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Supplementary Information for:

Polarity-Tunable and Wavelength-Tunable Bacteriochlorins Bearing a Single Carboxylic Acid (or NHS Ester) for Bioconjugation

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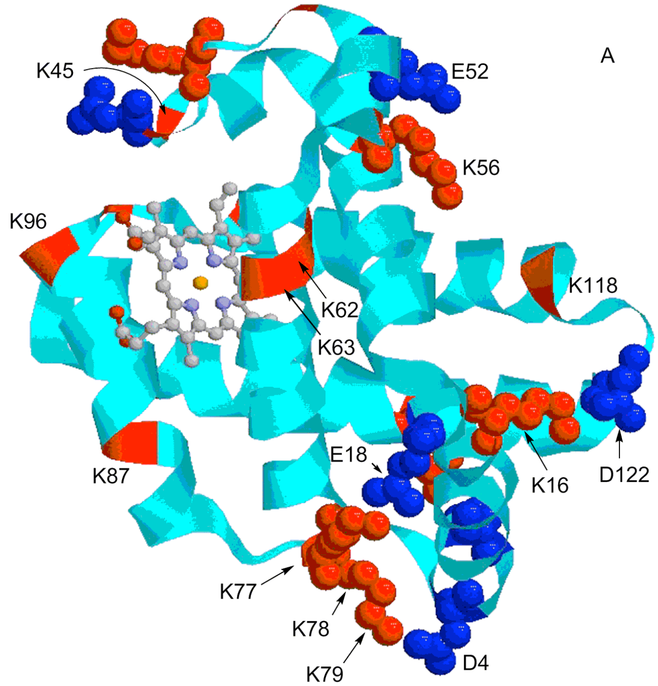
1. Sequence and Structure of Mb

	10	20	30	40	50	60
Equine	GLSDGEWQQV	LNVWGKVEAD	IAGHGQEVLI	RLFTGHPETL	EKFDKFKHLK	TEAEMKASED
Whale	VLSEGEWQLV	LHVWAKVEAD	VAGHGQNILI	RLFKSHPETL	EKFDRFKHLK	TEAEMKASED
Mouse	GLSDGEWQLV	LNVWGKVEAD	LAGHGQEVLI	GLFTGHPETL	DKFDKFKHLK	SEEDMKGSED
Rat	GLSDGEWQMV	LNVWGKVEAD	LAGHGQEVLI	SLFTGHPETL	EKFDKFKHLK	SEEEMKSSED
Human	GLSDGEWQLV	LNVWGKVEAD	IPGHGQEVLI	RLFTGHPETL	EKFDKFKHLK	SEDEMKASED
Pig	GLSDGEWQLV	LNVWGKVEAD	VAGHGQEVLI	RLFTGHPETL	EKFDKFKHLK	SEDEMKASED
Cow	GLSDGEWQLV	LNVWGKVEAD	VAGHGQEVLI	RLFTGHPETL	EKFDKFKHLK	TEAEMKASED

	70	80	90	100	110	120
Equine	LKKHGTVVLT	ALGGILKKKG	HHEAELKPLA	QSHATKHKIP	IKYLEFISDA	IIHVLHSKHP
Whale	LKKHGVTVLT	ALGAILKKKG	HHEAELKPLA	QSHATKHKIP	IKYLEFISEA	IIHVLHSRHP
Mouse	LKKHGCTVLT	ALGTILKKKG	QHAAEIQPLA	QSHATKHKIP	VKYLEFISEI	IIEVLKKRHS
Rat	LKKHGCTVLT	ALGTILKKKG	QHAAEIQPLA	QSHATKHKIP	VKYLEFISEV	IIQVLKKRYS
Human	LKKHGATVLT	ALGGILKKKG	HHEAEIKPLA	QSHATKHKIP	VKYLEFISEC	IIQVLQSKHP
Pig	LKKHGNTVLT	ALGGILKKKG	HHEAELTPLA	QSHATKHKIP	VKYLEFISEA	IIQVLQSKHP
Cow	LKKHGNTVLT	ALGGILKKKG	HHEAEVKHLA	ESHANKHKIP	VKYLEFISDA	IIHVLHAKHP

