Electronic Supplementary Information

to

Guanidinium–amino acid hydrogen-bonding interactions in protein crystal structures: Implications for guanidinium-induced protein denaturation

Indu Negi[1,¶], Raman Jangra[1,¶], Amit Gharu[1], John F. Trant[2,3,†*] and Purshotam Sharma[1,2*]

[1]*Computational Biochemistry Laboratory, Department of Chemistry and Centre for Advanced Studies in Chemistry, Panjab University, Chandigarh, 160014, India.*

[2]*Department of Chemistry and Biochemistry, University of Windsor, 401 Sunset Ave. Windsor ON, N9B 3P4, Canada*

[3]*Binary Star Research Services, LaSalle ON N9J 3X8, Canada*

[¶]Both authors contributed equally to this work.

[†]Dr. John F. Trant, a co-corresponding author on this work, is also affiliated to Binary Star Research Services as a Chief Executive Officer. However, Binary Star had no input into the paper.

**Email: j.trant@uwindsor.ca, psharma@pu.ac.in*

Table of Contents

Table S1. PDB codes of the 86 analyzed crystal structures of protein complexes containing at least one Gdm^+.

1JXM, 1KP2, 1KP3, 1O01, 1O02, 1O04, 1PXV, 1RBW, 1T8A, 1UMJ, 1XCL, 1ZUM, 229L, 2CEV, 2DDZ, 2DPK, 2EF5, 2F2Q, 2GV9, 2ONM, 2ONP, 2PNL, 2ZFZ, 3EQS, 3EQY, 3GNU, 3INJ, 3LAS, 3M6Z, 3MV1, 3N80, 3N81, 3N82, 3N83, 3SZ9, 3U4F, 3UHM, 4AM8, 4CEV, 4D50, 4F8L, 4F8N, 4F8O, 4GLL, 4HSE, 4ITC, 4KWF, 4KWG, 4LJA, 4LYP, 4N7H, 4PHL, 4PXJ, 4WQD, 5CEV, 5G2B, 5G57, 5G5V, 5GWB, 5L13, 5L8C, 5L8Y, 5SZD, 6A4N, 6A4O, 6A4P, 6A4Q, 6C1K, 6FDS, 6FDW, 6FDX, 6FE3, 6FRD, 6FTM, 6GXQ, 6P3L, 6P44, 6QGP, 6QGU, 6RB6, 6RFN, 6RFW, 6RGK, 6UW2, 6Y16, 7LOX.

Table S2. Non-redundant clusters of cystal structures with the analyzed dataset of Gdm^+:protein complexes.

S. No.	PDB File	Protein
1	1JXM	GMP bound SH3-HOOK-GK fragment of PSD-95
2	1KP2, 1KP3	Argininosuccinate synthetase
3	1O01, 1O02, 1O04, 1ZUM, 2ONM, 2ONP, 3INJ, 3N80, 3N81, 3N82, 3N83, 3SZ9, 4KWF, 4KWG, 5L13	Mitochondrial aldehyde dehydrogenase
4	1PXV	Staphostatin-Staphopain complex
5	1RBW	Ribonuclease A
6	1T8A, 229L, 2F2Q	T4 Lysozyme
7	1UMJ	Pyrococcus Horikoshii Cuta
8	1XCL	Guanidinoacetate methyltransferase
9	2CEV, 4CEV, 5CEV	Arginase
10	2DDZ	Protein from Pyrococcus Horikoshi
11	2DPK	Primary CA2+ sensor of the 2 NA+/CA2+ exchanger
12	2EF5	Arginase from Thermus Thermophilus
13	2GV9	Herpes simplex virus type 1 DNA polymerase
14	2PNL	VP4 protease
15	2ZFZ	C-terminal domain hexamer of ARGR
16	3EQS, 3EQY	Human MDM2
17	3GNU	NLP toxin
18	3LAS	Carbonic anhydrase
19	3M6Z	N-terminal 44 KDA fragment of topoisomerase V2
20	3MV1	Beta-galactosidase (R599A)
21	3U4F	Mandelate racemase
22	3UHM	N-acetylglucosamine deacetylase
23	4AM8	R54G mutant of putrescine transcarbamylase 2
24	4D50	Human deoxyhypusine hydroxylase
25	4F8L, 4F8N, 4F8O	PSAA from yersinia pestis
26	4GLL	Human UDP-xylose synthase
27	4HSE	CLPB NBD1
28	4ITC	K1 cleaved adhesin domain of LYS- 2 gingipain (KGP)
29	4LJA	CLPB NBD2 R621Q
30	4LYP	Glycoside hydrolase family 5 mannosidase
31	4N7H	3RD WW domain of human NEDD4 and 2 1ST PPXY motif of ARRDC3
32	4PXJ	LZII fragment

33	4WQD	Thiosulfate dehydrogenase (TSDA)
34	6A4N, 6A4O, 6A4P, 6A4Q, 5GWB	Hen egg-white lysozyme (HEWL)
35	5SZD	Aquifex aeolicus HFQ
36	6C1K	Hypopp mutant
37	6P3L, 6P44	Ketosteroid isomerase
38	6UW2	Acanthamoeba castellanii CYP51
39	6Y16	TMARGBP domain 1
40	7LOX	Agmatinase
41	6QGP, 6QGU, 6RB6, 6RFN, 6RFW, 6RGK, 6FDS, 6FDW, 6FDX, 6FE3, 6FRD, 6FTM, 6GXQ, 5G2B, 5G57, 5G5V, 5L8C, 5L8Y, 4PHL	T. brucei PDE-B1 catalytic domain

Table S3. The frequency of different protein types presents in the analyzed crystal structures, along with the total number of interactions identified for each protein type.

S.No.	Protein type	# of PDBs	PDB codes[a]	# of Gdm^+ hydrogen bonds
1	Binding protein	4	2ZFZ (2;474), 4N7H (2;50), 4PXJ (2;183), 5SZD (8;996)	13
2	Cell adhesion	3	4F8L (1;145), 4F8N (1;145), 4F8O (2;145)	8
3	Chaperone	2	4HSE (1;397), 4LJA (1;339)	4
4	Hydrolase	39	1PXV (1;588), 1RBW (4;124), 1T8A (1;175), 229L (1;164), 2CEV (6;1794), 2EF5 (6;1740), 2F2Q (1;175), 2PNL (17;2000), 3MV1 (4;4208), 3UHM (1;299), 4CEV (6;1794), 4ITC (3;173), 4LYP (1;339), 4PHL (1;694), 5CEV (6;1794), 5G2B (3;720), 5G57 (7;720), 5G5V (11;720), 5GWB (3;129), 5L8C (1;720), 5L8Y (1;720), 6A4N (5;129), 6A4O (6;129), 6A4P (10;129), 6A4Q (12;129), 6FDS (6;720), 6FDW (1;720), 6FDX (4;720), 6FE3 (7;720), 6FRD (7;720), 6FTM (10;720), 6GXQ (5;720), 6QGP (3;720), 6QGU (3;720), 6RB6 (12;720), 6RFN (4;720), 6RFW (4;720), 6RGK (5;720), 7LOX (4;918)	274
5	Isomerase	4	3M6Z (3;760), 3U4F (4;1504), 6P3L (2;246), 6P44 (2;246)	26
6	Ligase	3	1KP2 (1;455), 1KP3 (2:455), 3EQS (1;97)	9
7	Lyase	2	3LAS (2;332), 4GLL (2;674)	11
8	Oncoprotein	1	3EQY (2;194)	2
9	Oxido–reductase	18	1O01 (8;4000), 1O02 (16;4000), 1O04 (18;4000), 1ZUM (8;6000), 2ONM (9;6000), 2ONP (28;4000), 3INJ (9;4000), 3N80 (21;3992), 3N81 (21;4000), 3N82 (13;4000), 3N83 (16;4000), 3SZ9 (18;4000), 4D50 (5;588), 4KWF (7;3952), 4KWG (7;3952), 4WQD (1;252), 5L13 (16;4136), 6UW2 (3;2760)	650
10	Structural	3	1JXM (2;301), 1UMJ (4;204), 2DDZ (8;1140)	9
11	Toxin	1	3GNU (2;213)	2
12	Transferase	3	1XCL (1;235), 2GV9 (1;2386), 4AM8 (7;2130)	22
13	Transport	3	2DPK (1;152), 6C1K (2;570), 6Y16 (2;256)	14
	Total	86		1044

[a]First number in the bracket represents the number of Gdm^+ in crystal structure, whereas the second number represents the number of amino acid residues present in the protein.

Table S4. Frequency of Gdm^+–protein hydrogen bonding interactions in the analyzed Gdm^+–protein crystal structures.

# of Gdm^+ hydrogen bonds	# of crystal structures
0	7
1–10	57
11–20	7
21–30	6
31–40	2
41–50	1
51–100	5
100^+	1

Table S5. Summary of Gdm^+–protein hydrogen bonding interactions in the X-ray crystal structures containing a single Gdm^+.

S. No.	PDB Code	Gdm^+	Interacting amino acid	Heavy atoms involved in interaction (Gdm^+•••Amino acid)
1	1KP2	460(A)	SER211(A)	N1•••OG
			ASN210(A)	N1•••OD1 N2•••OD1
2	1PXV	464(B)	–	–
3	1T8A	300(A)	VAL68(A)	N2•••O
			GLU73(A)	N2•••OE1 N3•••OE2
4	1XCL	237(A)	VAL40(A)	N3•••O
			GLU45(A)	N1•••OE2 N2•••OE1
			ASP134(A)	N2•••OD2
5	2DPK	1008(A)	ASP498(A)	N1•••O
			ASP453(A)	N1•••OD1 N2•••OD2
6	2F2Q	500(A)	GLU73(A)	N2•••OE1 N3•••OE2
7	2G9V	1239(B)	GLY385(B)	N1•••O N3•••O
			ASP481(B)	N2•••OD1
8	3EQS	201(A)	HIS96(A)	N2•••ND1
9	3UHM	301(A)	ALA206(A)	N3•••O
			LEU205(A)	N2•••O
10	4F8L	235(A)	ASP47(A)	N2•••O
			LYS49(A)	N1•••O N2•••O
11	4F8N	201(A)	ASP47(A)	N2•••O
			LYS49(A)	N2•••O
12	4HSE	601(A)	PRO171(A)	N1•••O
			ASP170(A)	N3•••O
			GLU209(A)	N2•••OE1 N3•••OE1
13	4LJA	903(A)	–	–
14	4PHL	1004(A)	–	–
15	4WQD	1005(A)	–	–
16	5L8C	1006(A)	LEU915(A)	N3•••O
17	5L8Y	1004(A)	LEU915(A)	N2•••O N3•••O
18	6FDW	1004(A)	SER798(A)	N1•••O
19	229L	169(A)	ASP92(A)	N1•••OD1

				N2•••OD1
			PHE153(A)	N1•••O N3•••O

Table S6. Summary of Gdm^+–protein hydrogen bonding interactions in the X-ray crystal structures containing two Gdm^+.

S. No.	PDB Code	Gdm^+	Interacting amino acid	Heavy atoms involved in interaction (Gdm^+•••Amino acid)
1	1JXM	201(A)	–	–
		202(A)	ASP579(A)	N1•••OD1 N3•••OD2
2	1KP3	460(A)	ASN210(A)	N1•••OD1 N2•••OD1
			SER211(A)	N1•••OG
		461(A)	ASP399(A)	N2•••OD1 N3•••OD2
3	2ZFZ	400(E)	–	–
		400(A)	ASN168(A)	N1•••OD1 N3•••OD1
4	3EQY	301(B)	GLU45(B)	N3•••OE2
		302(A)	GLU45(A)	N3•••OE2
5	3GNU	215(P)	SER58(P)	N2•••OG
		214(P)	HIS128(P)	N3•••ND1
6	3LAS	169(B)	ASP68(B)	N1•••O
		170(A)	GLU164(B)	N2•••OE1 N3•••OE2
			ASP7(A)	N1•••OD2 N2•••OD1
7	4F8O	202(A)	ASP47(A)	N2•••O
			LYS49(a)	N1•••O N2•••O
		203(A)	–	–
8	4GLL	801(A)	THR288(A)	N3••• O
			ASP356(A)	N1•••OD1 N2•••OD2
		502(B)	THR288(B)	N1•••O
			ASP356(B)	N2•••OD2 N3•••OD1
9	4N7H	502(A)	–	–
		501(A)	THR446(A)	N3•••OG1
			THR447(A)	N3•••O
			ASP441(A)	N2•••OD2
10	4PXJ	501(B)	–	–
		502(B)	–	–
11	6C1K	2305(B)	–	–
		1301(A)	ARG1099(A)	N2••• O
			GLU1032(A)	N1••• OE1

12	6P3L	202(A)	GLU43(A)	N1•••OE1 N2•••OE2
		203(A)	ASP95(A)	N2•••OD1 N3•••OD2
13	6P44	204(A)	GLU43(A)	N1•••OE2 N3•••OE1
		205(A)	ASP95(A)	N3•••OD1 N3•••OD2
14	6Y16	301(A)	GLU23(A)	N3•••OE2
			ASP18(A)	N1•••OD1
			SER16(A)	N3•••O
			SER74(A)	N2•••O
		201(B)	GLU23(B)	N1•••OE2
			ASP18(B)	N2•••OD1
			SER16(B)	N1•••O
			SER74(B)	N1•••O N3•••O

Table S7. Summary of Gdm^+–protein hydrogen bonding interactions in the X-ray crystal structures containing three Gdm^+.

S. No.	PDB Code	Gdm^+	Interacting amino acid	Heavy atoms involved in interaction (Gdm^+•••Amino acid)
1	3M6Z	388(A)	–	–
		386(B)	VAL10(A)	N1•••O
			GLU169(B)	N1•••OE1 N3•••OE2
		389(A)	ASP160(A)	N3•••O
			VAL162(A)	N1•••O N3•••O
2	4ITC	1203(A)	AASN1054(A)	N1•••OD1 N3•••OD1
		1204(A)	ASP1139(A)	N3•••O
		1206(A)	THR999(A)	N1•••OG1
			PRO994(A)	N2•••O
			TRP997(A)	N1•••O
			ILE993(A)	N2•••O
3	5G2B	1004(B)	–	–
		1008(A)	GLU696(A)	N2•••OE1 N3•••OE1
		1007(A)	LEU753(A)	N3•••O
			ASP759(A)	N2•••OD2
			ASP762(A)	N2•••OD1
4	5GWB	208(A)	THR43(A)	N3•••OG1
		206(A)	ILE124(A)	N1•••O
			CYS127(A)	N1•••O N3•••O
		207(A)	GLN57(A)	N1•••O
5	6QGP	1003(B)	–	–
		1007(A)	GLU696(A)	N2•••OE1 N3•••OE1
		1006(A)	LEU753(A)	N1•••O
			ASP759(A)	N3•••OD2
			ASP762(A)	N3•••OD1
6	6QGU	1003(B)	–	–
		1007(A)	GLU696(A)	N2•••OE1 N3•••OE1
		1006(A)	LEU753(A)	N1•••O
			ASP759(A)	N3•••OD2
			ASP762(A)	N3•••OD1
7	6UW2	503(F)	–	–
		503(B)	–	–

		503(C)	–	–

Table S8. Summary of Gdm^+–protein hydrogen bonding interactions in the X-ray crystal structures containing four Gdm^+.

S. No.	PDB Code	Gdm^+	Interacting amino acid	Heavy atoms involved in interaction (Gdm^+•••Amino acid)
1	1RBW	131(A)	–	–
		132(A)	–	–
		135(A)	–	–
		133(A)	TYR76(A)	N3•••OH
2	1UMJ	1001(A)	ASP86(A)	N1•••OD2
		1003(B)	ASP86(B)	N1•••OD1
		1002(A)	ASP84(A)	N1•••O
			ASP86(A)	N1•••OD2
		1004(B)	ASP84(B)	N2•••O
			ASP86(B)	N2•••OD2
3	3MV1	2001(1)	–	–
		2001(2)	GLU797(2)	N1•••OE2
		2001(3)	VAL795(3)	N3•••O
		2001(4)	GLU797(4)	N2•••OE2
			VAL795(4)	N1•••O
4	3U4F	372(A)	GLU209(A)	N3•••OE2
			GLU311(A)	N1•••OE2
			GLU235(A)	N3•••OE1
		372(B)	GLU209(B)	N2•••OE2
			GLU311(B)	N1•••OE2
			GLU235(B)	N2•••OE1
		372(C)	GLU311(C)	N1•••OE2
			GLU209(C)	N2•••OE2
			GLU235(C)	N2•••OE1
		372(D)	GLU209(D)	N2•••OE2
			GLU311(D)	N1•••OE2
			GLU235(D)	N2•••OE1
5	4LYP	502(A)	LYS10(A)	N2•••O
		502(B)	ASP171(B)	N1•••OD1 N3•••OD1
		501(A)	GLU202(A)	N1•••OE2 N2•••OE1
		501(B)	GLU202(B)	N2•••OE1
6	6FDX	1003(B)	–	–
		1007(A)	ASP762(A)	N2•••OD1
		1008(A)	SER798(A)	N1•••O
		1007(B)	TYR691(B)	N1•••OH N3•••OH
7	6RFN	1006(A)	–	–

		1003(B)	–	–
		1005(A)	LEU915(A)	N3•••O
		1007(A)	GLU696(A)	N1•••OE1 N2•••OE1
8	6RFW	1004(A)	–	–
		1004(B)	–	–
		1001(B)	TYR686(B)	N2•••O
		1006(A)	LEU753(A)	N1•••O
			ASP759(A)	N2•••OD2
			ASP762(A)	N2•••OD1
9	7LOX	404(A)	–	–
		403(A)	ASP153(A)	N1•••OD2 N3•••OD1
			ASP232(A)	N2•••OD2
			ASP230(A)	N1•••OD2 N2•••OD2
		403(B)	THR244(B)	N2•••OG1
			HIS126(B)	N3•••ND1
			HIS163(B)	N1•••ND1
			ASP232(B)	N2•••OD2
			ASP153(B)	N3•••OD2
			ASP230(B)	N3•••OD2 N2•••OD2
		403(C)	HIS151(C)	N1•••ND1
			HIS163(C)	N2•••O
			ASP232(C)	N1•••OD2
			ASP230(C)	N3•••OD2 N1•••OD2

Table S9. Summary of Gdm^+–protein hydrogen–bonding interactions in the X–ray crystal structures containing five Gdm^+.

S. No.	PDB Code	Gdm^+	Interacting amino acid	Heavy atoms involved in interaction (Gdm^+•••Amino acid)
1	4D50	405(A)	–	–
		404(B)	–	–
		407(A)	–	–
		404(A)	ASP278(A)	N1•••OD1 N3•••OD1
		406(A)	THR233(A)	N3•••O
2	6A4N	207(A)	–	–
		206(A)	–	–
		203(A)	GLN57(A)	N1•••O
		204(A)	CYS127(A)	N1•••O N3•••O
		205(A)	ASP52(A)	N3•••OD2
			ASN46(A)	N2•••OD1 N3•••OD1
3	6GXQ	1005(B)	–	–
		1001(B)	TYR686(B)	N2•••O
		1006(A)	GLU692(A)	N3•••OE1
		1003(A)	GLU768(A)	N1•••OE1 N3•••OE2
		1004(A)	LEU753(A)	N1•••O
			ASP762(A)	N3•••OD1
			ASP759(A)	N3•••OD2
4	6RGK	1007(A)	–	–
		1005(B)	–	–
		1006(A)	GLU696(A)	N3•••OE1
		1006(B)	GLU696(B)	N1•••OE1 N2•••OE1
		1005(A)	LEU753(A)	N1•••O
			ASP759(A)	N3•••OD2
			ASP762(A)	N3•••OD1

Table S10. Summary of Gdm^+:protein hydrogen–bonding interactions in the X-ray crystal structures containing six Gdm^+.

S. No.	PDB Code	Gdm^+	Interacting amino acid	Heavy atoms involved in interaction (Gdm^+•••Amino acid)
1	2CEV	1001(A)	ASP199(B)	N2•••OD2 N3•••OD2
			GLU256(A)	N1•••OE2 N2•••OE1
		1003(A)	ASP199(A)	N2•••OD2 N3•••OD2
			GLU256(C)	N1•••OE2 N2•••OE1
		1002(B)	ASP199(C)	N2•••OD2 N3•••OD2
			GLU256(B)	N1•••OE2 N2•••OE1
		1004(D)	ASP199(E)	N2•••OD2 N3•••OD2
			GLU256(D)	N1•••OE2 N2•••OE1
		1005(E)	ASP199(F)	N2•••OD2 N3•••OD2
			GLU256(E)	N1•••OE2 N2•••OE1
		1006(F)	ASP199(D)	N2•••OD2 N3•••OD2
			GLU256(F)	N1•••OE2 N2•••OE1
2	2EF5	1001(A)	GLU248(A)	N1•••OE1 N3•••OE2
		1002(D)	GLU248(D)	N1•••OE1 N3•••OE2
		1003(E)	GLU248(E)	N1•••OE1 N3•••OE2
		1005(G)	GLU248(G)	N1•••OE1 N3•••OE2
		1004(A)	GLU248(F)	N1•••OE1 N3•••OE2
			ASP193(A)	N1•••OD2 N2•••OD2
		1006(B)	GLU248(B)	N1•••OE1 N3•••OE2
			ASP193(E)	N1•••OD2

				N2•••OD2
3	4CEV	407(A)	ASP199(B)	N2•••OD2 N3•••OD2
			GLU256(A)	N1•••OE1 N1•••OE2 N2•••OE1
		408(B)	ASP199(C)	N2•••OD2 N3•••OD2
			GLU256(B)	N1•••OE2 N2•••OE1
		409(C)	ASP199(A)	N2•••OD2 N3•••OD2
			GLU256(C)	N1•••OE2 N2•••OE1
		410(D)	ASP199(E)	N2•••OD2 N3•••OD2
			GLU256(D)	N1•••OE2 N2•••OE1
		411(F)	ASP199(F)	N2•••OD2 N3•••OD2
			GLU256(E)	N2•••OE1
		412(F)	GLU256(F)	N2•••OE1
4	5CEV	407(B)	ASP199(B)	N2•••OD2 N3•••OD2
			GLU256(A)	N1•••OE2 N2•••OE1
		408(B)	ASP199(C)	N2•••OD2 N3•••OD2
			GLU256(B)	N1•••OE2 N2•••OE1
		409(C)	ASP199(A)	N2•••OD2 N3•••OD2
			GLU256(C)	N1•••OE2 N2•••OE1
		412(D)	ASP199(D)	N2•••OD2 N3•••OD2
			GLU256(F)	N1•••OE2 N2•••OE1
		410(E)	ASP199(E)	N2•••OD2 N3•••OD2
			GLU256(D)	N1•••OE2 N2•••OE1
		411(E)	ASP199(F)	N2•••OD2 N3•••OD2
			GLU256(E)	N1•••OE1 N1•••OE2

				N2•••OE1
5	6A4O	204(A)	–	–
		206(A)	–	–
		205(A)	SER72(A)	N1•••O N2•••O
		201(A)	GLN57(A)	N1•••O
		202(A)	CYS127(A)	N1•••O N3•••O
		203(A)	ASN46(A)	N2•••OD1 N3•••OD1
6	6FDS	1004(A)	–	–
		1005(B)	–	–
		1007(A)	SER726(A)	N1•••OG
		1003(A)	SER798(A)	N3•••O
			ASP801(A)	N1•••O
		1004(B)	LEU764(B)	N2•••O
			ASP762(B)	N3•••OD1 N3•••O
		1001(A)	LEU764(A)	N2•••O
			ASP762(A)	N3•••OD1 N3•••O

Table S11. Summary of Gdm^+:–hydrogen bonding interactions in the X-ray crystal structures containing seven Gdm^+.

