

SUPPORTING INFORMATION

Photovoltaic Studies on Perylene Diimide-based Copolymers Containing Electronic Push-Pull Chromophores

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Sample code: **1,7-DPPDI-PFDA copolymer**

Sample Name:	S 18
Sample Type:	Broad Unknown
Vial:	18
Injection #:	1
Injection Volume:	80.00 ul
Run Time:	34.0 Minutes
Date Acquired:	10/23/2012 9:37:01 PM IST
Date Processed:	10/29/2012 12:10:05 PM IST

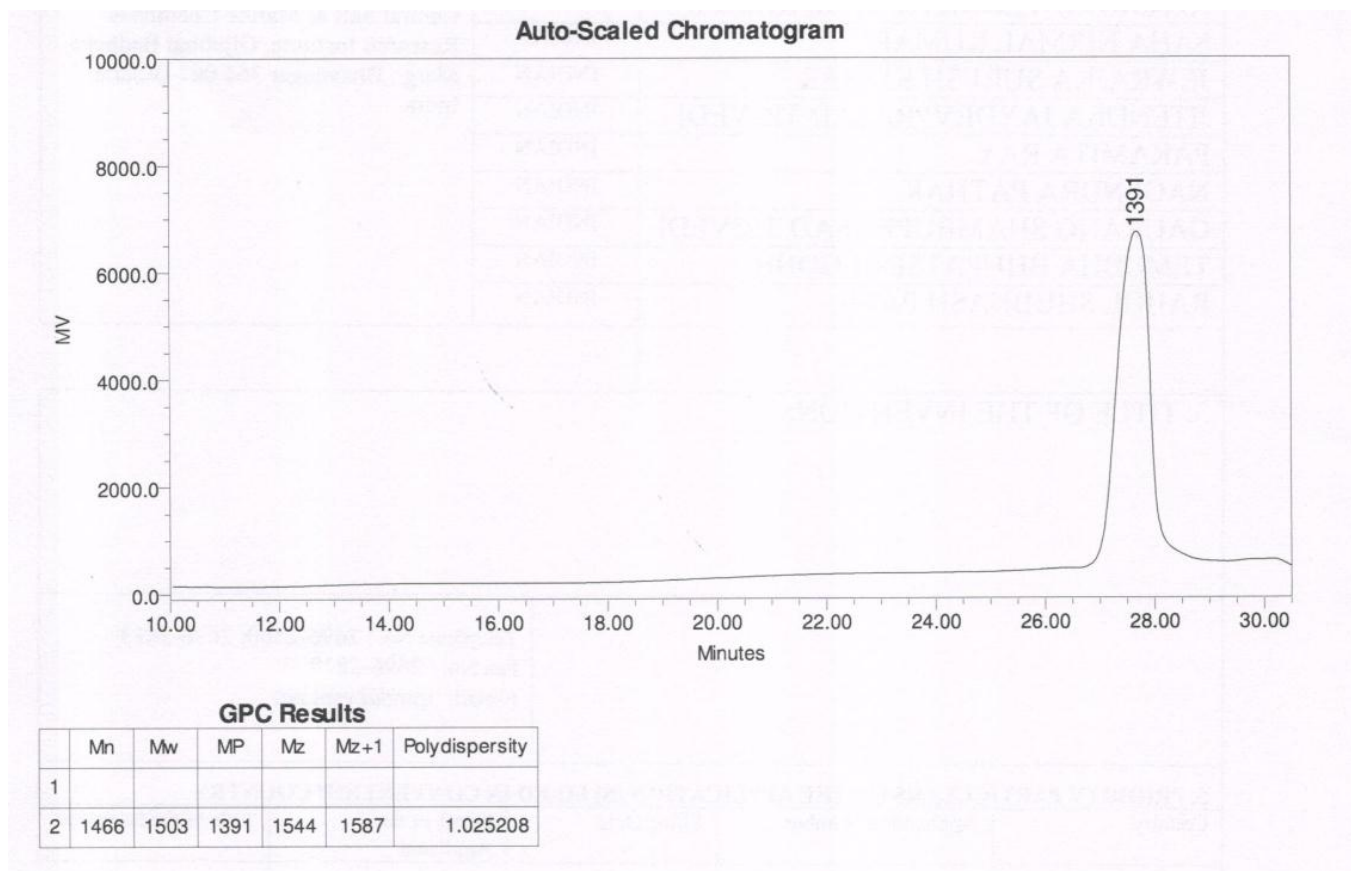


Figure S1. Gel permeation chromatogram of 1,7-DPPDI-PFDA copolymer in THF relative to low molecular weight polystyrene standard.