	130	140	150		total # of K's
Equine	GDFGADAQGA	MTKALELFRN	DIAAKYKELG	FQG	19
Whale	GDFGADAQGA	MNKALELFRK	DIAAKYKELG	YQG	19
Mouse	GDFGADAQGA	MSKALELFRN	DIAAKYKELG	FQG	19
Rat	GDFGADAQGA	MSKALELFRN	DIAAKYKELG	FQG	19
Human	GDFGADAQGA	MNKALELFRK	DMASNYKELG	FQG	19
Pig	GDFGADAQGA	MSKALELFRN	DMAAKYKELG	FQG	18
Cow	SDFGADAQAA	MSKALELFRN	DMAAQYKVLG	FHG	18

Figure S1. Sequence alignment of Mbs from different organisms.



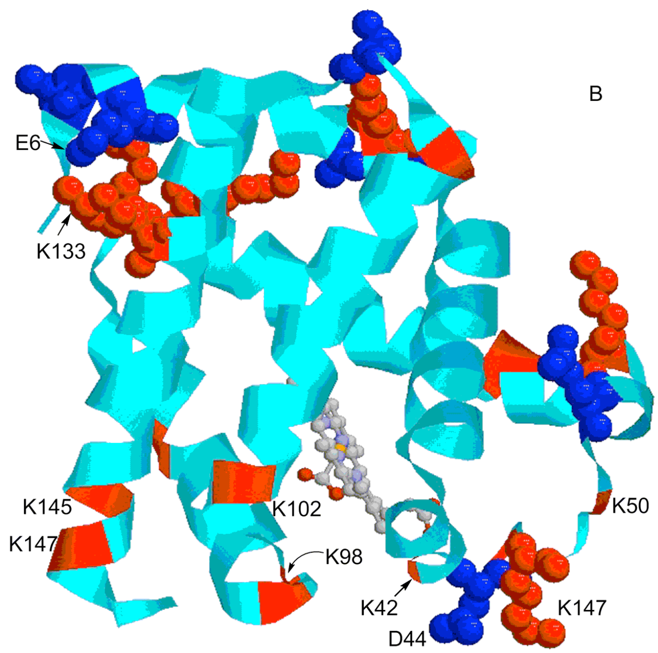


Figure S2. Views of equine Mb from different perspectives exhibiting all 19 Lys residues (red) and the ion-pair counterparts (blue). Residues forming the ion pairs are displayed in spacefill. The Mb crystal data ID is 1NPF, retrieved from Protein Data Bank, and visualized by Rasmol.

