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Supplementary Information

Table 1: Chemical shift assignments for mercury-bound merP (ppm).

	H_N (^{15}N)	H_α	H_β	Other
A1	8.19 (125.72)	4.32	1.32	
T2	7.67 (111.45)	4.50	3.94	0.92
Q3	8.43 (122.02)	4.41	1.43, 0.89	2.02, 6.64, 7.65
T4	8.28 (116.25)	5.65	3.71	0.99
V5	9.15 (122.98)	4.69	2.11	0.97
T6	8.73 (120.64)	5.02	3.97	0.96
L7	9.67 (125.45)	5.08	1.64, 1.55	1.18, 0.64, 0.54
A8	9.36 (126.27)	4.69	1.34	
V9	8.14 (121.19)	4.58	1.97	0.80, 0.66
G11	9.17 (106.09)	4.15, 3.87		
M12	6.91 (117.69)	4.81	2.41, 1.87	2.70, 2.14
T13	8.14 (111.17)	4.55	3.45	1.29
C14	7.37 (112.54)	4.72	3.56	
A16	8.22 (121.33)	4.39	1.36	
C17	7.79 (115.98)	4.34	3.43, 2.63	
I19	7.02 (115.29)	3.73	1.88	1.46, 1.22, 0.87
T20	7.72 (119.11)	3.76	4.20	1.36
V21	7.58 (121.47)	3.15	1.79	0.68, 0.42
K22	8.66 (119.96)	3.64	1.95	1.19, 1.64, 3.00
K23	8.21 (119.68)	3.85	1.83, 1.57	1.34, 1.57
A24	7.48 (119.55)	4.01	1.27	
L25	7.77 (115.98)	3.87	1.83, 1.08	1.46, 0.75, 0.47
S26	8.21 (111.17)	3.85	3.85	
K27	6.88 (117.21)	4.16	1.88	1.50, 1.74, 2.91
V28	7.25 (122.70)	3.66	2.14	0.89, 0.73
E29	8.63 (130.53)	3.94	1.95	2.28, 2.16

	H_N (^{15}N)	H_α	H_β	Other
G30	8.61 (110.07)	4.46, 3.64		
V31	7.86 (122.98)	3.99	2.18	0.71, 0.71
S32	9.04 (122.70)	4.67	3.73, 3.61	
K33	7.60 (122.29)	4.51	1.69	1.30, 1.69, 2.89
V34	8.45 (122.70)	4.72	1.83	0.77, 0.77
D35	8.77 (126.41)	5.02	2.56, 2.37	
V36	8.99 (124.08)	4.72	1.93	0.73, 0.73
G37	8.89 (116.11)	4.58, 3.62		
F38	9.09 (124.90)	4.23	3.17, 2.93	7.16, 7.27, 7.22
E39	9.18 (120.92)	3.40	1.95, 1.81	2.27, 2.13
K40	7.91 (114.33)	4.03	1.67, 1.34	1.22, 1.50, 2.83
R41	7.65 (115.98)	3.45	2.02, 1.81	1.60, 1.48, 3.29, 3.04, 6.68
E42	7.69 (116.25)	5.47	1.60	2.11, 1.83
A43	9.22 (122.43)	5.16	0.94	
V44	9.17 (125.04)	4.76	1.95	0.92, 0.75
V45	9.36 (129.15)	4.88	1.95	0.96, 0.87
T46	9.10 (124.90)	5.63	3.85	1.01
F47	9.48 (123.53)	5.44	2.75, 2.58	6.78, 7.00, 7.11
D48	8.17 (119.00)	4.74	2.84, 2.60	
D49	8.85 (128.88)	5.00	3.12, 2.23	
T50	8.92 (110.90)	4.46	4.27	1.25
K51	7.70 (120.64)	4.44	1.60	1.27, 1.60, 2.89
A52	8.28 (120.78)	4.56	1.29	
S53	6.36 (108.29)	4.79	4.16, 3.89	
V54	9.08 (119.82)	3.28	1.97	1.06, 0.89
Q55	8.26 (118.45)	4.04	1.97	2.35, 7.48, 6.79
K56	7.49 (118.45)	3.92	1.74	1.41, 1.50, 2.94
L57	7.61 (118.45)	3.83	1.90, 1.06	1.60, 0.38, 0.05
T58	8.33 (108.57)	4.03	4.23	1.08
K59	7.79 (125.45)	4.04	1.83	1.34, 1.83, 2.94

