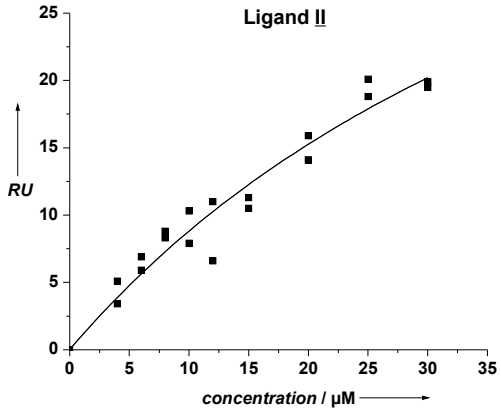
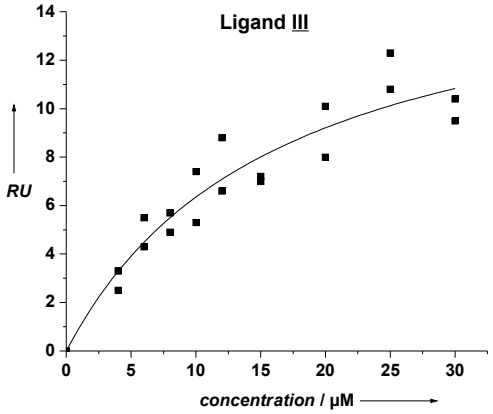
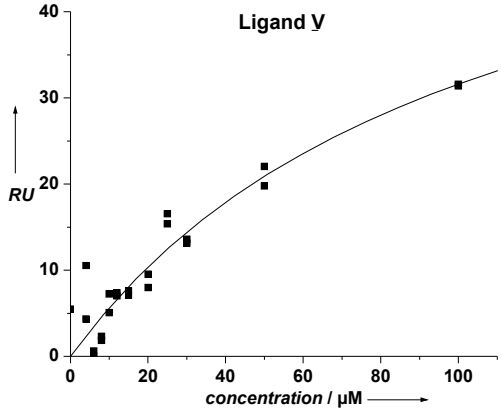
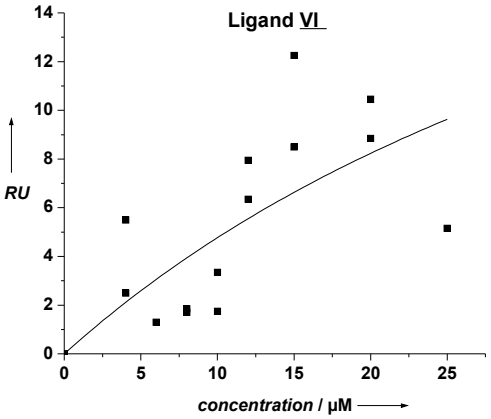
Supporting Information A.T. Neffe, M. Bilang, and B. Meyer.

