SUPPORTING INFORMATION TO:

NMR Mapping of Protein Conformational Landscapes using Coordinated Behavior of Chemical Shifts upon Ligand Binding

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Figure S1: Left Column: **Filtering** of the **synthetic data**. The residues were ordered by increasing SD_{PC1}/SD_{PC2} ratio (Black dots) and by increasing PC1 range (orange dots). Cutoffs are shown as horizontal lines. Right Column: scatterplots of the residues along the SD_{PC1}/SD_{PC2} ratio and the PC1 range. Only the residues on the top right quadrant are retained after filtering.

Figure S2: Hierarchical clustering analysis of the **synthetic data**. The square boxes show the clusters formed by cutting the tree at correlation of 0.99. The largest cluster is shown in blue.

Figure S3: Left Column: **Filtering** of the **data for PKA-C**. The residues were ordered by increasing SD_{PC1}/SD_{PC2} ratio (Black dots) and by increasing PC1 range (orange dots). Cutoffs are shown as horizontal lines. Right Column: scatterplots of the residues along the SD_{PC1}/SD_{PC2} ratio and the PC1 range. Only the residues on the top right quadrant are retained after filtering.

Figure S4: Hierarchical clustering analysis of the **data for PKA-C**. The square boxes show the clusters formed by cutting the tree at correlation of 0.99. The largest cluster is shown in blue.

Table S1: List of residues comprising the largest cluster of the PKA-C.

Figure S1

IDEAL + NOISE

RANDOM

MIX RANDOM/IDEAL

Figure S2

(a)

IDEAL

(b)

IDEAL + NOISE

(c)

RANDOM

(d)

