

Supporting Information

Using Hydrogen-Deuterium Exchange to Monitor Protein Structure in the Presence of Gold Nanoparticles

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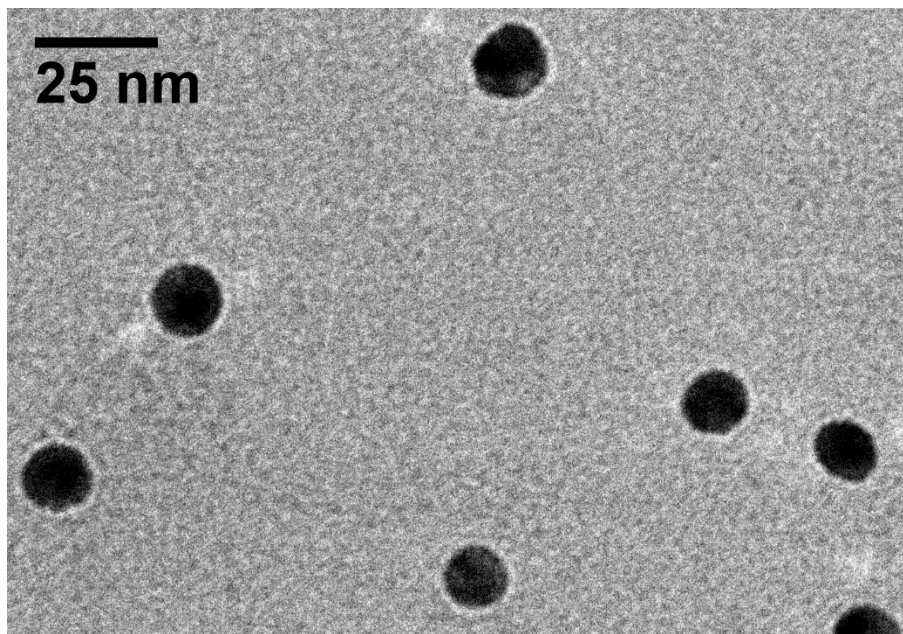


Figure S1. TEM image of 15 nM AuNPs after preparation.