S. No.	PDB Code	Gdm^+	Interacting amino acid	Heavy atoms involved in interaction (Gdm^+•••Amino acid)
1	4AM8	403(A)	SER51(A)	N2•••O
			GLN50(A)	N3•••OE1
		403(C)	SER51(C)	N2•••O
			GLN50(C)	N2•••OE1
		402(D)	SER51(D)	N1•••O
			GLN50(D)	N3•••OE1
		403(E)	SER51(E)	N1•••O N2•••O
			GLN50(E)	N2•••OE1
		403(B)	GLN50(B)	N1•••OE1
			SER51(B)	N1•••O
		403(D)	GLU84(D)	N1•••OE2
		403(F)	GLN50(F)	N1•••OE1
			SER51(F)	N1•••O N2•••O
2	4KWF	603(B)	PRO158(B)	N3•••O
		602(D)	PRO158(D)	N3•••O
		603(F)	PRO158(F)	N1•••O
		604(H)	GLU157(H)	N2•••OE1
		605(A)	GLU157(A)	N3•••OE1
			PRO158(A)	N2•••O
		604(C)	PRO158(C)	N1•••O N2•••O
		602(G)	PRO158(G)	N1•••O N2•••O
3	4KWG	604(B)	PRO158(B)	N3•••O
			GLU157(B)	N3•••OE1
		604(H)	PRO158(H)	N2•••O
		605(A)	PRO158(A)	N2•••O N3•••O
		602(C)	PRO158(C)	N1•••O N2•••O
		602(D)	GLU157(D)	N2•••OE1
			PRO158(D)	N2•••O N3•••O
		604(F)	VAL159(F)	N2•••O
			GLU157(F)	N1•••OE1
			PRO158(F)	N1•••O N2•••O

		602(G)	PRO158(G)	N1•••O N2•••O
4	5G57	1930(A)	–	–
		1921(B)	–	–
		1928(B)	GLY638(B)	N2•••O
		1929(A)	ALA799(A)	N3•••O
			SER798(A)	N2•••O
		1926(B)	ASP712(B)	N3•••OD2
		1928(A)	LEU753(A)	N3•••O
			ASP759(A)	N2•••OD2
			ASP762(A)	N2•••OD1
		1927(B)	LEU764(B)	N3•••O
			ASP762(B)	N3•••O N2•••OD1 N3•••OD1
5	6FE3	1007(B)	–	–
		1002(A)	–	–
		1010(A)	GLU815(A)	N1•••OE2
		1011(A)	GLU768(A)	N1•••OE1 N2•••OE2
		1012(A)	GLU692(A)	N3•••OE1
		1001(A)	LEU753(A)	N1•••O
			ASP759(A)	N3•••OD2
			ASP762(A)	N3•••OD1
		1006(B)	LEU764(B)	N2•••O
			ASP762(B)	N2•••O N1•••OD1 N2•••OD1
6	6FRD	1008(A)	–	–
		1004(A)	–	–
		1003(A)	GLY688(A)	N2•••O
		1005(A)	SER639(A)	N3•••O
			TYR686(A)	N2•••OH
		1004(B)	GLU696(B)	N1•••OE1
		1004(A)	SER754(A)	N2•••O
			ASP759(A)	N1•••OD2
			ASP762(A)	N1•••OD1
		1005(B)	SER754(B)	N1•••O
			ASP762(B)	N2•••OD1

Table S12. Summary of Gdm^+–protein hydrogen bonding interactions in the X-ray crystal structures containing eight Gdm^+.

S. No.	PDB Code	Gdm^+	Interacting amino acid	Heavy atoms involved in interaction (Gdm^+•••Amino acid)
1	1ZUM	3108(L)	ASP147(K)	N1•••O
			PHE459(L)	N2•••O N3•••O
		3101(A)	PHE459(B)	N2•••O N3•••O
			ASP147(A)	N1•••O N3•••O
		3102(E)	PHE459(F)	N2•••O N3•••O
			ASP147(E)	N1•••O N3•••O
		3104(F)	PHE459(E)	N2•••O N3•••O
			ASP147(F)	N1•••O N3•••O
		3105(G)	PHE459(H)	N2•••O N3•••O
			ASP147(G)	N1•••O N3•••O
		3106(H)	PHE459(G)	N2•••O N3•••O
			ASP147(H)	N1•••O N3•••O
		3107(I)	PHE459(J)	N2•••O N3•••O
			ASP147(I)	N1•••O N3•••O
		3103(F)	GLU157(F)	N3•••OE1
			PRO158(F)	N2•••O N3•••O
2	2DDZ	505(B)	–	–
		509(F)	–	–
		510(A)	–	–
		511(E)	–	–
		514(A)	–	–
		512(C)	–	–
		513(D)	–	–
		508(E)	TRP188(E)	N1•••O
3	5SZD	105(A)	–	–

		105(H)	–	–
		104(G)	–	–
		103(B)	–	–
		104(A)	ASN29(A)	N2•••O
			TYR6(J)	N2•••OH
		103(C)	ASN29(C)	N2•••O
			TYR6(L)	N2•••OH
		103(E)	ASN29(E)	N1•••O
			TYR6(H)	N1•••OH
		103(F)	ASN29(F)	N3•••O
			TYR6(I)	N3•••OH
4	1O01	4801(A)	PRO158(A)	N2•••O N3•••O
			GLU157(A)	N3•••OE1
		4802(B)	GLU157(B)	N3•••OE1
			PRO158(B)	N1•••O N3•••O
		4803(C)	GLU157(C)	N2•••OE1
			PRO158(C)	N1•••O N2•••O
		4804(D)	GLU157(D)	N2•••OE1
			PRO158(D)	N2•••O N3•••O
		4805(E)	GLU157(E)	N1•••OE1
			PRO158(E)	N1•••O N3•••O
		4806(F)	GLU157(F)	N1•••OE1
			PRO158(F)	N1•••O N2•••O
		4807(G)	GLU157(G)	N2•••OE1
			PRO158(G)	N1•••O N2•••O
		4808(H)	GLU157(H)	N2•••OE1
			PRO158(H)	N2•••O N3•••O

Table S13. Summary of Gdm^+–protein hydrogen bonding interactions in the X-ray crystal structures containing nine Gdm^+.

S. No.	PDB Code	Gdm^+	Interacting amino acid	Heavy atoms involved in interaction (Gdm^+•••Amino acid)
1	2ONM	906(E)	–	–
		910(I)	–	–
		906(E)	–	–
		905(D)	–	–
		902(A)	–	–
		909(H)	–	–
		611(J)	–	–
		907(E)	–	–
		5009(G)	–	–
2	3INJ	801(A)	GLU157(A)	N3•••OE1
			PRO158(A)	N2•••O N3•••O
		801(B)	VAL159(B)	N1•••O
			GLU157(B)	N3•••OE1
			PRO158(B)	N1•••O N3•••O
		801(C)	GLU157(C)	N2•••OE1
			PRO158(C)	N1•••O N2•••O
		801(D)	GLU157(D)	N2•••OE1
			PRO158(D)	N2•••O N3•••O
		801(E)	PRO158(E)	N1•••O N3•••O
		801(F)	GLU157(F)	N1•••OE1
			PRO158(F)	N1•••O N2•••O
		801(G)	GLU157(G)	N2•••OE1
			PRO158(G)	N1•••O N2•••O
		801(H)	PRO158(A)	N2•••O N3•••O
		802(G)	ALA326(G)	N1•••O
			ARG329(G)	N1•••O N2•••O

Table S14. Summary of Gdm^+–protein hydrogen bonding interactions in the X-ray crystal structures containing ten Gdm^+.

S. No.	PDB Code	Gdm^+	Interacting amino acid	Heavy atoms involved in interaction (Gdm^+•••Amino acid)
1	6A4P	204(A)	–	–
		205(A)	–	–
		207(A)	–	–
		209(A)	–	–
		208(A)	–	–
		210(A)	ARG21(A)	N1•••O
		201(A)	SER72(A)	N1•••O N3•••O
		202(A)	CYS127(A)	N1•••O N2•••O
		206(A)	GLN57(A)	N1•••O
		203(A)	ASN46(A)	N2•••OD1 N3•••OD1
2	6FTM	1017(A)	–	–
		1011(B)	–	–
		1016(A)	–	–
		1018(A)	–	–
		1019(A)	–	–
		1020(A)	GLU815(A)	N2•••OE1
		1011(B)	LEU915(B)	N2•••O
		1022(A)	MET861(A)	N3•••O
		1015(A)	ASP712(A)	N2•••O
		1021(A)	ASP778(A)	N2•••OD1

Table S15. Summary of Gdm^+–protein hydrogen bonding interactions in the X-ray crystal structures containing eleven Gdm^+.

S. No.	PDB Code	Gdm^+	Interacting amino acid	Heavy atoms involved in interaction (Gdm^+•••Amino acid)
1	5G5V	1931(A)	–	–
		1935(A)	–	–
		1922(B)	–	–
		1923(B)	–	–
		1928(B)	–	–
		1921(B)	–	–
		1920(A)	ASP712(A)	N1•••O
		1921(A)	SER604(A)	N1•••O
		1922(A)	GLN847(A)	N2•••OE1
		1934(A)	LEU694(A)	N1•••O
		1927(B)	LEU915(B)	N1•••O N2•••O

Table S16. Summary of Gdm^+–protein hydrogen-bonding interactions in the X-ray crystal structures containing twelve Gdm^+.

S. No.	PDB Code	Gdm^+	Interacting amino acid	Heavy atoms involved in interaction (Gdm^+•••Amino acid)
1	6A4Q	204(A)	–	–
		205(A)	–	–
		206(A)	–	–
		211(A)	–	–
		204(A)	–	–
		212(A)	–	–
		209(A)	CYS127(A)	N1•••O N2•••O
		213(A)	ARG45(A)	N2•••O
			ASN46(A)	N2•••OD1 N3•••OD1
		208(A)	ASP101(A)	N1•••OD2
		214(A)	ASP119(A)	N1•••OD1
		207(A)	SER72(A)	N1•••O N3•••O
		203(A)	GLN57(A)	N1•••O
2	6RB6	1003(A)	–	–
		1005(A)	–	–
		1007(A)	–	–
		1005(B)	–	–
		1006(A)	–	–
		1001(B)	–	–
		1006(B)	ASP712(B)	N1•••O
		1014(B)	GLU815(B)	N2•••OE1
		1008(A)	ASP712(A)	N2•••O
		1009(A)	SER639(A)	N1•••O
			GLU696(A)	N1•••OE2
		1013(B)	ASP649(B)	N2•••OD1 N3•••OD2
		1004(A)	LEU753(A)	N1•••O
			ASP759(A)	N3•••OD2
			ASP762(A)	N3•••OD1

Table S17. Summary of Gdm^+–protein hydrogen bonding interactions in the X-ray crystal structures containing thirteen Gdm^+.

S. No.	PDB Code	Gdm^+	Interacting amino acid	Heavy atoms involved in interaction (Gdm^+•••Amino acid)
1	3N82	814(D)	ASP147(D)	N3•••O
			PHE459(C)	N1•••O
		812(B)	ASP147(B)	N3•••O
		826(F)	GLY378(F)	N1•••O
		807(G)	PRO158(G)	N2•••O
			GLU157(G)	N2•••OE1
		817(G)	PHE459(H)	N1•••O
			ASP147(G)	N1•••O N2•••O
		801(A)	GLU157(A)	N3•••OE1
			VAL159(A)	N2•••O
			PRO158(A)	N2•••O N3•••O
		802(B)	GLU157(B)	N3•••OE1
			PRO158(B)	N1•••O N3•••O
		803(C)	GLU157(C)	N2•••OE1
			PRO158(C)	N1•••O N2•••O
		804(D)	GLU157(D)	N2•••OE1
			PRO158(D)	N2•••O N3•••O
		805(E)	GLU157(E)	N1•••OE1
			PRO158(E)	N1•••O N3•••O
		806(F)	GLU157(F)	N1•••OE1
			PRO158(F)	N1•••O N2•••O
		808(H)	GLU157(H)	N2•••OE1
			VAL159(H)	N3•••O
			PRO158(H)	N2•••O N3•••O
		815(E)	ASP147(E)	N3•••O
			PHE459(F)	N2•••O N3•••O

Table S18. Summary of Gdm^+–protein hydrogen bonding interactions in the X-ray crystal structures containing sixteen Gdm^+.

S. No.	PDB Code	Gdm^+	Interacting amino acid	Heavy atoms involved in interaction (Gdm^+•••Amino acid)
1	1O02	4603(A)	GLU157(A)	N3•••OE1
			PRO158(A)	N2•••O N3•••O
		603(B)	GLU157(B)	N3•••OE1
			PRO158(B)	N1•••O N3•••O
		603(C)	GLU157(C)	N2•••OE1
			PRO158(C)	N1•••O N2•••O
		603(D)	GLU157(D)	N2•••OE1
			PRO158(D)	N2•••O N3•••O
		603(E)	VAL159(E)	N3•••O
			GLU157(E)	N1•••OE1
			PRO158(E)	N1•••O N3•••O
		603(F)	GLU157(F)	N1•••OE1
			PRO158(F)	N1•••O N2•••O
		603(G)	GLU157(G)	N2•••OE1
			PRO158(G)	N1•••O N2•••O
		603(H)	GLU157(H)	N2•••OE1
			PRO158(H)	N2•••O N3•••O
		4604(A)	PHE459(B)	N2•••O N3•••O
			ASP147(A)	N1•••O N3•••O
		604(B)	PHE459(A)	N1•••O N3•••O
			ASP147(B)	N2•••O N3•••O
		604(C)	PHE459(D)	N1•••O N3•••O
			ASP147(C)	N1•••O N2•••O
		604(D)	PHE459(C)	N1•••O N3•••O

			ASP147(D)	N2•••O N3•••O
		604(E)	PHE459(F)	N2•••O N3•••O
			ASP147(E)	N1•••O N3•••O
		604(F)	PHE459(E)	N1•••O N2•••O
			ASP147(F)	N1•••O N3•••O
		604(G)	PHE459(H)	N1•••O N3•••O
			ASP147(G)	N1•••O N2•••O
		605(G)	PHE459(G)	N2•••O N3•••O
			ASP147(H)	N1•••O N2•••O
2		817(G)	PHE459(H)	N1•••O
			ASP147(G)	N1•••O N2•••O
		826(F)	GLY378(F)	N1•••O N3•••O
		833(D)	ARG329(D)	N1•••O N2•••O
		838(G)	ARG329(G)	N1•••O N2•••O
		801(A)	GLU157(A)	N3•••OE1
			PRO158(A)	N2•••O N3•••O
		802(B)	GLU157(B)	N3•••OE1
			PRO158(B)	N1•••O N3•••O
		803(C)	GLU157(C)	N2•••OE1
			PRO158(C)	N1•••O N2•••O
		804(D)	GLU157(D)	N2•••OE1
			PRO158(D)	N2•••O N3•••O
		805(E)	GLU157(E)	N1•••OE1
			PRO158(E)	N1•••O N3•••O
		806(F)	GLU157(F)	N1•••OE1
			PRO158(F)	N1•••O N2•••O

		807(G)	VAL159(G)	N1•••O
			GLU157(G)	N2•••OE1
			PRO158(G)	N1•••O N2•••O
		808(H)	VAL159(H)	N3•••O
			GLU157(H)	N2•••OE1
			PRO158(H)	N2•••O N3•••O
		812(B)	ASP147(B)	N2•••O N3•••O
			PHE459(A)	N1•••O N3•••O
		814(D)	ASP147(D)	N2•••O N3•••O
			PHE459(C)	N1•••O N3•••O
		815(E)	ASP147(E)	N1•••O
			PHE459(F)	N2•••O N3•••O
		816(F)	ASP147(F)	N1•••O N3•••O
			PHE459(E)	N1•••O N2•••O
3		606(E)	–	–
		605(D)	–	–
		607(G)	TYR203(G)	N1•••OH
		602(C)	PRO158(C)	N2•••O
		604(E)	VAL159(E)	N1•••O
			PRO158(E)	N3•••O
		605(G)	VAL159(G)	N3•••O
			PRO158(G)	N2•••O
			GLU157(G)	N2•••OE1
	5L13	605(A)	ASP147(B)	N2•••O
			PHE459(A)	N1•••O N3•••O
		603(D)	PHE459(C)	N1•••O
			ASP147(D)	N1•••O N3•••O
		606(D)	ASP147(C)	N3•••O
			PHE459(D)	N2•••O N3•••O
		604(A)	VAL159(A)	N1•••O
			PRO158(A)	N1•••O N3•••O
		604(B)	GLU157(B)	N3•••OE1

			PRO158(B)	N2•••O N3•••O
		604(D)	PRO158(D)	N1•••O N3•••O
		604(F)	VAL159(F)	N2•••O
			PRO158(F)	N2•••O N3•••O
		602(H)	PRO158(H)	N1•••O N3•••O
		605(E)	ASP147(E)	N2•••O N3•••O
			PHE459(F)	N1•••O N3•••O
		606(G)	PHE459(H)	N2•••O N3•••O
			ASP147(G)	N1•••O N2•••O

Table S19. Summary of Gdm^+–protein hydrogen bonding interactions in the X-ray crystal structures containing seventeen Gdm^+.

S. No.	PDB Code	Gdm^+	Interacting amino acid	Heavy atoms involved in interaction (Gdm^+•••Amino acid)
1	2PNL	2001(C)	–	–
		2015(E)	–	–
		2010(D)	–	–
		2014(C)	–	–
		2016(H)	–	–
		2007(E)	–	–
		2013(J)	–	–
		2002(A)	–	–
		2009(B)	–	–
		2006(C)	–	–
		2011(F)	–	–
		2008(H)	–	–
		2012(I)	–	–
		2004(B)	LEU610(B)	N1•••O
			GLU622(B)	N2•••OE2
		2005(A)	ASP644(A)	N1•••OD2 N3•••OD1
		2003(B)	ASN616(B)	N2•••O
			ASN618(B)	N2•••OD1
		2017(H)	CYS669(I)	N2•••O
			ALA716(H)	N2•••O N1•••OXT N2•••OXT

Table S20. Summary of Gdm^+–protein hydrogen bonding interactions in the X-ray crystal structures containing eighteen Gdm^+.

S. No.	PDB Code	Gdm^+	Interacting amino acid	Heavy atoms involved in interaction (Gdm^+•••Amino acid)
1	1O04	6801(A)	VAL159(A)	N2•••O
			GLU157(A)	N3•••OE1
			PRO158(A)	N2•••O N3•••O
		6802(B)	GLU157(B)	N3•••OE1
			PRO158(B)	N1•••O N3•••O
		6803(C)	GLU157(C)	N2•••OE1
			PRO158(C)	N1•••O N2•••O
		6804(D)	GLU157(D)	N2•••OE1
			PRO158(D)	N2•••O N3•••O
		6805(E)	GLU157(E)	N1•••OE1
			PRO158(E)	N1•••O N3•••O
		6806(F)	GLU157(F)	N1•••OE1
			PRO158(F)	N1•••O N2•••O
		6807(G)	GLU157(G)	N2•••OE1
			PRO158(G)	N1•••O N2•••O
		6808(H)	GLU157(H)	N2•••OE1
			PRO158(H)	N2•••O N3•••O
		6811(A)	PHE459(B)	N2•••O N3•••O
			ASP147(A)	N1•••O N3•••O
		6812(B)	PHE459(C)	N2•••O N3•••O
			ASP147(B)	N1•••O N3•••O
		6813(C)	PHE459(D)	N1•••O N3•••O
			ASP147(C)	N1•••O N2•••O
		6814(D)	PHE459(C)	N1•••O N3•••O

			ASP147(D)	N2•••O N3•••O
		6815(E)	PHE459(F)	N2•••O N3•••O
			ASP147(E)	N1•••O N3•••O
		6816(F)	PHE459(E)	N1•••O N2•••O
			ASP147(F)	N1•••O N3•••O
		6817(G)	PHE459(H)	N1•••O N3•••O
			ASP147(G)	N1•••O N2•••O
		6818(H)	PHE459(G)	N2•••O N3•••O
			ASP147(H)	N1•••O N2•••O
		6823(C)	ALA375(C)	N1•••O
			ASP376(C)	N1•••O
		6826(F)	GLY378(F)	N3•••O
			ALA375(F)	N1•••O
			ASP376(F)	N3•••O
2	3SZ9	6821(C)	GLY378(C)	N1•••O N2•••O
		6821(F)	GLY378(F)	N1•••O N3•••O
		6801(A)	GLU157(A)	N3•••OE1
			PRO158(A)	N2•••O N3•••O
		6801(B)	GLU157(B)	N3•••OE1
			PRO158(B)	N1•••O N3•••O
		6801(C)	GLU157(C)	N2•••OE1
			PRO158(C)	N1•••O N2•••O
		6801(D)	GLU157(D)	N2•••OE1
			PRO158(D)	N2•••O N3•••O
		6801(E)	GLU157(E)	N1•••OE1
			PRO158(E)	N1•••O N3•••O
		6801(F)	GLU157(F)	N1•••OE1
			PRO158(F)	N1•••O N2•••O

		6801(G)	GLU157(G)	N2•••OE1
			PRO158(G)	N1•••O N2•••O
		6801(H)	GLU157(H)	N2•••OE1
			PRO158(H)	N2•••O N3•••O
		6811(A)	ASP147(A)	N1•••O N3•••O
			PHE459(B)	N2•••O N3•••O
		6811(B)	ASP147(B)	N2•••O N3•••O
			PHE459(A)	N1•••O N3•••O
		6811(C)	ASP147(C)	N1•••O N2•••O
			PHE459(D)	N1•••O N3•••O
		502(C)	ASP147(D)	N2•••O N3•••O
			PHE459(C)	N1•••O N3•••O
		6811(E)	ASP147(F)	N1•••O N2•••O
			PHE459(E)	N1•••O N3•••O
		6811(F)	ASP147(E)	N3•••O
			PHE459(F)	N2•••O N3•••O
		6811(G)	ASP147(G)	N1•••O N2•••O
			PHE459(H)	N1•••O N3•••O
		6811(H)	ASP147(H)	N1•••O N2•••O
			PHE459(G)	N2•••O N3•••O

Table S21. Summary of Gdm^+–protein hydrogen bonding interactions in the X-ray crystal structures containing twenty-one Gdm^+.

S. No.	PDB Code	Gdm^+	Interacting amino acid	Heavy atoms involved in interaction (Gdm^+•••Amino acid)
1	3N80	833(D)	PRO15(D)	N1•••O N2•••O
		801(A)	GLU157(A)	N2•••OE1
			PRO158(A)	N2•••O N3•••O
		803(C)	GLU157(C)	N2•••OE1
			PRO158(C)	N1•••O N2•••O
		804(D)	GLU157(D)	N2•••OE1
			PRO158(D)	N2•••O N3•••O
		805(E)	GLU157(E)	N1•••OE1
			PRO158(E)	N1•••O N3•••O
		806(F)	GLU157(F)	N1•••OE1
			PRO158(F)	N1•••O N2•••O
		807(G)	GLU157(G)	N2•••OE1
			PRO158(G)	N1•••O N2•••O
		808(H)	GLU157(H)	N2•••OE1
			PRO158(H)	N2•••O N3•••O
		811(A)	ASP147(A)	N1•••O N3•••O
			PHE459(B)	N2•••O N3•••O
		812(B)	ASP147(B)	N2•••O N3•••O
			PHE459(A)	N1•••O N3•••O
		813(C)	ASP147(C)	N1•••O N2•••O
			PHE459(D)	N1•••O N3•••O
		814(D)	ASP147(D)	N2•••O N3•••O
			PHE459(C)	N1•••O N3•••O
		815(E)	ASP147(E)	N1•••O

				N3•••O
			PHE459(F)	N2•••O N3•••O
		816(F)	ASP147(F)	N1•••O N3•••O
			PHE459(E)	N1•••O N2•••O
		817(G)	ASP147(G)	N1•••O N2•••O
			PHE459(H)	N1•••O N3•••O
		818(H)	ASP147(H)	N1•••O N2•••O
			PHE459(G)	N2•••O N3•••O
		823(C)	ALA375(C)	N1•••O
			ASP376(C)	N1•••O N2•••O
		826(F)	ALA375(F)	N1•••O
			ASP376(F)	N3•••O
		839(F)	ALA326(F)	N2•••O
			ARG329(F)	N2•••O N3•••O
		838(G)	ALA326(G)	N1•••O
			ARG329(G)	N1•••O N2•••O
		802(B)	GLU157(B)	N3•••OE1
			PRO158(B)	N1•••O N3•••O
2	3N81	833(D)	PRO15(D)	N1•••O N2•••O
		813(C)	ASP147(C)	N1•••O N2•••O
			PHE459(D)	N3•••O
		823(C)	ASP376(C)	N1•••O N2•••O
		801(A)	GLU157(A)	N3•••OE1
			PRO158(A)	N2•••O N3•••O
		802(B)	GLU157(B)	N3•••OE1
			PRO158(B)	N1•••O N3•••O
		803(C)	GLU157(C)	N2•••OE1
			PRO158(C)	N1•••O N2•••O

		804(D)	GLU157(D)	N2•••OE1
			PRO158(D)	N2•••O N3•••O
		805(E)	GLU157(E)	N1•••OE1
			PRO158(E)	N1•••O N3•••O
		806(F)	GLU157(F)	N1•••OE1
			PRO158(F)	N1•••O N2•••O
		807(G)		
			GLU157(G)	N2•••OE1
			PRO158(G)	N1•••O N2•••O
		808(H)		
			GLU157(H)	N2•••OE1
			PRO158(H)	N2•••O N3•••O
		811(A)	ASP147(A)	N1•••O N3•••O
			PHE459(B)	N2•••O N3•••O
		812(B)	ASP147(B)	N2•••O N3•••O
			PHE459(A)	N1•••O N3•••O
		814(D)	ASP147(D)	N2•••O N3•••O
			PHE459(C)	N1•••O N3•••O
		815(E)	ASP147(E)	N1•••O N3•••O
			PHE459(F)	N2•••O N3•••O
		816(F)	ASP147(F)	N1•••O N3•••O
			PHE459(E)	N1•••O N2•••O
		817(G)	ASP147(G)	N1•••O N2•••O
			PHE459(H)	N1•••O N3•••O
		818(H)	ASP147(H)	N1•••O N2•••O
			PHE459(G)	N2•••O N3•••O

		838(G)	ARG329(G)	N1•••O N2•••O
		826(F)	ALA375(F)	N1•••O
			GLY378(F)	N3•••O
		845(F)	ARG329(F)	N1•••O N3•••O

Table S22. Summary of Gdm^+–protein hydrogen bonding interactions in the X-ray crystal structures containing twenty-eight Gdm^+.

