***Supporting information for***

# Rapid Synthesis of a BODIPY Derivative Serving as a Highly Selective and Sensitive Fluorescence Chemosensor for $Hg^{2+}$ Ion Detection

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## NMR spectra

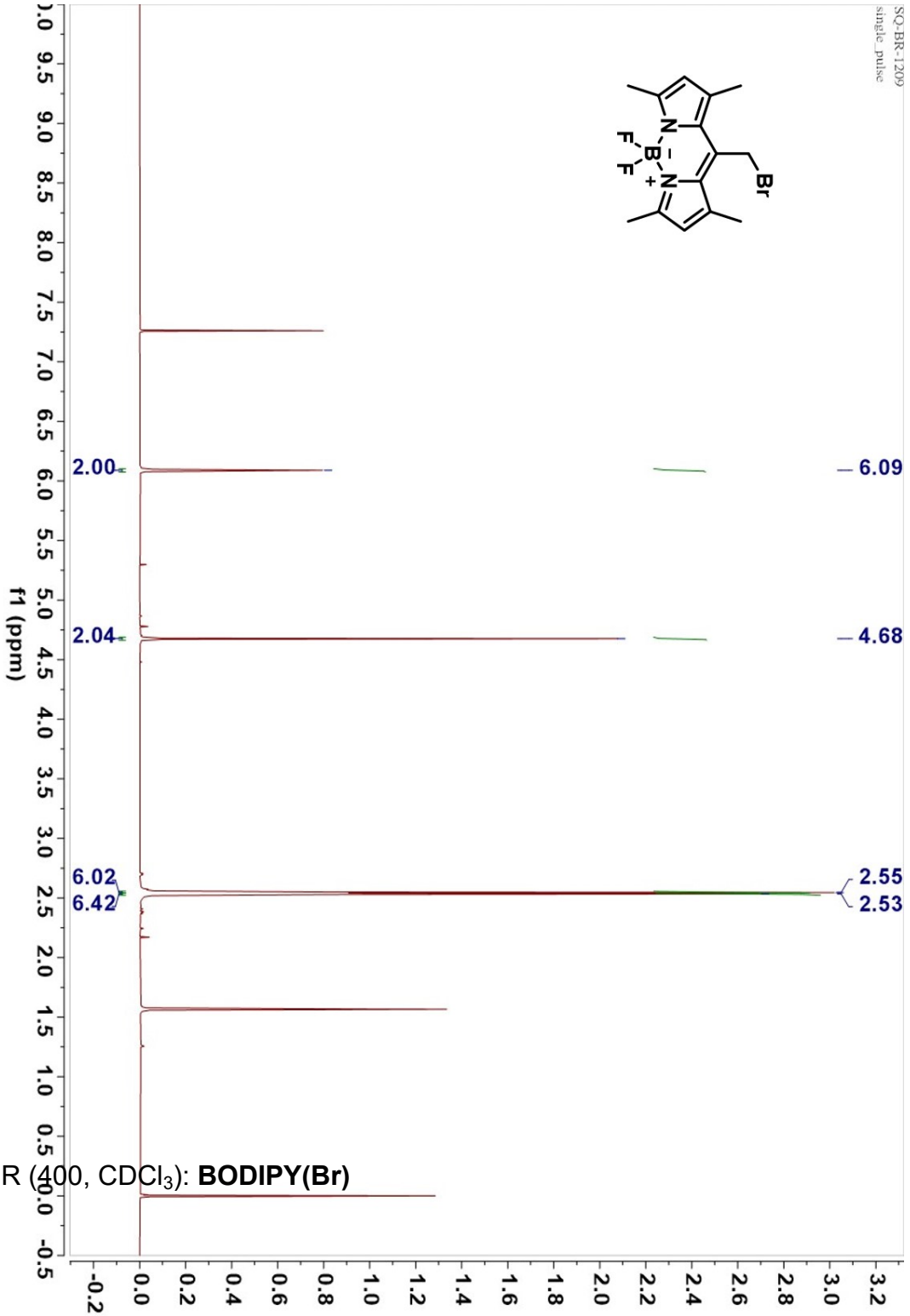



**Figure S1.** $^{1}H$ NMR (400, $CDCl_3$): **BODIPY(Br)**

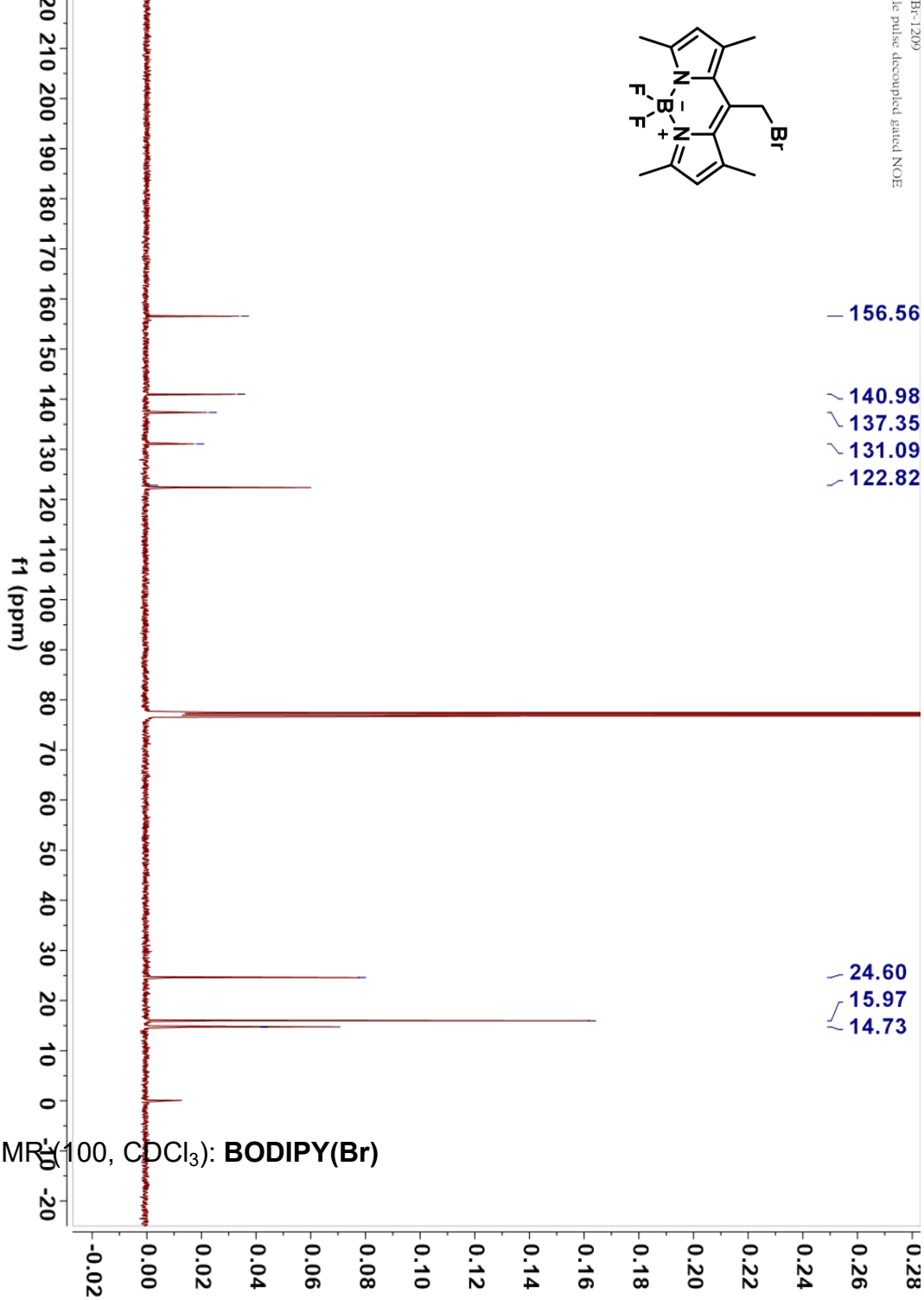



**Figure S2.