

File Name: Supplementary Data 1

Description: Backbone generation protocol, <thioether_backbone.py>

File Name: Supplementary Data 2

Description: Backbone to anchor docking protocol, <docking_protocol.py>

File Name: Supplementary Data 3

Description: Side chain rotamer design and filtering protocol, <kappa_peptide_design.xml>

File Name: Supplementary Data 4

Description: Residue and parameter files for scripts supplied in Supplementary Data 1 - 3, i.e. <CYY.params>, <CVV.params>, <l_res.txt>, <d_res.txt>