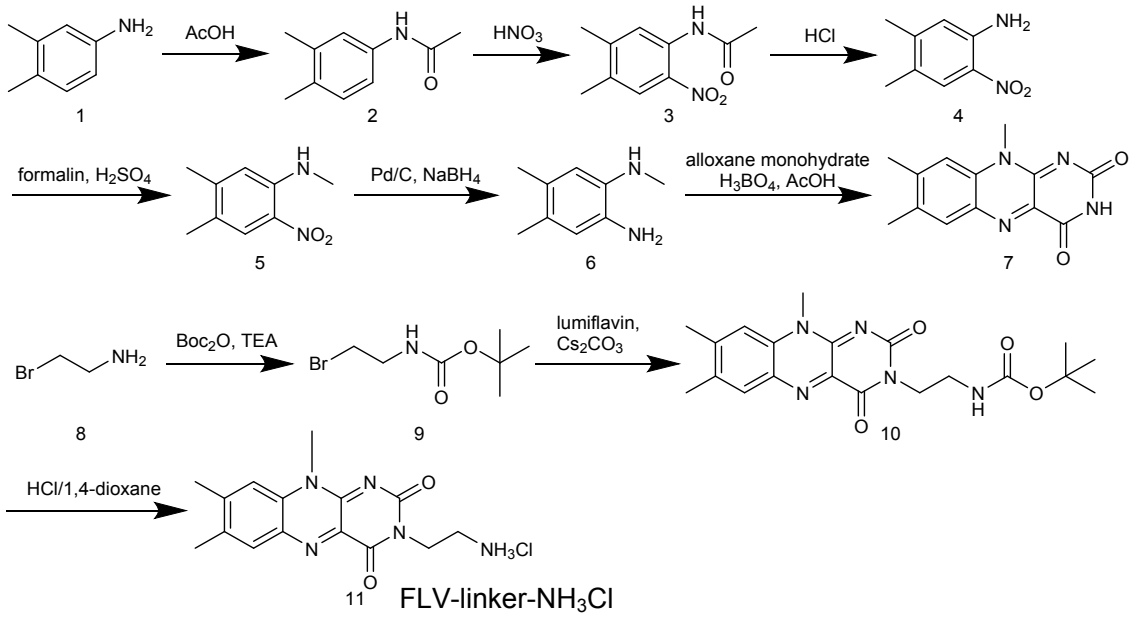
Supporting Information for

Chiral and random arrangements of flavin chromophores along cyclic peptide nanotubes on gold influencing differently on surface potential and piezoelectricity

Yusuke Kamano, Yuki Tabata, Hirotaka Uji, and Shunsaku Kimura

Department of Material Chemistry, Graduate School of Engineering, Kyoto University, Kyoto-Daigaku Katsura, Nishikyo-ku, Kyoto 615-8510, Japan

1. Synthesis section



Scheme 1. Synthetic schemes for FLV-linker-NH_3Cl. Compound 2, 3, and 4 were synthesized according to ref S1, compound 5, 6, and 7 were according to ref S2, compound 9 was according to ref S3, and compound 10 was according to ref S4 and S5.

***N*-(3,4-dimethylphenylene)acetamide (2)**

3,4-dimetylaniline (1) (11.284 g, 93.11 mmol) was dissolved in AcOH (27 mL) and refluxed and stirred under Ar for 3 h. The mixture was cooled to room temperature and poured into cold water. The mixture was centrifuged and the precipitate was washed with water. The residue was recrystallized from hot MeOH/water (1/6 = v/v) to afford *N*-(3,4-dimethylphenylene)acetamide (2) (11.673 g, 71.51 mmol, yield 77 %).

^{1}H-NMR (400 MHz, $CDCl_3$):δ (ppm) 2.15 (s, 3H, COCH_3), 2.21, 2.24 (s, 6H, aromatic CH_3) 7.05–7.07, 7.18–7.21, 7.27 (d, d, s, 3H, aromatic), 7.10 (br, 1H, amide)

***N*-(2-nitro-4,5-dimethylphenyl)acetamide (3)**

N-(3,4-dimethylphenylene)acetamide (2) (11.673 g, 71.52 mmol) was dissolved in AcOH (50 mL). HNO_3 (4 mL) was dropwised to the solution while stirred intensively. Then, H_2SO_4 (3 mL) was dropwised to the solution and stirred at -10°C with ice/NaCl. The solution was stirred at room temperature for 24 h. The reaction mixture was poured into crashed ice and the precipitate was filtered off. This precipitate was washed with water to afford *N*-(2-nitro-4,5-dimethylphenyl)acetamide (3) (2.975 g, 14.29 mmol, yield 20 %).

^{1}H-NMR (400 MHz, $CDCl_3$):δ (ppm) 2.27, 2.34 (s, 6H, COCH_3, aromatic CH_3), 7.97, 8.53 (s, 2H, aromatic), 10.29 (s, 1H, amide).

2-nitro-4,5-dimethylanilime (4)

N-(2-nitro-4,5-dimethylphenyl)acetamide (3) (2.975 g, 14.29 mmol) was dissolved in MeOH (70 mL) and concd. HCl aq. (30 mL) was added to the solution. The mixture was stirred at 80°C for 2 h. Then, this mixture was cooled to room temperature and adjusted to pH 10 with sat. $NaHCO_3$ aq. Thereafter, the product was extracted with AcOEt and the solvent was removed under reduced pressure to afford 2-nitro-4,5-dimethylanilime (4) (2.297 g, 13.82 mmol, yield 97 %).

^{1}H-NMR (400 MHz, $CDCl_3$):δ (ppm) 2.18, 2.22 (s, 6H, aromatic C*H*$_3$), 5.90 (s, 2H, amine), 6.59, 7.87 (s, 2H, aromatic).

***N*,4,5-trimethyl-2-nitroaniline (5)**

2-nitro-4,5-dimethylanilime (4) (2.000 g, 12.04 mmol) was dissolved in H_2SO_4 (20 mL). Formalin (20 mL) was dropwised to the solution and stirred at room temperature for 3 h. Then, the reaction mixture was heated and stirred at 70°C for 3 h. The resulting mixture was poured into water and the solid was collected by filtration and dissolved in AcOEt. The solution was washed with sat. $NaHCO_3$ aq. three times and dried over $MgSO_4$. The solvent was removed under reduced pressure to afford *N*,4,5-trimethyl-2-nitroaniline (5) (1.539 g, 8.54 mmol, 71 %).

^{1}H-NMR (400 MHz, $CDCl_3$):δ (ppm) 2.18, 2.28 (s, 6H, aromatic C*H*$_3$), 3.00 (s, 3H, N*H*), 6.61, 7.93 (s, 2H, aromatic).

Lumiflavin (7)

N,4,5-trimethyl-2-nitroaniline (5) (4.003 g, 22.20 mmol) was dissolved in MeOH and then, Pd/C (4 %, 500 mg) and $NaBH_4$ (2.549 g, 67.38 mmol) was added to the mixture. The mixture was stirred at room temperature for 2 h under Ar atmosphere. The reaction mixture was filtered and the filtrate was evaporated. Obtained residue was used in the next step without further purification. Reduced product, alloxane monohydrate (10.682 g, 66.76 mmol) and H_3BO_4 (3.501 g, 45.00 mmol) in AcOH (300 mL) was stirred at room temperature for 18 h under Ar atmosphere. The formed precipitate was centrifuged and washed with AcOH, MeOH, diethyl ether in this order to afford lumiflavin (7) (2.364 g, 9.23 mmol, 42%).

^{1}H-NMR (400 MHz, TFA-*d*):δ (ppm) 2.51, 2.63 (s, 6H, aromatic C*H*$_3$), 4.17 (s, 3H, NC*H*$_3$), 7.75, 8.16 (s, 2H, aromatic).

tert-butyl (2-bromoethyl)carbamate (**9**)

Boc_2O (1.075 g, 4.84 mmol) was dissolved in CH_2Cl_2 (26 mL) and 2-bromoethylamine hydrobromide (8) (393 mg, 3.38 mmol) was added to the mixture at 0°C. Then, TEA (960 μL, 6.88

mmol) was dropwised at 0°C and stirred for 10 min. The reaction mixture was stirred at room temperature for 18 h. The mixture was washed with 4 % $KHSO_4$ three times, sat. $NaHCO_3$ aq. three times and brine. The organic layer was dried over Na_2SO_4 and the solvent was removed under reduced pressure to afford tert-butyl (2-bromoethyl)carbamate (9).

^{1}H-NMR (400 MHz, $CDCl_3$):δ (ppm) 1.45 (s, 9H, Boc), 3.44–3,47, 3.52–3.54 (m 4H, C*H*$_2$ C*H*$_2$), 4.93 (br, 1H, CH_2CH_2N*H*).

FLV-linker-Boc (10)

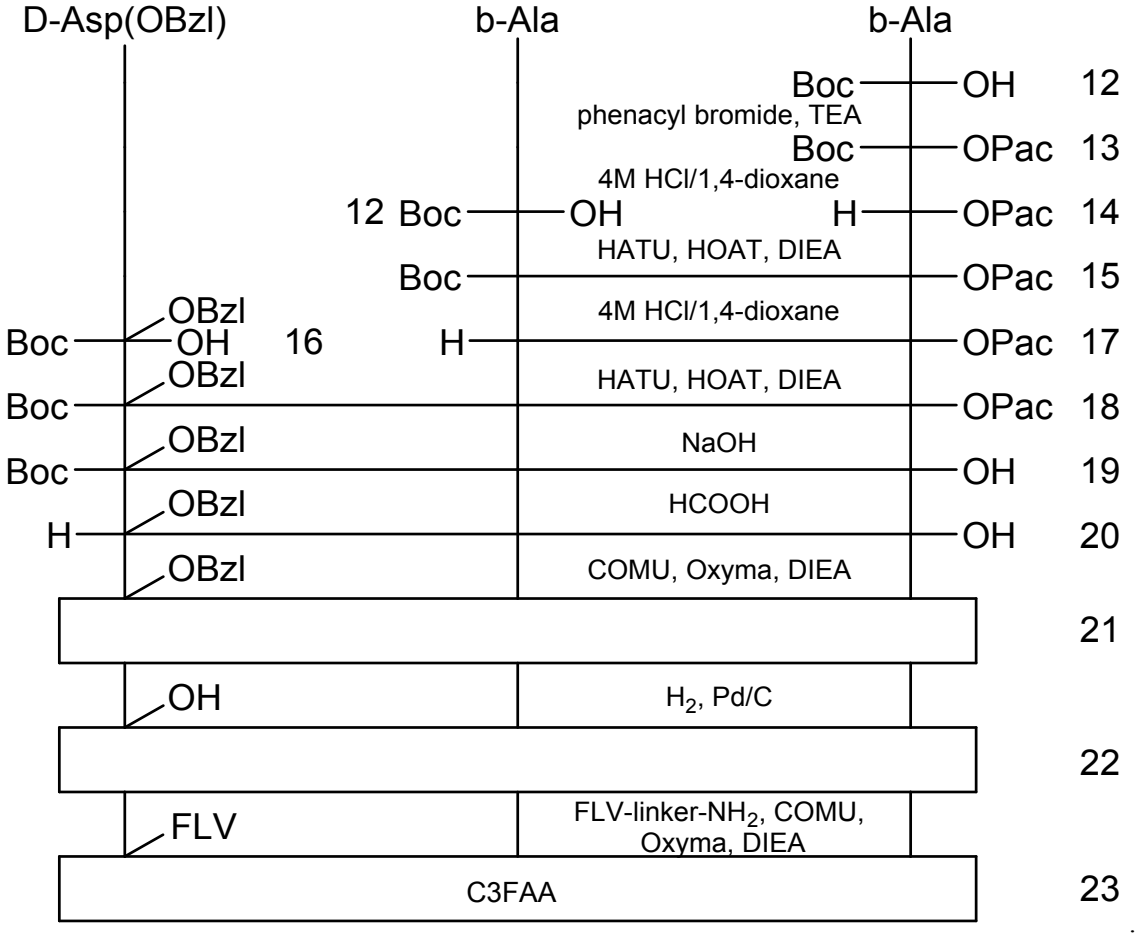
Lumiflavin (7) (806 mg, 3.15 mmol) and Cs_2CO_3 (1.522 g, 4.67 mmol) was suspended in dry DMF (50 mL). To the suspension, molecular sieves 20 Å was added. Thereafter, tert-butyl (2-bromoethyl)carbamate (9) (1050 mg, 4.68 mmol) in dry DMF (10 mL) was dropwised to the suspension and stirred at room temperature for 20 h under Ar atmosphere. Undissolved part was filtered off, and then, the solvent was removed under reduced pressure. The residue was dissolved in $CHCl_3$ and washed with water. The organic layer was dried over Na_2SO_4 and the solvent was removed under reduced pressure. The residue was purified by column chromatography (silica gel, eluent: $CHCl_3$/MeOH = 20/1 v/v) to afford FLV-linker-Boc (10) (332 mg, 0.83mmol, 27 %).

