

Synthesis and antimicrobial activity of aminoalkyl resveratrol derivatives inspired by cationic peptides.

Rubén Cebrián,^{a,b*} Ricardo Lucas,^c María Victoria Fernández-Cantos,^a Koen Slot,^a Pablo Peñalver,^d Marta Martínez-García,^a Antonio Párraga-Leo,^c María Violante de Paz,^c Federico García,^b Oscar P. Kuipers^{a,*} and Juan Carlos Morales^{d,*}

Affiliations

^aDepartment of Molecular Genetics, Groningen Biomolecular Sciences and Biotechnology Institute, University of Groningen, Nijenborgh 7, 9747AG, Groningen, The Netherlands.

^bDepartment of Clinical Microbiology, Instituto de Investigación Biosanitaria ibs. GRANADA, University Hospital Clínico San Cecilio, Av. de la Innovación s/n, 18061, Granada, Spain.

^cDepartment of Organic and Pharmaceutical Chemistry, School of Pharmacy, University of Seville, 41012, Seville, Spain.

^dDepartment of Biochemistry and Molecular Pharmacology and Department of Cellular Biology and Immunology. Instituto de Parasitología y Biomedicina López Neyra, CSIC, PTS Granada, Avda. del Conocimiento, 17, 18016 Armilla, Granada, Spain.

Corresponding Authors

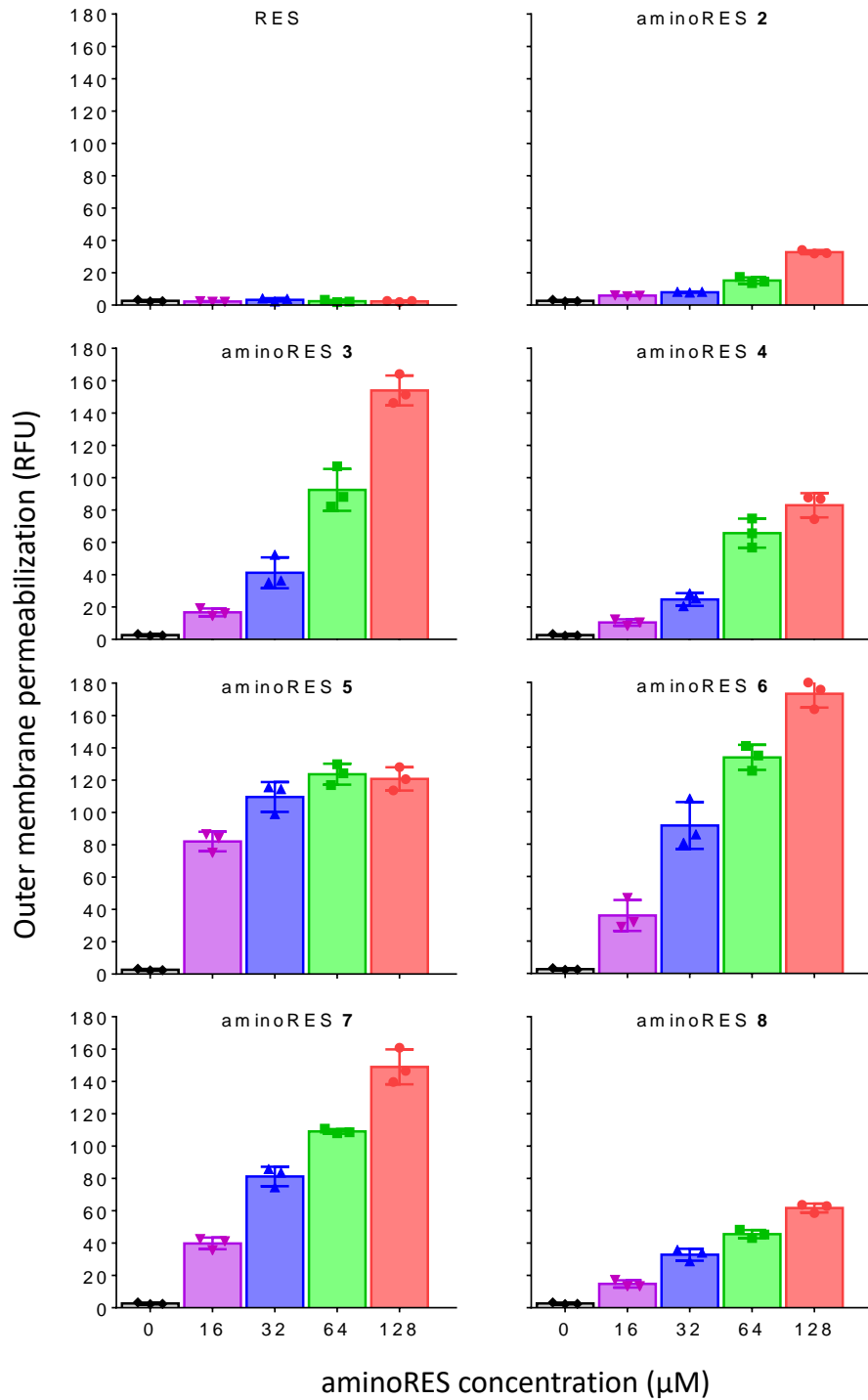
* R.C.: phone, +34-958021781 ; e-mail: rcebrian@ugr.es

* O.P.K.: phone, +31-503632093; email: o.p.kuipers@rug.nl

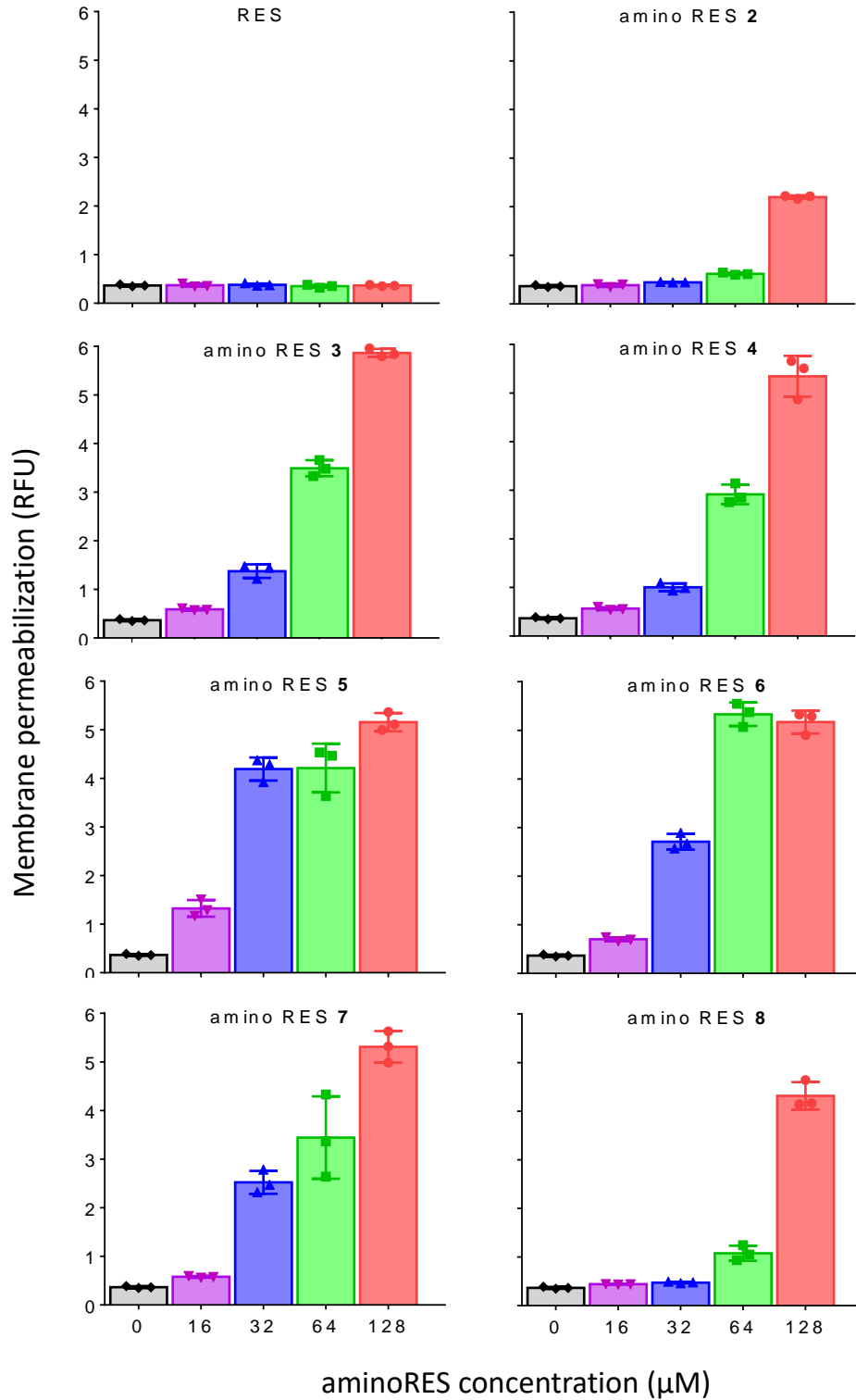
* J.C.M.: phone, +34-958181644; e-mail: jcmorales@ipb.csic.es

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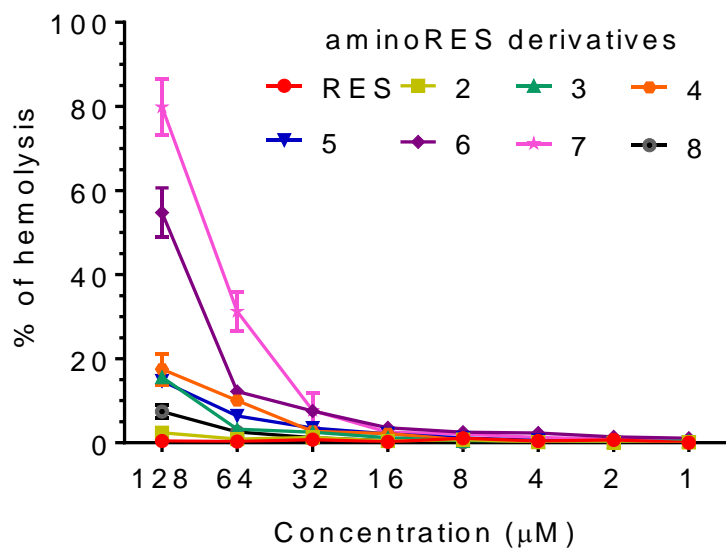
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Supplementary figure 1: *E. coli* LMG 8224 outer membrane permeabilization by the different amino RES designed.



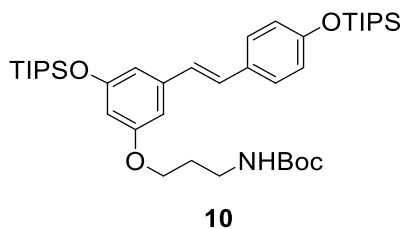
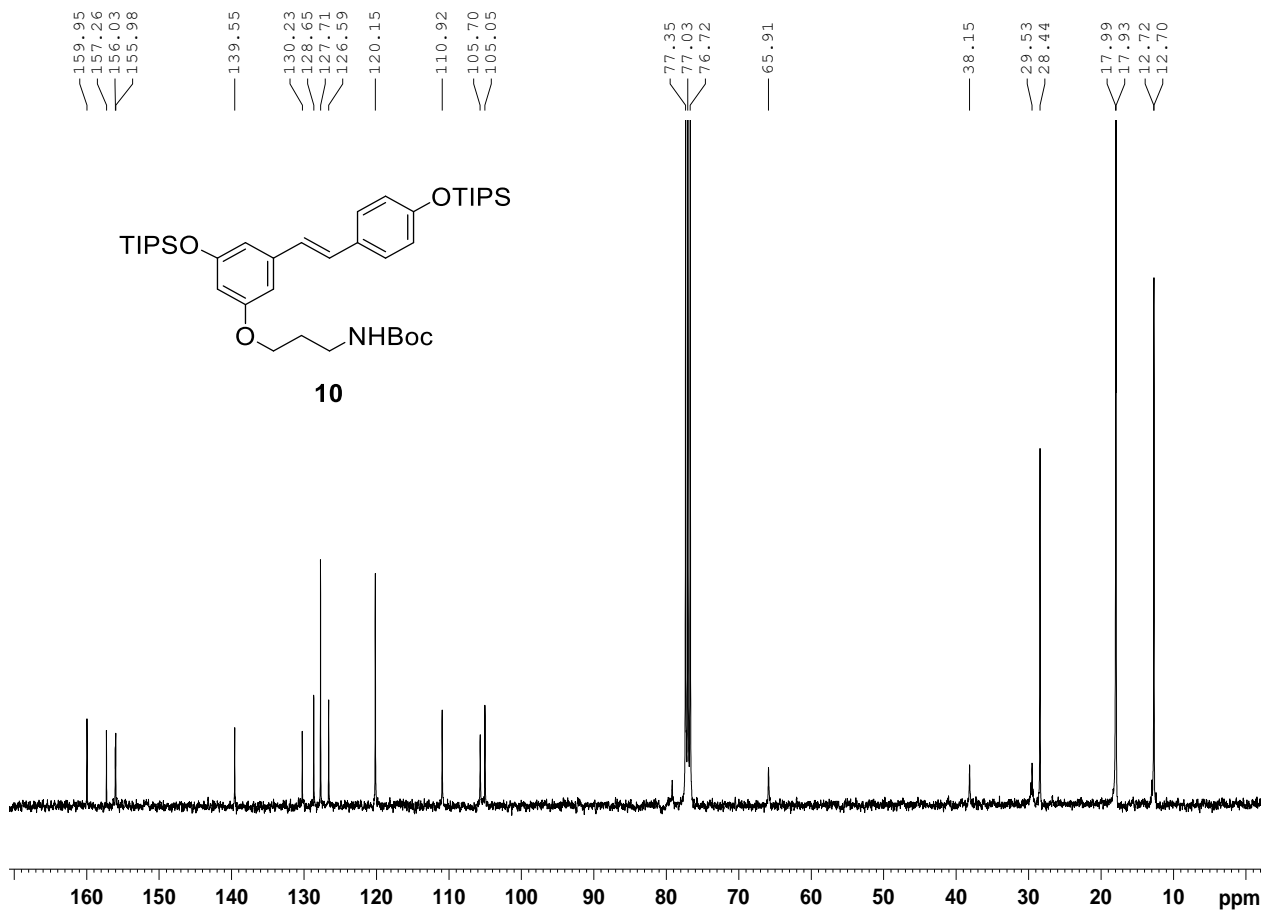
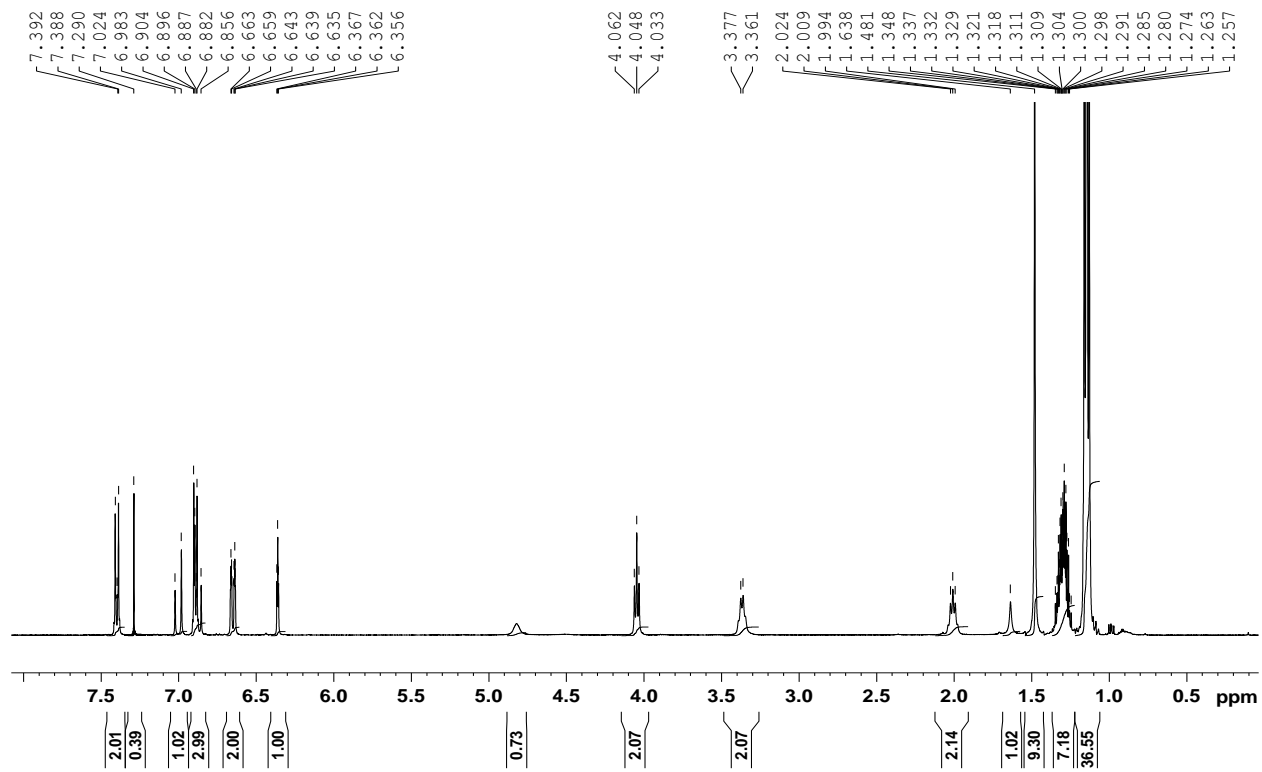
Supplementary figure 2: *E. coli* LMG 8224 inner membrane permeabilization by the different amino RES designed.

