

## Supporting Information

for

### **Supramolecular FRET photocyclodimerization of anthracenecarboxylate with naphthalene-capped $\gamma$ -cyclodextrin**

Qian Wang<sup>1,2</sup>, Cheng Yang\*<sup>1</sup>, Gaku Fukuhara<sup>1</sup>, Tadashi Mori<sup>1</sup>, Yu Liu<sup>2</sup>, and Yoshihisa Inoue\*<sup>1</sup>

Address: <sup>1</sup>Department of Applied Chemistry, Osaka University, 2-1 Yamada-oka, Suita 565-0871, Japan and <sup>2</sup>Department of Chemistry and State Key Laboratory of Elemento-Organic Chemistry, Nankai University Tianjin, 300071 (China)

Email: Cheng Yang - c.yang@chem.eng.osaka-u.ac.jp;

Yoshihisa Inoue - inoue@chem.eng.osaka-u.ac.jp

\*Corresponding author

**NMR and HR-MS data of compounds 6 and 7.**

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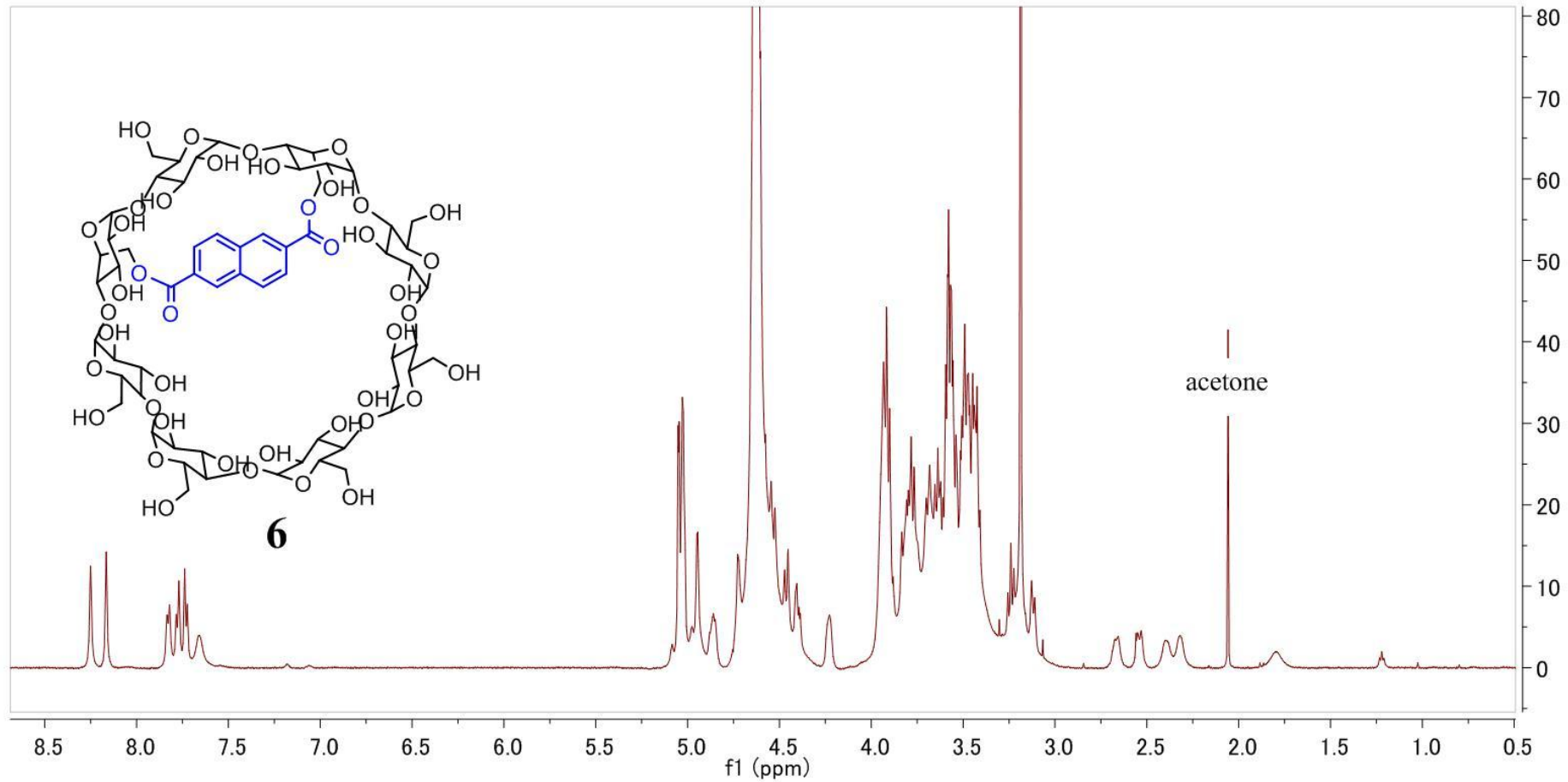
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## General