^{1}H-NMR (400 MHz, $CDCl_3$):δ (ppm) 1.37 (s, 9H, Boc), 2.46, 2.56 (s, 2H, aromatic C*H*$_3$), 3.52–3.53 (m, 2H, CH_2C*H*$_2$NH), 4.13 (s, 3H, NC*H*$_3$), 4.32 (m, 2H, C*H*$_2$$CH_2$NH), 5.15 (br, 1H, amide), 7.43, 8.08 (s, 2H, aromatic).

ESI-MS *m/z* : $[M+Na]^+$ calcd. for $C_{20}H_{25}N_5O_4$, 422.1799 ; found, 422.1789.

FLV-linker NH_3Cl (11)

FLV-linker-Boc (10) (90 mg, 0.22 mmol) was dissolved in 1,4-dioxane (3 mL) and 4 M HCl in 1,4-dioxane (40 mL) was dropwised to the solution. The mixture was stirred for 2 h and the solvent was removed under reduced pressure. Obtained product was used in the next step without further purification.



Scheme 2. Synthetic schemes for C3FAA

Boc-β-Ala-OPac (13)

Boc-β-Ala-OH (12) (5.095 g, 26.9 mmol) and 2-bromoacetophenone (7.891 g, 39.6 mmol) were dissolved in dry DMF. Then, TEA (5.52 mL, 39.6 mmol) was dropwised to the mixture at 0°C and stirred at room temperature for 20 h under Ar atmosphere. The solvent was removed under reduced pressure. The residue was taken up with $CHCl_3$ and washed with saturated $NaHCO_3$ aq. three times, 4 wt% $KHSO_4$ aq. three times and brine. The organic layer was dried over Na_2SO_4 and the solvent was removed under reduced pressure. The residue was washed with hexane and diisopropyl ether to afford Boc-β-Ala-OPac (**33**) (6.361g, 20.7 mmol, 77 %).

^{1}H-NMR (400 MHz, $CDCl_3$):δ (ppm) 1.45 (s, 9H, Boc), 2.68–2.71 (t, 2H, AlaC$^{\alpha}H_2$), 3.49–3.53 (q, 2H, AlaC$^{\beta}H_2$), 5.36 (s, 1H, AlaN*H*), 5.39 (s, 2H, OCH_2COPh), 7.48–7.52, 7.61–7.64, 7.91–7.93 (m, 5H, aromatic).

Boc-(β-Ala)$_2$-OPac (15)

Boc-β-Ala-OPac (13) (3.013 g, 9.8mmol) was dissolved in 1,4-dioxane (10 mL). To the solution, 4 M HCl in 1,4-dioxane (90 mL) was dropwised and stirred at room temperature for 2 h.The solvent was removed under reduced pressure. The residue was washed with diisopropyl ether to afford H-β-Ala-OPac (14). This deprotected product and Boc-β-Ala-OH (12) (2.098 g, 11.1 mmol), HATU (5.278 g, 13.9 mmol), and HOAt (1.883 g, 13.8 mmol) were dissolved in dry DMF (20 mL) and then, DIEA (9.62 mL, 55.2 mmol) was added to the mixture at 0°C and thereafter stirred at room temperature for 20 h under Ar atmosphere. The solvent was removed under reduced pressure. The residue was taken up with $CHCl_3$ and washed with saturated $NaHCO_3$ aq. three times, 4 wt% $KHSO_4$ aq. three times and brine. The organic layer was dried over Na_2SO_4 and the solvent was removed under reduced pressure. The residue was washed with diisopropyl ether to afford Boc-(β-Ala)$_2$-OMe (15) (2.447 g, 6.5 mmol, 70 %).

^{1}H-NMR (400 MHz, $CDCl_3$):δ (ppm) 1.40 (s, 9H, Boc), 2.45–2.48, 2.67–2.70 (t, 4H, AlaC$^{\alpha}H_2$), 3.40–3.45, 3.64–3.68 (q, 4H, AlaC$^{\beta}H_2$), 5.27 (s, 1H, AlaN*H*), 5.44 (s, 2H, OCH_2COPh), 6.94 (s, 1H, AlaN*H*), 7.49–7.53, 7.62–7.66, 7.91–7.94 (m, 5H, aromatic).

Boc-D-Asp(OBzl)- (β-Ala)$_2$-OPac (18)

Boc-(β-Ala)$_2$-OPac (15) (2.447 g, 6.5 mmol) was dissolved in 1,4-dioxane (14 mL). To the solution, 4 M HCl in 1,4-dioxane (130 mL) was dropwised and stirred at room temperature for 1 h. The solvent was removed under reduced pressure. The residue was washed with diisopropyl ether to afford H-(β-Ala)$_2$-OPac (17). Then, obtained deprotected product, Boc-D-Asp(OBzl)-OH (16) (2.445 g, 7.6 mmol), HATU (4.074 g, 10.7 mmol), and HOAt (1.471 g, 10.8 mmol) were dissolved in dry DMF (25 mL) and then, DIEA (2.4 mL, 13.9 mmol) was added to the mixture at 0°C and thereafter stirred at room temperature for 20 h under Ar atmosphere. The solvent was removed under reduced pressure. The residue was taken up with $CHCl_3$ and washed with sat. $NaHCO_3$ aq. three times, 4 wt% $KHSO_4$ aq. three times and brine. The organic layer was dried over Na_2SO_4 and the solvent was removed under reduced pressure. The residue was washed with diisopropyl ether to afford Boc-β-Asp(OBzl) -(β-Ala)$_2$-OMe (18) (2.998 g, 5.1 mmol, 82 %).

^{1}H-NMR (400 MHz, $CDCl_3$):δ (ppm) 1.41 (s, 9H, Boc), 2.39–2.43, 2.69–2.72 (t, 4H, AlaC$^{\alpha}H_2$), 2.60–2.65, 2.81–2.86 (m, 2H, D-AspC$^{\alpha}H_2$), 3.50–3.52, 3.64–3.66 (m, 4H, AlaC$^{\beta}H_2$), 4.53–4.56 (t, 1H, D-AspC$^{\beta}H$), 5.14 (s, 2H, COOCH_2Ph), 5.44 (s, 2H, COOCH_2COPh), 5.81–5.83 (d, 1H, D-AspN*H*), 6.56, 6.95 (br, 2H, AlaN*H*), 7.33 (m, 5H, COOCH$_2$*Ph*), 7.49–7.53, 7.63–7.67, 7.90–7.93 (m, 5H, COOCH$_2$CO*Ph*).

CP3OBzl (21)

Boc-D-Asp(OBzl)-(β-Ala)$_2$-OPac (18) (2.950 g, 5.05 mmol) was dissolved in DMF (10 mL). To the solution, zinc powder (3 g) was added and 90 % DMF solution of AcOH (30 mL) was dropwised and stirred at 0°C overnight under Ar atmosphere. Zinc powder was removed by filtration and the solution was evaporated. The residue was taken up with $CHCl_3$ and washed with 4 % $KHSO_4$ aq. four times. The organic layer was dried over Na_2SO_4 and the solvent was removed under reduced pressure to afford Boc-D-Asp(OBzl)-(β-Ala)$_2$-OH (19). Then, this deprotected product (927 mg, 1.99 mmol) was dissolved in TFA/anisole (11 mL, 10/1 = v/v) and stirred at room temperature for 2 h. The solvent was removed under reduced pressure. To the residue, 1 M HCl in diethyl ether was added and washed with diisopropyl ether to afford H-D-Asp(OBzl)-(β-Ala)$_2$-OH (20). Obtained deprotected product was separated into three round bottom flasks and COMU (2.901 g, 6.77 mmol), Oxyma (1.508 g, 10.61 mmol) were added to the each flasks, and thereafter dissolved in dry DMF (500 mL). To the solution was added 100 mL DMF solution of DIEA (2.08 mL, 11.92 mmol) at 0°C under Ar atmosphere and thereafter stirred at room temperature for 72 h under Ar atmosphere. The solvent was removed under reduced pressure. The precipitate was washed with MeCN and EtOH to afford CP3OBzl (21) (193 mg, 0.108 mmol, 28 %).

^{1}H-NMR (400 MHz, DMSO-d_6):δ (ppm) 2.11–2.50 (m, 6H, AlaC$^\alpha$*H*$_2$, D-AspC$^\alpha$*H*$_2$), 2.99–2.05, 3.21–3.23, 3.37–3.43 (m, 4H, AlaC$^\beta$*H*$_2$), 4.47–4.52 (m, 1H, D-AspC$^\beta$*H*), 5.13 (s, 2H, COOC*H*$_2$Ph), 7.32–7.40 (m, 5H, COOCH$_2$*Ph*), 7.62–7.67, 7.94–7.96 (m, d, 3H, AlaN*H*, D-AspN*H*).

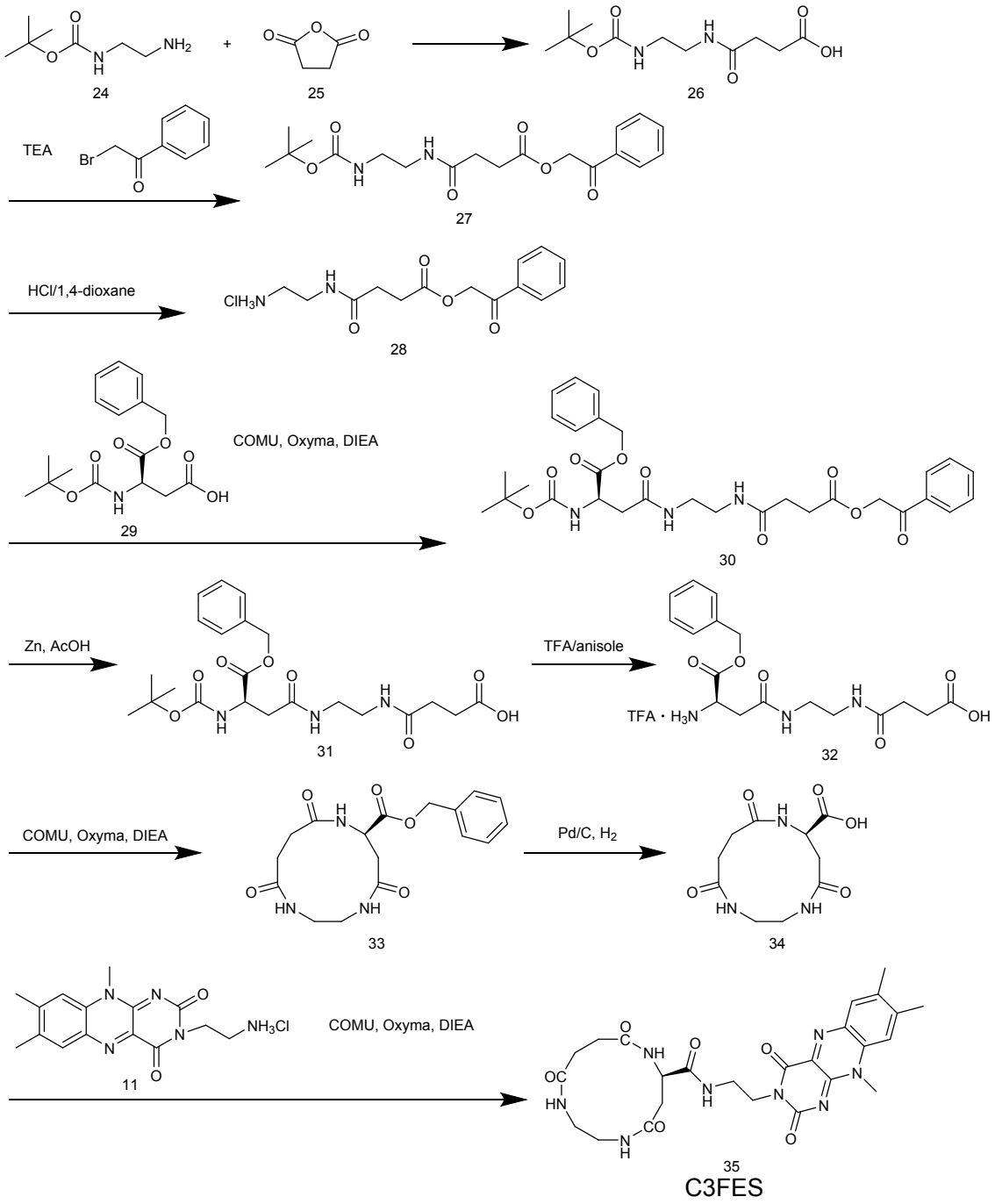
ESI-MS *m/z* : $[M+Na]^+$ calcd. for $C_{17}H_{21}N_3O_5$, 370.1373 ; found, 370.1378.

