

Supplementary Information

Resonance Assignment of the NMR Spectra of Disordered Proteins Using a Multi-Objective Non-Dominated Sorting Genetic Algorithm

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Mutation and crossover operators in the modified NSGA-II and combination NSGA-II/MC algorithms

The assignment result in our program is stored in an $N_{\text{res}} \times M$ matrix, where N_{res} is the number of residues in the sequence and M is the number of spectra. Name the matrix as \mathbf{p} , and $\mathbf{p}(i, j)$ is the number of the peak in the j^{th} spectrum that is assigned to the i^{th} residue in the sequence. If $\mathbf{p}(i, j) = 0$, then it means the i^{th} residue contributes to none of the cross peaks in the j^{th} spectrum.

The crossover operator, which is also called “recombination”, uses two parents to generate two children. For convenience, the two parents are represented by $\mathbf{p}_1(i, j)$ and $\mathbf{p}_2(i, j)$, where $i = 1, 2, \dots, N_{\text{res}}$; $j = 1, 2, \dots, M$. Randomly choose the k^{th} residue in the sequence, and the q^{th} spectrum, exchange the assignments of the two parents, i.e. $\mathbf{p}_1(k, q)$ and $\mathbf{p}_2(k, q)$ but keep other residues’ assignment the same, then two new children \mathbf{c}_1 and \mathbf{c}_2 are obtained. In doing so care must be taken that the maximum degeneracies of the newly assigned peaks are not exceeded.

The mutation operator uses one parent to generate one child. In our program, three mutation operators are designed. The first one is called simple mutation: randomly choose a spectrum index q and a residue k ; change the assigned peak number $\mathbf{p}(k, q)$ to another peak or 0. The second operator is called exchange mutation: randomly choose a spectrum index q , and two residues k_1 and k_2 ($k_1 \neq k_2$); exchange the two assignments $\mathbf{p}(k_1, q)$ and $\mathbf{p}(k_2, q)$. The third operator is called multi-exchange mutation: randomly choose two residues k_1 and k_2 ; exchange the assignments of the k_1^{th} residue and the k_2^{th} residue in each spectrum. While changing the assignment of a residue, all normal constraints must be satisfied. This means that the possible residue types of the assigned peak given in the peak list should include the residue that the peak is assigned to, and the maximum degeneracy of the assigned peak must not be exceeded. These three mutation operators are used for making multiple changes to the previous solution in a single step. Proper design of the operator can prevent the algorithm from being trapped in a local optimum. The users can also design their own operators to make the algorithm work more effectively.

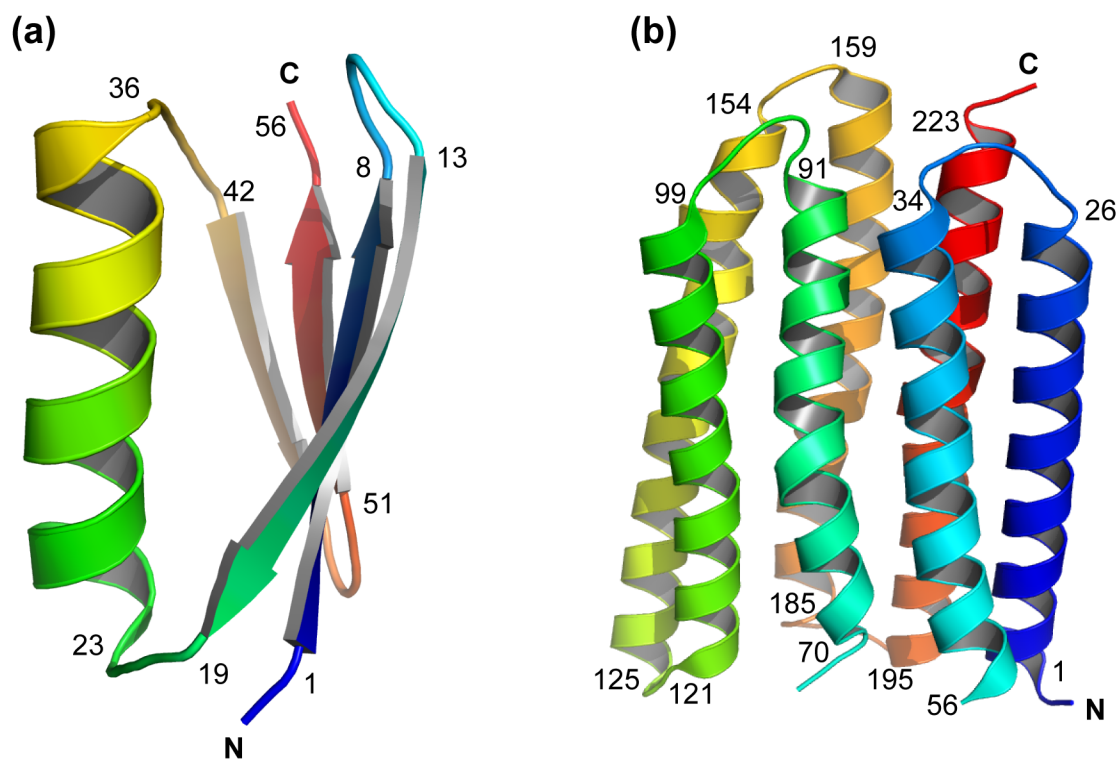


Figure S1. Cartoon representations of (a) GB1 (PDB: 2QMT) and (b) sensory rhodopsin (PDB: 1XIO). Key residue numbers are indicated to denote the positions of the deleted residues in the input peak lists.

Table S1. GB1 peak lists with 20% consecutive deletion.

NCACX

45	5										
39.5	54.6	171.7	32.8	30.6	0.5	0.3	0.3	0.3	0.3	1	K(C)M(C)
104.5	60.7	175.8	70.3		0.3	0.4	0.4	0.4	0.4	1	T(CH)
105.9	45.2	171.7			0.3	0.3	0.3	0.3	0.3	1	G(CSH)
109	60.7	174.5	72.9		0.2	0.2	0.2	0.2	0.2	1	T(CS)
112.4	62.9	174.8	72.1		0.4	0.4	0.4	0.4	0.4	1	T(CSH)
112.5	60.7	172.6	72.2	21.4	0.3	0.3	0.3	0.3	0.3	1	T(SC)
115.2	53.7	174.5	40.6	177.1	0.2	0.2	0.2	0.2	0.2	1	D(C)N(C)
115.6	60.5	172.4	70.9		0.4	0.4	0.4	0.4	0.4	1	T(SC)
116.4	60.7	174.7	73		0.3	0.4	0.4	0.4	0.4	1	T(SC)
116.6	61.6	171.6	71.1		0.3	0.3	0.3	0.3	0.3	1	T(SC)
116.6	59.4	178.1	29.4	35.8	0.2	0.3	0.3	0.3	0.3	1	E(HC)Q(H)R(H)
117.6	67.4	176.1	68		0.2	0.2	0.2	0.2	0.2	1	T(HC)
117	59.8	178.8	32.4	26.2	0.4	0.4	0.4	0.4	0.4	1	K(H)Q(H)R(H)E(H)M(H)
117.9	56.6	179.2	38.9	175.7	0.3	0.4	0.4	0.4	0.4	1	N(HC)D(H)
118.1	58.2	172.3	32.4	21.6	0.3	0.3	0.3	0.3	0.3	1	V(SC)K(C)
118.3	57.5	171.6	42.5	127.5	0.3	0.3	0.3	0.3	0.3	1	F(S)Y(S)
118.5	57.2	178.8	37.2	138.1	0.2	0.3	0.3	0.3	0.3	1	F(H)Y(CH)H(HC)
118.8	54.9	177.7	31.3	35.5	0.2	0.2	0.2	0.2	0.2	1	E(CS)K(CHS)R(C)M(C)Q(C)
118.8	53.8	179.5	18.8		0.2	0.2	0.2	0.2	0.2	1	A(HC)L(H)
119.6	66.7	179.4	32.4	22.6	0.3	0.4	0.4	0.4	0.4	1	V(HC)
120	55.9	175.8	28.3	24.7	0.3	0.3	0.3	0.3	0.3	1	K(C)R(C)Q(C)
121.3	55	182	18.7		0.5	0.5	0.5	0.5	0.5	1	A(HC)
121.3	60.5	179.7	32	27.7	0.5	0.4	0.4	0.4	0.4	1	K(H)E(H)R(H)Q(H)
121.4	62	179.2	37.4	130.2	0.4	0.4	0.4	0.4	0.4	1	Y(H)F(H)
121.4	54.2	174.4	34.5	35.4	0.3	0.3	0.3	0.3	0.3	1	K(SC)E(S)R(S)M(S)
121.4	56.2	176.5	38.6	178.1	0.3	0.3	0.3	0.3	0.3	1	N(H)D(CH)
121.6	59.2	177.9	29.3	34.5	0.3	0.3	0.3	0.3	0.3	1	E(HC)Q(H)R(H)K(HC)
122.9	55.1	173.5	36.5	25.9	0.2	0.2	0.2	0.2	0.2	1	K(SC)R(S)E(S)
122.3	56.6	179.2	17.7		0.4	0.4	0.4	0.4	0.4	1	A(H)
122.4	54.2	179.3	17.8		0.4	0.4	0.4	0.4	0.4	1	A(HC)
123	52.9	175.4	38.4	25.7	0.3	0.3	0.3	0.3	0.3	1	N(CH)L(CS)D(C)K(SC)
123	56.7	174.7	43.4	128.2	0.3	0.3	0.3	0.3	0.3	1	Y(S)F(SC)
123.1	54.3	177.2	42.7	179.5	0.3	0.3	0.3	0.3	0.3	1	D(CSH)
123.8	54.7	177	17.3		0.2	0.2	0.2	0.2	0.2	1	A(HC)
123.9	61.1	174	71.9		0.2	0.2	0.2	0.2	0.2	1	T(SC)
125.5	58	177.9	34.3	112.3	0.5	0.5	0.5	0.5	0.5	1	W(CSH)
125.5	51.1	176.8	38.8	177	0.4	0.4	0.4	0.4	0.4	1	D(C)N(CS)
125.5	56.2	175.4	30.6	35.3	0.3	0.3	0.3	0.3	0.3	1	E(CS)K(CS)R(CS)Q(C)
125.6	54.5	176.1	30.8	36	0.2	0.2	0.2	0.2	0.2	1	E(CS)K(CS)R(S)
126.5	60.1	175.4	38	27.6	0.2	0.1	0.1	0.1	0.1	1	I(SC)E(H)
125.9	50.5	175.9	42.2	179.8	0.4	0.4	0.4	0.4	0.4	1	D(CS)N(C)
126.7	52.7	174.5	42.2	27.1	0.3	0.3	0.3	0.3	0.3	1	L(SC)
126.9	54.5	174.9	42.7	27	0.2	0.2	0.2	0.2	0.2	1	L(SC)
130.7	56.9	176.1	43.4	140.3	0.4	0.3	0.3	0.3	0.3	1	F(SC)Y(S)
131.3	57.8	180.5	33.3	38.8	0.2	0.2	0.2	0.2	0.2	1	L(H)E(C)Q(H)

