Electronic Supplementary Information for:

Meso Bromination and Derivatization of Synthetic Bacteriochlorins

Haoyu Jing, Sijia Liu, Jianbing Jiang, Vy-Phuong Tran, Jie Rong, Pengzhi Wang, and Jonathan S. Lindsey*

Department of Chemistry
North Carolina State University
Raleigh, North Carolina 27695-8204

Contents **Pages**

X-ray structural data S1–S8

(1) X-ray structural data

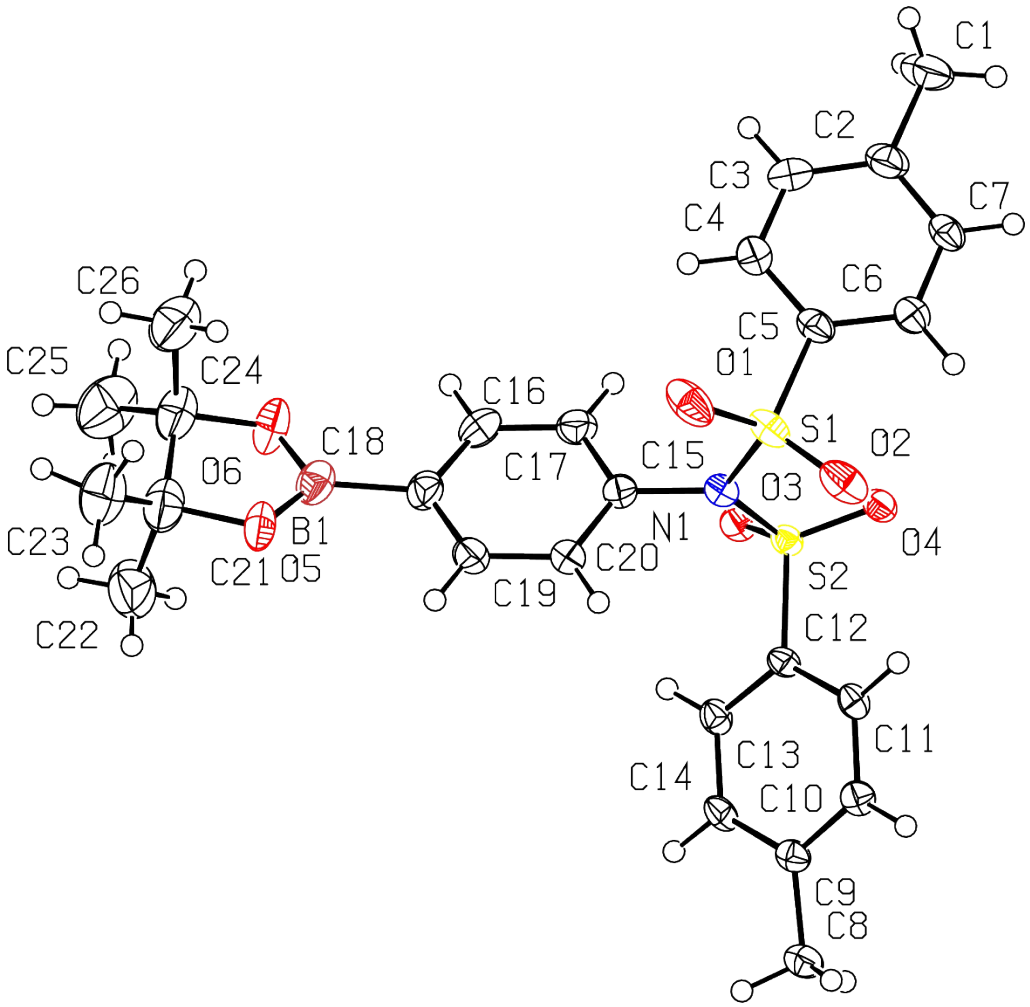

Figure S1. Single-crystal X-ray structure of **8**.

Table S1. Summary of Crystal Data for 8.

