Supporting Information

DFT/TDDFT in silico design of ullazine-derived D-π-A-π-A dye photosensitiser

Jing Huang[1*], Lei Yang[1], Zhangxu Chen[2], Yikun Zhou[3], Shasha Zeng[1]

1. Fujian Provincial Key Laboratory of Ecology-Toxicological Effects & Control for Emerging Contaminants, College of Environmental and Biological Engineering, Putian University, Putian, Fujian 351100, China.
2. Key Laboratory of Ecological Environment and Information Atlas, Fujian Provincial University, Putian, Fujian 351100, China.
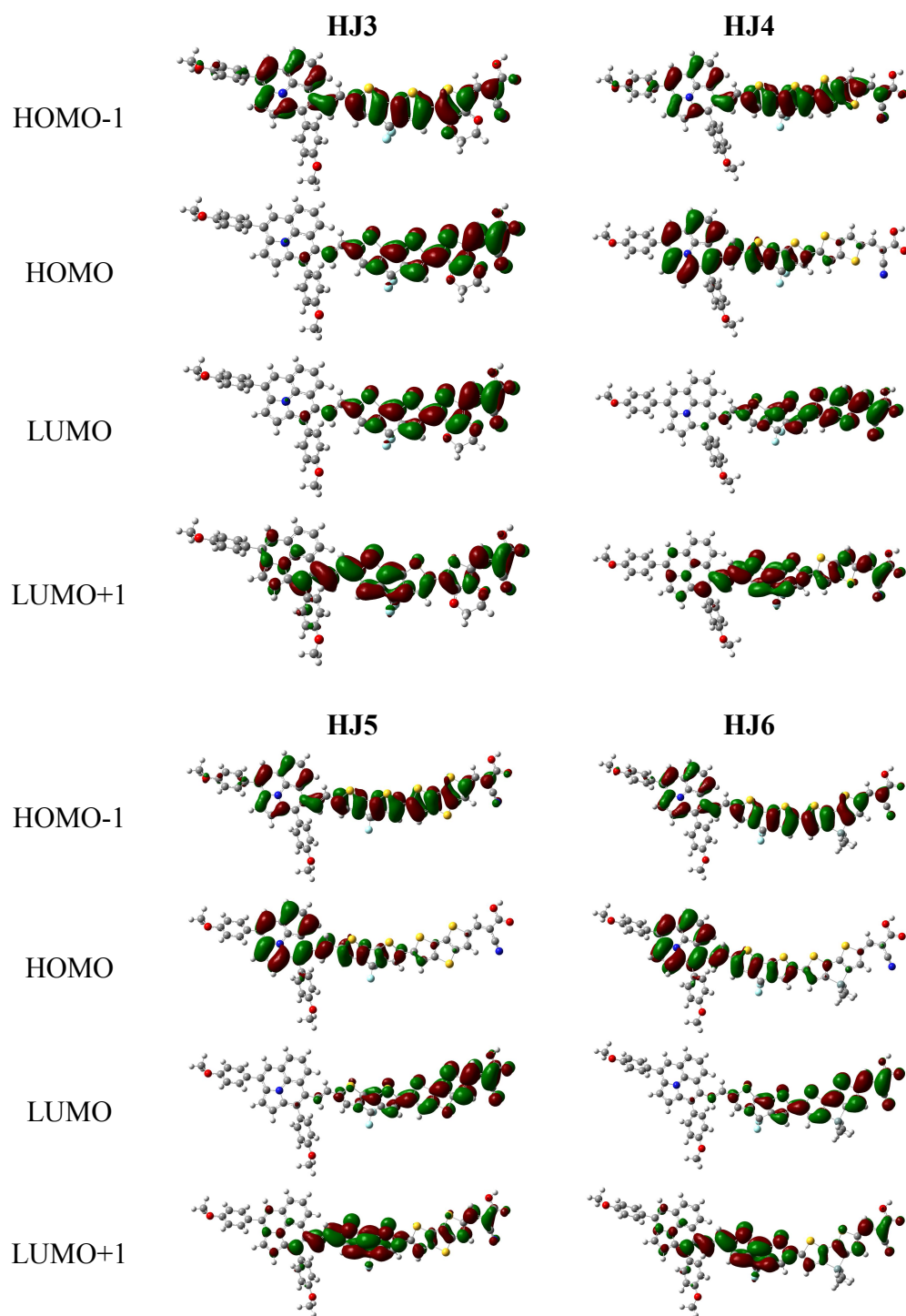*3. College of Chemical Engineering, Huaqiao University, Xiamen, Fujian, 361021, China.*