C3FAA (23)

CP3OBzl (21) (115 mg, 0.33 mmol) was dissolved in HCOOH (10 mL) and 10 % Pd/C (100 mg) was added. The mixture was stirred for 20 h under H_2 atomosphere. The reaction mixture was then filtered and the filtrate was evaporated. The residue was washed with diisopropyl ether to obtain deprotected product. A part of this deprotected product (15 mg, 0.058 mmol), FLV-linker-NH_3Cl (11) (15 mg, 0.045 mmol), COMU (48 mg, 0.112 mmol), and Oxyma (14 mg, 0.099 mmol) were dissolved in dry DMF (10 mL) and stirred under Ar atmosphere. Then, DIEA (62 μL, 0.357 mmol) was dropwised to the solution at 0°C and stirred at room temperature for 20 h under Ar atmosphere. The solvent was removed under reduced pressure and the residue was washed with MeCN, MeOH and DMF in this order to obtaine C3FAA (23) (8 mg, 15 μmol, yield 33 %).

^{1}H-NMR (400 MHz, TFA-*d*):δ (ppm) 2.58, 2.71 (s, 6H, aromatic C*H*$_3$), 2.75, 2.85–2.88, 3.01–3.04, (m, 6H, AlaC$^\alpha$*H*$_2$, D-AspC$^\alpha$*H*$_2$), 3.38–3.41, 3.59–3.62, 3.74, 3.91, 4.44 (m, 8H, NC*H*$_2$C*H*$_2$NH, AlaC$^\beta$*H*$_2$), 4.44 (s, 3H, NC*H*$_3$), 5.10–5.12 (d, 1H, D-AspC$^\beta$*H*), 8.05, 8.21 (s, 2H, aromatic).

ESI-MS *m/z* : $[M+Na]^+$ calcd. for $C_{25}H_{30}N_8O_6$, 561.2181 ; found, 561.2177.



Scheme 3. Synthetic schemes for C3FES

Boc-EDA-SA-OPac (27)

Succinic anhydride (25) (2.617g, 25.98 mmol) was dissolved in CH_2Cl_2. To this solution, Boc-ethylenediamine (24) (5 g, 31 mmol) in CH_2Cl_2 was added and the solution was stirred at room temperature for 18 h under Ar atmosphere. The solution was evaporated to afford Boc-EDA-SA-OH (26) and used in the next step without further purification. This product and phenacyl bromide (7.803g, 39.20 mmol) was dissolved in dry DMF (100 mL) and then, TEA (5.43 mL, 38.96 mmol) was dropwised to the mixture at 0°C and stirred at room temperature for 20 h under Ar atmosphere. The solvent was removed under reduced pressure. The residue was dissolved in $CHCl_3$ and washed with 4% $KHSO_4$ aq. three times, sat. $NaHCO_3$ aq. three times and brine. The organic layer was dried over Na_2SO_4 and the solvent was removed under reduced pressure. The residue was purified by column chromatography (silica gel, eluent: $CHCl_3$/MeOH = 20/1 v/v) and to afford Boc-EDA-SA-OPac (27) (7.629 g, 20.16 mmol, 78 %).

^{1}H-NMR (400 MHz, $CDCl_3$):δ (ppm) 1.41 (s, 9H, Boc), 2.56–2.59 (t, 2H, CH_2CH_2COOPac), 2.84–2.87 (t, 2H, CH_2CH_2COOPac), 3.26–3.27 (m, 2H, BocNHCH_2CH$_2$), 3.36–3.40 (m, 2H, BocNHCH$_2$CH_2), 5.03, 6.38 (br, 2H, amide), 5.38 (s, 2H, OPac CH_2), 7.48–7.51, 7.60–7.64, 7.90–7.92 (m, 5H, OPac aromatic).

ESI-MS *m/z* : $[M+Na]^+$ calcd. for $C_{19}H_{26}N_2O_6$, 401.1683 ; found, 401.1687.

Boc-D-Asp(OBzl)-EDA-SA-OPac (30)

Boc-EDA-SA-OPac (27) (7.629 g, 20.27 mmol) was dissolved in 1,4-dioxane (8 mL). To the solution, 4 M HCl in 1,4-dioxane (100 mL) was dropwised and stirred at room temperature for 1 h. The solvent was removed under reduced pressure. The residue was washed with diethyl ether to afford H-EDA-SA-OPac (28). Then, obtained deprotected product, Boc-D-Asp(OBzl)-OH (29) (5.411 g, 16.75 mmol), HATU (10.104 g, 26.59 mmol), and HOAt (3.902 g, 28.69 mmol) were dissolved in dry DMF (120 mL) and then, DIEA (6.4 mL, 36.74 mmol) was added to the mixture at 0°C and thereafter stirred at room temperature for 20 h under Ar atmosphere. The solvent was removed under reduced pressure. The residue was taken up with $CHCl_3$ and washed with saturated $NaHCO_3$ aq. three times, 4 wt% $KHSO_4$ aq. three times and brine. The organic layer was dried over Na_2SO_4 and the solvent was removed under reduced pressure. The residue was purified by column chromatography (silica gel, eluent: $CHCl_3$/MeOH = 20/1 v/v) to afford Boc-D-Asp(OBzl)-EDA-SA-OMe (30) (6.624 g, 11.36 mmol, 68 %).

^{1}H-NMR (400 MHz, $CDCl_3$):δ (ppm) 1.41 (s, 9H, Boc), 2.53–2.88 (m, 6H, CHCH_2, COCH_2CH_2CO), 3.34 (br, 4H, NHCH_2CH_2NH), 4.53–4.55 (t, 1H, C*H*CH$_2$), 5.13 (s, 2H, COOCH_2Ph), 5.37 (s, 2H, COOCH_2COPh), 5.79–5.81 (d, 1H, urethane), 6.51 (br, 2H, amide), 7.32 (m, 5H, COOCH$_2$*Ph*), 7.46–7.50, 7.60–7.64, 7.88–7.90 (m, 5H, COOCH$_2$CO*Ph*).

ESI-MS *m/z* : $[M+Na]^+$ calcd. for $C_{30}H_{37}N_3O_9$, 606.2422 ; found, 606.2421.

CP3ESOBzl (33)

Boc-D-Asp(OBzl)-EDA-SA-OPac (30) (6.624 g, 11.35 mmol) was dissolved in DMF (10 mL). To the solution, zinc powder (6 g) and 90 % aqueous solution of AcOH (60 mL) were added and stirred at 0°C overnight under Ar atmosphere. Zinc powder was removed by filtration and the solution was evaporated. The residue was taken up with $CHCl_3$ and washed with 4 % $KHSO_4$ aq. The organic layer was dried over Na_2SO_4 and the solvent was removed under reduced pressure to afford Boc-D-Asp(OBzl)-EDA-SA-OH (31). Then, this deprotected product (4.180 g, 8.99 mmol) was dissolved in TFA/anisole (22 mL, 10/1 = v/v) and stirred at room temperature for 2 h. The solvent was removed under reduced pressure. The residue was washed with 1 M HCl in diethyl ether to afford H-D-Asp(OBzl)-(β-Ala)$_2$-OH (32). Obtained deprotected product was separated into five round bottom flasks and dissolved in dry DMF (700 mL). COMU (7.59 g, 17.72 mmol) and Oxyma (3.78 g, 26.58 mmol) were added to each solutions. To the solution was added 50 mL DMF solution of DIEA (5.56 mL, 31.89 mmol) at 0°C under Ar atmosphere and thereafter stirred at room temperature for 72 h under Ar atmosphere. The solvent was removed under reduced pressure. The precipitate was washed with MeCN to afford CP3ESOBzl (33) (281 mg, 0.81 mmol, 7%).

^{1}H-NMR (400 MHz, DMSO-d_6):δ (ppm) 2.11–2.14 (m, 4H, COCH_2CH_2CO), 2.47 (m, 2H, D-AspC$^{\alpha}H_2$), 2.78–2.81, 3.58–3.63 (m, 4H, NHCH_2CH_2NH), 4.71–4.77 (m, 1H, D-AspC$^{\beta}H$), 5.13 (s, 2H, COOCH_2Ph), 7.27–7.29, 7.49–7.51, 8.22 (d, d, s, 3H, N*H*CH$_2$CH_2N*H*, D-AspN*H*), 7.33–7.40 (m, 5H, COOCH$_2$CO*Ph*), .

ESI-MS *m/z* : $[M+Na]^+$ calcd. for $C_{17}H_{21}N_3O_5$, 370.1373 ; found, 370.1377.

C3FES (35)

CP3ESOBzl (33) (76 mg, 0.22 mmol) was dissolved in HCOOH (50 mL). 10% Pd/C (50 mg) was added to the solution and the solution was stirred under H_2 atmosphere at room temperature for 18 h. Pd/C was removed by filtration and the filtrate was evaporated to afford deprotected product (34). This deprotected product and FLV-linker-NH_3Cl (11) (50 mg, 0.19 mmol) was dissolved in dry DMF (25 mL). To the solution was added COMU (171 mg, 0.40 mmol) and Oxyma (59 mg, 0.42 mmol), then, DIEA (102 μL, 0.58 mmol) were dropwised to the solution at 0°C. The solution was stirred at room temperature for 20 h under Ar atmosphere. The solvent was removed under reduced pressure and the residue was washed with MeCN, MeOH, DMF and diethyl ether in this order to afford CP3FES (35) (30 mg, 0.055 mmol, 28%).

^{1}H-NMR (400 MHz, TFA-*d*):δ (ppm) 2.59, 2.72 (s, 6H, aromatic CH_3), 2.62–2.66, 2.83–2.87, 2.98–3.01, (m, 6H, COCH_2CH_2CO, D-AspC$^{\alpha}H_2$), 3.19–3.20, 3.70–3.75, 3.92–4.04, 4.45–4.48(m, 8H, NCH_2CH_2NH, AlaC$^{\beta}H_2$), 4.50 (s, 3H, NCH_3), 5.24–5.26 (d, 1H, D-AspC$^{\beta}H$), 8.07, 8.22 (s, 2H, aromatic).

ESI-MS *m/z* : $[M+Na]^+$ calcd. for $C_{25}H_{30}N_8O_6$, 561.2181 ; found, 561.2180.

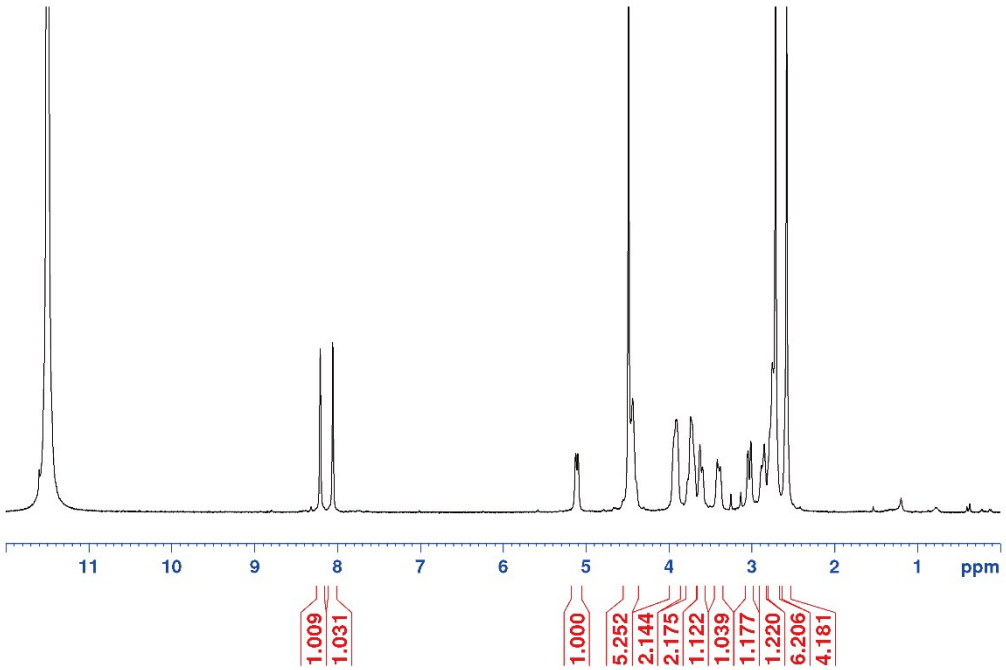


Figure S1 ^{1}H-NMR spectrum of C3FAA (23) in TFA-*d*.