NCOCX

44	5										
104.2	54	179.7	19		0.3	0.4	0.4	0.4	0.4	1	A(HC)
105.6	53.3	175.8	38.8	26.1	0.3	0.3	0.3	0.3	0.3	1	N(C)L(CS)R(C)K(SC)

108.4	53.5	174.3	40.4	176.9	0.3	0.3	0.3	0.3	0.3	1	D(C)N(C)
109.2	57.5	177.4	33.8	111.8	0.2	0.2	0.2	0.2	0.2	1	W(S)
109.6	50.7	176.4	38.4	176.6	0.2	0.2	0.2	0.2	0.2	1	N(CSH)D(C)
112	55.6	175.5	28	24.4	0.4	0.4	0.4	0.4	0.4	1	K(CS)R(C)L(HS)
112.2	56.6	175.8	43.1	140	0.3	0.3	0.3	0.3	0.3	1	F(SC)Y(S)
115	55.9	176.2	38.3	177.8	0.2	0.2	0.2	0.2	0.2	1	N(HC)D(HC)
115.2	53.9	174.1	34.2	35.1	0.4	0.4	0.4	0.4	0.4	1	E(SC)Q(S)K(C)M(SC)
116.1	60.1	172	70.5		0.3	0.4	0.4	0.4	0.4	1	T(SC)
116.3	60.3	174.3	72.6		0.3	0.3	0.3	0.3	0.3	1	T(SC)
116.4	55	177.3	17.6		0.2	0.3	0.3	0.3	0.3	1	A(HC)
117.4	54.5	181.5	18.2		0.2	0.2	0.2	0.2	0.2	1	A(HC)
117.4	59.1	177.8	29.1	35.5	0.4	0.4	0.4	0.4	0.4	1	E(HC)Q(H)R(H)
118.2	56.1	179.6	18.1		0.3	0.4	0.4	0.4	0.4	1	A(HC)
118.4	60.4	172.3	71.9	21.1	0.3	0.3	0.3	0.3	0.3	1	T(SC)
118.6	60.9	174.7	73.1		0.3	0.3	0.3	0.3	0.3	1	T(CS)
118.7	66.3	179	32	22.2	0.2	0.3	0.3	0.3	0.3	1	V(H)
119	54.6	177.5	43	179.8	0.2	0.2	0.2	0.2	0.2	1	D(CH)N(H)
119.3	60.2	179.2	32.8	26.5	0.3	0.4	0.4	0.4	0.4	1	K(HC)E(H)
119.7	60.3	175.4	69.9		0.3	0.3	0.3	0.3	0.3	1	T(CSH)
120.8	54.6	179.7	18.2		0.5	0.5	0.5	0.5	0.5	1	A(HC)
120.8	57.5	179.1	37.5	138.4	0.5	0.4	0.4	0.4	0.4	1	F(HC)Y(HC)
121	58.9	177.6	29	34.2	0.4	0.4	0.4	0.4	0.4	1	Q(HC)E(HC)
121.1	44.9	171.4			0.3	0.3	0.3	0.3	0.3	1	G(CS)
121.1	57	179.6	39.3	176.1	0.3	0.3	0.3	0.3	0.3	1	D(HC)N(H)
121.3	60.1	179.3	31.6	27.3	0.3	0.3	0.3	0.3	0.3	1	K(H)R(H)
122.7	57	175	43.7	128.5	0.2	0.2	0.2	0.2	0.2	1	F(SC)Y(S)
122.7	61.6	178.8	37	129.8	0.4	0.4	0.4	0.4	0.4	1	F(H)Y(HC)
123.3	55.9	175.1	30.3	35	0.3	0.3	0.3	0.3	0.3	1	E(CS)K(CS)Q(CSH)
123.4	50.9	176.3	42.6	180.2	0.3	0.3	0.3	0.3	0.3	1	D(CS)N(C)
124	67.2	175.9	67.8		0.2	0.2	0.2	0.2	0.2	1	T(HC)
124.1	58.5	172.6	32.7	21.9	0.2	0.2	0.2	0.2	0.2	1	V(SC)K(HC)
125	55.1	177.9	31.5	35.7	0.5	0.5	0.5	0.5	0.5	1	E(SCH)M(C)R(S)Q(C)
125.1	54.7	175.1	42.9	27.2	0.4	0.4	0.4	0.4	0.4	1	L(CSH)
125.2	54.3	171.4	32.5	30.3	0.3	0.3	0.3	0.3	0.3	1	K(CH)M(CH)
125.4	61.3	171.3	70.8		0.2	0.2	0.2	0.2	0.2	1	T(SC)
125.9	54.3	175.9	30.6	35.8	0.2	0.2	0.2	0.2	0.2	1	E(CS)
126.3	53	174.8	42.5	27.4	0.2	0.1	0.1	0.1	0.1	1	L(SC)
126.3	57.8	171.9	42.7	127.8	0.4	0.4	0.4	0.4	0.4	1	F(S)Y(S)
127	54.9	173.3	36.3	25.7	0.3	0.3	0.3	0.3	0.3	1	K(SC)
127.1	60	175.3	37.9	27.5	0.2	0.2	0.2	0.2	0.2	1	I(SCH)R(H)
130.3	62.5	174.4	71.7		0.4	0.3	0.3	0.3	0.3	1	T(SCH)
131.1	61.3	174.2	72.1		0.2	0.2	0.2	0.2	0.2	1	T(SC)

Table S2. GB1 peak lists with random deletion of 20% of the residues.

NCACX

44	5										
104.5	60.7	175.8	70.3		0.3	0.4	0.4	0.4	0.4	1	T(CH)
105.9	45.2	171.7			0.3	0.3	0.3	0.3	0.3	1	G(CSH)
106.6	62.1	173.6	69.7		0.2	0.2	0.2	0.2	0.2	1	T(CSH)
108.3	45.3	173			0.2	0.2	0.2	0.2	0.2	1	G(CS)
108.1	46.5	173.7			0.3	0.3	0.3	0.3	0.3	1	G(CHS)
109	60.7	174.5	72.9		0.2	0.2	0.2	0.2	0.2	1	T(CS)
109.4	44.5	173			0.2	0.2	0.2	0.2	0.2	1	G(CS)
112.4	62.9	174.8	72.1		0.4	0.4	0.4	0.4	0.4	1	T(CSH)
112.5	60.7	172.6	72.2	21.4	0.3	0.3	0.3	0.3	0.3	1	T(SC)
115.2	53.7	174.5	40.6	177.1	0.2	0.2	0.2	0.2	0.2	1	D(C)N(C)
115.6	60.5	172.4	70.9		0.4	0.4	0.4	0.4	0.4	1	T(SC)S(C)
116.6	63.8	175.4	32.3	20.5	0.3	0.3	0.3	0.3	0.3	1	V(CHS)
116.6	59.4	178.1	29.4	35.8	0.2	0.3	0.3	0.3	0.3	1	E(HC)Q(H)R(H)
117.6	67.4	176.1	68		0.2	0.2	0.2	0.2	0.2	1	T(HC)
117	59.8	178.8	32.4	26.2	0.4	0.4	0.4	0.4	0.4	1	K(H)Q(H)R(H)E(H)M(H)
117.9	56.6	179.2	38.9	175.7	0.3	0.4	0.4	0.4	0.4	1	N(HC)D(H)
118.1	58.2	172.3	32.4	21.6	0.3	0.3	0.3	0.3	0.3	1	V(SC)K(C)
118.3	57.5	171.6	42.5	127.5	0.3	0.3	0.3	0.3	0.3	1	F(S)Y(S)
118.5	57.2	178.8	37.2	138.1	0.2	0.3	0.3	0.3	0.3	1	F(H)Y(CH)H(HC)
118.8	54.9	177.7	31.3	35.5	0.2	0.2	0.2	0.2	0.2	1	E(CS)K(CHS)R(C)M(C)Q(C)
119.6	66.7	179.4	32.4	22.6	0.3	0.4	0.4	0.4	0.4	1	V(HC)
120	55.9	175.8	28.3	24.7	0.3	0.3	0.3	0.3	0.3	1	K(C)R(C)Q(C)
121.3	55	182	18.7		0.5	0.5	0.5	0.5	0.5	1	A(HC)
121.3	60.5	179.7	32	27.7	0.5	0.4	0.4	0.4	0.4	1	K(H)E(H)R(H)Q(H)
121.4	62	179.2	37.4	130.2	0.4	0.4	0.4	0.4	0.4	1	Y(H)F(H)
121.5	59.7	179.6	33.3	26.2	0.4	0.4	0.4	0.4	0.4	1	K(HC)Q(H)M(H)R(H)
121.4	54.2	174.4	34.5	35.4	0.3	0.3	0.3	0.3	0.3	1	K(SC)E(S)R(S)M(S)
121.4	56.2	176.5	38.6	178.1	0.3	0.3	0.3	0.3	0.3	1	N(H)D(CH)
121.6	59.2	177.9	29.3	34.5	0.3	0.3	0.3	0.3	0.3	1	E(HC)Q(H)R(H)K(HC)
122	61.9	175.4	32.2	22.2	0.2	0.2	0.2	0.2	0.2	1	V(SCH)
122.9	55.1	173.5	36.5	25.9	0.2	0.2	0.2	0.2	0.2	1	K(SC)R(S)E(S)
122.3	56.6	179.2	17.7		0.4	0.4	0.4	0.4	0.4	1	A(H)
123	56.7	174.7	43.4	128.2	0.3	0.3	0.3	0.3	0.3	1	Y(S)F(SC)
123.1	54.3	177.2	42.7	179.5	0.3	0.3	0.3	0.3	0.3	1	D(CSH)
123.8	54.7	177	17.3		0.2	0.2	0.2	0.2	0.2	1	A(HC)
125.5	58	177.9	34.3	112.3	0.5	0.5	0.5	0.5	0.5	1	W(CSH)
125.5	51.1	176.8	38.8	177	0.4	0.4	0.4	0.4	0.4	1	D(C)N(CS)
125.5	56.2	175.4	30.6	35.3	0.3	0.3	0.3	0.3	0.3	1	E(CS)K(CS)R(CS)Q(C)
126.1	50.9	178	23.9		0.2	0.2	0.2	0.2	0.2	1	A(SC)
126.5	60.1	175.4	38	27.6	0.2	0.1	0.1	0.1	0.1	1	I(SC)E(H)
127.6	54.2	173.7	42.9	27.7	0.2	0.2	0.2	0.2	0.2	1	L(SC)
130.7	56.9	176.1	43.4	140.3	0.4	0.3	0.3	0.3	0.3	1	F(SC)Y(S)
131.4	53	175.1	41.9	180.9	0.3	0.2	0.2	0.2	0.2	1	D(CS)
131.3	57.8	180.5	33.3	38.8	0.2	0.2	0.2	0.2	0.2	1	L(H)E(C)Q(H)