* corresponding author: jinghuang@ptu.edu.cn

SUMMARY

S1. Frontier molecular orbitals

HJ3 **HJ4**

HOMO-1

HOMO

LUMO

LUMO+1

HJ5 **HJ6**

HOMO-1

HOMO

LUMO

LUMO+1

HJ7   **HJ9**

HOMO-1

HOMO

LUMO

LUMO+1

HJ10   **HJ11**

HOMO-1

HOMO

LUMO

LUMO+1

	HJ12	HJ13
HOMO-1		
HOMO		
LUMO		
LUMO+1		

S2. UV-Vis spectroscopy

YZ7

HJ1

HJ2

HJ3

HJ4

HJ5

HJ6

HJ7

HJ8

HJ9

HJ10

HJ11

HJ12

HJ13
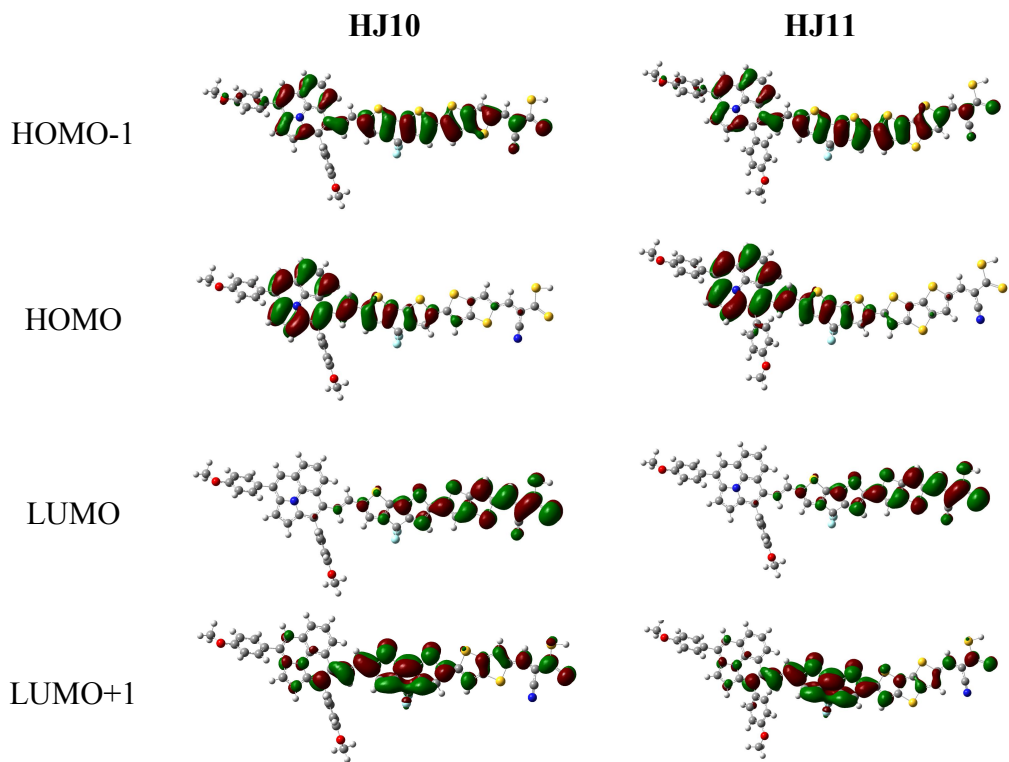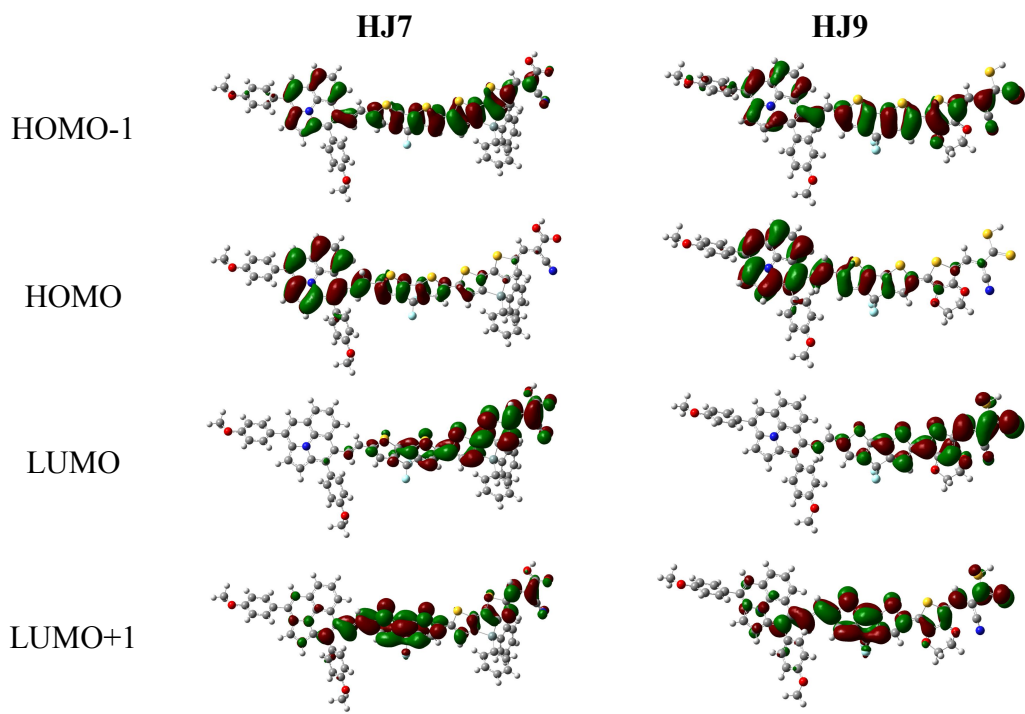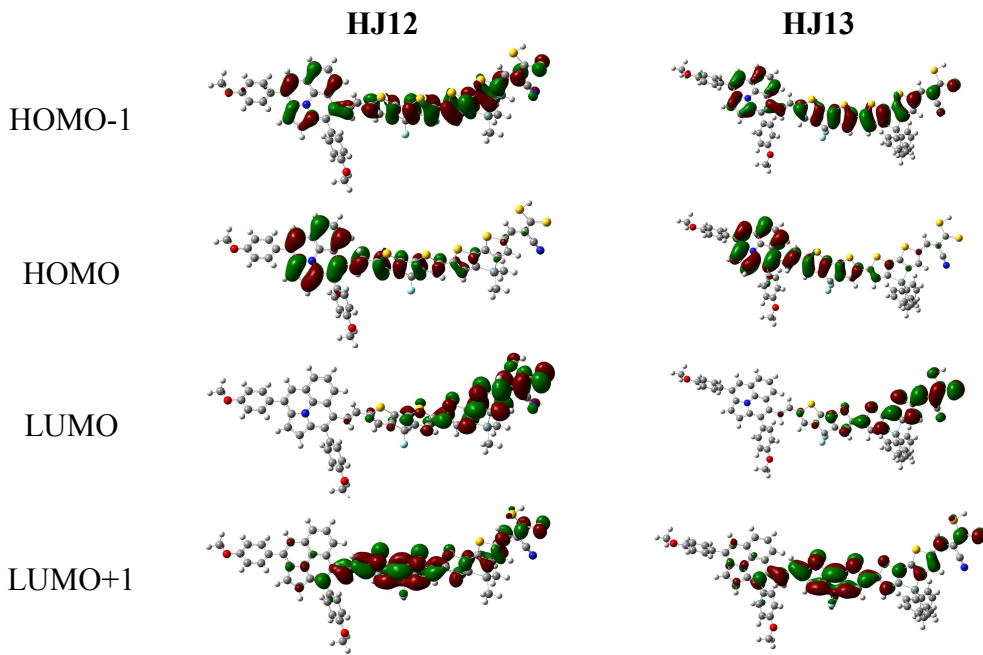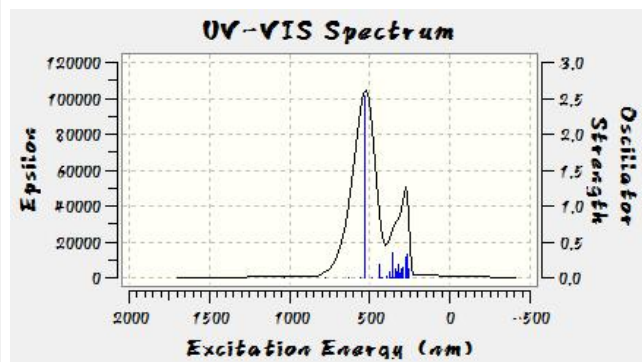