

Electronic Supplementary Information for:

Thienyl-Substituted Methanofullerene Derivatives for Organic Photovoltaic Cells

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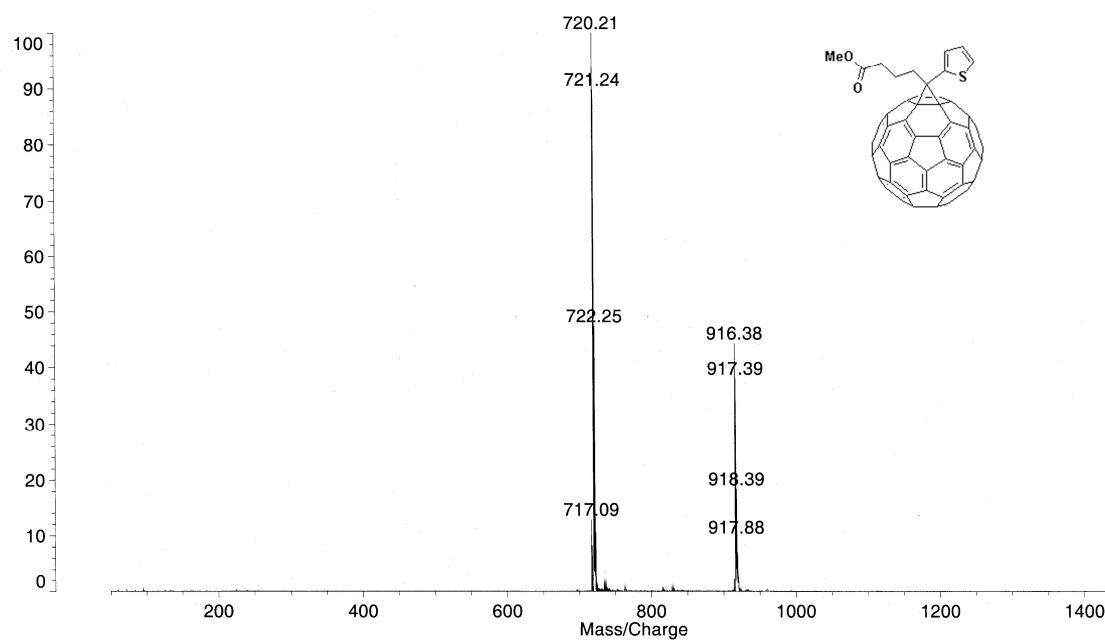
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MALDI-TOF mass spectra

(a) the monoadduct **1**

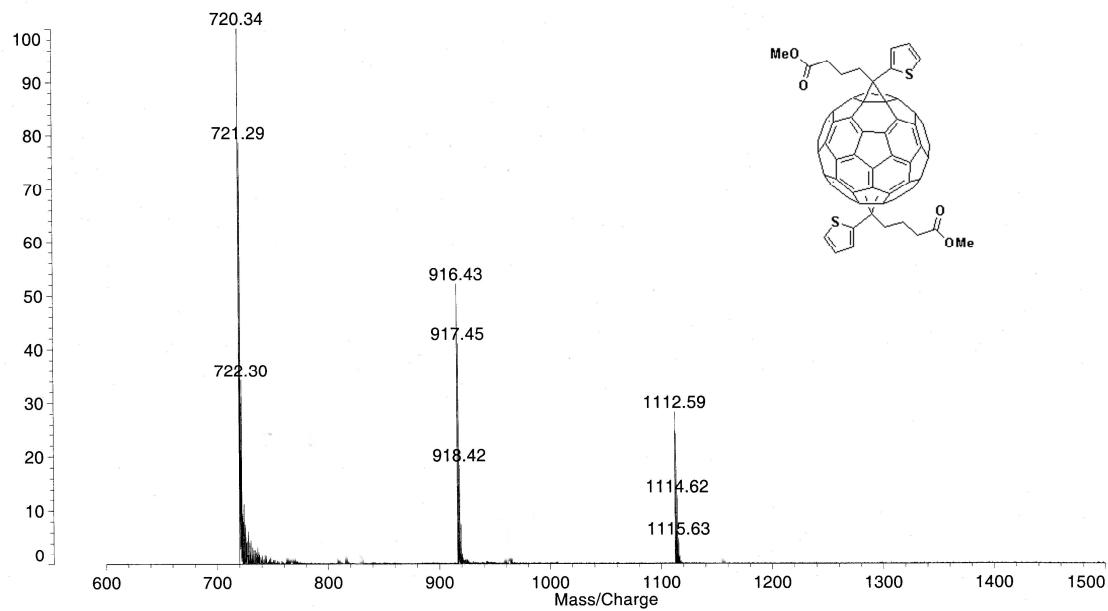
Data: H4a20001.H4 25 Jul 2008 1:29 Cal: InsulinB_CHCA 21 Jun 2007 11:27
Kratos PC Axima CFR V2.3.5: Mode Linear_neg, Power: 77, P.Ext. @ 916 (bin 52)
%Int. 1795 mV[sum= 53842 mV] Profiles 1-30 Smooth Gauss 1 -Baseline 20



(b) the bisadduct **2**

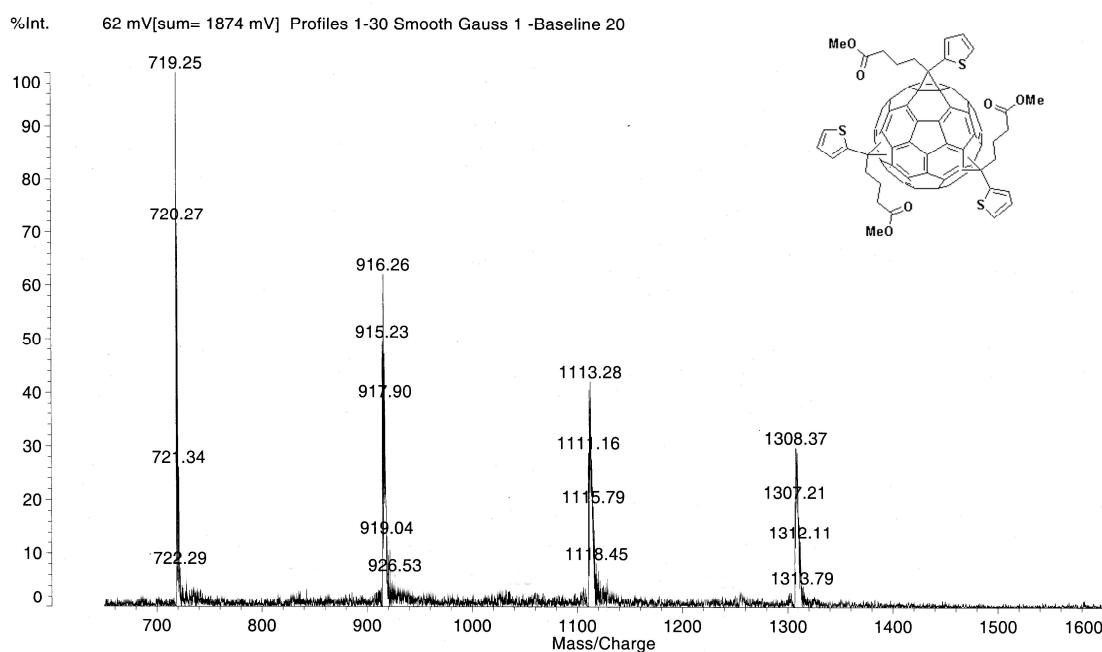
Data: Column20001.A2 30 Apr 2009 20:56 Cal: InsulinB_CHCA 21 Jun 2007 13:05
Kratos PC Axima CFR V2.3.5: Mode Reflectron_neg, Power: 39, P.Ext. @ 2500 (bin 128)