S. No.	PDB Code	Gdm^+	Interacting amino acid	Heavy atoms involved in interaction (Gdm^+•••Amino acid)
1	2ONP	6823(C)	GLY378(C)	N1•••O N3•••O
		6826(F)	GLY378(F)	N3•••O
		6824(D)	ALA375(D)	N1•••O
			GLY378(D)	N3•••O
		6811(A)	ASP147(A)	N1•••O
			PHE459(B)	N1•••O N2•••O
		6813(C)	PHE459(D)	N2•••O
			ASP147(C)	N1•••O N3•••O
		6801(A)	GLU157(A)	N1•••OE1
			VAL159(A)	N2•••O
			PRO158(A)	N1•••O N2•••O
		6802(B)	GLU157(B)	N1•••OE1
			PRO158(B)	N1•••O N2•••O
		6803(C)	GLU157(C)	N1•••OE1
			PRO158(C)	N1•••O N2•••O
		6804(D)	GLU157(D)	N1•••OE1
			VAL159(D)	N2•••O
			PRO158(D)	N1•••O N2•••O
		6805(E)	GLU157(E)	N1•••OE1
			PRO158(E)	N1•••O N2•••O
		6806(F)	GLU157(F)	N1•••OE1
			PRO158(F)	N1•••O N2•••O
		6807(G)	VAL159(G)	N2•••O
			PRO158(G)	N1•••O N2•••O
		6808(H)	GLU157(H)	N1•••OE1
			VAL159(H)	N2•••O
			PRO158(H)	N1•••O N2•••O
		6812(B)	ASP147(B)	N1•••O

				N3•••O
			PHE459(A)	N2•••O
		6814(D)	ASP147(D)	N1•••O N3•••O
			PHE459(C)	N1•••O N2•••O
		6815(E)	ASP147(E)	N1•••O N3•••O
			PHE459(F)	N1•••O N2•••O
		6816(F)	ASP147(F)	N1•••O
			PHE459(E)	N1•••O N2•••O
		6817(G)	ASP147(G)	N1•••O N3•••O
			PHE459(H)	N1•••O N2•••O
		6818(H)	ASP147(H)	N1•••O N3•••O
			PHE459(G)	N1•••O N2•••O
		6821(A)	ALA A 375	N1•••O
			GLY A 378	N1•••O
		6832(A)	GLY467(A)	N3•••O
			GLY472(A)	N2•••O N3•••O
			GLU487(B)	N1•••O N3•••O
		6831(B)	GLY467(B)	N3•••O
			GLY472(B)	N2•••O N3•••O
			GLU487(A)	N1•••OE2
		6834(C)	LYS469(C)	N2•••O
			GLY467(C)	N3•••O
			GLY472(C)	N2•••O
			GLU487(D)	N1•••OE2 N3•••OE1
		6833(D)	GLY467(D)	N3•••O
			GLY472(D)	N3•••O N2•••O
			GLU487(C)	N1•••OE1
		6835(E)	LYS469(F)	N2•••O
			GLY467(F)	N3•••O
			GLY472(F)	N2•••O N3•••O

			GLU487(E)	N1•••OE2 N3•••OE1
		6836(E)	GLY467(E)	N3•••O
			GLY472(E)	N2•••O N3•••O
			GLU487(F)	N1•••OE2 N3•••OE1
		6837(H)	GLY467(H)	N1•••O
			GLY472(H)	N1•••O N3•••O
			GLU487(G)	N1•••OE1 N2•••OE2
		6838(G)	GLY467(G)	N1•••O
			GLY472(G)	N1•••O N3•••O
			GLU487(H)	N1•••OE1 N2•••OE2

Table S23. Frequency distribution of Gdm^+ according to the total number of hydrogen bonding interactions formed by Gdm^+.

# of hydrogen bonding interactions formed by a single Gdm^+	**# of Gdm^+ involved in forming a particular number of hydrogen bonding interactions with protein**	**Total number of hydrogen bonding interactions**
0	109	0
1	64	64
2	90	180
3	125	375
4	93	372
5	8	40
6	1	6
7	1	7
Total	491	1044

Table S24. Distribution of Gdm^+ according to the number of interacting amino acid with each Gdm^+.

Type of Gdm^+	**Number of Gdm^+**
Interacting with a single amino acid	121
Interacting with multiple amino acids	261
Total	382

Table S25: Atom-wise comparison of average B-factors of interacting and non-interacting Gdm+ and unbound[b] state calculated from PDB files.

Atom name	Residue	Average B-factor	
		Interacting	Non-interacting
N1	Gdm^+	32.695	32.922
N2	Gdm^+	33.457	32.730
N3	Gdm^+	33.152	32.549
	Average	33.101	32.734
ND1	His	62.054	84.242
O	Ala	22.202	15.851
O	Arg	26.654	17.245
O	Asn	14.752	21.773
O	Asp	20.586	22.633
O	Cys	19.933	18.819
O	Gln	10.922	14.685
O	Gly	35.269	28.790
O	His	87.770	82.206
O	Ile	18.675	15.178
O	Leu	35.58	34.371
O	Lys	19.078	26.903
O	Met	20.130	30.189
O	Phe	25.705	22.449
O	Pro	17.543	22.184
O	Ser	25.868	31.228
O	Thr	28.948	30.794
O	Trp	28.625	39.245
O	Tyr	50.600	42.317
O	Val	21.764	22.779
OD1	Asn	19.536	25.398
OD1	Asp	38.948	46.059
OD2	Asp	33.271	42.150
OE1	Gln	25.456	28.546
OE1	Glu	23.175	33.902
OE2	Glu	24.739	37.996
OG	Ser	40.790	48.830
OG1	Thr	31.260	59.995
OH	Tyr	24.761	24.588
OXT	Ala	28.960	30.500
	Average	29.452	33.395

Table S26. Distribution of Gdm^+:protein hydrogen bonds in terms of the interacting portion of amino acid residue (main chain or side chain).

Amino acids	Total no. of interactions	Main chain interactions	Side chain interactions
GLY	41	41	0
ALA	15	15	0
SER	31	27	4
THR	8	4	4
CYS	11	11	0
VAL	23	23	0
LEU	23	23	0
ILE	2	2	0
MET	1	1	0
PRO	199	199	0
PHE	131	131	0
TYR	11	2	9
TRP	2	2	0
ASP	274	154	120
GLU	207	0	207
ASN	22	5	17
GLN	12	5	7
HIS	6	1	5
LYS	8	8	0
ARG	17	17	0
Total	1044	671	373

Table S27. Distribution of the Gdm^+:protein hydrogen bonding interactions as a function of the protein type and the identity of the interacting amino acid.

Protein type	# of PDBs	# of hydrogen bonding interactions																			Total
		GLY	ALA	SER	THR	CYS	VAL	LEU	ILE	MET	PRO	PHE	TYR	TRP	ASP	GLU	ASN	GLN	HIS	LYS	ARG	
Binding protein	4	0	0	0	2	0	0	0	0	0	0	0	4	0	1	0	6	0	0	0	0	13
Cell adhesion	3	0	0	0	0	0	0	0	0	0	0	0	0	0	3	0	0	0	0	5	0	8
Chaperone	2	0	0	0	0	0	0	0	0	0	1	0	0	0	1	2	0	0	0	0	0	4
Hydrolases	39	2	5	15	2	11	3	23	1	1	0	2	6	0	102	78	10	6	4	1	2	274
Isomerase	4	0	0	0	0	0	3	0	0	0	0	0	0	0	5	18	0	0	0	0	0	26
Ligase	3	0	0	2	0	0	0	0	0	0	0	0	0	0	2	0	4	0	1	0	0	9
Lyase	2	0	0	0	2	0	0	0	0	0	0	0	0	0	7	2	0	0	0	0	0	11
Onco-protein	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	2
Oxido-reductase	18	37	10	0	2	0	16	0	1	0	198	129	1	1	138	99	2	0	0	2	14	650
Structural	3	0	0	0	0	0	0	0	0	0	0	0	0	1	8	0	0	0	0	0	0	9
Toxin	1	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	2
Transferase	3	2	0	8	0	0	1	0	0	0	0	0	0	0	2	3	0	6	0	0	0	22
Transport	3	0	0	5	0	0	0	0	0	0	0	0	0	0	5	3	0	0	0	0	1	14
Total	86	41	15	31	8	11	23	23	2	1	199	131	11	2	274	207	22	12	6	8	17	1044

Table S28. Occurrence of different Gdm^+–amino acid pairs present in the analyzed crystal structures.

S. No.	Motif	Occurrence
1	Gly–Gdm^+	29
2	Ala–Gdm^+	13
3	Ser–Gdm^+	25
4	Thr–Gdm^+	8
5	Cys–Gdm^+	6
6	Val–Gdm^+	22
7	Leu–Gdm^+	21
8	Ile–Gdm^+	2
9	Met–Gdm^+	1
10	Pro–Gdm^+	106
11	Phe–Gdm^+	69
12	Tyr–Gdm^+	10
13	Trp–Gdm^+	2
14	Asp–Gdm^+	168
15	Glu–Gdm^+	163
16	Asn–Gdm^+	14
17	Gln–Gdm^+	12
18	His–Gdm^+	6
19	Lys–Gdm^+	6
20	Arg–Gdm^+	10
Total		693

Table S29. Distribution of the Gdm^+–protein hydrogen bonding interactions as a function of the identity of the interacting amino acid and the number of Gdm^+ present in the crystal structure.

# of Gdm^+	# of PDBs	# of hydrogen bonding interactions																				Total
		GLY	ALA	SER	THR	CYS	VAL	LEU	ILE	MET	PRO	PHE	TYR	TRP	ASP	GLU	ASN	GLN	HIS	LYS	ARG	
1	19	2	1	2	0	0	2	4	0	0	1	2	0	0	10	8	2	0	1	3	0	38
2	14	0	0	7	4	0	0	0	0	0	0	0	0	0	19	11	4	0	1	2	1	49
3	7	0	0	0	2	2	3	3	2	0	1	0	0	1	8	8	2	1	0	0	0	33
4	9	0	0	1	1	0	2	2	0	0	0	0	4	0	23	19	0	0	4	1	0	57
5	4	0	0	0	1	2	0	2	0	0	0	0	1	0	7	6	2	1	0	0	0	22
6	6	0	0	4	0	2	0	2	0	0	0	0	0	0	45	46	2	1	0	0	0	102
7	6	2	1	11	0	0	1	4	0	0	20	0	1	0	14	11	0	6	0	0	0	71
8	4	0	0	0	0	0	0	0	0	0	17	14	4	1	13	9	4	0	0	0	0	62
9	2	0	1	0	0	0	1	0	0	0	16	0	0	0	0	6	0	0	0	0	2	26
10	2	0	0	2	0	2	0	1	0	1	0	0	0	0	2	1	2	1	0	0	1	13
11	1	0	0	1	0	0	0	3	0	0	0	0	0	0	1	0	0	1	0	0	0	6
12	2	0	0	3	0	2	0	1	0	0	0	0	0	0	8	2	2	1	0	0	1	20
13	1	1	0	0	0	0	2	0	0	0	15	4	0	0	5	8	0	0	0	0	0	35
16	3	2	0	0	0	0	7	0	0	0	45	34	1	0	33	18	0	0	0	0	4	144
17	1	0	3	0	0	1	0	1	0	0	0	0	0	0	2	1	2	0	0	0	0	10
18	2	5	2	0	0	0	1	0	0	0	32	32	0	0	33	16	0	0	0	0	0	121
21	2	1	5	0	0	0	0	0	0	0	36	31	0	0	37	16	0	0	0	0	8	134
28	1	28	2	0	0	0	4	0	0	0	16	14	0	0	14	21	0	0	0	2	0	101
Total	86	41	15	31	8	11	23	23	2	1	199	131	11	2	274	207	22	12	6	8	17	1044

Table S30. Frequency of Gdm^+–protein hydrogen bonding interactions involving the main chain acceptor atoms of amino acids.

Amino acids	**# of interactions of main chain atoms**			**Total**
	N	**O**	**OXT**	
GLY	0	41	0	41
ALA	0	13	2	15
SER	0	27	0	27
THR	0	4	0	4
CYS	0	11	0	11
VAL	0	23	0	23
LEU	0	23	0	23
ILE	0	2	0	2
MET	0	1	0	1
PRO	0	199	0	199
PHE	0	131	0	131
TYR	0	2	0	2
TRP	0	2	0	2
ASP	0	154	0	154
GLU	0	0	0	0
ASN	0	5	0	5
GLN	0	5	0	5
HIS	0	1	0	1
LYS	0	8	0	8
ARG	0	17	0	17
Total	0	669	2	671

Table S31. Frequency of Gdm^+–protein hydrogen bonding interactions involving the side chain acceptor atoms of amino acids.

Hydrogen bond type		**Number of contacts**
Amino acids	**Interacting atoms**	**Number of contacts**
SER	OG	4
THR	OG1	4
TYR	OH	9
ASP	OD1	42
	OD2	78
GLU	OE1	150
	OE2	57
ASN	OD1	17
GLN	OE1	7
HIS	ND1	5
Total		373

Table S32. Distribution of Gdm^+–protein hydrogen bonding interactions present in the analyzed crystal structures of Gdm^+:protein complexes in terms of hydrogen-bnding type.

N–H•••O	1039
N–H•••N	5
Total	1044

Table S33. Cartesian coordinates of the ωB97X-D/6-31G(d,p) optimized Leu–Gdm^+ complex (binding energy: –35.9 kcal mol^{-1}).

Energy (Hartrees) = –650.909632			
Atom	X	Y	Z
N	–0.10797700	0.08694200	1.13209900
C	–1.03208800	–0.73394800	0.35328400
C	–0.31089700	–1.85386100	–0.38559300
O	0.90368600	–1.89454100	–0.48319600
C	–1.79091800	0.11862000	–0.68338600
C	–2.61275600	1.28579200	–0.10937200
C	–3.35502700	1.98819600	–1.24940800
C	–3.58695000	0.83176500	0.97984500
H	–0.63494000	0.89003300	1.46494700
H	–1.77037600	–1.22423000	1.01039200
H	–2.47448000	–0.53832900	–1.23363900
H	–1.06788000	0.50595400	–1.41254700
H	–1.92279500	2.02410600	0.32598700
H	–3.89235200	2.86598500	–0.88141700
H	–4.08865900	1.31494100	–1.70579900
H	–2.66709500	2.31775300	–2.03403100
H	–4.20152300	1.66929400	1.31931100
H	–4.26220400	0.05800200	0.59789800
H	–3.07693000	0.42635400	1.86056200
C	3.22254200	0.82849900	–0.25984200
N	4.33101600	1.54675200	–0.49802100
N	2.04741500	1.42602600	–0.10794300
N	3.29152900	–0.49533200	–0.16479600
H	4.32848100	2.54982800	–0.42355000
H	1.22108500	0.89196200	0.25926300
H	2.42642200	–1.04353100	–0.20182200
H	1.95661000	2.41036900	–0.29731100
H	4.17705600	–0.97200200	–0.18737000
H	5.19496200	1.10242500	–0.75937700
C	–1.16415800	–2.90685600	–1.04092500
H	–1.30280300	–2.63746600	–2.09375800
H	–0.64317700	–3.86468300	–1.01207800
H	–2.14995100	–2.99663700	–0.58081400
C	0.44465500	–0.59722600	2.30933100
H	1.09083300	–1.41611600	1.99014700

H	1.04675500	0.11001200	2.88333600
H	–0.33683500	–1.00430700	2.96426000

Table S34. Cartesian coordinates of the ωB97X-D/6-31G(d,p) optimized Leu–Gdm^+ complex (binding energy: –27.1 kcal mol^{-1}).

Energy (Hartrees) = –650.900870			
Atom	X	Y	Z
N	2.32418700	1.56070100	–0.41245900
C	1.27948600	0.59221800	–0.18239300
C	0.07598300	1.23974900	0.48436200
O	–1.04252500	0.75580300	0.31671500
C	1.74299000	–0.54522100	0.75234200
C	2.90873600	–1.39614300	0.21916800
C	3.19468800	–2.53046300	1.20688600
C	2.64043600	–1.94276900	–1.18375700
C	–3.92442000	–0.56025300	–0.17674100
N	–3.78923800	0.46989700	0.65306600
N	–5.12819800	–1.10706900	–0.38791100
N	–2.84856500	–1.04138500	–0.79337300
H	0.88383400	–1.20346700	0.93149100
H	2.02777400	–0.11686700	1.72120000
H	3.81197100	–0.77219200	0.17690600
H	4.06550700	–3.11084900	0.89114100
H	2.34116500	–3.21501500	1.26927500
H	3.39323000	–2.14627500	2.21187200
H	2.56090300	–1.14679700	–1.93106000
H	3.45038600	–2.60566100	–1.49897000
H	1.71034300	–2.52346800	–1.20335000
H	0.89880600	0.13841300	–1.11525800
H	3.23063000	1.11186100	–0.41332400
H	–4.56602400	0.81603100	1.18995900
H	–5.95706700	–0.72895500	0.03909400
H	–1.94503900	–0.60226600	–0.60821400
C	2.15141800	2.34660500	–1.62514000
H	2.04735100	1.73538400	–2.53620800
H	1.25623100	2.97373800	–1.54424000
H	3.00473400	3.01537800	–1.75051100
C	0.28974600	2.42503900	1.36954600
H	1.16928000	2.27603900	1.99971400
H	0.51759400	3.29697600	0.74795600
H	–0.59919600	2.62338100	1.96825300
H	–2.85993200	0.87172200	0.78316500

H	–2.92359500	–1.76630200	–1.48635000
H	–5.24036700	–1.91479900	–0.97716800

Table S35. Cartesian coordinates of the ωB97X-D/6-31G(d,p) optimized Lys–Gdm^+ complex (binding energy: –37.3 kcal mol^{-1}).

Energy (Hartrees) = –706.260254			
Atom	X	Y	Z
N	1.16465000	1.32439600	–1.23344900
C	–0.17257000	1.36978400	–0.63027000
C	–0.07581100	1.46313100	0.89354500
O	0.75267800	0.81746000	1.51275100
C	–0.94830000	0.09805800	–1.01682200
C	–2.38038800	0.03569800	–0.48973300
C	–3.14603900	–1.18001000	–1.00869200
C	–4.53247500	–1.30437300	–0.37539400
N	–4.42210700	–1.44661100	1.07497600
H	1.02264600	1.24656500	–2.23838200
H	–0.73014600	2.25216200	–0.98308700
H	–0.96089700	0.03875600	–2.11340300
H	–0.37810900	–0.76740600	–0.65673800
H	–2.39453900	–0.00935500	0.60439500
H	–2.91971700	0.94857100	–0.77792600
H	–3.25108500	–1.12662400	–2.09908700
H	–2.57105100	–2.09205300	–0.79517700
H	–5.09972100	–0.38914900	–0.58117800
H	–5.07630400	–2.12710700	–0.86468700
H	–5.33077700	–1.33135200	1.50982600
H	–4.11192500	–2.38525800	1.30706400
C	3.26385600	–1.47511000	0.18966600
N	2.85360200	–0.97426700	1.34777600
N	2.76088300	–0.99816300	–0.94279400
N	4.17885600	–2.45781200	0.16654200
H	2.07301900	–0.30774400	1.37129400
H	2.13613300	–0.15505400	–0.95605700
H	2.96350300	–1.46257200	–1.81249600
H	4.60333100	–2.75535500	–0.69524700
H	4.48026600	–2.90982200	1.01313300
H	3.30529800	–1.22522400	2.21084600
C	1.96855600	2.52714000	–0.98111000
H	2.24631400	2.56612200	0.07460800
H	2.88758300	2.47494800	–1.56779200
H	1.44004700	3.45411400	–1.24047600

C	–1.03101900	2.38220100	1.59231800
H	–2.04351400	2.27719100	1.19398300
H	–1.02040700	2.19918300	2.66606900
H	–0.71741300	3.41485800	1.39609700

Table S36. Cartesian coordinates of the ωB97X-D/6-31G(d,p) optimized Lys–Gdm^+ complex (binding energy: –27.0 kcal mol^{-1}).

Energy (Hartrees) = –611.580977			
Atom	X	Y	Z
N	–2.64382400	–0.93857600	0.68763000
C	–1.65284200	–0.46191700	–0.26550400
C	–0.46644700	–1.42616700	–0.22820200
O	0.69086300	–1.01549600	–0.20107400
C	–1.22023200	0.99805500	–0.09999100
C	–2.36868900	2.00248300	–0.19742900
C	–1.88519800	3.44517600	–0.07221900
C	3.64312900	0.21765500	0.07929500
N	2.57665300	1.01189000	0.05917700
N	3.47243900	–1.09806200	–0.01253800
N	4.87270900	0.73506900	0.19215800
H	–2.57937900	–0.41532500	1.55261700
H	–2.07517400	–0.58488900	–1.27542500
H	–0.47572600	1.23315500	–0.87119100
H	–0.71642500	1.11170600	0.87115200
H	–3.10551600	1.79662400	0.58698700
H	–2.88852000	1.86816200	–1.15365100
H	–2.71932600	4.14734400	–0.13788600
H	–1.38572200	3.61201300	0.88808900
H	–1.17744000	3.69517600	–0.86965400
H	2.66284200	2.00958500	0.15053800
H	1.65343400	0.58534700	–0.03589200
H	4.25539900	–1.72904900	–0.02844200
H	2.52357800	–1.46327900	–0.09548100
H	5.01986000	1.72894600	0.24490000
C	–0.76452500	–2.89403900	–0.20725700
H	–1.05800900	–3.16974100	0.80954600
H	–1.61848200	–3.13125300	–0.84564400
H	0.11364800	–3.46648100	–0.50703300
C	–4.02101600	–0.99864300	0.21407300
H	–4.41297100	–0.04347500	–0.16464900
H	–4.09934700	–1.73978200	–0.58708200
H	–4.66249800	–1.33490600	1.03104900
H	5.68793400	0.14622600	0.22416500

Table S37. Cartesian coordinates of the ωB97X-D/6-31G(d,p) optimized Met–Gdm^+ complex (binding energy: –24.2 kcal mol^{-1}).

Energy (Hartrees) = –1009.77389			
Atom	X	Y	Z
N	–3.44909500	–0.01673400	–0.76924500
C	–2.04779400	–0.19743200	–0.48730700
C	–1.69388800	–0.99465600	0.77793500
O	–0.62070300	–1.57857300	0.86242800
C	–1.33871700	1.17629500	–0.43229400
C	0.17626000	1.02982200	–0.35383900
S	1.17563600	2.53632800	–0.53784000
C	0.78564100	3.38640200	1.01696700
C	3.12519800	–1.46071400	–0.13642300
N	3.28951000	–0.16582600	0.13359600
N	4.20954500	–2.24031900	–0.25071900
N	1.91818000	–1.99168900	–0.29796300
H	–1.71283100	1.75505100	0.42138900
H	–1.62523400	1.71478600	–1.33866200
H	0.51064300	0.37896100	–1.17064000
H	0.45763100	0.55535500	0.59196100
H	1.43708100	4.25944100	1.07502400
H	0.97757800	2.74250900	1.87872800
H	–0.25094700	3.72656400	1.02706900
H	–1.61129000	–0.76078500	–1.32316100
H	–3.92625200	0.49749000	–0.03873300
H	4.19997000	0.17905300	0.39181500
H	5.12839300	–1.84486500	–0.36389300
H	1.04879700	–1.58882300	0.06896300
H	4.13418300	–3.24406700	–0.23565700
H	2.58243500	0.54287500	–0.05023000
H	1.84397300	–2.94164400	–0.62605400
C	–4.17764900	–1.21072800	–1.16372500
H	–4.16560400	–2.03256100	–0.42806700
H	–5.21906000	–0.94661300	–1.35563600
H	–3.75864300	–1.59628100	–2.09835200
C	–2.65528900	–0.98293900	1.93254500
H	–3.57997100	–1.50350800	1.66551300
H	–2.20319900	–1.46676900	2.79738200
H	–2.93176000	0.04683400	2.18442300

Table S38. Cartesian coordinates of the ωB97X-D/6-31G(d,p) optimized Phe–Gdm^+ complex (binding energy: –27.1 kcal mol^{-1}).