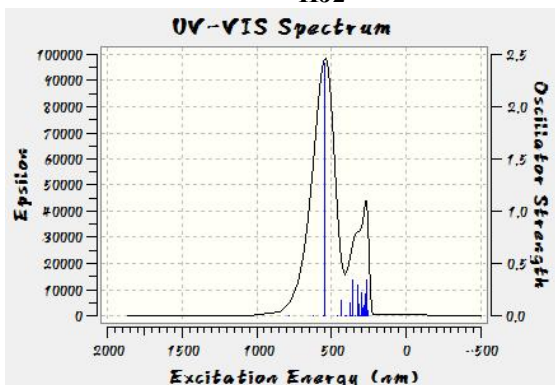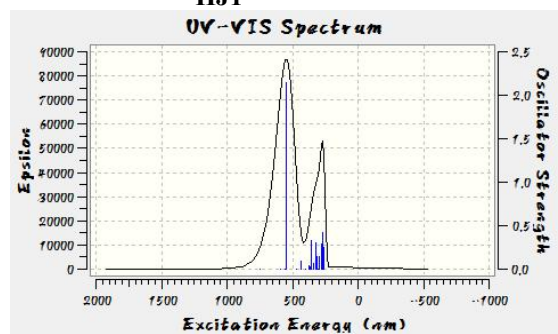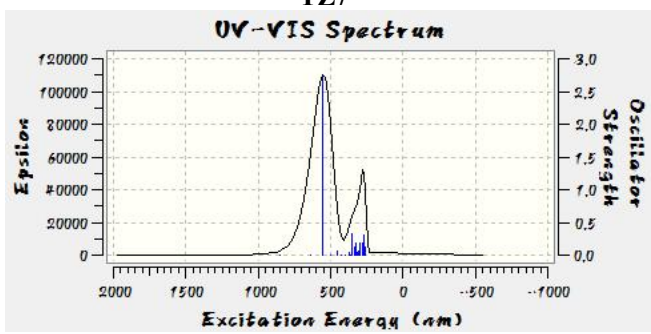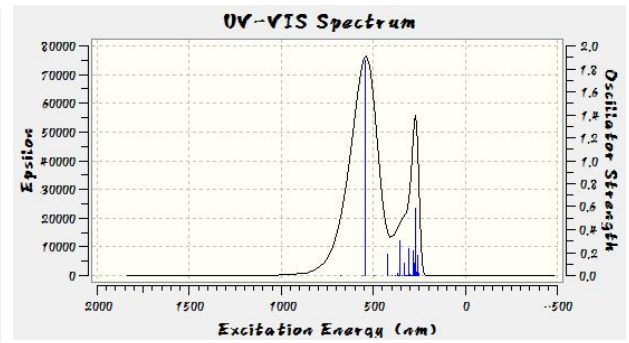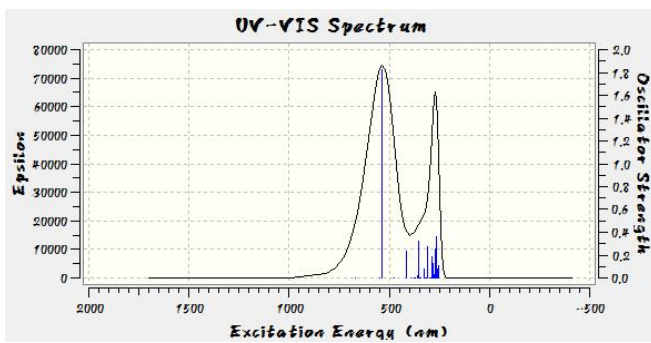
Figure S1. The TDDFT calculated UV-Vis spectroscopy of YZ7, HJ1~HJ3.

