Electronic Supplementary Information

Highly efficient light-converting films based on diketopyrrolopyrrole with deep-red aggregation-induced emission for enhancing lipid productivity of *Chlorella* sp.

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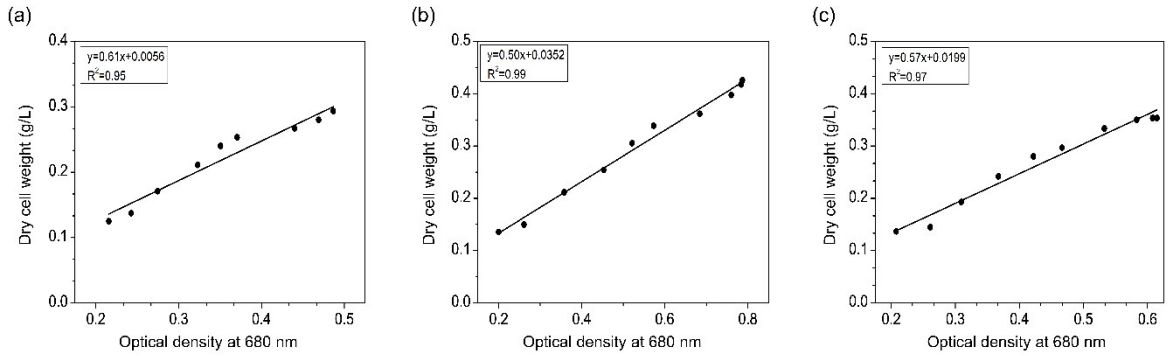


Fig S1. Relationship between optical density and dry cell weight in different culture conditions.

Synthesis and characterization.

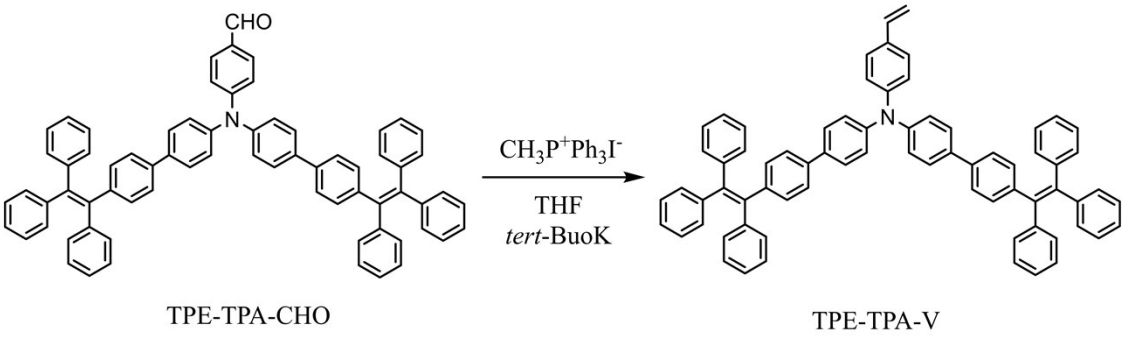
A series of diketopyrrolopyrrole (DPP) compounds and triphenylamine (TPA) derivatives (MTPA-BO, TPE-TPA-CHO, TPE-TPA-V) were synthesized efficiently according to literature procedures. All other reagents were purchased from commercial suppliers and used as received without further purification. Synthesized 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.

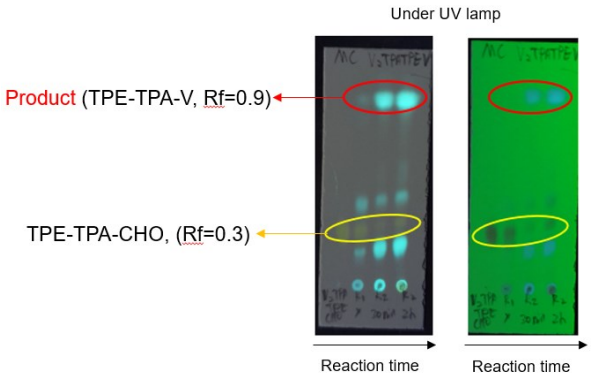
*3-(4'-(bis(4-methoxyphenyl)amino)-[1,1'-biphenyl]-4-yl)-6-(4-bromophenyl)-2,5-dihexyl-2,5-dihydropyrrolo[3,4-c]pyrrole-1,4-dione (**M2**).*

A mixture of $Pd(PPh_3)_4$ (100 mg, 0.091 mmol), D6C (0.28 g, 0.46 mmol), and MTPA-BO (480 mg, 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 brine 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:methanol (400:1, *v/v*) as the eluent to produce dark red crystals of isolated **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.

*4'-(1,2,2-triphenylvinyl)-N-(4'-(1,2,2-triphenylvinyl)-[1,1'-biphenyl]-4-yl)-N-(4-vinylphenyl)-[1,1'-biphenyl]-4-amine (**TPE-TPA-V**).*



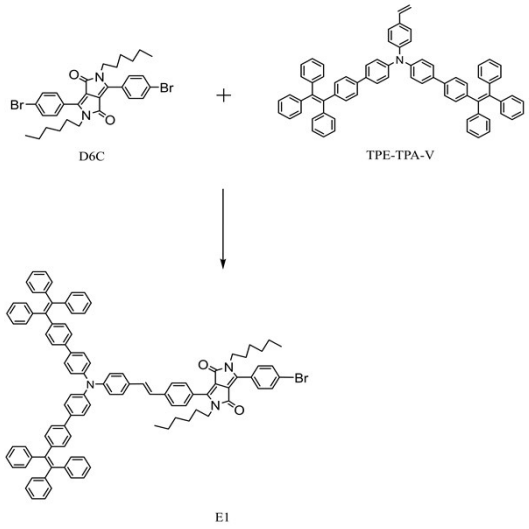
TPE-TPA-CHO TPE-TPA-V



A mixture of methyltriphenylphosphonium iodide (3.63g, 9 mmol), and the TPE-TPA-CHO (5.4g, 6.0 mmol) were solved in anhydrous THF (40 mL). Then the mixtures were stirred under nitrogen atmosphere at 40°C. After 30 min, potassium *tert*-butyloxide (1.05g, 9 mmol) was added and the mixture was stirred for another 4 h. The mixture was extracted with dichloromethane and washed several times with brine. The combined organic layer