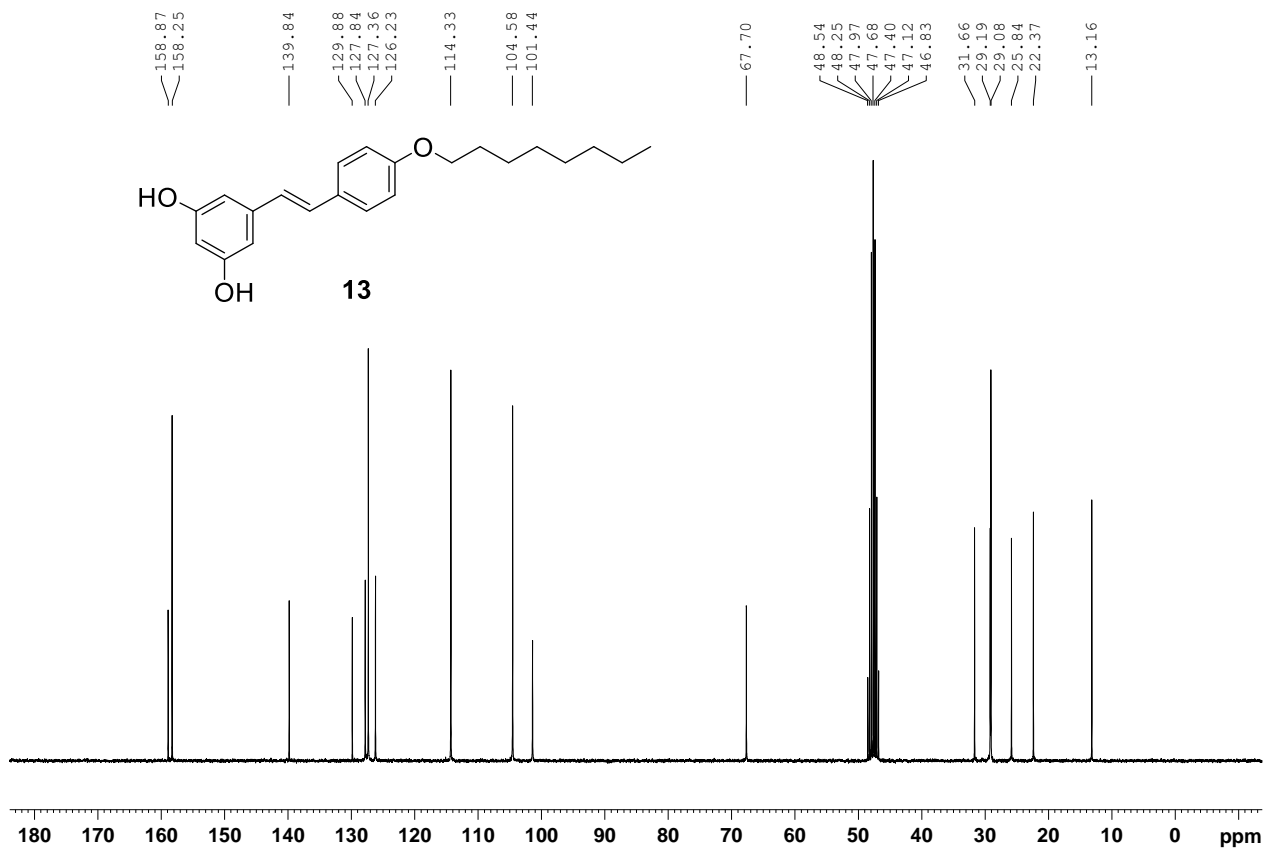
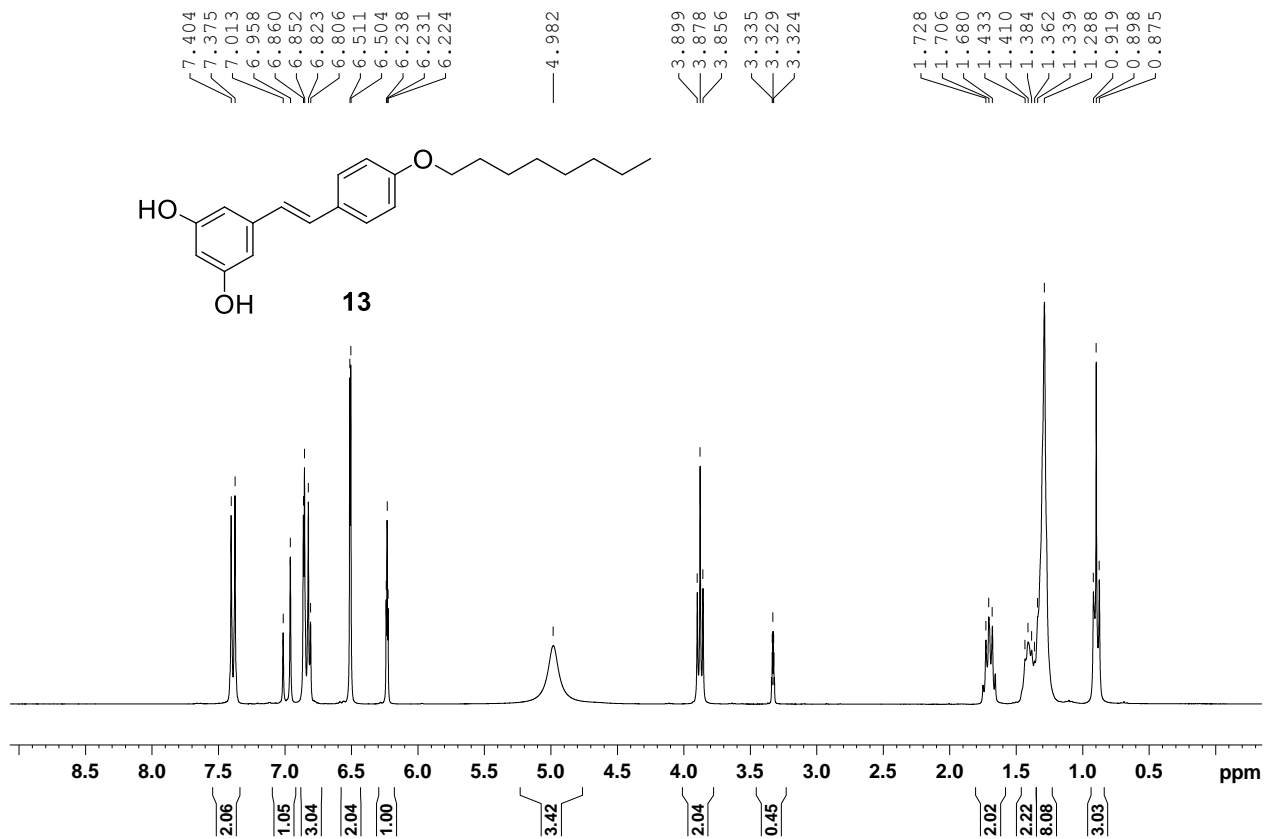


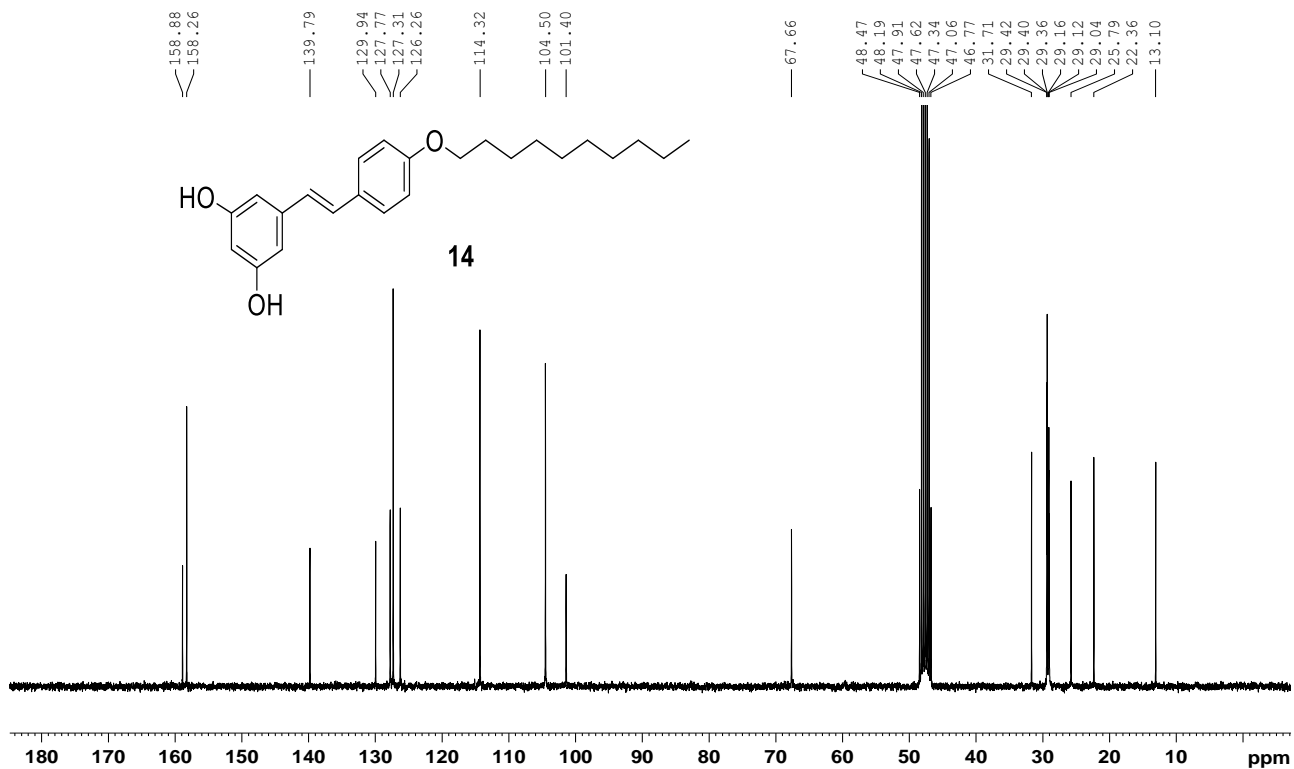
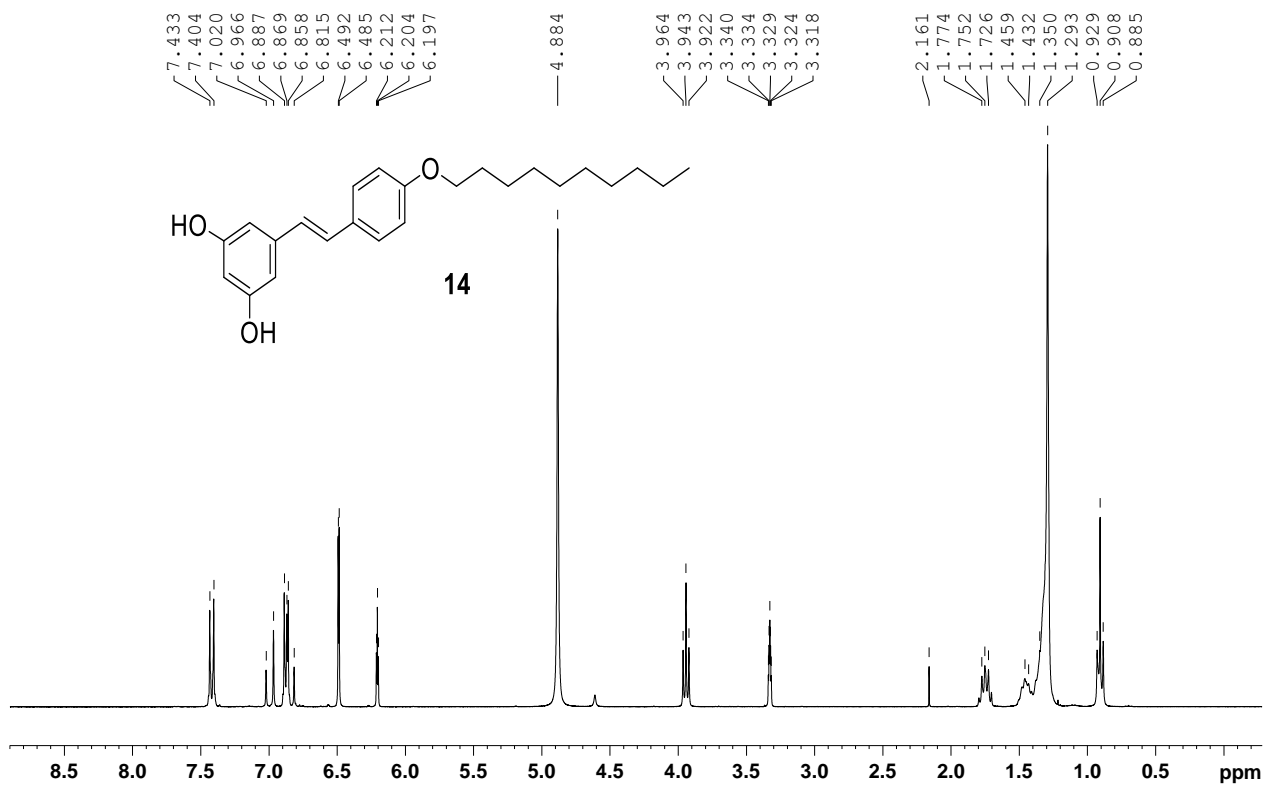
Supplementary Figure 3: Haemolytic activity of the different amino RES derivatives.

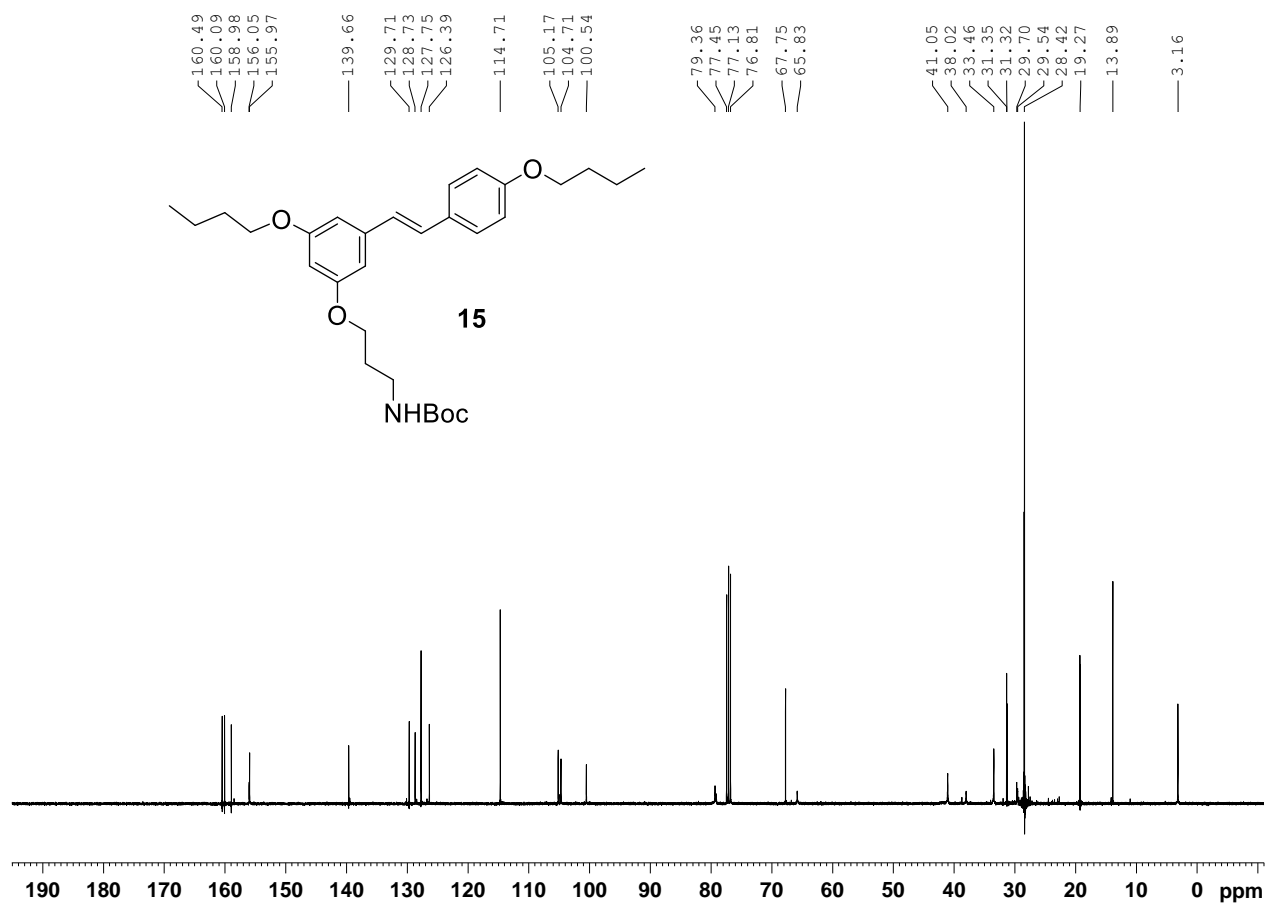
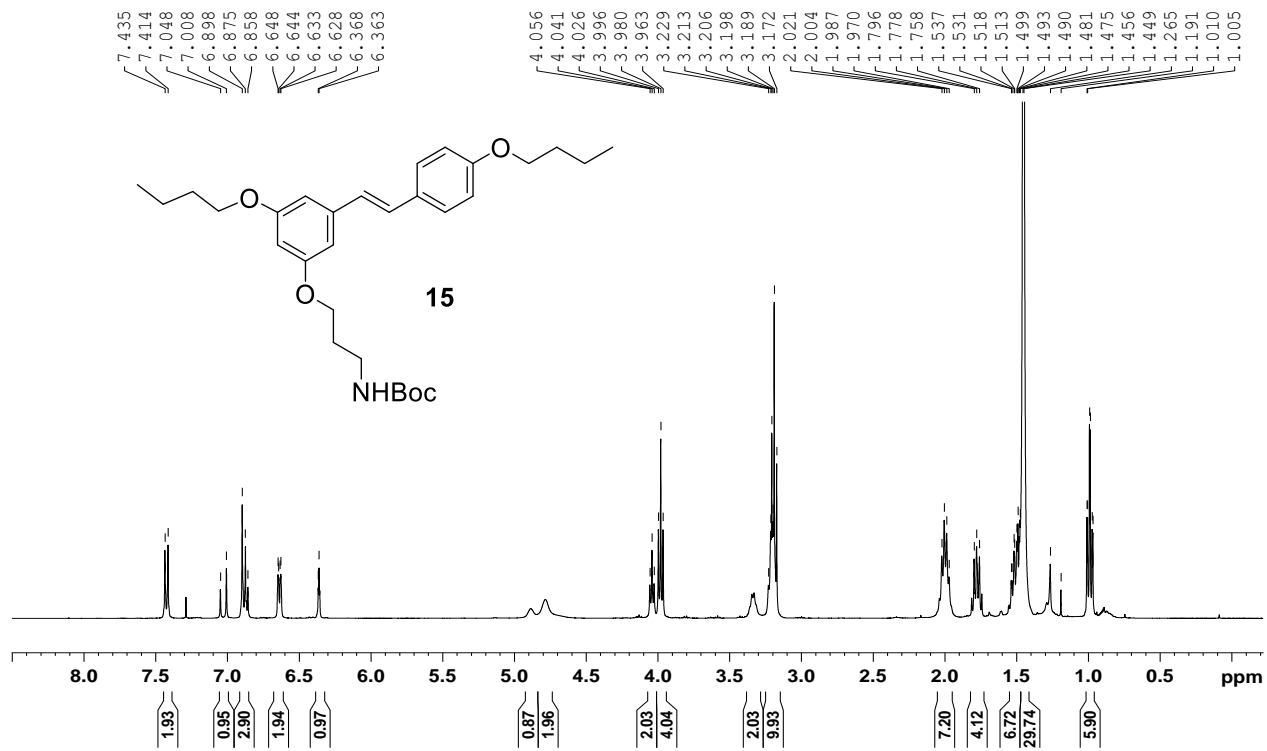
	RES	2	3	4	5	6	7	8
HC ₅₀	>128	>128	>128	>128	>128	124.43	79.90	>128
<i>A. baumannii</i> LMG 01041	-	-	2	2	8	-	-	-
<i>K. aerogenes</i> LMG 02094	-	-	-	-	4	-	-	-
<i>E. cloacae</i> LMG 02783	-	-	2	2	8	-	-	-
<i>E. coli</i> LMG 8224	-	-	2	2	16	0.97	-	2
<i>E. coli</i> NCTC 13846	-	-	-	-	19.20	-	-	2
<i>K. pneumoniae</i> LMG 20218	-	-	-	-	4	-	-	-
<i>P. aeruginosa</i> PAO1	-	-	-	-	4	-	-	-
<i>S. enterica</i> LMG 07233	-	-	-	-	8	-	-	2
<i>B. cereus</i> LMG 10987	-	-	2	3	9.60	1.46	0.62	-
<i>B. cereus</i> LMG 14574	-	-	2.4	4	8	3.89	0.62	2
<i>E. faecalis</i> V583	-	-	-	-	9.60	-	-	-
<i>E. faecalis</i> LMG 8222	-	-	4.80	6	16	7.78	-	2
<i>E. faecalis</i> LMG 16716	-	-	4	4	19.20	7.78	-	-
<i>E. faecium</i> LMG 11423	-	-	4	8	16	15.55	-	2
<i>E. faecium</i> LMG 16003	-	-	2	2	16	-	-	2
<i>S. aureus</i> LMG 15975	-	-	4.80	8	76.80	7.78	0.62	2
<i>S. aureus</i> LMG 8223	-	2	6	6	32	15.55	1.25	2
<i>S. aureus</i> LMG 10147	-	-	-	-	19.20	0.97	-	2
<i>Bacteroides ovatus</i> 3_8_47FAA	-	-	12.02	8	16	15.55	2.50	-
<i>B. fragilis</i> NCTC 9343	-	-	8	8	16	6.69	1.25	-
<i>B. salyersiae</i> DMS 18765	-	-	8	8	16	9.36	1.50	-
<i>B. xylanisolvens</i> DMS 18836	-	2	16	16	32	15.55	2.50	2
<i>Parabacteroides merdae</i> CL03T12C32	-	-	-	-	4	-	-	-
<i>C. botulinum</i> CECT 551	2	2	32	16	128	124.43	9.99	2
<i>C. difficile</i> CECT 531	-	2	16	16	64	31.11	4.99	-
<i>C. perfringens</i> CECT 376	-	2	16	16	12	62.22	-	-
<i>C. tetani</i> CECT 462	-	-	19.20	16	32	124.43	3.75	-

