附 錄 A

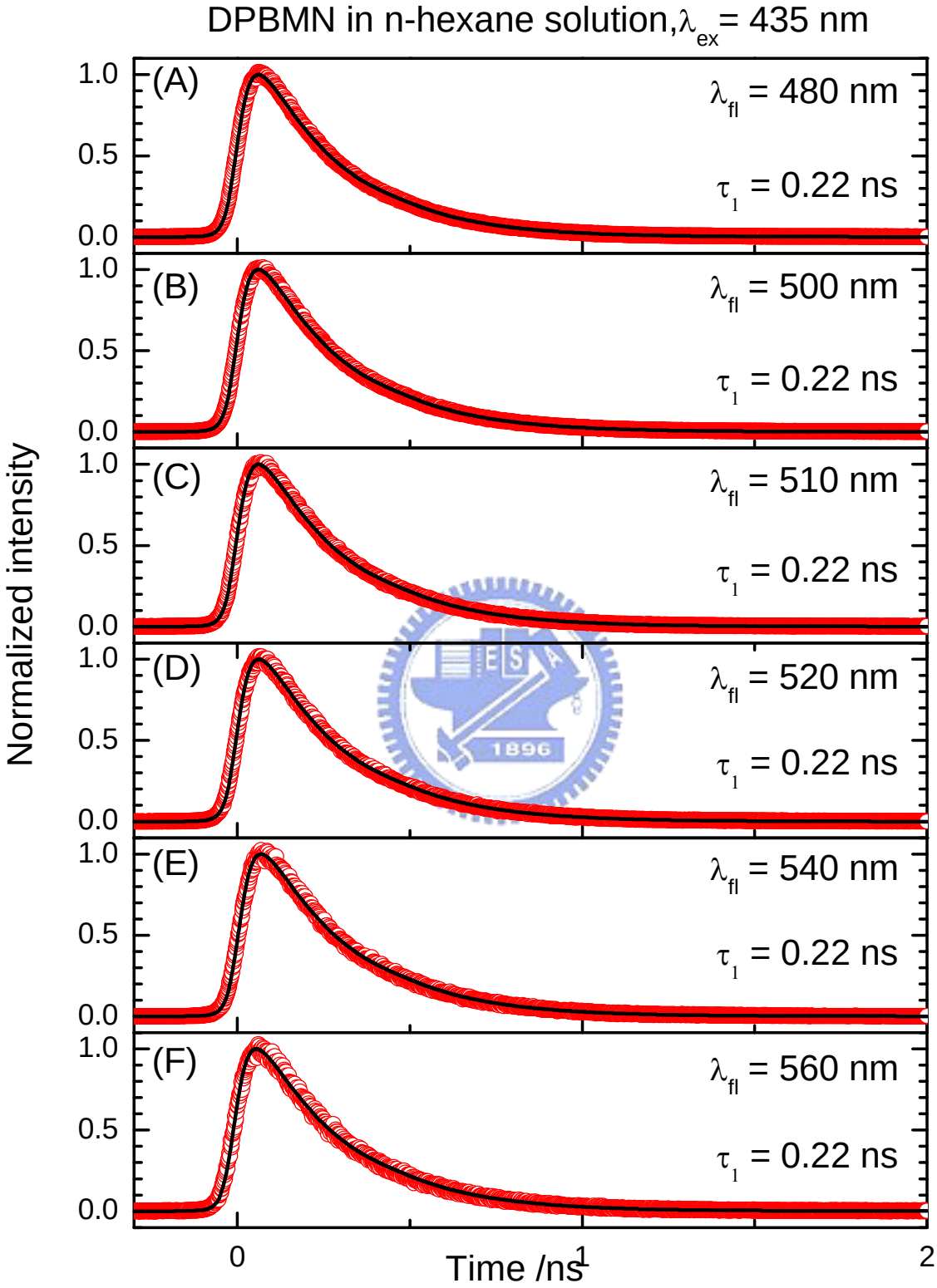

圖 A-1. 激發 DPBMN 在 n-hexane 溶劑中，螢光波長為 (A) 480、(B) 500、(C) 510、(D) 520、(E) 530 及(F) 560 nm 的時間-解析螢光光譜，激發波長為 435 nm。圓圈為實驗值，黑線為擬合結果。

