# **Supplemental Materials**

# Structure-activity study of an all-D antimicrobial octapeptide D2D

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| Peptide | Molecular weight | MALDI mass (MH <sup>+</sup> ) | Retention time (min) | Purity |
|---------|------------------|-------------------------------|----------------------|--------|
| D2-D    | 1184.54          | 1185.77                       | 15.45                | 100 %  |
| 1       | 1127.45          | 1128.54                       | 16.48                | 96 %   |
| 2       | 1127.45          | 1128.56                       | 16.48                | 98 %   |
| 3       | 1058.38          | 1059.49                       | 14.45                | 96 %   |
| 4       | 1108.44          | 1109.54                       | 14.72                | 99 %   |
| 5       | 1127.45          | 1128.62                       | 16.49                | 98 %   |
| 6       | 1058.38          | 1059.76                       | 13.39                | 100 %  |
| 7       | 1127.45          | 1128.75                       | 16.45                | 99 %   |
| 8       | 1142.46          | 1143.64                       | 14.47                | 98 %   |
| 9       | 1253.60          | 1253.92                       | 18.24                | 98 %   |
| 10      | 1142.46          | 1143.48                       | 16.00                | 98 %   |
| 11      | 1169.53          | 1170.46                       | 17.45                | 98 %   |
| 12      | 1203.54          | 1204.46                       | 17.43                | 98 %   |
| 13      | 1143.45          | 1144.48                       | 17.90                | 96 %   |
| 14      | 1157.47          | 1158.44                       | 18.03                | 96 %   |
| 15      | 1219.54          | 1220.76                       | 17.11                | 95 %   |
| 16      | 1155.50          | 1156.51                       | 17.31                | 97 %   |
| 17      | 1253.60          | 1255.13                       | 18.45                | 98 %   |
| 18      | 1142.46          | 1143.97                       | 15.63                | 95 %   |
| 19      | 1169.53          | 1170.93                       | 17.41                | 97 %   |
| 20      | 1203.54          | 1204.75                       | 17.50                | 96 %   |
| 21      | 1143.45          | 1145.08                       | 16.34                | 96 %   |
| 22      | 1157.47          | 1158.80                       | 16.44                | 96 %   |
| 23      | 1219.54          | 1220.84                       | 16.66                | 93 %   |
| 24      | 1155.50          | 1156.79                       | 16.84                | 95 %   |
| 25      | 1184.54          | 1186.18                       | 15.48                | 98 %   |
| 26      | 1184.54          | 1186.04                       | 15.46                | 99 %   |
| 27      | 1056.37          | 1057.97                       | 16.42                | 97 %   |
| 28      | 928.19           | 929.63                        | 17.22                | 97 %   |
| 29      | 730.96           | 732.30                        | 15.56                | 99 %   |
| 30      | 1071.38          | 1072.89                       | 14.47                | 94 %   |
| 31      | 943.21           | 944.60                        | 15.59                | 96 %   |
| 32      | 745.97           | 747.30                        | 13.05                | 98 %   |
| 33      | 1212.56          | 1213.95                       | 15.72                | 97 %   |
| 34      | 1212.56          | 1213.98                       | 15.77                | 98 %   |
| 35      | 1212.56          | 1214.06                       | 15.71                | 97 %   |
| 36      | 1212.56          | 1214.13                       | 15.73                | 97 %   |

# Table S1: Peptide mass, retention time and purity

## Peptide structures









Molecular Weight: 1127,45



Molecular Weight: 1127,45











Molecular Weight: 1127,45



















Molecular Weight: 1142,46













Molecular Weight: 1143,45



Molecular Weight: 1157,47







Molecular Weight: 1155,50











Molecular Weight: 1169,53



Molecular Weight: 1203,54









Molecular Weight: 1157,47











Molecular Weight: 1184,54













Molecular Weight: 928,19



Molecular Weight: 730,96









Molecular Weight: 943,21



Molecular Weight: 745,97







Molecular Weight: 1212,56



Molecular Weight: 1212,56





#### Analytical chromatograms

#### D2-D

Retention time: 15.45 min Purity: 100 %







#### **2** Retention time: 16.48 min Purity: 98 %







# **4** Retention time: 14.72 min



#### 5 Retention time: 16.49 min

Purity: 98 %



#### **6** Retention time: 13.39 min Purity: 100 %





![](_page_18_Figure_3.jpeg)

![](_page_18_Figure_4.jpeg)

19

#### **8** Retention time: 14.47 min Purity: 98 %

![](_page_19_Figure_1.jpeg)

Retention time: 18.24 min Purity: 98 %

![](_page_19_Figure_4.jpeg)

10 Retention time: 16.00 min Purity: 98 %

![](_page_20_Figure_1.jpeg)

11 Retention time: 17.45 min Purity: 98 %

![](_page_20_Figure_3.jpeg)