	H_N (^{15}N)	H_α	H_β	Other
A60	7.44 (119.13)	4.08	1.32	
T61	7.68 (106.50)	3.87	4.56	1.10
A62	7.79 (129.15)	3.54	1.58	
D63	8.94 (120.37)	4.28	2.65	
A64	7.06 (119.27)	4.41	1.46	
G65	7.68 (103.90)	3.96, 3.38		
Y66	8.12 (117.90)	4.62	2.56	6.45, 6.78
S68	9.29 (117.35)	5.49	3.80, 3.68	
S69	8.10 (109.66)	4.65	3.80	
V70	8.78 (122.15)	4.01	1.88	0.89, 0.89
K71	8.89 (130.80)	4.27	1.67	1.34, 1.46
Q72	8.10 (129.15)	4.16	2.04, 1.88	2.25, 7.49, 6.79

Table 2: Chemical shift assignments for reduced merP (ppm).

	H_N (^{15}N)	H_α ($^{13}C_\alpha$)	H_β ($^{13}C_\beta$)	Other
A1	8.19 (125.62)	4.32 (51.80)	1.32 (18.64)	
T2	7.65 (111.39)	4.48 (60.37)	3.92 (70.26)	0.91
Q3	8.45(121.99)	4.41 (53.55)	1.41, 0.87 (30.93)	2.00, 6.64, 7.75
T4	8.27 (116.17)	5.64 (60.61)	3.69 (71.11)	0.97
V5	9.15 (122.90)	4.67 (59.04)	2.11 (35.22)	0.97
T6	8.75 (120.69)	4.98 (61.67)	3.99 (68.70)	0.94
L7	9.62 (125.48)	5.08 (51.60)	1.64, 1.55 (43.01)	1.15, 0.63, 0.54
A8	9.37 (126.10)	4.67 (50.93)	1.34 (19.09)	
V9	8.14 (121.31)	4.57 (58.19)	1.95	0.78, 0.61
P10		(64.10)	(31.38)	
G11	9.10 (106.03)	4.11, 3.83 (44.99)		
M12	6.91 (117.69)	4.81 (56.84)	2.14, 1.87	2.70, 2.14
T13	10.49 (118.45)	4.27 (71.11[6])	3.50 (62.32)	1.20
C14	9.13 (123.57)	5.05 (55.98)	3.19, 3.08 (30.71)	
A15	8.35 (120.14)	3.50 (54.01)	1.24 (17.55)	
A16	7.91 (118.63)	4.22 (53.35)	1.41 (18.43)	

[6] C_α and C_β assignments for T13 may be reversed

	H_N (^{15}N)	H_α ($^{13}C_\alpha$)	H_β ($^{13}C_\beta$)	Other
C17	7.79 (120.14)	3.92 (64.83)	3.28, 2.61	
P18		(65.43)	(30.94)	
I19	6.71 (117.40)	3.64 (63.65)	2.02 (36.64)	1.53, 1.18, 0.85
T20	7.20 (119.11)	3.76 (66.07)	4.20	1.36
V21	8.17 (121.44)	3.07 (66.97)	1.71 (31.60)	0.59, 0.22
K22	8.22 (119.32)	3.64 (59.93)	1.95 (31.60)	1.19, 1.64, 3.00
K23	8.23 (120.07)	3.85 (59.26)	1.81, 1.55 (31.60)	1.29, 1.55
A24	7.76 (119.80)	3.97 (54.22)	1.24 (17.54)	
L25	7.74 (115.98)	3.87 (56.64)	1.81, 1.06 (43.25)	1.45, 0.75, 0.45
S26	8.16 (111.03)	3.90 (60.79)	3.90 (62.56)	
K27	6.90 (117.13)	4.16 (55.54)	1.88 (32.04)	1.48, 1.74, 2.91
V28	7.21 (122.74)	3.64 (62.77)	2.14 (30.07)	0.89, 0.73
E29	8.63 (130.42)	3.92 (57.74)	1.93 (28.30)	2.26, 2.14
G30	8.61 (110.07)	4.46, 3.64 (44.55)		
V31	7.86 (123.02)	4.02 (63.66)	2.18 (30.94)	0.71, 0.71
S32	9.05 (122.68)	4.67 (64.10)	3.75, 3.59 (57.53)	
K33	7.58 (122.33)	4.51 (56.40)	1.69 (35.33)	1.31, 1.69, 2.89
V34	8.43 (122.95)	4.72 (60.58)	1.81 (34.66)	0.75, 0.75

