

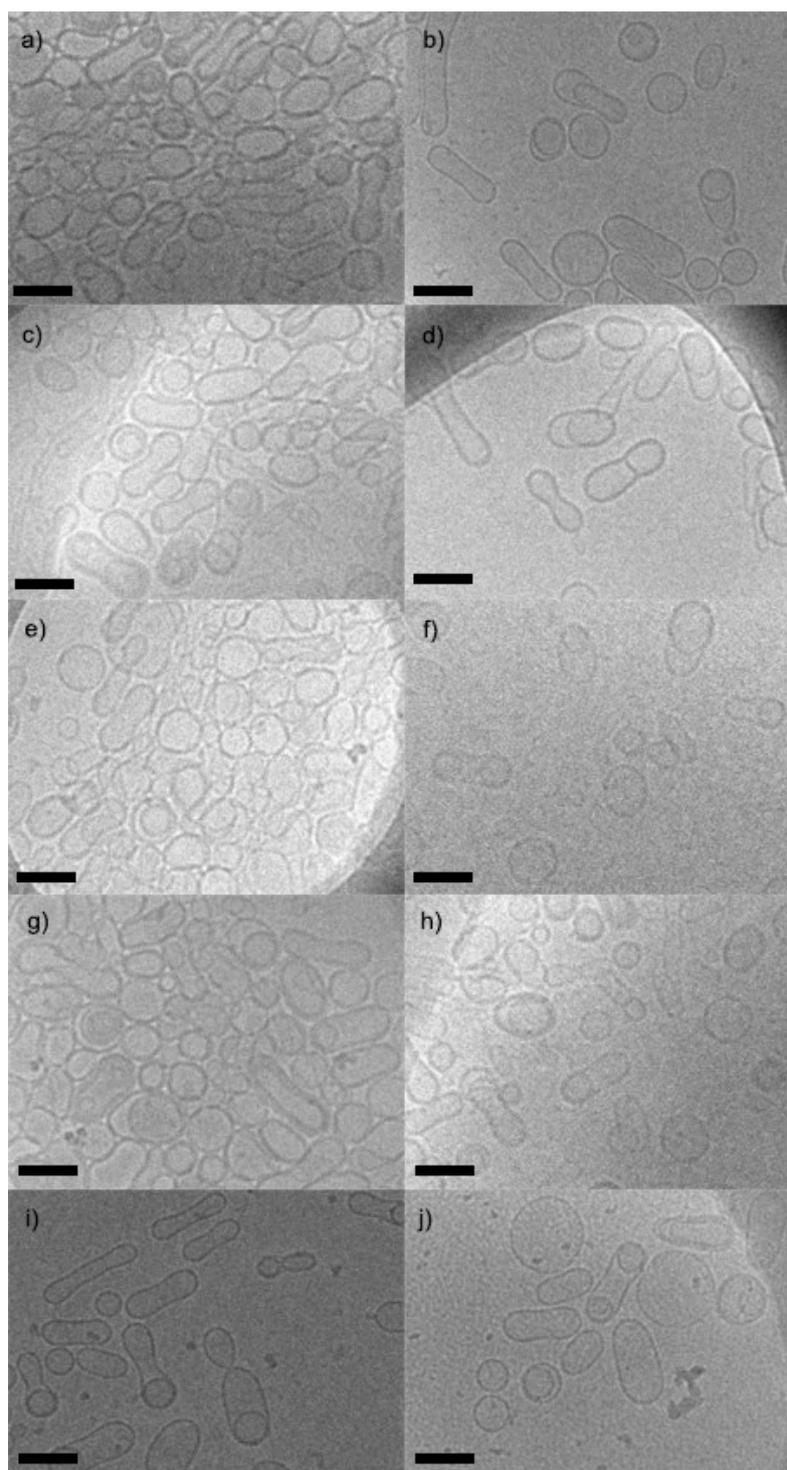
## **Supporting Information**

**S1. Cryo-TEM of Liposomes Before and After Irradiation**

**S2. Photolysis of NB-PC containing Liposomes**

**S3. Synthesis Data**

**S4. MS and NMR data**



**Figure S1. Cryo-TEM image of the liposome. a) Blank liposome before NIR irradiation; b) Blank liposome after NIR irradiation; c) Liposome 1 before NIR irradiation; d) Liposome 1 after NIR irradiation; e) Liposome 2 before NIR irradiation; f) Liposome 2 after NIR irradiation; g) Liposome 4 before UV irradiation; h) Liposome 4 after UV irradiation; i) Liposome 5 before UV irradiation; j) Liposome 5 after UV irradiation (bar = 100 nm).**