Sample code: **1,7-DBPDI-PFDA copolymer**

Sample Name: S 20
Sample Type: Broad Unknown
Vial: 20
Injection #: 1
Injection Volume: 80.00 ul
Run Time: 34.0 Minutes

Date Acquired: 10/23/2012 10:47:36 PM IST
Date Processed: 10/29/2012 12:10:05 PM IST

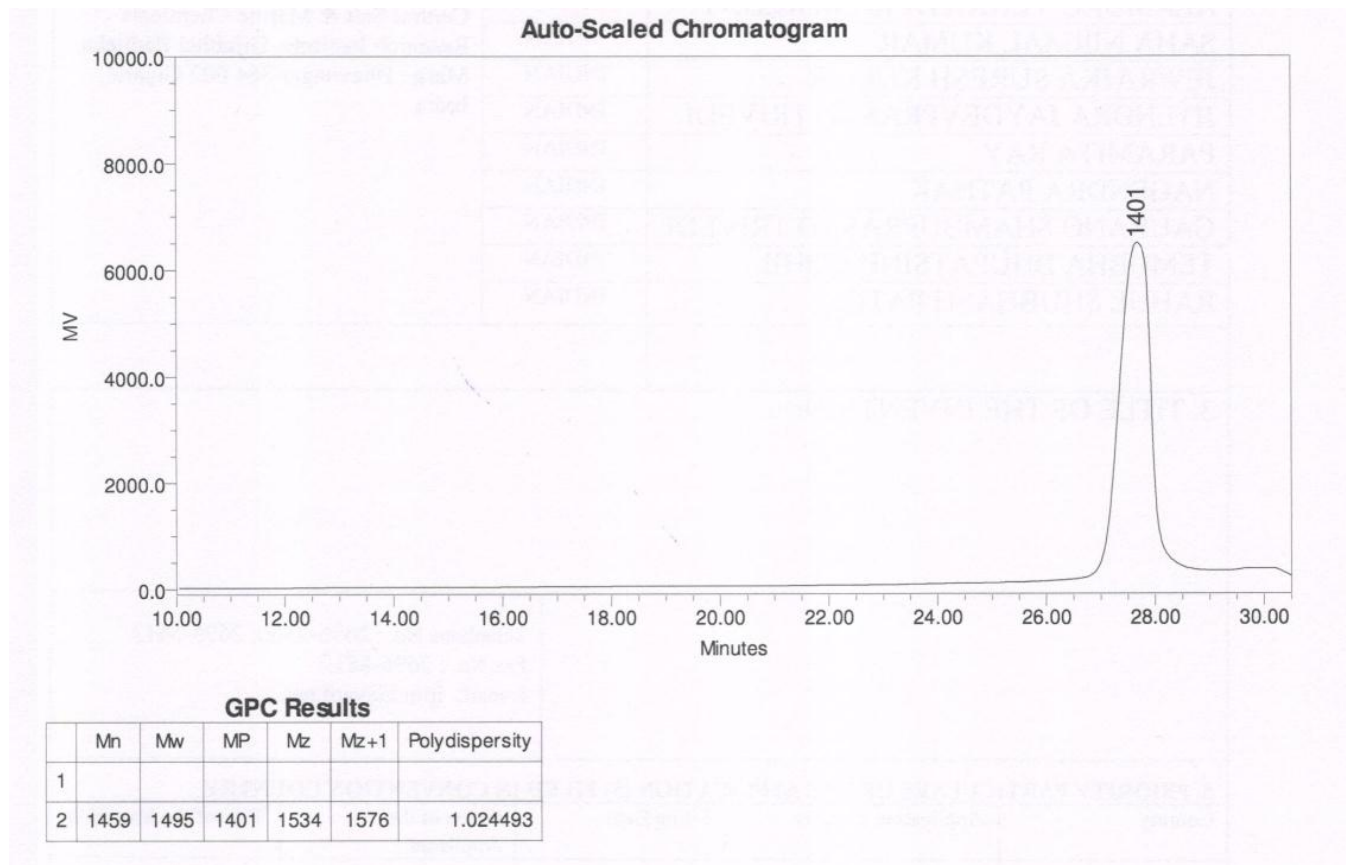


Figure S2. Gel permeation chromatogram of 1,7-DBPDI-PFDA copolymer in THF relative to low molecular weight polystyrene standard.