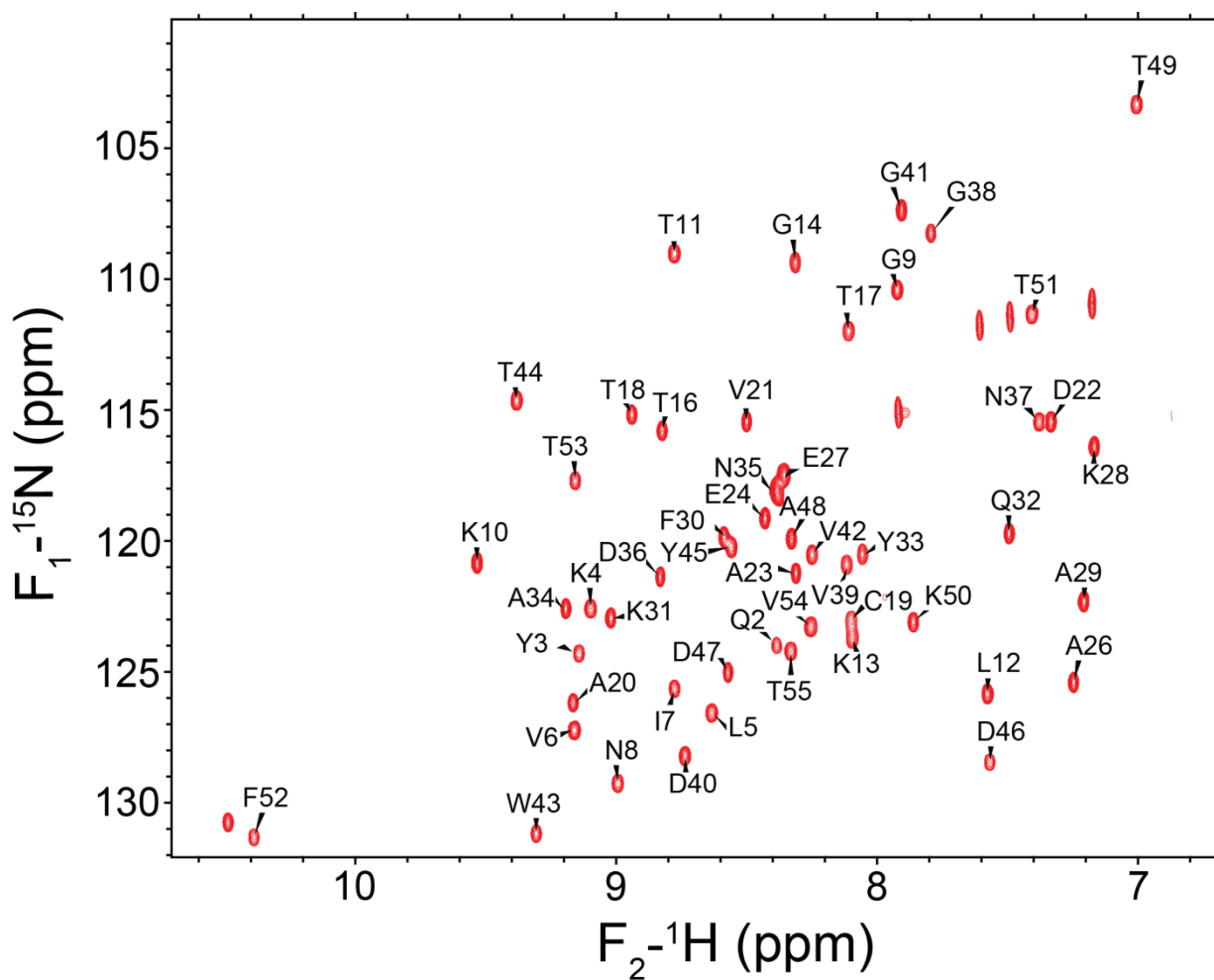


Figure S2. ^{15}N - ^1H HSQC spectrum of K19C GB3. Each cross peak represents the amide protons of K19C GB3 which contains 500 μM of protein, 20mM PIPES pH6.5 and 500 μM , tris(2-carboxyethyl)phosphine (TCEP).