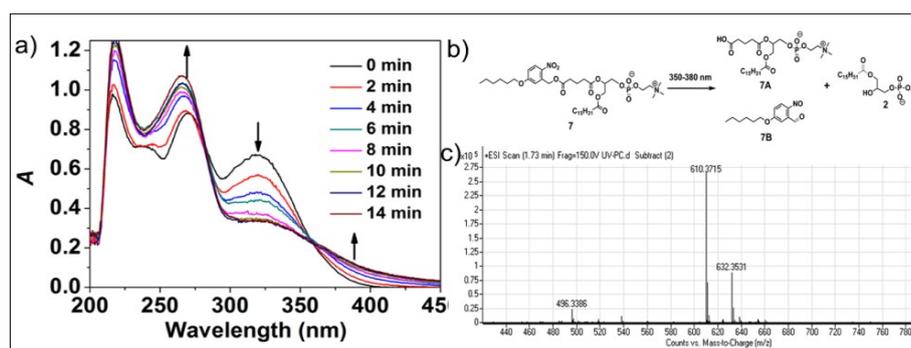


Figure S2. a) UV-vis absorption of liposome 6 exposed to UV light (50 mW/cm<sup>2</sup>); b) Photolysis route of Liposome 6 upon UV irradiation (50 mW/cm<sup>2</sup>); c) ESI-MS data of photolyzed product from NB-PC.

### S3. Synthesis Data

#### Compound 3

In a sealed tube, **Compound 1** (454 mg, 1 mmol), LPC (494 mg, 1 mmol), DCC (230 mg, 1.1 mmol), and DMAP (134 mg, 1.1 mmol) were dispersed in 20 mL anhydrous chloroform under N<sub>2</sub>, along with 5.0 g crushed glass. After 6 h of sonication, Dowex 50W×8 residue was added and the mixture was sonicated for 30 min before filtration through a fritted filter. After filtration and concentration, the crude product was purified by column chromatography through a silica gel using chloroform/methanol/water (100:30:2) to yield 371 mg (0.4 mmol, 40% yield) of **Compound 3** as a yellow solid. <sup>1</sup>H-NMR (MeOD, 400 MHz): δ = 0.92 (s, CH<sub>3</sub>, 6H), 1.31 (m, CH<sub>2</sub>, 24H), 1.42 (m, CH<sub>2</sub>, 4H), 1.87-1.89 (m, CH<sub>2</sub>, 6H), 2.28 (m, CH<sub>3</sub>CH<sub>2</sub>, 2H), 3.26 (m, NCH<sub>3</sub>, 9H), 3.69-3.70 (m, OCH<sub>2</sub>, 2H), 4.03-4.04 (m, COOCH<sub>2</sub>, 4H), 4.16-4.17 (m, OCH<sub>2</sub>, 4H), 5.38-5.39 (m, ArCH<sub>2</sub>O, 2H), 6.36 (m, ArH, 1H), 6.93 (m, ArH, 1H), 7.61 (m,

ArH, 1H). ESI MS calculated for  $C_{44}H_{71}BrNO_{13}P$ , 931.38, 933.38; found 934.42 (M+H<sup>+</sup>), 854.51 (M-Br<sup>-</sup>+2H<sup>+</sup>).

### Compound 5

1.67 g (10 mmol) 5-hydroxy-2-nitrobenzylaldehyde, 1.65 g (10 mmol) 1-bromohexane, and 10 g  $K_2CO_3$  were dissolved in 40 mL DMF, and heated at 90°C for 6 h. The solution was poured in water and extracted with ethyl acetate (60 mL), after which the organic phase was dried with  $Na_2SO_4$  and the crude product was purified by column chromatography with hexane as the eluent; 2.4 g yellow solid was obtained, yielding 96%. <sup>1</sup>H NMR ( $CDCl_3$ , 400 MHz):  $\delta$  = 0.91-0.92 (t,  $J$  = 4.0 Hz,  $CH_3$ , 3H), 1.35-1.37 (m,  $CH_2$ , 4H), 1.46-1.49 (m,  $CH_2$ , 2H), 1.80-1.87 (m,  $CH_2$ , 2H), 4.09-4.12 (t,  $J$  = 6.0 Hz,  $CH_2$ , 2H), 7.15-7.17 (dd,  $J$  = 4.0 Hz,  $J$  = 8.0 Hz, ArH, 1H), 7.30-7.31 (d, ArH,  $J$  = 4.0 Hz, 1H), 8.14-8.16 (d,  $J$  = 8.0 Hz, ArH, 1H), 10.48 (s, CHO); ESI MS: calculated for  $C_{13}H_{17}NO_4$  251.28, found, 250.11 (M-H<sup>+</sup>).