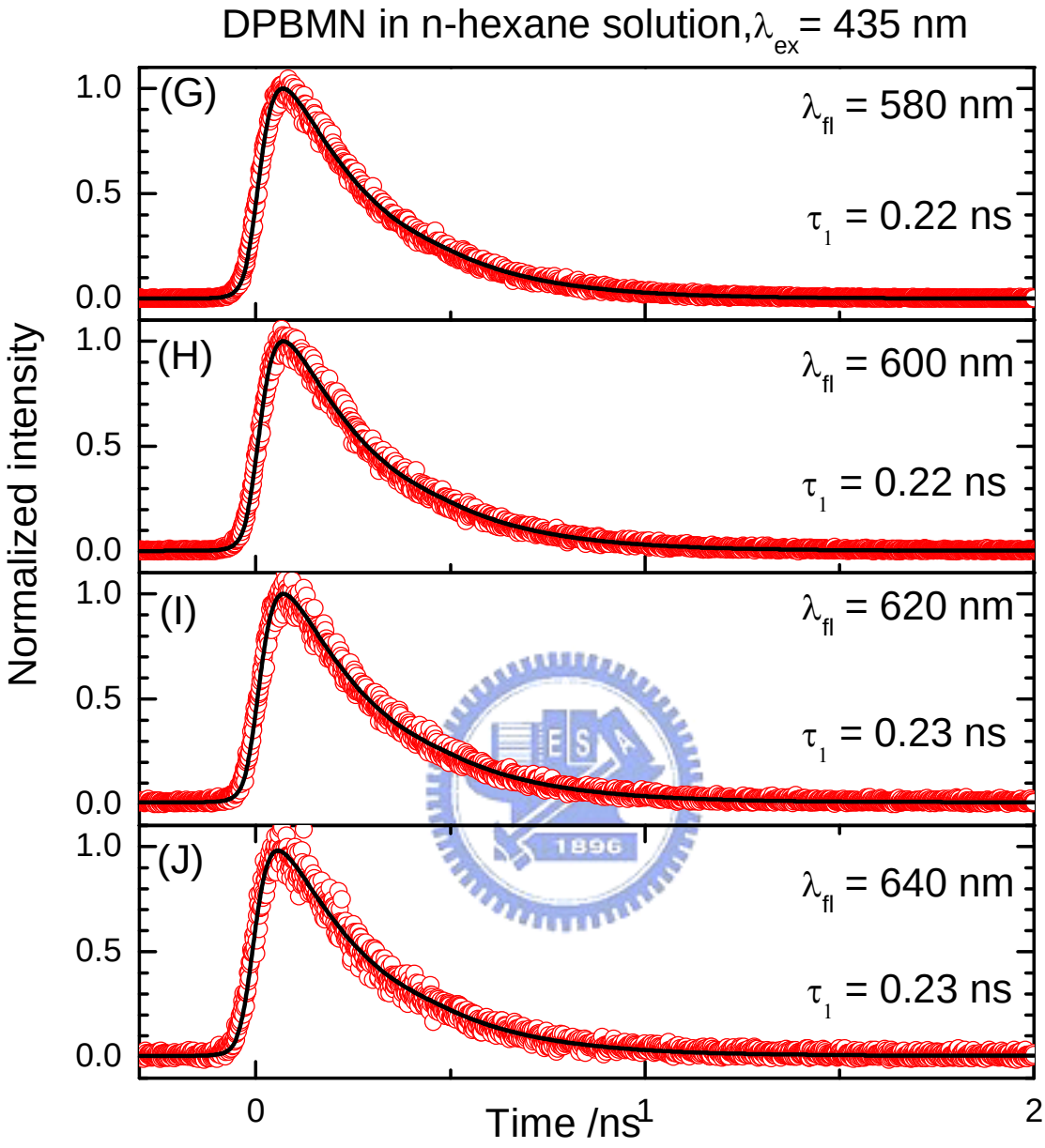

圖 A-2. 激發 DPBMN 在 n-hexane 溶劑中，螢光波長為 (G) 580、(H) 600、(I) 620、及(J) 640 nm 的時間-解析螢光光譜，激發波長為 435 nm。圓圈為實驗值，黑線為擬合結果。

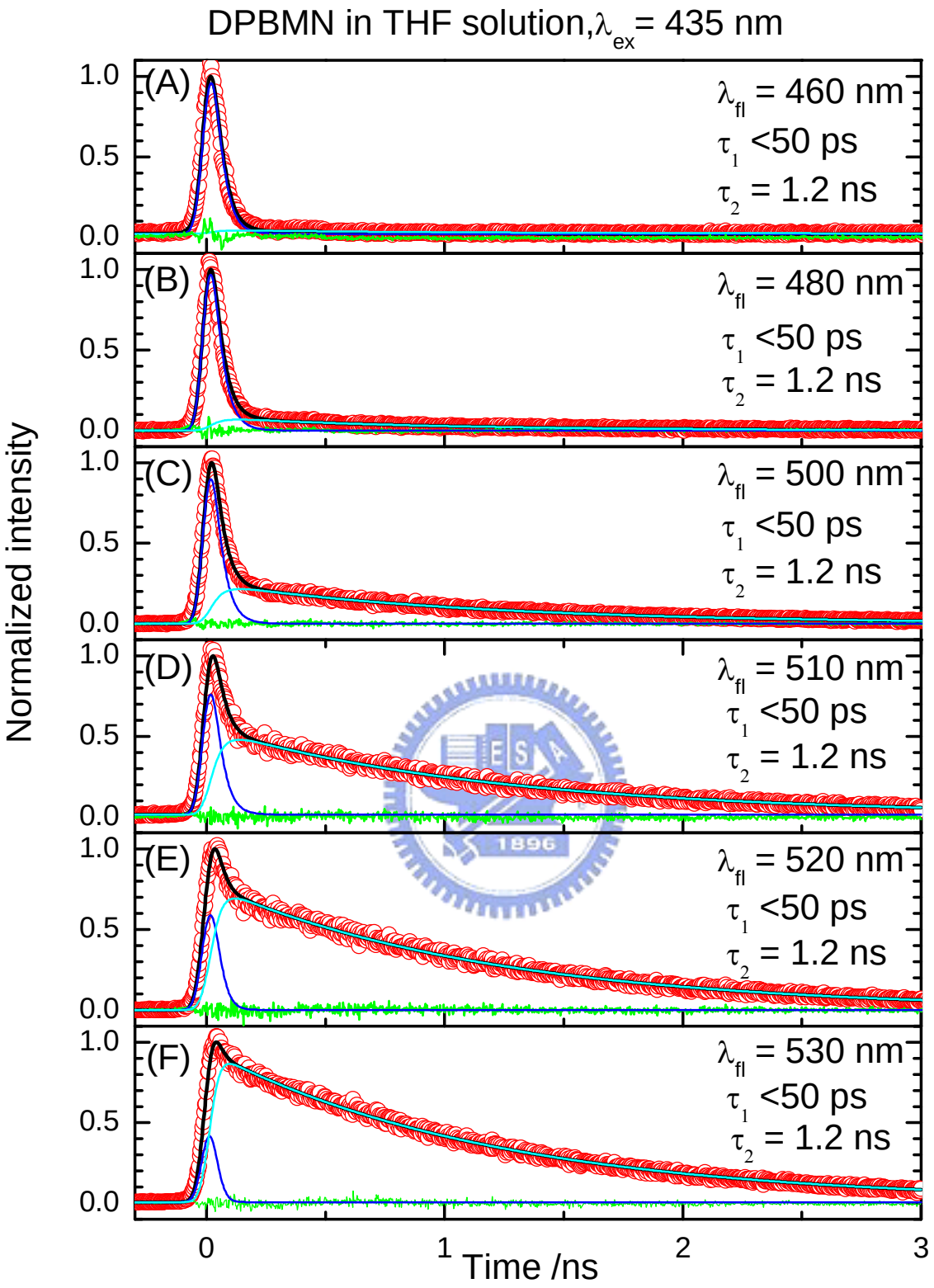

圖 A-3. 激發 DPBMN 在 THF 溶劑中，螢光波長為 (A) 460、(B) 480、(C) 500、(D) 510、(E) 520 及(F) 530 nm 的時間-解析螢光光譜，激發波長為 435 nm。圓圈為實驗值，黑線為擬合結果，綠線為 residual。