2. MALDI-MS and Spectral Data for Mb–Bacteriochlorin Conjugates

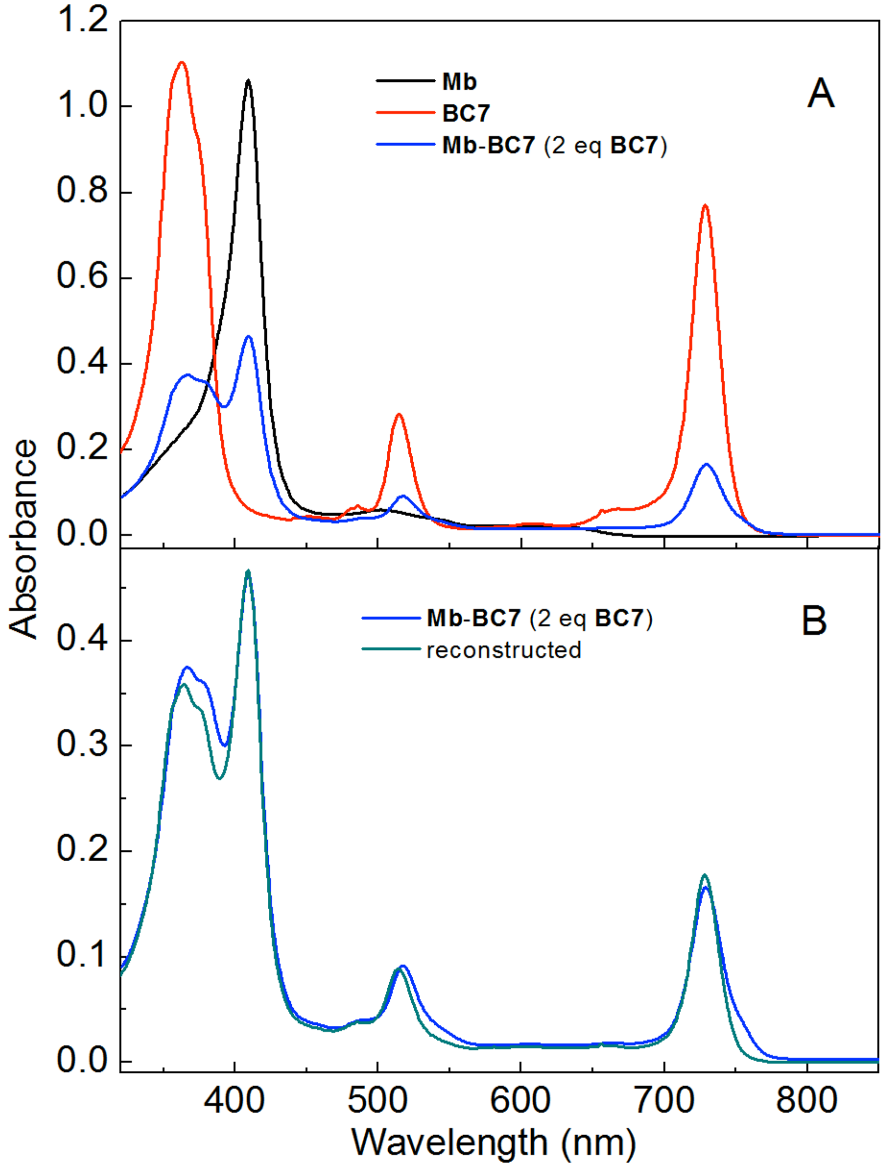


Figure S3. Absorption spectra of Mb, **BC7** and conjugate **Mb-BC7** derived from 2 equiv of **BC7** in potassium phosphate buffer (500 mM, pH 7.0). The concentration of each component is chosen arbitrarily (A). The experimental (blue) and reconstructed (cyan) absorption spectra of conjugate **Mb-BC7** (B).

