

## Supplementary Materials

# Peptide-Tetrapyrrole Supramolecular Self-Assemblies: State of the Art

Paolo Dognini <sup>1</sup>, Christopher R. Coxon <sup>2</sup>, Wendel A. Alves <sup>3</sup> and Francesca Giuntini <sup>1,\*</sup>

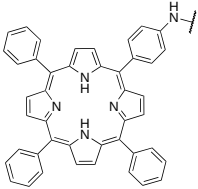
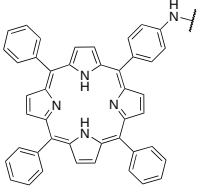
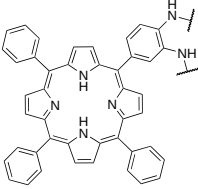
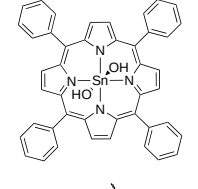
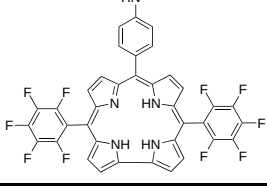
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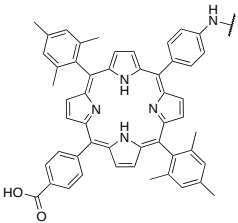
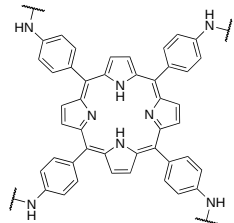
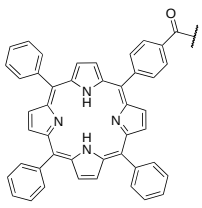
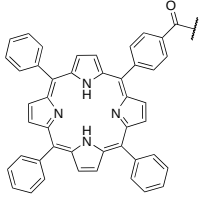
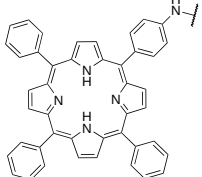
<sup>2</sup> Institute of Chemical Sciences, School of Engineering and Physical Sciences, Heriot-Watt University, Edinburgh, EH14 4AS, UK; C.Coxon@hw.ac.uk

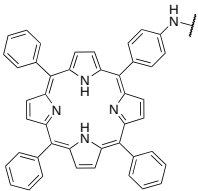
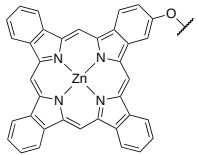
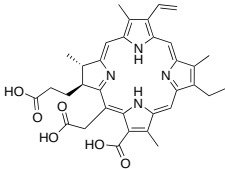
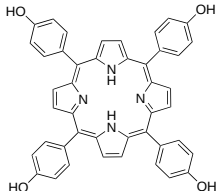
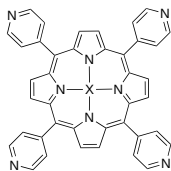
<sup>3</sup> Centro de Ciências Naturais e Humanas, Universidade Federal do ABC, 09210-380, Santo André, São Paulo, Brazil; wendel.alves@ufabc.edu.br

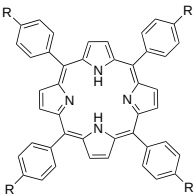
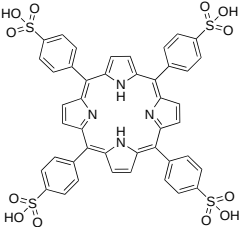
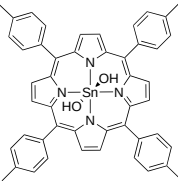
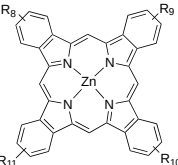
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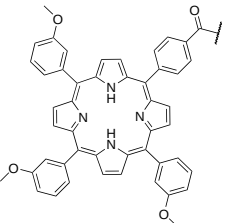
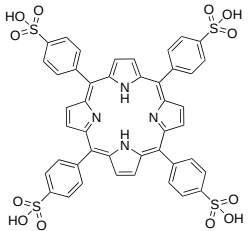
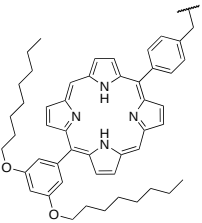
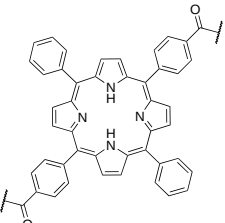
**Table S1.** Peptide-tetrapyrroles conjugates, complexes and non-covalent assembling systems. For references, please refer to the main article.  
*DSSC= Dye Sensitised Solar Cell; PAI= Photoacoustic imaging; PTT= Photothermal therapy; PDT= Photodynamic therapy; FI= Fluorescence imaging.*