** $^{13}C$ NMR (100, $CDCl_3$): **BODIPY(Br)**

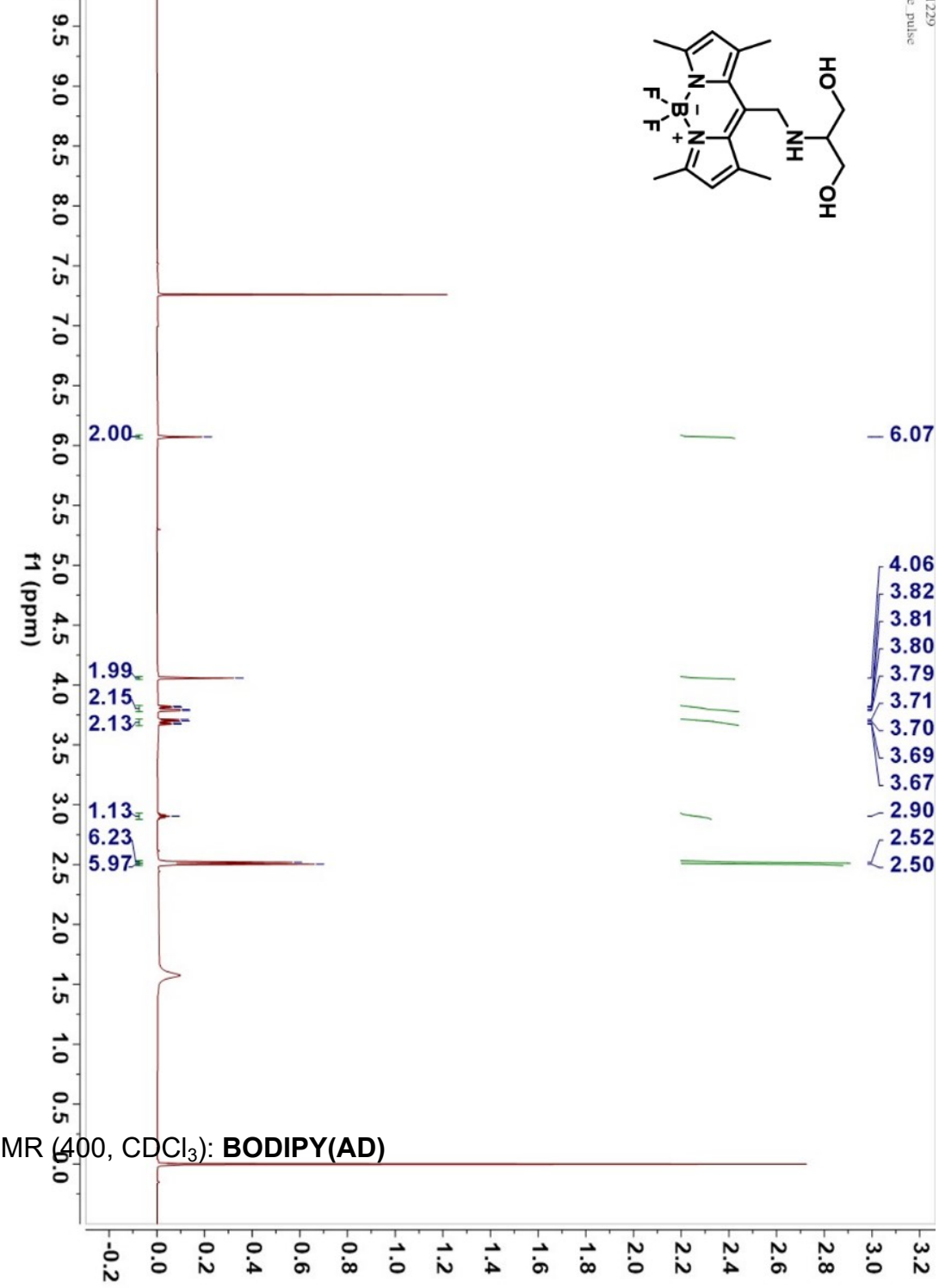



**Figure S3.** $^{1}H$ NMR (400, $CDCl_3$): **BODIPY(AD)**

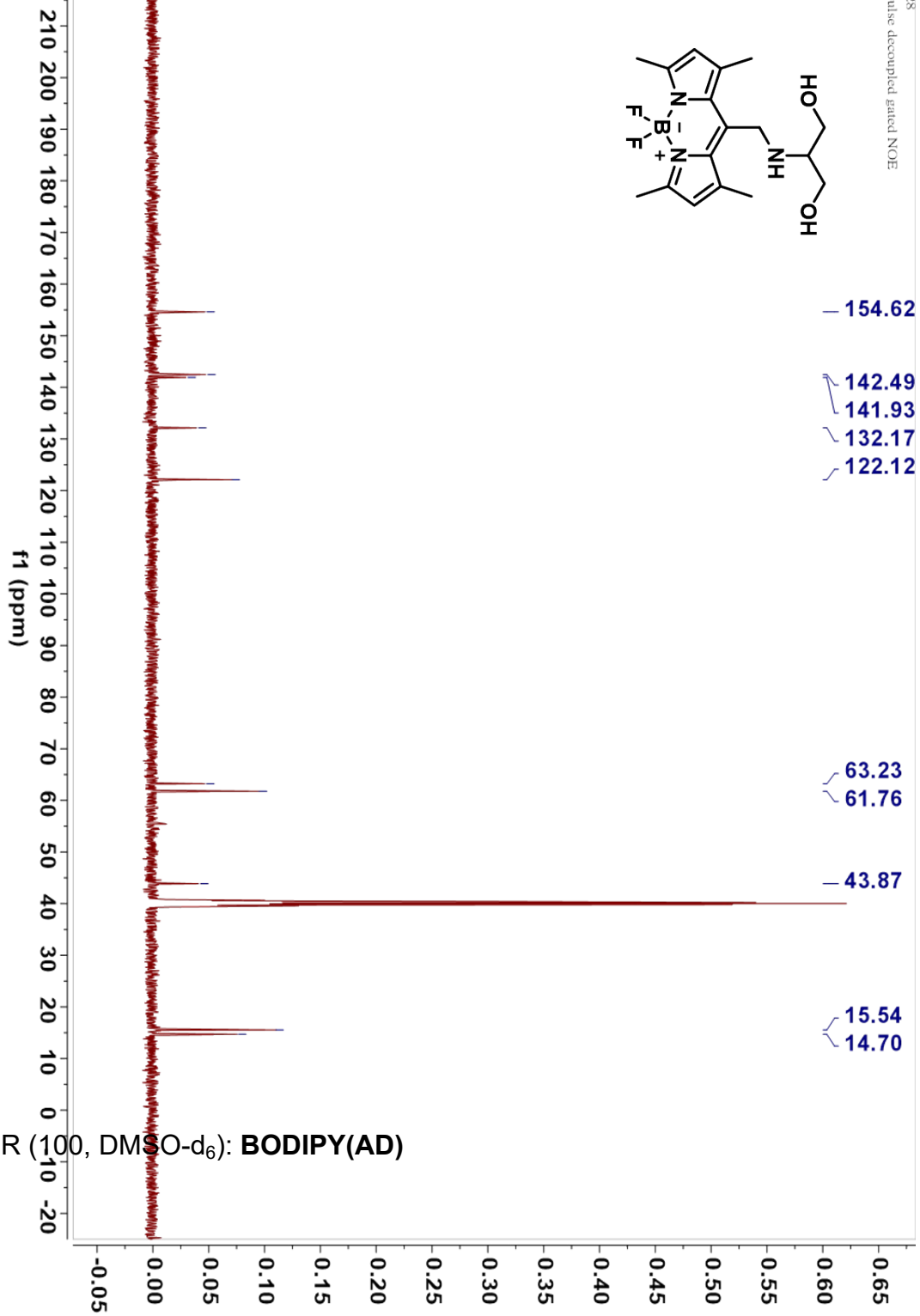
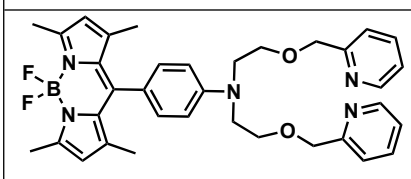
