Supporting Information

Ultrafast broadband optical limiting in simple pyrene-based molecules with high transmittance from visible to infrared regions

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Figure S1: ^{1}H NMR for **P1**(top panel) and **P2** (bottom panel)

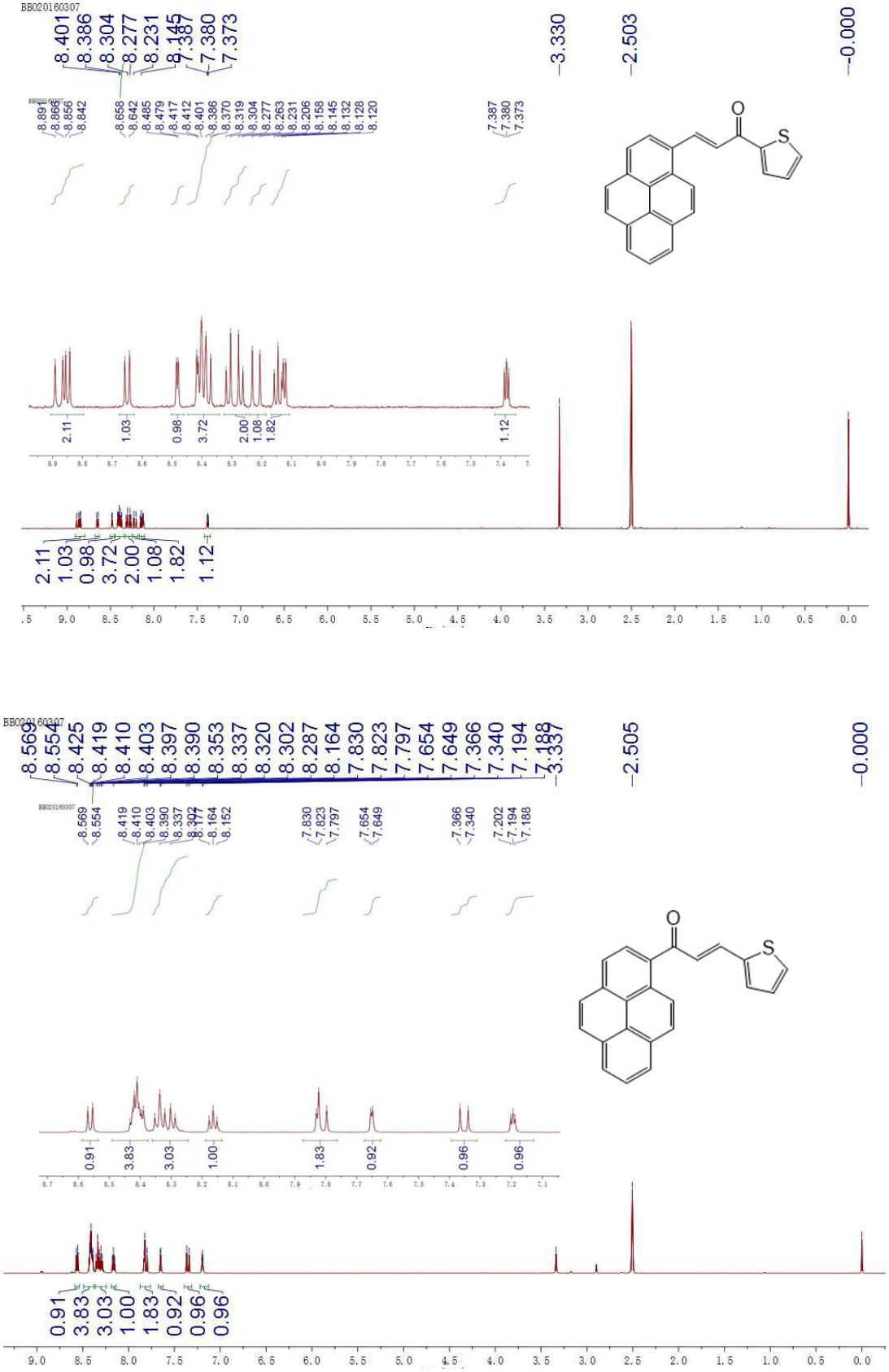


Figure S2: ^{13}C NMR for **P1**(top panel) and **P2** (bottom panel)

