

## Electronic Supplementary Information (ESI)

### **Enhanced AIE and different stimuli-responses in red fluorescent (1,3-dimethyl)barbituric acid-functionalized anthracenes**

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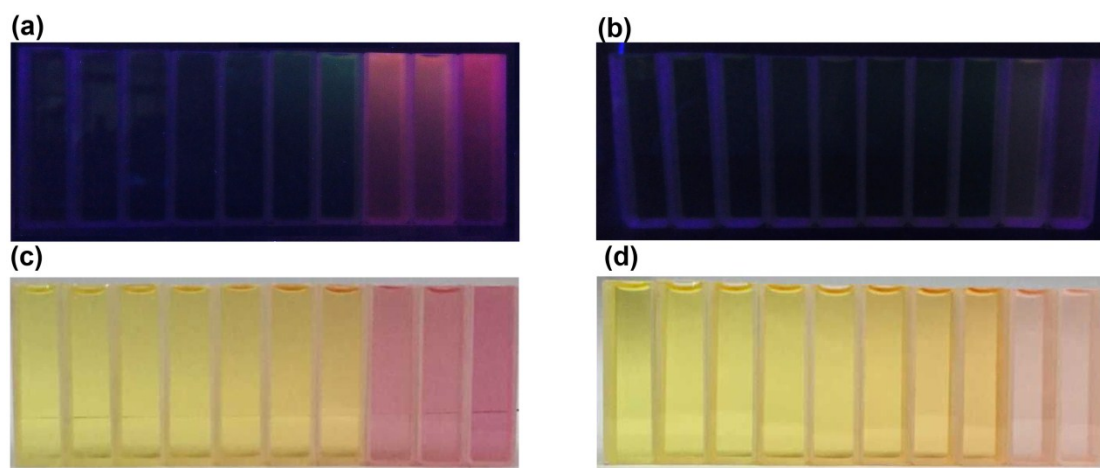


Fig. S1 The photographs of (a, c) **B-A** and (b, d) **DMB-A** (100  $\mu$ M) in 1,4-dioxane–water mixtures with different water fractions ( $f_w$ : 0 to 90%, from left to right) under 365 nm (top) and natural (bottom) light

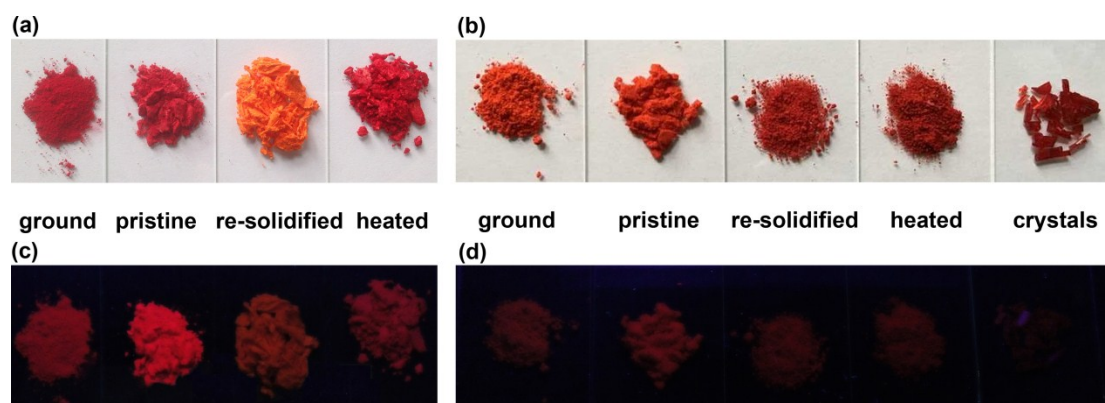


Fig. S2 The photographs of (a, c) **B-A** and (b, d) **DMB-A** in different states under natural (top) and 365 nm (bottom) light.