### Compound 6

2.0 g **Compound 5** (8 mmol) was dissolved in 30 mL THF, and 0.38 g  $NaBH_4$  (10 mmol) was added to one portion to the solution, after which solution was stirred at 25°C for 1 h and quenched with 1 M HCl. The organic phase was separated and dried with  $Na_2SO_4$ , and recrystallized from hexane. The yellow crystal was obtained with a quantitative yield. <sup>1</sup>H NMR ( $CDCl_3$ , 400 MHz):  $\delta$  = 0.93-0.94 (t,  $J$  = 4.0 Hz,  $CH_3$ , 3H), 1.33-1.37 (m,  $CH_2$ , 4H), 1.45-1.49 (m,  $CH_2$ , 2H), 1.78-1.84 (m,  $CH_2$ , 2H), 2.67 (s,  $CH_2OH$ , 1H), 4.05-4.08 (t,  $J$  = 6.0 Hz,  $ArOCH_2$ , 2H), 4.98 (s,  $ArCH_2OH$ , 2H), 6.86-6.89 (dd,  $J$  = 4.0 Hz,  $J$  = 8.0 Hz, ArH, 1H), 7.19-7.20 (d, ArH,  $J$  = 4.0 Hz, 1H),

8.15-8.18 (d,  $J = 8.0$  Hz, ArH, 1H); ESI MS: calcd for  $C_{13}H_{19}NO_4$  253.29, found, 254.14 (M-H<sup>+</sup>), 276.12 (M+Na<sup>+</sup>).

### Compound 7

1.0 g **Compound 6** (4 mmol) and 5.7 g glutaric anhydride (4 mmol) were dissolved in 20 mL pyridine and heated at 50°C for 6 h. The solution was removed by rotated evaporation, and the residue was dissolved in ethyl ether (30 mL) and washed with 1 M HCl (20 mL). Organic phase was dried with Na<sub>2</sub>SO<sub>4</sub>, and the crude product was purified by column chromatography with ethyl acetate as the eluent; 1.1 g yellow solid was obtained, yielding 74%. <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz):  $\delta = 0.93-0.94$  (t,  $J = 4.0$  Hz, CH<sub>3</sub>, 3H), 1.35-1.37 (m, CH<sub>2</sub>, 4H), 1.45-1.47 (m, CH<sub>2</sub>, 2H), 1.82-1.84 (m, CH<sub>2</sub>, 2H), 2.01-2.04 (m, CH<sub>2</sub>, 2H), 2.67 (s, CH<sub>2</sub>OH, 1H), 2.46-2.57 (m, CH<sub>2</sub>, 4H), 4.04-4.07 (t,  $J = 6.0$  Hz, ArOCH<sub>2</sub>, 2H), 5.54 (s, ArCH<sub>2</sub>OH, 2H), 6.88-6.91 (dd,  $J = 4.0$  Hz,  $J = 8.0$  Hz, ArH, 1H), 7.01-7.02 (d, ArH,  $J = 4.0$  Hz, 1H), 8.16-8.18 (d,  $J = 8.0$  Hz, ArH, 1H); ESI MS: calculated for  $C_{18}H_{25}NO_7$  367.39, found, 366.16 (M-H<sup>+</sup>).

