

Supporting Information

A Feasible Scalable Porphyrin Dye for Dye-Sensitized Solar Cells under One Sun and Dim Light Environments

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Keywords: porphyrin, dye, solar cells, dim light, synthesis

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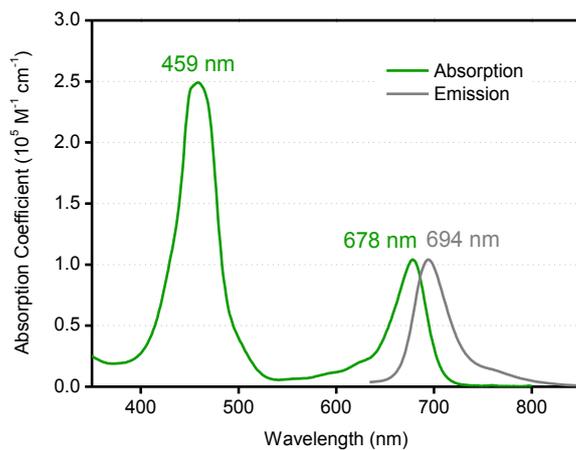


Figure S1. UV-vis absorption and emission spectra of **Y1A1** in THF.

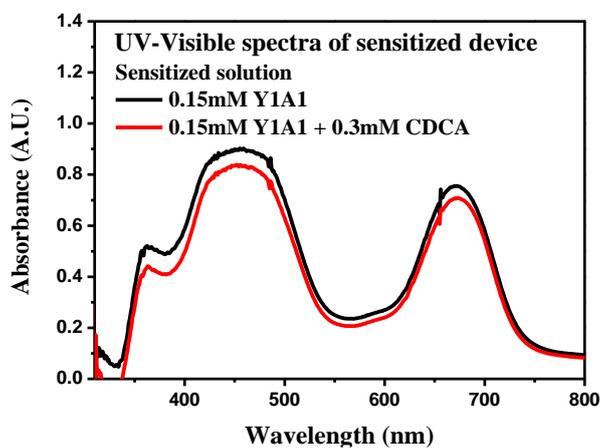


Figure S2. Thin-film absorption spectra of **Y1A1** on TiO_2 with and without the presence of CDCA.

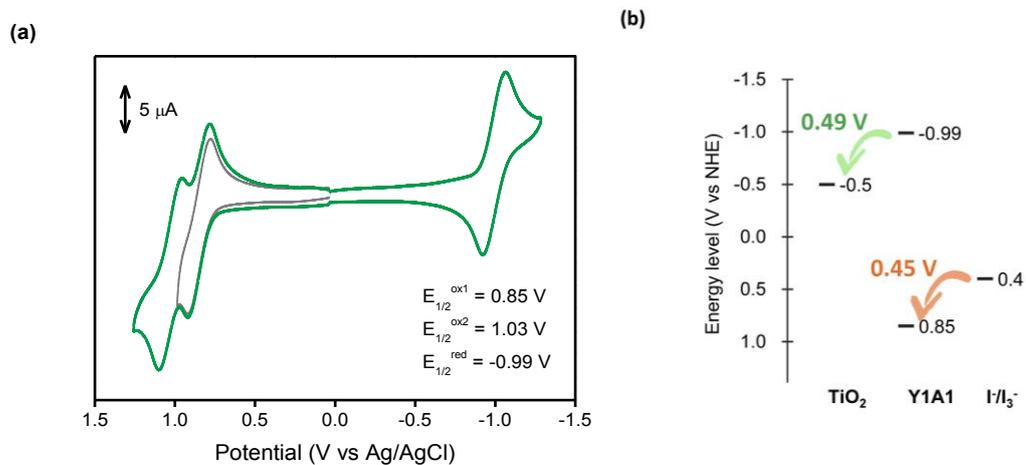


Figure S3. (a) Cyclic voltammogram of **Y1A1** and (b) energy level diagram of **Y1A1**-based DSC.

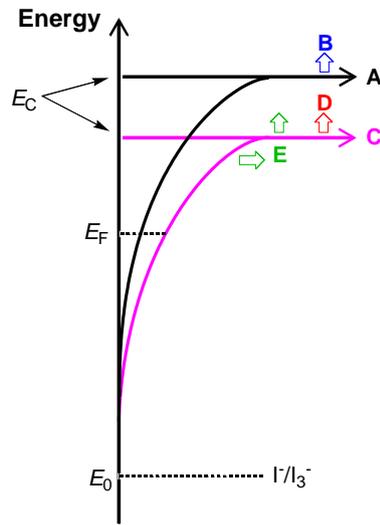


Figure S4. Representation of proposed density of states showing the influence of additives and CDCA.