%Int. 196 mV[sum= 5887 mV] Profiles 1-30 Smooth Gauss 1 -Baseline 20



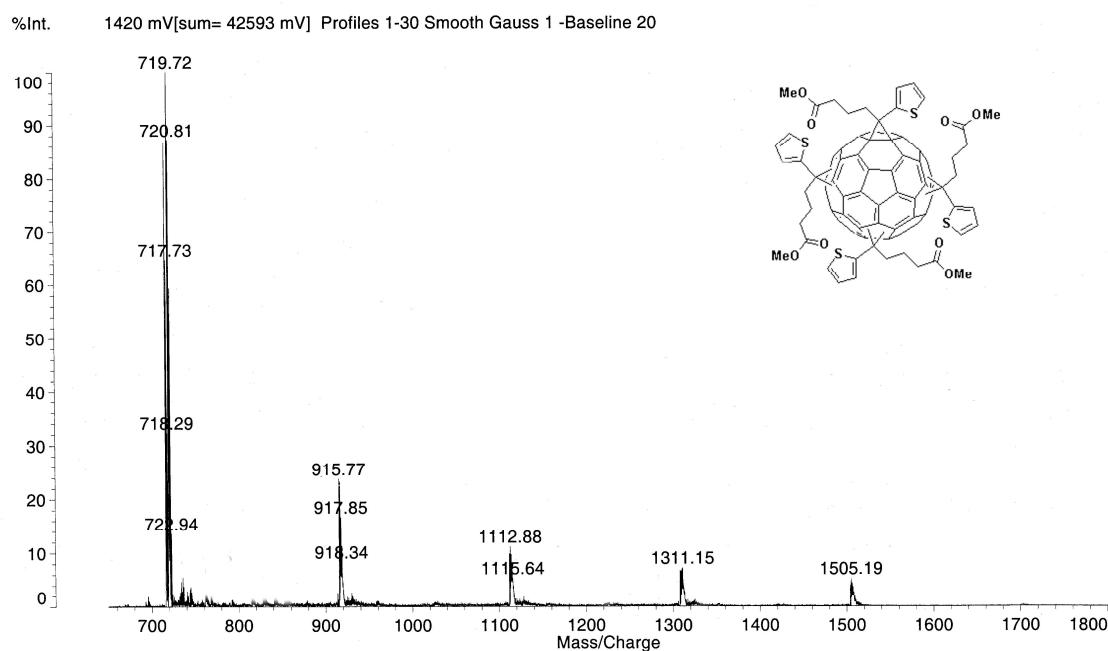
(c) the trisadduct 3

Data: <Untitled>.B1 1 May 2009 17:26 Cal: InsulinB_CHCA 21 Jun 2007 11:27
 Kratos PC Axima CFR V2.3.5: Mode Linear_neg, Power: 37, P.Ext. @ 670 (bin 47)



(d) the tetrakisadduct 4

Data: Tetra0002.B4 12 May 2009 17:48 Cal: InsulinB_CHCA 21 Jun 2007 11:27
 Kratos PC Axima CFR V2.3.5: Mode Linear_neg, Power: 80, P.Ext. @ 760 (bin 47)



(e) the monoadduct with dimethoxy group **5**

Data: <Untitled>.C5 11 May 2009 14:37 Cal: InsulinB_CHCA 21 Jun 2007 11:27
Kratos PC Axima CFR V2.3.5: Mode Linear_neg, Power: 80, P.Ext. @ 760 (bin 47)