NCOCX

43	5										
106.4	59.3	179.2	32.9	25.8	0.2	0.2	0.2	0.2	0.2	1	K(HC)
108.1	52.8	174.9	41.7	180.7	0.2	0.2	0.2	0.2	0.2	1	D(CS)N(CS)
108.4	53.5	174.3	40.4	176.9	0.3	0.3	0.3	0.3	0.3	1	D(C)N(C)

109.2	57.5	177.4	33.8	111.8	0.2	0.2	0.2	0.2	0.2	1	W(S)
109.6	50.7	176.4	38.4	176.6	0.2	0.2	0.2	0.2	0.2	1	N(CSH)D(C)
112	55.6	175.5	28	24.4	0.4	0.4	0.4	0.4	0.4	1	K(CS)R(C)L(HS)
112.2	56.6	175.8	43.1	140	0.3	0.3	0.3	0.3	0.3	1	F(SC)Y(S)
115	55.9	176.2	38.3	177.8	0.2	0.2	0.2	0.2	0.2	1	N(HC)D(HC)
115.2	53.9	174.1	34.2	35.1	0.4	0.4	0.4	0.4	0.4	1	E(SC)Q(S)K(C)M(SC)
115.5	63.5	175.1	32	20.2	0.4	0.4	0.4	0.4	0.4	1	V(CSH)P(C)
116.1	60.1	172	70.5		0.3	0.4	0.4	0.4	0.4	1	T(SC)
116.3	50.7	177.8	23.7		0.3	0.3	0.3	0.3	0.3	1	A(SC)
116.4	55	177.3	17.6		0.2	0.3	0.3	0.3	0.3	1	A(HC)
117.4	54.5	181.5	18.2		0.2	0.2	0.2	0.2	0.2	1	A(HC)
117.4	59.1	177.8	29.1	35.5	0.4	0.4	0.4	0.4	0.4	1	E(HC)Q(H)R(H)
118.2	56.1	179.6	18.1		0.3	0.4	0.4	0.4	0.4	1	A(HC)
118.4	60.4	172.3	71.9	21.1	0.3	0.3	0.3	0.3	0.3	1	T(SC)
118.6	60.9	174.7	73.1		0.3	0.3	0.3	0.3	0.3	1	T(CS)
118.7	66.3	179	32	22.2	0.2	0.3	0.3	0.3	0.3	1	V(H)
119	45.1	172.8			0.2	0.2	0.2	0.2	0.2	1	G(CS)
119	54.6	177.5	43	179.8	0.2	0.2	0.2	0.2	0.2	1	D(CH)N(H)
119.3	60.2	179.2	32.8	26.5	0.3	0.4	0.4	0.4	0.4	1	K(HC)E(H)
119.7	60.3	175.4	69.9		0.3	0.3	0.3	0.3	0.3	1	T(CSH)
120.8	57.5	179.1	37.5	138.4	0.5	0.4	0.4	0.4	0.4	1	F(HC)Y(HC)
121	58.9	177.6	29	34.2	0.4	0.4	0.4	0.4	0.4	1	Q(HC)E(HC)
121.1	44.7	173.2			0.4	0.4	0.4	0.4	0.4	1	G(CS)
121.1	44.9	171.4			0.3	0.3	0.3	0.3	0.3	1	G(CS)
121.1	57	179.6	39.3	176.1	0.3	0.3	0.3	0.3	0.3	1	D(HC)N(H)
121.3	60.1	179.3	31.6	27.3	0.3	0.3	0.3	0.3	0.3	1	K(H)R(H)
121.8	46.8	174			0.2	0.2	0.2	0.2	0.2	1	G(CHS)
122.7	57	175	43.7	128.5	0.2	0.2	0.2	0.2	0.2	1	F(SC)Y(S)
122.7	61.6	178.8	37	129.8	0.4	0.4	0.4	0.4	0.4	1	F(H)Y(HC)
123.3	55.9	175.1	30.3	35	0.3	0.3	0.3	0.3	0.3	1	E(CS)K(CS)Q(CSH)
123.3	54.4	173.9	43.1	27.9	0.3	0.3	0.3	0.3	0.3	1	L(SC)R(SC)
124	67.2	175.9	67.8		0.2	0.2	0.2	0.2	0.2	1	T(HC)
124.1	58.5	172.6	32.7	21.9	0.2	0.2	0.2	0.2	0.2	1	V(SC)K(HC)
125	55.1	177.9	31.5	35.7	0.5	0.5	0.5	0.5	0.5	1	E(SCH)M(C)R(S)Q(C)
126.3	57.8	171.9	42.7	127.8	0.4	0.4	0.4	0.4	0.4	1	F(S)Y(S)
127	54.9	173.3	36.3	25.7	0.3	0.3	0.3	0.3	0.3	1	K(SC)
127.1	60	175.3	37.9	27.5	0.2	0.2	0.2	0.2	0.2	1	I(SCH)R(H)
127.8	61.9	173.4	69.5		0.2	0.2	0.2	0.2	0.2	1	T(CSH)
130.3	62.5	174.4	71.7		0.4	0.3	0.3	0.3	0.3	1	T(SCH)
131.1	61.7	175.2	32	22	0.3	0.2	0.2	0.2	0.2	1	V(SCH)

Table S3. Residues in GB1 that are randomly and independently deleted from the NCOCX and NCACX peak lists.

Residues corresponding to the deleted peaks in the NCACX list	3	8	24	25	34	37	45	48	49	50	52	55
Residues corresponding to the deleted peaks in the NCOCX list	8	12	16	22	26	30	31	36	39	42	45	53

Table S4. GB1 peak lists with random and independent deletion of 20% of the peaks.

NCACX

44	5										
39.5	54.6	171.7	32.8	30.6	0.5	0.3	0.3	0.3	0.3	1	K(C)M(C)
105.9	45.2	171.7			0.3	0.3	0.3	0.3	0.3	1	G(CSH)
106.6	62.1	173.6	69.7		0.2	0.2	0.2	0.2	0.2	1	T(CSH)
108.3	45.3	173			0.2	0.2	0.2	0.2	0.2	1	G(CS)
108.1	46.5	173.7			0.3	0.3	0.3	0.3	0.3	1	G(CHS)
109	60.7	174.5	72.9		0.2	0.2	0.2	0.2	0.2	1	T(CS)
109.4	44.5	173			0.2	0.2	0.2	0.2	0.2	1	G(CS)
112.4	62.9	174.8	72.1		0.4	0.4	0.4	0.4	0.4	1	T(CSH)
112.5	60.7	172.6	72.2	21.4	0.3	0.3	0.3	0.3	0.3	1	T(SC)
115.6	60.5	172.4	70.9		0.4	0.4	0.4	0.4	0.4	1	T(SC)
115.9	52.9	175.5	42.7	180.3	0.4	0.4	0.4	0.4	0.4	1	D(CS)N(C)
116.4	60.7	174.7	73		0.3	0.4	0.4	0.4	0.4	1	T(SC)
116.6	61.6	171.6	71.1		0.3	0.3	0.3	0.3	0.3	1	T(SC)
116.6	63.8	175.4	32.3	20.5	0.3	0.3	0.3	0.3	0.3	1	V(CHS)
116.6	59.4	178.1	29.4	35.8	0.2	0.3	0.3	0.3	0.3	1	E(HC)Q(H)R(H)
117	59.8	178.8	32.4	26.2	0.4	0.4	0.4	0.4	0.4	1	K(H)Q(H)R(H)E(H)M(H)
117.9	56.6	179.2	38.9	175.7	0.3	0.4	0.4	0.4	0.4	1	N(HC)D(H)
118.1	58.2	172.3	32.4	21.6	0.3	0.3	0.3	0.3	0.3	1	V(SC)K(C)
118.5	57.2	178.8	37.2	138.1	0.2	0.3	0.3	0.3	0.3	1	F(H)Y(CH)H(HC)
118.8	54.9	177.7	31.3	35.5	0.2	0.2	0.2	0.2	0.2	1	E(CS)K(CHS)R(C)M(C)Q(C)
119.6	66.7	179.4	32.4	22.6	0.3	0.4	0.4	0.4	0.4	1	V(HC)
121.3	60.5	179.7	32	27.7	0.5	0.4	0.4	0.4	0.4	1	K(H)E(H)R(H)Q(H)
121.4	62	179.2	37.4	130.2	0.4	0.4	0.4	0.4	0.4	1	Y(H)F(H)
121.5	59.7	179.6	33.3	26.2	0.4	0.4	0.4	0.4	0.4	1	K(HC)Q(H)M(H)R(H)
121.4	54.2	174.4	34.5	35.4	0.3	0.3	0.3	0.3	0.3	1	K(SC)E(S)R(S)M(S)
121.4	56.2	176.5	38.6	178.1	0.3	0.3	0.3	0.3	0.3	1	N(H)D(CH)
121.6	59.2	177.9	29.3	34.5	0.3	0.3	0.3	0.3	0.3	1	E(HC)Q(H)R(H)K(HC)
122	61.9	175.4	32.2	22.2	0.2	0.2	0.2	0.2	0.2	1	V(SCH)
122.9	55.1	173.5	36.5	25.9	0.2	0.2	0.2	0.2	0.2	1	K(SC)R(S)E(S)
122.4	54.2	179.3	17.8		0.4	0.4	0.4	0.4	0.4	1	A(HC)
123	52.9	175.4	38.4	25.7	0.3	0.3	0.3	0.3	0.3	1	N(CH)L(CS)D(C)K(SC)
123.1	54.3	177.2	42.7	179.5	0.3	0.3	0.3	0.3	0.3	1	D(CSH)
123.8	54.7	177	17.3		0.2	0.2	0.2	0.2	0.2	1	A(HC)
125.5	58	177.9	34.3	112.3	0.5	0.5	0.5	0.5	0.5	1	W(CSH)
125.5	56.2	175.4	30.6	35.3	0.3	0.3	0.3	0.3	0.3	1	E(CS)K(CS)R(CS)Q(C)
125.6	54.5	176.1	30.8	36	0.2	0.2	0.2	0.2	0.2	1	E(CS)K(CS)R(S)
126.1	50.9	178	23.9		0.2	0.2	0.2	0.2	0.2	1	A(SC)
126.5	60.1	175.4	38	27.6	0.2	0.1	0.1	0.1	0.1	1	I(SC)E(H)
125.9	50.5	175.9	42.2	179.8	0.4	0.4	0.4	0.4	0.4	1	D(CS)N(C)
126.7	52.7	174.5	42.2	27.1	0.3	0.3	0.3	0.3	0.3	1	L(SC)

