

## Supporting Information for

### **Achieving tricolor luminescence switching from a stimuli-responsive luminophore based on bisarylic methanone derivative**

Xiucun Feng,<sup>a</sup> Ningning Zhou,<sup>a</sup> Hongke Zhou,<sup>a</sup> Fuhua Song,<sup>a</sup> Shengjie Fu,<sup>a</sup> Weidong Zhang,<sup>a</sup> Xingliang Liu,<sup>a\*</sup> Defang Xu<sup>b\*</sup>

<sup>a</sup>School of Chemical Engineering, Qinghai University, Xining 810016, China

<sup>b</sup>State Key Laboratory of Plateau Ecology and Agriculture, Qinghai University, Xining 810016, China

E-mail address: [liuxl1219@163.com](mailto:liuxl1219@163.com), [xudefang123@163.com](mailto:xudefang123@163.com).

**Table S1** UV-vis absorption and fluorescence properties of **DBF-BZ-TPA** in different solvents.

| Solvent       | $\Delta f$ | $\lambda_{\text{abs}}/\text{nm}$ ( $\epsilon/\text{M}^{-1} \text{ cm}^{-1}$ ) | $\lambda_{\text{em}}/\text{nm}$ | $\Delta\nu_{\text{st}}^a/\text{cm}^{-1}$ | $\Phi_{\text{f}}^b$ |
|---------------|------------|-------------------------------------------------------------------------------|---------------------------------|------------------------------------------|---------------------|
| hexane        | $\sim 0$   | 293 (33700), 388 (21000)                                                      | 438, 464                        | 2942                                     | 0.58                |
| cyclohexane   | $\sim 0$   | 293 (41300), 390 (24600)                                                      | 441, 467                        | 2965                                     | 0.56                |
| toluene       | 0.014      | 296 (31800), 393 (23900)                                                      | 478                             | 4525                                     | 0.54                |
| ethyl acetate | 0.201      | 293 (33800), 393 (26700)                                                      | 518                             | 6140                                     | 0.51                |
| THF           | 0.210      | 296 (36800), 396 (27500)                                                      | 525                             | 6205                                     | 0.48                |
| DCM           | 0.218      | 296 (33400), 398 (28800)                                                      | 561                             | 7300                                     | 0.42                |
| DMF           | 0.275      | 295 (31000), 399 (29100)                                                      | 580                             | 7821                                     | 0.27                |

<sup>a</sup> $\Delta\nu_{\text{st}} = \nu_{\text{abs}} - \nu_{\text{em}}$ . <sup>b</sup>The fluorescence quantum yield ( $\Phi_{\text{f}}$ ) was measured using 9,10-diphenylanthracene ( $\Phi_{\text{f}} = 0.85$  in benzene) as a standard excited at 390 nm.

**Table S2.** Cartesian coordinates of DFT-optimized structure of **DBF-BZ-TPA** by B3LYP/6-31G(d,p)/CH<sub>2</sub>Cl<sub>2</sub>.