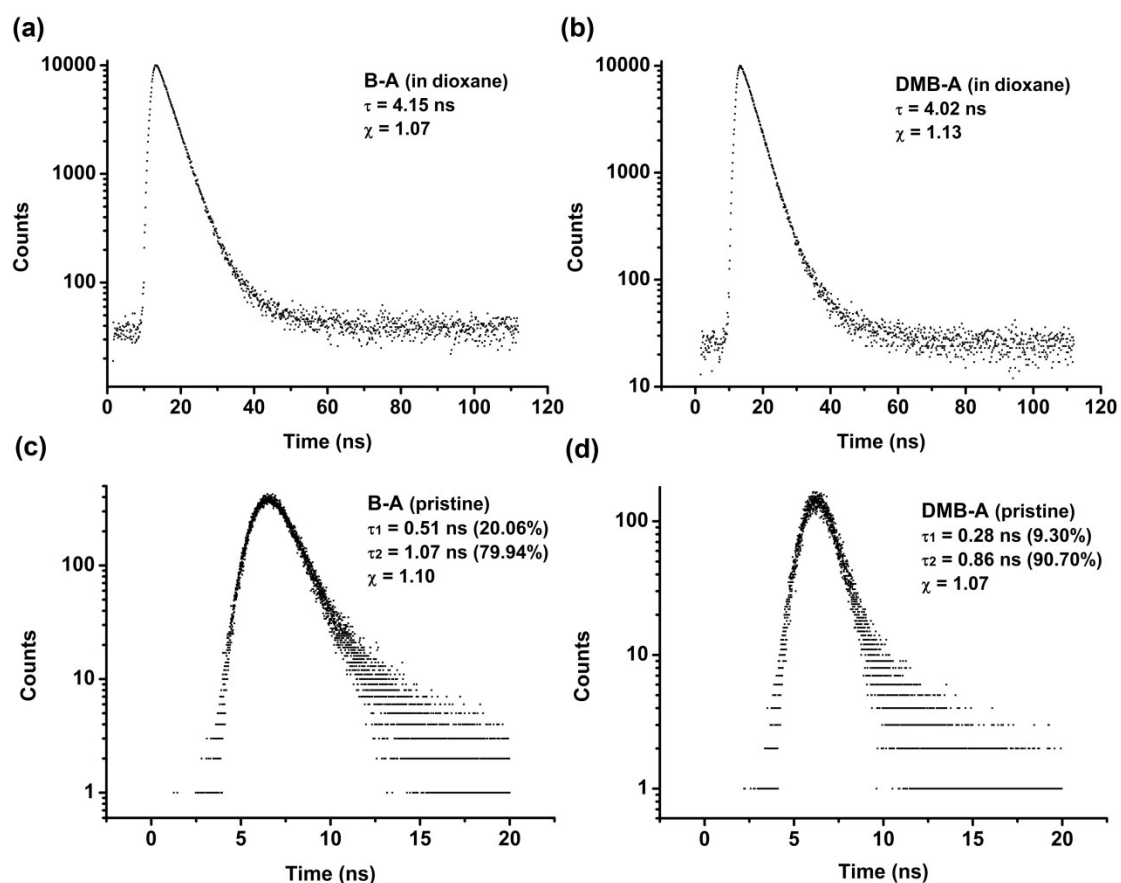


Fig. S3 Time-resolved fluorescence spectra of **B-A** and **DMB-A** in (a, b) dioxane solution (10  $\mu\text{M}$ ) and (c, d) solid state.

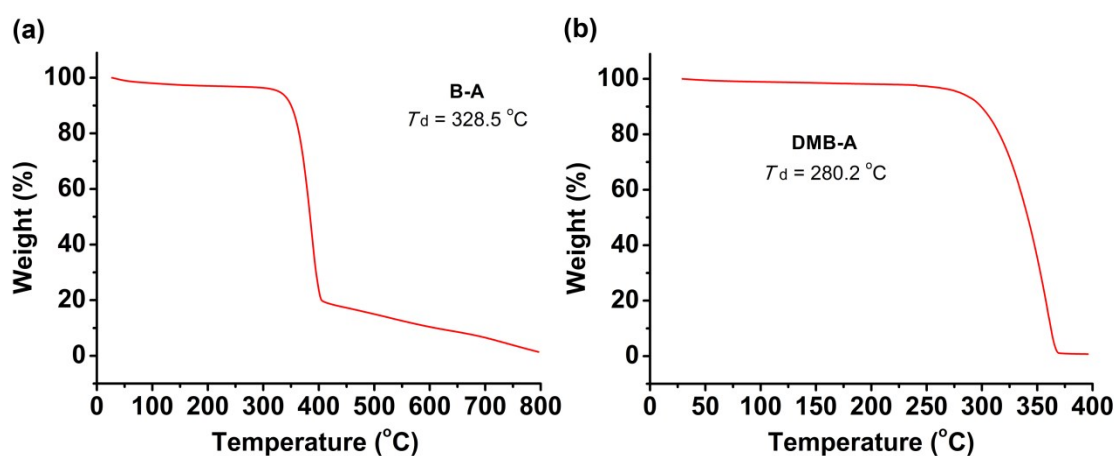


Fig. S4 TGA curves of (a) **B-A** and (b) **DMB-A**.

