

# Nerve Targeting via Myelin Protein Zero and the Impact of Dimerization on Binding Affinity

Nataliia Berehova <sup>1</sup>, Tessa Buckle <sup>1</sup>, Maarten P. van Meerbeek <sup>1</sup>, Anton Bunschoten <sup>2</sup>,  
Aldrik H. Velders <sup>2</sup>, and Fijs W.B. van Leeuwen <sup>1,2,\*</sup>

<sup>1</sup> Interventional Molecular Imaging Laboratory, Department of Radiology, Leiden University Medical Center, Albinusdreef 2, 2300 RC Leiden, The Netherlands

<sup>2</sup> Laboratory of BioNanoTechnology, Wageningen University & Research, Bornse Weiland 9, 6708 WG Wageningen, The Netherlands

\* Correspondence: f.w.b.van\_leeuwen@lumc.nl

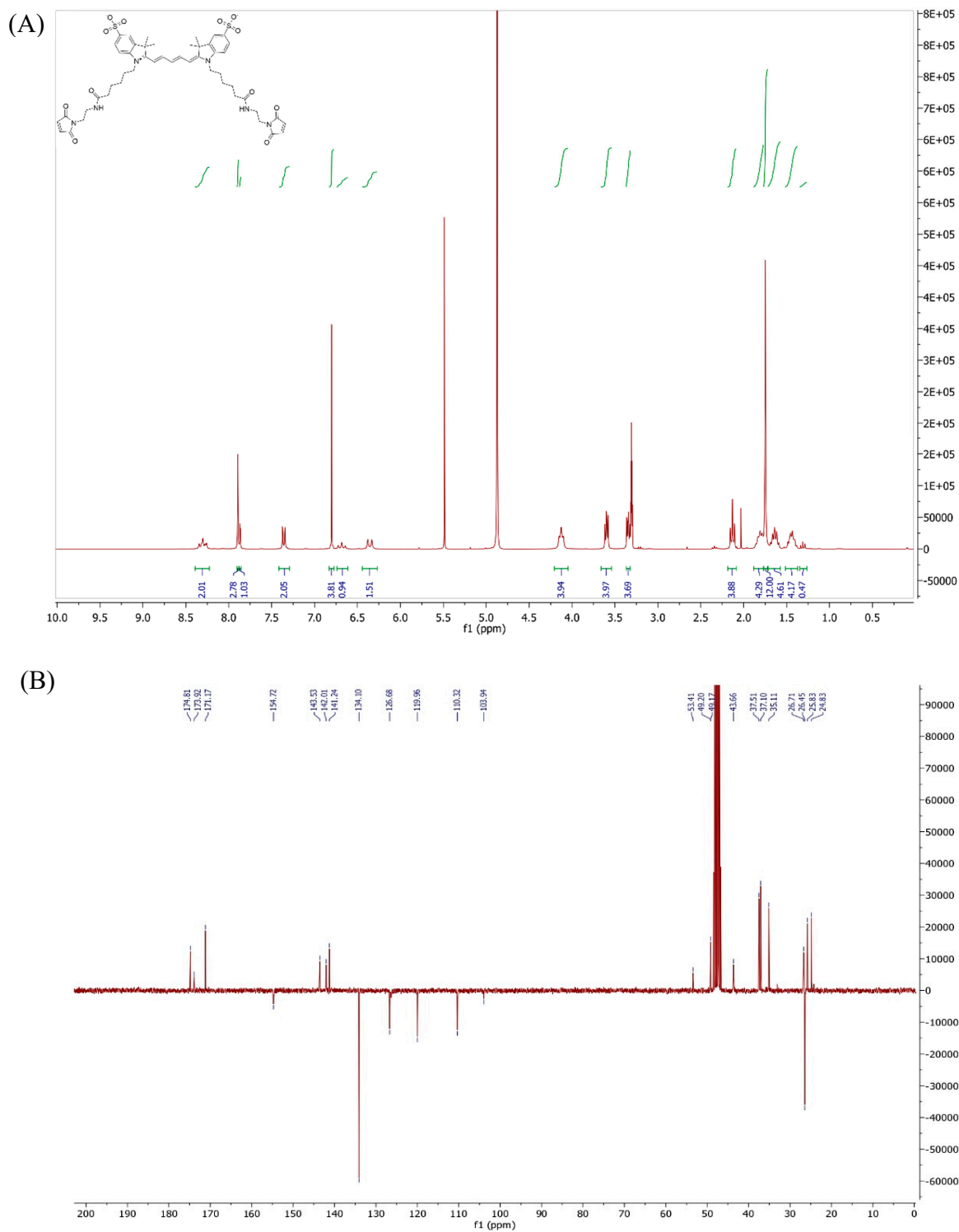
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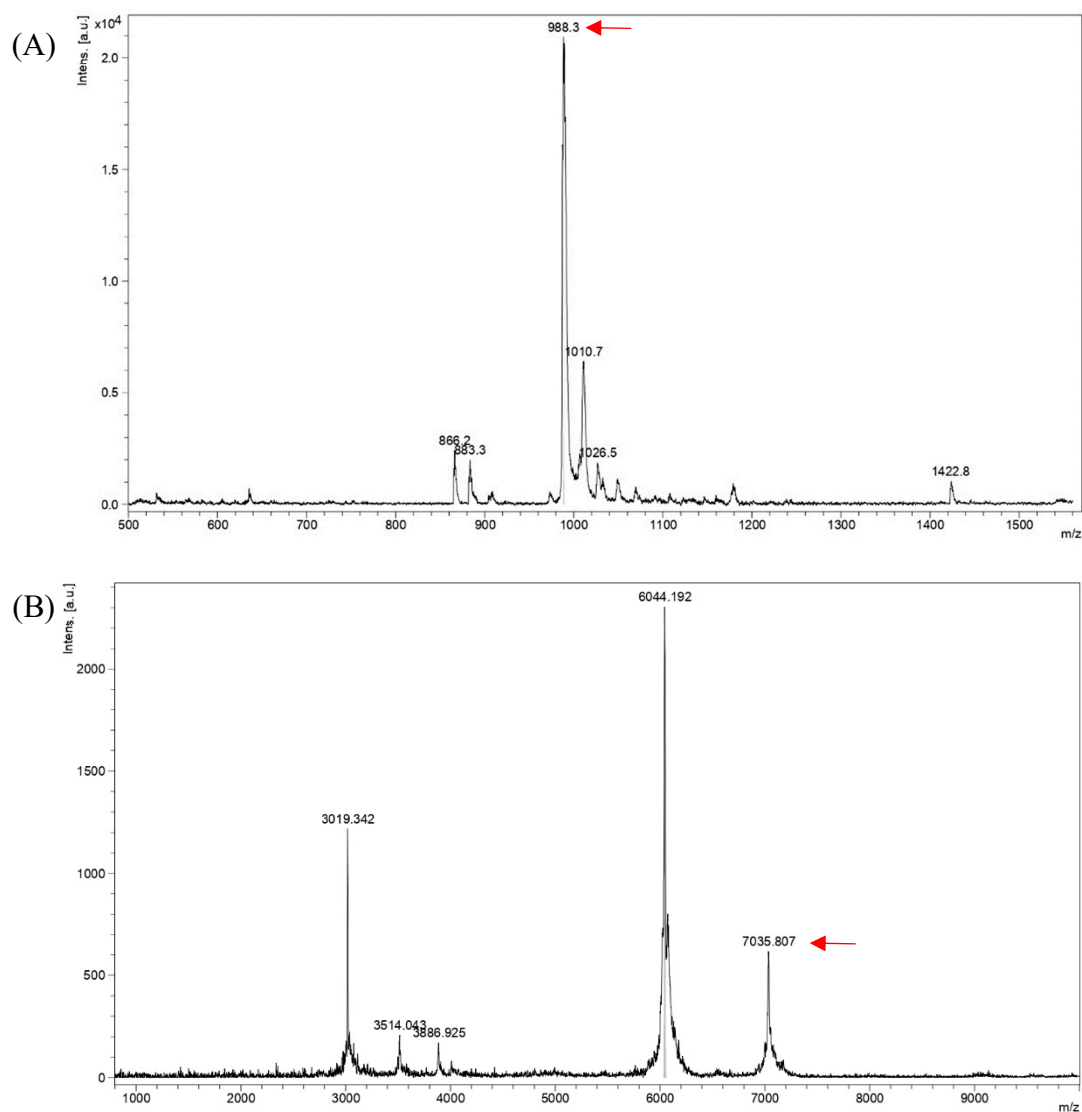
**Figure S2:** MALDI-TOF mass spectra of *Maleimide-(SO<sub>3</sub>)Cy5(SO<sub>3</sub>)-Maleimide (1)* and *Cy5-(P0<sub>101-125</sub>)<sub>2</sub> (2)*