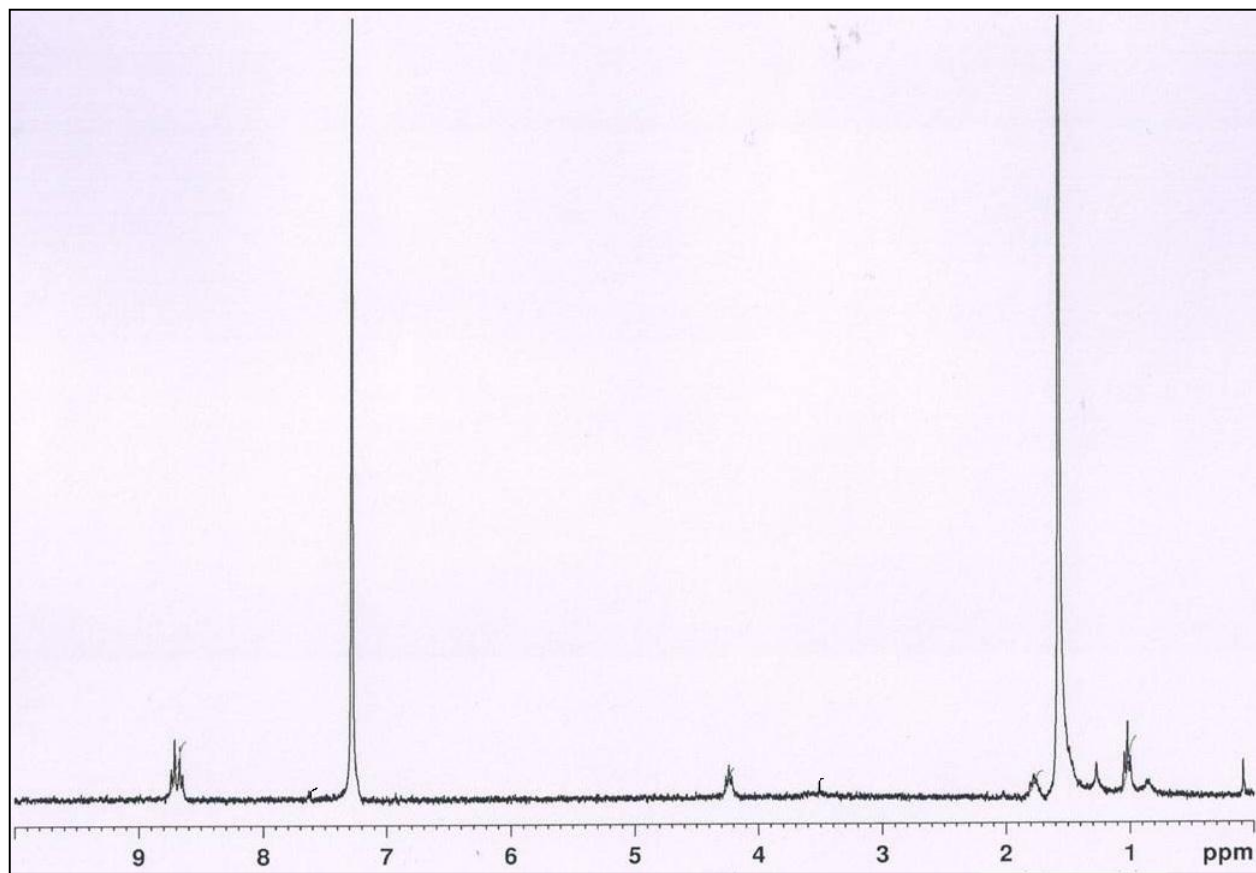


Figure S3. ¹H-NMR spectrum of compound **3** in CDCl₃ and TMS as internal standard.