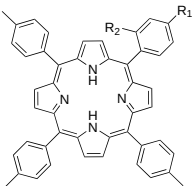
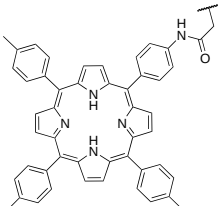
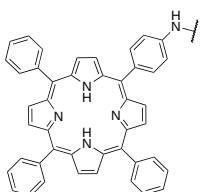
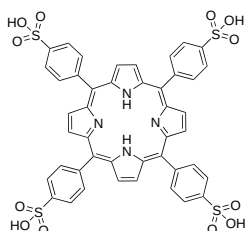
| Entry | Peptide                             | Tetrapyrrole                                                                        | Interaction (linker/bond)             | Structure (aggregate)                                      | Application | Ref     |
|-------|-------------------------------------|-------------------------------------------------------------------------------------|---------------------------------------|------------------------------------------------------------|-------------|---------|
| 1     | (a) FF<br>(b) Boc-FF<br>(c) Fmoc-FF |    | Covalent (amide)                      | Nanosphere<br>Microfibril<br>Platelet<br>(J-/H-aggregates) | DSSC        | [52,53] |
| 2     | FF-OMe                              |    | Covalent (triazine)                   | Nanosphere                                                 | -           | [54]    |
| 3     | Boc-FF                              |    | Covalent (amide)                      | Nanosphere                                                 | -           | [54]    |
| 4     | Boc-FF                              |  | Metal coordination                    | Nanosphere                                                 | -           | [54]    |
| 5     | (a) Fmoc-FF<br>(b) FF-OMe           |  | Covalent<br>(a) amide<br>(b) triazine | Nanosphere                                                 | -           | [54]    |

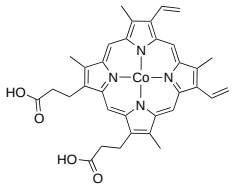
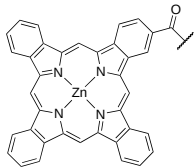
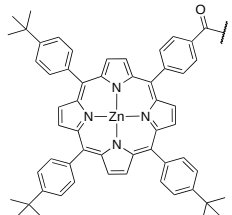
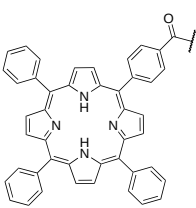
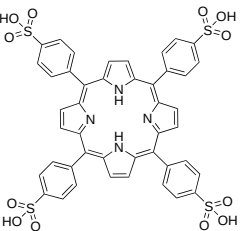
| Entry | Peptide                             | Tetrapyrrole                                                                        | Interaction (linker/bond) | Structure (aggregate)                                    | Application                                            | Ref  |
|-------|-------------------------------------|-------------------------------------------------------------------------------------|---------------------------|----------------------------------------------------------|--------------------------------------------------------|------|
| 6     | Boc-FF                              |    | Covalent (amide)          | -                                                        | DSSC                                                   | [55] |
| 7     | (a) FF<br>(b) Boc-FF<br>(c) Fmoc-FF |    | Covalent (amide)          | Nanosphere<br>Microfibril<br>Plaque<br>(J-aggregate)     | -                                                      | [56] |
| 8     | FF-BODIPY                           |    | Covalent (amide)          | Microsphere<br>(J-aggregate)                             | -                                                      | [56] |
| 9     | FF                                  |   | Covalent (amide)          | Microsphere                                              | Light harvesting and energy transfer<br>Photocatalysis | [57] |
| 10    | FF                                  |  | Covalent (triazine)       | Nanosphere<br>Nanoparticle<br>Nanosheet<br>(J-aggregate) | Light harvesting and energy transfer                   | [58] |