was dried over anhydrous $MgSO_4$ and concentrated using a rotary evaporator. The crude product was purified by column chromatography using *n*-hexane:CH_2Cl_2 (3:1, *v/v*) as the eluent to produce yellow flake (Rf=0.9) of isolated **TPE-TPA-V** (3.7 g, 69% yield). ^{1}H NMR (500 MHz, CD_2Cl_2), δ (ppm): 7.37-7.39 (d, *J* = 9 Hz, 3H), 7.27 (d, *J* = 8.5 Hz, 4H), 7.23 (d, *J* = 9 Hz, 2H),7.07-6.88 (m, 41H), 6.60 (dd, *J* = 11, 6.5 Hz, 1H), 5.56 (d, *J* = 17.5 Hz, 1H), 5.09 (d, *J* = 11 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$), δ (ppm): 147.62, 147.23, 144.40, 144.34, 143.01, 141.65, 141.17, 138.74, 136.70, 135.44, 132.93, 132.24, 131.82, 131.75, 128.28, 128.21, 128.16, 128.03, 127.65, 127.02, 126.98, 126.92, 126.14, 124.89, 124.57, 112.72. MALDI-TOF MS: *m/z* calcd for $C_{72}H_{53}N$ (100%, [M^+]), 931.42; found 931.7560.

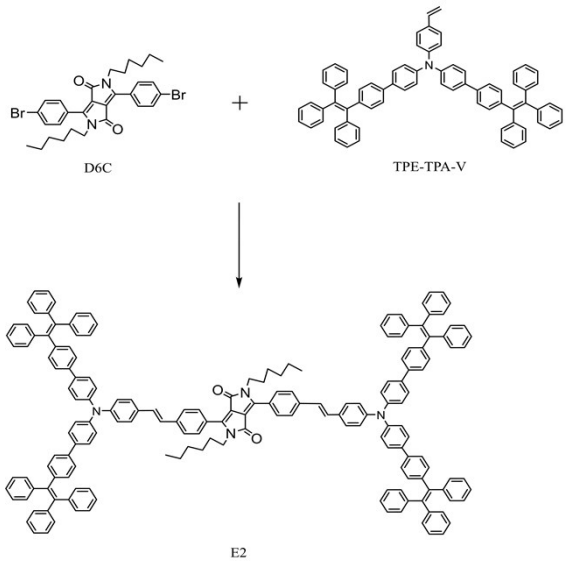
*(E)-3-(4-(4-(bis(4'-(1,2,2-triphenylvinyl)-[1,1'-biphenyl]-4-yl)amino)styryl)phenyl)-6-(4-bromophenyl)-2,5-dihexyl-2,5-dihydropyrrolo[3,4-c]pyrrole-1,4-dione (**E1**).*



A mixture of D6C (0.75 g, 1.23 mmol), TPE-TPA-V (1.15g, 1.23 mmol), $Pd(OAc)_2$ (111.5mg, 0.5 mmol) tetrabutylammonium bromide (275mg, 0.85mmol) were dissolved in 20mL anhydrous DMF under N_2 atmosphere and stirred at 100 °C. Then, K_2CO_3 (0.2g ,2mmol) was added to the reaction mixture and stirred for 12h at 100 °C. The mixture was extracted with ethyl acetate and washed several times with brine. The combined organic layer was dried over anhydrous $MgSO_4$ and concentrated using a rotary evaporator. The crude product was purified by column chromatography using *n*-hexane:CH_2Cl_2 (1:3, *v/v*) as the eluent to produce dark red flake (Rf=0.8) of isolated **E1** (0.45 g, 25% yield). ^{1}H NMR (500 MHz, CD_2Cl_2), δ (ppm): 7.75-7.76 (d, *J* = 8.5 Hz, 2H), 7.57-7.63 (m, 6H), 7.38-7.42 (t, *J* = 10 Hz, 6H), 7.27-7.29 (d, *J* = 8.5 Hz, 4H), 7.17 (s, 1H) 7.14 (s, 1H), 6.95-7.07

(m, 40H), 3.68 (t, *J* = 7.5 Hz, 2H), 3.64 (t, *J* = 8 Hz, 2H), 1.47-1.51 (m, 4H), 1.12-1.19 (m, 12H), 0.74-0.76 (t, *J* = 7 Hz, 6H). ^{13}C NMR (125 MHz, CD_2Cl_2), δ (ppm): 163.09, 162.80, 148.97, 148.07, 147.03, 146.75, 144.39, 144.34, 143.10, 141.69, 141.15, 138.70, 135.81, 132.62, 132.27, 131.82, 131.75, 130.90, 130.76, 129.75, 128.32, 128.30, 128.22, 128.17, 128.12, 127.98, 127.34, 127.00, 126.94, 126.40, 126.18, 125.72, 125.25, 124.15, 110.83, 110.21, 42.45, 42.20, 31.78, 29.89, 26.89, 26.85, 23.03, 14.28. MALDI-TOF MS: *m/z* calcd for $C_{102}H_{86}BrN_3O_2$ (100%, [$(M+2H)^{2+}$]), 1465.59; found 1465.4246. Elemental analysis: calcd for $C_{102}H_{86}BrN_3O_2$: C, 83.58; H, 5.91; Br, 5.45; N, 2.87; O, 2.18. Found: C, 83.38; H, 5.94; N, 2.80; O, 2.29.