	H_N (^{15}N)	H_α ($^{13}C_\alpha$)	H_β ($^{13}C_\beta$)	Other
D35	8.82 (126.38)	5.02 (52.46)	2.54, 2.37 (43.02)	
V36	8.99 (124.66)	4.72 (61.45)	1.95 (32.26)	0.75, 0.75
G37	9.06 (117.47)	4.51, 3.50 (45.22)		
F38	9.04 (125.55)	4.08 (60.82)	3.10, 2.94 (38.83)	6.97, 7.04, 6.86
E39	9.22 (120.14)	3.54 (59.72)	1.99, 1.86 (27.85)	2.25
K40	7.72 (114.73)	4.01 (55.53)	1.67, 1.34 (32.03)	1.22, 1.50, 2.91
R41	7.74 (116.03)	3.43 (55.10)	1.97, 1.78 (25.93)	1.57, 1.43, 3.19, 2.96, 6.70
E42	7.82 (116.44)	5.49 (53.34)	1.60 (34.34)	2.07, 1.83
A43	9.15 (121.92)	5.07 (49.62)	0.92 (21.06)	
V44	9.08 (125.00)	4.76 (61.68)	1.95 (32.04)	0.91, 0.75
V45	9.38 (129.32)	4.86 (60.58)	1.95 (34.22)	0.96, 0.87
T46	9.09 (124.66)	5.61 (61.23)	3.85 (69.39)	1.01
F47	9.48 (123.43)	5.44 (54.44)	2.75, 2.58 (41.29)	6.78, 7.00, 7.10
D48	8.17 (118.91)	4.74 (51.79)	2.84, 2.59 (40.83)	
D49	8.85 (128.84)	5.00 (54.44)	3.12, 2.23 (39.71)	
T50	8.92 (110.82)	4.44 (62.55)	4.27 (68.95)	1.24
K51	7.70 (120.55)	4.44 (55.99)	1.60 (35.99)	1.27, 1.60, 2.89
A52	8.28 (120.69)	4.56 (49.83)	1.27 (19.78)	

	H_N (^{15}N)	H_α ($^{13}C_\alpha$)	H_β ($^{13}C_\beta$)	Other
S53	6.36 (108.29)	4.79 (54.65)	4.15, 3.87 (66.09)	
V54	9.08 (119.66)	3.27 (66.52)	1.97 (30.72)	1.04, 0.89
Q55	8.27 (118.43)	4.04 (58.82)	1.97 (26.97)	2.35, 7.48, 6.79
K56	7.49 (118.43)	3.90 (58.62)	1.74 (32.69)	1.41, 1.48, 2.94
L57	7.61 (118.43)	3.85 (57.08)	1.90, 1.04 (40.60)	1.60, 0.36, 0.05
T58	8.30 (108.43)	4.01 (67.83)	4.23 (63.65)	1.06
K59	7.79 (125.35)	4.06 (58.38)	1.81 (31.60)	1.34, 1.81, 2.94
A60	7.44 (119.18)	4.08 (54.23)	1.31 (17.32)	
T61	7.70 (106.37)	3.83 (65.85)	4.56 (57.08)	1.08
A62	7.79 (129.32)	3.54 (55.54)	1.57 (17.34)	
D63	8.92 (120.28)	4.30 (56.20)	2.63 (39.27)	
A64	7.07 (119.32)	4.44 (50.92)	1.44 (18.64)	
G65	7.77 (104.39)	4.04, 3.45 (43.67)		
Y66	8.12 (118.43)	4.67 (54.66)	2.53, 2.28	6.45, 6.98
P67		(63.44)	(30.94)	
S68	9.32 (117.68)	5.44 (56.41)	3.82, 3.68 (68.04)	
S69	8.09 (109.66)	4.65 (55.99)	3.80 (65.19)	
V70	8.77 (122.06)	4.01 (63.44)	1.88 (31.38)	0.89, 0.89

	H_N (^{15}N)	H_α ($^{13}C_\alpha$)	H_β ($^{13}C_\beta$)	Other
K71	8.89 (130.76)	4.27 (56.20)	1.67 (32.91)	1.34, 1.46
Q72	8.10 (129.05)	4.16 (56.58)	2.04, 1.88	2.23, 7.49, 6.79