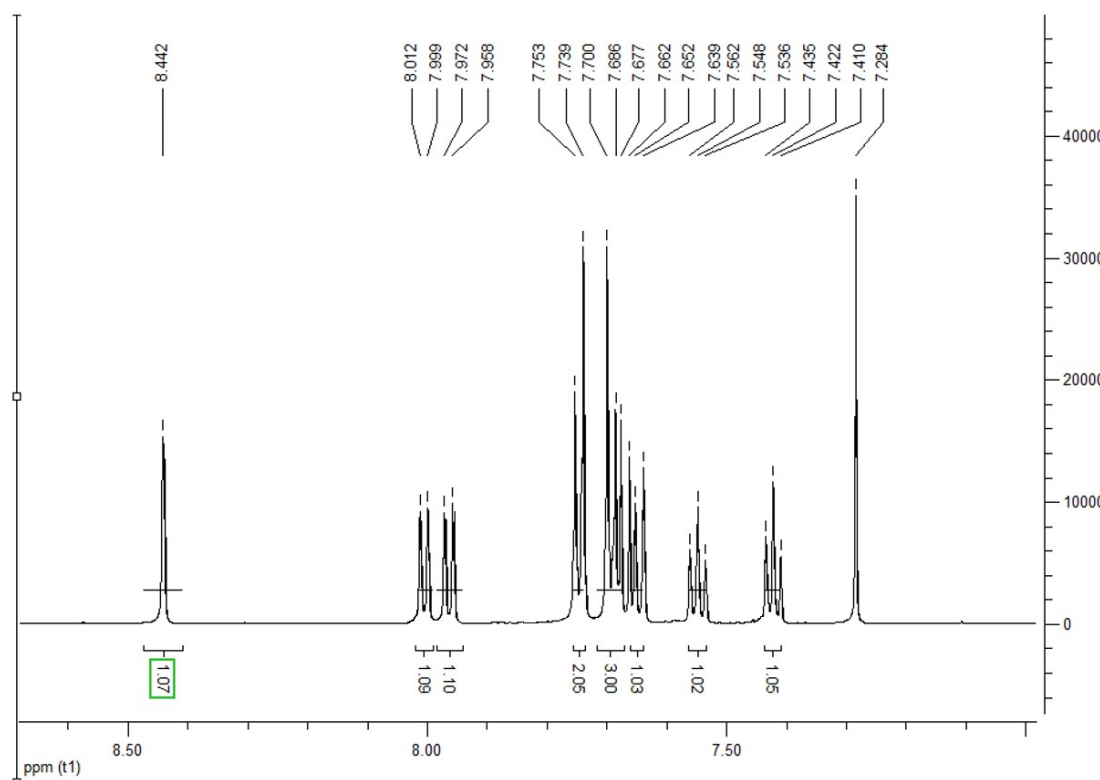
Charge = 0 Multiplicity = 1

|   |           |          |          |
|---|-----------|----------|----------|
| C | -9.47457  | 0.09955  | 3.47099  |
| C | -8.25754  | 0.5887   | 2.99689  |
| C | -7.39627  | -0.29393 | 2.33469  |
| C | -7.78664  | -1.63561 | 2.17131  |
| C | -8.99146  | -2.14483 | 2.63391  |
| C | -9.83565  | -1.24696 | 3.29207  |
| C | -5.80424  | -1.49008 | 1.22674  |
| C | -6.08693  | -0.19522 | 1.71083  |
| C | -5.15479  | 0.82014  | 1.50989  |
| H | -5.33702  | 1.83492  | 1.84752  |
| C | -3.94765  | 0.52268  | 0.85756  |
| C | -3.70435  | -0.78588 | 0.38298  |
| C | -4.63309  | -1.81161 | 0.55452  |
| H | -10.15602 | 0.76918  | 3.98731  |
| H | -7.98516  | 1.63041  | 3.1389   |
| H | -9.25819  | -3.18631 | 2.48903  |
| H | -10.79001 | -1.5994  | 3.67217  |
| H | -2.78649  | -0.99777 | -0.15399 |
| H | -4.45408  | -2.81277 | 0.17773  |
| O | -6.82389  | -2.36622 | 1.49958  |
| C | -2.99537  | 1.65327  | 0.61894  |
| O | -3.42562  | 2.80465  | 0.53436  |
| C | -1.52763  | 1.4012   | 0.48643  |
| C | -0.86287  | 0.34978  | 1.13829  |
| C | -0.7612   | 2.31361  | -0.25894 |
| C | 0.51814   | 0.20986  | 1.03449  |
| H | -1.4217   | -0.35456 | 1.74578  |
| C | 0.61365   | 2.16338  | -0.37454 |
| H | -1.26438  | 3.14599  | -0.74036 |
| H | 1.00202   | -0.62359 | 1.5346   |
| H | 1.18178   | 2.89382  | -0.94276 |
| C | 2.37543   | 0.98396  | 0.17907  |
| C | 3.13198   | 1.80824  | -0.53244 |
| H | 2.78572   | 0.1241   | 0.72541  |
| H | 2.72169   | 2.6681   | -1.07878 |
| C | 1.28771   | 1.10578  | 0.26978  |
| C | 7.24141   | -0.19546 | -0.41477 |
| C | 6.12891   | -0.5846  | 0.35516  |
| C | 7.11541   | 0.9449   | -1.22904 |
| C | 4.95047   | 0.13927  | 0.31091  |
| H | 6.19312   | -1.46499 | 0.98264  |