S3. Fragmentation Scheme of TDM analysis
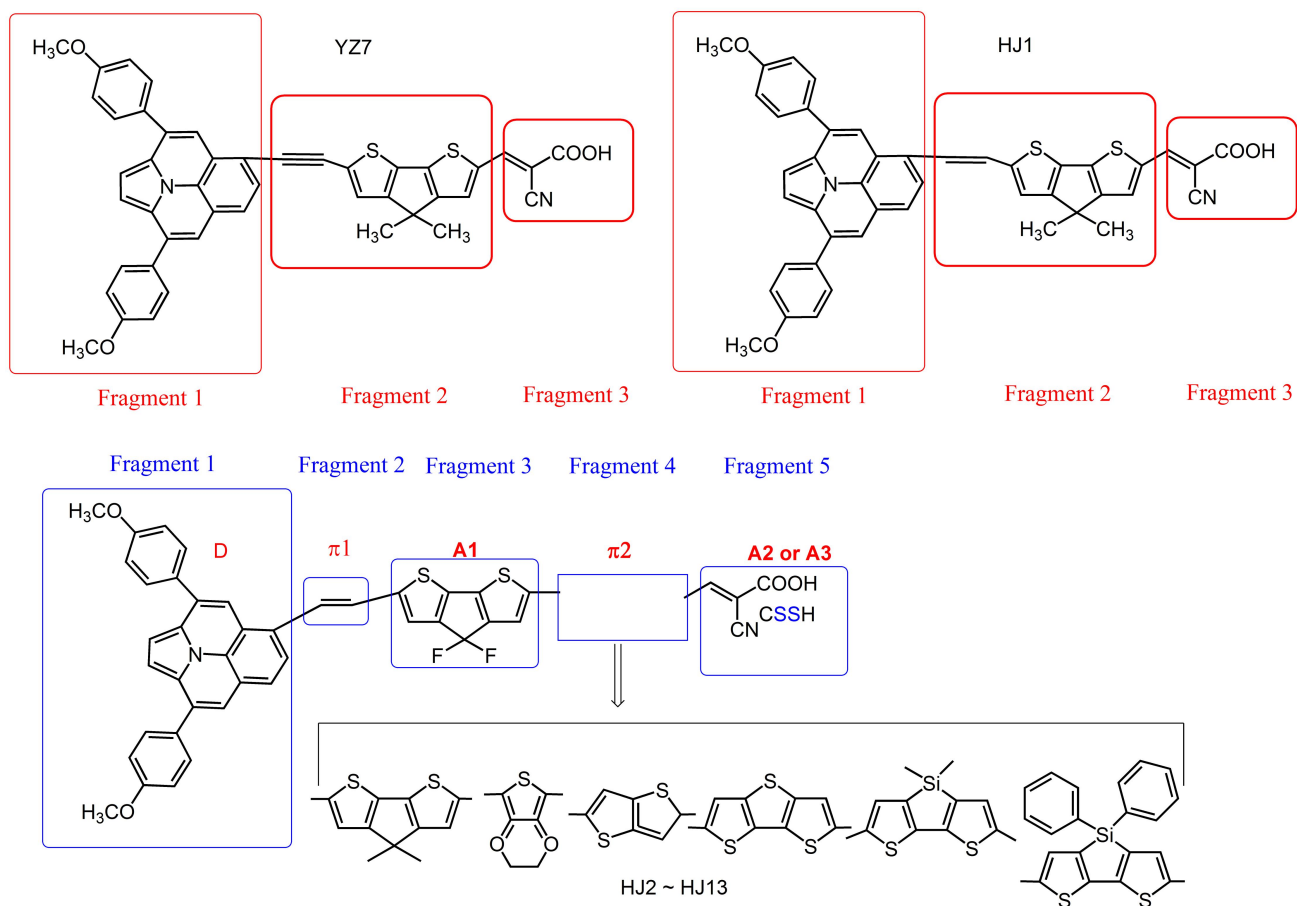
Figure S2. The fragmentation scheme of YZ7, HJ1~HJ3.

