Supporting Information

Automated Sequence- and Stereo-Specific Assignment of Methyl-Labeled Proteins by Paramagnetic Relaxation and Methyl-Methyl Nuclear Overhauser Enhancement Spectroscopy

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Table S1. Assignments obtained at each of the three steps of the assignment protocol (see main text). If the analysis of the PRE data resulted in multiple possible assignments for a single cross-peak, only the two most probable assignments are listed. Inconsistencies between PRE and NOE data are highlighted in red. Cross-peaks for which the correct assignment does not correspond to the most probable PRE assignment are highlighted in yellow (note that these correspond to highly ambiguous assignments). In green, methyl groups for which the expected agreement between PRE and NOE data is restored when considering the effect of transient intra- and inter-molecular interactions in predicting the PREs are highlighted. In the fifth column the PRE/NOE assignments are compared to the reference assignments obtained by conventional means.[S1] Methyl assignments of Ile, Val and Leu were further verified by acquisition of a 4D HC(CO)NH-TOCSY experiment.[S2] Empty entries in the fifth column involve methyl groups whose assignments are missing in the previously deposited data[S1] and could not be assigned directly from the 4D HC(CO)NH-TOCSY spectrum (either because of incompleteness of the backbone assignment or because of fast exchange of exposed backbone amide groups). In the last column the assignment obtained simply by combining the NOE data with chemical shift predictions using the automated procedure described by Xu et al.[S3] is reported; correct assignments obtained using this method are highlighted in cyan. The correctness of the stereospecific assignments for Val and Leu was checked by comparison of the methyl-methyl NOE data to the 3D structure of EIN. The experimental $^{1}H_{M}$-Γ_2 values are listed in Table S2. The chemical shifts for the 140 methyl cross-peaks are listed in Table S3.

	STEP1		STEP 2		STEP 3			
Peak index	Assignment	Selected	Assignment	Selected	Assignment	NOE check	Reference	MAP-XS[S3]
M1	M239	M239	M239	M239	M239		M239	
M2	M1	M1	M1	M1	M1			
M3	M193	M193	M193	M193	M193		M193	
M4	M98	M98	M98	M98	M98			
M5	M78	M78	M78	M78	M78			
I1	I2, I180...		I180, I2...		I180, I157...	I180	I180	I180
I2	I236, I11...		I219, I236		I219, I236	I219	I219	I133
I3	I31	I31	I31	I31	I31	I31	I31	I236
I4	I202, I180...		I202, I180		I202	I157	I157	I157
I5	I2, I180...		I2, 180		I2, I180	I2		I2
I6	I89		I89	I89	I89	I89		I93
I7	I141, I133		I141	I141	I141	I141		I141
I8	I108		I108	I108	I108	I108	I108	I89
I9	I26, I24		I26	I26	I26	I26	I26	I26
I10	I72, I192		I72	I72	I72	I72	I72	I5
I11	I5, I180...		I5		I5	I5	I5	I219
I12	I90	I90	I90	I90	I90	I90	I90	I11
I13	I133, I141		I133	I133	I133	I133	I133	I108
I14	I93	I93	I93	I93	I93	I93	I93	I72
I15	I24, I26		I24	I24	I24	I24	I24	I24
I16	I152	I152	I152	I152	I152	I152		I152
I17	I57	I57	I57	I57	I57	I57	I57	I90
I18	I157, I202...		I157, I180		I157, I180	I202	I202	I202
I19	I236, I219...		I236, I219		I236, I219	I236	I236	I192
I20	I77	I77	I77	I77	I77	I77	I77	I147
I21	I192, I72		I192	I192	I192	I192	I192	I57

Table S1 (continued)