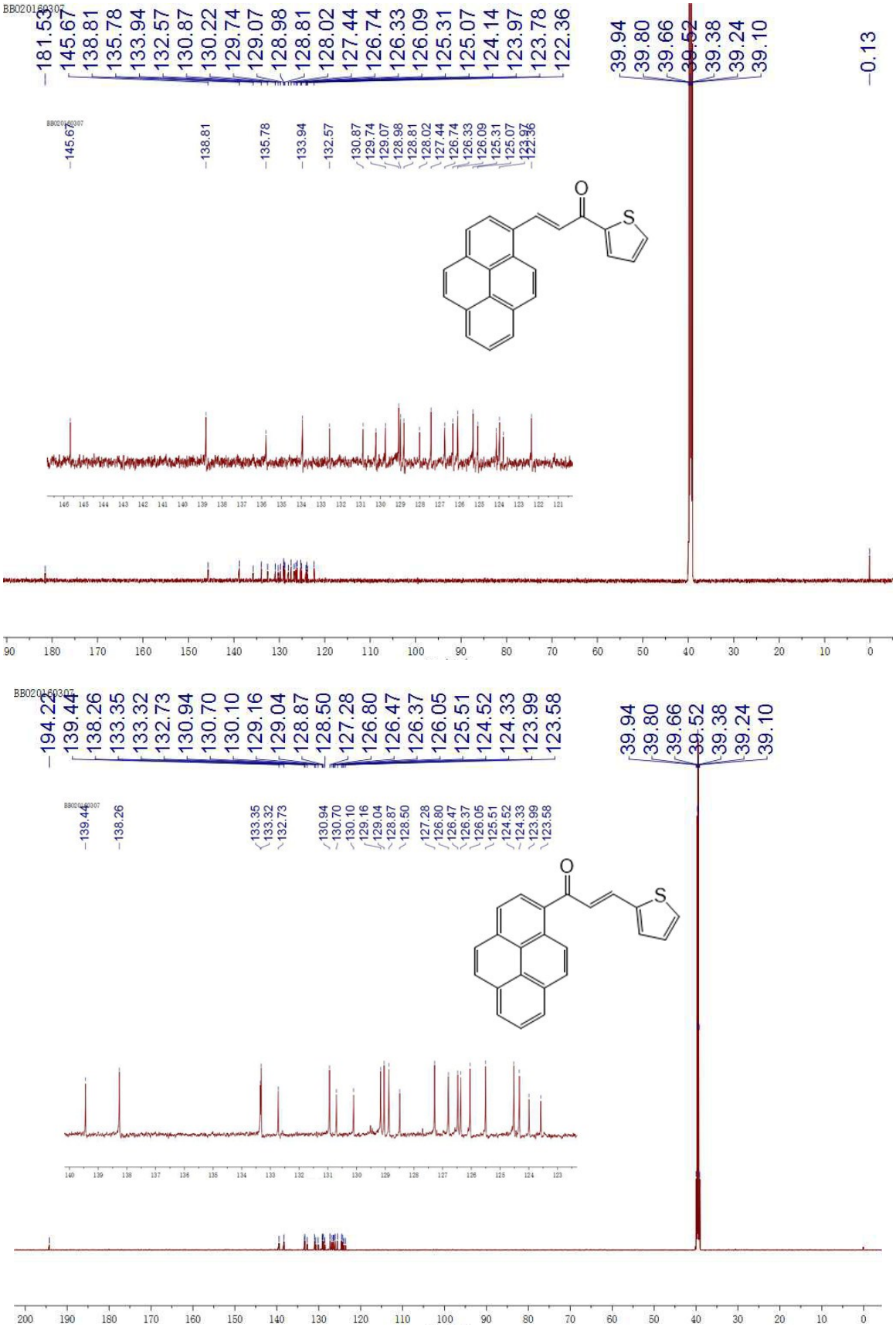


Figure S3: MALDI-TOF mass spectroscopes for **P1**(left panel) and **P2** (right panel)

