Aza-BODIPY Probe for Selective Visualization of Cyclooxygenase-2 in Cancer Cell

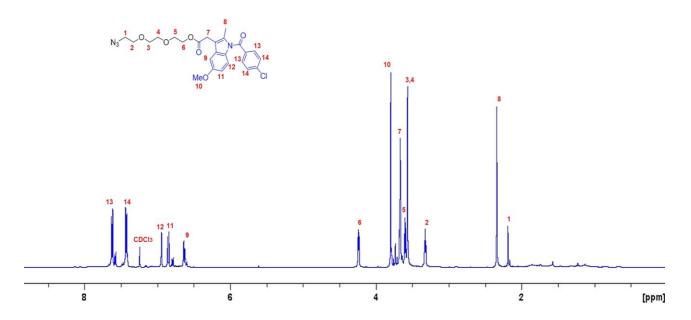
Supporting Information

Thitima Pewklang,^{a,‡} Kantapat Chansaenpak,^{b,‡} Rung-Yi Lai,^a Parinya Noisa^c and Anyanee Kamkaew^{*a}

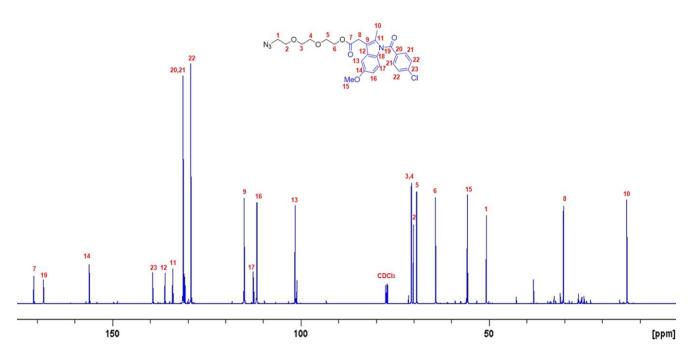
- ^a School of Chemistry, Institute of Science, Suranaree University of Technology, Nakhon Ratchasima, Thailand 30000
- ^b National Nanotechnology Center, National Science and Technology Development Agency, Thailand Science Park, Pathum Thani, Thailand 12120
- ^c Laboratory of Cell-Based Assays and Innovations, School of Biotechnology, Institute of Agricultural Technology, Suranaree University of Technology, Nakhon Ratchasima, Thailand 30000

- 3. Fluorescence spectroscopic data of AZB-IMC₂ in aqueous with and without 3% tween-80....8

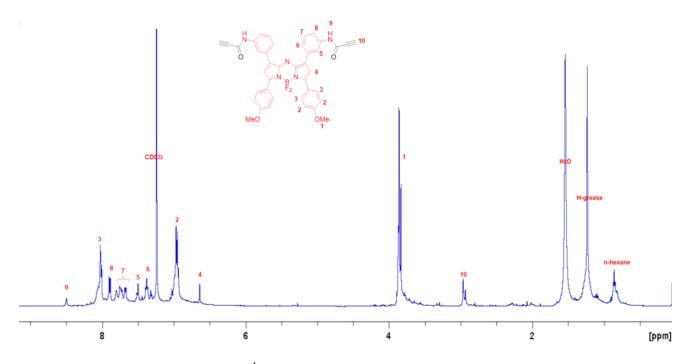
1. ¹H NMR, ¹³C NMR, and MS results of compound 3, 5, and AZB-IMC₂