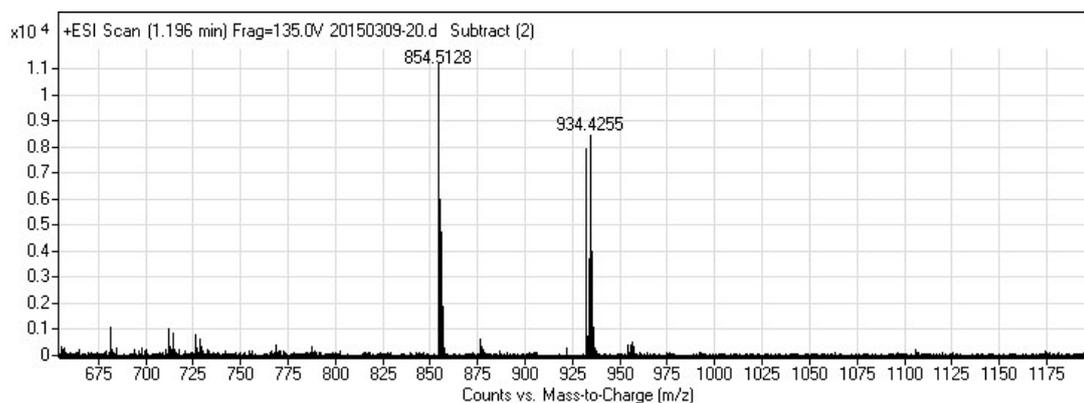
### Compound 8

In a sealed tube, **Compound 7** (368 mg, 1 mmol), LPC (494 mg, 1 mmol), DCC (230 mg, 1.1 mmol), and DMAP (134 mg, 1.1 mmol) were dispersed in 20 mL anhydrous chloroform under N<sub>2</sub>, along with 5.0 g crushed glass. After 6 h of sonication, Dowex 50W×8 residue was added and the mixture was sonicated for 30 min before filtration through a fritted filter. After filtration and concentration, the crude product was purified by column chromatography through a silica gel using chloroform/methanol/water (100:30:2) to yield 443 mg (0.4 mmol, 51% yield) of

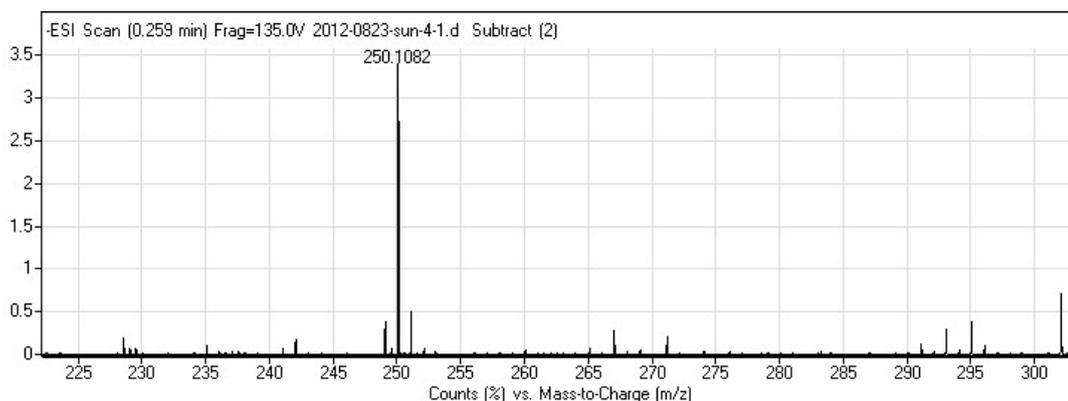
compound **8** as yellow solid.  $^1\text{H-NMR}$  ( $d^6$ -DMSO, 400 MHz):  $\delta$  = 0.86-0.88 (s,  $\text{CH}_3$ , 6H), 1.20-1.31 (m,  $\text{CH}_2$ , 34H), 1.42-1.48 (m,  $\text{CH}_2$ , 4H), 1.73-1.88 (m,  $\text{CH}_2$ , 4H), 2.26-2.37 (m,  $\text{CH}_2\text{CO}$ , 6H), 3.13 (s,  $\text{NCH}_3$ , 9H), 3.50-3.52 (m,  $\text{CH}_2\text{O}$ , 2H), 3.71-3.75 (m,  $\text{CH}_2\text{O}$ , 2H), 4.25-4.33 (m,  $\text{CHO}$ , 1H), 5.43 (s,  $\text{ArCH}_2$ , 2H), 6.88-6.91 (dd,  $\text{ArH}$ , 1H,  $J_1$  = 2.0 Hz,  $J_2$  = 8.0 Hz), 7.01-7.02 (d,  $\text{ArH}$ , 1H,  $J$  = 2.0 Hz), 8.17-8.19 (d,  $\text{ArH}$ , 1H,  $J$  = 8.0 Hz). ESI MS calculated for  $\text{C}_{42}\text{H}_{73}\text{N}_2\text{O}_{13}\text{P}$ , 844.4850; found 845.4883 ( $\text{M}+\text{H}^+$ ), 867.4671 ( $\text{M}+\text{Na}^+$ ).