12 Retention time: 17.43 min Purity: 98 %

![](_page_21_Figure_1.jpeg)

**13** Retention time: 17.90 min Purity: 96 %

![](_page_21_Figure_3.jpeg)

14 Retention time: 18.03 min Purity: 96 %

![](_page_22_Figure_1.jpeg)

![](_page_22_Figure_2.jpeg)

![](_page_22_Figure_3.jpeg)

**16** Retention time: 17.31 min Purity: 97 %

![](_page_23_Figure_1.jpeg)

![](_page_23_Figure_2.jpeg)

![](_page_23_Figure_3.jpeg)

#### **18** Retention time: 15.63 min Purity: 95 %

![](_page_24_Figure_1.jpeg)

**19** Retention time: 17.41 min Purity: 97 %

![](_page_24_Figure_3.jpeg)

**20** Retention time: 17.50 min Purity: 96 %

![](_page_25_Figure_1.jpeg)

![](_page_25_Figure_2.jpeg)

![](_page_25_Figure_3.jpeg)

**22** Retention time: 16.44 min Purity: 96 %

![](_page_26_Figure_1.jpeg)

#### 23 Retention time: 16.66 min Purity: 93 %

![](_page_26_Figure_3.jpeg)

27

#### 24 Retention time: 16.84 min Purity: 95 %

![](_page_27_Figure_1.jpeg)

25 Retention time: 15.48 min Purity: 98 %

![](_page_27_Figure_3.jpeg)

**26** Retention time: 15.46 min Purity: 99 %

![](_page_28_Figure_1.jpeg)

27 Retention time: 16.42 min Purity: 97 %

![](_page_28_Figure_3.jpeg)

#### **28** Retention time: 17.22 min Purity: 97 %

![](_page_29_Figure_1.jpeg)

**29** Retention time: 15.56 min

![](_page_29_Figure_3.jpeg)

#### **30** Retention time: 14.47 min Purity: 94 %

![](_page_30_Figure_1.jpeg)

![](_page_30_Figure_2.jpeg)

![](_page_30_Figure_3.jpeg)

**32** Retention time: 13.05 min Purity: 98 %

![](_page_31_Figure_1.jpeg)

![](_page_31_Figure_2.jpeg)

![](_page_31_Figure_3.jpeg)

**34** Retention time: 15.77 min Purity: 98 %

![](_page_32_Figure_1.jpeg)

![](_page_32_Figure_2.jpeg)

![](_page_32_Figure_3.jpeg)

**36** Retention time: 15.73 min Purity: 97 %

![](_page_33_Figure_1.jpeg)

## **MALDI-TOF-MS spectra**

#### **D2-D**

Mw: 1184.54 [MH<sup>+</sup>]: 1185.77

![](_page_34_Figure_3.jpeg)

2 Mw: 1127.45

![](_page_35_Figure_1.jpeg)

![](_page_35_Figure_2.jpeg)

Mw: 1058.38 [MH<sup>+</sup>]: 1059.49

![](_page_35_Figure_4.jpeg)

#### 4 Mw: 1108.44 [MH<sup>+</sup>]: 1109.54

![](_page_36_Figure_1.jpeg)

![](_page_36_Figure_2.jpeg)

Mw: 1127.45 [MH<sup>+</sup>]: 1128.62

![](_page_36_Figure_4.jpeg)

![](_page_37_Figure_0.jpeg)

![](_page_37_Figure_1.jpeg)

Mw: 1127.45 [MH<sup>+</sup>]: 1128.75

![](_page_37_Figure_3.jpeg)

![](_page_38_Figure_1.jpeg)

![](_page_38_Figure_2.jpeg)

Mw: 1253.60 [MH<sup>+</sup>]: 1253.92

![](_page_38_Figure_4.jpeg)

#### **10** Mw: 1142.46 [MH<sup>+</sup>]: 1143.48

![](_page_39_Figure_1.jpeg)

![](_page_39_Figure_2.jpeg)

Mw: 1169.53 [MH<sup>+</sup>]: 1170.46

![](_page_39_Figure_4.jpeg)

#### **12** Mw: 1203.54 [MH<sup>+</sup>]: 1204.46

![](_page_40_Figure_1.jpeg)

#### **13** Mw: 1143.45 [MH<sup>+</sup>]: 1144.48

![](_page_40_Figure_3.jpeg)

#### 14 M

![](_page_41_Figure_1.jpeg)

![](_page_41_Figure_2.jpeg)

Mw: 1219.54 [MH<sup>+</sup>]: 1220.76

![](_page_41_Figure_5.jpeg)

#### **16** Mw: 1155.50

![](_page_42_Figure_1.jpeg)

![](_page_42_Figure_2.jpeg)

Mw: 1253.60 [MH<sup>+</sup>]: 1255.13

![](_page_42_Figure_4.jpeg)

#### **18** Mw: 1142.46 [MH<sup>+</sup>]: 1143.97

![](_page_43_Figure_1.jpeg)