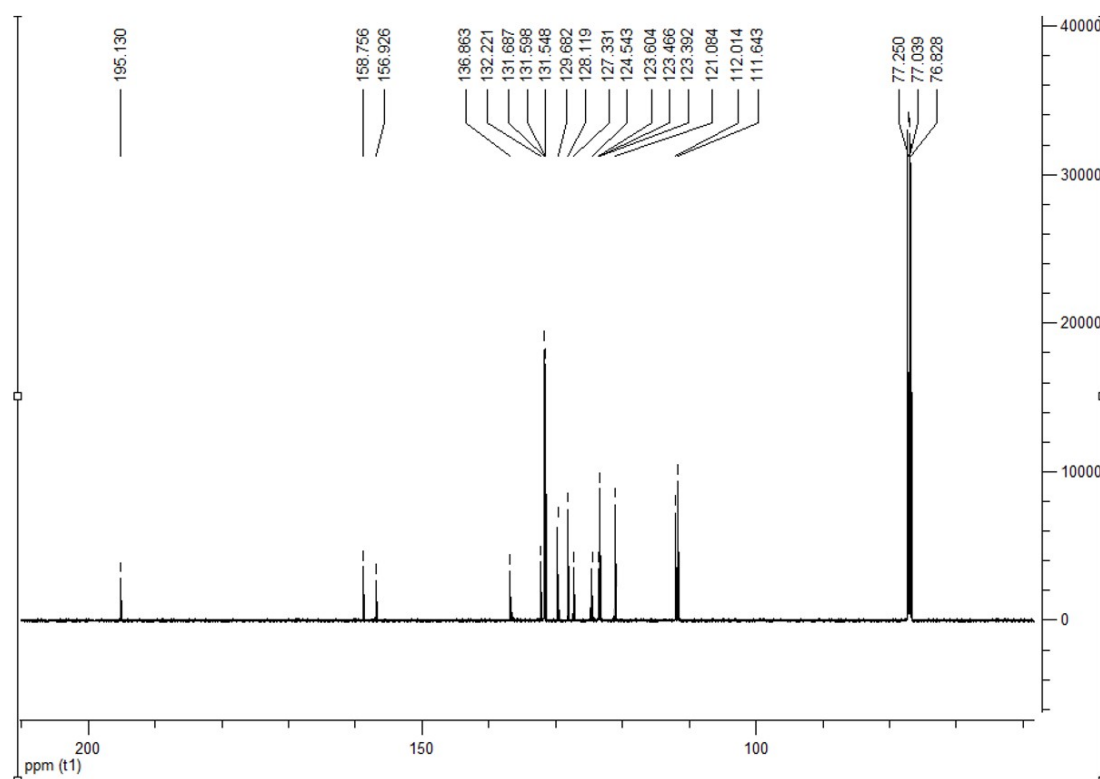
|   |          |          |          |
|---|----------|----------|----------|
| C | 5.93801  | 1.67237  | -1.25296 |
| H | 7.95134  | 1.26581  | -1.83788 |
| C | 4.82552  | 1.29631  | -0.48013 |
| H | 4.10934  | -0.18935 | 0.91073  |
| H | 5.88098  | 2.54394  | -1.89353 |
| C | 9.30148  | -0.98425 | -1.51049 |
| C | 8.79066  | -1.28069 | -2.7799  |
| C | 10.67496 | -0.76156 | -1.36098 |
| C | 9.6401   | -1.33881 | -3.88042 |
| H | 7.72875  | -1.46515 | -2.89866 |
| C | 11.52046 | -0.83734 | -2.46363 |
| H | 11.07374 | -0.52977 | -0.37984 |
| C | 11.00859 | -1.12114 | -3.72842 |
| H | 9.2308   | -1.56931 | -4.85879 |
| H | 12.58335 | -0.66113 | -2.33352 |
| H | 11.66941 | -1.17331 | -4.58713 |
| N | 8.43778  | -0.92881 | -0.3749  |
| C | 8.8254   | -1.62713 | 0.80882  |
| C | 8.78927  | -0.99032 | 2.05532  |
| C | 9.26507  | -2.95352 | 0.72992  |
| C | 9.17252  | -1.67766 | 3.20285  |
| H | 8.4622   | 0.04151  | 2.11908  |
| C | 9.66125  | -3.62906 | 1.88023  |
| H | 9.29611  | -3.44854 | -0.23423 |
| C | 9.6125   | -2.99802 | 3.12189  |
| H | 9.14087  | -1.17202 | 4.16258  |
| H | 9.99994  | -4.65741 | 1.8051   |
| H | 9.91748  | -3.52865 | 4.0176   |