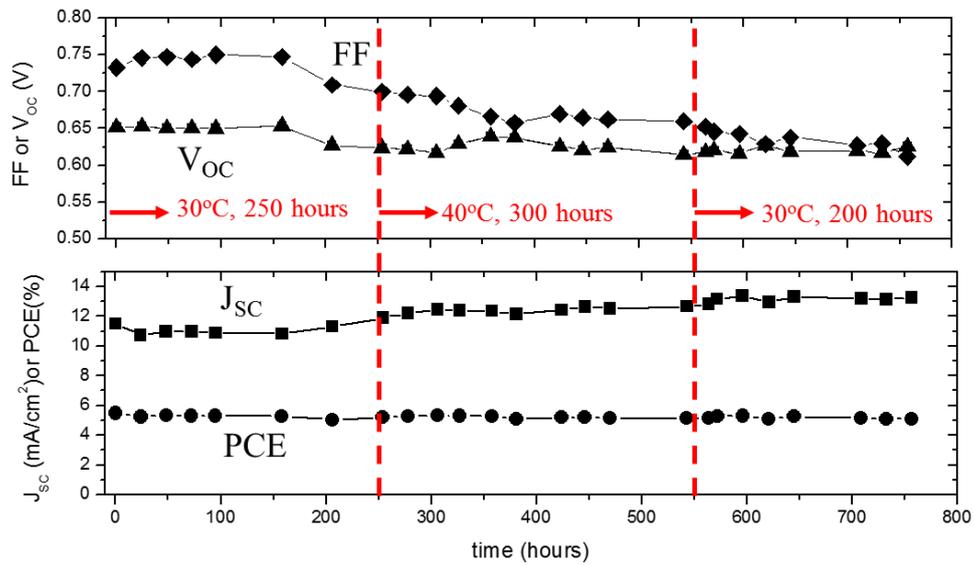
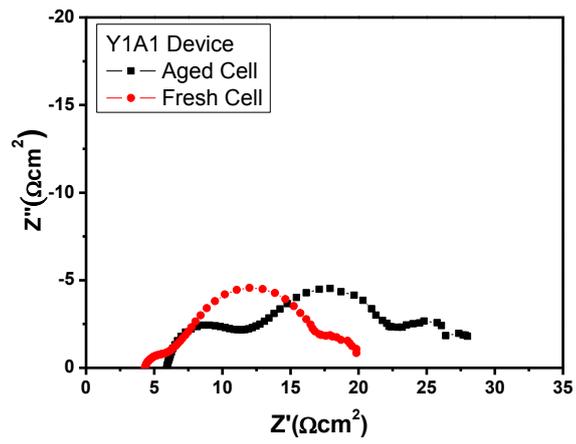


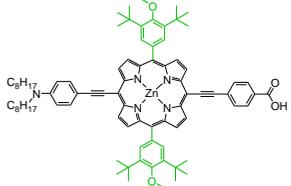
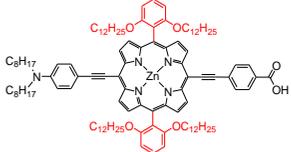
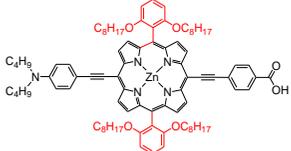
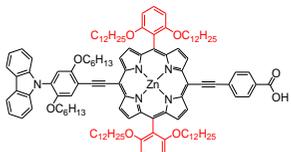
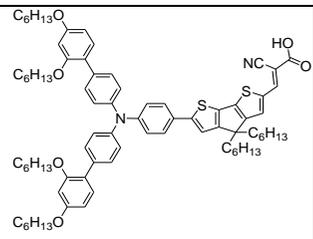
Figure S5. Preliminary thermal aging test on Y1A1-sensitized cells by a simulated indoor condition profile