%Int. 1451 mV[sum= 58035 mV] Profiles 1-40 Smooth Gauss 1 -Baseline 20

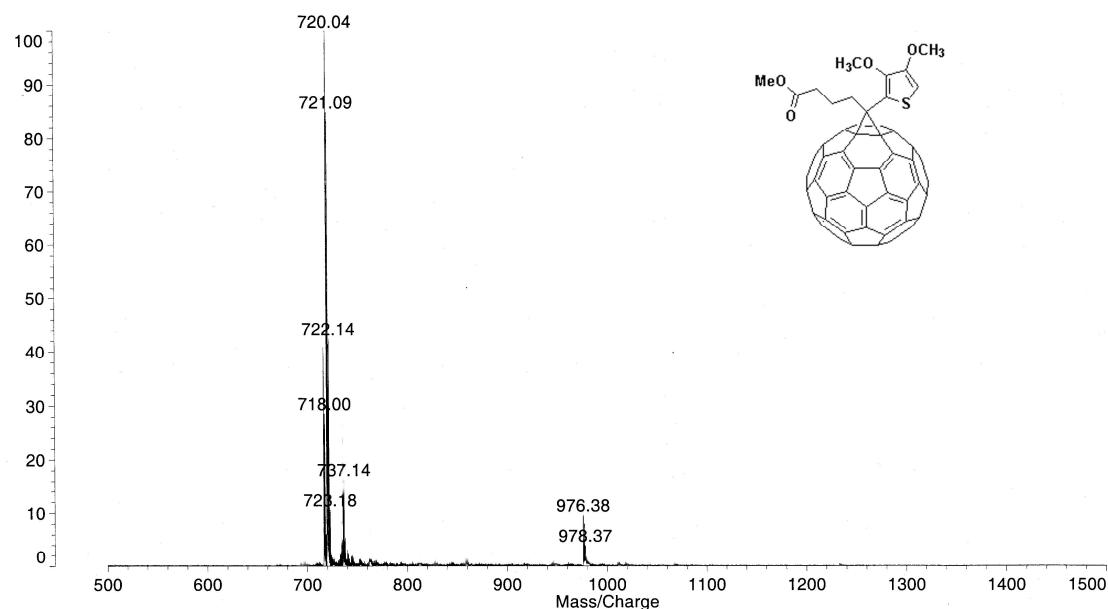
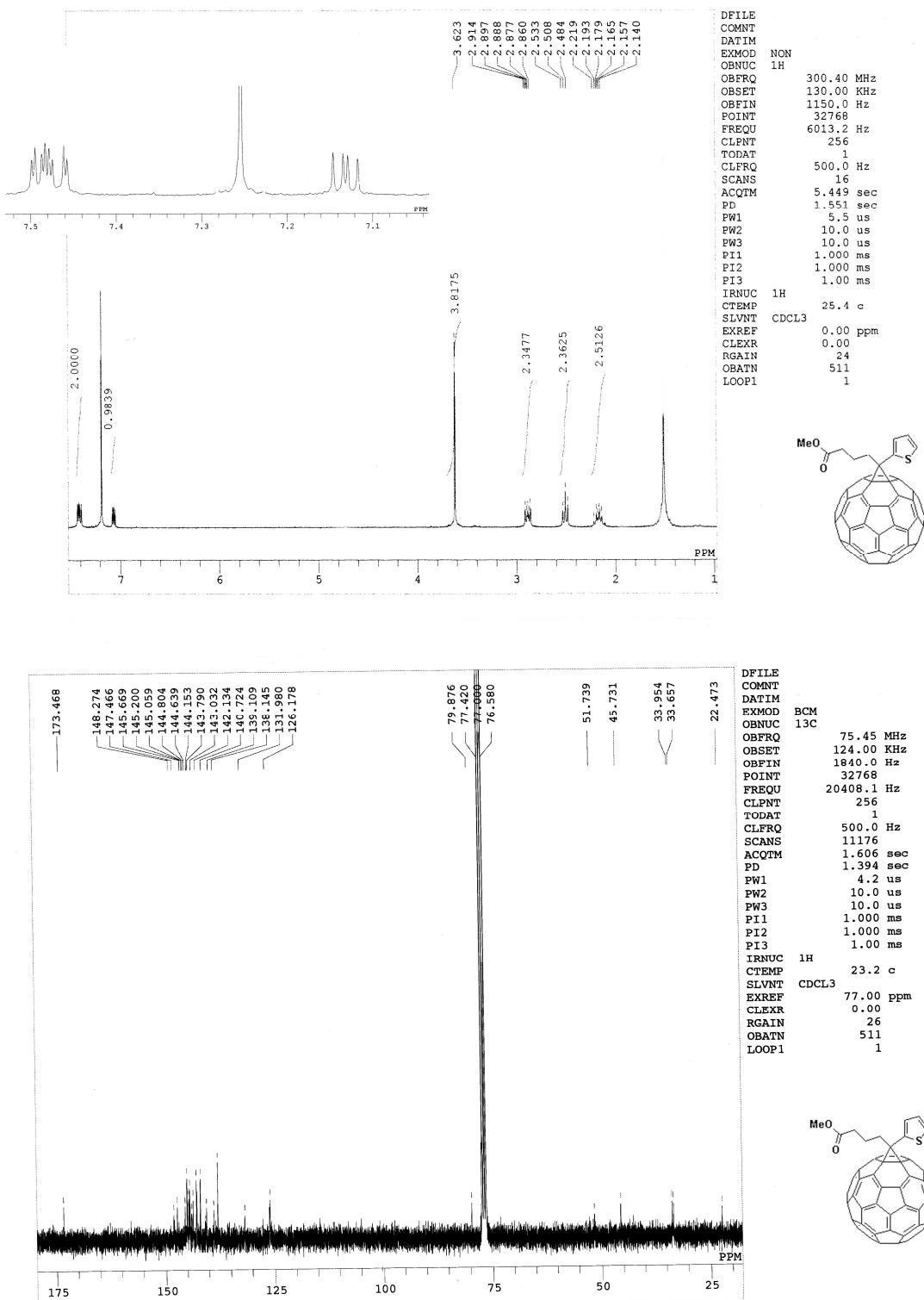


Figure S1. MALDI-TOF mass spectra of (a) the monoadduct **1**, (b) the bisadduct **2**, (c) the trisadduct **3**, (d) the tetrakisadduct **4** and (e) the monoadduct with dimethoxy group **5** using dithiranol as the matrix.