**Table S3** Crystallographic experimental details for **DBF-BZ-TPA** (CCDC 2119347).

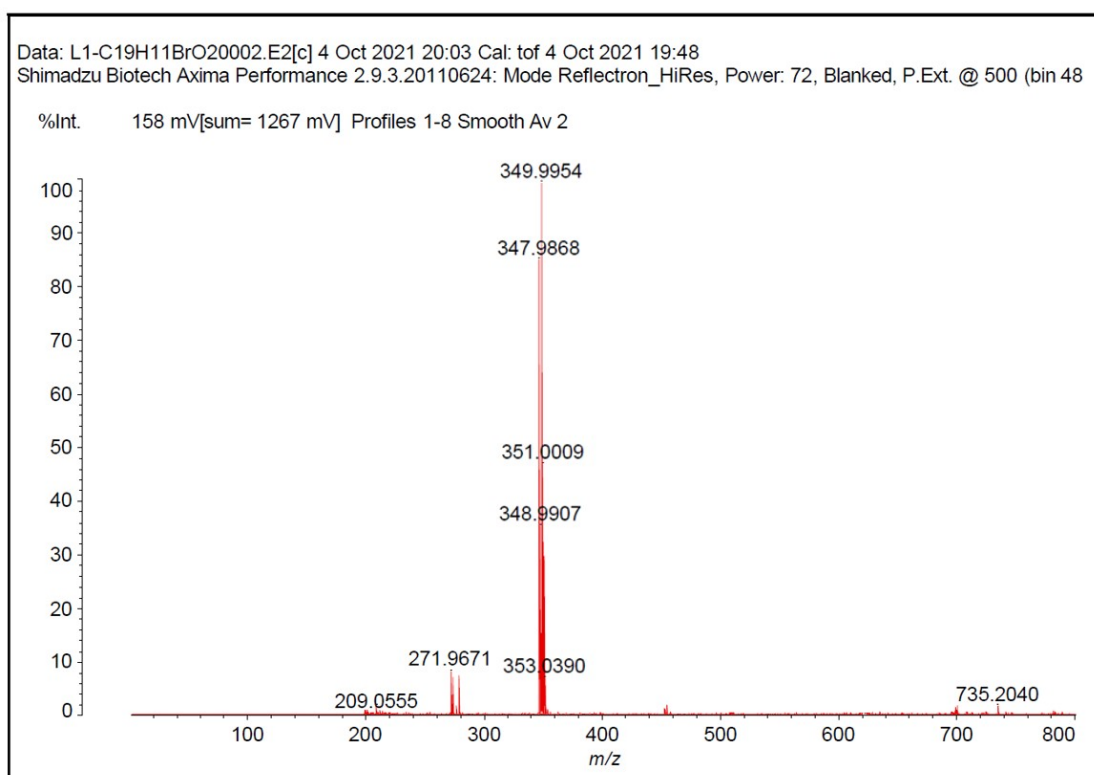
|                                             |                                                               |
|---------------------------------------------|---------------------------------------------------------------|
| Empirical formula                           | C <sub>39</sub> H <sub>27</sub> NO <sub>2</sub>               |
| Formula weight                              | 541.61                                                        |
| Temperature/K                               | 150.00(10)                                                    |
| Crystal system                              | triclinic                                                     |
| Space group                                 | P-1                                                           |
| a/Å                                         | 6.0022(3)                                                     |
| b/Å                                         | 7.5070(4)                                                     |
| c/Å                                         | 30.8256(13)                                                   |
| α/°                                         | 84.861(4)                                                     |
| β/°                                         | 89.533(3)                                                     |
| γ/°                                         | 89.472(4)                                                     |
| Volume/Å <sup>3</sup>                       | 1383.28(12)                                                   |
| Z                                           | 2                                                             |
| ρ <sub>calc</sub> /g/cm <sup>3</sup>        | 1.300                                                         |
| μ/mm <sup>-1</sup>                          | 0.622                                                         |
| F(000)                                      | 568.0                                                         |
| Crystal size/mm <sup>3</sup>                | 0.13 × 0.1 × 0.08                                             |
| Radiation                                   | Cu Kα (λ = 1.54184)                                           |
| 2Θ range for data collection/°              | 5.758 to 147.852                                              |
| Index ranges                                | -7 ≤ h ≤ 4, -9 ≤ k ≤ 9, -34 ≤ l ≤ 38                          |
| Reflections collected                       | 9298                                                          |
| Independent reflections                     | 5375 [R <sub>int</sub> = 0.0265, R <sub>sigma</sub> = 0.0390] |
| Data/restraints/parameters                  | 5375/0/379                                                    |
| Goodness-of-fit on F <sup>2</sup>           | 1.050                                                         |
| Final R indexes [I ≥ 2σ (I)]                | R <sub>1</sub> = 0.0489, wR <sub>2</sub> = 0.1327             |
| Final R indexes [all data]                  | R <sub>1</sub> = 0.0570, wR <sub>2</sub> = 0.1389             |
| Largest diff. peak/hole / e Å <sup>-3</sup> | 0.19/-0.24                                                    |