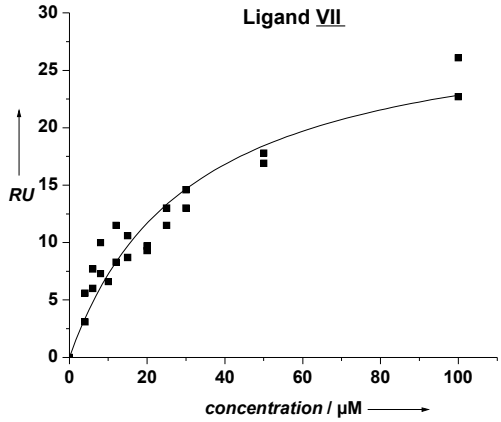
a) SPR graphs

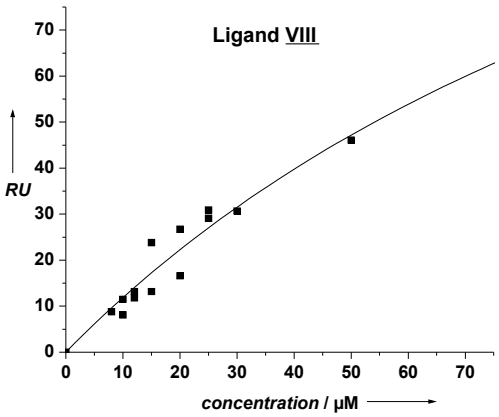


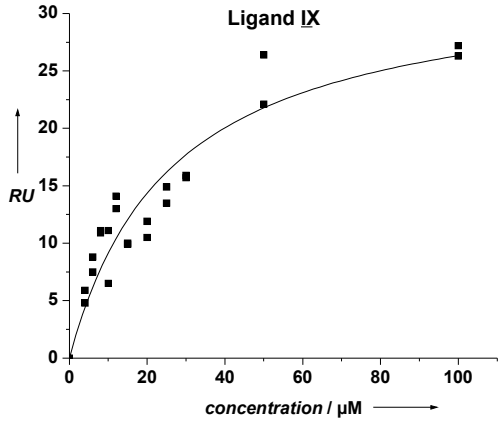


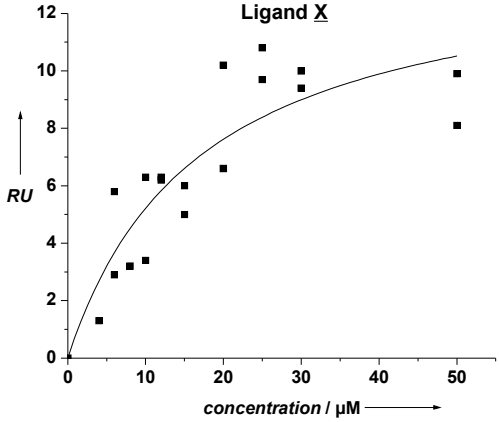


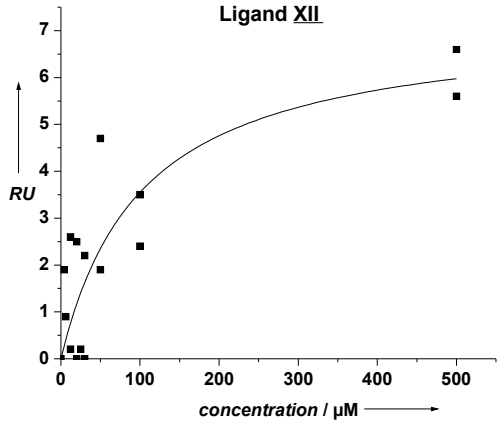












b) Characterization

b1) Ligand **II**
Yield: 1.8 mg (2.3 µmol) white solid, 3 % (of 90 µmol resin bound prolinol).
MALDI-TOF MS: 796 ($M+H^+$), 818 ($M+Na^+$), 834 ($M+K^+$)
NMR:
500 MHz, T = 295K, pH = 2, H_2O/D_2O 9:1,
calibrated on Lys-Hα = 4.384 ppm and Lys-Cε = 39.691 ppm.

Spin system	***N*H**	**Hα/α'**	**Hβ/β'**	**Hγ/γ'**	**Miscellaneous**
α-NOA					H2: 6.817, H3: 7.369, H4: 7.516, H5: 7.844, H6: 7.523, H7: 7.513, H8: 8.237, O-CH_2: 4.835
Lys	8.302	4.384	1.715/1.619	1.141	Hδ: 1.470, Hε: 2.742, *N*H-Z: 7.395
Val	8.221	4.006	1.950	0.840	
Gly	8.504	3.908/3.805			
Thr	7.899	4.416	3.903	0.997	
Prolinol		4.141	1.885/1.783	1.936/1.793	Hδ/ δ': 3.429, H1/1': 4.005
Cyclohexyl	6.683				H1: 3.188, H2/2': 1.687/1.057, H3/3': 1.583/1.175, H4/4': 1.460/1.057

Table 1: ^{1}H NMR chemical shifts of the *trans* rotamere of Ligand II (determined from ^{1}H, TOCSY, ROESY, COSY, HSQC).

Spinsystem	Cα	Cβ	Cγ	Miscellaneous
α-NOA				C2: 106.245, C3: 126.450, C4: 121.991, C5: 128.029, C6: 127.432, C7: 126.437, C8: 121.760
Lys	53.475	30.850	22.207	Cδ: 26.601, Cε: 39.691
Val	60.407	30.293	18.595	
Gly	42.667			
Thr	57.979	67.769	?	
Prolinol	56.843	27.01	24.097	Cδ: 48.584, C1: 65.05
Cyclohexyl				C1: 50.398, C2/6: 32.822, C3/5: 24.882, C4: 25.324

Table 2: ^{13}C NMR chemical shifts of the *trans* rotamere of Ligand II (determined from a HSQC).

Spin system	*N*H	Hα/α'	Hβ/β'	Hγ/γ'	Miscellaneous
α-NOA					
Lys	8.341	4.378	1.721/1.613	1.129	Hd : 1.47 6, He : 2.736, NH-Z : 7.379
Val	8.113	4.064	1.969	0.826	
Gly	8.423	3.911			
Thr	7.798	4.938	3.968	1.045	
Prolinol					
Cyclohexyl	6.388				H1: 3.138, H2/2': 1.684/1.008, H3/3': 1.556/1.149, H4/4': 1.435

Table 3: ^{1}H NMR chemical shifts of the *cis* rotamere of Ligand II (determined from ^{1}H, TOCSY, ROESY, COSY, HSQC).