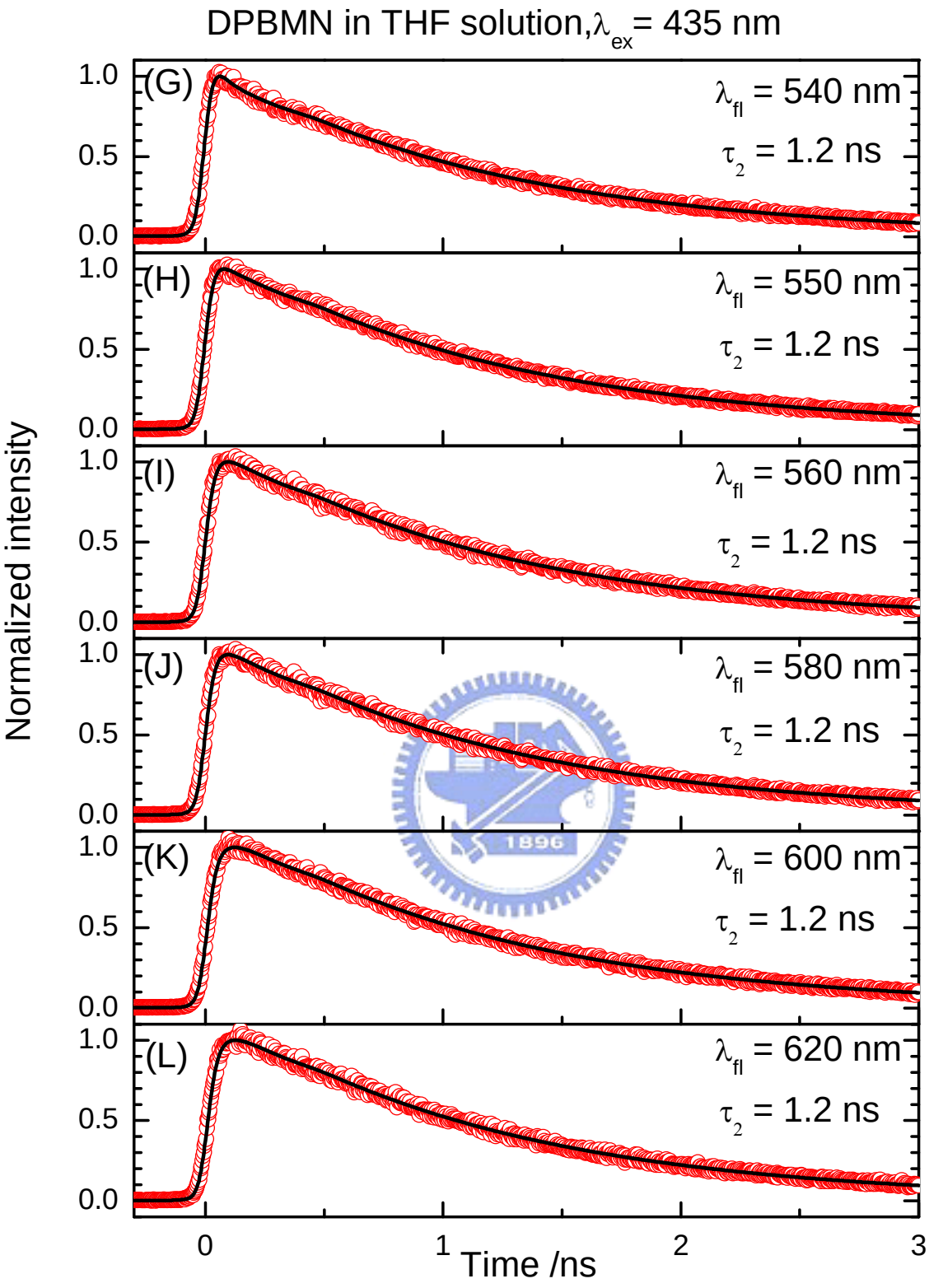

圖 A-4. 激發 DPBMN 在 THF 溶劑中，螢光波長為 (G) 540、(H) 550、(I) 560、(J) 580、(K) 600 及(L)620 nm 的時間-解析螢光光譜，激發波長為 435 nm。圓圈為實驗值，黑線為擬合結果。

