Supporting information

Enhancement of lipid productivity of *Chlorella* sp. using light-converting red fluorescent films based on aggregation-induced emission

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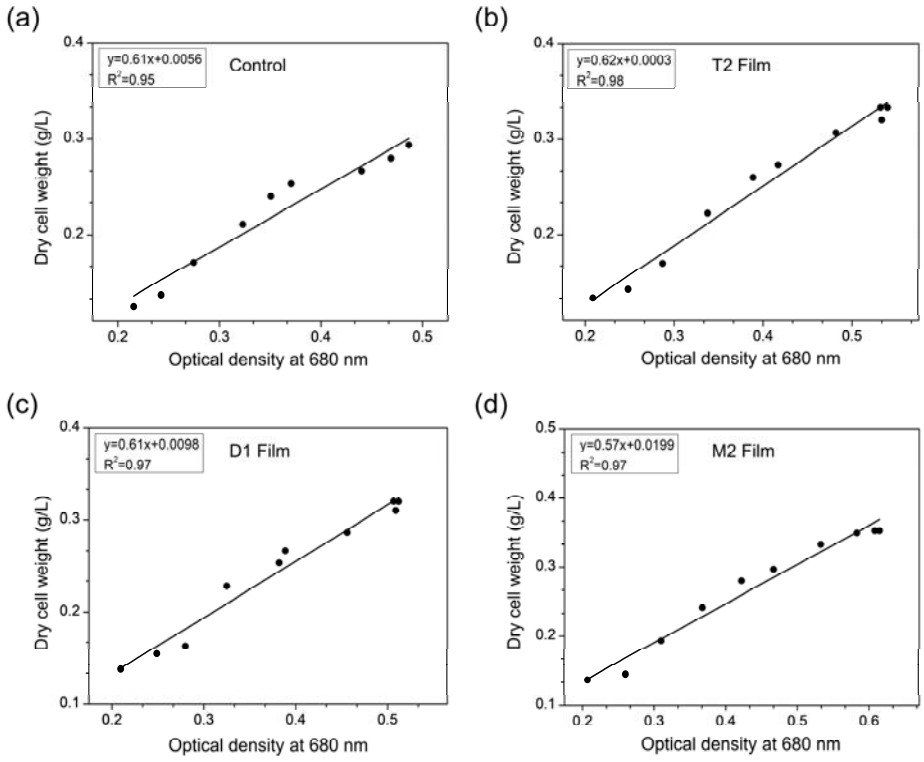


Figure S1. Relationship between optical density and dry cell weight in different culture conditions.

Synthesis and characterization.

A series of diketopyrrolopyrrole (DPP) compounds and triphenylamine (TPA) derivatives (MTPA-BO, BTPA-BO) were synthesized efficiently according to literature procedures. TPA-BO was purchased from Tokyo Chemical Industry (TCI) and was used as received. All other reagents were purchased from commercial suppliers and used as received without further purification. Synthesized DPP compounds were characterized using ^{1}H and ^{13}C NMR, elemental analysis (EA), and matrix-assisted laser desorption/ionization time-of-flight (MALDI-TOF) mass analysis. ^{1}H and ^{13}C NMR spectra were recorded on a Bruker Avance III 500 spectrometer at 500 MHz in chloroform-*d* or dichloromethane-*d* with tetramethylsilane (TMS) as an internal standard. EA was performed with a Thermo Scientific Flash EA 1112 elemental analyzer. MALDI-TOF mass spectra were recorded on an Applied Biosystems Voyager-DE STR Biospectrometry Workstation using cyano-4-hydroxycinnamic acid (CHCA) as a matrix.

3,6-Bis(4'-(diphenylamino)-1,1'-biphenyl-4-yl)-2,5-dihexyl-2,5-dihydropyrrolo3,4-c pyrrole -1,4-dione (T2). A mixture of $Pd(PPh_3)_4$ (100 mg, 0.091 mmol), D6C (0.28 g, 0.46 mmol), and TPA-BO (0.40 g, 1.38 mmol) in dry THF (40 mL) was stirred for 30 min at room temperature under a nitrogen atmosphere. After increasing the temperature of the mixture to 60 °C, an aqueous solution of K_2CO_3 (3.65 M, 5 mL) was added dropwise and the resulting mixture was maintained at this temperature for 16 h. The reaction mixture was then poured into water and extracted with CH_2Cl_2. The combined organic layers were dried over anhydrous $MgSO_4$ and then evaporated to dryness. The crude product was purified by column chromatography using CH_2Cl_2:hexane (3:1, v/v) as the eluent to obtain red crystals of T2 (0.35 g, 80% yield). ^{1}H NMR (500 MHz, CD_2Cl_2), δ (ppm): 7.88–7.89 (m, 4H), 7.73–7.75 (m, 4H), 7.55–7.57 (m, 4H), 7.26–7.30 (m, 8H), 7.11–7.14 (m, 12H), 7.04–7.07 (m, 4H), 3.78 (t, *J* = 7.5 Hz, 4H), 1.56–1.62 (m, 4H), 1.19–1.26 (m, 12H), 0.83 (d, *J* = 7 Hz, 6H). ^{13}C NMR (125 MHz, CD_2Cl_2), δ (ppm): 163.13, 148.62, 148.23, 148.03, 143.56, 133.77, 129.91, 129.84, 128.30, 127.22, 127.14, 125.35, 123.90, 123.79, 110.40, 42.39, 31.82, 29.93, 26.91, 23.05, 14.31. MALDI-TOF MS: *m/z* calcd for $C_{66}H_{63}N_4O_2$ (100%, $[(M+H)^+]$), 943.49; found 943.7191. Elemental analysis: Calcd for $C_{66}H_{62}N_4O_2$: C, 84.04; H, 6.63; N, 5.94; O, 3.39. Found: C, 84.04; H, 6.62; N, 5.97; O, 3.38.

3-(4-bromophenyl)-6-(4'-(di([1,1'-biphenyl]-4-yl)amino)-[1,1'-biphenyl]-4-yl)-2,5-dihexyl-2,5-dihydropyrrolo[3,4-c]pyrrole-1,4-dione (D1). D1 was prepared according to the procedure of T2, using BTPA-BO instead of TPA-BO to obtain orange crystals of D1 (126 mg, 29% yield). ^{1}H NMR (500 MHz, CD_2Cl_2), δ (ppm): 7.88–7.89 (d, *J* = 8.5 Hz , 2H), 7.76–7.77 (d, *J* = 8.5 Hz, 2H), 7.66–7.70 (m, 4H), 7.59–7.63 (m, 6H), 7.55–7.57 (d, *J* = 8.5 Hz, 4H), 7.41–7.44 (t, *J* = 7.75 Hz, 4H), 7.30-7.33(t, *J* = 7.5 Hz, 2H), 7.23-7.25(d, *J* = 8.5Hz, 6H), 3.77-3.78 (t, *J* = 7.75 Hz, 2H), 3.70-3.73 (t, *J* = 7.5 Hz, 2H), 1.52–1.57 (m, 8H), 1.19–1.24 (m, 10H), 0.80-0.83 (m, 4H). ^{13}C NMR (125 MHz, $CDCl_3$), δ (ppm): 163.00, 162.77, 149.06, 147.95, 146.77, 143.60, 140.72, 136.27, 133.89, 132.43, 130.31, 129.48, 128.99, 128.21, 128.13, 127.36, 127.20, 127.06, 126.94, 126.55, 125.76, 125.02, 124.04, 110.40, 109.80, 42.34, 42.14, 31.42, 29.65, 26.62, 26.60, 22.67, 14.17. MALDI-TOF MS: *m/z* calcd for $C_{60}H_{57}BrN_3O_2$ (100%, $[(M+H)^+]$), 930.36 ; found 930.3344. Elemental analysis: Calcd for $C_{60}H_{56}BrN_3O_2$: C, 77.40; H, 6.06; Br, 8.58; N, 4.51; O, 3.44. Found: C, 77.23; H, 6.17; N, 4.53; O, 3.50.

3-(4'-(bis(4-methoxyphenyl)amino)-[1,1'-biphenyl]-4-yl)-6-(4-bromophenyl)-2,5-dihexyl-2,5-dihydropyrrolo[3,4-c]pyrrole-1,4-dione (M2). M2 was prepared according to the procedure of T2, using MTPA-BO (480 mg, 1.38 mmol) instead of TPA-BO and CH_2Cl_2:methanol (400:1, *v/v*) instead of CH_2Cl_2:hexane (3:1, *v/v*) as the eluent to produce deep red crystals to produce dark red crystals of M2 (340 mg, 70% yield). ^{1}H NMR (500 MHz, $CDCl_3$), δ (ppm): 7.88–7.90 (d, J = 8.5 Hz, 4H), 7.69–7.71 (d, J = 8.5 Hz, 4H), 7.48 (d, J = 2 Hz, 2H), 7.47 (d, J = 2 Hz, 2H), 7.09–7.13 (m, 8H), 6.99–7.00 (t, J = 1.5 Hz, 4H), 6.85–6.88 (m, 8H), 3.79–3.82 (m, 16H), 0.82–1.69 (m, 22H). ^{13}C NMR (125 MHz, $CDCl_3$), δ (ppm): 163.12, 156.35, 149.13, 148.22, 143.61, 140.72, 131.43, 129.42, 127.76, 127.14, 126.71, 126.30, 120.34, 114.99, 109.90, 55.71, 42.35, 31.45, 29.67, 26.65, 22.69, 14.17. MALDI-TOF MS: *m/z* calcd for $C_{70}H_{71}N_4O_{62}$ (100%, $[(M+H)^+]$), 1063.53; found 1063.5001. Elemental analysis: Calcd. for $C_{70}H_{70}N_4O_6$: C, 79.07; H, 6.64; N, 5.27; O, 9.03. Found: C, 79.05; H, 6.74; N, 5.26; O, 8.98.