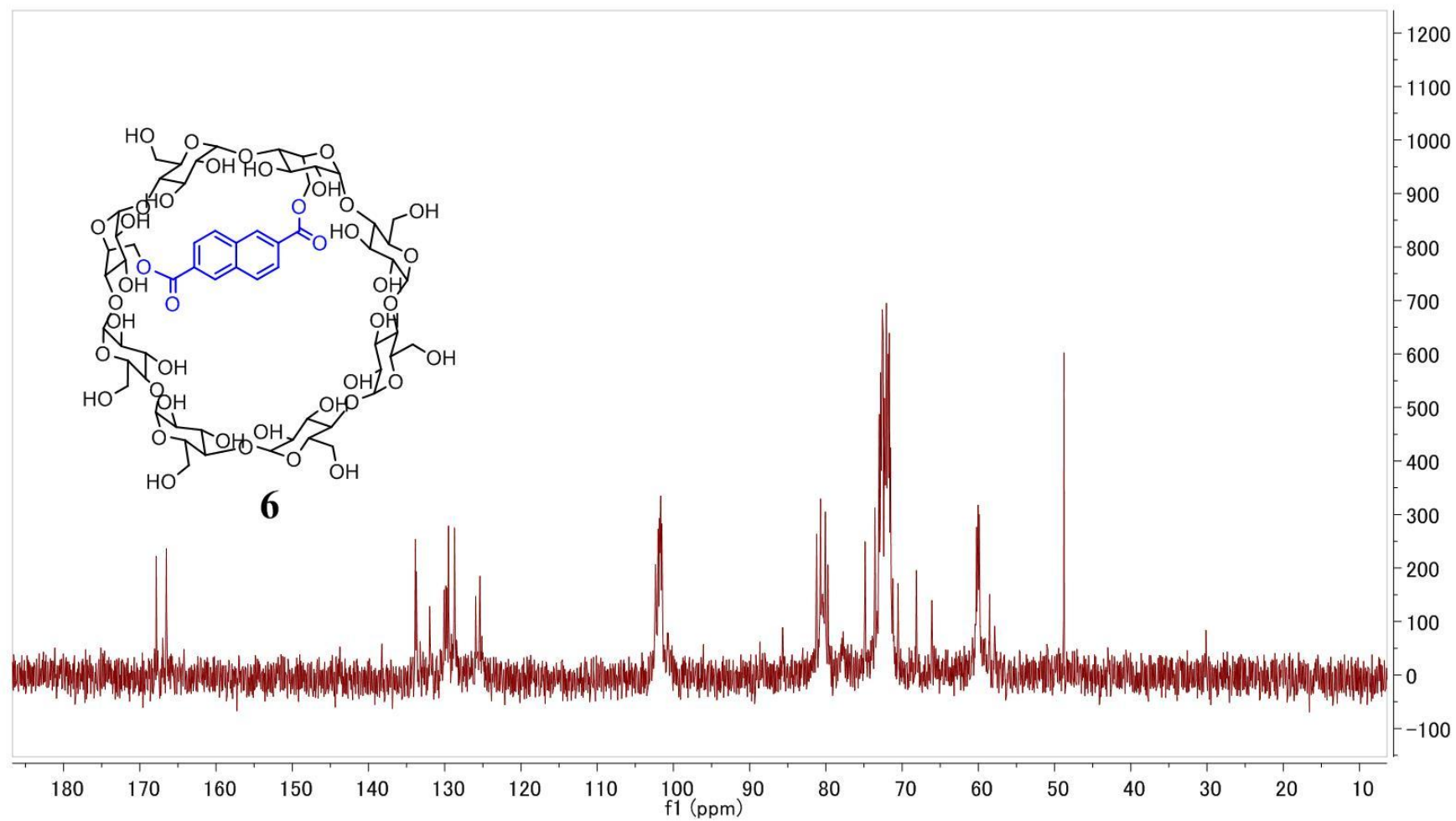
**Materials.**  $\gamma$ -CD (Aldrich) and other reagents (Tokyo Chemical Industry) were used without further purification.