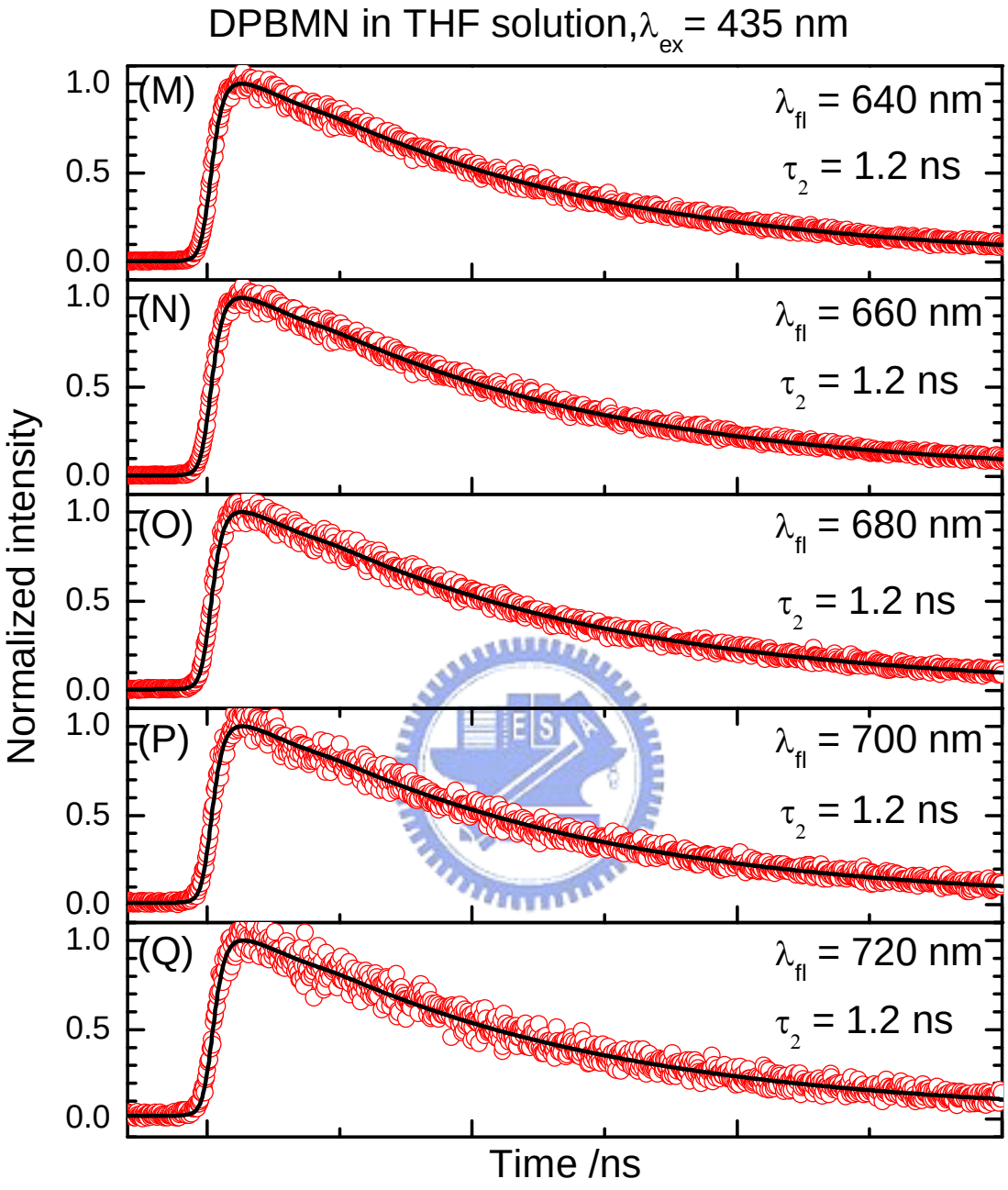

圖 A-5. 激發 DPBMN 在 THF 溶劑中，螢光波長為 (M) 640、(N) 660、(O) 680、(P) 700 及(Q)720 nm 的時間-解析螢光光譜，激發波長為 435 nm。圓圈為實驗值，黑線為擬合結果。