Energy (Hartrees) = –764.004430			
Atom	X	Y	Z
N	–0.26329900	0.20739800	0.98092100
C	0.19529700	1.38017600	0.24575100
C	–0.95909700	2.24366800	–0.24539500
O	–2.11476800	1.85660500	–0.22537700
C	1.04017700	0.94634100	–0.97821100
C	2.18732600	0.04776800	–0.58033500
C	2.14341000	–1.32311900	–0.84135600
C	3.29370500	0.57026400	0.09559000
C	3.18414200	–2.15716200	–0.43947700
C	4.33284500	–0.25991300	0.49924300
C	4.27932900	–1.62656500	0.23348600
C	–3.25460000	–1.57580300	–0.16910700
N	–3.76689600	–0.37255400	0.06834500
N	–1.93604800	–1.72313800	–0.18785500
N	–4.06636600	–2.62373000	–0.38049500
H	1.42088700	1.84192000	–1.47835800
H	0.38592000	0.42944100	–1.68901700
H	3.34779500	1.63731700	0.29716700
H	1.29632400	–1.73638200	–1.38408300
H	5.18953700	0.16004500	1.01547900
H	3.14328900	–3.21878100	–0.65993500
H	5.09304100	–2.27293600	0.54405700
H	0.82608000	2.02201500	0.88454900
H	0.55750000	–0.38065000	1.11895200
H	–3.15592800	0.45000500	0.03956700
H	–1.31058000	–0.95232000	0.16123200
H	–5.05714400	–2.50058400	–0.50389800
H	–3.70550800	–3.56101800	–0.43303800
H	–1.53266500	–2.60888900	–0.44403800
H	–4.75968000	–0.24016600	0.16124600
C	–0.61318300	3.59323900	–0.81454000
H	–0.49199800	3.49283300	–1.89904200
H	–1.43660900	4.28578700	–0.63688700
H	0.31655900	3.99492500	–0.40695600
C	–0.83160100	0.51593600	2.29909400
H	–1.76401200	1.07031800	2.18024000
H	–1.05351500	–0.41865600	2.81818100

H	–0.14938000	1.10811900	2.92273500

Table S39. Cartesian coordinates of the ωB97X-D/6-31G(d,p) optimized Phe–Gdm^+ complex (binding energy: –26.1 kcal mol^{-1}).

Energy (Hartrees) = –763.992859			
Atom	X	Y	Z
C	4.17938100	–1.32721800	–0.08278600
N	5.12282900	–2.26188800	–0.25090900
N	2.89110700	–1.64897200	–0.15304300
N	4.51906500	–0.06337200	0.15520400
H	6.10149300	–2.03124600	–0.21371100
H	2.19719200	–0.91346100	–0.01052300
H	5.48209400	0.21517800	0.23538700
N	–1.27069200	2.18247400	–0.30377800
C	–0.46962700	1.23570500	0.44720100
C	0.97933100	1.70705300	0.45622100
O	1.90428400	0.90667900	0.34336500
C	–0.60708800	–0.25655500	0.08094600
C	–2.04861900	–0.70933500	0.11130600
C	–2.71035700	–1.08555900	–1.05768100
C	–2.75381600	–0.73401800	1.31837800
C	–4.04765100	–1.47252200	–1.02641300
C	–4.08968500	–1.11761600	1.35349800
C	–4.74113700	–1.48596600	0.17885000
H	–0.77644300	1.34833000	1.49934600
H	–0.02014100	–0.84130700	0.79940300
H	–0.17782200	–0.43532200	–0.91150700
H	–2.17408500	–1.08476700	–2.00341000
H	–2.25209200	–0.46076700	2.24405800
H	–4.54611200	–1.76416500	–1.94490200
H	–4.62193100	–1.13401400	2.29883900
H	–5.78314000	–1.78612500	0.20524400
H	2.59358400	–2.59049500	–0.34376800
H	3.77943100	0.62711700	0.28087000
H	4.88230400	–3.22375500	–0.42197200
H	–2.24554100	2.07465900	–0.04928200
C	–1.12098600	2.12034700	–1.75158500
H	–1.71346900	2.91884600	–2.20198300
H	–0.07454700	2.29733200	–2.02688700
H	–1.43184900	1.16815200	–2.20317700
C	1.23850300	3.17169800	0.62853100
H	0.54284000	3.60927100	1.34689100
H	2.27359500	3.34189200	0.92584400

H 1.04471800 3.67744000 –0.32279800

Table S40. Cartesian coordinates of the ωB97X-D/6-31G(d,p) optimized Pro–Gdm^+ complex (binding energy: –35.3 kcal mol^{-1}).

Energy (Hartrees) = –610.378551			
Atom	X	Y	Z
N	0.63182500	–0.74987800	0.71427300
C	1.73951900	0.02899300	0.16542300
C	1.40576700	1.48744700	–0.08817900
O	0.26609800	1.91526000	–0.02715500
C	2.11967400	–0.71156000	–1.14415600
C	1.55555700	–2.13929700	–0.95119600
C	1.02738100	–2.14786500	0.48440600
H	2.60296800	0.00332600	0.85447700
H	1.66692700	–0.22618000	–2.01303400
H	3.20048900	–0.70538700	–1.29160500
H	0.74651500	–2.32701000	–1.66187800
H	2.31108600	–2.90993400	–1.10865700
H	0.17199500	–2.81266600	0.63872200
H	1.81477600	–2.44834300	1.19345000
C	–2.81727300	0.11957200	–0.25393000
N	–4.11344300	–0.11703400	–0.50821200
N	–2.43785100	1.28716100	0.25508500
N	–1.89845800	–0.80719800	–0.49570300
H	–4.79662300	0.62045800	–0.46817100
H	–3.11451700	1.97775400	0.53276700
H	–2.14846300	–1.64193400	–0.99918000
H	–0.91703900	–0.69124400	–0.13501300
H	–4.43780600	–1.03786900	–0.75028000
H	–1.44404800	1.53547600	0.24130000
C	0.33988500	–0.45944200	2.11599000
H	0.04792100	0.58667000	2.22506300
H	–0.49161800	–1.08564400	2.44882600
H	1.20591600	–0.65816200	2.76480900
C	2.56250100	2.38637000	–0.42088200
H	2.19922100	3.34062200	–0.80034300
H	3.14668500	2.56226700	0.48949100
H	3.23424400	1.91906100	–1.14645600

Table S41. Cartesian coordinates of the ωB97X-D/6-31G(d,p) optimized Pro–Gdm^+ complex (binding energy: –26.8 kcal mol^{-1}).

Energy (Hartrees) = –610.364675			
Atom	X	Y	Z
N	1.72818800	–0.87202200	0.79343500
C	2.06688200	0.42477800	0.26784900
C	0.92070100	1.41414600	0.13936000
O	–0.24295200	1.03378500	0.03810600
C	2.60013900	0.13559600	–1.17379000
C	2.62423600	–1.39949000	–1.26868800
C	1.54846300	–1.83048300	–0.27454200
H	2.84055200	0.89973300	0.88851700
H	1.91811600	0.54766600	–1.92525000
H	3.57894300	0.58751700	–1.33833000
H	3.59255600	–1.78321000	–0.94003000
H	2.43950800	–1.75272200	–2.28474300
H	0.54756400	–1.79411300	–0.74932700
H	1.69702200	–2.84823100	0.10027800
C	–3.19907000	–0.19547100	–0.18832400
N	–4.43003200	–0.71536600	–0.26772100
N	–2.13723800	–0.98869400	–0.08043500
N	–3.02172300	1.12249200	–0.21895700
H	–5.24595700	–0.12751200	–0.30122500
H	–1.21180900	–0.55825600	–0.02111400
H	–3.78961300	1.75139800	–0.38119600
H	–2.23405100	–1.98212800	0.04291500
H	–2.07348700	1.48857700	–0.13824800
H	–4.57623000	–1.71026500	–0.30172300
C	0.99213800	–0.99208600	2.02427600
H	–0.08450000	–0.76137400	1.94621300
H	1.09323000	–2.01158100	2.40770200
H	1.41883400	–0.31796300	2.77396300
C	1.27001900	2.87181400	0.12515800
H	2.16121200	3.04919900	–0.48403800
H	0.43717500	3.47369500	–0.23781200
H	1.51913600	3.18160500	1.14655300

Table S42. Cartesian coordinates of the ωB97X-D/6-31G(d,p) optimized Ser–Gdm^+ complex (binding energy: –37.2 kcal mol^{-1}).

Energy (Hartrees) = –608.183686			
Atom	X	Y	Z
N	0.58731300	0.98980600	–0.95945700
C	1.74592700	0.30439800	–0.40182100
C	1.46850500	–1.19980200	–0.36418200
O	0.44633700	–1.65323900	–0.84781000
C	2.10759600	0.82415500	0.98815900
O	1.02328400	0.54195700	1.84825400
C	–2.66712800	–0.13771000	0.13115100
N	–1.77129000	0.71326500	0.60496700
N	–2.31462000	–0.99126400	–0.82978600
N	–3.92713200	–0.13420800	0.59494500
H	2.31761200	1.90021400	0.93421600
H	3.03117600	0.33203100	1.31873100
H	1.27513700	0.77540100	2.74583900
H	2.64563600	0.43647900	–1.03194100
H	0.30694800	0.48299800	–1.79442200
H	–1.92542700	1.17447000	1.48575800
H	–1.32546100	–1.20331800	–0.97185500
H	–4.26937000	0.62872400	1.15429500
H	–3.00420300	–1.55370600	–1.29913300
H	–0.83844000	0.80499300	0.14308100
H	–4.56904400	–0.87569700	0.37102600
C	2.49726000	–2.09181900	0.26703400
H	2.36845800	–2.04278600	1.35419300
H	2.33975800	–3.11980000	–0.05749300
H	3.51635200	–1.77144500	0.03609000
C	0.81284600	2.39536600	–1.30321800
H	–0.04399400	2.75966200	–1.87243100
H	0.88650800	2.99997400	–0.39634700
H	1.72144700	2.55134800	–1.90056900

Table S43. Cartesian coordinates of the ωB97X-D/6-31G(d,p) optimized Ser–Gdm^+ complex (binding energy: –27.3 kcal mol^{-1}).

Energy (Hartrees) = –608.173278			
Atom	X	Y	Z
N	–1.46622500	1.62352400	0.03092100
C	–2.11890400	0.37951800	0.32549000
C	–1.18645100	–0.79957600	0.62729300
O	0.02737600	–0.68113100	0.51080100
C	–3.02285600	–0.02315200	–0.84425100
O	–2.15502000	–0.38155000	–1.90241100
H	–0.91669600	1.54909300	–0.81582000
H	–2.75925000	0.51547600	1.20875500
H	–3.64578800	0.84284300	–1.09296300
H	–3.67796700	–0.85764200	–0.55791000
H	–2.66678700	–0.48080300	–2.70927800
C	3.09763600	–0.08948400	–0.19046600
N	2.72497600	–1.31157700	0.17936000
N	2.18089100	0.86944100	–0.28425800
N	4.38171700	0.17140500	–0.46535500
H	3.36250200	–2.08829100	0.13455300
H	2.44600200	1.83131400	–0.41175000
H	4.66605300	1.06291000	–0.83518700
H	1.74677300	–1.47351100	0.41531400
H	1.20726700	0.63058700	–0.08079400
H	5.09813500	–0.52111100	–0.32518800
C	–1.79497100	–2.11156800	1.02471900
H	–2.04568700	–2.65018500	0.10346700
H	–1.07965600	–2.70902700	1.59085300
H	–2.71657300	–1.98150000	1.59596500
C	–0.78734900	2.29043300	1.12612300
H	–0.38505600	3.24212800	0.76992300
H	–1.51344200	2.52586500	1.91052600
H	0.02918700	1.71670800	1.59428000

Table S44. Cartesian coordinates of the ωB97X-D/6-31G(d,p) optimized Ser–Gdm^+ complex (binding energy: –32.8 kcal mol^{-1}).

Energy (Hartrees) = –608.176665			
Atom	X	Y	Z
N	0.43041000	0.89054800	–0.26624100
C	1.34077200	–0.16407100	0.17591500
C	2.81286000	0.27276600	–0.00386300
O	3.05054500	1.26281700	–0.65938000
C	1.09839100	–1.46453100	–0.58338300
O	–0.17453100	–1.97086400	–0.20633500
C	–3.02783900	0.02440500	–0.00367300
N	–2.25813000	0.55081900	–0.94444400
N	–4.33695400	0.30887200	0.06366200
N	–2.47611200	–0.79729200	0.89028000
H	1.88051200	–2.19249500	–0.33691800
H	1.13544100	–1.26680400	–1.66285600
H	–0.34689600	–2.78320900	–0.69042900
H	1.16692800	–0.36816300	1.24006200
H	0.91892600	1.35881200	–1.03257700
H	–1.21329200	0.55570900	–0.80766600
H	–4.73752100	1.04833700	–0.48878400
H	–1.57086600	–1.22049100	0.66859900
H	–2.67061900	1.07613500	–1.69793300
H	–2.99655100	–1.11774200	1.68926100
H	–4.95879800	–0.22443500	0.64799200
C	3.89431100	–0.57540200	0.61185900
H	4.26040800	–1.28536100	–0.13836000
H	4.73376600	0.06025500	0.89659000
H	3.53993600	–1.14366600	1.47505500
C	0.20575000	1.90542800	0.77555600
H	–0.39139500	2.71916800	0.35887900
H	–0.35561500	1.45723800	1.60064500
H	1.13754900	2.32887900	1.16689500

Table S45. Cartesian coordinates of the ωB97X-D/6-31G(d,p) optimized Ser–Gdm^+ complex (binding energy: –30.1 kcal mol^{-1}).

Energy (Hartrees) = –608.169497			
Atom	X	Y	Z
N	–0.40608000	–0.69675800	–0.53652500
C	–1.30175800	0.12643800	0.28800300
C	–2.65349200	–0.59341400	0.50050800
O	–2.74410700	–1.75725700	0.17673000
C	–1.46060500	1.55361800	–0.22471400
O	–0.17272800	2.13508900	–0.34581000
C	3.18148500	–0.18877700	0.31166200
N	2.02820800	0.39879900	0.08447500
N	3.25219000	–1.52928100	0.33084900
N	4.30292200	0.51523700	0.52858800
H	–2.07524000	2.11413000	0.48966500
H	–1.98442100	1.55629100	–1.18993600
H	–0.27787300	3.01901900	–0.70841800
H	–0.84959200	0.19900300	1.28966100
H	–0.63516500	–1.65652100	–0.27565500
H	1.90687900	1.39670600	0.17249500
H	2.41751300	–2.07426400	0.19256100
H	4.29595000	1.51972500	0.47450400
H	4.13522500	–2.00927200	0.28748700
H	1.14289900	–0.12973300	–0.17678400
H	5.13996900	0.07518900	0.87246400
C	–3.78137600	0.15927000	1.15266800
H	–4.20287600	0.88343000	0.44630700
H	–4.56290700	–0.54144700	1.44468200
H	–3.43317700	0.71851000	2.02656800
C	–0.63489400	–0.59053500	–1.98681300
H	–1.68532600	–0.73096400	–2.26585600
H	–0.28878100	0.38298400	–2.34009400
H	–0.04524100	–1.36101500	–2.48661600

Table S46. Cartesian coordinates of the ωB97X-D/6-31G(d,p) optimized Ser–Gdm^+ complex (binding energy: –31.2 kcal mol^{-1}).

Energy (Hartrees) = –608.174172			
Atom	X	Y	Z
N	2.58345700	0.55356400	–1.08376400
C	1.80947200	0.51596500	0.14626700
C	1.39010200	–0.92259600	0.46439700
O	0.31381500	–1.35930200	0.08388800
C	0.60290400	1.43681600	–0.01153700
O	–0.24385600	1.41144200	1.13507000
C	–3.23102700	–0.12909200	–0.23608500
N	–2.27437100	–0.86208500	–0.79395800
N	–2.92426000	0.79154100	0.67094800
N	–4.50973500	–0.30673400	–0.60135000
H	–0.00639800	1.09938200	–0.85469200
H	0.95105600	2.44867100	–0.23697100
H	0.11181400	1.98830600	1.81607200
H	2.44705500	0.88669900	0.95801500
H	2.20373500	–0.06659500	–1.78861800
H	–1.31868600	–0.89911000	–0.41831300
H	–1.94667900	1.02089500	0.89242400
H	–5.23015300	0.33164600	–0.30884500
C	4.03223500	0.47624000	–0.99842200
H	4.44943100	0.62646400	–1.99611700
H	4.40010600	1.28617400	–0.36228600
H	4.43061400	–0.47211500	–0.60688700
C	2.37466500	–1.80250000	1.17762300
H	1.99805200	–2.82306600	1.23743800
H	3.34322500	–1.78966700	0.66884400
H	2.54570400	–1.41088600	2.18629300
H	–2.49749500	–1.50113600	–1.53900500
H	–3.65280100	1.25305400	1.18940800
H	–4.78399400	–1.07884100	–1.18501500

Table S47. Cartesian coordinates of the ωB97X-D/6-31G(d,p) optimized Thr–Gdm^+ complex (binding energy: –36.6 kcal mol^{-1}).

Energy (Hartrees) = –647.496518			
Atom	X	Y	Z
N	–0.38064900	0.40321700	1.18196400
C	–1.52095500	–0.17645400	0.48304800
C	–1.19293600	–1.61255700	0.09559000
O	–0.04241800	–2.01622800	0.04641200
C	–1.90635100	0.62295900	–0.81645300
O	–0.76367100	1.21126100	–1.40131400
C	–2.94205600	1.71128300	–0.57416100
C	2.94132900	0.05023400	–0.16378800
N	2.65557500	–1.17473600	0.27390100
N	1.95698000	0.92692300	–0.29637700
N	4.20716500	0.38061200	–0.46197700
H	–2.35653500	–0.09101000	–1.52035600
H	–3.18396500	2.19257600	–1.52345600
H	–2.58368200	2.47812900	0.11370700
H	–3.85781300	1.27927000	–0.16211500
H	–0.29027400	0.54168700	–1.90335900
H	–2.42262000	–0.21083300	1.11761900
H	–0.09141700	–0.25480500	1.89995800
H	1.68147800	–1.48815300	0.28131400
H	2.11260600	1.81340500	–0.74709300
H	1.02149100	0.73088200	0.13767000
H	4.46611100	1.33646900	–0.63890900
H	4.93043500	–0.31632800	–0.51993900
C	–2.34835200	–2.52702800	–0.20064100
H	–2.03928700	–3.31955300	–0.88226300
H	–2.65412800	–2.99085800	0.74466900
H	–3.21768800	–1.99619600	–0.59488700
C	–0.61973200	1.70820800	1.80578200
H	–1.56540400	1.75426600	2.36151700
H	0.19881300	1.92028600	2.49633400
H	–0.62332000	2.48433700	1.03830000
H	3.38472900	–1.83580000	0.48167000

Table S48. Cartesian coordinates of the ωB97X-D/6-31G(d,p) optimized Thr–Gdm^+ complex (binding energy: –26.7 kcal mol^{-1}).

Energy (Hartrees) = –647.483218			
Atom	X	Y	Z
N	–2.54490300	0.75001800	1.08068000
C	–1.48111400	–0.03631500	0.49352700
C	–0.38002600	0.90808600	0.01631200
O	0.79158600	0.53162600	0.04493600
C	–1.87297700	–0.88877000	–0.74790900
O	–2.66279300	–0.07527300	–1.58733600
C	–2.53558200	–2.22573200	–0.41849200
C	3.90023000	–0.25484200	0.10983300
N	5.19937000	–0.57667900	0.14580400
N	3.50623400	0.90251600	–0.41143900
N	2.98619700	–1.09183800	0.59443400
H	–0.91618000	–1.12942100	–1.24244100
H	–3.51158900	–2.10634100	0.04999700
H	–2.66995100	–2.80008700	–1.34089300
H	–1.89949500	–2.81864400	0.24453200
H	–2.92439800	–0.58986300	–2.35618500
H	–0.99835400	–0.74554000	1.18993700
H	–2.21334000	1.13723100	1.95669900
H	5.50873600	–1.46879400	0.49319600
H	4.15835900	1.52782300	–0.85334300
H	3.25185800	–1.93602600	1.07205300
C	–3.85273100	0.14548900	1.29066000
H	–4.32393200	–0.04262800	0.32509800
H	–3.83666900	–0.78709000	1.87594600
H	–4.47404400	0.86718900	1.82467500
C	–0.76815600	2.23783900	–0.53446600
H	–1.22032400	2.84788500	0.25144900
H	0.09407600	2.74551400	–0.96697400
H	–1.55889800	2.07973800	–1.27462900
H	2.00383300	–0.81878200	0.55069900
H	5.90600200	0.06377800	–0.17489600
H	2.50781200	1.12057900	–0.40886200

Table S49. Cartesian coordinates of the ωB97X-D/6-31G(d,p) optimized Thr–Gdm^+ complex (binding energy: –35.9 kcal mol^{-1}).

Energy (Hartrees) = –647.497718			
Atom	X	Y	Z
N	2.04131600	–0.52841100	1.18260000
C	1.89689600	–0.33420600	–0.26464400
C	1.56441900	1.13639100	–0.56923600
O	0.48391600	1.60712200	–0.26706000
C	0.73182800	–1.25175500	–0.72674300
C	1.16570800	–2.69960900	–0.91277400
O	–0.29873500	–1.15305900	0.25061800
H	2.81007500	–0.59965800	–0.81739700
H	0.32272000	–0.87093200	–1.66884900
H	0.19024600	–0.94918200	1.07773000
H	0.30932400	–3.31101000	–1.20500100
H	1.92685100	–2.78106300	–1.69374600
H	1.57101000	–3.11894900	0.01346000
C	–3.27270500	0.26955100	0.12041400
N	–4.53125700	0.73378900	0.11451500
N	–3.04383000	–1.03987600	0.15755100
N	–2.25046000	1.11445400	0.08621600
H	–5.31904400	0.10905900	0.08948200
H	–3.79652900	–1.69518900	0.28047700
H	–2.07145200	–1.36161200	0.17609600
H	–1.28120700	0.78989300	0.08899600
H	–2.39598500	2.10361100	–0.02625400
H	2.46295300	–1.43976300	1.33597300
H	–4.72373000	1.72093200	0.12806500
C	2.61648100	1.94391500	–1.27185400
H	2.82325500	1.50236100	–2.25335100
H	2.28869100	2.97564500	–1.39313500
H	3.55562700	1.90840900	–0.70963300
C	2.83686900	0.47230800	1.89521500
H	2.92123200	0.17073500	2.94031100
H	3.85036800	0.59665400	1.48843200
H	2.32678700	1.43830200	1.87143900

Table S50. Cartesian coordinates of the ωB97X-D/6-31G(d,p) optimized Thr–Gdm^+ complex (binding energy: –40.1 kcal mol^{-1}).

Energy (Hartrees) = –647.501573			
Atom	X	Y	Z
N	–0.76007300	0.08282600	–1.44751800
C	–1.62281400	0.22517900	–0.28162100
C	–1.03318900	1.25059500	0.70109400
O	0.15080600	1.51128000	0.68628300
C	–1.82985100	–1.11287300	0.45130200
C	–2.45320200	–2.19710700	–0.42037100
O	–0.56126400	–1.52555500	0.95331500
H	–1.07827800	–0.71605400	–1.98673600
H	–2.63028900	0.57949400	–0.56222100
H	–2.50769700	–0.91353800	1.29279400
H	–0.65613100	–2.39363900	1.35649000
H	–2.69873100	–3.07430600	0.18533300
H	–3.38193200	–1.84650100	–0.87805800
H	–1.76654400	–2.52557300	–1.20575800
C	2.74174800	–0.26381100	0.06320900
N	2.04746300	–0.20706900	–1.06188900
N	4.06325200	–0.02318600	0.06500500
N	2.14294400	–0.60931800	1.20290700
H	2.53335900	–0.10496100	–1.93755700
H	4.63151500	–0.26097900	0.86034600
H	4.52360200	0.36737200	–0.73919300
H	2.55139600	–0.32381500	2.07772200
H	1.13703900	–0.77953800	1.18485600
H	1.00372100	–0.13851600	–1.06413600
C	–0.77481100	1.26392600	–2.31862300
H	–1.79055100	1.57434300	–2.59925000
H	–0.27964500	2.09479000	–1.81223100
H	–0.21959200	1.04215800	–3.23251900
C	–1.99622800	1.91979000	1.64520200
H	–2.76031200	1.23350600	2.01999200
H	–1.45268000	2.37067800	2.47489800
H	–2.51961800	2.71231500	1.09775800

Table S51. Cartesian coordinates of the ωB97X-D/6-31G(d,p) optimized Trp–Gdm^+ complex (binding energy: –44.9 kcal mol^{-1}).

Energy (Hartrees) = –895.582533			
Atom	X	Y	Z
N	–2.35391100	1.18300000	0.33389200
C	–2.59861300	–0.15095500	–0.20798000
C	–2.21597200	–1.19481500	0.83394400
O	–1.52006800	–0.90537900	1.79092900
C	–1.86831600	–0.38546900	–1.56057300
C	–0.40941800	–0.05087900	–1.56825900
C	0.15295400	1.05435000	–2.14323200
C	0.67812300	–0.79918000	–0.98669000
N	1.51106500	1.07259700	–1.91910500
C	1.86167100	–0.06353600	–1.22440900
C	0.76980300	–2.02207600	–0.30373600
C	3.11201700	–0.48545500	–0.76413700
C	2.00340500	–2.44774300	0.15593200
C	3.16507800	–1.67969400	–0.06414300
C	1.25632000	1.47381400	1.55085500
N	1.07396900	0.25681200	2.05949600
N	2.48146100	2.02093800	1.58982900
N	0.22982100	2.15447000	1.06135100
H	–2.37932900	0.21229900	–2.32086500
H	–2.02332900	–1.42778600	–1.85867100
H	–0.31836400	1.84207700	–2.71457000
H	2.15928600	1.68358400	–2.38676200
H	–0.10892200	–2.63746900	–0.14178100
H	2.08560300	–3.39507300	0.67777400
H	4.01062500	0.09053100	–0.96121200
H	4.12139400	–2.04782500	0.29250800
H	–3.67295900	–0.30568700	–0.41417800
H	–2.74622900	1.21092300	1.27165500
H	1.83237700	–0.40889600	1.99959500
H	3.22000900	1.57965200	2.11096900
H	–0.65673500	1.68084300	0.77351400
H	0.34703000	3.12499900	0.82241400
H	2.69380600	2.86564800	1.08881400
H	0.13250000	–0.13353900	2.03197000
C	–2.94914900	2.25854100	–0.46113400
H	–2.89089100	3.19252800	0.10186600
H	–2.38802000	2.39039700	–1.38914500

H	–4.00177600	2.07512700	–0.71689900
C	–2.78879800	–2.57640000	0.67373700
H	–2.21213800	–3.28981600	1.26240000
H	–3.81641100	–2.56611400	1.05516700
H	–2.83845200	–2.89110500	–0.37129200

Table S52. Cartesian coordinates of the ωB97X-D/6-31G(d,p) optimized Tyr–Gdm^+ complex (binding energy: –19.60kcal mol^{-1}).