	STEP1		STEP 2		STEP 3			
Peak index	**Assignment**	**Selected**	**Assignment**	**Selected**	**Assignment**	**NOE check**	**Reference**	**MAP-XS[S3]**
I22	I147	I147	I147	I147	I147	I147	I147	I77
I23	I146	I146	I146	I146	I146	I146	I146	I146
I24	I11, I219...		I11	I11	I11	I11	I11	I31
A1	A247	A247	A247	A247	A247	A247		A33
A2	A169, A161		A169	A169	A169	A169	A169	A7
A3	A112, A102		A127	A127	A127	A127	A127	A103
A4	A151	A151	A151	A151	A151	A151	A151	A91
A5	A61, A169		A61	A61	A61	A61	A61	A194
A6	A7		A201, A7...		A7	A194	A194	A128
A7	A102, A112		A112	A112	A112	A112	A112	A100
A8	A50		A50	A50	A50	A50	A50	A201
A9	A33		A33	A33	A33	A33	A33	A241
A10	A128		A102	A102	A102	A102	A102	A102
A11	A71, A194...		A71	A71	A71	A71	A71	A52
A12	A222, A12		A222	A222	A222	A222	A222	A222
A13	A161, A160...		A161	A161	A161	A161	A161	A169
A14	A91	A91	A91	A91	A91	A91	A91	A161
A15	A241	A241	A241	A241	A241	A241	A241	A183
A16	A52	A52	A52	A52	A52	A52	A52	A151
A17	A104		A104	A104	A104	A104	A104	A104
A18	A48	A48	A48	A48	A48	A48	A48	A114
A19	A100		A100	A100	A100	A100	A100	A61
A20	A103		A103	A103	A103	A103	A103	A160
A21	A160, A183...		A183	A183	A183	A183	A183	A71
A22	A16	A16	A16	A16	A16	A16	A16	A16
A23	A201, A194...		A7, A201...		A201, A194	A7	A7	A112
A24	A194, A201...		A194, A201...		A194, A201	A201	A201	A127
A25	A183, A160		A160	A160	A160	A160	A160	A50
A26	A12, A222		A12	A12	A12	A12	A12	A12
A27	A114	A114	A114	A114	A114	A114	A114	A48
A28	A127		A128		A128	A128	A128	A247
VL1					V203G2	V203G2	V203	V235G1
VL2					V156G2	V156G2	V156	V156G2
VL3					V203G1, V85G2...	V203G1	V203	V130G2
VL4					V159G1, V156G1...	V208G2	V208	V208G1
VL5					V223G2, V246G1...	V223G1	V223	V25G1
VL6					V25G2, V25G1	V25G2	V25	V235G2
VL7					V242G1, V246G2...	V246G2		V36G2
VL8					V25G1, V25G2	V25G1	V25	V229G1
VL9					V223G1, V246G2...	V246G1		V25G2

Table S1 (continued)

	STEP1		STEP 2		STEP 3			
Peak index	**Assignment**	**Selected**	**Assignment**	**Selected**	**Assignment**	**NOE check**	**Reference**	**MAP-XS[S3]**
VL10					V235G1, V242G1...	V242G1	V242	V36G1
VL11					V208G2, V212G2...	V229G1	V229	V208G2
VL12					V40G1	V40G1	V40	V223G2
VL13					L144D1	L144D1	L144	L18D1
VL14					V246G1, V223G2...	V223G2	V223	V40G2
VL15					V159G2, V159G1...	V159G2	V159	V159G2
VL16					V229G1, V208G2	V229G2	V229	V159G1
VL17					V229G2	V227G1	V227	V227G1
VL18					V235G2, V235G1...	V235G1	V235	V130G1
VL19					L44D1, L44D2	L44D1	L44	L197D2
VL20					L220D2	L177D2	L177	L19D2
VL21					V107G1	V107G1		V40G1
VL22					V36G1, V36G2	V36G1	V36	V246G2
VL23					V235G1, V242G1...	V242G2	V242	V203G1
VL24					L137D1	L137D1	L137	L6D2
VL25					L199D2, L199D1...		L197	V107G1
VL26					L137D2	V130G1		L163D1
VL27					V156G1, V159G1...	V156G1	V156	V212G2
VL28					V227G1	V227G2	V227	V227G2
VL29					V176G1, V176G2...	V176G1	V176	V203G2
VL30					V176G2, L173D1...	V176G2	V176	V223G1
VL31					L123D2	L123D2	L123	L163D2
VL32					L118D2, L118D1	L118D2	L118	L171D2
VL33					V212G2, V208G1...	V212G2		V246G1
VL34					L92D2, L92D1...	L92D2	L92	L79D1
VL35					V176G1, V176G2...	V208G1	V208	V156G1
VL36					L177D2, L19D1	V212G1		V212G1
VL37					L173D1, V176G2...			L144D2
VL38					L142D2, L144D2	L142D2	L142	L173D2
VL39					L54D2	L54D2		L92D2
VL40					V223G1, V246G2...	V235G2	V235	V229G2
VL41					L115D2	L115D2	L115	L149D1
VL42					L19D2, L17D2	L149D2	L149	L54D2
VL43					V227G2	L6D1	L6	L173D1
VL44					V208G1, V212G1...	V159G1	V159	V176G1
VL45					V212G1, V208G1...	L18D2	L18	L177D2
VL46					V130G1	L79D1	L79	L79D2
VL47					V130G2	V130G2		V107G2
VL48					V36G2, V36G1	V36G2	V36	V242G2
VL49					V40G2	V40G2	V40	V242G1