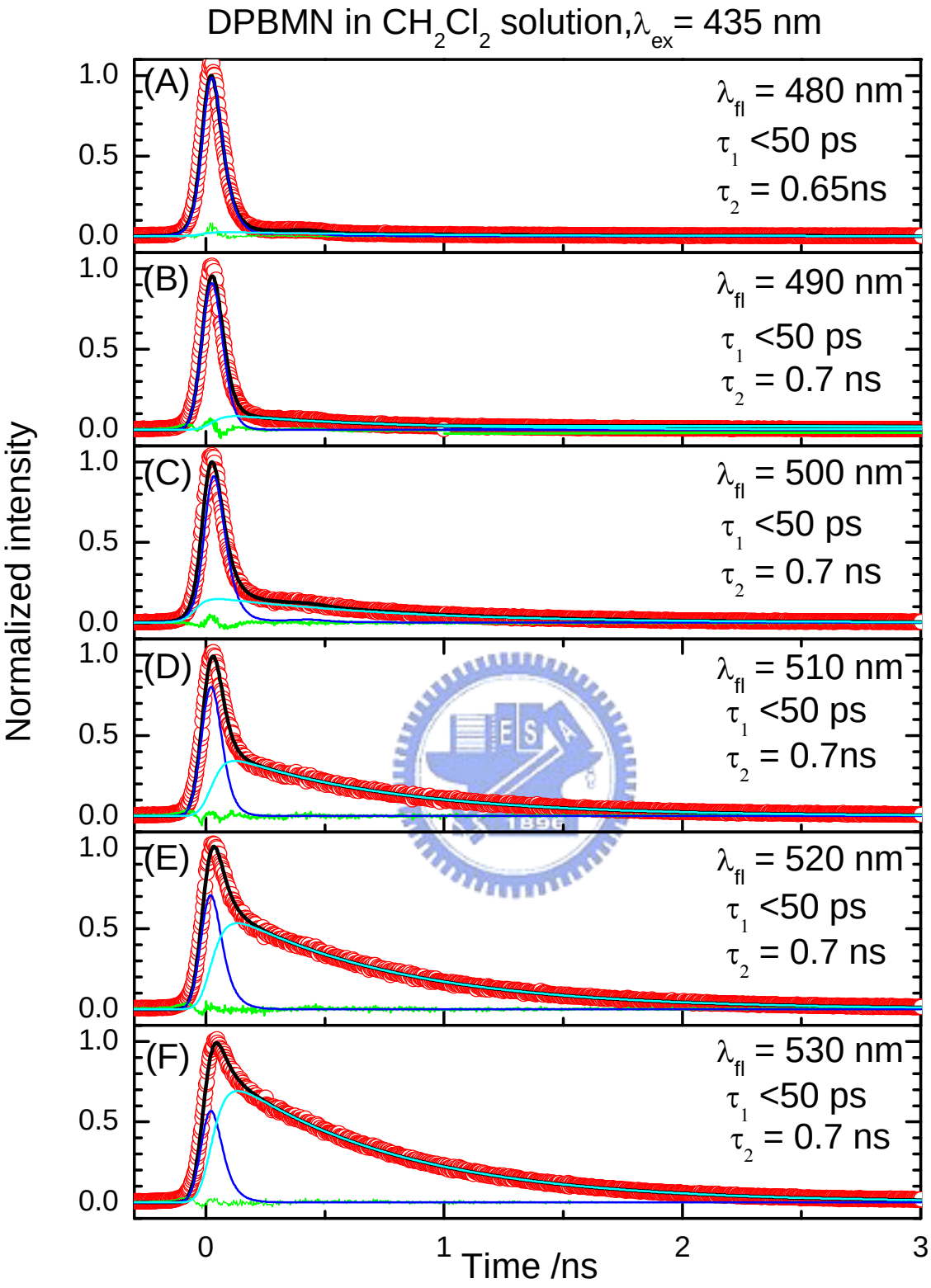

圖 A-6. 激發 DPBMN 在 CH_2Cl_2 溶劑中，螢光波長為 (A) 480、(B) 490、(C) 500、(D) 510、(E) 520 及(F) 530 nm 的時間-解析螢光光譜，激發波長為 435 nm。圓圈為實驗值，黑線為擬合結果，綠線為 residual。

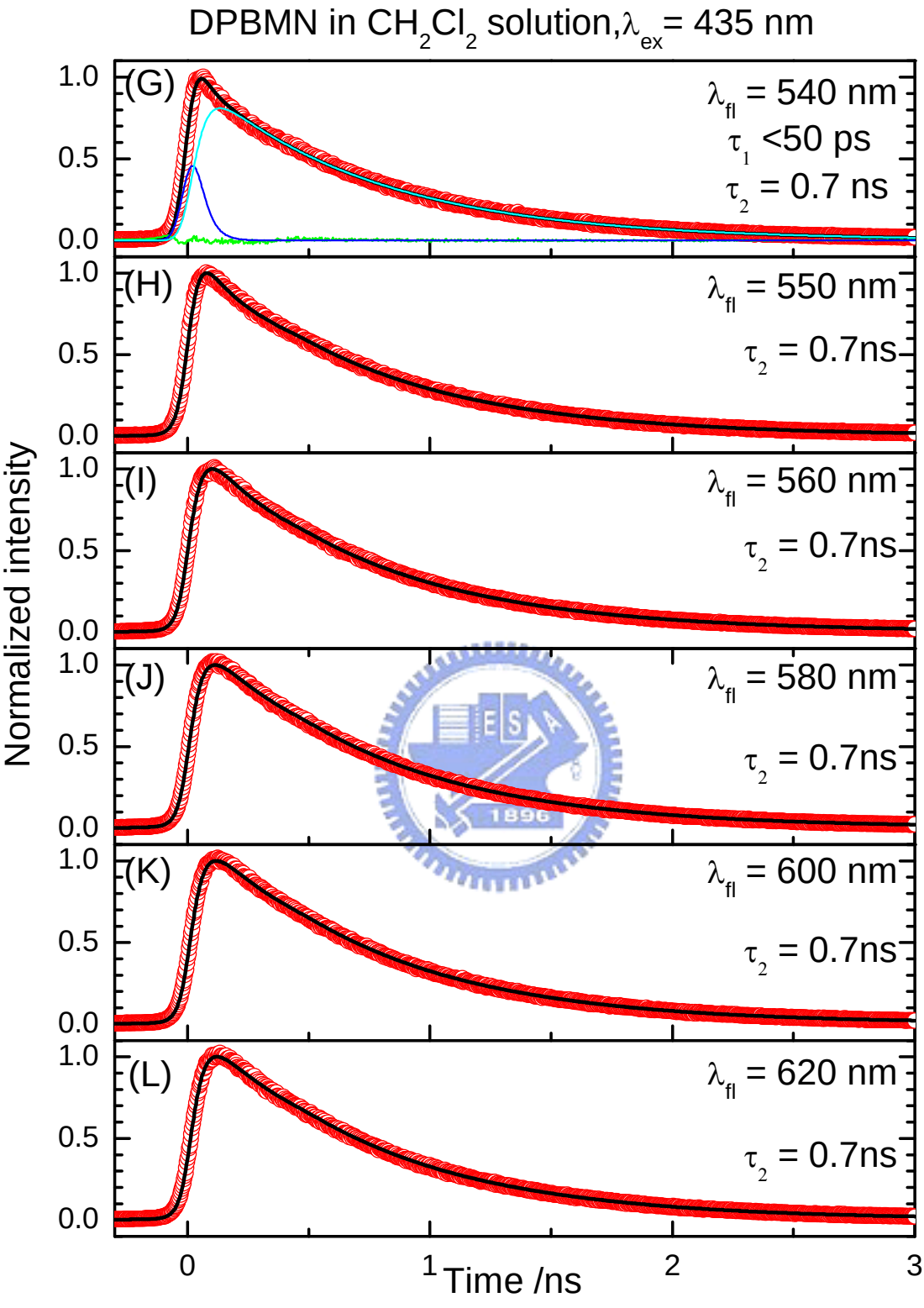

圖 A-7. 激發 DPBMN 在 CH_2Cl_2 溶劑中，螢光波長為 (G) 540、(H) 550、(I) 560、(J) 580、(K) 600 及(L)620 nm 的時間-解析螢光光譜，激發波長為 435 nm。圓圈為實驗值，黑線為擬合結果，綠線為 residual。