**Instruments.** FAB mass spectra were measured on a JEOL JMS-DX303 mass spectrometer. NMR spectra were recorded on a Bruker DRX-600 or a JEOL JNM-EX 400 spectrometer. UV–vis, fluorescence, and circular dichroism spectra were recorded in a UNISOKU USP-203CD cryostat with a JASCO V-560 spectrophotometer, JASCO FP-6500 spectrofluorimeter, and JASCO J-810 spectropolarimeter, respectively.

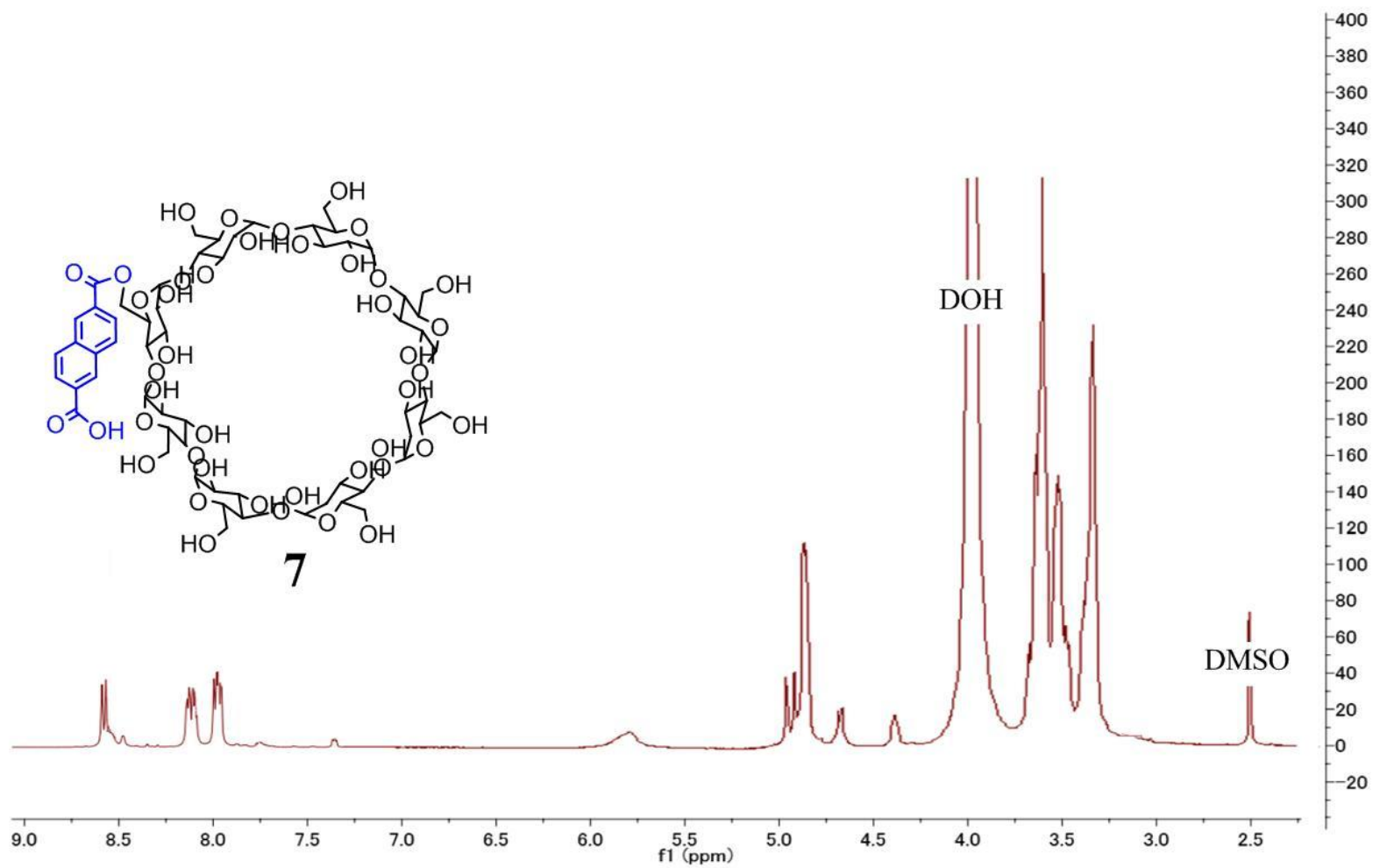
**Photolysis.** Photoirradiations were performed in a UNISOKU USP-203 cryostat with an appropriate interference filter for 300 nm or 360 nm. Irradiated samples were subjected to chiral HPLC analysis on a tandem column of Intersil ODS-2(GL Science) and Chiralcel OJ-R (Daicel) with a 36:64 mixture of acetonitrile and water as eluent.