Table S1 (continued)

Peak index	STEP1 Assignment	STEP1 Selected	STEP 2 Assignment	STEP 2 Selected	STEP 3 Assignment	STEP 3 NOE check	Reference	MAP-XS[S3]
VL50					L177D1, V156G1...	L17D2	L17	L158D1
VL51					L17D2, L19D2	L19D2	L19	L115D1
VL52					L163D2, L163D1...	L163D2	L163	L137D1
VL53					L80D1	L80D2	L80	L6D1
VL54					L138D2	L138D2	L138	L138D2
VL55					L85D1	L85D1		L85D1
VL56					L149D2, L177D1		L171	L142D2
VL57					L85D2	L85D2		L80D1
VL58					L218D1	L218D2	L218	L218D2
VL59					L218D2	L220D1	L220	L220D1
VL60					L163D2, L163D1...	L163D1	L163	L123D2
VL61					L18D2, L18D1	L218D1	L218	L218D1
VL62					L6D1	L220D2	L220	L220D2
VL63					L199D1, L199D2...			L44D2
VL64					L17D1, L177D1	L17D1	L17	L17D2
VL65					L220D1, L6D2	L177D1	L177	L177D1
VL66					L142D1	L142D1	L142	L142D1
VL67					L144D2, L142D2	L144D2	L144	L199D2
VL68					L158D2, L199D1...		L197	L115D2
VL69					L80D2	L80D1	L80	L118D2
VL70					L92D1, L92D2	L92D1	L92	L158D2
VL71					L118D1, L118D2	L118D1	L118	L44D1
VL72					L123D1, L118D1	L123D1	L123	L171D1
VL73					L79D1	L137D2	L137	L137D2
VL74					L138D1	L138D1	L138	L138D1
VL75					L171D1, L171D2...			L118D1
VL76					L197D2, L197D1...	L158D1	L158	L17D1
VL77					L18D1, L18D2	L18D1	L18	L18D2
VL78					L115D1	L115D1	L115	L92D1
VL79					L158D1, L171D2		L171	L144D1
VL80					L171D1, L163D2...	L19D1	L19	L80D2
VL81					L149D1	L149D1	L149	L54D1
VL82					L79D2	L79D2	L79	L85D2
VL83					L6D2, L220D1	L6D2	L6	L123D1
VL84					L44D2, L44D1	L44D2	L44	L19D1
VL85					L54D1	L54D1		L149D2
VL86					V107G2, L92D2...	V107G2		V176G2
VL87					L19D1, L177D2			L199D1
VL88					L197D2, L197D1...		L158	L197D1

Table S2. $^{1}H_{M}$-Γ_2 PRE rates and associated standard deviations measured for the five EIN mutants. PRE too big to be measured accurately are reported as NAN.

