

A highly selective fluorescent chemosensor for Al³⁺ imaging in living cells *via* through-bond energy transfer

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1. Fig. S1

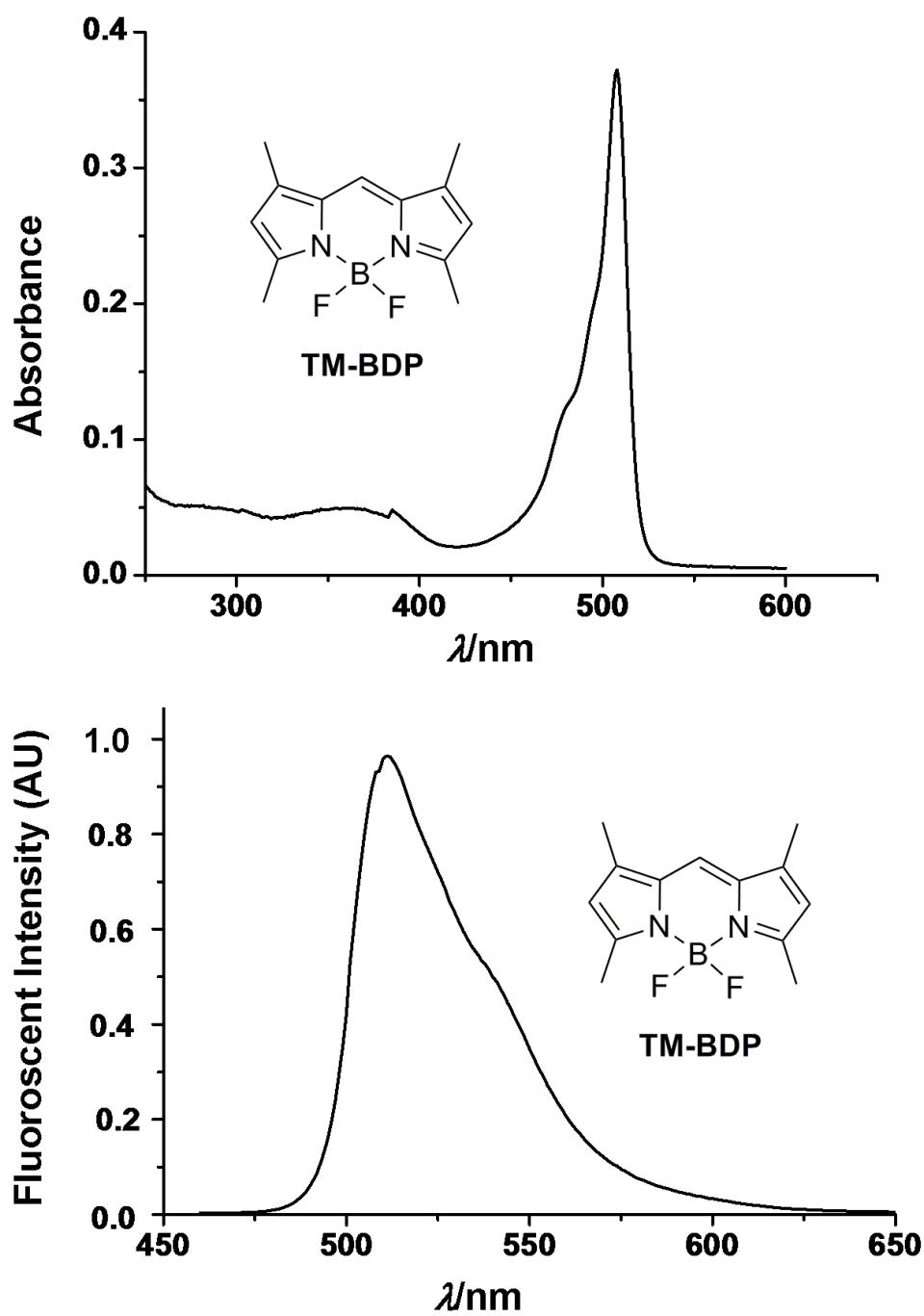


Fig. S1 The spectra of absorption and fluorescence of **TM-BDP** ($\lambda_{\text{abs}} = 508$ nm; $\lambda_{\text{em}} = 511$ nm) in MeOH/H₂O (v/v = 1: 1).

