

## Supplementary Information

### **Solution-processable Phenothiazine and Phenoxazine Substituted Fluorene Cored Nanotextured Hole Transporting Materials for Achieving High-efficiency OLEDs**

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**Figure S13** MS Spectrum of DNFPhe.

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**Figure S17** MS Spectrum of DNFPhe.

**Figure S18** MS Spectrum of DDPPFPhe.

**Figure S19**  $^1\text{H}$  NMR spectrum of DNFPhe.

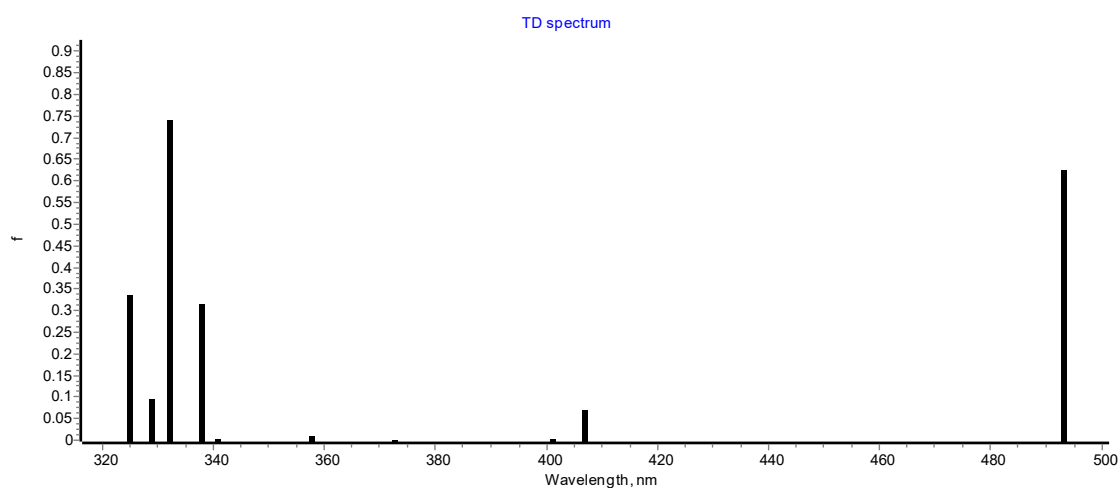
**Figure S20**  $^1\text{H}$  NMR spectrum of DDPFPhe.

**Figure S21**  $^1\text{H}$  NMR spectrum of DFPPFPhe.

**Figure S22**  $^1\text{H}$  NMR spectrum of DPFPh.

**Figure S23**  $^1\text{H}$  NMR spectrum of DNFPhe.

**Figure S24**  $^1\text{H}$  NMR spectrum of DDPPFPhe.



**Figure S1** TD Spectrum of DNFPhe.

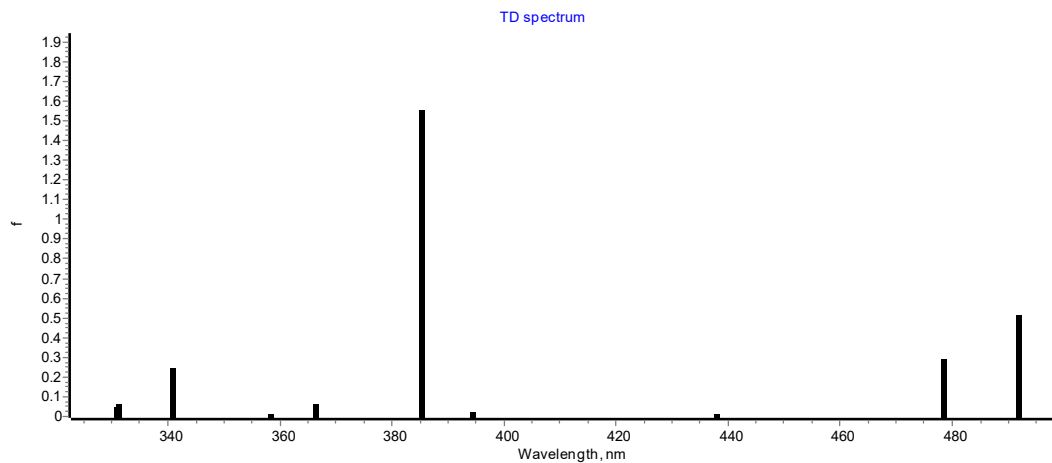


Figure S2 TD Spectrum of DDPFPhe.

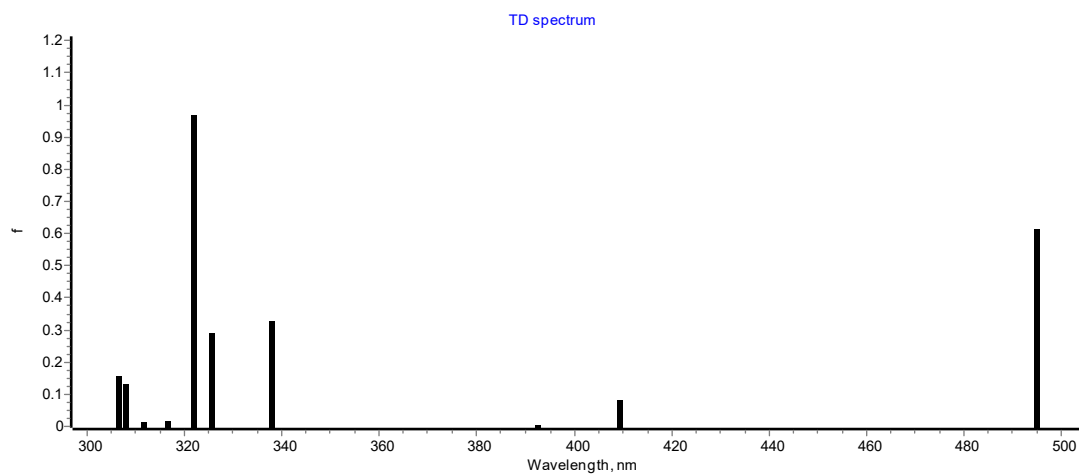


Figure S3 TD Spectrum of DFPFPhe.

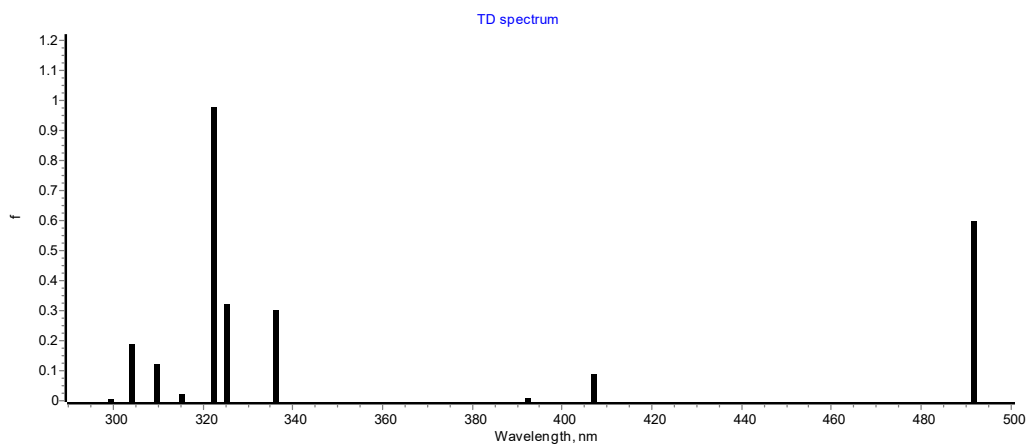


Figure S4 TD Spectrum of DPFPhе.

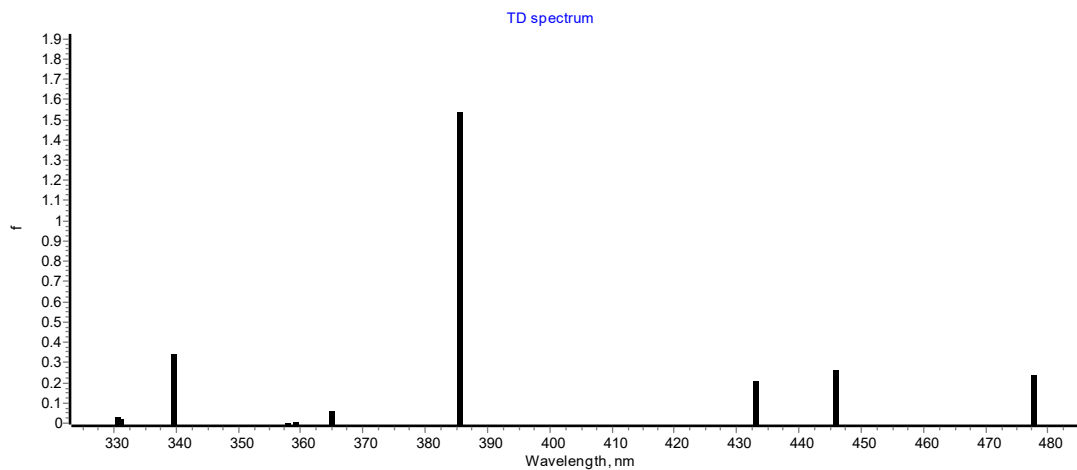


Figure S5 TD Spectrum of DDPPFPh.