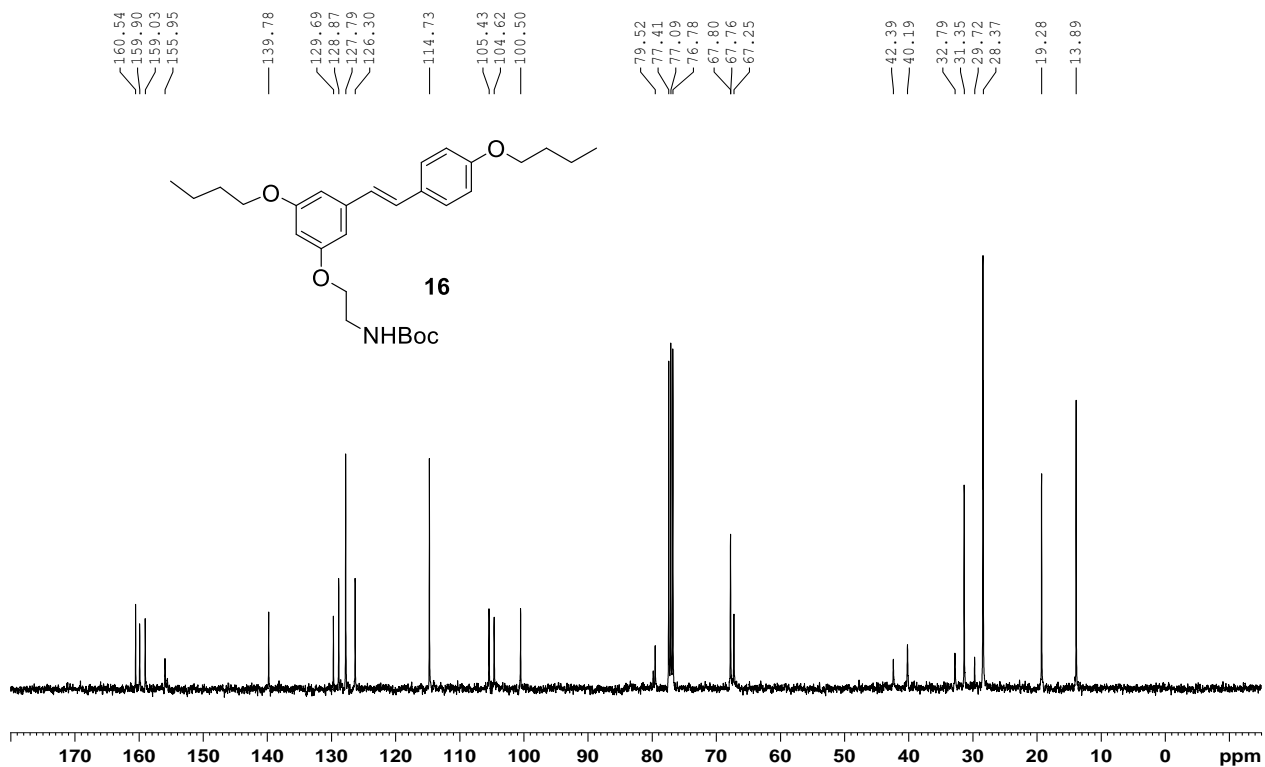
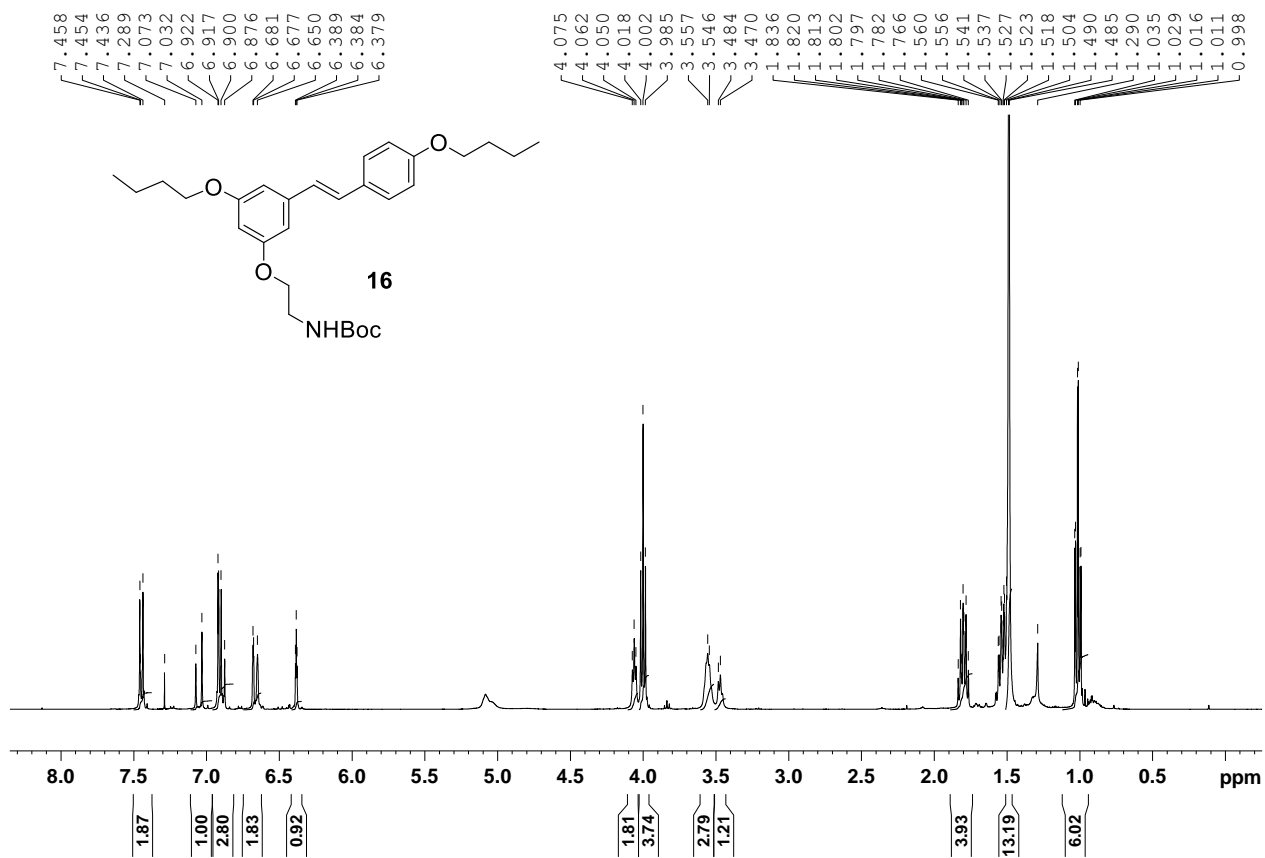
Supplementary table 1: Selective index HC₅₀/MIC. For the compounds in which HC₅₀ was not detected in the assay 2X the higher tested concentration was used in the calculations.

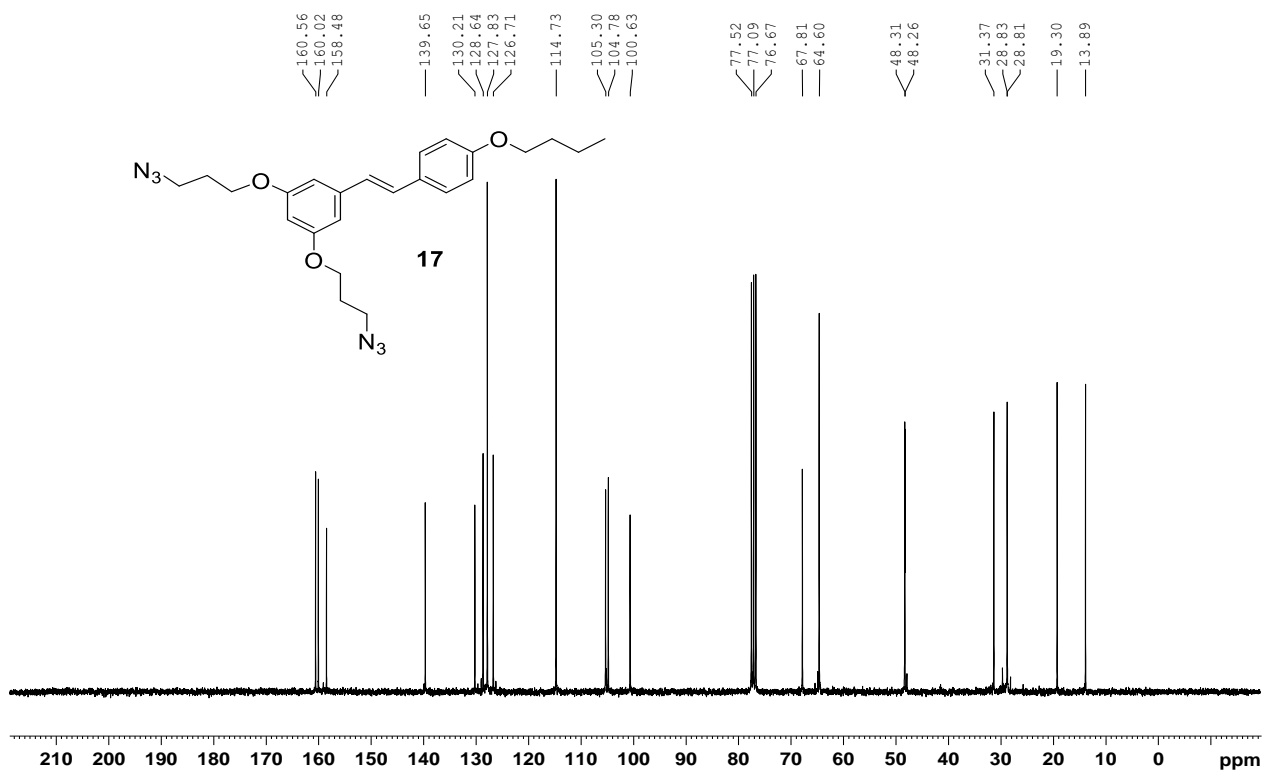
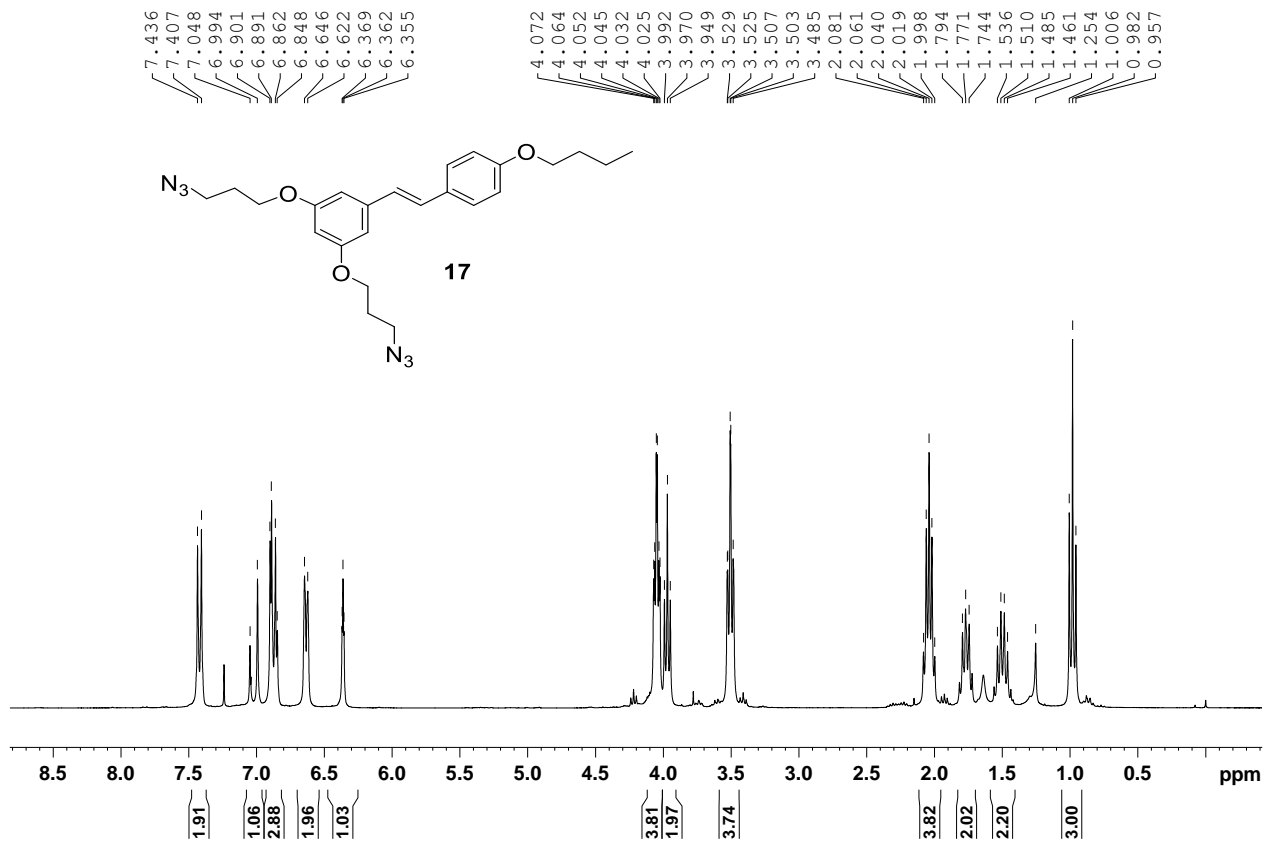