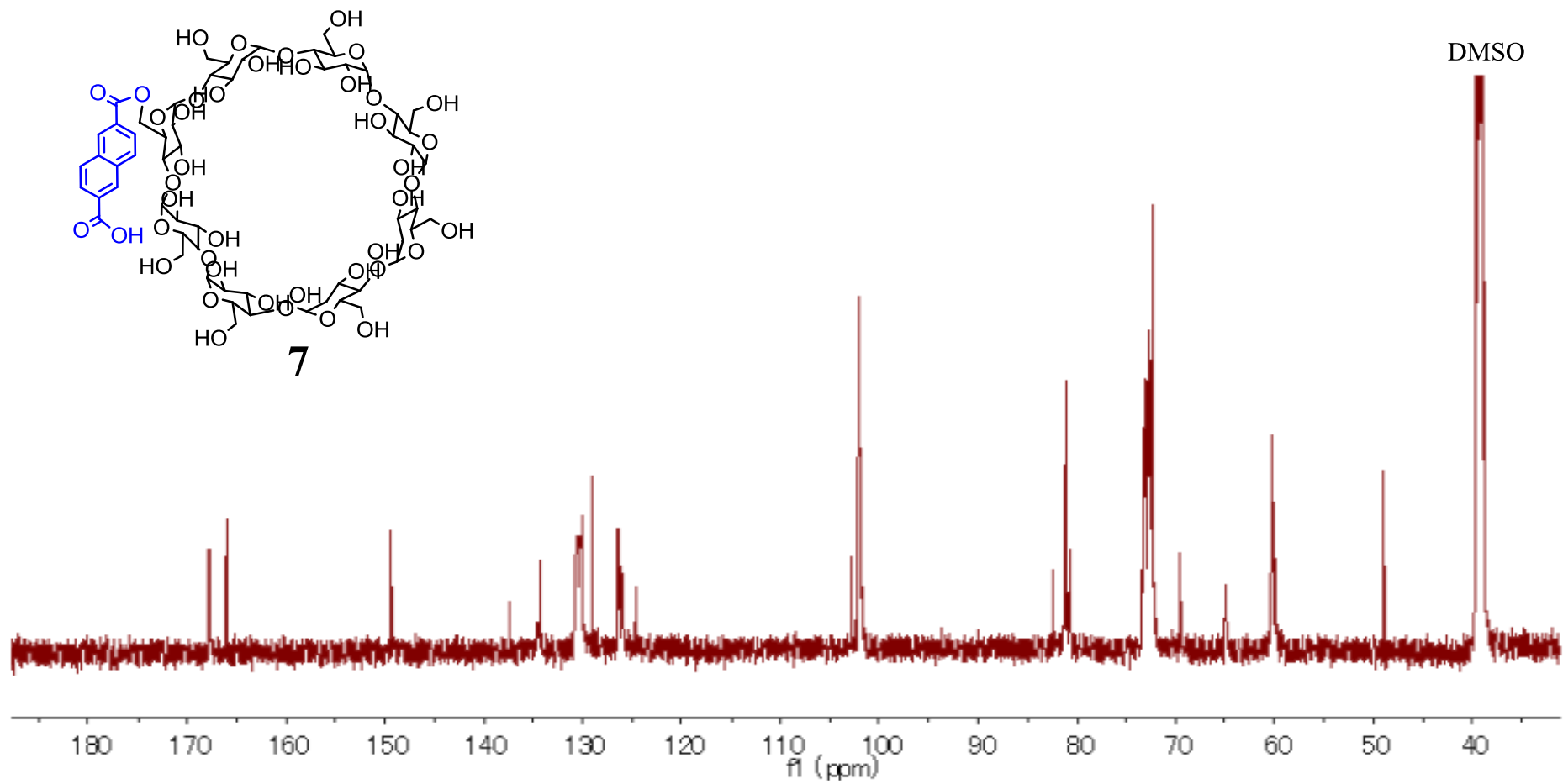
**Figure S1:**  $^1\text{H}$  NMR of **6** in  $\text{D}_2\text{O}$  at  $20\text{ }^\circ\text{C}$ .