	A52C		Q87C		S113C		S196C		A241C	
Peak Index	PRE (s^{-1})	St. Dev.	PRE (s^{-1})	St. Dev.	PRE (s^{-1})	St. Dev.	PRE (s^{-1})	St. Dev.	PRE (s^{-1})	St. Dev.
M1	1.55	0.35	0.75	1.02	0.71	0.94	2.01	1.30	NAN	
M2	0.64	0.41	0.36	0.40	0.59	0.55	0.97	0.32	14.98	0.60
M3	4.71	0.55	1.16	0.35	1.69	0.19	NAN		5.81	0.41
M4	1.55	0.48	22.69	1.74	NAN		0.29	0.70	0.50	0.59
M5	11.48	0.59	11.70	0.75	6.69	0.40	5.42	0.37	2.99	0.25
I1	0.36	0.56	0.41	0.50	-0.27	0.50	2.89	3.55	8.03	1.04
I2	2.90	0.58	0.51	0.85	1.35	0.64	0.60	1.09	NAN	
I3	2.15	1.29	24.93	1.32	3.25	0.41	0.21	0.71	0.41	0.63
I4	0.68	0.58	0.28	0.53	0.47	0.63	8.41	0.49	21.81	2.02
I5	0.34	0.93	0.23	0.54	0.92	0.72	2.05	0.54	4.91	1.00
I6	14.89	0.67	NAN		28.72	2.54	1.56	0.91	1.63	0.51
I7	16.88	2.14	15.95	1.23	9.97	1.18	-1.24	1.54	0.40	0.91
I8	12.21	1.22	23.84	0.58	NAN	11.16	3.17	0.34	1.77	0.74
I9	2.62	0.58	4.63	0.40	NAN	1.80	-0.46	0.46	0.28	0.35
I10	5.57	0.66	2.05	0.57	4.47	0.88	NAN		3.85	0.59
I11	1.02	0.77	1.34	1.21	4.76	0.91	6.41	0.52	3.64	1.03
I12	7.67	0.56	NAN		3.09	0.65	0.10	0.59	0.66	0.54
I13	20.91	1.29	12.57	0.59	25.11	1.53	Overlap		5.70	0.45
I14	7.17	0.70	NAN		7.54	1.35	Overlap		0.72	0.51
I15	5.70	0.35	2.29	0.52	NAN		1.73	0.91	0.52	0.53
I16	8.42	0.71	0.60	0.66	0.79	0.62	16.29	1.00	1.97	0.35
I17	NAN		1.44	0.32	1.74	0.50	NAN		0.88	0.33
I18	0.19	0.61	0.63	0.58	0.91	1.01	4.41	0.82	16.91	1.37
I19	1.02	0.94	0.49	1.05	0.51	1.50	0.08	1.64	NAN	
I20	NAN		3.79	1.57	1.93	1.04	14.25	1.76	0.57	0.96
I21	1.71	0.85	4.41	0.95	3.94	0.53	NAN		3.38	0.56
I22	12.01	0.64	1.05	0.81	2.20	0.81	5.71	1.23	1.73	0.65
I23	NAN		1.58	0.36	2.88	0.36	3.35	0.13	0.43	0.40
I24	0.53	0.59	0.50	0.77	0.48	0.62	5.23	0.99	NAN	
A1	0.71	0.54	0.19	0.85	0.16	0.98	2.81	0.57	NAN	6.10
A2	18.30	1.62	2.69	0.61	2.38	0.62	NAN		2.66	0.42
A3	1.20	0.55	4.37	0.50	NAN		6.86	0.72	0.97	0.69
A4	NAN		0.85	1.05	0.94	0.88	3.74	0.94	1.55	1.01
A5	19.13	1.90	0.69	1.21	1.03	1.34	NAN		1.04	1.27
A6	0.51	0.72	1.11	1.28	1.89	0.46	NAN		5.52	1.32
A7	2.07	0.90	8.08	0.64	NAN		1.82	1.59	0.78	0.65
A8	NAN		7.17	0.88	3.63	1.68	3.38	1.20	0.57	0.70
A9	0.81	1.09	17.11	1.48	1.43	1.54	0.62	0.62	0.33	0.97

Table S2 (continued)