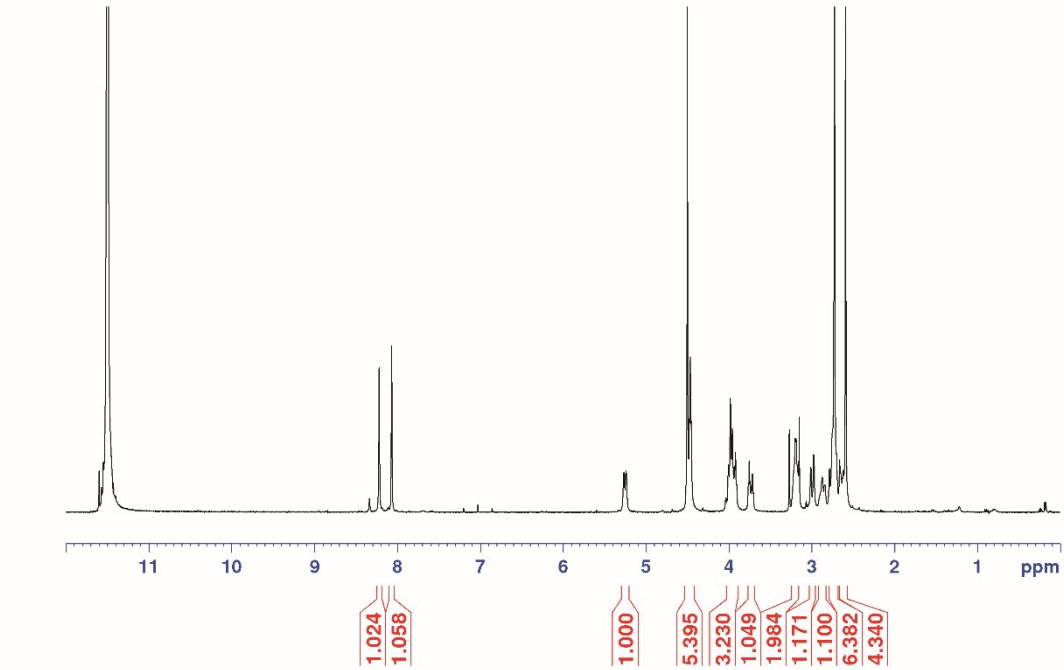


Figure S2 ^{1}H-NMR spectrum of C3FES (35) in TFA-*d*.

2. Supporting Figures section

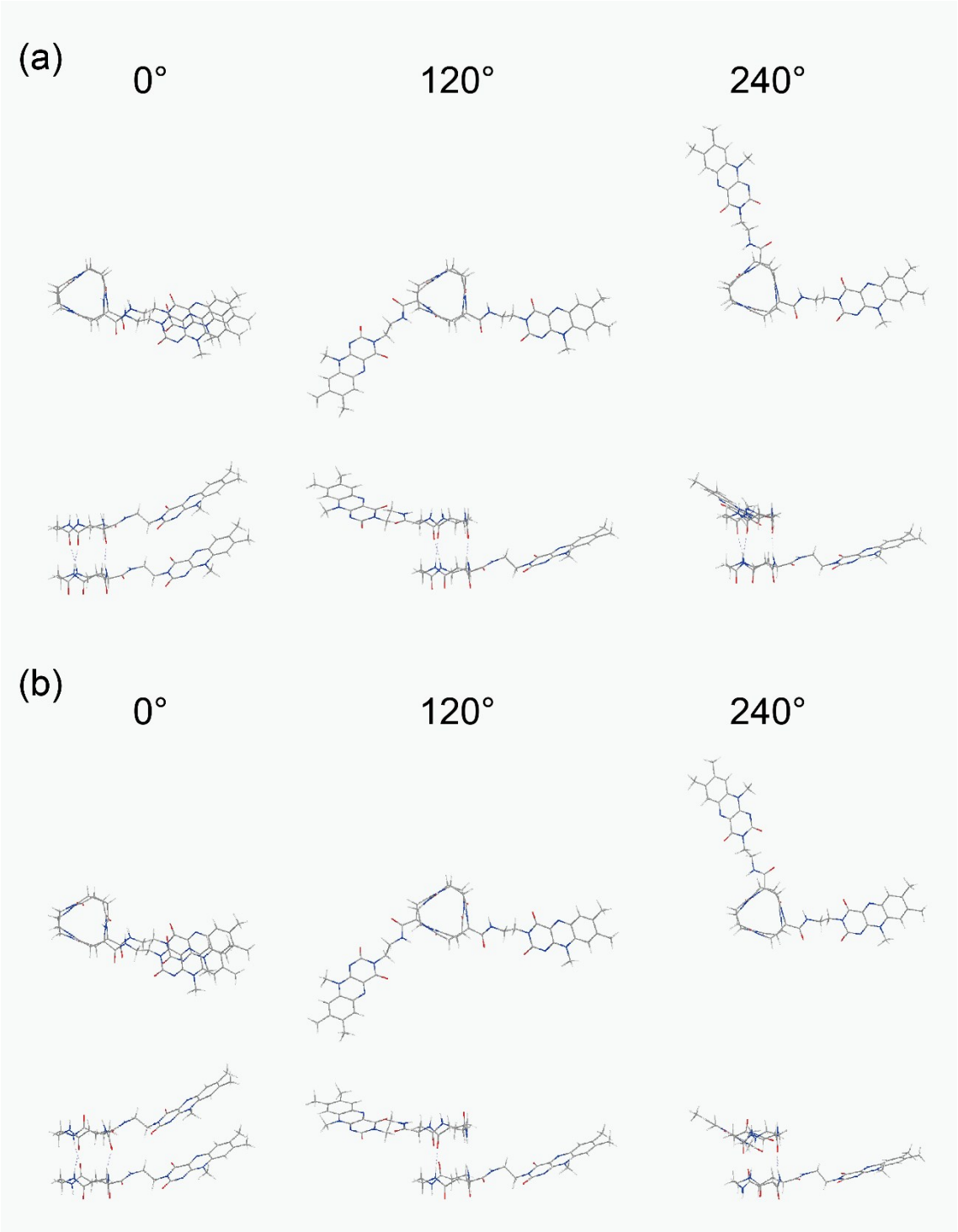


Figure S3 (a) C3FAA and (b) C3FES optimized dimer structures with initial rotation of 0°, 120°, 240°.

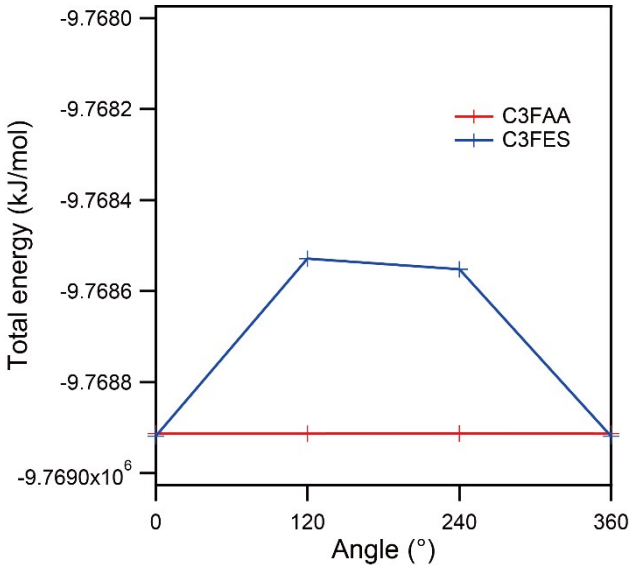


Figure S4 The total energy of C3FAA (red) and C3FES (blue) dimers with initial rotation of 0°, 120°, 240°.

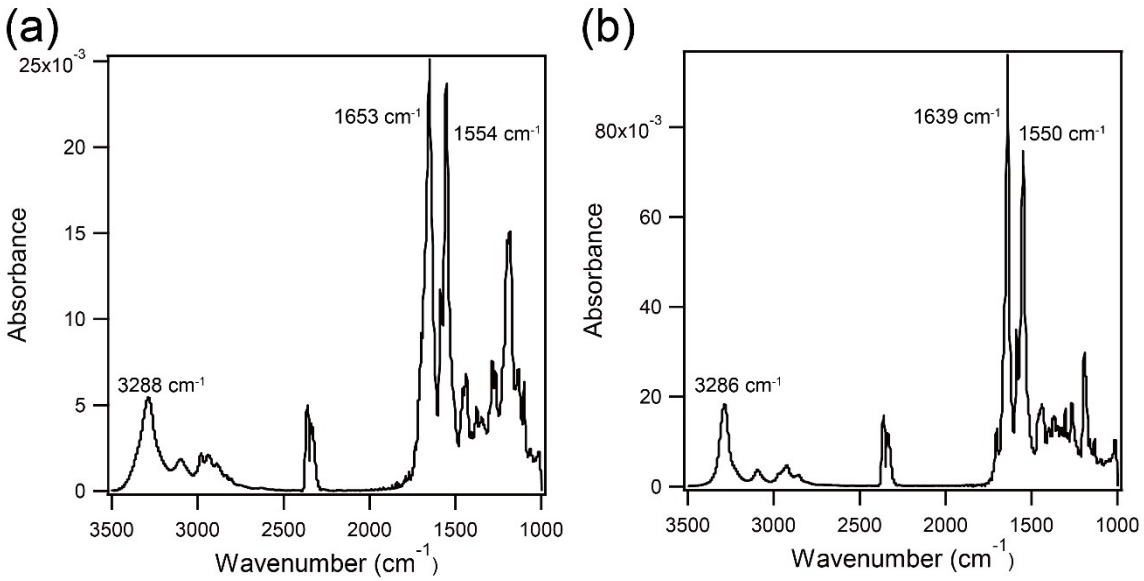


Figure S5 ATR-FTIR spectra of the (a) C3FAA and (b) C3FES crystals.

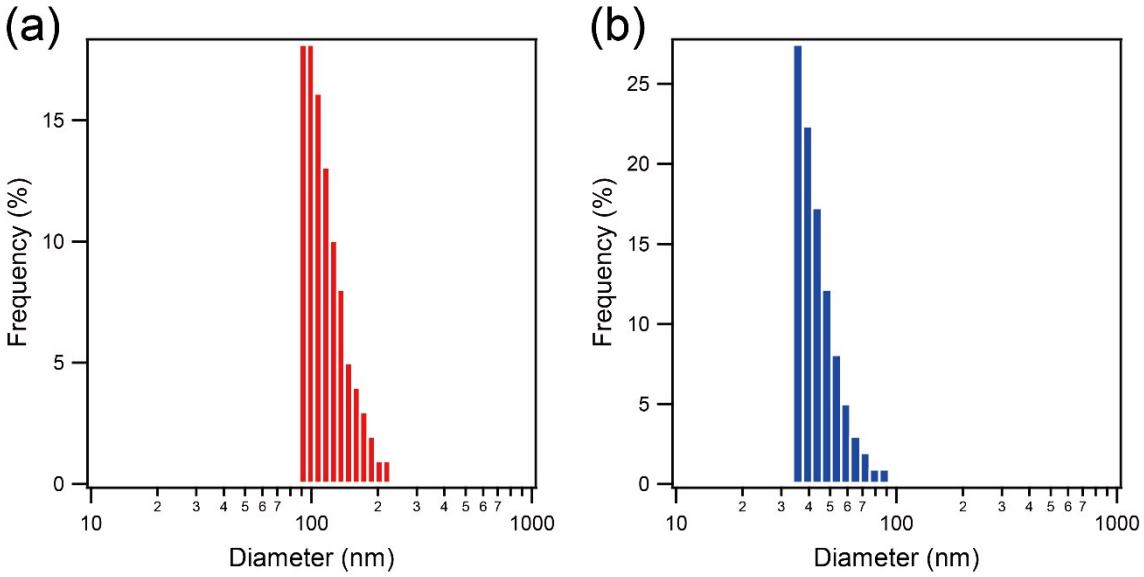


Figure S6 DLS results of the peptide nanotubes of (a) C3FAA and (b)C3FES in mixed solution of HFIP and water (1/39 v/v).