No individual ^{13}C NMR chemical shifts could be determined for the cis rotamere.

b2) Ligand **III**
Yield: 3 mg (3.7 µmol) white solid, 4 % (of 90 µmol resin bound prolinol).
MALDI-TOF MS: 797 ($M+H^+$), 819 ($M+Na^+$), 835 ($M+K^+$)
NMR:
500 MHz, T = 290K, pH = 2, H_2O/D_2O 9:1,
calbrated on HDO = 4.7 ppm and MeOH = 49.2 ppm.

Spin system	*N*H	Hα/α'	Hβ/β'	Hγ/γ'	Miscellaneous
QuinOA					H2: 8.963, H3: 7.936, H4: 8.902, H5: 7.701, H6: 7.741, H7: 7.353, O-CH_2: 4.903
Lys	8.704	4.308	1.663	1.25	Hδ: 1.508, Hε: 2.792, *N*H-Z: 7.401
Val	8.331	3.946	1.882	0.753	
Gly	8.491	3.817			
Thr	7.919	4.391	3.882	0.986	
Prolinol		4.075	1.879/1.754	1.837/1.709	Hδ/ δ': 3.434, H1/1': 4.13/3.765
Cyclohexyl	6.673				H1: 3.088, H2/2': 1.586/0.953, H3/3': 1.379/0.93, H4/4': 1.502/1.076

Table 4: ^{1}H NMR chemical shifts of the *trans* rotamere of Ligand III (determined from ^{1}H, TOCSY, ROESY, COSY, HSQC).

Spin system	Cα	Cβ	Cγ	Miscellaneous
QuinOA				C2: 147.401, C3: 122.714, C4: 143.644, C5: 126.001, C6: 121.841, C7: 114.328, O-CH_2: 67.696
Lys	53.91	30.634	22.323	Cδ: 26.621, Cε: 39.676
Val	60.12	30.443	17.93	
Gly	42.589			
Thr	57.779	67.619	18.857	
Prolinol	56.919	24.138	26.813	Cδ: 48.274, C1: 64.295
Cyclohexyl				C1: 50.375, C2/6: 32.672, C3/5: 25.061, C4: 24.681

Table 5: ^{13}C NMR chemical shifts of the *trans* rotamere of Ligand III (determined from a HSQC).

Spin system	*N*H	Hα/α'	Hβ/β'	Hγ/γ'	Miscellaneous
ChinOA					
Lys					
Val	8.19	4.011	1.863	0.741	
Gly	8.491	3.869			
Thr	7.783	4.869	3.908	0.992	
Prolinol					
Cyclohexyl	6.616				H1: 3.121, H2/2': 1.476/1.063, H3/3': 1.34/0.953, H4/4': 1.618

Table 6: ^{1}H NMR chemical shifts of the *cis* rotamere of Ligand III (determined from ^{1}H, TOCSY, ROESY, COSY, HSQC).

^{13}C NMR chemical shifts of the *cis* rotamer could be determined only for some of the carbons.

Spin system	Cα	Cβ	Cγ	Miscellaneous
ChinOA				
Lys				
Val	59.69	30.76	18.692	
Gly	41.232			
Thr		67.9798	18.925	
Prolinol				
Cyclohexyl				C1: 49.181, C2/6:

Table 7: ^{13}C NMR chemical shifts of the *cis* rotamere of Ligand III (determined from a HSQC).

b3) Ligand V
Yield: 1.3 mg (1,7 µmol) white solid, 3.3 % (of 50 µmol resin bound prolinol).
MALDI-TOF MS: 779 ($M+H^+$), 801 ($M+Na^+$), 817 ($M+K^+$)
NMR: 700 MHz, T = 285 K, pH = 2, H_2O/D_2O 9:1,
calibrated on HDO = 4.7 und Lys-Hε = 38.820 ppm.