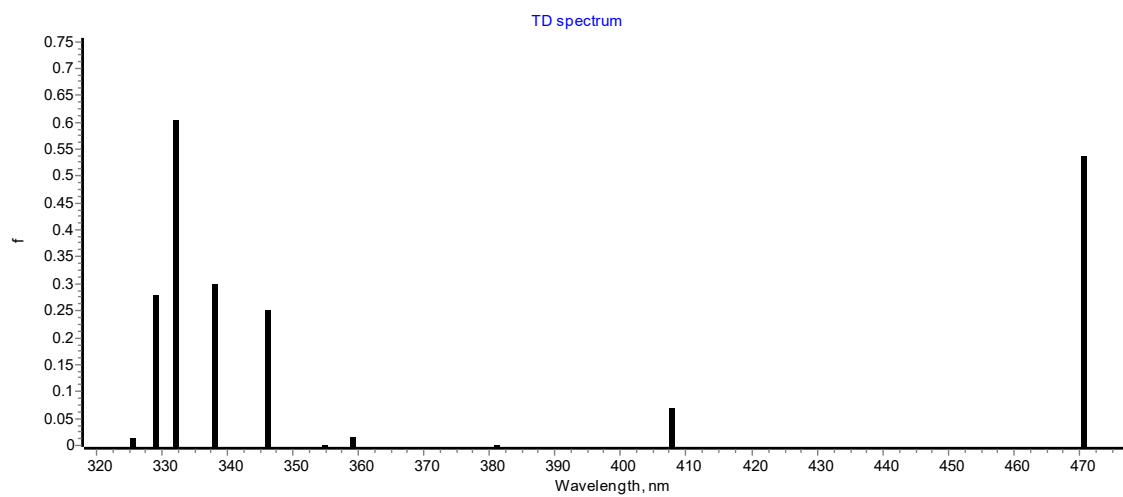
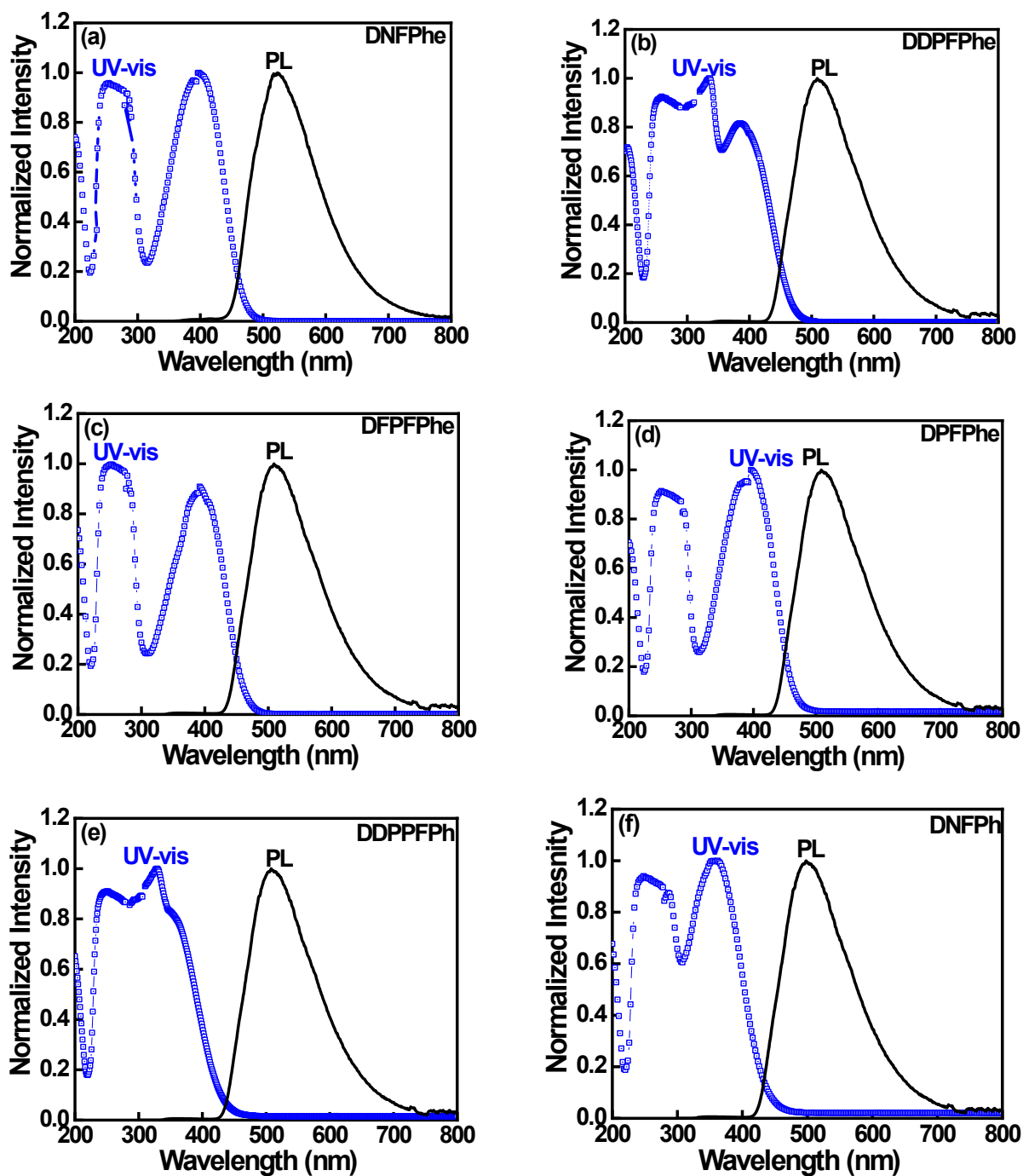
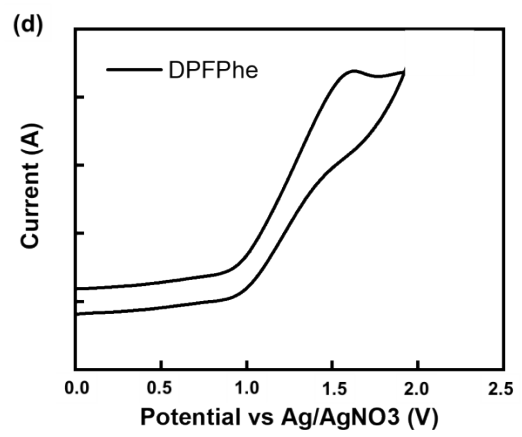
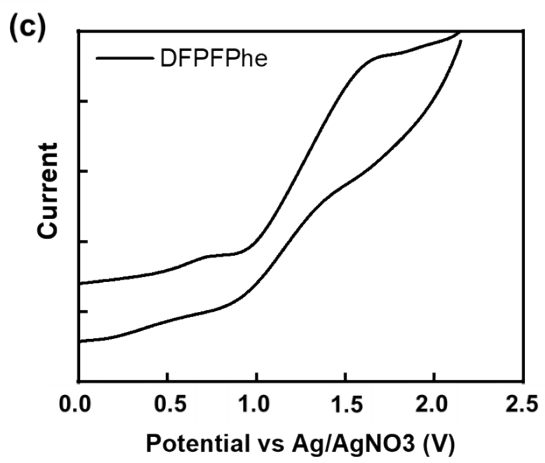
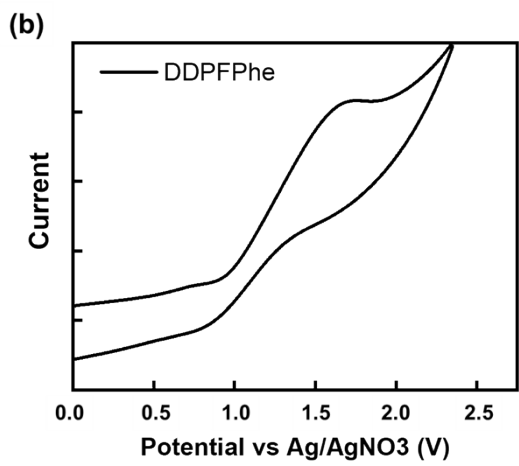
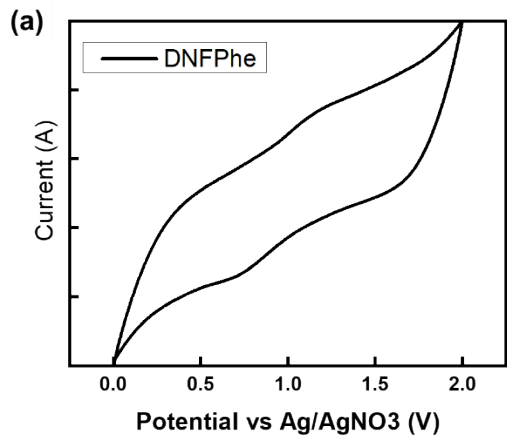
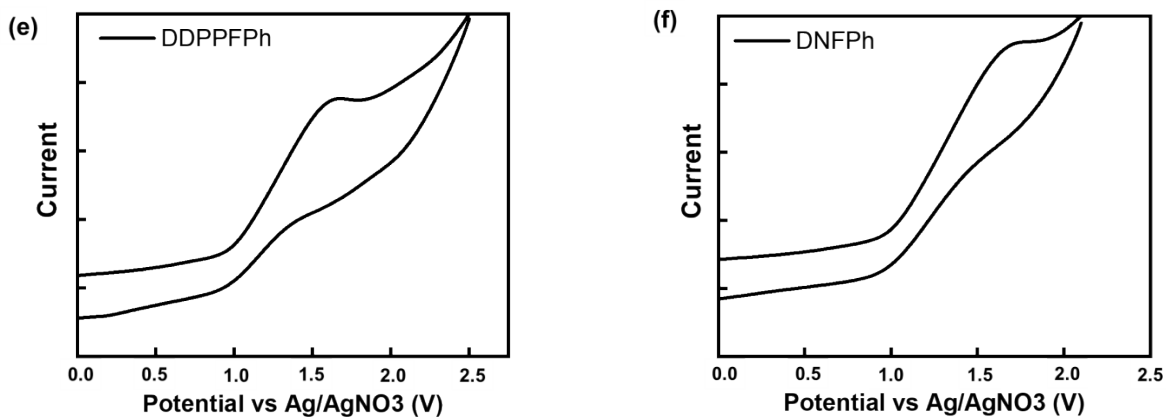


Figure S6 TD Spectrum of DNFPh.

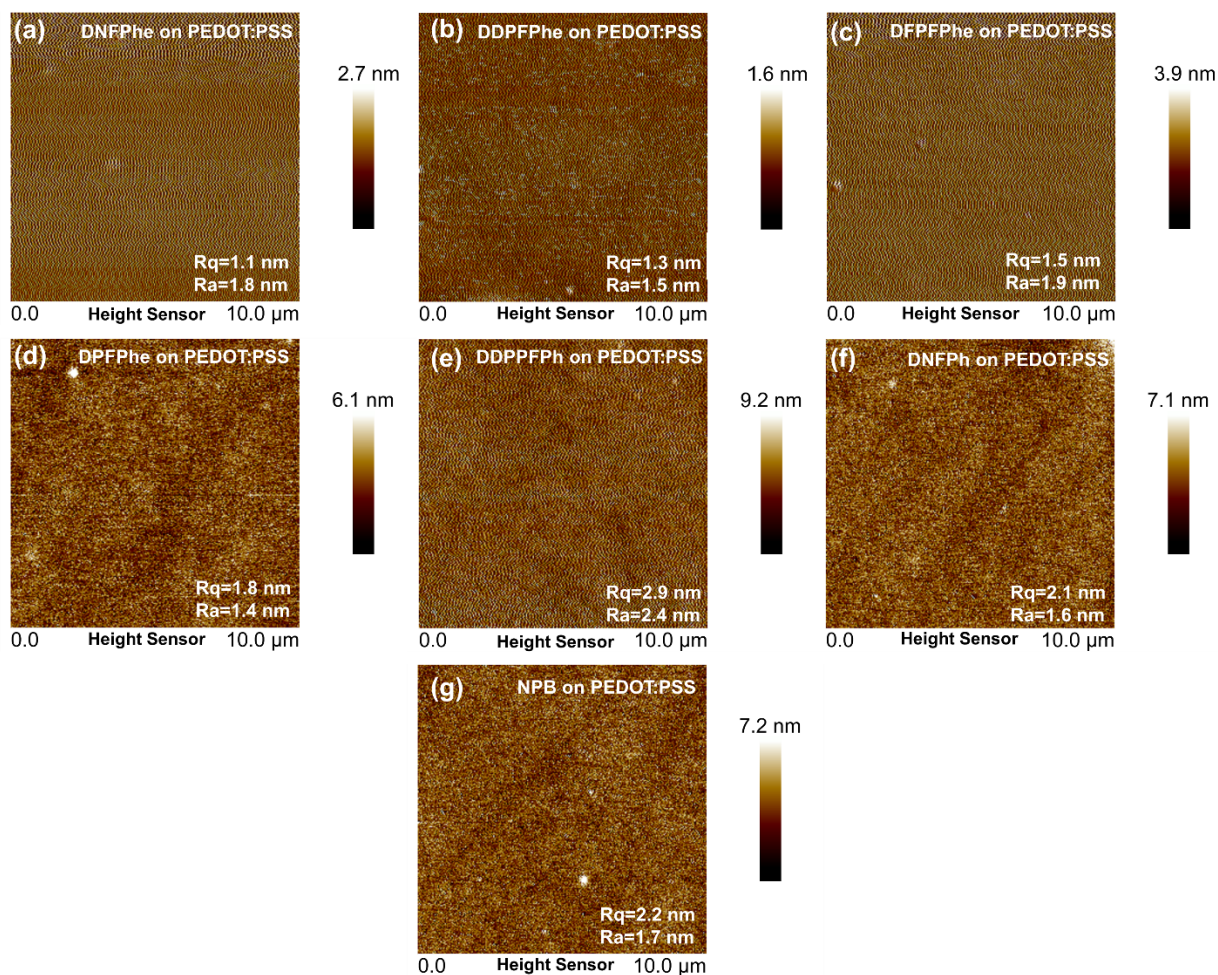


**Figure S7 (a-f).** Normalized ultraviolet-visible (UV-vis) absorption and photoluminescence (PL) spectra of thin-films for **DNFPh**, **DDPFPh**, **DFPFPh**, **DPFPh**, **DDPPFPh**, and **DNFPh**.



