Supplementary data

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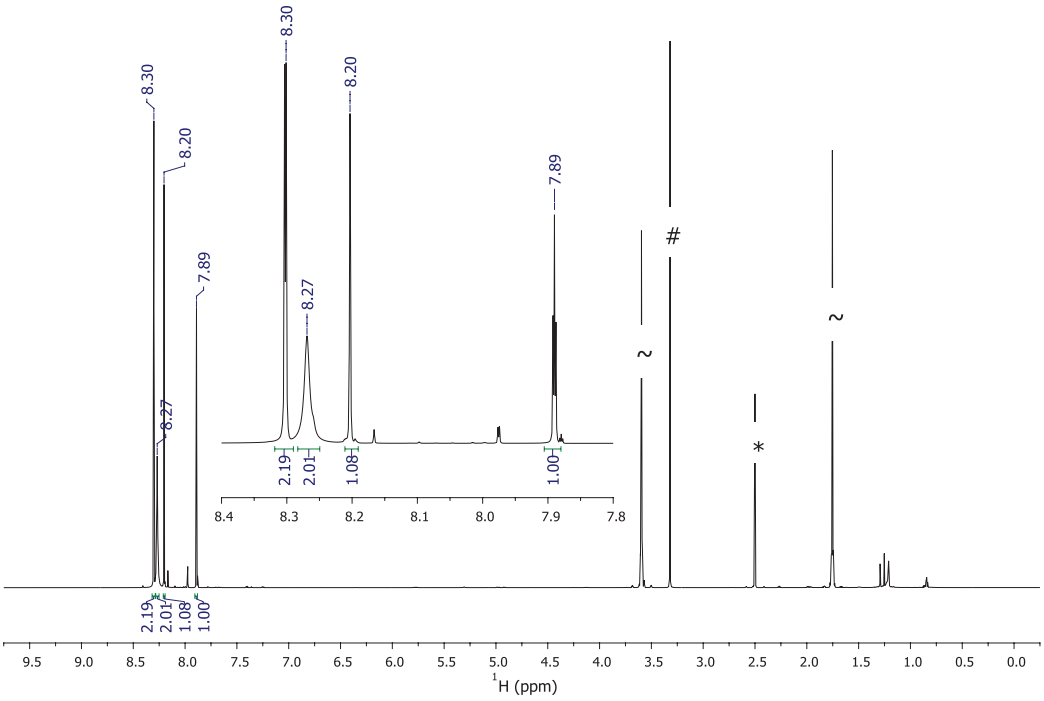
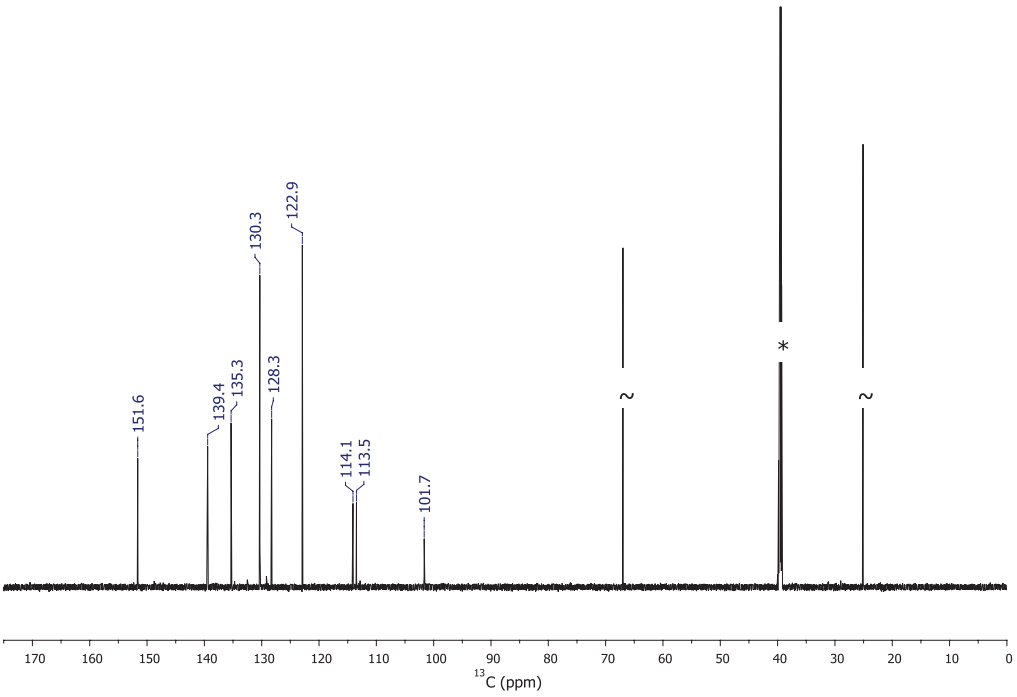
NMR data of 2

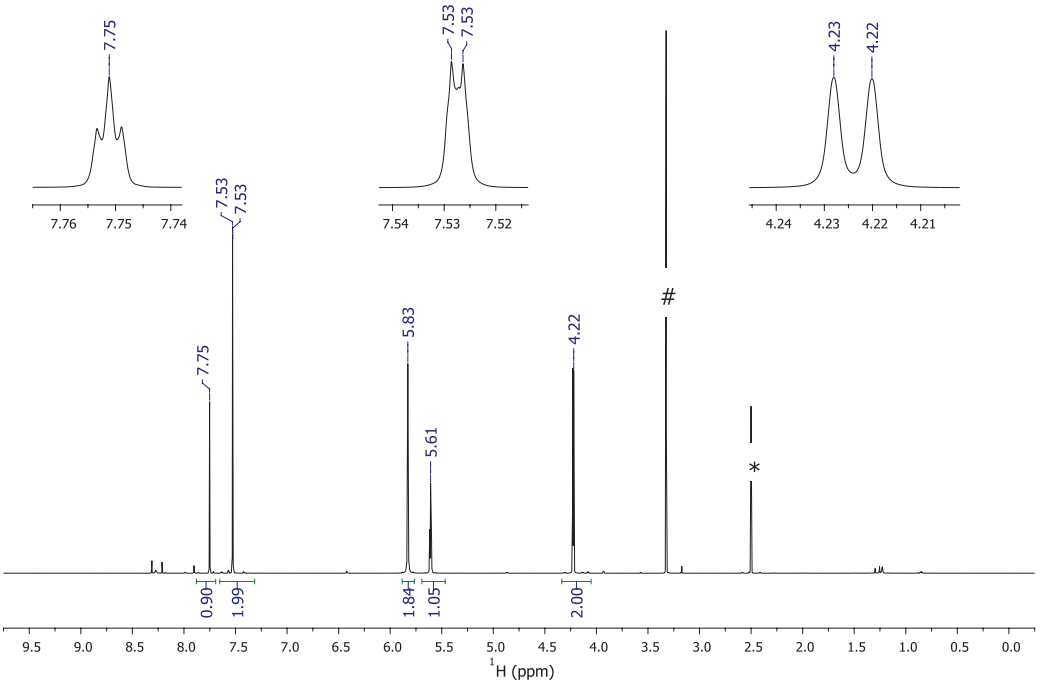


^{1}H NMR spectrum of **2** (DMSO-d_6, 298 K). The symbols ~, * and # indicate THF, DMSO and water residual peaks, respectively.