**Figure S2:**  $^{13}\text{C}$  NMR of **6** in  $\text{D}_2\text{O}$  at  $20\text{ }^\circ\text{C}$ .

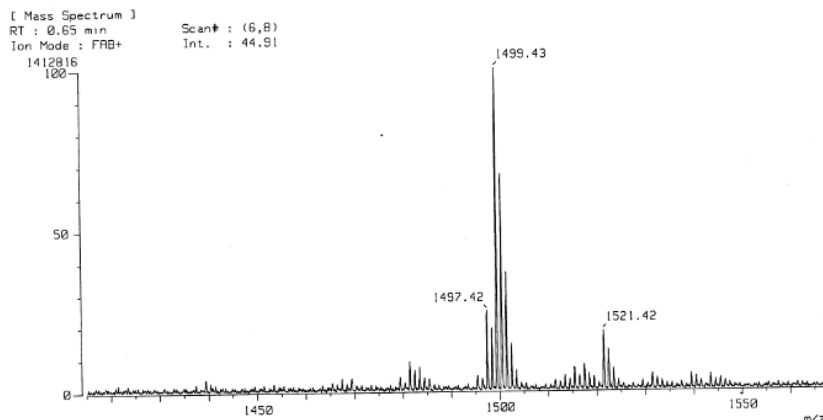
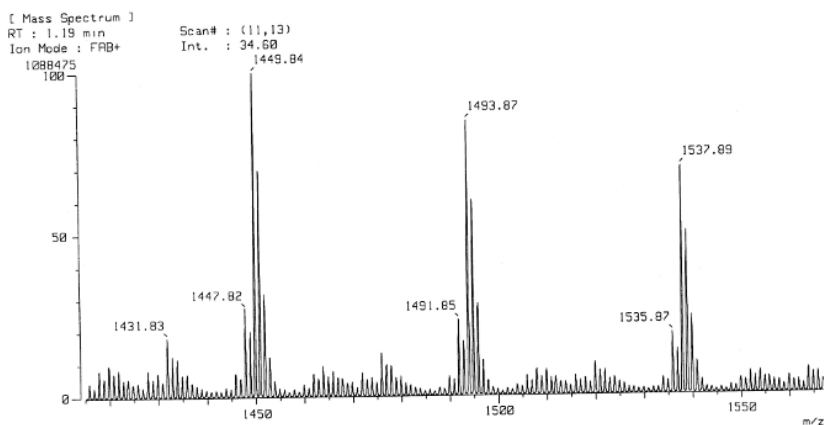
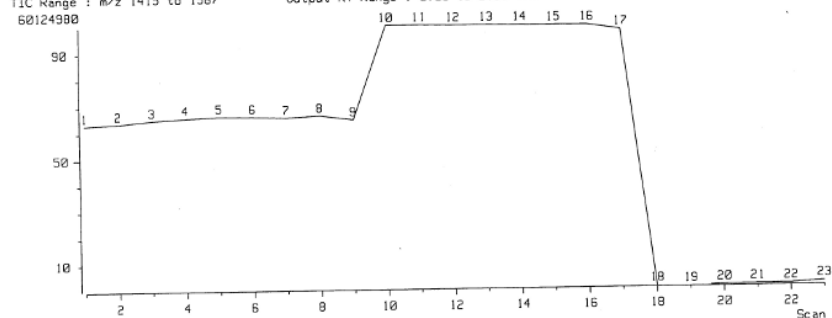


**Figure S3:**  $^1\text{H}$  NMR of **7** in 4:1 DMSO- $d_6$ -D $_2$ O at 20 °C.



**Figure S4:**  $^{13}\text{C}$  NMR of **7** in 4:1 DMSO- $d_6$ -D $_2$ O at 20 °C.

[ TIC ]  
 Date : HR003016 Date : 29-Nov-2010 13:16  
 Sample: 2  
 Note :  
 Inlet : Direct Ion Mode : FAB+  
 Ion Species : Normal Ion [EF-Linear] Output RT Range : 0.00 to 2.39 min  