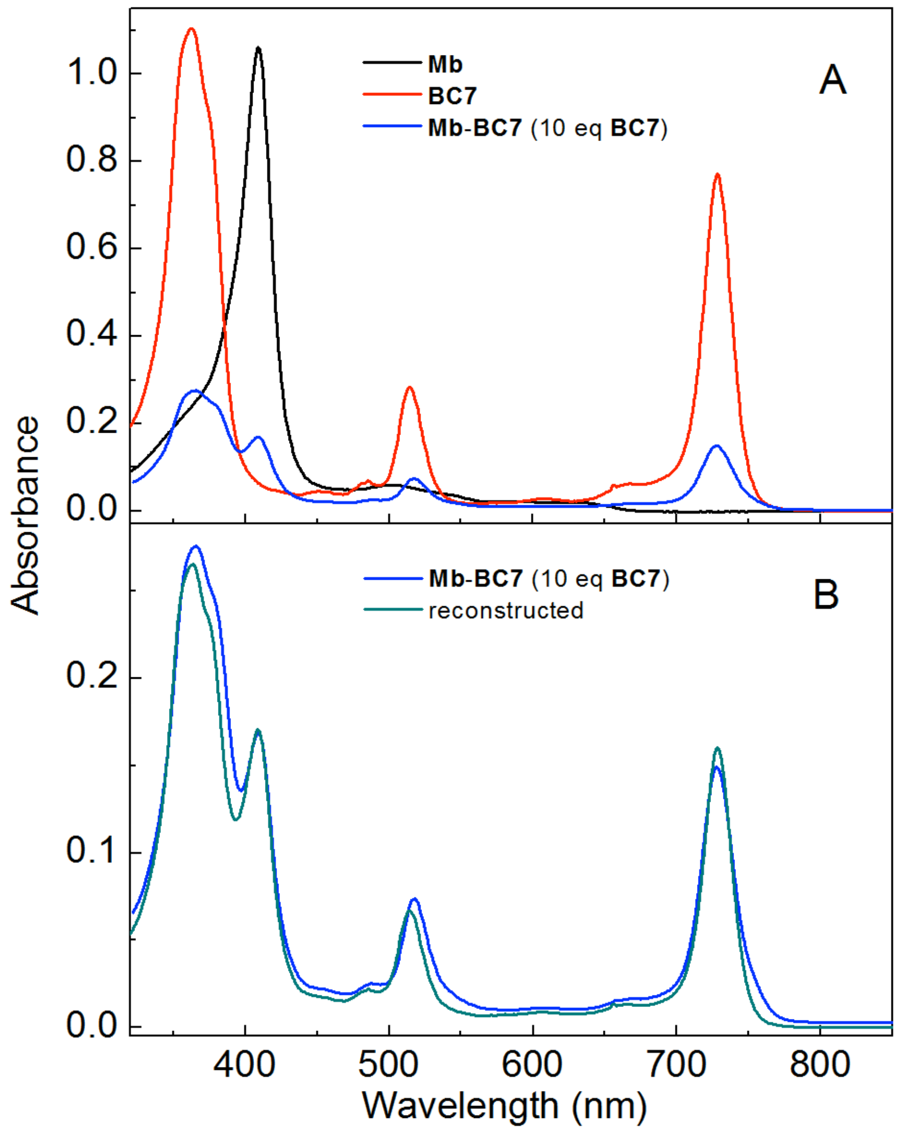


Figure S4. Absorption spectra of Mb, **BC7** and conjugate **Mb-BC7** derived from 10 equiv of **BC7** in potassium phosphate buffer (500 mM, pH 7.0). The concentration of each component is chosen arbitrarily (A). The experimental (blue) and reconstructed (cyan) absorption spectra of conjugate **Mb-BC7** (B).

