Electronic Supplementary Information for

Development of an Open-Type Water-Soluble Near-Infrared Chemiluminescent Material Inspired by Luciferin

Dongyue Zhang ,[a] Shuo Wang ,*[b] Xue Li ,*[c d] Yuewei Zhang ,*[a] and Leqin Cheng [a*]

[a] School of Chemistry and Pharmaceutical Engineering, Jilin Institute of Chemical Technology, Jilin， 132022, China;.

[b] Zhejiang Engineering Research Center for Fabrication and Application of Advanced Photovoltaic Materials, NingboTech University, Ningbo, 315100, China

[c] Department of Materials Science and Engineering, Luoyang Institute of Science and Technology, Luoyang,Henan, 471023, China;

[d] Department of Materials Science and Engineering, Luoyang Institute of Science and Technology, Luoyang, Henan, 471023, China;

* To whom correspondence should be addressed. Tel: +86 15044693511; Email: zhangyueweichem@163.com

Contents

Experimental section

^{1}H NMR and ^{13}C NMR spectra analysis of TM6.

Zeta potential and particle size distribution over time

Experimental section

The synthetic route of S2

Route S2 ：2-Hydroxy acetophenone (2.65 mL, 22 mmol) and ethyl acetate (60 mL) were added to a flask, and then sodium (2.3 g, 102 mmol) was added. The reaction mixture was stirred vigorously for 4 h under ambient temperature. Then the greyish green solid was obtained after the filtration. The solid was dissolved in deionized water, neutralized and then extracted with ethyl acetate (150 mL). The organics was then dried with anhydrous sodium sulfate and filtered. Remove the solvent under vacuum to afford the crude product as brown solid (1.9 g, yield = 45 %).

The synthetic route of S3

Route S3 ：The crude product (compound 2, 1.9 g) was dissolved with acetic acid (25 mL), then concentrated sulfuric acid (1.2 mL) was added dropwise. The reaction mixture was then refluxed for 30 min. The reaction mixture was poured into ice water (300 mL), then the mixture was neutralized with sodium carbonate. Extract th eaqueous phase with dichloromethane twice, combine the organics and dry with anhydrous sodium sulfate. The solvent was then removed under vacuum, and compound 3 was obtained as colourless crystal (1.12 g, yield = 78%).

The synthetic route of S4

Route S4 ：Compound 3 (2.25 g, 14 mmol) and malononitrile (1.38 g, 21 mmol) were dissolved in acetic anhydride (20 mL), then the reaction mixture was refluxed for 17 h. The solvent was removed under vacuum. Then deionized water (40 mL) was added to the flask, the mixture was refluxed for 0.5 h. After cooled to ambient temperature, the mixture was extracted with dichloromethane, the organic phase was collected, dried with anhydrous sodium sulfate, and then concentrated under vacuum. Then column chromatography was performed to afford compound 4 as orange red solid (1.1 g, yield = 38%).

The synthetic route of S5

Route S5 ： Compound 4 (500 mg, 2.4 mmol) and 4- hydroxybenzaldehyde (300 mg, 2.5 mmol) were dissolved into toluene (34 mL). Piperidine (0.6 mL) and acetic acid (0.6 mL) were added to the reaction mixture. Then the reaction was carried out at reflux for 17 h. After the mixture cooled down, the solvent was evaporated under vacuum. The product was purified further through column chromatography to afford compound 5 as red solid (242 mg, yield = 40%).

^{1}H NMR and ^{13}C NMR spectra analysis of TM6.