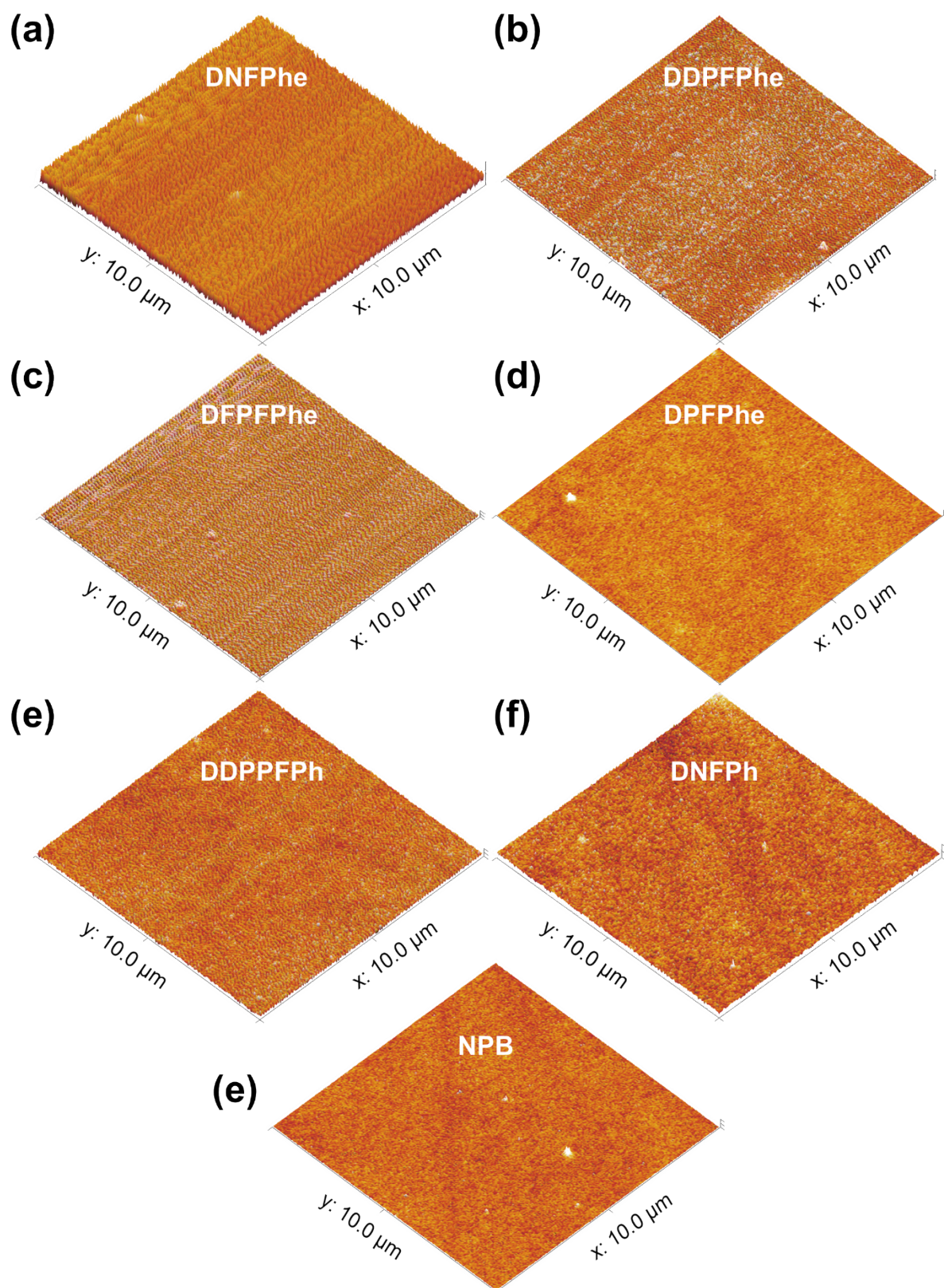


**Figure S8 (a-f)** cyclic voltammetry measurement of newly synthesized HTMs.



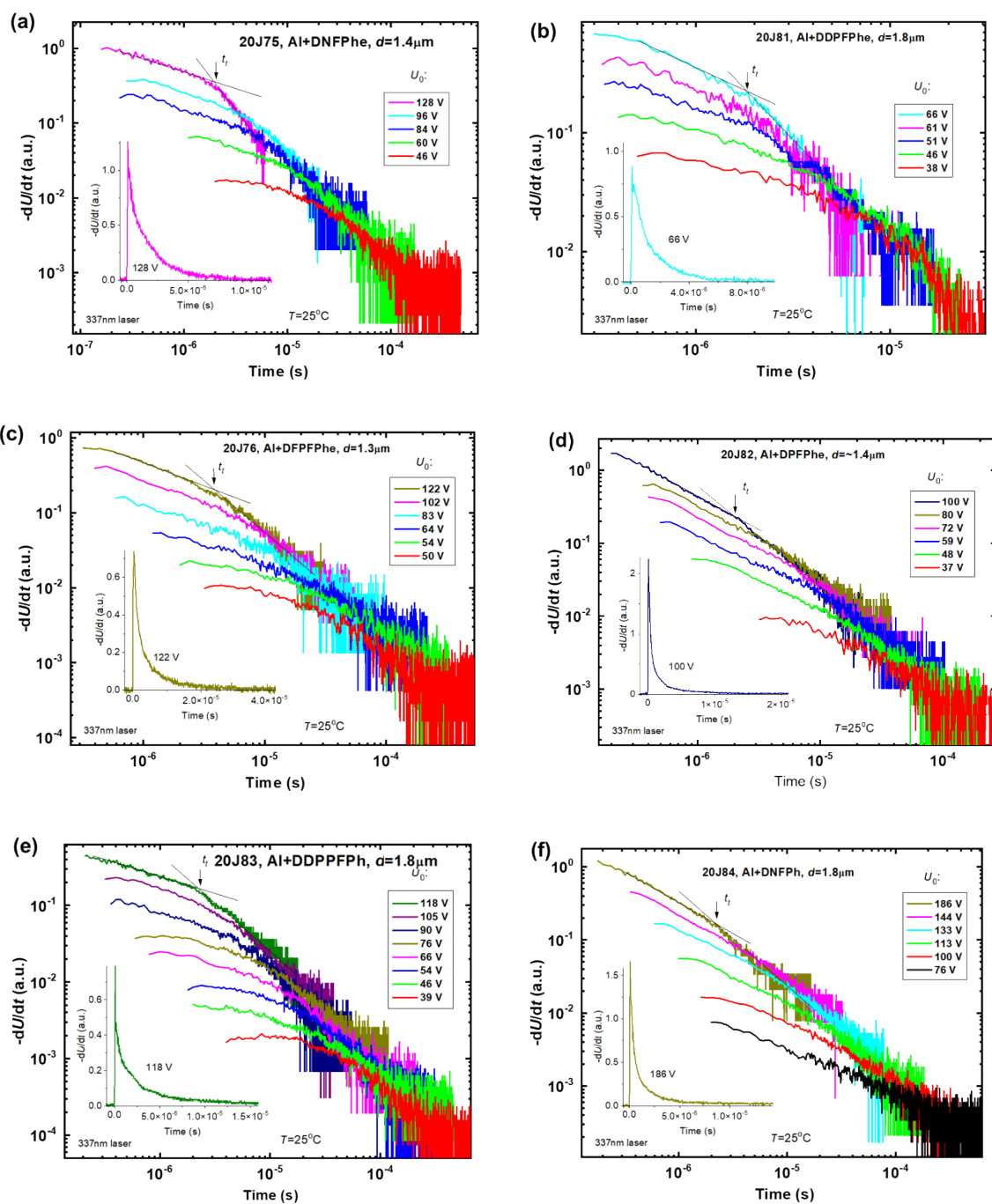
**Figure S9** Atomic force microscopic images of newly synthesized HTMs thin-films prepared on PEDOT:PSS.





**Figure S10** 3D topographies of newly synthesized HTMs thin-films prepared on PEDOT:PSS.

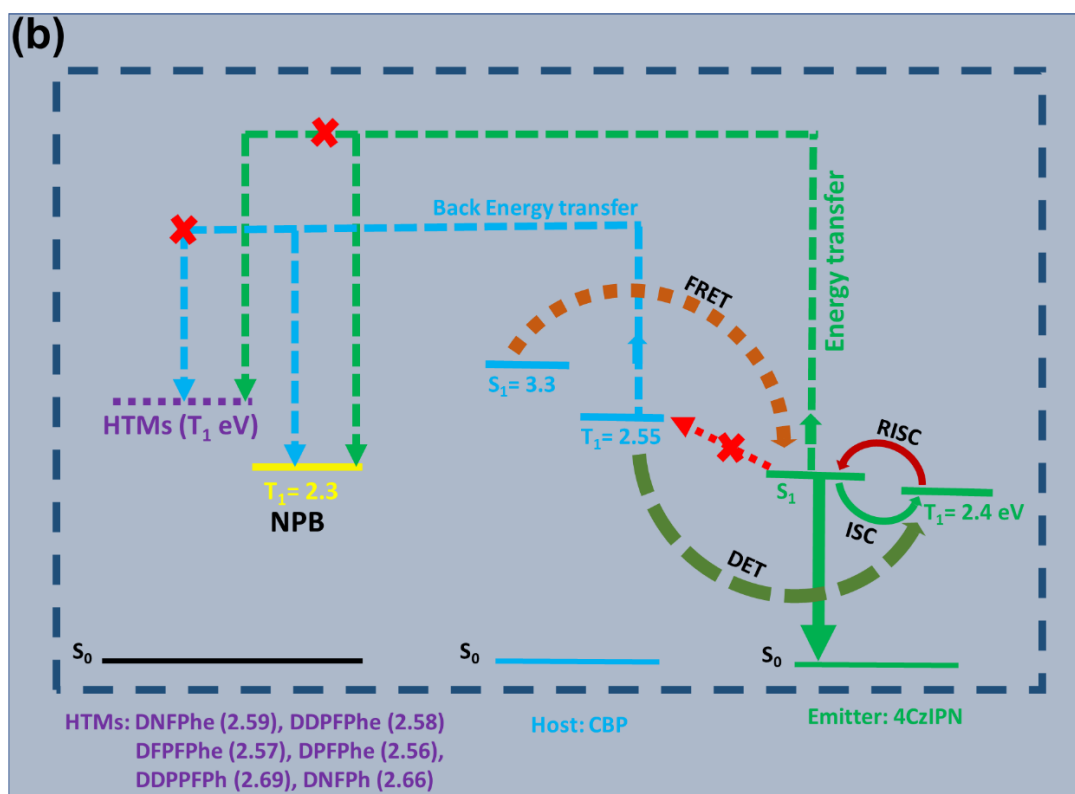
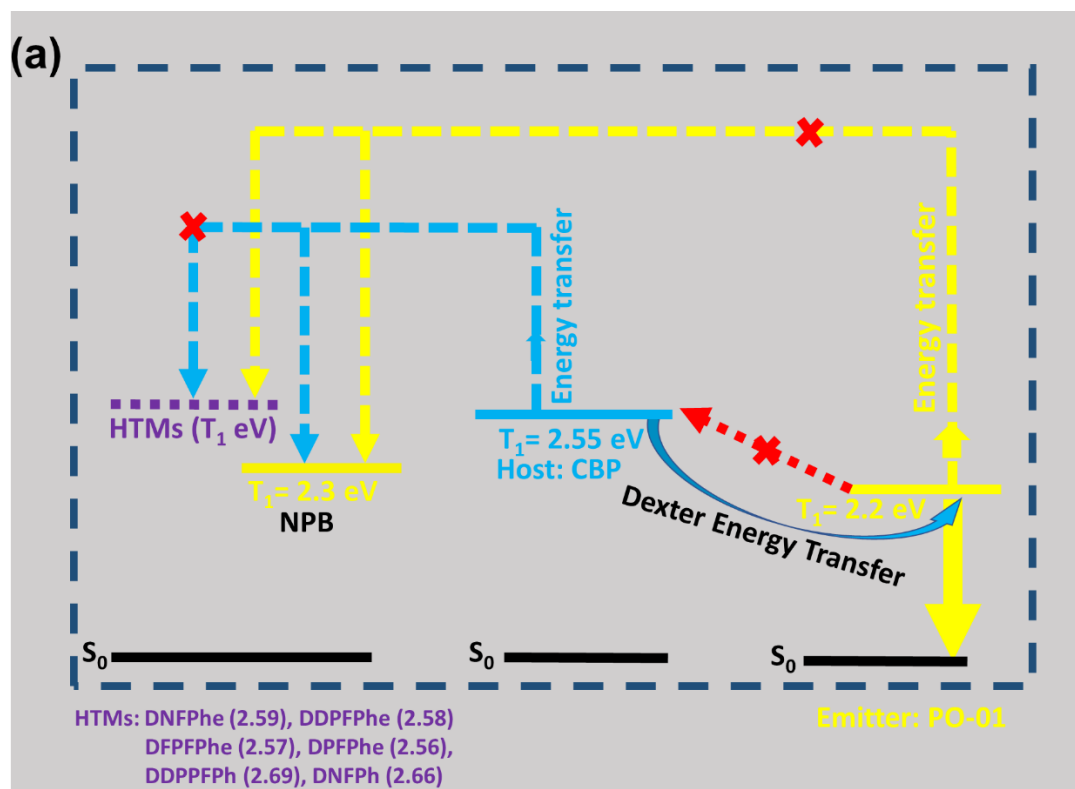




**Figure S11** Double-logarithmic representation of transient photocurrents curves of the newly synthesized HTMs, (a) DNFPhe, (b) DDPPFPh, (c) DFPFPh, (d) DPFPhe, (e) DDPPFPh, and (f) DNFPhe, and inset show the TOF transient curves.

**Table S1.** Reported characteristics of yellow phosphorescent and green TADF OLED in papers.

HTLs	Operation Voltage (V)	Power efficacy (lmW <sup>-1</sup> )	Current efficacy (cdA <sup>-1</sup> )	EQE (%)	CIE @100 cdm <sup>-2</sup>	L <sub>max</sub> (cdm <sup>-2</sup> )	Ref.
	@ 100 cdm <sup>-2</sup> /1,000 cdm <sup>-2</sup> / maximum values						
FI-PyEyF	4.9/6.1/-	27.4/17.9/29.0	46.6/34.7/49.4	16.7/10.7/-	(0.53, 0.46)	10,913	1
di-FI-PyEyF	4.7/6.1/-	33.2/21.9/38.2	53.4/39.0/58.7	17.1/12.2/-	(0.53, 0.47)	12,060	
tri-FI-PyEyF	4.6/5.8/-	35.3/25.6/39.5	56.3/42.1/61.0	17.4/12.4/-	(0.53, 0.47)	13,400	
Compound 3	5.4/7.2/-	14.8/8.5/23.1	25.4/19.4/29.4	7.7/5.9/9.0	(0.49,0.51)	12,120	2
Compound 4	5.4/7.3/-	14.0/8.6/22.8	24.1/20/29.2	7.4/6.1/9.0	(0.49,0.51)	16,700	
Compound 5	5.5/7.5/-	16.6/9.2/27.9	29.3/22.0/35.7	9.0/6.7/10.9	(0.49,0.51)	14,800	
Py-Br	-/-	-/11.7/12.3	-/22.4/27.6	-/7.4/9.0	(0.50, 0.49)	17 300	3
Py-MeO	-/-	-/10.3/11.8	-/19.2/25.7	-/6.9/8.8	(0.51, 0.49)	15 270	
PVK	-/-	-/14.2	-/31.6	-/16.8	(0.45,0.51)	3180	4
PEDOT:PSS	4.3/5.1/-	4.3/5.1/-	32.3/25.2/-	44.0/40.9/-	(0.51, 0.49)	19870	5
DDPPFPh	<b>3.7/ 4.4/ 6.4/ 3.5</b>	<b>41.4/ 24.3/ 7.7/ 45.4</b>	<b>48.2/ 33.8/ 15.6/ 50.6</b>	<b>18.7/ 12.9/ 5.8/ 19.6</b>	<b>(0.51, 0.48)</b>	<b>19,409</b>	<b>This work</b>
PVK	4.0/-	-/33.6	-/51.4	-/20.6	(0.24,0.50)	2816	6
PVK	3.8/-	-/17.2	-/25.8	-/11.2	(0.27,0.52)	951	
PVK	-/-	-/8.9	-/-	-/8.1	(0.20, 0.43)	-	7
PEDOT:PSS	-/-	-/17.6	-/43	-/15	-	-	8
PEDOT:PSS:PFI	-/3.8	-/58	-/73	-/24	-	-	
PEDOT:PSS	5.2/6.8/-	22.0/16.6/32.6	36.4/34.9/41.5	12.3/11.7/13.9	(0.23,0.54)	-	9
PEDOT:PSS:InCl <sub>3</sub>	-/-	-/-	-/53.7	-/16.4	-	-	10
PEDOT:PSS	-/-	-/-	-/-	-/18.6	-	-	11
PVK:TFB	-/-	-/47.2	-/55.6	-/18.9	(0.35,0.56)	-	12
DDPPFPh	<b>4.2/ 5.5/ 7.0/ 3.6</b>	<b>53.2/ 36.3/ 22.5/ 69.1</b>	<b>71.6/ 64.0/ 50.0/ 78.0</b>	<b>25.0/ 22.4/ 17.6/ 27.2</b>	<b>(0.29, 0.58)</b>	<b>44278</b>	<b>This work</b>



**Figure S12.** Energy-transfer route of (a) yellow phosphorescent and (b) green TADF OLED fabricated with newly synthesized HTMs. As observed, their high triplet energy indicates that they are more capable to confine excitons as comparing with NPB