126.9	54.5	174.9	42.7	27	0.2	0.2	0.2	0.2	0.2	1	L(SC)
127.6	54.2	173.7	42.9	27.7	0.2	0.2	0.2	0.2	0.2	1	L(SC)
131.4	53	175.1	41.9	180.9	0.3	0.2	0.2	0.2	0.2	1	D(CS)
131.3	57.8	180.5	33.3	38.8	0.2	0.2	0.2	0.2	0.2	1	L(H)E(C)Q(H)

NCOCX

43	5										
104.2	54	179.7	19		0.3	0.4	0.4	0.4	0.4	1	A(HC)
105.6	53.3	175.8	38.8	26.1	0.3	0.3	0.3	0.3	0.3	1	N(C)L(CS)R(C)K(SC)
106.4	59.3	179.2	32.9	25.8	0.2	0.2	0.2	0.2	0.2	1	K(HC)
108.1	52.8	174.9	41.7	180.7	0.2	0.2	0.2	0.2	0.2	1	D(CS)N(CS)
108.4	53.5	174.3	40.4	176.9	0.3	0.3	0.3	0.3	0.3	1	D(C)N(C)
109.2	57.5	177.4	33.8	111.8	0.2	0.2	0.2	0.2	0.2	1	W(S)
112	55.6	175.5	28	24.4	0.4	0.4	0.4	0.4	0.4	1	K(CS)R(C)L(HS)
112.2	56.6	175.8	43.1	140	0.3	0.3	0.3	0.3	0.3	1	F(SC)Y(S)
115.2	53.9	174.1	34.2	35.1	0.4	0.4	0.4	0.4	0.4	1	E(SC)Q(S)K(C)M(SC)
115.5	63.5	175.1	32	20.2	0.4	0.4	0.4	0.4	0.4	1	V(CSH)P(C)
116.3	60.3	174.3	72.6		0.3	0.3	0.3	0.3	0.3	1	T(SC)
116.3	50.7	177.8	23.7		0.3	0.3	0.3	0.3	0.3	1	A(SC)
117.4	54.5	181.5	18.2		0.2	0.2	0.2	0.2	0.2	1	A(HC)
117.4	59.1	177.8	29.1	35.5	0.4	0.4	0.4	0.4	0.4	1	E(HC)Q(H)R(H)
118.2	56.1	179.6	18.1		0.3	0.4	0.4	0.4	0.4	1	A(HC)
118.6	60.9	174.7	73.1		0.3	0.3	0.3	0.3	0.3	1	T(CS)
118.7	66.3	179	32	22.2	0.2	0.3	0.3	0.3	0.3	1	V(H)
119	45.1	172.8			0.2	0.2	0.2	0.2	0.2	1	G(CS)
119	54.6	177.5	43	179.8	0.2	0.2	0.2	0.2	0.2	1	D(CH)N(H)
119.3	60.2	179.2	32.8	26.5	0.3	0.4	0.4	0.4	0.4	1	K(HC)E(H)
119.7	60.3	175.4	69.9		0.3	0.3	0.3	0.3	0.3	1	T(CSH)
120.8	54.6	179.7	18.2		0.5	0.5	0.5	0.5	0.5	1	A(HC)
121	58.9	177.6	29	34.2	0.4	0.4	0.4	0.4	0.4	1	Q(HC)E(HC)
121.1	44.7	173.2			0.4	0.4	0.4	0.4	0.4	1	G(CS)
121.1	44.9	171.4			0.3	0.3	0.3	0.3	0.3	1	G(CS)
121.1	57	179.6	39.3	176.1	0.3	0.3	0.3	0.3	0.3	1	D(HC)N(H)
121.8	46.8	174			0.2	0.2	0.2	0.2	0.2	1	G(CHS)
122.7	57	175	43.7	128.5	0.2	0.2	0.2	0.2	0.2	1	F(SC)Y(S)
122.7	61.6	178.8	37	129.8	0.4	0.4	0.4	0.4	0.4	1	F(H)Y(HC)
123.3	55.9	175.1	30.3	35	0.3	0.3	0.3	0.3	0.3	1	E(CS)K(CS)Q(CSH)
123.4	50.9	176.3	42.6	180.2	0.3	0.3	0.3	0.3	0.3	1	D(CS)N(C)
124	67.2	175.9	67.8		0.2	0.2	0.2	0.2	0.2	1	T(HC)
124.1	58.5	172.6	32.7	21.9	0.2	0.2	0.2	0.2	0.2	1	V(SC)K(HC)
125.1	54.7	175.1	42.9	27.2	0.4	0.4	0.4	0.4	0.4	1	L(CSH)
125.2	54.3	171.4	32.5	30.3	0.3	0.3	0.3	0.3	0.3	1	K(CH)M(CH)
125.4	61.3	171.3	70.8		0.2	0.2	0.2	0.2	0.2	1	T(SC)
125.9	54.3	175.9	30.6	35.8	0.2	0.2	0.2	0.2	0.2	1	E(CS)
126.3	53	174.8	42.5	27.4	0.2	0.1	0.1	0.1	0.1	1	L(SC)
127	54.9	173.3	36.3	25.7	0.3	0.3	0.3	0.3	0.3	1	K(SC)
127.1	60	175.3	37.9	27.5	0.2	0.2	0.2	0.2	0.2	1	I(SCH)R(H)
127.8	61.9	173.4	69.5		0.2	0.2	0.2	0.2	0.2	1	T(CSH)
130.3	62.5	174.4	71.7		0.4	0.3	0.3	0.3	0.3	1	T(SCH)
131.1	61.3	174.2	72.1		0.2	0.2	0.2	0.2	0.2	1	T(SC)

Table S5. HET-s peak lists.