*3,6-bis(4-((E)-4-(bis(4'-(1,2,2-triphenylvinyl)-[1,1'-biphenyl]-4-yl)amino)styryl)phenyl)-2,5-dihexyl-2,5-dihydropyrrolo[3,4-c]pyrrole-1,4-dione (**E2**).*



A mixture of D6C (0.38 g, 0.62 mmol), TPE-TPA-V (1.15g, 1.23 mmol), $Pd(OAc)_2$ (111.5mg, 0.5 mmol) tetrabutylammonium bromide (275mg, 0.85mmol) were dissolved in 20mL anhydrous DMF under N_2 atmosphere and stirred at 100 °C. Then, K_2CO_3 (0.2g ,2mmol) was added to the reaction mixture and stirred for 24h at 100 °C. The mixture was extracted with ethyl acetate and washed several times with brine. The combined organic layer was dried over anhydrous $MgSO_4$ and concentrated using a rotary evaporator. The crude product was purified by column chromatography using *n*-hexane:CH_2Cl_2 (1:3, *v/v*) as the eluent to produce dark red flake (Rf=0.8) of isolated **E2** (0.63 g, 44% yield). ^{1}H NMR (500 MHz, CD_2Cl_2), δ (ppm): 7.76 (d, *J* = 8 Hz, 4H), 7.57

(d, J = 8 Hz, 4H), 7.38-7.42 (t, J = 8.5 Hz, 12H), 7.27-7.29 (d, J = 8.5 Hz, 8H), 7.23 (s, 2H) 7.22 (s, 2H), 6.65-7.08 (m, 80H), 3.70 (t, J = 7 Hz, 4H), 1.50-1.53 (m, 4H), 1.15-1.18 (m, 12H), 0.74-0.77 (t, J = 7 Hz, 6H). . ^{13}C NMR (125 MHz, CD_2Cl_2), δ (ppm): 163.12, 148.08, 148.04, 147.04, 144.39, 144.34, 143.10, 141.68, 141.15, 140.91, 138.70, 135.78, 132.27, 131.82, 131.75, 130.76, 129.74, 128.30, 128.22, 128.17, 128.12, 127.53, 127.15, 127.02, 126.99, 126.94, 126.48, 126.18, 125.23, 124.19, 110.47, 42.44, 31.82, 29.92, 26.92, 23.05, 14.30. MALDI-TOF MS: *m/z* calcd for $C_{174}H_{140}N_4O_2$ (100%, $[(M+2H)^{2+}]$), 2317.08; found 2317.0234. Elemental analysis: calcd for $C_{174}H_{138}N_4O_2$: C, 90.20; H, 6.00; N, 2.42; O, 1.38. Found: C, 89.94; H, 6.05; N, 2.41; O, 1.50.

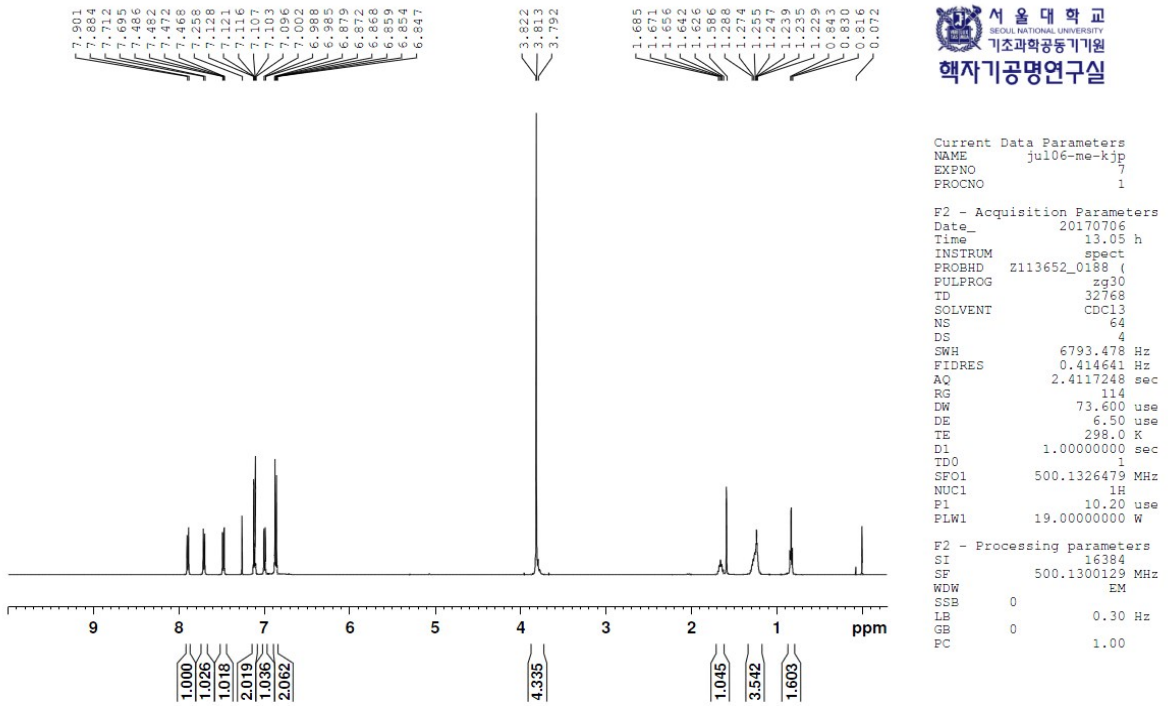


Figure S2 ^{1}H NMR spectrum of M2 in $CDCl_3$.