CCDC registry	2125372
Chemical formula	$C_{26}H_{30}BNO_6S_2$
Formula weight (g/mol)	527.44
Temperature (K)	100.00
Wavelength (Å)	1.54178
Crystal size (mm)	0.62 × 0.43 × 0.02
Crystal habit	Clear light colorless plate
Crystal system	Orthorhombic
Space group	*P*bca
Unit cell dimension, *a* (Å)	13.1157(3)
Unit cell dimension, *b* (Å)	13.2742(4)
Unit cell dimension, *c* (Å)	29.9769(8)
α, deg	90
β, deg	90
γ, deg	90
Volume (Å^3)	5219.0(2)
Z	8
Density (calculated) (g/cm^3)	1.343
Absorption coefficient (mm^{-1})	2.197
F(000)	2224
Theta range for data collection, deg	4.479 to 66.589
Index ranges	-15 <=h<=15, -13<=k<=15, -35<=l<=35
Reflections collected	47668
Independent reflections	4592 [R(int) = 0.055]
R_1	0.0692
wR_2	0.1753
R_1 (all data)	0.0741
wR_2 (all data)	0.1782
Largest diff. peak and hole (eÅ^3)	0.76 and −0.48
R.M.S. deviation from mean (eÅ^3)	0.086

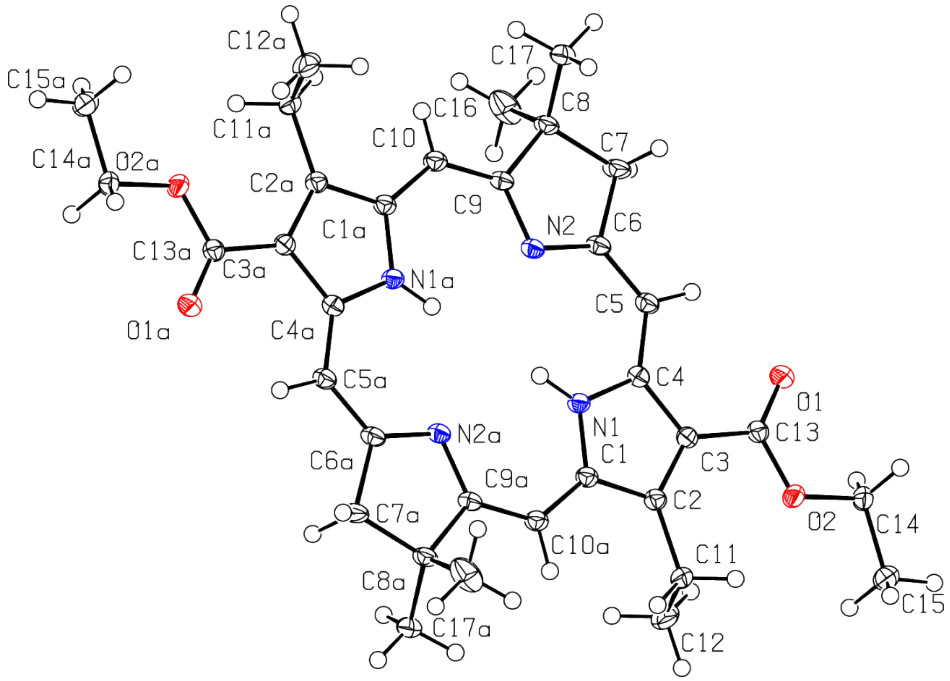

Figure S2. Single-crystal X-ray structure of **BC-6**.

Table S2. Summary of Crystal Data for BC-6.

CCDC registry	2120236
Chemical formula	$C_{34}H_{42}N_4O_4$
Formula weight (g/mol)	570.71
Temperature (K)	110
Wavelength (Å)	0.71073
Crystal size (mm)	0.42 × 0.25 × 0.15
Crystal habit	Purple block
Crystal system	Triclinic
Space group	*P*1
Unit cell dimension, *a* (Å)	6.9814(3)
Unit cell dimension, *b* (Å)	9.7210(5)
Unit cell dimension, *c* (Å)	11.6464(5)
α, deg	75.978(3)
β, deg	85.771(2)
γ, deg	75.899(3)
Volume (Å^3)	743.65(6)
Z	1
Density (calculated) (g/cm^3)	1.274
Absorption coefficient (mm^{-1})	0.084
F(000)	306
Theta range for data collection, deg	1.80 to 32.88
Index ranges	-10 <=h<=6, -14<=k<=14, -17<=l<=17
Reflections collected	20131
Independent reflections	5461 [R(int) = 0.031]
R_1	0.0440
wR_2	0.1027
R_1 (all data)	0.1093
wR_2 (all data)	0.1202
Largest diff. peak and hole (eÅ^3)	0.44 and −0.29
R.M.S. deviation from mean (eÅ^3)	0.051