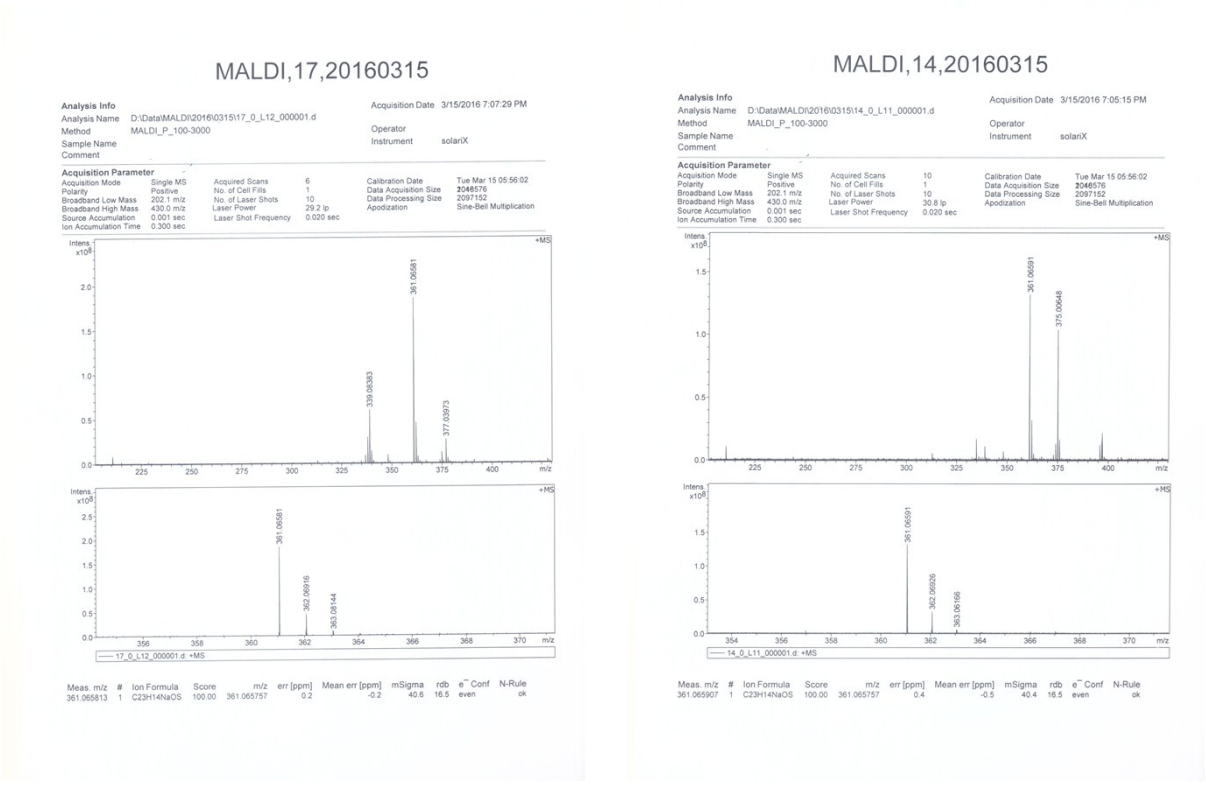


Figure S4: The degenerate pump-probe data of **P1** at 532 nm wavelength

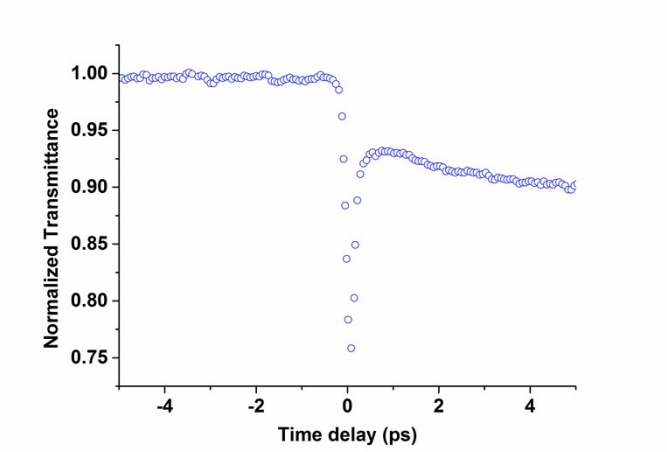


Figure S5: The degenerate pump-probe data of **P1** at 800 nm wavelength

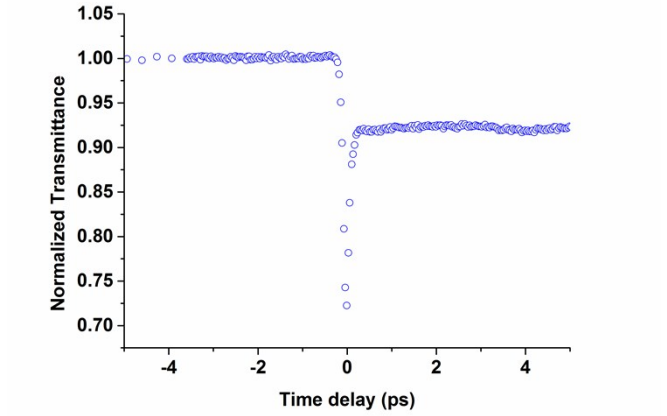


Figure S6: Open-aperture Z-scans of **P1** at different energies under 515 nm, 532 nm, 600 nm, 650 nm, 750 nm, 800 nm, 850 nm, 900 nm, respectively. The different color circles are the experimental data and the corresponding color solid lines represent the theoretical fitting.