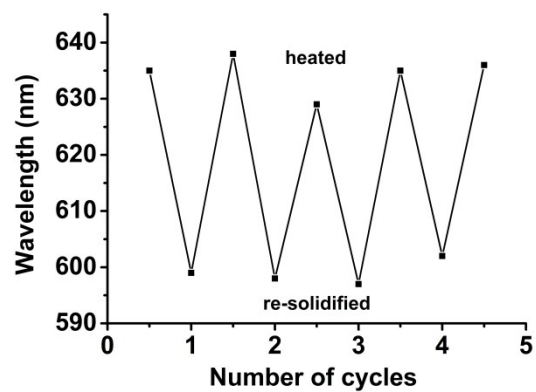


Fig. S5 Reversibility of the fluorescence wavelengths of **B-A** by re-solidifying and heating treatments.

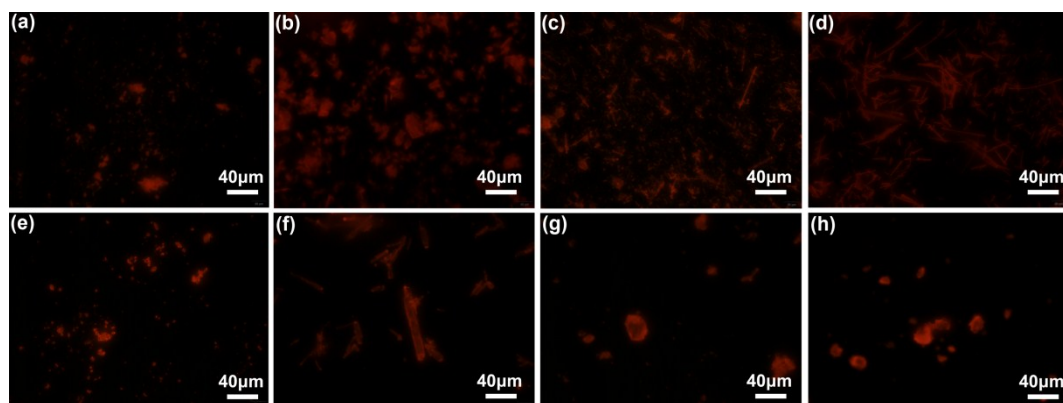
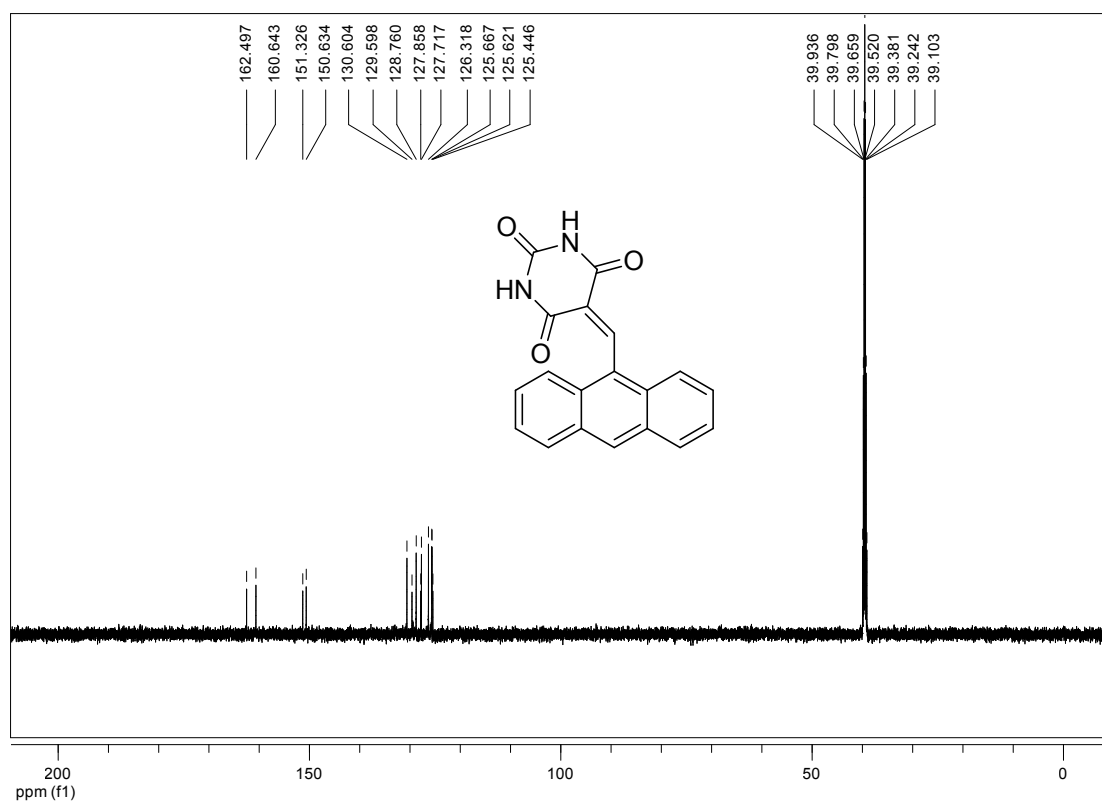