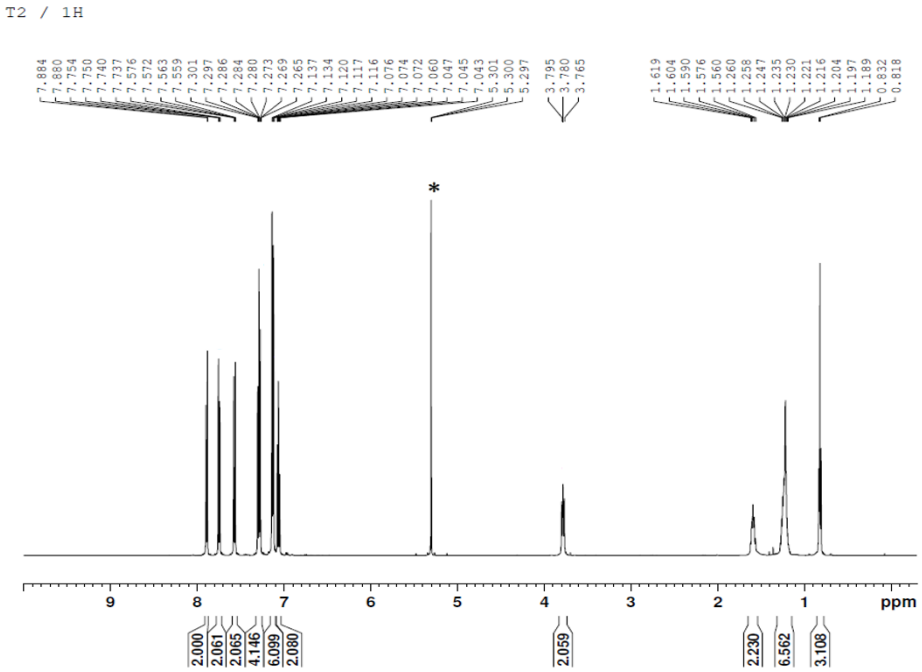


Figure S2. ^{1}H NMR spectrum of T2 in CD_2Cl_2. The solvent peak is marked with asterisk.

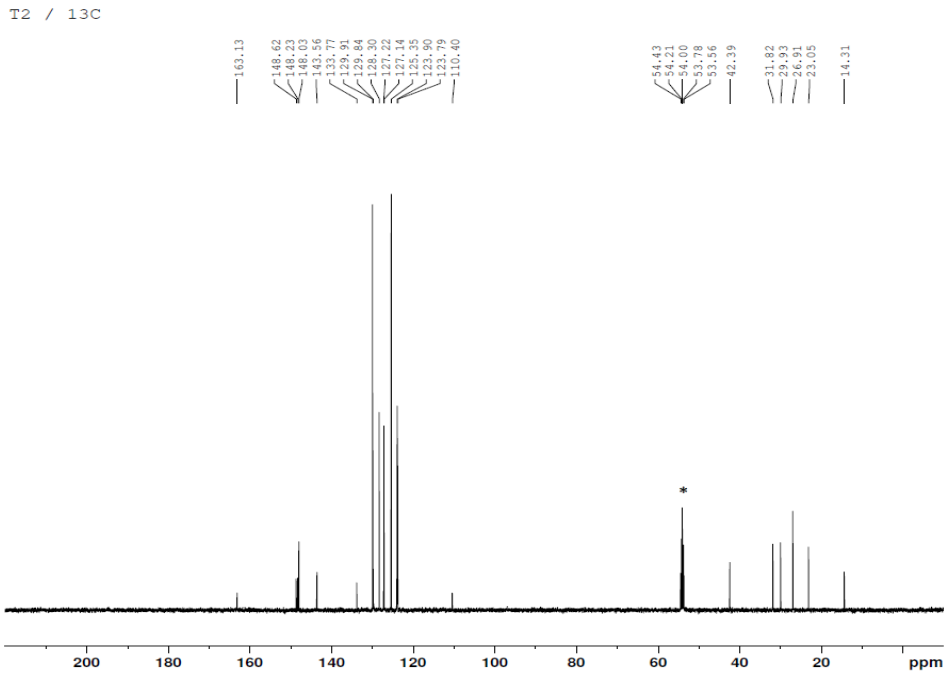


Figure S3. ^{13}C NMR spectrum of T2 in CD_2Cl_2. The solvent peak is marked with asterisk.

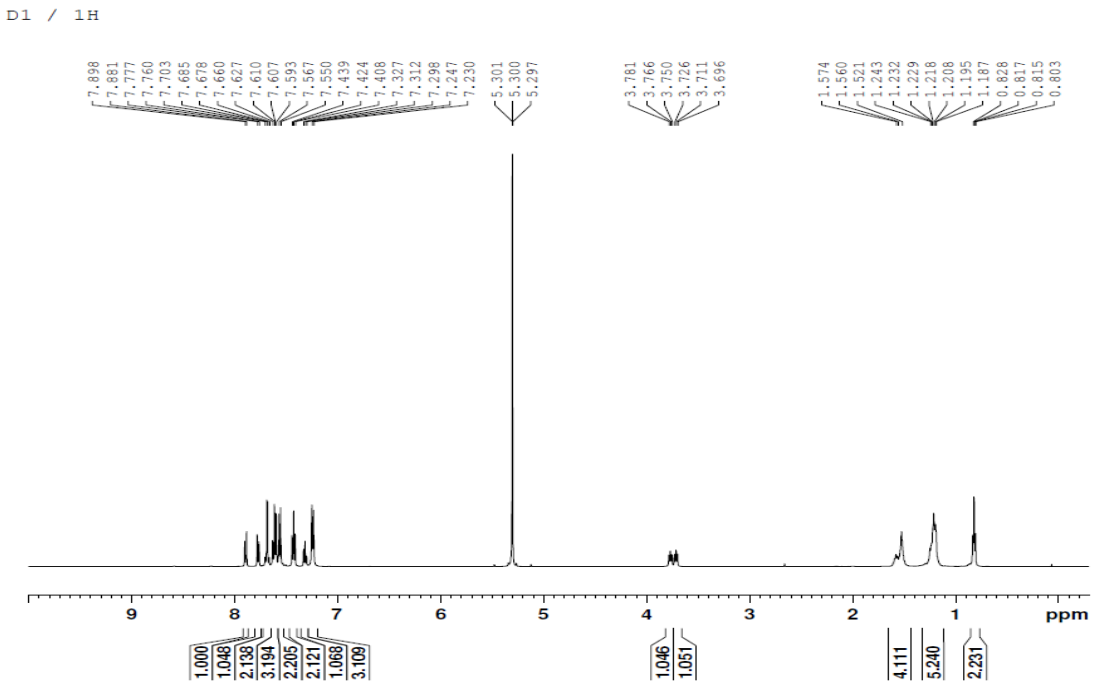


Figure S4. ^{1}H NMR spectrum of D1 in CD_2Cl_2.

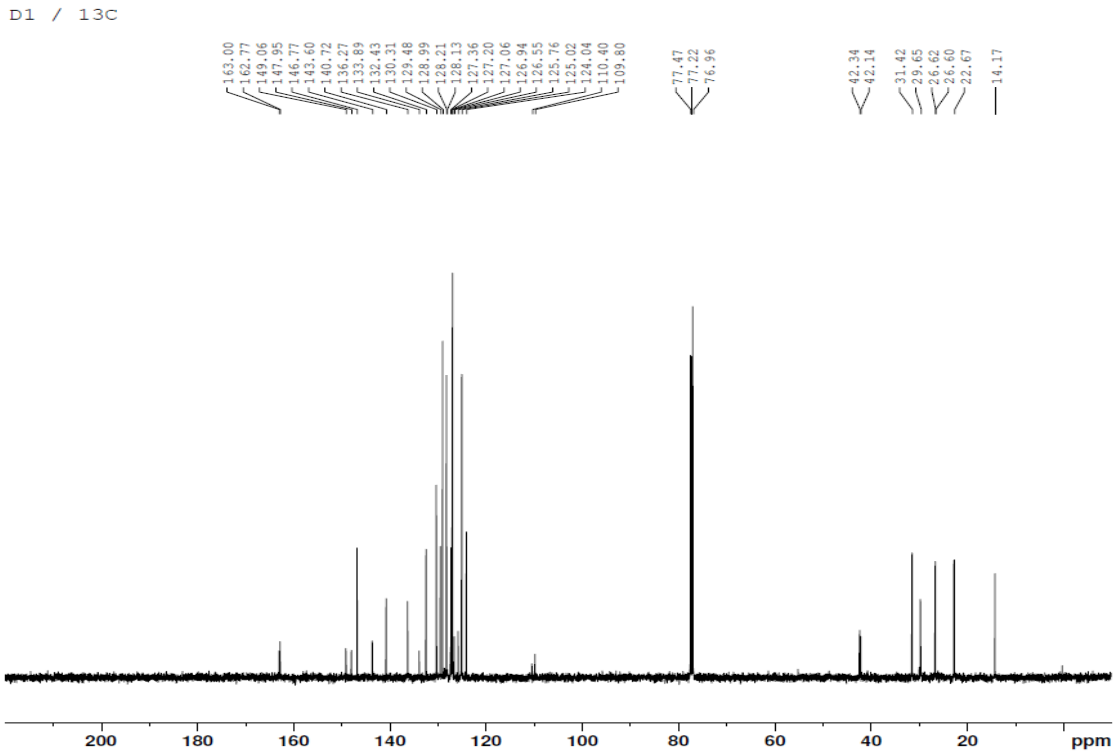


Figure S5. ^{13}C NMR spectrum of D1 in $CDCl_3$.