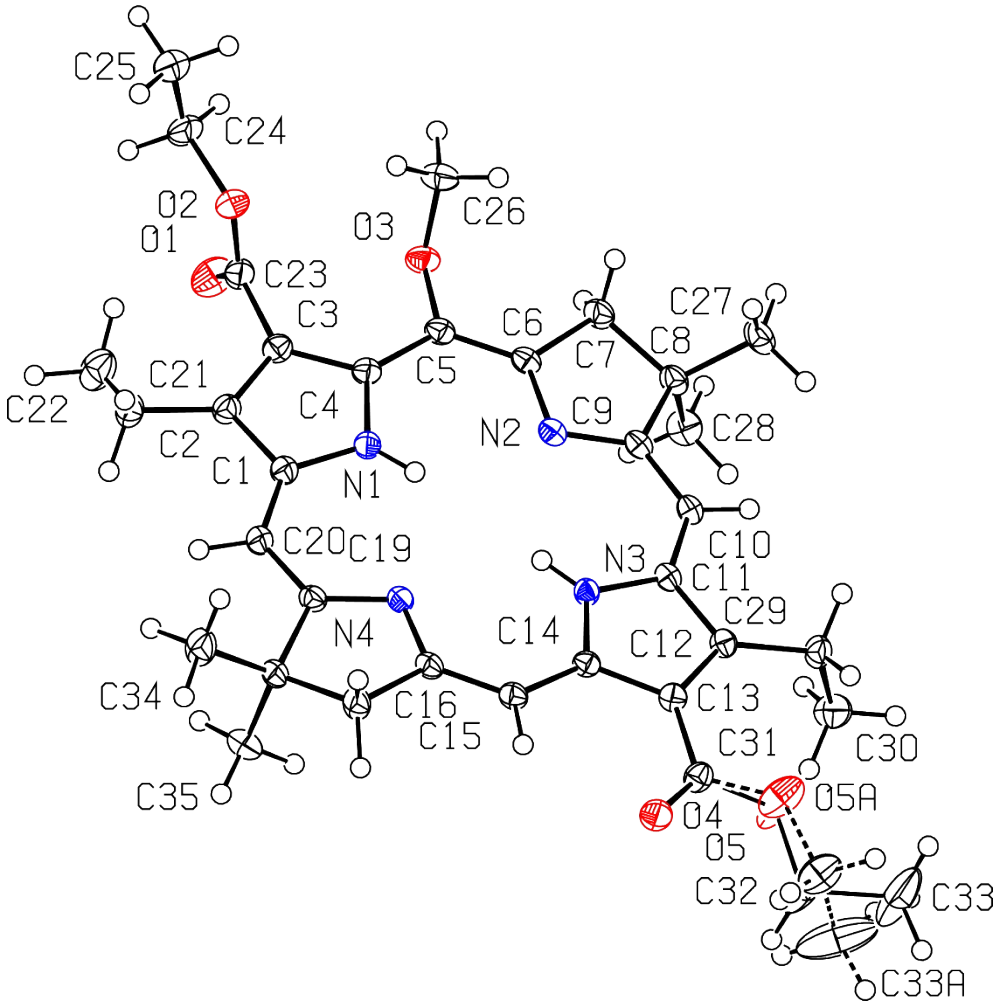

Figure S3. Single-crystal X-ray structure of **BC-7**.

Table S3. Summary of Crystal Data for BC-7.

CCDC registry	2120266
Chemical formula	$C_{35}H_{44}N_4O_5$
Formula weight (g/mol)	600.74
Temperature (K)	110
Wavelength (Å)	0.71073
Crystal size (mm)	0.60 × 0.33 × 0.23
Crystal habit	Dark green parallelapiped
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimension, *a* (Å)	13.9883(3)
Unit cell dimension, *b* (Å)	11.3135(3)
Unit cell dimension, *c* (Å)	20.5010(5)
α, deg	90
β, deg	92.5280(10)
γ, deg	90
Volume (Å^3)	3241.26(14)
Z	4
Density (calculated) (g/cm^3)	1.231
Absorption coefficient (mm^{-1})	0.072
F(000)	1288
Theta range for data collection, deg	1.99 to 30.51
Index ranges	-19 <=h<=19, -14<=k<=16, -29<=l<=25
Reflections collected	58352
Independent reflections	9892 [R(int) = 0.038]
R_1	0.0479
wR_2	0.1173
R_1 (all data)	0.0692
wR_2 (all data)	0.1296
Largest diff. peak and hole (eÅ^3)	0.45 and −0.25
R.M.S. deviation from mean (eÅ^3)	0.050