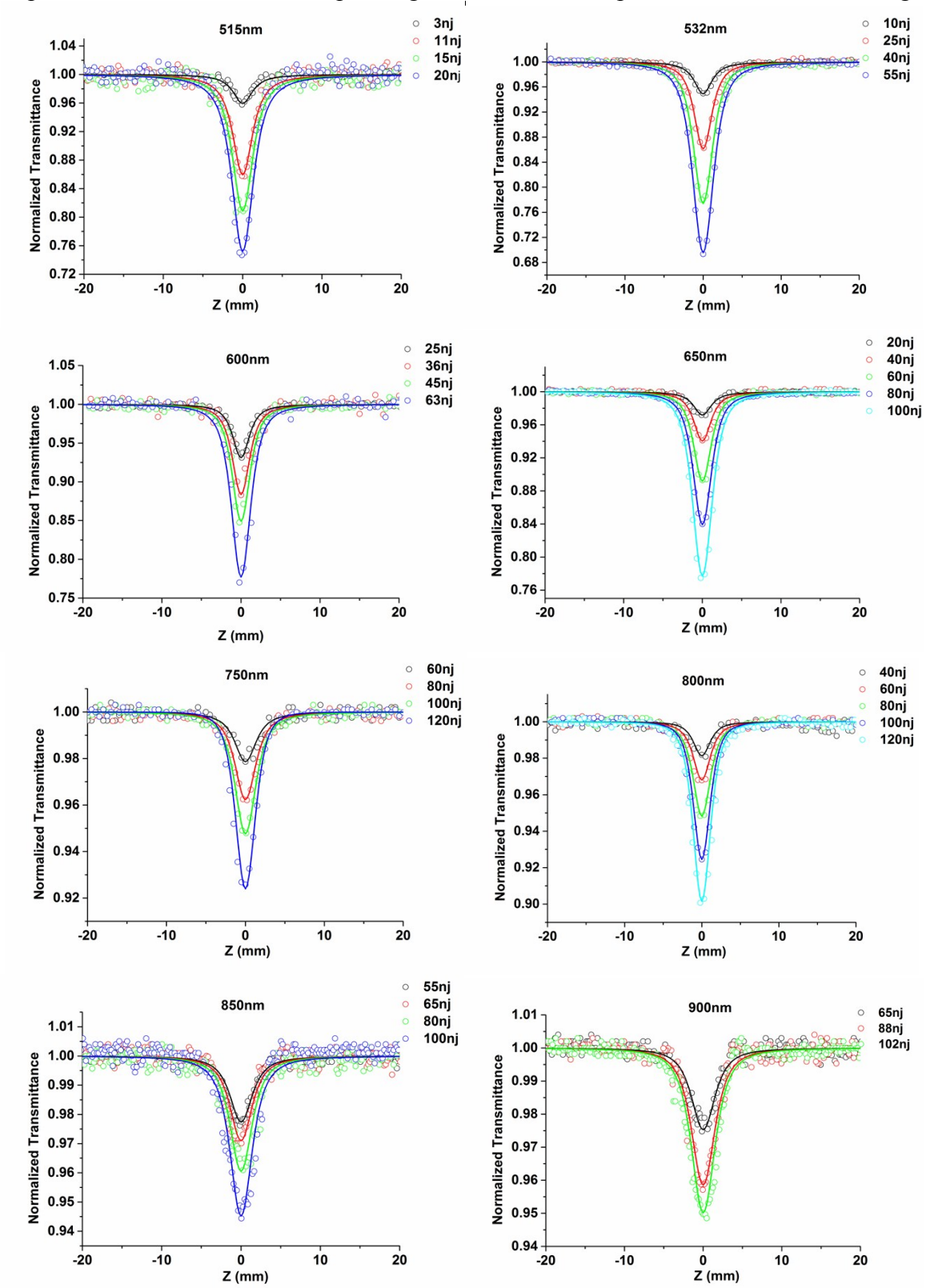