**Figure S3:** <sup>1</sup>H NMR spectra of *Cy5-P0<sub>101-125</sub>* in D<sub>2</sub>O and *Cy5-(P0<sub>101-125</sub>)<sub>2</sub>* in D<sub>2</sub>O and DMSO

**Figure S4:** Concentration dependent stacking behavior of *Cy5-P0<sub>101-125</sub>* and *Cy5-(P0<sub>101-125</sub>)<sub>2</sub>* and corresponding free dyes measured in H<sub>2</sub>O.



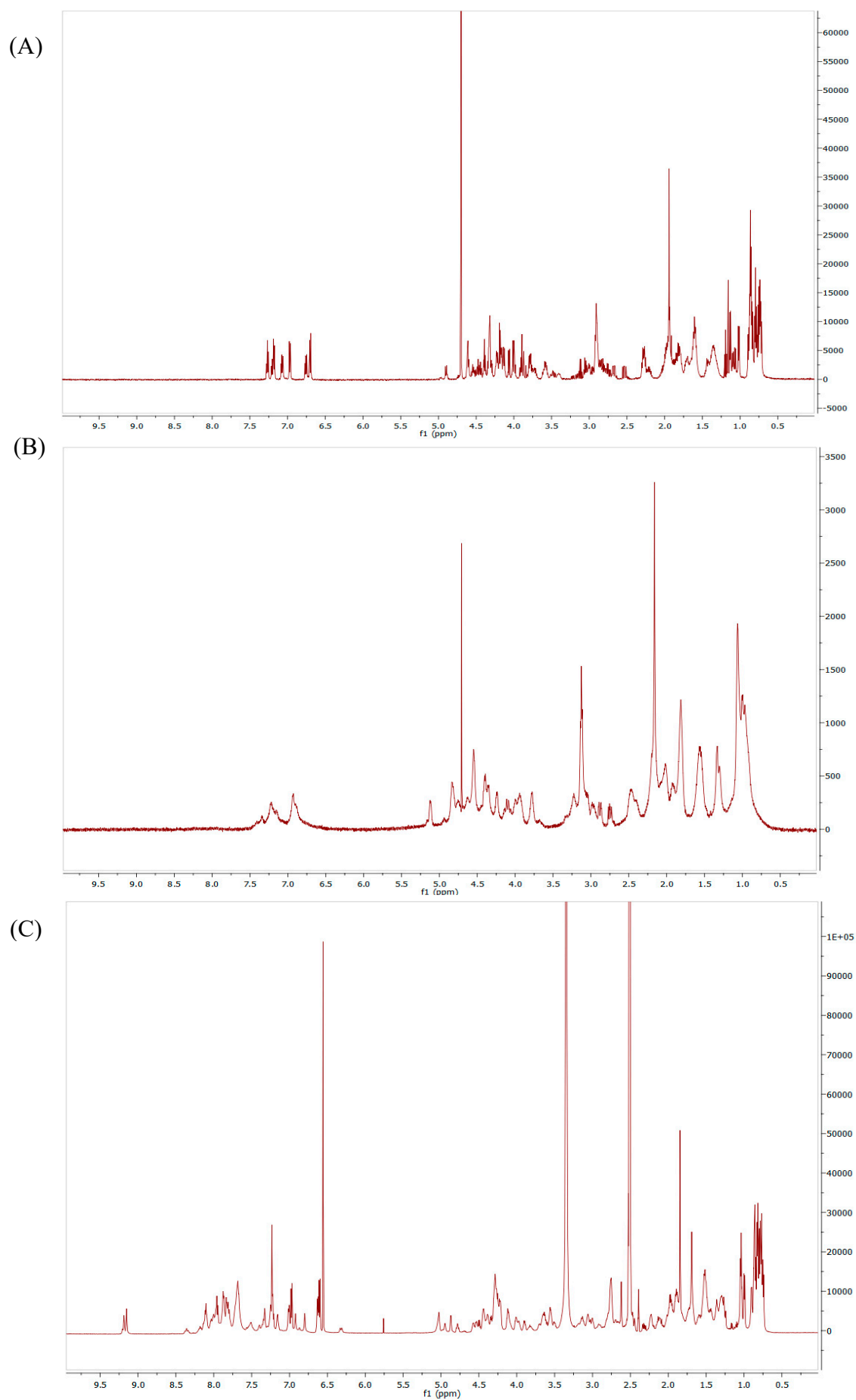
**Figure S1: NMR characterization of Maleimide-(SO<sub>3</sub>)Cy5(SO<sub>3</sub>)-Maleimide (1).** (A) <sup>1</sup>H NMR spectra (300MHz, MeOD); (B) <sup>13</sup>C NMR spectra (75 MHz, MeOD).