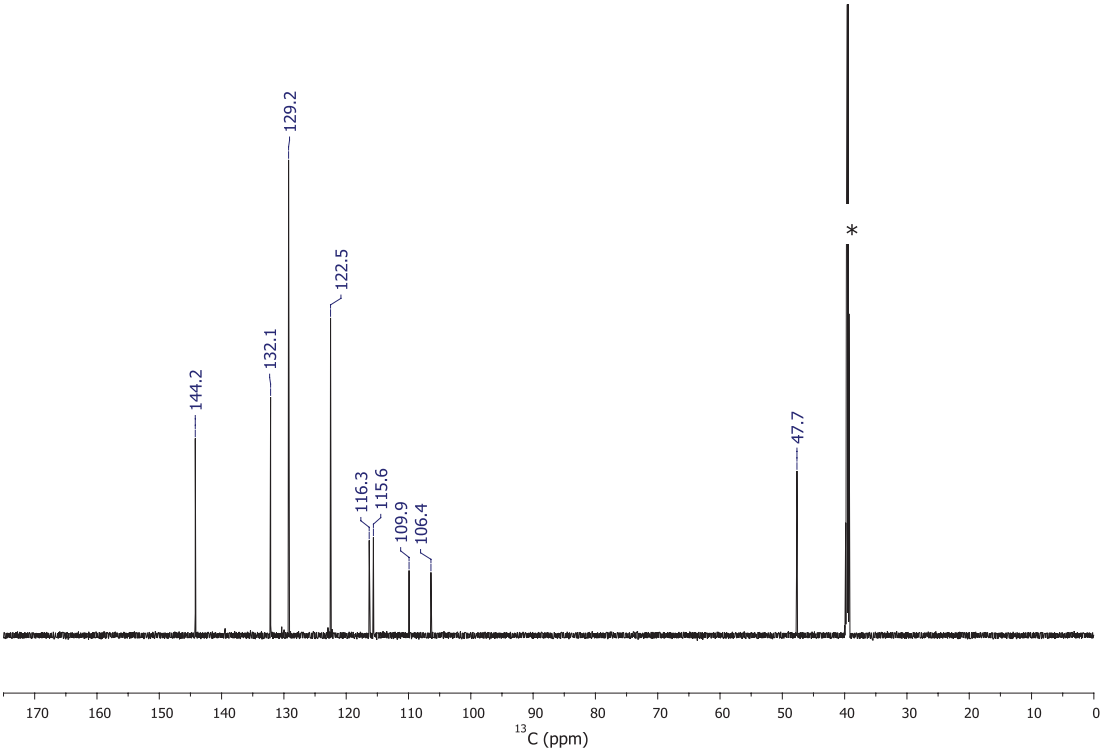


^{13}C NMR spectrum of **2** (DMSO-d_6, 298 K). The symbols * and ~ indicate DMSO and THF peaks, respectively.

NMR data of 3

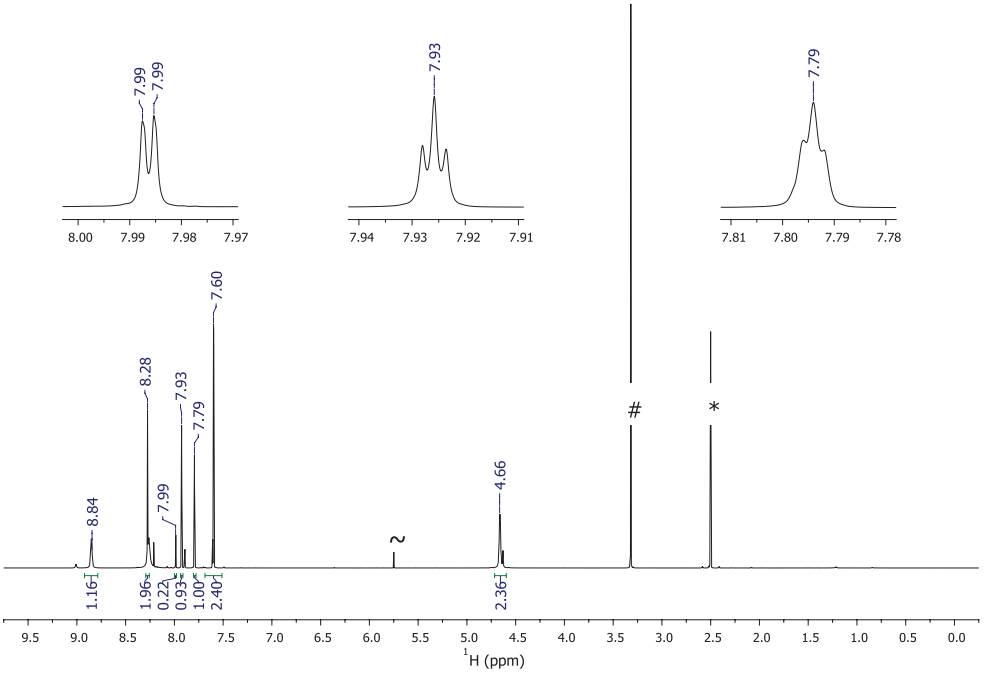


^{1}H NMR spectrum of **3** (DMSO-d_6, 298 K). The symbols * and # indicate DMSO and water residual peaks, respectively.

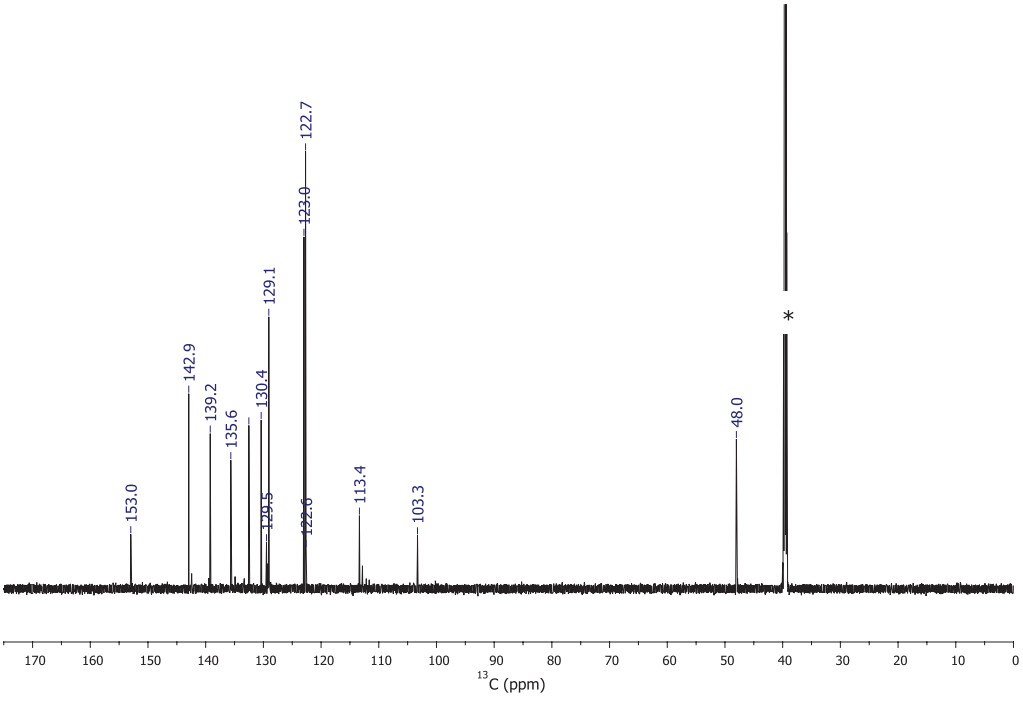


^{13}C NMR spectrum of **3** (DMSO-d_6, 298 K). The symbol * indicates DMSO peak.

NMR data of 4

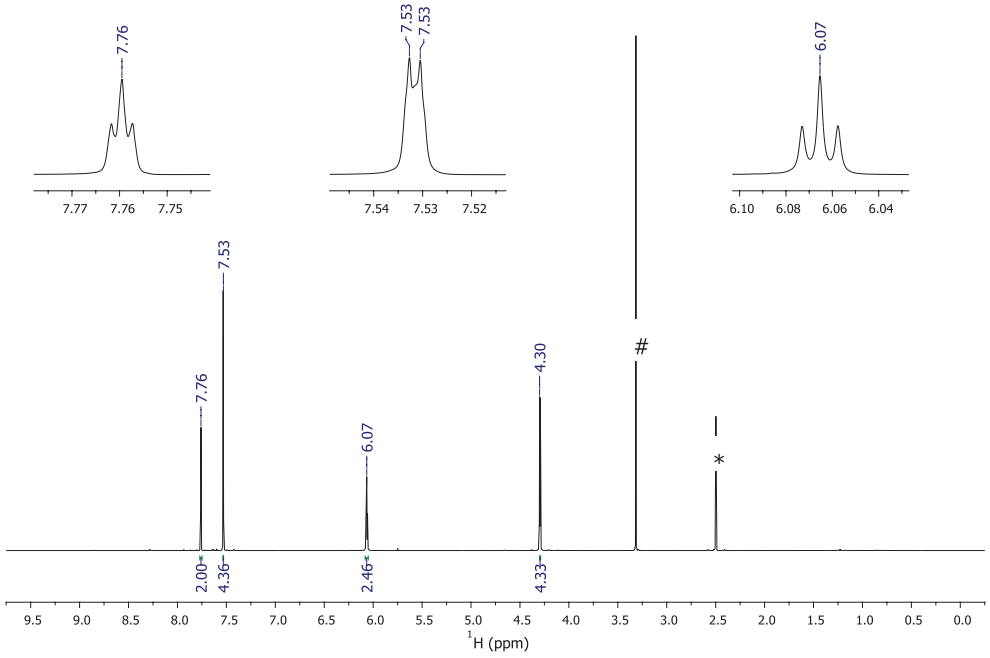


^{1}H NMR spectrum of **4** (DMSO-d_6, 298 K). The symbols *, ~ and # indicate DMSO, dichloromethane and water residual peaks, respectively.