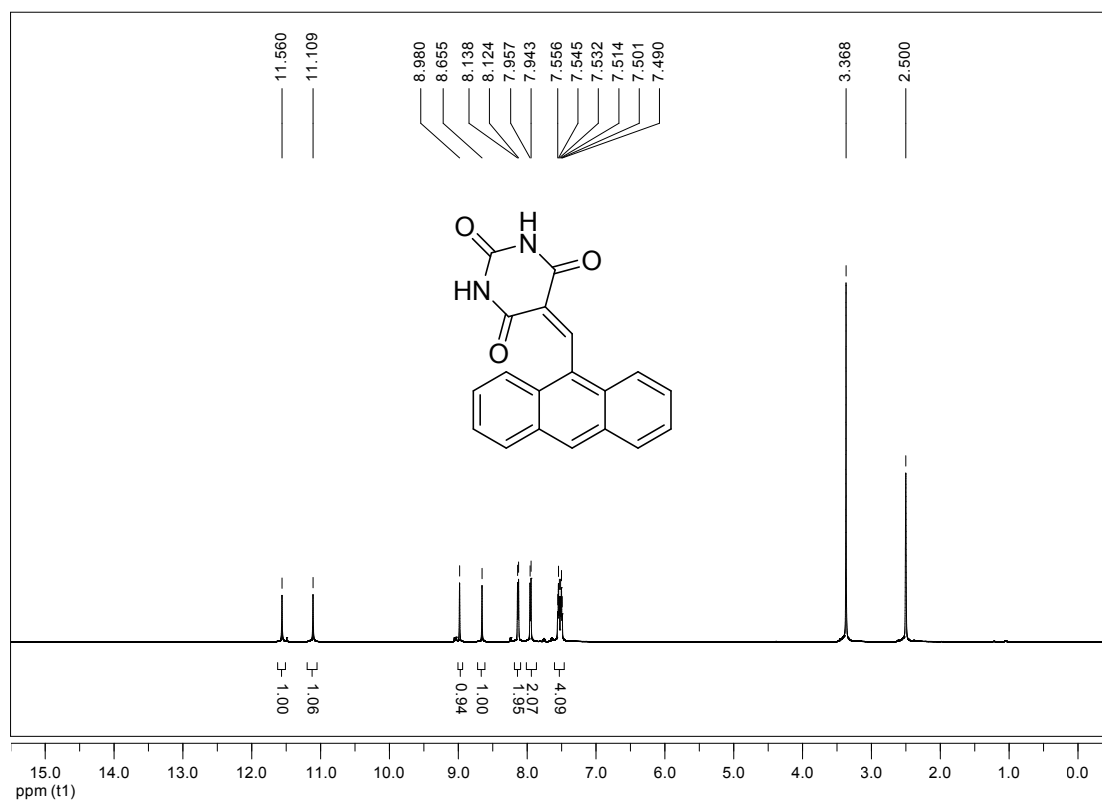


Fig. S6 Fluorescence microscopy images of **B-A** (top) and **DMB-A** (bottom): (a, e) ground, (b, f) pristine, (c, g) re-solidified and (d, h) heated samples.