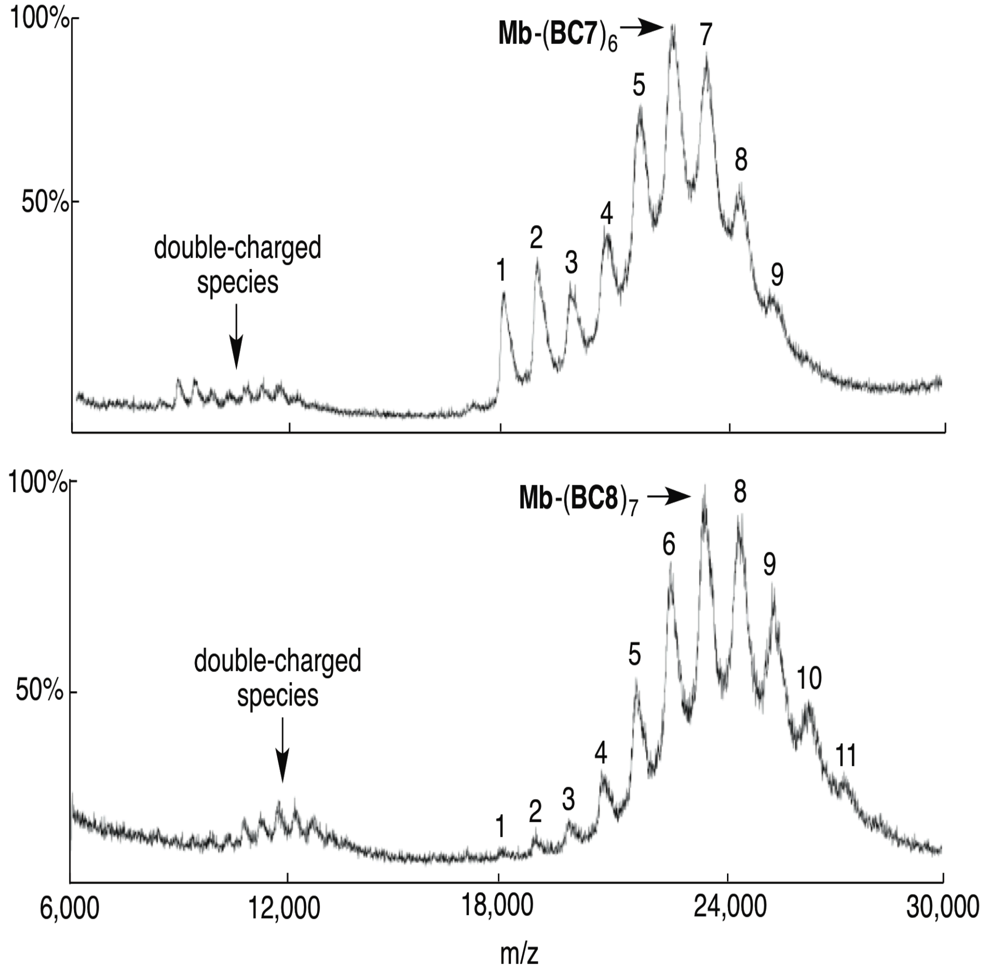


Figure S5. MALDI-MS data for bacteriochlorin–Mb conjugates derived from 60 equiv of **BC7** (top) and **BC8** (bottom). The number of appended bacteriochlorins is shown above the individual peaks in the monomolecular ion manifold.

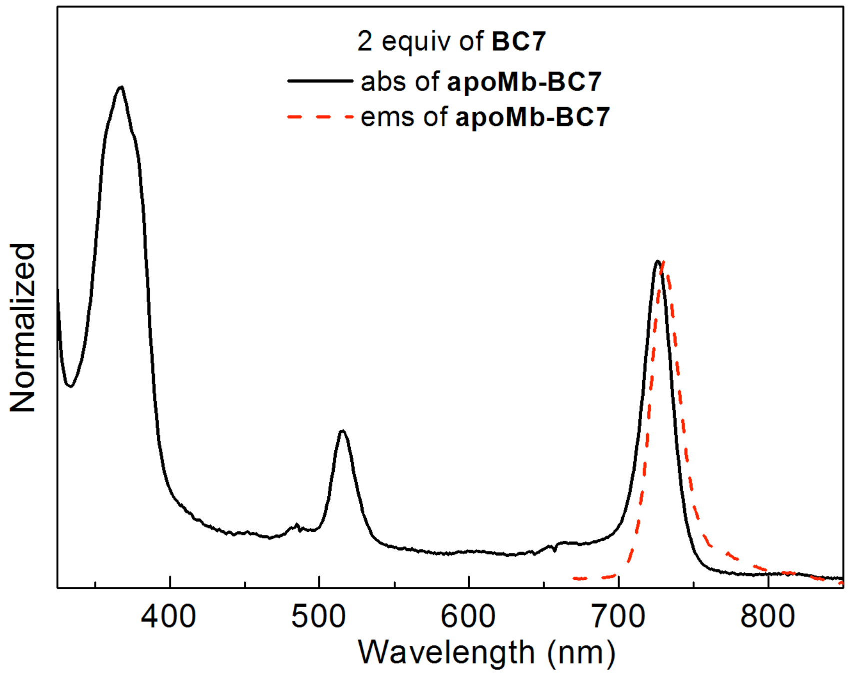


Figure S6. Absorption and fluorescence spectra of **apoMb-BC7** derived from 2 equiv of **BC7** in potassium phosphate buffer (500 mM, pH 7.0).