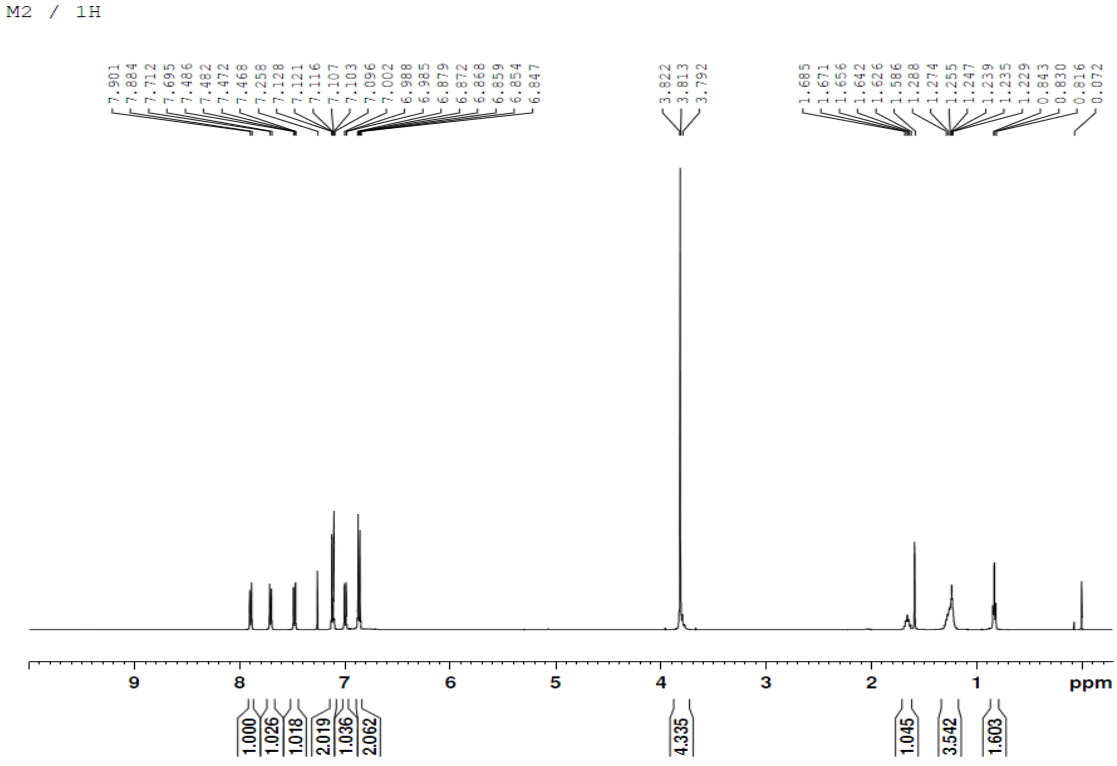


Figure S6. ^{1}H NMR spectrum of M2 in $CDCl_3$.

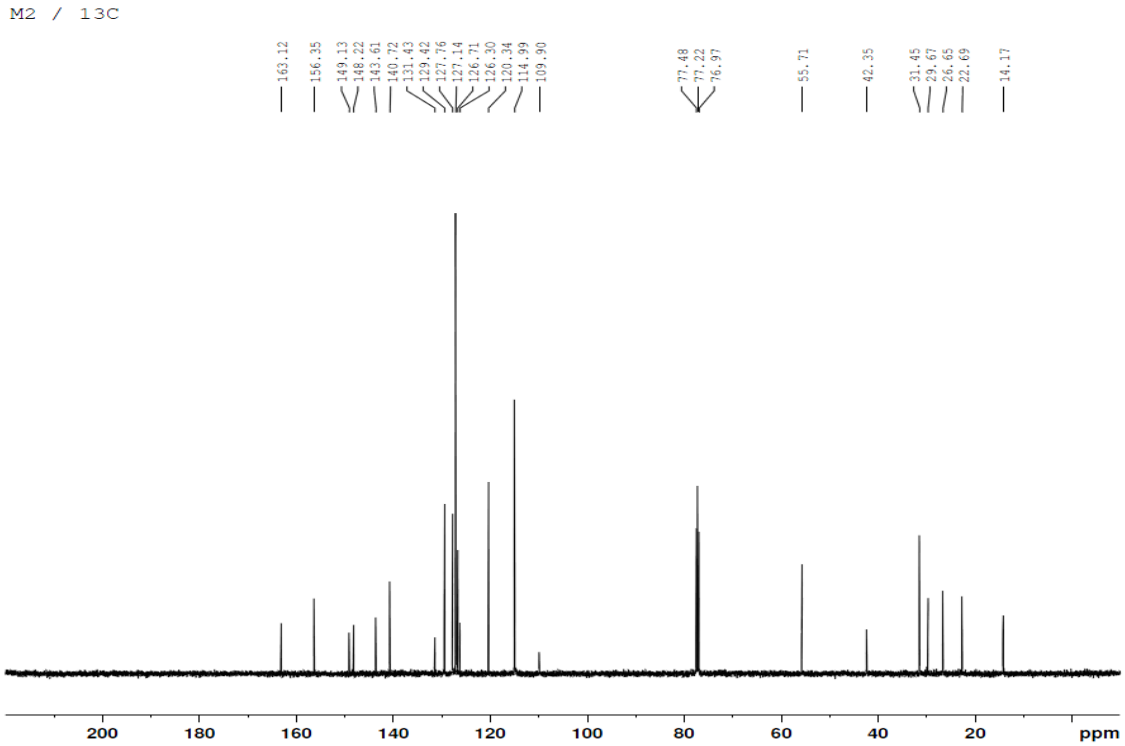


Figure S7. ^{13}C NMR spectrum of M2 in $CDCl_3$.

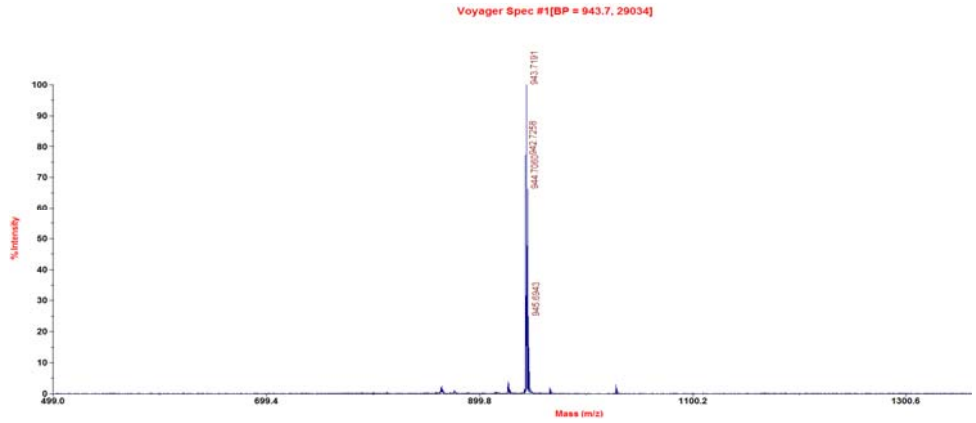
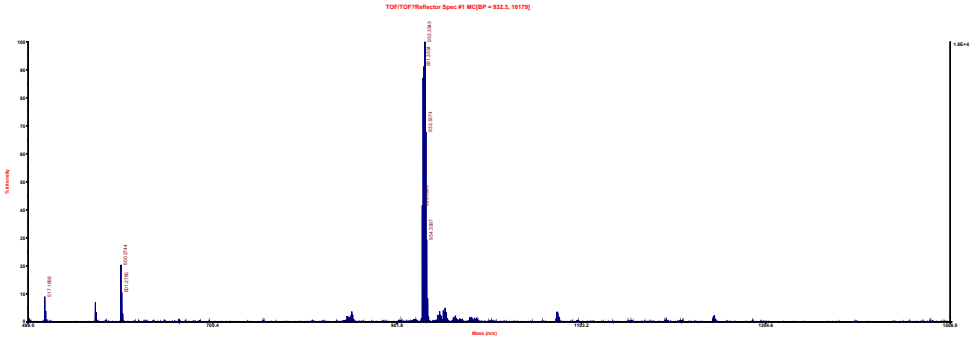


Figure S8. MALDI-TOF mass spectrum of T2.



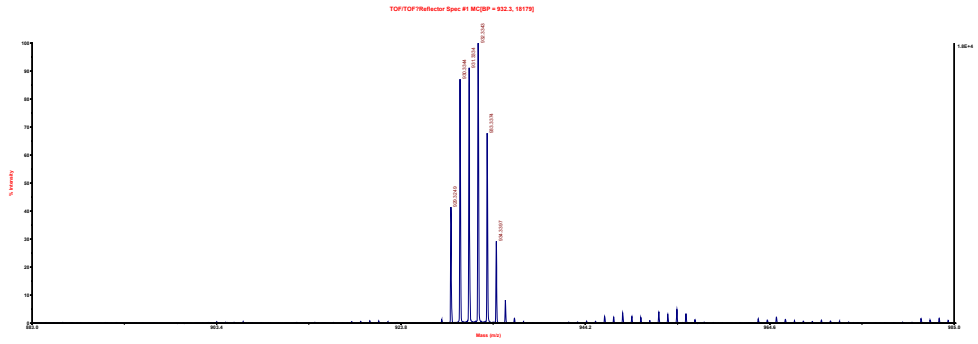


Figure S9. MALDI-TOF mass spectrum of D1.

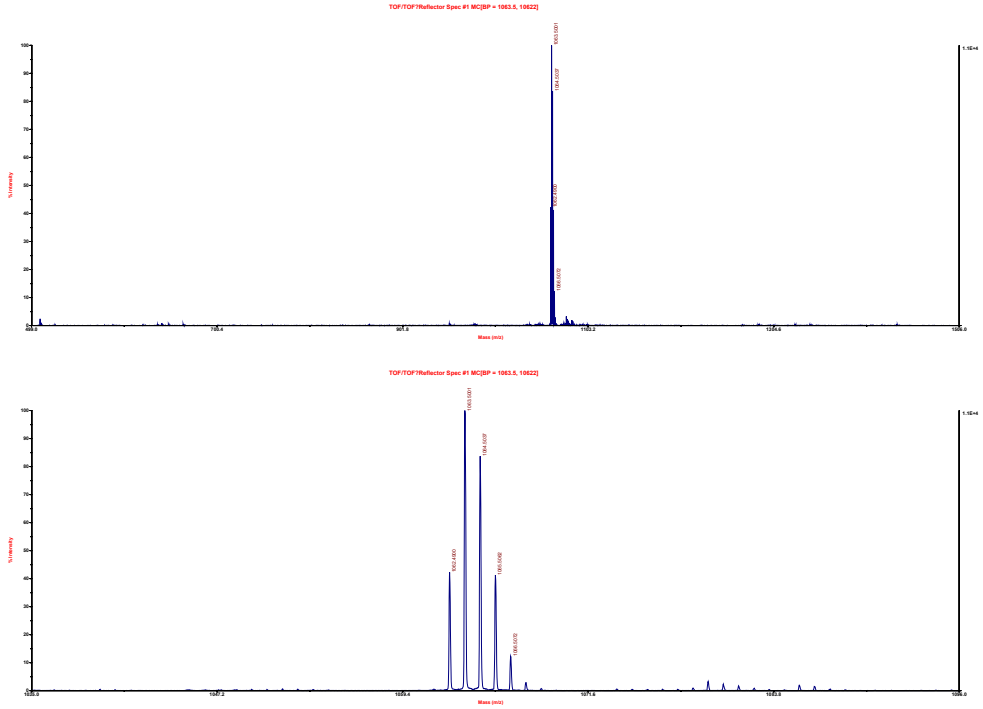


Figure S10. MALDI-TOF mass spectrum of M2.