	A52C		Q87C		S113C		S196C		A241C	
Peak Index	**PRE (s^{-1})**	**St. Dev.**	**PRE (s^{-1})**	**St. Dev.**	**PRE (s^{-1})**	**St. Dev.**	**PRE (s^{-1})**	**St. Dev.**	**PRE (s^{-1})**	**St. Dev.**
A10	2.10	0.96	12.47	1.25	30.37	4.32	1.85	0.96	0.84	0.80
A11	6.47	1.17	1.98	0.55	2.06	1.05	NAN		2.06	0.65
A12	0.47	1.47	0.70	1.65	0.93	1.33	16.69	2.58	26.45	5.10
A13	1.97	0.86	0.31	0.59	10.02	1.14	6.69	1.77	0.93	1.06
A14	Overlap		NAN		14.48	0.77	Overlap		Overlap	
A15	0.76	0.59	0.44	1.13	0.57	0.82	0.79	0.55	A241C	
A16	A52C		2.79	0.79	0.87	1.18	2.82	0.81	1.00	0.69
A17	8.87	1.32	22.89	1.46	27.70	1.38	3.14	1.19	0.65	0.82
A18	NAN		10.28	0.93	1.37	1.15	0.92	0.68	0.61	0.81
A19	9.55	0.63	23.94	2.09	6.10	0.78	2.19	0.94	1.14	0.34
A20	3.72	1.10	NAN		29.94	11.71	2.55	3.73	3.73	0.88
A21	1.49	1.16	1.36	0.80	15.58	1.58	11.76	1.56	1.81	0.71
A22	1.17	0.73	0.66	1.29	0.12	0.79	2.53	1.32	4.21	1.02
A23	1.32	0.34	0.93	0.51	2.23	0.45	NAN		4.84	0.43
A24	2.31	1.44	1.77	1.30	0.12	1.70	NAN		3.85	1.24
A25	2.24	0.81	1.15	0.60	3.03	0.61	18.55	3.03	2.00	0.48
A26	0.74	1.17	-0.02	1.35	0.89	0.90	10.76	1.67	13.84	5.10
A27	Overlap		21.72	1.20	NAN		Overlap		Overlap	
A28	2.05	0.80	1.92	0.89	NAN		17.83	2.57	0.39	0.78
VL1	1.15	1.03	0.99	0.90	4.10	1.82	29.07	11.94	2.83	0.99
VL2	3.05	1.06	1.17	1.07	0.53	1.54	19.47	1.82	4.70	0.91
VL3	0.68	1.02	0.83	0.76	2.25	0.54	NAN		2.55	0.93
VL4	0.66	0.73	0.20	1.12	1.70	0.61	7.71	1.16	2.62	0.48
VL5	2.37	0.86	0.73	0.74	1.05	0.87	5.05	1.47	NAN	
VL6	1.79	0.87	1.06	1.09	11.48	1.25	0.45	0.80	0.45	1.04
VL7	1.05	0.60	0.03	0.64	0.32	1.02	2.86	0.71	NAN	
VL8	1.48	0.89	1.27	0.54	11.95	0.67	0.00	0.65	0.60	0.49
VL9	1.33	0.46	0.31	0.46	0.45	0.54	2.94	0.55	NAN	
VL10	1.90	1.33	1.11	0.83	0.66	0.82	2.14	1.53	NAN	
VL11	0.40	0.53	0.34	0.99	0.62	1.03	0.91	0.77	5.50	0.84
VL12	14.26	0.57	NAN		2.19	0.65	1.59	0.75	0.93	0.48
VL13	9.19	0.88	1.00	0.67	3.35	1.05	0.97	1.49	0.68	0.71
VL14	1.41	0.56	0.72	0.67	0.97	1.07	4.25	0.48	NAN	
VL15	0.20	1.47	0.24	1.49	0.62	0.83	7.70	1.96	5.77	1.22
VL16	1.16	0.52	0.80	0.87	0.99	0.92	0.38	1.69	8.94	0.80
VL17	-0.40	0.95	0.73	1.98	0.82	1.55	4.41	2.07	11.79	1.45
VL18	1.51	0.94	0.14	0.96	0.83	0.77	0.08	1.67	NAN	
VL19	NAN		NAN	8.93	2.89	0.70	2.01	0.73	0.24	0.80
VL20	1.08	0.63	0.20	0.44	0.52	0.61	18.18	3.22	17.57	1.65
VL21	8.73	1.21	NAN		NAN		2.02	0.81	1.15	0.86

