

SUPPORTING INFORMATION

Designing Bodipy-Based Probes for Fluorescence Imaging of β -amyloid Plaques

Fazli Sozmen,^{‡a} Safacan Kolemen,^{‡a} Henri-Obadja Kumada,^b Masahiro Ono,^b Hideo Saji^b and Engin U. Akkaya^{*ac}

^aUNAM-National Nanotechnology Research Center

^bDepartment of Patho-Functional Bioanalysis, Graduate School of Pharmaceutical Sciences, Kyoto University, 46-29 Yoshida Shimoadachi-cho, Sakyo-ku, Kyoto 606-8501, Japan.

^cDepartment of Chemistry, Bilkent University, 06800 Ankara, Turkey

[‡] These two authors made equal contributions

*eua@fen.bilkent.edu.tr

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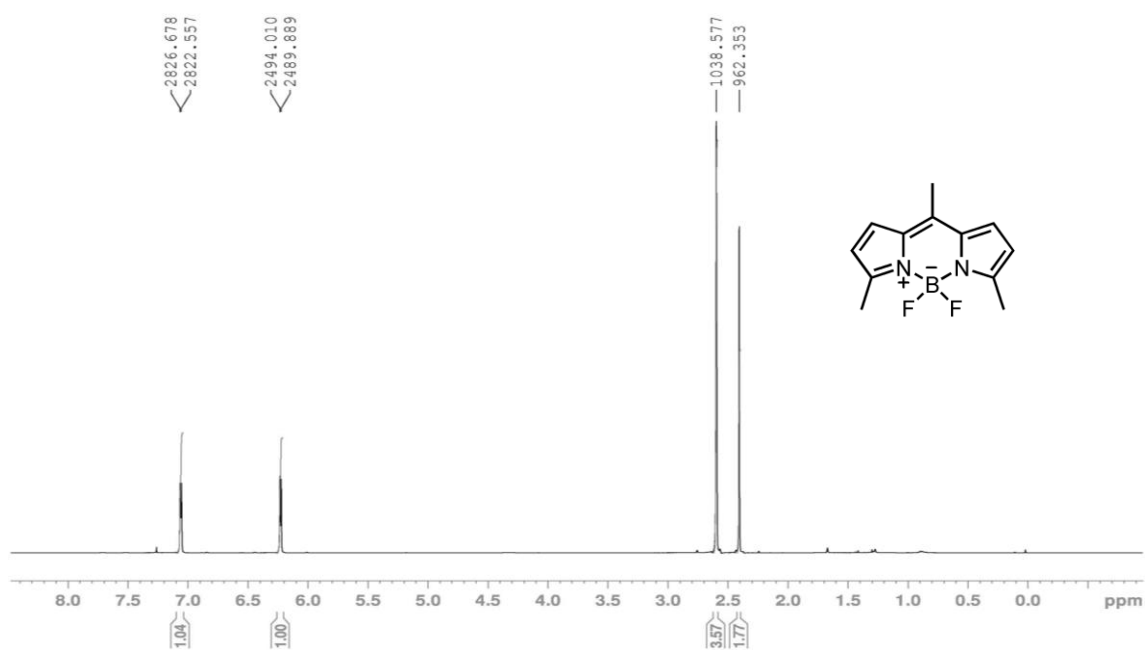