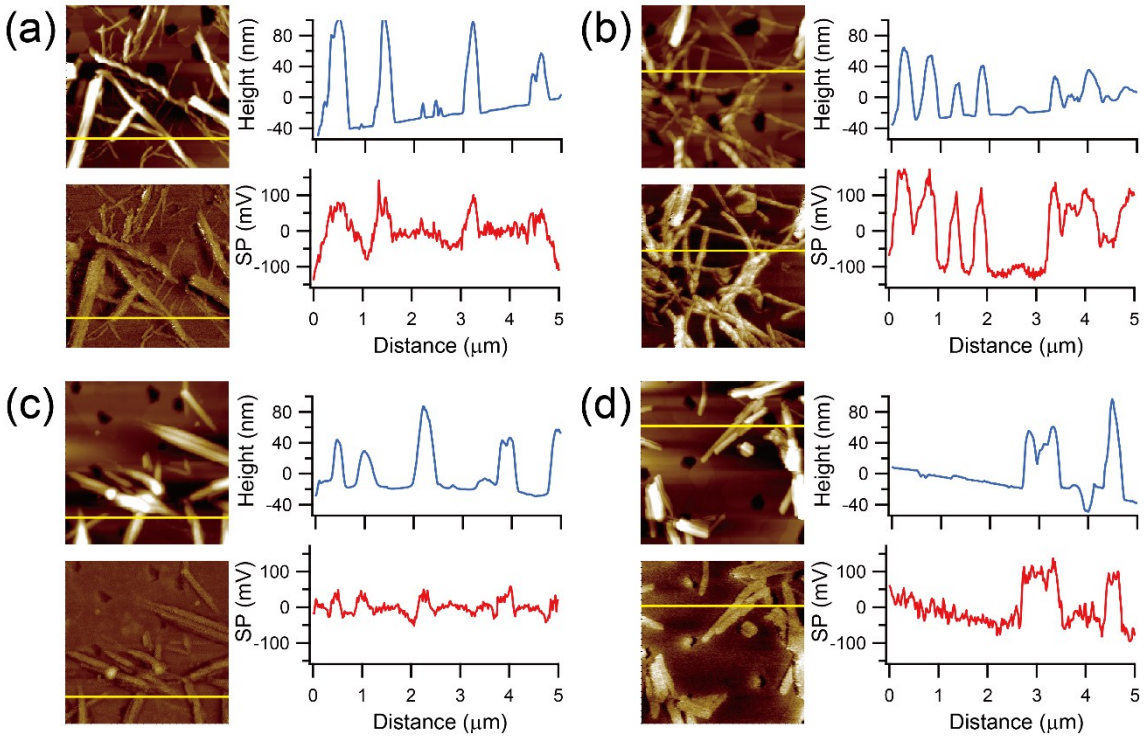


Figure S7 AFM (upper) and KFM (lower) images and cross sectional profiles of C3FAA nanotube bundles (a) before and (c) after the thermal anneal treatments, and C3FES nanotube bundles (b) before and (d) after the thermal anneal treatments. The sizes of AFM images are 5×5 μm^2.

Table S1. The coordinates of the optimized geometry of C3FAA (0°)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-6.461844	-3.556662	2.423746
2	6	0	-8.227149	-4.049922	0.807792
3	7	0	-6.653841	-3.912976	-1.120457
4	6	0	-4.424755	-3.275224	-1.889073
5	6	0	-4.117553	-2.783243	2.788314
6	6	0	-5.581285	-2.756702	3.268746
7	6	0	-7.474094	-3.053824	1.679274
8	8	0	-7.776784	-1.850033	1.675225
9	6	0	-5.865494	-2.907279	-1.560166
10	8	0	-6.258320	-1.736610	-1.686275
11	1	0	-6.299435	-4.554438	2.387805
12	1	0	-9.292610	-3.958633	1.043356
13	1	0	-7.928586	-5.080400	1.025368
14	1	0	-6.250573	-4.838885	-1.064733
15	1	0	-4.227751	-2.978120	-2.921818
16	1	0	-4.248515	-4.353007	-1.810970
17	1	0	-3.513820	-2.221791	3.508779
18	1	0	-3.743651	-3.811885	2.779048
19	1	0	-5.620967	-3.137843	4.293589
20	1	0	-5.966646	-1.736873	3.268371
21	6	0	-8.040782	-3.752325	-0.692128
22	1	0	-8.334499	-2.726825	-0.916477
23	1	0	-8.676438	-4.428358	-1.271768
24	8	0	-4.108254	-0.901460	1.281244
25	6	0	-3.934524	-2.117286	1.432332
26	7	0	-3.562971	-2.939854	0.410325
27	1	0	-3.540965	-3.935273	0.597504
28	6	0	-3.445149	-2.508191	-0.977783
29	1	0	-3.712394	-1.447813	-0.993977
30	6	0	-2.009414	-2.592671	-1.542572
31	8	0	-1.814316	-2.386851	-2.746078
32	7	0	-1.028375	-2.874865	-0.659198

33	1	0	-1.288037	-3.005269	0.309583
34	6	0	0.381208	-2.964633	-1.014454
35	1	0	0.815451	-3.821396	-0.492240
36	1	0	0.449164	-3.135996	-2.089773
37	6	0	1.139239	-1.680375	-0.632231
38	1	0	0.775074	-0.839215	-1.219246
39	1	0	1.010166	-1.471654	0.430373
40	6	0	3.369678	-2.334434	0.128587
41	6	0	3.087409	-1.410115	-2.156866
42	6	0	4.821526	-2.423342	-0.188409
43	6	0	5.244727	-1.976338	-1.498969
44	6	0	6.954436	-2.982302	0.433180
45	6	0	7.840683	-3.494936	1.409869
46	6	0	7.470960	-2.568385	-0.827814
47	6	0	9.197693	-3.608171	1.175941
48	1	0	7.410155	-3.799716	2.358771
49	6	0	8.851483	-2.681627	-1.066437
50	6	0	9.709042	-3.189523	-0.094111
51	1	0	9.269088	-2.373294	-2.016150
52	7	0	2.582582	-1.810863	-0.883930
53	7	0	4.424594	-1.502779	-2.416820
54	7	0	6.587910	-2.070005	-1.772853
55	7	0	5.627893	-2.899013	0.723287
56	8	0	2.288240	-0.985686	-2.995663
57	8	0	2.897075	-2.695497	1.204919
58	6	0	10.119204	-4.160360	2.234504
59	1	0	10.634964	-5.061882	1.884243
60	1	0	10.894542	-3.435479	2.507398
61	1	0	9.562726	-4.418168	3.138348
62	6	0	11.182180	-3.296023	-0.388486
63	1	0	11.769055	-2.705651	0.324778
64	1	0	11.527382	-4.332462	-0.298631
65	1	0	11.413203	-2.944087	-1.395865
66	6	0	7.096806	-1.639789	-3.086565
67	1	0	7.579143	-2.483674	-3.584050
68	1	0	6.255460	-1.293570	-3.677588

69	1	0	7.815281	-0.828683	-2.951497
70	7	0	-8.008141	1.118011	1.834035
71	6	0	-9.508946	0.681670	-0.035256
72	7	0	-7.626604	0.920670	-1.657438
73	6	0	-5.324775	1.655204	-2.002960
74	6	0	-5.788182	1.905823	2.661385
75	6	0	-7.315780	1.878657	2.867755
76	6	0	-8.940920	1.642797	1.003439
77	8	0	-9.311575	2.827904	1.051274
78	6	0	-6.814500	1.969905	-1.918371
79	8	0	-7.221243	3.133004	-2.074582
80	1	0	-7.814396	0.120888	1.767424
81	1	0	-10.601119	0.753219	0.010129
82	1	0	-9.228160	-0.350174	0.194265
83	1	0	-7.210419	-0.005276	-1.581365
84	1	0	-4.966433	1.992671	-2.978896
85	1	0	-5.136230	0.580928	-1.921275
86	1	0	-5.341248	2.434229	3.510511
87	1	0	-5.387831	0.888147	2.650389
88	1	0	-7.526772	1.436637	3.847812
89	1	0	-7.718461	2.892150	2.857780
90	6	0	-9.068125	1.042514	-1.468016
91	1	0	-9.344828	2.070477	-1.704576
92	1	0	-9.581559	0.378585	-2.171705
93	8	0	-5.600964	3.873810	1.281299
94	6	0	-5.396974	2.658518	1.397578
95	7	0	-4.823198	1.906917	0.414241
96	1	0	-4.718340	0.906838	0.576276
97	6	0	-4.544287	2.427019	-0.918603
98	1	0	-4.888220	3.466099	-0.922362
99	6	0	-3.043967	2.491459	-1.270532
100	8	0	-2.692293	2.802010	-2.416025
101	7	0	-2.176751	2.226385	-0.269209
102	1	0	-2.564032	1.988484	0.634636
103	6	0	-0.730951	2.292042	-0.418657
104	1	0	-0.287159	1.421157	0.070518

105	1	0	-0.502847	2.251227	-1.484931
106	6	0	-0.158491	3.583658	0.193123
107	1	0	-0.581436	4.454975	-0.303425
108	1	0	-0.378575	3.626197	1.260770
109	6	0	2.083003	3.013413	0.988074
110	6	0	1.834635	4.335681	-1.096225
111	6	0	3.552077	3.119261	0.769731
112	6	0	3.999174	3.861283	-0.390483
113	6	0	5.693686	2.641831	1.427739
114	6	0	6.573123	2.019531	2.344921
115	6	0	6.233973	3.358283	0.321924
116	6	0	7.945707	2.085959	2.200156
117	1	0	6.124938	1.482807	3.175379
118	6	0	7.630010	3.427092	0.173944
119	6	0	8.480787	2.808627	1.086296
120	1	0	8.065372	3.965409	-0.657896
121	7	0	1.303468	3.648278	0.036041
122	7	0	3.186854	4.429657	-1.259731
123	7	0	5.358061	3.959820	-0.567990
124	7	0	4.351371	2.541368	1.627045
125	8	0	1.046004	4.835402	-1.902822
126	8	0	1.590138	2.411014	1.940195
127	6	0	8.857949	1.411251	3.193896
128	1	0	9.487476	0.655888	2.709643
129	1	0	9.533120	2.130897	3.670839
130	1	0	8.280070	0.917667	3.978420
131	6	0	9.970900	2.907277	0.892567
132	1	0	10.449062	3.383735	1.756244
133	1	0	10.421453	1.913150	0.791681
134	1	0	10.218463	3.487504	0.001384
135	6	0	5.891661	4.710558	-1.717800
136	1	0	6.474543	4.040284	-2.353104
137	1	0	5.053446	5.112634	-2.277051
138	1	0	6.524264	5.524467	-1.358008

Table S2. The coordinates of the optimized geometry of C3FAA (120°)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.196206	-0.302080	2.817997
2	6	0	-1.934490	-2.329511	3.960980
3	7	0	0.371982	-3.275189	3.949719
4	6	0	2.642029	-3.060820	3.068675
5	6	0	0.598105	0.902793	1.574318
6	6	0	-0.907269	0.607349	1.714065
7	6	0	-1.766425	-1.521477	2.681285
8	8	0	-2.122294	-1.983407	1.585038
9	6	0	1.203618	-3.538331	2.917163
10	8	0	0.843110	-4.124908	1.884698
11	1	0	-0.968834	0.008829	3.753240
12	1	0	-2.981559	-2.644264	4.018909
13	1	0	-1.722428	-1.722962	4.847122
14	1	0	0.754508	-2.798718	4.755784
15	1	0	3.297272	-3.929460	2.967183
16	1	0	2.825642	-2.616070	4.052199
17	1	0	0.726140	1.642725	0.777730
18	1	0	0.983512	1.344965	2.498473
19	1	0	-1.438450	1.550740	1.873371
20	1	0	-1.292314	0.147360	0.803882
21	6	0	-1.053052	-3.592839	3.963893
22	1	0	-1.259912	-4.203966	3.085296
23	1	0	-1.279604	-4.183619	4.856337
24	8	0	1.235956	-0.864212	0.068084
25	6	0	1.390067	-0.332836	1.174808
26	7	0	2.269115	-0.808522	2.102058
27	1	0	2.270821	-0.367699	3.014153
28	6	0	3.004344	-2.059975	1.952779
29	1	0	2.696506	-2.484097	0.992606
30	6	0	4.535967	-1.883188	1.862225
31	8	0	5.267876	-2.879829	1.881115
32	7	0	4.991579	-0.618665	1.739097