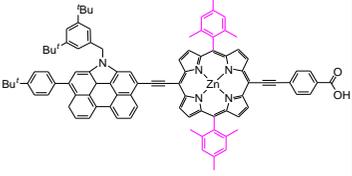
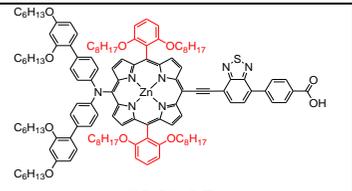
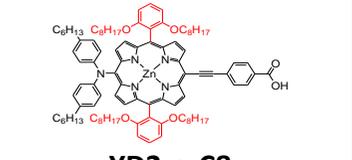
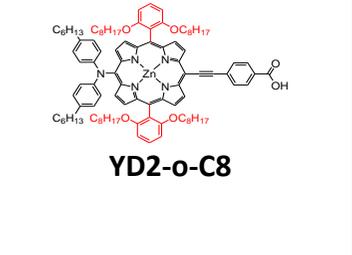
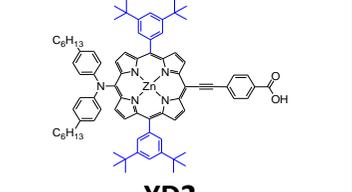
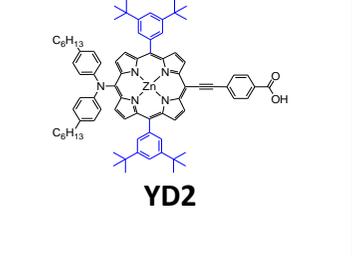


| Y1A1 Device | R_{CT} (Ωcm^2) | R_{TiO_2} (Ωcm^2) |
|-------------|----------------------------------|-------------------------------------|
| Aged Cell | 5.68 | 12.38 |
| Fresh Cell | 2.88 | 10.56 |

Figure S6. Nyquist plot and impedance elements of **Y1A1** aged cell and fresh cell after a simulated indoor condition profile.

Table S1. Comparison of photophysical and electrochemical properties for several porphyrin dyes.

| Entry | Porphyrin dye | Photophysical properties | | | Energy levels | | Best device performance | | | | | Ref. | |
|-------|---|---|-------------------------------|-------------------|-----------------------------|--------------------|-------------------------|--|------|-----------|-------|---|---------------|
| | | λ_{abs} (ϵ), nm (10^3 $\text{M}^{-1} \text{cm}^{-1}$) | λ_{em} , nm | E_{0-0} , eV | $E_{1/2(\text{ox})}$, V | E_{0-0}^* , V | V_{oc} , V | J_{sc} , mA cm^{-2} | FF | PCE, % | E^a | | Co-sensitizer |
| 1 |  <p>Y1A1</p> | 459 (300), 678 (12.8) | 694 | 1.81 | +0.85 | -0.99 | 0.66 | 18.60 | 0.75 | 9.22 | A | × | This work |
| 2 |  <p>LD16</p> | 461 (224), 671 () | 683, 746 | - | +0.72 | - | 0.71 | 20.59 | 0.70 | 10.24 | A | × | 1 |
| 3 |  <p>YD22</p> | 459 (22.3), 671 (6.8) | 676 | 1.84 | +0.78 | -1.06 | 0.70 | 14.92 | 0.72 | 7.56 | A | × | 2 |
| 4 |  <p>XW-4</p> | 457 (314), 611 (10.7), 663 (77.3) | 675 | 1.86 | +0.83 | -1.03 | 0.70 | 16.22 | 0.70 | 7.94 | A | × | |
| | | | | | | | 0.73 | 20.0 | 0.74 | 10.75 | A |  <p>XS-3</p> | 3, 4 |