Figure S1: ^1H NMR spectrum of Compound **1**

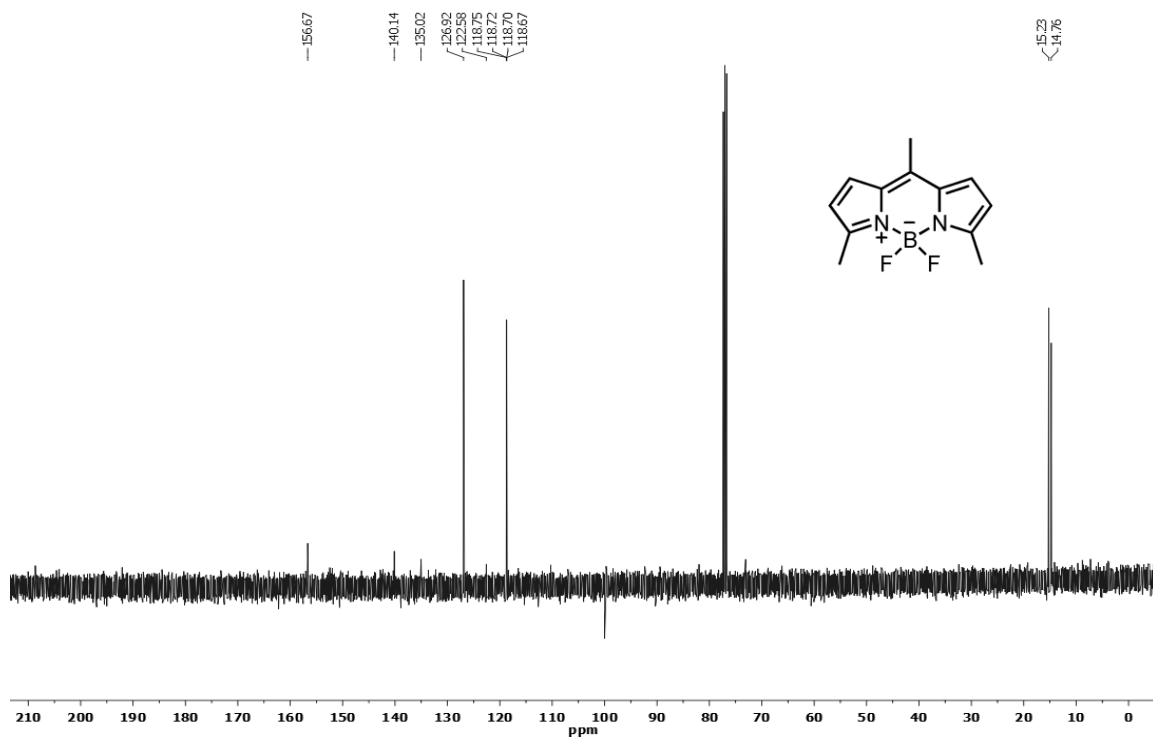


Figure S2: ^{13}C NMR spectrum of Compound **1**

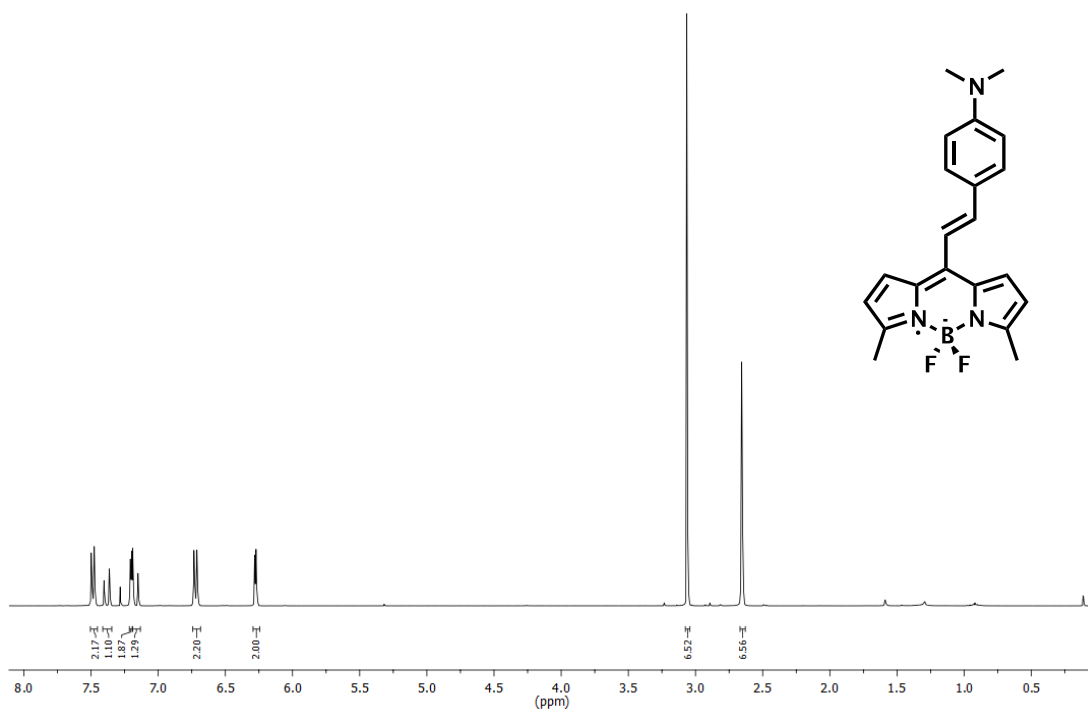


Figure S3: ^1H NMR spectrum of **EUA-1**

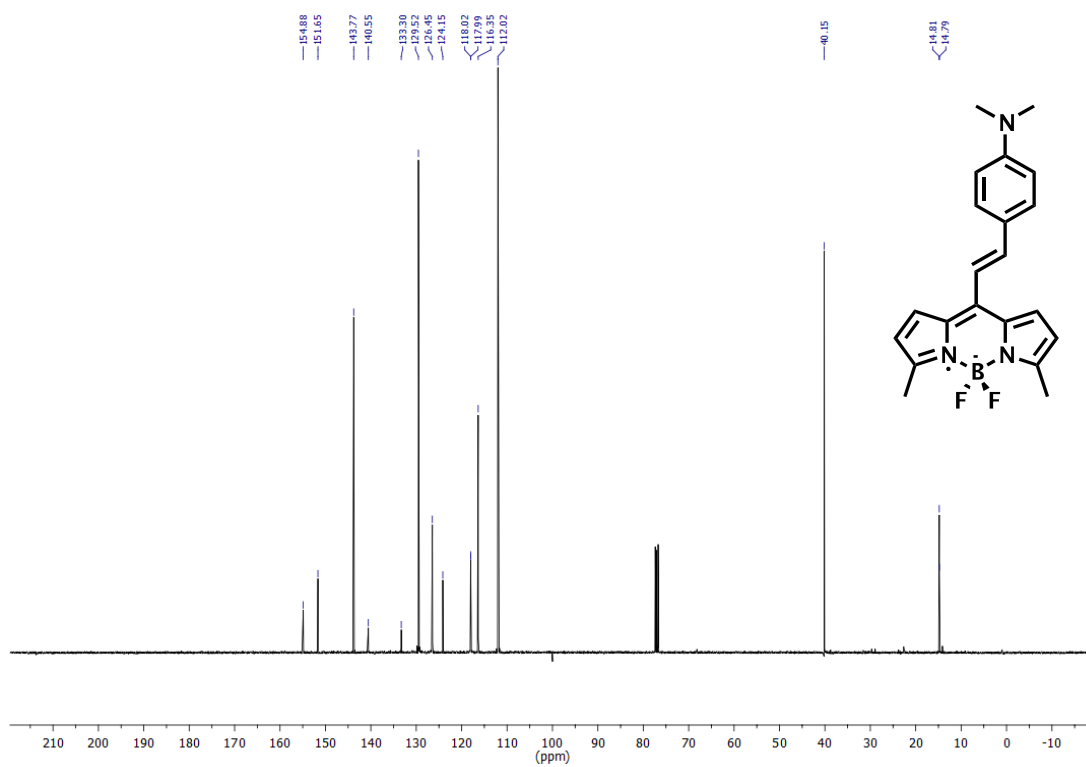


Figure S4: ^{13}C NMR spectrum of **EUA-1**

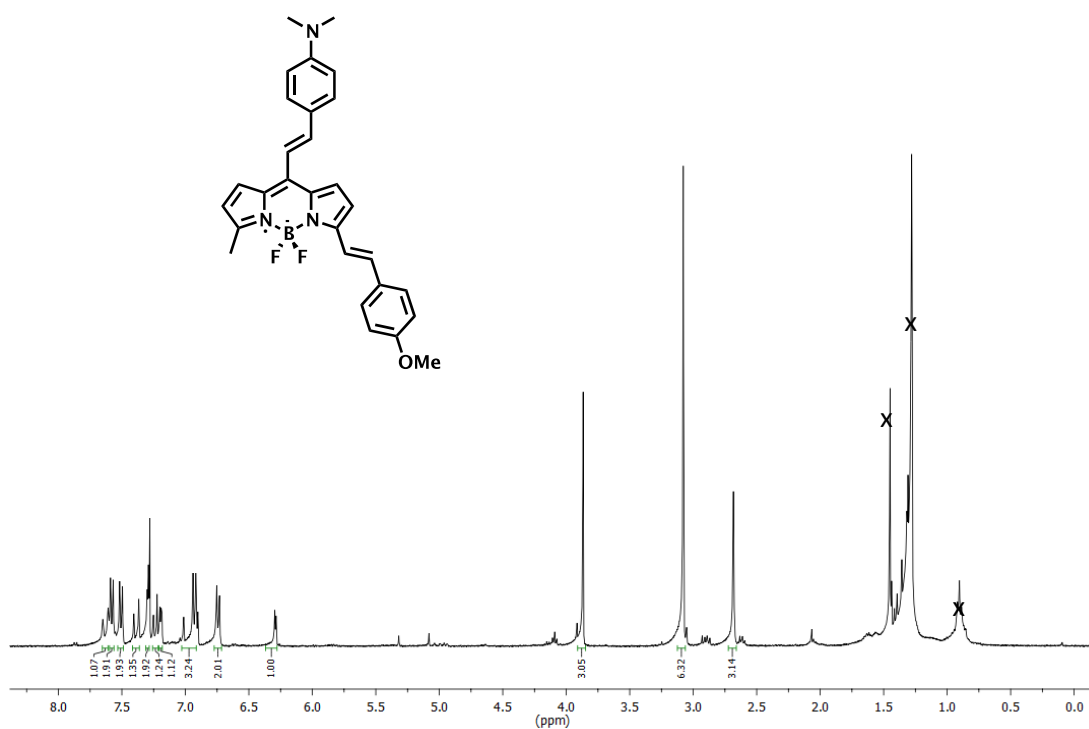


Figure S5: ¹H NMR spectrum of EUA-2

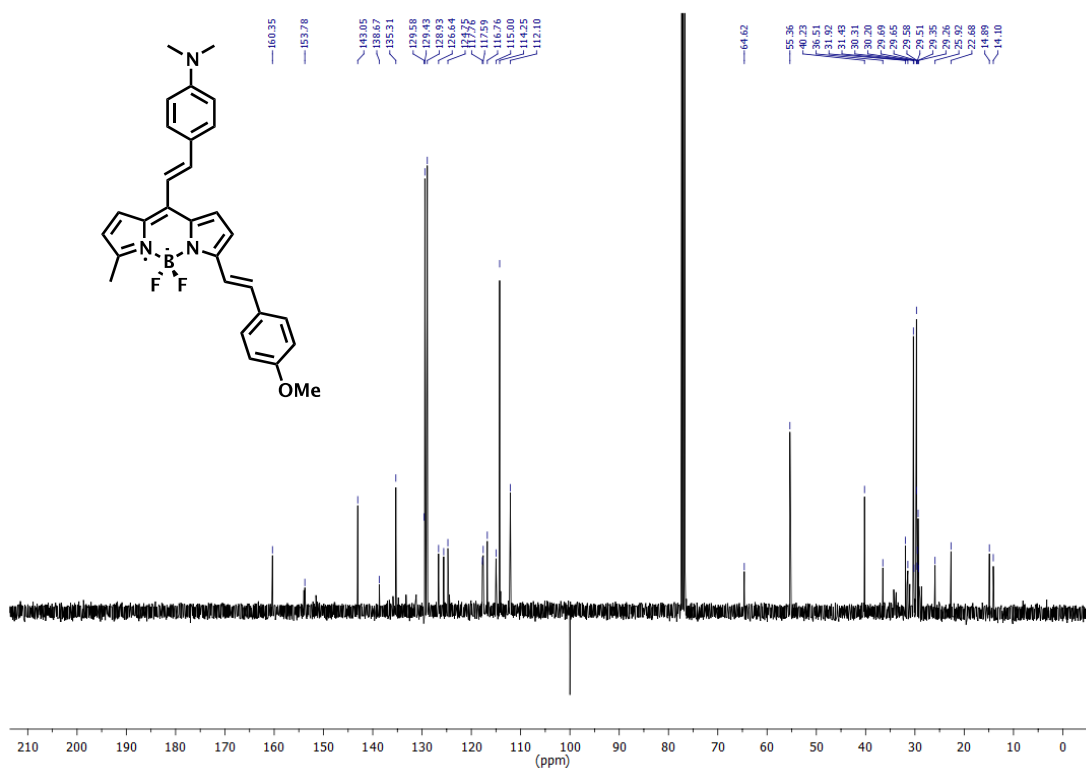


Figure S6: ¹³C NMR spectrum of EUA-2

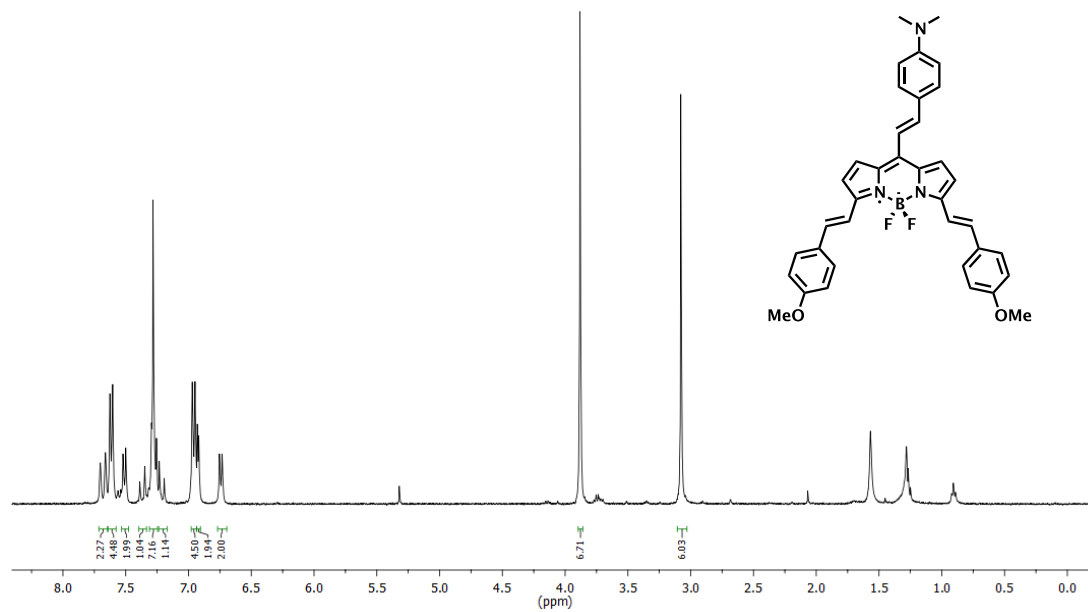


Figure S7: ^1H NMR spectrum of EUA-3