S4. Heat maps of fragment transition density matrix
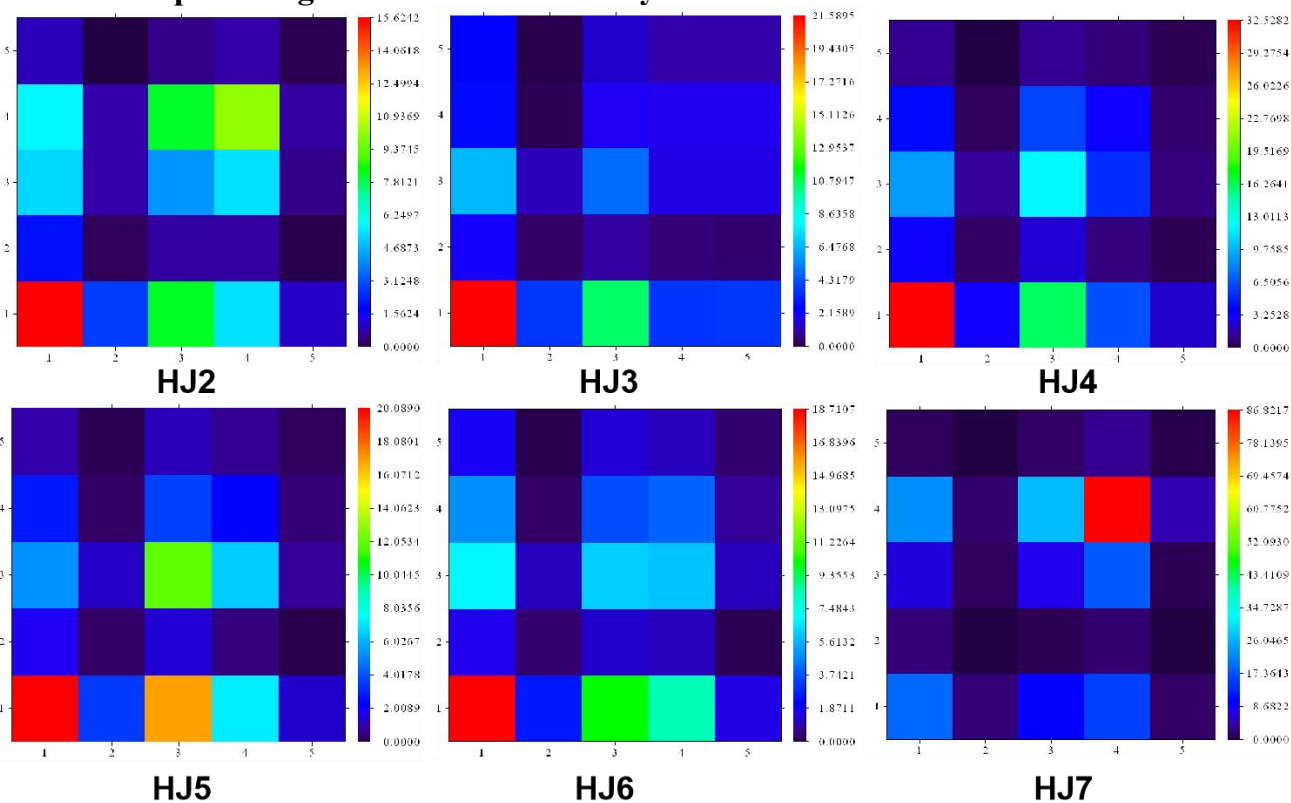
Figure S3. fragment transition density matrix heatmaps of HJ2~HJ7
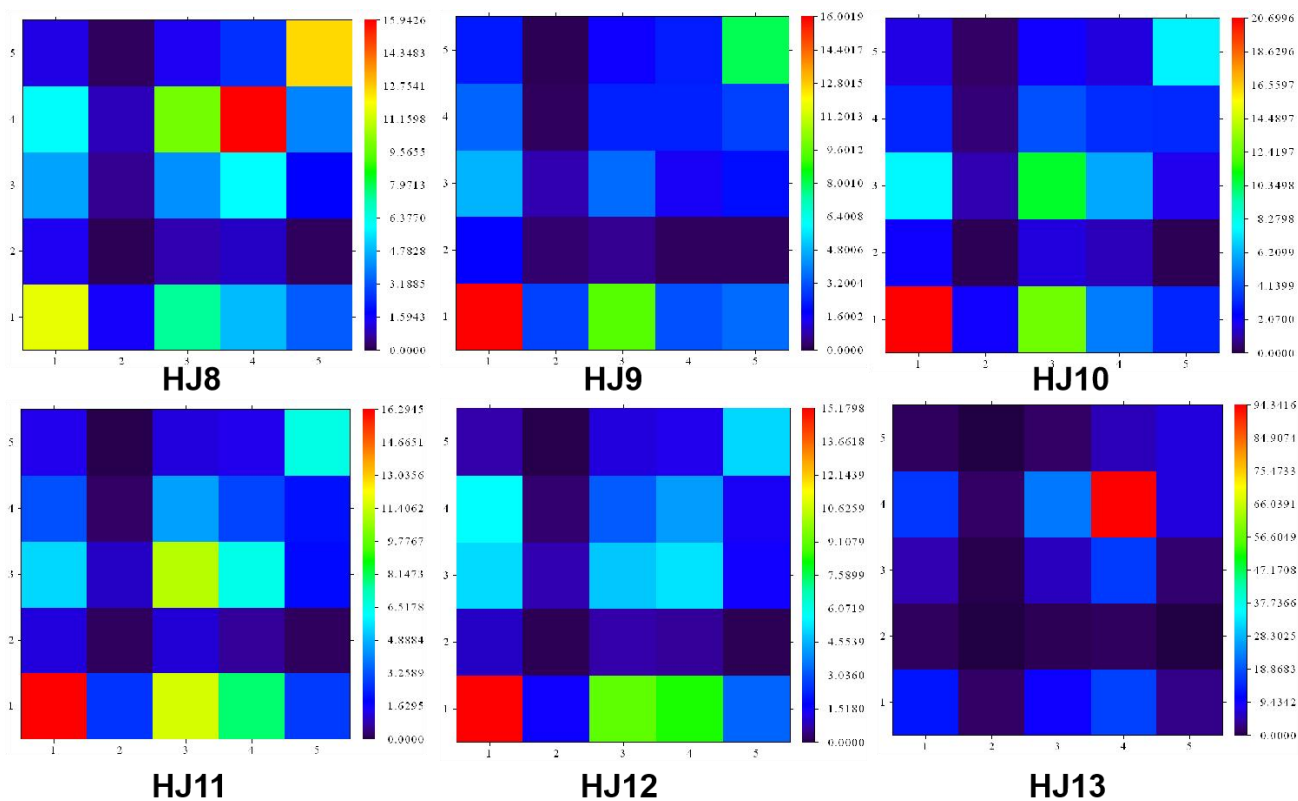
Figure S4. fragment transition density matrix heatmaps of HJ8~HJ13