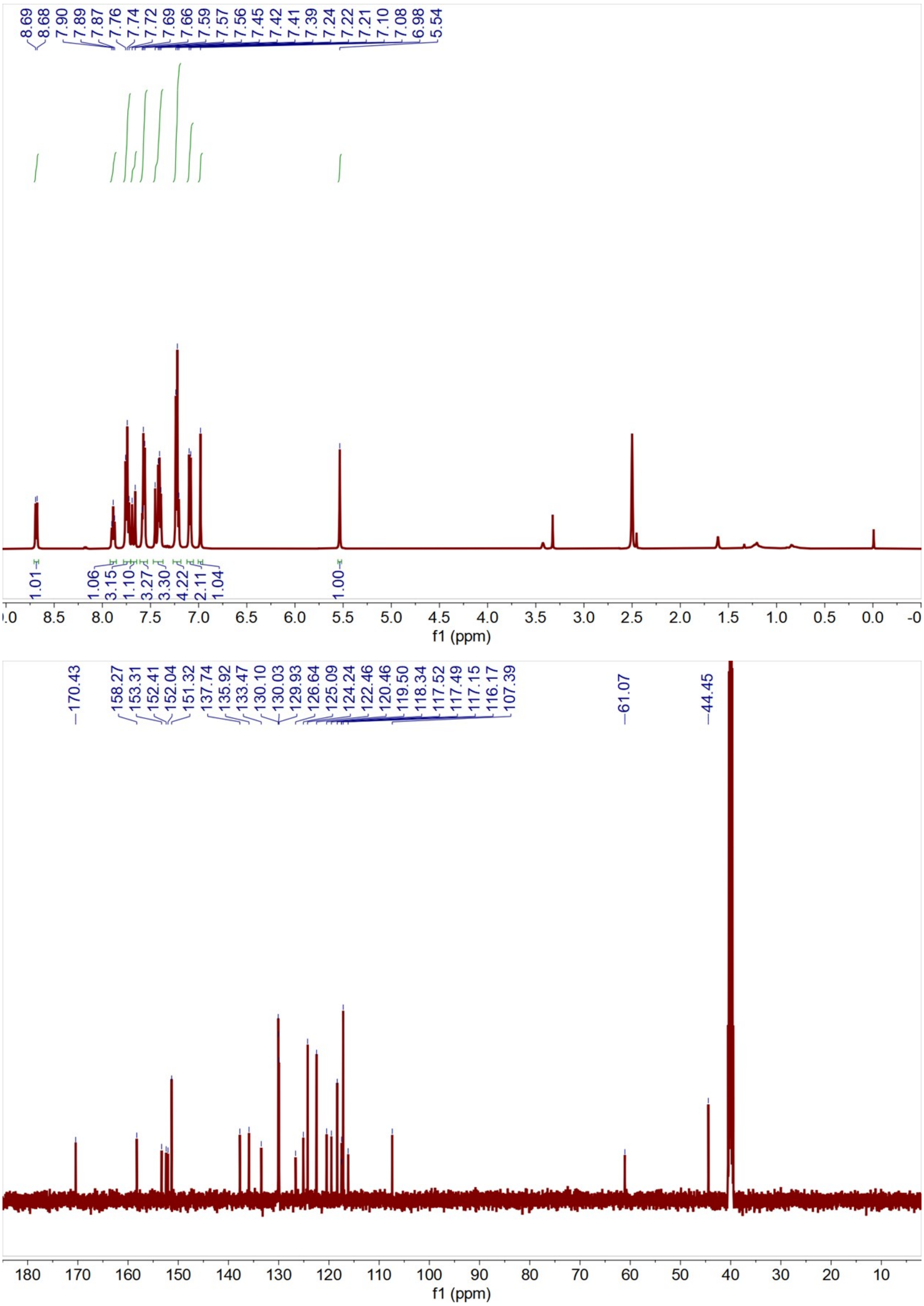

Fig. S1. ^{1}H NMR (500 MHz, DMSO-d_6, top) and ^{13}C NMR (125 MHz,DMSO-d_6, bottom) of TM6

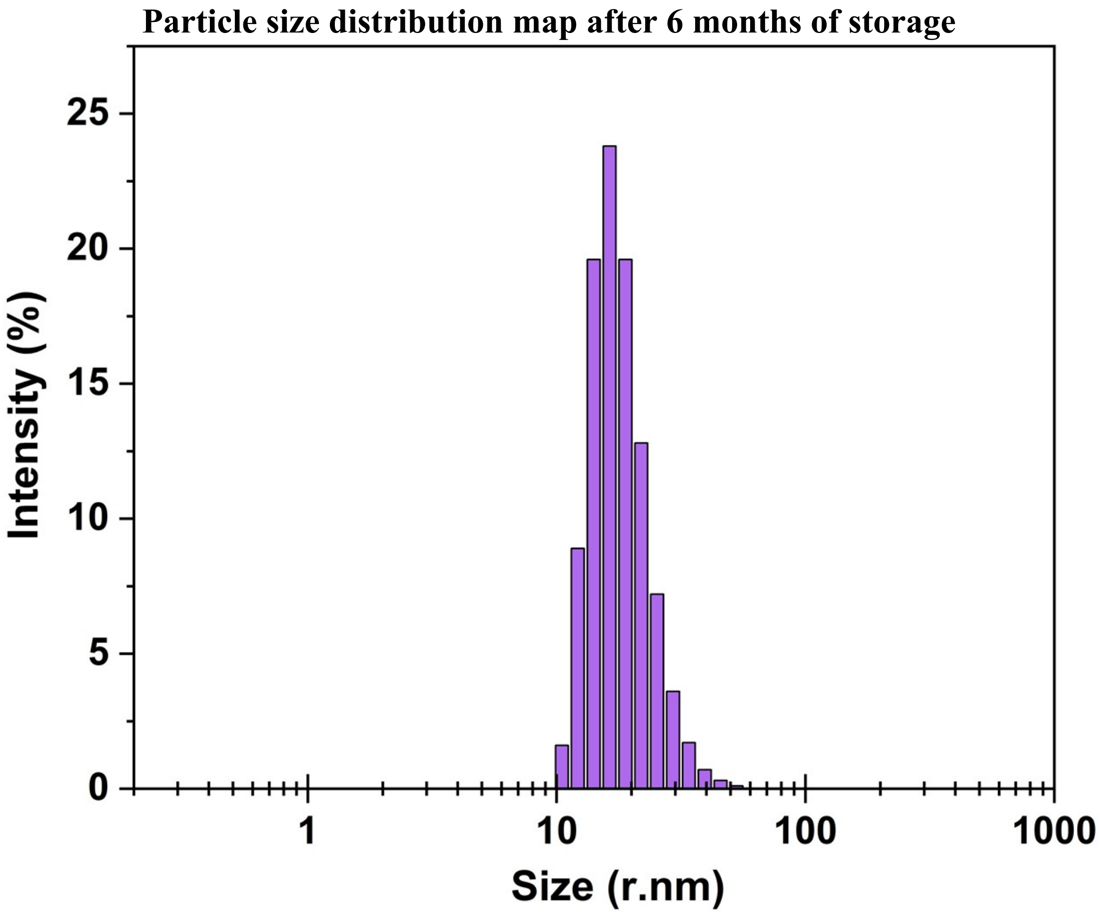

Fig. S2. The particle size distribution of TM and PSMA nanoparticles after 6 months