(Unit: wt%)

Sample name	Nitrogen	Carbon	Hydrogen	Sulphur	Oxygen
D1	4.5265	77.2294	6.1709	n.d.	3.4985
T2	5.9707	84.0411	6.6186	n.d.	3.3798
M2	5.2562	79.0506	6.7356	n.d.	8.9788

Figure S11. Elemental analysis of T2, D1, and M2.

TDDFT Calculation results of T2, D1, and M2.

- **Excitation energies and oscillator strengths of T2 (B3LYP functional with 6-31G(d.p) basis set of Gaussian 16 software package).**

Excited State 1: Triplet-A 1.1538 eV 1074.55 nm f=0.0000 <S**2>=2.000

249 -> 252 0.36999

251 -> 252 0.60269

251 <- 252 0.12374

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-DFT) = -2921.93564261

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 2.2577 eV 549.16 nm f=1.2254 <S**2>=0.000

249 -> 252 -0.10474

251 -> 252 0.69643

Excited State 3: Triplet-A 2.2791 eV 544.01 nm f=0.0000 <S**2>=2.000

246 -> 252 0.11880

250 -> 252 0.64150

250 -> 254 0.10013

251 -> 253 0.20383

Excited State 4: Triplet-A 2.3116 eV 536.37 nm f=0.0000 <S**2>=2.000

247 -> 252 0.10595

249 -> 252 0.55260

250 -> 253 -0.15012

251 -> 252 -0.35058

251 -> 254 -0.12506

Excited State 5: Singlet-A 2.4749 eV 500.96 nm f=0.0024 <S**2>=0.000

250 -> 252 0.70436

Excited State 6: Singlet-A 2.6610 eV 465.93 nm f=0.0847 <S**2>=0.000

249 -> 252 0.69532

251 -> 252 0.10393

Excited State 7: Triplet-A 2.7117 eV 457.22 nm f=0.0000 <S**2>=2.000

246 -> 252 0.15963

248 -> 252 0.24088

249 -> 253 0.18307

249 -> 261 -0.12854

250 -> 252 -0.22662

251 -> 253 0.49775

251 -> 261 -0.13282

Excited State 8: Triplet-A 2.9786 eV 416.25 nm f=0.0000 <S**2>=2.000

247 -> 252 0.26221

248 -> 252 0.29292

249 -> 252 -0.12887

249 -> 253 0.14687

250 -> 252 0.11802

250 -> 253 -0.27153

250 -> 254 -0.18368

251 -> 253 -0.17502

251 -> 254 -0.23053

251 -> 261 -0.11017

Excited State 9: Triplet-A 2.9912 eV 414.50 nm f=0.0000 <S**2>=2.000

246 -> 253 0.11748

248 -> 252 0.37518

249 -> 252 0.17451

249 -> 253 0.12959

249 -> 254 -0.11404

250 -> 253 0.29119

250 -> 254 -0.12868

250 -> 261 0.10617

251 -> 253 -0.15437

251 -> 254 0.26247

Excited State 10: Triplet-A 3.1275 eV 396.44 nm f=0.0000 <S**2>=2.000

245 -> 252 0.41579

246 -> 252 0.18359

247 -> 252 0.25238

248 -> 252 -0.29770

249 -> 253 0.17061

249 -> 254 -0.11255

250 -> 253 0.10613

250 -> 254 -0.11986

Excited State 11: Triplet-A 3.1535 eV 393.17 nm f=0.0000 <S**2>=2.000

245 -> 252 0.18940

247 -> 252 0.35391

248 -> 252 0.21412

249 -> 253 -0.33448

250 -> 254 0.26092

251 -> 261 0.19385

Excited State 12: Triplet-A 3.1861 eV 389.14 nm f=0.0000 <S**2>=2.000

238 -> 265 0.11216

242 -> 256 0.13465

247 -> 258 0.12396

249 -> 258 -0.27452

250 -> 256 -0.12580

250 -> 258 0.42876

251 -> 258 0.30160

Excited State 13: Triplet-A 3.1890 eV 388.79 nm f=0.0000 <S**2>=2.000

241 -> 255 0.13660

246 -> 257 -0.13712

249 -> 257 0.33211

250 -> 257 0.39932

251 -> 257 -0.30221

Excited State 14: Singlet-A 3.2364 eV 383.09 nm f=0.0002 <S**2>=0.000

247 -> 252 0.24551

248 -> 252 0.59875

251 -> 253 -0.23652

Excited State 15: Triplet-A 3.2921 eV 376.61 nm f=0.0000 <S**2>=2.000

233 -> 252 -0.15361

241 -> 252 0.11063

242 -> 252 0.10987

245 -> 252 0.43181

246 -> 253 0.11555

247 -> 252 -0.22601

248 -> 252 0.11938

249 -> 254 0.20992

250 -> 253 -0.15081

250 -> 261 -0.12639

251 -> 266 0.13992

Excited State 16: Singlet-A 3.3672 eV 368.22 nm f=0.0031 <S**2>=0.000

245 -> 252 -0.25717

246 -> 252 -0.14433

248 -> 252 0.24779

251 -> 253 0.57394

Excited State 17: Singlet-A 3.3845 eV 366.33 nm f=0.0053 <S**2>=0.000

239 -> 252 -0.10324

245 -> 252 0.51841

247 -> 252 0.33449

251 -> 253 0.27806

Excited State 18: Triplet-A 3.4209 eV 362.43 nm f=0.0000 <S**2>=2.000

232 -> 252 0.11140

246 -> 252 0.50811

247 -> 252 -0.13454

247 -> 253 -0.14771

248 -> 252 0.12589

249 -> 253 -0.15041

249 -> 261 0.10142

251 -> 253 -0.21323

Excited State 19: Triplet-A 3.4628 eV 358.04 nm f=0.0000 <S**2>=2.000

249 -> 255 0.30744

250 -> 255 0.43104

251 -> 255 -0.40951

Excited State 20: Triplet-A 3.4658 eV 357.74 nm f=0.0000 <S**2>=2.000

249 -> 256 -0.24857

250 -> 256 0.45568

250 -> 258 0.12959

251 -> 256 0.40566

251 -> 258 0.10403

Excited State 21: Triplet-A 3.5293 eV 351.30 nm f=0.0000 <S**2>=2.000

234 -> 252 0.38721

240 -> 252 0.52160

245 -> 253 -0.12335

Excited State 22: Singlet-A 3.5976 eV 344.63 nm f=0.9248 <S**2>=0.000

247 -> 252 -0.13582

249 -> 254 -0.13214

250 -> 253 0.64506

251 -> 254 0.13329

Excited State 23: Triplet-A 3.6671 eV 338.10 nm f=0.0000 <S**2>=2.000

239 -> 252 -0.36162

245 -> 252 -0.13315

247 -> 252 0.10964

249 -> 254 0.14441

250 -> 253 -0.26247

251 -> 254 0.40823

251 -> 260 0.11513

Excited State 24: Triplet-A 3.6829 eV 336.65 nm f=0.0000 <S**2>=2.000

234 -> 252 -0.13920

239 -> 252 0.46006

240 -> 253 -0.10021

247 -> 252 0.11060

249 -> 254 0.12473

250 -> 253 -0.19399

251 -> 254 0.32047

251 -> 259 -0.12057

251 -> 260 -0.13468

Excited State 25: Singlet-A 3.6960 eV 335.45 nm f=0.0135 <S**2>=0.000

246 -> 252 -0.29735

247 -> 252 0.14486

249 -> 253 0.57238

250 -> 254 -0.15632

251 -> 253 -0.11146

Excited State 26: Triplet-A 3.7079 eV 334.38 nm f=0.0000 <S**2>=2.000

234 -> 252 0.36114

236 -> 258 -0.13983

239 -> 252 0.12504

239 -> 253 0.11668

240 -> 252 -0.27826

242 -> 265 0.12274

250 -> 253 -0.12398

250 -> 261 0.10744

251 -> 259 0.14904

251 -> 260 -0.12696

Excited State 27: Triplet-A 3.7123 eV 333.99 nm f=0.0000 <S**2>=2.000

234 -> 252 0.28897

236 -> 258 0.18479

238 -> 256 -0.12398

240 -> 252 -0.17402

242 -> 265 -0.16250

247 -> 252 0.13923

249 -> 253 -0.10351

249 -> 261 0.14280

250 -> 266 0.16534

251 -> 253 0.12124

251 -> 259 0.10312

251 -> 267 -0.12438

Excited State 28: Triplet-A 3.7209 eV 333.21 nm f=0.0000 <S**2>=2.000

233 -> 252 -0.11172

234 -> 252 -0.11737

235 -> 257 -0.23573

237 -> 255 0.16501

241 -> 262 -0.11502

241 -> 263 -0.16662

243 -> 255 -0.10894

243 -> 257 -0.10793

246 -> 252 -0.13684

249 -> 261 0.12419

249 -> 266 0.12904

250 -> 253 -0.11385

250 -> 261 0.12411

250 -> 266 0.12221

250 -> 267 0.14332

251 -> 266 -0.11939

251 -> 267 -0.11116

Excited State 29: Singlet-A 3.7485 eV 330.75 nm f=0.0209 <S**2>=0.000

234 -> 252 -0.16553

240 -> 252 -0.15942

245 -> 252 -0.27273

246 -> 252 0.10701

247 -> 252 0.39368

248 -> 252 -0.20845

249 -> 253 -0.10106

251 -> 254 0.33338

Excited State 30: Singlet-A 3.7806 eV 327.95 nm f=0.0011 <S**2>=0.000

234 -> 252 0.43387

240 -> 252 0.42549

245 -> 252 -0.10183

246 -> 252 0.10167

247 -> 252 0.11763

249 -> 253 0.10178

251 -> 254 0.17123

Excited State 31: Singlet-A 3.8169 eV 324.83 nm f=0.0090 <S**2>=0.000

249 -> 255 -0.24434

250 -> 255 -0.39652

251 -> 255 0.49448

Excited State 32: Singlet-A 3.8221 eV 324.39 nm f=0.0107 <S**2>=0.000

249 -> 256 -0.19849

250 -> 256 0.42191

251 -> 256 0.49172

Excited State 33: Singlet-A 3.8751 eV 319.95 nm f=0.2950 <S**2>=0.000

240 -> 252 -0.10062

246 -> 252 0.29311

247 -> 252 -0.30478

248 -> 252 0.11725

249 -> 253 0.20821

250 -> 253 -0.17186

251 -> 254 0.43613

Excited State 34: Singlet-A 3.8885 eV 318.85 nm f=0.2427 <S**2>=0.000

245 -> 252 -0.12810

246 -> 252 0.48821

249 -> 253 0.26348

250 -> 253 0.14326

251 -> 254 -0.35145

Excited State 35: Singlet-A 3.9849 eV 311.13 nm f=0.0196 <S**2>=0.000

239 -> 252 0.49030

251 -> 257 0.11404

251 -> 259 0.18044

251 -> 260 0.35995

Excited State 36: Singlet-A 3.9970 eV 310.19 nm f=0.0130 <S**2>=0.000

234 -> 252 0.37316

240 -> 252 -0.31410

251 -> 257 -0.12303

251 -> 258 -0.10074

251 -> 259 -0.34730

251 -> 260 0.16948

Excited State 37: Singlet-A 4.0193 eV 308.47 nm f=0.1362 <S**2>=0.000

249 -> 257 -0.23183

250 -> 257 -0.37565

251 -> 257 0.50431

251 -> 259 -0.11043

Excited State 38: Singlet-A 4.0256 eV 307.99 nm f=0.1742 <S**2>=0.000

249 -> 258 -0.18758

250 -> 258 0.40259

251 -> 258 0.50828

Excited State 39: Singlet-A 4.0846 eV 303.54 nm f=0.0002 <S**2>=0.000

249 -> 253 0.13834

250 -> 254 0.65273

251 -> 253 -0.11894

251 -> 261 0.10845

Excited State 40: Singlet-A 4.1470 eV 298.97 nm f=0.0010 <S**2>=0.000

238 -> 252 0.13516

244 -> 252 0.65075

251 -> 256 -0.15511

- **Excitation energies and oscillator strengths of D1 (B3LYP functional with 6-31G(d.p) basis set of Gaussian 16 software package).**

Excited State 1: Triplet-A 1.1683 eV 1061.24 nm f=0.0000 <S**2>=2.000

243 -> 245 0.51070

244 -> 245 -0.49298

243 <- 245 0.12078

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-DFT) = -5206.64169115

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Triplet-A 2.1988 eV 563.88 nm f=0.0000 <S**2>=2.000