![](_page_43_Figure_2.jpeg)

Mw: 1169.53 [MH<sup>+</sup>]: 1170.93

![](_page_43_Figure_4.jpeg)

![](_page_44_Figure_0.jpeg)

![](_page_44_Figure_1.jpeg)

![](_page_44_Figure_2.jpeg)

#### **22** Mw: 1157.47 [MH<sup>+</sup>]: 1158.80

![](_page_45_Figure_1.jpeg)

![](_page_45_Figure_2.jpeg)

Mw: 1219.54 [MH<sup>+</sup>]: 1220.84

![](_page_45_Figure_4.jpeg)

#### **24** Mw: 1155.50 [MH<sup>+</sup>]: 1156.79

![](_page_46_Figure_1.jpeg)

![](_page_46_Figure_2.jpeg)

Mw: 1184.54 [MH<sup>+</sup>]: 1186.18

![](_page_46_Figure_4.jpeg)

#### **26** Mw: 1184.54 [MH<sup>+</sup>]: 1186.04

![](_page_47_Figure_1.jpeg)

![](_page_47_Figure_2.jpeg)

Mw: 1056.37

![](_page_47_Figure_4.jpeg)

Mw: 928.19 [MH<sup>+</sup>]: 929.63

![](_page_48_Figure_2.jpeg)

Mw: 730.96

![](_page_48_Figure_5.jpeg)

#### **30** Mw: 1071.38 [MH<sup>+</sup>]: 1072.89

![](_page_49_Figure_1.jpeg)

![](_page_49_Figure_2.jpeg)

Mw: 943.21

![](_page_49_Figure_4.jpeg)

![](_page_50_Figure_0.jpeg)

![](_page_50_Figure_1.jpeg)

![](_page_50_Figure_2.jpeg)

Mw: 1212.56 [MH<sup>+</sup>]: 1213.95

![](_page_50_Figure_4.jpeg)

#### **34** Mw: 1212.56 [MH<sup>+</sup>]: 1213.98

![](_page_51_Figure_1.jpeg)

![](_page_51_Figure_2.jpeg)

Mw: 1212.56

![](_page_51_Figure_4.jpeg)

#### **36** Mw: 1212.56 [MH<sup>+</sup>]: 1214.13

![](_page_52_Figure_1.jpeg)

Figure S1:

![](_page_53_Figure_1.jpeg)

**Figure S1.** SAXS data for peptide 5 shows that the nanotube structure is retained over full temperature range (25-45 °C).

Figure S2:

![](_page_54_Figure_1.jpeg)

**Figure S2.** SAXS data for peptide 2 shows how the anisotropy (seen in the detector image) increases over time even though the scattering pattern does not change. The effect can be explained by the elongated structures being partly broken up during injection of the sample into the capillary and then reformed over time, however they are not visible in the scattering as the length of these structures are outside the measured q-range.

# Figure S3:

![](_page_55_Figure_1.jpeg)

![](_page_55_Figure_2.jpeg)

#### Table S2:

**Table S2.** Important fit parameters from the analysis of liposomes-peptide mixes. Values outside of the experimental q-range noted with \* and joint SAXS/SANS fits noted with §. The error of the fits is found to be less than 5 %.

|                                  | Liposomes<br>- | D2D peptide       |                   | Peptide 5         |                   |                   |                   |
|----------------------------------|----------------|-------------------|-------------------|-------------------|-------------------|-------------------|-------------------|
| Fraction                         |                | 1.20              | 1.10              | 1.5               | 1.20              | 1.10§             | 1.5               |
| peptide                          |                | 1.20              | 1.10              | 1.5               | 1.20              | 1.10              | 1.5               |
| ULV radius[Å]                    | 380            | *                 | *                 | *                 | *                 | *                 | *                 |
| Bilayer                          | 38 5+0 5       | 38 5+0 5          | 38 5+0 5          | 38 5+0 5          | 38 5+0 5          | 37 8+0 5          | 37 /+0 5          |
| thickness[Å]                     | 38.J±0.J       | 38. <u>5</u> ±0.5 | 38. <u>5</u> ±0.5 | 38. <u>3</u> ±0.3 | 30. <u>31</u> 0.J | 57.8 <u>-</u> 0.5 | 57.4 <u>-</u> 0.5 |
| Z <sub>peptide</sub> [Å]         | -              | 11                | 12                | 14                | 17                | 17                | 16                |
| σ <sub>peptide</sub> [Å]         | -              | 3                 | 3                 | 3                 | 3                 | 3                 | 3                 |
| <b>f</b> <sub>free peptide</sub> |                | 0.5               | 0.51              | 0.7               | 0.5               | 0.5               | 0.4               |
| $\sigma_{\text{SD}}$             | 0.22           | 0.22              | 0.3               | 0.3               | 0.3               | 0.3               | 0.3               |