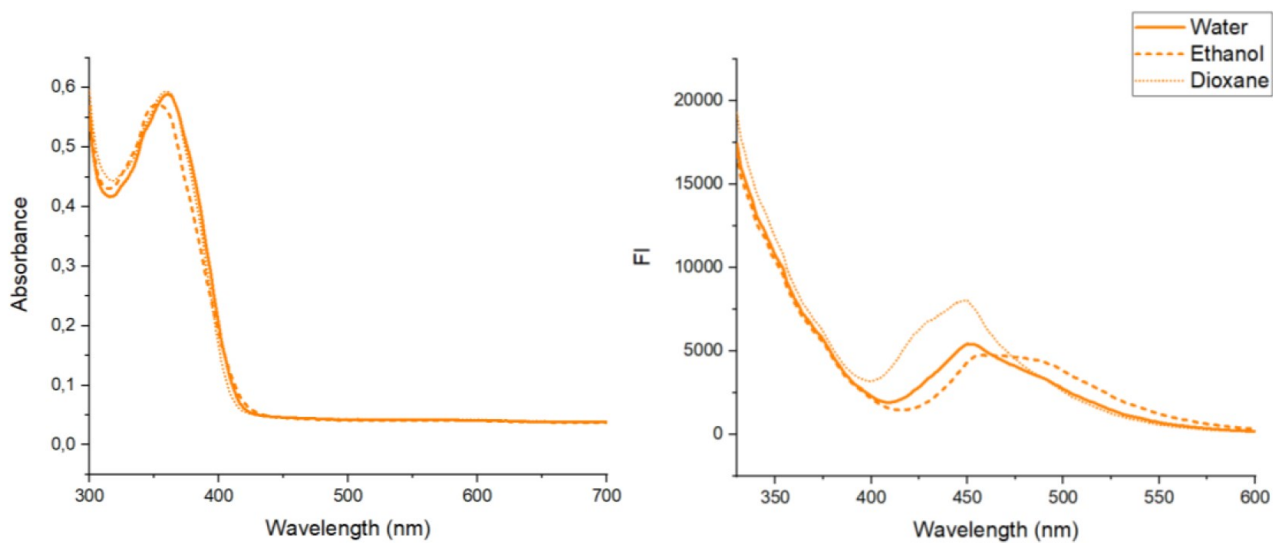


Figure S8

Absorption Spectrum and Fluorescence Emission Spectrum with Excitation at 300 nm of Naphthalimide-Based Isocyanide 12(Figure S9)

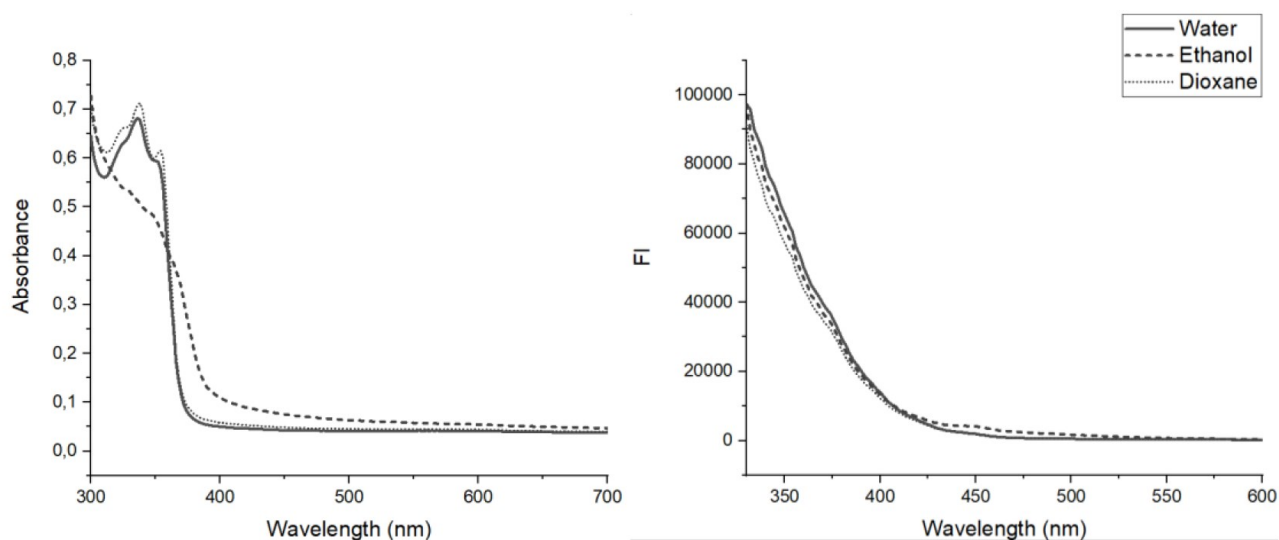


Figure S9

Absorption Spectrum and Fluorescence Emission Spectrum with Excitation at 380 nm of Naphthalimide-Based GBB adduct 17(Figure S10)

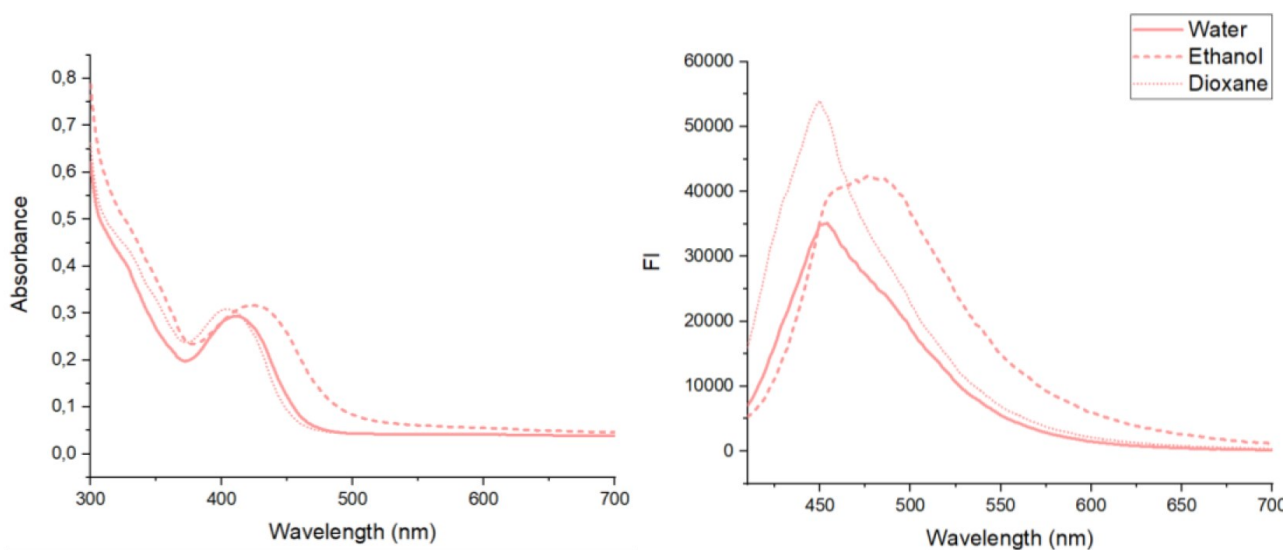


Figure S10