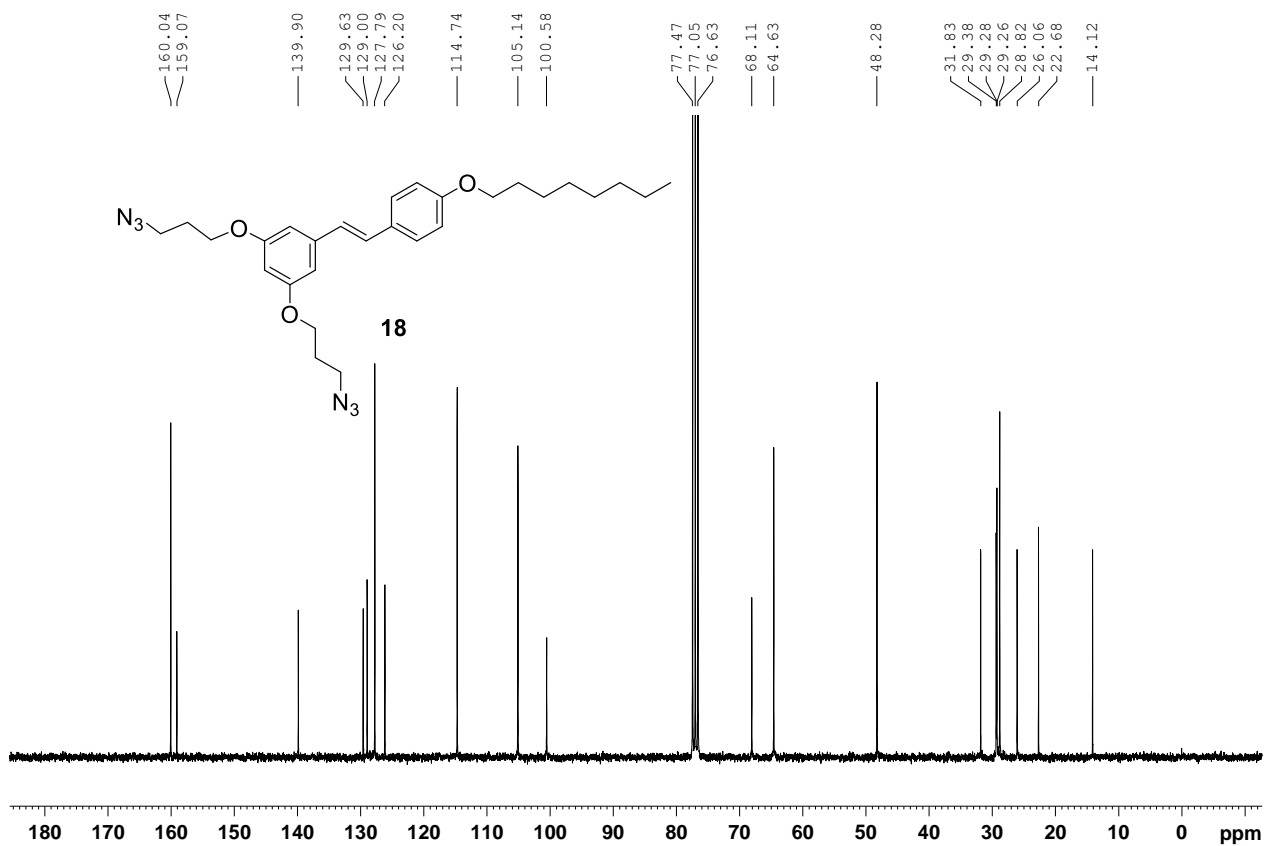
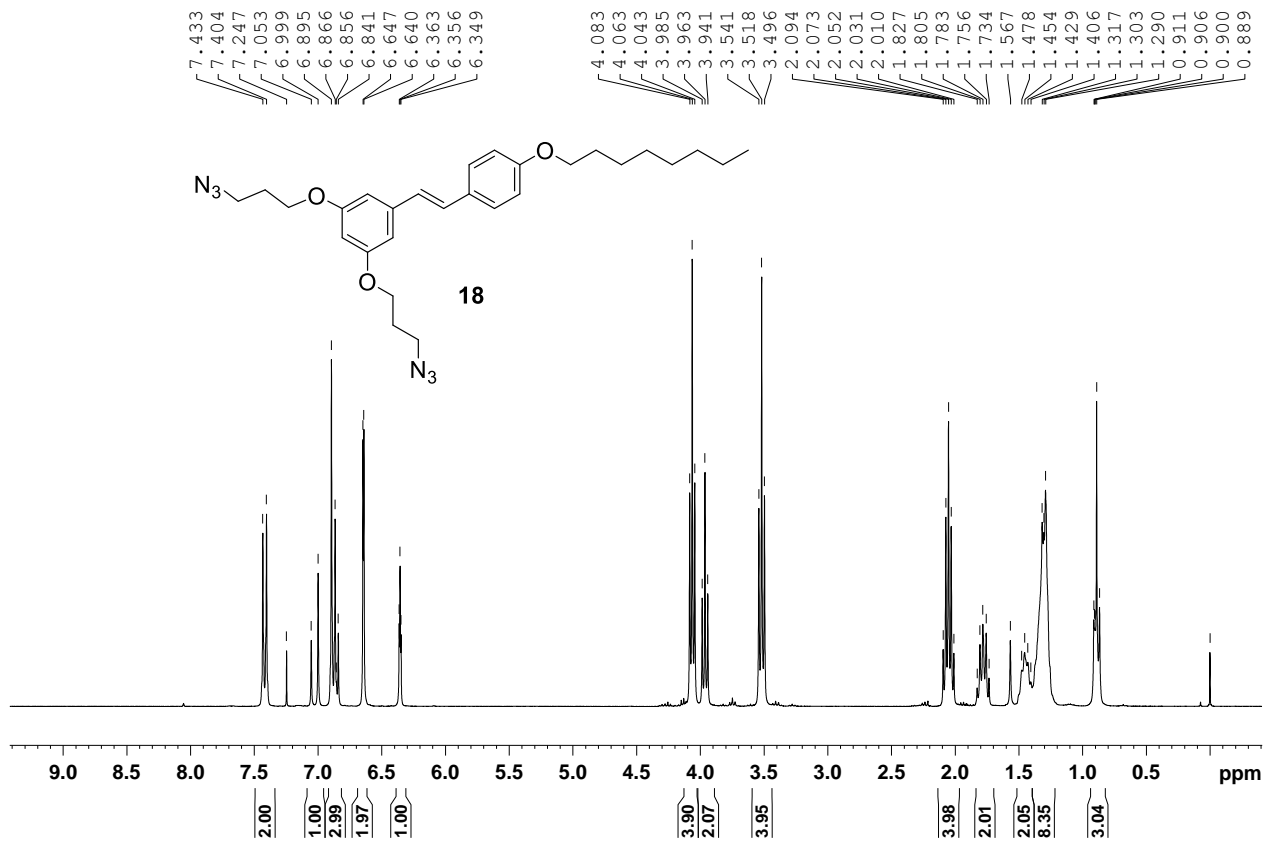


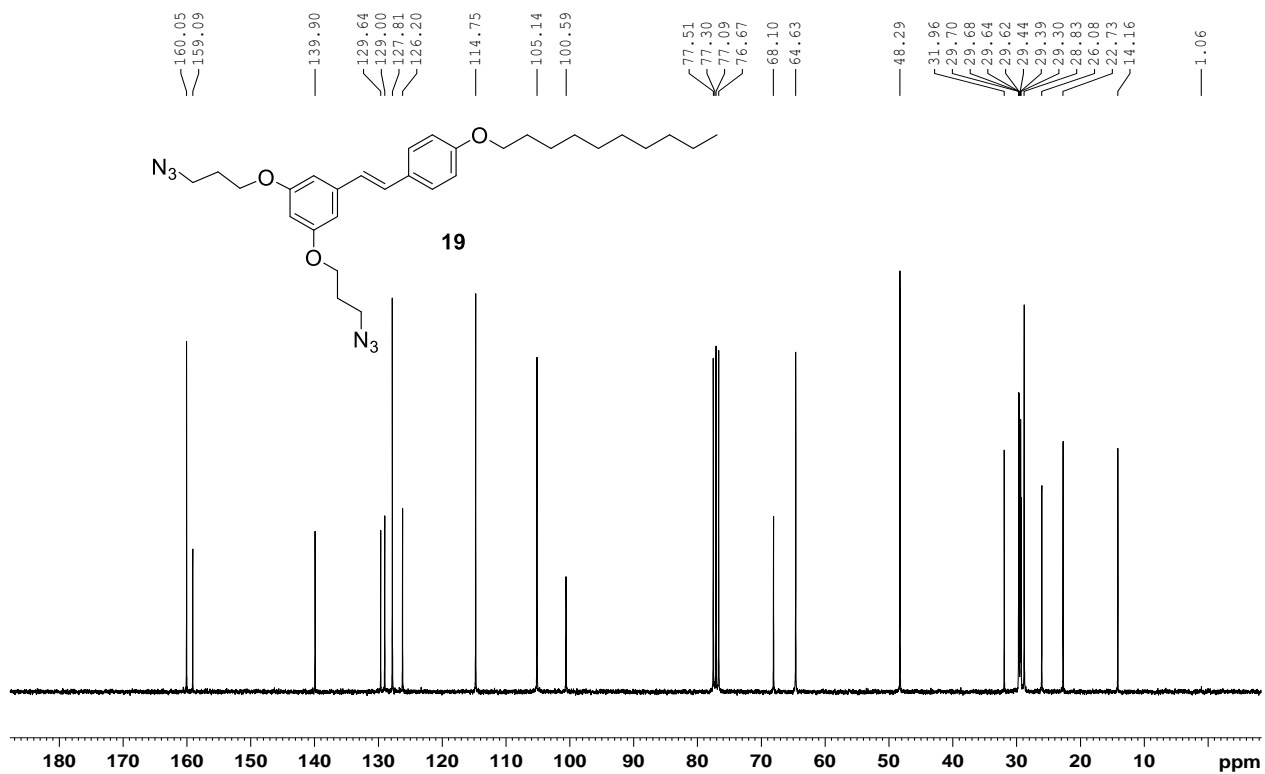
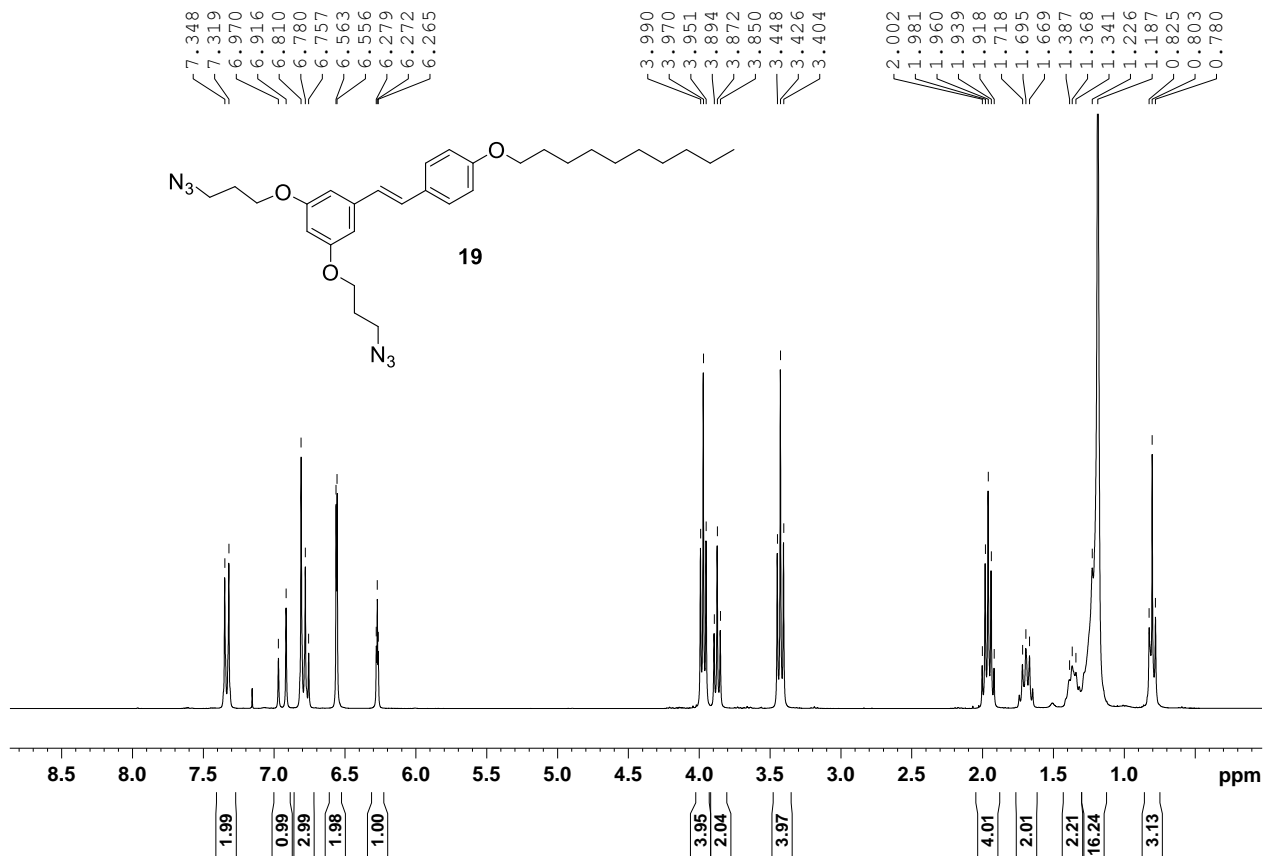


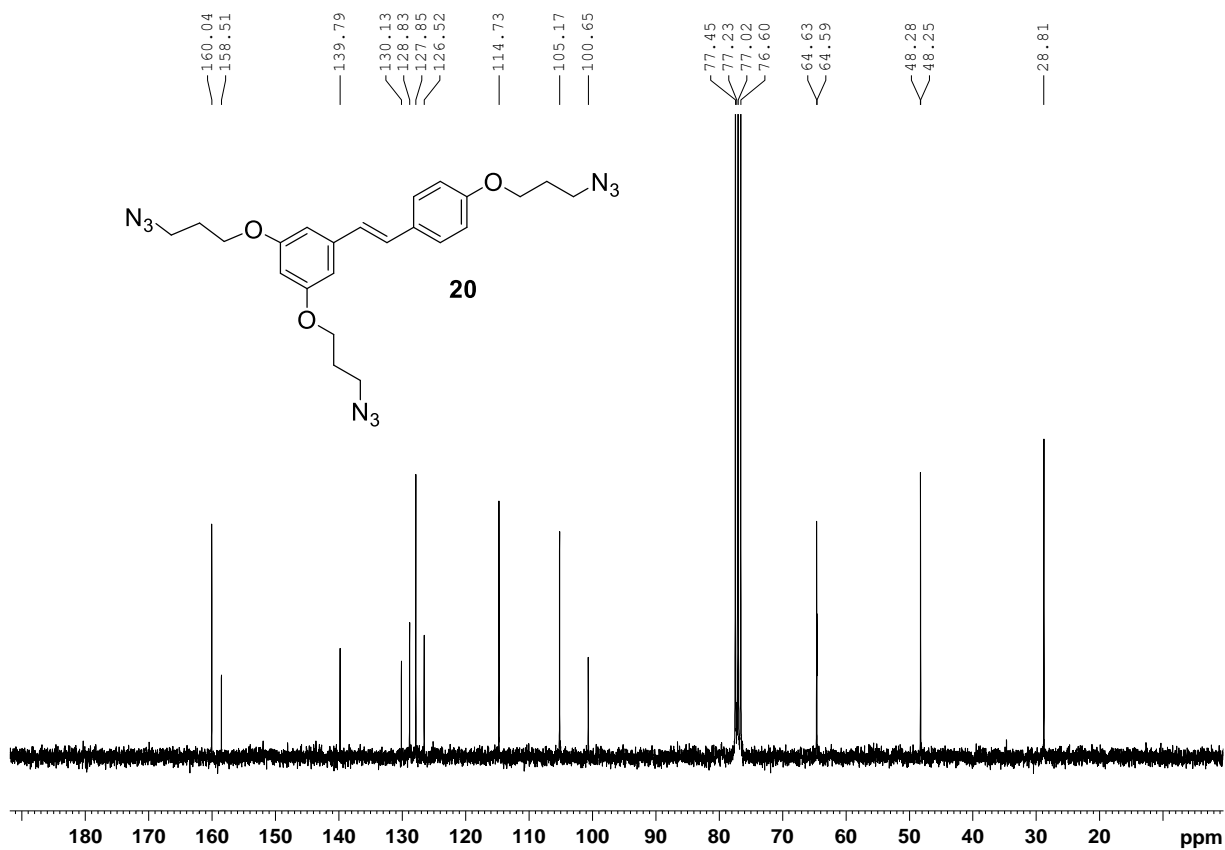
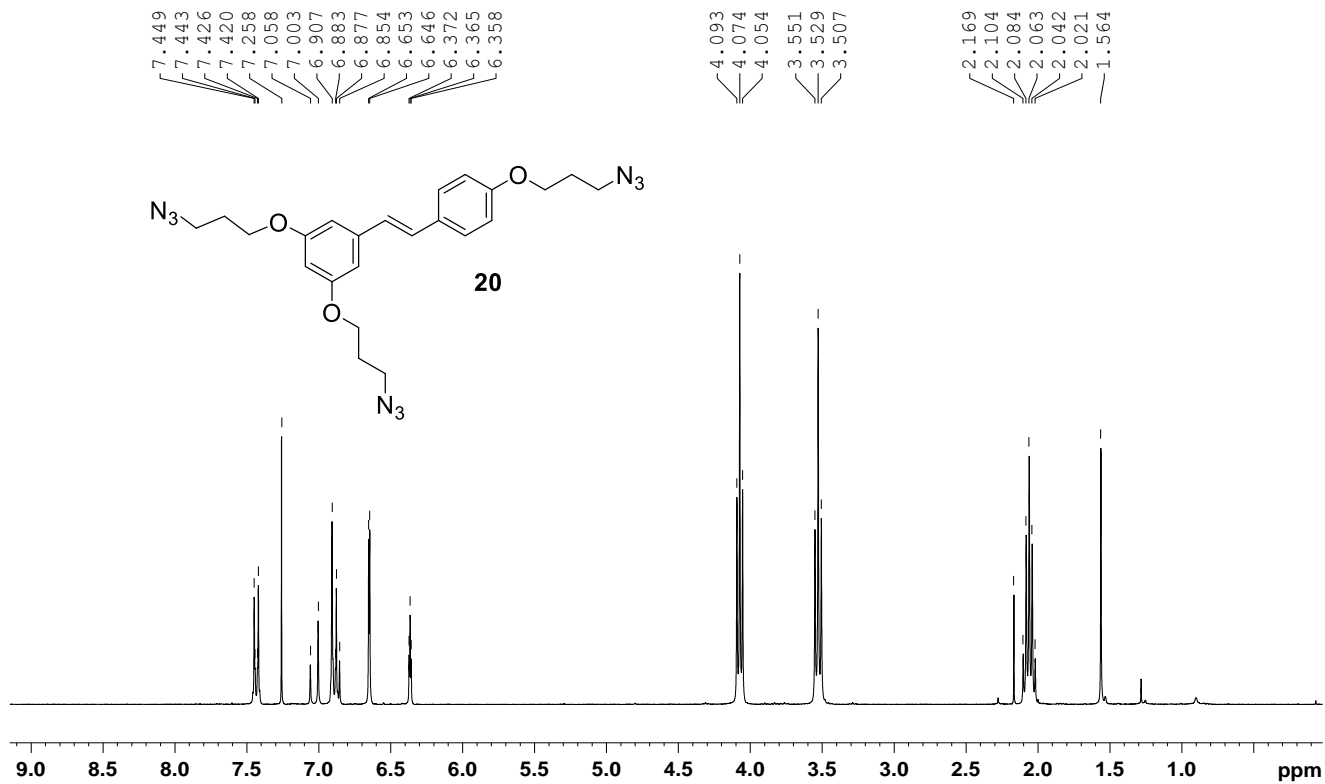


