Supplementary Materials

Peptide-Tetapyrrole Supramolecular Self-Assemblies: State of the Art

Paolo Dognini 1, Christopher R. Coxon 2, Wendel A. Alves 3 and Francesca Giuntini 1, *

1 School of Pharmacy and Biomolecular Sciences, Byrom Street Campus, Liverpool John Moores University, Liverpool, L3 3AF, UK; P.Dognini@ljmu.ac.uk
2 Institute of Chemical Sciences, School of Engineering and Physical Sciences, Heriot-Watt University, Edinburgh, EH14 4AS, UK; C.Coxon@hw.ac.uk
3 Centro de Ciências Naturais e Humanas, Universidade Federal do ABC, 09210-380, Santo André, São Paulo, Brazil; wendel.alves@ufabc.edu.br
* Correspondence: F.Giuntini@ljmu.ac.uk; Tel.: +441512312072
Table S1. Peptide-tetapyrroles conjugates, complexes and non-covalent assembling systems. For references, please refer to the main article.

| Entry | Peptide | Tetapyrrole | Interaction (linker/bond) | Structure (aggregate) | Application | Ref |
|-------|---------|-------------|--------------------------|----------------------|-------------|-----|
| 1     | (a) FF  | ![Covalent (amide)](image1) | Covalent (amide) | Nanosphere Microfibril Platelet (J-/H-aggregates) | DSSC | [52,53] |
|       | (b) Boc-FF | ![Covalent (amide)](image2) | | | | |
|       | (c) Fmoc-FF | ![Covalent (amide)](image3) | | | | |
| 2     | FF-OMe  | ![Covalent (triazine)](image4) | Covalent (triazine) | Nanosphere | | [54] |
| 3     | Boc-FF  | ![Covalent (amide)](image5) | Covalent (amide) | Nanosphere | | [54] |
| 4     | Boc-FF  | ![Metal coordination](image6) | Metal coordination | Nanosphere | | [54] |
| 5     | (a) Fmoc-FF | ![Covalent (amide)](image7) | Covalent (a) amide (b) triazine | Nanosphere | | [54] |
|       | (b) FF-OMe | ![Covalent (triazine)](image8) | | | | |

DSSC = Dye Sensitised Solar Cell; PAI = Photoacoustic imaging; PTT = Photothermal therapy; PDT = Photodynamic therapy; FIM = Fluorescence imaging.
| Entry | Peptide   | Tetrapyrrole | Interaction (linker/bond) | Structure (aggregate)                  | Application                                      | Ref  |
|-------|-----------|--------------|---------------------------|----------------------------------------|--------------------------------------------------|------|
| 6     | Boc-FF    | ![Boc-FF](image) | Covalent (amide)          | -                                      | DSSC                                             | [55] |
| 7     | (a) FF    | ![FF](image)  | Covalent (amide)          | Nanosphere, Microfibril, Plaque (J-aggregate) | -                                                | [56] |
|       | (b) Boc-FF| ![Boc-FF](image) | Covalent (amide)          | Nanosphere, Microfibril, Plaque (J-aggregate) | -                                                | [56] |
|       | (c) Fmoc-FF| ![Fmoc-FF](image) | Covalent (amide)          | Nanosphere, Microfibril, Plaque (J-aggregate) | -                                                | [56] |
| 8     | FF-BODIPY | ![FF-BODIPY](image) | Covalent (amide)          | Microsphere (J-aggregate)              | -                                                | [56] |
| 9     | FF        | ![FF](image)  | Covalent (amide)          | Microsphere                            | Light harvesting and energy transfer, Photocatalysis | [57] |
| 10    | FF        | ![FF](image)  | Covalent (triazine)       | Nanosphere, Nanoparticle, Nanosheet (J-aggregate) | Light harvesting and energy transfer              | [58] |
| Entry | Peptide   | Tetrahydrofolate | Interaction (linker/bond) | Structure (aggregate)   | Application                      | Ref  |
|-------|-----------|------------------|---------------------------|-------------------------|----------------------------------|------|
| 11    | FF        | ![image1](image1.png) | Covalent (glutaric acid) | Nanodots               | PTT, PAI                         | [59] |