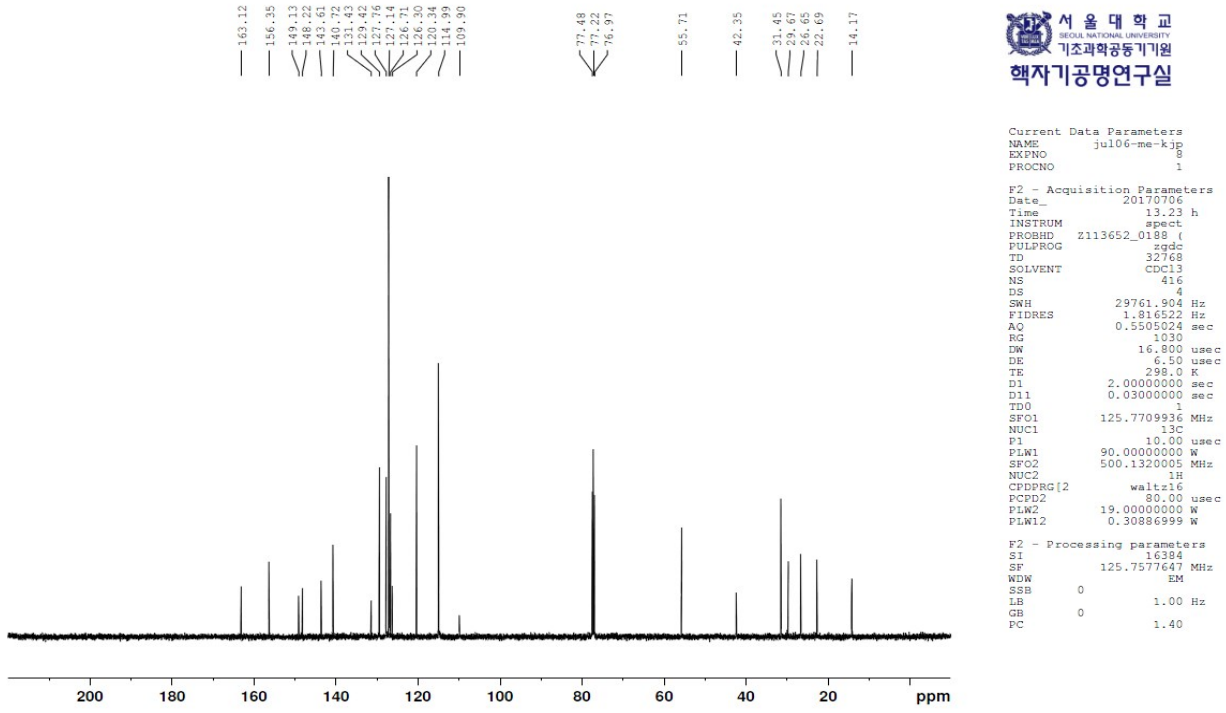


Figure S3 ^{13}C NMR spectrum of M2 in $CDCl_3$.

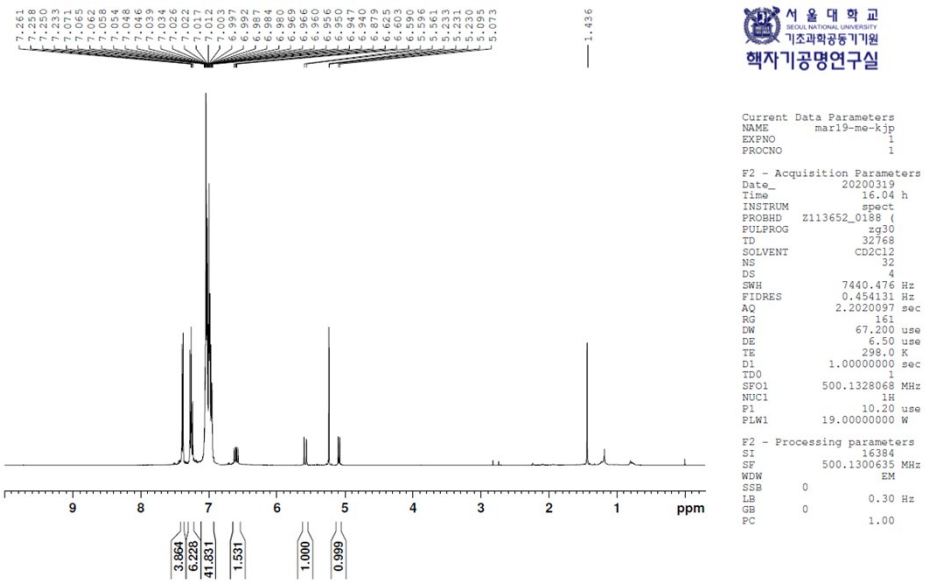


Figure S4 ^{1}H NMR spectrum of TPE-TPA-V in CD_2Cl_2.

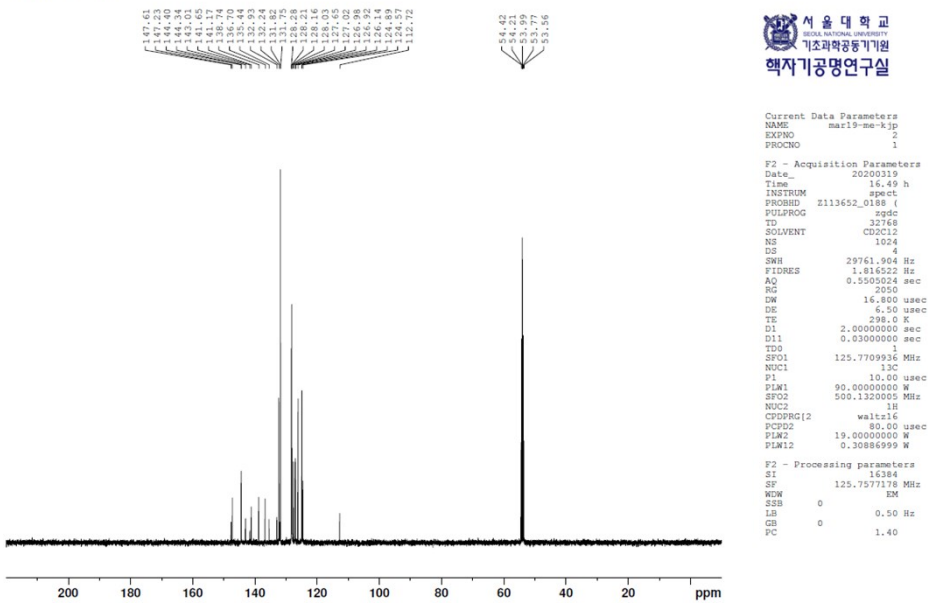


Figure S5 ^{13}C NMR spectrum of TPE-TPA-V in CD_2Cl_2.