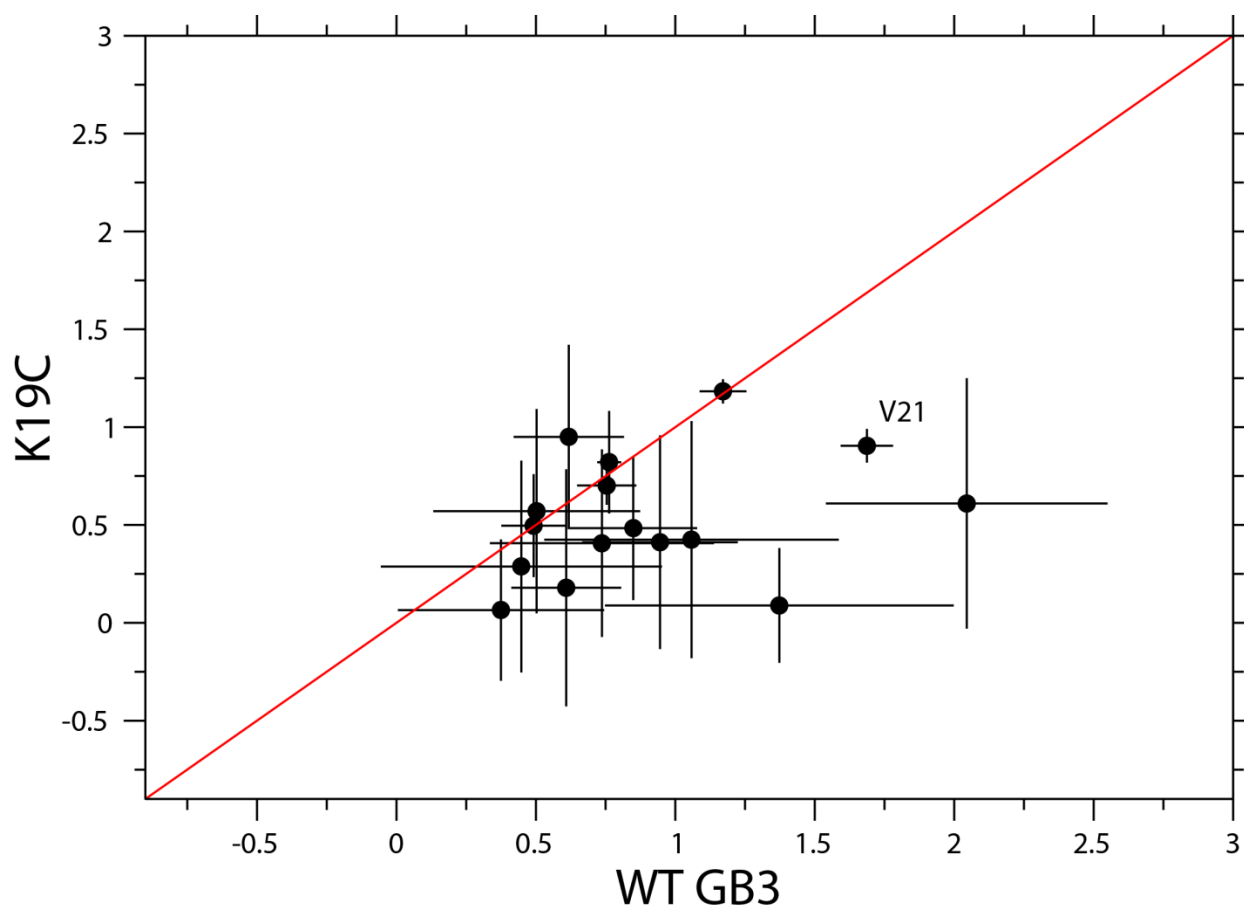


Figure S3. Correlation of SOLEXSY profiles between wild-type and K19C GB3. 500uM of wild-type and K19C GB3 was prepared in 50%H₂O-50%D₂O containing 20mM sodium phosphate pH*6.5 and 20mM PIPES pH*6.5 respectively. For K19C sample, tris(2-carboxyethyl)phosphine (TCEP) was added in equimolar amounts to prevent disulfide formation. The error bars are estimated from the spectral noise, as described in the main text.

Table S1. Hydrogen exchange rates of wild-type GB3.

residue	Real-time Hydrogen Exchange		SOLEXSY	
	GB3 $k_{\text{ex}} \text{ s}^{-1}$	GB3-AuNP $k_{\text{ex}} \text{ s}^{-1}$	GB3 $k_{\text{DH}} \text{ s}^{-1}$	GB3-AuNP $k_{\text{DH}} \text{ s}^{-1}$
1 MET	-	-	-	-
2 GLN	-	-	9.55 ± 0.72	9.01 ± 0.67
3 TYR	0.0153 ± 0.0014	0.0167 ± 0.0082	-	-
4 LYS	0.0051 ± 0.0003	0.0048 ± 0.0023	-	-
5 LEU	0.0025 ± 0.0006	0.0027 ± 0.0009	-	-
6 VAL	0.0012 ± 0.0002	0.0012 ± 0.0009	-	-
7 ILE	0.0025 ± 0.0005	0.0028 ± 0.0012	-	-
8 ASN	-	-	0.38 ± 0.37	0.61 ± 0.47
9 GLY	-	-	0.61 ± 0.20	-
10 LYS	-	-	-	-
11 THR	-	-	0.76 ± 0.04	0.31 ± 0.17
12 LEU	-	-	0.30 ± 0.15	-
13 LYS	-	-	0.74 ± 0.40	0.83 ± 0.70
14 GLY	-	-	0.24 ± 0.36	-
15 GLU	-	-	-	-
16 THR	-	-	0.50 ± 0.37	-
17 THR	-	-	1.07 ± 0.07	-
18 THR	-	-	-	-
19 LYS	-	-	1.17 ± 0.08	0.65 ± 0.32
20 ALA	-	-	0.78 ± 0.19	-
21 VAL	-	-	1.69 ± 0.09	1.19 ± 0.27
22 ASP	-	-	-	-
23 ALA	-	-	0.51 ± 0.10	-
24 GLU	-	-	0.85 ± 0.23	0.88 ± 0.22
25 THR	0.0034 ± 0.0010	0.0039 ± 0.0013	-	-
26 ALA	0.0094 ± 0.0006	0.0093 ± 0.0022	-	-
27 GLU	-	-	0.49 ± 0.12	0.57 ± 0.66
28 LYS	0.0041 ± 0.0003	0.0039 ± 0.0011	-	-
29 ALA	0.0191 ± 0.0013	0.0176 ± 0.0066	-	-
30 PHE	0.0023 ± 0.0004	0.0029 ± 0.0013	-	-
31 LYS	0.0031 ± 0.0003	0.0033 ± 0.0011	-	-
32 GLN	0.0338 ± 0.0082	0.0350 ± 0.0172	-	-
33 TYR	0.0077 ± 0.0004	0.0067 ± 0.0026	-	-
34 ALA	0.0052 ± 0.0002	0.0046 ± 0.0020	-	-
35 ASN	0.0187 ± 0.0021	0.0151 ± 0.0069	-	-
36 ASP	0.0403 ± 0.0081	0.0370 ± 0.0151	-	-