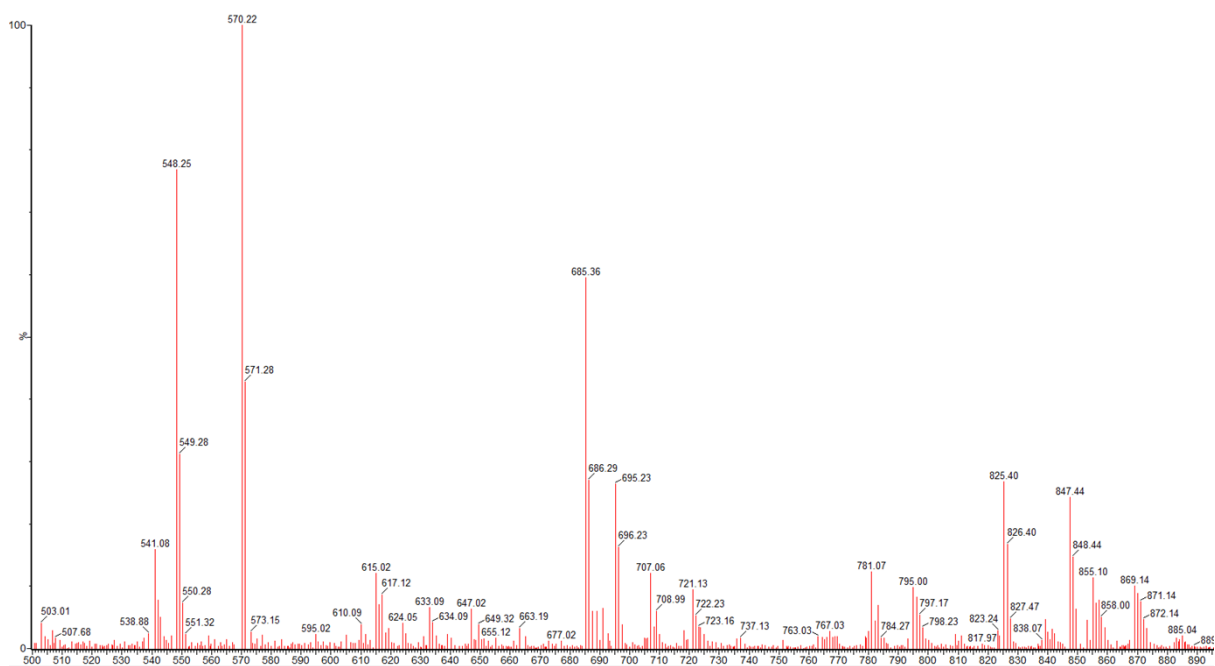


Figure S13 MS Spectrum of DNFPhE.

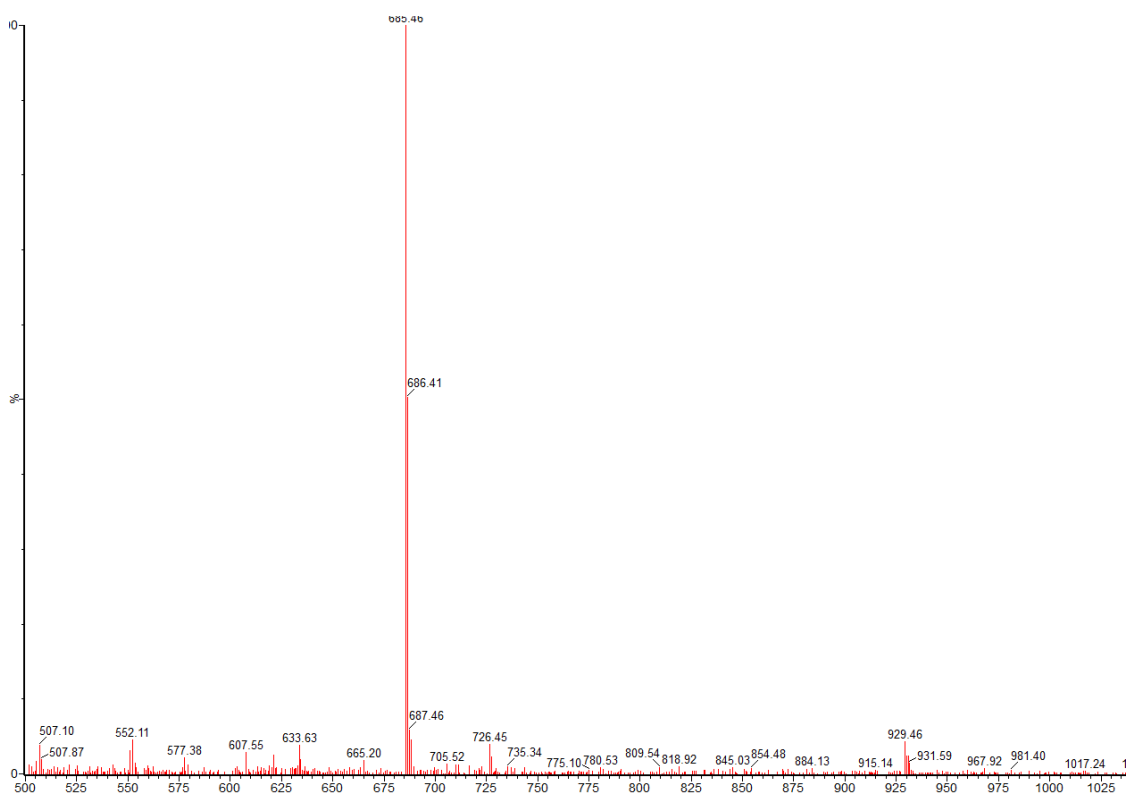
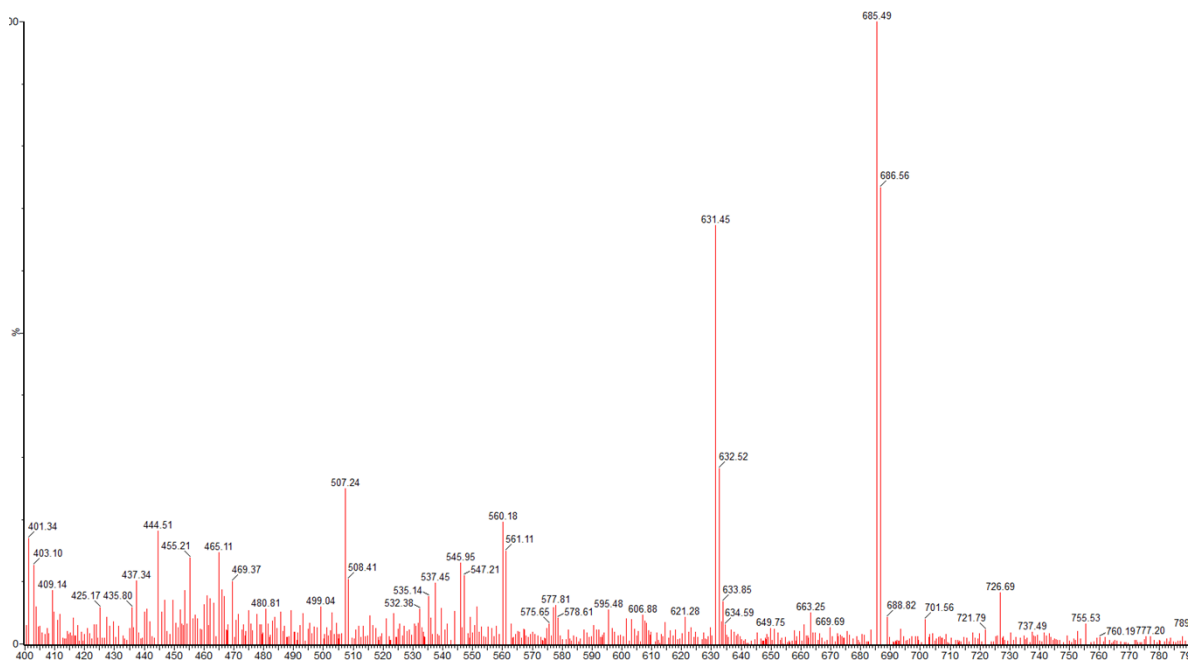
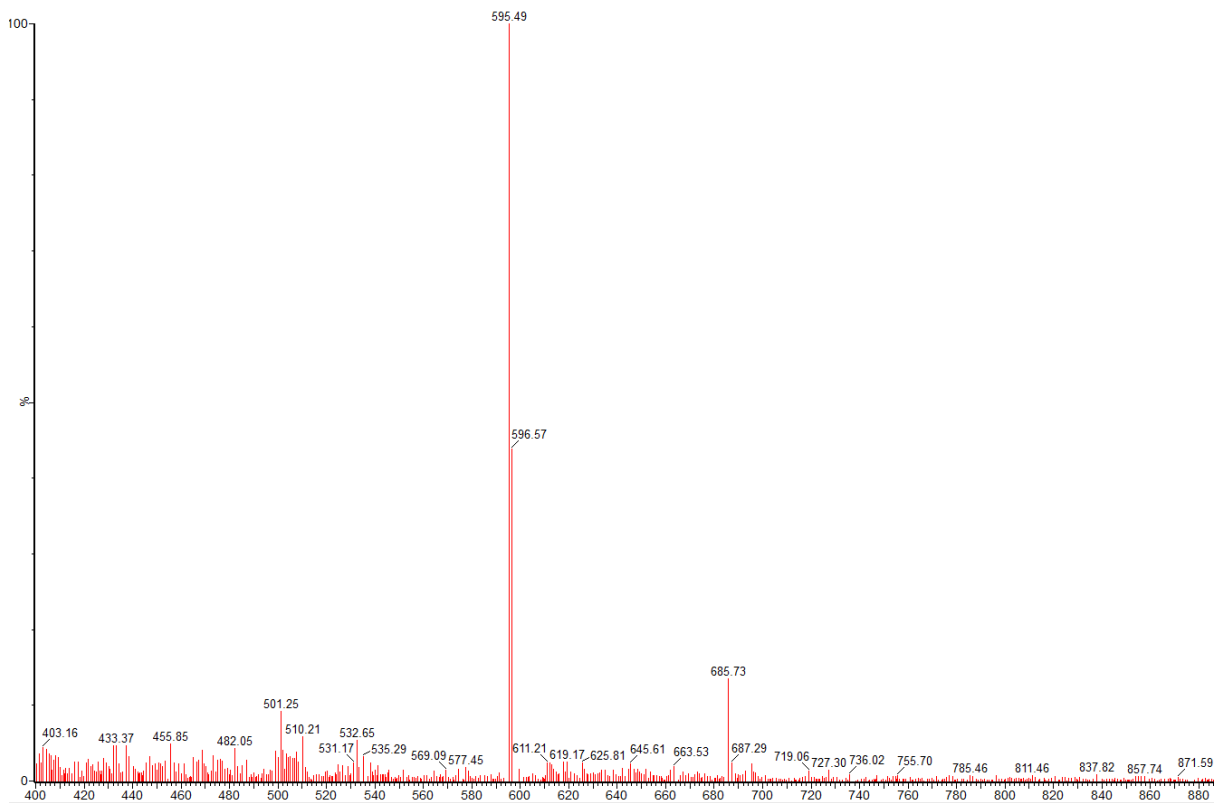


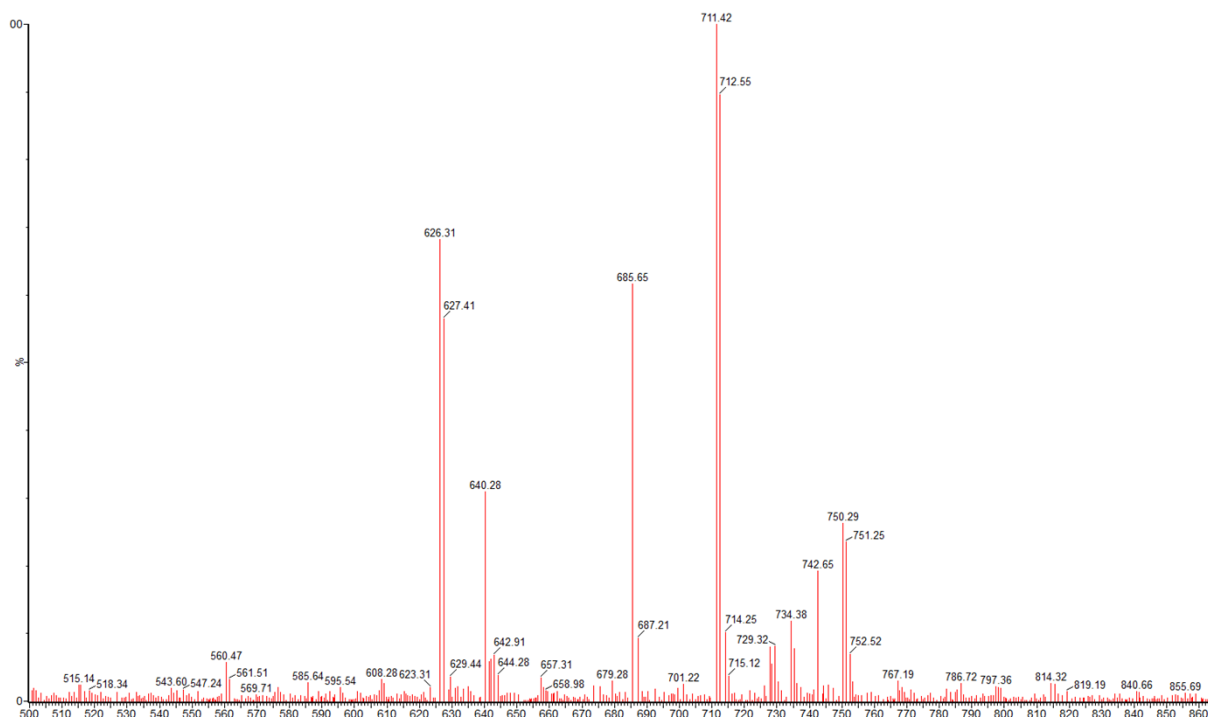
Figure S14 MS Spectrum of DDPFPhE.