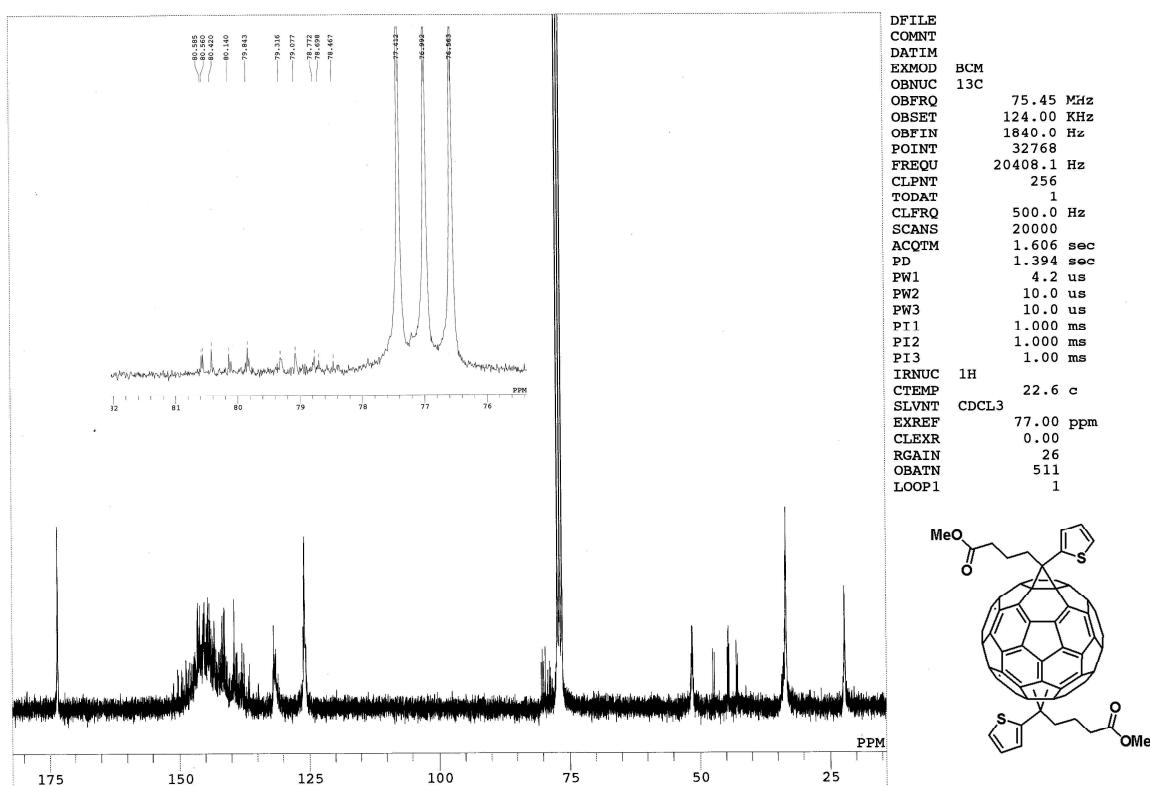
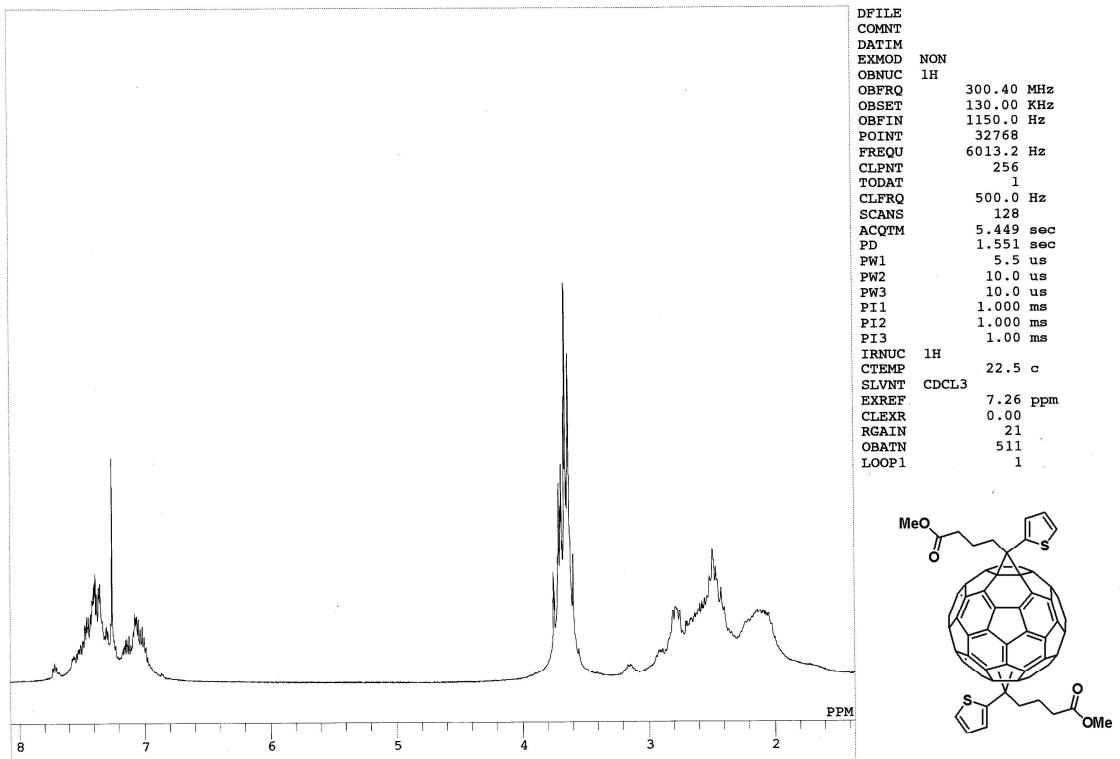


Figure S2. (b) ¹H NMR and ¹³C NMR spectra of compound 2.