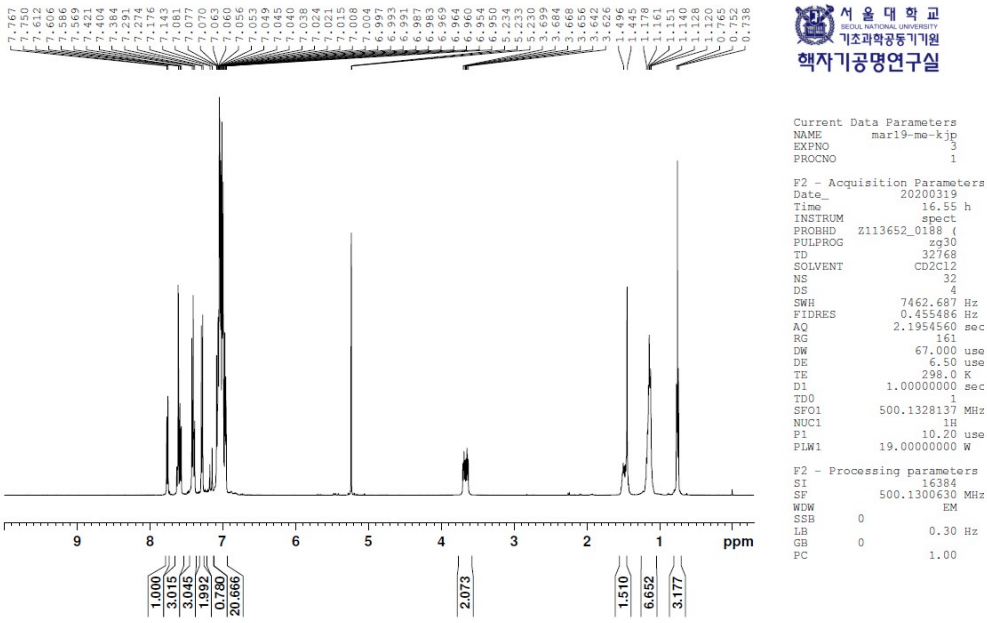


Figure S6 ^{1}H NMR spectrum of E1 in CD_2Cl_2.

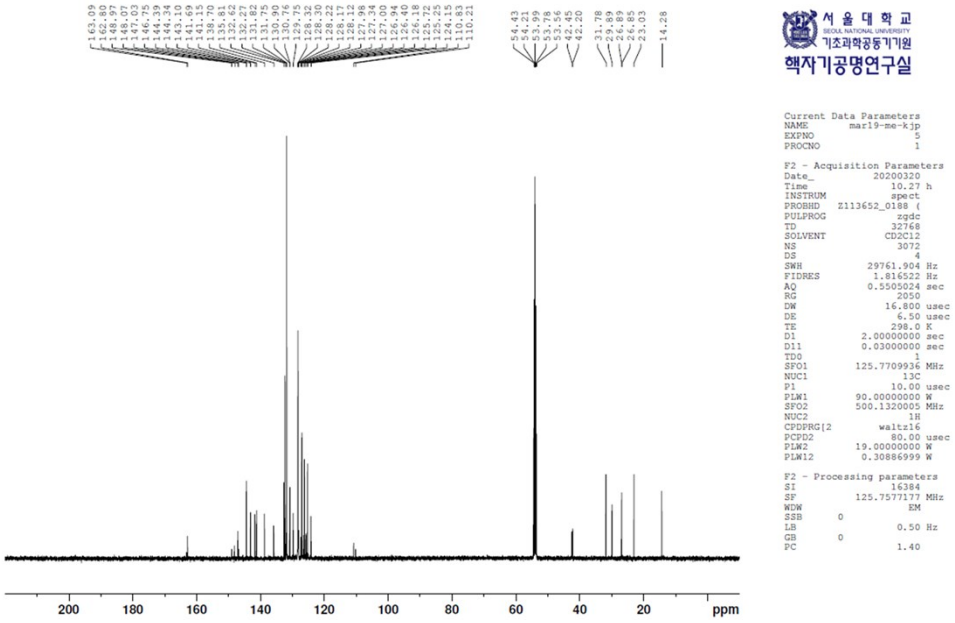


Figure S7 ^{13}C NMR spectrum of E1 in CD_2Cl_2.

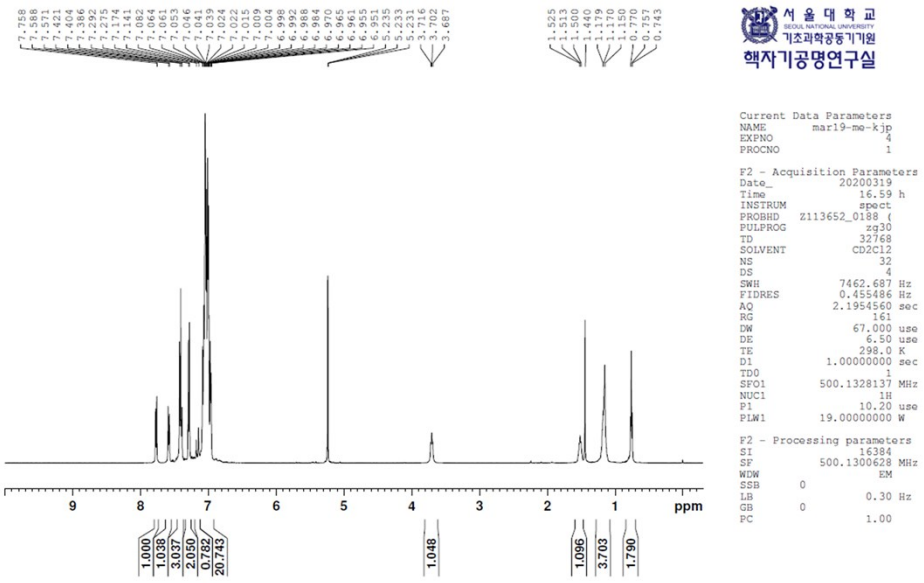


Figure S8 ^{1}H NMR spectrum of E2 in CD_2Cl_2.