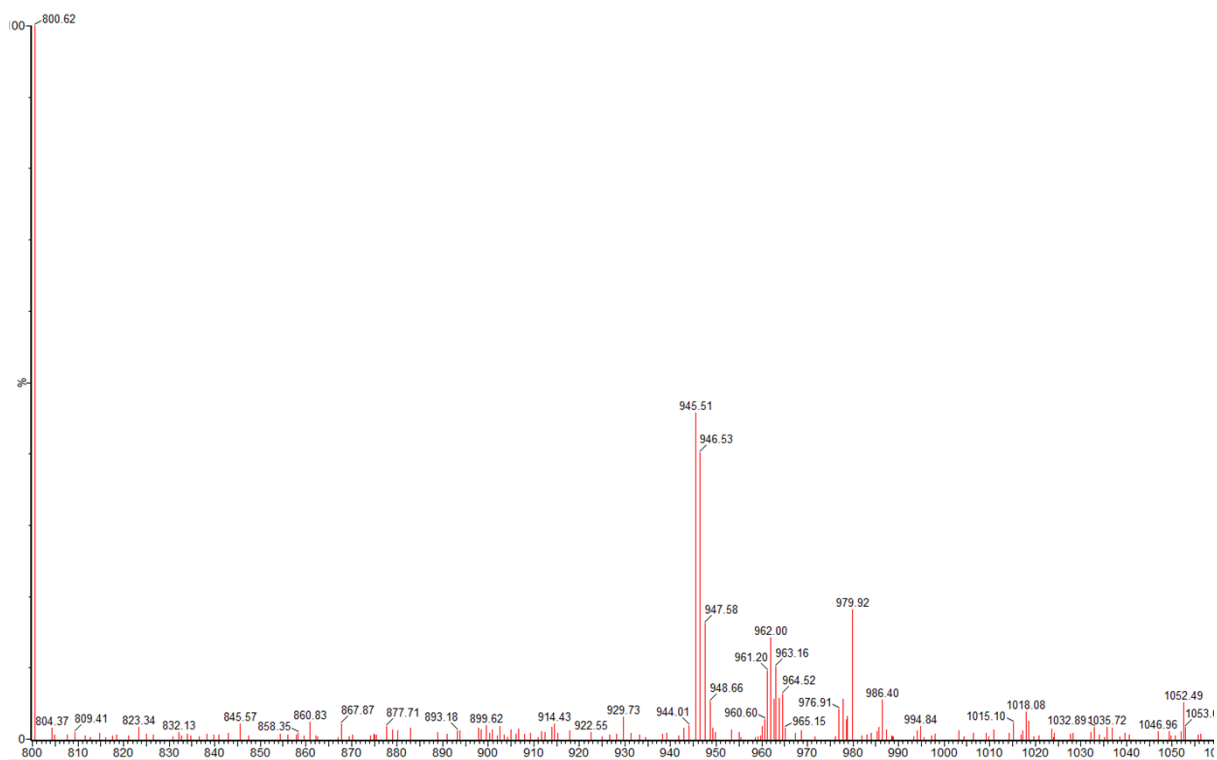
**Figure S15** MS Spectrum of DFPFPhe.