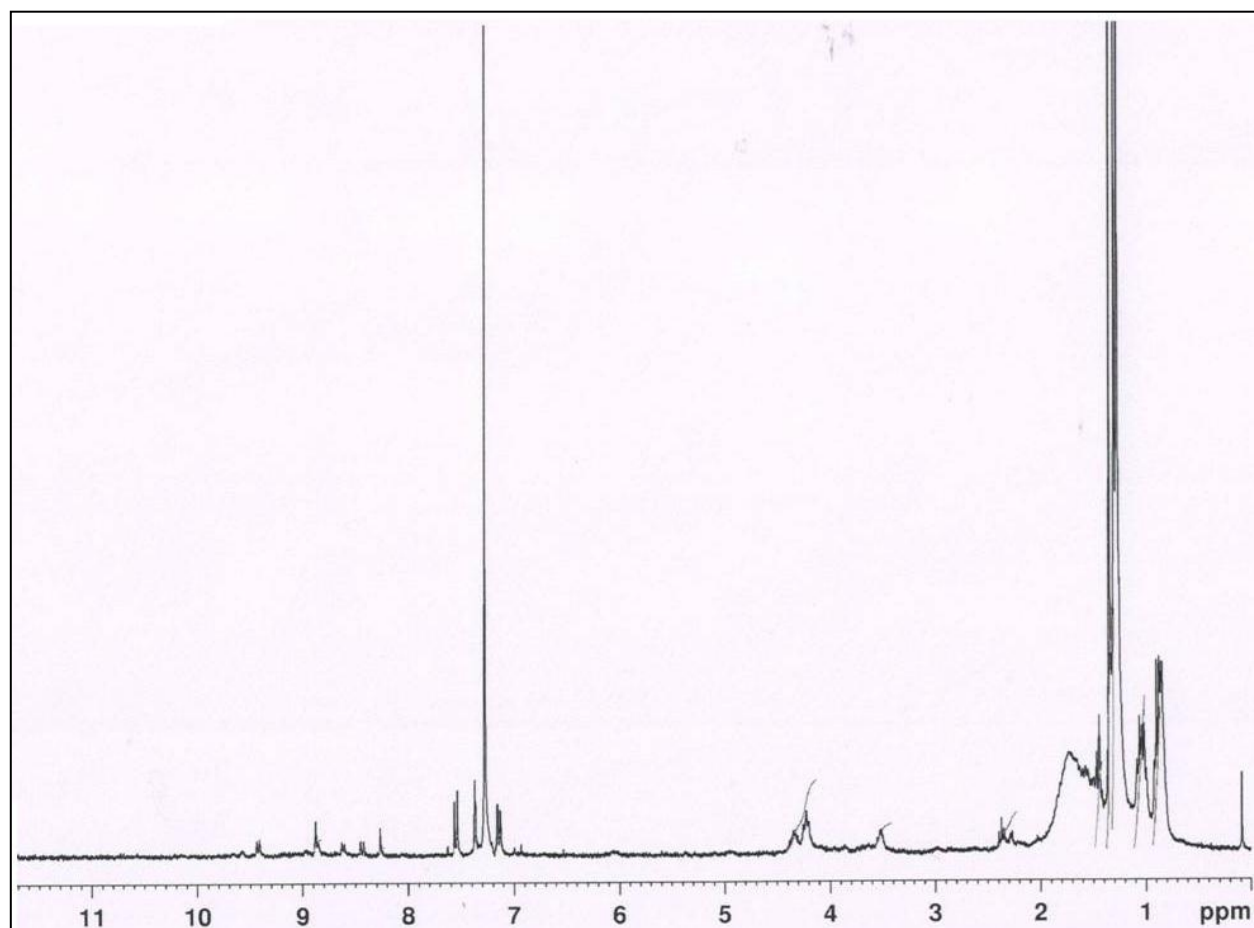


Figure S4. ¹H-NMR spectrum of compound **4** in CDCl₃ and TMS as internal standard.

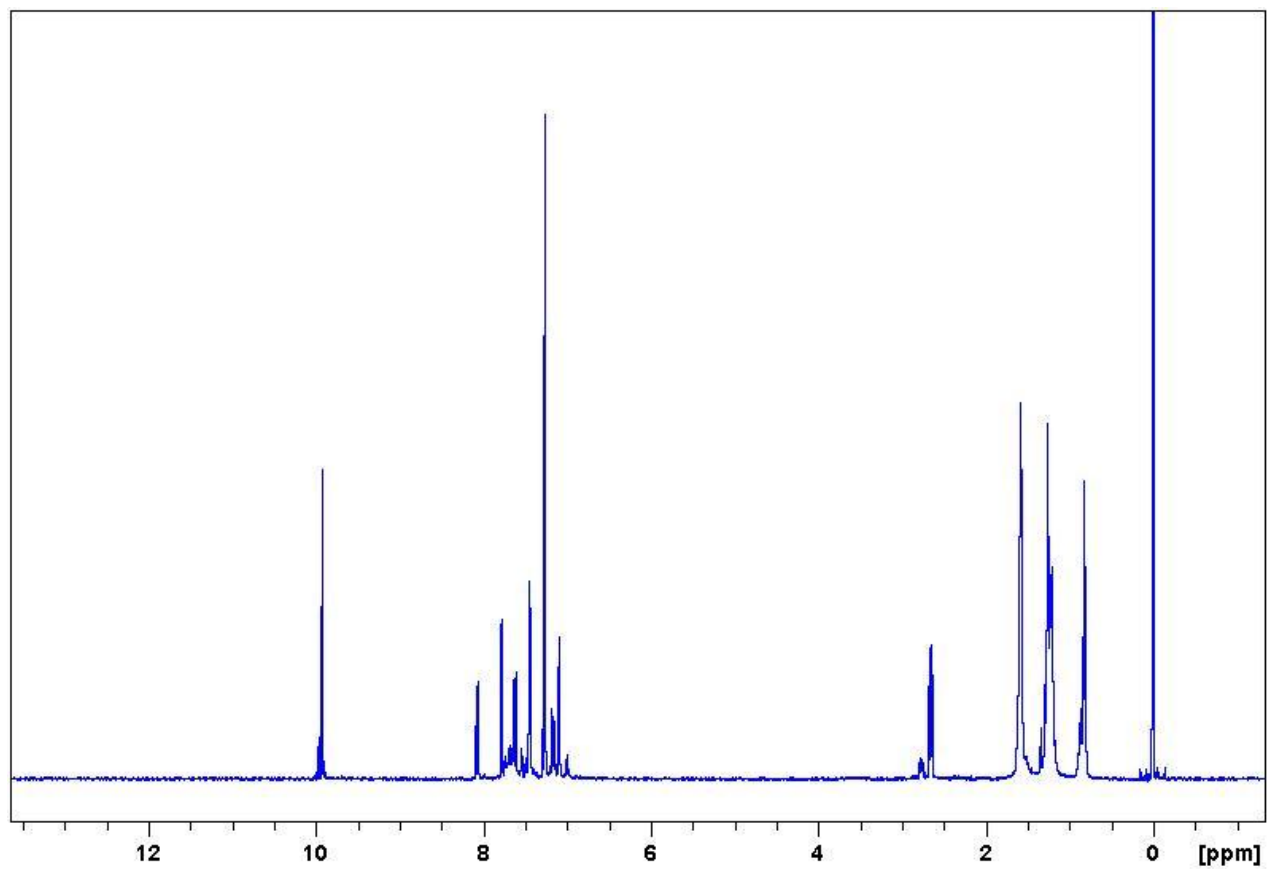


Figure S5. ¹H-NMR spectrum of compound **5** in CDCl₃ and TMS as internal standard.

