

SUPPLEMENTARY MATERIAL FOR MICROFILM EDITION.

Table 1. ^1H , ^{15}N and ^{13}C chemical shifts for MMOB in 25 mM potassium phosphate, pH 6.8 at 40°C. Chemical shifts are expressed in parts per million downfield from sodium 4,4-dimethyl-4-silapentane-1-sulfonate.

<u>Residue</u>	<u>^{15}N</u>	<u>NH</u>	<u>Hα</u>	<u>Hβ</u>	<u>H others</u>	<u>$^{13}\text{C}\alpha$</u>	<u>$^{13}\text{C}\beta$</u>	<u>^{13}C others</u>
M1								
S2	122.66	7.19	4.72	3.09				
S3	122.32	7.24	4.72	3.09				
A4			4.26	0.98		61.46	17.46	
H5	122.77	8.33		2.11		55.82	32.83	
N6								
A7				1.36		52.68	19.33	
Y8	118.28	8.07	4.72	3.18		57.83	39.67	
N9								
A10				1.48		53.16	19.08	
G11	106.72	8.3	4.02			45.63		
I12	119.07	7.84	4.26	2	H γ 11.00	61.46	38.65	

Q30		4.41			H γ 2.40		56.12	29.48	C γ 33.77
V31	120.8	8.08	4.15	2.1	H γ 1 0.95		62.42	32.94	C γ 1 20.87
V32	123.41	8.14	4.16	2.12	H γ 1 1.41 H γ 2 0.98		62.23	32.82	C γ 1 20.59
H33	123.12	8.45	4.73	3.25 3.15			55.9	30.63	
E34	122.27	8.56	4.39		H γ 2.33		56.59	30.5	C γ 36.30
S35	116.25	8.47	4.52	4			58.86	63.88	
N36	120.73	8.68	5.03	2.98 2.81			52.64	39.25	
A37	123.05	7.77	4.94	1.46			52.64	20.34	
V38	114.46	8.81	4.73	2.12	H γ 1 0.82 H γ 2 0.67		59.45	34.95	C γ 1 22.96 C γ 2 18.80
V39	119.56	8.47	5.2	1.77	H γ 1 0.92 H γ 2 0.82		60.63	36.46	
L40	127.57	9.36	4.81	1.87 1.35	H γ 1.55 H δ 1 1.14 H δ 2 0.92		53.39	46.39	
V41	126.28	8.37	5.22	1.69	H γ 1 0.16 H γ 2 0.00		60.86	32.11	C γ 1 20.35 C γ 2 20.25
L42	126.93	9.39	5.5	1.84	H γ 1.66 H δ 1 0.87		52.81	47.14	C γ 26.18
M43	121.79	9.09	4.36		H γ 2.25 2.76		56.79	34.07	C γ 32.81
K44	119.26	7.48	4.26	2.12	H γ 1 0.63 H δ 1 1.14 1.05 H ϵ 1.38		58.41	33.39	C γ 24.79 C δ 29.19
S45	114.03	7.86	4.69	4.35			57.55	65.88	
D46	120.67	9.1	4.43	2.77 2.69			58.43	40	

E47	117.4	8.7	4.05	2.17	1.75	Hy 2.59 2.53	60.25	29.55	Cy 37.53
I48	119.05	7.79	3.72	2.5		Hy1 1.77 1.72 Hy2 1.22 Hδ1 0.96	62.25	36	Cy1 28.69 Cy2 19.45 Cδ1 9.85
D49	120.95	9.41	4.34	2.99			57.87	39.74	
A50	120.6	7.13	4.26	1.55			54.92	18.29	
I51	118.47	7.68	3.44	2.14		Hy1 0.64 Hy2 0.75 Hδ1 0.41	65.04	38.28	Cy1 29.19 Cy2 16.22 Cδ1 14.85
I52	122.37	8.66	3.4	1.55		Hy1 1.18 -0.30 Hy2 -0.13 Hδ1 0.26	62.52	34.82	Cy1 25.43 Cy2 16.37 Cδ1 9.13
E53	116.07	7.63	3.92	2.09	1.99	Hy 2.34 2.31	59.69	29.98	Cy 35.70
D54	112.42	8.34	4.99	2.73			55.44	43.2	
I55	117.74	7.87	4.47	2.39		Hy1 1.52 1.19 Hy2 1.0 Hδ1 0.83	63.87	38.39	Cy1 27.80 Cy2 16.73 Cδ1 13.09
V56	121.69	8.45	3.7	2.5		Hy1 0.93 Hy2 0.88	67.55	30.96	Cy1 21.36
L57	113.05	8.13	4.23	2.07		Hy 1.69 Hδ1 0.91	55.98	41.68	Cy 25.64
K58	117.64	6.85	4.62	1.81		Hy 1.47	56.51	32.68	Cy 25.15 Cδ 29.24
G59	111.49	8.59	4.73	4.06			47.21		
G60	110.1	8.79	4.05				47.83		
K61	123.81	7.51	4.73	1.8		He 4.43	56.88	33.08	Cy 25.65 Cδ 29.88
A62	120.05	7.75	4.26	1.57			54.41	18.17	
K63	115.67	7.42	4.73	1.67		Hy 2.01 He 4.36	57.68	33.37	Cy 25.37 Cδ 29.24
N64	114.75	8.22	5.26	3.34	2.87		49.79	38.26	