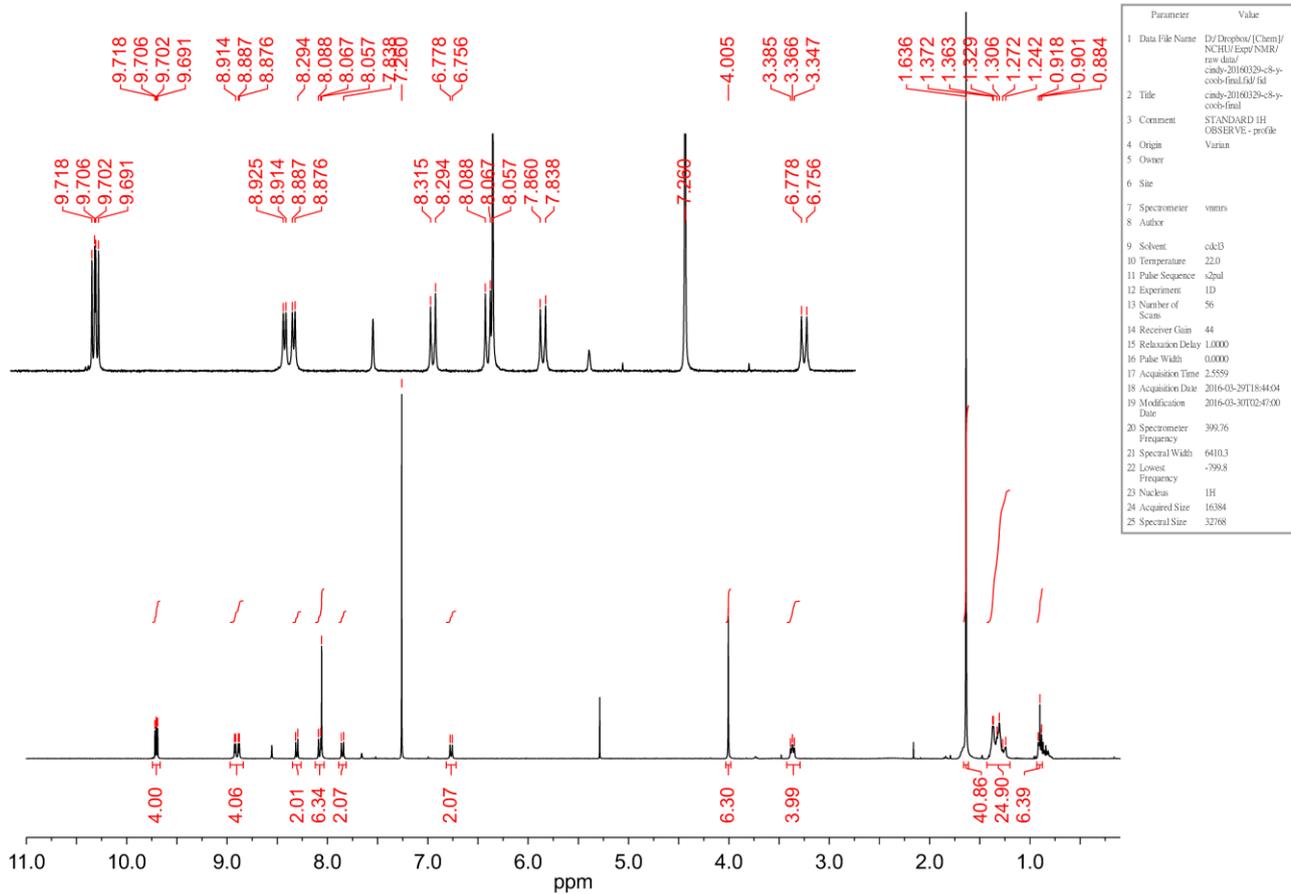
| | | | | | | | | | | | | | |
|---|--|---|-----|------|-------|-------|------|-------|------|------|---|---|---|
| 5 |  <p>WW5</p> | 441 (159), 466 (115), 502 (61.5), 679 (75.4) | - | 1.71 | +0.74 | -0.97 | 0.77 | 18.43 | 0.73 | 10.3 | B | x | 5 |
| 6 |  <p>SM315</p> | 440 (105), 454 (117), 581 (12), 668 (53) | 732 | 1.79 | +0.88 | -0.91 | 0.91 | 18.1 | 0.78 | 13.0 | B | x | 6 |
| 7 |  <p>YD2-o-C8</p> | 448 (212), 581 (12), 645 (31) | 663 | - | +0.82 | - | 0.83 | 15.8 | 0.71 | 9.4 | A | x | 7 |
| | | | | | | | 0.97 | 17.3 | 0.71 | 11.9 | B | x | |
| | | | | | | | 0.94 | 17.7 | 0.74 | 12.3 | B |  <p>Y123</p> | |
| 8 |  <p>YD2</p> | 444 (217), 589 (10.8), 648 (33.7) | 676 | 1.81 | +0.89 | -1.09 | 0.74 | 16.7 | 0.72 | 8.8 | A | x | 8 |
| | | | | | | | 0.77 | 18.6 | 0.76 | 11 | A |  <p>D205</p> | |
| | | | | | | | 0.83 | 14.9 | 0.69 | 8.4 | B | x | |

^a E denotes to electrolyte where electrolyte A is based on I⁻/I₃⁻ and electrolyte B is based on Co(bpy)^{2+/3+}.