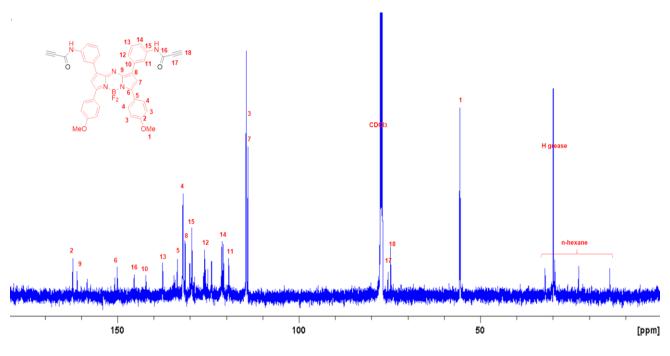
¹H NMR of compound 3



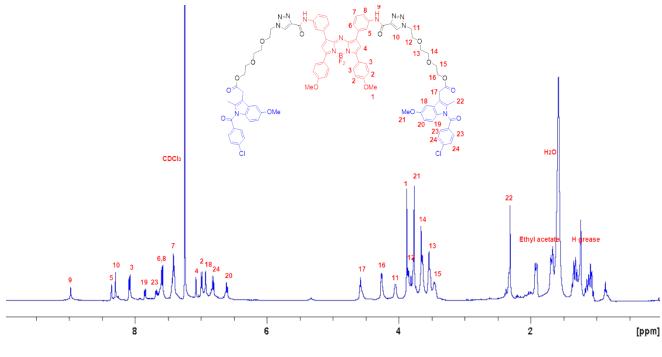
¹³C NMR of compound **3**



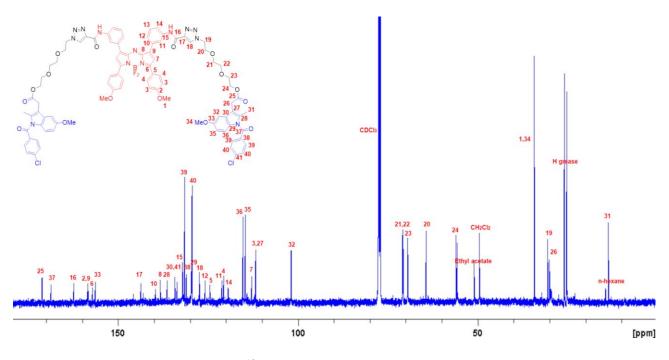
¹H NMR of compound **5**



¹³C NMR of compound **5**



¹H NMR of **AZB-IMC**₂



¹³C NMR of **AZB-IMC**₂

BIORESOURCES RESEARCH UNIT

High resolution report Acquisition Date 11/27/2018 1:54:49 PM Analysis Name D:\Data\customer\PEG N3 Indomethacin.d NaFormate_pos.m Method Ext: 3560 Operator Sutichai Sample Name PEG N3 Indomethacin Instrument micrOTOF Bruker Calibrate by Sodium Formate **Acquisition Parameter** Set Nebulizer Set Dry Heater Set Dry Gas 0.3 Bar 180 ?C 4.0 l/min Source Type Ion Polarity Positive Focus Scan Begin Scan End Not active Set Capillary Set End Plate Offset 4500 V -500 V 100 m/z 1500 m/z Set Divert Valve Source Intens. x10⁶ 1.0-+MS, 0.1min #8 $[M+Na]^{+}$ 537.1515 0.8 0.6 304.2626 0.4 Exact Mass: 514.96 g/mol 198.0860 0.2 761.3327 100 400 700 800 1000 500 900 1100 600 Intens. x10⁶ +MS, 0.1min #8 1.0 537.1515 0.8 0.6 0.4 0.2 528.4480 532.1848 553.1366 559.5139 563.5501