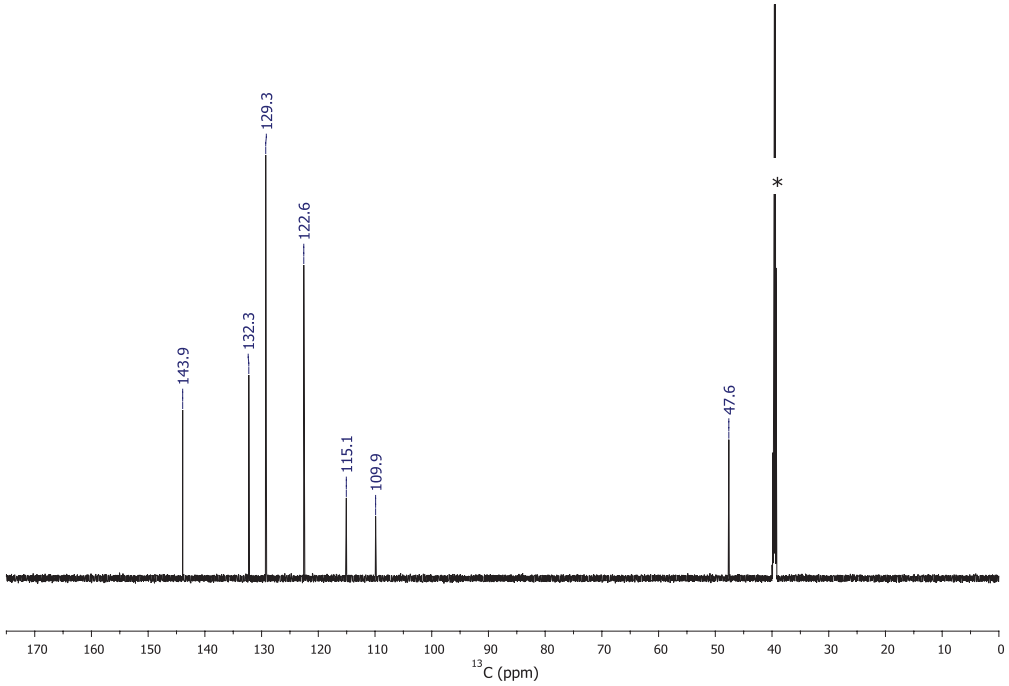


^{13}C NMR spectrum of **4** (DMSO-d_6, 298 K). The symbol * indicates DMSO peak.

NMR data of 5

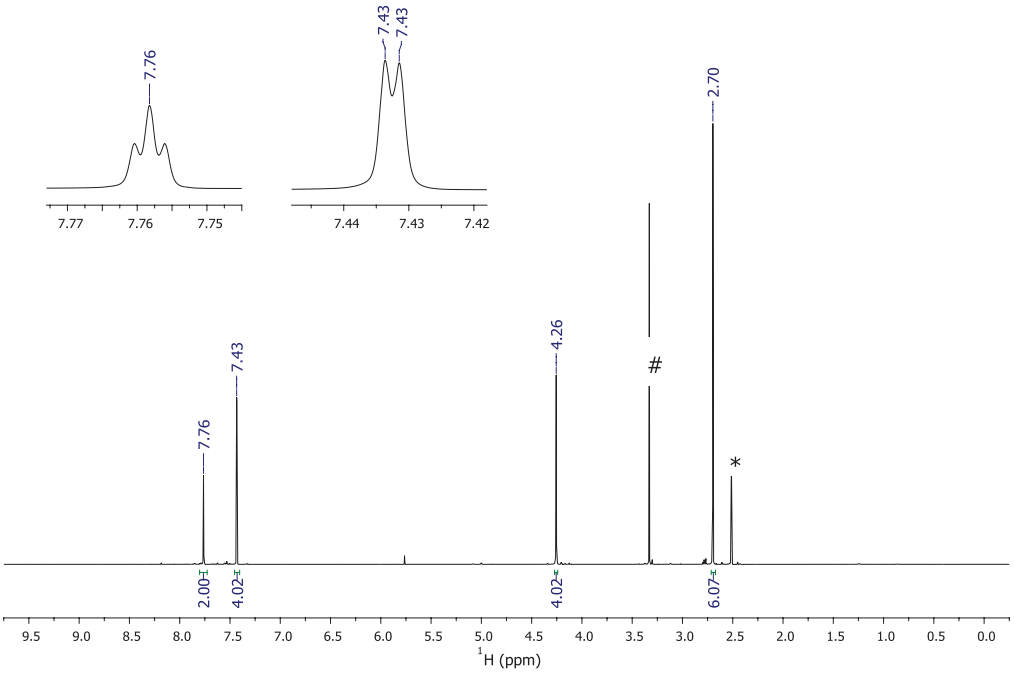


^{1}H NMR spectrum of **5** (DMSO-d_6, 298 K). The symbols * and # indicate DMSO and water residual peaks, respectively.

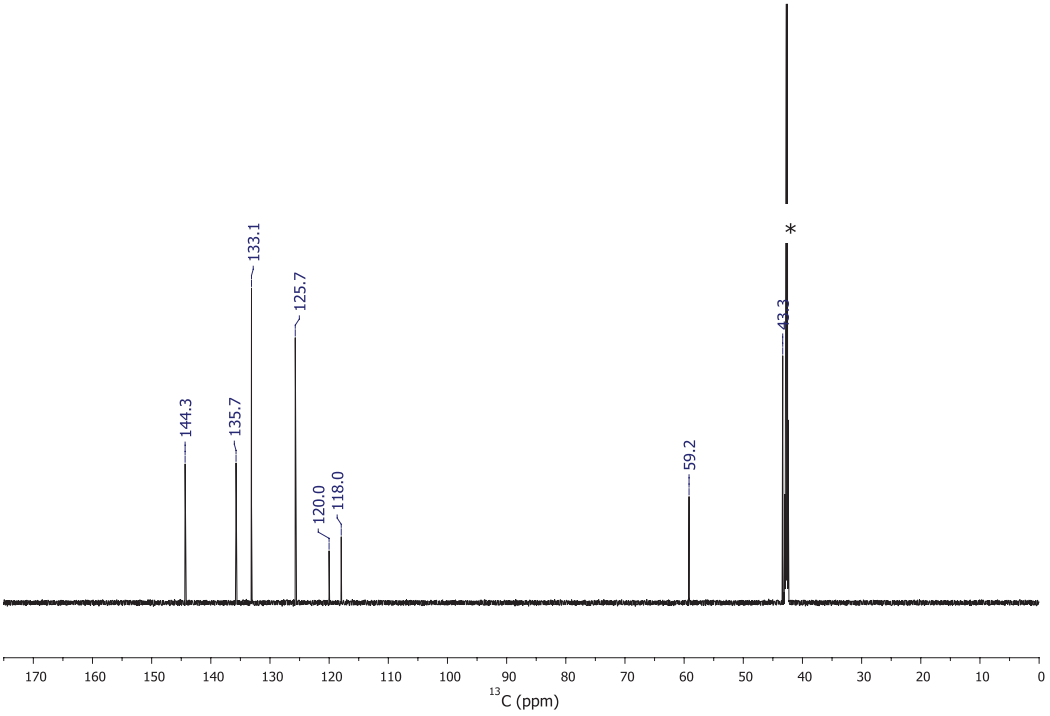


^{13}C NMR spectrum of **5** (DMSO-d_6, 298 K). The symbol * indicates DMSO peak.