MIX RANDOM/IDEAL
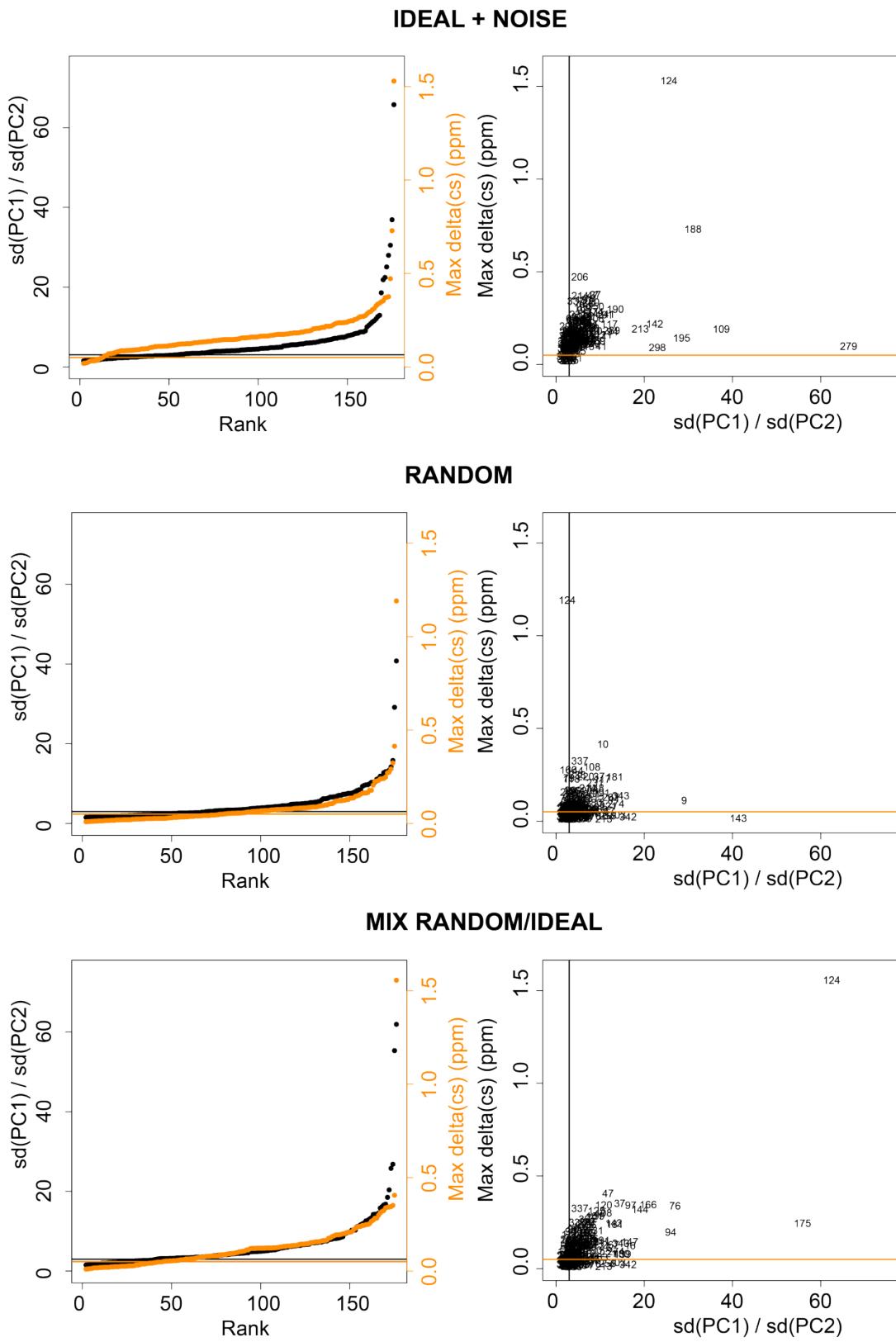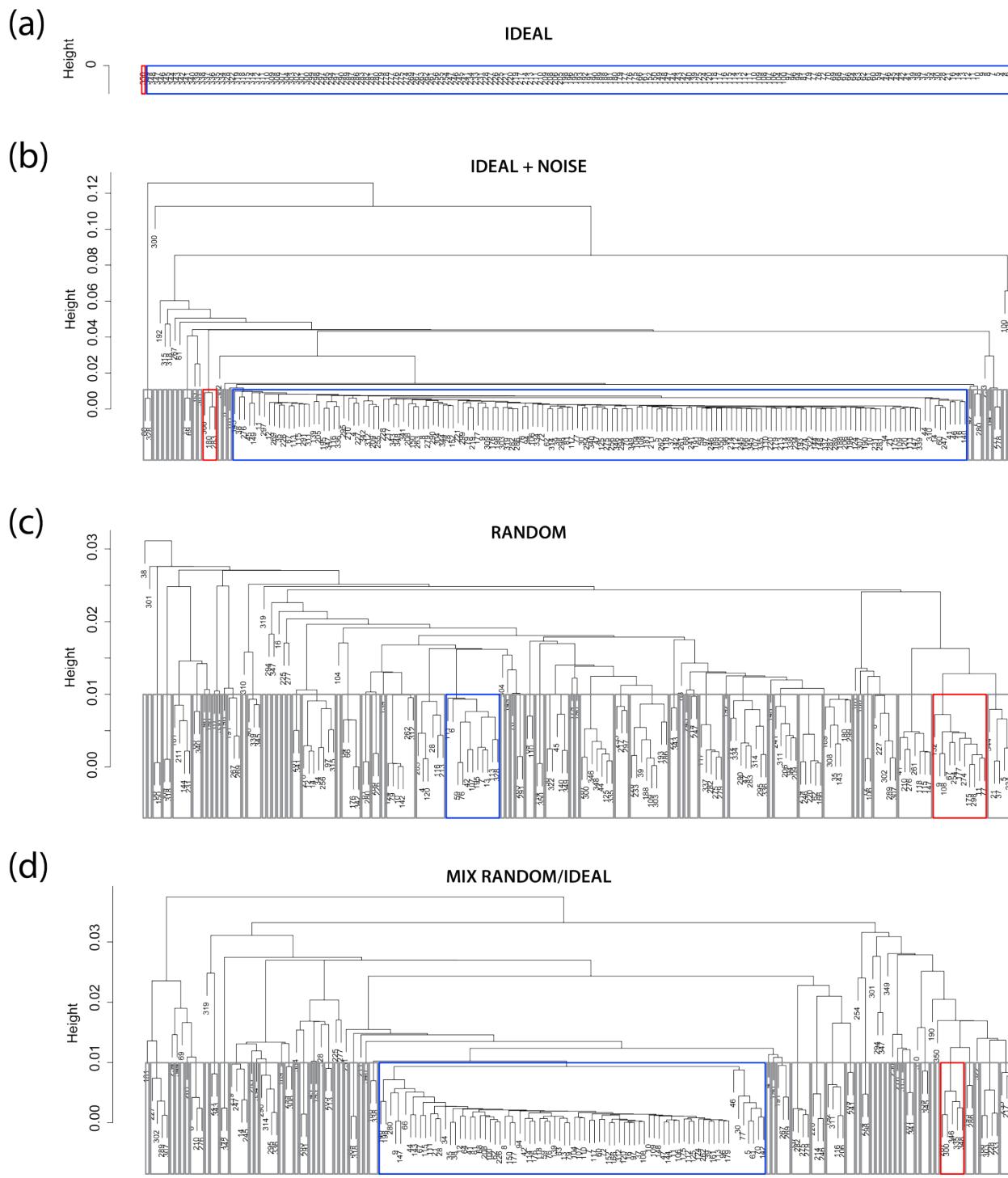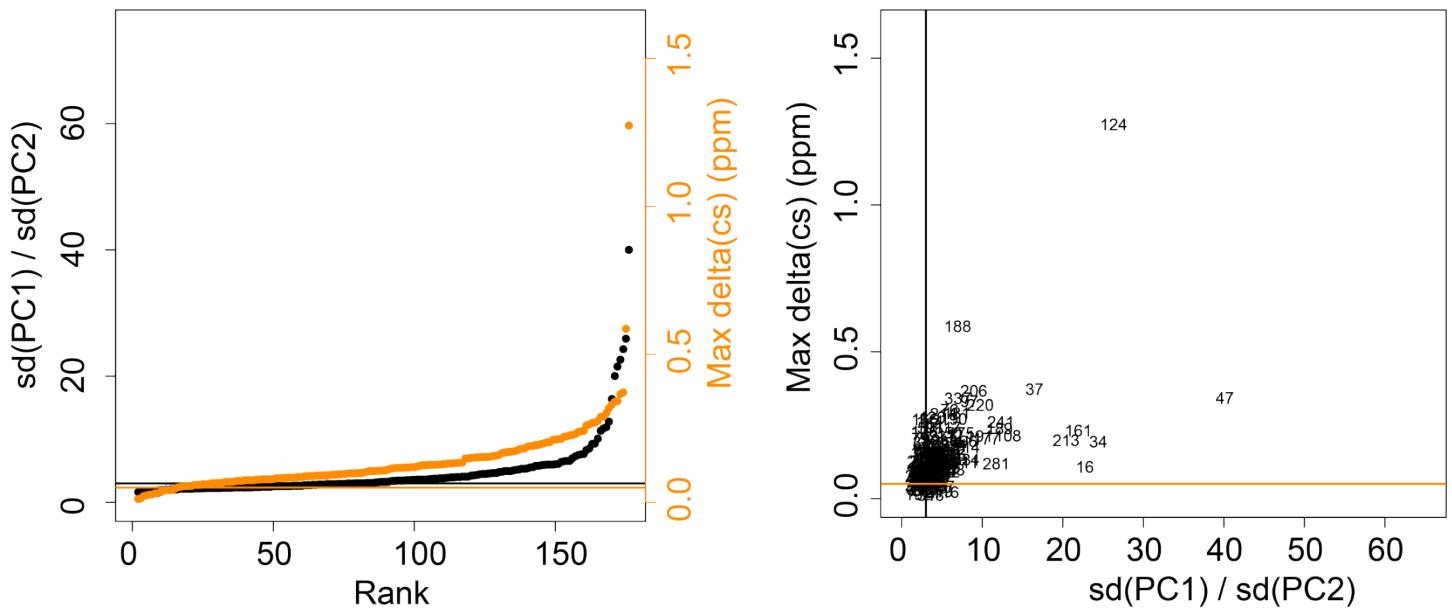
Figure S3