NCACX

57	4								
116.2	59.4	173.5	66.8	0.6	0.5	0.5	0.5	1	S(C)T(C)
125.6	52.2	174.7	39.6	0.6	0.5	0.5	0.5	1	D(C)N(C)
128.0	52.5	174.8	41.1	0.6	0.5	0.5	0.5	1	D(C)L(CS)N(S)
109.2	44.2	174.9		0.6	0.5	0.5	0.5	1	G(C)
114.3	43.7	170.7		0.6	0.5	0.5	0.5	1	G(SC)
118.1	54.8	174.8	35.4	0.6	0.5	0.5	0.5	1	K(SC)R(S)E(S)
127.3	59.3	175.7	29.7	0.6	0.5	0.5	0.5	1	E(CHS)C(C)I(S)
118.1	54.5	173.7		0.6	0.5	0.5	0.5	1	N(C)R(SC)D(C)E(SC)K(CS)Q(S) C(H(CS)L(SH))
120.6	58.4	178.6	41.7	0.6	0.5	0.5	0.5	1	L(H)
130.1	58.5	173.1	35.5	0.6	0.5	0.5	0.5	1	V(S)I(S)
128.9	61.3	175.1	32.1	0.6	0.5	0.5	0.5	1	V(S)
123.2	61.9	174.2	34.6	0.6	0.5	0.5	0.5	1	V(S)
116.1	48.3	172.0		0.6	0.5	0.5	0.5	1	G(C)
131.4	52.6	172.6	44.8	0.6	0.5	0.5	0.5	1	L(S)
125.8	57.1	177.4	33.3	0.6	0.5	0.5	0.5	1	K(C)
113.5	59.8	174.3	72.1	0.6	0.5	0.5	0.5	1	T(SC)
129.0	54.2	176.6	29.9	0.6	0.5	0.5	0.5	1	E(CS)
110.2	45.8	174.4		0.6	0.5	0.5	0.5	1	G(C)
119.5	56.9	171.6	67.4	0.6	0.5	0.5	0.5	1	S(S)
123.2	49.8	177.1	24.1	0.6	0.5	0.5	0.5	1	A(S)
124.0	60.9	175.1	35.5	0.6	0.5	0.5	0.5	1	V(S)
113.7	44.9	172.1		0.6	0.5	0.5	0.5	1	G(C)
122.0	54.5	176.7	35.4	0.6	0.5	0.5	0.5	1	K(SC)
125.7	59.3	175.8	32.2	0.6	0.5	0.5	0.5	1	V(SC)K(HC)
109.7	43.6	178.8		0.6	0.5	0.5	0.5	1	G(CS)
128.8	56.2	176.7	40.2	0.6	0.5	0.5	0.5	1	D(C)L(C)Y(S)
130.1	54.0	175.3	33.2	0.6	0.5	0.5	0.5	1	R(S)K(SC)E(S)
126.7	52.5	173.2	32.7	0.6	0.5	0.5	0.5	1	R(S)E(S)V(S)K(C)Q(S)
119.5	55.0	179.0	18.6	0.6	0.5	0.5	0.5	1	A(H)
113.0	60.9	172.7	71.7	0.6	0.5	0.5	0.5	1	T(SC)
122.5	66.0	175.4	70.2	0.6	0.5	0.5	0.5	1	T(CHS)
128.4	61.1	174.9	34.0	0.6	0.5	0.5	0.5	1	V(S)
120.3	54.8	175.0	33.4	0.6	0.5	0.5	0.5	1	E(SC)K(CS)R(S)
123.4	59.7	175.1	32.5	0.6	0.5	0.5	0.5	1	V(SC)K(HCS)
122.7	60.1	172.7	35.8	0.6	0.5	0.5	0.5	1	V(S)
116.3	62.5	175.4	70.9	0.6	0.5	0.5	0.5	1	T(CS)
118.0	57.4	175.5	29.4	0.6	0.5	0.5	0.5	1	E(CH)Q(CH)K(C)R(CH)W(C)
123.8	61.3	172.2	70.6	0.6	0.5	0.5	0.5	1	T(S)
123.1	59.9	173.0	36.8	0.6	0.5	0.5	0.5	1	V(S)
120.8	54.0	178.3	18.9	0.6	0.5	0.5	0.5	1	A(HC)
122.6	54.8	176.2	30.5	0.6	0.5	0.5	0.5	1	E(C)R(C)
129.1	62.0	175.1	38.3	0.6	0.5	0.5	0.5	1	I(SC)
126.3	53.3	176.1	20.1	0.6	0.5	0.5	0.5	1	A(C)
125.2	57.0	174.4	35.7	0.6	0.5	0.5	0.5	1	V(S)K(CS)
113.3	44.2	173.0		0.6	0.5	0.5	0.5	1	G(CS)
117.7	58.9	174.0	27.3	0.6	0.5	0.5	0.5	1	E(CH)I(S)R(H)Q(H)L(H)
120.5	54.1	173.7	33.8	0.6	0.5	0.5	0.5	1	E(S)R(S)K(CS)Q(S)
127.4	59.7	175.3	41.4	0.6	0.5	0.5	0.5	1	I(S)F(C)
115.1	52.0	173.0	40.3	0.6	0.5	0.5	0.5	1	N(CS)D(C)

117.5	56.6	171.9	66.3	0.6	0.5	0.5	0.5	1	S(SC)
109.9	51.2	175.8	40.1	0.6	0.5	0.5	0.5	1	D(C)N(CS)F(H)
121.6	56.4	179.1	17.2	0.6	0.5	0.5	0.5	1	A(H)
111.5	43.8	172.0		0.6	0.5	0.5	0.5	1	G(CS)
118.2	54.6	175.5	33.1	0.6	0.5	0.5	0.5	1	E(S)K(C)R(S)
130.8	52.7	173.6	43.7	0.6	0.5	0.5	0.5	1	L(S)
123.0	60.6	174.8	41.8	0.6	0.5	0.5	0.5	1	I(S)
118.4	53.1	174.3	45.0	0.6	0.5	0.5	0.5	1	L(SC)N(C)D(S)

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122.8	54.8	174.5	35.2	0.6	0.5	0.5	0.5	1	K(SC)E(S)R(S)
124.3	66.0	175.4	69.7	0.6	0.5	0.5	0.5	1	T(CH)
130.9	60.5	172.7	36.2	0.6	0.5	0.5	0.5	1	V(S)
118.7	53.4	176.1	20.1	0.6	0.5	0.5	0.5	1	A(CS)
130.1	60.6	174.7	41.7	0.6	0.5	0.5	0.5	1	I(S)
118.2	59.0	173.4	66.8	0.6	0.5	0.5	0.5	1	S(CS)T(C)
119.0	52.4	174.5	40.0	0.6	0.5	0.5	0.5	1	N(CS)D(C)L(C)
123.4	51.4	176.1	40.2	0.6	0.5	0.5	0.5	1	D(C)N(CS)
131.6	53.1	173.3	33.3	0.6	0.5	0.5	0.5	1	R(S)K(CS)E(SC)Q(CS)H(S)
122.7	53.0	174.3	44.9	0.6	0.5	0.5	0.5	1	L(SC)D(S)
120.6	59.8	174.4	71.9	0.6	0.5	0.5	0.5	1	T(SC)
127.6	57.4	174.7	35.6	0.6	0.5	0.5	0.5	1	V(S)K(CS)I(S)E(CSH)Y(H)R(S)M(C)F(C)
113.9	61.2	175.0	34.3	0.6	0.5	0.5	0.5	1	V(SC)
118.0	59.8	175.3	41.3	0.6	0.5	0.5	0.5	1	I(SC)F(C)
130.5	52.7	174.0	43.5	0.6	0.5	0.5	0.5	1	L(SC)D(SC)N(S)
113.5	46.4	174.2		0.6	0.5	0.5	0.5	1	G(CHS)
109.5	59.0	176.1	32.6	0.6	0.5	0.5	0.5	1	K(CH)V(CS)C(C)
128.0	61.2	172.6	70.7	0.6	0.5	0.5	0.5	1	T(SC)
118.2	44.1	178.5		0.6	0.5	0.5	0.5	1	L(HSC)G(C)D(CS)
113.8	54.0	175.7	33.3	0.6	0.5	0.5	0.5	1	K(C)E(SC)R(SC)Q(SC)M(C)
128.9	54.5	174.7	33.3	0.6	0.5	0.5	0.5	1	E(SC)R(SC)K(CS)Q(SC)M(C)
123.7	49.6	176.8	24.1	0.6	0.5	0.5	0.5	1	A(S)
125.8	56.4	171.3	66.1	0.6	0.5	0.5	0.5	1	S(SC)
120.8	53.9	178.3	18.9	0.6	0.5	0.5	0.5	1	A(HC)
126.9	59.8	173.3	37.3	0.6	0.5	0.5	0.5	1	I(SCH)V(SC)Y(HC)E(H)F(CH)T(S)C)N(C)M(S)S(C)
126.1	54.9	174.0		0.6	0.5	0.5	0.5	1	K(SC)E(SC)R(SC)N(C)H(CS)Q(S)C)D(C)L(S)F(SC)C(C)Y(CS)Q(C)M(S)
121.9	44.6	172.2		0.6	0.5	0.5	0.5	1	G(CSH)
121.5	62.6	175.4	70.6	0.6	0.5	0.5	0.5	1	T(CSH)
117.6	52.2	174.7	41.2	0.6	0.5	0.5	0.5	1	D(CS)N(SC)L(C)
118.0	59.9	175.0	33.0	0.6	0.5	0.5	0.5	1	V(SC)K(C)
123.2	55.0	175.8	32.8	0.6	0.5	0.5	0.5	1	E(SC)K(CH)M(C)R(SC)Q(S)
111.9	58.4	173.6	35.5	0.6	0.5	0.5	0.5	1	V(SC)S(C)I(CS)
116.8	54.0	176.5	30.1	0.6	0.5	0.5	0.5	1	E(CS)R(CS)Q(CS)K(C)
125.6	55.1	176.0	31.0	0.6	0.5	0.5	0.5	1	R(CS)E(SC)Q(CS)K(C)
123.0	56.6	171.6	67.2	0.6	0.5	0.5	0.5	1	S(SC)
110.3	55.9	176.3	40.2	0.6	0.5	0.5	0.5	1	D(CH)Y(S)L(HC)
123.0	59.0	173.9	27.5	0.6	0.5	0.5	0.5	1	R(CH)C(CS)L(H)E(C)Q(H)V(S)
117.2	53.7	173.6	33.9	0.6	0.5	0.5	0.5	1	Q(CS)E(S)R(SC)K(CS)M(S)
129.5	62.2	174.8	34.3	0.6	0.5	0.5	0.5	1	V(SC)

120.5	51.6	172.8	40.8	0.6	0.5	0.5	0.5	1	N(CS)D(C)L(C)F(S)Y(S)
124.1	61.2	172.7	71.7	0.6	0.5	0.5	0.5	1	T(SC)
125.3	62.1	175.2	38.3	0.6	0.5	0.5	0.5	1	I(CSH)Y(H)
128.6	60.6	175.5	35.8	0.6	0.5	0.5	0.5	1	V(S)I(CS)
127.6	44.0	174.6		0.6	0.5	0.5	0.5	1	G(CS)
115.9	54.2	176.9	35.4	0.6	0.5	0.5	0.5	1	K(SC)E(SC)R(S)
119.4	56.4	178.9	17.0	0.6	0.5	0.5	0.5	1	A(H)
116.6	61.1	175.1	32.0	0.6	0.5	0.5	0.5	1	V(SC)P(C)
128.8	48.4	172.2		0.6	0.5	0.5	0.5	1	G(CSH)A(S)N(CS)
114.9	43.9	172.2		0.6	0.5	0.5	0.5	1	G(CSH)
113.5	59.8	176.2	29.6	0.6	0.5	0.5	0.5	1	E(CH)R(H)Q(H)H(H)K(H)C(C)
114.1	52.9	172.5	44.7	0.6	0.5	0.5	0.5	1	L(S)D(S)
120.8	55.2	179.1	18.3	0.6	0.5	0.5	0.5	1	A(H)
126.0	43.8	173.2		0.6	0.5	0.5	0.5	1	G(CSH)
109.9	43.7	170.9		0.6	0.5	0.5	0.5	1	G(CS)
108.5	57.3	177.6	33.7	0.6	0.5	0.5	0.5	1	K(CH)M(H)Q(H)E(H)

Table S6. Rhodopsin peak lists for the first 98 residues.