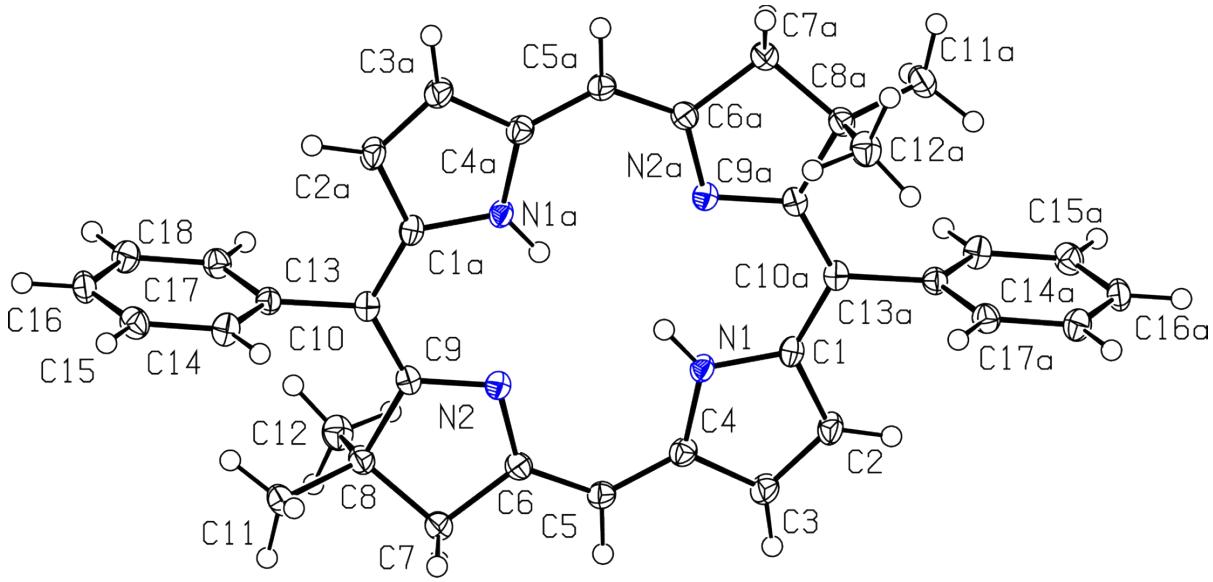

Figure S4. Single-crystal X-ray structure of **BC-8**.

Table S3. Summary of Crystal Data for BC-8.

CCDC registry	2120133
Chemical formula	$C_{36}H_{34}N_4$
Formula weight (g/mol)	522.67
Temperature (K)	100
Wavelength (Å)	1.54178
Crystal size (mm)	0.35 × 0.10 × 0.04
Crystal habit	Dark red plate
Crystal system	Triclinic
Space group	*P*1
Unit cell dimension, *a* (Å)	6.95760(10)
Unit cell dimension, *b* (Å)	8.7932(2)
Unit cell dimension, *c* (Å)	12.4732(2)
α, deg	106.0936(6)
β, deg	105.0837(6)
γ, deg	98.5367(6)
Volume (Å^3)	687.64(2)
Z	1
Density (calculated) (g/cm^3)	1.262
Absorption coefficient (mm^{-1})	0.575
F(000)	278
Theta range for data collection, deg	3.89 to 72.10
Index ranges	-8 <=h<=8, -10<=k<=10, -15<=l<=15
Reflections collected	18219
Independent reflections	2709 [R(int) = 0.022]
R_1	0.0349
wR_2	0.0859
R_1 (all data)	0.0357
wR_2 (all data)	0.0865
Largest diff. peak and hole (eÅ^3)	0.25 and −0.22
R.M.S. deviation from mean (eÅ^3)	0.039