243 -> 245 0.45768

244 -> 245 0.48291

244 -> 246 0.16658

Excited State 3: Singlet-A 2.2621 eV 548.09 nm f=0.6871 <S**2>=0.000

243 -> 245 0.10971

244 -> 245 0.69668

Excited State 4: Singlet-A 2.5869 eV 479.28 nm f=0.2800 <S**2>=0.000

243 -> 245 0.69614

244 -> 245 -0.11029

Excited State 5: Triplet-A 2.7373 eV 452.94 nm f=0.0000 <S**2>=2.000

238 -> 245 0.11269

239 -> 245 0.13191

240 -> 245 0.27034

243 -> 245 -0.12343

243 -> 246 -0.23677

243 -> 248 0.13552

243 -> 249 -0.11930

244 -> 245 -0.11050

244 -> 246 0.44426

Excited State 6: Triplet-A 2.8685 eV 432.22 nm f=0.0000 <S**2>=2.000

240 -> 245 -0.13534

241 -> 247 0.10740

241 -> 248 0.14958

243 -> 246 0.24272

243 -> 247 0.20727

243 -> 248 0.15351

244 -> 246 0.21108

244 -> 247 0.31739

244 -> 248 0.29777

Excited State 7: Triplet-A 2.9715 eV 417.25 nm f=0.0000 <S**2>=2.000

240 -> 245 0.34343

241 -> 245 0.10678

241 -> 246 0.12164

242 -> 247 -0.13264

243 -> 246 -0.16898

243 -> 247 0.16098

244 -> 246 -0.23626

244 -> 247 0.22921

244 -> 249 0.19662

244 -> 250 0.11194

244 -> 251 0.12357

Excited State 8: Triplet-A 3.0855 eV 401.83 nm f=0.0000 <S**2>=2.000

238 -> 245 -0.19651

239 -> 245 -0.16580

240 -> 245 0.45732

242 -> 247 0.13274

243 -> 246 0.22918

244 -> 247 -0.12364

244 -> 248 0.11652

244 -> 249 -0.13046

Excited State 9: Triplet-A 3.1609 eV 392.24 nm f=0.0000 <S**2>=2.000

238 -> 245 0.38573

239 -> 245 -0.14846

240 -> 245 -0.13963

241 -> 245 0.20869

242 -> 245 -0.18678

242 -> 247 0.13561

243 -> 248 0.12724

243 -> 249 -0.10626

244 -> 247 -0.11913

244 -> 255 0.11506

Excited State 10: Triplet-A 3.2148 eV 385.67 nm f=0.0000 <S**2>=2.000

233 -> 245 -0.11068

234 -> 245 0.19625

236 -> 245 0.47970

238 -> 245 -0.25856

239 -> 245 -0.20667

240 -> 245 -0.15555

243 -> 246 -0.12375

Excited State 11: Singlet-A 3.2573 eV 380.64 nm f=0.0084 <S**2>=0.000

240 -> 245 0.68227

244 -> 246 -0.13453

Excited State 12: Triplet-A 3.2999 eV 375.72 nm f=0.0000 <S**2>=2.000

238 -> 245 -0.17399

239 -> 245 0.10366

243 -> 246 -0.14340

243 -> 247 -0.12050

243 -> 248 0.23680

243 -> 249 0.10846

244 -> 247 -0.26078

244 -> 248 0.36027

244 -> 249 0.21323

244 -> 250 0.12593

Excited State 13: Triplet-A 3.3772 eV 367.12 nm f=0.0000 <S**2>=2.000

235 -> 253 0.13044

236 -> 245 -0.15588

238 -> 245 -0.20139

241 -> 247 0.12728

242 -> 247 0.24724

242 -> 248 -0.18593

243 -> 246 -0.20388

244 -> 247 0.18645

244 -> 248 -0.14525

244 -> 251 0.14013

244 -> 258 0.10408

Excited State 14: Singlet-A 3.4064 eV 363.97 nm f=0.0426 <S**2>=0.000

234 -> 245 0.15474

236 -> 245 0.36564

238 -> 245 -0.36032

239 -> 245 -0.20860

241 -> 245 0.11946

242 -> 245 -0.13754

244 -> 246 0.32217

Excited State 15: Triplet-A 3.4068 eV 363.94 nm f=0.0000 <S**2>=2.000

234 -> 245 0.15552

236 -> 245 0.26154

238 -> 245 0.17568

239 -> 245 0.14512

241 -> 245 -0.24031

242 -> 245 0.27228

242 -> 247 0.15728

242 -> 248 -0.12996

243 -> 246 0.13169

244 -> 246 -0.21420

Excited State 16: Singlet-A 3.4402 eV 360.40 nm f=0.3559 <S**2>=0.000

234 -> 245 -0.11132

236 -> 245 -0.26129

238 -> 245 0.12472

240 -> 245 0.13742

244 -> 246 0.58435

Excited State 17: Singlet-A 3.4833 eV 355.94 nm f=0.1190 <S**2>=0.000

236 -> 245 0.11787

238 -> 245 -0.13021

241 -> 245 -0.16496

242 -> 245 0.62725

243 -> 246 0.14333

Excited State 18: Triplet-A 3.5340 eV 350.83 nm f=0.0000 <S**2>=2.000

239 -> 245 -0.12391

241 -> 245 0.32091

242 -> 245 0.58466

Excited State 19: Triplet-A 3.5455 eV 349.70 nm f=0.0000 <S**2>=2.000

229 -> 245 -0.20204

231 -> 245 0.37783

232 -> 245 0.21199

233 -> 245 0.43997

236 -> 246 0.10008

Excited State 20: Singlet-A 3.5535 eV 348.91 nm f=0.0952 <S**2>=0.000

241 -> 245 -0.21554

243 -> 247 0.21684

244 -> 247 0.58058

244 -> 248 -0.17198

Excited State 21: Singlet-A 3.5792 eV 346.40 nm f=0.0814 <S**2>=0.000

241 -> 245 0.51051

242 -> 245 0.27855

243 -> 246 -0.23134

244 -> 247 0.14984

244 -> 248 -0.22316

Excited State 22: Triplet-A 3.5968 eV 344.71 nm f=0.0000 <S**2>=2.000

235 -> 253 0.20084

237 -> 254 -0.15230

239 -> 247 -0.12459

241 -> 246 -0.10837

241 -> 248 -0.18998

242 -> 247 0.22872

242 -> 248 -0.14555

242 -> 251 -0.10286

243 -> 249 0.11144

244 -> 247 0.16793

244 -> 249 0.17336

244 -> 250 0.10859

244 -> 251 -0.16844

244 -> 255 -0.10166

Excited State 23: Triplet-A 3.6595 eV 338.80 nm f=0.0000 <S**2>=2.000

229 -> 245 -0.16312

231 -> 245 0.45102

232 -> 245 -0.13902

233 -> 245 -0.36879

233 -> 246 -0.13308

244 -> 251 0.11746

244 -> 252 -0.10843

Excited State 24: Singlet-A 3.6799 eV 336.92 nm f=0.2813 <S**2>=0.000

238 -> 245 0.10589

241 -> 245 0.26141

243 -> 246 0.15214

243 -> 248 0.13807

244 -> 247 0.24821

244 -> 248 0.51808

Excited State 25: Triplet-A 3.6995 eV 335.14 nm f=0.0000 <S**2>=2.000

231 -> 245 -0.10077

237 -> 254 -0.11882

239 -> 248 -0.11100

241 -> 248 -0.12273

243 -> 251 0.20909

243 -> 255 -0.13246

244 -> 248 0.14318

244 -> 249 -0.15269

244 -> 251 0.40546

244 -> 252 0.10753

244 -> 255 -0.21745

Excited State 26: Singlet-A 3.7249 eV 332.85 nm f=0.0309 <S**2>=0.000

239 -> 245 0.13705

241 -> 245 0.24591

243 -> 246 0.54765

243 -> 248 -0.12814

244 -> 248 -0.19309

244 -> 249 -0.13123

Excited State 27: Triplet-A 3.7335 eV 332.09 nm f=0.0000 <S**2>=2.000

239 -> 245 0.35191

239 -> 246 0.12005

241 -> 245 0.46562

242 -> 245 -0.10012

243 -> 249 0.10218

Excited State 28: Triplet-A 3.7450 eV 331.07 nm f=0.0000 <S**2>=2.000

229 -> 245 -0.33769

238 -> 250 -0.10032

243 -> 249 0.19825

243 -> 250 -0.31533

244 -> 249 -0.22405

244 -> 250 0.36727

Excited State 29: Singlet-A 3.7926 eV 326.91 nm f=0.0123 <S**2>=0.000

229 -> 245 -0.26713

231 -> 245 0.46129

232 -> 245 0.15435

233 -> 245 0.29699

236 -> 245 0.17782

238 -> 245 0.15767

239 -> 245 -0.10183

Excited State 30: Triplet-A 3.8237 eV 324.25 nm f=0.0000 <S**2>=2.000

243 -> 246 0.37085

243 -> 255 -0.13487

244 -> 247 -0.12320

244 -> 248 -0.27390

244 -> 249 0.26685

244 -> 250 0.17261

244 -> 251 0.20048

Excited State 31: Triplet-A 3.8334 eV 323.43 nm f=0.0000 <S**2>=2.000

237 -> 254 -0.10199

243 -> 254 -0.11628

243 -> 256 0.21467

244 -> 252 0.30878

244 -> 254 -0.18878

244 -> 256 0.37137

Excited State 32: Singlet-A 3.9044 eV 317.55 nm f=0.1943 <S**2>=0.000

231 -> 245 -0.15404

233 -> 245 -0.16366

236 -> 245 0.16675

238 -> 245 0.44678

239 -> 245 -0.37504

241 -> 245 -0.11917

Excited State 33: Singlet-A 3.9414 eV 314.57 nm f=0.0175 <S**2>=0.000

231 -> 245 -0.19101

233 -> 245 0.16268

236 -> 245 0.23690

239 -> 245 0.28662

243 -> 246 -0.18710

244 -> 248 0.15369

244 -> 249 -0.27076

244 -> 250 -0.27930

244 -> 251 0.19950

Excited State 34: Singlet-A 3.9664 eV 312.58 nm f=0.0015 <S**2>=0.000

229 -> 245 0.22753

243 -> 249 0.18470

243 -> 250 -0.32751

244 -> 249 -0.35495

244 -> 250 0.40146

Excited State 35: Singlet-A 3.9826 eV 311.32 nm f=0.0176 <S**2>=0.000

231 -> 245 -0.26691

232 -> 245 0.17046

233 -> 245 0.38603

239 -> 245 -0.26924

243 -> 246 0.14929

243 -> 248 0.13650

244 -> 251 0.12004

244 -> 252 -0.24159

Excited State 36: Singlet-A 4.0257 eV 307.98 nm f=0.0246 <S**2>=0.000

239 -> 245 -0.10123

243 -> 247 0.62035

244 -> 247 -0.23817

Excited State 37: Singlet-A 4.0443 eV 306.56 nm f=0.0081 <S**2>=0.000

232 -> 245 -0.10282

233 -> 245 -0.11409

234 -> 245 -0.16011

236 -> 245 -0.17272

238 -> 245 -0.11507

239 -> 245 -0.26818

243 -> 246 0.11079

243 -> 247 -0.18728

243 -> 249 -0.12464

243 -> 251 0.13729

244 -> 249 -0.19309

244 -> 250 -0.16286

244 -> 251 0.31403

244 -> 252 0.17538

Excited State 38: Singlet-A 4.0939 eV 302.85 nm f=0.1064 <S**2>=0.000

232 -> 245 -0.16659

234 -> 245 -0.23666

236 -> 245 0.23477

238 -> 245 0.12970

239 -> 245 0.12878

243 -> 248 0.44158

244 -> 248 -0.18904

244 -> 249 0.14910

244 -> 250 0.10607

244 -> 251 0.16096

Excited State 39: Singlet-A 4.1281 eV 300.34 nm f=0.0651 <S**2>=0.000

232 -> 245 0.10675

234 -> 245 0.33969

236 -> 245 -0.13576

243 -> 248 0.43413

244 -> 249 -0.27378

244 -> 250 -0.15511

244 -> 251 -0.11793

Excited State 40: Singlet-A 4.1635 eV 297.79 nm f=0.0389 <S**2>=0.000

232 -> 245 0.15333

234 -> 245 0.36749

237 -> 245 -0.11221

238 -> 245 0.12913

243 -> 251 0.10278

244 -> 249 0.18483

244 -> 250 0.11990

244 -> 251 0.42038 Excited State 1: Triplet-A 1.1683 eV 1061.24 nm f=0.0000 <S**2>=2.000

243 -> 245 0.51070

244 -> 245 -0.49298

243 <- 245 0.12078

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-DFT) = -5206.64169115

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Triplet-A 2.1988 eV 563.88 nm f=0.0000 <S**2>=2.000