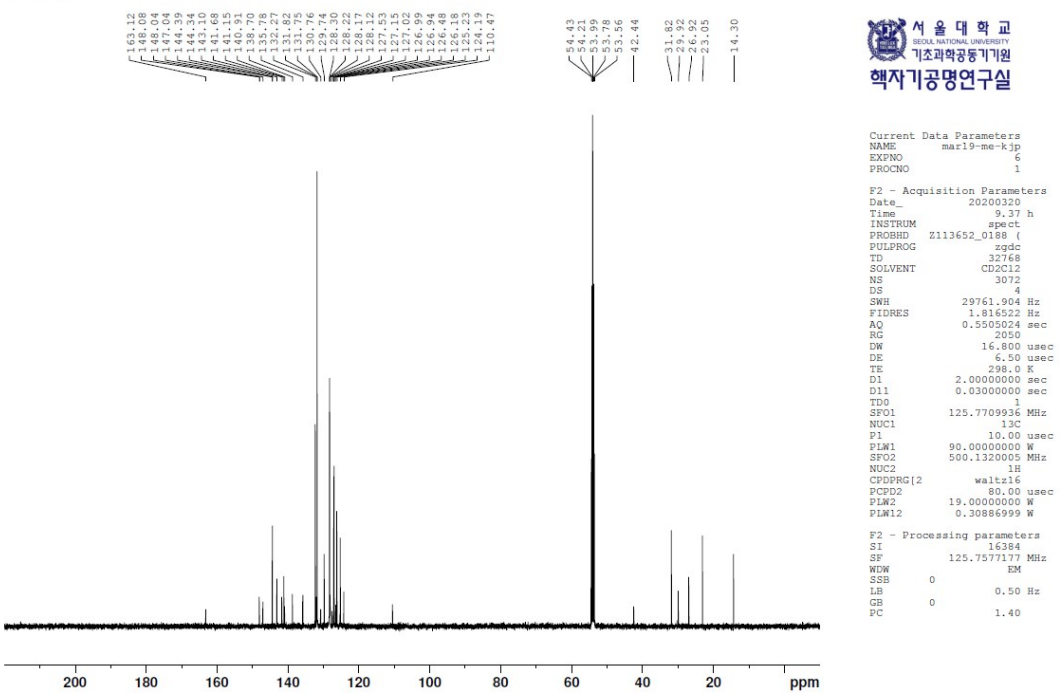


Figure S9 ^{13}C NMR spectrum of E2 in CD_2Cl_2.

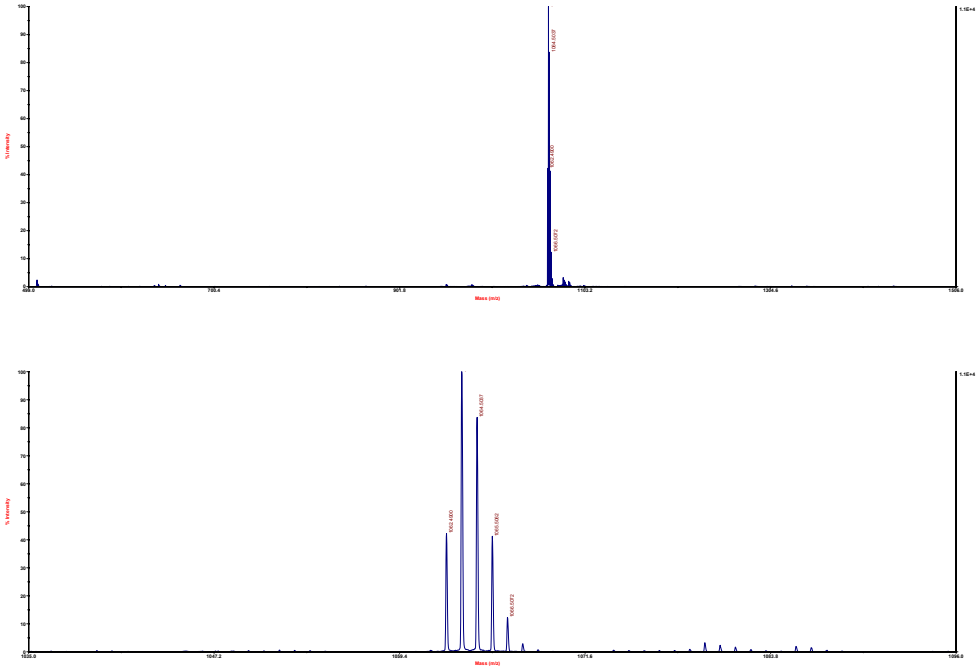


Figure S10. MALDI-TOF mass spectrum of M2.

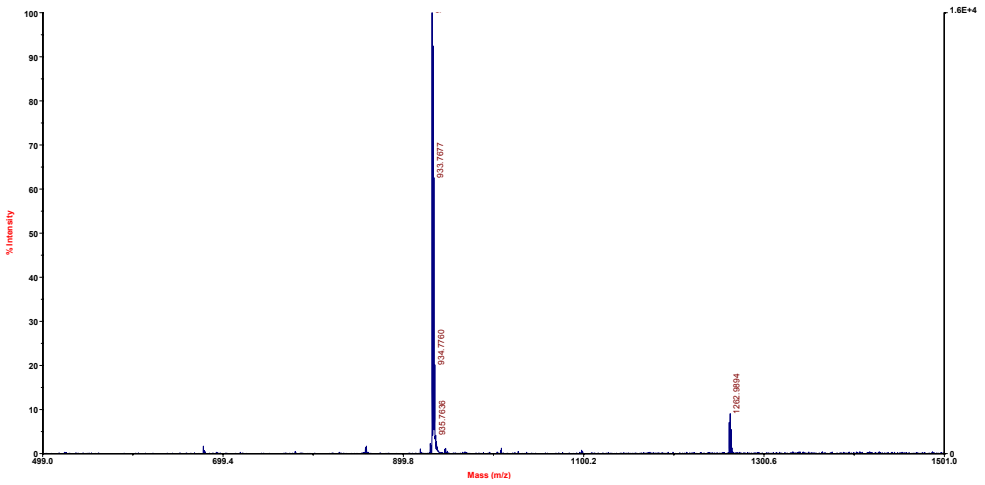
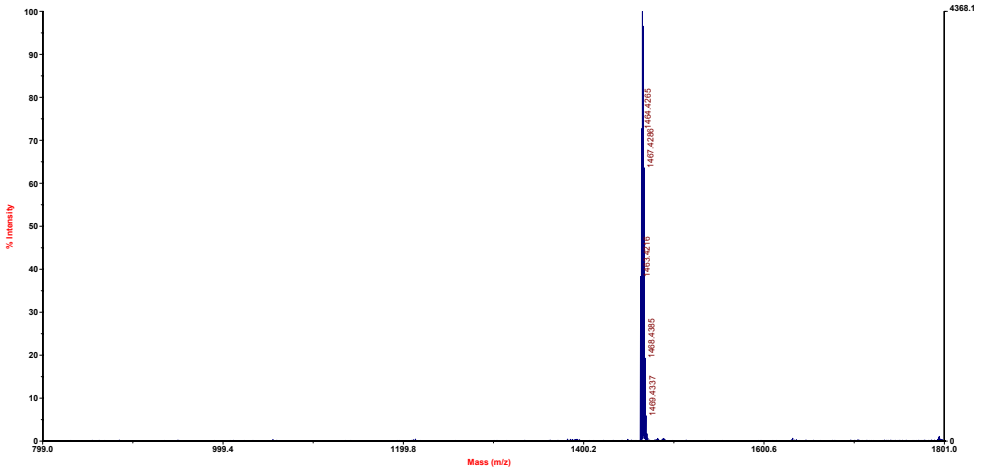