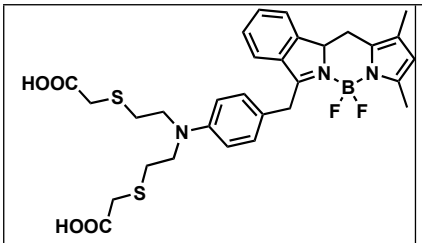
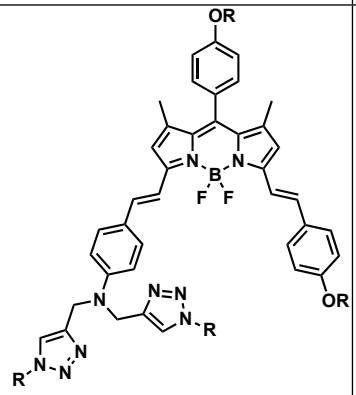
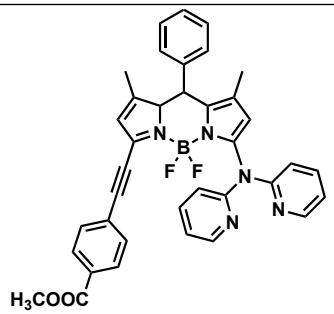
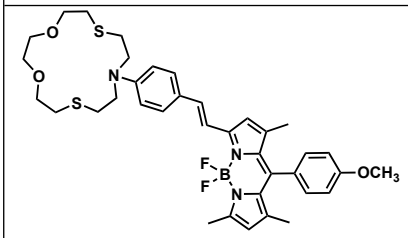
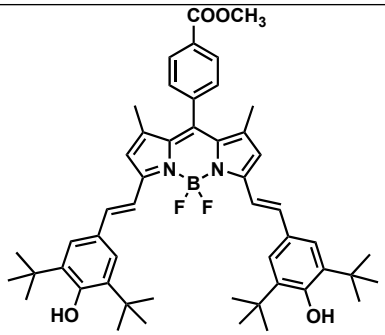