243 -> 245 0.45768

244 -> 245 0.48291

244 -> 246 0.16658

Excited State 3: Singlet-A 2.2621 eV 548.09 nm f=0.6871 <S**2>=0.000

243 -> 245 0.10971

244 -> 245 0.69668

Excited State 4: Singlet-A 2.5869 eV 479.28 nm f=0.2800 <S**2>=0.000

243 -> 245 0.69614

244 -> 245 -0.11029

Excited State 5: Triplet-A 2.7373 eV 452.94 nm f=0.0000 <S**2>=2.000

238 -> 245 0.11269

239 -> 245 0.13191

240 -> 245 0.27034

243 -> 245 -0.12343

243 -> 246 -0.23677

243 -> 248 0.13552

243 -> 249 -0.11930

244 -> 245 -0.11050

244 -> 246 0.44426

Excited State 6: Triplet-A 2.8685 eV 432.22 nm f=0.0000 <S**2>=2.000

240 -> 245 -0.13534

241 -> 247 0.10740

241 -> 248 0.14958

243 -> 246 0.24272

243 -> 247 0.20727

243 -> 248 0.15351

244 -> 246 0.21108

244 -> 247 0.31739

244 -> 248 0.29777

Excited State 7: Triplet-A 2.9715 eV 417.25 nm f=0.0000 <S**2>=2.000

240 -> 245 0.34343

241 -> 245 0.10678

241 -> 246 0.12164

242 -> 247 -0.13264

243 -> 246 -0.16898

243 -> 247 0.16098

244 -> 246 -0.23626

244 -> 247 0.22921

244 -> 249 0.19662

244 -> 250 0.11194

244 -> 251 0.12357

Excited State 8: Triplet-A 3.0855 eV 401.83 nm f=0.0000 <S**2>=2.000

238 -> 245 -0.19651

239 -> 245 -0.16580

240 -> 245 0.45732

242 -> 247 0.13274

243 -> 246 0.22918

244 -> 247 -0.12364

244 -> 248 0.11652

244 -> 249 -0.13046

Excited State 9: Triplet-A 3.1609 eV 392.24 nm f=0.0000 <S**2>=2.000

238 -> 245 0.38573

239 -> 245 -0.14846

240 -> 245 -0.13963

241 -> 245 0.20869

242 -> 245 -0.18678

242 -> 247 0.13561

243 -> 248 0.12724

243 -> 249 -0.10626

244 -> 247 -0.11913

244 -> 255 0.11506

Excited State 10: Triplet-A 3.2148 eV 385.67 nm f=0.0000 <S**2>=2.000

233 -> 245 -0.11068

234 -> 245 0.19625

236 -> 245 0.47970

238 -> 245 -0.25856

239 -> 245 -0.20667

240 -> 245 -0.15555

243 -> 246 -0.12375

Excited State 11: Singlet-A 3.2573 eV 380.64 nm f=0.0084 <S**2>=0.000

240 -> 245 0.68227

244 -> 246 -0.13453

Excited State 12: Triplet-A 3.2999 eV 375.72 nm f=0.0000 <S**2>=2.000

238 -> 245 -0.17399

239 -> 245 0.10366

243 -> 246 -0.14340

243 -> 247 -0.12050

243 -> 248 0.23680

243 -> 249 0.10846

244 -> 247 -0.26078

244 -> 248 0.36027

244 -> 249 0.21323

244 -> 250 0.12593

Excited State 13: Triplet-A 3.3772 eV 367.12 nm f=0.0000 <S**2>=2.000

235 -> 253 0.13044

236 -> 245 -0.15588

238 -> 245 -0.20139

241 -> 247 0.12728

242 -> 247 0.24724

242 -> 248 -0.18593

243 -> 246 -0.20388

244 -> 247 0.18645

244 -> 248 -0.14525

244 -> 251 0.14013

244 -> 258 0.10408

Excited State 14: Singlet-A 3.4064 eV 363.97 nm f=0.0426 <S**2>=0.000

234 -> 245 0.15474

236 -> 245 0.36564

238 -> 245 -0.36032

239 -> 245 -0.20860

241 -> 245 0.11946

242 -> 245 -0.13754

244 -> 246 0.32217

Excited State 15: Triplet-A 3.4068 eV 363.94 nm f=0.0000 <S**2>=2.000

234 -> 245 0.15552

236 -> 245 0.26154

238 -> 245 0.17568

239 -> 245 0.14512

241 -> 245 -0.24031

242 -> 245 0.27228

242 -> 247 0.15728

242 -> 248 -0.12996

243 -> 246 0.13169

244 -> 246 -0.21420

Excited State 16: Singlet-A 3.4402 eV 360.40 nm f=0.3559 <S**2>=0.000

234 -> 245 -0.11132

236 -> 245 -0.26129

238 -> 245 0.12472

240 -> 245 0.13742

244 -> 246 0.58435

Excited State 17: Singlet-A 3.4833 eV 355.94 nm f=0.1190 <S**2>=0.000

236 -> 245 0.11787

238 -> 245 -0.13021

241 -> 245 -0.16496

242 -> 245 0.62725

243 -> 246 0.14333

Excited State 18: Triplet-A 3.5340 eV 350.83 nm f=0.0000 <S**2>=2.000

239 -> 245 -0.12391

241 -> 245 0.32091

242 -> 245 0.58466

Excited State 19: Triplet-A 3.5455 eV 349.70 nm f=0.0000 <S**2>=2.000

229 -> 245 -0.20204

231 -> 245 0.37783

232 -> 245 0.21199

233 -> 245 0.43997

236 -> 246 0.10008

Excited State 20: Singlet-A 3.5535 eV 348.91 nm f=0.0952 <S**2>=0.000

241 -> 245 -0.21554

243 -> 247 0.21684

244 -> 247 0.58058

244 -> 248 -0.17198

Excited State 21: Singlet-A 3.5792 eV 346.40 nm f=0.0814 <S**2>=0.000

241 -> 245 0.51051

242 -> 245 0.27855

243 -> 246 -0.23134

244 -> 247 0.14984

244 -> 248 -0.22316

Excited State 22: Triplet-A 3.5968 eV 344.71 nm f=0.0000 <S**2>=2.000

235 -> 253 0.20084

237 -> 254 -0.15230

239 -> 247 -0.12459

241 -> 246 -0.10837

241 -> 248 -0.18998

242 -> 247 0.22872

242 -> 248 -0.14555

242 -> 251 -0.10286

243 -> 249 0.11144

244 -> 247 0.16793

244 -> 249 0.17336

244 -> 250 0.10859

244 -> 251 -0.16844

244 -> 255 -0.10166

Excited State 23: Triplet-A 3.6595 eV 338.80 nm f=0.0000 <S**2>=2.000

229 -> 245 -0.16312

231 -> 245 0.45102