P65		4.83	2.58	H γ 2.16 H δ 3.97 3.65	63.9	32.42	C γ 26.80	
S66	113.44	7.87	4.46	4.21 4.12	59.61	64.39		
I67	122.33	7.44	4.52	1.66	H γ 1 1.88 0.97 H γ 2 0.80 H δ 1 0.97	63.32	39.59	C γ 1 30.52 C γ 2 17.11 C δ 1 13.76
V68	128.23	9.28	4.43	2.12	H γ 1 1.10	61.39	35.77	C γ 1 21.17
V69	123.28	8.51	5.42	2.07	H γ 1 1.05 H γ 2 0.94	60.62	34.85	C γ 1 22.60
E70	126.4	9.67	4.97	2.18 2.11	H γ 2.34 2.29	55.11	34.2	C γ 36.52
D71	124.67	8.75	4.96	2.79 2.41		52.87	41.2	
K72	125.34	8.85	4.64	1.71 1.58	H γ 1.53 1.20	55.65	34.6	C γ 24.31 C δ 28.78
A73	126.64	8.88	4.13	1.64		53.49	17.58	
G74	105.76	8.87	4.03 3.49			45.26		
F75	117.57	7.81	5.09	2.98 2.82		56.49	43.28	
W76	118.83	9.36	5.59	3.18 3.11		55.73	32.36	
W77	124.67	9.87	5.07	3.35 3.25		56.87	29.41	
I78	125.67	9.4	5.15	2.14	H γ 1 1.81 1.08 H γ 2 0.88 H δ 1 0.88	60.55	39.75	C γ 1 27.43 C γ 2 18.66 C δ 1 15.03
K79	126.56	9.08	5.5	1.89 1.70	H γ 1.59 H δ 1 1.74 He 2.96	54.22	35.97	C γ 25.31 C δ 29.64 C ϵ 41.95
A80	121.62	8.46	4.53	1.41		50.94	24.4	
D81	117.81	8.8	5.07	2.68		53.76	41.66	

G82	113.6	8.9	4.37	3.58			47.8	
A83	122.94	7.81	5.43	1.36			52	22.39
I84	119.5	8.67	4.25	1.47	Hy2 0.76 Hδ1 0.67		60.59	42.2 Cy1 28.05 Cy2 0.76 Cδ1 14.75
E85	124.59	8.46	5.47	1.91	Hy 2.14 2.08		54.37	34.1 Cy 36.47
I86	122.94	9.26	4.17	1.78	Hy1 1.55 0.92 Hy2 0.78 Hδ1 0.69		61.08	42.21 Cy1 27.52 Cy2 17.01 Cδ1 12.90
D87	127.26	9.27	5.18	3.20	2.52		52.75	42.31
A88	129.82	9.68	4.17	1.68			55.19	18.44
A89	120	8.8	4.48	1.63			55.01	18.36
E90	119.2	7.23	4.17		Cy 2.32		58.62	30.08 Cy 36.59
A91	121.29	7.81	3.89	1.11			55.11	18.2
G92	105.06	8.63	4.22				47.91	
E93	120.89	7.52	4.16	2.27	2.18 Hy 2.45 2.35		59	29.5 Cy 36.12
L94	120.32	7.67	4.2	2.01	1.72 Hy 1.69 Hδ1 0.90		57.73	42.63 Cy 26.11 Cδ1 23.84
L95	115.32	8.37	4.17	1.81	1.47 Hy 1.76 Hδ1 0.93 Hδ2 0.41		55.45	43.25 Cy 25.76 Cδ1 22.26 Cδ2 25.49
G96	107.83	8.09	4.04	3.95			46.33	
K97	116.34	7.94	4.96	1.95	1.84 Hy 1.34		53.36	32.91
P98		4.44		2.33	1.45 Hy 2.19 2.02 Hδ 3.85 3.71		63.51	31.44 Cy 27.88 Cδ 50.25