2. Fig. S2

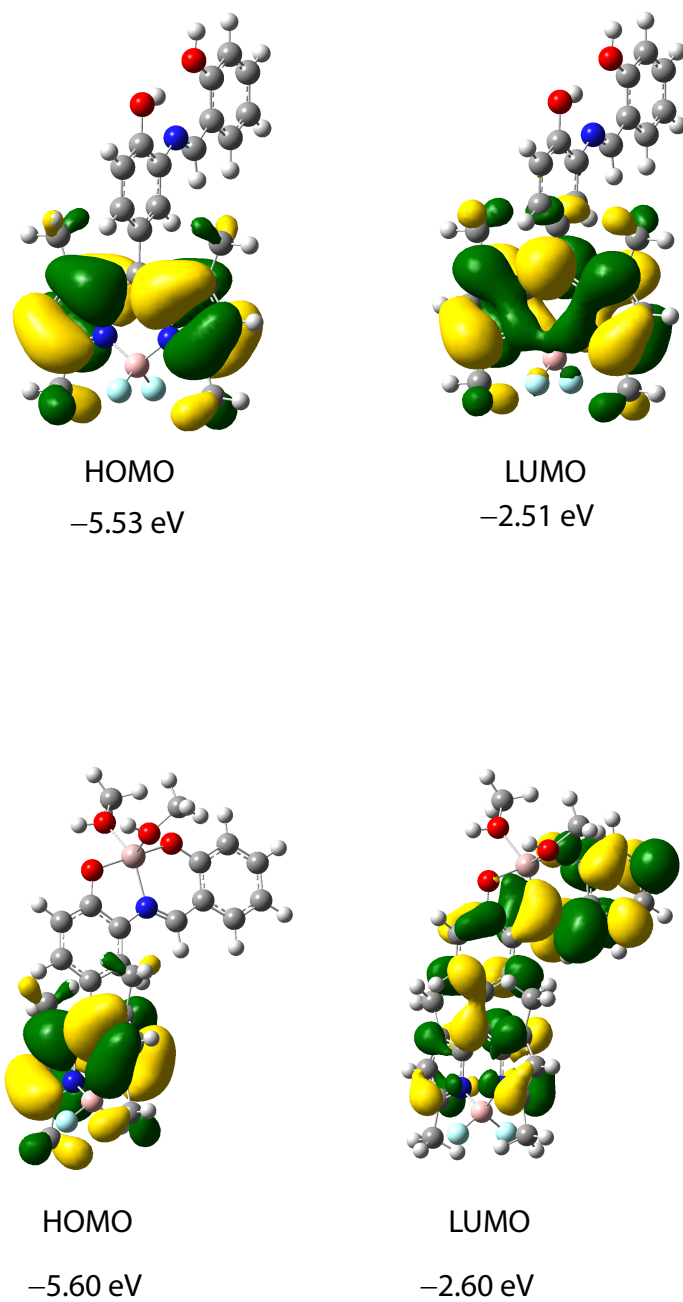


Fig. S2 HOMO and LUMO of **PSI-BDP** (upper row) and **PSI-BDP+ Al³⁺** (bottom row). Calculated at B3LYP/6-31G(d) level with Gaussian 09W. MeOH was used as solvent.¹