**Figure S16** MS Spectrum of DPFPhE.

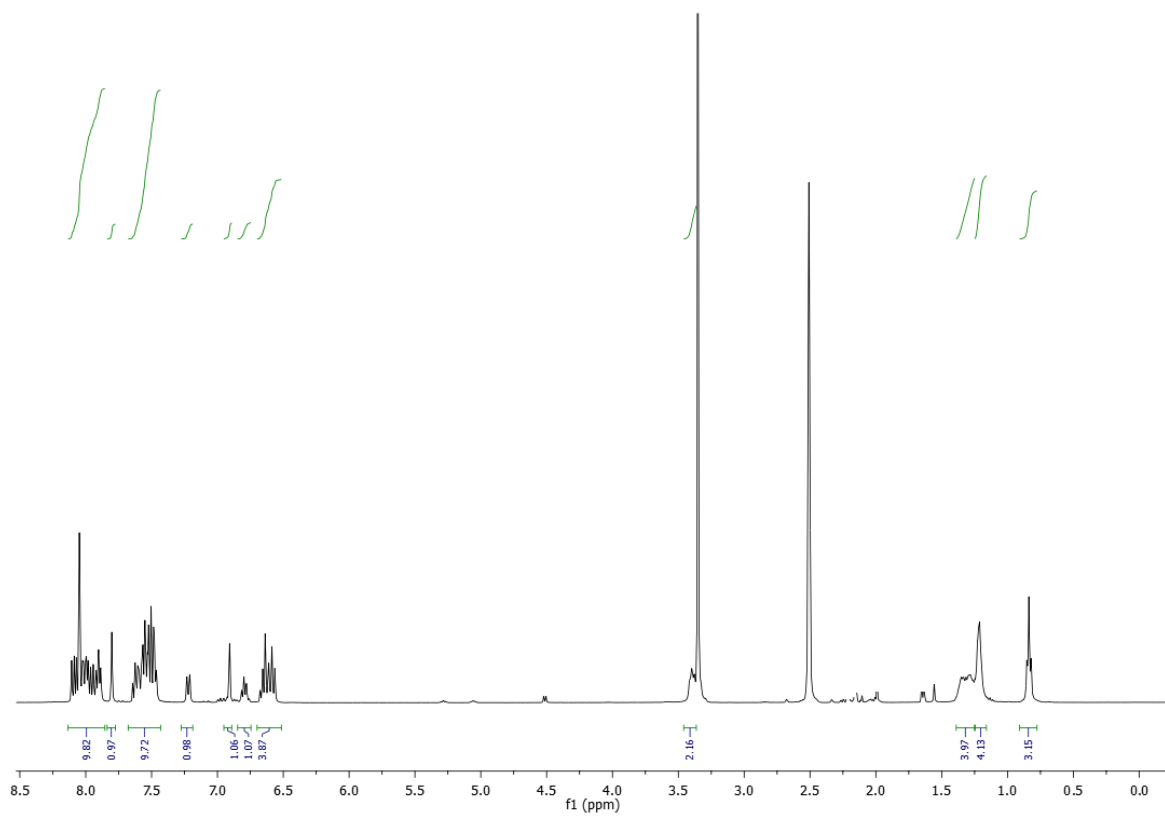


**Figure S17** MS Spectrum of DNFPh.

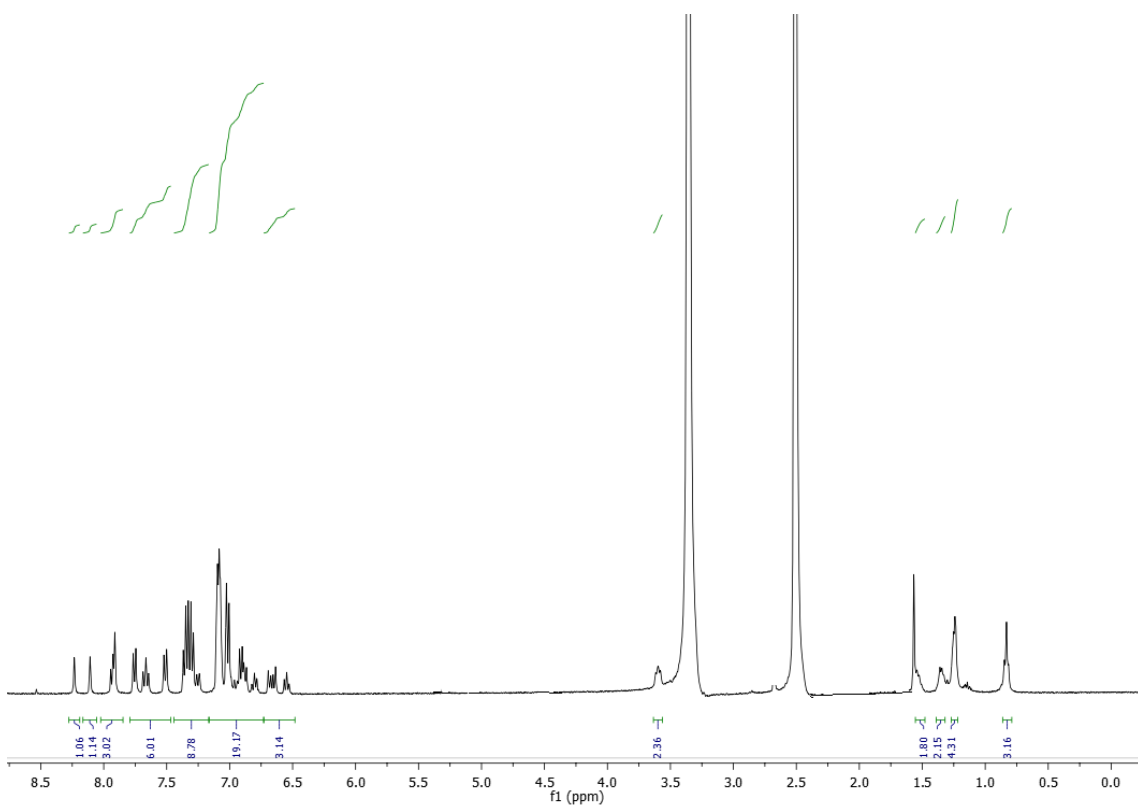


**Figure S18** MS Spectrum of DDPPFPh.

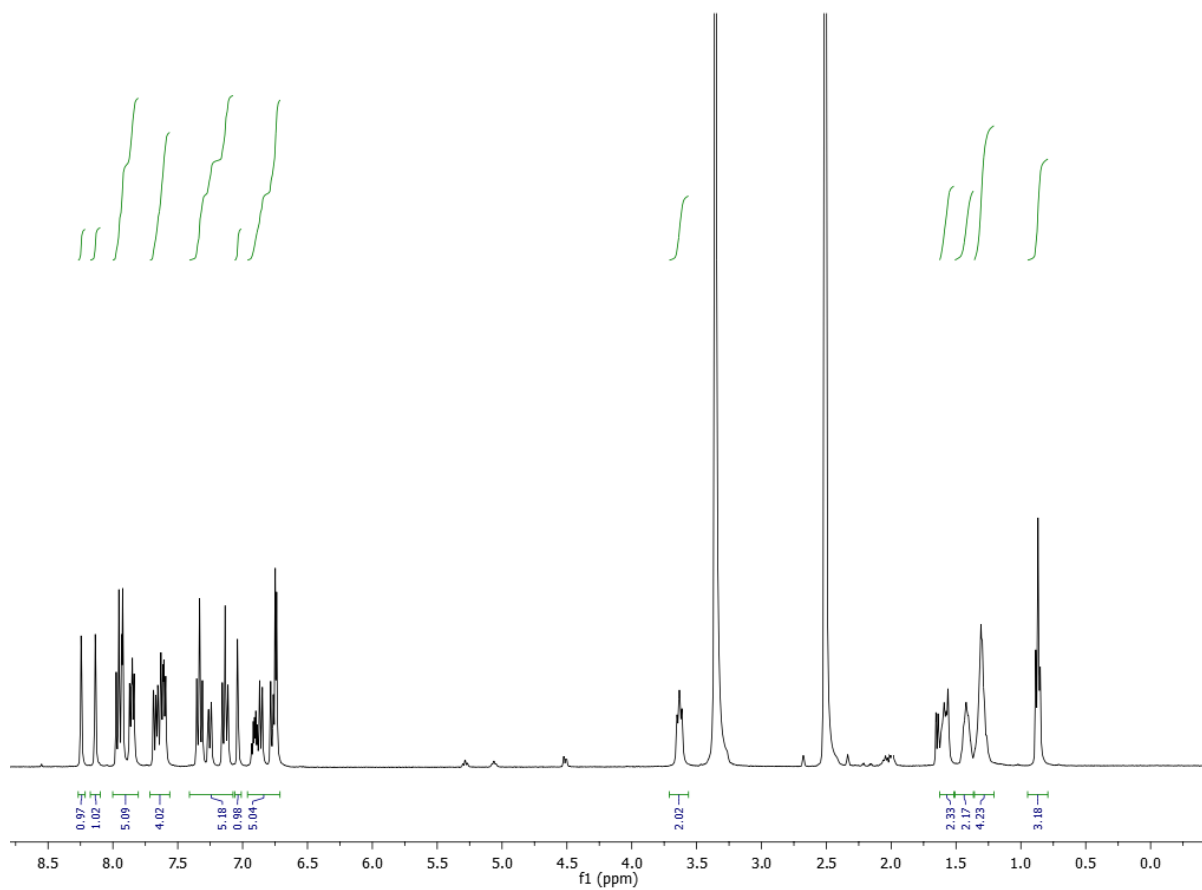




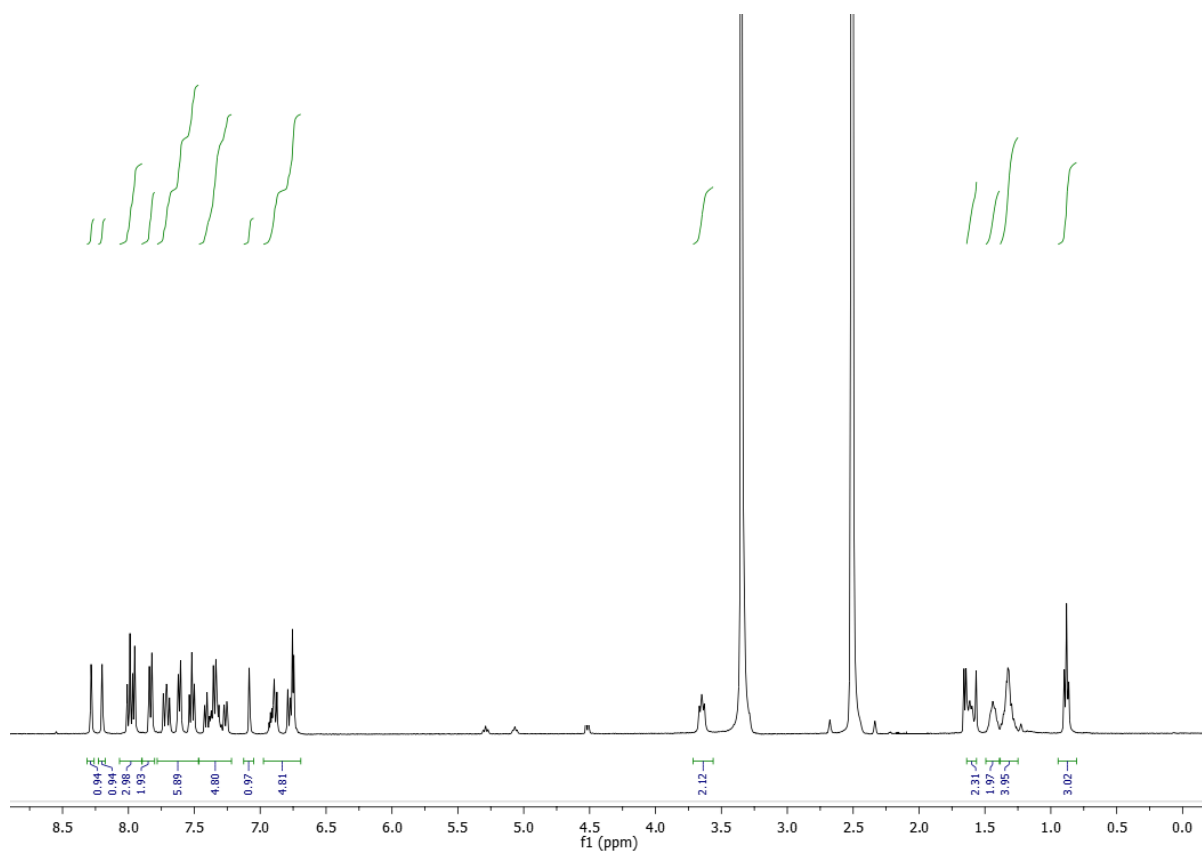
**Figure S19**  $^1\text{H}$  NMR spectrum of DNFPhe



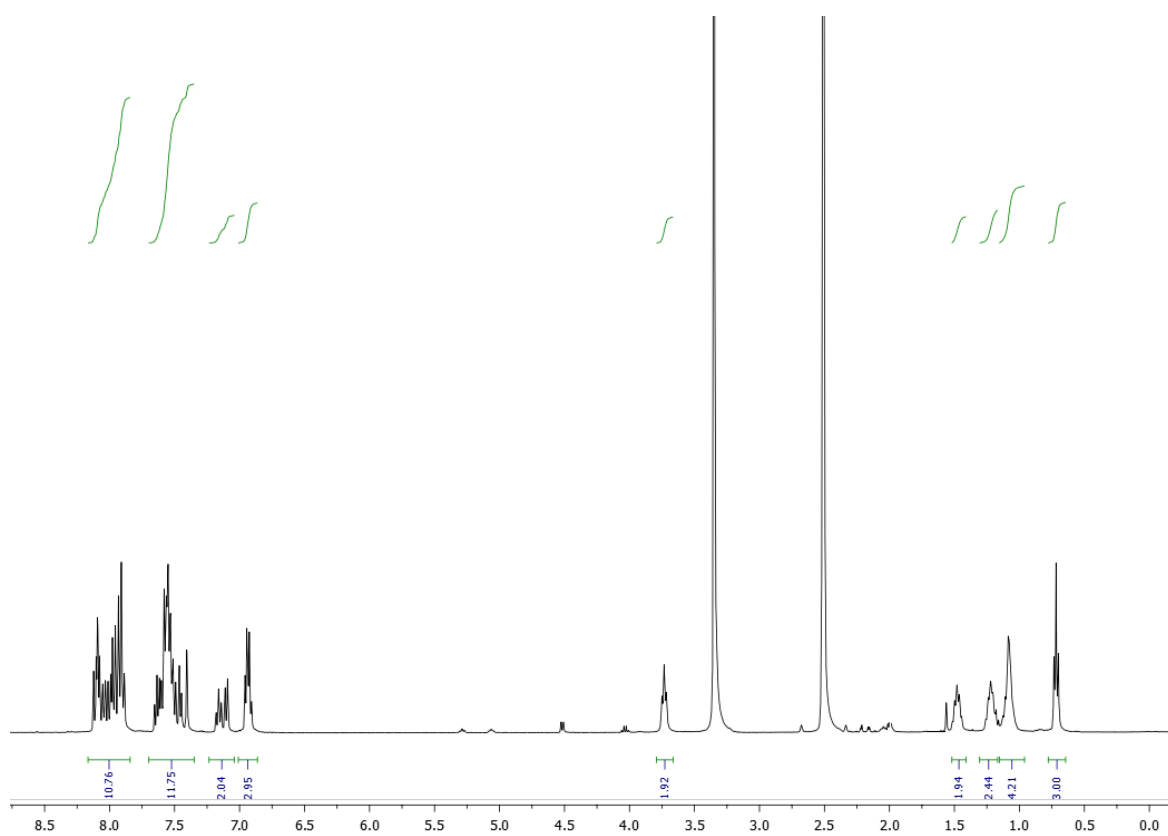
**Figure S20**  $^1\text{H}$  NMR spectrum of DDPFphe.



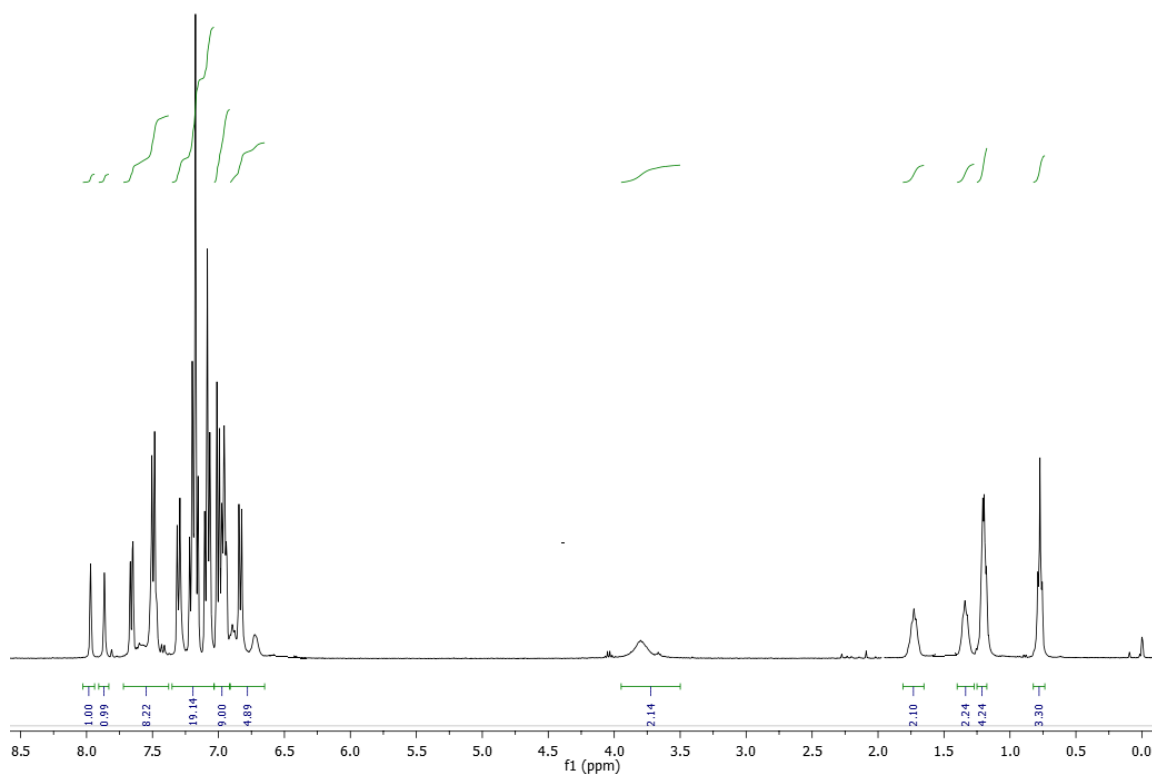
**Figure S21**  $^1\text{H}$  NMR spectrum of DFPFPh.



**Figure S22**  $^1\text{H}$  NMR spectrum of DPFPh.



**Figure S23**  $^1\text{H}$  NMR spectrum of DNFPh.



**Figure S24**  $^1\text{H}$  NMR spectrum of DDPPFPh.

Coordinates of the optimized structures:

1. Coordinates of the optimized structure of DNFPhе

6	-4.795512000	6.237315000	-1.582638000
6	-3.683665000	6.635828000	-2.312108000
6	-2.463993000	5.987549000	-2.104561000
6	-2.367770000	4.970266000	-1.170933000
6	-3.479472000	4.553826000	-0.416352000
6	-4.697924000	5.201602000	-0.649974000
8	-1.122005000	4.400321000	-0.989570000
7	-3.316465000	3.525396000	0.529829000
6	-4.421186000	3.150440000	1.414223000
6	-5.378937000	2.104869000	0.823679000
6	-6.508639000	1.736913000	1.792109000
6	-7.478166000	0.697417000	1.218566000
6	-8.609307000	0.317016000	2.180987000
6	-9.576625000	-0.716304000	1.596324000
6	6.797283000	0.979719000	-1.382471000
6	7.230451000	1.870994000	-2.335740000
6	8.392145000	2.646559000	-2.118842000
6	9.107122000	2.497480000	-0.956030000
6	-1.773887000	-5.058726000	-2.094655000
6	-2.315521000	-5.817041000	-3.105762000
6	-3.702786000	-6.086193000	-3.137871000
6	-4.522174000	-5.572447000	-2.163047000
6	-1.049309000	3.226537000	-0.266805000
6	-2.136230000	2.781644000	0.514282000
6	0.142637000	2.535963000	-0.310283000
6	0.324934000	1.339432000	0.415261000
6	-0.740254000	0.911028000	1.215754000
6	-1.943631000	1.608992000	1.258521000

6	1.629817000	0.686688000	0.370965000
6	1.997204000	-0.617686000	0.453195000
6	3.417827000	-1.033496000	0.555409000
6	3.488112000	-2.441739000	0.630649000
6	2.128329000	-2.969561000	0.532170000
6	1.222965000	-1.883033000	0.423170000
6	4.581476000	-0.272441000	0.619295000
6	5.827216000	-0.905190000	0.749285000
6	5.876824000	-2.308724000	0.827380000
6	4.718187000	-3.079810000	0.768927000
6	1.669800000	-4.283969000	0.493613000
6	0.310372000	-4.526051000	0.321080000
6	-0.601843000	-3.466880000	0.171068000
6	-0.133127000	-2.145776000	0.223840000
6	-2.061916000	-3.730014000	0.018559000
6	7.082905000	-0.108847000	0.864491000
6	7.497679000	0.813138000	-0.155749000
6	8.693768000	1.579555000	0.046325000
6	9.450757000	1.397846000	1.232653000
6	9.051428000	0.488618000	2.179649000
6	7.869320000	-0.259820000	1.991942000
6	-2.585892000	-4.528086000	-1.054456000
6	-3.997743000	-4.778330000	-1.108327000
6	-4.847083000	-4.219359000	-0.118575000
6	-4.327594000	-3.435789000	0.881126000
6	-2.937850000	-3.195541000	0.945767000
1	-5.753121000	6.721396000	-1.733119000
1	-3.753360000	7.436472000	-3.038087000
1	-1.571925000	6.266659000	-2.652257000
1	-5.583515000	4.902491000	-0.107677000
1	-3.992609000	2.786313000	2.350081000
1	-4.964882000	4.060961000	1.673616000

1	-5.802668000	2.488786000	-0.110093000
1	-4.812912000	1.205999000	0.557767000
1	-6.077472000	1.353614000	2.725777000
1	-7.067557000	2.641981000	2.062261000
1	-7.911649000	1.083253000	0.287114000
1	-6.918374000	-0.205560000	0.943279000
1	-8.176433000	-0.072693000	3.110269000
1	-9.165278000	1.220579000	2.458976000
1	-10.369985000	-0.966432000	2.306029000
1	-10.051684000	-0.340334000	0.684753000
1	-9.055453000	-1.643819000	1.339106000
1	5.913802000	0.383548000	-1.569594000
1	6.680890000	1.976260000	-3.264401000
1	8.720543000	3.349145000	-2.876367000
1	10.008599000	3.077121000	-0.787004000
1	-0.711856000	-4.851389000	-2.092425000
1	-1.675322000	-6.207054000	-3.889032000
1	-4.116655000	-6.689041000	-3.938230000
1	-5.590427000	-5.760755000	-2.187389000
1	0.941359000	2.939388000	-0.921933000
1	-0.626348000	0.037447000	1.843222000
1	-2.736000000	1.231924000	1.888882000
1	2.451955000	1.389573000	0.252724000
1	4.540435000	0.810480000	0.589807000
1	6.840120000	-2.796049000	0.925313000
1	4.783369000	-4.160732000	0.828016000
1	2.359804000	-5.114825000	0.591193000
1	-0.053913000	-5.546746000	0.308655000
1	-0.840066000	-1.339711000	0.087795000
1	10.351219000	1.986066000	1.373976000
1	9.632550000	0.347549000	3.083925000
1	7.555104000	-0.952990000	2.764037000