**Figure S4.** $^{13}C$ NMR (100, DMSO-$d_6$): **BODIPY(AD)**

**Table S1.** Recent BODIPY-based fluorophores for detecting Hg(II) ions.

| Structures | Detection Limit | Number of Synthetic Steps | Reaction time and overall yield | References |
|---|---|---|---|---|
|  | 0.18 μM | 4 steps | 48 h, 17.8% | 1 |

| | | | | |
|---|---|---|---|---|
|  | 5.7 nM | 7 steps | 76 h, 9.2% | 2 |
|  | 0.09 μM | 4 steps | 53 h, 1.5% | 3 |
|  | 0.07 μM | 5 steps | 70 h, 7.6% | 4 |
|  | 99 ppm | 3 steps | 6.5 h, 7.9% | 5 |
|  | 0.7 μM | 2 steps | 19 h, 16.8% | 6 |

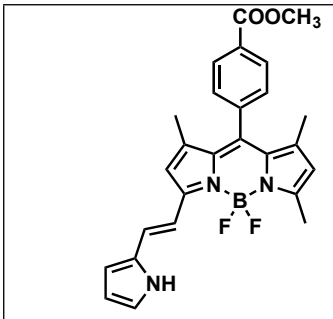
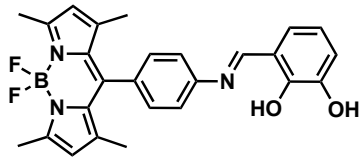
| | | | | |
|---|---|---|---|---|
|  | 0.05 μM | 2 steps | 22 h, 3.4% | 7 |
|  | 0.9 μM | 3 steps | 36 h, 24.0% | 8 |