**Table S1** Crystal data and structure refinement for **DMB-A**.

|                                   |                                                                                                                        |
|-----------------------------------|------------------------------------------------------------------------------------------------------------------------|
| Empirical formula                 | C21 H16 N2 O3                                                                                                          |
| Formula weight                    | 344.36                                                                                                                 |
| Temperature                       | 113(2) K                                                                                                               |
| Wavelength                        | 0.71073 Å                                                                                                              |
| Crystal system, space group       | Monoclinic, P2(1)/n                                                                                                    |
| Unit cell dimensions              | a = 8.2837(17) Å    alpha = 90 deg.<br>b = 15.617(6) Å    beta = 91.261(16) deg.<br>c = 25.025(7) Å    gamma = 90 deg. |
| Volume                            | 3236.7(16) Å <sup>3</sup>                                                                                              |
| Z, Calculated density             | 8, 1.413 Mg/m <sup>3</sup>                                                                                             |
| Absorption coefficient            | 0.096 mm <sup>-1</sup>                                                                                                 |
| F(000)                            | 1440                                                                                                                   |
| Crystal size                      | 0.20 x 0.18 x 0.12 mm                                                                                                  |
| Theta range for data collection   | 2.09 to 30.70 deg.                                                                                                     |
| Limiting indices                  | -11<=h<=11, -20<=k<=21, -35<=l<=34                                                                                     |
| Reflections collected / unique    | 34463 / 9670 [R(int) = 0.0321]                                                                                         |
| Completeness to theta = 30.70     | 96.2 %                                                                                                                 |
| Absorption correction             | Semi-empirical from equivalents                                                                                        |
| Max. and min. transmission        | 0.9886 and 0.9811                                                                                                      |
| Refinement method                 | Full-matrix least-squares on F <sup>2</sup>                                                                            |
| Data / restraints / parameters    | 9670 / 0 / 473                                                                                                         |
| Goodness-of-fit on F <sup>2</sup> | 1.045                                                                                                                  |
| Final R indices [I>2sigma(I)]     | R1 = 0.0425, wR2 = 0.1221                                                                                              |
| R indices (all data)              | R1 = 0.0560, wR2 = 0.1296                                                                                              |
| Largest diff. peak and hole       | 0.474 and -0.240 e.Å <sup>-3</sup>                                                                                     |