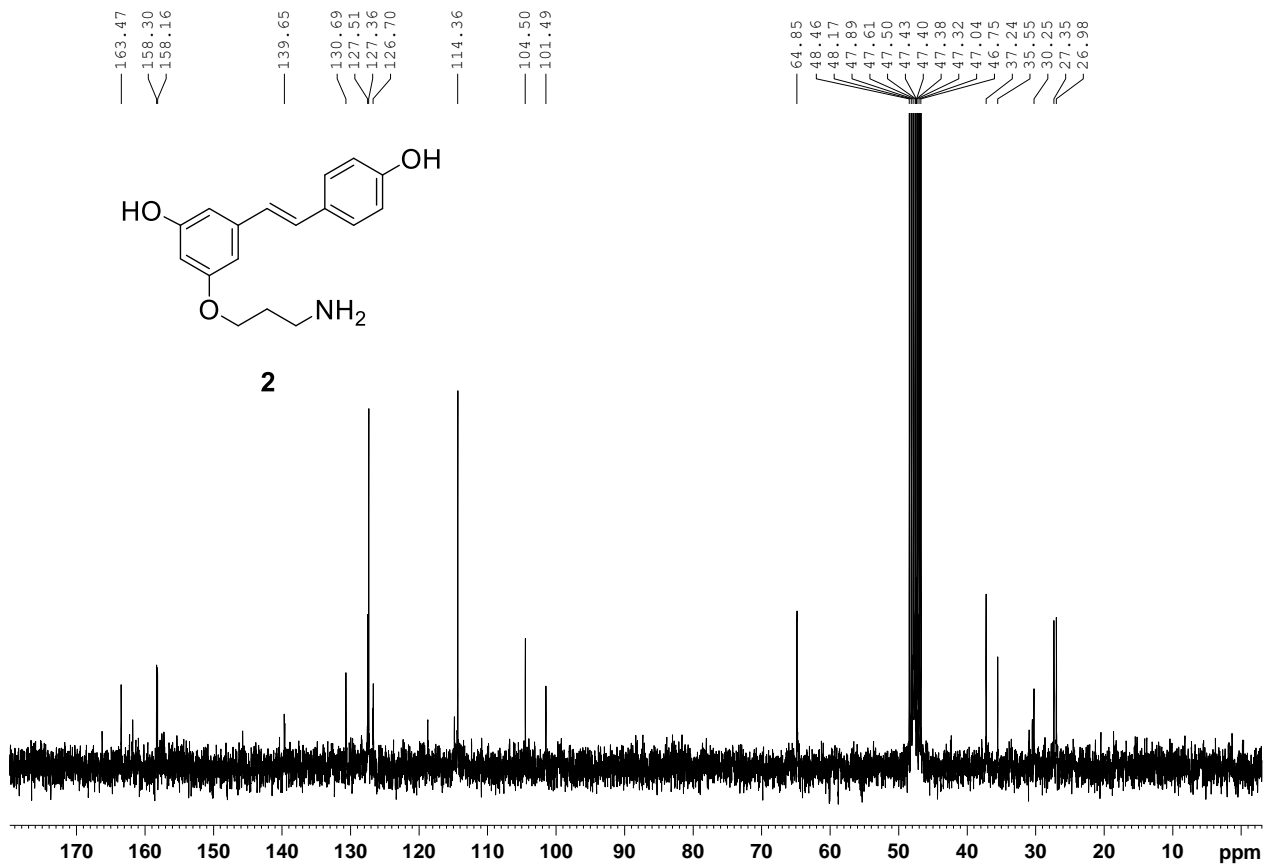
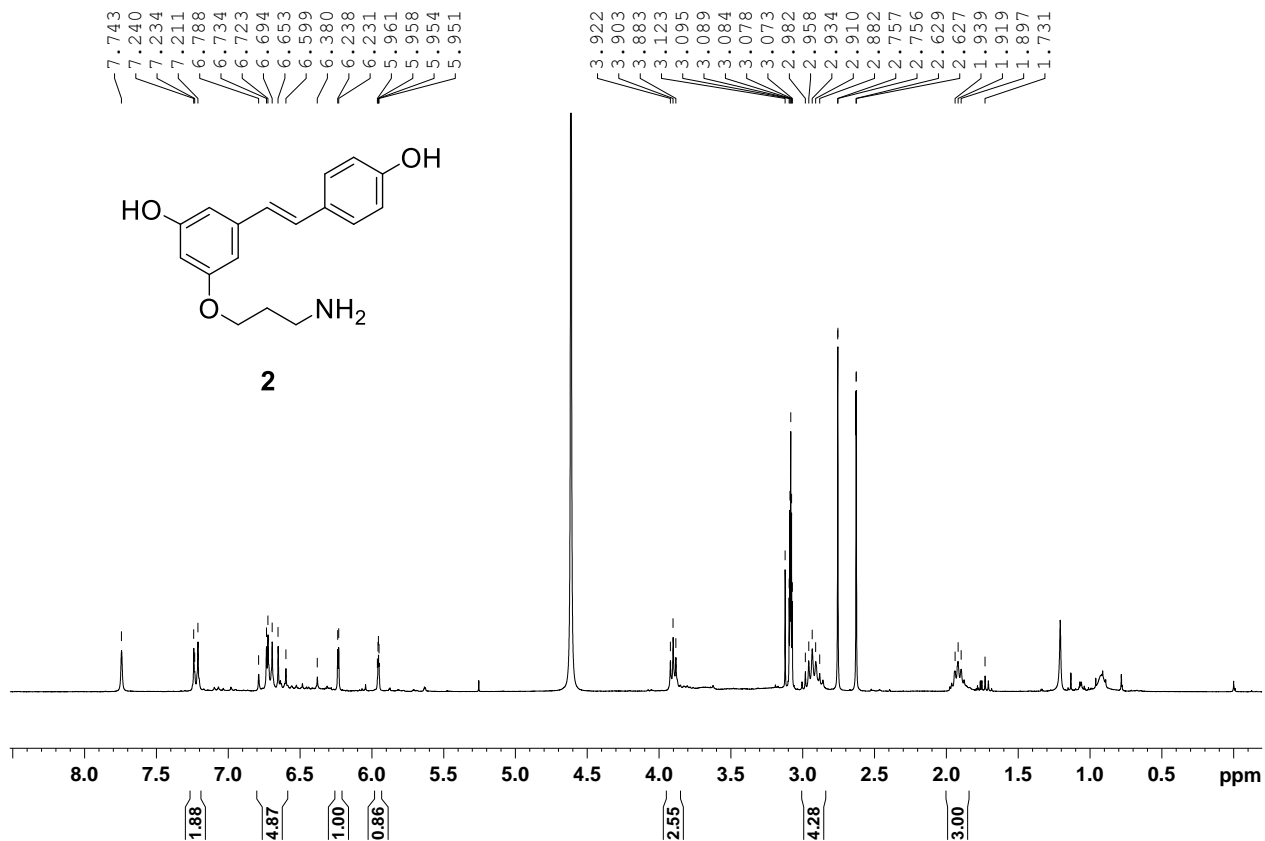


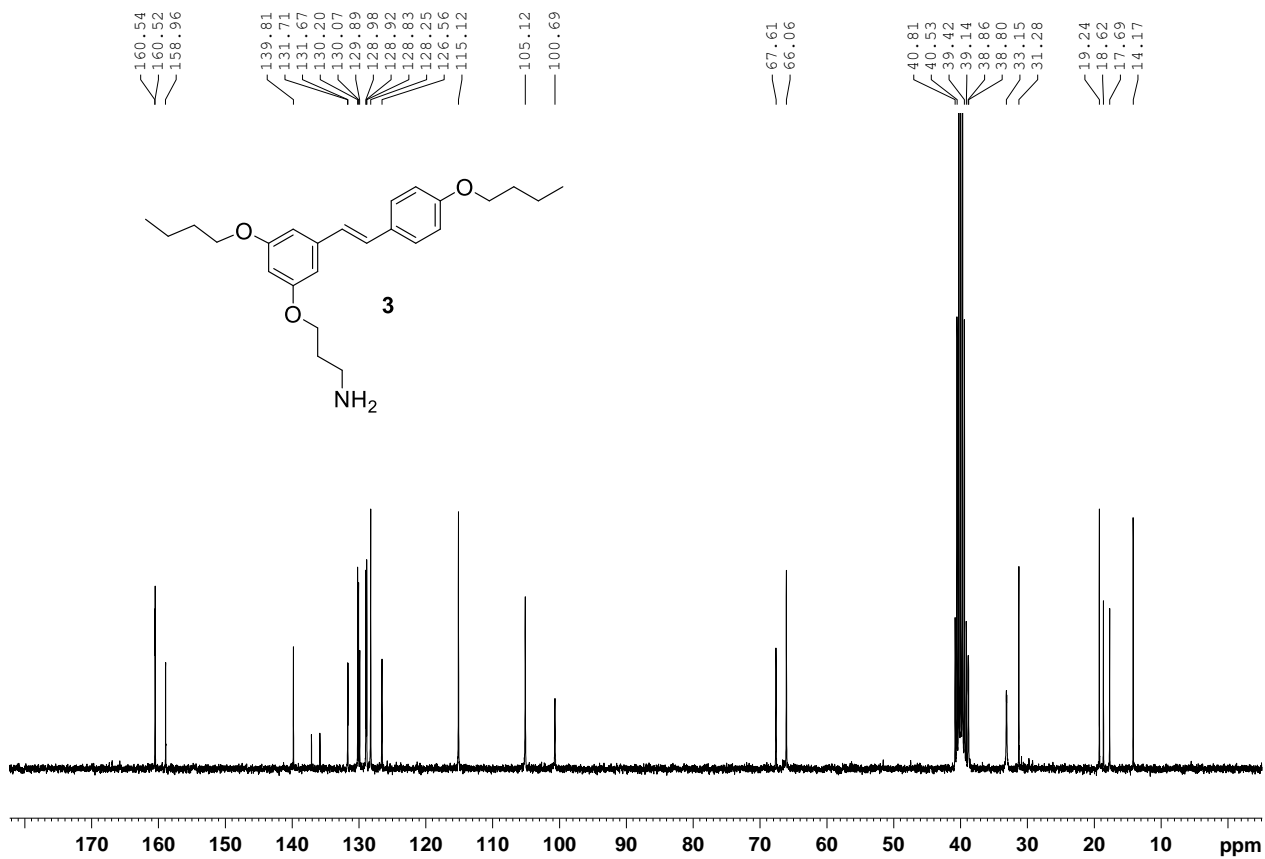
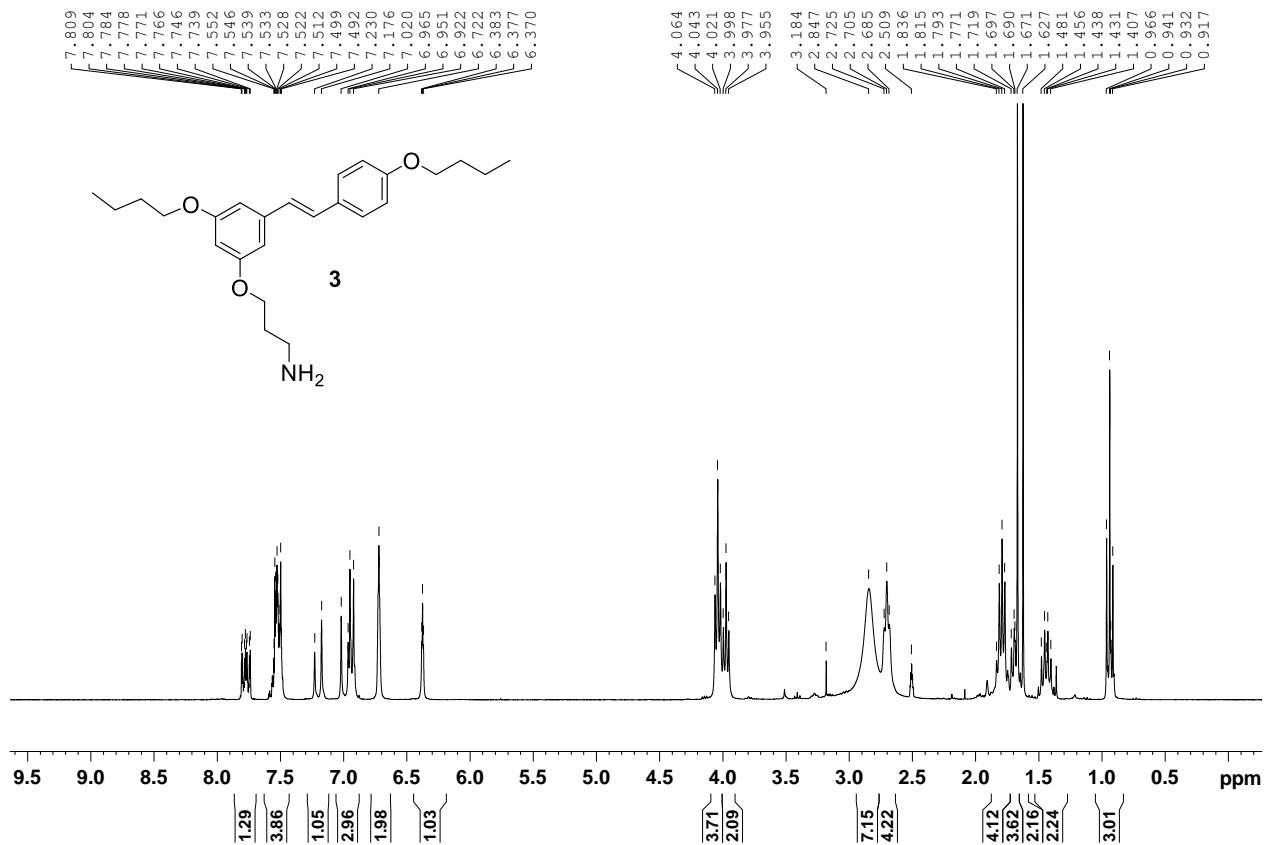