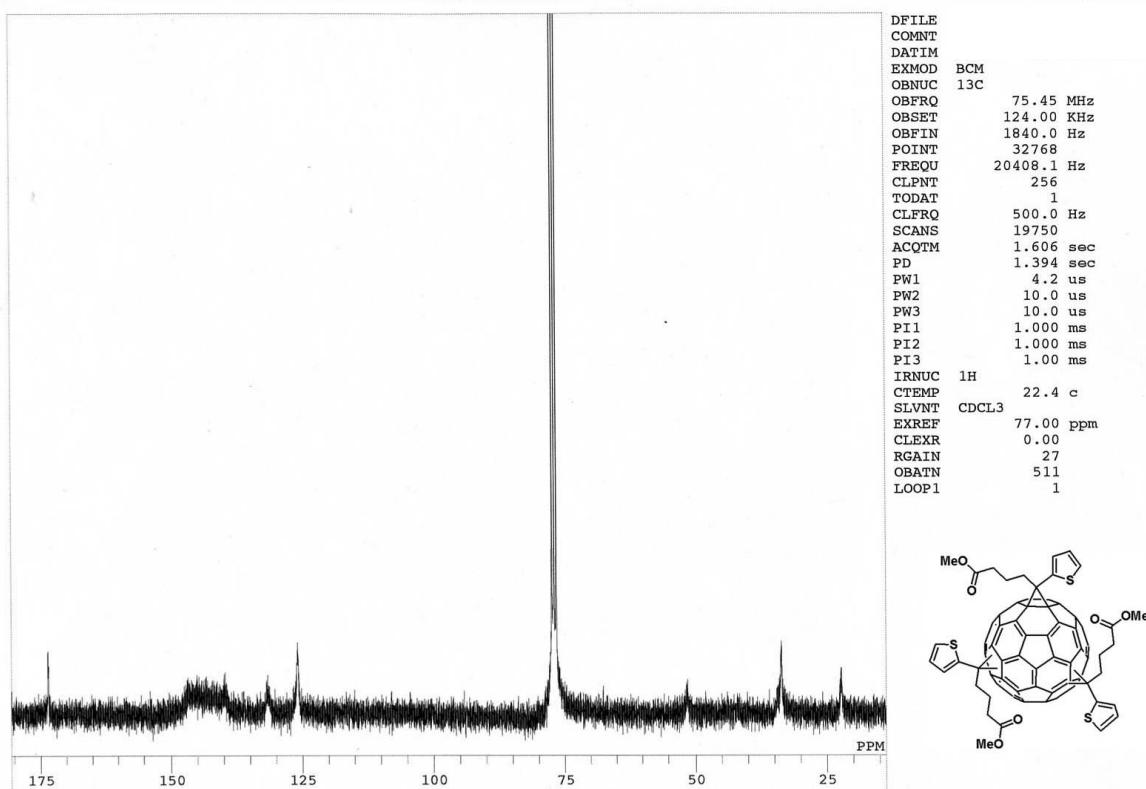
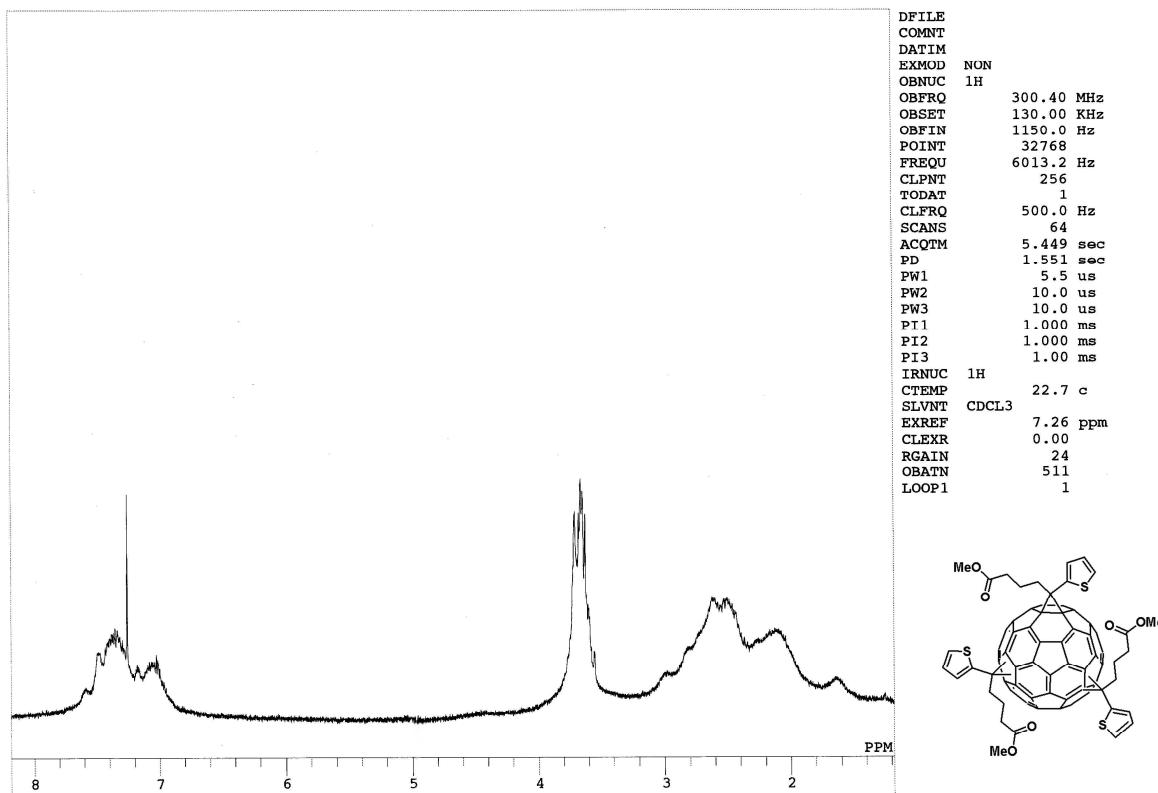


Figure S2. (c) ¹H NMR and ¹³C NMR spectra of compound 3.

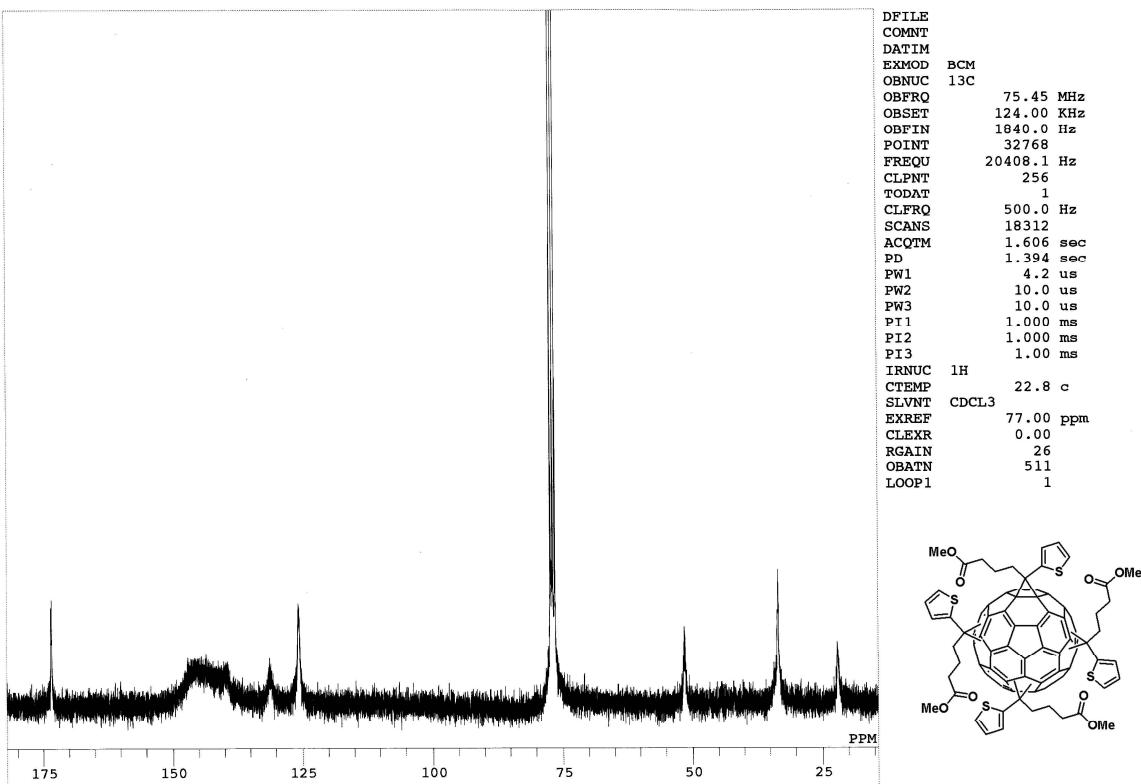
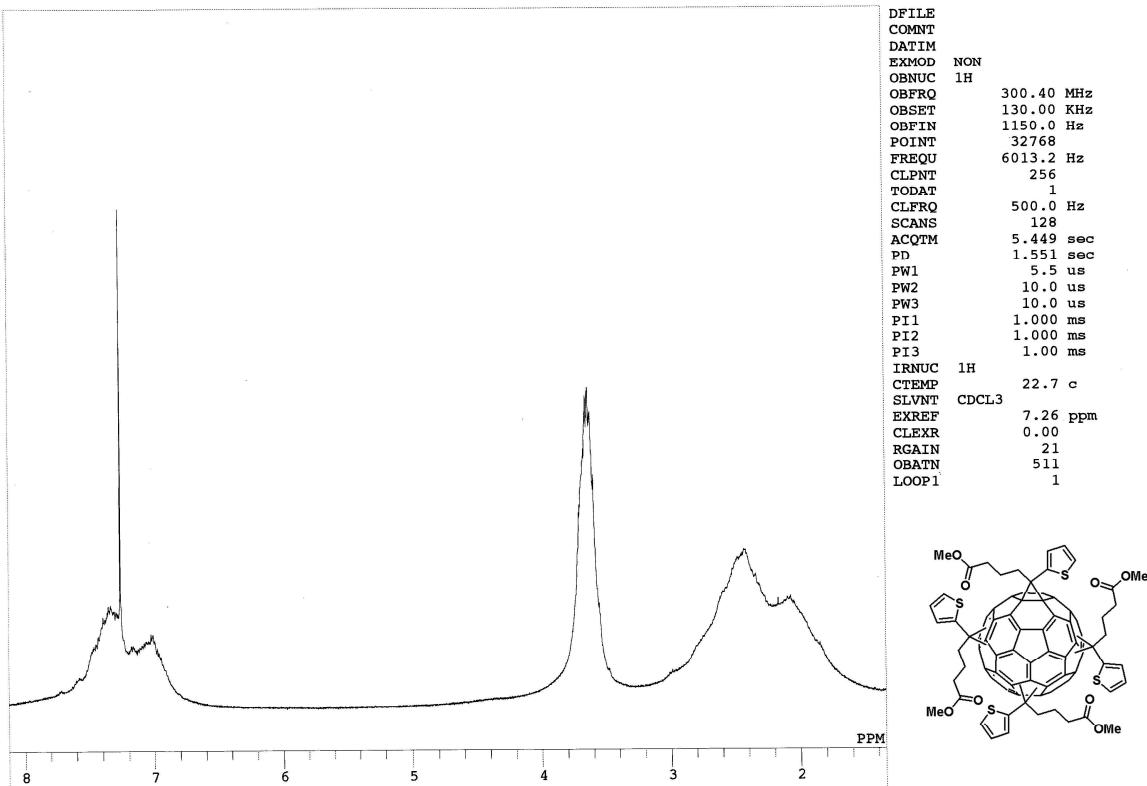