232 -> 245 -0.13902

233 -> 245 -0.36879

233 -> 246 -0.13308

244 -> 251 0.11746

244 -> 252 -0.10843

Excited State 24: Singlet-A 3.6799 eV 336.92 nm f=0.2813 <S**2>=0.000

238 -> 245 0.10589

241 -> 245 0.26141

243 -> 246 0.15214

243 -> 248 0.13807

244 -> 247 0.24821

244 -> 248 0.51808

Excited State 25: Triplet-A 3.6995 eV 335.14 nm f=0.0000 <S**2>=2.000

231 -> 245 -0.10077

237 -> 254 -0.11882

239 -> 248 -0.11100

241 -> 248 -0.12273

243 -> 251 0.20909

243 -> 255 -0.13246

244 -> 248 0.14318

244 -> 249 -0.15269

244 -> 251 0.40546

244 -> 252 0.10753

244 -> 255 -0.21745

Excited State 26: Singlet-A 3.7249 eV 332.85 nm f=0.0309 <S**2>=0.000

239 -> 245 0.13705

241 -> 245 0.24591

243 -> 246 0.54765

243 -> 248 -0.12814

244 -> 248 -0.19309

244 -> 249 -0.13123

Excited State 27: Triplet-A 3.7335 eV 332.09 nm f=0.0000 <S**2>=2.000

239 -> 245 0.35191

239 -> 246 0.12005

241 -> 245 0.46562

242 -> 245 -0.10012

243 -> 249 0.10218

Excited State 28: Triplet-A 3.7450 eV 331.07 nm f=0.0000 <S**2>=2.000

229 -> 245 -0.33769

238 -> 250 -0.10032

243 -> 249 0.19825

243 -> 250 -0.31533

244 -> 249 -0.22405

244 -> 250 0.36727

Excited State 29: Singlet-A 3.7926 eV 326.91 nm f=0.0123 <S**2>=0.000

229 -> 245 -0.26713

231 -> 245 0.46129

232 -> 245 0.15435

233 -> 245 0.29699

236 -> 245 0.17782

238 -> 245 0.15767

239 -> 245 -0.10183

Excited State 30: Triplet-A 3.8237 eV 324.25 nm f=0.0000 <S**2>=2.000

243 -> 246 0.37085

243 -> 255 -0.13487

244 -> 247 -0.12320

244 -> 248 -0.27390

244 -> 249 0.26685

244 -> 250 0.17261

244 -> 251 0.20048

Excited State 31: Triplet-A 3.8334 eV 323.43 nm f=0.0000 <S**2>=2.000

237 -> 254 -0.10199

243 -> 254 -0.11628

243 -> 256 0.21467

244 -> 252 0.30878

244 -> 254 -0.18878

244 -> 256 0.37137

Excited State 32: Singlet-A 3.9044 eV 317.55 nm f=0.1943 <S**2>=0.000

231 -> 245 -0.15404

233 -> 245 -0.16366

236 -> 245 0.16675

238 -> 245 0.44678

239 -> 245 -0.37504

241 -> 245 -0.11917

Excited State 33: Singlet-A 3.9414 eV 314.57 nm f=0.0175 <S**2>=0.000

231 -> 245 -0.19101

233 -> 245 0.16268

236 -> 245 0.23690

239 -> 245 0.28662

243 -> 246 -0.18710

244 -> 248 0.15369

244 -> 249 -0.27076

244 -> 250 -0.27930

244 -> 251 0.19950

Excited State 34: Singlet-A 3.9664 eV 312.58 nm f=0.0015 <S**2>=0.000

229 -> 245 0.22753

243 -> 249 0.18470

243 -> 250 -0.32751

244 -> 249 -0.35495

244 -> 250 0.40146

Excited State 35: Singlet-A 3.9826 eV 311.32 nm f=0.0176 <S**2>=0.000

231 -> 245 -0.26691

232 -> 245 0.17046

233 -> 245 0.38603

239 -> 245 -0.26924

243 -> 246 0.14929

243 -> 248 0.13650

244 -> 251 0.12004

244 -> 252 -0.24159

Excited State 36: Singlet-A 4.0257 eV 307.98 nm f=0.0246 <S**2>=0.000

239 -> 245 -0.10123

243 -> 247 0.62035

244 -> 247 -0.23817

Excited State 37: Singlet-A 4.0443 eV 306.56 nm f=0.0081 <S**2>=0.000

232 -> 245 -0.10282

233 -> 245 -0.11409

234 -> 245 -0.16011

236 -> 245 -0.17272

238 -> 245 -0.11507

239 -> 245 -0.26818

243 -> 246 0.11079

243 -> 247 -0.18728

243 -> 249 -0.12464

243 -> 251 0.13729

244 -> 249 -0.19309

244 -> 250 -0.16286

244 -> 251 0.31403

244 -> 252 0.17538

Excited State 38: Singlet-A 4.0939 eV 302.85 nm f=0.1064 <S**2>=0.000

232 -> 245 -0.16659

234 -> 245 -0.23666

236 -> 245 0.23477

238 -> 245 0.12970

239 -> 245 0.12878

243 -> 248 0.44158

244 -> 248 -0.18904

244 -> 249 0.14910

244 -> 250 0.10607

244 -> 251 0.16096

Excited State 39: Singlet-A 4.1281 eV 300.34 nm f=0.0651 <S**2>=0.000

232 -> 245 0.10675

234 -> 245 0.33969

236 -> 245 -0.13576

243 -> 248 0.43413

244 -> 249 -0.27378

244 -> 250 -0.15511

244 -> 251 -0.11793

Excited State 40: Singlet-A 4.1635 eV 297.79 nm f=0.0389 <S**2>=0.000

232 -> 245 0.15333

234 -> 245 0.36749

237 -> 245 -0.11221

238 -> 245 0.12913

243 -> 251 0.10278

244 -> 249 0.18483

244 -> 250 0.11990

244 -> 251 0.42038

- **Excitation energies and oscillator strengths of M2 (B3LYP functional with 6-31G(d.p) basis set of Gaussian 16 software package).**

Excited State 1: Triplet-A 1.1659 eV 1063.44 nm f=0.0000 <S**2>=2.000

281 -> 284 0.43501

283 -> 284 0.55763

281 <- 284 0.10606

283 <- 284 0.10803

Excited State 2: Triplet-A 2.1980 eV 564.07 nm f=0.0000 <S**2>=2.000

282 -> 284 0.65891

283 -> 285 -0.17747

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-KS) = -3380.00014858

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 3: Singlet-A 2.1984 eV 563.97 nm f=1.2604 <S**2>=0.000