Energy (Hartrees) = –839.208665			
Atom	X	Y	Z
N	3.55087400	1.10432600	0.47642000
C	3.19330800	–0.27916800	0.22885800
C	4.35830900	–1.27929300	0.08595000
O	4.19482900	–2.43527500	0.40873300
C	2.30680800	–0.38789700	–1.03342200
C	0.91503100	0.14920100	–0.81140800
C	–0.16373300	–0.72574200	–0.67294900
C	0.67209300	1.52079000	–0.70202700
C	–1.45158600	–0.25708300	–0.43555200
C	–0.60829100	2.00788400	–0.46361900
C	–1.65859700	1.11033600	–0.33350000
O	–2.96223300	1.54678200	–0.09214800
C	–5.35751200	–0.67240800	0.34887300
N	–6.30265800	–1.60160800	0.52168600
N	–4.64610500	–0.23216800	1.38363100
N	–5.11265400	–0.17503900	–0.86103500
H	2.24768200	–1.43938300	–1.32885300
H	2.79510300	0.14941300	–1.85596700
H	0.00251500	–1.79609100	–0.75036000
H	1.50207300	2.21268700	–0.78040500
H	–2.28190800	–0.94914400	–0.33424500
H	–0.77745900	3.07850700	–0.38025800
H	–2.97783900	2.50950700	–0.06310700
H	2.60770800	–0.63809900	1.08300200
H	4.17965300	1.44090100	–0.24589300
H	–6.51230900	–1.97278200	1.43352900
H	–4.77169600	–0.60637000	2.30905800
H	–5.63635600	–0.46736300	–1.66878800
H	–4.37893100	0.52285300	–0.96293700
H	–6.84150100	–1.95202700	–0.25290300
H	–3.93214500	0.47430600	1.21970600
C	4.11160900	1.35403200	1.79647100
H	4.99877000	0.74767100	2.04200400
H	4.38678400	2.40771400	1.87974500
H	3.35053800	1.14659300	2.55474000
C	5.65311100	–0.78430300	–0.51898400
H	6.14103900	–0.06454400	0.14646400
H	6.32095300	–1.62924200	–0.68338300
H	5.46707100	–0.27382800	–1.47088200

Table S53. Cartesian coordinates of the ωB97X-D/6-31G(d,p) optimized Tyr–Gdm^+ complex (binding energy: –21.0 kcal mol^{-1}).

Energy (Hartrees) = –839.208226			
Atom	X	Y	Z
N	–4.22594600	1.41213200	–0.12505600
C	–3.14116600	0.45671100	–0.22892200
C	–3.57805200	–0.96428100	0.15543500
O	–2.89057700	–1.90769800	–0.17593900
C	–1.87885900	0.84780600	0.60262900
C	–0.63165500	0.09100500	0.22656300
C	0.11940500	0.48027300	–0.88443300
C	–0.22104200	–1.04247300	0.93222500
C	1.23914100	–0.24179700	–1.29444700
C	0.90074900	–1.76832700	0.55125500
C	1.61880800	–1.37067500	–0.57217500
O	2.76743400	–2.01842900	–0.97979800
C	4.57841400	0.87882600	0.37504400
N	4.82479500	–0.13251600	–0.45019700
N	5.58390700	1.64809700	0.81169500
N	3.33388500	1.13230300	0.77303300
H	–2.10119500	0.70884300	1.66769900
H	–1.71227100	1.91985400	0.45235200
H	–0.18561700	1.35082600	–1.45893100
H	–0.79558200	–1.37547100	1.79007400
H	1.79684400	0.03926800	–2.18203900
H	1.20203000	–2.64532900	1.11725300
H	2.79149000	–2.90879700	–0.61362900
H	–2.84662500	0.40135600	–1.28325400
H	–4.41084900	1.64734300	0.84434800
H	4.11840900	–0.84636300	–0.66015200
H	6.54399200	1.37821100	0.67498800
H	2.54254300	0.69265400	0.30950700
C	–4.05652700	2.62068400	–0.91403600
H	–4.90936800	3.28153200	–0.74587400
H	–3.13825900	3.19357900	–0.69762500
H	–4.04560200	2.35984800	–1.97678200
C	–4.83605300	–1.12646700	0.96985700
H	–5.68541800	–0.70922800	0.42314000
H	–4.99551100	–2.18213700	1.18663100
H	–4.76023200	–0.56638200	1.90963100
H	3.15030400	1.77057800	1.52918400
H	5.72227700	–0.21093200	–0.90021200
H	5.40831700	2.52194500	1.27929800

Table S54. Cartesian coordinates of the ωB97X-D/6-31G(d,p) optimized Tyr–Gdm^+ complex (binding energy: –31.4 kcal mol^{-1}).

Energy (Hartrees) = –839.221372			
Atom	X	Y	Z
N	–1.61971200	1.04927300	–0.12139700
C	–2.19479800	–0.29185300	–0.37536400
C	–3.73555900	–0.28969100	–0.24573700
O	–4.30233200	–1.11165000	0.43495900
C	–1.58758600	–1.39765300	0.49762700
C	–0.09115500	–1.51128000	0.35919100
C	0.48590200	–1.98674000	–0.82069100
C	0.76229800	–1.11202100	1.39071700
C	1.86764500	–1.98150100	–1.00601400
C	2.14174200	–1.11045800	1.23263100
C	2.69081300	–1.50981600	0.01730000
O	4.03692500	–1.30862300	–0.14947300
C	2.04112600	2.03548400	–0.31094700
N	1.14476700	1.23897500	–0.87003400
N	1.64835400	3.22561400	0.17010000
N	3.33149500	1.69581300	–0.23703500
H	–2.07419500	–2.33325100	0.21007800
H	–1.86736600	–1.23822400	1.54252800
H	0.34142300	–0.79143700	2.33950500
H	–0.14970500	–2.35136900	–1.62303600
H	2.80186000	–0.78810800	2.03023000
H	2.29552200	–2.33457900	–1.94061900
H	4.36903900	–1.83725800	–0.88280000
H	–1.97316800	–0.51410800	–1.42908200
H	–2.06482500	1.69344500	–0.77068900
H	1.46643100	0.34534600	–1.22151500
H	0.13885000	1.24689000	–0.57925800
H	2.26918900	3.81268600	0.70080100
H	0.74734800	3.59558300	–0.08070200
H	3.64250500	0.73627000	–0.35795300
C	–4.49056300	0.78397800	–1.00132600
H	–4.47112300	1.72270200	–0.43529900
H	–4.05859700	0.97436200	–1.98887100
H	–5.53155500	0.47959100	–1.10730000
C	–1.83779800	1.54574100	1.24366100
H	–2.87272800	1.43602900	1.59344700
H	–1.18614000	1.01243200	1.93811300
H	–1.57436900	2.60520500	1.28545900
H	4.02813000	2.37712800	0.01534200

Table S55. Cartesian coordinates of the ωB97X-D/6-31G(d,p) optimized Tyr–Gdm^+ complex (binding energy: –26.1 kcal mol^{-1}).

Energy (Hartrees) = –839.214854			
Atom	X	Y	Z
N	0.81958300	2.36001100	–0.91033600
C	–0.11932500	1.34212600	–0.53550700
C	–1.55861000	1.77416900	–0.22206800
O	–2.43717600	0.91271700	–0.21358000
C	0.37956200	0.47712000	0.64987900
C	1.70506900	–0.19780800	0.38992200
C	1.88025100	–1.05152900	–0.70351500
C	2.78289700	–0.01125700	1.25111800
C	3.08575100	–1.69143600	–0.93593900
C	4.00211900	–0.64678300	1.03570000
C	4.15879000	–1.48931000	–0.06314100
O	5.31160200	–2.14058900	–0.34115400
C	–4.27711400	–1.70862400	0.08595700
N	–2.99835800	–1.80754200	–0.26428800
N	–4.80050700	–0.50312000	0.29453500
N	–5.02988800	–2.80629000	0.22751600
H	–0.39342200	–0.27067900	0.86131100
H	0.45137000	1.09916900	1.54905400
H	2.67577300	0.63795400	2.11657200
H	1.06002700	–1.22179600	–1.39753000
H	4.82737100	–0.48417100	1.72370200
H	3.22189000	–2.34933500	–1.78675500
H	5.98078700	–1.92021200	0.31315200
H	–0.23625600	0.66972600	–1.39741700
H	0.56142500	2.84693400	–1.75546600
H	–2.46102200	–0.94475500	–0.37524300
H	–4.20185700	0.31529300	0.19465100
H	–4.66546500	–3.72071900	0.01903400
H	–2.54324800	–2.70103500	–0.34383800
H	–5.98347700	–2.75046300	0.54373100
H	–5.78356700	–0.38230700	0.46944200
C	–1.88929100	3.20205800	0.08167700
H	–1.39351100	3.87695300	–0.61927500
H	–2.96785200	3.35707900	0.06844000
H	–1.50384700	3.44437600	1.07847100
C	1.43681100	3.21423900	0.08553700
H	0.73989700	3.78605900	0.71851800
H	2.08531800	2.62385600	0.73811600
H	2.07698700	3.93185500	–0.43050600

Table S56. Cartesian coordinates of the ωB97X-D/6-31G(d,p) optimized Tyr–Gdm^+ complex (binding energy: –30.1 kcal mol^{-1}).

Energy (Hartrees) = –875.159169			
Atom	X	Y	Z
N	0.68465200	–0.05605200	–0.47130000
C	0.29223200	–1.25537500	0.28302700
C	1.42010400	–2.28020300	0.26983000
O	2.56945000	–2.05446200	–0.04562800
C	–1.08359800	–1.84552900	–0.10613700
C	–2.16531600	–0.79419600	–0.02219400
C	–2.61290100	–0.33586600	1.21915800
C	–2.72444500	–0.22412100	–1.16992900
C	–3.57897500	0.65782600	1.31869500
C	–3.69023200	0.76912800	–1.08955200
C	–4.12266900	1.21675800	0.15974500
O	–5.06297000	2.18812800	0.17896300
O	1.01256300	–3.47173800	0.69968900
H	0.22075900	–0.94312400	1.33452300
H	–1.29908600	–2.67528800	0.57119000
H	–1.04007600	–2.27178700	–1.11298300
H	–2.21473600	–0.77362000	2.13173800
H	–2.41883300	–0.57917400	–2.15078000
H	–3.91955900	0.98826500	2.29642800
H	–4.13193400	1.19880100	–1.98140700
H	–5.33588400	2.36895600	1.08307900
C	3.86675300	1.81002200	0.22278000
N	5.19761800	1.97621400	0.22402100
N	3.32098100	0.61834000	0.12667000
N	3.08360200	2.89534700	0.32605200
H	5.61623200	2.85037000	0.49454500
H	2.28980600	0.45798100	–0.03017300
H	2.08474200	2.78807500	0.38137700
H	5.81133900	1.19046000	0.08750600
H	3.44977900	3.82272900	0.19298200
H	3.87296200	–0.22649500	0.13870400
H	1.77890900	–4.06371200	0.70537600
C	0.81903100	–0.25341800	–1.92355900
H	1.62841000	–0.95899900	–2.11748200
H	–0.09535700	–0.61827200	–2.40140300
H	1.08334500	0.70230100	–2.38139800
H	–0.06104000	0.62001000	–0.31529500

Table S57. Cartesian coordinates of the ωB97X-D/6-31G(d,p) optimized Val–Gdm^+ complex (binding energy: –36.6 kcal mol^{-1}).

Energy (Hartrees) = –611.579679			
Atom	X	Y	Z
N	0.24369900	1.30578600	–0.01644600
C	0.89486100	0.02337600	–0.38448200
C	0.88557000	–0.87817800	0.86579300
O	–0.17359300	–1.40282300	1.17311700
C	2.19658100	0.17303600	–1.20604400
C	3.33052300	0.98588800	–0.57429000
C	2.68317600	–1.18593900	–1.72230900
H	0.44460000	1.96819200	–0.76162300
H	0.18895800	–0.48222300	–1.05769400
H	1.87161200	0.73649500	–2.09338700
H	4.14374400	1.09075200	–1.29713100
H	3.75154200	0.51015100	0.31438700
H	3.01199200	1.99691900	–0.30624300
H	3.46917800	–1.04420000	–2.46775400
H	1.87391200	–1.74925900	–2.19748800
H	3.10435100	–1.80907100	–0.92804900
C	–3.25475700	–0.05110800	–0.27272000
N	–2.64369500	–1.22308300	–0.12847000
N	–4.55745300	–0.01349700	–0.59613600
N	–2.57370800	1.07674000	–0.11228400
H	–1.73534000	–1.28875600	0.35043500
H	–5.13057000	–0.83914300	–0.55032200
H	–1.52581200	1.10077600	–0.04391100
H	–3.12737500	–2.07734700	–0.35066300
H	–5.00199900	0.84568500	–0.87205800
H	–3.07167800	1.95116000	–0.07624800
C	2.09451500	–1.08064400	1.73081100
H	1.83341900	–1.73660800	2.56055400
H	2.91922700	–1.51523000	1.16128700
H	2.44644300	–0.11896900	2.11581700
C	0.60585100	1.91513600	1.27093100
H	0.21133900	1.30669500	2.08905600
H	1.68255900	2.05033000	1.42018600
H	0.12881700	2.89520700	1.33312500

Table S58. Cartesian coordinates of the ωB97X-D/6-31G(d,p) optimized Val–Gdm^+ complex (binding energy: –27.1 kcal mol^{-1}).

Energy (Hartrees) = –611.580134			
Atom	X	Y	Z
N	–2.49613800	–0.79543100	–1.22173800
C	–1.56256300	0.03332600	–0.46512600
C	–0.52717400	–0.87261600	0.19221400
O	0.67102800	–0.63477900	0.05109800
C	–2.17073700	1.03497700	0.54993500
C	–1.09606400	1.68075500	1.42962000
C	–2.96581500	2.10544500	–0.20067500
H	–0.98796800	0.62245200	–1.19011800
H	–2.85654900	0.48210500	1.20433900
H	–1.54557100	2.43243600	2.08304300
H	–0.58357400	0.95601400	2.06997600
H	–0.33824400	2.18389000	0.81763900
H	–3.49705900	2.75437600	0.50014200
H	–3.70361300	1.67049900	–0.87960400
H	–2.29375600	2.73481000	–0.79509900
C	3.77975100	0.11370400	–0.21214900
N	3.40534500	–0.97735700	0.44940300
N	5.07670000	0.42549900	–0.32688100
N	2.84870600	0.89245300	–0.75575700
H	2.40838300	–1.18534100	0.51956100
H	5.79000900	–0.13267200	0.11125000
H	1.86983000	0.61556900	–0.66493300
H	4.08110600	–1.62575600	0.81597000
H	3.08968600	1.75180400	–1.21905900
H	5.37795500	1.22750600	–0.85438000
H	–2.64808800	–0.39922200	–2.13839300
C	–0.97953000	–2.04979500	0.99927900
H	–1.49138000	–2.75325100	0.33621000
H	–0.13039800	–2.54014200	1.47481100
H	–1.70001200	–1.73311500	1.75961100
C	–3.76546800	–1.18601900	–0.62127300
H	–4.29571500	–1.82073900	–1.33403000
H	–3.60163400	–1.78530500	0.27798200
H	–4.42832500	–0.35248900	–0.34983600

Table S59. Cartesian coordinates of the ωB97X-D/6-31G(d,p) optimized Val–Gdm^+ complex (binding energy: –27.1 kcal mol^{-1}).

Energy (Hartrees) = –611.575692			
Atom	X	Y	Z
N	0.28876200	1.03931000	0.53348600
C	1.07654000	0.10780400	–0.30426800
C	0.93653000	–1.28273400	0.34883800
O	0.08570100	–2.04697000	–0.07076000
C	2.50788400	0.56226100	–0.67669000
C	3.38952600	1.00871900	0.49333700
C	3.19849900	–0.49820700	–1.54016300
H	0.52207700	0.01266000	–1.24626200
H	2.36304200	1.44046700	–1.31834400
H	2.88583100	1.73107200	1.14489000
H	3.72522000	0.17224900	1.11061100
H	4.28616300	1.49990100	0.10726400
H	2.57725500	–0.78798400	–2.39305700
H	4.14307800	–0.11292400	–1.93142100
H	3.43004300	–1.40482300	–0.97134900
C	–3.39260800	–0.04202800	–0.09282800
N	–4.26130400	–0.86217200	–0.69943200
N	–3.84802100	1.09715300	0.44791600
N	–2.11168200	–0.33769200	–0.03138300
H	–3.93959200	–1.70236700	–1.15120400
H	–4.78605600	1.42177400	0.28474800
H	–1.74227100	–1.23351200	–0.33484500
H	–5.25537500	–0.73943300	–0.60275900
H	–3.23025800	1.69217300	0.97347200
H	–1.37424500	0.30134800	0.33860200
H	0.70018100	1.09673000	1.46153100
C	0.17546900	2.39264300	–0.02118800
H	1.13247700	2.91665900	–0.12087100
H	–0.28694800	2.33419900	–1.01105900
H	–0.46981700	2.99045000	0.62761300
C	1.79202300	–1.66618700	1.52692200
H	1.89791900	–0.84379600	2.23997600
H	1.35854500	–2.53766700	2.01682400
H	2.79966200	–1.92124000	1.18385800

Table S60. Cartesian coordinates of the ωB97X-D/6-31G(d,p) optimized Ala–Gdm^+ complex (binding energy: –24.9 kcal mol^{-1}).

Energy (in hartrees) = –532.795122

Atom	X	Y	Z
N	–1.72730100	–1.57380700	0.16116200
C	–2.34895100	–0.28697900	0.00375600
C	–1.38891400	0.87734400	–0.23498600
O	–0.18351800	0.74571900	–0.04146600
C	–3.21665100	0.04630100	1.22987200
H	–3.00682700	–0.33450400	–0.87529900
H	–3.77869700	0.97340700	1.09624000
H	–2.59602400	0.14555300	2.12634300
H	–3.92085200	–0.77110900	1.38783000
C	2.94677000	0.05100500	0.14399500
N	2.55304100	1.30637300	–0.05083600
N	2.02990600	–0.90273300	0.28802400
N	4.24972700	–0.24956700	0.19667000
H	3.20873600	2.06904500	–0.03105100
H	2.28609100	–1.87550000	0.27672200
H	4.56335900	–1.17454300	0.43903600
H	1.55465200	1.49891700	–0.12428200
H	1.04380600	–0.63665500	0.25473800
H	4.95496700	0.44454100	0.01336600
H	–1.13538100	–1.60438900	0.98230300
C	–1.95368200	2.20499300	–0.65089700
H	–2.10713900	2.81170400	0.24883000
H	–1.24639100	2.73189000	–1.29360400
H	–2.91709500	2.10373500	–1.15358400
C	–1.09534700	–2.13794100	–1.01800000
H	–1.84990600	–2.27835700	–1.79784800
H	–0.28145900	–1.53232200	–1.45141600
H	–0.70065000	–3.12734700	–0.77417100

Table S61. Cartesian coordinates of the ωB97X-D/6-31G(d,p) optimized Ala–Gdm^+ complex (binding energy: –34.6 kcal mol^{-1}).

Energy (in hartrees) = –532.808511			
Atom	X	Y	Z
N	–0.66381900	1.34807300	0.41098400
C	–1.87746400	0.66696400	–0.03675000
C	–1.74706100	–0.85016100	0.06128400
O	–0.68645200	–1.39700800	0.30735200
C	–2.19299900	1.05197900	–1.48805900
H	–2.73971300	0.94438000	0.59335800
H	–3.11489900	0.58074400	–1.83358300
H	–2.32946500	2.13366200	–1.57008800
H	–1.37714900	0.75130900	–2.15157800
C	2.63858300	–0.18710900	–0.23132700
N	1.87535200	0.78577000	–0.71381600
N	2.08401200	–1.13160800	0.52163700
N	3.95479600	–0.21662700	–0.49007900
H	0.89373000	0.91622700	–0.36936700
H	1.06424100	–1.22369000	0.53382400
H	4.41827600	0.56222000	–0.92648100
H	2.25366700	1.43480900	–1.38371200
H	2.64654500	–1.83192900	0.97446400
H	4.51496700	–1.01932100	–0.25740100
H	–0.75803200	2.32532800	0.14473600
C	–0.45434900	1.29733200	1.86482800
H	–0.26473300	0.26785700	2.17206400
H	0.42175200	1.89688400	2.12007000
H	–1.31565700	1.67734800	2.42924600
C	–2.98662200	–1.66265500	–0.19979500
H	–3.00051600	–1.94638200	–1.25808900
H	–2.95047400	–2.58046700	0.38800200
H	–3.90384300	–1.11026600	0.01354700

Table S62. Cartesian coordinates of the ωB97X-D/6-31G(d,p) optimized Arg–Gdm^+ complex (binding energy: –25.4 kcal mol^{-1}).

Energy (in hartrees) = –815.513168			
Atom	X	Y	Z
N	1.05343500	2.26197500	–0.16383200
C	0.08273400	1.31242000	0.32333500
C	0.69193000	0.02072800	0.87121400
O	1.69949900	–0.45002500	0.34694400
C	–0.90966100	0.97535200	–0.80821000
C	–2.06596100	0.05505900	–0.42227800
C	–3.15588500	0.01452200	–1.49926900
N	–4.26056200	–0.87835600	–1.18309100
C	–4.98382500	–0.72595400	0.00262700
N	–5.19438900	0.60708200	0.35146600
N	–5.43383000	–1.65454100	0.75529700
H	1.46360600	1.95340500	–1.03690600
H	–0.47678000	1.78414900	1.14237300
H	–0.34366500	0.53578300	–1.64096700
H	–1.29513300	1.93833900	–1.15812100
H	–1.71048500	–0.96847700	–0.24593000
H	–2.53513500	0.40597900	0.50432900
H	–2.73757300	–0.31175900	–2.45698000
H	–3.53645600	1.02806600	–1.66143100
H	–5.50787900	1.18747800	–0.41587100
H	–5.11005300	–2.57078700	0.45194500
C	4.77891400	–0.94961800	–0.38274900
N	4.13528500	0.11790300	–0.84904600
N	4.12251600	–1.82347300	0.37461000
N	6.07163600	–1.14018100	–0.67206900
H	4.62867700	0.85968800	–1.31592700
H	4.53865000	–2.69903000	0.64326300
H	6.55994800	–0.53469400	–1.31043500
H	3.14237500	0.22100300	–0.62955100
H	6.59080700	–1.90308400	–0.27063400
H	3.14530400	–1.63533600	0.59919200
C	2.04740200	2.71693100	0.79117700
H	2.66855800	3.48609400	0.32646100
H	1.54103700	3.18233800	1.64222300
H	2.71077800	1.92764000	1.18572800
C	0.07062700	–0.62621000	2.06884700
H	0.38805000	–1.66464700	2.16707600
H	0.40345700	–0.06745700	2.95281100
H	–1.01894600	–0.55726700	2.04634300

H	–4.07423500	–1.84780300	–1.39494900
H	–5.82718700	0.65834000	1.13889700

Table S63. Cartesian coordinates of the ωB97X-D/6-31G(d,p) optimized Arg–Gdm^+ complex (binding energy: –33.6 kcal mol^{-1}).