33	1	0	4.310239	0.128290	1.714535
34	6	0	6.400149	-0.277332	1.596818
35	1	0	6.596865	0.624421	2.182586
36	1	0	6.991239	-1.098482	2.005022
37	6	0	6.776463	-0.037737	0.122954
38	1	0	6.655960	-0.955204	-0.450743
39	1	0	6.150039	0.747157	-0.302091
40	6	0	8.440618	1.753748	0.050349
41	6	0	9.182362	-0.603621	-0.166805
42	6	0	9.874362	2.121120	-0.107604
43	6	0	10.822393	1.040996	-0.282163
44	6	0	11.508585	3.722625	-0.218157
45	6	0	11.875272	5.088908	-0.186308
46	6	0	12.518491	2.733996	-0.394656
47	6	0	13.189187	5.494675	-0.319643
48	1	0	11.078084	5.813312	-0.051193
49	6	0	13.855511	3.145651	-0.530235
50	6	0	14.198615	4.494493	-0.494348
51	1	0	14.642056	2.414542	-0.664119
52	7	0	8.176158	0.395428	-0.009926
53	7	0	10.489411	-0.234920	-0.307426
54	7	0	12.140802	1.400790	-0.424588
55	7	0	10.197813	3.387084	-0.076808
56	8	0	8.834608	-1.787619	-0.171765
57	8	0	7.552116	2.586726	0.220229
58	6	0	13.551507	6.958155	-0.282410
59	1	0	14.253142	7.175881	0.530952
60	1	0	14.035534	7.273861	-1.213867
61	1	0	12.662117	7.575427	-0.137078
62	6	0	15.642818	4.895057	-0.640536
63	1	0	15.782087	5.558058	-1.502224
64	1	0	15.988718	5.447384	0.240968
65	1	0	16.286542	4.022952	-0.771820
66	6	0	13.166108	0.359195	-0.609576
67	1	0	13.882180	0.402082	0.213766
68	1	0	12.669799	-0.605500	-0.617518

69	1	0	13.681457	0.520936	-1.558482
70	7	0	-0.493533	-5.510250	-0.409395
71	6	0	1.634134	-4.966045	-1.467770
72	7	0	0.740462	-2.758374	-2.221714
73	6	0	-1.233612	-1.356465	-2.520734
74	6	0	-2.914696	-4.999878	-0.085804
75	6	0	-1.829182	-6.078638	-0.268315
76	6	0	0.295091	-5.694611	-1.495145
77	8	0	-0.035354	-6.389469	-2.470825
78	6	0	-0.311185	-2.463032	-3.019782
79	8	0	-0.543715	-3.041538	-4.093618
80	1	0	-0.117723	-4.978360	0.372724
81	1	0	2.412541	-5.693875	-1.720953
82	1	0	1.847636	-4.578287	-0.467518
83	1	0	0.882062	-2.199324	-1.383777
84	1	0	-1.277837	-0.583215	-3.292000
85	1	0	-0.852545	-0.899866	-1.602497
86	1	0	-3.869930	-5.506764	0.088801
87	1	0	-2.693864	-4.385576	0.791586
88	1	0	-1.851628	-6.746576	0.599962
89	1	0	-2.029763	-6.673273	-1.160117
90	6	0	1.696595	-3.824026	-2.502397
91	1	0	1.480972	-4.203931	-3.501663
92	1	0	2.709003	-3.406659	-2.505111
93	8	0	-3.501831	-4.606141	-2.391676
94	6	0	-3.077963	-4.134408	-1.328199
95	7	0	-2.723409	-2.825649	-1.185834
96	1	0	-2.355695	-2.523586	-0.283970
97	6	0	-2.664898	-1.891043	-2.302109
98	1	0	-2.962757	-2.452335	-3.193408
99	6	0	-3.662853	-0.719884	-2.190888
100	8	0	-3.602978	0.223831	-2.989866
101	7	0	-4.590303	-0.805758	-1.212438
102	1	0	-4.573010	-1.623307	-0.617278
103	6	0	-5.623721	0.197057	-0.997782
104	1	0	-5.818745	0.264419	0.075463

105	1	0	-5.244103	1.158934	-1.347674
106	6	0	-6.921069	-0.157452	-1.747511
107	1	0	-6.736014	-0.190435	-2.819849
108	1	0	-7.299598	-1.122377	-1.409128
109	6	0	-8.820230	0.643864	-0.426685
110	6	0	-8.061712	1.957432	-2.389501
111	6	0	-9.887149	1.670993	-0.270013
112	6	0	-9.909785	2.757076	-1.226967
113	6	0	-11.715057	2.475660	0.853135
114	6	0	-12.646435	2.344702	1.910339
115	6	0	-11.823269	3.581456	-0.037606
116	6	0	-13.662680	3.260375	2.105355
117	1	0	-12.532134	1.488926	2.568318
118	6	0	-12.855739	4.514313	0.160362
119	6	0	-13.764361	4.368995	1.205285
120	1	0	-12.960302	5.364798	-0.500784
121	7	0	-7.976294	0.839708	-1.507337
122	7	0	-9.046087	2.887173	-2.214793
123	7	0	-10.902415	3.693507	-1.067186
124	7	0	-10.738208	1.538895	0.713046
125	8	0	-7.232780	2.050016	-3.298784
126	8	0	-8.694665	-0.311387	0.337614
127	6	0	-14.642571	3.094721	3.239670
128	1	0	-14.621947	3.957588	3.915183
129	1	0	-15.670409	3.004183	2.869927
130	1	0	-14.413446	2.201122	3.824772
131	6	0	-14.857402	5.390061	1.380795
132	1	0	-15.846640	4.921989	1.318608
133	1	0	-14.796075	5.867592	2.365567
134	1	0	-14.798898	6.169187	0.618065
135	6	0	-10.993103	4.827762	-2.002617
136	1	0	-10.887743	5.764058	-1.450827
137	1	0	-10.191155	4.733188	-2.727198
138	1	0	-11.958937	4.803643	-2.511379

Table S3. The coordinates of the optimized geometry of C3FAA (240°)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.600224	-5.083294	3.621340
2	6	0	1.691277	-4.326732	3.997502
3	7	0	1.123759	-1.992235	3.334109
4	6	0	-0.561330	-0.538713	2.323771
5	6	0	-2.870613	-4.607814	2.710218
6	6	0	-1.748310	-5.642687	2.915256
7	6	0	0.648555	-4.990512	3.107965
8	8	0	0.946422	-5.396725	1.973286
9	6	0	0.590838	-1.524844	2.183805
10	8	0	0.989801	-1.868432	1.059761
11	1	0	-0.747062	-4.756152	4.567230
12	1	0	2.547251	-5.005758	4.068254
13	1	0	1.311103	-4.167582	5.011545
14	1	0	0.740906	-1.651416	4.206074
15	1	0	-0.274035	0.388796	1.822295
16	1	0	-0.773325	-0.300428	3.371341
17	1	0	-3.722718	-5.116129	2.247587
18	1	0	-3.204382	-4.219005	3.677329
19	1	0	-2.147941	-6.486922	3.485472
20	1	0	-1.391288	-6.016042	1.955209
21	6	0	2.184792	-2.992814	3.405767
22	1	0	2.562132	-3.141186	2.394000
23	1	0	2.999556	-2.606833	4.025203
24	8	0	-2.207443	-3.700791	0.580754
25	6	0	-2.450616	-3.484686	1.774164
26	7	0	-2.362315	-2.242425	2.329883
27	1	0	-2.489646	-2.171534	3.332100
28	6	0	-1.827548	-1.079506	1.630271
29	1	0	-1.553050	-1.424494	0.629067
30	6	0	-2.850796	0.054752	1.409931
31	8	0	-2.466770	1.143462	0.966321
32	7	0	-4.141017	-0.225450	1.691747

33	1	0	-4.363751	-1.153531	2.026715
34	6	0	-5.231224	0.711229	1.452515
35	1	0	-5.958507	0.610430	2.261715
36	1	0	-4.818728	1.721196	1.472162
37	6	0	-5.908010	0.444846	0.095620
38	1	0	-5.185297	0.557247	-0.710632
39	1	0	-6.327616	-0.561666	0.075879
40	6	0	-8.263868	1.063738	0.324279
41	6	0	-6.717548	2.587535	-0.876993
42	6	0	-9.334816	2.045211	-0.002197
43	6	0	-8.954058	3.214306	-0.766603
44	6	0	-11.530158	2.691993	0.103324
45	6	0	-12.851603	2.439884	0.541959
46	6	0	-11.259435	3.868272	-0.652680
47	6	0	-13.892286	3.302689	0.256339
48	1	0	-13.019265	1.533625	1.115614
49	6	0	-12.317417	4.746632	-0.943987
50	6	0	-13.612006	4.481744	-0.505643
51	1	0	-12.139507	5.647136	-1.517563
52	7	0	-7.007541	1.388545	-0.159454
53	7	0	-7.723001	3.463904	-1.168139
54	7	0	-9.959088	4.099868	-1.072239
55	7	0	-10.550028	1.800049	0.411486
56	8	0	-5.551171	2.796315	-1.221276
57	8	0	-8.470751	0.037152	0.969046
58	6	0	-15.291643	3.008266	0.735379
59	1	0	-15.666368	3.804550	1.388802
60	1	0	-15.992369	2.928493	-0.103624
61	1	0	-15.322275	2.069627	1.293229
62	6	0	-14.718205	5.447135	-0.840154
63	1	0	-15.507915	4.954912	-1.419645
64	1	0	-15.190519	5.835196	0.069730
65	1	0	-14.345099	6.293542	-1.420197
66	6	0	-9.652473	5.308717	-1.856387
67	1	0	-9.905220	6.196126	-1.272616
68	1	0	-8.591298	5.304533	-2.081933

69	1	0	-10.229847	5.297253	-2.783033
70	7	0	-1.100416	-3.838856	-2.221064
71	6	0	-1.166285	-6.230490	-1.750808
72	7	0	1.173934	-6.194537	-0.890941
73	6	0	3.255510	-4.940584	-0.689680
74	6	0	0.272545	-1.764722	-2.445413
75	6	0	-0.895479	-2.613784	-2.985841
76	6	0	-0.978721	-5.084561	-2.738867
77	8	0	-0.711374	-5.306570	-3.931331
78	6	0	2.343810	-5.868297	-1.485632
79	8	0	2.680775	-6.270256	-2.611631
80	1	0	-1.381954	-3.748480	-1.248107
81	1	0	-1.902487	-6.920366	-2.177610
82	1	0	-1.560337	-5.866137	-0.797617
83	1	0	1.006474	-5.862317	0.056594
84	1	0	4.227501	-5.430206	-0.589806
85	1	0	2.860777	-4.754709	0.313581
86	1	0	0.308308	-0.833758	-3.021759
87	1	0	0.098806	-1.503669	-1.397696
88	1	0	-1.808705	-2.009687	-2.955124
89	1	0	-0.710243	-2.898278	-4.022361
90	6	0	0.142535	-7.011468	-1.520566
91	1	0	0.540942	-7.371095	-2.469850
92	1	0	-0.070027	-7.878813	-0.886327
93	8	0	2.083853	-2.691016	-3.739811
94	6	0	1.616835	-2.458945	-2.616952
95	7	0	2.256189	-2.803784	-1.463002
96	1	0	1.790547	-2.608579	-0.577111
97	6	0	3.470420	-3.609443	-1.439925
98	1	0	3.709951	-3.836780	-2.483775
99	6	0	4.703397	-2.866285	-0.884250
100	8	0	5.746617	-3.486965	-0.641517
101	7	0	4.580370	-1.531024	-0.720468
102	1	0	3.695383	-1.106803	-0.964780
103	6	0	5.671182	-0.676018	-0.273653
104	1	0	5.244540	0.155512	0.292413