NMR data of 6

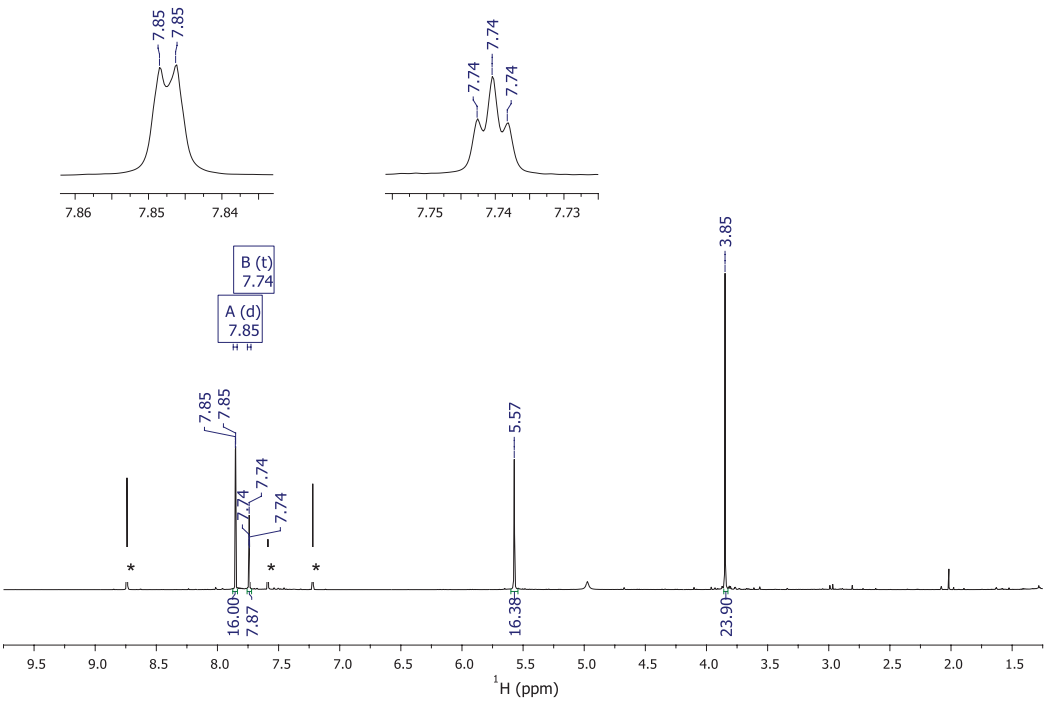


^{1}H NMR spectrum of **6** (DMSO-d_6, 298 K). The symbols * and # indicate DMSO and water residual peaks, respectively.

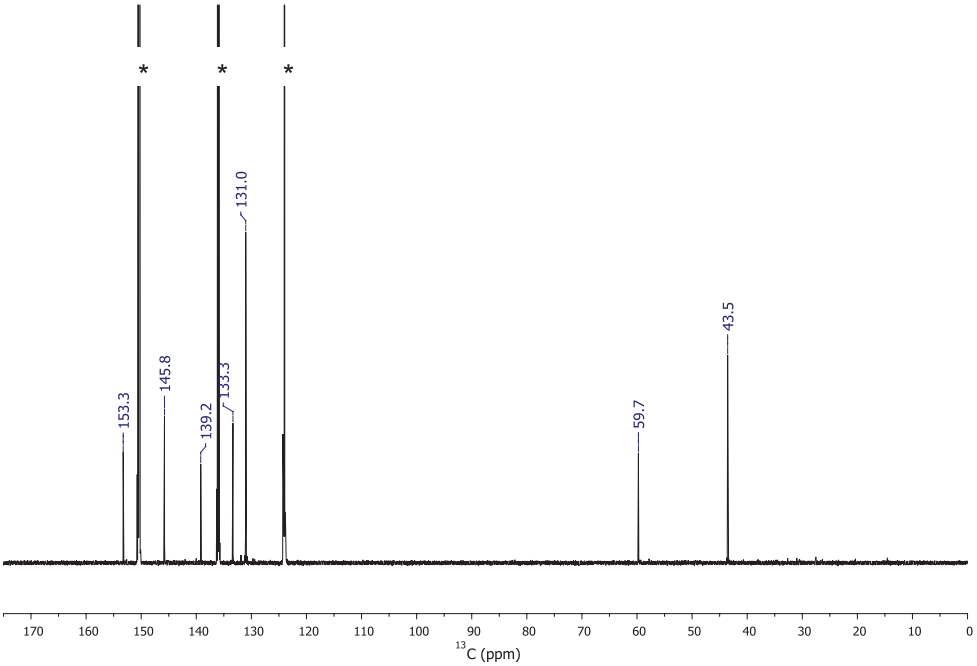


^{13}C NMR spectrum of **6** (DMSO-d_6, 298 K). The symbol * indicates DMSO peak.