| 12    | FF        | ![image2](image2.png) | Covalent (butanoic acid) | Nanofibrils (J-aggregate)<br>Nanosphere (H-aggregate) | PTT, PAI, PDT, FI                     | [60,61] |
| 13    | FF-NH₂·HCl | ![image3](image3.png) | Noncovalent                | Nanosphere               | PDT                              | [62] |
| 14    | FF        | ![image4](image4.png) | Noncovalent                | Nanotube (J-aggregate)  | Light harvesting and energy transfer | [63] |
| 15    | Fmoc-FF   | ![image5](image5.png) | Noncovalent                | Hydrogel (J-aggregate)  | Photocatalysis                     | [64] |
| Entry | Peptide | Tetrapyrrole | Interaction (linker/bond) | Structure (aggregate) | Application | Ref |
|-------|---------|--------------|--------------------------|-----------------------|-------------|-----|
| 16    | Fmoc-FF | ![Tetrapyrrole](image1) | Noncovalent | Hydrogel (J-/H-aggregates) | Light harvesting and energy transfer | [65] |
| 17    | FF      | ![Tetrapyrrole](image2) | Noncovalent | Microsphere (J-aggregate) | Photocatalysis | [66] |
| 18    | D-F-D-F-NH₂ | ![Tetrapyrrole](image3) | Noncovalent | Nanoribbon | DNA sensor | [67] |
| 19    | FF      | ![Tetrapyrrole](image4) | Noncovalent | Sharp-edged structure | PDT | [68] |
| Entry | Peptide | Tetapyrrole | Interaction (linker/bond) | Structure (aggregate) | Application | Ref |
|-------|---------|-------------|---------------------------|----------------------|-------------|-----|
| 20    | GG      |             | Covalent (amide)          | Rod                  | -           | [69]|
|       |         |             |                           | Sphere               |             |     |
|       |         |             |                           | (J-/H-aggregate)      |             |     |
| 21    | KK      |             | Noncovalent               | Fibre                | Light       | [70,71]|
|       |         |             |                           | (J-aggregate)        | harvesting and energy transfer |     |
|       |         |             |                           |                      | Photocatalysis |     |
| 22    | YY      |             | Covalent (ether)          | Nanofibre            | -           | [72]|
|       |         |             |                           | Toroid               |             |     |
|       |         |             |                           | (H-aggregate)        |             |     |
| 23    | WG      |             | Covalent (amide)          | Nanoparticle         | PDT         | [73]|
|       |         |             |                           | Nanofibre            |             |     |
| Entry | Peptide                  | Tetrapyrole | Interaction (linker/bond)     | Structure (aggregate) | Application                              | Ref   |
|-------|--------------------------|-------------|--------------------------------|-----------------------|------------------------------------------|-------|
| 24    | Ac-CKVKV-NH₂              | ![Tetrapyrole](image1.png) | Covalent (thioether) | β-sheet                | -                                        | [74,75] |
|       | (a) R₁= R₂= H            |             |                                |                       |                                          |       |
|       | (b) R₁= H R₂= H          |             |                                |                       |                                          |       |
| 25    | Ac-CKVSVKV-NH₂            | ![Tetrapyrole](image2.png) | Covalent (thioether) | β-sheet                | -                                        | [74,75] |
| 26    | Ac-NAEASAESAY-NH₂         | ![Tetrapyrole](image3.png) | Covalent (amide)             | Extended array (J-aggregate) | Light harvesting and energy transfer     | [76]  |
| 27    | (a) Ac-IQQLKNQIKQLL KQ-NH₂ | ![Tetrapyrole](image4.png) | Noncovalent                  | Mesoscale fibrils (J-aggregate) | -                                        | [77-79] |