**Analysis Info**

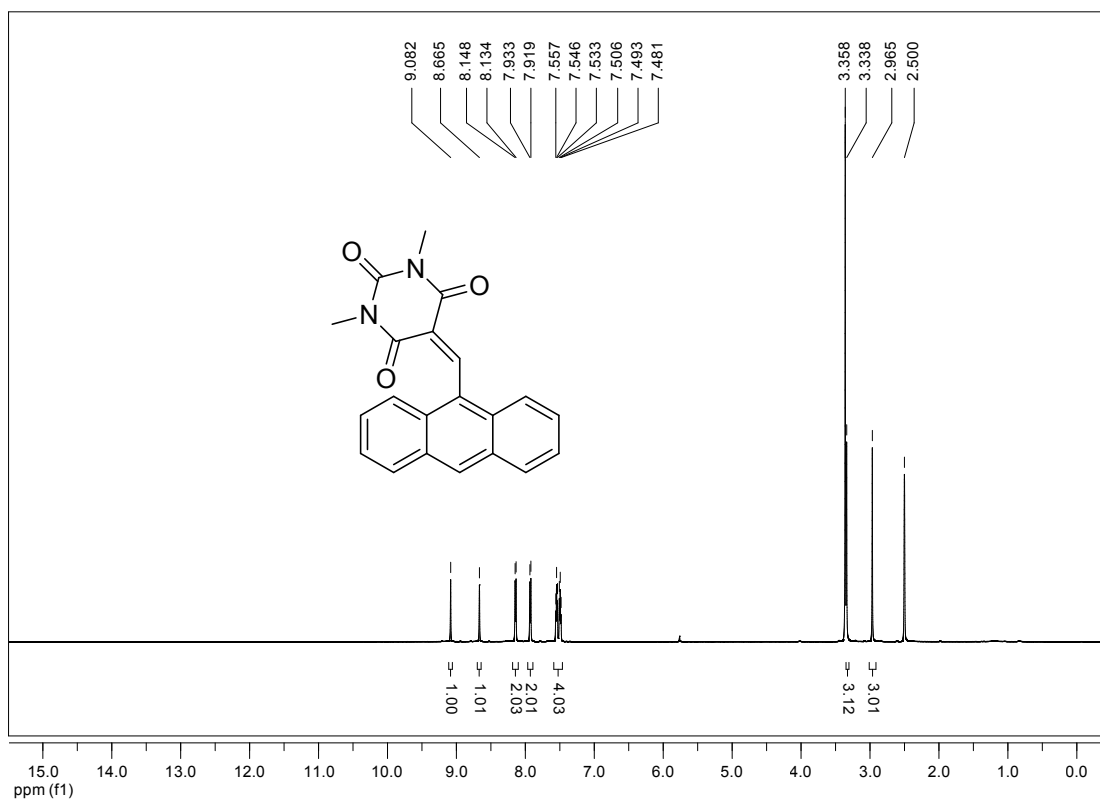
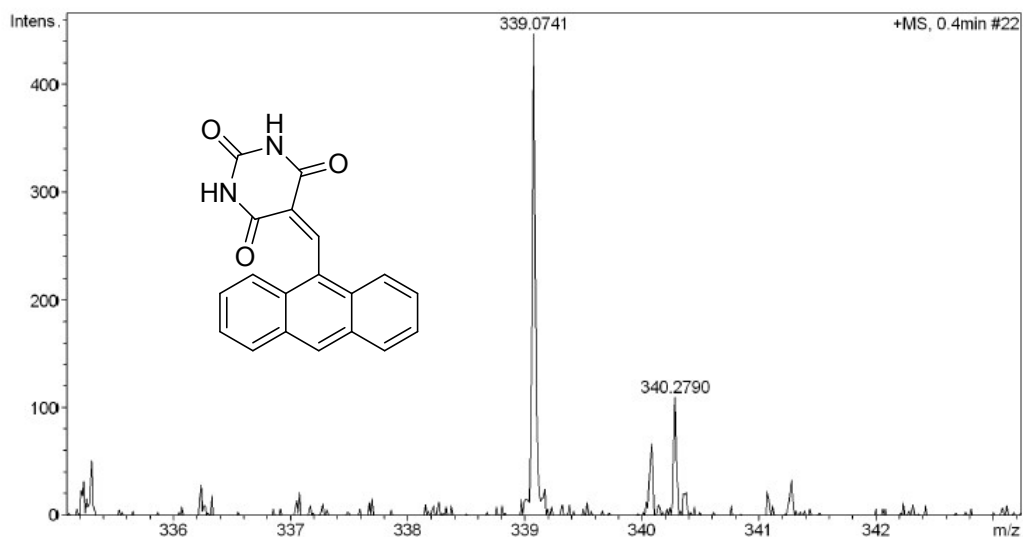
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