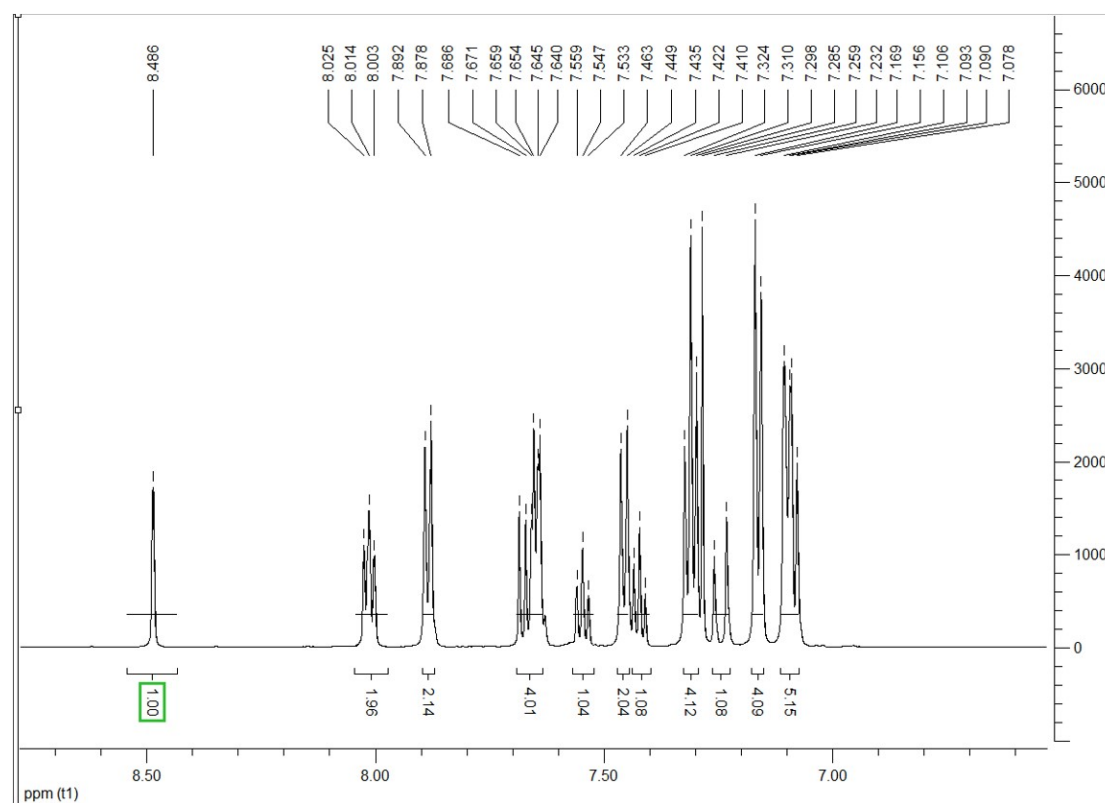
**Fig. S1**  $^1\text{H}$  NMR (600 MHz) spectrum of **3**.