Figure S11. MALDI-TOF mass spectrum of TPE-TPA-V.



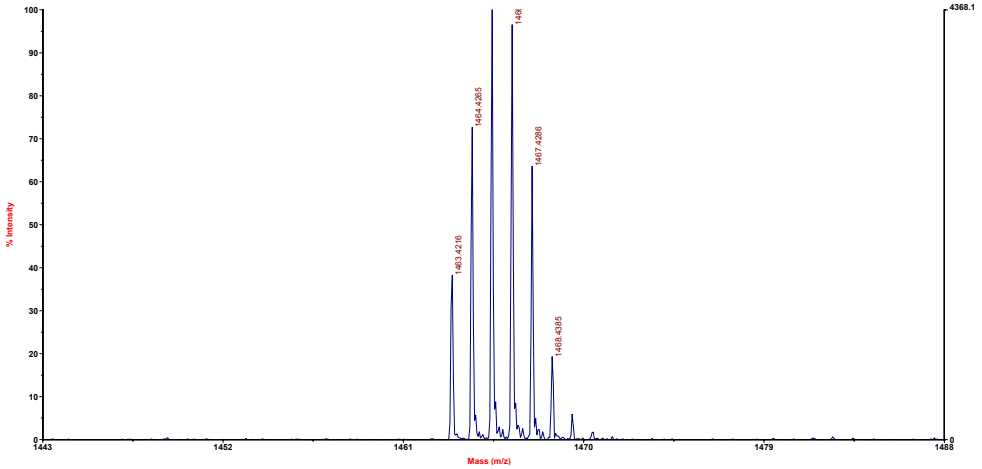
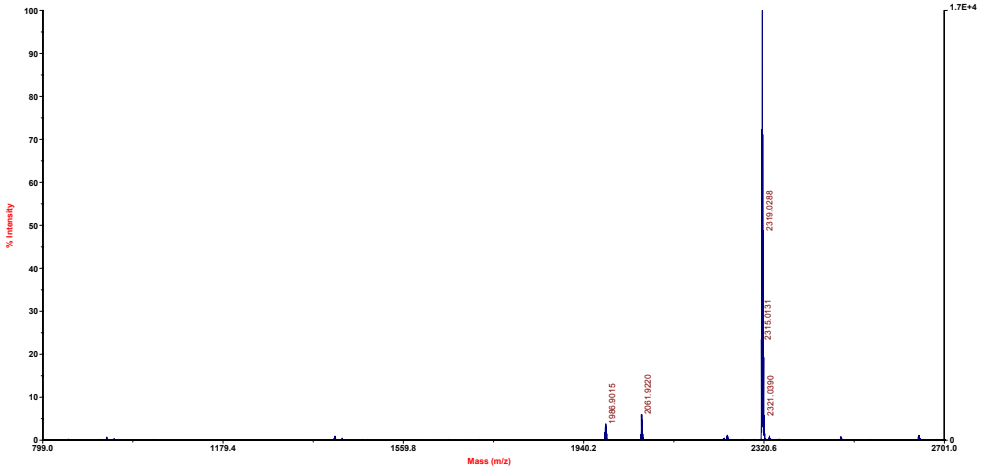


Figure S12. MALDI-TOF mass spectrum of E1.



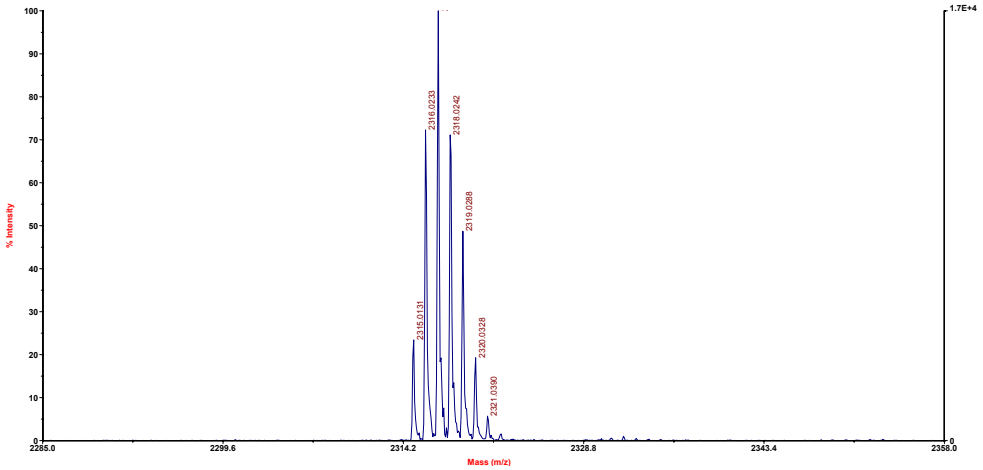


Figure S13. MALDI-TOF mass spectrum of E2.

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Operator ID: SNU-EA2000
Company name: Thermo Fisher

(Unit: wt%)

Sample name	Nitrogen	Carbon	Hydrogen	Sulphur	Oxygen
M2	5.2562	79.0506	6.7356	n.d.	8.9788

* n.d. : not detected

Figure S14. Elemental analysis of M2.