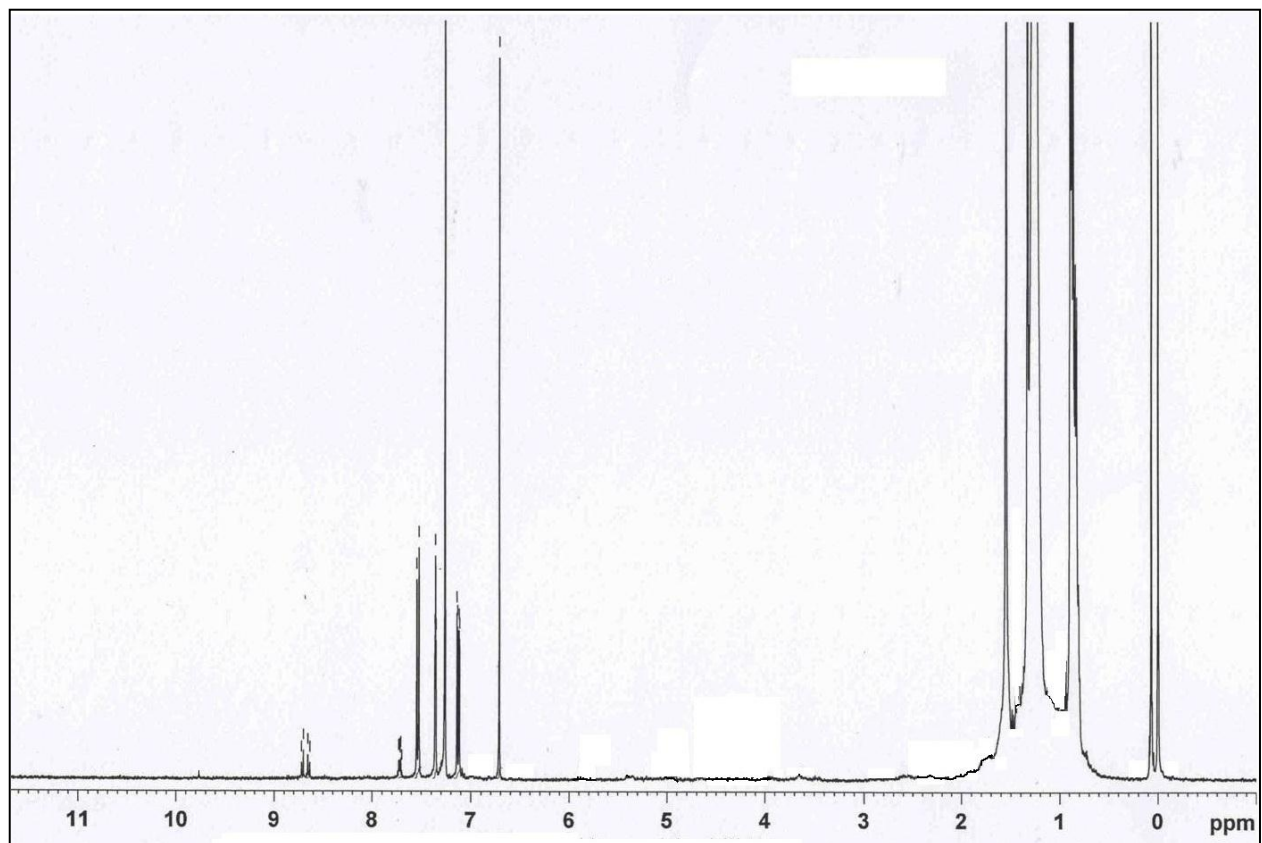


Figure S6. ¹H-NMR spectrum of compound **6** in CDCl₃ and TMS as internal standard.