Spin system	*N*H	Hα/α'	Hβ/β'	Hγ/γ'	Miscellaneous
β-NA					H1: 7.569, H3: 7.200, H4: 7.688, H5: 7.308, H6: 7.684, H7: 7.274, H8: 7.656, -CH_2: 3.58
Lys	8.353	4.129	1.578/1.513	1.151	Hδ: 1.394, Hε: 2.658, *N*H-Z: 7.309
Val	8.007	3.844	1.762	0.636	
Gly	8.382	3.718			
Thr	7.822	4.284	3.775	0.900	
Prolinol		4.028	1.77/1.667	1.829/1.686	Hδ/ δ': 3.524/3.376, H1/1': 4.116/3.741
Cyclohexyl	6.645				H1: 3.04, H2/2': 1.536/0.901, H3/3': 1.441/1.028, H4/4': 1.441/1.315

Table 8: ^{1}H NMR chemical shifts of the *trans* rotamere of Ligand V (determined from ^{1}H, TOCSY, ROESY, COSY, HSQC).

Spin system	Cα	Cβ	Cγ	Miscellaneous
β-NA				C1: 126.948, C3: 126.099, C4: ca. 127, C5: 125.642, C6: ca. 127, C7: ca. 125, C8: ca. 127, -CH_2: 41.229
Lys	52.886	29.516	21.397	Cδ: 24.836, Cε: 38.819
Val	57.784	29.516	17.799	
Gly	41.269			
Thr	56.455	66.981	17.831	
Prolinol	55.85	25.95	22.957	Cδ: 47.137, C1: 53.472
Cyclohexyl				C1: 49.436, C2/6: 31.776, C3/5: 23.785, C4: 24.332

Table 9: ^{13}C NMR chemical shifts of the *trans* rotamere of Ligand V (determined from a HSQC).

Spin system	*N*H	Hα/α'	Hβ/β'	Hγ/γ'	Miscellaneous
β-NA					
Lys	8.418	4.127	1.605/1.529	1.164	Hd : 1.403
Val	7.858	3.894	1.781	0.63	
Gly	8.282	3.756			
Thr	7.713	4.857	3.85	0.932	
Prolinol	XXX				XXX
Cyclohexyl	6.237				H1: 2.941, H2/2': 1.532/0.869, H3/3': 1.361/0.984, H4/4': 1.532

Table 10: ^{1}H NMR chemical shifts of the *cis* rotamere of Ligand V (determined from ^{1}H, TOCSY, ROESY, COSY, HSQC).

No individual ^{13}C NMR chemical shifts could be determined for the cis rotamere.

b4) Ligand **VI**
Yield: 2.3 mg (2.8 µmol) white solid, 5.6 % (of 50 µmol resin bound prolinol).
MALDI-TOF MS: 826 ($M+H^+$), 848 ($M+Na^+$), 864 ($M+K^+$)
NMR:
700 MHz, T = 285 K, pH = 2, H_2O/D_2O 9:1,
calibrated on HDO = 4.7 ppm and Lys-Hε = 38.848 ppm.

Spin system	*N*H	Hα/α'	Hβ/β'	Hγ/γ'	Miscellaneous
β-NTP					H1: 7.649, H3: 7.265, H4: 7.635, H5: 7.616, H6: 7.290, H7: 7.328, H8: 7.669, S-CH_2: 3.075, CH_2: 2.420
Lys	8.084	3.868	1.423	1.001	Hδ: 1.276, Hε: 2.655, *N*H-Z: 7.303
Val	7.989	3.804	1.787	0.708/0.692	
Gly	8.348	3.746/3.67			
Thr	7.822	4.263	3.765	0.867	
Prolinol		3.964	1.712/1.615	1.778/1.639	Hδ/ δ': 3.458/3.329, H1/1': 4.056/3.685
Cyclohexyl	6.625				H1: 3.017, H2/2': 1.527/0.895, H3/3': 1.43/1.297, H4/4': 1.015

Table 11: ^{1}H NMR chemical shifts of the *trans* rotamere of Ligand VI (determined from ^{1}H, TOCSY, ROESY, COSY, HSQC).

Spin system	Cα	Cβ	Cγ	Miscellaneous
β-NTP				C1: 126.479, C3: 126.749, C4: 128.054, C5: 126.542, C6: 125.587, C7: 126.717, C8: 127.720, S-CH_2: 27.3. CH_2: 34.263
Lys	52.943	26.661	21.419	Cδ: 25.937, Cε: 38.848
Val	59.247	29.349	17.882/16.691	
Gly	41.228			
Thr	56.568	67.022	17.917	
Prolinol	55.993	26.042	22.61	Cδ: 47.217, C1: 63.397
Cyclohexyl				C1: 49.476, C2/6: 31.926, C3/5: 29.474, C4: 23.696

Table 12: ^{13}C NMR chemical shifts of the *trans* rotamere of Ligand VI (determined from a HSQC).