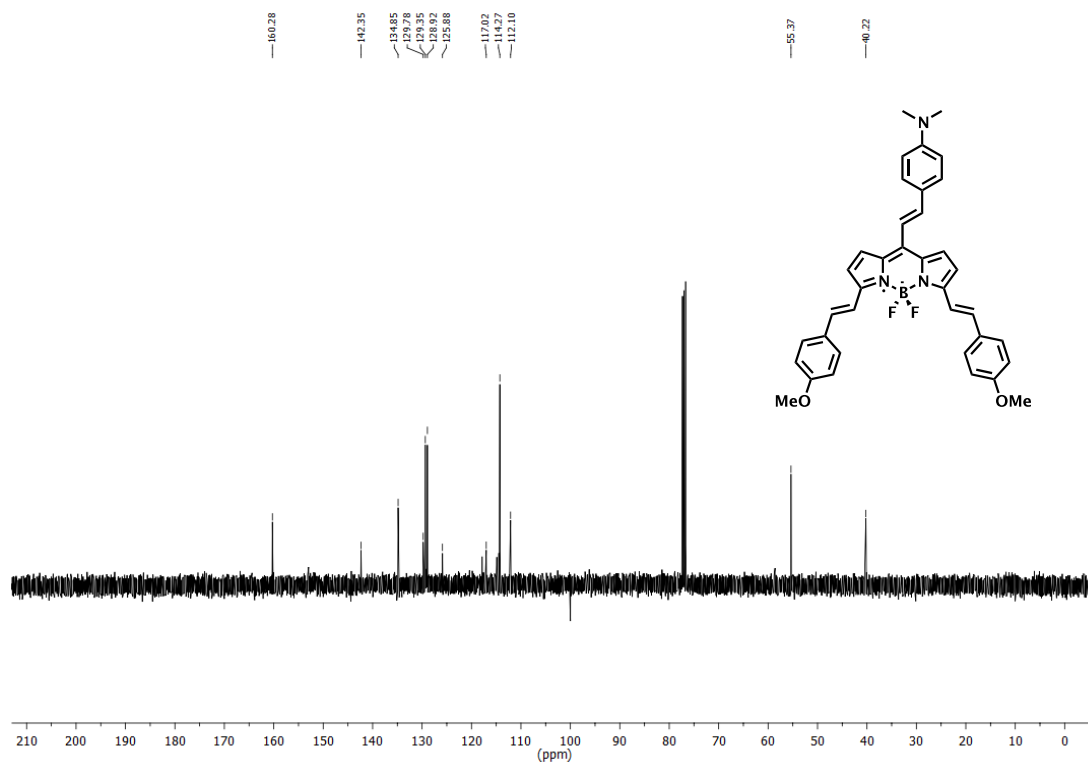


Figure S8: ^{13}C NMR spectrum of EUA-3

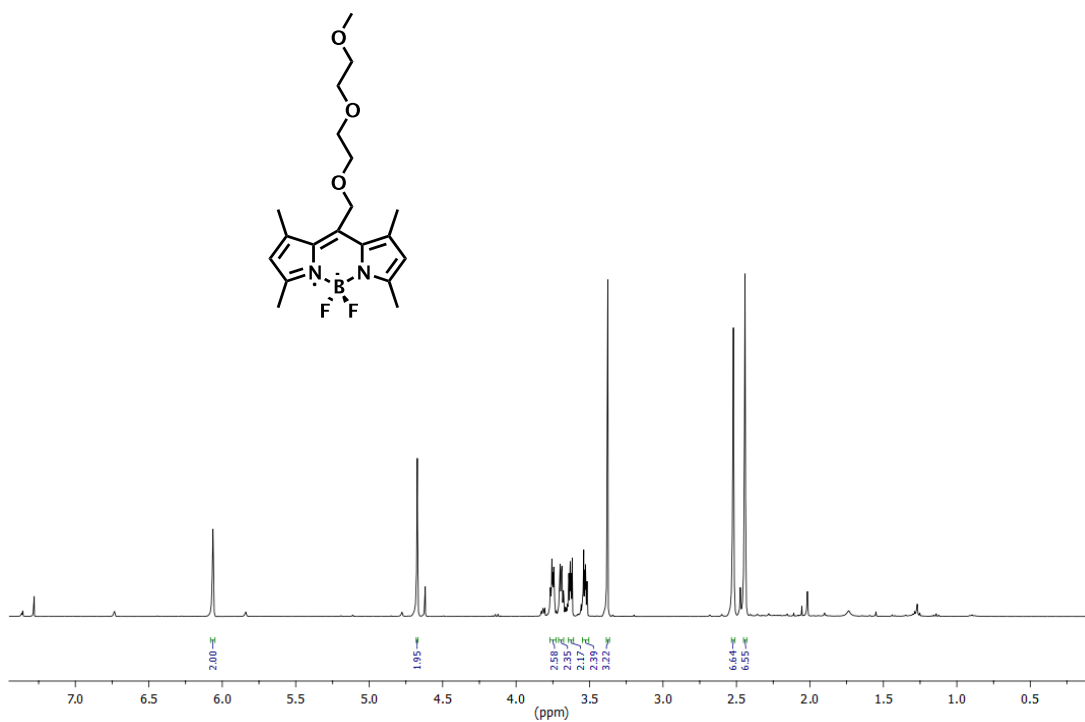


Figure S9: ^1H NMR spectrum of Compound 3

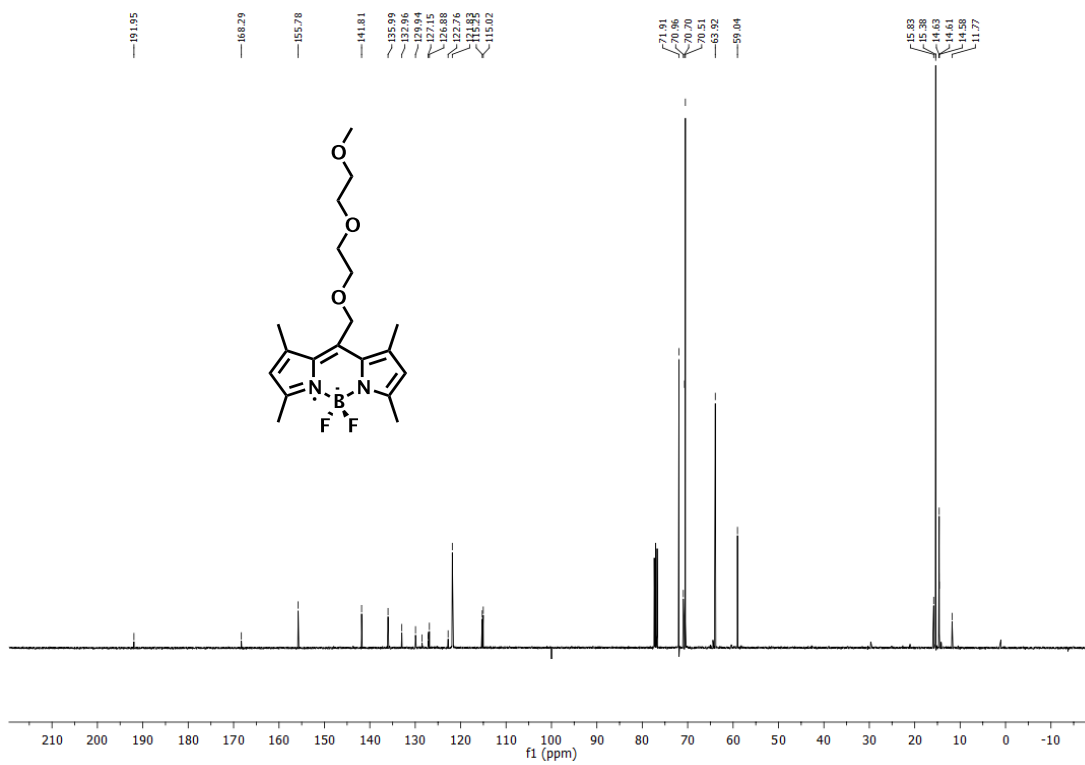


Figure S10: ^{13}C NMR spectrum of Compound 3

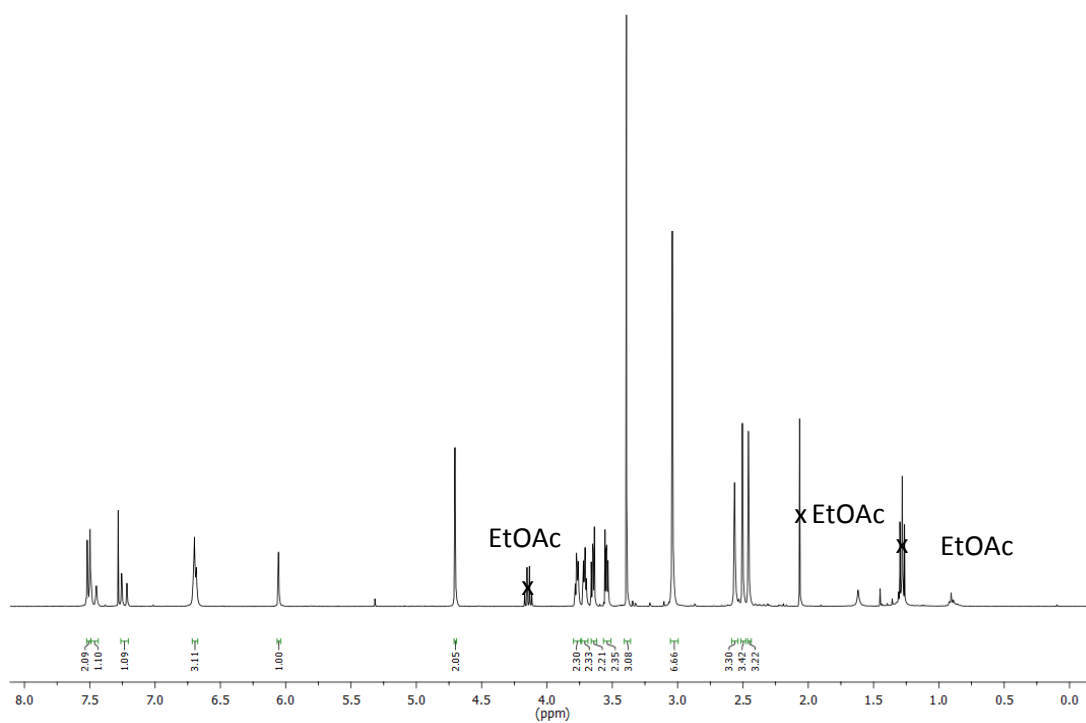


Figure S11: ^1H NMR spectrum of **EUA-4**

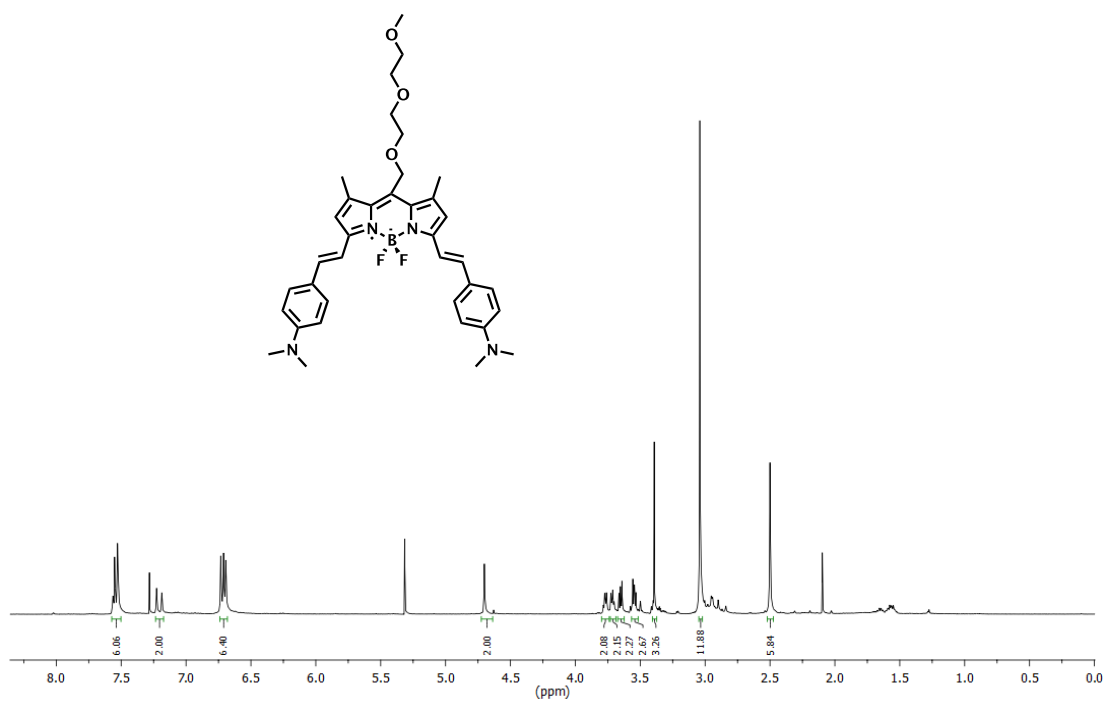


Figure S12: ^1H NMR spectrum of **EUA-5**

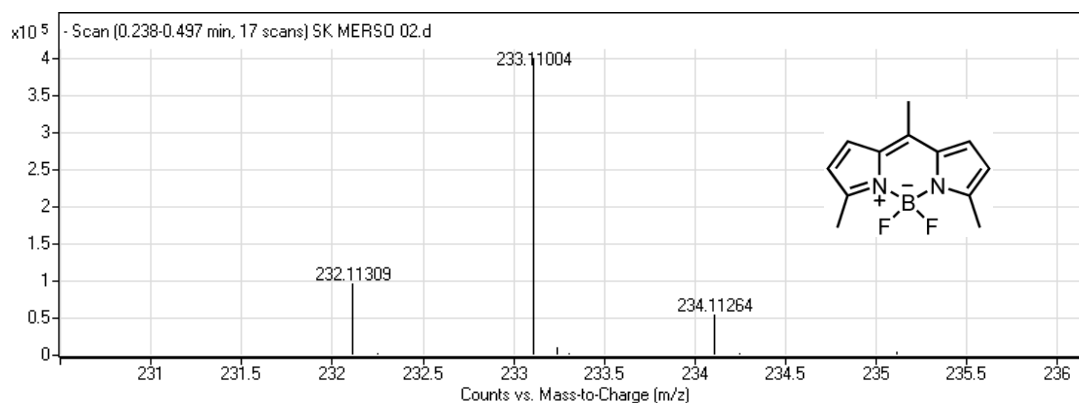


Figure S13: Mass spectrum of Compound 1