residue	Real-time Hydrogen Exchange				SOLEXSY			
	GB3 $k_{\text{ex}} \text{ s}^{-1}$		GB3-AuNP $k_{\text{ex}} \text{ s}^{-1}$		GB3 $k_{\text{DH}} \text{ s}^{-1}$		GB3-AuNP $k_{\text{DH}} \text{ s}^{-1}$	
37 ASN	0.0257	± 0.0017	0.0179	± 0.0086	-		-	
38 GLY	-		-		-		-	
39 VAL	0.0043	± 0.0003	0.0037	± 0.0019	-		-	
40 ASP	-		-		-		-	
41 GLY	-		-		0.31	± 0.25	-	
42 VAL	0.0034	± 0.0003	0.0029	± 0.0007	-		-	
43 TRP	-		-		1.19	± 0.45	-	
44 THR	0.0016	± 0.0007	0.0016	± 0.0013	-		-	
45 TYR	-		-		0.77	± 0.06	-	
46 ASP	0.0019	± 0.0003	0.0025	± 0.0012	-		-	
47 ASP	-		-		0.75	± 0.11	1.17	± 0.65
48 ALA	-		-		0.34	± 0.26	0.59	± 0.47
49 THR	-		-		0.48	± 0.38	0.55	± 0.28
50 LYS	0.0255	± 0.0023	0.0181	± 0.0049	0.47	± 0.23	2.15	± 0.68
51 THR	0.0035	± 0.0006	0.0037	± 0.0013	-		-	
52 PHE	0.0029	± 0.0006	0.0027	± 0.0014	-		-	
53 THR	0.0031	± 0.0003	0.0036	± 0.0020	-		-	
54 VAL	0.0011	± 0.0003	0.0017	± 0.0013	-		-	
55 THR	0.0023	± 0.0002	0.0024	± 0.0015	-		-	
56 GLU	-		-		0.49	± 0.32	-	

Table S2. Hydrogen exchange rates of ubiquitin.