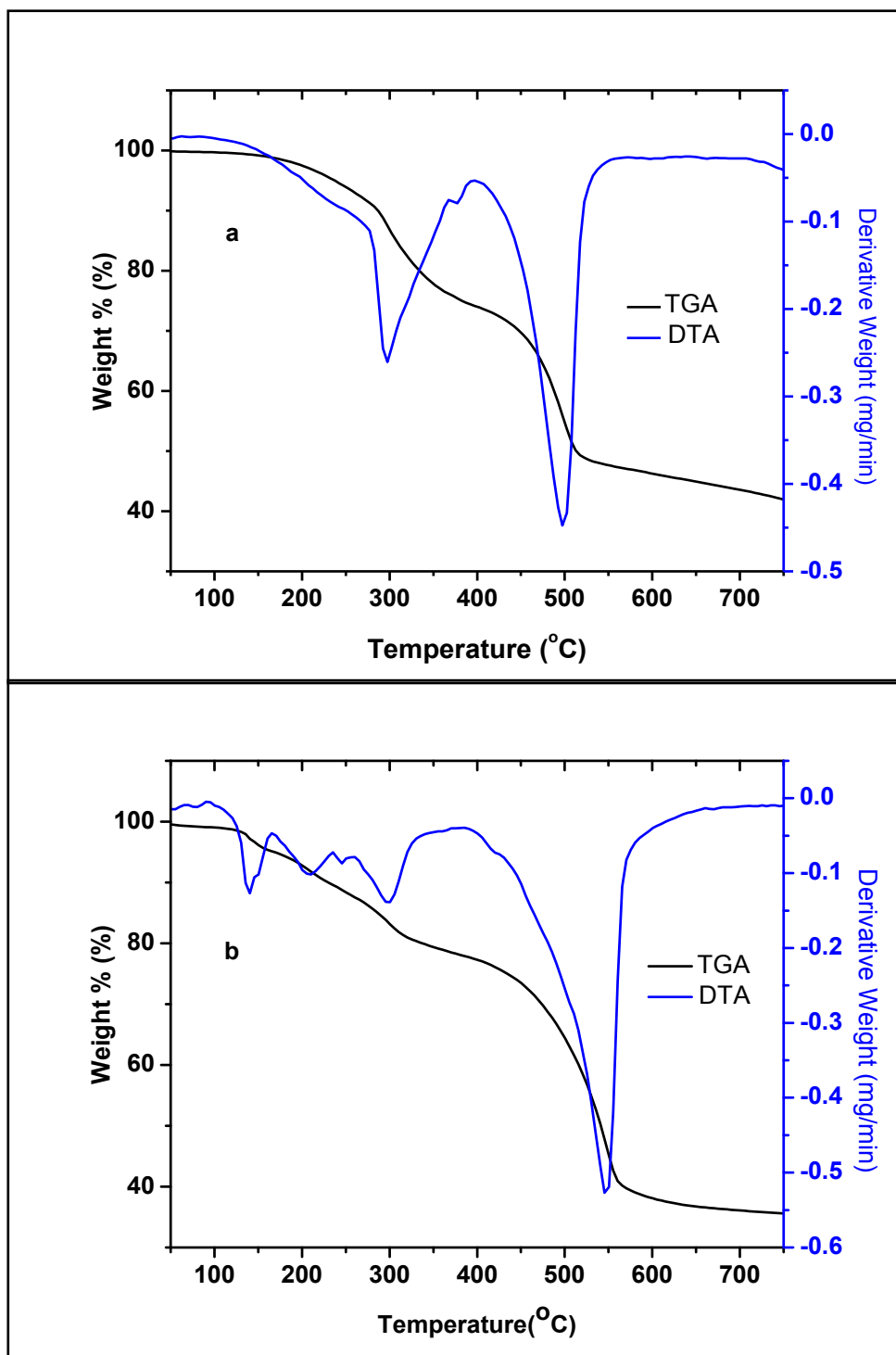


Figure S7. Thermogravimetric (black) and its corresponding derivative weight curves (blue) for (a) 1,7-DPPDI-PFDA and (b) 1,7-DBPDI-PFDA copolymer.

Data: XYZ coordinates of 1,7-DPPDI-PFDA copolymer optimized at RB3LYP/6-31G(d) basis set.

H	-13.14836200	-0.67904800	-1.17697000
C	-13.81133100	-0.13091000	-0.51624600
C	-15.51504600	1.28160300	1.18158200
C	-13.26160700	0.67555900	0.49713500
C	-15.19185400	-0.22575700	-0.67390300
C	-16.05149600	0.47830800	0.17149700
C	-14.13699400	1.38035000	1.34493400
H	-15.59777500	-0.85343000	-1.46288500
H	-17.12799500	0.40251600	0.04601900
H	-13.73423200	2.00598100	2.13637100
H	-16.17400100	1.83346100	1.84667900
C	-11.82094500	0.78464800	0.66929300
C	-11.01637500	1.50968600	1.51626800
C	-9.66948500	1.19107700	1.19304600
C	-9.72412200	0.28491900	0.16192600
O	-11.02826300	0.03192000	-0.16310400
H	-11.34851200	2.19653500	2.28175800
H	-8.77121900	1.57537700	1.65383500
C	-8.72341300	-0.40642400	-0.59485000
O	-7.41876500	-0.14651500	-0.27856200
C	-6.62819600	-0.89951600	-1.11287400
C	-7.43475400	-1.63249600	-1.95126600
C	-8.78056100	-1.31799300	-1.62132500
H	-7.10415700	-2.32080700	-2.71606500
H	-9.67997300	-1.70802300	-2.07496700
C	-5.18781700	-0.77868600	-0.95675600
C	-2.40265900	-0.54862400	-0.67412200
C	-4.31598300	-1.48625500	-1.80531800
C	-4.63098600	0.04528300	0.03783100
C	-3.25202100	0.15611200	0.17819200
C	-2.93914100	-1.37027300	-1.66724900
H	-4.71855200	-2.12843400	-2.58276600
H	-5.28658500	0.59893800	0.70065800
H	-2.83185800	0.79797100	0.94537900
H	-2.27585400	-1.92004000	-2.32672400
N	-0.97060500	-0.42586000	-0.53797200
C	1.08149800	0.92242000	-0.71351400