Energy (in hartrees) = – 815.525334			
Atom	X	Y	Z
N	1.65474400	–0.72786500	1.48274900
C	0.46094900	–1.06770300	0.68928800
C	0.86833000	–1.96168100	–0.47695500
O	1.94055000	–1.79559100	–1.03551600
C	–0.18527000	0.22750000	0.15013300
C	–1.54849300	0.08809000	–0.52959400
C	–2.65171300	–0.46296000	0.38986000
N	–3.99108900	–0.27283900	–0.11540200
C	–4.54744100	1.00671300	–0.17061300
N	–4.10311900	2.08548100	0.35567900
N	–5.71783800	1.02864700	–0.91556900
C	3.96158200	1.32075000	–0.53169100
N	3.16950600	1.46213100	0.52400700
N	3.91010000	0.19893200	–1.24249600
N	4.81083600	2.29846000	–0.88287900
H	0.52896100	0.69111300	–0.53958400
H	–0.29155300	0.91457400	0.99812800
H	–1.47803100	–0.52473400	–1.43637600
H	–1.85501000	1.08290400	–0.86684800
H	–2.58664100	0.01505800	1.37534800
H	–2.51758500	–1.53508900	0.57088700
H	–4.23189800	–0.84571600	–0.91201600
H	–6.35086800	0.26153300	–0.73532900
H	–6.17422100	1.92768100	–0.84854500
H	–3.19377000	1.95599300	0.78967100
H	–0.26781100	–1.61505500	1.30613900
H	2.29293500	–1.51936000	1.47191200
H	2.58582400	0.65839400	0.86175400
H	3.18566100	–0.50536900	–1.06758000
H	4.96108400	3.09675100	–0.28960400
H	5.33101200	2.25533300	–1.74295800
H	4.57914900	0.01931000	–1.97221800
H	3.10456100	2.35232400	0.98921000
C	–0.06677200	–3.05815100	–0.89091900
H	–0.00464900	–3.86181900	–0.14731800
H	–1.10491200	–2.71730600	–0.89967100
H	0.21745100	–3.45240600	–1.86593700
C	1.34319200	–0.40526700	2.88073500
H	2.27330300	–0.20786000	3.41755600

H	0.72838400	0.49669500	2.92865200
H	0.80605500	–1.21258600	3.39476800

Table S64. Cartesian coordinates of the ωB97X-D/6-31G(d,p) optimized Arg–Gdm^+ complex (binding energy: –38.0 kcal mol^{-1}).

Energy (in hartrees) = –815.552355			
Atom	X	Y	Z
N	–2.14325800	–0.02269000	1.18992700
C	–1.55884000	0.41433600	–0.06758900
C	–1.53202900	1.93432100	–0.29334300
O	–0.48695900	2.48441700	–0.60426900
C	–2.24671800	–0.26354700	–1.26600400
C	–2.32884200	–1.79590700	–1.20347400
C	–0.98453300	–2.51372000	–1.07824100
N	–0.43089500	–2.36662400	0.26347100
C	0.86856700	–2.03683000	0.49011200
N	1.86020900	–2.10570600	–0.35263800
N	1.11549600	–1.49154800	1.73415700
C	3.06942700	1.02171900	–0.34342000
N	3.53840000	2.25561700	–0.11214400
N	1.86898900	0.86452500	–0.89361200
N	3.78925400	–0.05660800	–0.04436000
H	–1.71384100	0.03549300	–2.17644100
H	–3.26643800	0.13011800	–1.36255900
H	–2.81114600	–2.14229500	–2.12218000
H	–2.98221600	–2.10892800	–0.38180700
H	–0.28376100	–2.09171000	–1.81070300
H	–1.10588800	–3.57415500	–1.32034600
H	–1.09509400	–1.98144500	0.93215500
H	1.60986500	–2.59016100	–1.20766800
H	0.45949000	–1.72417000	2.46505500
H	2.07708200	–1.57742000	2.02732300
H	–0.50464500	0.12406900	–0.03939600
H	–3.15708500	0.01987200	1.15846900
H	3.04153700	3.06069700	–0.45589800
H	4.40227100	2.40532700	0.38007700
H	1.57891100	–0.10200300	–1.01598600
H	1.13567200	1.57580800	–0.82820200
H	4.77267900	0.01365800	0.15552000
H	3.32299900	–0.97931700	–0.15014000
C	–2.81316000	2.71442200	–0.18036300
H	–2.59562000	3.75502500	0.06056600
H	–3.31940700	2.69116600	–1.15230400
H	–3.49539800	2.28780000	0.55811500
C	–1.62760500	0.66752000	2.36940800
H	–2.05673800	0.21885800	3.26773200

H	–0.54151900	0.53897800	2.40303900
H	–1.84099800	1.74676000	2.39362100

Table S65. Cartesian coordinates of the ωB97X-D/6-31G(d,p) optimized Asn–Gdm^+ complex (binding energy: –29.1 kcal mol^{-1}).

Energy (in hartrees) = –701.456605

Atom	X	Y	Z
N	–2.97238700	0.78646600	0.51531200
C	–1.59986500	0.44304900	0.77908300
C	–0.54035600	0.88655100	–0.24708500
O	0.64344800	0.64744100	–0.00039200
C	–1.46720800	–1.07033300	1.00170300
C	–1.68761300	–1.79086800	–0.31980800
N	–2.05418200	–3.08592000	–0.25341300
O	–1.50029200	–1.20499300	–1.38203600
H	–3.27437300	0.43830500	–0.38676000
H	–1.30770700	0.94035000	1.71428100
H	–2.18875600	–1.38013300	1.76119100
H	–0.46384500	–1.32371400	1.35924600
H	–2.29163200	–3.53252300	0.61591900
H	–2.21730400	–3.58369100	–1.11474900
C	3.77679500	0.04684700	0.15253800
N	5.09111000	–0.20304800	0.21317500
N	3.23858600	0.57593100	–0.94019700
N	2.99132800	–0.23391400	1.19068000
H	5.71016100	0.07541900	–0.52949400
H	5.49692100	–0.68218300	0.99925500
H	2.23324700	0.77206000	–0.93156700
H	1.99270100	–0.04197700	1.10499400
H	3.38011800	–0.48276800	2.08419600
C	–3.35652300	2.17076000	0.73255700
H	–4.42654500	2.27569600	0.54350300
H	–3.18234600	2.43430600	1.78055600
H	–2.82956600	2.90808900	0.10634400
C	–0.90339400	1.70263600	–1.44975300
H	–1.91989800	1.51381100	–1.78785400
H	–0.81223600	2.76259500	–1.18568500
H	–0.20414000	1.48676500	–2.25800600
H	3.76776100	0.67155400	–1.79026700

Table S66. Cartesian coordinates of the ωB97X-D/6-31G(d,p) optimized Asn–Gdm^+ complex (binding energy: –35.5 kcal mol^{-1}).

Energy (in hartrees) = –701.463530			
Atom	X	Y	Z
N	2.73635900	–0.44477600	–0.76724100
C	2.01353600	–0.76837300	0.45010500
C	0.74148800	–1.59137500	0.18521500
O	0.00572100	–1.84593700	1.12029800
C	1.62556600	0.51248800	1.21227800
C	0.82583600	1.44449000	0.32708500
N	1.34487100	2.65057900	0.06932900
O	–0.27548500	1.10119700	–0.12909100
H	2.60894400	–1.37866800	1.15531300
H	2.51675500	1.00311500	1.60956100
H	0.99867600	0.22361200	2.05968900
H	2.25284300	2.92372100	0.40580300
H	0.85108400	3.28016500	–0.54414000
C	–3.36938900	0.15127700	–0.07962600
N	–2.44359900	–0.52778800	0.58047400
N	–3.01338500	1.25311700	–0.74002500
N	–4.64531100	–0.25836000	–0.08661800
H	–1.48236200	–0.18521800	0.56116100
H	–2.02927800	1.51919600	–0.73793900
H	–4.94405200	–1.03015500	0.48542800
H	–2.60148000	–1.45128700	0.94871700
H	–5.34098200	0.20142300	–0.64899400
H	–3.70149000	1.87706300	–1.12483900
H	2.86524200	–1.28625200	–1.31722500
C	4.04757300	0.15451300	–0.54494100
H	4.59677500	0.16595600	–1.48772100
H	3.94669900	1.19568200	–0.22390500
H	4.65526000	–0.37450400	0.20624200
C	0.44420200	–2.05534200	–1.21428800
H	1.18356000	–2.79588200	–1.54016300
H	–0.54213200	–2.51757700	–1.24025200
H	0.49864000	–1.20794800	–1.90278600

Table S67. Cartesian coordinates of the ωB97X-D/6-31G(d,p) optimized Asn–Gdm^+ complex (binding energy: –32.7 kcal mol^{-1}).

Energy (in hartrees) = –701.466260			
Atom	X	Y	Z
N	0.48198900	–1.00777700	0.53026900
C	1.43750000	–0.16285600	–0.18032900
C	2.85746200	–0.74661800	–0.05532200
O	3.15780300	–1.46764200	0.85839100
C	1.45174200	1.25746300	0.39016500
C	0.21660400	2.05343800	–0.00384800
N	0.03624800	3.21041300	0.65638800
O	–0.55020600	1.68252600	–0.89024700
O	3.75819100	–0.36305800	–0.96749900
H	0.93736600	–1.25432500	1.41061600
H	1.12965100	–0.11030100	–1.23097200
H	1.55183300	1.21899800	1.48048900
H	2.32839300	1.80434900	0.02181600
H	0.69668600	3.55111100	1.33586600
H	–0.71875800	3.81582900	0.37279600
C	–3.07089700	–0.49800600	–0.01962900
N	–4.35160700	–0.87152400	0.11912400
N	–2.60429900	–0.12865800	–1.21077900
N	–2.24714600	–0.50024400	1.02158700
H	–5.02512100	–0.71010400	–0.61089200
H	–1.76707200	0.46240900	–1.24168800
H	–1.20996700	–0.50886400	0.87081200
H	–2.60991200	–0.66787400	1.94575500
H	–3.18879900	–0.18599300	–2.02809800
H	–4.67272700	–1.33265400	0.95381600
H	3.35351600	0.14374800	–1.68042800
C	0.21853400	–2.26728400	–0.18492300
H	–0.43170300	–2.89452800	0.42813600
H	–0.30261400	–2.04619800	–1.12087700
H	1.13095600	–2.83250100	–0.40510900

Table S68. Cartesian coordinates of the ωB97X-D/6-31G(d,p) optimized Asn–Gdm^+ complex (binding energy: –36.8 kcal mol^{-1}).

Energy (in hartrees) = –701.465832

Atom	X	Y	Z
N	2.84594500	0.61250900	0.47757500
C	1.91592600	0.56853400	–0.63073600
C	0.51953600	1.08797700	–0.25901100
O	–0.30945300	1.17511200	–1.15662200
C	1.76391500	–0.86109700	–1.17849900
C	1.20123800	–1.80361100	–0.12983500
N	1.93117500	–2.89223100	0.16538500
O	0.12397700	–1.57776100	0.42511800
H	3.50779800	–0.15101900	0.41106900
H	2.23896200	1.19572500	–1.48010700
H	2.72712500	–1.20473800	–1.56708100
H	1.05814000	–0.83630100	–2.01277800
H	2.79743800	–3.10605800	–0.29893400
H	1.57209800	–3.54668000	0.84366100
C	–3.41360400	0.04853100	0.04195000
N	–3.01686600	1.09608700	–0.66996900
N	–2.53256400	–0.84787500	0.47155500
N	–4.71303200	–0.10187800	0.34583200
H	–2.01469100	1.23867700	–0.87335900
H	–2.81004700	–1.55726400	1.12928100
H	–1.54264900	–0.85239400	0.21064300
H	–5.05436000	–0.94282600	0.77929300
H	–5.38342300	0.61842100	0.13749100
H	–3.69328600	1.68196800	–1.13046600
C	3.57323800	1.86982400	0.60718200
H	2.88188700	2.68634700	0.83469200
H	4.27371500	1.79682600	1.44091100
H	4.13171100	2.14953100	–0.29961400
C	0.22211700	1.46720400	1.15916200
H	0.73528000	2.40329600	1.40257000
H	–0.85026700	1.61239300	1.29604000
H	0.61157300	0.70483200	1.83479300

Table S69. Cartesian coordinates of the ωB97X-D/6-31G(d,p) optimized Asn–Gdm^+ complex (binding energy: –35.7 kcal mol^{-1}).

Energy (in hartrees) = –701.673664			
Atom	X	Y	Z
N	2.65817500	–0.39642200	0.91601800
C	1.36392900	–0.48632700	0.26811800
C	1.09556100	–1.90286000	–0.25700800
O	–0.05637000	–2.26356400	–0.44176800
C	1.28410000	0.48282900	–0.94028700
C	0.70931400	1.84560000	–0.58632600
N	1.40297100	2.92371000	–0.98073900
O	–0.37052200	1.95264400	0.00503000
H	2.72984800	–1.12809300	1.61539100
H	0.52574600	–0.24641000	0.94508700
H	2.27563100	0.55412900	–1.39585000
H	0.60100600	0.07269700	–1.69297700
H	2.28979400	2.85196400	–1.45072900
H	1.02650800	3.84003200	–0.79047100
C	–3.29458100	–0.12767300	0.19480200
N	–2.00003300	–0.26523000	0.00043900
N	–4.11040200	–1.19044700	0.19215300
N	–3.80242200	1.09552500	0.39875700
H	–1.38813100	0.56720300	0.00228900
H	–3.74516800	–2.11122500	0.01374400
H	–3.18595200	1.89290800	0.42121600
H	–4.78577300	1.25024200	0.53954000
H	–5.10008600	–1.10126800	0.34666900
H	–1.53277100	–1.16443600	–0.13622700
C	2.91362300	0.88402000	1.56789800
H	3.08921200	1.66295100	0.82112300
H	2.09349100	1.22002200	2.22250900
H	3.82320500	0.80133700	2.16475600
C	2.25975400	–2.79477800	–0.57025100
H	3.05478000	–2.23364000	–1.06708500
H	2.69118600	–3.17863600	0.36102800
H	1.92439700	–3.63722500	–1.17418600

Table S70. Cartesian coordinates of the ωB97X-D/6-31G(d,p) optimized Cys–Gdm^+ complex (binding energy: –23.4 kcal mol^{-1}).

Energy (in hartrees) = – 930.961709			
Atom	X	Y	Z
N	2.77703100	0.99897300	0.19982800
C	1.68354000	0.38491300	–0.52167400
C	0.46400500	1.30257400	–0.45793700
O	–0.66443800	0.84135200	–0.30904000
C	1.32272300	–1.06605800	–0.16423400
S	2.70204600	–2.23337500	–0.39344800
H	1.96729500	0.39970300	–1.58505700
H	0.93589600	–1.14122900	0.85577800
H	0.54086100	–1.42178400	–0.83988200
C	–3.62093300	–0.39046100	0.14274300
N	–2.54583500	–1.17203100	0.20074600
N	–4.84355700	–0.90527800	0.31627100
N	–3.46318100	0.90989600	–0.08770400
H	–2.61928300	–2.15350700	0.40769300
H	–1.62926600	–0.75102700	0.05161000
H	–5.66426700	–0.32342600	0.29943900
H	–4.98067500	–1.89071700	0.46709500
H	–4.25260200	1.52631100	–0.18019800
H	3.66286600	0.64348800	–0.13718500
H	3.39715300	–1.88120900	0.70011000
H	–2.51927900	1.27341400	–0.21495100
C	0.69091900	2.77437700	–0.60685500
H	1.45020900	2.97685100	–1.36476900
H	–0.24509000	3.28173200	–0.84156700
H	1.09347100	3.16603800	0.33277300
C	2.69959300	0.93575100	1.65162500
H	1.78963300	1.43803400	1.99988200
H	2.69674800	–0.08118900	2.07506500
H	3.54880000	1.47419400	2.07565200

Table S71. Cartesian coordinates of the ωB97X-D/6-31G(d,p) optimized Cys–Gdm^+ complex (binding energy: –33.4 kcal mol^{-1}).

Energy (in hartrees) = –930.971475			
Atom	X	Y	Z
N	0.34890600	–0.81581200	–0.02790400
C	1.24222000	0.26217700	0.39141300
C	0.64253800	1.64084200	0.10503200
O	–0.48585600	1.76971700	–0.33467400
C	2.69415800	0.14946400	–0.12850000
S	3.47914200	–1.44390800	0.29602600
H	1.29731700	0.20994800	1.48857300
H	2.75159500	0.30997100	–1.20758100
H	3.31596300	0.91423000	0.33960700
C	–3.30249200	–0.38267800	0.19324100
N	–2.32832300	–0.97215700	0.87434300
N	–4.58168700	–0.74221000	0.37688400
N	–2.99511100	0.56529000	–0.68764700
H	–2.55058500	–1.59595100	1.63249700
H	–5.33694200	–0.20498500	–0.01464900
H	–3.69949100	0.97143100	–1.27999700
H	–4.82259600	–1.55014100	0.92574700
H	–2.06277400	0.98530700	–0.66213400
H	–1.32531200	–0.82248100	0.60907200
H	3.14360700	–2.10062900	–0.82556400
H	0.72833700	–1.66977700	0.37862000
C	0.23552600	–1.01363900	–1.47993900
H	1.18126100	–1.28806300	–1.96353600
H	–0.48292500	–1.81452600	–1.66729600
H	–0.13920500	–0.10272700	–1.94788700
C	1.48768100	2.84609900	0.41273800
H	2.22739900	2.98492600	–0.38388400
H	0.85384900	3.73115600	0.45485500
H	2.03678900	2.72773100	1.35088400

Table S72. Cartesian coordinates of the ωB97X-D/6-31G(d,p) optimized Gln–Gdm^+ complex (binding energy: –30.6 kcal mol^{-1}).

Energy (in hartrees) = –740.761442			
Atom	X	Y	Z
N	2.18785900	–1.89810100	–0.37981000
C	2.19960300	–0.45013800	–0.47246800
C	3.20467800	0.29574500	0.42649000
O	3.58539300	1.40284600	0.10646400
C	0.78005100	0.08290200	–0.19942400
C	0.60003300	1.56298900	–0.51907600
C	–0.80137700	2.06388800	–0.25191300
N	–0.96493900	3.39370800	–0.26074100
O	–1.75684600	1.29862000	–0.05042800
C	–3.89267900	–1.06566000	0.17544000
N	–4.78235000	–2.06433000	0.24669800
N	–2.59548300	–1.32079700	0.04474400
N	–4.29537300	0.20106600	0.23929300
H	0.50748900	–0.10903400	0.84718500
H	0.11345700	–0.51858400	–0.82423600
H	0.81787100	1.74487800	–1.57899800
H	1.31599800	2.17590000	0.03616300
H	–1.88172300	3.78591500	–0.11550000
H	–0.19123800	4.02037600	–0.41240600
H	2.46834400	–0.18260600	–1.50154800
H	2.06860600	–2.19136700	0.58446000
H	–4.48746500	–3.02609100	0.25680900
H	–2.25638300	–2.25231500	–0.12545800
H	–5.25145500	0.43761400	0.44190000
H	–3.59088100	0.93539400	0.16430200
H	–5.77113500	–1.88316000	0.28641500
H	–1.95787000	–0.52028200	–0.01229700
C	3.62774100	–0.35196900	1.72474700
H	4.22107000	–1.25182400	1.53437100
H	4.22368000	0.35451900	2.30148600
H	2.75334200	–0.65721000	2.31110900
C	3.35639400	–2.54699700	–0.96181100
H	4.32312100	–2.21451200	–0.55066300
H	3.27894200	–3.62631600	–0.81535100
H	3.37319300	–2.35839900	–2.03923000

Table S73. Cartesian coordinates of the ωB97X-D/6-31G(d,p) optimized Gln–Gdm^+ complex (binding energy: –28.4 kcal mol^{-1}).

Energy (in hartrees) = –740.758992			
Atom	X	Y	Z
N	2.03024700	1.57651300	0.91533100
C	1.10639300	0.79305300	0.11680300
C	–0.17810500	1.54549900	–0.21099900
O	–1.28230400	1.05712700	0.01819400
C	0.83241100	–0.57307700	0.75747800
C	2.11152700	–1.38339600	0.92857200
C	2.67390100	–1.84167200	–0.41387800
N	3.83197500	–2.54139700	–0.34605900
O	2.11818400	–1.59443900	–1.47548800
H	1.58367700	0.59702800	–0.85315000
H	0.14916300	–1.13222100	0.11091300
H	0.35208300	–0.43093900	1.73261200
H	1.92370000	–2.26744800	1.54816600
H	2.86029500	–0.77752900	1.45034700
H	4.24423300	–2.87117300	–1.20393900
H	4.29039800	–2.74493800	0.52540400
C	–3.99413400	–0.66685800	0.05063800
N	–4.01596400	0.60671600	–0.33256000
N	–5.11377300	–1.40056700	0.02395000
N	–2.84928500	–1.19986000	0.46654800
H	–3.14184500	1.13189700	–0.33079800
H	–5.12889400	–2.34361600	0.37422000
H	–2.76555600	–2.18736200	0.63825000
H	–4.87966100	1.07270400	–0.55248300
H	–2.01264700	–0.61342400	0.46771300
H	–5.97268300	–1.03183100	–0.34831600
H	1.58613600	2.05796400	1.68635300
C	–0.06892500	2.91835100	–0.81195900
H	–1.05147900	3.28039500	–1.11404000
H	0.36061800	3.61155500	–0.08201900
H	0.60622800	2.90269200	–1.67159400
C	3.03843900	2.37793700	0.24525300
H	3.59554600	1.74136300	–0.44855400
H	2.65718600	3.24119800	–0.32164400
H	3.74501300	2.75331300	0.98898000

Table S74. Cartesian coordinates of the ωB97X-D/6-31G(d,p) optimized Gln–Gdm^+ complex (binding energy: –45.7 kcal mol^{-1}).

Energy (in hartrees) = –740.782965			
Atom	X	Y	Z
N	–0.19134600	0.58675200	–1.23386300
C	–0.66883500	1.48269900	–0.19649500
C	0.49940800	2.28120900	0.39762900
O	1.62533000	1.82233100	0.44232600
C	–1.34199600	0.71997100	0.96378900
C	–2.69472900	0.07226000	0.63120100
C	–2.60117800	–1.36289600	0.12467000
N	–3.72898400	–2.09088500	0.23767900
O	–1.57718300	–1.82585800	–0.37483800
H	–0.90044500	–0.11655800	–1.42578000
H	–1.39473400	2.21602100	–0.59293600
H	–0.64473000	–0.03745800	1.33462700
H	–1.50439500	1.42897500	1.78110000
H	–3.22751100	0.65842200	–0.12896500
H	–3.33268800	0.08694200	1.52047200
H	–4.57429100	–1.72479900	0.64226100
H	–3.73574100	–3.02926600	–0.13044700
C	2.52528900	–1.63865900	0.19343500
N	3.08934800	–2.82627000	0.47099600
N	3.24106000	–0.52016400	0.30694800
N	1.26616500	–1.55957400	–0.19434300
H	2.62093500	–3.68433600	0.23528300
H	2.75670500	0.37730100	0.27628000
H	0.62124600	–2.33212000	–0.11989300
H	0.85858500	–0.66534100	–0.55333400
H	4.23679600	–0.54533100	0.44267800
H	3.99040700	–2.88789800	0.91306500
C	0.18923700	3.65513900	0.92105800
H	–0.78655200	3.69446500	1.41261900
H	0.97356500	3.99111700	1.59848000
H	0.14271000	4.34083200	0.06664200
C	0.21913900	1.26229600	–2.46257400
H	1.10722300	1.87030000	–2.27145200
H	0.48117000	0.51389500	–3.21240700
H	–0.56514200	1.91193400	–2.87638800

Table S75. Cartesian coordinates of the ωB97X-D/6-31G(d,p) optimized Gln–Gdm^+ complex (binding energy: –39.6 kcal mol^{-1}).

Energy (in hartrees) = –740.771662			
Atom	X	Y	Z
N	2.74811500	0.42674700	–0.89431500
C	2.05268200	–0.02962400	0.30053300
C	1.95642600	–1.56937900	0.38077900
O	0.87619300	–2.13746700	0.35967100
C	0.64423100	0.54677800	0.36609100
C	0.53333900	2.05921600	0.30762200
C	–0.92398200	2.48633600	0.21356500
N	–1.14785900	3.80045600	0.05762900
O	–1.86067000	1.67838600	0.27556400
H	2.46457500	–0.09296300	–1.71670600
H	2.63885000	0.30814100	1.16595700
H	0.17363400	0.18271800	1.28390500
H	0.08500600	0.12978600	–0.47602200
H	0.97548400	2.53029500	1.19404100
H	1.08327900	2.43962600	–0.56010000
H	–2.09683600	4.13729400	0.01602400
H	–0.39477000	4.46620100	0.00569300
C	–3.11502300	–1.37029700	–0.17549900
N	–1.95606000	–1.13336600	0.41636000
N	–3.50191400	–2.61946900	–0.46176200
N	–3.90544600	–0.33479000	–0.47436900
H	–1.16835400	–1.77644100	0.39081200
H	–4.31747500	–2.80323000	–1.02092700
H	–4.87664200	–0.46230700	–0.70227700
H	–1.73533800	–0.14656100	0.57261200
H	–2.96125800	–3.40554500	–0.14124400
H	–3.55223700	0.60362800	–0.31402100
C	3.24050000	–2.35613900	0.42274700
H	3.95308700	–1.91483000	1.12418200
H	3.03011000	–3.39013900	0.69511600
H	3.71027000	–2.34285000	–0.56686200
C	4.19046900	0.60047600	–0.83001600
H	4.43164000	1.29451100	–0.01919600
H	4.77078300	–0.31996900	–0.66963200
H	4.53230200	1.05402900	–1.76296700

Table S76. Cartesian coordinates of the ωB97X-D/6-31G(d,p) optimized Gly–Gdm^+ complex (binding energy: –33.0 kcal mol^{-1}).