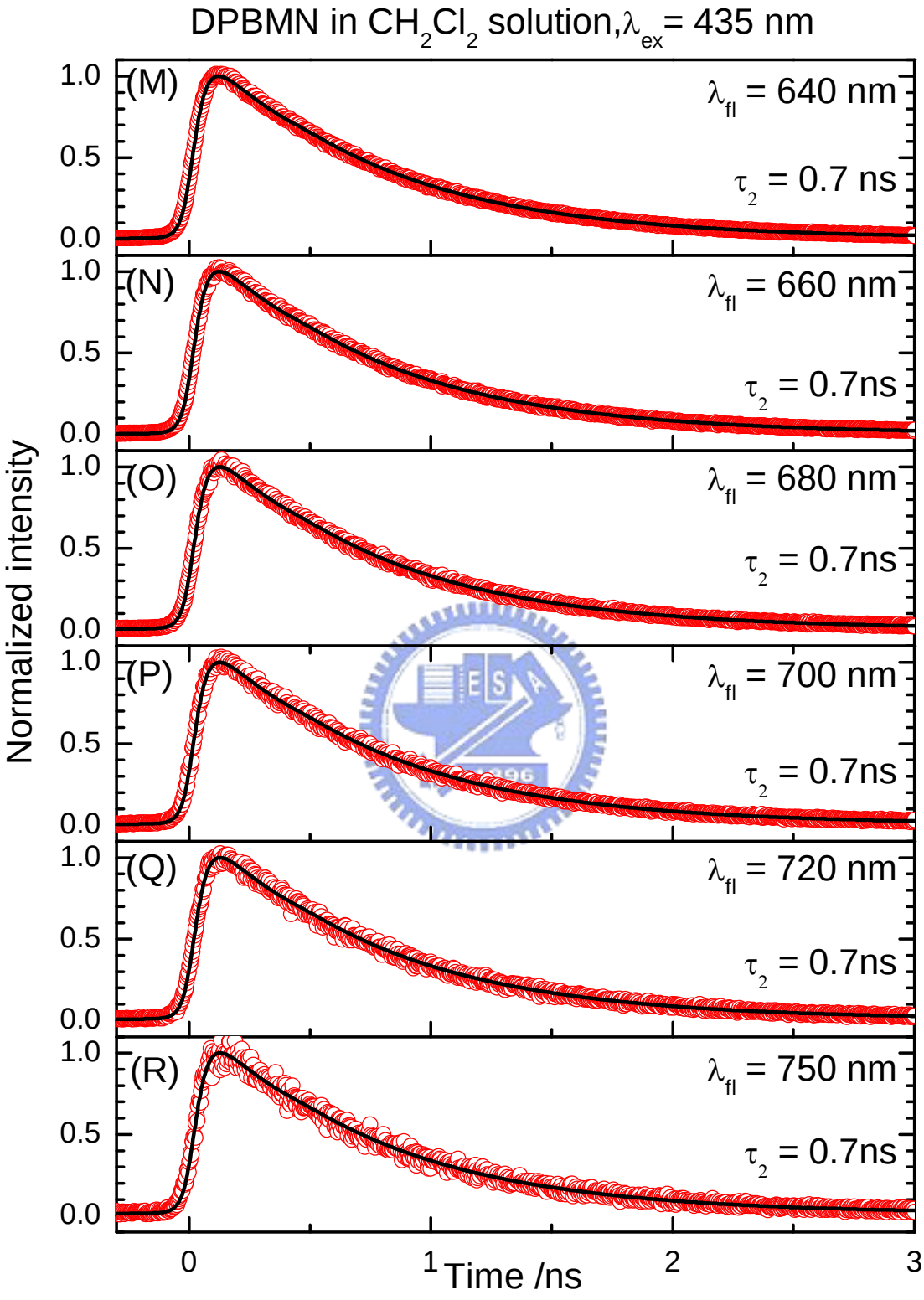

圖 A-7. 激發 DPBMN 在 CH_2Cl_2 溶劑中，螢光波長為 (M) 640、(N) 660、(O)680、(P) 700、(Q) 720 及(R)750 nm 的時間-解析螢光光譜，激發波長為 435 nm。圓圈為實驗值，黑線為擬合結果。

附 錄 B

附錄 B. DPBMN正己烷溶液之理論計算：

A. S_0 state：

1. S_0 optimization Cartesian Coordinates：

command：b3lyp/6-311+G(d,p) opt freq SCRF(pcm,read)
nosymmcav
eps=1.9
epsinf=1.8903
rsolv=4.60

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.208976	-0.221182	-0.090016
2	6	0	-5.113643	1.170173	0.580571
3	6	0	-0.682240	0.779888	0.363942
4	6	0	-0.342305	-1.417852	-0.599916
5	6	0	2.487004	-1.145113	0.039644
6	6	0	2.158939	1.282554	-0.054710
7	6	0	-2.051046	0.598853	0.308514
8	6	0	-1.712667	-1.590249	-0.649707
9	6	0	-2.614456	-0.595388	-0.202953
10	6	0	1.775675	2.207375	-1.036388
11	6	0	3.125902	1.641279	0.893845
12	6	0	2.344106	3.480169	-1.054915
13	6	0	3.310310	3.836442	-0.111664
14	6	0	3.700991	2.910631	0.858008
15	6	0	2.301366	-2.144931	1.004948
16	6	0	3.575477	-1.226086	-0.839186
17	6	0	3.187831	-3.218541	1.076533
18	6	0	4.274247	-3.297498	0.202532
19	6	0	4.465668	-2.295300	-0.750809
20	6	0	-4.022174	-0.882478	-0.306920
21	6	0	-5.133684	-0.145011	0.020572
22	6	0	-6.433141	-0.705202	-0.202983
23	1	0	4.449229	3.179110	1.598633
24	1	0	0.313240	-2.199036	-0.966681
25	1	0	-2.690186	1.389913	0.681044
26	1	0	-4.249926	-1.862216	-0.722020
27	1	0	5.306340	-2.348534	-1.437074
28	1	0	4.967090	-4.131603	0.265802
29	1	0	3.035411	-3.987705	1.828697
30	1	0	3.718935	-0.449325	-1.583843
31	1	0	1.465947	-2.074470	1.694816
32	1	0	-0.284977	1.700381	0.775805
33	1	0	3.755909	4.826734	-0.133182
34	1	0	2.039228	4.190007	-1.818864
35	1	0	3.421313	0.923198	1.652401

36	1	0	1.035971	1.924696	-1.779105
37	1	0	-2.109861	-2.515952	-1.059380
38	7	0	-7.485512	-1.167767	-0.387841
39	7	0	1.590992	-0.031332	-0.033122
40	7	0	-5.111262	2.241900	1.036577