|       | (b) Ac-IQQLKNQIKQLLKQA AIQQLQNQIQQLQQ-NH₂ | ![Tetrapyrole](image5.png) |                                |                       |                                          |       |
| Entry | Peptide | Tetrapyrrole | Interaction (linker/bond) | Structure (aggregate) | Application | Ref |
|-------|---------|--------------|---------------------------|-----------------------|-------------|-----|
| 28    | (a) Ac-K(I EALEGK)²(IEALE HK)(IEALEGK)G-NH₂ | ![Tetrapyrrole](image) | Metal coordination | Rod | - | [80,81] |
|       | (b) Ac-Q(I AALEQK)(I AALE-4-Pal-K)(I AALEQK)²G-NH₂ | ![Tetrapyrrole](image) | Covalent (amide) | Nanodot | PDT, FI | [82] |
| 29    | KKKKK | ![Tetrapyrrole](image) | Covalent (amide) | Nanofibre Nanotube (J-aggregate) | Semiconductor | [83] |
| 30    | GAGAG-NH₂ | ![Tetrapyrrole](image) | Covalent (amide) | Microfibril (J-aggregate) | - | [84] |
| 31    | (a) GIGKFLHSAKKFGKA FVGEILNS | ![Tetrapyrrole](image) | Covalent (amide) | Microfibril (J-aggregate) | - | [84] |
|       | (b) GIGKALHSAKKFGKA FVGEILNS | ![Tetrapyrrole](image) | Noncovalent | Nanofibre (J-aggregate) | Light harvesting and energy transfer Photocatalysis | [85-87] |
| Entry | Peptide | Tetrapyrrole | Interaction (linker/bond) | Structure (aggregate) | Application | Ref |
|-------|---------|--------------|--------------------------|----------------------|-------------|-----|
| 33    | PLG     | ![Peptide](image1.png) | Covalent (amide)         | Fibre                | PAI         | [88]|
| 34    | YVHD    | ![Peptide](image2.png) | Covalent (amide)         | Fibre                | PAI         | [89]|
| 35    | (a) QRLGVGFPK (b) QKVPHVGQK | ![Peptide](image3.png) | Covalent (amide)         | Nanoparticle         | -           | [90]|
| 36    | GTFG    | ![Peptide](image4.png) | Covalent (amide)         | Nanofibre            | PAI         | [91]|
| 37    | AKC     | ![Peptide](image5.png) | Covalent (amide)         | Fibre (J-aggregate)  | PAI         | [92]|
| Entry | Peptide               | Tetrapyrrole | Interaction (linker/bond) | Structure (aggregate) | Application                      | Ref   |
|-------|-----------------------|--------------|---------------------------|-----------------------|----------------------------------|-------|
| 38    | (a) RRR              | Covalent     | Fibre                     |                       | PAI                              | [93]  |
|       | (b) RRRRRRRRR        | (amide)      | (J-aggregate)             |                       |                                  |       |
| 39    | KLVFF                 | Covalent     | Nanosphere                |                       | Prevention of Aβ aggregation    | [94]  |
|       |                       | (amide)      |                           |                       |                                  |       |
| 40    | FFYSV                 | Covalent     | Nanorod                   |                       | PTT, PAI                         | [95]  |
|       |                       | (amide)      |                           |                       |                                  |       |
| 41    | (a) c16-AHLLLKKK     | Metal coordination | Fibre             | Light harvesting and energy transfer Photocatalysis | [97-100] |
|       | (b) c16-AHALLLKKK    |              | Micelle                  |                       |                                  |       |
|       | (c) c16-AHWWWKKK      |              |                           |                       |                                  |       |
|       | (d) c16-AHFFFKKK      |              |                           |                       |                                  |       |
|       | (e) c16-AHIWKKK       |              |                           |                       |                                  |       |