C	1.21930100	-1.41738500	-0.01517300
C	1.85377200	-0.19134200	-0.30780300
C	-0.25268800	-1.56455500	-0.11454300
C	-0.38746800	0.82745300	-0.84650100
O	-0.82851400	-2.60989600	0.14901300
O	-1.08124600	1.76726800	-1.20402400
C	1.96617700	-2.49561600	0.41536600
H	1.42125400	-3.38657900	0.69842600
C	3.37639500	-2.45856700	0.48396600
C	4.05241100	-1.27766400	0.06047700
C	3.27533000	-0.10265500	-0.20497100
C	1.71537400	2.11845700	-1.00907200
H	1.11841600	2.95476900	-1.35718800
C	3.09484100	2.24554600	-0.83170300
H	3.56752200	3.19634500	-1.04498200
C	3.89367900	1.17953200	-0.39634200
C	5.49222700	-1.18546500	-0.23705200
C	6.10826600	0.10787300	-0.34506600
C	5.34154300	1.31139300	-0.21730400
C	6.27946200	-2.31688300	-0.49190300
H	5.81433700	-3.29116000	-0.43231900
C	7.63543100	-2.22545100	-0.81127500
H	8.21925800	-3.11608600	-1.01968900
C	8.26347800	-0.99112900	-0.84589900
C	7.51015400	0.18295700	-0.60473400
C	6.02665600	2.55093800	-0.05033800
C	7.41393400	2.59558500	-0.34381200
H	7.96118600	3.52898400	-0.31476500
C	8.13014200	1.45935200	-0.64284500
C	9.71017300	-0.91038400	-1.14493200
N	10.23940000	0.38259000	-1.16771700
C	9.57886900	1.58637000	-0.93737700
H	11.23140700	0.45125200	-1.37129200
O	10.42539600	-1.87669100	-1.36554000
O	10.18095200	2.65011000	-0.97913900
N	4.07477400	-3.59215300	0.95995800
C	5.88756800	-4.50742400	2.40204600
C	4.33830000	-6.04125200	1.15532300
C	5.19270000	-5.87384500	2.41688000
C	3.35894500	-4.87407900	0.98789500

C	4.87970100	-3.37622900	2.18233700
H	6.63743100	-4.48063700	1.60122000
H	4.98684700	-6.09262400	0.27081800
H	4.54809400	-5.94676900	3.30509400
H	2.61934900	-4.90469700	1.80969100
H	4.20557200	-3.30595200	3.05566400
H	6.41854000	-4.32903100	3.34522000
H	3.76716100	-6.97692300	1.19223600
H	5.93003800	-6.68158200	2.49448700
H	2.80961700	-4.98420500	0.04856700
H	5.39920000	-2.42082400	2.09629900
N	5.39416000	3.70465800	0.39903200
C	5.06065000	6.14027400	0.53045500
C	4.72071400	4.67265600	2.57872000
C	4.63527900	6.10718400	2.01633500
C	4.41534400	3.62758700	1.50060300
C	6.04137700	5.01162400	0.20351800
H	5.52540200	7.09939000	0.27751900
H	5.72321800	4.48086800	2.98119800
H	3.61336400	6.49161500	2.11244800
H	3.39050800	3.76665100	1.12697600
H	6.36586200	5.08247500	-0.83965300
H	4.18348600	6.03667100	-0.11987900
H	4.01922500	4.53809800	3.40991900
H	5.27454900	6.77028000	2.61055800
H	4.45687600	2.61966400	1.92308000
H	6.94227400	5.11746900	0.83044400

Data: XYZ coordinates of 1,7-DBPDI-PFDA copolymer optimized at RB3LYP/6-31G(d) basis set.

H	13.60435500	-2.29593200	-1.07246200
C	14.23129600	-2.15616800	-0.19841700
C	15.84229200	-1.79661700	2.05015400
C	13.64450100	-1.74033600	1.01083600
C	15.60252500	-2.38721600	-0.27649500
C	16.41581500	-2.20965700	0.84441600
C	14.47331300	-1.56391500	2.13501100
H	16.03759200	-2.70808500	-1.21935300
H	17.48514800	-2.39067300	0.78053200
H	14.04170700	-1.24198800	3.07843900
H	16.46508900	-1.65448500	2.92937000
C	12.21313100	-1.49615200	1.10436400
C	11.37905000	-1.10982600	2.12687900
C	10.06330200	-1.04169600	1.59398800
C	10.16491500	-1.39157500	0.26938400
O	11.46845700	-1.66968700	-0.03710000
H	11.67142800	-0.89882900	3.14568700
H	9.15442200	-0.77150600	2.11150800
C	9.21058500	-1.51140200	-0.79224500
O	7.90809800	-1.22807100	-0.48772100
C	7.16432100	-1.40108700	-1.63002900
C	7.99804400	-1.79295600	-2.65081600
C	9.31256900	-1.86457800	-2.11624000
H	7.70576600	-2.00623200	-3.66917200
H	10.22101000	-2.13936900	-2.63204700
C	5.73543100	-1.14900300	-1.53977100
C	2.97455200	-0.66001700	-1.38093100
C	4.90842300	-1.30998200	-2.66721700
C	5.14564100	-0.73845500	-0.33060600
C	3.77812800	-0.49974000	-0.25264200
C	3.54364500	-1.06532900	-2.58957000
H	5.33644600	-1.62822900	-3.61290300
H	5.76646700	-0.60813000	0.54869500
H	3.33308100	-0.18021400	0.68378500
H	2.91494700	-1.19526000	-3.46402500
N	1.55490200	-0.40615800	-1.30126300
C	-0.77130100	-1.21958000	-1.36829400
C	-0.32802400	1.15235500	-1.00868400
C	-1.25283600	0.09279800	-1.15387800
C	1.13716000	0.92059200	-1.07229700
C	0.67956200	-1.50567400	-1.46045300
O	1.94703800	1.82387000	-0.93454400
O	1.11603000	-2.62719800	-1.66448000