**Table S2.** Crystal data and structure refinement for BODIPY(AD)

| | |
|---|---|
| Identification code | K10911-CHL-A(SQ-dioxide) |
| Empirical formula | $C_{34}H_{48}B_2F_4N_6O_4$ |
| Formula weight | 704.42 |
| Temperature/K | 113(2) |
| Crystal system | monoclinic |
| Space group | $P2_1/n$ |
| a/Å | 9.00305(16) |

| | |
|---|---|
| b/Å | 17.8739(4) |
| c/Å | 21.0833(3) |
| α/° | 90 |
| β/° | 91.3815(15) |
| γ/° | 90 |
| Volume/Å$^3$ | 3391.73(10) |
| Z | 4 |
| $\rho_{calc}$mg/mm$^3$ | 1.379 |
| μ/mm$^{-1}$ | 0.105 |
| F(000) | 1496.0 |
| Crystal size/mm$^3$ | 0.15 × 0.15 × 0.13 |
| 2Θ range for data collection | 4.558 to 50° |
| Index ranges | -10 ≤ h ≤ 10, -19 ≤ k ≤ 21, -25 ≤ l ≤ 25 |
| Reflections collected | 32271 |
| Independent reflections | 5960[R(int) = 0.0325] |
| Data/restraints/parameters | 5960/0/475 |
| Goodness-of-fit on F$^2$ | 1.045 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0435, $wR_2$ = 0.1160 |
| Final R indexes [all data] | $R_1$ = 0.0537, $wR_2$ = 0.1212 |
| Largest diff. peak/hole / e Å$^{-3}$ | 0.73/-0.67 |
| CCDC number | 2272046 |

**Table S3.** Absorption and fluorescence data of BODIPY(AD).

| Solvents | $\lambda_{ab}$ (nm) | Ɛ (L/mol·cm) | $\lambda_{em}$ (nm) | Φ[a] | $\Delta_{st}$ (cm$^{-1}$) | Ɛ[b] |
|---|---|---|---|---|---|---|
| Toluene | 512 | 66000 | 522 | 84.5% | 374 | 2.38 |
| DCM | 511 | 111800 | 520 | 51.2% | 338 | 8.93 |
| Acetone | 506 | 86400 | 513 | 1.96% | 307 | 20.7 |
| MeOH | 506 | 101600 | 515 | 6.85% | 345 | 32.7 |
| DMSO | 508 | 78600 | 522 | 6.48% | 528 | 46.68 |

| | | | | | | |
|---|---|---|---|---|---|---|
| DMSO ($Hg^{2+}$) | 520 | 54900 | 536 | 118% | 574 | 46.68 |

*a*: The Φ of DCM was absolute quantum yield, and the Φ of the others were relative quantum yields by using the DCM sample as standard. *b*: Dielectric constant of each solvent