| Entry | Peptide                 | Tetrapyrrole                                                                                                      | Interaction (linker/bond) | Structure (aggregate)                                 | Application                          | Ref     |
|-------|-------------------------|-------------------------------------------------------------------------------------------------------------------|---------------------------|-------------------------------------------------------|--------------------------------------|---------|
| 11    | FF                      |                                  | Covalent (glutaric acid)  | Nanodots                                              | PTT, PAI                             | [59]    |
| 12    | FF                      |                                  | Covalent (butanoic acid)  | Nanofibrils (J-aggregate)<br>Nanosphere (H-aggregate) | PTT, PAI, PDT, FI                    | [60,61] |
| 13    | FF-NH <sub>2</sub> ·HCl |                                  | Noncovalent               | Nanosphere                                            | PDT                                  | [62]    |
| 14    | FF                      |                                 | Noncovalent               | Nanotube (J-aggregate)                                | Light harvesting and energy transfer | [63]    |
| 15    | Fmoc-FF                 | <br>X= H <sub>2</sub> , Zn, Sn | Noncovalent               | Hydrogel (J-aggregate)                                | Photocatalysis                       | [64]    |

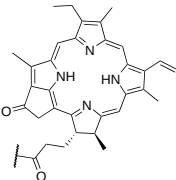
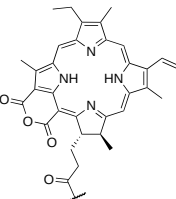
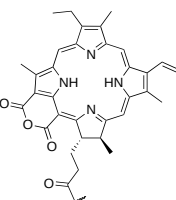
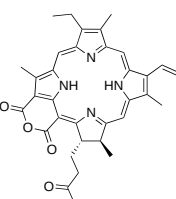
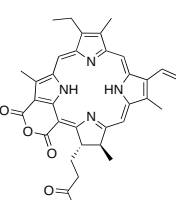
| Entry | Peptide                 | Tetrapyrrole                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | Interaction (linker/bond) | Structure (aggregate)         | Application                                | Ref  |
|-------|-------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------|-------------------------------|--------------------------------------------|------|
| 16    | Fmoc-FF                 |  <p>(a) R= COOH<br/>(b) R= NH<sub>2</sub></p>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | Noncovalent               | Hydrogel<br>(J-/H-aggregates) | Light<br>harvesting and<br>energy transfer | [65] |
| 17    | FF                      |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 | Noncovalent               | Microsphere<br>(J-aggregate)  | Photocatalysis                             | [66] |
| 18    | D-F-D-F-NH <sub>2</sub> |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 | Noncovalent               | Nanoribbon                    | DNA sensor                                 | [67] |
| 19    | FF                      |  <p>(a) R<sub>8</sub>, R<sub>9</sub>, R<sub>10</sub>, R<sub>11</sub>= <br/>(b) R<sub>8</sub>, R<sub>9</sub>, R<sub>10</sub>, R<sub>11</sub>= <br/>(c) R<sub>8</sub>, R<sub>9</sub>, R<sub>10</sub>= ; R<sub>11</sub>= CH<sub>3</sub><br/>(d) R<sub>8</sub>, R<sub>9</sub>, R<sub>10</sub>= ; R<sub>11</sub>= CH<sub>3</sub></p> | Noncovalent               | Sharp-edged structure         | PDT                                        | [68] |

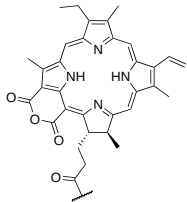
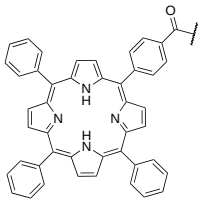
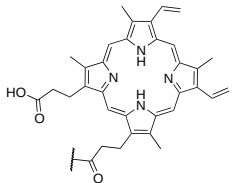
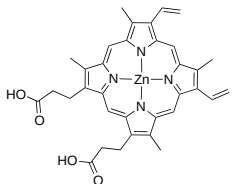
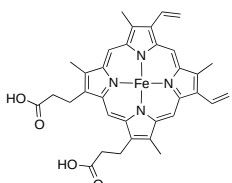
| Entry | Peptide | Tetrapyrrole                                                                        | Interaction (linker/bond) | Structure (aggregate)                | Application                                            | Ref     |
|-------|---------|-------------------------------------------------------------------------------------|---------------------------|--------------------------------------|--------------------------------------------------------|---------|
| 20    | GG      |    | Covalent (amide)          | Rod<br>Sphere<br>(J-/H-aggregate)    | -                                                      | [69]    |
| 21    | KK      |    | Noncovalent               | Fibre<br>(J-aggregate)               | Light harvesting and energy transfer<br>Photocatalysis | [70,71] |
| 22    | YY      |   | Covalent (ether)          | Nanofibre<br>Toroid<br>(H-aggregate) | -                                                      | [72]    |
| 23    | WG      |  | Covalent (amide)          | Nanoparticle<br>Nanofibre            | PDT                                                    | [73]    |