## S4. MS and NMR data

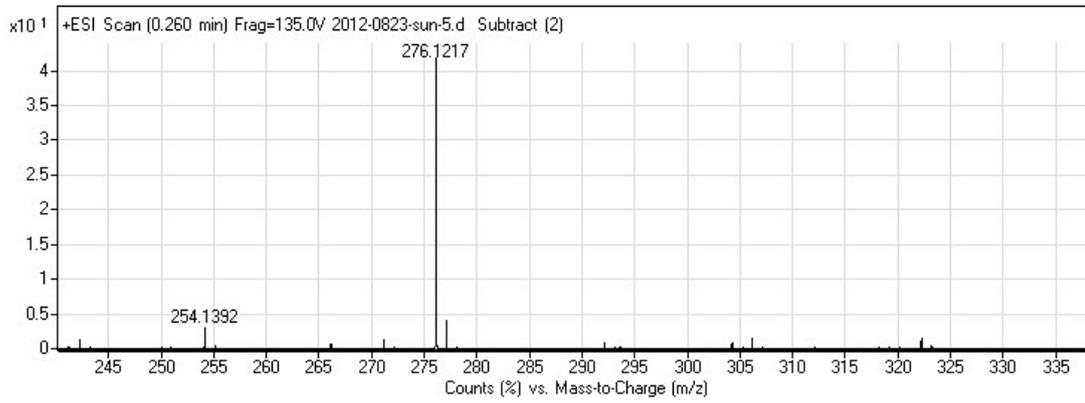
### Compound 3



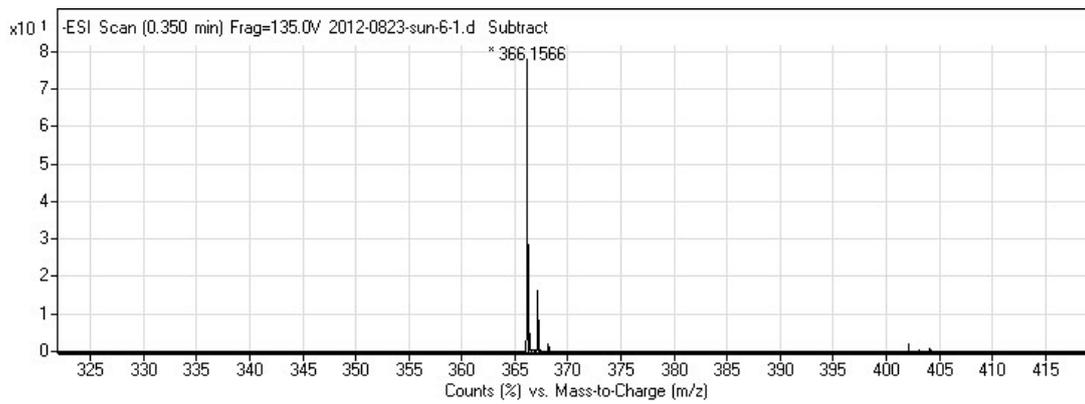
### Compound 5



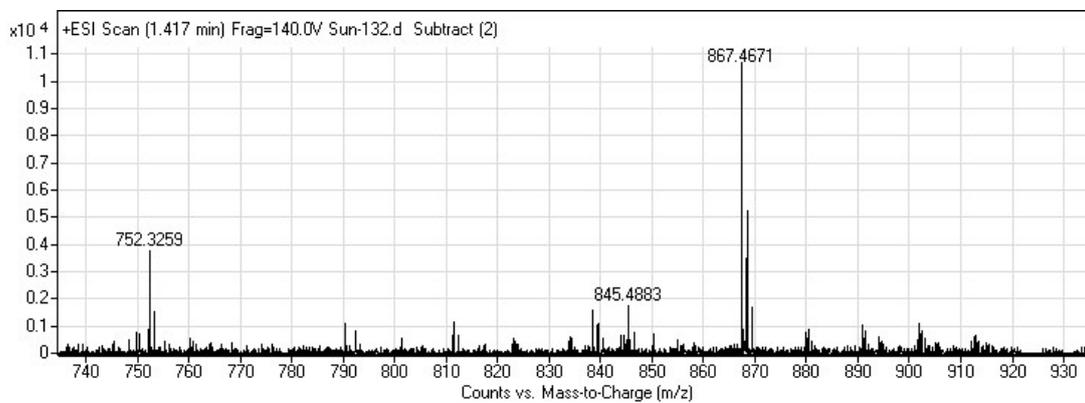