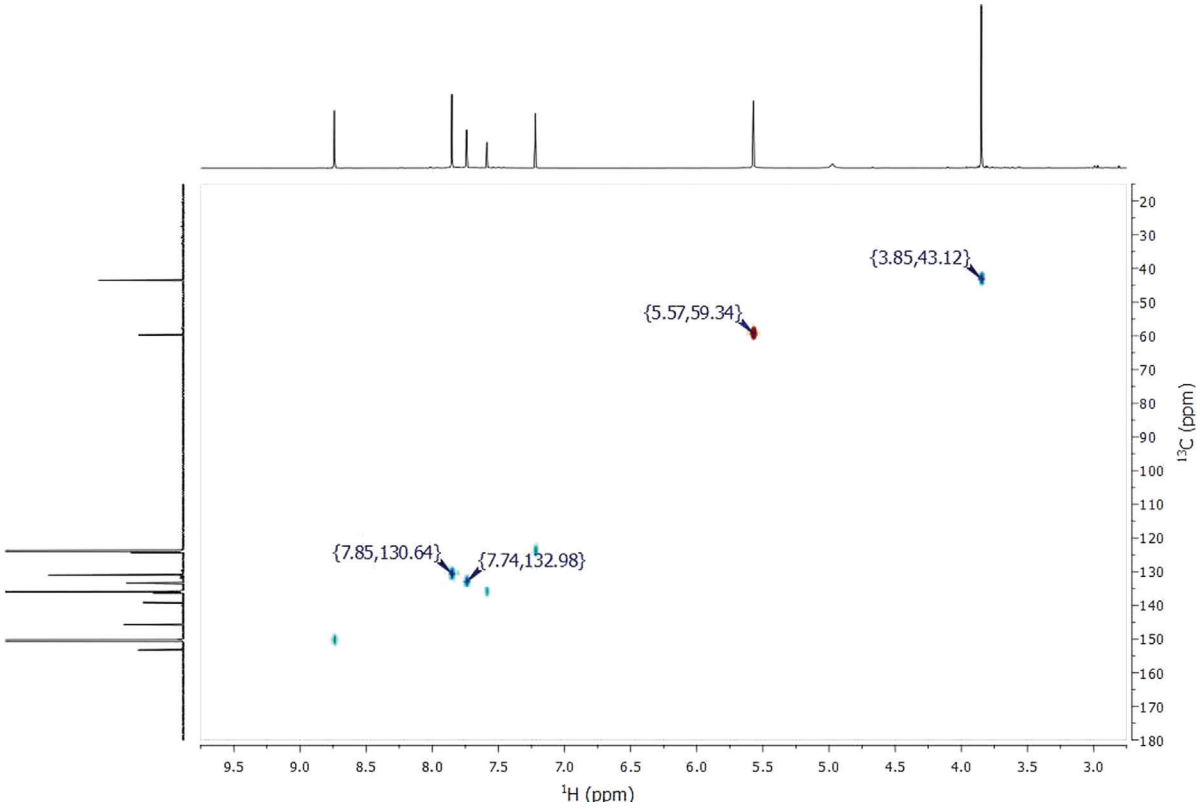
NMR data of 7



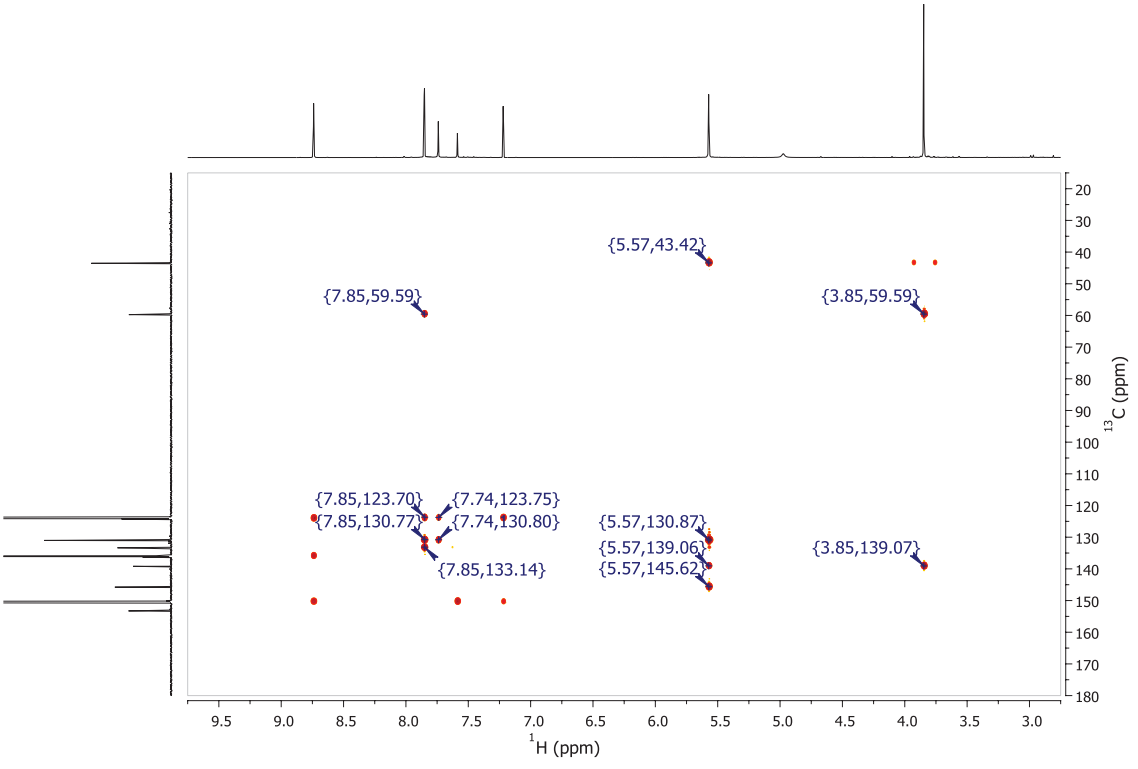
^{1}H NMR spectrum of **7** (pyridine-d_5, 298 K). The symbol * indicates pyridine residual peaks.



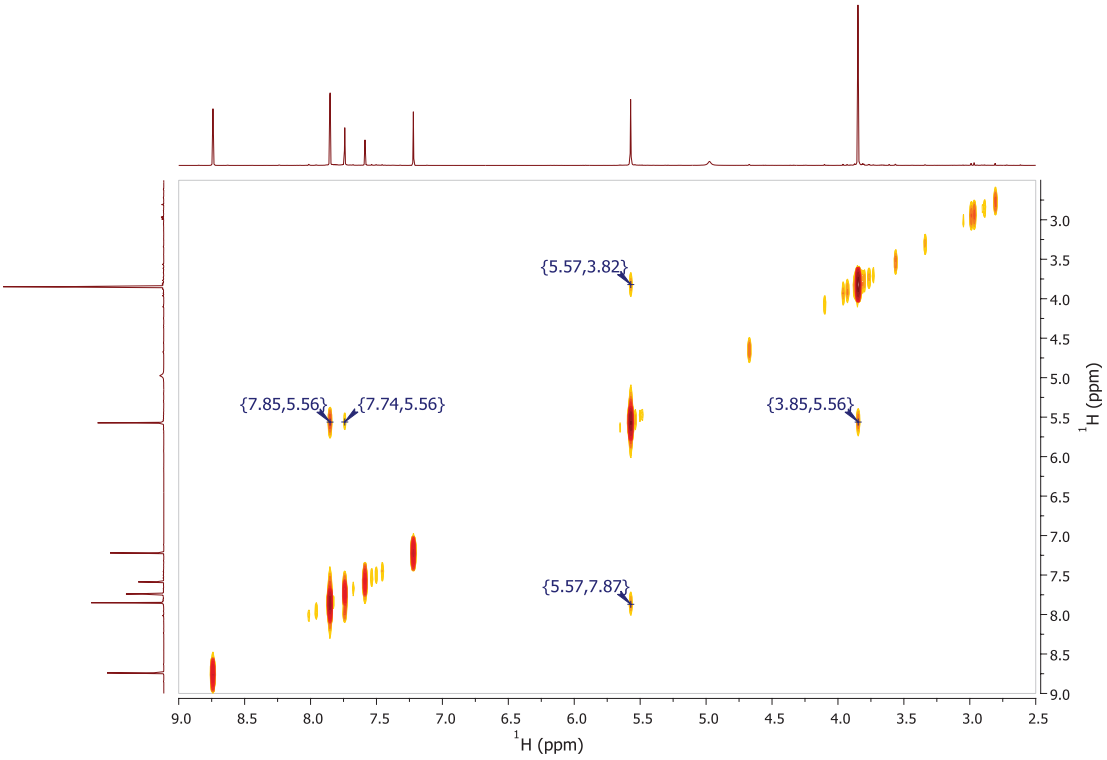
^{13}C NMR spectrum of **7** (pyridine-d_5, 298 K). The symbol * indicates pyridine peaks.



^{1}H-^{13}C HSQC spectrum of **7** (pyridine-d_5, 298 K).



^{1}H-^{13}C HMBC spectrum of **7** (pyridine-d_5, 298 K).



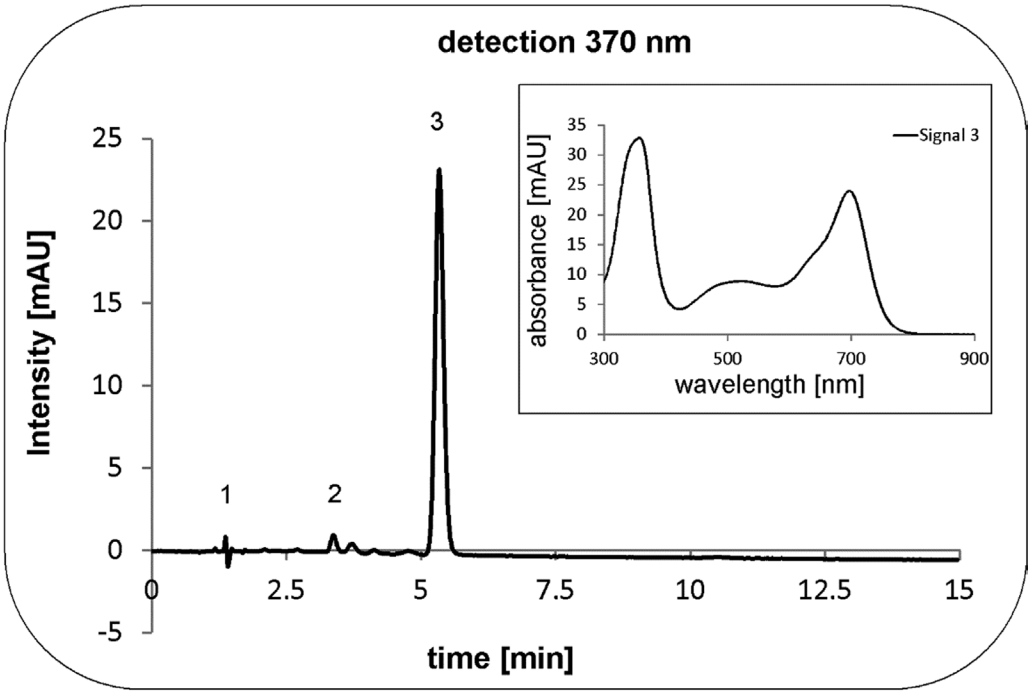
^{1}H-^{1}H COSY spectrum of **7** (pyridine-d_5, 298 K).