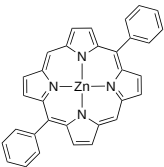
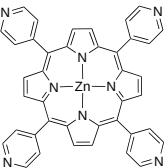
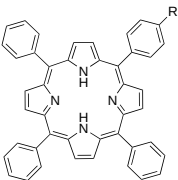
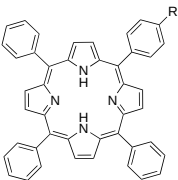
| Entry | Peptide                                                                                                | Tetrapyrrole                                                                                                                                                                                                                                                                                                                              | Interaction (linker/bond) | Structure (aggregate)              | Application                                | Ref     |
|-------|--------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------|------------------------------------|--------------------------------------------|---------|
| 24    | Ac-CKVKV-NH <sub>2</sub>                                                                               |  <p>(a) R<sub>1</sub>=  R<sub>2</sub>= H<br/> (b) R<sub>1</sub>= H R<sub>2</sub>= </p> | Covalent<br>(thioether)   | β-sheet                            | -                                          | [74,75] |
| 25    | Ac-CKVSVKV-NH <sub>2</sub>                                                                             |                                                                                                                                                                                                                                                          | Covalent<br>(thioether)   | β-sheet                            | -                                          | [74,75] |
| 26    | Ac-NAEASAESAY-NH <sub>2</sub>                                                                          |                                                                                                                                                                                                                                                         | Covalent<br>(amide)       | Extended array<br>(J-aggregate)    | Light<br>harvesting and<br>energy transfer | [76]    |
| 27    | (a) Ac-IQQLKNQIKQLL<br>KQ-NH <sub>2</sub><br>(b) Ac-IQQLKNQIKQLLKQA<br>AIQQLQNQIQQLLQQ-NH <sub>2</sub> |                                                                                                                                                                                                                                                        | Noncovalent               | Mesoscale fibrils<br>(J-aggregate) | -                                          | [77-79] |

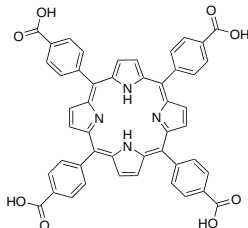
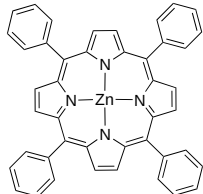
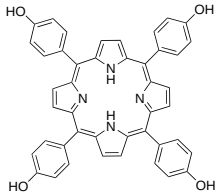
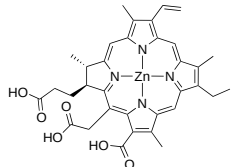
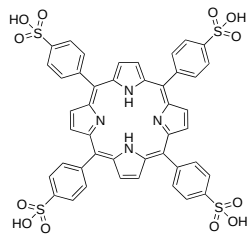
| Entry | Peptide                                                                                                                                        | Tetrapyrrole                                                                        | Interaction (linker/bond) | Structure (aggregate)                  | Application                                                  | Ref     |
|-------|------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|---------------------------|----------------------------------------|--------------------------------------------------------------|---------|
| 28    | (a) Ac-K(IEALEGK) <sub>2</sub> (IEALEHK)(IEALEGK)G-NH <sub>2</sub><br>(b) Ac-Q(IAALEQK)(IAALE-4-Pal-K)(IAALEQK) <sub>2</sub> G-NH <sub>2</sub> |    | Metal coordination        | Rod<br>Sphere                          | -                                                            | [80,81] |
| 29    | KKKKK                                                                                                                                          |    | Covalent<br>(amide)       | Nanodot                                | PDT, FI                                                      | [82]    |
| 30    | GAGAG-NH <sub>2</sub>                                                                                                                          |    | Covalent<br>(amide)       | Nanofibre<br>Nanotube<br>(J-aggregate) | Semiconductor                                                | [83]    |
| 31    | (a) GIGKFLHSAKKFGKA<br>FVGEILNS<br>(b) GIGKALHSAKKFGKA<br>FVGEILNS                                                                             |   | Covalent<br>(amide)       | Microfibril<br>(J-aggregate)           | -                                                            | [84]    |
| 32    | Ac-IIIKK-NH <sub>2</sub>                                                                                                                       |  | Noncovalent               | Nanofibre<br>(J-aggregate)             | Light<br>harvesting and<br>energy transfer<br>Photocatalysis | [85-87] |