### Compound 6



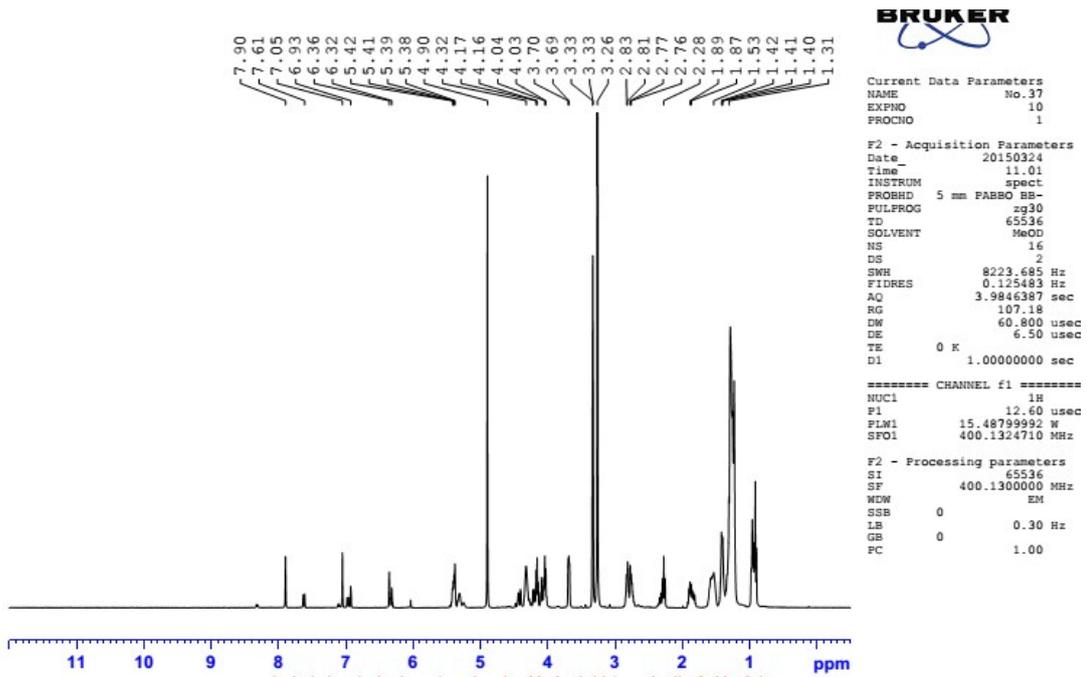
### Compound 7



### Compound 8

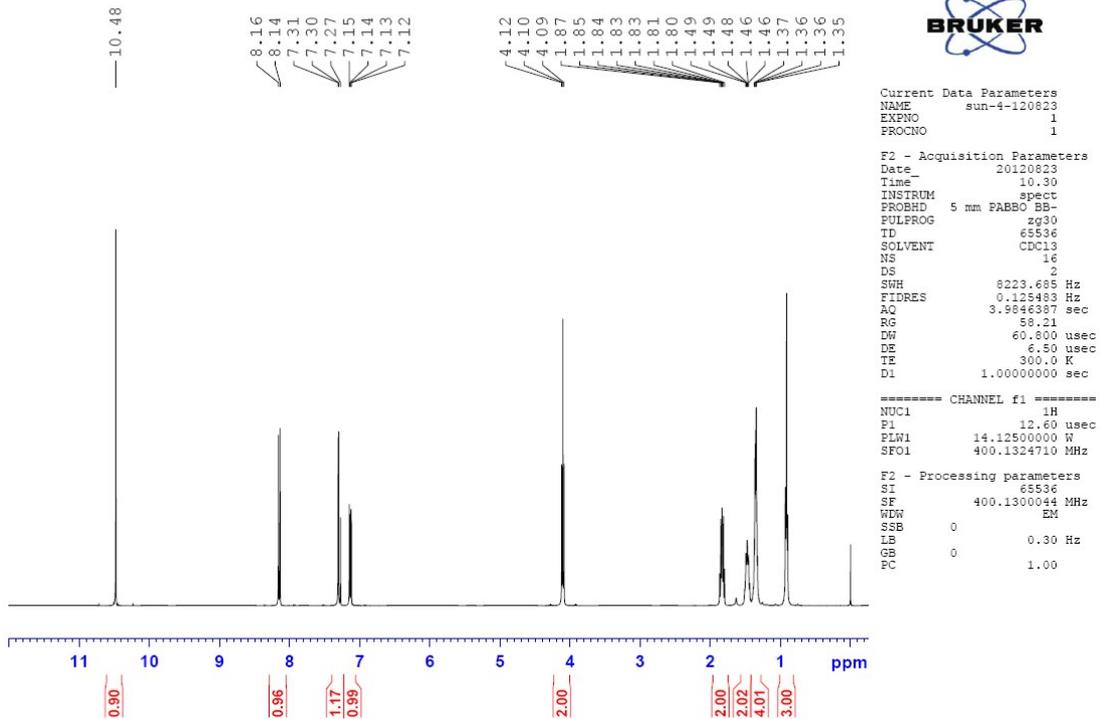


### Compound 3



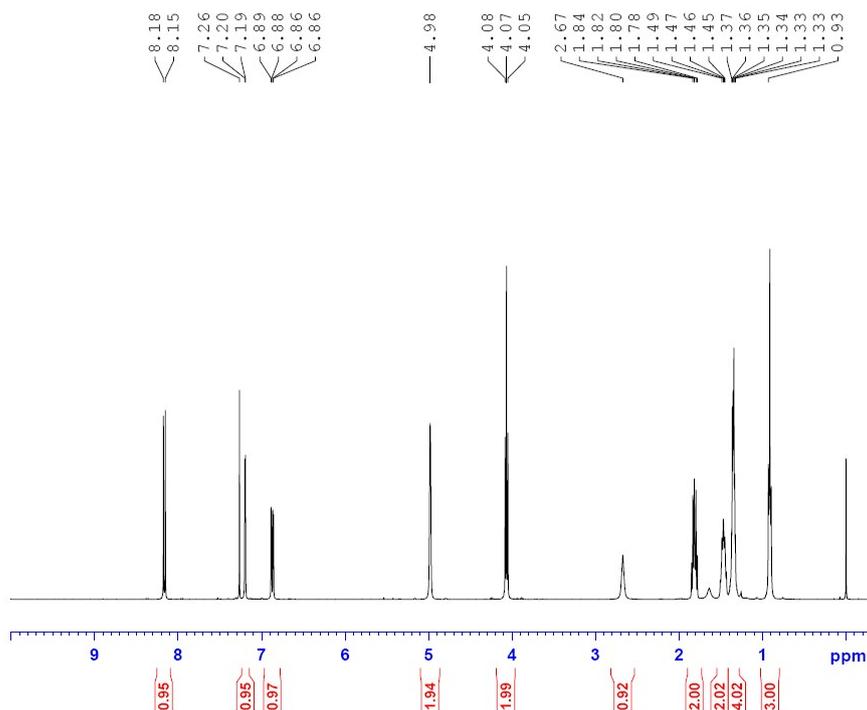
### Compound 5

<sup>1</sup>H  
 PROTON CDCl<sub>3</sub>



### Compound 6

<sup>1</sup>H  
PROTON CDCl<sub>3</sub>



Current Data Parameters  
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PROCNO 1

