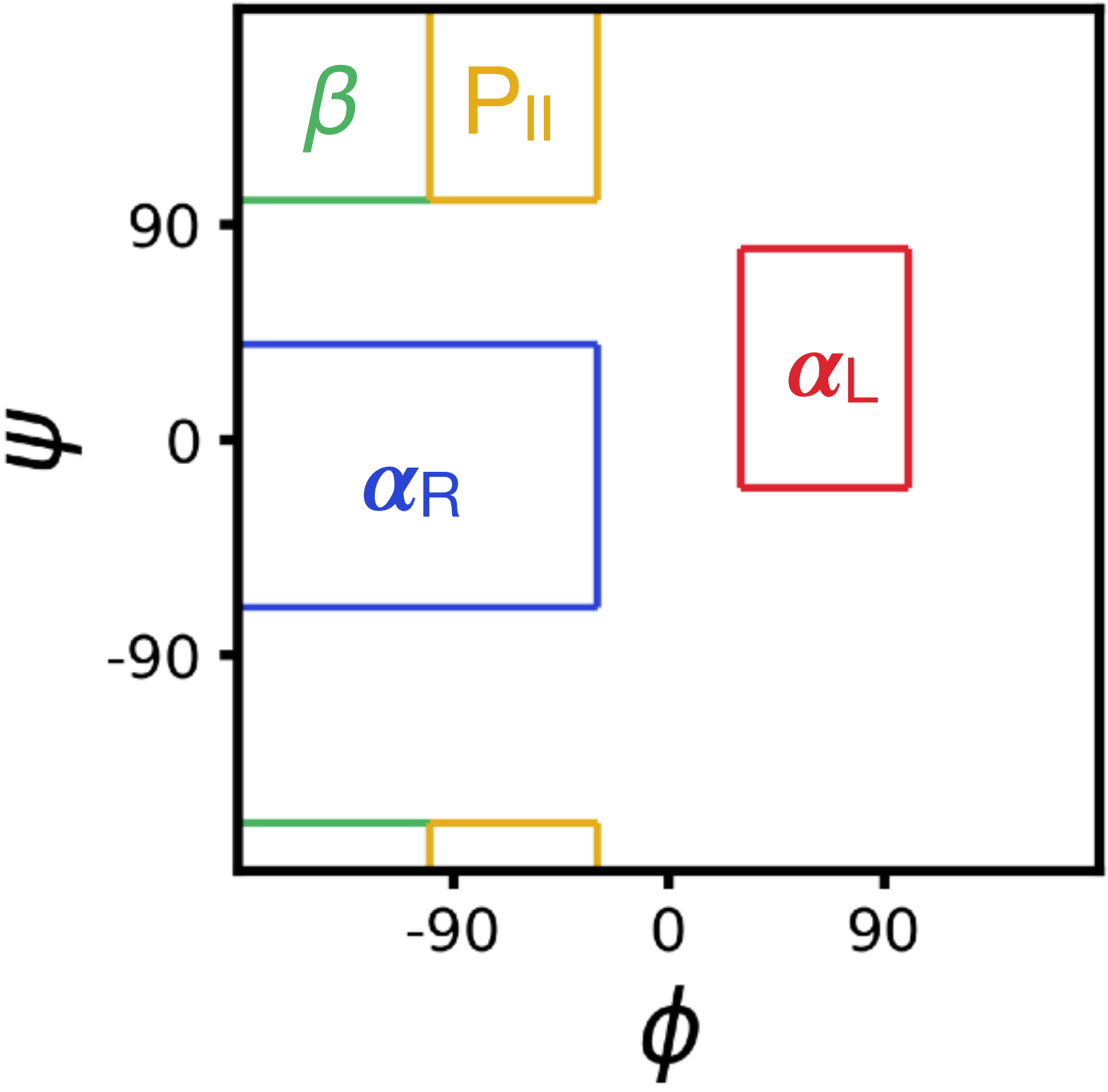
Desired SESE conformation

Target cyclo-(SESEX$_1$X$_2$X$_3$X$_4$) structure

Target cyclo-(SESE$X_1X_2X_3X_4X_5$) structure


β
PII
αL
αR
90
0
-90
ψ
-90
0
90
ϕ

Conformer Probability

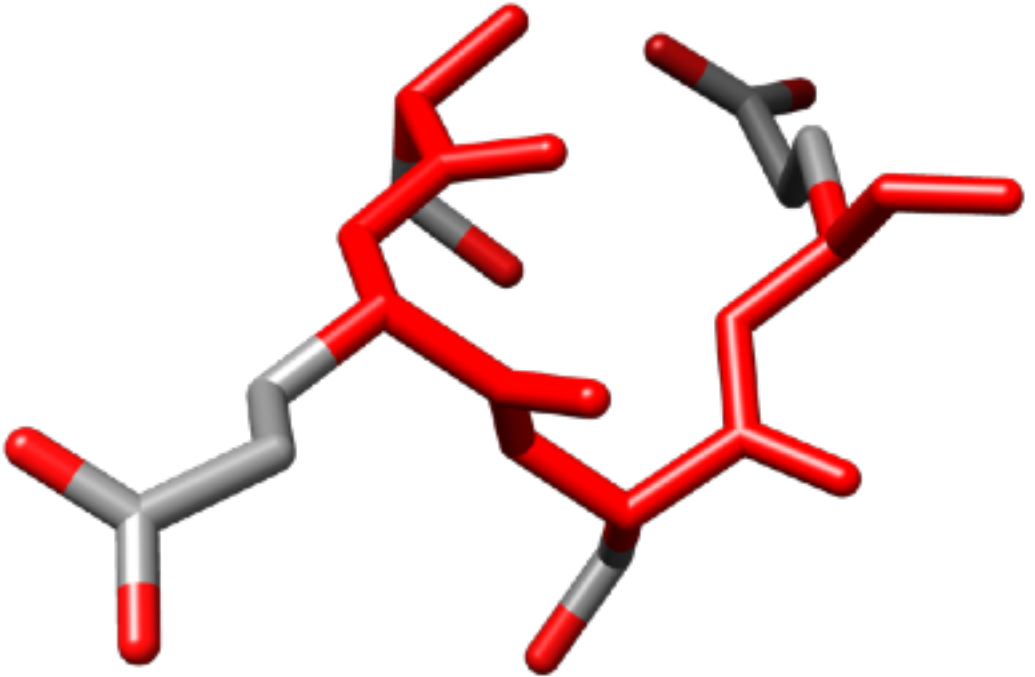
AA	P_{II}	β	α_R	α_L
P	0.80	0.00	0.15	0.00
A	0.46	0.23	0.21	0.02
L	0.43	0.21	0.26	0.02
M	0.40	0.24	0.21	0.03
E	0.40	0.22	0.28	0.03
I	0.39	0.36	0.20	0.00