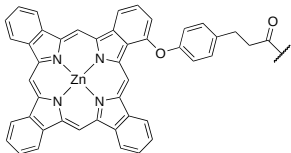
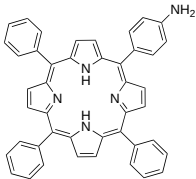
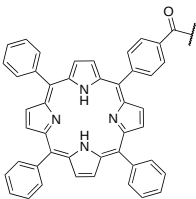
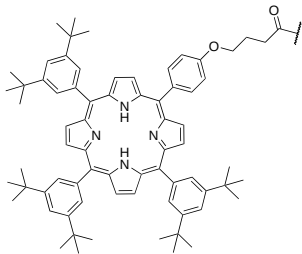
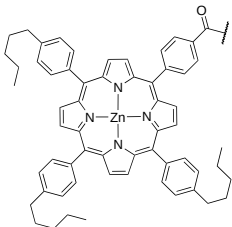


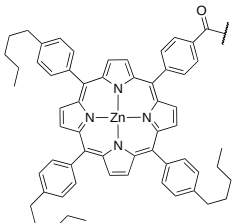
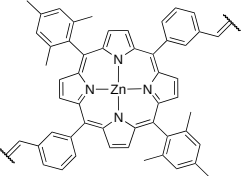
| Entry | Peptide                        | Tetrapyrrole                                                                        | Interaction (linker/bond) | Structure (aggregate)  | Application | Ref  |
|-------|--------------------------------|-------------------------------------------------------------------------------------|---------------------------|------------------------|-------------|------|
| 33    | PLG                            |    | Covalent<br>(amide)       | Fibre                  | PAI         | [88] |
| 34    | YVHD                           |    | Covalent<br>(amide)       | Fibre                  | PAI         | [89] |
| 35    | (a) QRLGVGFPK<br>(b) QKVPHVGQK |    | Covalent<br>(amide)       | Nanoparticle           | -           | [90] |
| 36    | GTFG                           |   | Covalent<br>(amide)       | Nanofibre              | PAI         | [91] |
| 37    | AKC                            |  | Covalent<br>(amide)       | Fibre<br>(J-aggregate) | PAI         | [92] |

| Entry | Peptide                                                                                                                               | Tetrapyrrole                                                                        | Interaction (linker/bond) | Structure (aggregate)  | Application                                                  | Ref      |
|-------|---------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|---------------------------|------------------------|--------------------------------------------------------------|----------|
| 38    | (a) RRR<br>(b) RRRRRRR                                                                                                                |    | Covalent<br>(amide)       | Fibre<br>(J-aggregate) | PAI                                                          | [93]     |
| 39    | KL VFF                                                                                                                                |    | Covalent<br>(amide)       | Nanosphere             | Prevention of<br>A $\beta$ aggregation                       | [94]     |
| 40    | FFYSV                                                                                                                                 |    | Covalent<br>(amide)       | Nanorod                | PTT, PAI                                                     | [95]     |
| 41    | (a) c16-AHLLLKKK<br>(b) c16-AHALLLKKK<br>(c) c16-AHWWKKK<br>(d) c16-AHFFFKKK<br>(e) c16-AHIIKKK<br>(f) c16-AHVVKKK<br>(g) c16-AHAAKKK |   | Metal coordination        | Fibre<br>Micelle       | Light<br>harvesting and<br>energy transfer<br>Photocatalysis | [97-100] |
| 42    | (a) c16-AALLLKKK<br>(b) c16-AHLLLKKK<br>(c) c16-HHLLLKKK<br>(d) c16-MHLLLKKK                                                          |  | Metal coordination        | Fibre<br>Micelle       | Photocatalysis                                               | [101]    |