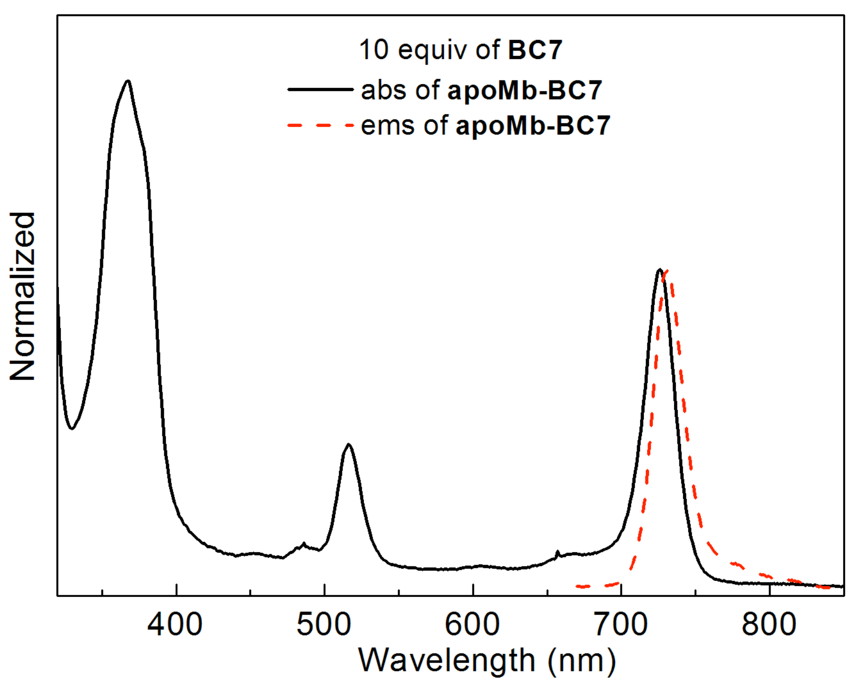


Figure S7. Absorption and fluorescence spectra of **apoMb-BC7** derived from 10 equiv of **BC7** in potassium phosphate buffer (500 mM, pH 7.0).

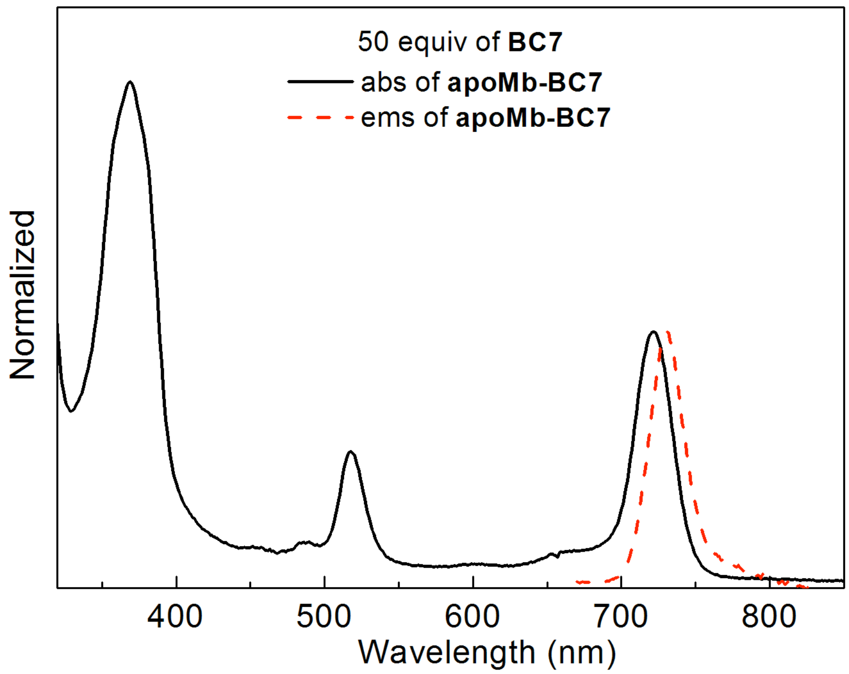


Figure S8. Absorption and fluorescence spectra of **apoMb-BC7** derived from 50 equiv of **BC7** in potassium phosphate buffer (500 mM, pH 7.0).