Spin system	*N*H	Hα/α'	Hβ/β'	Hγ/γ'	Miscellaneous
β-NTP					
Lys	8.123	3.861	1.442	1.027	Hd : 1.289, He : 2.648, NH-Z : 7.303
Val	7.890	3.868	1.825	0.708	
Gly	8.290	3.74			
Thr	7.675	4.819	3.797	0.887	
Prolinol	XXX				XXX
Cyclohexyl	6.255				H1: 2.963 H2/2': 1.430/1.003, H3/3': 1.538/0.847, H4/4': 1.291

Table 13: ^{1}H NMR chemical shifts of the *cis* rotamere of Ligand VI (determined from ^{1}H, TOCSY, ROESY, COSY, HSQC).

No individual ^{13}C NMR chemical shifts could be determined for the cis rotamere.

b5) Ligand **VII**
Yield: 1.4 mg (1,7 µmol) white solid, 2 % (of 90 µmol resin bound prolinol).
MALDI-TOF MS: 825 ($M+H^+$), 847 ($M+Na^+$), 863 ($M+K^+$)
NMR:
500 MHz, T = 295 K, pH = 2, H_2O/D_2O 9:1,
calibrated on HDO = 4.725 ppm and MeOH = 49.4 ppm. Due to a lack of substance, the probe had a low concentration, so not all signals could be determined.

Spin system	*N*H	Hα/α'	Hβ/β'	Hγ/γ'	Miscellaneous
β-NOA					H1: 7.18, H3: 7.214, H4: 7.819, H5: 7.802, H6: 7.356, H7: 7.445, H8: 7.746, O-CH_2: 4.781
Cit	8.395	4.368	1.693/1.602	1.252	Hδ: 1.252
Val	8.182	3.986	1.913	0.786	
Gly	8.424	3.856			
Thr	7.911	4.433	3.927	1.045	
Prolinol		4.152	1.954/1.795		Hδ/ δ': 3.400
Cyclohexyl	6.698				H1: 3.175, H4/4': 1.584/1.182

Table 14: ^{1}H NMR chemical shifts of the *trans* rotamere of Ligand VII (determined from ^{1}H, TOCSY, ROESY, COSY, HSQC).

Spin system	Cα	Cβ	Cγ	Miscellaneous
β-NOA				C1: 107.708, C3: 118.537, C4: 128.231, C5: 128.001, C6: 124.896, C7: 127.368, C8: 127.311
Cit	53.54	28.461	25.717	Cδ: 39.526
Val	60.369			
Gly	42.673			
Thr	58.112	67.851		
Prolinol	57.044	24.26		
Cyclohexyl				C4: 24.709

Table 15: ^{13}C NMR chemical shifts of the *trans* rotamere of Ligand VII (determined from a HSQC).

Spin system	*N*H	Hα/α'	Hβ/β'	Hγ/γ'	Miscellaneous
β-NOA					
Cit	8.425	4.361	1.693/1.608	1.252	Hδ: 2.846
Val	8.08			0.786	
Gly	8.331	3.889			
Thr	7.799	4.944	3.979	1.071	
Prolinol					
Cyclohexyl	6.378				H1: 3.148

Table 16: ^{1}H NMR chemical shifts of the *cis* rotamere of Ligand VII (determined from ^{1}H, TOCSY, ROESY, COSY, HSQC).

For the ^{13}C NMR chemical shifts of the *cis* rotamere, no individual signals could be determined.

b6) Ligand **VIII**
Yield: 2.5 mg (3 µmol) white solid, 3.3 % (of 90 µmol resin bound prolinol).
MALDI-TOF MS: 835 ($M+H^+$), 857 ($M+Na^+$), 873 ($M+K^+$)
NMR:
500 MHz, T = 290K, pH = 2, H_2O/D_2O 9:1,
calibrated on HDO = 4.7 ppm and Lys-Hε = 39.468 ppm

Spin system	*N*H	Hα/α'	Hβ/β'	Hγ/γ'	Miscellaneous
β-NOA					H1: 7.077, H3: 7.137, H4: 7.752, H5: 7.743, H6: 7.298, H7: 7.383, H8: 7.682, O-CH_2: 4.678
Lys	8.371	4.287	1.629/1.543	1.014	Hδ: 1.1.348, Hε: 2.481, *N*H-Z: 7.277
Chg	8.088	3.925	1.486	Siehe rechts	Hγ/δ/δ'/ε/ε': 1.446/1.405/0.968/0.818/0.738
Gly	8.425	3.798			
Thr	7.856	4.367	3.873	0.991	
Prolinol		4.095	1.835/1.727	1.884/1.758	Hδ/ δ': 3.586/3.441, H1/1': 4.176/3.798
Cyclohexyl	6.687				H1: 3.125, H2/2': 1.635/0.991, H3/3': 1.405/0.991, H4/4': 1.514/1.106

Table 17: ^{1}H NMR chemical shifts of the *trans* rotamere of Ligand VIII (determined from ^{1}H, TOCSY, ROESY, COSY, HSQC).