W	0.39	0.26	0.23	0.03
C	0.38	0.31	0.18	0.03
V	0.37	0.39	0.19	0.00
F	0.35	0.33	0.20	0.03
Q	0.35	0.26	0.26	0.04
Y	0.34	0.32	0.21	0.03
R	0.34	0.27	0.26	0.04
K	0.34	0.26	0.29	0.04
S	0.33	0.25	0.33	0.02
H	0.30	0.30	0.22	0.06
T	0.29	0.28	0.38	0.00
D	0.29	0.09	0.43	0.05
N	0.24	0.15	0.30	0.13
G	0.21	0.09	0.09	0.27

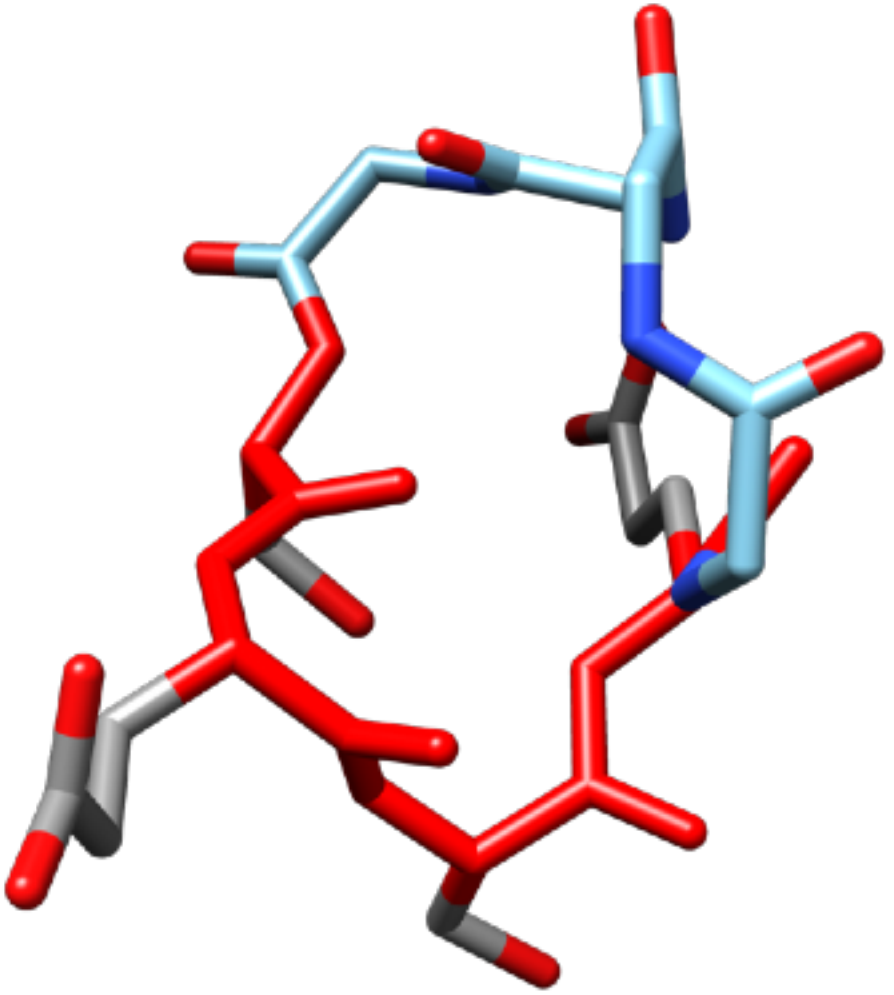
Zhou, C.-Y., Jiang, F. & Wu, Y.-D. *J. Phys. Chem. B.* **119**, 1035-1047 (2015)