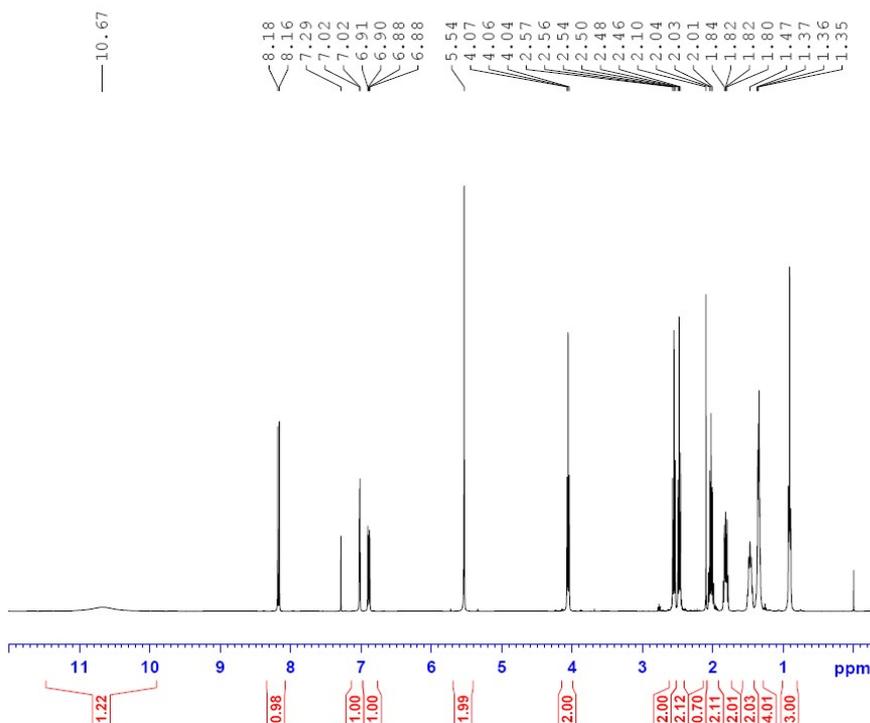
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FIDRES 0.125483 Hz  
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DE 6.50 usec  
TE 300.0 K  
D1 1.00000000 sec

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SFO1 400.1324710 MHz

F2 - Processing parameters  
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### Compound 7

<sup>1</sup>H  
PROTON CDCl<sub>3</sub>



Current Data Parameters  
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PROCNO 1

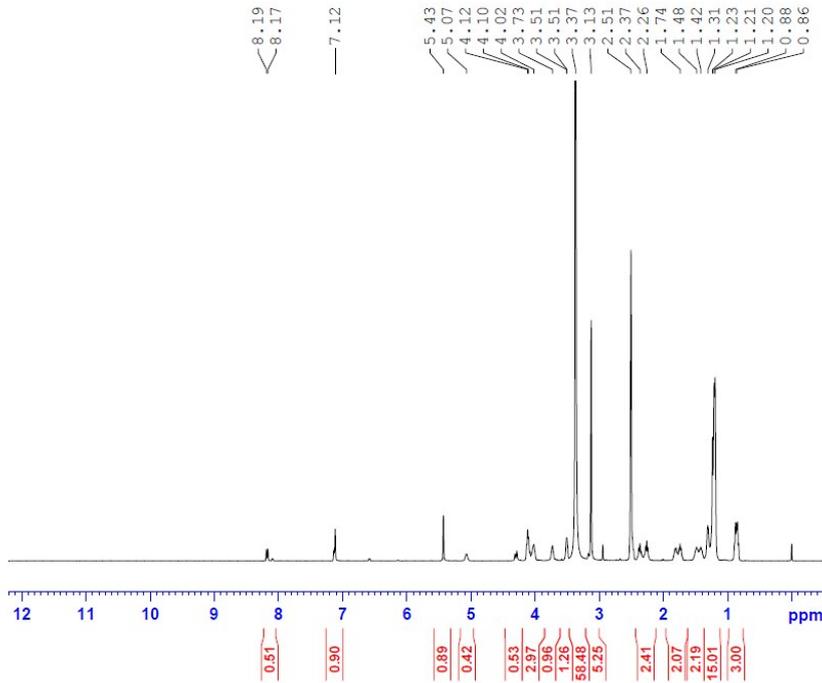
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DS 2  
SWH 8223.685 Hz  
FIDRES 0.125483 Hz  
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TE 300.0 K  
D1 1.00000000 sec

===== CHANNEL f1 =====  
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### Compound 8

1H  
PROTON DMSO D:\NMR10\SYW nmr.su



Current Data Parameters  
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PROCNO 1

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Time\_ 16.03  
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DW 60.800 usec  
DE 6.50 usec  
TE 0 K  
DI 1.00000000 sec

===== CHANNEL f1 =====  
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PLH1 15.4879992 W  
SF01 400.1324710 MHz

F2 - Processing parameters  
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SF 400.1300027 MHz  
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SSB 0  
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GB 0  
PC 1.00