residue	Real-time Hydrogen Exchange			SOLEXSY		
	Ubq		Ubq-AuNP	Ubq		Ubq-AuNP
	$k_{\text{ex}} \text{ s}^{-1}$		$k_{\text{ex}} \text{ s}^{-1}$	$k_{\text{DH}} \text{ s}^{-1}$		$k_{\text{DH}} \text{ s}^{-1}$
1 MET	-		-	-		-
2 GLN	-		-	1.30 ± 0.61		-
3 ILE	0.0000 ± 0.0001		0.0000 ± 0.0000	-		-
4 PHE	0.0001 ± 0.0000		-	-		-
5 VAL	0.0000 ± 0.0000		0.0123 ± 0.0147	-		-
6 LYS	0.0018 ± 0.0007		0.0014 ± 0.0004	-		-
7 THR	-		-	1.34 ± 0.58		-
8 LEU	-		-	1.39 ± 0.13	2.25 ± 0.47	
9 THR	-		-	5.00 ± 0.10	5.78 ± 0.55	
10 GLY	-		-	0.95 ± 0.07	1.04 ± 0.15	
11 LYS	-		-	-		-
12 THR	-		-	1.07 ± 0.05	1.86 ± 0.24	
13 ILE	0.0038 ± 0.0004		0.0031 ± 0.0005	-		-
14 THR	-		-	0.91 ± 0.38		-
15 LEU	0.0000 ± 0.0001		0.0000 ± 0.0002	-		-
16 GLU	-		-	-		-
17 VAL	0.0001 ± 0.0001		0.0001 ± 0.0000	-		-
18 GLU	0.0074 ± 0.0032		0.0065 ± 0.0011	-		-
19 PRO	-		-	-		-
20 SER	-		-	1.28 ± 0.46		-
21 ASP	0.0002 ± 0.0000		0.0010 ± 0.0015	-		-
22 THR	0.0097 ± 0.0008		0.0078 ± 0.0007	-		-
23 ILE	0.0015 ± 0.0008		0.0014 ± 0.0017	-		-
24 GLU	-		-	-		-
25 ASN	0.0237 ± 0.0036		0.0182 ± 0.0035	-		-
26 VAL	0.0000 ± 0.0001		0.0000 ± 0.0001	-		-
27 LYS	-		-	1.88 ± 0.49		-
28 ALA	0.0036 ± 0.0007		0.0030 ± 0.0004	-		-
29 LYS	0.0004 ± 0.0001		0.0008 ± 0.0009	-		-
30 ILE	0.0000 ± 0.0000		0.0000 ± 0.0000	-		-
31 GLN	-		-	0.83 ± 0.70		-
32 ASP	-		-	0.36 ± 0.41		-
33 LYS	-		-	1.68 ± 0.24	1.70 ± 0.75	
34 GLU	-		-	-		-
35 GLY	-		-	1.06 ± 0.29		-
36 ILE	0.0334 ± 0.0076		0.0390 ± 0.0209	-		-

residue		Real-time Hydrogen Exchange				SOLEXSY			
		Ubq		Ubq-AuNP		Ubq		Ubq-AuNP	
		$k_{\text{ex}} \text{ s}^{-1}$		$k_{\text{ex}} \text{ s}^{-1}$		$k_{\text{DH}} \text{ s}^{-1}$		$k_{\text{DH}} \text{ s}^{-1}$	
37	PRO	-		-		-		-	
38	PRO	-		-		-		-	
39	ASP	-		-		-		-	
40	GLN	-		-		0.80	±	0.33	-
41	GLN	-		-		0.76	±	0.62	-
42	ARG	0.0264	±	0.0112	0.0349	±	0.0119	-	-
43	LEU	-		-		-		-	
44	ILE	0.0001	±	0.0001	0.0001	±	0.0001	-	-
45	PHE	0.0087	±	0.0005	0.0097	±	0.0040	-	-
46	ALA	-		-		3.02	±	0.17	3.51 ± 0.85
47	GLY	-		-		0.58	±	0.07	-
48	LYS	-		-		-		-	
49	GLN	-		-		0.45	±	0.29	-
50	LEU	0.0117	±	0.0014	0.0106	±	0.0035	-	-
51	GLU	-		-		1.84	±	0.56	1.89 ± 0.52
52	ASP	-		-		-		-	
53	GLY	-		-		-		-	
54	ARG	0.0217	±	0.0064	0.0193	±	0.0015	-	-
55	THR	0.0043	±	0.0007	0.0033	±	0.0009	-	-
56	LEU	0.0009	±	0.0007	0.0002	±	0.0001	-	-
57	SER	-		-		0.88	±	0.48	-
58	ASP	-		-		-		-	
59	TYR	0.0024	±	0.0002	0.0019	±	0.0008	-	-
60	ASN	-		-		1.68	±	0.44	-
61	ILE	0.0214	±	0.0064	0.0175	±	0.0007	-	-
62	GLN	-		-		-		-	
63	LYS	-		-		0.42	±	0.27	-
64	GLU	-		-		1.95	±	0.69	-
65	SER	-		-		1.82	±	0.61	-
66	THR	-		-		1.16	±	0.43	-
67	LEU	0.0328	±	0.0048	0.0283	±	0.0131	-	-
68	HIS	-		-		-		-	
69	LEU	0.0083	±	0.0010	0.0071	±	0.0017	-	-
70	VAL	0.0026	±	0.0004	0.0031	±	0.0009	-	-
71	LEU	-		-		0.36	±	0.30	-
72	ARG	-		-		0.26	±	0.05	-
73	LEU	-		-		0.88	±	0.04	0.47 ± 0.24