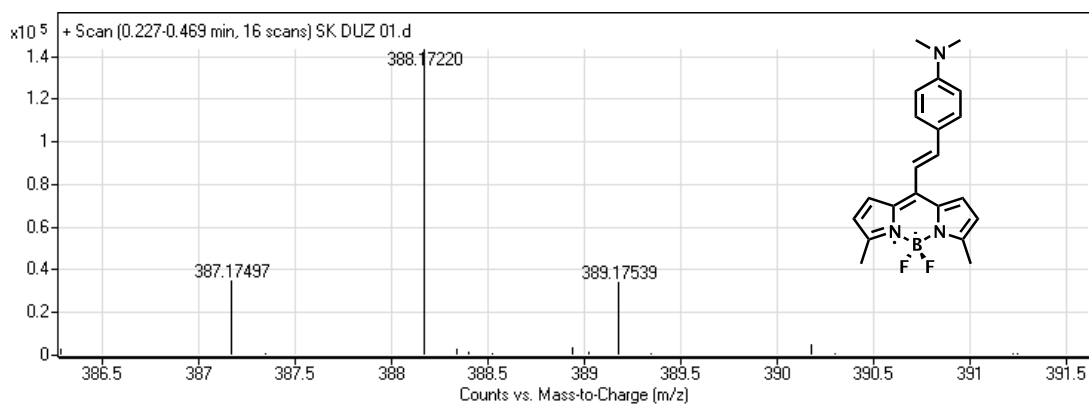


Figure S14: Mass spectrum of EUA-1

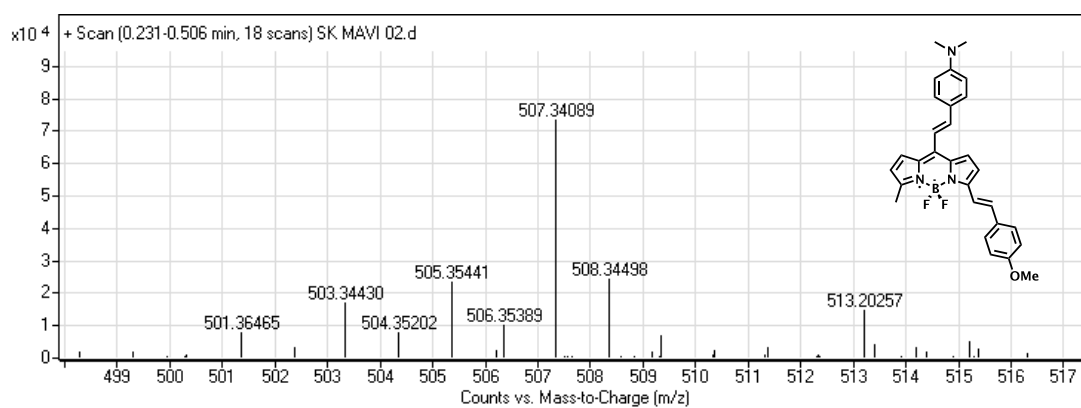


Figure S15: Mass spectrum of EUA-2

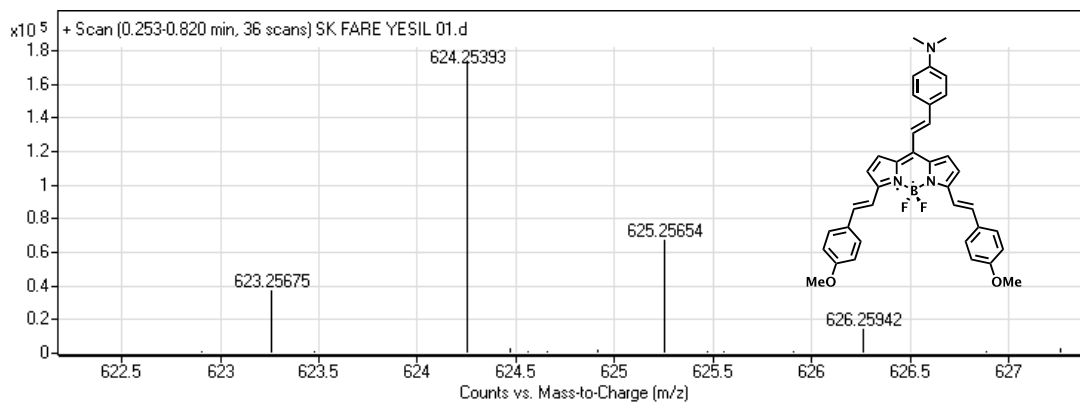


Figure S16: Mass spectrum of **EUA-3**

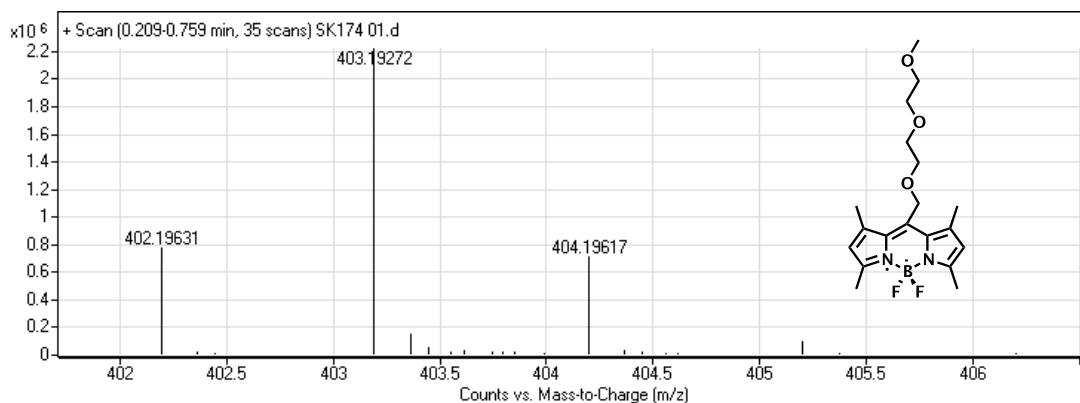


Figure S17: Mass spectrum of **Compound 3**

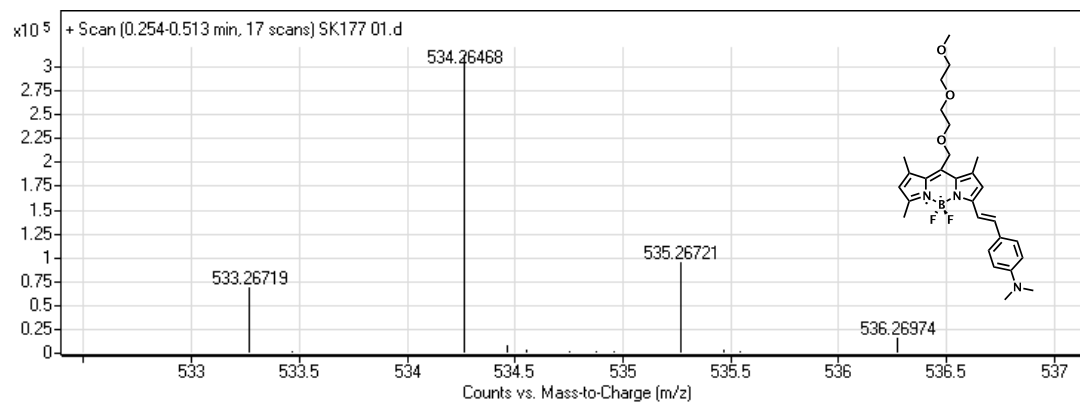


Figure S18: Mass spectrum of **EUA-4**

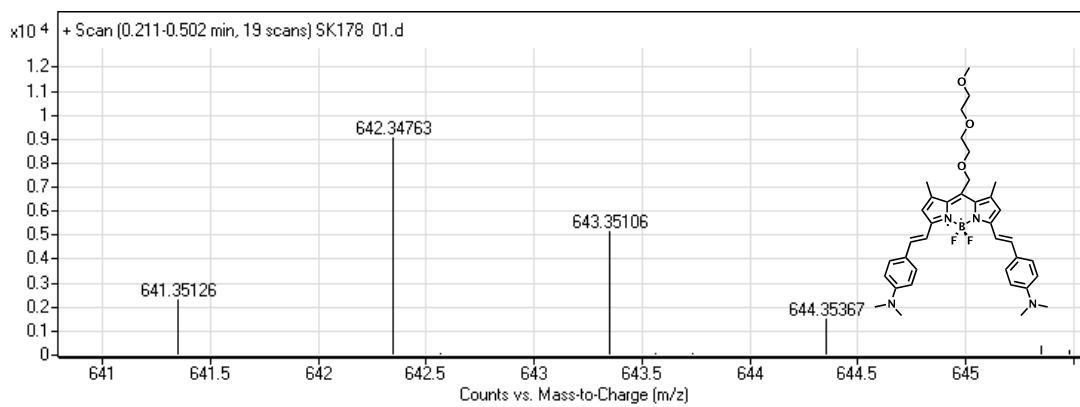


Figure S19: Mass spectrum of **EUA-5**

Measurement and calculation of log P of the probe compounds with HPLC