---

2. S_0 state frequency：

22	30	34	46	54	66	82	89	101	133
173	186	227	251	258	268	315	349	371	409
421	422	426	449	461	480	523	531	550	617
629	632	637	638	651	657	710	712	723	737
775	778	794	831	847	853	854	878	914	920
943	949	950	969	970	976	985	995	996	1018
1018	1025	1056	1058	1112	1114	1162	1190	1193	1194
1200	1208	1214	1231	1275	1294	1325	1335	1360	1364
1365	1371	1374	1416	1485	1499	1503	1540	1541	1553
1586	1618	1638	1643	1652	1654	1669	2326	2341	3179
3187	3188	3189	3196	3197	3208	3208	3214	3215	3218
3219	3227	3231	3249						

3. S_0 state TD：

command：#B3LYP/6-311+G** TD(50-50,nstates=4) SCRF(pcm,read)
nosymmcav
eps=1.9
epsinf=1.8903
rsolv=4.60

Excited State 1: Triplet-A 1.9015 eV 652.05 nm f=0.0000
83 -> 85 -0.22841
84 -> 85 0.73831
This state for optimization and/or second-order correction.
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 2.7503 eV 450.80 nm f=0.9568
84 -> 85 0.64682

Excited State 3: Triplet-A 3.0134 eV 411.44 nm f=0.0000
78 -> 85 0.28827
81 -> 85 0.16725
82 -> 85 -0.19579
83 -> 85 0.60492
84 -> 85 0.17642

Excited State 4: Triplet-A 3.3108 eV 374.49 nm f=0.0000
80 -> 85 -0.10669
80 -> 88 0.18243
81 -> 86 0.11918
81 -> 89 0.15103
82 -> 86 -0.14113
82 -> 90 -0.16217

83 -> 87	-0.22792				
84 -> 86	0.44901				
84 -> 87	-0.43020				
Excited State	5:	Triplet-A	3.5363 eV	350.61 nm	f=0.0000
79 -> 85	-0.20173				
80 -> 87	0.10377				
82 -> 85	0.11145				
83 -> 87	0.10143				
84 -> 86	0.46716				
84 -> 87	0.38824				
84 -> 88	-0.18709				
Excited State	6:	Singlet-A	3.6394 eV	340.67 nm	f=0.0195
79 -> 85	-0.11794				
81 -> 85	0.12855				
82 -> 85	0.12060				
84 -> 86	0.64487				
Excited State	7:	Singlet-A	3.6538 eV	339.33 nm	f=0.1531
81 -> 85	-0.11344				
82 -> 85	0.10317				
83 -> 85	0.61935				
84 -> 88	0.12692				
Excited State	8:	Singlet-A	3.8063 eV	325.74 nm	f=0.1113
79 -> 85	-0.12351				
82 -> 85	0.12139				
84 -> 86	-0.10849				
84 -> 87	0.61960				

B.S_1(min) state：

1. S_1(min) state optimization Cartesian Coordinates：

command：#CIS(singlets,root=1,nstates=2)/6-31g* opt freq

standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.328517	-1.415295	-0.717090
2	6	0	-0.220267	-0.222825	-0.119838
3	6	0	0.695792	0.751834	0.396322
4	6	0	2.033881	0.563196	0.332700
5	6	0	2.609337	-0.626659	-0.268271
6	6	0	1.662269	-1.599306	-0.788119
7	1	0	-0.351005	-2.143996	-1.137924
8	1	0	0.294398	1.635937	0.873156
9	1	0	2.693324	1.307921	0.753803
10	1	0	2.059055	-2.490498	-1.259741
11	7	0	-1.601388	-0.026092	-0.050811
12	6	0	-2.160356	1.308260	-0.080651

13	6	0	-3.214362	1.646848	0.774200
14	6	0	-1.649252	2.264463	-0.963509
15	6	0	-3.743125	2.923445	0.741309
16	1	0	-3.605710	0.908355	1.461880
17	6	0	-2.186115	3.539313	-0.983392
18	1	0	-0.843455	1.997739	-1.635292
19	6	0	-3.231731	3.874035	-0.133823
20	1	0	-4.556624	3.182299	1.408450
21	1	0	-1.789140	4.274960	-1.672724
22	1	0	-3.648950	4.873576	-0.153655
23	6	0	-2.502976	-1.152299	0.060555
24	6	0	-3.692312	-1.174194	-0.675249
25	6	0	-2.189086	-2.223428	0.902496
26	6	0	-4.548311	-2.253846	-0.566312
27	1	0	-3.932464	-0.347361	-1.331160
28	6	0	-3.053534	-3.299358	0.998967
29	1	0	-1.276709	-2.198422	1.484451
30	6	0	-4.232966	-3.319986	0.267394
31	1	0	-5.466547	-2.268020	-1.141213
32	1	0	-2.807605	-4.124348	1.656857
33	1	0	-4.907119	-4.164157	0.347404
34	6	0	3.983154	-0.894747	-0.379028
35	1	0	4.234845	-1.836193	-0.854181
36	6	0	5.096461	-0.137432	0.034015
37	6	0	5.053485	1.139662	0.676739
38	6	0	6.410126	-0.671826	-0.196960
39	7	0	7.467415	-1.113534	-0.388478
40	7	0	5.049964	2.178636	1.200027

---

2. S_1(min) state frequency：

25	29	42	59	64	83	93	112	112	153
177	208	255	276	280	299	349	356	386	456
474	481	486	489	499	536	542	588	596	692
696	697	706	709	710	713	801	802	825	826
884	884	890	928	939	955	1019	1019	1019	1031
1051	1104	1108	1110	1148	1149	1151	1168	1167	1186
1186	1195	1203	1203	1203	1205	1269	1271	1279	1327
1359	1361	1370	1370	1373	1396	1402	1451	1501	1520
1534	1546	1551	1611	1662	1709	1723	1730	1743	1770
1773	1779	1893	1901	1903	1915	1959	2597	2644	3709
3780	3714	3716	3728	3728	3734	3736	3736	3742	3742
3744	3748	3748	3767						