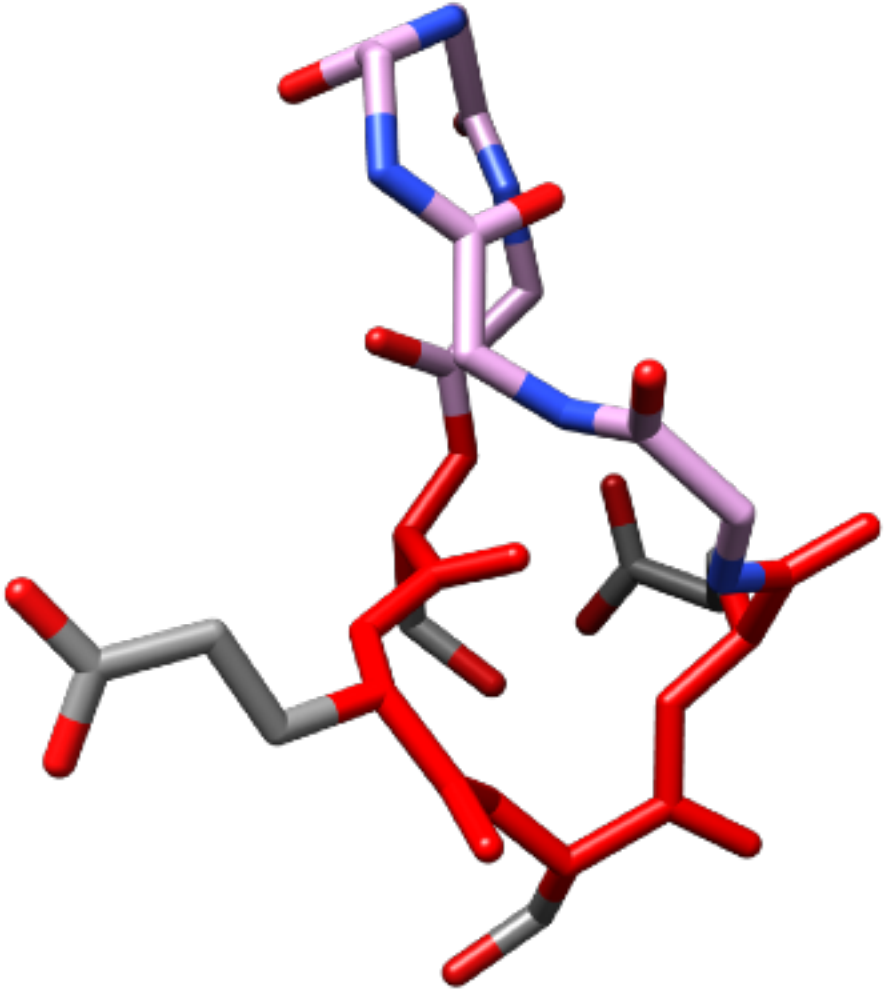
Linker sequence selection is

informed by aa's intrinsic propensity

SESEG4 and SESEG5 adopt target conformation with high population







Conformer Definition