Figure S2. (d) ^1H NMR and ^{13}C NMR spectra of compound 4.

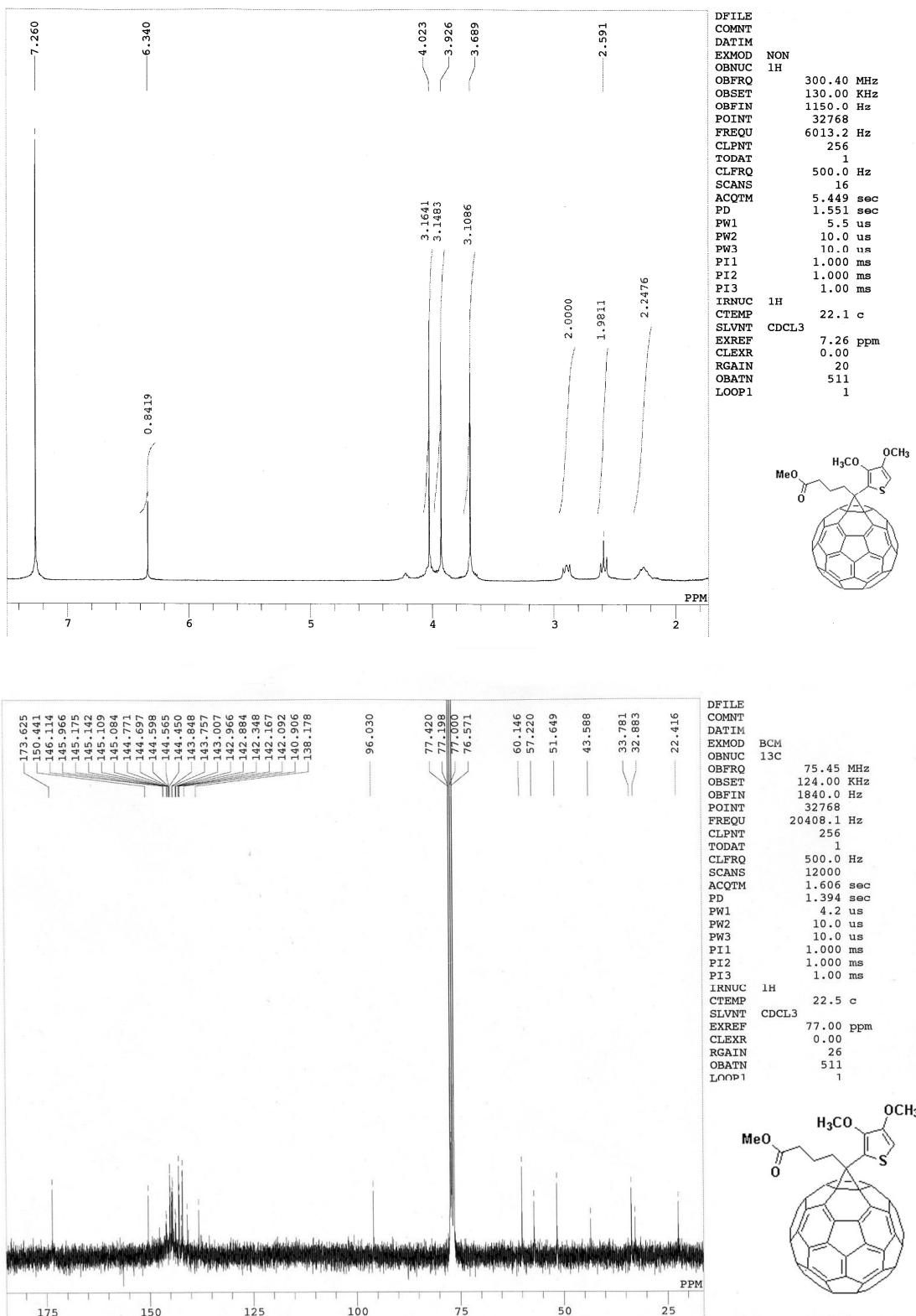


Figure S2. (e) ¹H NMR and ¹³C NMR spectra of compound 5.