1	-5.912077000	-4.419239000	-0.168939000
1	-4.977333000	-3.008993000	1.636796000
1	-2.542684000	-2.599266000	1.760431000

2. Coordinates of the optimized structure of DDPFPhe-

6	-1.038511000	-1.139681000	0.007417000
6	-3.630056000	-1.460198000	0.016446000
6	-4.686930000	-2.383900000	0.082596000
6	-4.380533000	-3.755262000	0.189390000
6	-3.064782000	-4.207031000	0.224947000
6	0.206393000	-4.598840000	0.169488000
6	1.036795000	3.314370000	-0.686184000
6	2.133436000	3.157163000	0.172828000
6	0.037313000	2.349630000	-0.762006000
6	0.090598000	1.173440000	-0.002110000
6	1.169383000	1.035664000	0.893736000
6	2.157041000	1.995319000	0.971946000
6	-1.004781000	0.212915000	-0.099743000
6	-2.311382000	-1.901360000	0.045781000
6	-2.026521000	-3.280420000	0.151886000
6	-0.575314000	-3.446660000	0.146640000
6	0.031371000	-2.166943000	0.053751000
6	1.589892000	-4.486634000	0.077342000
6	2.215212000	-3.232628000	-0.053141000
6	1.416796000	-2.075622000	-0.064726000
6	3.689553000	-3.129920000	-0.176630000
6	-6.096196000	-1.923903000	0.045284000
6	-6.489818000	-0.721283000	0.654415000
6	-7.808869000	-0.288667000	0.626218000
6	-8.793850000	-1.040079000	-0.030505000
6	-8.412216000	-2.239774000	-0.648026000

6	-7.093331000	-2.671650000	-0.601755000
6	4.544630000	-4.005154000	0.512252000
6	5.925846000	-3.902974000	0.411827000
6	6.513173000	-2.922710000	-0.400825000
6	5.669418000	-2.050433000	-1.103324000
6	4.289904000	-2.150593000	-0.984602000
7	-10.141079000	-0.598692000	-0.068194000
6	-10.433696000	0.777104000	-0.277235000
6	-11.201248000	-1.530624000	0.103876000
6	-12.342903000	-1.468562000	-0.707598000
6	-13.381493000	-2.377992000	-0.530546000
6	-13.295133000	-3.372519000	0.443342000
6	-12.157551000	-3.441704000	1.247137000
6	-11.121738000	-2.525912000	1.088167000
6	-9.733817000	1.515065000	-1.242432000
6	-10.017161000	2.863429000	-1.438480000
6	-11.011179000	3.495138000	-0.691678000
6	-11.715619000	2.761741000	0.262761000
6	-11.427223000	1.417090000	0.477057000
8	3.187089000	1.757929000	1.859341000
6	4.071373000	2.786989000	2.119753000
6	4.088716000	3.955508000	1.336491000
7	3.174557000	4.080468000	0.275244000
7	7.922870000	-2.814066000	-0.508255000
6	8.725183000	-3.986494000	-0.575362000
6	8.540528000	-1.533091000	-0.526748000
6	9.593457000	-1.264568000	-1.412876000
6	10.204211000	-0.014008000	-1.420673000
6	9.767212000	0.994000000	-0.561592000
6	8.713870000	0.733429000	0.314496000
6	8.109330000	-0.519915000	0.341345000
6	8.346430000	-5.063121000	-1.389617000

6	9.131363000	-6.210980000	-1.447129000
6	10.312392000	-6.300324000	-0.710736000
6	10.696175000	-5.227882000	0.093890000
6	9.908352000	-4.083088000	0.170316000
6	4.957023000	2.602610000	3.167543000
6	5.904474000	3.584716000	3.466578000
6	5.935869000	4.748445000	2.709968000
6	5.032617000	4.936650000	1.660805000
6	3.256129000	5.213256000	-0.647889000
6	2.477154000	6.460576000	-0.204583000
6	2.597979000	7.605009000	-1.216793000
6	1.813609000	8.857992000	-0.811948000
6	1.930433000	10.005593000	-1.821559000
6	1.137959000	11.251113000	-1.414517000
1	-3.855514000	-0.404403000	-0.080494000
1	-5.188082000	-4.473195000	0.271792000
1	-2.860271000	-5.268013000	0.317846000
1	-0.252993000	-5.578956000	0.235602000
1	0.949322000	4.201584000	-1.296794000
1	-0.797317000	2.513614000	-1.434318000
1	1.239205000	0.186168000	1.559876000
1	-1.965956000	0.685434000	-0.291148000
1	2.193969000	-5.386249000	0.068901000
1	1.897269000	-1.112312000	-0.154002000
1	-5.759719000	-0.129589000	1.194664000
1	-8.083162000	0.632593000	1.125401000
1	-9.152737000	-2.829341000	-1.174498000
1	-6.827664000	-3.590162000	-1.112383000
1	4.125124000	-4.756412000	1.171599000
1	6.556744000	-4.578638000	0.976174000
1	6.099406000	-1.296324000	-1.750974000
1	3.667967000	-1.475319000	-1.560890000

1	-12.411534000	-0.706718000	-1.474504000
1	-14.256700000	-2.315538000	-1.167696000
1	-14.102819000	-4.083079000	0.574183000
1	-12.079268000	-4.204563000	2.013804000
1	-10.247838000	-2.577462000	1.726031000
1	-8.969827000	1.028265000	-1.836346000
1	-9.466269000	3.418320000	-2.189802000
1	-11.233936000	4.543586000	-0.851345000
1	-12.486721000	3.240658000	0.855947000
1	-11.970196000	0.857446000	1.228961000
1	9.929720000	-2.038419000	-2.092134000
1	11.017367000	0.175896000	-2.112484000
1	10.240475000	1.968829000	-0.575005000
1	8.366089000	1.504999000	0.992302000
1	7.299856000	-0.717595000	1.033205000
1	7.437359000	-4.995589000	-1.974788000
1	8.823638000	-7.033725000	-2.082943000
1	10.924751000	-7.192871000	-0.763325000
1	11.607964000	-5.285491000	0.677993000
1	10.206286000	-3.259234000	0.807297000
1	4.897223000	1.680142000	3.732397000
1	6.599046000	3.434293000	4.283809000
1	6.657122000	5.526631000	2.929524000
1	5.071068000	5.858847000	1.098562000
1	4.311958000	5.455529000	-0.785397000
1	2.900605000	4.872994000	-1.623084000
1	1.422860000	6.199379000	-0.065701000
1	2.843302000	6.790228000	0.773296000
1	3.656156000	7.866000000	-1.345905000
1	2.246491000	7.260443000	-2.197847000
1	0.755416000	8.596359000	-0.684215000
1	2.163265000	9.203472000	0.169381000

1	2.987585000	10.269680000	-1.945921000
1	1.585455000	9.658063000	-2.802920000
1	1.242210000	12.049609000	-2.154283000
1	0.071353000	11.025631000	-1.316421000
1	1.483307000	11.641980000	-0.452159000

### 3. Coordinates of the optimized structure of DFPPPh-

6	-5.161107000	5.617407000	-1.387854000
6	-4.125063000	6.157790000	-2.137430000
6	-2.841823000	5.620355000	-2.013763000
6	-2.609587000	4.570831000	-1.141888000
6	-3.642742000	4.010528000	-0.369281000
6	-4.925680000	4.549371000	-0.518453000
8	-1.308749000	4.115562000	-1.039078000
7	-3.341940000	2.954624000	0.510768000
6	-4.355939000	2.450230000	1.437623000
6	-5.255484000	1.346313000	0.861706000
6	-6.292675000	0.857342000	1.878433000
6	-7.202694000	-0.247439000	1.329707000
6	-8.243539000	-0.741767000	2.340636000
6	-9.148929000	-1.844012000	1.783198000
6	-1.094719000	2.917412000	-0.388481000
6	-2.100716000	2.326933000	0.404545000
6	0.155686000	2.351329000	-0.512893000
6	0.480311000	1.140357000	0.134210000
6	-0.506988000	0.562384000	0.940364000
6	-1.768869000	1.136706000	1.067925000
6	1.842409000	0.627416000	0.016883000
6	2.337402000	-0.635963000	-0.004415000
6	3.793177000	-0.916758000	0.042268000
6	4.000584000	-2.312766000	0.004866000

6	2.697310000	-2.962368000	-0.114601000
6	1.687905000	-1.964908000	-0.121474000
6	4.878207000	-0.052605000	0.149773000
6	6.184196000	-0.564913000	0.206132000
6	6.370073000	-1.960224000	0.166252000
6	5.291217000	-2.833933000	0.069048000
6	2.365705000	-4.306965000	-0.258651000
6	1.033036000	-4.664404000	-0.434667000
6	0.017976000	-3.692050000	-0.488230000
6	0.361077000	-2.339315000	-0.328835000
6	-1.395860000	-4.089098000	-0.711981000
6	7.349551000	0.350058000	0.310403000
6	7.380533000	1.563998000	-0.394227000
6	8.466301000	2.429444000	-0.299499000
6	9.532564000	2.070868000	0.509823000
6	9.546677000	0.882223000	1.222282000
6	8.452406000	0.028743000	1.117605000
6	-1.722483000	-5.132011000	-1.593466000
6	-3.043827000	-5.511152000	-1.810277000
6	-4.048012000	-4.834842000	-1.135955000
6	-3.773423000	-3.798863000	-0.257388000
6	-2.446528000	-3.433688000	-0.050502000
9	10.595057000	2.908690000	0.607528000
9	-5.338849000	-5.197724000	-1.341747000
1	-6.165579000	6.014499000	-1.473456000
1	-4.301927000	6.984152000	-2.814739000
1	-2.004812000	6.012013000	-2.579145000
1	-5.754435000	4.139686000	0.041134000
1	-3.842578000	2.091245000	2.332088000
1	-4.959620000	3.299409000	1.764129000
1	-5.762481000	1.721300000	-0.033378000
1	-4.633569000	0.507016000	0.533347000



1	-5.778225000	0.490016000	2.775632000
1	-6.909086000	1.704461000	2.205158000
1	-7.716795000	0.119825000	0.432433000
1	-6.586467000	-1.094793000	1.002629000
1	-7.729294000	-1.109526000	3.236791000
1	-8.858366000	0.105402000	2.667799000
1	-9.878482000	-2.175433000	2.527226000
1	-9.702994000	-1.493590000	0.906693000
1	-8.564917000	-2.717775000	1.477329000
1	0.887331000	2.865589000	-1.125300000
1	-0.284837000	-0.331817000	1.507567000
1	-2.495128000	0.650343000	1.703647000
1	2.587536000	1.416513000	-0.062345000
1	4.726775000	1.018675000	0.216321000
1	7.376297000	-2.361859000	0.189678000
1	5.463394000	-3.904052000	0.035323000
1	3.133366000	-5.072583000	-0.239850000
1	0.772240000	-5.712614000	-0.522552000
1	-0.414786000	-1.590361000	-0.401717000
1	6.555641000	1.829009000	-1.044692000
1	8.496076000	3.361934000	-0.849344000
1	10.394041000	0.640925000	1.851986000
1	8.448443000	-0.890204000	1.691375000
1	-0.936112000	-5.641863000	-2.136725000
1	-3.297835000	-6.309208000	-2.496811000
1	-4.585043000	-3.300101000	0.257652000
1	-2.225758000	-2.639762000	0.652528000

#### 4. Coordinates of the optimized structure of DPFPh-

6	-5.600560000	4.925390000	-1.465103000
6	-4.629500000	5.576120000	-2.214101000

6	-3.292765000	5.194743000	-2.077025000
6	-2.945000000	4.188402000	-1.192729000
6	-3.911270000	3.518266000	-0.421014000
6	-5.247623000	3.900639000	-0.583418000
8	-1.600382000	3.891395000	-1.074292000
7	-3.494908000	2.513494000	0.470847000
6	-4.439506000	1.930321000	1.424408000
6	-5.229566000	0.722842000	0.897004000
6	-6.209594000	0.180008000	1.942861000
6	-7.011746000	-1.031323000	1.454116000
6	-8.003142000	-1.566577000	2.493609000
6	-8.799446000	-2.778506000	2.001332000
6	-1.253671000	2.727679000	-0.417875000
6	-2.190406000	2.028678000	0.371314000
6	0.054781000	2.308508000	-0.531243000
6	0.509078000	1.143535000	0.120907000
6	-0.412078000	0.455391000	0.918495000
6	-1.731375000	0.884101000	1.038050000
6	1.922399000	0.784565000	0.024032000
6	2.541109000	-0.421581000	-0.018244000
6	4.014880000	-0.565801000	0.068053000
6	4.354157000	-1.934396000	-0.005544000
6	3.122284000	-2.698981000	-0.189498000
6	2.024079000	-1.800752000	-0.198345000
6	5.008487000	0.392857000	0.238650000
6	6.355245000	0.004828000	0.324396000
6	6.673092000	-1.365021000	0.247594000
6	5.686183000	-2.332890000	0.085804000
6	2.922339000	-4.062421000	-0.390141000
6	1.635115000	-4.533740000	-0.627077000
6	0.535211000	-3.658502000	-0.684222000
6	0.745124000	-2.287106000	-0.464346000