Table S2 (continued)

	A52C		Q87C		S113C		S196C		A241C	
Peak Index	**PRE (s^{-1})**	**St. Dev.**	**PRE (s^{-1})**	**St. Dev.**	**PRE (s^{-1})**	**St. Dev.**	**PRE (s^{-1})**	**St. Dev.**	**PRE (s^{-1})**	**St. Dev.**
VL22	3.67	1.19	NAN		2.40	0.63	-0.21	1.39	0.55	0.72
VL23	2.65	0.68	1.48	0.43	1.07	0.40	2.29	0.55	NAN	
VL24	NAN		16.99	1.74	8.67	1.45	0.00	2.26	2.42	0.54
VL25	4.63	0.91	1.43	1.57	1.45	0.99	NAN		8.33	0.91
VL26	16.83	1.95	17.81	2.26	NAN		5.16	1.46	4.72	1.38
VL27	2.68	0.52	0.46	0.74	1.05	0.65	6.34	0.97	3.50	0.80
VL28	0.33	0.94	0.28	0.65	1.43	0.97	2.98	1.76	15.75	0.64
VL29	2.89	0.94	0.65	0.81	1.07	1.06	NAN		4.66	0.92
VL30	3.33	1.26	0.81	0.56	0.29	1.59	NAN		3.38	0.91
VL31	2.15	1.24	5.19	1.21	NAN		11.99	1.00	5.75	1.06
VL32	0.71	0.75	6.73	0.90	NAN		1.90	1.13	1.53	0.96
VL33	0.30	0.47	0.30	0.82	1.25	0.59	1.50	0.54	3.05	0.75
VL34	1.57	1.01	NAN		NAN		0.34	1.23	0.04	1.16
VL35	1.00	1.39	0.58	1.97	1.47	1.50	NAN		3.87	1.61
VL36	0.58	1.26	Overlap		Overlap		Overlap		Overlap	
VL37	3.53	0.69	0.75	0.65	0.14	0.56	NAN		2.12	0.88
VL38	6.62	0.50	3.36	0.61	7.71	0.47	0.13	0.92	-0.21	0.73
VL39	NAN		2.47	0.83	3.61	0.63	29.68	8.15	1.09	0.51
VL40	2.42	0.25	1.61	0.41	2.38	0.54	2.64	0.50	NAN	
VL41	4.32	0.94	14.67	1.09	NAN		2.01	1.74	7.15	0.92
VL42	9.62	0.34	0.85	0.32	1.29	0.19	9.36	5.29	2.51	0.30
VL43	0.84	0.79	1.44	0.39	5.11	0.97	8.81	1.81	23.28	2.81
VL44	1.25	1.01	0.84	0.76	1.73	0.97	2.64	1.42	2.13	0.97
VL45	1.32	0.75	-0.10	1.01	1.50	0.87	2.82	0.91	1.57	0.58
VL46	8.94	1.04	18.76	0.89	NAN		8.71	1.47	8.03	0.65
VL47	11.87	0.65	16.23	1.26	NAN		8.16	1.41	9.61	0.86
VL48	1.65	0.61	NAN		2.84	1.40	0.16	0.84	0.31	0.95
VL49	6.70	1.88	NAN		3.02	1.49	0.21	0.94	1.47	0.58
VL50	Overlap		-0.06	0.81	1.10	0.67	1.66	0.93	3.46	0.80
VL51	6.15	0.72	0.48	0.70	2.10	0.90	12.22	1.50	1.36	1.42
VL52	2.51	0.76	1.17	0.50	3.11	0.74	NAN		1.93	0.67
VL53	NAN		17.79	1.24	10.56	1.24	1.25	2.09	2.04	0.58
VL54	7.10	1.16	8.95	0.87	NAN		1.89	1.52	1.05	0.35
VL55	15.80	1.09	NAN		NAN		3.69	1.20	3.68	0.64
VL56	6.47	1.23	0.86	0.56	0.05	0.82	Overlap		1.00	0.97
VL57	11.90	0.75	NAN		NAN		Overlap		3.45	0.82
VL58	0.51	0.71	-0.48	0.87	0.07	0.82	2.15	1.13	10.64	1.70
VL59	1.31	0.87	0.17	0.51	0.74	1.01	2.92	7.43	15.35	1.38
VL60	3.51	0.90	0.95	1.04	2.20	1.10	NAN		1.79	1.15
VL61	0.71	0.79	0.30	1.02	0.36	1.38	2.16	4.31	6.75	1.06