Spin system	**Cα**	**Cβ**	**Cγ**	**Miscellaneous**
β-NOA				C1: 107.421, C3: 118.712, C4: 128.013, C5: 128.054, C6: 125.0074, C7: 127.282, C8: 127.363, O-CH_2: n.b.
Lys	56.881	30.657	22.298	Cδ: 26.618, Cε: 39.496
Chg	59.574	39.536	Siehe rechts	Cγ/δ/ε: 25.587/28.777/29.337
Gly	42.603			
Thr	57.904	67.764	18.899	
Prolinol	56.934	26.938	24.178	Cδ: 48.529, C1: 64.424
Cyclohexyl				C1: 50.469, C2/6: 32.697, C3/5: 25.698, C4: 24.898

Table 18: ^{13}C NMR chemical shifts of the *trans* rotamere of Ligand VIII (determined from a HSQC).

Spin system	***N*H**	**Hα/α'**	**Hβ/β'**	**Hγ/γ'**	**Miscellaneous**
β-NOA					
Lys	8.412	4.275	1.635/1.56	1.02	Hδ : 1.353, Hε : 2.498
Chg	7.98	3.959	1.48		
Gly	8.324	3.827			
Thr	7.772	4.891	3.919	1.014	
Prolinol					H1/1': 3.921/3.811
Cyclohexyl	6.343				H1: 3.085, H2/2': 1.642/0.962, H3/3': 1.394/0.962, H4/4': 1.514/1.106

Table 19: ^{1}H NMR chemical shifts of the *cis* rotamere of Ligand VIII (determined from ^{1}H, TOCSY, ROESY, COSY, HSQC).

Only for some of the carbons of the *cis* rotamere, individual ^{13}C NMR chemical shifts could be determined.

Spin system	Cα	Cβ	Cγ	Miscellaneous
ChinOA				
Lys				
Val	59.69	30.76	18.692	
Gly	41.232			
Thr		67.9798	18.925	
Prolinol				
Cyclohexyl				C1: 49.181

Table 20: ^{13}C NMR chemical shifts of the *cis* rotamere of Ligand VIII (determined from a HSQC).

b7) Ligand **IX**
Yield: 0.7 mg (0.9 µmol) white solid, 1 % (of 90 µmol resin bound prolinol).
MALDI-TOF MS: 809 ($M+H^+$), 831 ($M+Na^+$), 847 ($M+K^+$)
NMR:
500 MHz, T = 300 K, pH = 2, H_2O/D_2O 9:1,
calibreated on HDO = 4.725 ppm and Naph-C1 = 107.725 ppm

Spin system	***N*H**	**Hα/α'**	**Hβ/β'**	**Hγ/γ'**	**Miscellaneous**
β-NOA					H1: 7.23, H3: 7.275, H4: 7.886, H5: 7.868, H6: 7.408, H7: 7.488, H8: 7.813, O-CH_2: 4.812
Lys	8.424	4.406	1.741/1.644	1.113	Hδ: 1.455, Hε: 2.599, *N*H-Z: 7.340
Val	8.110	4.371	1.985	0.834	
Sar		3.709			N-CH_3: 3.139
Thr	8.004	4.497	4.009	1.141	
Prolinol		4.263	2.034/1.91	2.004/1.917	Hδ/ δ': 3.761/3.645, H1/1': 4.371/4.065
Cyclohexyl	6.745				H1: 3.255, H2/6, H3/5: , H4:

Table 21: ^{1}H NMR chemical shifts of the *trans* rotamere of Ligand IX (determined from ^{1}H, TOCSY, ROESY, COSY, HSQC).

Spin system	**Cα**	**Cβ**	**Cγ**	**Miscellaneous**
β-NOA				C1: 107.725, C3: 118.924, C4: 128.16, C5: 128.16 , C6: 125.080, C7: 127.522, C8 : 127.415, CH_2: 66.947
Lys	53.561	30.769	22.529	Cδ: 26.606, Cε: 39.627
Val	55.58	30.537	18.813	
Sar	48637			N-CH_3 : ca. 37.8
Thr	57.903	67.727	19.007	
Prolinol	67.955	27.139	24.331	Cδ: 55.864, C1: 55.631
Cyclohexyl				C1: ca. 38, C2/6: 32.947, C3/5: 24.96, C6: 22.6

Table 22: ^{13}C NMR chemical shifts of the *trans* rotamere of Ligand IX (determined from a HSQC).