3. Fig. S3

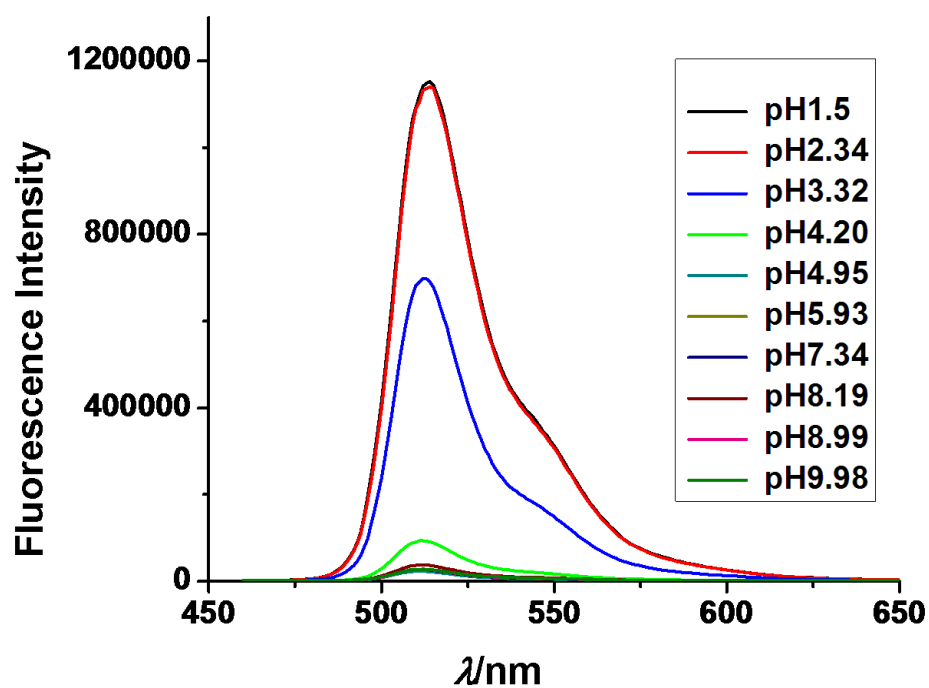


Fig. S3 Effect of pH on fluorescence intensity of **PSI-BDP** (1 μM) in MeOH/H₂O (v/v = 1:1). $\lambda_{em} = 513$ nm. $\lambda_{ex} = 450$ nm.