Table S2 (continued)

	A52C		Q87C		S113C		S196C		A241C	
Peak Index	**PRE (s^{-1})**	**St. Dev.**	**PRE (s^{-1})**	**St. Dev.**	**PRE (s^{-1})**	**St. Dev.**	**PRE (s^{-1})**	**St. Dev.**	**PRE (s^{-1})**	**St. Dev.**
VL62	1.33	0.80	0.73	0.84	-0.11	0.58	10.27	1.21	17.63	1.38
VL63	1.73	0.58	-0.34	0.44	0.51	0.49	NAN		5.98	0.15
VL64	6.46	0.69	0.54	1.14	1.47	0.77	6.82	2.08	2.71	0.73
VL65	0.92	1.58	0.40	0.72	-0.18	0.92	9.84	3.67	25.40	8.99
VL66	7.99	1.70	3.33	1.61	15.37	4.11	-0.24	1.47	-0.84	1.30
VL67	8.75	1.29	1.56	1.01	7.97	1.18	1.11	0.96	1.20	1.06
VL68	3.60	0.92	0.83	0.77	1.05	1.11	NAN		5.87	1.24
VL69	NAN		12.23	2.31	6.87	0.96	0.85	4.79	1.45	0.56
VL70	1.80	0.76	NAN		NAN		2.09	1.84	0.45	1.07
VL71	1.15	0.42	8.28	0.58	NAN		2.29	1.88	1.96	0.41
VL72	1.91	0.53	6.72	0.81	NAN		10.40	0.41	2.79	0.71
VL73	13.79	4.04	20.09	3.84	NAN		4.76	3.92	1.97	1.64
VL74	6.09	1.65	6.72	1.04	NAN		2.16	0.76	0.93	0.97
VL75	6.31	0.33	1.11	0.30	1.28	0.28	NAN		4.72	0.62
VL76	Overlap		Overlap		Overlap		NAN		Overlap	
VL77	4.71	1.83	0.43	1.15	1.89	1.87	2.66	0.52	1.77	1.59
VL78	4.18	0.66	11.82	0.34	NAN		5.36	1.77	6.72	0.84
VL79	1.65	0.89	0.38	0.69	1.34	1.70	21.39	3.40	1.58	0.85
VL80	5.87	1.35	0.57	0.48	2.58	1.23	21.03	4.99	0.77	0.61
VL81	10.91	1.31	0.97	1.16	2.12	0.99	NAN		0.98	1.13
VL82	9.52	0.63	17.04	4.60	NAN		11.99	2.92	8.13	1.16
VL83	1.34	0.88	2.24	0.89	4.55	0.81	7.21	1.41	26.42	4.45
VL84	NAN		NAN		1.59	0.81	0.99	2.34	1.37	1.17
VL85	NAN		4.89	1.34	3.07	0.96	3.71	3.05	0.92	1.18
VL86	Overlap		NAN		NAN		6.84	1.25	0.01	0.69
VL87	1.46	1.02	Overlap		Overlap		Overlap		Overlap	
VL88	Overlap		Overlap		Overlap		NAN		Overlap	

Table S3. $^{1}H/^{13}C$ chemical shifts for the 140 ^{1}H-^{13}C HMQC cross-peaks.