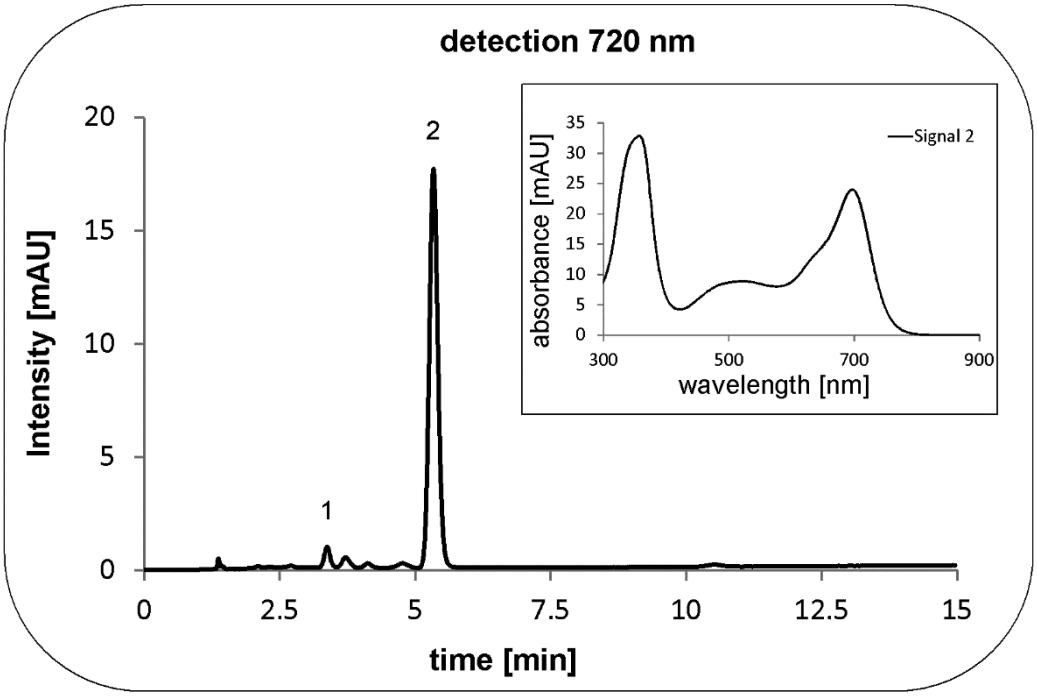
HPLC purity of 7

The purity of macrocycle **7** was determined by HPLC analysis using an Agilent 1200 instrument equipped with UV-DAD detector. The chromatographic separation was obtained on an octadecylsilane coated column, 150 mm × 4.6 mm, 5 µm (Eclipse XDB-C18, Agilent), using both isocratic and gradient elution conditions at a flow rate of 1.0 mL/min. Band dispersion, and additional peaks from aggregates significantly hampered HPLC analysis. The best conditions are shown below. Peaks of minor components were detected, but the impurity content did not exceed 5% of the total signal intensity.

Configuration 1

phase			
time [min]	acetonitrile	tetrahydrofuran	triethylamine
0	60	30	10
15	60	30	10

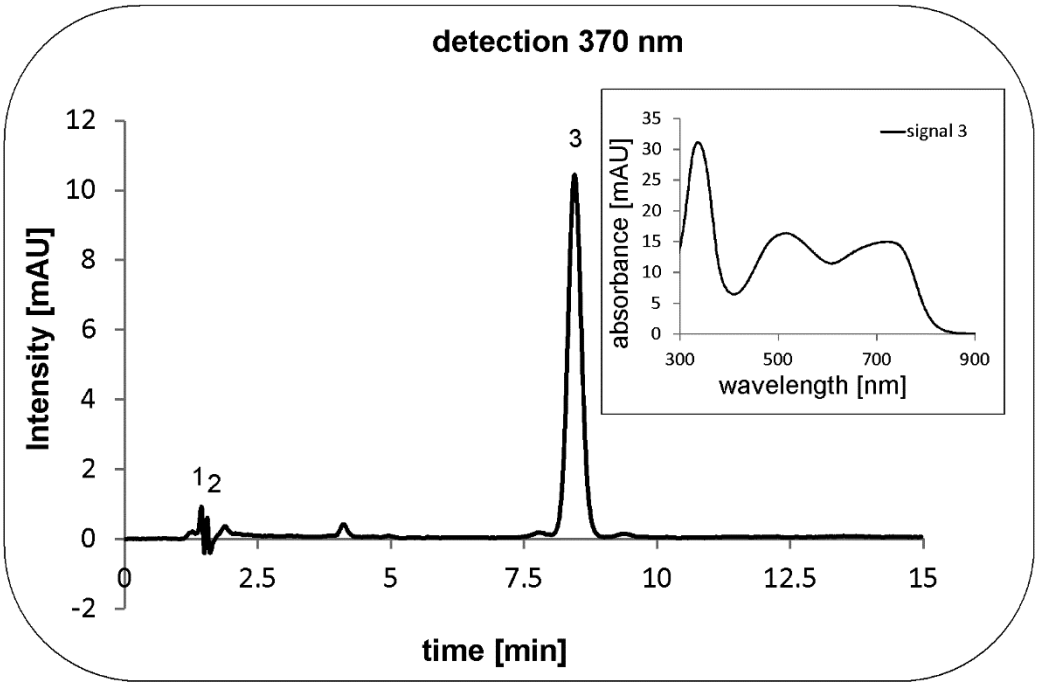


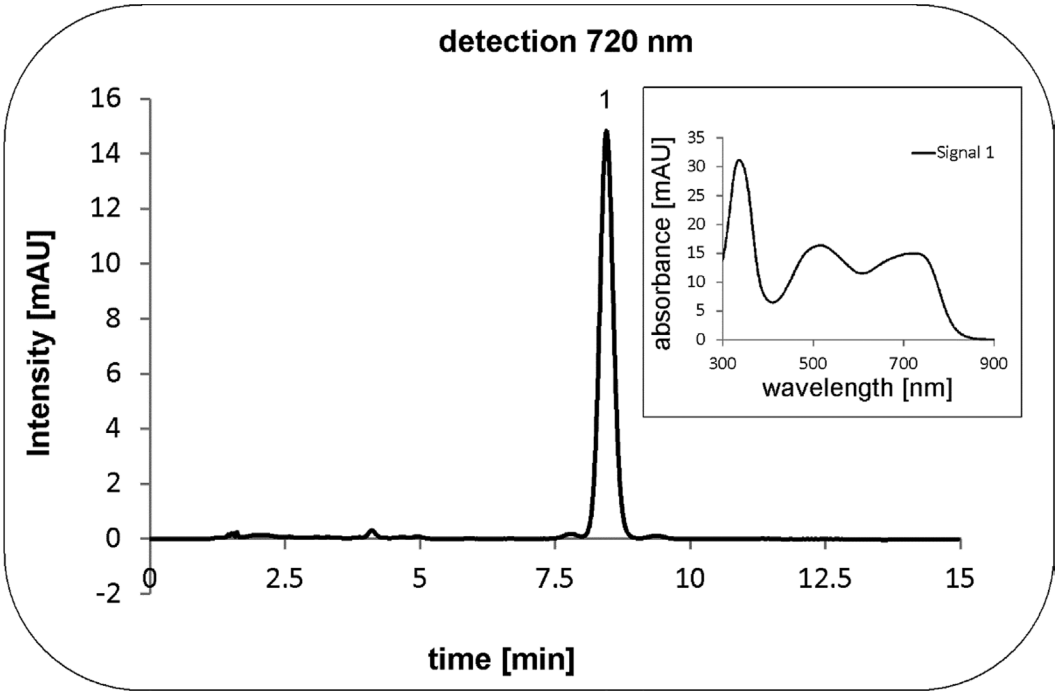


results			
signal	retention time [min]	area	purity [%]
detection 370 nm			
1	1.4	4.9	1.8
2	3.4	7.9	2.9
3	5.3	260.0	95.3
detection 720 nm			
1	3.4	6.5	3.2
2	5.3	195.6	96.8