4. Fig. S4

Print of window 80: MS Spectrum

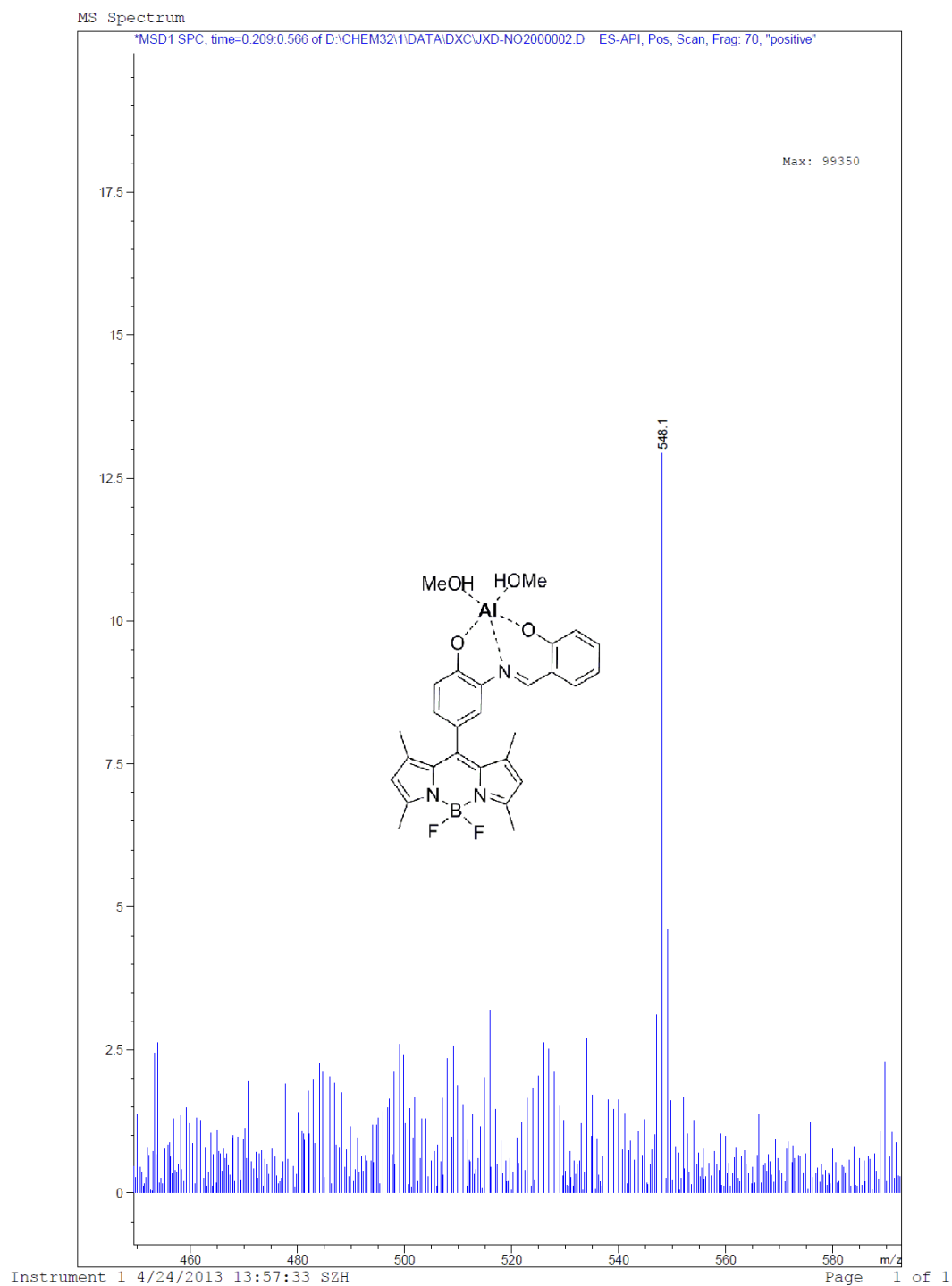