Spin system	***N*H**	**Hα/α'**	**Hβ/β'**	**Hγ/γ'**	**Miscellaneous**
β-NOA					
Lys	8.358	4.512	1.728/1.639	1.167	Hδ: 1.460. Hε: 2.620, *N*H-Z: 7.346
Val	8.031	4.557	1.989	0.842/0.779	
Sar					
Thr	7.841	5.003	4.047	1.129	
Prolinol					
Cyclohexyl					

Table 23: ^{1}H NMR chemical shifts of the *cis* rotamere of Ligand IX (determined from ^{1}H, TOCSY, ROESY, COSY, HSQC).

No individual ^{13}C NMR chemical shifts could be detected for the *cis* rotamere.

b8) Ligand **X**
Yield: 0.8 mg (0.9 µmol) white solid, 1 % (of 90 µmol resin bound prolinol).
MALDI-TOF MS: 868 ($M+H^+$), 890 ($M+Na^+$), 906 ($M+K^+$)
NMR:
500 MHz, T = 285 K, pH = 2, H_2O/D_2O 9:1,
calibrated on HDO = 4.700 and Lys-Hε: 39.433 ppm

Spin system	***N*H**	**Hα/α'**	**Hβ/β'**	**Hγ/γ'**	**Miscellaneous**
β-NOA					H1: 7.019, H3: 7.074, H4: 7.686, H5: 7.673, H6: 7.223, H7: 7.310, H8: 7.618, O-CH_2: 4.610
Lys	8.314	4.194	1.542/1.459	0.871	Hδ: 1.227, Hε: 2.325, *N*H-Z: 7.188
Val	8.067	3.826	1.720	0.616	
Glu	8.374	4.206	1.844/1.702	2.189	
Thr	8.081	4.295	3.826	0.966	
Prolinol		4.033	1.830/1.710	1.847/1.713	Hδ/ δ': 3.529/3.403, H1/1': 4.166/3.744
Cyclohexyl	6.615				H1: 3.120, H2/2': 1.581/0.959, H3/3': 1.356, H4/4': 1.466/1.078

Table 24: ^{1}H NMR chemical shifts ofthe *trans* rotamere of Ligand X (determined from ^{1}H, TOCSY, ROESY, COSY, HSQC).

Spin system	**Cα**	**Cβ**	**Cγ**	**Miscellaneous**
β-NOA				C1: 107.248, C3: 118.508, C4: 127.5, C5: 127.5, C6: 124.803, C7: 126.997, C8: 127.228, O-CH_2: 67.696
Lys	53.300	30.536	22.131	Cδ: 26.548, Hε: 39.433
Val	59.869	30.291	18.082	
Glu	53.191	26.855	30.107	
Thr	57.772	67.486	19.002	
Prolinol	56.723	26.794	24.278	Cδ: 48.554, C1: 64.285
Cyclohexyl				C1: 49.195, C2/6: 32.745, C3/5: 25.505, C4: 24.953

Table 25: ^{13}C NMR chemical shifts of the *trans* rotamere of Ligand X (determined from a HSQC).

Even though double signals in the 2D NMR spectra could be found only for valine (*N*H: 8.031, Hα: 3.838, Hβ: 30.291, Hγ: 18.082), this indicates a cis trans equilibrium for **X**.

b9) Ligand **XI**
Yield: 4.9 mg (6.4 µmol) white solid, 7 % (of 90 µmol resin bound alaninol).
MALDI-TOF MS: 769 ($M+H^+$), 791 ($M+Na^+$), 807 ($M+K^+$)
NMR:
700 MHz, T = 285K, pH = 2, H_2O/D_2O 9:1,
calibrated on HDO = 4.7 ppm and MeOH = 48.711 ppm.
No *cis*/*trans* rotameres could be detected.

Spin system	***N*H**	**Hα/α'**	**Hβ/β'**	**Hγ/γ'**	**Miscellaneous**
β-NOA					H1: 7.298, H3: 7.341, H4: 7.936, H5: 7.92, H6: 7.484, H7: 7.566, H8: 7.865, O-CH_2: 4.865
Lys	8.443	4.536	1.86/1.76	1.231	Hδ: 1.578, Hε: 2.701, *N*H-Z: 7.588
Val	8.31	4.131	2.06	0.949	
Gly	8.645	4.084/3.966			
Thr	7.968	4.272	4.178	1.207	
Alaninol	8.316	4.201	1.201		H1/1': 4.078/3.972
Cyclohexyl	6.873				H1: 3.337, H2/2': 1.825/1.178, H3/3': 1.602, H4/4': 1.713/1.3

Table 26: ^{1}H NMR chemical shifts of Ligand XI (determined from ^{1}H, TOCSY, ROESY, COSY, HSQC).