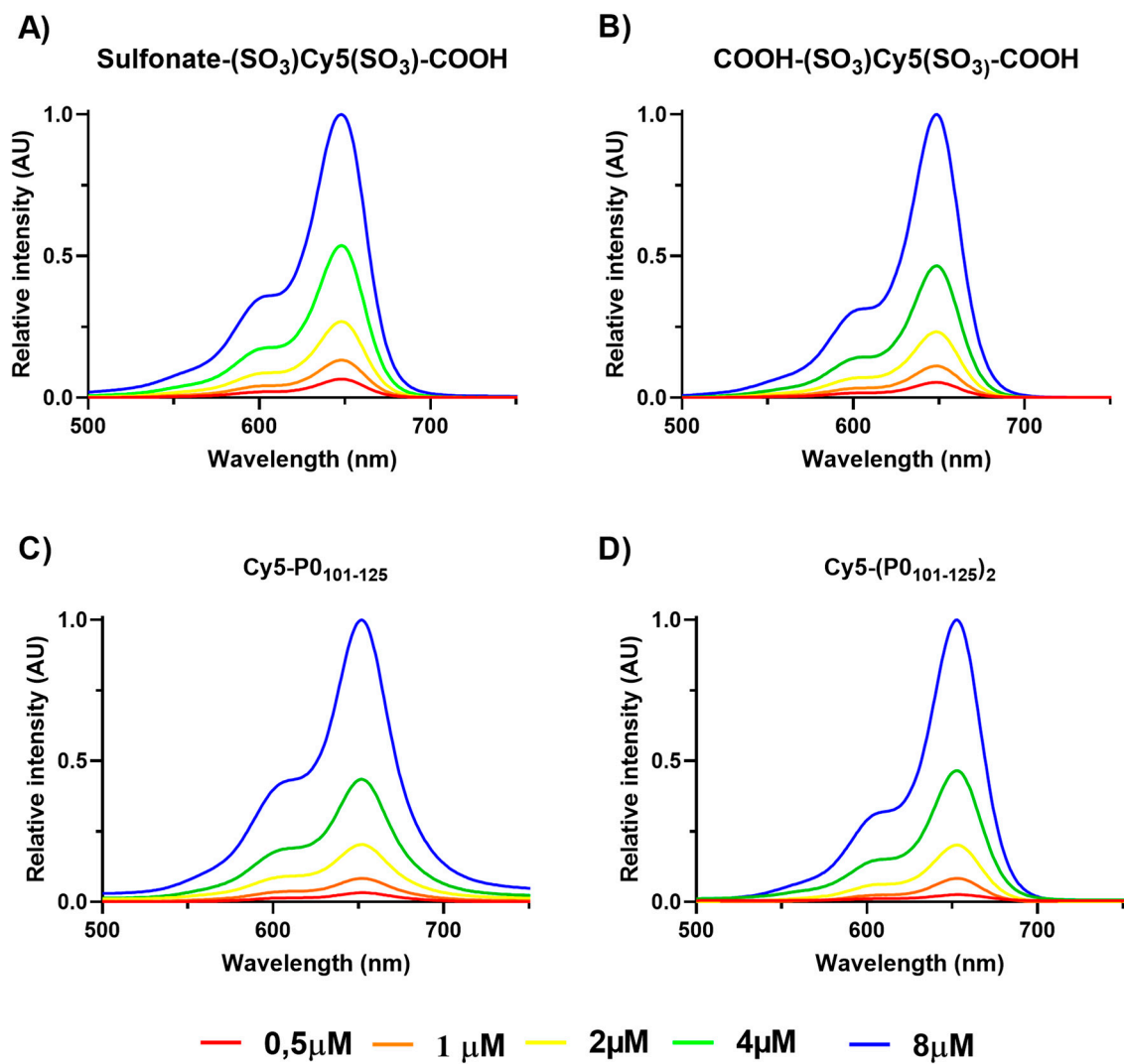
**Figure S2: MALDI-TOF mass spectra of (A) Maleimide-(SO<sub>3</sub>)Cy5(SO<sub>3</sub>)-Maleimide - 988.3 (1) and (B) Cy5-(P<sub>0101-125</sub>)<sub>2</sub> – 7035,8 (2).**