283 -> 284 0.69900

Excited State 4: Triplet-A 2.2381 eV 553.96 nm f=0.0000 <S**2>=2.000

281 -> 284 0.52168

282 -> 285 0.13252

283 -> 284 -0.41494

283 -> 286 -0.10095

Excited State 5: Singlet-A 2.3838 eV 520.12 nm f=0.0014 <S**2>=0.000

282 -> 284 0.70495

Excited State 6: Singlet-A 2.6255 eV 472.24 nm f=0.1578 <S**2>=0.000

281 -> 284 0.69798

Excited State 7: Triplet-A 2.6981 eV 459.52 nm f=0.0000 <S**2>=2.000

275 -> 284 -0.10072

276 -> 284 -0.21630

278 -> 284 0.12503

281 -> 285 0.22450

281 -> 293 -0.13280

282 -> 284 0.20590

283 -> 285 0.49762

Excited State 8: Triplet-A 2.9559 eV 419.45 nm f=0.0000 <S**2>=2.000

277 -> 284 -0.15245

278 -> 285 -0.11488

281 -> 284 -0.17775

282 -> 285 0.40221

282 -> 293 0.13123

283 -> 284 0.13552

283 -> 286 -0.33427

283 -> 288 0.11561

Excited State 9: Triplet-A 2.9917 eV 414.43 nm f=0.0000 <S**2>=2.000

276 -> 284 0.47987

281 -> 285 -0.23403

282 -> 284 0.12037

282 -> 286 -0.23628

283 -> 285 0.21314

283 -> 293 0.16217

Excited State 10: Triplet-A 3.1330 eV 395.74 nm f=0.0000 <S**2>=2.000

273 -> 284 -0.15066

275 -> 284 -0.24244

276 -> 284 0.38181

278 -> 284 0.15418

281 -> 285 0.27994

282 -> 286 0.24220

283 -> 293 -0.14705

Excited State 11: Triplet-A 3.2072 eV 386.58 nm f=0.0000 <S**2>=2.000

265 -> 284 -0.12141

274 -> 284 0.26162

277 -> 284 0.31175

279 -> 284 -0.21196

280 -> 284 -0.12462

281 -> 286 0.20248

282 -> 285 0.16881

282 -> 287 0.14909

282 -> 289 0.11784

283 -> 298 0.10926

Excited State 12: Triplet-A 3.2274 eV 384.16 nm f=0.0000 <S**2>=2.000

273 -> 284 0.41921

275 -> 284 0.29559

276 -> 284 0.15410

278 -> 284 -0.10914

281 -> 285 0.13805

282 -> 286 0.11275

282 -> 289 0.10413

282 -> 290 0.13742

283 -> 287 -0.10902

283 -> 289 -0.13234

Excited State 13: Triplet-A 3.2435 eV 382.25 nm f=0.0000 <S**2>=2.000

277 -> 284 0.11644

278 -> 290 0.10023

281 -> 290 -0.23007

282 -> 289 -0.11614

282 -> 290 0.32939

282 -> 293 0.10606

283 -> 290 0.28917

Excited State 14: Triplet-A 3.2482 eV 381.71 nm f=0.0000 <S**2>=2.000

273 -> 284 -0.15771

275 -> 284 -0.12924

281 -> 285 -0.12716

281 -> 289 0.21723

282 -> 289 0.31018

282 -> 290 0.12205

283 -> 289 -0.24845

283 -> 293 0.11215

Excited State 15: Singlet-A 3.2601 eV 380.30 nm f=0.0003 <S**2>=0.000

276 -> 284 0.62331

283 -> 285 0.29726

Excited State 16: Triplet-A 3.3418 eV 371.01 nm f=0.0000 <S**2>=2.000

273 -> 284 0.23187

276 -> 284 -0.12587

278 -> 284 0.29029

279 -> 284 -0.22251

280 -> 284 0.34450

281 -> 285 -0.14913

282 -> 288 0.10840

283 -> 285 -0.18040

Excited State 17: Singlet-A 3.3555 eV 369.50 nm f=0.0019 <S**2>=0.000

273 -> 284 0.11281

275 -> 284 0.15187

276 -> 284 -0.29394

278 -> 284 -0.13677

280 -> 284 -0.14120

283 -> 285 0.55685

Excited State 18: Triplet-A 3.3850 eV 366.28 nm f=0.0000 <S**2>=2.000

280 -> 284 0.11714

281 -> 288 0.19410

282 -> 287 0.34128

282 -> 288 -0.22106

282 -> 290 0.12719

283 -> 286 -0.13056

283 -> 287 0.17505

283 -> 288 -0.33530

283 -> 290 0.11871

Excited State 19: Triplet-A 3.3908 eV 365.65 nm f=0.0000 <S**2>=2.000

279 -> 284 -0.11461

280 -> 284 0.10159

281 -> 287 -0.19552

281 -> 288 -0.10355

282 -> 286 -0.10967

282 -> 287 -0.23400

282 -> 288 -0.32098

282 -> 289 0.13168

283 -> 287 0.33272

283 -> 288 0.16387

283 -> 289 -0.13547

Excited State 20: Singlet-A 3.4319 eV 361.27 nm f=0.0012 <S**2>=0.000

269 -> 284 -0.10741

273 -> 284 0.46657

274 -> 284 -0.14000

275 -> 284 0.35461

276 -> 284 0.11368

278 -> 284 -0.11023

279 -> 284 0.11256

280 -> 284 -0.11341

283 -> 285 -0.22508

Excited State 21: Singlet-A 3.4693 eV 357.37 nm f=0.1762 <S**2>=0.000

277 -> 284 -0.11156

279 -> 284 0.39756

280 -> 284 0.54112

282 -> 285 0.14059

Excited State 22: Singlet-A 3.4890 eV 355.35 nm f=0.0353 <S**2>=0.000

273 -> 284 -0.16481

275 -> 284 -0.12139

279 -> 284 0.52607

280 -> 284 -0.38646

283 -> 285 -0.11452

Excited State 23: Triplet-A 3.5043 eV 353.81 nm f=0.0000 <S**2>=2.000

274 -> 284 0.13835

277 -> 284 0.16505

278 -> 284 -0.11745

279 -> 284 0.44118

280 -> 284 0.42913

Excited State 24: Triplet-A 3.5418 eV 350.06 nm f=0.0000 <S**2>=2.000

266 -> 284 -0.14767

270 -> 284 0.21199

273 -> 284 -0.13953

275 -> 284 0.10208

278 -> 284 -0.32936

279 -> 284 -0.31852

280 -> 284 0.34279

Excited State 25: Singlet-A 3.5469 eV 349.56 nm f=0.6860 <S**2>=0.000

277 -> 284 -0.12543

279 -> 284 -0.15747

282 -> 285 0.62904

283 -> 286 -0.14845

Excited State 26: Triplet-A 3.5535 eV 348.91 nm f=0.0000 <S**2>=2.000

266 -> 284 -0.30781

270 -> 284 0.38447

271 -> 284 -0.27956

273 -> 285 0.10438

277 -> 284 0.10792

278 -> 284 0.12993

279 -> 284 0.24596

Excited State 27: Singlet-A 3.6567 eV 339.06 nm f=0.0019 <S**2>=0.000

273 -> 284 -0.15552

278 -> 284 -0.43349

281 -> 285 0.46302

282 -> 286 0.14713

283 -> 285 -0.10635

Excited State 28: Triplet-A 3.6602 eV 338.74 nm f=0.0000 <S**2>=2.000

269 -> 284 0.57292

270 -> 285 0.12027

272 -> 284 -0.10636

283 -> 291 -0.10890

283 -> 292 -0.19079

Excited State 29: Triplet-A 3.6690 eV 337.93 nm f=0.0000 <S**2>=2.000

266 -> 284 -0.19515

277 -> 284 -0.12692

281 -> 286 0.12874

282 -> 285 0.36094

283 -> 286 0.37826

283 -> 288 -0.16490

283 -> 291 -0.11960

Excited State 30: Triplet-A 3.6850 eV 336.45 nm f=0.0000 <S**2>=2.000

266 -> 284 0.16538

270 -> 284 0.12249

275 -> 290 -0.11171

278 -> 290 -0.11017

280 -> 297 -0.18470

281 -> 293 0.11200

282 -> 285 0.15703

282 -> 293 -0.13617

282 -> 298 -0.10808

282 -> 299 -0.10527

283 -> 285 0.10658

283 -> 291 0.14338

Excited State 31: Singlet-A 3.6912 eV 335.90 nm f=0.0429 <S**2>=0.000

274 -> 284 0.12608

277 -> 284 0.61925

279 -> 284 0.10477

282 -> 285 0.13811

283 -> 286 -0.18376

Excited State 32: Singlet-A 3.7536 eV 330.31 nm f=0.0382 <S**2>=0.000

281 -> 288 0.14472

282 -> 285 -0.13680

282 -> 287 0.37520

282 -> 288 -0.10752

283 -> 286 -0.34818

283 -> 288 -0.36826

Excited State 33: Singlet-A 3.7617 eV 329.60 nm f=0.0074 <S**2>=0.000

278 -> 284 -0.16368

281 -> 287 -0.17420

282 -> 286 -0.21403

282 -> 287 -0.12806

282 -> 288 -0.33029

283 -> 287 0.47904

Excited State 34: Singlet-A 3.7869 eV 327.40 nm f=0.0022 <S**2>=0.000

278 -> 284 0.47837

281 -> 285 0.47089

Excited State 35: Singlet-A 3.8064 eV 325.73 nm f=0.0139 <S**2>=0.000

266 -> 284 0.45955

270 -> 284 -0.36292

271 -> 284 0.23165

274 -> 284 0.11117

277 -> 284 -0.13754

Excited State 36: Singlet-A 3.8896 eV 318.76 nm f=0.3687 <S**2>=0.000

266 -> 284 0.13229

277 -> 284 0.12497

282 -> 285 0.13627

282 -> 287 0.14203

283 -> 286 0.51526

283 -> 288 -0.34869

Excited State 37: Singlet-A 3.9719 eV 312.15 nm f=0.0058 <S**2>=0.000

269 -> 284 0.48880

272 -> 284 -0.11144

283 -> 289 0.10541

283 -> 291 0.21035

283 -> 292 0.32594

Excited State 38: Singlet-A 3.9864 eV 311.02 nm f=0.0118 <S**2>=0.000

266 -> 284 0.36210

270 -> 284 0.24891

271 -> 284 -0.21679

281 -> 291 -0.10337

283 -> 291 -0.35142

283 -> 292 0.19440

Excited State 39: Singlet-A 4.0176 eV 308.60 nm f=0.1202 <S**2>=0.000

266 -> 284 -0.12207

274 -> 284 0.57700

275 -> 284 0.19273

277 -> 284 -0.13131

281 -> 286 -0.10386

282 -> 289 -0.10718

283 -> 290 0.12910

Excited State 40: Singlet-A 4.0294 eV 307.70 nm f=0.0241 <S**2>=0.000

273 -> 284 -0.21324

275 -> 284 0.27585

281 -> 285 -0.14770

281 -> 289 0.10202

282 -> 286 0.37083

282 -> 288 -0.18496

282 -> 289 0.14015

282 -> 290 0.14515

283 -> 289 -0.26466