Column: Cosmosil 5C18-MS-II Waters 4.6x150mm (Nacalai)

Wavelength: 254nm

Mobile phase: MeOH:0.04M Britton-Robinson buffer=5:2 (pH=7.5)

Britton-Robinson buffer: boric acid, acetic acid, phosphate (each 0.04M)

Standards:

t_0 confirmation solution: NaNO₃ 1g/ 50ml H₂O (1)

Benzene 10mg/ 20ml acetonitrile (2)

Bromobenzene 10mg/ 20ml acetonitrile (3)

Hexachlorobenzen 10mg/ 20ml acetonitrile (4)

Biphenyl 10ml/ 50 ml acetonitrile (5)

(5) 5 ml/ 50 ml acetonitrile (5)'

samples:

(1) 1ml, (2)or(3)or(4) 2ml, acetonitrile 7ml (total 10 ml)

(1) 1ml, (5)' 1ml, acetonitrile 8ml (total 10 ml)

(1) 10 ul, 1mM EUA(1-5) 20 ul, acetonitrile 80 ul (total 100ul)

Inject quantity for HPLC: 25 ul

Table. 1 Retention Times and logPow of Standard Reagents

	t_0 (min)	t_R (min)	$k'(t_R-t_0/t_0)$ (min)	logk'	logPow
Benzene	3.233	9.6	1.969	0.294	2.13
Bromobenzen	3.251	15.709	4.832	0.684	2.99
Biphenyl	3.231	33.834	9.472	0.976	3.76
Hexachlorobenzene	3.195	92.301	27.889	1.445	6.18
	(measured)	(measured)	(calculated)	(calc.)	(known)

t_0 : retention time of NaNO₃