Spin system	**Cα**	**Cβ**	**Cγ**	**Miscellaneous**
β-NOA				C1: 107.633, C3: 118.727, C4: 128.103, C5: 128.057, C6: 124.993, C7: 127.268, C8: 127.361, O-CH_2: 67.155
Lys	53.206	31.14	22.652	Cδ: 26.879, Cε: 39.554
Val	60.369	30.394	18.305	
Gly	42.762			
Thr	60.091	67.716	16.121	
Alaninol	45.488	16.121		C1: 67.162
Cyclohexyl				C1: 50.433, C2/6: 33.004, C3/5: 25.355, C4: 24.855

Table 27: ^{13}C NMR chemical shifts of Ligand XI (determined from an HSQC).

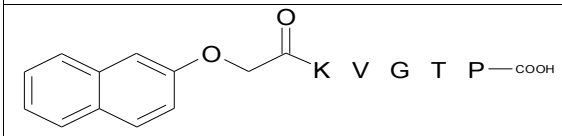
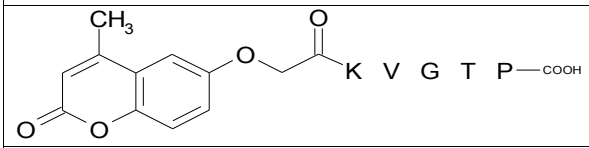
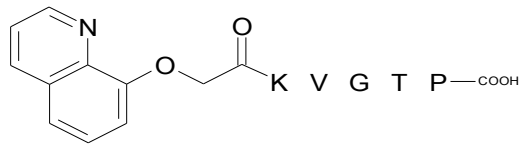
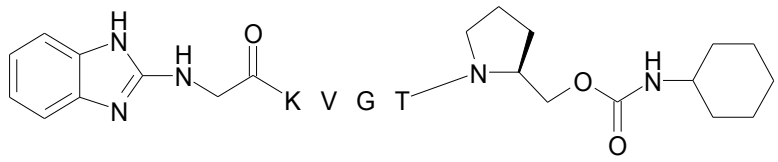
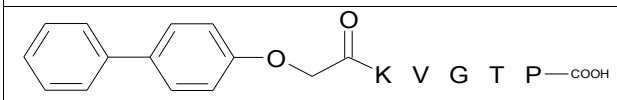
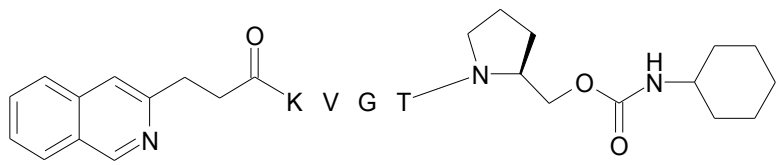
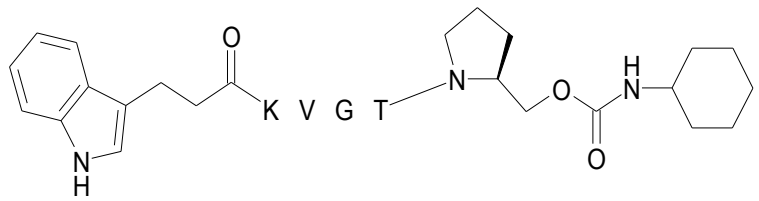
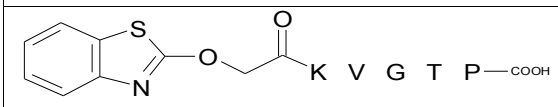
Compound	Binding energy [kcal/mol]	Δ E [kcal/mol]
	-274	0
	-277	-3
	-270	7
	-264*	10*
	-263	14
	-250*	24*
	-234*	40*
	§	---

Table 1: Total calculated binding energy of the ligand protein complexes of peptidomimetics with different aromatics and energy difference to the β-naphthyl system (*: for these compounds, binding activity could only be determined if there was the connection to a cyclohexylcarbamoyl subunit. This group dramatically increases binding affinity in all docked compounds. §: for this compound, no binding energy could be determined, because of separation of the ligand protein complex during docking.).