F99	126.1	8.3	4.71	3.05 2.90		58.8	42.24	
S100	124.65	9.18	4.88	4.28 3.91		56.3	67.25	
V101	119.17	9.08	3.66	2.02	H γ 1 0.95 H γ 2 0.86	65.94	31.7	C γ 1 21.28
Y102	119.55	7.51	4.06	2.94		61.35	37.71	
D103	118.12	7.23	4.14	1.97 1.76		56.93	40.28	
L104	117.97	6.97	4.12	1.78	H γ 1.59 H δ 1 0.86	57.57	42.25	
L105	117.17	8.01	3.71	1.74 1.48	H γ 1.62 H δ 1 0.77 H δ 2 0.54	57.83	42.1	
I106	115.23	7.54	4.07	1.94	H γ 1 1.34 H γ 2 0.91	63.32	38.31	
N107	117.38	7.71	5.06	3.26 2.71	H δ 7.27 6.99	53.93	40.93	
V108	122.26	7.6	4.15	2.3	H γ 1 0.90	63.86	39.77	
S109	123.69	9.21	4.67	3.69 3.54		59.23	64.54	
S110	111.31	7.55	4.58	3.97		58.22	64.66	
T111	110.91	8.05	5.07	4.1	H γ 2 1.23	59.77	72.66	C γ 2 23.13
V112	123.76	9.06	4.22	1.98	H γ 1 0.97	63.82	33.85	C γ 1 20.51
G113	111.6	8.14	4.59 3.84			43.17		
R114	120.68	8.89	4.57	1.82 1.75	H γ 1.64 H δ 3.28	55.35	31.11	C γ 27.49
A115	128.25	8.44	5.42	1.36		50.25	21.59	

Y116	119.85	9.14	4.98	3.10 2.93			57.01	41	
T117	112.74	8.46	5.31	4.16	Hy2 1.25		60.07	70.45	Cy2 22.47
L118	126.57	8.66	4.73	1.80 1.66	Hy 1.04		54.38	43.59	
G119			4.28 3.81				47.25		
T120	117.47	8.67	4.51	4.86	Hy2 1.38		62.23	68.18	Cy2 21.68
K121	121.21	8.27	4.95	2.03	Hy 1.46 1.26 H8 1.74 He 3.10		56.49	34.69	Cy 25.92 C8 29.63
F122	127.41	9.03	5.09	3.11 2.89			56.39	41.61	
T123	123.47	8.36	5.1	3.21	Hy2 1.01		60.53	71.53	Cy2 21.84
I124	122.88	8.55	5.07	1.58	Hy1 1.18 0.98 Hy2 0.88 H61 0.75		58.8	40.23	Cy1 27.86 Cy2 18.06 C81 15.06
T125	117.93	8.96	5.41	4.28	Hy2 1.40		58.96	71.28	Cy2 21.53
S126	118.6	8.36	4.53	4.27 3.90			58.09	64.24	
E127	123.2	8.77	4.34	2.09	Hy 2.36		57.54	30.45	Cy 36.47
L128	121.35	8.27	4.35	1.68	Hy 0.95		55.79	42.17	Cy 27.29 C81 24.66 C82 23.81
M129	119.34	8.06	4.49	2.06	Hy 2.60 He 1.43		55.89	33.1	
G130	108.57	8.31	4.01				45.59		
L131	121.16	8	4.37	1.67	Hy 0.91		55.42	42.49	Cy 27.16 C81 24.87 C82 23.59
D132	120.04	8.37	4.61	2.82 2.70			54.68	41.06	
R133	120.77	8.07	4.72	1.77	H8 3.23		56.1	30.89	Cy 29.21

A134	123.93	8.33	4.38	1.47		55.69	19.28
L135	120.12	8.16	4.47	1.77 1.70	H γ 0.98	55.37	42.27 C γ 27.26 C δ 1 25.03
T136	111.88	7.9	4.46	4.34	H γ 2 1.27	61.54	69.94 C γ 2 21.52
D137	122.81	8.28	4.77	2.82 2.70		54.6	41.09
I138	124	7.6	4.17	1.91	H γ 1 1.49 1.21 H γ 2 0.91	62.8	39.9