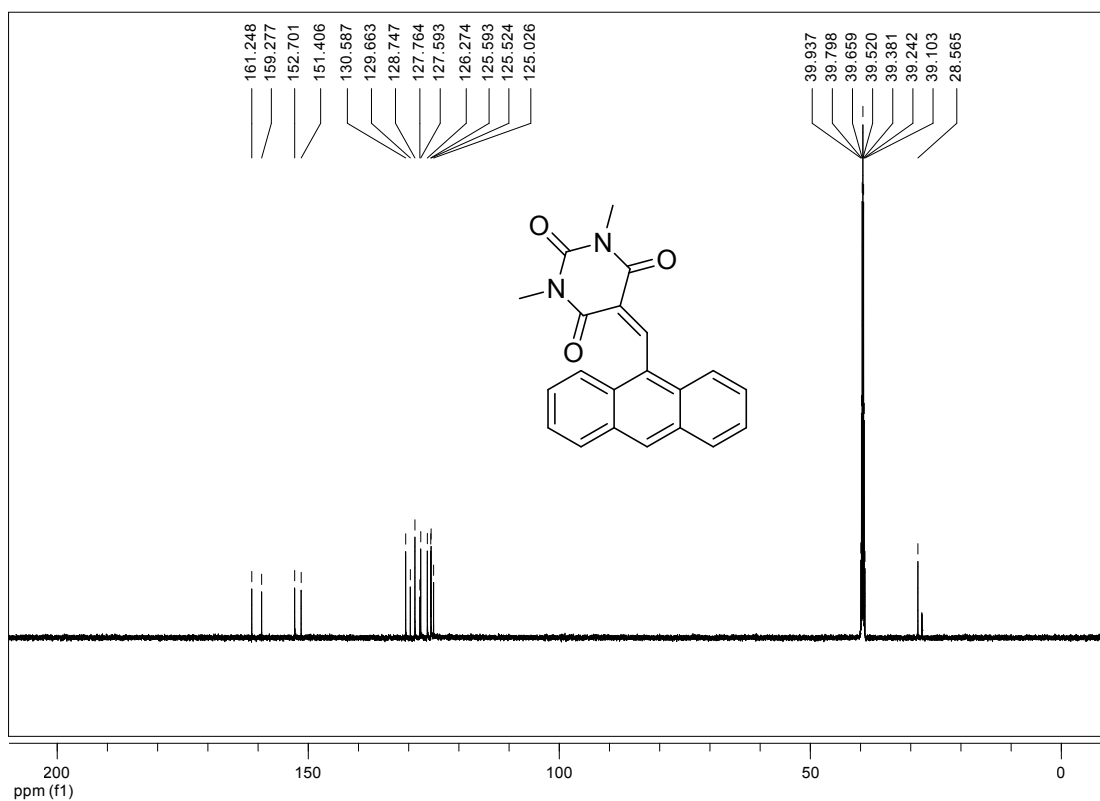
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Operator TJU  
Instrument / Ser# microTOF-Q II 10204