|       | (f) c16-AHVVKKK       |              |                           |                       |                                  |       |
|       | (g) c16-AHAASKK       |              |                           |                       |                                  |       |
| 42    | (a) c16-AALLLKKK     | Metal coordination | Fibre             | Photocatalysis        | [101]  |
|       | (b) c16-AHLLLKKK     |              | Micelle                  |                       |                                  |       |
|       | (c) c16-HHLLLKKK     |              |                           |                       |                                  |       |
|       | (d) c16-MHLLLKKK     |              |                           |                       |                                  |       |
| Entry | Peptide | Tetrapyrrole | Interaction (linker/bond) | Structure (aggregate) | Application | Ref |
|-------|---------|--------------|---------------------------|-----------------------|-------------|----|
| 43    | (a) c16-AHLLLKKK  
(b) c16-AHLLLKKKKKKKKK | Metal coordination | Fibre | DSSC  
Photocatalysis | [102] |
| 44    | (a) c14-FFK  
(b) c14-FK  
(c) c14-YYK  
(d) c14-YK | Noncovalent | Nanoribbon  
Nanofibre  
(J-aggregate) | - | [103] |
| 45    | (a) Boc-II  
(b) Fmoc-II  
(c) Cbz-II  
(d) II-OMe | Covalent  
(amide) | Spheres  
Flakes  
Spikes  
(J-aggregate) | - | [104] |
| 46    | (a) Boc-Al  
(b) Fmoc-Al  
(c) Cbz-Al  
(d) Al-OMe | Covalent  
(amide) | Sphere  
(J-aggregate) | - | [104] |
| Entry | Peptide         | Tetrapyrrole | Interaction (linker/bond) | Structure (aggregate) | Application                                   | Ref  |
|-------|-----------------|--------------|---------------------------|-----------------------|-----------------------------------------------|------|
| 47    | Fmoc-TL-NH₂     | ![Tetrapyrrole](image1.png) | Noncovalent               | Hydrogel              | Light harvesting and energy transfer          | [105]|
| 48    | Fmoc-LLL-OMe    | ![Tetrapyrrole](image2.png) | Noncovalent               | Hydrogel (J-aggregate) | Light harvesting and energy transfer          | [106]|
| 49    | Fmoc-LLL-OMe    | ![Tetrapyrrole](image3.png) | Noncovalent               | Nanoparticle           | PDT                                           | [107, 108]|
| 50    | Cbz-HF          | ![Tetrapyrrole](image4.png) | Metal coordination        | Nanosphere             | PDT                                           | [109]|
| 51    | (a) Fmoc-ChaChaGK-NH₂  
(b) Fmoc-FFGK-NH₂  
(c) Ac-ChaChaGK-NH₂  
(d) Ac-FFGK-NH₂ | ![Tetrapyrrole](image5.png) | Noncovalent               | Nanoribbons            | Light harvesting and energy transfer          | [110, 111]|
|       |                 |              |                           | Nanorods               |                                               |      |
| Entry | Peptide | TetraPyrole | Interaction (linker/bond) | Structure (aggregate) | Application | Ref |
|-------|---------|-------------|--------------------------|----------------------|-------------|-----|
| 52    | (a) GGK(Biotin)-COOH  
(b) GGK(Biotin)-CONH₂ | ![Image](image1.png) | Covalent (amide) | Nanosphere | PDT | [112] |
|       |         |             |                          |                      |             |     |
| 53    | Thy-AAibAAibAibAAibAib-Ade | ![Image](image2.png) | Noncovalent | Vesicle  
Fibre | - | [113] |
| 54    | Ac-VE(NDI)VKVE(NDI)VN-H₂ | ![Image](image3.png) | Covalent (amide) | Fibre  
(J-/H-aggregate) | - | [114] |
| 55    | (a) KK  
(b) KKKK  
(c) KKKKKKKK  
(d) KKKKKKKKKKKKKKKK | ![Image](image4.png) | Covalent (amide) | Cluster | DSSC | [115, 116] |
| 56    | c[(S-D₁₆-N-γ-Ach-F-D₁₆-N-γ-Ach)₂] | ![Image](image5.png) | 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)]₂ | Covalent (ester) | Dimer | - | [120] |
| 58    | c[(L-MeN-γ-Acp-L-NH₂AcmN-γ-Acp)]₂ | Covalent (hydrazone) | Dimer | Molecular capsule | [121] |