 525
 530
 535
 540
 545
 550
 555
 560
 565
 570
 m/z

 Bruker Daltonics DataAnalysis 3.4
 printed:
 11/27/2018 2:10:37 PM
 Page 1 of 1

537.1511

x106 1.2

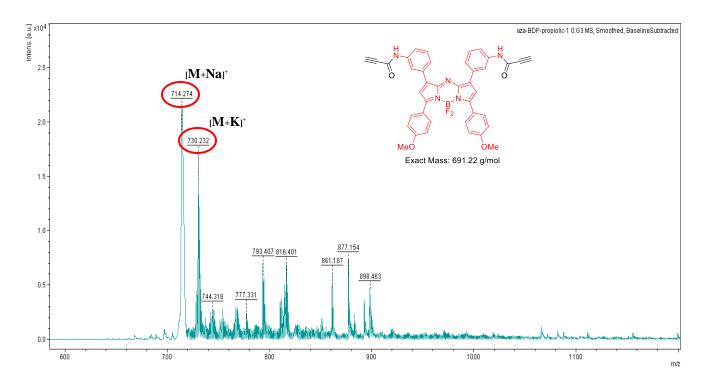
1.0-

0.8

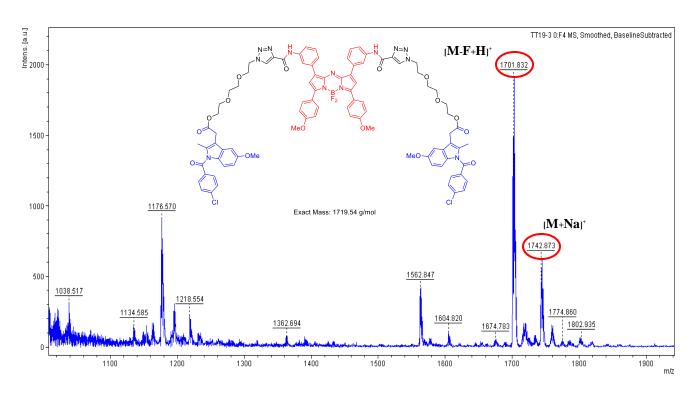
0.2

ESI MS of compound 3

C 25 H 27 Cl 1 N 4 Na 1 O 6 ,537.15



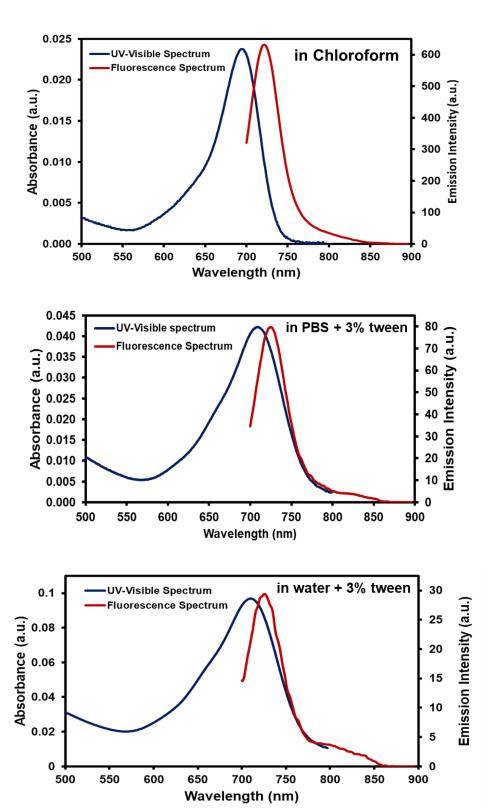
MALDI-TOF MS of compound 5



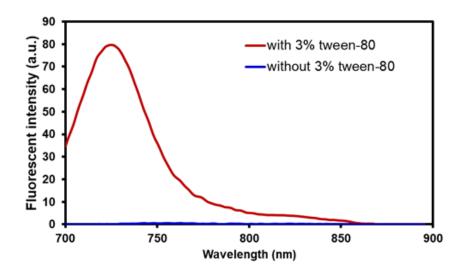
MALDI-TOF MS of AZB-IMC2

S6

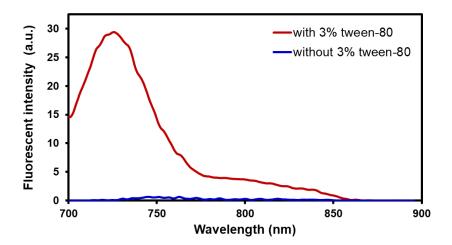
2. UV/Vis and fluorescence spectroscopic data of AZB-IMC $_2$ in various solvents



3. Fluorescence spectroscopic data of AZB-IMC $_2$ in aqueous with and without 3% tween-80



Fluorescent spectra of AZB-IMC2 (2.9 μ M) excited at 670 nm in PBS solution with and without 3% tween-80



Fluorescent spectra of AZB-IMC2 (2.9 μ M) excited at 670 nm in water with and without 3% tween-80