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* n.d. : not detected

Operator ID: SNU-EA2000
Company name: Thermo Fisher

(Unit: wt%)

Sample name	Nitrogen	Carbon	Hydrogen	Oxygen
E1	2.8075	83.3826	5.9446	2.2941

* n.d. : not detected

Figure S15. Elemental analysis of E1.

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Operator ID: SNU-EA2000
Company name: Thermo Fisher

(Unit: wt%)

Sample name	Nitrogen	Carbon	Hydrogen	Oxygen
E2	2.4065	89.9376	6.0526	1.4972

* n.d. : not detected

Figure S16. Elemental analysis of E2.

TDDFT Calculation results of M2, E1, and E2.

- **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

- **Excitation energies and oscillator strengths of E1 (B3LYP functional with 6-31G(d.p) basis set of Gaussian 16 software package).**

Excited State 1: Singlet-A 2.0933 eV 592.29 nm f=1.1528 <S**2>=0.000

385 -> 386 0.70194

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

Total Energy, E(TD-HF/TD-DFT) = -6825.17383461

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

Excited State 2: Singlet-A 2.4485 eV 506.38 nm f=0.4001 <S**2>=0.000

384 -> 386 0.69770

385 -> 387 -0.10097

Excited State 3: Singlet-A 2.6870 eV 461.42 nm f=0.0063 <S**2>=0.000

383 -> 386 0.70466

Excited State 4: Singlet-A 2.7741 eV 446.94 nm f=0.0217 <S**2>=0.000

382 -> 386 0.69102

Excited State 5: Singlet-A 2.9762 eV 416.58 nm f=0.5478 <S**2>=0.000

385 -> 387 0.67548

Excited State 6: Singlet-A 3.0166 eV 411.01 nm f=0.7490 <S**2>=0.000

384 -> 388 0.17361

385 -> 388 0.66596

385 -> 390 -0.10284

Excited State 7: Singlet-A 3.1693 eV 391.21 nm f=0.1287 <S**2>=0.000

378 -> 386 0.39439

381 -> 386 0.34908

384 -> 387 -0.35367

385 -> 389 0.23926

Excited State 8: Singlet-A 3.2180 eV 385.28 nm f=0.0460 <S**2>=0.000

378 -> 386 0.55187

381 -> 386 -0.33856

384 -> 387 0.15978

385 -> 389 -0.17649

Excited State 9: Singlet-A 3.2642 eV 379.83 nm f=0.0646 <S**2>=0.000

381 -> 386 -0.15678

384 -> 387 0.24982

384 -> 389 0.12107

385 -> 389 0.62012

Excited State 10: Singlet-A 3.3735 eV 367.53 nm f=0.0205 <S**2>=0.000

368 -> 386 -0.12529

370 -> 386 0.28073

371 -> 386 -0.10338

372 -> 386 0.43712

381 -> 386 -0.20198

384 -> 387 -0.32551

- **Excitation energies and oscillator strengths of E2 (B3LYP functional with 6-31G(d.p) basis set of Gaussian 16 software package).**

Excited State 1: Singlet-A 2.0109 eV 616.56 nm f=2.3473 <S**2>=0.000

613 -> 614 0.69794

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

Total Energy, E(TD-HF/TD-DFT) = -7083.29410517

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

Excited State 2: Singlet-A 2.2293 eV 556.15 nm f=0.0001 <S**2>=0.000

612 -> 614 0.70155

Excited State 3: Singlet-A 2.4469 eV 506.71 nm f=0.1595 <S**2>=0.000

611 -> 614 0.69792

Excited State 4: Singlet-A 2.7630 eV 448.73 nm f=0.0069 <S**2>=0.000

610 -> 614 0.70576

Excited State 5: Singlet-A 2.7651 eV 448.39 nm f=0.0054 <S**2>=0.000

609 -> 614 0.70283

Excited State 6: Singlet-A 2.7838 eV 445.37 nm f=0.0010 <S**2>=0.000

606 -> 614 0.10317

608 -> 614 -0.40097

613 -> 615 0.54616

Excited State 7: Singlet-A 2.8445 eV 435.88 nm f=0.0990 <S**2>=0.000

607 -> 614 0.63462

608 -> 614 -0.22410

613 -> 615 -0.15416

Excited State 8: Singlet-A 2.8474 eV 435.44 nm f=0.0156 <S**2>=0.000

607 -> 614 0.27206

608 -> 614 0.51933

613 -> 615 0.36521

Excited State 9: Singlet-A 2.9749 eV 416.77 nm f=0.8372 <S**2>=0.000

612 -> 615 0.48816

612 -> 617 -0.23114

613 -> 616 -0.10642

613 -> 617 -0.35411

613 -> 618 0.14588

Excited State 10: Singlet-A 2.9765 eV 416.54 nm f=0.6273 <S**2>=0.000

611 -> 616 -0.14505

612 -> 616 -0.37179

613 -> 616 0.55187

Experimental details of harvest, extraction, and FAME analysis.

In order to prepare dry biomass for FAME analysis, microalgal samples were centrifuged at 4,000 rpm for 20 min

and washed once with deionized water. These cells were then re-centrifuged under the same conditions and freeze-dried at −70 ℃ for 96 h.

Afterwards, lipid extraction from the dry biomass and subsequent FAME analysis were conducted at the National Instrumentation Center for Environmental Management (NICEM) in Seoul National University (SNU) following the previous literatures.[29] Agilent 7890A gas chromatography (GC) with flame ionization detector (FID) and Agilent DB-23 column (60 mm × 0.25 mm × 0.25 μm) were used for the analysis. Besides, FAME contents and its compositions were determined by using Supelco 37 Componet FAME Mix as a standard and pentadecanoic acid (Sigma-aldrich) as an internal standard. Following are the details of the GC instrumentation and methods; column injector temperature:250 ℃ and FID detector temperature:280 ℃ with H_2 (35 mL/min), Air (350 mL/min), and He (35 mL/min); GC oven program: 50 ℃ (1 min hold), 25 ℃/min to 130 ℃ (0 min hold), 8 ℃/min to 170 ℃ (0 min hold), 1.5 ℃/min to 215 ℃ (0 min hold), and 5 ℃/min to 250 ℃ (5 min hold); injection: 1 μL (spilt ratio of 1:10).