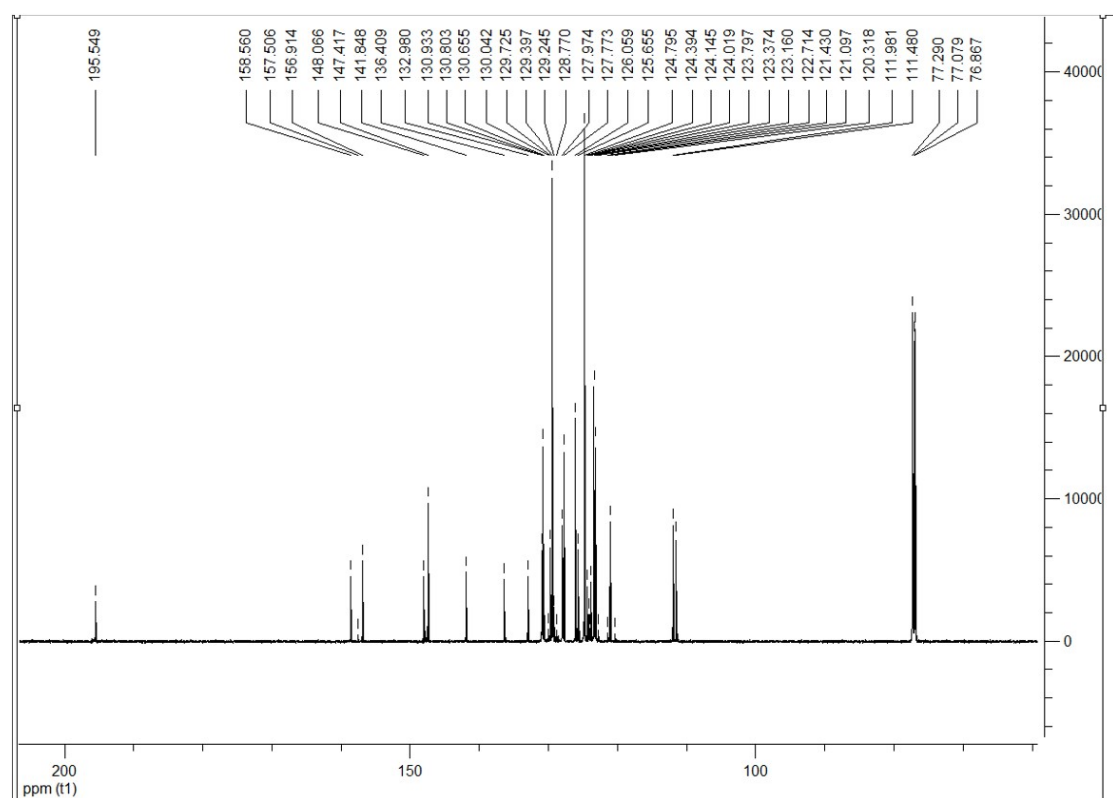
**Fig. S2**  $^{13}\text{C}$  NMR (150 MHz) spectrum of **3**.



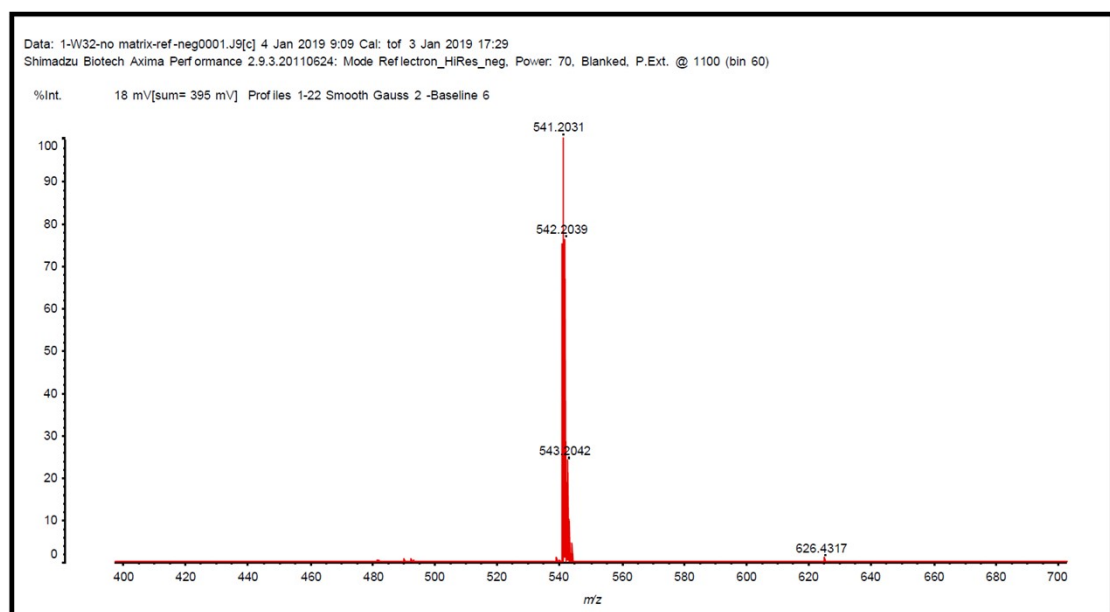
**Fig. S3** MALDI/TOF MS spectrum of **3**



**Fig. S4**  $^1\text{H}$  NMR (600 MHz) spectrum of **DBF-BZ-TPA**.



**Fig. S5**  $^{13}\text{C}$  NMR (150 MHz) spectrum of DBF-BZ-TPA.



**Fig. S6** MALDI/TOF MS spectrum of DBF-BZ-TPA.