3. S_1(min) state TD：

command：#B3LYP/6-311+G** TD(50-50,nstates=3 SCRF(pcm,read)
nosymmcav
eps=1.9
epsinf=1.8903
rsolv=4.60

Excited State 1: Triplet-A 1.6242 eV 763.37 nm f=0.0000
83 -> 85 0.23941
84 -> 85 0.76479
This state for optimization and/or second-order correction.
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 2.5729 eV 481.89 nm f=1.0061
84 -> 85 0.63359

Excited State 3: Triplet-A 2.7870 eV 444.87 nm f=0.0000
78 -> 85 0.19819
82 -> 85 0.12220
83 -> 85 0.69000
84 -> 85 -0.16423

Excited State 4: Triplet-A 3.3048 eV 375.16 nm f=0.0000
80 -> 85 -0.12916
80 -> 88 0.11202
80 -> 90 -0.14027
81 -> 85 0.11608
81 -> 88 -0.15975
82 -> 86 0.16983
82 -> 89 0.10856
83 -> 87 -0.24222
84 -> 86 -0.28246
84 -> 87 0.54743

Excited State 5: Singlet-A 3.5508 eV 349.18 nm f=0.0148
79 -> 85 -0.10772
81 -> 85 0.18578
84 -> 86 0.63529

Excited State 6: Singlet-A 3.6943 eV 335.61 nm f=0.1764
83 -> 85 0.63740
84 -> 88 -0.12200

C.P state：

1.P state optimization Cartesian Coordinates：

command：#CIS(singlets,root=1,nstates=2)/6-31g* opt=z-matirx freq

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.207032	-0.754996	-1.102673
2	6	0	-0.259075	-0.255472	0.165430

3	6	0	0.704752	0.278278	1.072332
4	6	0	2.033812	0.203174	0.815189
5	6	0	2.530956	-0.357186	-0.428717
6	6	0	1.528800	-0.800669	-1.377802
7	1	0	-0.525547	-1.074044	-1.833179
8	1	0	0.349143	0.712870	1.997921
9	1	0	2.741618	0.570696	1.544026
10	1	0	1.866464	-1.154751	-2.344160
11	7	0	-1.639577	-0.000237	0.392211
12	6	0	-2.504058	-1.151436	0.235716
13	6	0	-3.686128	-1.123185	-0.512637
14	6	0	-2.112347	-2.346720	0.852652
15	6	0	-4.457620	-2.264666	-0.625944
16	1	0	-3.987458	-0.214239	-1.013564
17	6	0	-2.891382	-3.481760	0.729215
18	1	0	-1.199407	-2.365667	1.433523
19	6	0	-4.067831	-3.445935	-0.007592
20	1	0	-5.368256	-2.235743	-1.211282
21	1	0	-2.582121	-4.398858	1.214749
22	1	0	-4.677616	-4.335486	-0.102730
23	6	0	-2.176620	1.315181	0.093261
24	6	0	-3.364752	1.729217	0.711799
25	6	0	-1.490038	2.202214	-0.738078
26	6	0	-3.866679	2.991453	0.469596
27	1	0	-3.878884	1.052225	1.381041
28	6	0	-2.002443	3.468769	-0.968886
29	1	0	-0.567039	1.894355	-1.209370
30	6	0	-3.188613	3.867076	-0.372907
31	1	0	-4.786968	3.303239	0.947487
32	1	0	-1.469044	4.146966	-1.623230
33	1	0	-3.584151	4.857925	-0.557288
34	6	0	3.890690	-0.475230	-0.774693
35	1	0	4.083846	-0.913195	-1.747386
36	6	0	5.045079	-0.122764	-0.061167
37	6	0	5.077882	0.479420	1.238585
38	6	0	6.326876	-0.375576	-0.664743
39	7	0	7.353976	-0.585911	-1.165402
40	7	0	5.130696	0.968802	2.292593

2.P state frequency：

22	28	35	49	67	72	88	92	113	153
178	206	242	267	274	309	342	361	389	439
473	478	482	493	509	534	539	580	598	684
696	698	701	707	709	710	796	805	822	824
871	901	902	927	934	952	1016	1017	1019	1036
1041	1094	1106	1109	1147	1147	1150	1166	1181	1186
1187	1195	1202	1203	1204	1208	1269	1273	1276	1318
1350	1361	1366	1371	1372	1392	1414	1447	1479	1502
1512	1543	1548	1573	1648	1702	1708	1721	1730	1766

1770	1771	1890	1896	1901	1910	1954	2593	2637	3707
3708	3714	3714	3723	3729	3729	3733	3737	3737	3745
3746	3751	3752	3763						

3.P state TD：

command：#B3LYP/6-311+G** TD(50-50,nstates=3) SCRF(pcm,read)
nosymmcav
eps=1.9
epsinf=1.8903
rsolv=4.60

Excited State 1: Triplet-A 1.8421 eV 673.06 nm f=0.0000
80 -> 85 0.24690
83 -> 85 0.12250
84 -> 85 0.68026
This state for optimization and/or second-order correction.
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 2.0600 eV 601.86 nm f=0.1670
84 -> 85 0.68947

Excited State 3: Triplet-A 2.3734 eV 522.38 nm f=0.0000
77 -> 85 0.13228
78 -> 85 -0.11654
79 -> 86 -0.10978
80 -> 85 0.62522
81 -> 85 -0.12851
82 -> 85 0.18885
83 -> 85 0.29213
84 -> 85 -0.22370

Excited State 4: Triplet-A 3.1738 eV 390.65 nm f=0.0000
79 -> 85 -0.12809
80 -> 85 -0.10146
81 -> 91 0.14097
81 -> 93 -0.12822
82 -> 85 0.20785
82 -> 91 0.14021
82 -> 93 0.13459
83 -> 86 0.10634
83 -> 89 0.14262
83 -> 90 0.13468
84 -> 86 -0.27200
84 -> 88 0.55333

Excited State 5: Singlet-A 3.2676 eV 379.43 nm f=0.0526
83 -> 85 0.67580

Excited State 6: Singlet-A 3.4240 eV 362.10 nm f=0.0230
82 -> 85 0.68427