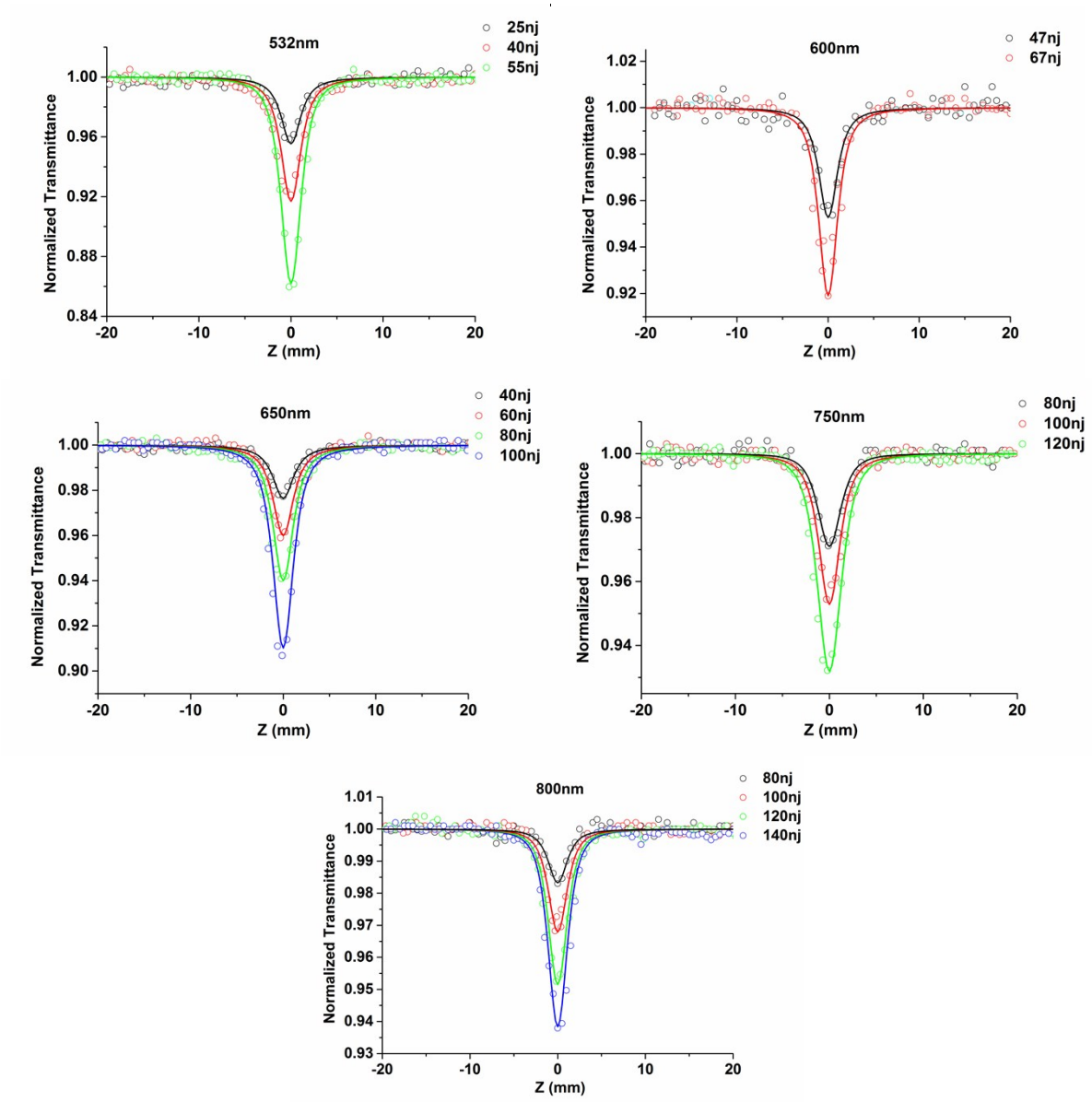