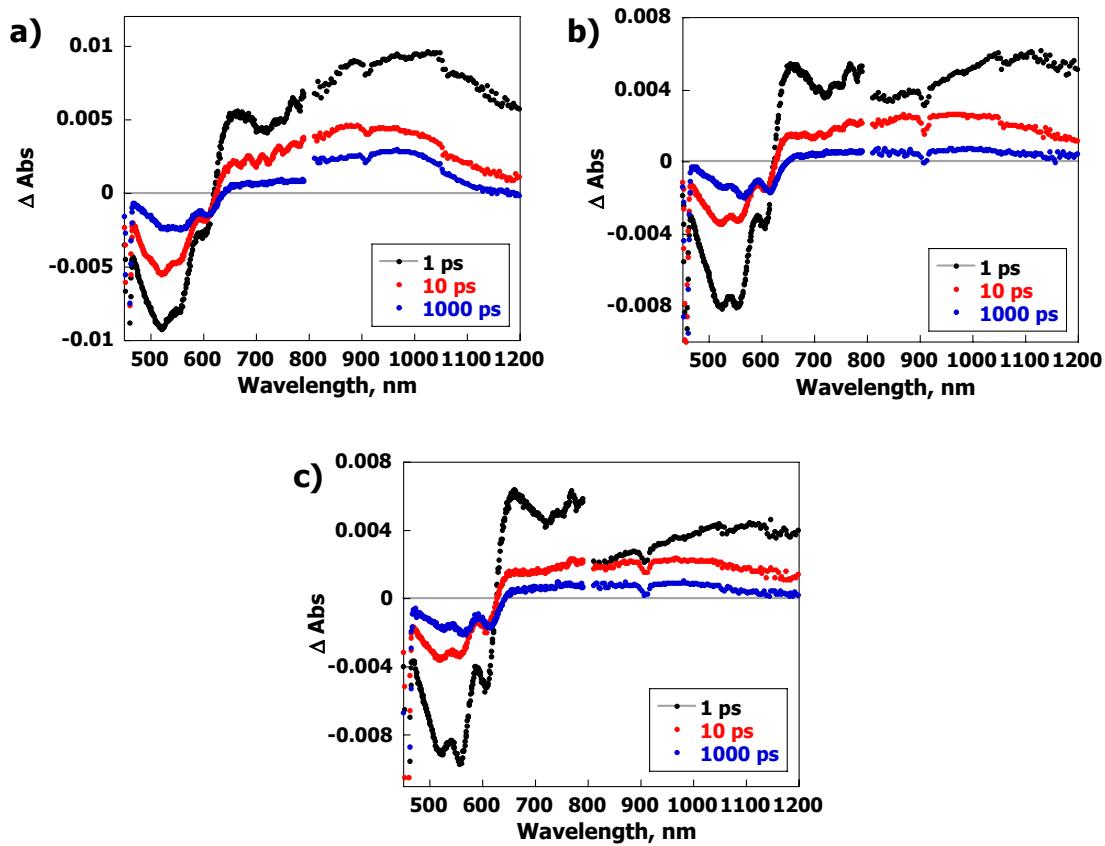


Figure S3. Transient absorption spectra of (a) P3HT:PCBM film, (b) P3HT:**2** film and (c) P3HT:**5** film obtained by femtosecond laser flash photolysis taken at 1 and 1000 ps after laser excitation (450 nm) at 298K.

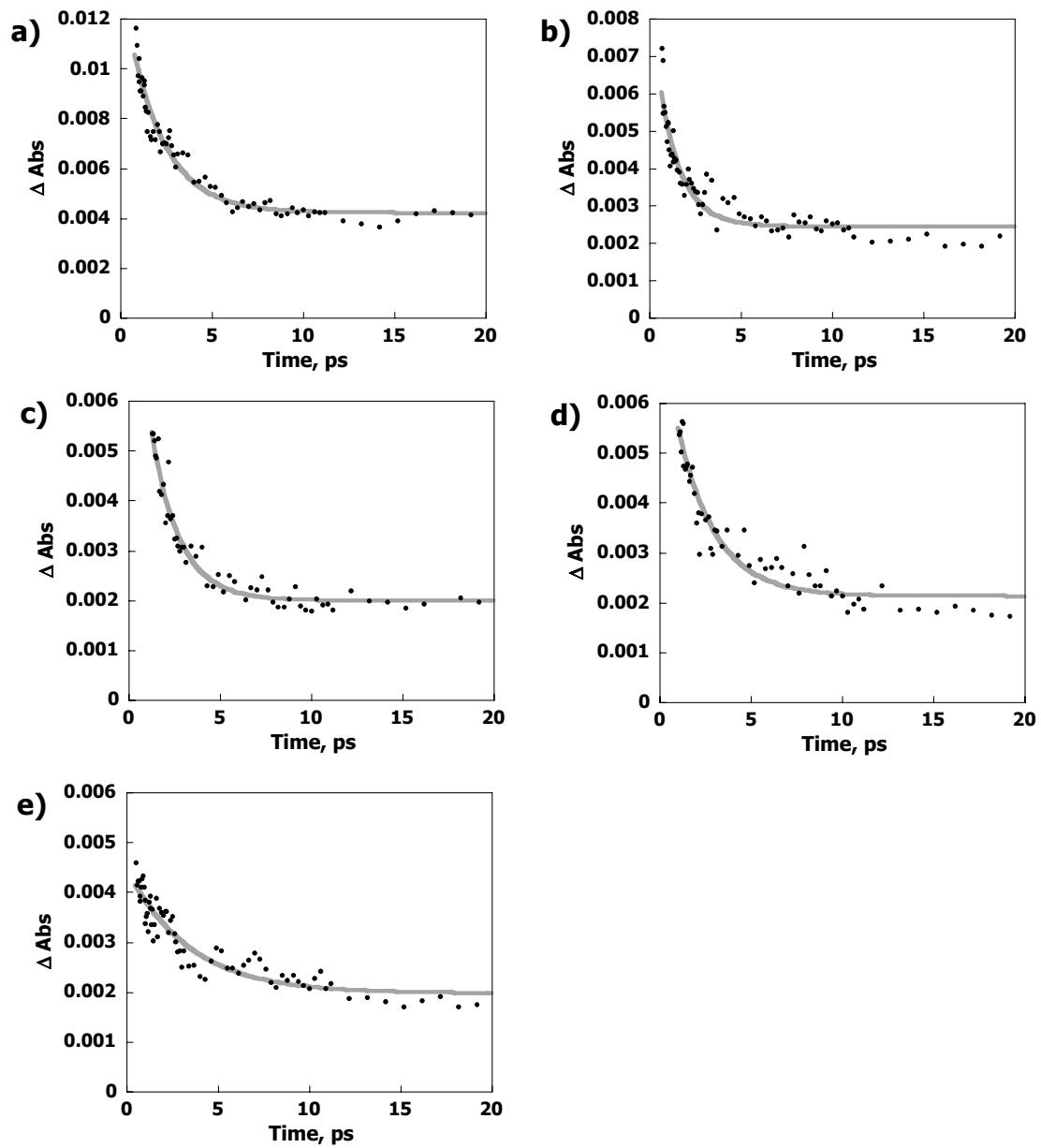


Figure S4. Time profiles of absorbance (a) P3HT:PCBM film, (b) P3HT:**2** film, (c) P3HT:**3** film, (d) P3HT:**4** film and (e) P3HT:**5** film of at 1000 nm in the 20 ps range.