C	-0.77896700	2.43711700	-0.80106700
H	-0.05517100	3.23384600	-0.67810000
C	-2.15363100	2.71919200	-0.77925200
C	-3.12377000	1.71270300	-0.98004400
C	-2.65656200	0.36027700	-1.09081300
C	-1.67290600	-2.25737100	-1.51361300
H	-1.29646600	-3.25576600	-1.70842700
C	-3.04535300	-2.02602900	-1.38684800
H	-3.71446800	-2.86447200	-1.48641000
C	-3.56821300	-0.74967200	-1.13604000
C	-4.56759200	1.96376800	-1.08691600
C	-5.47637300	0.85299400	-0.99065000
C	-5.00131200	-0.50102100	-0.92654200
C	-5.10154100	3.24423900	-1.28677800
H	-4.43766200	4.08173700	-1.42268500
C	-6.47850100	3.47982700	-1.31328800
H	-6.86540000	4.48152400	-1.46828000
C	-7.36990000	2.44288300	-1.11737700
C	-6.88184800	1.12119600	-0.95293900
C	-5.95211600	-1.51269000	-0.66837400
C	-7.32543600	-1.23396100	-0.59472200
H	-8.03849400	-2.03350900	-0.43146600
C	-7.79130500	0.05108900	-0.75688100
C	-8.82354200	2.72546700	-1.09847000
N	-9.64175100	1.61309200	-0.89539400
C	-9.25584500	0.28815700	-0.71716800
H	-10.64046800	1.79338100	-0.87664700
O	-9.31082700	3.83617600	-1.24589800
O	-10.08653100	-0.59093500	-0.54179900
O	-2.56148700	4.01998700	-0.61344100
C	-1.78327300	4.91693600	0.11585500
C	-0.36582900	6.86135400	1.58151400
C	-1.41719200	6.11028800	-0.49354700
C	-1.45939500	4.67483200	1.45148800
C	-0.75515500	5.64107200	2.16344800
C	-0.71709600	7.07051400	0.24130100
H	-1.68154400	6.28370000	-1.53210200
H	-1.76131500	3.74536800	1.92436500
H	-0.51125200	5.43625700	3.20170600
H	-0.44387400	7.99305800	-0.25756600
C	0.40795900	7.89803700	2.41612000
C	-0.45025300	8.32381000	3.63121500
H	-0.69629400	7.47357800	4.27615600
H	-1.39206400	8.78022700	3.30606100
H	0.09094900	9.05762500	4.24064400
C	0.75188700	9.16161000	1.60504200

H	-0.14744200	9.67478100	1.24575700
H	1.38565300	8.93264500	0.74068100
H	1.30154600	9.86665400	2.23828800
C	1.73162700	7.27241100	2.91690300
H	1.55684500	6.39038900	3.54201700
H	2.29200000	7.99919400	3.51743000
H	2.36418900	6.96551300	2.07639200
O	-5.52980500	-2.81325000	-0.54197400
C	-6.25528200	-3.72097900	0.22697900
C	-7.57109600	-5.68617900	1.75880500
C	-6.51600300	-3.48431600	1.57742900
C	-6.63330600	-4.91969400	-0.36450800
C	-7.28206100	-5.89027500	0.40300300
C	-7.17142500	-4.46045900	2.32192600
H	-6.20526500	-2.55079100	2.03632000
H	-6.41807900	-5.08888700	-1.41503900
H	-7.56539200	-6.81689200	-0.08262300
H	-7.36820200	-4.25859400	3.37080100
C	-8.29163300	-6.73270300	2.62809700
C	-7.37967500	-7.13671100	3.81100500
H	-7.88237400	-7.87971300	4.44179400
H	-7.12759000	-6.27994900	4.44484000
H	-6.44145200	-7.57464000	3.45190600
C	-9.60601100	-6.12778800	3.17652300
H	-10.12826200	-6.85927700	3.80501700
H	-10.27730800	-5.84037500	2.35943000
H	-9.42285300	-5.23674700	3.78620100
C	-8.64334400	-8.00643800	1.83659300
H	-9.15306100	-8.71925900	2.49403400
H	-7.74931000	-8.50323700	1.44264800
H	-9.31603100	-7.79373300	0.99791600