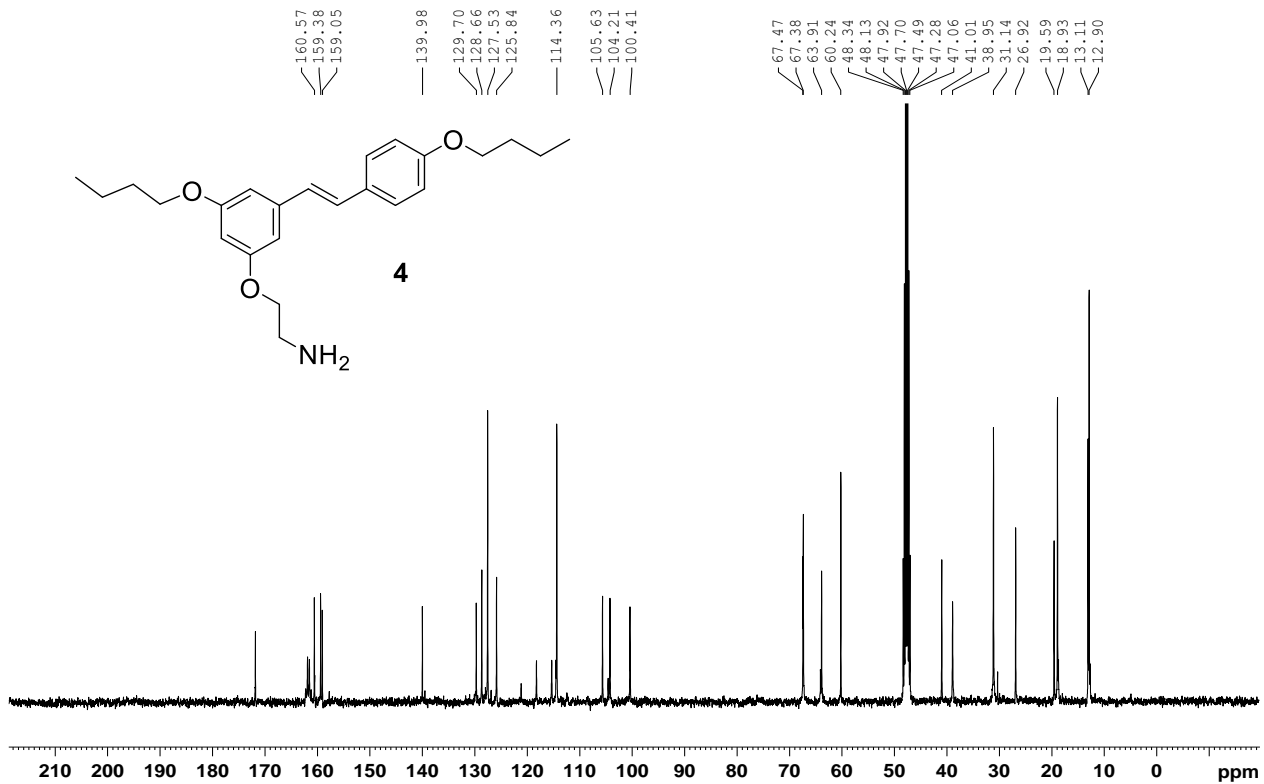
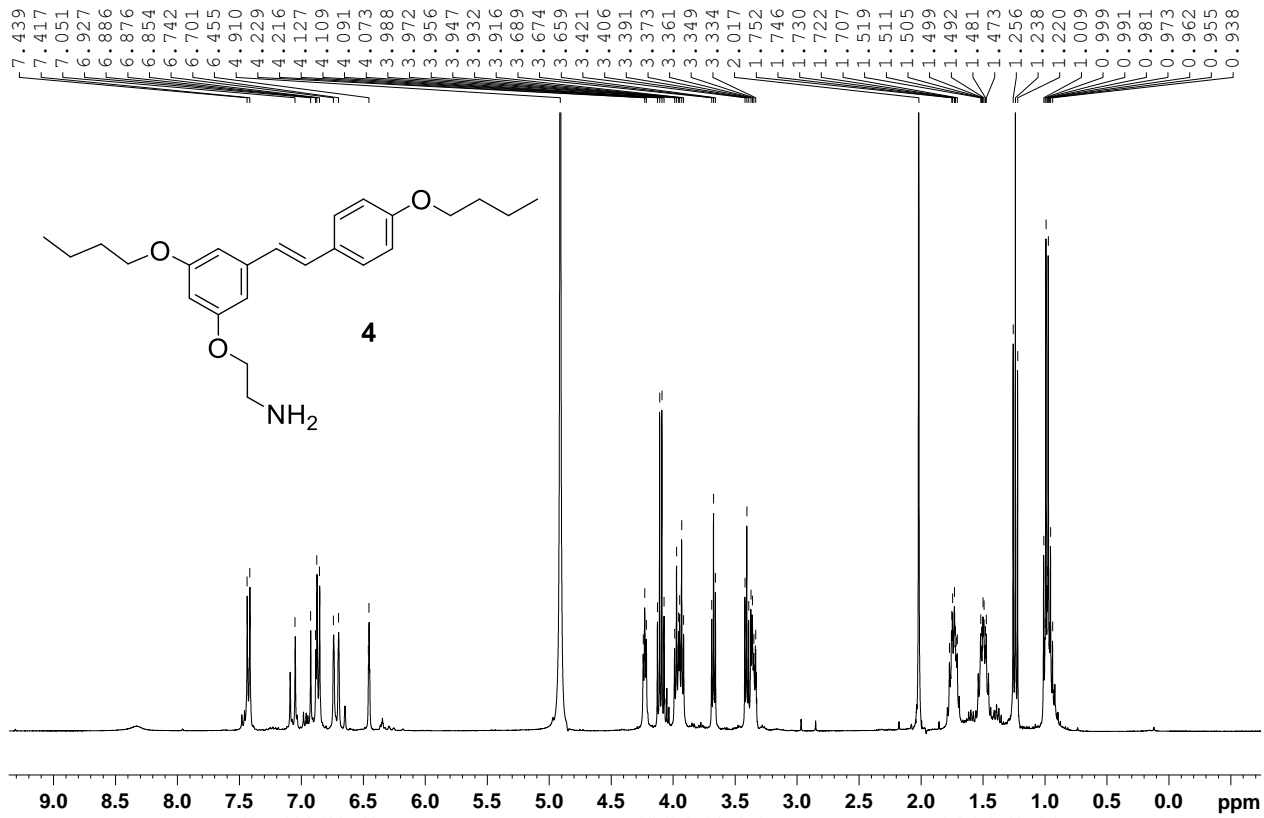


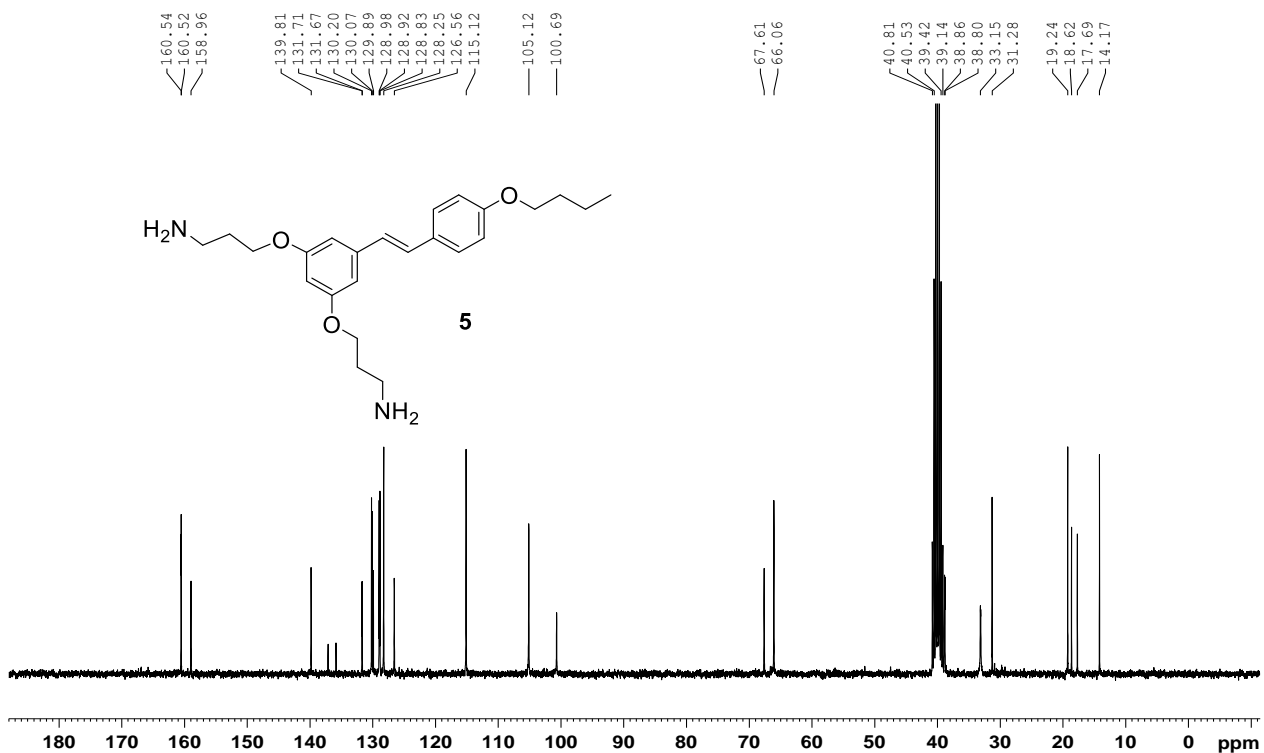
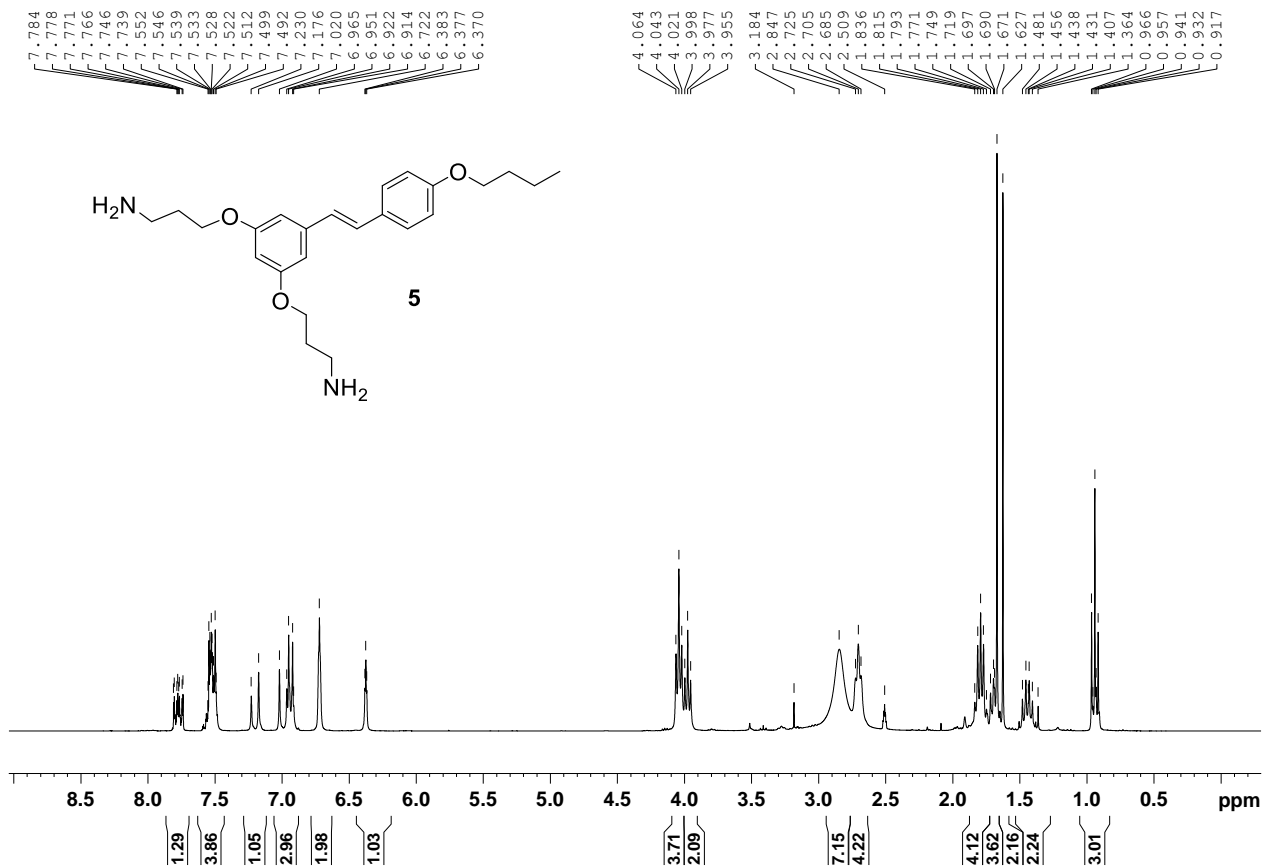


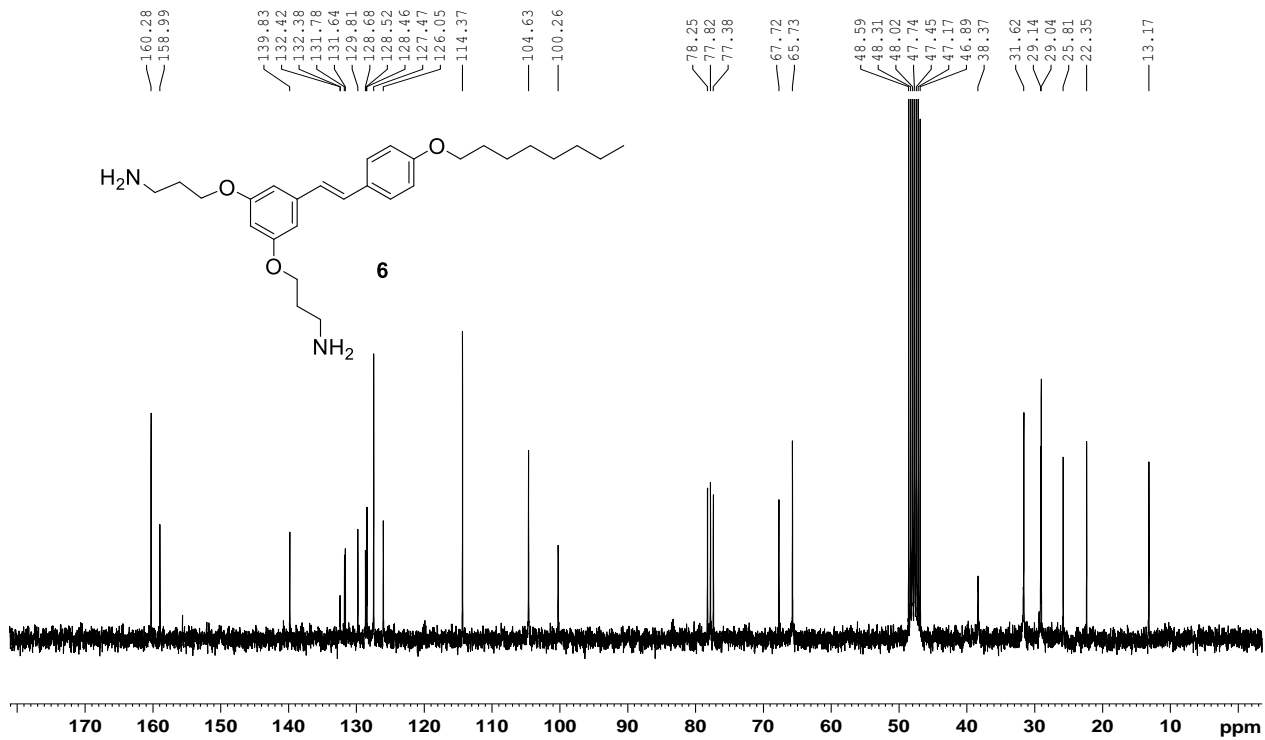
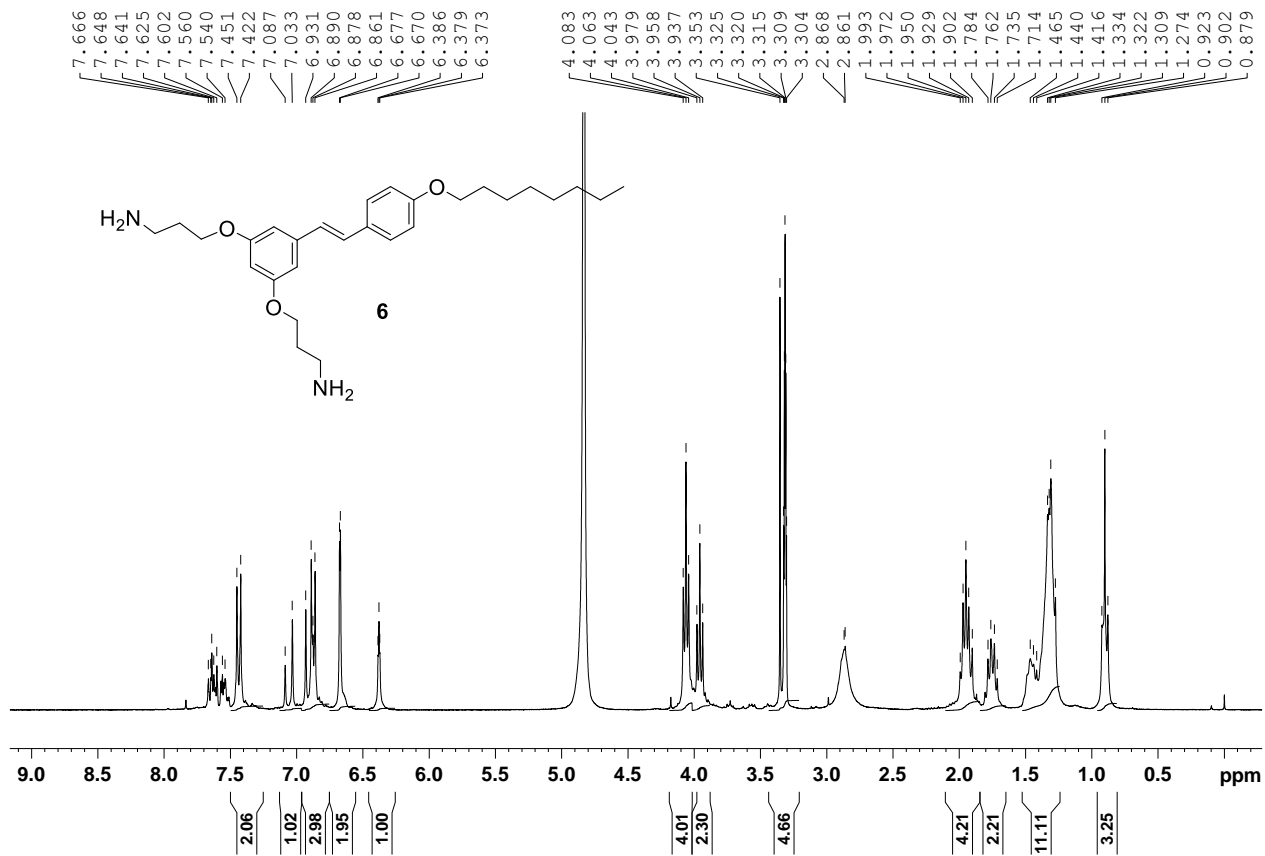