t_R : retention time of each compounds

k' : capacity factor

$(t_R-t_0)/t_0$

logk': natural logarithm of k'

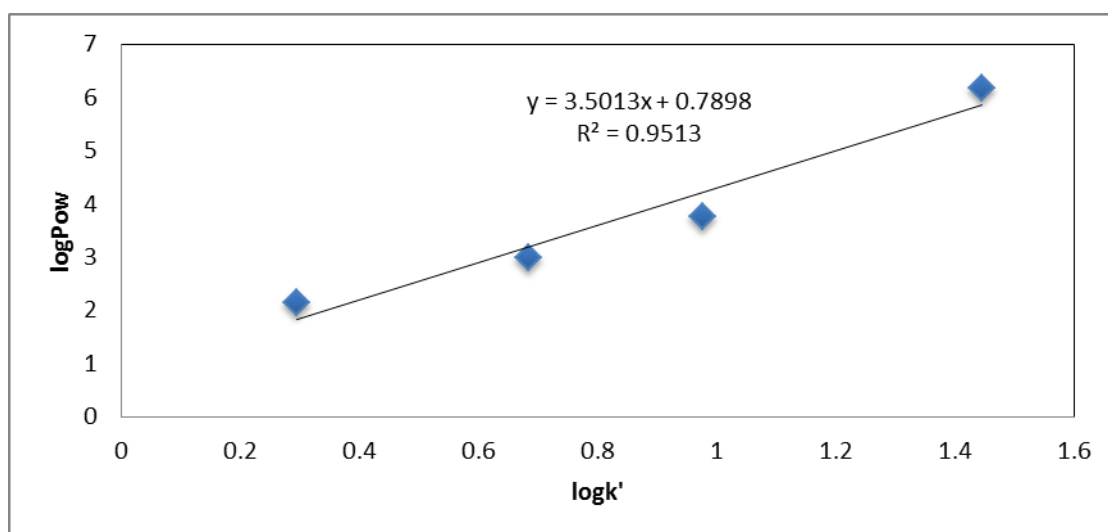


Fig.1 A regression line, $\log\text{Pow}=3.501k'+0.790$ ($r=0.951$) is obtained from data of table 1.

Some of $\text{LogP}_{(\text{HPLC})}$ of **EUA(1-5)** are calculated from the measured and calculated data.

Table. 2 Retention Times and $\log\text{P}(\text{HPLC})$ of BODIPY compounds

	$t_0(\text{min})$	$t_R(\text{min})$	$k'(t_R-t_0/t_0)(\text{min})$	$\log k'$	$\log\text{P}(\text{HPLC})$
EUA1	3.158	116.299	36.827	1.566	6.273
EUA2	3.867	112.753	28.158	1.449	5.863
EUA3	3.885	116.456	28.986	1.462	5.908
EUA4	3.938	111.807	27.392	1.438	5.824
EUA5	3.981	63.909	15.054	1.178	4.914
	(measured)	(measured)	(calculated)	(calc.)	(calc.)

References:

K. Matsumoto., A. Takeyasu., K. Oizumi., and T. Furubayashi
 Studies of Novel 1,4-Dihydropyridine Ca Antagonist CS-905. I.
 Measurement of Partition Coefficient (LogP)
 by High Performance Liquid Chromatography (HPLC)
 YAKUGAKU ZASSHI 115(3)213-220 (1995)