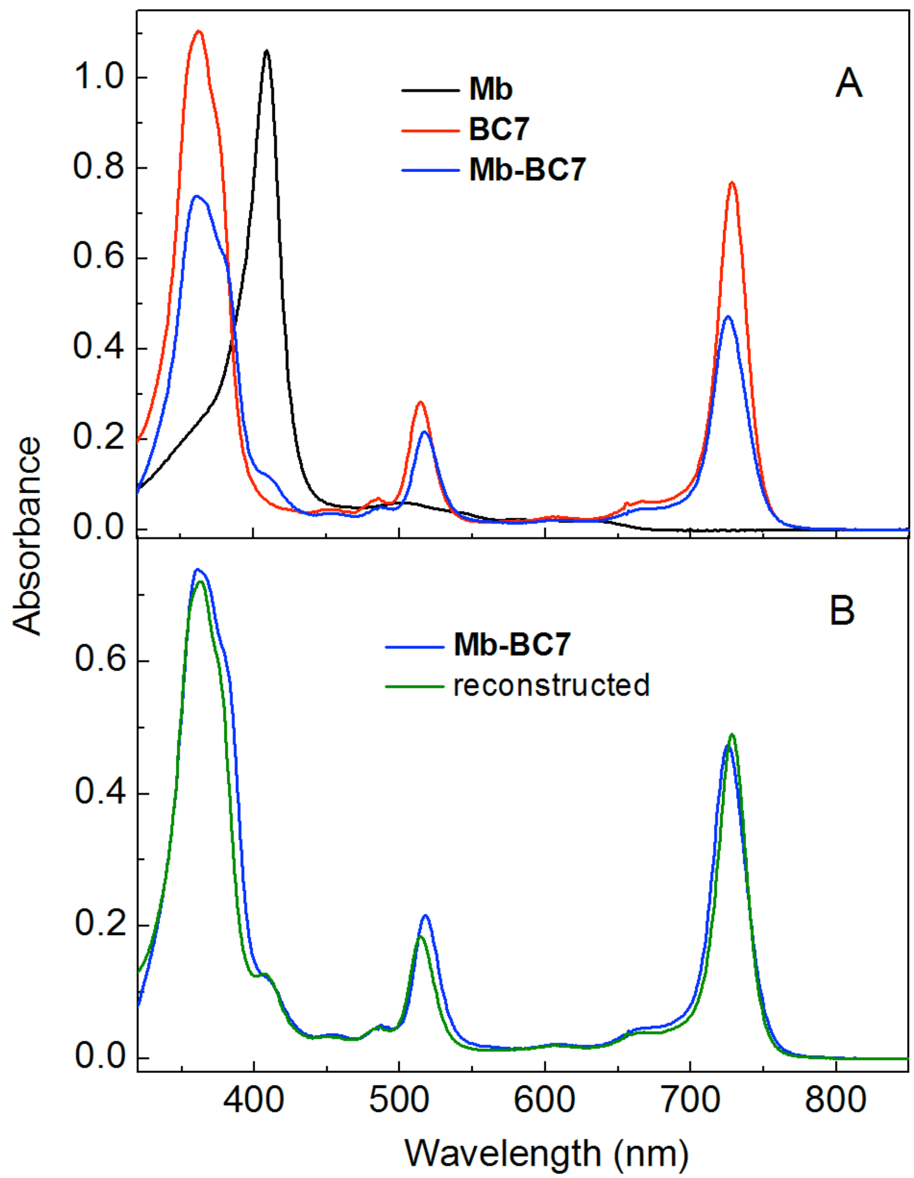


Figure S9. Absorption spectra of Mb, **BC7** and conjugate **Mb-BC7** derived from 60 equiv of **BC7** in potassium phosphate buffer (500 mM, pH 7.0). The concentration of each component is chosen arbitrarily (A). The experimental (blue) and reconstructed (cyan) absorption spectra of conjugate **Mb-BC7** (B).