 TIC Range : m/z 1415 to 1567



[ Elemental Composition ]

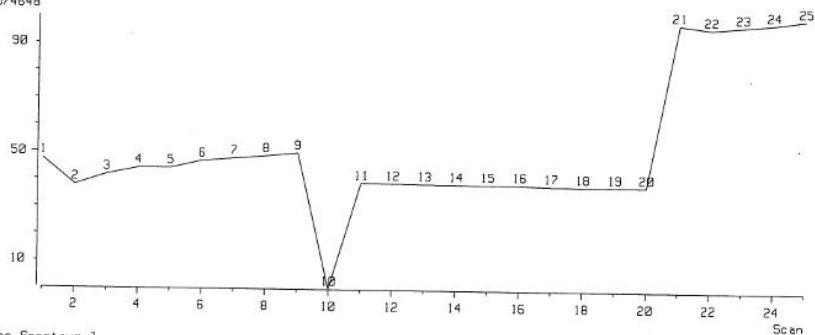
Data : HR003016 Date : 29-Nov-2010 13:16  
 Sample: 2 + Na  
 Note :  
 Inlet : Direct Ion Mode : FAB+  
 RT : 0.65 min Scan#: (6,8)  
 Elements : C 100/0, H 120/0, O 43/0, Na 1/0  
 Mass Tolerance : 10mmu  
 Unsaturation (U.S.) : -1.0 - 20.0

Observed m/z	Int%	Err[ppm / mmu]	U.S. Composition
1499.4318	100.0	-1.2 / -1.7	18.5 C 60 H 84 O 42 Na

Figure S5: HR-MS of 6. Calc. for  $[6+Na]^+$ ,  $C_{60}H_{86}NaO_{42}$  1499.43, found: 1499.43.