NCACX

87	5										
125.0	55.4	178.9	17.1		0.6	0.5	0.5	0.5	0.5	1	A(H)
122.3	57.8	178.0	42.0	26.2	0.6	0.5	0.5	0.5	0.5	1	L(HC)K(C)
114.5	56.6	179.3	30.3	113.8	0.6	0.5	0.5	0.5	0.5	1	W(HS)
113.8	58.8	180.5	30.9	32.8	0.6	0.5	0.5	0.5	0.5	1	K(H)E(H)M(H)
116.6	60.9	174.6	63.0		0.6	0.5	0.5	0.5	0.5	1	S(CH)
122.8	58.5	180.2	28.2	115.5	0.6	0.5	0.5	0.5	0.5	1	W(H)
117.1	57.1	176.8	42.5	26.6	0.6	0.5	0.5	0.5	0.5	1	L(HC)
115.3	50.8	173.4	39.2	178.5	0.6	0.5	0.5	0.5	0.5	1	N(CH)D(C)
110.8	59.3	174.5	41.9	24.6	0.6	0.5	0.5	0.5	0.5	1	I(SC)L(H)
122.6	60.5	177.9	29.0	33.4	0.6	0.5	0.5	0.5	0.5	1	K(HC)E(H)Q(H)R(H)
109.6	63.6	178.9	34.5	22.1	0.6	0.5	0.5	0.5	0.5	1	V(SCH)
121.9	67.7	179.5	32.1	22.4	0.6	0.5	0.5	0.5	0.5	1	V(HCS)
116.5	61.7	178.3			0.6	0.5	0.5	0.5	0.5	1	S(H)Y(H)R(H)F(H)
119.0	58.9	176.6	35.8	26.2	0.6	0.5	0.5	0.5	0.5	1	I(SC)
130.7	64.7	178.4	33.8	26.8	0.6	0.5	0.5	0.5	0.5	1	P(C)
127.0	58.1	176.8	40.6	25.1	0.6	0.5	0.5	0.5	0.5	1	L(H)
117.7	61.4	179.3	29.7	38.7	0.6	0.5	0.5	0.5	0.5	1	E(H)R(H)
128.3	56.7	175.9	29.8	36.1	0.6	0.5	0.5	0.5	0.5	1	E(CSH)K(CS)Q(C)R(C)
132.1	65.8	178.6	32.6	27.7	0.6	0.5	0.5	0.5	0.5	1	P(HCS)
117.7	58.5	178.2	41.1	26.9	0.6	0.5	0.5	0.5	0.5	1	L(H)
119.8	58.1	177.9	37.1	138.0	0.6	0.5	0.5	0.5	0.5	1	F(HC)Y(H)
120.8	60.1	171.8	35.8	21.2	0.6	0.5	0.5	0.5	0.5	1	V(SC)
120.2	54.3	177.3	18.7		0.6	0.5	0.5	0.5	0.5	1	A(HC)
112.9	56.1	175.4		140.9	0.6	0.5	0.5	0.5	0.5	1	H(C)F(S)
139.8	62.5	177.8	32.1	27.6	0.6	0.5	0.5	0.5	0.5	1	P(CSH)
117.2	67.9	176.0			0.6	0.5	0.5	0.5	0.5	1	T(HC)V(H)
120.9	55.4	178.8	18.1		0.6	0.5	0.5	0.5	0.5	1	A(HC)
120.9	58.0	179.3	43.2	28.3	0.6	0.5	0.5	0.5	0.5	1	L(H)
121.3	60.1	177.5	37.2	126.5	0.6	0.5	0.5	0.5	0.5	1	Y(H)F(H)
115.8	64.6	178.5	63.4		0.6	0.5	0.5	0.5	0.5	1	S(CH)
114.2	59.4	176.3	28.6	27.9	0.6	0.5	0.5	0.5	0.5	1	R(HC)
129.2	52.5	176.5	21.4		0.6	0.5	0.5	0.5	0.5	1	A(SC)
120.2	61.0	179.7	30.5	111.7	0.6	0.5	0.5	0.5	0.5	1	H(H)W(H)Y(H)
118.4	54.9	179.2	17.6		0.6	0.5	0.5	0.5	0.5	1	A(HC)
118.4	68.7	176.0	32.6	25.9	0.6	0.5	0.5	0.5	0.5	1	K(CH)V(CS)
106.5	47.6	175.2			0.6	0.5	0.5	0.5	0.5	1	G(HC)
121.4	58.9	177.9	41.3	27.1	0.6	0.5	0.5	0.5	0.5	1	L(HC)
126.3	59.2	177.5	33.0	31.5	0.6	0.5	0.5	0.5	0.5	1	K(CH)M(H)V(SC)
115.4	68.0	174.4	36.7	31.5	0.6	0.5	0.5	0.5	0.5	1	I(H)
117.2	62.6	178.1		130.2	0.6	0.5	0.5	0.5	0.5	1	Y(H)
113.9	53.8	175.0	36.4	24.4	0.6	0.5	0.5	0.5	0.5	1	K(C)
125.5	60.0	174.2	32.5	23.2	0.6	0.5	0.5	0.5	0.5	1	V(SC)K(CH)
117.2	63.0	176.4	62.9		0.6	0.5	0.5	0.5	0.5	1	S(HC)T(C)
115.7	56.7	174.9	38.7	181.7	0.6	0.5	0.5	0.5	0.5	1	N(HC)D(CH)E(C)
106.6	60.3	177.8	65.4		0.6	0.5	0.5	0.5	0.5	1	S(C)T(C)
120.3	60.9	176.7	29.5	111.8	0.6	0.5	0.5	0.5	0.5	1	H(H)W(H)
122.2	56.4	179.9	18.0		0.6	0.5	0.5	0.5	0.5	1	A(H)
104.2	46.0	173.3			0.6	0.5	0.5	0.5	0.5	1	G(C)
129.5	55.2	176.2	25.6	128.3	0.6	0.5	0.5	0.5	0.5	1	H(C)W(C)
119.4	60.8	178.3	38.2	133.4	0.6	0.5	0.5	0.5	0.5	1	Y(HC)F(H)
114.0	57.8	178.0	41.2	26.2	0.6	0.5	0.5	0.5	0.5	1	L(HC)I(S)
121.1	57.0	178.3	33.6	35.3	0.6	0.5	0.5	0.5	0.5	1	K(CH)S)E(HCS)M(HC)V(S))L(H)
119.9	64.4	176.2	37.1		0.6	0.5	0.5	0.5	0.5	1	I(HC)

110.6	59.2	176.9	34.3	35.3	0.6	0.5	0.5	0.5	0.5	1	V(SC)Q(H)E(HC)K(CHS) M(H)
124.2	56.1	179.3	18.3		0.6	0.5	0.5	0.5	0.5	1	A(H)
134.4	50.6	177.4	17.4		0.6	0.5	0.5	0.5	0.5	1	A(C)
120.2	57.0	179.1	42.1	26.3	0.6	0.5	0.5	0.5	0.5	1	L(HC)
107.5	66.0	177.8	70.2		0.6	0.5	0.5	0.5	0.5	1	T(HS)
127.0	55.7	179.7	15.3		0.6	0.5	0.5	0.5	0.5	1	A(H)
115.8	58.1	179.4	42.6	26.8	0.6	0.5	0.5	0.5	0.5	1	L(H)
106.5	47.8	175.8			0.6	0.5	0.5	0.5	0.5	1	G(HC)
118.7	55.0	177.7	18.9		0.6	0.5	0.5	0.5	0.5	1	A(HC)
125.6	58.2	172.7	31.1	32.1	0.6	0.5	0.5	0.5	0.5	1	R(C)K(H)E(C)M(H)
119.9	65.8	177.7	37.2	29.8	0.6	0.5	0.5	0.5	0.5	1	I(HC)
115.7	63.4	177.7	28.8	129.2	0.6	0.5	0.5	0.5	0.5	1	W(H)H(H)Y(H)
119.9	56.5	176.8	32.8		0.6	0.5	0.5	0.5	0.5	1	K(CHS)M(CH)Q(CSH)R(C)V(CS)W(S)
115.9	63.4	175.7		132.0	0.6	0.5	0.5	0.5	0.5	1	Y(CS)
120.2	63.0	177.2	40.2	139.5	0.6	0.5	0.5	0.5	0.5	1	F(HC)
118.3	57.7	179.6	41.6	27.7	0.6	0.5	0.5	0.5	0.5	1	L(H)
120.3	59.4	177.7	27.9	127.9	0.6	0.5	0.5	0.5	0.5	1	H(H)Q(H)W(H)
112.8	67.1	176.4	68.0		0.6	0.5	0.5	0.5	0.5	1	T(HC)
102.8	45.7	173.7			0.6	0.5	0.5	0.5	0.5	1	G(CH)
112.8	59.9	177.5	37.8	128.6	0.6	0.5	0.5	0.5	0.5	1	Y(HC)F(H)
118.2	53.2	172.5	29.6	29.9	0.6	0.5	0.5	0.5	0.5	1	Q(CH)K(H)
137.8	66.6	178.8	31.9	29.0	0.6	0.5	0.5	0.5	0.5	1	P(HC)
127.0	53.1	178.0	18.1		0.6	0.5	0.5	0.5	0.5	1	A(CH)
121.3	63.7	177.5	38.6	129.0	0.6	0.5	0.5	0.5	0.5	1	F(H)Y(H)
119.0	69.4	175.2	66.8		0.6	0.5	0.5	0.5	0.5	1	T(CHS)
117.5	54.8	175.4	31.6	35.4	0.6	0.5	0.5	0.5	0.5	1	E(SC)R(CS)Q(CS)
109.0	53.2	176.6	33.0	34.2	0.6	0.5	0.5	0.5	0.5	1	M(C)
111.5	60.2	174.1	35.8	23.8	0.6	0.5	0.5	0.5	0.5	1	I(SC)
120.4	66.3	177.5	37.7	28.9	0.6	0.5	0.5	0.5	0.5	1	I(H)
119.3	65.5	178.0	38.4	29.7	0.6	0.5	0.5	0.5	0.5	1	I(H)
101.9	46.2	172.1			0.6	0.5	0.5	0.5	0.5	1	G(CSH)
105.5	47.8	172.7			0.6	0.5	0.5	0.5	0.5	1	G(CHS)
121.9	58.5	178.5	41.2	27.5	0.6	0.5	0.5	0.5	0.5	1	L(HC)
116.4	56.1	178.3	40.7	178.3	0.6	0.5	0.5	0.5	0.5	1	D(HC)N(H)