Configuration 2

phase			
time [min]	methanol	dichloromethane	triethylamine
0	55	40	5
15	55	40	5

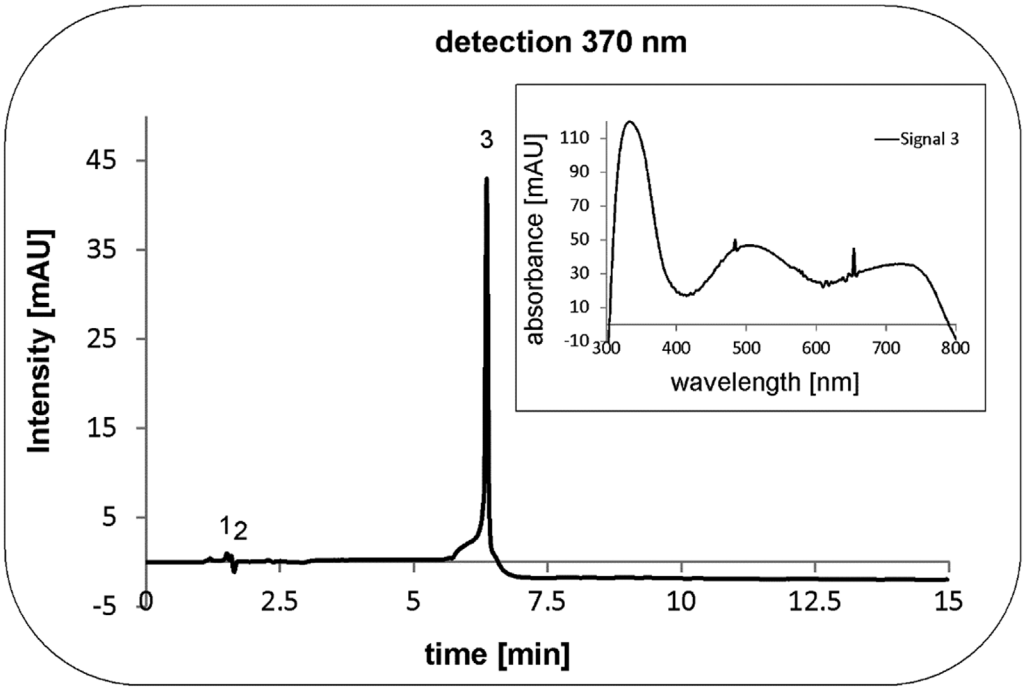

detection 370 nm
Intensity [mAU]
time [min]
1
2
3
absorbance [mAU]
wavelength [nm]
signal 3

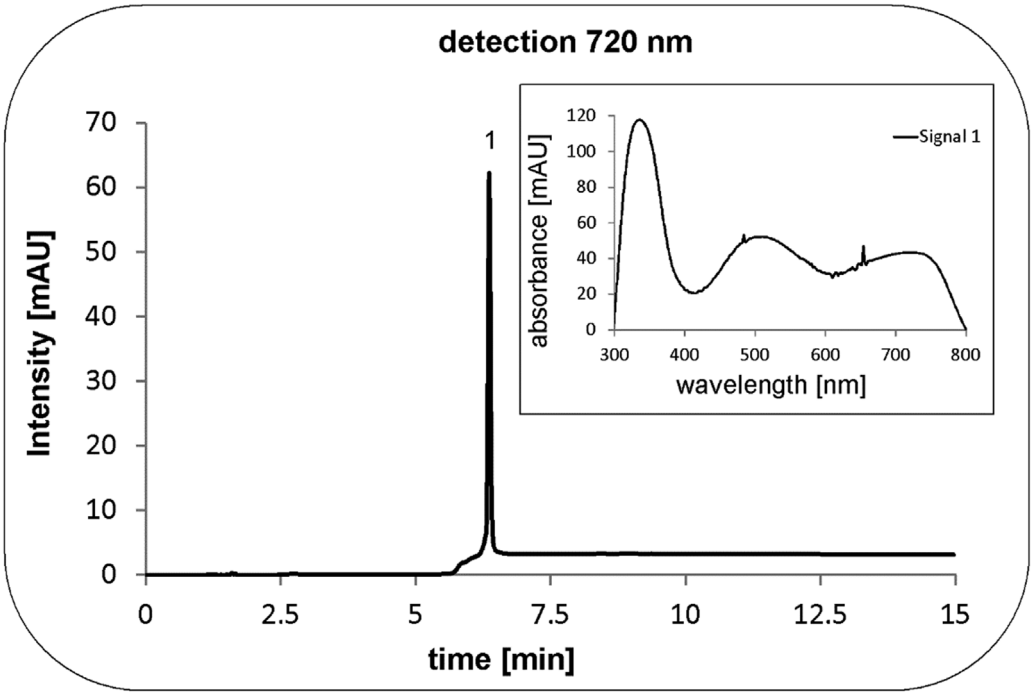

detection 720 nm
Intensity [mAU]
time [min]
1
absorbance [mAU]
wavelength [nm]
Signal 1

results			
signal	retention time [min]	area	purity [%]
detection 370 nm			
1	1.4	5.1	2.7
2	1.6	2.9	1.5
3	8.5	185.2	95.9
detection 720 nm			
1	8.5	264.8	100.0

Configuration 3

phase			
time [min]	acetonitrile	dichloromethane	triethylamine
0	90	5	5
3	90	5	5
4	5	90	5
15	5	90	5

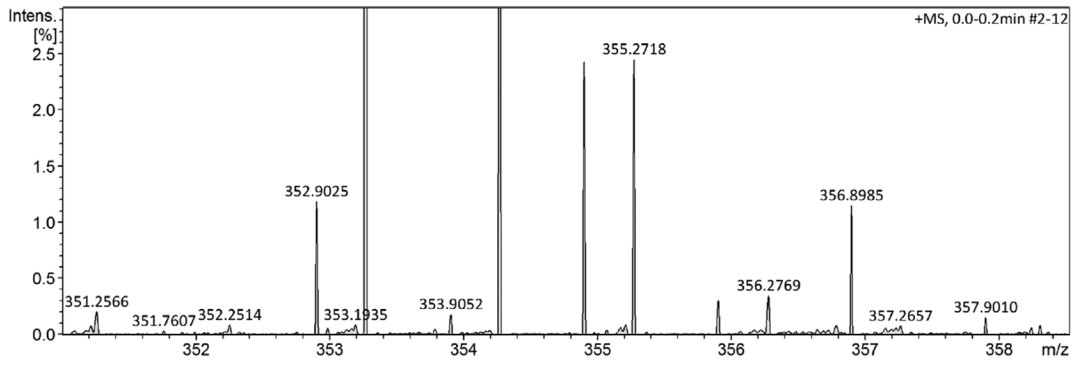




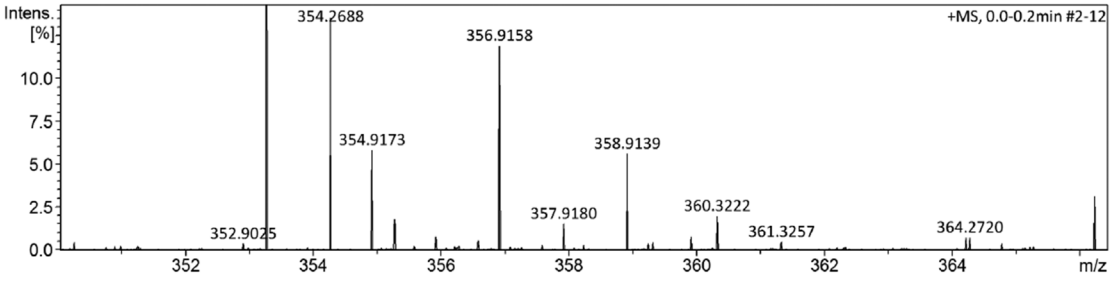
results			
signal	retention time [min]	area	purity [%]
detection 370 nm			
1	1.5	6.2	1.9
2	1.6	5.2	2.2
3	6.4	267.7	95.9
detection 720 nm			
1	6.4	246.9	100.0