Others MS peaks in Figure S2 (A) can be contributed to: 1) side products : 866,2 - Maleimide-(SO<sub>3</sub>)Cy5(SO<sub>3</sub>)-COOH, 2) Maleimide-(SO<sub>3</sub>)Cy5(SO<sub>3</sub>)-Maleimide + salts : 1010,7 - Maleimide-(SO<sub>3</sub>)Cy5(SO<sub>3</sub>)-Maleimide and Na<sup>+</sup> and 1026,5 - Maleimide-(SO<sub>3</sub>)Cy5(SO<sub>3</sub>)-Maleimide and K<sup>+</sup>, and 3) 1422.8 – matrix (reference peak).

Others MS peaks in Figure S2 (B): 3019.3 – free P<sub>0101-125</sub> peptide peak; 6044,19 – mass of two P<sub>0101-125</sub> peptides.



**Figure S3.**  $^1\text{H}$  NMR spectra of (A)  $\text{Cy5-P0}_{101-125}$  (600MHz,  $\text{D}_2\text{O}$ ), (B)  $\text{Cy5-(P0}_{101-125})_2$  (600MHz,  $\text{D}_2\text{O}$ ), (C)  $\text{Cy5-(P0}_{101-125})_2$  (600MHz, DMSO).



**Figure S4.** Concentration dependent stacking behavior of **Cy5-P0<sub>101-125</sub>** and **Cy5-(P0<sub>101-125</sub>)<sub>2</sub>** and corresponding free dyes measured in H<sub>2</sub>O.