Energy (in hartrees) = –493.499090			
Atom	X	Y	Z
N	–0.83141500	–1.29173000	–0.35942700
C	–1.98778800	–0.62152000	0.21400900
C	–1.92523400	0.88444300	0.04939000
O	–0.95406400	1.42807900	–0.44689700
H	–0.74501300	–1.00451800	–1.33160700
H	–2.04060900	–0.84101700	1.28858000
H	–2.94480300	–0.97086800	–0.20900300
C	2.43562700	0.27832200	0.08511900
N	1.72460500	–0.67277500	0.67770200
N	3.75462000	0.38539800	0.30476700
N	1.82651200	1.12323500	–0.74238200
H	0.74378400	–0.86984700	0.36240900
H	4.26018500	–0.32853000	0.80147700
H	0.80506700	1.18838600	–0.73720800
H	2.14339500	–1.24197400	1.39440900
H	4.27472400	1.18485200	–0.01572400
H	2.35218700	1.79851000	–1.27149900
C	–3.13177200	1.66258200	0.48810200
H	–3.89156100	1.60286300	–0.29957200
H	–3.57298300	1.24576000	1.39716400
H	–2.86795100	2.70939700	0.63588500
C	–0.94413900	–2.75349600	–0.30001000
H	–0.07115700	–3.20186800	–0.77828000
H	–0.96475700	–3.07264400	0.74566100
H	–1.84840500	–3.13401600	–0.79179700

Table S77. Cartesian coordinates of the ωB97X-D/6-31G(d,p) optimized Gly–Gdm^+ complex (binding energy: –24.5 kcal mol^{-1}).

Energy (in hartrees) = –493.484029

Atom	X	Y	Z
N	3.48759800	–0.65882000	0.30917400
C	2.13005800	–0.61943100	0.77131300
C	1.24700600	0.53979700	0.31722800
O	0.03616200	0.37511600	0.19536600
C	–3.13665700	–0.17268100	–0.08320900
N	–2.31036200	–1.15148000	0.27423000
N	–2.64048100	1.03779700	–0.32412200
N	–4.44997700	–0.40190300	–0.19899700
H	2.12019900	–0.57698200	1.87045000
H	1.61736800	–1.54789000	0.49376500
H	4.05400800	0.09749300	0.66862700
H	–1.31381600	–0.94611000	0.34788400
H	–1.63690300	1.18420200	–0.22173300
H	–4.83728600	–1.31804000	–0.04662800
C	1.87954200	1.87879800	0.08874200
H	2.47273700	2.16601400	0.96312000
H	2.57119600	1.82402400	–0.75780900
H	1.12219100	2.63672300	–0.10867000
C	3.66707000	–0.87489900	–1.11469200
H	3.20842400	–0.11130500	–1.76708400
H	4.73401000	–0.91186200	–1.34084000
H	3.23895700	–1.84438100	–1.38871100
H	–3.22645000	1.79204100	–0.63925500
H	–2.65234100	–2.06805100	0.50775600
H	–5.09113900	0.33452900	–0.44209000

Table S78. Cartesian coordinates of the ωB97X-D/6-31G(d,p) optimized His–Gdm^+ complex (binding energy: –30.1 kcal mol^{-1}).

Energy (in hartrees) = –757.762119

Atom	X	Y	Z
N	–0.75243200	–2.48929100	–0.47069400
C	–1.07012300	–1.12744400	–0.07298600
C	–2.59213100	–1.05291500	0.17218900
O	–3.29552900	–0.35030800	–0.52200000
C	–0.61708700	–0.03852000	–1.06355000
C	–0.63556600	1.34212600	–0.48788000
N	0.48120900	1.88516900	0.12983900
C	–1.66171600	2.24221900	–0.42842500
C	0.12633100	3.09051700	0.54118200
N	–1.15709900	3.34310100	0.22304500
C	3.12438800	–0.17336300	0.21622000
N	4.09405700	–1.09593100	0.20002200
N	2.28253100	–0.08368500	1.24076600
N	2.97402700	0.67742100	–0.79485000
H	–1.27061600	–0.07947000	–1.93861700
H	0.40037100	–0.26607400	–1.39712000
H	–2.67993300	2.17734700	–0.77468100
H	–1.65956500	4.19337900	0.42526900
H	0.75848000	3.79632200	1.05877000
H	–0.58243300	–0.96155400	0.89934000
H	–1.12599400	–2.68229300	–1.39399400
H	4.22707800	–1.72675100	0.97254800
H	2.34571400	–0.69475300	2.03657600
H	1.53511500	0.61593500	1.16284900
H	3.56502900	0.65098500	–1.60801900
H	2.19425300	1.33930500	–0.73117200
C	0.64714000	–2.85725700	–0.39367400
H	1.33151200	–2.22233300	–0.98447600
H	0.97174600	–2.81838800	0.65260000
H	0.76768000	–3.88694700	–0.73693000
C	–3.13334400	–1.90049200	1.29213200
H	–2.82065300	–1.46970000	2.25044300
H	–4.22187100	–1.92306900	1.25048900
H	–2.71878900	–2.90916500	1.23394800
H	4.76370000	–1.13702800	–0.54997400

Table S79. Cartesian coordinates of the ωB97X-D/6-31G(d,p) optimized His–Gdm^+ complex (binding energy: –46.5 kcal mol^{-1}).

Energy (in hartrees) = –757.784221

Atom	X	Y	Z
N	0.41117000	0.66455300	–1.23264500
C	0.09480800	1.62584200	–0.18401800
C	1.38210000	2.22023500	0.40812500
O	2.41282200	1.57992800	0.41774100
C	–0.66419000	0.92455800	0.96960100
C	–1.90596900	0.22317500	0.51989600
N	–1.85214300	–1.01963500	–0.08494300
C	–3.20563400	0.64567400	0.57564900
C	–3.09644200	–1.33358500	–0.38107200
N	–3.94729000	–0.35672900	0.00022700
C	1.68509200	–2.48699100	0.20494200
N	2.07651400	–1.24821500	–0.03433100
N	0.41455700	–2.83838000	0.00822000
N	2.56733600	–3.40542100	0.63952400
H	–0.91941500	1.66556200	1.73212800
H	0.01105200	0.19909900	1.43576800
H	–3.65499700	1.54239400	0.97097000
H	–4.94950000	–0.36940100	–0.10609500
H	–3.42473300	–2.24334700	–0.86106200
H	–0.52950700	2.45200100	–0.56421700
H	–0.44568500	0.18388700	–1.49319900
H	2.95457300	–0.90098500	0.31692600
H	1.45130400	–0.54599100	–0.50082400
H	0.15590700	–3.81008000	0.04042100
H	–0.34152200	–2.13921900	–0.09161600
H	3.55509200	–3.21653200	0.62439300
C	1.28520100	3.60949900	0.97791300
H	0.35617300	3.75492200	1.53695000
H	2.14627800	3.81736500	1.61219200
H	1.27294500	4.32565400	0.14809500
C	1.01655000	1.26262100	–2.42481700
H	2.01728700	1.62700800	–2.18441900
H	1.11285900	0.49795300	–3.19755000
H	0.42448400	2.09571500	–2.82824100
H	2.26473000	–4.29481700	0.99777600

Table S80. Cartesian coordinates of the ωB97X-D/6-31G(d,p) optimized His–Gdm^+ complex (binding energy: –37.6 kcal mol^{-1}).

Energy (in hartrees) = –757.769193

Atom	X	Y	Z
N	–2.84693800	–1.03775300	0.30570400
C	–1.65480000	–1.26659000	–0.49259900
C	–0.46527400	–1.68214500	0.36838300
O	0.52504100	–2.14645000	–0.18330300
C	–1.25399300	–0.00087400	–1.29037800
C	–0.89877200	1.19830700	–0.46166800
N	0.33592000	1.81233600	–0.56405000
C	–1.67291600	1.88333200	0.43733900
C	0.29824500	2.84520600	0.25018200
N	–0.89624200	2.92651200	0.87743900
C	3.21222200	–0.36578800	–0.22412000
N	4.09028000	0.59838600	0.08064500
N	3.27307100	–1.55308700	0.37866500
N	2.28462400	–0.12883100	–1.14814400
H	–2.07553300	0.24184200	–1.97023800
H	–0.41046200	–0.25411000	–1.93579900
H	–2.67381600	1.70909200	0.79565100
H	–1.17491100	3.63907900	1.53308400
H	1.09552000	3.55448600	0.41428400
H	–1.78285200	–2.07082600	–1.23882400
H	–3.03407700	–1.86246000	0.86583300
H	4.19831300	1.38396300	–0.53983500
H	4.73345400	0.50395800	0.84838600
H	2.44801100	–2.14814700	0.33826100
H	4.08758900	–1.85069600	0.88910900
H	1.78191100	0.77892000	–1.13223600
C	–0.51635600	–1.47192200	1.85204600
H	–1.20350700	–2.19164000	2.31046800
H	0.47486800	–1.61095600	2.28401400
H	–0.91347700	–0.47714000	2.06854600
C	–4.04620000	–0.74349300	–0.47506000
H	–4.91594800	–0.80562200	0.18123700
H	–4.00947400	0.27703000	–0.86754900
H	–4.20222900	–1.42890400	–1.32258600
H	1.67834400	–0.91540200	–1.35194400

Table S81. Cartesian coordinates of the ωB97X-D/6-31G(d,p) optimized Ile–Gdm^+ complex (binding energy: –26.0 kcal mol^{-1}).

Energy (in hartrees) = –650.712745			
Atom	X	Y	Z
N	–2.74354900	–1.04214500	–0.47818400
C	–1.41266900	–0.49340400	–0.49232700
C	–0.41678800	–1.09010600	0.50469300
O	0.78563900	–0.89283900	0.33760400
C	–1.41486500	1.05761500	–0.34586300
C	–1.96973300	1.50773400	1.01532100
C	–2.16467600	1.68003300	–1.52344800
C	–1.89691000	3.01671400	1.24570300
H	–3.19507800	–0.97156000	0.42361500
H	–0.98285600	–0.71150400	–1.47975600
H	–0.36281700	1.37393400	–0.39355400
H	–3.01395200	1.18299000	1.10738300
H	–1.41042400	1.01116400	1.81975400
H	–2.08946800	2.76940700	–1.50656900
H	–3.21999600	1.39943800	–1.49514000
H	–1.75406800	1.33368300	–2.47706600
H	–0.87803000	3.38932400	1.09504900
H	–2.55860100	3.56282100	0.56935100
H	–2.19564500	3.26518100	2.26689100
C	3.79783900	0.07727000	–0.22469600
N	3.53164200	–0.69417500	0.82598900
N	2.80522900	0.43233300	–1.03491000
N	5.04872700	0.49133100	–0.46060900
H	2.56957000	–0.99133900	0.98374900
H	4.26242300	–1.02387000	1.43331100
H	2.95998800	1.04458900	–1.81757700
H	1.86533200	0.08675600	–0.83027100
H	5.27173500	1.05064200	–1.26669700
H	5.80526700	0.25282100	0.15838300
C	–0.90539600	–1.88161100	1.67952100
H	–1.38166500	–2.80413000	1.33255600
H	–0.07819600	–2.12812600	2.34447500
H	–1.66801900	–1.31925700	2.22680100
C	–2.91534200	–2.34931700	–1.08508200
H	–2.65561700	–2.29293400	–2.14675300
H	–2.31264700	–3.15847800	–0.63775500
H	–3.96546500	–2.63981800	–1.01993800

Table S82. Cartesian coordinates of the ωB97X-D/6-31G(d,p) optimized Asp–Gdm^+ complex (binding energy: –34.9 kcal mol^{-1}).

Energy (in hartrees) = –721.310056			
Atom	X	Y	Z
N	–3.54685800	–0.11835300	–0.11552800
C	–2.16872200	–0.23431700	0.32366500
C	–1.44789200	1.11991100	0.49793500
O	–0.36260600	1.33356400	–0.00656300
C	–1.38488700	–1.16417400	–0.62620100
C	–0.16149200	–1.77202900	0.01609300
O	–0.35391900	–2.72906400	0.92107400
O	0.97574200	–1.42566000	–0.23659300
C	3.59312300	0.47272900	–0.16343500
N	3.66916600	–0.82587000	0.11668800
N	4.70215100	1.22692500	–0.15047500
N	2.41949200	1.02072700	–0.45032400
H	–1.05318200	–0.61858800	–1.50952200
H	–2.06752100	–1.96121000	–0.93822200
H	–2.19851200	–0.68309400	1.32755400
H	–4.13175900	0.25965600	0.61905900
H	4.55654700	–1.29845200	0.14781100
H	5.58135300	0.85795300	0.16993700
H	1.57704600	0.44858300	–0.48515100
C	–2.16739800	2.16539900	1.31052800
H	–1.47467800	2.95935300	1.58785400
H	–2.97542900	2.60133600	0.71305800
H	–2.62094400	1.73310000	2.20729300
H	–1.28548900	–2.97004200	0.99239600
H	2.29219900	2.01888100	–0.44130400
H	4.68952600	2.17348800	–0.49069900
H	2.80993800	–1.37239600	0.14422800
C	–3.75962600	0.58409000	–1.37468500
H	–4.83277200	0.65673900	–1.55703300
H	–3.33542100	1.60068500	–1.41586500
H	–3.33093700	0.00963800	–2.20065900

Table S83. Cartesian coordinates of the ωB97X-D/6-31G(d,p) optimized Asp–Gdm^+ complex (binding energy: –22.2 kcal mol^{-1}).

Energy (in hartrees) = –721.296787			
Atom	X	Y	Z
N	0.85103000	1.14068100	0.24957900
C	1.27335600	–0.16209600	–0.19496000
C	0.18202000	–1.22207200	–0.21186900
O	–0.96827000	–0.93429100	0.10586900
C	2.51997800	–0.59924700	0.58913200
C	3.70236200	0.24826700	0.11223600
O	3.74917800	0.72591600	–0.98936200
O	4.71814300	0.39346700	0.97040800
H	0.24581000	1.07707000	1.05927800
H	1.61164800	–0.07153400	–1.23826500
H	2.78295400	–1.64946200	0.41726900
H	2.34450900	–0.47242700	1.66297100
C	–3.97932100	0.23597100	0.17794000
N	–3.77514500	–1.07815300	0.14501300
N	–5.22313100	0.72830200	0.17594100
N	–2.93116700	1.05500300	0.21570800
H	–2.81769800	–1.42366300	0.10587700
H	–6.02381800	0.12839700	0.06682000
H	–1.99583100	0.64676400	0.22697300
H	–5.39582700	1.71247100	0.29632000
H	–3.03792100	2.04585800	0.07720100
H	–4.53524500	–1.72860900	0.25119000
H	4.53178400	–0.02600500	1.81681700
C	0.32896500	2.02712800	–0.77669800
H	–0.54147700	1.63390400	–1.33113000
H	0.05193400	2.98013800	–0.31908600
H	1.12150700	2.23272100	–1.50074800
C	0.53169500	–2.61978500	–0.63429000
H	0.84432900	–3.18823200	0.24920700
H	–0.34253300	–3.11344500	–1.06026300
H	1.35801900	–2.63451300	–1.34838200

Table S84. Cartesian coordinates of the ωB97X-D/6-31G(d,p) optimized Asp–Gdm^+ complex (binding energy: –36.1 kcal mol^{-1}).

Energy (in hartrees) = –721.324515			
Atom	X	Y	Z
N	–0.49418400	–0.16612400	1.33116100
C	–1.36907700	–0.62172000	0.24926900
C	–0.96666300	–2.03880200	–0.16476000
O	0.16669900	–2.43365900	0.04817400
C	–1.23303500	0.26076500	–1.02098800
C	–1.41012100	1.73125200	–0.72256800
O	–2.69657400	2.05851900	–0.58377200
O	–0.50307900	2.52294800	–0.59158800
C	2.86895900	0.18856500	–0.08302900
N	2.76879400	–1.12510800	0.12926600
N	4.02094600	0.70667100	–0.53363100
N	1.83026000	0.96872000	0.16584600
H	–1.98102500	–0.04066500	–1.75851100
H	–0.23691500	0.13254100	–1.44900500
H	–2.42463600	–0.62736000	0.55886300
H	–0.14414200	–0.98611400	1.81890400
H	3.58303200	–1.71603600	0.11783100
H	4.75994200	0.12011600	–0.88283800
H	0.98130500	0.57948200	0.62979500
C	–2.00352000	–2.89945300	–0.82110100
H	–1.53073900	–3.73403600	–1.33763900
H	–2.66283000	–3.29550900	–0.03967500
H	–2.63290400	–2.32812400	–1.50813000
H	–2.74689600	3.00737000	–0.39515000
H	1.74067900	1.89051000	–0.23586400
H	4.17738900	1.70059800	–0.51537900
H	1.85281400	–1.56304800	0.22924200
C	–1.13504700	0.72653700	2.30472700
H	–0.43680100	0.90807000	3.12341800
H	–1.36230800	1.68983000	1.84677200
H	–2.06201600	0.30792700	2.71705300

Table S85. Cartesian coordinates of the ωB97X-D/6-31G(d,p) optimized Asp–Gdm^+ complex (binding energy: –32.5 kcal mol^{-1}).

Energy (in hartrees) = –721.321047			
Atom	X	Y	Z
N	–3.14946100	–0.43267700	0.11208400
C	–1.90984100	–0.42553100	–0.62712800
C	–0.89713800	–1.37109600	0.02084500
O	0.28160000	–1.05071600	0.06337800
C	–1.26431100	0.95018600	–0.94143300
C	–0.70536100	1.65199000	0.26535700
O	–1.64324700	1.92421900	1.17914200
O	0.45634900	1.96465800	0.43998600
C	3.62026400	–0.12376100	–0.12167900
N	2.89616100	0.92923900	–0.48005800
N	3.03566000	–1.19672000	0.40097700
N	4.95106300	–0.11068600	–0.29603500
H	–2.02990100	1.59287400	–1.38665800
H	–0.45376800	0.83155900	–1.66026700
H	–2.12211900	–0.88988800	–1.60262000
H	–3.05066900	0.11027300	0.96324100
H	3.33234000	1.69937400	–0.95965600
H	1.92875800	1.07304100	–0.17114000
H	3.59012200	–1.93238000	0.80506000
H	2.01762400	–1.29143500	0.38898300
H	5.43745800	0.73566300	–0.53925600
C	–4.31596300	0.01988400	–0.63417300
H	–5.19343900	–0.03786500	0.01211800
H	–4.24237100	1.05055600	–1.01457500
H	–4.48603500	–0.64717100	–1.48453300
C	–1.40325500	–2.67007300	0.56716300
H	–2.12342300	–3.12414000	–0.11743300
H	–0.57196500	–3.34596400	0.76734900
H	–1.95450900	–2.47376800	1.49164600
H	–1.21364700	2.38044700	1.91816000
H	5.49759000	–0.95014500	–0.20296600

Table S86. Cartesian coordinates of the ωB97X-D/6-31G(d,p) optimized Asp–Gdm^+ complex (binding energy: –35.5 kcal mol^{-1}).

Energy (in hartrees) = –721.323723

Atom	X	Y	Z
C	2.89150900	–0.41754500	–0.10638800
N	1.80864100	–1.06351200	0.30239300
N	2.85281400	0.90262700	–0.26667600
N	4.02359300	–1.08967900	–0.36624100
N	–0.66229900	–0.19767800	1.36567400
C	–1.58135800	–0.27322400	0.23170300
C	–1.71915300	–1.74363500	–0.19631900
O	–0.88797700	–2.54950500	0.16941800
C	–1.04428500	0.50733700	–0.99723200
C	–0.71039100	1.93463700	–0.65687300
O	–1.78505300	2.71287000	–0.61425200
O	0.40789800	2.34724200	–0.40976700
H	–1.79208700	0.50519600	–1.79353300
H	–0.13309600	0.02826800	–1.36217000
H	–2.57852000	0.11902300	0.48450100
H	–0.70907900	–1.09257500	1.84733100
H	0.98092600	–0.57258400	0.70308700
H	1.96083400	1.40713500	–0.27119600
H	4.13316900	–2.04784600	–0.07947700
H	3.70007600	1.42859600	–0.40132000
H	1.74447200	–2.06734900	0.23651400
H	4.79588500	–0.65094200	–0.83880400
C	–2.90435600	–2.12120800	–1.03940600
H	–3.17676700	–1.34288400	–1.75603300
H	–2.71191300	–3.06250700	–1.55352100
H	–3.76368300	–2.25891800	–0.37278500
H	–1.50661900	3.61069400	–0.37895200
C	–0.93475200	0.87621300	2.32630400
H	–1.98266900	0.89676900	2.65294800
H	–0.30011800	0.72883200	3.20173300
H	–0.68227200	1.84848800	1.90170300

Table S87. Cartesian coordinates of the ωB97X-D/6-31G(d,p) optimized Asp–Gdm^+ complex (binding energy: –32.5 kcal mol^{-1}).

Energy (in hartrees) = –721.320083			
Atom	X	Y	Z
N	3.49032800	1.12144000	0.08329900
C	2.27470400	0.34174200	0.15627700
C	2.52407700	–1.14119200	–0.17115800
O	1.57667800	–1.92244600	–0.12597700
C	1.20291600	0.90652400	–0.81005700
C	–0.24627700	0.61450400	–0.46271500
O	–0.55714400	–0.58165400	0.01057200
O	–1.11024800	1.45607900	–0.62809600
H	3.30332100	2.05041700	–0.27069800
H	1.85009900	0.34791800	1.17795600
H	1.27417200	1.99524900	–0.83482000
H	1.38069200	0.55633800	–1.83393000
C	–4.27277700	–0.10986800	0.21351400
N	–5.58193700	–0.31863700	0.41570800
N	–3.39447800	–1.05335000	0.54787300
N	–3.84730000	1.02790500	–0.31560200
H	–5.92942000	–1.21399800	0.71484300
H	–3.68354700	–1.86672400	1.06430400
H	–4.50122700	1.70424900	–0.67289800
H	–6.25764000	0.40683300	0.24510100
H	–2.83849200	1.21254500	–0.42260400
H	–2.39970500	–0.92830100	0.36209100
H	0.24754900	–1.20463400	0.02414400
C	4.22951500	1.21197600	1.33681900
H	4.58614800	0.22379800	1.64125400
H	5.10844200	1.84140800	1.18897100
H	3.63580900	1.62450100	2.16759800
C	3.88551600	–1.60541400	–0.56227300
H	4.54883000	–1.57440400	0.30854800
H	3.83308300	–2.62548200	–0.94006300
H	4.31525400	–0.91667200	–1.29317800

Table S88. Cartesian coordinates of the ωB97X-D/6-31G(d,p) optimized Asp–Gdm^+ complex (binding energy: –29.9 kcal mol^{-1}).

Energy (in hartrees) = –721.320896

Atom	X	Y	Z
N	2.12774400	0.01401100	1.17043700
C	2.04092800	0.25566500	–0.25737500
C	1.49584400	1.69283300	–0.39467800
O	0.31278600	1.90538300	–0.60189000
C	1.24089000	–0.73617900	–1.17025300
C	0.83420600	–2.01812300	–0.47695700
O	1.78574800	–2.92211200	–0.24884800
O	–0.29713400	–2.24885800	–0.09824300
H	2.69857100	–0.79186500	1.38526900
H	3.07662300	0.27700000	–0.61276200
H	1.84927900	–0.97943100	–2.04792700
H	0.33477000	–0.26121900	–1.54488600
C	–3.14869800	0.26080400	–0.01701500
N	–1.85357500	0.07729400	–0.18105800
N	–3.94038000	–0.77529600	0.28592200
N	–3.68369900	1.48103600	–0.15046400
H	–1.20583800	0.85293300	–0.32967900
H	–3.54535600	–1.69278800	0.41725400
H	–3.10618000	2.26279800	–0.41376700
H	–4.94307100	–0.69440300	0.27914700
H	–4.64207100	1.66762400	0.09176000
H	–1.42979000	–0.85839500	–0.15086700
H	2.61845500	–2.67462100	–0.66638000
C	0.92802000	0.07224500	1.99550700
H	1.22317700	–0.10574300	3.03081500
H	0.49167900	1.07435600	1.95414700
H	0.14903100	–0.65460000	1.73532500
C	2.48320800	2.79762400	–0.17980700
H	3.16694200	2.84085600	–1.03519800
H	1.97165400	3.75380000	–0.07814200
H	3.08391900	2.57986200	0.70736500

Table S89. Cartesian coordinates of the ωB97X-D/6-31G(d,p) optimized Glu–Gdm^+ complex (binding energy: –28.1 kcal mol^{-1}).