HRMS reports

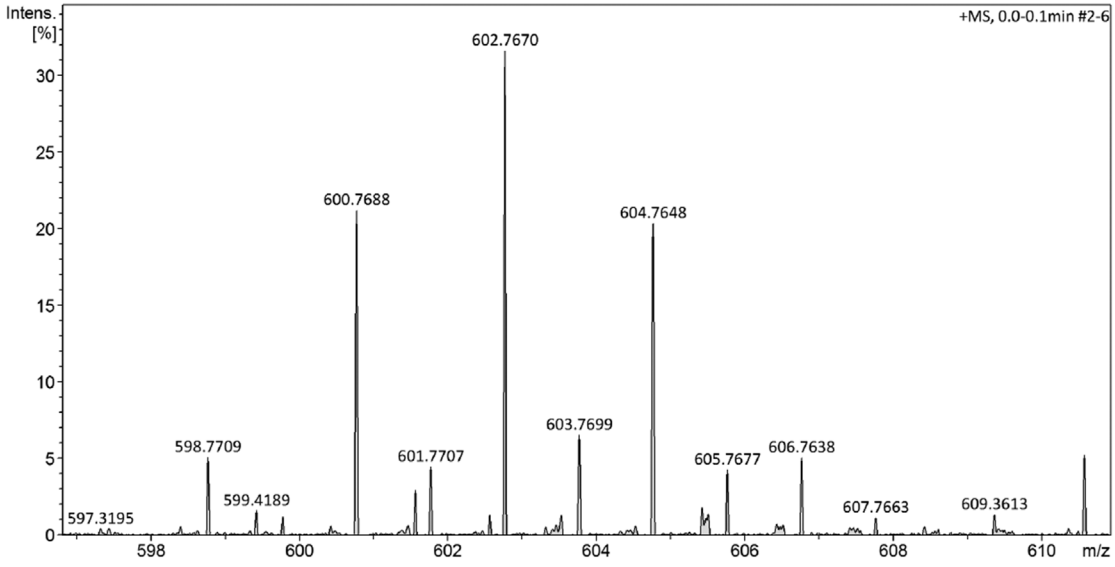
HRMS report of 2



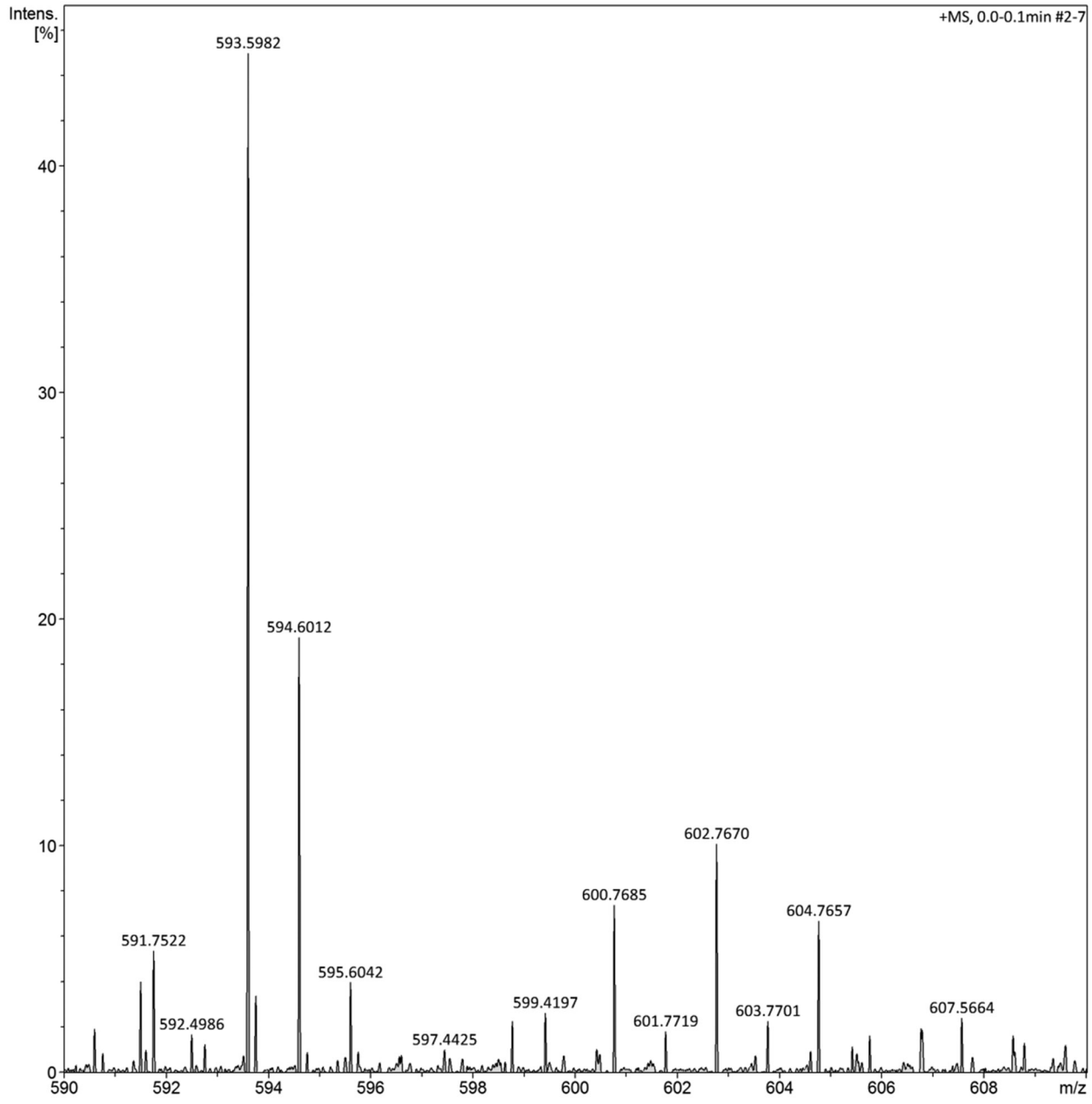
HRMS report of 3



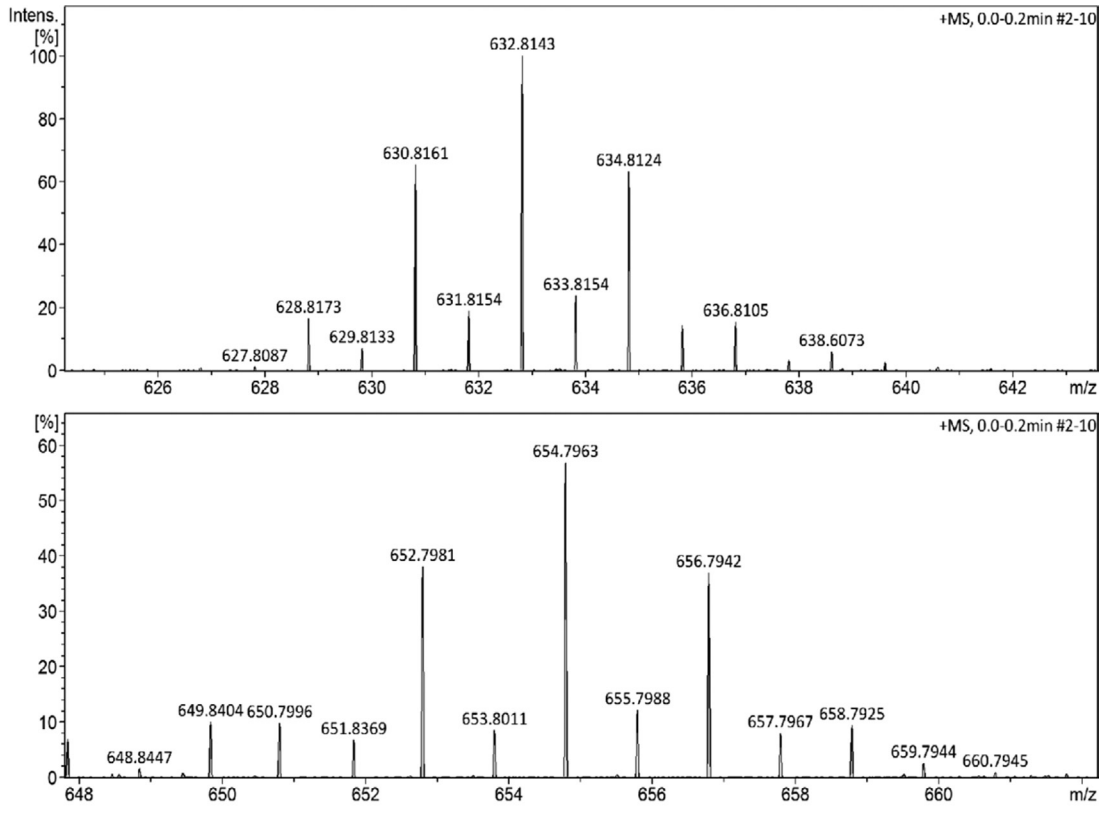
HRMS report of 4



HRMS report of 5



HRMS report of 6



MS (MALDI) report of 7