105	1	0	6.315074	-1.258298	0.388242
106	6	0	6.491159	-0.140027	-1.461808
107	1	0	6.944026	-0.967331	-2.005582
108	1	0	5.850550	0.434345	-2.131503
109	6	0	7.295139	2.100562	-0.893855
110	6	0	8.845533	0.172170	-0.719318
111	6	0	8.447589	2.944557	-0.473240
112	6	0	9.704588	2.273578	-0.216099
113	6	0	9.319073	5.004807	0.021318
114	6	0	9.138968	6.402743	0.144176
115	6	0	10.596971	4.440434	0.297410
116	6	0	10.169526	7.240819	0.524671
117	1	0	8.151209	6.796502	-0.074463
118	6	0	11.646066	5.291724	0.684827
119	6	0	11.451190	6.665544	0.800155
120	1	0	12.626957	4.887513	0.898516
121	7	0	7.575412	0.749787	-1.016379
122	7	0	9.881717	0.971901	-0.330475
123	7	0	10.755356	3.069299	0.171871
124	7	0	8.264674	4.233408	-0.358699
125	8	0	8.971920	-1.050456	-0.827464
126	8	0	6.178149	2.561335	-1.122655
127	6	0	9.947100	8.727607	0.646098
128	1	0	10.153343	9.081582	1.662715
129	1	0	10.607229	9.287216	-0.026469
130	1	0	8.914875	8.987071	0.400376
131	6	0	12.601357	7.543548	1.217555
132	1	0	12.818197	8.298136	0.452648
133	1	0	12.366446	8.087658	2.139733
134	1	0	13.507179	6.957986	1.387226
135	6	0	12.065880	2.460171	0.457575
136	1	0	12.347497	2.670668	1.491406
137	1	0	11.979843	1.389046	0.308245
138	1	0	12.815164	2.871895	-0.221739

Table S4. The coordinates of the optimized geometry of C3FES (0°)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	8.240232	3.772399	1.165639
2	7	0	6.670191	3.917127	-0.763091
3	6	0	4.414101	3.400040	-1.536578
4	6	0	4.038530	2.022178	2.958624
5	6	0	5.547205	2.069952	3.279030
6	6	0	5.851362	2.971011	-1.268397
7	8	0	6.217561	1.810351	-1.518635
8	1	0	9.293427	3.576756	1.392269
9	1	0	8.000650	4.779041	1.514928
10	1	0	6.272318	4.823213	-0.554502
11	1	0	4.225579	3.294637	-2.608213
12	1	0	4.247095	4.449196	-1.271272
13	1	0	3.565386	1.266484	3.590364
14	1	0	3.583880	2.990605	3.182810
15	1	0	5.661899	2.274230	4.349833
16	1	0	6.013754	1.103658	3.074805
17	6	0	8.049819	3.679443	-0.358829
18	1	0	8.328658	2.690157	-0.723952
19	1	0	8.702885	4.415955	-0.839616
20	8	0	3.821117	0.445887	1.138717
21	6	0	3.785509	1.626315	1.513047
22	7	0	3.533481	2.656721	0.655659
23	1	0	3.635819	3.595834	1.024819
24	6	0	3.418770	2.492891	-0.788844
25	1	0	3.669619	1.449912	-1.002177
26	6	0	1.990389	2.700111	-1.337483
27	8	0	1.795992	2.666716	-2.558681
28	7	0	1.013823	2.891229	-0.425782
29	1	0	1.275583	2.887126	0.551400
30	6	0	-0.389979	3.065664	-0.770622
31	1	0	-0.810722	3.842425	-0.126805
32	1	0	-0.444602	3.399795	-1.807953

33	6	0	-1.179215	1.755174	-0.595353
34	1	0	-0.806091	0.996775	-1.281305
35	1	0	-1.091342	1.397802	0.431161
36	6	0	-3.423384	2.358697	0.167626
37	6	0	-3.075504	1.726916	-2.206306
38	6	0	-4.860639	2.523968	-0.184601
39	6	0	-5.244601	2.253484	-1.554180
40	6	0	-7.002266	3.060280	0.427405
41	6	0	-7.912281	3.476576	1.427755
42	6	0	-7.481038	2.814397	-0.890975
43	6	0	-9.257029	3.652978	1.163304
44	1	0	-7.510626	3.654443	2.420551
45	6	0	-8.849108	2.990972	-1.160619
46	6	0	-9.730592	3.401471	-0.164011
47	1	0	-9.238393	2.809874	-2.154059
48	7	0	-2.610549	1.947724	-0.875722
49	7	0	-4.400954	1.879756	-2.496325
50	7	0	-6.575139	2.410335	-1.859075
51	7	0	-5.689732	2.905699	0.750756
52	8	0	-2.254067	1.398922	-3.066563
53	8	0	-2.982736	2.568969	1.296303
54	6	0	-10.203315	4.100065	2.249208
55	1	0	-10.696356	5.043009	1.986592
56	1	0	-10.995827	3.362010	2.418273
57	1	0	-9.671327	4.247391	3.191769
58	6	0	-11.189003	3.580072	-0.494478
59	1	0	-11.816365	2.935755	0.132242
60	1	0	-11.511459	4.611175	-0.308379
61	1	0	-11.391303	3.342145	-1.540635
62	6	0	-7.045515	2.151475	-3.231042
63	1	0	-7.490152	3.060450	-3.641506
64	1	0	-6.191549	1.854688	-3.830808
65	1	0	-7.786842	1.349874	-3.216200
66	6	0	9.618282	-0.688882	-0.171836
67	7	0	7.693408	-0.763283	-1.764338
68	6	0	5.409155	-1.555792	-2.105053

69	6	0	5.998519	-2.487407	2.447000
70	6	0	7.540570	-2.424345	2.548628
71	6	0	6.908799	-1.828028	-2.049353
72	8	0	7.353629	-2.968278	-2.259107
73	1	0	10.706801	-0.809930	-0.147254
74	1	0	9.381781	0.310468	0.195423
75	1	0	7.251783	0.143156	-1.620257
76	1	0	5.065793	-1.776709	-3.119678
77	1	0	5.186397	-0.506590	-1.890722
78	1	0	5.628758	-3.167793	3.219355
79	1	0	5.573892	-1.497681	2.633323
80	1	0	7.810442	-2.225314	3.590732
81	1	0	7.970645	-3.391359	2.273652
82	6	0	9.138308	-0.862975	-1.624531
83	1	0	9.437542	-1.839819	-2.008993
84	1	0	9.621943	-0.094556	-2.237770
85	8	0	5.744422	-4.232827	0.807851
86	6	0	5.550071	-3.046157	1.102643
87	7	0	4.958192	-2.159165	0.254468
88	1	0	4.826496	-1.198254	0.566768
89	6	0	4.650667	-2.482879	-1.133353
90	1	0	4.998400	-3.507496	-1.293595
91	6	0	3.146011	-2.499158	-1.467342
92	8	0	2.779646	-2.704401	-2.632272
93	7	0	2.292014	-2.305296	-0.439724
94	1	0	2.687754	-2.135365	0.475490
95	6	0	0.843654	-2.318594	-0.583145
96	1	0	0.425108	-1.525971	0.042376
97	1	0	0.604409	-2.107261	-1.626585
98	6	0	0.251014	-3.679024	-0.173622
99	1	0	0.629914	-4.464393	-0.825619
100	1	0	0.507707	-3.905093	0.861885
101	6	0	-1.943185	-3.276639	0.831966
102	6	0	-1.808379	-4.082486	-1.510109
103	6	0	-3.422044	-3.345881	0.671984
104	6	0	-3.931627	-3.793387	-0.607326

105	6	0	-5.524569	-3.075829	1.540771
106	6	0	-6.352217	-2.715614	2.630347
107	6	0	-6.124340	-3.504969	0.322612
108	6	0	-7.730592	-2.768343	2.548518
109	1	0	-5.859098	-2.394193	3.542489
110	6	0	-7.526337	-3.557292	0.237410
111	6	0	-8.325602	-3.199694	1.319970
112	1	0	-8.007047	-3.880624	-0.676817
113	7	0	-1.217062	-3.683750	-0.274818
114	7	0	-3.167975	-4.132129	-1.627456
115	7	0	-5.298394	-3.856560	-0.733453
116	7	0	-4.173372	-3.005313	1.685516
117	8	0	-1.062362	-4.379752	-2.446900
118	8	0	-1.399902	-2.895716	1.867341
119	6	0	-8.587896	-2.382420	3.727922
120	1	0	-9.259105	-1.552233	3.480182
121	1	0	-9.219840	-3.217062	4.052578
122	1	0	-7.969307	-2.076803	4.574768
123	6	0	-9.824072	-3.273265	1.189083
124	1	0	-10.250352	-3.956874	1.932414
125	1	0	-10.283317	-2.293150	1.362227
126	1	0	-10.119896	-3.619402	0.196680
127	6	0	-5.894327	-4.307938	-2.002714
128	1	0	-6.522651	-3.514812	-2.413066
129	1	0	-5.088330	-4.535020	-2.692571
130	1	0	-6.494824	-5.202407	-1.824601
131	7	0	7.412949	2.834297	1.910620
132	7	0	9.003331	-1.637259	0.748649
133	1	0	9.208497	-2.619775	0.624179
134	1	0	7.672322	1.848965	1.905995
135	8	0	7.810733	-0.110312	1.951453
136	8	0	5.809235	4.346788	2.517625
137	6	0	6.264443	3.189723	2.529986
138	6	0	8.129607	-1.289715	1.719280

Table S5. The coordinates of the optimized geometry of C3FES (120°)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.929035	-3.606740	3.703557
2	7	0	0.445989	-4.278620	3.465087
3	6	0	2.637241	-3.716727	2.576196
4	6	0	0.168157	0.198982	1.815709
5	6	0	-1.279852	-0.289890	1.929671
6	6	0	1.246294	-4.296812	2.391455
7	8	0	0.908470	-4.738552	1.311782
8	1	0	-2.927182	-4.028641	3.740504
9	1	0	-1.734529	-3.133355	4.659166
10	1	0	0.813146	-3.912991	4.314685
11	1	0	3.346466	-4.488112	2.310550
12	1	0	2.822678	-3.429723	3.605317
13	1	0	0.188869	1.063274	1.161883
14	1	0	0.534029	0.511609	2.787148
15	1	0	-1.899218	0.538950	2.251529
16	1	0	-1.640954	-0.628048	0.971806
17	6	0	-0.929438	-4.745503	3.471784
18	1	0	-1.120211	-5.229929	2.527904
19	1	0	-1.049188	-5.478741	4.259844
20	8	0	0.976595	-1.147536	0.027514
21	6	0	1.074063	-0.847220	1.196220
22	7	0	1.983477	-1.411328	2.022269
23	1	0	1.946694	-1.161719	2.986045
24	6	0	2.841035	-2.515074	1.642537
25	1	0	2.563777	-2.804454	0.639371
26	6	0	4.328823	-2.154510	1.561398
27	8	0	5.137755	-3.034805	1.349447
28	7	0	4.660212	-0.869988	1.702755
29	1	0	3.931684	-0.209793	1.847730
30	6	0	6.021780	-0.381853	1.600133
31	1	0	6.116045	0.479038	2.248625
32	1	0	6.694691	-1.150190	1.950375

33	6	0	6.363145	0.004790	0.161477
34	1	0	6.297303	-0.854568	-0.483487
35	1	0	5.683842	0.764245	-0.191496
36	6	0	7.889276	1.895558	0.214873
37	6	0	8.779238	-0.354931	-0.186866
38	6	0	9.288105	2.377316	0.048121
39	6	0	10.294185	1.368974	-0.233167
40	6	0	10.831951	4.058760	-0.008955
41	6	0	11.127124	5.429865	0.102761
42	6	0	11.860570	3.161110	-0.282634
43	6	0	12.403966	5.898607	-0.051870
44	1	0	10.314156	6.100345	0.314541
45	6	0	13.168421	3.623604	-0.443209
46	6	0	13.446735	4.967566	-0.331785
47	1	0	13.955233	2.922119	-0.653621
48	7	0	7.725028	0.545176	0.056583
49	7	0	10.053997	0.100518	-0.335633
50	7	0	11.538037	1.829576	-0.383725
51	7	0	9.548290	3.619896	0.151384
52	8	0	8.522583	-1.530348	-0.261687
53	8	0	6.978532	2.635941	0.464173
54	6	0	12.699911	7.374821	0.071980
55	1	0	13.409649	7.570426	0.869480
56	1	0	13.122819	7.771679	-0.845491
57	1	0	11.793479	7.925951	0.288299
58	6	0	14.865337	5.447966	-0.508019
59	1	0	14.933877	6.157596	-1.326030
60	1	0	15.217236	5.949300	0.387757
61	1	0	15.530750	4.621146	-0.718469
62	6	0	12.589538	0.842064	-0.666685
63	1	0	12.849026	0.328883	0.235652
64	1	0	12.231979	0.137025	-1.387774
65	1	0	13.452989	1.341485	-1.053896
66	6	0	1.608012	-5.296313	-1.706191
67	7	0	0.919563	-2.980015	-2.262817
68	6	0	-0.919809	-1.410280	-2.507933