NCOCX

82	5										
124.2	67.9	180.1	32.0	22.5	0.6	0.5	0.5	0.5	0.5	1	V(H)
119.9	57.9	179.3	42.4	27.1	0.6	0.5	0.5	0.5	0.5	1	L(HC)I(S)
117.7	62.6	178.4		130.1	0.6	0.5	0.5	0.5	0.5	1	Y(H)F(H)H(HC)
120.0	64.6	175.9	37.3		0.6	0.5	0.5	0.5	0.5	1	I(HC)
115.9	66.0	177.1	37.7	29.1	0.6	0.5	0.5	0.5	0.5	1	I(HCS)
125.4	59.7	177.6	37.0	126.5	0.6	0.5	0.5	0.5	0.5	1	Y(H)F(H)
117.9	46.0	173.0			0.6	0.5	0.5	0.5	0.5	1	G(CSH)
114.6	56.3	178.3	40.6	178.7	0.6	0.5	0.5	0.5	0.5	1	D(HC)N(HC)
119.7	59.8	177.3	37.7	128.5	0.6	0.5	0.5	0.5	0.5	1	F(H)Y(HC)
119.7	62.1	178.2			0.6	0.5	0.5	0.5	0.5	1	Y(H)P(CS)F(HC)S(H)I(HC) W(H)T(C)R(H)E(H)
113.9	67.0	179.1	32.1	29.0	0.6	0.5	0.5	0.5	0.5	1	P(HC)E(H)
119.5	65.3	178.7	32.3	28.0	0.6	0.5	0.5	0.5	0.5	1	P(CHS)
118.8	58.6	179.8	28.3	115.3	0.6	0.5	0.5	0.5	0.5	1	W(H)
104.2	52.8	177.7	17.8		0.6	0.5	0.5	0.5	0.5	1	A(CHS)
119.5	59.6	174.8	41.9	24.5	0.6	0.5	0.5	0.5	0.5	1	I(SC)
113.1	65.8	177.4	70.4		0.6	0.5	0.5	0.5	0.5	1	T(H)
125.5	45.5	174.0			0.6	0.5	0.5	0.5	0.5	1	G(CHS)
127.4	58.9	180.6	31.2	33.3	0.6	0.5	0.5	0.5	0.5	1	Q(HC)M(H)E(H)K(C)

113.0	59.5	176.0	28.7	27.5	0.6	0.5	0.5	0.5	0.5	1	R(HC)
109.2	54.0	177.4	19.0		0.6	0.5	0.5	0.5	0.5	1	A(CH)
121.4	58.3	178.4	41.5	27.2	0.6	0.5	0.5	0.5	0.5	1	L(HC)
120.4	63.6	177.7	29.0	129.0	0.6	0.5	0.5	0.5	0.5	1	H(H)
121.5	63.4	175.5		132.1	0.6	0.5	0.5	0.5	0.5	1	Y(CS)
120.5	68.9	175.3	66.4		0.6	0.5	0.5	0.5	0.5	1	T(HCS)
125.4	56.7	179.8	30.0	113.4	0.6	0.5	0.5	0.5	0.5	1	W(H)
120.2	59.3	176.4	34.2	35.2	0.6	0.5	0.5	0.5	0.5	1	Q(H)V(S)K(CS)E(C)M(HC)R(C)
119.9	59.2	178.0	27.8	128.2	0.6	0.5	0.5	0.5	0.5	1	H(H)
121.1	66.2	177.6	37.4	30.1	0.6	0.5	0.5	0.5	0.5	1	I(H)
110.8	55.2	179.4	15.8		0.6	0.5	0.5	0.5	0.5	1	A(H)
122.7	47.8	172.7			0.6	0.5	0.5	0.5	0.5	1	G(CS)A(CS)D(C)
107.5	63.3	178.7	34.4	22.0	0.6	0.5	0.5	0.5	0.5	1	V(SC)
106.1	60.0	178.0	65.5		0.6	0.5	0.5	0.5	0.5	1	T(CS)S(HC)
140.4	59.8	173.9	32.2	23.2	0.6	0.5	0.5	0.5	0.5	1	V(SC)
121.6	48.2	175.7			0.6	0.5	0.5	0.5	0.5	1	G(HC)
122.5	53.5	176.7	33.1	33.9	0.6	0.5	0.5	0.5	0.5	1	K(CSH)E(SC)M(CSH)R(SC)Q(SC)
113.0	60.5	177.6	28.7	33.1	0.6	0.5	0.5	0.5	0.5	1	K(HC)E(H)Q(H)
128.9	56.6	175.9	29.9	36.0	0.6	0.5	0.5	0.5	0.5	1	E(CH)Q(C)
117.2	57.3	176.8	42.5	26.2	0.6	0.5	0.5	0.5	0.5	1	L(HC)
115.4	63.2	177.3	40.4	139.2	0.6	0.5	0.5	0.5	0.5	1	F(H)
109.6	58.2	172.6	31.6	31.9	0.6	0.5	0.5	0.5	0.5	1	K(CH)M(HC)R(C)Q(C)
118.4	59.3	178.3	41.9	27.1	0.6	0.5	0.5	0.5	0.5	1	L(HC)
116.0	58.0	177.0	40.5	25.1	0.6	0.5	0.5	0.5	0.5	1	L(HC)
130.6	51.1	173.1	39.2	178.2	0.6	0.5	0.5	0.5	0.5	1	N(C)D(C)
121.7	63.4	177.1	38.6	128.7	0.6	0.5	0.5	0.5	0.5	1	Y(H)F(H)
122.1	64.2	178.4	63.6		0.6	0.5	0.5	0.5	0.5	1	S(H)
127.1	58.0	179.5	41.8	27.8	0.6	0.5	0.5	0.5	0.5	1	L(HC)
113.7	54.9	179.3	17.6		0.6	0.5	0.5	0.5	0.5	1	A(HC)
118.8	68.8	176.0	32.7	25.9	0.6	0.5	0.5	0.5	0.5	1	V(H)
127.1	52.1	176.5	21.7		0.6	0.5	0.5	0.5	0.5	1	A(CS)
118.3	59.2	177.5	32.8	31.4	0.6	0.5	0.5	0.5	0.5	1	K(HC)M(H)
122.8	62.9	176.6	62.7		0.6	0.5	0.5	0.5	0.5	1	S(H)
119.6	53.1	172.3	30.0	29.9	0.6	0.5	0.5	0.5	0.5	1	E(CH)Q(S)
106.7	55.6	179.4	18.1		0.6	0.5	0.5	0.5	0.5	1	A(HC)
111.4	56.0	175.2		140.7	0.6	0.5	0.5	0.5	0.5	1	F(SC)
119.6	55.4	178.6	17.8		0.6	0.5	0.5	0.5	0.5	1	A(HC)
101.9	54.6	175.0	31.6	35.5	0.6	0.5	0.5	0.5	0.5	1	Q(SC)
105.2	65.5	178.1	38.2	29.5	0.6	0.5	0.5	0.5	0.5	1	I(H)
126.6	60.9	178.5	38.4	133.7	0.6	0.5	0.5	0.5	0.5	1	Y(HC)F(H)
121.2	55.3	176.2	25.5	128.2	0.6	0.5	0.5	0.5	0.5	1	H(C)
115.5	61.3	179.1	30.1	38.6	0.6	0.5	0.5	0.5	0.5	1	E(H)
137.8	66.6	176.2	67.9		0.6	0.5	0.5	0.5	0.5	1	T(HC)
114.0	46.0	172.4			0.6	0.5	0.5	0.5	0.5	1	G(CS)
116.7	56.9	178.0	33.8	35.1	0.6	0.5	0.5	0.5	0.5	1	K(CH)E(CH)M(HC)Q(H)
134.4	58.8	176.5	36.2	26.4	0.6	0.5	0.5	0.5	0.5	1	I(SC)
120.9	53.7	175.4	36.7	23.9	0.6	0.5	0.5	0.5	0.5	1	K(SC)L(C)
106.4	61.2	176.8	29.4	111.7	0.6	0.5	0.5	0.5	0.5	1	W(CH)
116.2	57.1	178.8	42.1	25.8	0.6	0.5	0.5	0.5	0.5	1	L(HC)
115.5	60.2	174.1	36.0	23.3	0.6	0.5	0.5	0.5	0.5	1	I(SC)
121.1	57.9	177.5	41.1	26.0	0.6	0.5	0.5	0.5	0.5	1	L(HC)
113.8	55.3	179.0	17.1		0.6	0.5	0.5	0.5	0.5	1	A(H)
111.1	55.5	177.9	18.7		0.6	0.5	0.5	0.5	0.5	1	A(HC)
129.5	51.1	177.2	17.6		0.6	0.5	0.5	0.5	0.5	1	A(CHS)
117.2	57.9	178.4	41.7	26.0	0.6	0.5	0.5	0.5	0.5	1	L(HC)
118.3	57.8	179.6	43.1	28.2	0.6	0.5	0.5	0.5	0.5	1	L(H)
119.8	61.1	179.7	30.6	112.0	0.6	0.5	0.5	0.5	0.5	1	W(C)
115.7	56.3	179.7	17.9		0.6	0.5	0.5	0.5	0.5	1	A(HC)
115.6	58.4	178.1	40.8	26.9	0.6	0.5	0.5	0.5	0.5	1	L(HC)
132.4	67.8	174.8	36.7	31.4	0.6	0.5	0.5	0.5	0.5	1	I(H)

119.8	68.2	176.3			0.6	0.5	0.5	0.5	0.5	1	T(H)V(H)
127.9	60.1	171.6	35.8	21.2	0.6	0.5	0.5	0.5	0.5	1	V(SC)
117.5	56.4	174.8	38.9	181.7	0.6	0.5	0.5	0.5	0.5	1	D(C)N(HC)
121.2	47.5	174.9			0.6	0.5	0.5	0.5	0.5	1	G(CHS)

Table S7. HNP-1 peak lists.