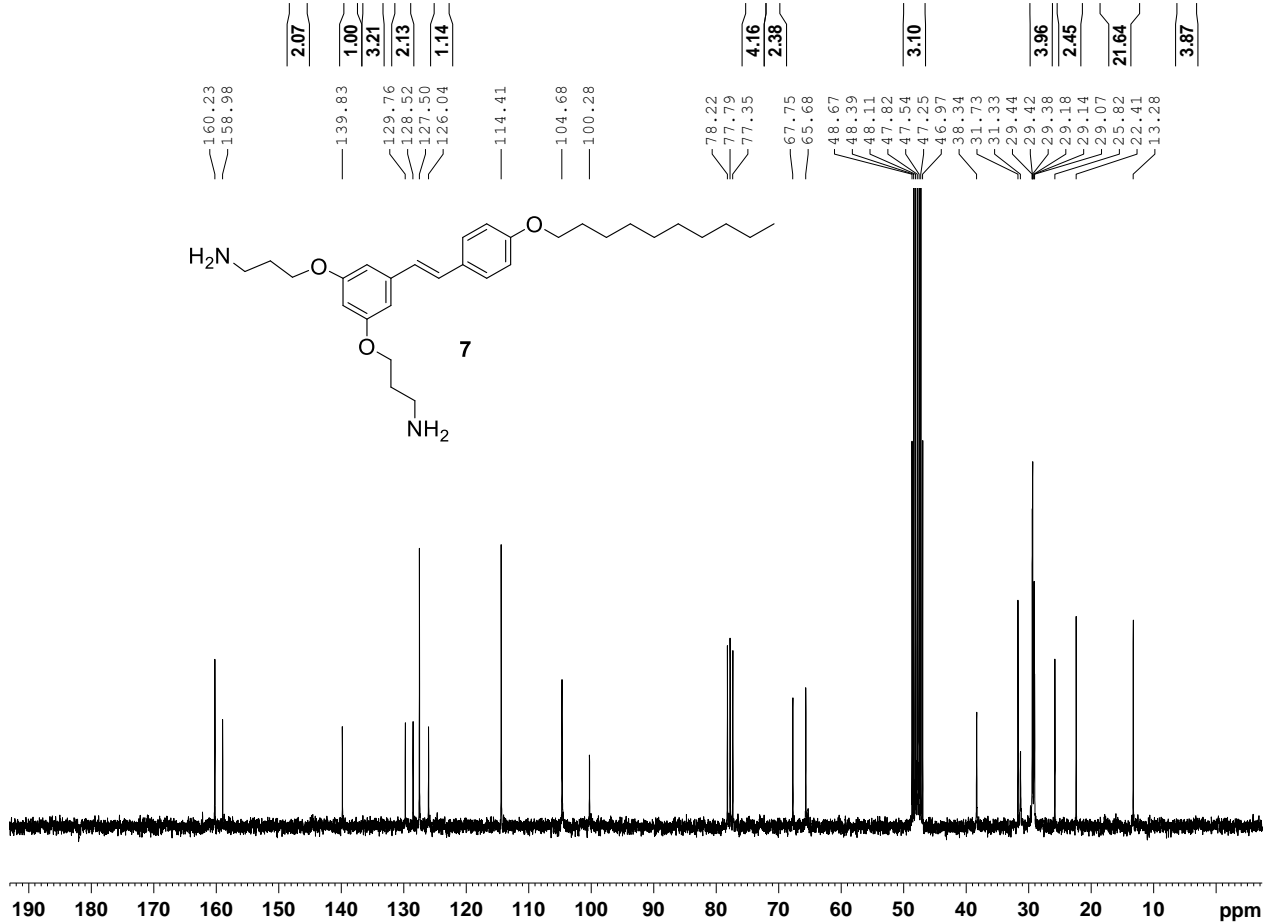
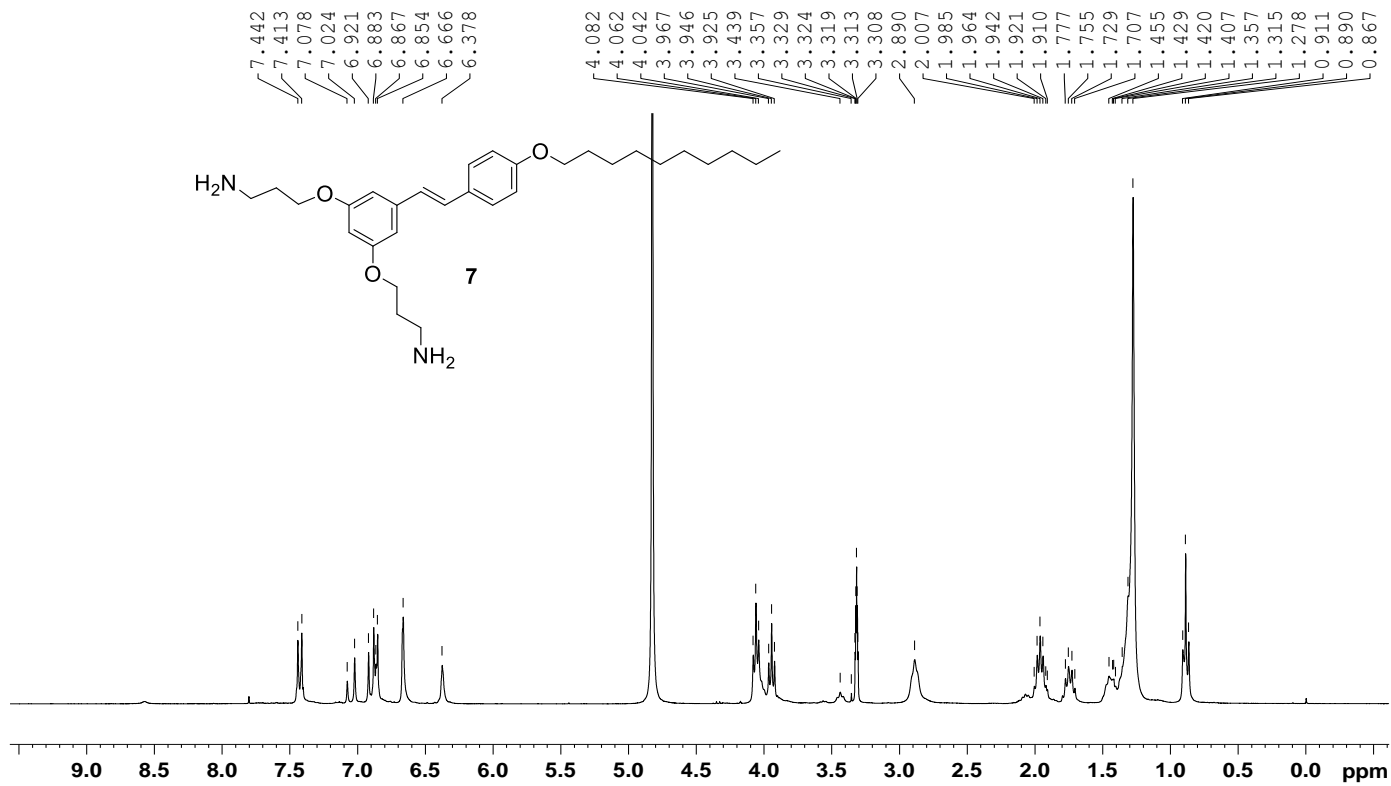


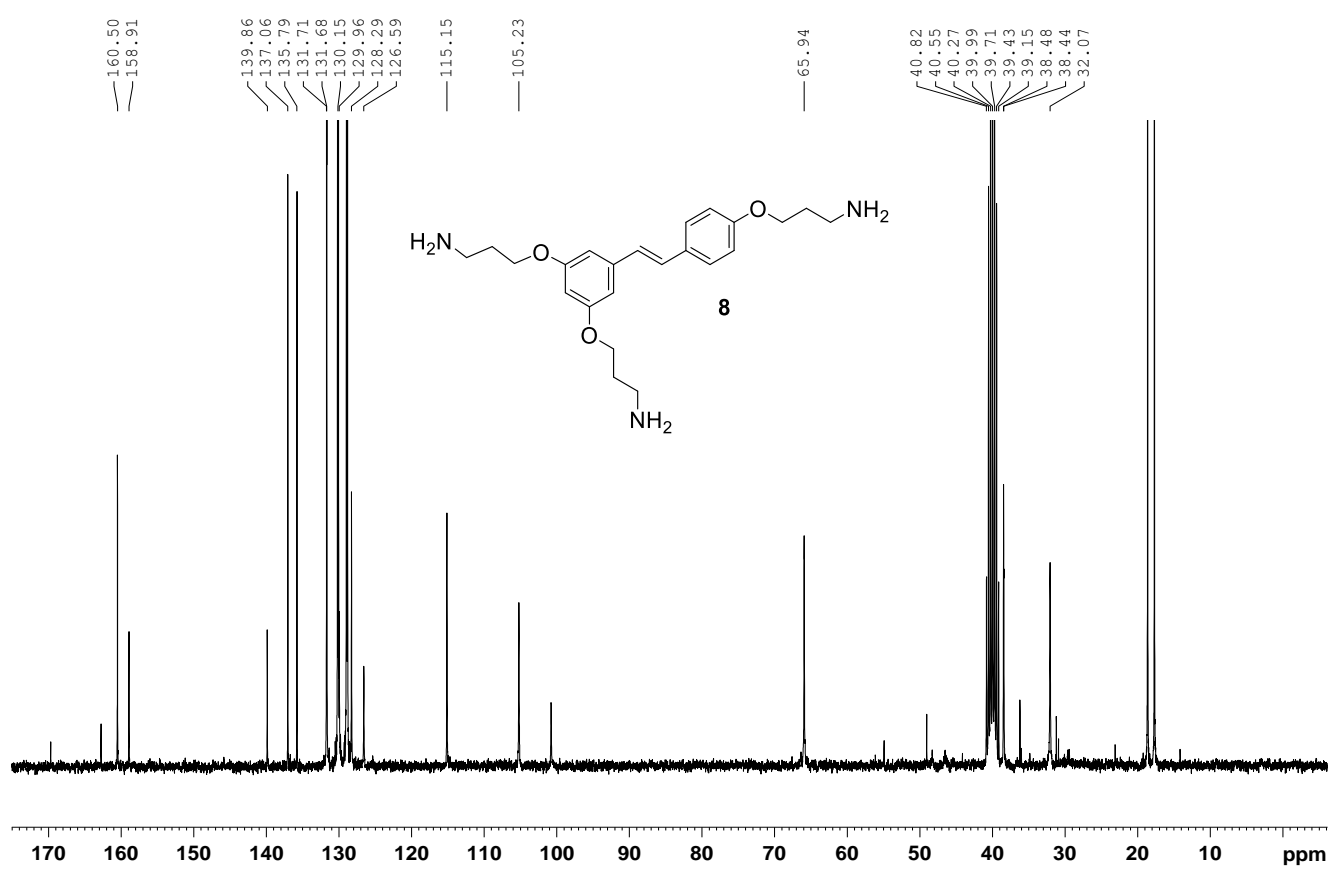
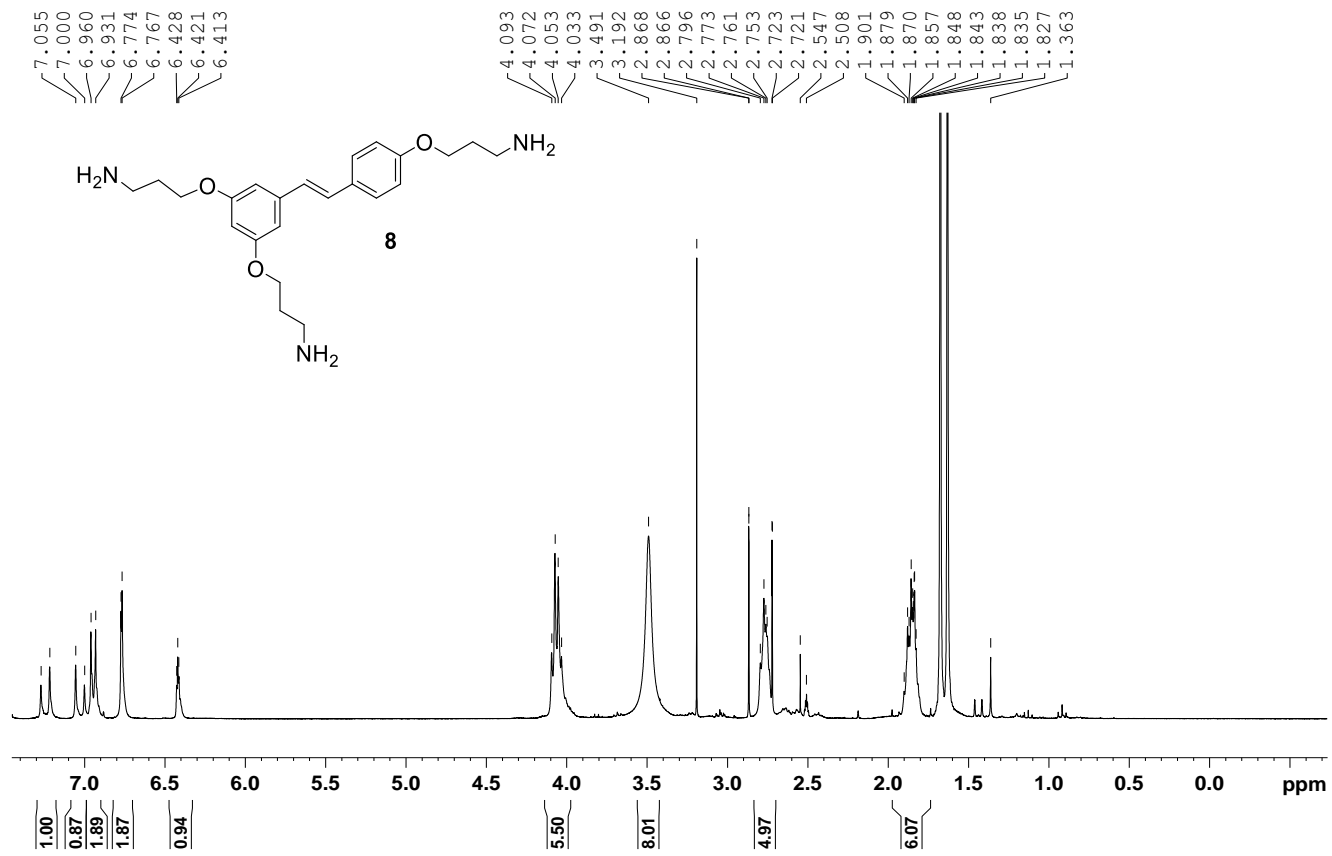