6	-0.826579000	-4.175280000	-0.977799000
6	7.425537000	1.020575000	0.497067000
6	7.359790000	2.259187000	-0.160902000
6	8.362719000	3.211314000	0.001279000
6	9.456159000	2.947302000	0.824822000
6	9.536157000	1.721865000	1.484941000
6	8.532716000	0.770307000	1.323408000
6	-1.021383000	-5.203425000	-1.914079000
6	-2.296730000	-5.687162000	-2.193244000
6	-3.408966000	-5.153957000	-1.543521000
6	-3.232400000	-4.132141000	-0.611640000
6	-1.956711000	-3.649434000	-0.331768000
1	-6.643952000	5.201336000	-1.560868000
1	-4.897152000	6.369480000	-2.901026000
1	-2.503625000	5.677564000	-2.640777000
1	-6.025954000	3.400724000	-0.024459000
1	-3.880535000	1.652459000	2.320747000
1	-5.125023000	2.721493000	1.735407000
1	-5.775438000	1.011884000	-0.007080000
1	-4.532660000	-0.066265000	0.596117000
1	-5.657840000	-0.094924000	2.850936000
1	-6.903250000	0.977935000	2.237033000
1	-7.556881000	-0.760134000	0.541007000
1	-6.319099000	-1.833756000	1.169480000
1	-7.458119000	-1.834451000	3.406859000
1	-8.695843000	-0.764613000	2.775844000
1	-9.497436000	-3.133755000	2.764419000
1	-9.380972000	-2.532312000	1.107274000
1	-8.135349000	-3.610123000	1.745346000
1	0.728435000	2.901878000	-1.138621000
1	-0.094536000	-0.412068000	1.482198000
1	-2.403132000	0.319880000	1.669093000

1	2.583500000	1.648259000	-0.011049000
1	4.753307000	1.442338000	0.331679000
1	7.711602000	-1.671141000	0.294576000
1	5.961601000	-3.379971000	0.024532000
1	3.756603000	-4.754901000	-0.370060000
1	1.475844000	-5.597170000	-0.761769000
1	-0.093833000	-1.609457000	-0.537225000
1	6.527973000	2.469257000	-0.823534000
1	8.293676000	4.157559000	-0.523774000
1	10.237300000	3.688298000	0.950925000
1	10.377728000	1.508579000	2.134652000
1	8.596756000	-0.168286000	1.861860000
1	-0.169264000	-5.610655000	-2.446090000
1	-2.422146000	-6.476074000	-2.926553000
1	-4.402068000	-5.529926000	-1.761451000
1	-4.089300000	-3.714860000	-0.094336000
1	-1.833263000	-2.870266000	0.411514000

##### 5. Coordinates of the optimized structure of DDPPFPh-

6	5.689994000	4.949457000	-2.522367000
6	4.845873000	5.213955000	-3.597037000
6	3.471700000	5.042246000	-3.443174000
6	2.947553000	4.650913000	-2.213733000
6	3.788064000	4.388784000	-1.117044000
6	5.171677000	4.521335000	-1.301673000
16	1.180720000	4.534265000	-1.982862000
7	3.221448000	3.983041000	0.116815000
6	1.173639000	3.124001000	-0.887669000
6	2.186875000	3.027030000	0.085785000
6	0.148849000	2.190469000	-0.951952000
6	0.078895000	1.119361000	-0.043920000

6	1.074433000	1.040880000	0.940576000
6	2.111685000	1.963640000	0.997806000
6	-1.067275000	0.207509000	-0.101927000
6	-1.149584000	-1.130914000	0.088829000
6	-2.444969000	-1.853718000	0.152110000
6	-2.200317000	-3.229968000	0.349293000
6	-0.753773000	-3.435492000	0.385504000
6	-0.109481000	-2.182190000	0.225337000
6	-3.749066000	-1.378119000	0.074492000
6	-4.832893000	-2.266210000	0.183719000
6	-4.566788000	-3.636004000	0.378624000
6	-3.265101000	-4.121449000	0.462224000
6	-0.005201000	-4.603479000	0.504864000
6	1.382881000	-4.531963000	0.445492000
6	2.045837000	-3.305606000	0.253458000
6	1.280026000	-2.131834000	0.142709000
6	3.525479000	-3.250883000	0.169261000
6	-6.228374000	-1.770970000	0.106618000
6	-6.593341000	-0.526677000	0.645495000
6	-7.901290000	-0.064143000	0.589222000
6	-8.903691000	-0.826743000	-0.027519000
6	-8.549017000	-2.066304000	-0.579568000
6	-7.241563000	-2.527484000	-0.504100000
6	4.332896000	-4.094891000	0.948904000
6	5.718688000	-4.043208000	0.880614000
6	6.358961000	-3.149016000	0.010500000
6	5.563120000	-2.306254000	-0.778928000
6	4.178124000	-2.354077000	-0.691951000
7	-10.240092000	-0.358677000	-0.090232000
6	-10.504095000	1.015934000	-0.343102000
6	-11.321961000	-1.259313000	0.114148000
7	7.773568000	-3.099950000	-0.069375000

6	8.530911000	-4.303736000	-0.027196000
6	8.441095000	-1.849978000	-0.186353000
6	-12.456469000	-1.205536000	-0.707596000
6	-13.517143000	-2.082322000	-0.499617000
6	-13.460074000	-3.035827000	0.516567000
6	-12.329873000	-3.096457000	1.331387000
6	-11.271972000	-2.212418000	1.141049000
6	-9.792723000	1.707542000	-1.333684000
6	-10.049450000	3.054317000	-1.572796000
6	-11.028077000	3.730064000	-0.844296000
6	-11.743719000	3.042731000	0.135588000
6	-11.481551000	1.700228000	0.392850000
6	8.128574000	-5.424389000	-0.767089000
6	8.866875000	-6.603042000	-0.715098000
6	10.024998000	-6.680418000	0.058026000
6	10.433414000	-5.564164000	0.787453000
6	9.691537000	-4.387029000	0.754507000
6	8.036465000	-0.749702000	0.582921000
6	8.690753000	0.472535000	0.460392000
6	9.767383000	0.616414000	-0.414375000
6	10.178395000	-0.478481000	-1.174022000
6	9.518958000	-1.699626000	-1.070405000
6	3.975522000	4.187933000	1.363062000
6	3.107281000	4.714666000	2.516731000
6	2.450601000	6.081108000	2.259805000
6	3.408692000	7.271545000	2.085913000
6	4.247738000	7.609395000	3.325067000
6	5.112338000	8.859972000	3.137909000
1	6.762960000	5.056197000	-2.632481000
1	5.248511000	5.537819000	-4.549176000
1	2.799063000	5.224523000	-4.273302000
1	5.851787000	4.283218000	-0.494824000

1	-0.614007000	2.295750000	-1.715503000
1	1.030385000	0.258453000	1.687544000
1	2.861956000	1.856696000	1.769278000
1	-2.005878000	0.707281000	-0.332493000
1	-3.942655000	-0.324487000	-0.090944000
1	-5.395513000	-4.324805000	0.493268000
1	-3.092346000	-5.179712000	0.624293000
1	-0.492486000	-5.565101000	0.622230000
1	1.962646000	-5.444975000	0.513414000
1	1.787155000	-1.187542000	0.007329000
1	-5.850245000	0.076061000	1.155050000
1	-8.153160000	0.889724000	1.036096000
1	-9.301677000	-2.665117000	-1.077502000
1	-6.997573000	-3.478974000	-0.962539000
1	3.871374000	-4.779685000	1.651194000
1	6.312596000	-4.692516000	1.512079000
1	6.034115000	-1.619299000	-1.471171000
1	3.593720000	-1.706818000	-1.335743000
1	-12.502074000	-0.475758000	-1.506735000
1	-14.386604000	-2.027200000	-1.145230000
1	-14.284856000	-3.721442000	0.671619000
1	-12.274703000	-3.826965000	2.130863000
1	-10.403644000	-2.256229000	1.787093000
1	-9.040475000	1.186438000	-1.913377000
1	-9.489881000	3.573127000	-2.343220000
1	-11.230179000	4.777017000	-1.037631000
1	-12.502968000	3.556174000	0.715029000
1	-12.032978000	1.176816000	1.164451000
1	7.237377000	-5.366926000	-1.380150000
1	8.541160000	-7.460161000	-1.293927000
1	10.601312000	-7.597553000	0.091367000
1	11.328294000	-5.611584000	1.398014000

1	10.008069000	-3.528233000	1.333823000
1	7.210012000	-0.857355000	1.274712000
1	8.365094000	1.312255000	1.064314000
1	10.279195000	1.567569000	-0.502322000
1	11.009892000	-0.380529000	-1.863094000
1	9.836514000	-2.541755000	-1.673121000
1	4.495817000	3.271875000	1.669656000
1	4.749175000	4.921551000	1.146452000
1	2.324705000	3.989536000	2.753951000
1	3.750368000	4.760832000	3.401890000
1	1.816881000	6.004828000	1.370595000
1	1.776037000	6.295006000	3.097201000
1	4.075753000	7.100013000	1.232181000
1	2.811111000	8.151296000	1.818427000
1	3.577810000	7.753343000	4.181886000
1	4.893781000	6.763012000	3.583363000
1	5.810904000	8.736211000	2.304172000
1	4.494765000	9.737801000	2.923065000
1	5.699928000	9.077588000	4.034199000

#### 6. Coordinates of the optimized structure of DNFPh-

6	-5.605067000	5.099398000	-2.024948000
6	-4.683199000	5.678666000	-2.888711000
6	-3.324564000	5.492968000	-2.644665000
6	-2.894460000	4.756126000	-1.544042000
6	-3.814611000	4.129916000	-0.680569000
6	-5.179702000	4.325312000	-0.947247000
16	-1.156140000	4.743233000	-1.159299000
7	-3.379554000	3.349331000	0.416611000



6	-4.347603000	3.026132000	1.477674000
6	-5.246404000	1.796153000	1.251316000
6	-6.197121000	1.575566000	2.433952000
6	-7.127400000	0.371363000	2.248819000
6	-8.082984000	0.151649000	3.427197000
6	-9.012751000	-1.049988000	3.234866000
6	-1.056203000	3.154823000	-0.360928000
6	-2.144152000	2.680942000	0.404444000
6	0.151080000	2.473430000	-0.394669000
6	0.362207000	1.299174000	0.350163000
6	-0.693745000	0.867672000	1.162804000
6	-1.913942000	1.530729000	1.181179000
6	1.683062000	0.672630000	0.328700000
6	2.062952000	-0.626972000	0.403075000
6	3.483540000	-1.034152000	0.537750000
6	3.562261000	-2.442866000	0.586659000
6	2.209342000	-2.978744000	0.439500000
6	1.298913000	-1.897071000	0.330420000
6	4.637292000	-0.265161000	0.655134000
6	5.883687000	-0.890621000	0.813164000
6	5.942267000	-2.295008000	0.861722000
6	4.792723000	-3.074010000	0.749767000
6	1.761591000	-4.294904000	0.359378000
6	0.408774000	-4.541248000	0.145092000
6	-0.507350000	-3.485387000	-0.003229000
6	-0.050032000	-2.162534000	0.092566000
6	-1.960222000	-3.756318000	-0.203363000
6	7.127193000	-0.087363000	0.992933000
6	7.567116000	0.868797000	0.015609000
6	8.747328000	1.640157000	0.281930000
6	9.465131000	1.429623000	1.487697000
6	9.043314000	0.488184000	2.392541000

6	7.876181000	-0.265180000	2.141854000
6	-2.446036000	-4.526270000	-1.314151000
6	-3.853322000	-4.787486000	-1.414866000
6	-4.735257000	-4.265671000	-0.433321000
6	-4.251544000	-3.507859000	0.603372000
6	-2.866511000	-3.257848000	0.714509000
6	6.907915000	1.065842000	-1.229254000
6	7.364034000	1.989941000	-2.139643000
6	8.509099000	2.769797000	-1.859290000
6	9.185147000	2.592042000	-0.677401000
6	-1.600244000	-5.017851000	-2.346606000
6	-2.106093000	-5.750129000	-3.394720000
6	-3.489207000	-6.030784000	-3.473611000
6	-4.340317000	-5.554126000	-2.507177000
1	-6.668187000	5.231824000	-2.188709000
1	-5.008734000	6.268145000	-3.737081000
1	-2.584722000	5.943051000	-3.296757000
1	-5.928515000	3.875418000	-0.313534000
1	-3.780947000	2.901309000	2.403083000
1	-4.968686000	3.912333000	1.624605000
1	-5.826725000	1.916488000	0.332467000
1	-4.634117000	0.902932000	1.100554000
1	-5.611142000	1.442262000	3.352331000
1	-6.802044000	2.478490000	2.586580000
1	-7.712259000	0.504188000	1.329766000
1	-6.524618000	-0.533468000	2.098626000
1	-7.498426000	0.017828000	4.345438000
1	-8.683156000	1.057193000	3.576985000
1	-9.681696000	-1.177726000	4.090356000
1	-9.633894000	-0.929364000	2.341734000
1	-8.441950000	-1.976659000	3.118087000
1	0.957952000	2.871249000	-1.000589000

1	-0.559218000	0.012111000	1.811782000
1	-2.689965000	1.143867000	1.823666000
1	2.496596000	1.390195000	0.243652000
1	4.587000000	0.817730000	0.648182000
1	6.905877000	-2.776929000	0.980871000
1	4.865446000	-4.155285000	0.788885000
1	2.454425000	-5.123546000	0.455592000
1	0.052429000	-5.563716000	0.097539000
1	-0.759034000	-1.357561000	-0.040887000
1	10.353981000	2.021781000	1.677730000
1	9.594642000	0.325318000	3.311681000
1	7.542844000	-0.983923000	2.881877000
1	-5.796580000	-4.472627000	-0.520143000
1	-4.926309000	-3.108711000	1.352202000
1	-2.499764000	-2.683046000	1.557342000
1	6.038025000	0.467102000	-1.465596000
1	6.845695000	2.117867000	-3.083282000
1	8.855896000	3.498292000	-2.583390000
1	10.074168000	3.174732000	-0.459899000
1	-0.540833000	-4.800758000	-2.308343000
1	-1.440616000	-6.110284000	-4.171190000
1	-3.874804000	-6.612832000	-4.302957000
1	-5.405559000	-5.751224000	-2.567009000

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