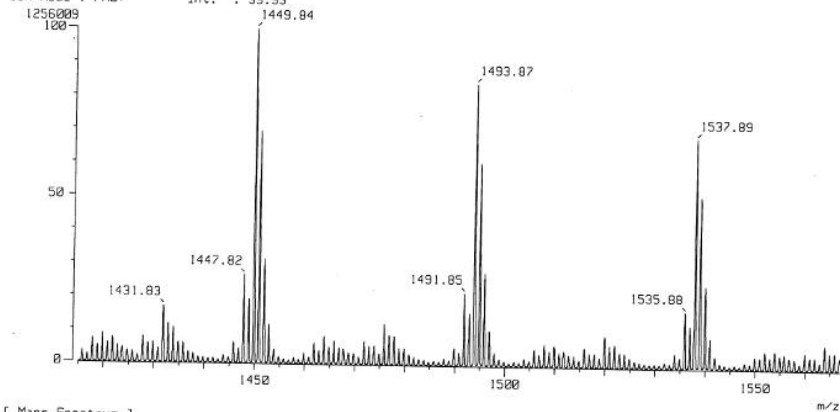


TIC  
 Data : HR003015 Date : 29-Nov-2010 12:59  
 Sample: 1  
 Note :  
 Inlet : Direct Ion Mode : FAB+  
 Ion Species : Normal Ion [EF-Linear]  
 TIC Range : m/z 1415 to 1567 Output RT Range : 0.00 to 2.60 min  
 69074648



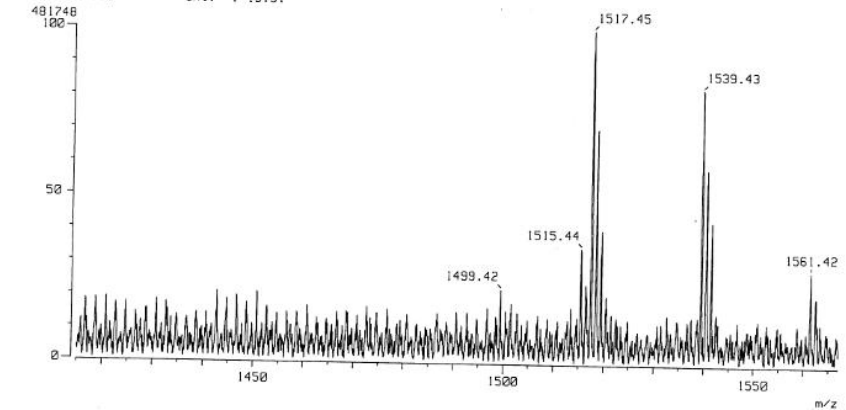
[ Mass Spectrum ]

RT : 1.30 min Scan# : (12,14)  
 Ion Mode : FAB+ Int. : 39.93



[ Mass Spectrum ]

RT : 0.76 min Scan# : (7,9)  
 Ion Mode : FAB+ Int. : 15.31



[ Elemental Composition ]

Data : HR003015 Date : 29-Nov-2010 12:59 Page:  
 Sample: 1 + [Na]  
 Note :  
 Inlet : Direct Ion Mode : FAB+  
 RT : 0.76 min Scan# : (7,9)  
 Elements : C 100/0, H 120/0, O 43/0, Na 1/0  
 Mass Tolerance : 10mmu  
 Unsaturation (U.S.) : -1.0 - 20.0

Observed m/z	Int%	Err [ppm / mmu]	U.S. Composition
1517.4495	100.0	+3.6 / +5.4	17.5 C 60 H 86 O 43 Na

**Figure S6:** HR-MS of **7**. Calc. for  $[7+Na]^+$ ,  $C_{60}H_{86}NaO_{43}$  1517.44, found: 1517.45.