residue	Real-time Hydrogen Exchange		SOLEXSY			
	Ubq	Ubq-AuNP	Ubq		Ubq-AuNP	
	$k_{\text{ex}} \text{ s}^{-1}$	$k_{\text{ex}} \text{ s}^{-1}$	$k_{\text{DH}} \text{ s}^{-1}$		$k_{\text{DH}} \text{ s}^{-1}$	
74 ARG	-	-	2.13	± 0.04	2.13	± 0.11
75 GLY	-	-	4.64	± 0.06	4.82	± 0.14
76 GLY	-	-	-		-	

Table S3. Fast hydrogen exchange rates (from SOLEXY) of K19C GB3.

Note that colors correspond to the data points (and residue spheres) in Figure 5C in the main text.

residue		K19C			K19C-AuNP		
		$k_{DH} \text{ s}^{-1}$			$k_{DH} \text{ s}^{-1}$		
1	MET	-			-		
2	GLN	4.29	±	0.10	3.57	±	1.80
3	TYR	0.28	±	0.35	-		
4	LYS	0.99	±	0.29	-		
5	LEU	0.18	±	0.57	-		
6	VAL	-			-		
7	ILE	0.51	±	0.49	-		
8	ASN	-			-		
9	GLY	-			-		
10	LYS	-			-		
11	THR	0.82	±	0.26	0.53	±	0.37
12	LEU	-			-		
13	LYS	0.41	±	0.48	-		
14	GLY	1.87	±	0.64	-		
15	GLU	-			-		
16	THR	0.57	±	0.52	2.15	±	0.25
17	THR	0.91	±	0.18	-		
18	THR	-			-		
19	LYS	1.18	±	0.06	0.95	±	1.35
20	ALA	0.84	±	0.58	-		
21	VAL	0.90	±	0.09	2.14	±	0.61
22	ASP	1.40	±	0.35	-		
23	ALA	1.51	±	0.59	-		
24	GLU	0.48	±	0.37	-		
25	THR	-			-		
26	ALA	0.95	±	0.49	-		
27	GLU	0.50	±	0.26	0.79	±	0.15
28	LYS	1.15	±	0.28	-		
29	ALA	0.71	±	0.43	-		
30	PHE	0.41	±	0.55	1.90	±	0.74
31	LYS	1.71	±	0.58	-		
32	GLN	0.30	±	0.22	1.16	±	0.67
33	TYR	0.95	±	0.47	-		
34	ALA	0.43	±	0.61	1.23	±	0.47
35	ASN	1.44	±	0.36	-		

residue		K19C			K19C-AuNP		
		$k_{DH} \text{ s}^{-1}$			$k_{DH} \text{ s}^{-1}$		
36	ASP	0.61	±	0.64	-		
37	ASN	1.31	±	0.49	-		
38	GLY	0.38	±	0.34	-		
39	VAL	-			-		
40	ASP	0.52	±	0.26	-		
41	GLY	-			-		
42	VAL	-			-		
43	TRP	-			-		
44	THR	1.29	±	0.51	-		
45	TYR	0.82	±	0.14	-		
46	ASP	1.45	±	0.38	-		
47	ASP	0.70	±	0.10	0.43	±	0.33
48	ALA	1.10	±	0.49	-		
49	THR	0.21	±	0.50	-		
50	LYS	0.79	±	0.22	-		
51	THR	0.91	±	0.30	-		
52	PHE	0.09	±	0.29	2.34	±	0.44
53	THR	0.74	±	0.34	0.61	±	0.26
54	VAL	0.29	±	0.54	1.92	±	0.46
55	THR	1.06	±	0.27	-		
56	GLU	2.04	±	0.38	-		