NCACX																		
27	8																	
109.3	172.8	42.5							1.0	0.5	0.4	0.4	0.3	0.3	0.3	0.3	1	G(CS)
103.7	170.7	44.0							1.0	0.5	0.4	0.4	0.3	0.3	0.3	0.3	1	G(CSH)
107.0	171.9	45.0							1.0	0.5	0.4	0.4	0.3	0.3	0.3	0.3	1	G(CH)
123.0	172.4	48.7	20.5						1.0	0.5	0.4	0.4	0.3	0.3	0.3	0.3	1	A(SC)
107.0		49.3	17.5						1.0	0.5	0.4	0.4	0.3	0.3	0.3	0.3	1	A(H)
115.8	173.1	50.7	33.4						1.0	0.5	0.4	0.4	0.3	0.3	0.3	0.3	1	R(SC)E(SC)Y(C)F(C)C(C)
115.9		50.7	32.7						1.0	0.5	0.4	0.4	0.3	0.3	0.3	0.3	1	E(SC)R(S)Y(C)
116.4	172.4	50.9							1.0	0.5	0.4	0.4	0.3	0.3	0.3	0.3	1	L(SC)E(S)R(CS)Q(S)C(CH)
126.6	173.0	51.0	17.0						1.0	0.5	0.4	0.4	0.3	0.3	0.3	0.3	1	A(CSH)
118.2	172.3	51.5		25.4					1.0	0.5	0.4	0.4	0.3	0.3	0.3	0.3	1	L(SC)Q(CS)R(CS)E(S)
122.5	171.7	51.5	43.0						1.0	0.5	0.4	0.4	0.3	0.3	0.3	0.3	1	C(SC)L(SC)F(S)
120.4		51.9	16.8						1.1	0.5	0.4	0.4	0.3	0.3	0.3	0.3	1	A(HC)
119.9	174.3	51.9		25.4		23.2	22.3		1.0	0.5	0.4	0.4	0.3	0.3	0.3	0.3	1	L(CSH)
120.5		52.1	29.0						1.0	0.5	0.4	0.4	0.3	0.3	0.3	0.3	1	R(CSH)E(CSH)Q(SC)L(CSH)W(C)
120.5	172.8	52.6	39.2						1.0	0.5	0.4	0.4	0.3	0.3	0.3	0.3	1	C(C)L(CHS)Q(C)F(SC)Y(S)
130.5	171.5	52.7	43.5						1.0	0.5	0.4	0.4	0.3	0.3	0.3	0.3	1	C(S)L(S)
130.4	172.6	52.9	44.6						1.0	0.5	0.4	0.4	0.3	0.3	0.3	0.3	1	C(S)L(S)
117.2	171.4	53.0	46.6						1.0	0.5	0.4	0.4	0.3	0.3	0.3	0.3	1	L(CS)C(SC)
121.9	173.0	53.8	33.8	26.6		41.4			1.5	0.5	0.4	0.4	0.3	0.3	0.3	0.3	1	R(C)
117.3	172.5	54.8							1.0	0.5	0.4	0.4	0.3	0.3	0.3	0.3	1	Y(SC)F(SC)E(CSH)R(CHS)Q(CH)L(CH)
)
124.5	172.6	54.8	37.8						1.0	0.5	0.4	0.4	0.3	0.3	0.3	0.3	1	F(SC)Y(SC)I(SC)L(CHS)E(CS)C(S)
127.4	173.6	56.2	39.1	131.0					1.0	0.5	0.4	0.4	0.3	0.3	0.3	0.3	1	F(S)Y(S)
122.5	172.6	56.3	41.2		15.3				1.0	0.5	0.4	0.4	0.3	0.3	0.3	0.3	1	I(S)
115.8	173.0	57.9	37.3		15.9				1.0	0.5	0.4	0.4	0.3	0.3	0.3	0.3	1	I(SC)
123.6	171.6	59.5							1.0	0.5	0.4	0.4	0.3	0.3	0.3	0.3	1	T(SC)I(SC)
124.0	173.5	59.8	35.8	24.4	16.3	11.5			1.0	0.5	0.4	0.4	0.3	0.3	0.3	0.3	1	I(CSH)
123.0		54.5	28.0						1.0	0.5	0.4	0.4	0.3	0.3	0.3	0.3	1	E(CH)R(C)

NCOCX																		
25	8																	
120.5	172.8	42.3							1.0	0.5	0.4	0.4	0.3	0.3	0.3	0.3	1	G(CSH)
118.3	171.1	44.1							1.0	0.5	0.4	0.4	0.3	0.3	0.3	0.3	1	G(CS)
123.8	172.0	45.0							1.0	0.5	0.4	0.4	0.3	0.3	0.3	0.3	1	G(CH)L(S)
115.6	173.1	48.8	20.6						1.0	0.5	0.4	0.4	0.3	0.3	0.3	0.3	1	A(SC)
117.3	170.9	49.4	17.8						1.0	0.5	0.4	0.4	0.3	0.3	0.3	0.3	1	A(CS)
123.9	173.9	50.8							1.0	0.5	0.4	0.4	0.3	0.3	0.3	0.3	1	L(SC)A(CSH)E(S)

115.5	173.1	50.8	33.1					1.0	0.5	0.4	0.4	0.3	0.3	0.3	0.3	1	E(S)R(S)Y(C)L(H)W(S)C(C)Q(SC)
122.1	172.1	51.0						1.0	0.5	0.4	0.4	0.3	0.3	0.3	0.3	1	L(SC)R(SC)E(SC)Q(S)F(S)W(S)A(C)
124.2	173.2	51.2	17.0					1.0	0.5	0.4	0.4	0.3	0.3	0.3	0.3	1	A(CHS)
120.3	172.4	51.6						1.0	0.5	0.4	0.4	0.3	0.3	0.3	0.3	1	L(SCH)Q(SC)E(SC)R(SC)C(CS)F(S)A(C)W(S)
123.5	171.8	51.6	43.1					1.0	0.5	0.4	0.4	0.3	0.3	0.3	0.3	1	L(SC)F(S)C(S)
118.9	175.2	51.9		23.4				1.0	0.5	0.4	0.4	0.3	0.3	0.3	0.3	1	L(CS)R(CS)Q(C)A(S)
120.8	173.9	52.0	42.1					1.0	0.5	0.4	0.4	0.3	0.3	0.3	0.3	1	L(SCH)
125.0	174.0	52.0	16.8					1.0	0.5	0.4	0.4	0.3	0.3	0.3	0.3	1	A(CH)
127.0	174.8	52.1	29.3					1.0	0.5	0.4	0.4	0.3	0.3	0.3	0.3	1	R(CSH)E(CS)Q(CS)W(S)C(C)
124.0	171.5	52.5						1.5	0.5	0.4	0.4	0.3	0.3	0.3	0.3	1	E(SC)R(SC)Q(SC)L(SC)C(SC)Y(SC)F(SC)W(CS)
121.2	173.0	52.8	39.0					1.0	0.5	0.4	0.4	0.3	0.3	0.3	0.3	1	L(CSH)F(SC)Y(SC)E(SC)C(C)
117.6	171.6	52.9	46.9					1.0	0.5	0.4	0.4	0.3	0.3	0.3	0.3	1	L(SH)C(S)
122.5	173.1	54.2	33.8	26.6		41.4		1.0	0.5	0.4	0.4	0.3	0.3	0.3	0.3	1	R(C)
126.7	173.1	54.6						1.0	0.5	0.4	0.4	0.3	0.3	0.3	0.3	1	Q(C)F(SC)Y(SC)R(CS)E(SH)L(C)W(S)C)
130.5	172.6	54.6	37.6					1.0	0.5	0.4	0.4	0.3	0.3	0.3	0.3	1	Y(SC)F(SC)I(S)L(C)
106.8	173.9	56.7	38.7	130.9				1.0	0.5	0.4	0.4	0.3	0.3	0.3	0.3	1	Y(SC)F(CSH)
122.7	171.7	59.7						1.0	0.5	0.4	0.4	0.3	0.3	0.3	0.3	1	T(CS)I(SC)P(C)
125.5	173.7			24.6	16.6	11.4		1.0	0.5	0.4	0.4	0.3	0.3	0.3	0.3	1	I(SC)
127.7	175	54.2	28.0					1.0	0.8	0.4	0.4	0.3	0.3	0.3	0.3	1	E(CH)R(C)

Table S8. Amino acid sequences of the four proteins investigated here.

GB1	MQYKLILNGKTLKGETTTEAVDAATAEKVFKQYANDNGVDGEWTYDDATKTFTVT E
HET-s	MKIDAIVGRNSAKDIRTEERARVQLGNVVTAALHGGIRISDQTTNSVETVVGKGESR VLIGNEYGGKGFWDNHHHHHH
Truncated Sensory Rhodopsin	MNLESLHWHYVAGMTIGALHFWLSRNPGRVGPQYEYLVAMFIPIWSGLAYMAMAI DQKVEAAGQIAHYARYIDWMVTTPLLLSLSWTAMQFIKKD
HNP-1	ACYCRIPACIAGERRYGTCTIYQGRWAFCC