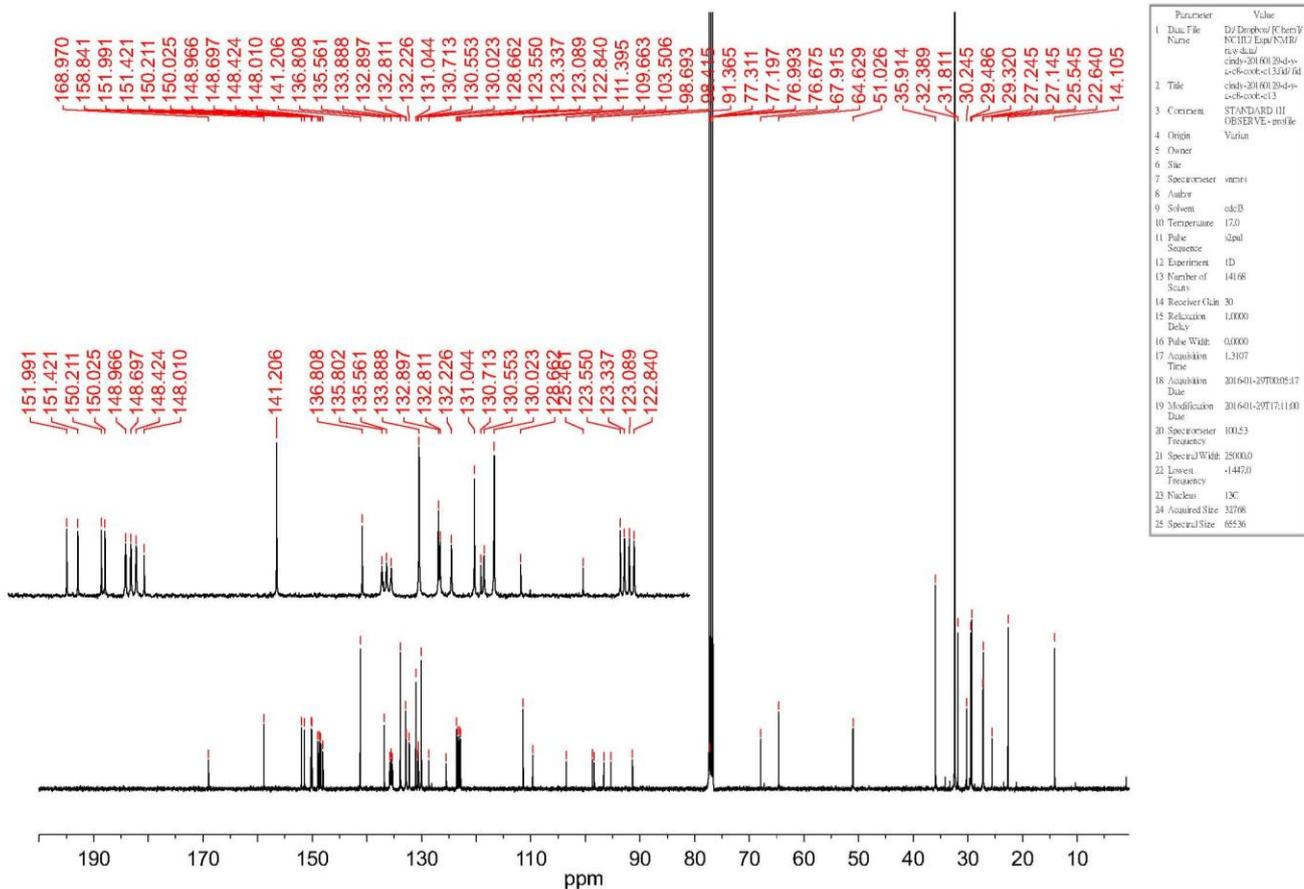
Table S2. Performance of **Y1A1** device illuminated under different light source at varied light intensity.