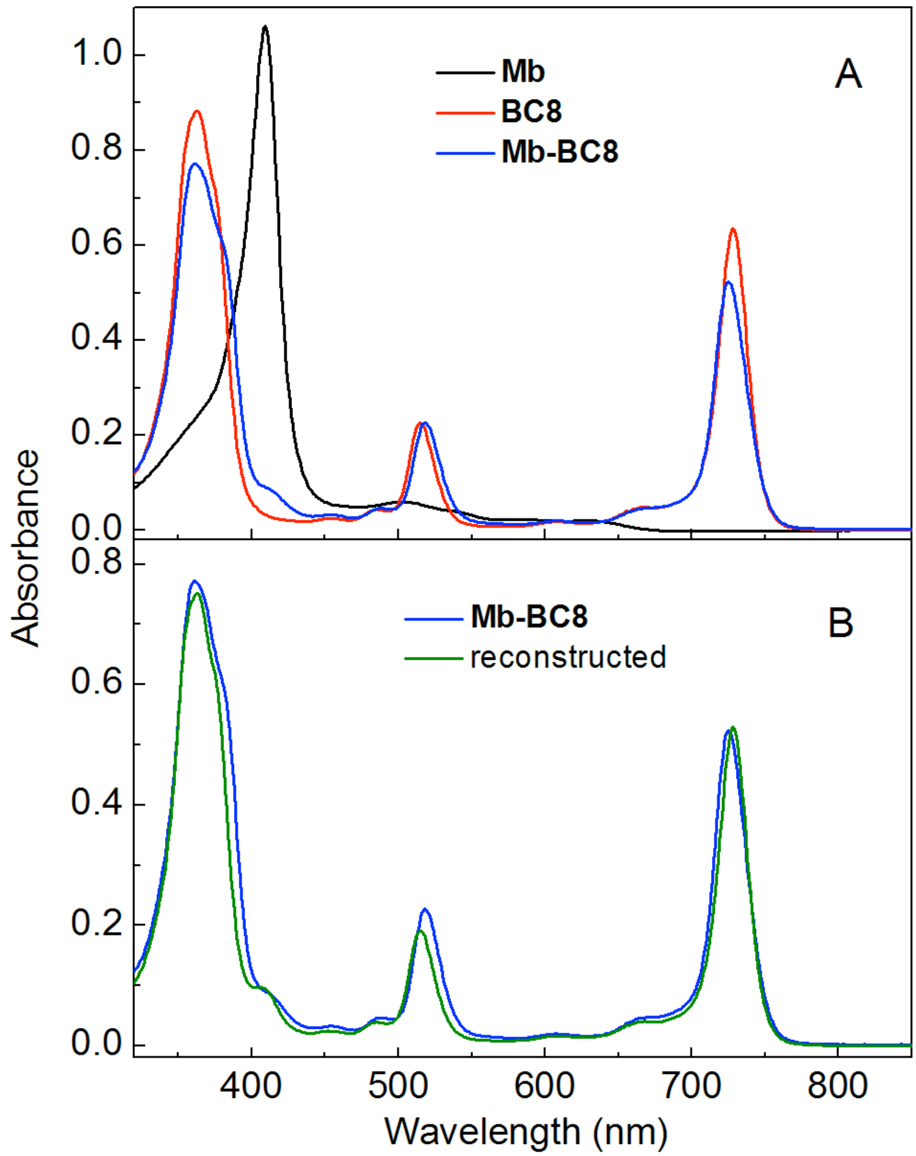


Figure S10. Absorption spectra of Mb, **BC8** and conjugate **Mb-BC8** derived from 60 equiv of **BC8** in potassium phosphate buffer (500 mM, pH 7.0). The concentration of each component is chosen arbitrarily (A). The experimental (blue) and reconstructed (cyan) absorption spectra of conjugate **Mb-BC8** (B).