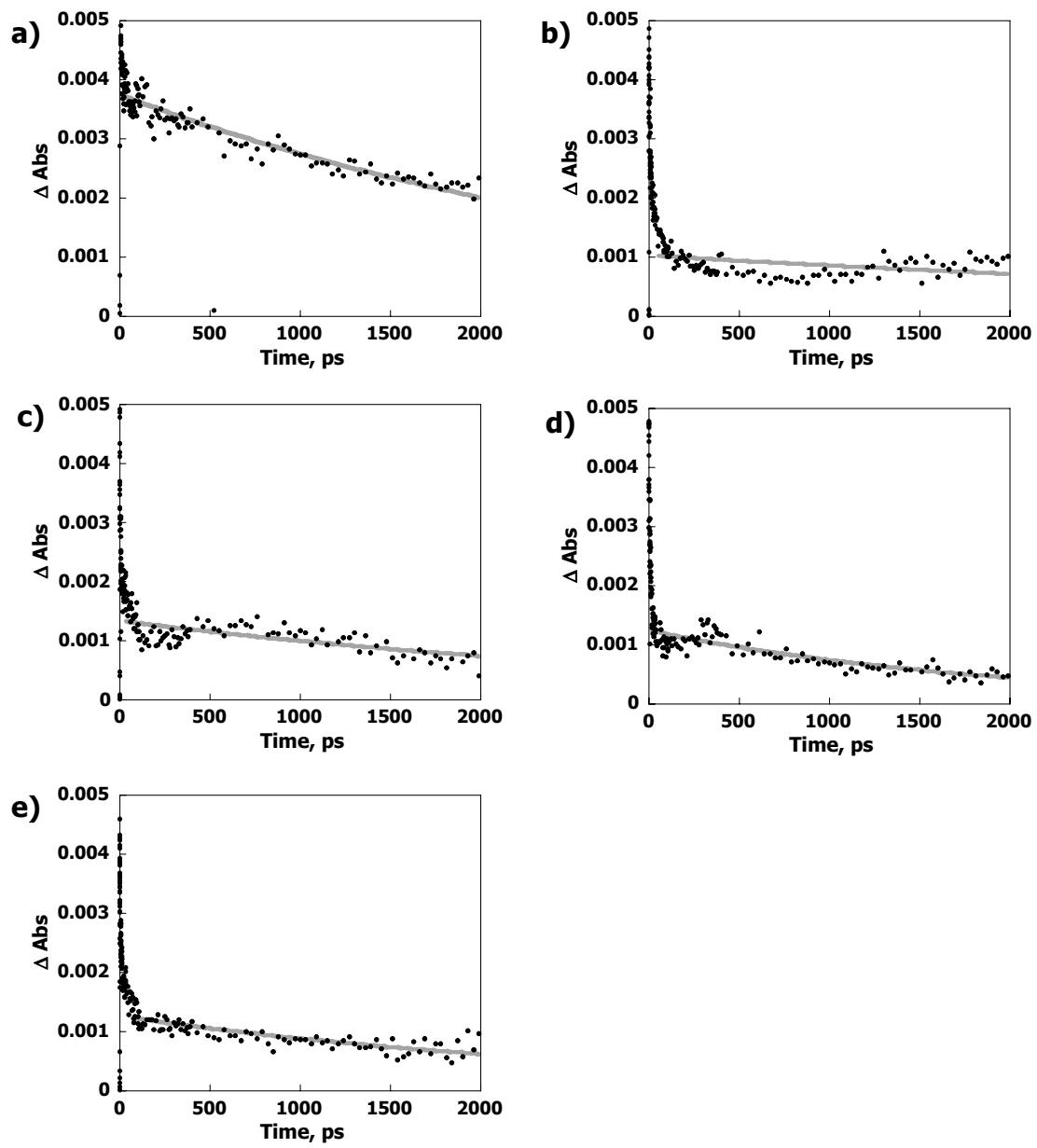


Figure S5. Time profiles of absorbance (a) P3HT:PCBM film, (b) P3HT:**2** film, (c) P3HT:**3** film, (d) P3HT:**4** film and (e) P3HT:**5** film of at 1000 nm in the 2000 ps range.

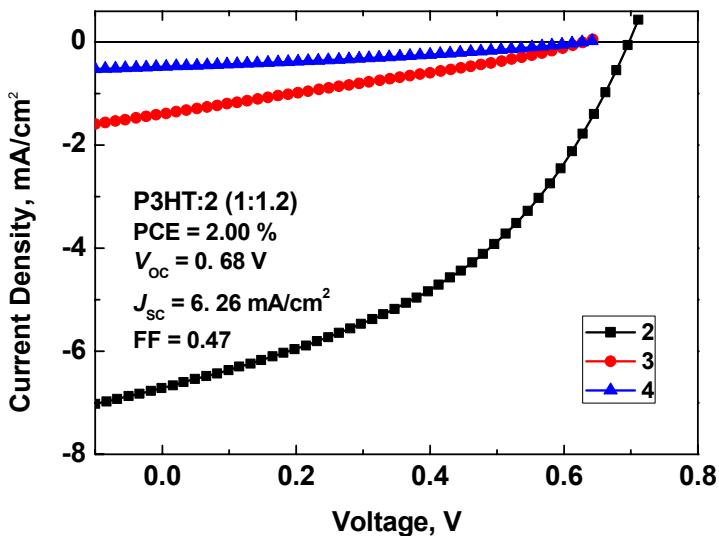


Figure S6. Current density-voltage (J - V) characteristics of P3HT:**2** (1:1.2), P3HT:**3** (1:1.4) and P3HT:**4** (1:1.6) blend solar cells under AM 1.5 G simulated solar illumination (100 mW/cm²).