**Acquisition Parameter**

|             |          |                       |           |                  |           |
|-------------|----------|-----------------------|-----------|------------------|-----------|
| Source Type | ESI      | Ion Polarity          | Positive  | Set Nebulizer    | 0.8 Bar   |
| Focus       | Active   | Set Capillary         | 4500 V    | Set Dry Heater   | 180 °C    |
| Scan Begin  | 100 m/z  | Set End Plate Offset  | -500 V    | Set Dry Gas      | 6.0 l/min |
| Scan End    | 2000 m/z | Set Collision Cell RF | 600.0 Vpp | Set Divert Valve | Source    |





#### Analysis Info

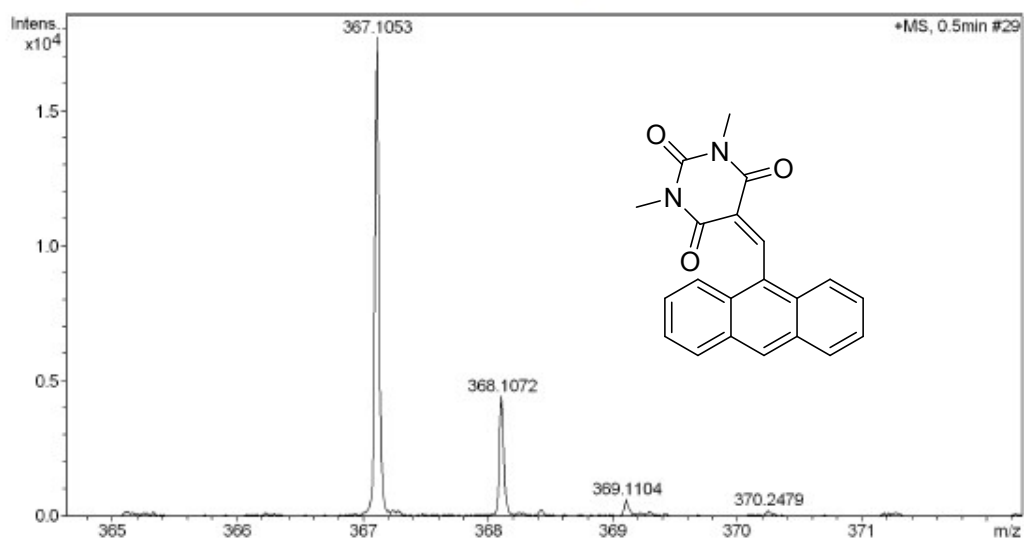
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| Focus       | Active   | Set Capillary         | 4500 V    | Set Dry Heater   | 180 °C    |
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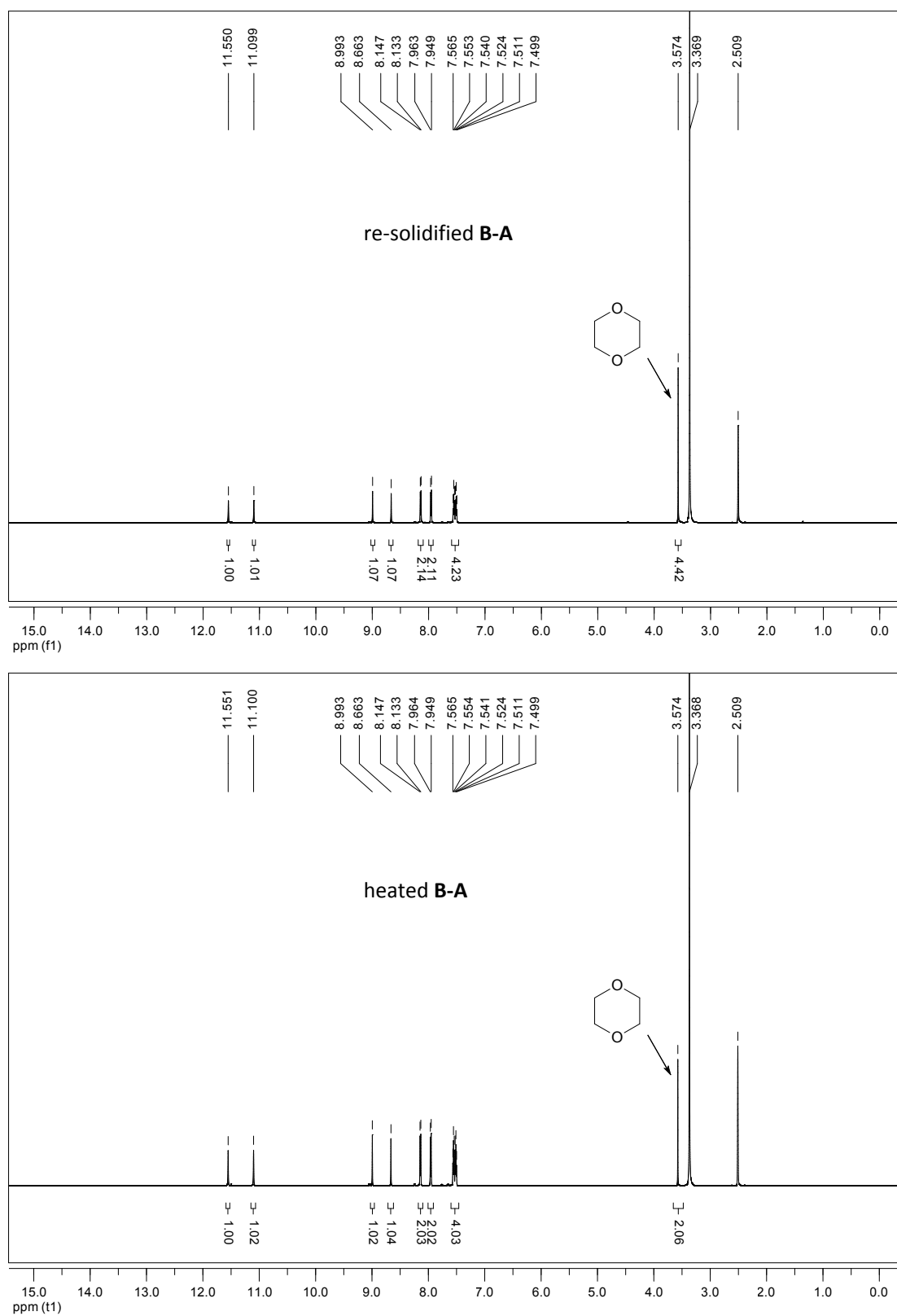


Fig. S7  $^1\text{H}$  NMR,  $^{13}\text{C}$  NMR and HRMS spectra of B-A and DMB-A.