Figure S7: Open-aperture Z-scans of **P2** at different energies under 532 nm, 600 nm, 650 nm, 750 nm, 800 nm, respectively. The different color circles are the experimental data and the corresponding color solid lines represent the theoretical fitting.



The input structure data of **P1** for quantum chemical calculations:

```
%chk=P1.chk
%mem=3000mb
%nproc=8
#p b3lyp/6-31+g** opt freq SCRF=(CPCM,Solvent=DMSO) test

syl P1 in DMSO 20150316

 0  1
   6         0      -3.388333   -1.469645    0.281358
   6         0      -1.532893    0.153116   -0.260430
   6         0      -2.004873   -0.940044    0.373969
   6         0      -0.163716    0.686791   -0.253660
   6         0      -0.052729    2.090211   -0.270129
   6         0       1.168257    2.734637   -0.156263
   6         0       2.357314    1.997168   -0.044866
   6         0       2.290453    0.570414   -0.093531
   6         0       1.026388   -0.094826   -0.215768
   6         0       3.500719   -0.187084   -0.020931
   6         0       3.463604   -1.611109   -0.103657
   6         0       2.193085   -2.245072   -0.297091
   6         0       1.036801   -1.526799   -0.353580
   6         0       3.634287    2.635585    0.100316
   6         0       4.782094    1.909259    0.189816
   6         0       4.758794    0.474975    0.129409
   6         0       5.931729   -0.292857    0.209905
   6         0       5.882352   -1.683751    0.135892
   6         0       4.662888   -2.337916   -0.022706
   6         0      -4.563792   -0.587598    0.069944
   6         0      -5.809069   -1.046168   -0.301722
   6         0      -6.796054   -0.028254   -0.359924
   6         0      -6.302185    1.203565   -0.011897
  16         0      -4.620785    1.137734    0.380698
   8         0      -3.565870   -2.681818    0.387723
   1         0      -2.242330    0.765629   -0.814465
   1         0      -1.346002   -1.588015    0.943957
   1         0      -0.962279    2.681990   -0.337307
   1         0       1.212001    3.820748   -0.144772
   1         0       2.166277   -3.325688   -0.414565
   1         0       0.103180   -2.042147   -0.539531
   1         0       3.664307    3.721737    0.138907
   1         0       5.742146    2.406871    0.303522
   1         0       6.886463    0.213349    0.329864
   1         0       6.800920   -2.260647    0.199020
   1         0       4.628605   -3.422637   -0.087550
   1         0      -5.982754   -2.094285   -0.514499
   1         0      -7.829609   -0.199656   -0.640169
   1         0      -6.832153    2.145958    0.037901
```

The input structure data of **P2** for quantum chemical calculations:

```
%chk=P2.chk
%mem=3000mb
%nproc=8
#p b3lyp/6-31+g** opt freq SCRF=(CPCM,Solvent=DMSO) test

syl P2 in DMSO 20150316

 0  1
  6         0       3.018899    0.005468    0.053384
  6         0       1.226578   -1.322117   -1.128553
  6         0       2.624569   -0.981628   -0.782283
  8         0       0.988119   -2.447015   -1.567214
  6         0       0.133855   -0.306644   -0.943540
  6         0       0.361758    1.015919   -1.354185
  6         0      -0.629214    1.985986   -1.277286
  6         0      -1.894842    1.674645   -0.760244
  6         0      -2.156317    0.336697   -0.329249
  6         0      -1.143247   -0.670155   -0.435642
  6         0      -3.443287    0.012150    0.200896
  6         0      -3.724070   -1.316919    0.636107
  6         0      -2.688011   -2.301778    0.524500
  6         0      -1.462253   -2.000548    0.012959
  6         0      -2.933989    2.660629   -0.653531
  6         0      -4.157400    2.346191   -0.147402
  6         0      -4.457560    1.014162    0.298407
  6         0      -5.713323    0.669335    0.822666
  6         0      -5.977100   -0.632357    1.246083
  6         0      -4.995000   -1.615932    1.154591
  6         0       4.367329    0.292153    0.483767
  6         0       4.749995    1.293098    1.355944
  6         0       6.149998    1.341169    1.592929
  6         0       6.831780    0.376051    0.899636
 16         0       5.774687   -0.609438   -0.054954
  1         0       2.266202    0.666587    0.478839
  1         0       3.345279   -1.692743   -1.182137
  1         0       1.329273    1.277241   -1.770861
  1         0      -0.428251    2.997303   -1.621877
  1         0      -2.902317   -3.315106    0.855898
  1         0      -0.709472   -2.771781   -0.081672
  1         0      -2.718730    3.672354   -0.988526
  1         0      -4.933919    3.103679   -0.072111
  1         0      -6.483831    1.433167    0.894279
  1         0      -6.955089   -0.881106    1.648963
  1         0      -5.205235   -2.630342    1.484561
  1         0       4.034427    1.970937    1.810102
  1         0       6.630179    2.059087    2.248490
  1         0       7.896643    0.184392    0.893316
```