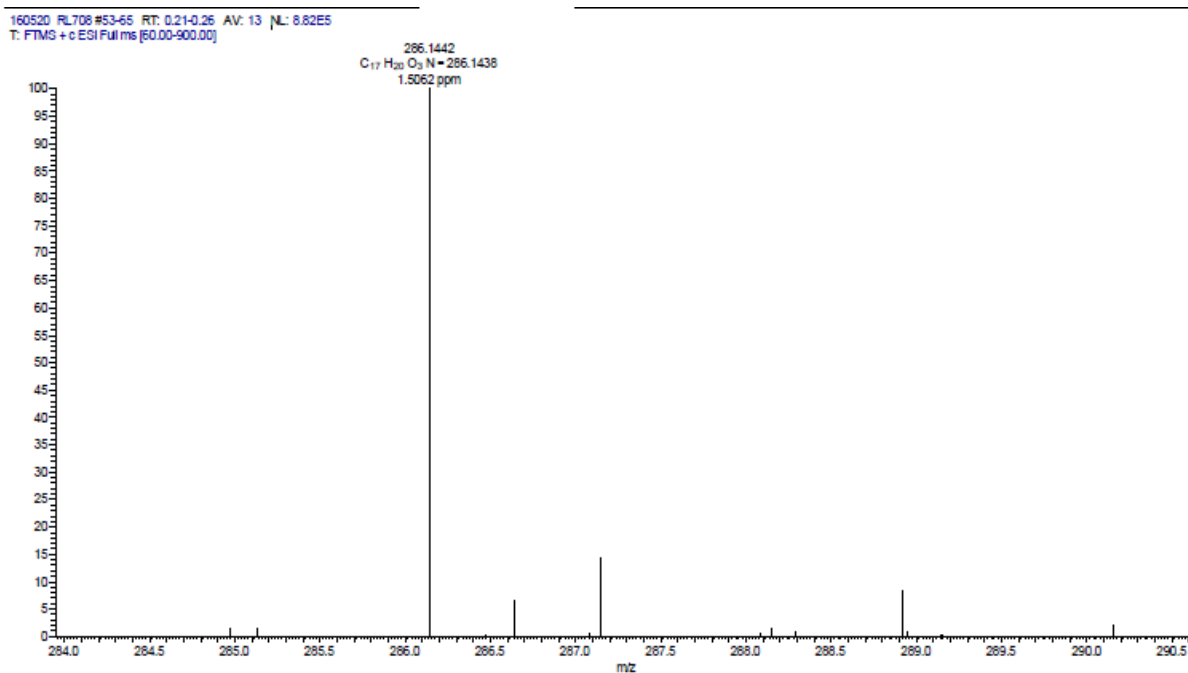




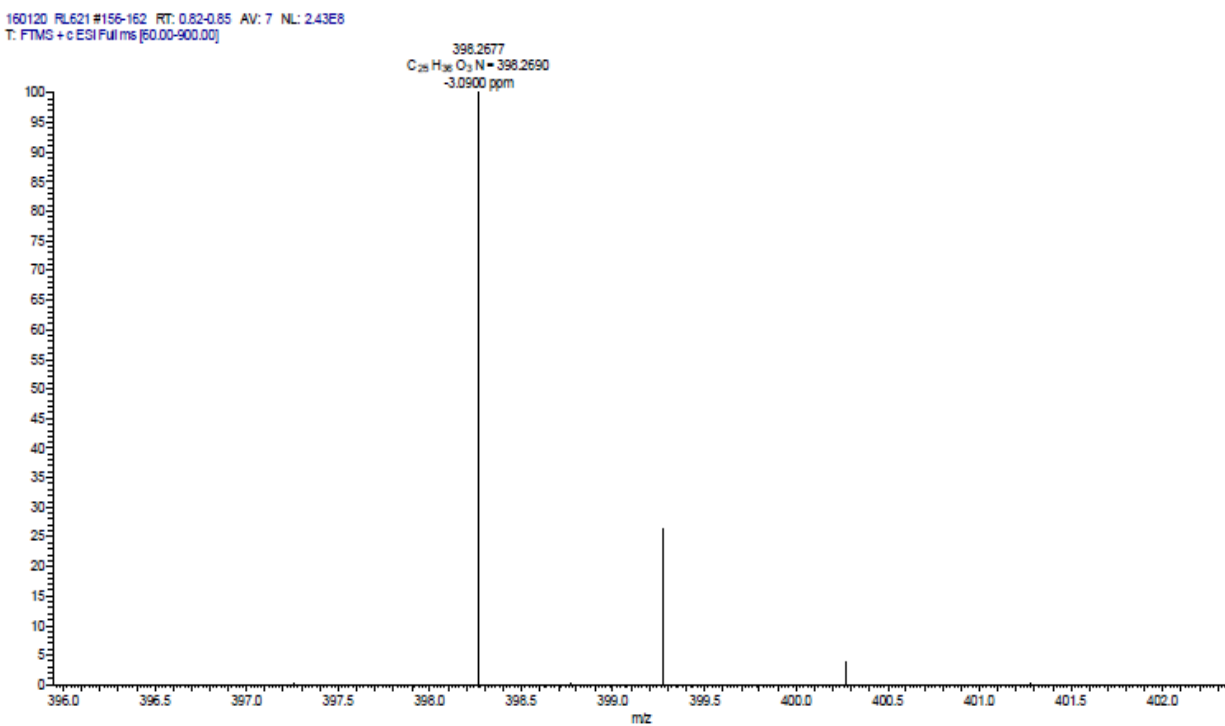


High resolution MS of final products

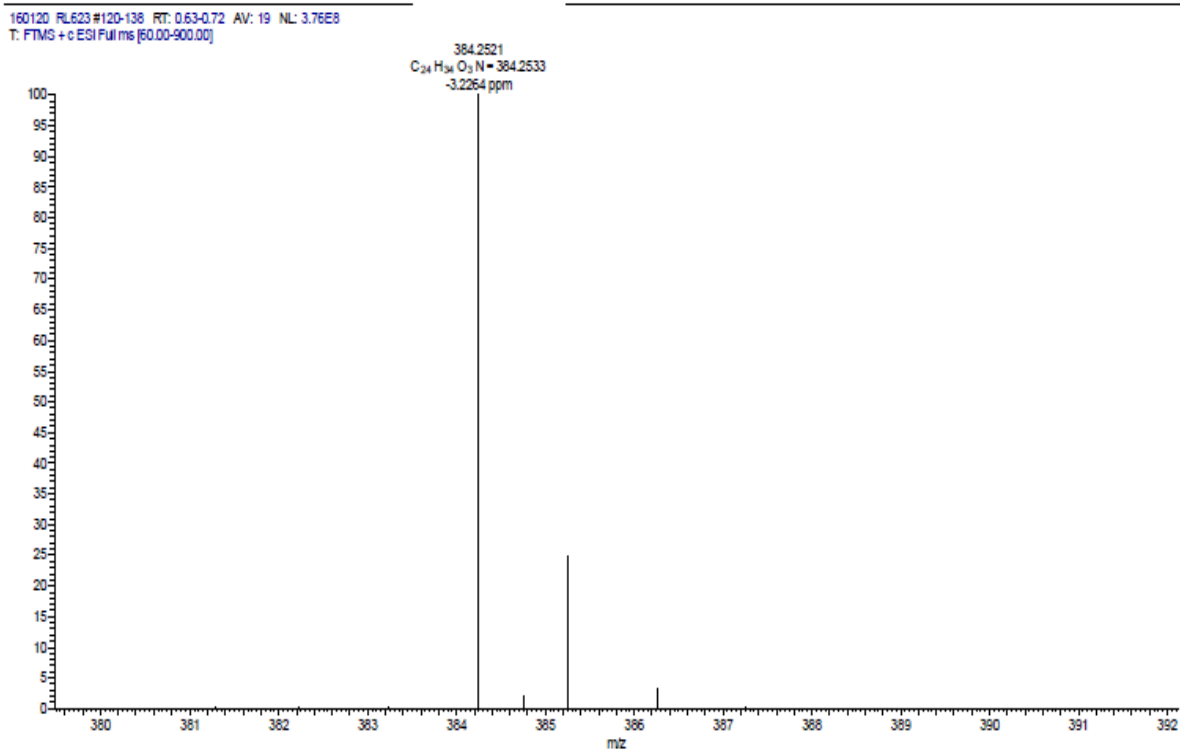
Compound 2 ($C_{17}H_{20}NO_3$ $[M+H]^+$)



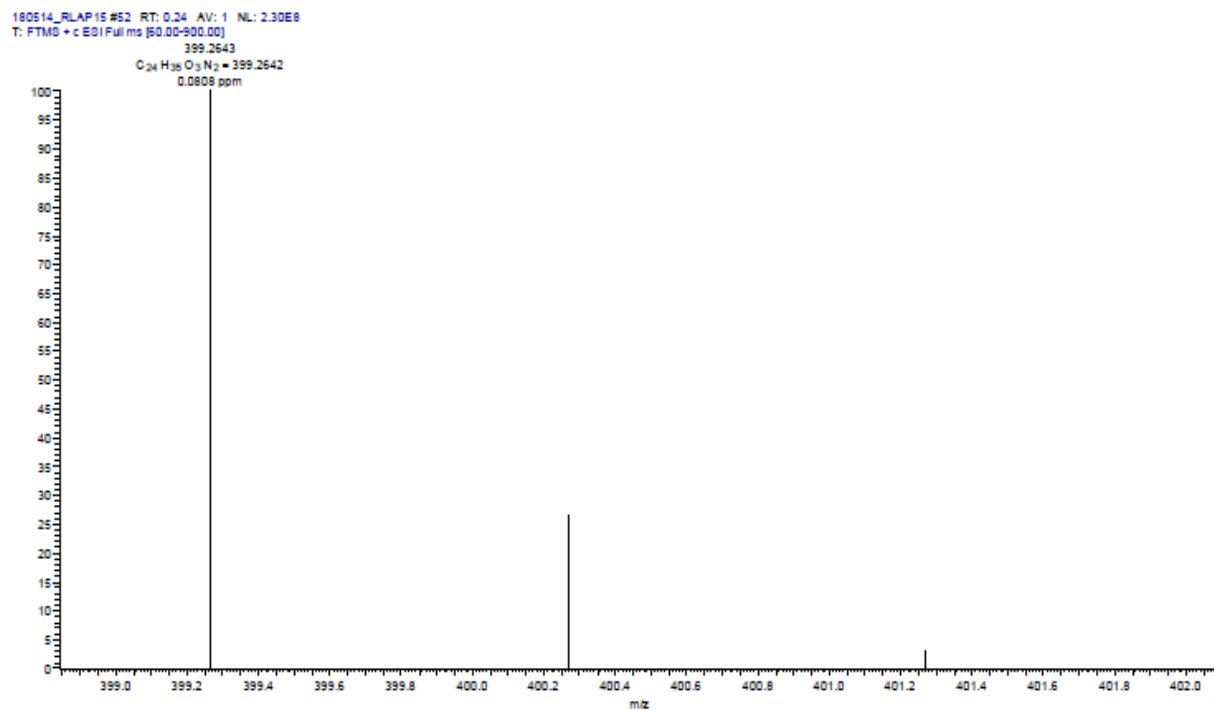
Compound 3 ($C_{25}H_{36}NO_3$ $[M+H]^+$):



Compound 4 (C₂₄H₃₄N₂O₃ [M+H]⁺):

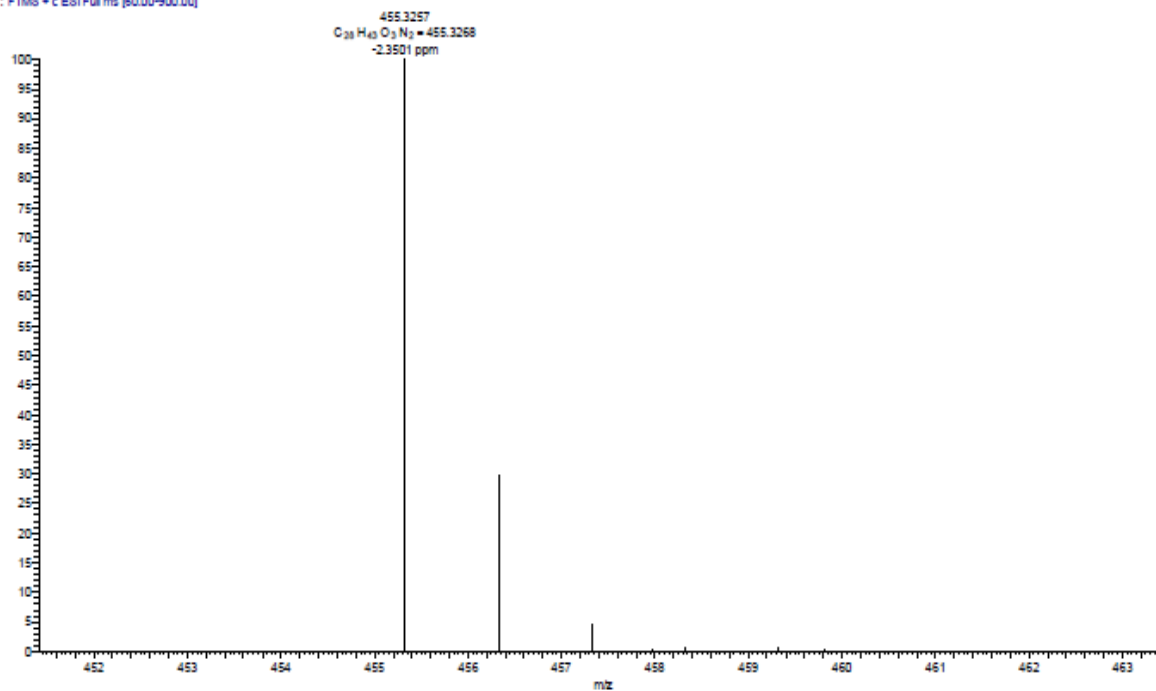


Compound 5 (C₂₄H₃₅N₂O₃ [M+H]⁺):



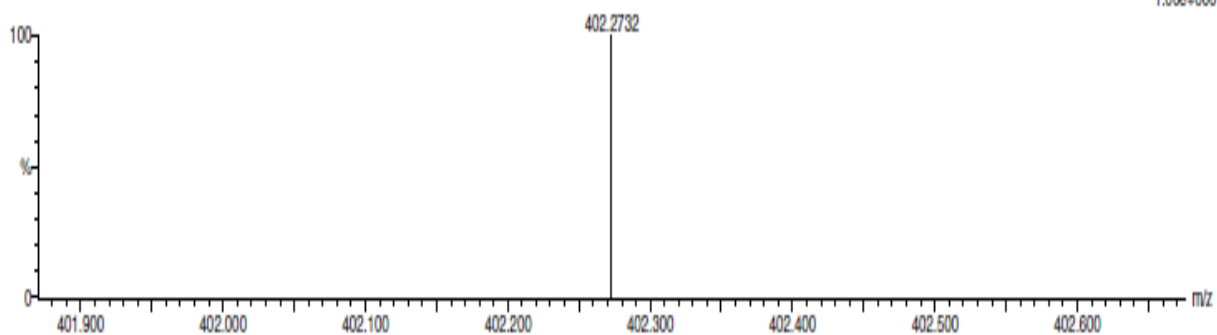
Compound **6** (C₂₈H₄₃N₂O₃ [M+H]⁺):

190604_RL784 #84-100 RT: 0.41-0.50 AV: 17 NL: 4.02E8
T: FTMS + c ESI Full ms [50.00-900.00]



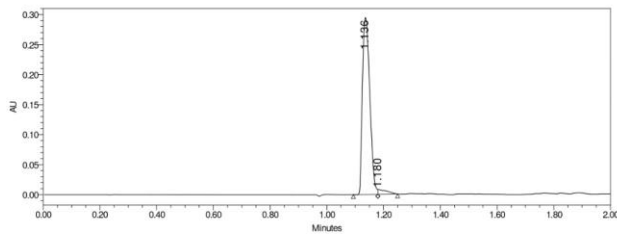
Compound **8** (C₂₃H₃₆N₃O₃ [M+H]⁺):

1: TOF MS ES+



HPLC chromatograms of final compounds 2-8

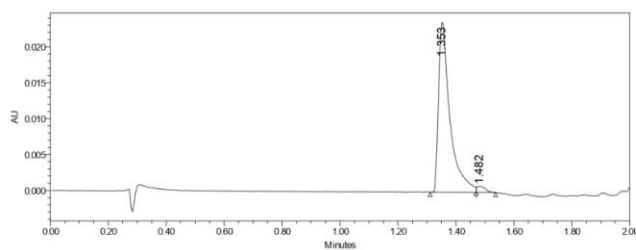
Compound 2



Peak Name:

	Injection	RT	Area	% Area	Height
1	1	1.180	17104	3.10	8009
2	1	1.136	534821	96.90	294818
Mean		1.158			
Std. Dev.		0.031			
% RSD		2.68			

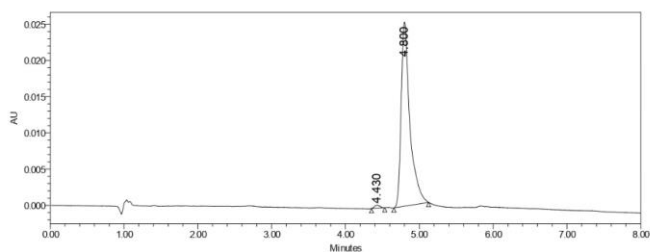
Compound 3



Peak Name:

	Injection	RT	Area	% Area	Height
1	1	1.482	1717	2.58	856
2	1	1.353	64818	97.42	23638
Mean		1.417			
Std. Dev.		0.091			
% RSD		6.44			

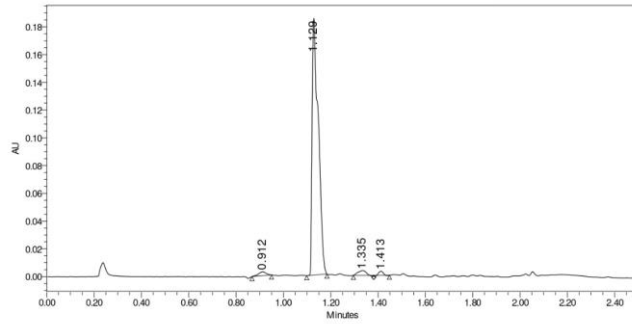
Compound 4



Peak Name:

	Injection	RT	Area	% Area	Height
1	1	4.800	207639	99.00	25433
2	1	4.430	2094	1.00	401
Mean		4.615			
Std. Dev.		0.282			
% RSD		5.68			

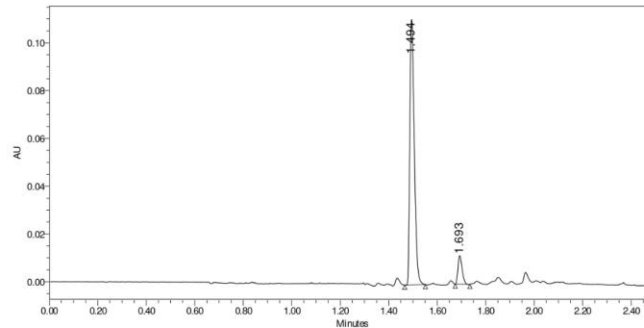
Compound 5



Processed Channel: PDA 280.0 nm

SampleName	Processed Channel	Retention Time (min)	Area	% Area	Height
1 220517_API5_Puro	PDA 280.0 nm	0.912	6537	1.84	2879
2 220517_API5_Puro	PDA 280.0 nm	1.129	334751	94.45	185138
3 220517_API5_Puro	PDA 280.0 nm	1.335	8716	2.46	3441
4 220517_API5_Puro	PDA 280.0 nm	1.413	4422	1.25	2911

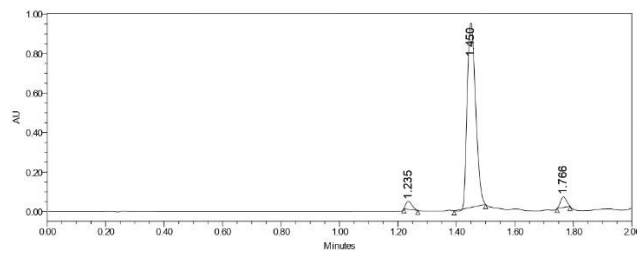
Compound 6



Processed Channel: PDA 280.0 nm

SampleName	Processed Channel	Retention Time (min)	Area	% Area	Height
1 220517_RL784_C	PDA 280.0 nm	1.494	143085	90.98	11114
2 220517_RL784_C	PDA 280.0 nm	1.693	14194	9.02	11872

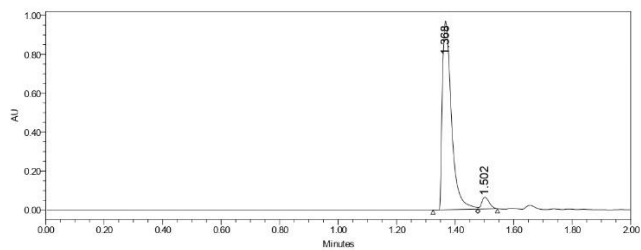
Compound 7



Peak Name:

	Injection	RT	Area	% Area	Height
1	1	1.450	1880293	93.29	934434
2	1	1.235	59416	2.95	40181
3	1	1.766	75826	3.76	53543
Mean		1.484			
Std. Dev.		0.267			
% RSD		18.00			

Compound 8



Peak Name:

	Injection	RT	Area	% Area	Height
1	1	1.502	106773	4.82	59711
2	1	1.368	2107288	95.18	970188
Mean		1.435			
Std. Dev.		0.095			
% RSD		6.61			