| Entry | Peptide                                                | Tetrapyrrole                                                                                                                      | Interaction (linker/bond) | Structure (aggregate)                        | Application            | Ref   |
|-------|--------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------|---------------------------|----------------------------------------------|------------------------|-------|
| 43    | (a) c16-AHLLLKKK<br>(b) c16-AHLLLKKKKKKKKK             |                                                  | Metal coordination        | Fibre                                        | DSSC<br>Photocatalysis | [102] |
| 44    | (a) c14-FFK<br>(b) c14-FK<br>(c) c14-YYK<br>(d) c14-YK |                                                  | Noncovalent               | Nanoribbon<br>Nanofibre<br>(J-aggregate)     | -                      | [103] |
| 45    | (a) Boc-II<br>(b) Fmoc-II<br>(c) Cbz-II<br>(d) II-OMe  | <br>(a, b, c) R= NH <sub>2</sub><br>(d) R= COOH  | Covalent<br>(amide)       | Spheres<br>Flakes<br>Spikes<br>(J-aggregate) | -                      | [104] |
| 46    | (a) Boc-AI<br>(b) Fmoc-AI<br>(c) Cbz-AI<br>(d) AI-OMe  | <br>(a, b, c) R= NH <sub>2</sub><br>(d) R= COOH | Covalent<br>(amide)       | Sphere<br>(J-aggregate)                      | -                      | [104] |

| Entry | Peptide                                                                                                                              | Tetrapyrrole                                                                        | Interaction (linker/bond) | Structure (aggregate)   | Application                          | Ref        |
|-------|--------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|---------------------------|-------------------------|--------------------------------------|------------|
| 47    | Fmoc-TL-NH <sub>2</sub>                                                                                                              |    | Noncovalent               | Hydrogel                | Light harvesting and energy transfer | [105]      |
| 48    | Fmoc-LLL-OMe                                                                                                                         |    | Noncovalent               | Hydrogel (J-aggregate)  | Light harvesting and energy transfer | [106]      |
| 49    | Fmoc-LLL-OMe                                                                                                                         |    | Noncovalent               | Nanoparticle            | PDT                                  | [107, 108] |
| 50    | Cbz-HF                                                                                                                               |   | Metal coordination        | Nanosphere              | PDT                                  | [109]      |
| 51    | (a) Fmoc-ChaChaGK-NH <sub>2</sub><br>(b) Fmoc-FFGK-NH <sub>2</sub><br>(c) Ac-ChaChaGK-NH <sub>2</sub><br>(d) Ac-FFGK-NH <sub>2</sub> |  | Noncovalent               | Nanoribbons<br>Nanorods | Light harvesting and energy transfer | [110, 111] |

| Entry | Peptide                                                                | Tetrapyrrole                                                                        | Interaction (linker/bond) | Structure (aggregate)     | Application | Ref           |
|-------|------------------------------------------------------------------------|-------------------------------------------------------------------------------------|---------------------------|---------------------------|-------------|---------------|
| 52    | (a) GGK(Biotin)-COOH<br>(b) GGK(Biotin)-CONH <sub>2</sub>              |   | Covalent<br>(amide)       | Nanosphere                | PDT         | [112]         |
| 53    | Thy-AAibAAibAAibAAib-Ade                                               |    | Noncovalent               | Vesicle<br>Fibre          | -           | [113]         |
| 54    | Ac-VE(NDI)VKVE(NDI)V-NH <sub>2</sub>                                   |    | Covalent<br>(amide)       | Fibre<br>(J-/H-aggregate) | -           | [114]         |
| 55    | (a) KK<br>(b) KKKK<br>(c) KKKKKKKK<br>(d) KKKKKKKKKKKKKKKKKK           |  | Covalent<br>(amide)       | Cluster                   | DSSC        | [115,<br>116] |
| 56    | c[(S-D <sup>Me</sup> N-γ-Ach-F-D <sup>Me</sup> N-γ-Ach) <sub>2</sub> ] |  | Covalent (ester)          | Dimer                     | -           | [119]         |

| Entry | Peptide                                        | Tetrapyrrole                                                                      | Interaction (linker/bond) | Structure (aggregate) | Application       | Ref   |
|-------|------------------------------------------------|-----------------------------------------------------------------------------------|---------------------------|-----------------------|-------------------|-------|
| 57    | c[S-D-MeN-γ-Acp-(F-D-MeN-γ-Acp) <sub>2</sub> ] |  | Covalent (ester)          | Dimer                 | -                 | [120] |
| 58    | c[(I-MeN-γ-Acp-I-NHNHAcN-γ-Acp) <sub>2</sub> ] |  | Covalent (hydrazone)      | Dimer                 | Molecular capsule | [121] |