69	6	0	-2.992810	-5.153455	-0.584707
70	6	0	-1.982848	-6.273438	-0.857337
71	6	0	-0.051998	-2.525004	-3.064402
72	8	0	-0.260694	-2.961794	-4.178230
73	1	0	2.336700	-6.050683	-1.981144
74	1	0	1.780871	-5.031994	-0.669191
75	1	0	1.028894	-2.550470	-1.371837
76	1	0	-0.855579	-0.577917	-3.194701
77	1	0	-0.572480	-1.072948	-1.537667
78	1	0	-3.981409	-5.592015	-0.512211
79	1	0	-2.773600	-4.675967	0.363578
80	1	0	-2.090011	-7.029056	-0.088091
81	1	0	-2.178582	-6.734570	-1.811955
82	6	0	1.819424	-4.069182	-2.600143
83	1	0	1.659543	-4.323404	-3.635411
84	1	0	2.841755	-3.729626	-2.488077
85	8	0	-3.497728	-4.431189	-2.795524
86	6	0	-3.038279	-4.142094	-1.713447
87	7	0	-2.541183	-2.916254	-1.434482
88	1	0	-2.114275	-2.784719	-0.543992
89	6	0	-2.382829	-1.867719	-2.421071
90	1	0	-2.674236	-2.280815	-3.375736
91	6	0	-3.302780	-0.660331	-2.206588
92	8	0	-3.174357	0.312660	-2.921434
93	7	0	-4.228062	-0.752821	-1.249979
94	1	0	-4.281477	-1.596608	-0.727679
95	6	0	-5.194285	0.291963	-0.971573
96	1	0	-5.426953	0.256757	0.084451
97	1	0	-4.745776	1.249067	-1.192063
98	6	0	-6.466935	0.101546	-1.796109
99	1	0	-6.245151	0.162918	-2.847706
100	1	0	-6.908375	-0.859084	-1.583666
101	6	0	-8.359420	0.866899	-0.477145
102	6	0	-7.450511	2.322433	-2.230267
103	6	0	-9.375650	1.931073	-0.250364
104	6	0	-9.285221	3.107732	-1.096161

105	6	0	-11.200236	2.753988	0.848576
106	6	0	-12.186823	2.592089	1.838511
107	6	0	-11.189763	3.916043	0.081598
108	6	0	-13.135548	3.553144	2.062672
109	1	0	-12.171400	1.685523	2.415757
110	6	0	-12.150894	4.905767	0.298007
111	6	0	-13.112153	4.737581	1.269500
112	1	0	-12.133457	5.799336	-0.299204
113	7	0	-7.470085	1.128567	-1.485202
114	7	0	-8.385815	3.287553	-2.010436
115	7	0	-10.212081	4.042650	-0.875133
116	7	0	-10.265457	1.778235	0.648107
117	8	0	-6.590591	2.463349	-3.063187
118	8	0	-8.327605	-0.142006	0.171599
119	6	0	-14.186410	3.359940	3.130609
120	1	0	-14.137481	4.143471	3.880062
121	1	0	-15.186332	3.374314	2.708650
122	1	0	-14.047972	2.409701	3.630649
123	6	0	-14.141504	5.817693	1.488758
124	1	0	-15.144305	5.431885	1.337244
125	1	0	-14.089929	6.199944	2.503058
126	1	0	-13.987985	6.643085	0.806223
127	6	0	-10.155912	5.253092	-1.707343
128	1	0	-9.373650	5.892350	-1.354757
129	1	0	-9.961751	4.978803	-2.723200
130	1	0	-11.091449	5.769195	-1.649827
131	7	0	-1.907874	-2.595897	2.571765
132	7	0	0.231909	-5.906596	-1.898800
133	1	0	-0.100450	-6.517523	-3.067520
134	1	0	-2.352951	-2.931532	1.331259
135	8	0	-0.311742	-5.416782	-0.127502
136	8	0	-1.187561	-1.231363	3.708497
137	6	0	-1.411493	-1.386104	2.871652
138	6	0	-0.616689	-5.783683	-0.866955

Table S6. The coordinates of the optimized geometry of C3FES (240°)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.700436	-4.467961	3.805188
2	7	0	1.141007	-2.113893	3.207321
3	6	0	-0.538152	-0.627183	2.236161
4	6	0	-2.860374	-4.698450	2.504098
5	6	0	-1.741529	-5.742164	2.681340
6	6	0	0.611217	-1.612507	2.069959
7	8	0	1.010799	-1.925387	0.937201
8	1	0	2.554235	-5.151352	3.857895
9	1	0	1.319245	-4.336390	4.822796
10	1	0	0.757900	-1.796699	4.088044
11	1	0	-0.247294	0.313251	1.761530
12	1	0	-0.750975	-0.417976	3.289757
13	1	0	-3.713334	-5.190844	2.026081
14	1	0	-3.194392	-4.336128	3.481356
15	1	0	-2.144572	-6.600956	3.226883
16	1	0	-1.384221	-6.089309	1.711613
17	6	0	2.198884	-3.119365	3.252121
18	1	0	2.577271	-3.240218	2.237089
19	1	0	3.013899	-2.753575	3.883367
20	8	0	-2.191290	-3.733597	0.402078
21	6	0	-2.435574	-3.550591	1.600784
22	7	0	-2.344319	-2.324826	2.191551
23	1	0	-2.472920	-2.281923	3.195194
24	6	0	-1.804980	-1.144235	1.525870
25	1	0	-1.530048	-1.461606	0.515690
26	6	0	-2.824445	-0.001049	1.336282
27	8	0	-2.436451	1.098586	0.924190
28	7	0	-4.115929	-0.285132	1.608256
29	1	0	-4.341981	-1.221627	1.916519
30	6	0	-5.202925	0.661296	1.394100
31	1	0	-5.931711	0.539888	2.199108
32	1	0	-4.787388	1.669027	1.442891

33	6	0	-5.878506	0.435493	0.029267
34	1	0	-5.154259	0.568429	-0.772472
35	1	0	-6.301142	-0.568759	-0.019530
36	6	0	-8.232806	1.054929	0.272056
37	6	0	-6.680078	2.607325	-0.883461
38	6	0	-9.300278	2.048541	-0.028015
39	6	0	-8.914833	3.237614	-0.758504
40	6	0	-11.493797	2.698844	0.092699
41	6	0	-12.816652	2.438502	0.522179
42	6	0	-11.218376	3.895199	-0.629343
43	6	0	-13.854280	3.312246	0.259633
44	1	0	-12.987920	1.516899	1.069728
45	6	0	-12.273248	4.784706	-0.897158
46	6	0	-13.569285	4.511515	-0.468292
47	1	0	-12.091749	5.700523	-1.444776
48	7	0	-6.974781	1.389416	-0.200539
49	7	0	-7.682428	3.494675	-1.151098
50	7	0	-9.916710	4.134562	-1.040365
51	7	0	-10.516843	1.795522	0.376869
52	8	0	-5.512562	2.822164	-1.220070
53	8	0	-8.443767	0.011156	0.887229
54	6	0	-15.255236	3.008704	0.728196
55	1	0	-15.628505	3.787336	1.403364
56	1	0	-15.954956	2.954859	-0.113705
57	1	0	-15.289550	2.054759	1.259222
58	6	0	-14.672045	5.489389	-0.776899
59	1	0	-15.462389	5.016193	-1.371187
60	1	0	-15.144525	5.853009	0.142940
61	1	0	-14.295506	6.350712	-1.332240
62	6	0	-9.605256	5.364159	-1.789567
63	1	0	-9.856168	6.235473	-1.181275
64	1	0	-8.543766	5.363086	-2.013659
65	1	0	-10.181288	5.380694	-2.716972
66	6	0	-1.154376	-6.199523	-1.998670
67	7	0	1.184664	-6.195124	-1.134863
68	6	0	3.269744	-4.953789	-0.895297

69	6	0	0.299061	-1.720349	-2.564633
70	6	0	-0.870738	-2.550178	-3.130498
71	6	0	2.356407	-5.855799	-1.718451
72	8	0	2.693817	-6.226780	-2.854901
73	1	0	-1.892040	-6.874776	-2.445847
74	1	0	-1.548731	-5.861068	-1.036102
75	1	0	1.016810	-5.889327	-0.178542
76	1	0	4.240092	-5.449035	-0.807959
77	1	0	2.874091	-4.795154	0.112269
78	1	0	0.338510	-0.773568	-3.114357
79	1	0	0.124563	-1.488505	-1.510193
80	1	0	-1.782167	-1.944379	-3.083977
81	1	0	-0.684831	-2.805805	-4.174393
82	6	0	0.151719	-6.990733	-1.788789
83	1	0	0.550438	-7.324587	-2.747311
84	1	0	-0.064421	-7.875013	-1.179642
85	8	0	2.109460	-2.615234	-3.882191
86	6	0	1.641486	-2.413582	-2.753868
87	7	0	2.278076	-2.792897	-1.609246
88	1	0	1.811716	-2.621397	-0.718837
89	6	0	3.489815	-3.602626	-1.607278
90	1	0	3.730201	-3.801079	-2.656807
91	6	0	4.724221	-2.879289	-1.029077
92	8	0	5.765187	-3.509801	-0.802546
93	7	0	4.605014	-1.548823	-0.827753
94	1	0	3.721685	-1.115134	-1.061200
95	6	0	5.697758	-0.710166	-0.355403
96	1	0	5.272809	0.106329	0.233367
97	1	0	6.338894	-1.312920	0.290651
98	6	0	6.521123	-0.143308	-1.526771
99	1	0	6.972277	-0.956290	-2.093102
100	1	0	5.883258	0.451752	-2.180840
101	6	0	7.331072	2.077828	-0.894528
102	6	0	8.875332	0.140500	-0.772458
103	6	0	8.485459	2.906030	-0.448593
104	6	0	9.740028	2.224173	-0.208785

105	6	0	9.362472	4.948768	0.105276
106	6	0	9.186438	6.343217	0.267386
107	6	0	10.638236	4.372874	0.367073
108	6	0	10.218976	7.167013	0.672879
109	1	0	8.200207	6.746047	0.058596
110	6	0	11.689341	5.209625	0.779885
111	6	0	11.498474	6.580227	0.933766
112	1	0	12.668679	4.796509	0.983422
113	7	0	7.607416	0.730202	-1.054831
114	7	0	9.913366	0.925713	-0.359697
115	7	0	10.792636	3.005357	0.203011
116	7	0	8.306296	4.191682	-0.297887
117	8	0	8.998159	-1.078961	-0.914977
118	8	0	6.215829	2.548331	-1.111759
119	6	0	10.000894	8.650450	0.836014
120	1	0	10.206705	8.974886	1.862526
121	1	0	10.663719	9.226823	0.180472
122	1	0	8.969828	8.919942	0.596291
123	6	0	12.650686	7.442521	1.377446
124	1	0	12.870955	8.217774	0.634499
125	1	0	12.416064	7.961047	2.314321
126	1	0	13.554470	6.849604	1.531746
127	6	0	12.100875	2.384353	0.473195
128	1	0	12.381598	2.564650	1.512960
129	1	0	12.011802	1.318152	0.293499
130	1	0	12.852415	2.812818	-0.193151
131	7	0	0.657020	-5.103093	2.895771
132	7	0	-0.961862	-5.026684	-2.953647
133	8	0	-1.425264	-3.718102	-1.212392
134	8	0	-0.773289	-4.837907	4.574679
135	6	0	-0.592795	-5.206511	3.404571
136	6	0	-1.080535	-3.795757	-2.400976
137	1	0	-0.741417	-5.181901	-3.937371
138	1	0	0.902117	-5.411089	1.954779

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