S5. DFT optimized cartesian coordinates

YZ7

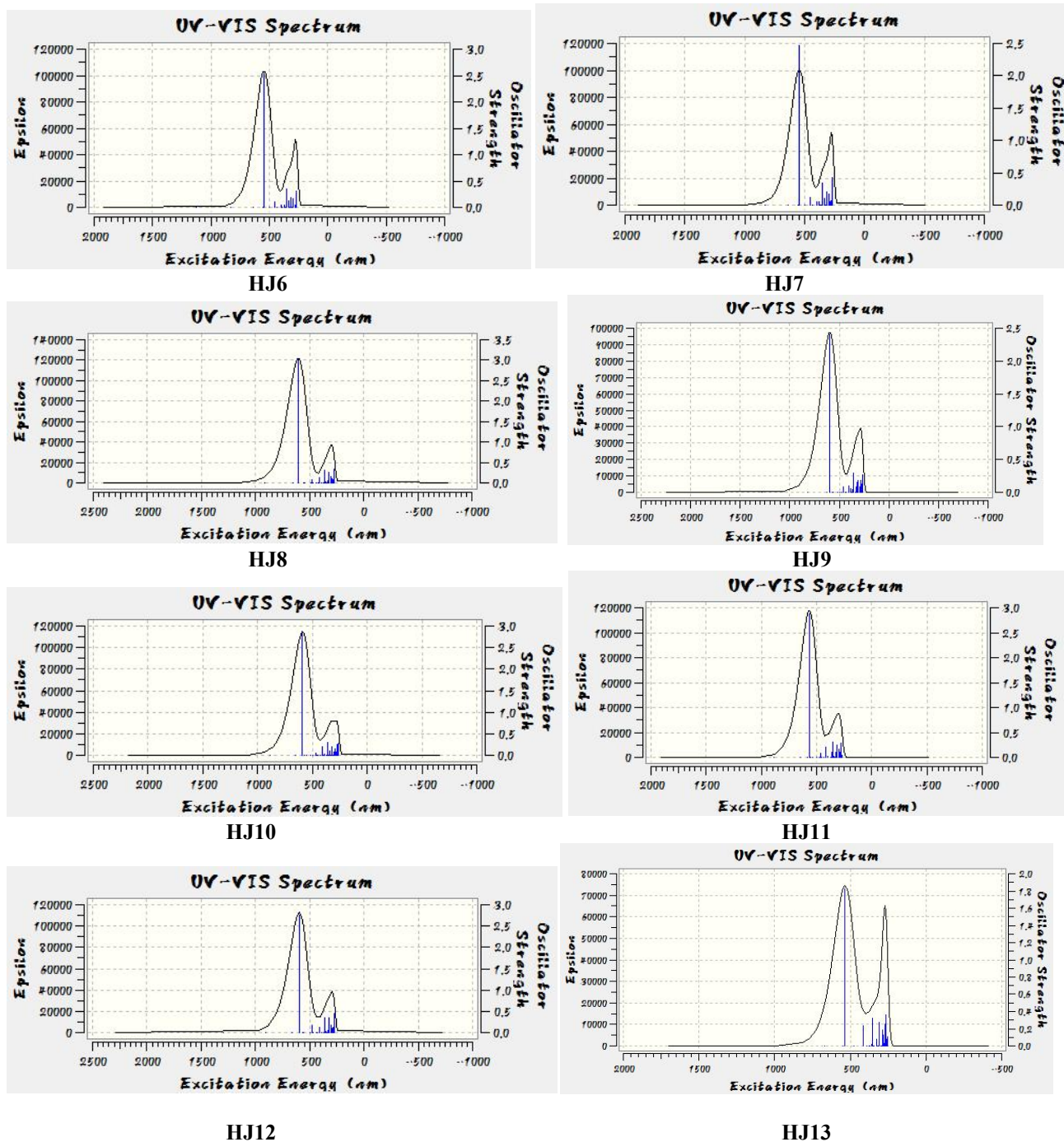|			
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6	4.854438	-2.585217	-0.016084
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6	2.706837	-1.344633	-0.053597
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6	2.798454	1.128777	-0.017200
6	6.948022	-1.299226	0.071864
6	6.283529	-2.496457	0.030918
6	2.172777	2.466836	-0.030098
6	8.422421	-1.240872	0.110975
6	2.457082	3.401644	0.974055
6	1.875017	4.655868	0.965488
6	0.999339	5.017777	-0.062645
6	0.713398	4.103065	-1.076281
6	1.296169	2.840563	-1.047328
6	9.100152	-0.399982	1.004767