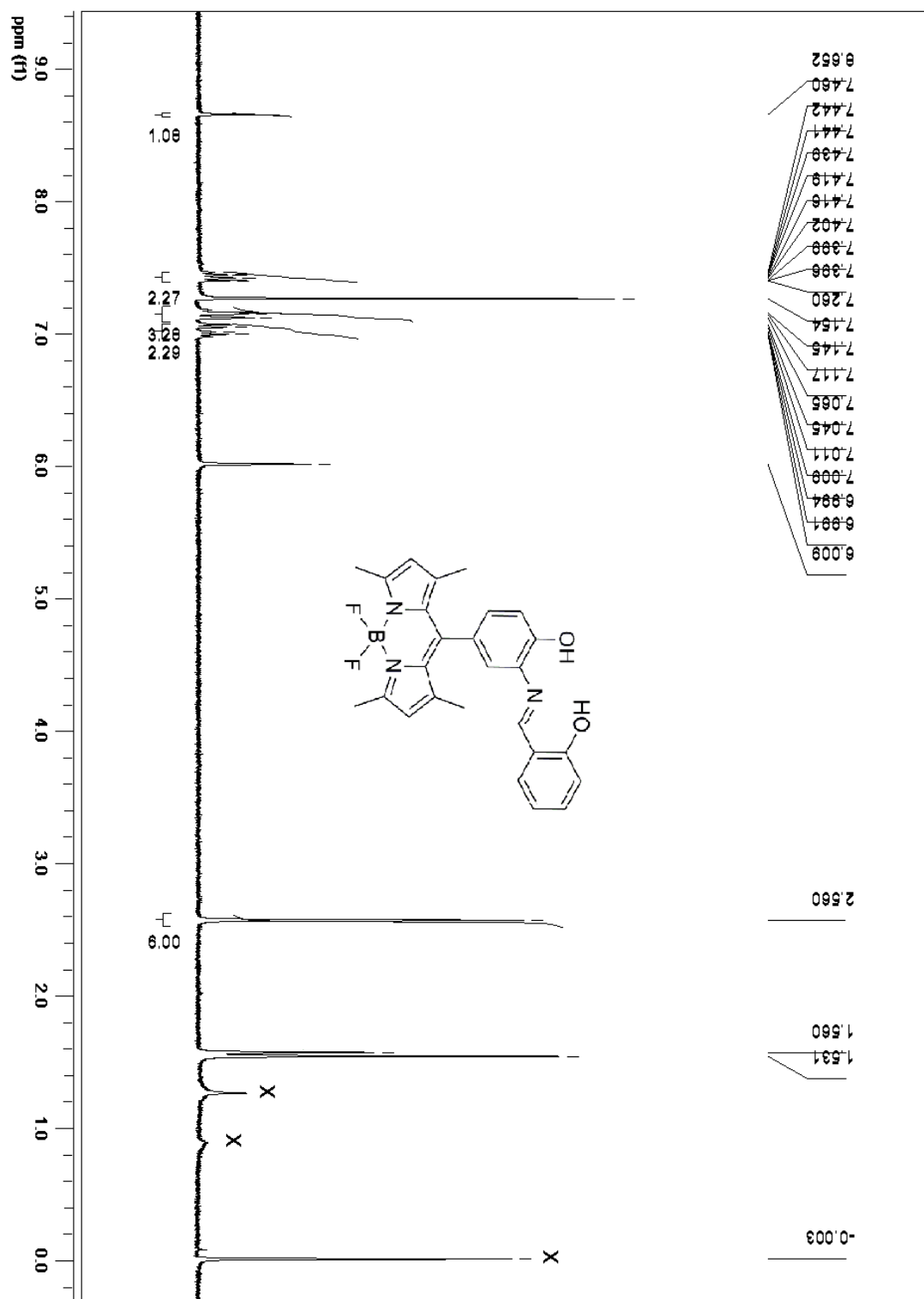
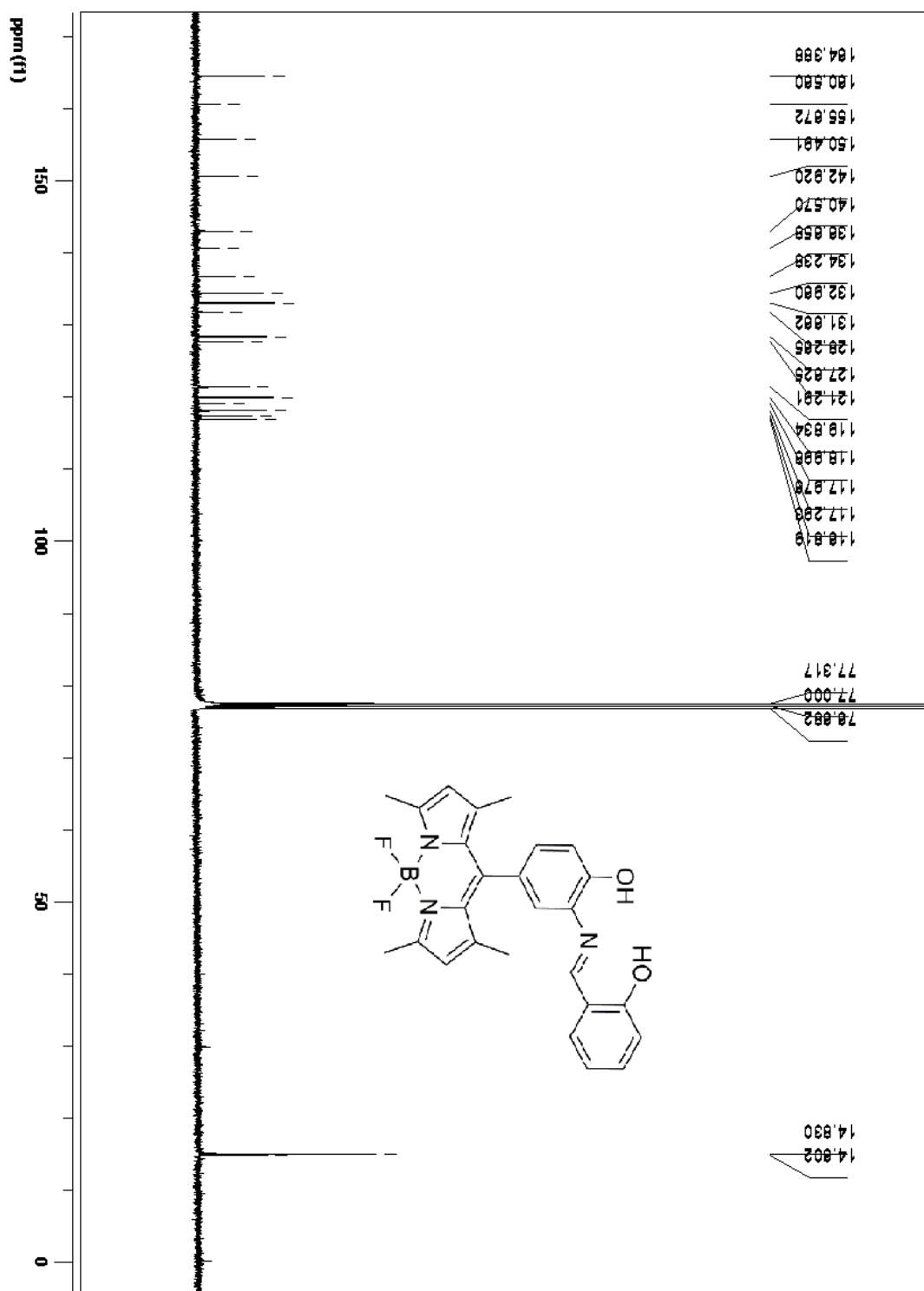