Energy (in hartrees) = –760.847652

Atom	X	Y	Z
N	2.80262300	0.54163600	–1.17442900
C	2.56445600	0.06758700	0.17613000
C	2.88473400	–1.43050400	0.34596400
O	2.63769300	–2.18742200	–0.56902100
C	1.07747800	0.25689000	0.52718900
C	0.66174600	1.71540500	0.39156800
C	–0.82645000	1.92496000	0.37439900
O	–1.64718800	1.02166900	0.34356300
O	–1.27434800	3.17486600	0.37422900
C	–4.09109000	–0.99346200	–0.22980200
N	–2.84893900	–1.46228100	–0.13380500
N	–5.10665200	–1.82552900	–0.49242000
N	–4.31075200	0.30585000	–0.06043600
H	0.86550700	–0.11415300	1.53564900
H	0.49429000	–0.35338700	–0.17157100
H	1.07719100	2.09665900	–0.55243100
H	1.09310400	2.32663000	1.19426600
H	3.17907700	0.65697200	0.86904600
H	2.42301000	–0.16457600	–1.80243800
H	–2.63185000	–2.41984900	–0.35192700
H	–4.96465700	–2.81906700	–0.56330000
H	–3.51250200	0.91749500	0.11639700
H	–5.24339600	0.68204800	–0.04293500
H	–6.04425200	–1.48284300	–0.61802500
H	–2.09488400	–0.81080700	0.07217800
H	–0.54896100	3.81141000	0.38602000
C	3.46883400	–1.88526100	1.65641000
H	2.94346800	–1.43009100	2.50231700
H	3.44054000	–2.97211600	1.73170900
H	4.51016900	–1.54768200	1.71210300
C	4.21896000	0.72179100	–1.48475000
H	4.31979600	1.03725600	–2.52501000
H	4.63210100	1.51539200	–0.85484800
H	4.82703300	–0.18438000	–1.34237800

Table S90. Cartesian coordinates of the ωB97X-D/6-31G(d,p) optimized Glu–Gdm^+ complex (binding energy: –26.1 kcal mol^{-1}).

Energy (in hartrees) = –760.845310			
Atom	X	Y	Z
N	2.39096700	–1.60393400	–0.68791700
C	1.40826000	–1.14274800	0.27614700
C	0.20540200	–2.09503500	0.22831300
O	–0.94203600	–1.66272500	0.17938200
C	0.95324300	0.31312100	0.13649400
C	2.07845000	1.33712800	0.19955000
C	1.63937800	2.78054800	0.07935500
O	0.29050600	2.94607800	0.02862700
O	2.39281600	3.71543200	0.03632900
H	2.28430300	–1.12419200	–1.57349000
H	1.83860400	–1.28444900	1.27933200
H	0.42110600	0.42489300	–0.81651000
H	0.23849000	0.53240300	0.93541500
H	2.81506200	1.17817100	–0.59370300
H	2.63232800	1.26188100	1.14199000
C	–3.59562600	0.22134700	–0.09105600
N	–2.36710300	0.72103100	–0.05967400
N	–3.75051800	–1.10050800	–0.02074700
N	–4.66271300	1.02247800	–0.19279400
H	–1.59099000	0.06276500	0.02831900
H	–4.66051000	–1.52759500	–0.04962000
H	–5.59794000	0.65208800	–0.21535800
H	–2.16988600	1.70783300	–0.08960200
H	–4.55944200	2.02120000	–0.25546600
H	–2.92643400	–1.69001700	0.06081300
H	0.16324800	3.90425700	–0.03668800
C	0.48423800	–3.56568300	0.21992500
H	1.31115100	–3.81256000	0.88986000
H	–0.41272800	–4.12399400	0.48745900
H	0.81069700	–3.84771800	–0.78516000
C	3.78122800	–1.62216600	–0.25127800
H	3.89644800	–2.33988300	0.56625300
H	4.40679800	–1.96703700	–1.07664900
H	4.16752800	–0.65086500	0.09133100

Table S91. Cartesian coordinates of the ωB97X-D/6-31G(d,p) optimized Glu–Gdm^+ complex (binding energy: –41.4 kcal mol^{-1}).

Energy (in hartrees) = – 760.629263			
Atom	X	Y	Z
N	0.41577300	–0.44346500	–1.14473100
C	1.51140700	–0.68685400	–0.21618600
C	1.40652700	–2.11376000	0.35634900
O	0.32940600	–2.65961900	0.46860400
C	1.48339900	0.28766200	0.97799200
C	1.94436600	1.72060300	0.68766300
C	0.88620700	2.63737100	0.10164000
O	–0.22380300	2.27728000	–0.22963500
O	1.22290900	3.91359700	–0.05398300
H	0.34840300	0.55040800	–1.33639700
H	2.49361100	–0.60191000	–0.71532700
H	2.14250400	–0.10937800	1.75570100
H	0.47305700	0.29727000	1.39870900
H	2.28984000	2.18452100	1.61953600
H	2.80995400	1.72392400	0.01193300
C	–3.01542700	–0.23376400	0.22990600
N	–4.23679500	–0.65001600	0.60444300
N	–2.00975700	–1.08341300	0.13750600
N	–2.82394900	1.05641200	–0.05232000
H	–4.95310200	0.00356100	0.87167500
H	–1.10302000	–0.83205400	–0.32665200
H	–3.60372400	1.67969200	–0.17495600
H	–2.06914400	–2.01424500	0.51841000
H	–1.88565500	1.43547100	–0.15372600
H	–4.44828800	–1.63118600	0.67019300
H	2.12312900	4.09071900	0.24386600
C	0.52828500	–1.19173500	–2.39802500
H	0.41189500	–2.25950800	–2.19904700
H	–0.27502800	–0.88579900	–3.07049100
H	1.48942600	–1.03116600	–2.90568900
C	2.69541600	–2.77837000	0.75951200
H	3.40053000	–2.07452700	1.21038800
H	2.49632900	–3.60614900	1.43942200
H	3.17320400	–3.17324700	–0.14482800

Table S92. Cartesian coordinates of the ωB97X-D/6-31G(d,p) optimized Glu–Gdm^+ complex (binding energy: –39.6 kcal mol^{-1}).

Energy (in hartrees) = –760.865950			
Atom	X	Y	Z
N	–0.69895400	–0.25529200	1.34292500
C	–1.62339500	–0.95716300	0.46267300
C	–0.88684700	–1.96867000	–0.41667100
O	0.32831900	–2.04265500	–0.42711500
C	–2.42321800	0.03362000	–0.40797500
C	–1.55886300	1.05195800	–1.16550300
C	–1.09443800	2.24533300	–0.36292100
O	–0.02576500	2.80500000	–0.49267100
O	–2.01689600	2.67713500	0.50583200
C	2.90819000	0.11937600	–0.13924800
N	1.75199700	0.72417900	0.06775600
N	2.99777700	–1.20385900	0.00494500
N	3.99544200	0.83276500	–0.46954400
H	–3.13782100	0.56377100	0.22664400
H	–3.02082900	–0.53272000	–1.12638600
H	–2.14905200	1.47231700	–1.98827200
H	–0.67301700	0.59514500	–1.61442800
H	–2.36022400	–1.54845500	1.03548800
H	–1.18045300	0.55831600	1.71633500
H	0.93193000	0.22606300	0.45522400
H	2.13831000	–1.74415100	–0.03340100
H	3.98049200	1.83804000	–0.42687000
C	–1.72243500	–2.86811000	–1.28939500
H	–1.80701500	–2.41447900	–2.28333900
H	–1.21935500	–3.82842700	–1.40740300
H	–2.73124500	–3.01528600	–0.89840000
C	–0.22232400	–1.06168900	2.47260800
H	0.39350900	–1.88356100	2.10343000
H	0.39683100	–0.43732800	3.11959100
H	–1.04185100	–1.48229600	3.07086800
H	–1.67457000	3.48437900	0.91749000
H	1.56822700	1.66629200	–0.25955400
H	3.88565800	–1.67459200	–0.02987500
H	4.83136800	0.38863500	–0.80949900

Table S93. Cartesian coordinates of the ωB97X-D/6-31G(d,p) optimized Glu–Gdm^+ complex (binding energy: –38.6 kcal mol^{-1}).

Energy (in hartrees) = –760.624040

Atom	X	Y	Z
N	1.01085900	0.71940900	–1.40525300
C	0.88884600	1.54201600	–0.19791500
C	2.03657300	1.21260200	0.75944100
O	2.61483600	0.14284200	0.66643000
C	–0.42995600	1.25858700	0.56749000
C	–1.68556900	1.33990800	–0.31516500
C	–2.82017900	0.51428200	0.27606200
O	–3.91142700	1.13999600	0.70475200
O	–2.74750400	–0.69281100	0.36930200
H	1.94992500	0.32900300	–1.41286100
H	0.93933200	2.61334800	–0.44397600
H	–0.36836100	0.25177300	0.99048200
H	–0.52471400	1.95300300	1.40788400
H	–1.47979700	0.88099100	–1.28590500
H	–1.96998000	2.38096000	–0.49803700
C	0.40763500	–2.72824800	–0.06476700
N	–0.30944900	–1.76707800	–0.62720400
N	1.72806700	–2.58229100	0.07771100
N	–0.18760700	–3.86085100	0.33111700
H	0.16504600	–0.93708900	–1.02061800
H	2.12747100	–1.64635900	0.11760700
H	0.27549600	–4.51414200	0.94010000
H	2.30725500	–3.35966700	0.34819800
H	–1.29244800	–1.64049600	–0.37523800
H	–1.14690000	–4.04153700	0.08351700
H	–3.85558100	2.09236900	0.57235100
C	0.80679300	1.45057900	–2.66080600
H	0.96017100	0.76794800	–3.49841100
H	–0.21541600	1.82992700	–2.72250700
H	1.49042800	2.30268400	–2.77195600
C	2.41655500	2.23370200	1.78960000
H	1.54184600	2.73673400	2.20911600
H	3.00806200	1.77204900	2.57951000
H	3.02364500	3.00340200	1.29863000

Table S94. Cartesian coordinates of the ωB97X-D/6-31G(d,p) optimized Glu–Gdm^+ complex (binding energy: –26.1 kcal mol^{-1}).

Energy (in hartrees) = –760.621113			
Atom	X	Y	Z
N	3.02119200	–0.85837600	–0.46104800
C	1.93046400	–0.78174600	0.48829100
C	0.89958200	–1.86300800	0.16842000
O	–0.29664900	–1.67142600	0.36415700
C	1.31473400	0.60640600	0.73898000
C	0.78237300	1.28939600	–0.53129300
C	0.30175000	2.68064800	–0.20101300
O	–1.05705800	2.77846400	–0.13539200
O	1.01187900	3.62094000	0.02782700
H	2.72348600	–0.56337200	–1.38477100
H	2.34154000	–1.12066000	1.45453200
H	2.08185000	1.25014200	1.17805900
H	0.52321100	0.51789900	1.49047100
H	1.59633100	1.40947700	–1.25154700
H	–0.01274700	0.70615100	–1.00263500
C	–3.33663600	–0.56872300	0.01829700
N	–2.33911300	0.21954100	0.39981900
N	–3.12789400	–1.88176600	–0.07919000
N	–4.54138200	–0.05482000	–0.25622300
H	–1.44487500	–0.23103300	0.59384700
H	–2.18204700	–2.23498100	0.04106600
H	–4.75082300	0.90603600	–0.04289300
H	–3.89220800	–2.53092100	–0.16020900
H	–2.31796900	1.21418900	0.20609100
H	–5.27742000	–0.61954400	–0.64581000
H	–1.24520700	3.69903300	0.10243100
C	1.39979700	–3.17447600	–0.35190400
H	2.31670000	–3.47195000	0.16065300
H	0.62605300	–3.93636100	–0.25672000
H	1.67285100	–3.05941600	–1.40575900
C	4.23567300	–0.15141200	–0.07161300
H	4.11537200	0.93549000	0.04707900
H	4.59953400	–0.55938000	0.87604800
H	5.00495600	–0.32919000	–0.82515900

Table S95. Cartesian coordinates of the ωB97X-D/6-31G(d,p) optimized Glu–Gdm^+ complex (binding energy: –31.8 kcal mol^{-1}).

Energy (in hartrees) = –760.619249

Atom	X	Y	Z
N	2.77220800	0.38839500	–0.87457300
C	2.06229100	–0.07243600	0.31011300
C	1.92455100	–1.61062300	0.36525600
O	0.82836600	–2.14576700	0.32931000
C	0.66700200	0.53561000	0.37708700
C	0.59026000	2.05046500	0.30814900
C	–0.85372800	2.50103800	0.20053700
O	–1.80250700	1.73753300	0.24992200
O	–1.08411700	3.79818400	0.04208400
H	2.48607000	–0.11794100	–1.70462400
H	2.65174800	0.23702600	1.18360000
H	0.18473400	0.18671100	1.29495100
H	0.09944700	0.13020600	–0.46511300
H	1.03474300	2.52463600	1.19262300
H	1.15225600	2.41161200	–0.56161400
C	–3.19294400	–1.29584200	–0.16828900
N	–3.62560600	–2.53052800	–0.44829700
N	–2.00175400	–1.09999000	0.37597000
N	–3.96512800	–0.23677400	–0.42482300
H	–3.09928800	–3.33534600	–0.15107800
H	–1.24150800	–1.77336300	0.33695700
H	–4.94389300	–0.33622000	–0.63461200
H	–1.74018400	–0.12887800	0.54081000
H	–4.47758900	–2.68688000	–0.95977500
H	–3.58933200	0.69370100	–0.27657400
H	–0.26215600	4.30207900	0.00907700
C	3.18660300	–2.43152300	0.40207700
H	3.90422900	–2.02295800	1.11813400
H	2.94700200	–3.46476400	0.65210200
H	3.66537200	–2.41104600	–0.58313200
C	4.21844200	0.52939300	–0.79763600
H	4.46905900	1.21018400	0.02141100
H	4.77518100	–0.40588100	–0.64152000
H	4.57727400	0.98330200	–1.72384700

Table S96. Cartesian coordinates of the ωB97X-D/6-31G(d,p) optimized Glu–Gdm^+ complex (binding energy: –31.8 kcal mol^{-1}).

Energy (in hartrees) = –760.609422

Atom	X	Y	Z
N	1.77148700	–0.30538500	1.55569700
C	2.05854600	–0.75066200	0.20673600
C	2.41542100	0.54687800	–0.54749700
O	1.56407400	1.17997500	–1.15431300
C	1.00529100	–1.57117300	–0.58578500
C	0.03253000	–2.44134200	0.25196600
C	–1.38540000	–1.97757300	0.01622400
O	–1.85094000	–2.07906400	–1.24780800
O	–2.08437800	–1.43070900	0.83805300
H	2.97349700	–1.34629500	0.28576400
H	1.55008200	–2.20189300	–1.29400800
H	0.43624800	–0.87091100	–1.19820300
H	0.12108000	–3.49874700	–0.01683300
H	0.22762500	–2.35778500	1.32167700
C	–1.95119100	1.73043500	–0.21415100
N	–1.51643900	2.96282600	0.06917600
N	–1.31099200	1.01819000	–1.13781300
N	–3.02039500	1.22344800	0.39549500
H	–0.84078700	3.41119500	–0.52898500
H	–0.30968700	1.15929400	–1.29711900
H	–3.09008300	0.20994700	0.48356900
H	–1.73207300	0.15956000	–1.46667300
H	–3.60979600	1.80007000	0.97337600
H	–1.84433800	3.46376400	0.87801500
H	1.91518800	–1.03213100	2.24170800
H	–1.25482500	–2.59143900	–1.80781300
C	3.82529100	1.03521200	–0.41788400
H	4.48939200	0.36780800	–0.97881200
H	3.91906900	2.04846900	–0.80663100
H	4.13019200	0.99218500	0.63102000
C	0.59177200	0.49926500	1.82087800
H	0.57931500	0.74525300	2.88459500
H	0.65388900	1.44455600	1.27252500
H	–0.36323300	0.01569700	1.57457500

Table S97. Cartesian coordinates of the ωB97X-D/6-31G(d,p) optimized Glu–Gdm^+ complex (binding energy: –20.6 kcal mol^{-1}).

Energy (in hartrees) = –760.605895			
Atom	X	Y	Z
N	–1.16721300	0.36025000	1.22224600
C	–1.00055700	1.55692800	0.36707300
C	–2.04233200	1.55877400	–0.76494400
O	–2.78876100	2.49855900	–0.89325200
C	0.40495700	1.59171700	–0.25076900
C	1.55149300	1.55054500	0.77532800
C	2.86783400	1.26174700	0.09802200
O	2.93398800	–0.04073800	–0.32425300
O	3.76629800	2.02982600	–0.09307800
H	–0.61608100	0.52321300	2.06192500
H	–1.19073800	2.47442600	0.93939600
H	0.49758000	2.50368700	–0.84826100
H	0.50760800	0.74955100	–0.94346200
H	1.64459000	2.50242500	1.29988500
H	1.39427700	0.76018700	1.51762500
C	0.09572000	–2.92781900	–0.05305800
N	0.49701500	–1.69595100	0.19371700
N	0.95146600	–3.87082800	–0.46453700
N	–1.19779200	–3.24416800	0.10420900
H	1.43575600	–1.38047600	–0.03619300
H	0.63561500	–4.77936700	–0.76077900
H	–1.51453600	–4.19916500	0.08782000
H	–0.17688100	–0.98278600	0.56348200
H	–1.85492100	–2.53834800	0.39487500
H	1.93802900	–3.68046800	–0.52044900
H	3.78918200	–0.13496700	–0.76903000
C	–2.55491400	0.15836700	1.67115600
H	–3.18015900	–0.16071400	0.83201200
H	–2.57383300	–0.62300900	2.43441100
H	–3.00161300	1.06728600	2.09112500
C	–2.06020600	0.38633700	–1.72469400
H	–3.08136400	0.21875700	–2.06955100
H	–1.45386700	0.64050100	–2.60063700
H	–1.64714400	–0.52660100	–1.28766200

Table S98. Cartesian coordinates of the ωB97X-D/6-31G(d,p) optimized Glu–Gdm^+ complex (binding energy: –34.2 kcal mol^{-1}).

Energy (in hartrees) = –760.617691			
Atom	X	Y	Z
N	3.03912800	–0.41578500	–0.67780100
C	1.96393200	–0.55228800	0.28536500
C	1.41957500	–1.99667900	0.22725400
O	0.22083800	–2.22760100	0.16841200
C	0.79188300	0.41899500	0.15719100
C	1.08659900	1.91039100	0.19980900
C	–0.21028100	2.70054900	0.09106900
O	–1.30699400	2.18959900	–0.02112900
O	–0.11749800	4.02616600	0.12166700
C	–3.40890000	–0.85389100	–0.10380200
N	–3.79927400	–2.13423900	–0.12708500
N	–4.32580400	0.12152300	–0.11134300
N	–2.12783400	–0.54451300	–0.07604300
H	0.08876700	0.19336400	0.96254700
H	0.28073000	0.20256100	–0.78723000
H	1.74399200	2.21665800	–0.62311000
H	1.59165300	2.19817800	1.13061000
H	2.41234400	–0.45585200	1.28528000
H	2.68359300	–0.17461600	–1.59516600
H	–4.76741100	–2.39426200	–0.04549900
H	–5.30346100	–0.06960300	–0.24947600
H	–1.38894900	–1.24632300	0.01064800
H	–3.11341400	–2.87172500	–0.12957700
H	–4.03149100	1.08579900	–0.08848200
H	–1.83599900	0.43672200	–0.08630900
H	0.79684600	4.31836900	0.21418200
C	2.43162800	–3.10420300	0.22825500
H	3.23381900	–2.90163300	0.94253400
H	1.94566900	–4.05395500	0.44972400
H	2.90312400	–3.14882500	–0.75740000
C	4.16375200	0.42353100	–0.29473000
H	4.66014800	–0.01073800	0.57803500
H	4.89106300	0.43693000	–1.10884400
H	3.90558900	1.46629300	–0.05062300

Table S99. Cartesian coordinates of the ωB97X-D/6-31G(d,p) optimized Glu–Gdm^+ complex (binding energy: –27.2 kcal mol^{-1}).

Energy (in hartrees) = –760.606000			
Atom	X	Y	Z
N	–3.61642100	1.13063300	0.75634900
C	–3.04446700	0.16584500	–0.16986100
C	–3.84657700	–1.15595900	–0.14472900
O	–3.27961700	–2.22080800	–0.25853100
C	–1.56563800	–0.11350600	0.13954000
C	–0.58334100	0.64950100	–0.75296800
C	0.87305200	0.38876100	–0.46485400
O	1.20583900	–0.81790500	0.03741000
O	1.76051000	1.18367500	–0.68282700
C	4.98455800	–0.23091700	0.18115900
N	4.12618400	–1.15183400	0.61945600
N	6.29749500	–0.39666300	0.38978100
N	4.53299300	0.83867200	–0.45670100
H	–1.44720300	–1.19638300	–0.00360800
H	–1.39448300	0.11169600	1.19754100
H	–0.71696100	1.73135800	–0.69944800
H	–0.73936900	0.37143700	–1.80381000
H	–3.11896300	0.50878500	–1.22558300
H	–4.61232900	1.21119800	0.58816800
H	3.13265500	–1.07291800	0.42144300
H	6.66524200	–1.25874900	0.75580600
H	3.52215800	1.00288500	–0.54741700
H	6.95765500	0.32516100	0.15380100
H	5.16845800	1.48191900	–0.89883800
H	4.42969200	–1.88934400	1.23278200
C	–5.34682100	–1.06622900	–0.02724400
H	–5.75983700	–0.31964800	–0.71357000
H	–5.78206200	–2.04195600	–0.23930900
H	–5.61515400	–0.77099100	0.99278300
C	–3.03151400	2.46147000	0.67827700
H	–3.62760600	3.14828900	1.28185600
H	–2.02227700	2.45969700	1.10208400
H	–2.97329700	2.86387000	–0.34814000
H	0.42255900	–1.36545700	0.18692200

Table S100. Cartesian coordinates of the ωB97X-D/6-31G(d,p) optimized Glu–Gdm^+ complex (binding energy: –26.3 kcal mol^{-1}).

Energy (in hartrees) = –760.620535

Atom	X	Y	Z
N	0.77791600	1.29861000	1.39864500
C	1.83055800	0.92687800	0.45359300
C	1.58416500	1.65102100	–0.87345700
O	0.62976900	2.39473900	–1.00492800
C	1.91013000	–0.60126300	0.26947000
C	0.52953400	–1.19081900	0.02615800
C	0.50706700	–2.67071900	–0.24733200
O	1.45012500	–3.38255000	–0.45686500
O	–0.77554900	–3.11326800	–0.23206900
H	0.67815700	2.30963600	1.35480900
H	2.82353700	1.26600900	0.79971800
H	2.58312200	–0.84982800	–0.55436600
H	2.35188000	–1.05713600	1.15944900
H	0.03237500	–0.69709500	–0.81962300
H	–0.09876800	–1.01873300	0.90619200
C	–2.87190600	0.57155700	–0.10678900
N	–3.96671000	1.15835300	–0.61049700
N	–2.94134600	–0.71216800	0.26643400
N	–1.75392800	1.26382900	0.02508300
H	–4.02056300	2.16050600	–0.69221400
H	–2.12210500	–1.30442300	0.29639900
H	–0.93776600	1.00014900	0.61022500
H	–1.60402500	2.10908100	–0.50777800
H	–3.83509000	–1.16996100	0.33981700
H	–4.74468900	0.61661700	–0.94887700
C	1.05734200	0.90466000	2.78117900
H	0.30643300	1.34816900	3.43736100
H	0.99170400	–0.18168300	2.88740200
H	2.05207400	1.21988500	3.12423000
H	–0.76119900	–4.06279400	–0.42118600
C	2.56476800	1.41404900	–1.99125400
H	2.26015200	0.52373900	–2.55342300
H	2.55051800	2.26501700	–2.67219600
H	3.57803100	1.23892800	–1.62210800

Table S101. Cartesian coordinates of the ωB97X-D/6-31G(d,p) optimized Glu–Gdm^+ complex (binding energy: –23.1 kcal mol^{-1}).

Energy (in hartrees) = –760.610403			
Atom	X	Y	Z
N	–3.00564200	0.53197200	–0.32292300
C	–1.75429900	–0.11676400	–0.65702500
C	–1.78848700	–1.57300100	–0.15476800
O	–0.82259000	–2.08611100	0.39120900
C	–0.45895100	0.56984200	–0.20521300
C	–0.29537300	2.00325000	–0.69237700
C	0.88781600	2.73727000	–0.10721600
O	1.91120700	1.91695800	0.32804300
O	0.98993700	3.92620300	–0.00748400
H	–3.20882400	1.29874100	–0.94996600
H	–1.73614700	–0.21034300	–1.75376800
H	0.37663900	–0.02708600	–0.57180500
H	–0.41386000	0.54777300	0.88917400
H	–0.18245400	2.03512200	–1.78340400
H	–1.16701200	2.62010700	–0.45840600
C	2.61593000	–1.55894000	0.13419300
N	1.78325400	–1.20124000	1.11254900
N	2.67792000	–2.83889800	–0.23310500
N	3.39039600	–0.64406000	–0.45136800
H	1.79007100	–0.22323700	1.37076700
H	3.15470700	–3.12804700	–1.07109700
H	4.16965000	–0.90152900	–1.03475100
H	2.19099300	–3.53938800	0.30390700
H	3.13791300	0.33364600	–0.36636600
H	0.85676900	–1.63948600	1.11576200
H	2.56035800	2.53293200	0.70335700
C	–3.17806700	0.91732000	1.06931400
H	–4.18346400	1.31964500	1.20457600
H	–3.09239400	0.03347300	1.71140200
H	–2.45959500	1.66659400	1.43690600
C	–3.05867800	–2.34023500	–0.37485300
H	–3.48212600	–2.12953200	–1.35933700
H	–2.87587500	–3.40633600	–0.24265900
H	–3.80462800	–2.00632100	0.35316300