6	10.481479	-0.377893	1.058102
6	11.233221	-1.195323	0.208650
6	10.577697	-2.036314	-0.689965
6	9.187157	-2.050597	-0.728683
8	0.484049	6.266130	0.007925
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6  -10.947662   -0.004266    0.160480        6   -8.332663   -1.119433   -0.184844
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1    0.952057   -2.579702   -0.133167        6   -8.866721   -0.453498   -1.296915
1    6.851368   -3.421020    0.055225        6  -10.230826   -0.410813   -1.518019
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HJ2
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HJ3

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6	-6.127650	-1.377974	0.551530
6	-6.826584	-2.569102	0.850136
6	-6.095136	-3.630311	1.397729
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6	-3.449360	2.622990	-1.383411
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6	-10.909007	-1.184942	-1.434482

6	-12.259581	-1.300940	-1.706501
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6	-12.604807	-2.341440	0.441262
6	-11.242693	-2.221882	0.698533
8	-2.892575	6.190247	-1.403873
8	-14.425710	-1.943826	-1.119819
6	-3.319218	7.361694	-0.731587
6	-15.334582	-2.527662	-0.203993
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1	-6.602662	-4.559437	1.635424
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6	3.618199	-0.276886	0.278398
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6   1.296973    1.134231    0.877432
6   2.685716    1.293122    0.930737
6   3.346605    0.204081    0.386784
6   0.888455   -0.055491    0.311121
1   3.201111    2.142719    1.359658
9   0.011696    3.141924    0.691405
9   0.072156    2.185582    2.641759
16  -1.791264   -1.202622   -0.147560
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HJ8

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6  14.823892  -2.611613   0.846626
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6  -5.121018   4.042379  -1.658325        1   6.351796   2.970201   0.399194
6  -5.688937   5.099966  -0.941657        1  12.494911   1.122084  -0.119034
6  -6.606052   4.827831   0.073319        1  12.772987  -2.827144  -0.466312
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6 -12.460491  -1.863840  -1.487737        1  -4.312135   1.529987   0.777958
6 -13.790857  -2.123016  -1.760705        1  -3.463071  -1.276560  -0.093873
6 -14.578809  -2.814718  -0.835827        6  -2.007511   0.221095   0.418172
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6  -4.458532   0.485820   0.512593        6   3.588781   2.012344   0.944272
6  -3.358023  -0.260842   0.275171        6   4.326409   0.967709   0.411531
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6   6.652533   1.933905   0.324956        1   4.042297   2.896426   1.373514
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6   8.103027   0.101389   0.087610        9   0.912863   2.728892   2.635881
16  6.557994  -0.666321   0.132486       16  -0.696201  -0.791704  -0.149264
6  10.331500   0.780191  -0.005533       16   3.285497  -0.319519  -0.165422
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HJ12

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7   -8.773654   -0.647276   0.036658
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6   -8.488126   -2.826172   0.930208
6   -7.642727   -3.763385   1.536693
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6   -5.793207   -2.200442   1.434743
6   -6.577168   -1.233055   0.786955
6   -6.121655   0.095125   0.385133
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6 -12.908911   -3.029020   0.718280
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8 -16.076489   -3.222545   -1.137610
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6   5.479766   1.001082   0.392555
6   6.380401   2.052651   0.486386
6   7.721012   1.659122   0.357567
6   7.837742   0.286085   0.155382
16   6.308575   -0.511193   0.144465
6   10.208270   0.707263   0.063762
6   9.161499   -0.231137   -0.005319
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6   11.390137   -1.281244   -0.300376
16   9.715632   -1.822922   -0.271817
6   9.737840   3.595188   -1.068790
6   9.930881   3.159247   2.002804

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HJ13

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6	-14.237863	-2.682832	0.786309
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6	6.682734	-0.567336	0.054699
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6	7.979954	-1.150094	-0.110311
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6	10.154740	-2.305129	-0.415483
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9	-0.399511	2.393955	2.582036
16	-2.154665	-1.161242	-0.065875
16	1.845931	-0.857763	-0.094942
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6	8.696274	2.635556	-1.235440
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S20

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6    9.197066   4.289894   -3.444233        6    9.703049    3.343332    4.296948
1   11.021712   4.820168   -2.434859        1    9.018044    5.212672    3.481344
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