Fig. S4 Positive-ion electrospray ionization mass spectrum of **PSI-BDP** upon addition of $\text{Al}(\text{NO}_3)_3$ (1 equiv) in CH_3OH .

5. NMR of PSI-BDP



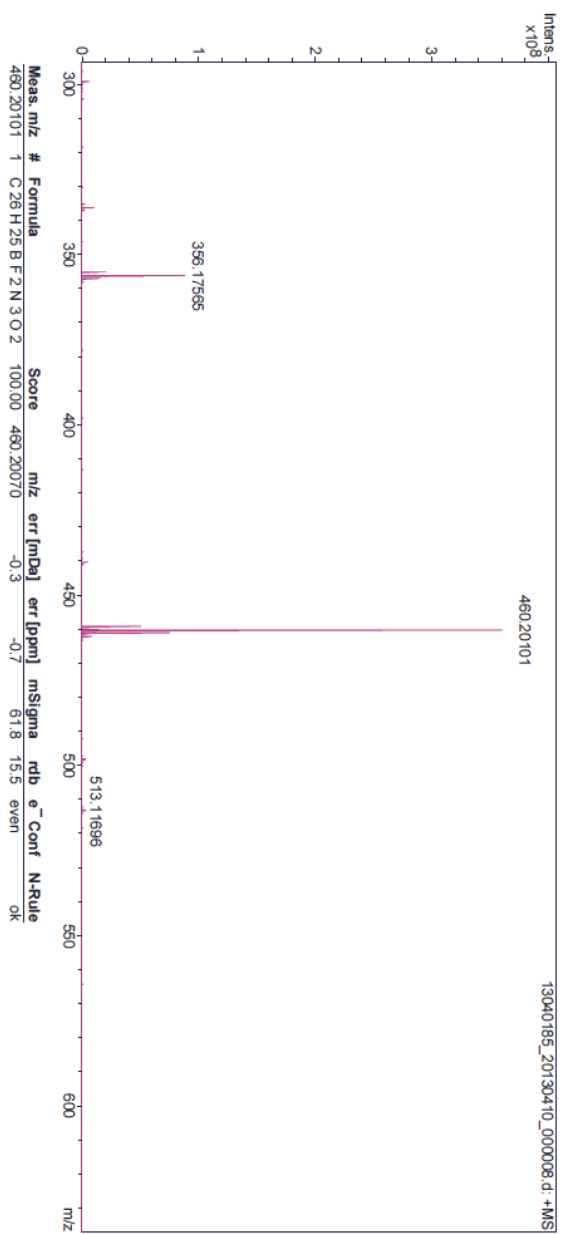


^{13}C NMR of PSI-BDP

6. HRMS of PSI-BDP

Peking University Mass Spectrometry Sample Analysis Report

Analysis Info	
Analysis Name	13040185_20130410_000008.d
Sample	BDP
Comment	ESI Positive
Acquisition Date	4/10/2013 3:17:56 PM
Instrument	Bruker Apex IV FTMS
Operator	Peking University



7 References

1. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A., Jr. Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, *Gaussian 09W*, revision A.1; Gaussian Inc.: Wallingford, CT, 2009.