| Photon flux, lux | T5-White Fluorescent lamp | | | | | | T8-White Fluorescent lamp | | | | | | LED planar light | | | | | |
|------------------|---------------------------------|--------------|-------|------------|---------------------------------|----------------------------------|---------------------------------|--------------|-------|------------|---------------------------------|----------------------------------|---------------------------------|--------------|-------|------------|---------------------------------|----------------------------------|
| | J_{sc} , μAcm^{-2} | V_{oc} , V | FF | η , % | P_{in} , μWcm^{-2} | P_{Max} , μWcm^{-2} | J_{sc} , μAcm^{-2} | V_{oc} , V | FF | η , % | P_{in} , μWcm^{-2} | P_{Max} , μWcm^{-2} | J_{sc} , μAcm^{-2} | V_{oc} , V | FF | η , % | P_{in} , μWcm^{-2} | P_{Max} , μWcm^{-2} |
| 300 | 52.6 | 0.467 | 0.739 | 19.3 | 94.01 | 18.2 | 45.8 | 0.471 | 0.765 | 17.0 | 96.8 | 16.5 | – | – | – | – | – | – |
| 350 | 50.9 | 0.471 | 0.754 | 16.4 | 10.11 | 18.1 | 47.3 | 0.472 | 0.744 | 14.2 | 117.0 | 16.6 | 56.6 | 0.476 | 0.755 | 19.5 | 104.3 | 20.3 |
| 600 | 81 | 0.486 | 0.768 | 16.1 | 18.81 | 30.2 | 75.1 | 0.487 | 0.753 | 14.3 | 192.2 | 27.6 | 83 | 0.490 | 0.772 | 17.5 | 179.2 | 31.4 |
| 900 | 117 | 0.500 | 0.779 | 16.1 | 28.24 | 45.5 | 114 | 0.501 | 0.761 | 15.0 | 289.3 | 43.5 | 117 | 0.502 | 0.768 | 16.7 | 269.0 | 45 |
| 1200 | 148 | 0.508 | 0.761 | 15.2 | 37.67 | 57.2 | 150 | 0.510 | 0.763 | 15.0 | 3889 | 58.4 | 144 | 0.510 | 0.769 | 15.7 | 358.4 | 56.3 |
| 1750 | 211 | 0.520 | 0.762 | 15.3 | 54.95 | 83.8 | 205 | 0.521 | 0.766 | 14.1 | 5818 | 81.9 | 215 | 0.523 | 0.760 | 16.4 | 522.3 | 85.5 |
| 2400 | 293 | 0.530 | 0.766 | 15.8 | 75.54 | 119 | 293 | 0.532 | 0.754 | 15.3 | 7671 | 117 | 299 | 0.534 | 0.755 | 16.9 | 716.6 | 121 |
| 5250 | 653 | 0.558 | 0.769 | 17.0 | 1650 | 280 | 581 | 0.556 | 0.765 | 13.5 | 1835 | 247 | 634 | 0.560 | 0.768 | 17.4 | 1567 | 272 |
| 6000 | 755 | 0.561 | 0.771 | 17.4 | 1882 | 327 | 687 | 0.560 | 0.765 | 14.5 | 2029 | 295 | 735 | 0.564 | 0.762 | 17.7 | 1783 | 316 |
| 7000 | 876 | 0.566 | 0.765 | 17.4 | 2186 | 380 | 741 | 0.562 | 0.765 | 13.8 | 2315 | 319 | 873 | 0.570 | 0.763 | 18.2 | 2086 | 380 |

S5. NMR spectra of Y1A1



| Parameter | Value |
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| 3 Comment | STANDARD IH OBSERVE - profile |
| 4 Origin | Varian |
| 5 Owner | Varian |
| 6 Site | |
| 7 Spectrometer | varius |
| 8 Author | |
| 9 Solvent | cdcl3 |
| 10 Temperature | 22.0 |
| 11 Pulse Sequence | s2pul |
| 12 Experiment | 1D |
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| 14 Receiver Gain | 44 |
| 15 Relaxation Delay | 1.0000 |
| 16 Pulse Width | 0.0000 |
| 17 Acquisition Time | 2.5559 |
| 18 Acquisition Date | 2016-03-29T18:44:04 |
| 19 Modification Date | 2016-03-30T02:47:00 |
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| 23 Nucleus | 1H |
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| Parameter | Value |
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| 6 Site | |
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| 8 Author | |
| 9 Solvent | cdcl3 |
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