Figure S4
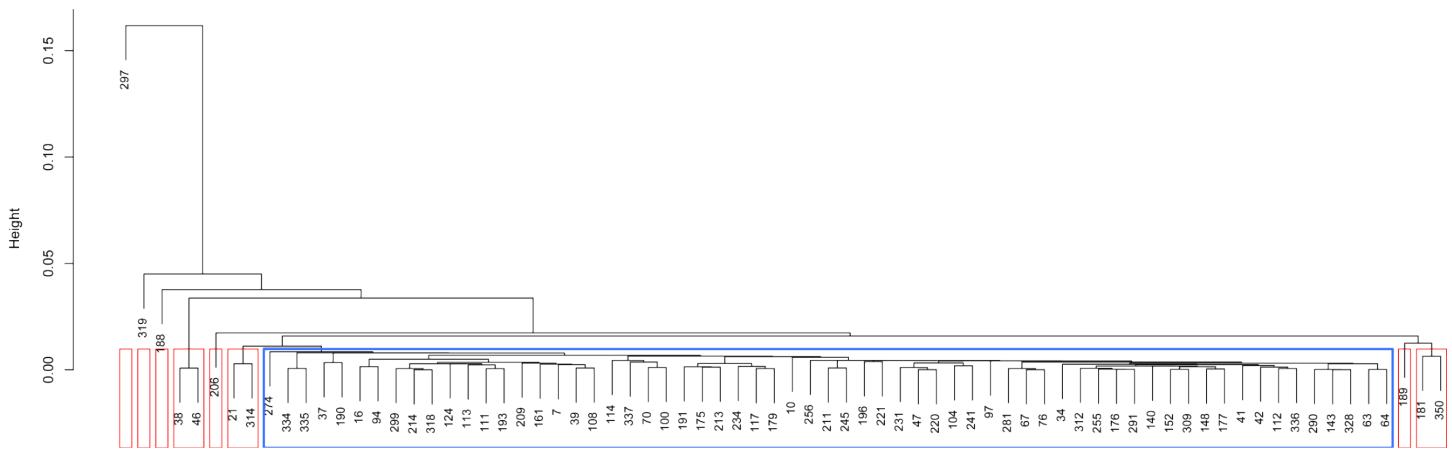
Table S1:

K 7	N 113	D 220
S 10	S 114	W 221
K 16	Y 117	M 231
S 34	A 124	G 234
T 37	E 140	D 241
Q 39	A 143	Q 245
D 41	A 148	V 255
Q 42	L 152	R 256
K 47	D 161	Q 274
K 63	D 175	F 281
E 64	Q 176	D 290
N 67	Q 177	I 291
A 70	Y 179	T 299
K 76	R 190	K 309
I 94	V 191	A 312
A 97	G 193	F 318
F 100	W 196	D 328
V 104	I 209	E 334
F 108	L 211	I 335
K 111	K 213	R 336
D 112	G 214	V 337