## Computational data

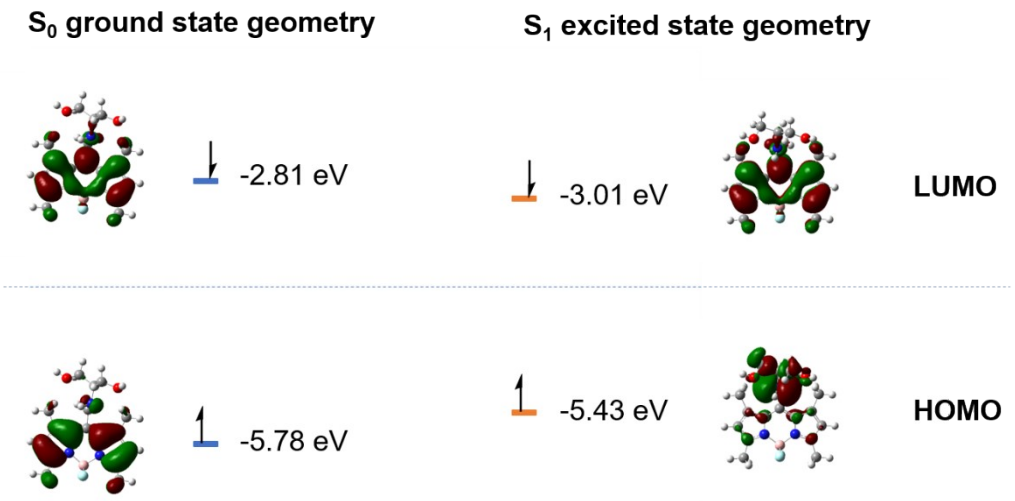



**Figure S5.** TD-DFT calculations for BODIPY(AD) in DMSO. The dominant configuration of $S_1$ excited states at $S_0$ ground state geometry (left) and at $S_1$ excited state geometry (right) showed that ICT process occurred when the molecule was excited. The poor overlap of wavefunctions between the excited state and the ground state at $S_1$ geometry caused the diminishment of fluorescence.

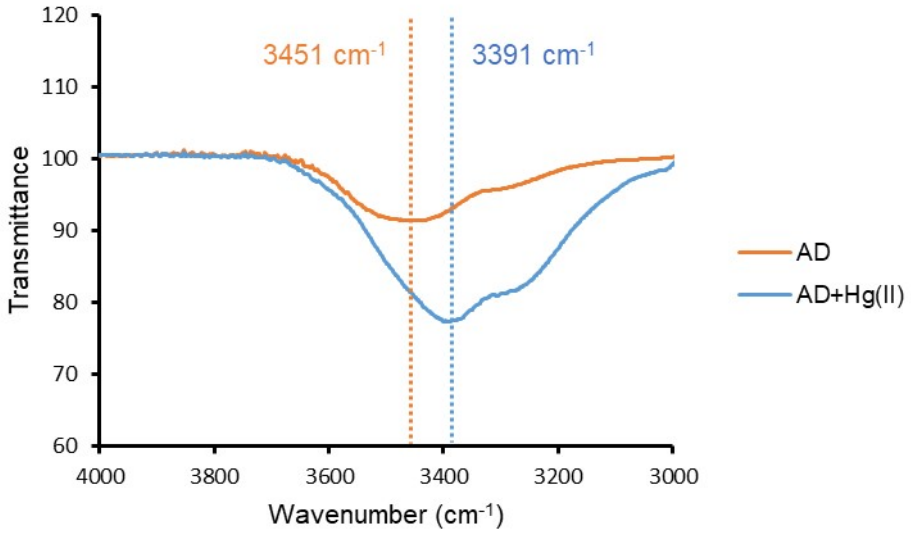



**Figure S6.** FI-IR spectra demonstrated that N-H and O-H peak shifted after adding $Hg^{2+}$ ion to BODIPY(AD).

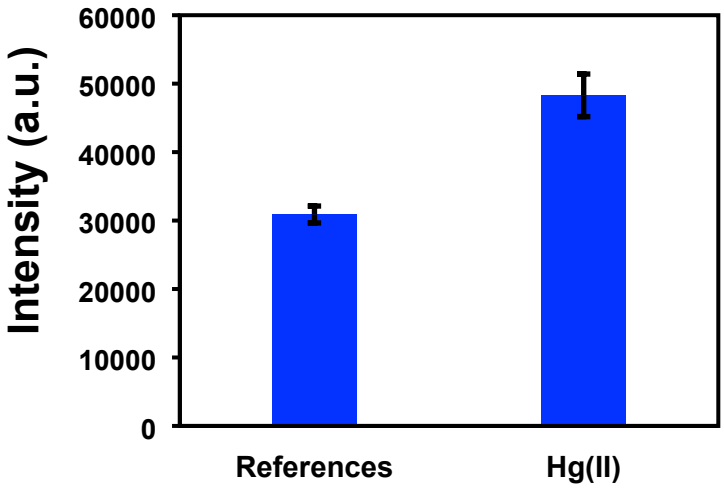



**Figure S7.** Fluorescence of BODIPY(AD) in the buffer solution with and without $Hg^{2+}$ ions.

## References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