Peak index	Assignment	^{1}H (ppm)	^{13}C (ppm)
M1	M239	1.988	15.93
M2	M1	1.967	16.63
M3	M193	1.803	17.01
M4	M98	2.041	17.41
M5	M78	2.138	17.06
I1	I180	0.69	16.18
I2	I219	0.53	14.92
I3	I31	0.647	14.88
I4	I157	0.407	14.01
I5	I2	0.659	14.50
I6	I89	0.569	14.21
I7	I141	0.972	14.63
I8	I108	0.737	10.76
I9	I26	0.481	11.27
I10	I72	0.647	12.68
I11	I5	0.936	13.13
I12	I90	1.057	13.88
I13	I133	0.734	14.57
I14	I93	0.736	14.40
I15	I24	0.92	14.01
I16	I152	0.833	13.62
I17	I57	0.692	13.58
I18	I202	0.681	13.49
I19	I236	0.704	13.47
I20	I77	0.838	13.33
I21	I192	0.773	12.73
I22	I147	0.834	12.85
I23	I146	0.809	13.04
I24	I11	0.784	13.97
A1	A247	1.484	19.18
A2	A169	1.409	19.16
A3	A127	1.638	19.11
A4	A151	1.377	18.97
A5	A61	1.543	18.46
A6	A194	1.42	18.39
A7	A112	1.379	18.38
A8	A50	1.432	18.32
A9	A33	1.523	18.28
A10	A102	1.446	18.21
A11	A71	1.48	18.16
A12	A222	1.518	18.08
A13	A161	1.567	18.06
A14	A91	1.494	18.00
A15	A241	1.544	17.81
A16	A52	1.56	17.77
A17	A104	1.392	17.72
A18	A48	1.54	17.69
A19	A100	1.721	19.69
A20	A103	1.42	20.78
A21	A183	1.554	20.68
A22	A16	1.237	20.49
A23	A7	1.292	21.31
A24	A201	0.981	22.16
A25	A160	1.337	24.35
A26	A12	1.208	23.60
A27	A114	1.49	17.94
A28	A128	1.569	17.73
VL1	V203G2	0.449	17.21
VL2	V156G2	0.776	17.10
VL3	V203G1	0.679	19.64
VL4	V208G2	0.78	19.60
VL5	V223G1	0.868	20.32
VL6	V25G2	0.835	20.38
VL7	V246G2	1.025	20.78
VL8	V25G1	0.828	20.81
VL9	V246G1	0.991	21.04
VL10	V242G1	0.931	20.96
VL11	V229G1	0.946	21.41
VL12	V40G1	1.111	21.38
VL13	L144D1	0.881	21.37
VL14	V223G2	0.886	21.14
VL15	V159G2	0.711	21.13
VL16	V229G2	0.736	21.02
VL17	V227G1	0.668	21.01
VL18	V235G1	0.477	21.10
VL19	L44D1	0.619	21.75
VL20	L177D2	0.81	21.64
VL21	V107G1	0.911	21.55
VL22	V36G1	1.037	21.73
VL23	V242G2	1.117	21.98

Table S3 (continued)

Peak index	Assignment	^{1}H (ppm)	^{13}C (ppm)
VL24	L137D1	0.986	22.02
VL25		0.926	22.04
VL26	V130G1	0.928	22.16
VL27	V156G1	0.782	22.04
VL28	V227G2	0.768	21.88
VL29	V176G1	0.55	22.09
VL30	V176G2	0.864	22.00
VL31	L123D2	0.863	22.04
VL32	L118D2	0.895	22.39
VL33	V212G2	0.786	22.76
VL34	L92D2	0.865	22.69
VL35	V208G1	0.872	22.80
VL36	V212G1	0.875	22.94
VL37		0.914	22.86
VL38	L142D2	1.013	22.83
VL39	L54D2	1.101	23.12
VL40	V235G2	0.998	23.05
VL41	L115D2	0.926	23.03
VL42	L149D2	0.8	23.15
VL43	L6D1	0.705	23.00
VL44	V159G1	0.66	23.39
VL45	L18D2	0.75	23.39
VL46	L79D1	0.853	23.40
VL47	V130G2	0.988	23.33
VL48	V36G2	1.205	23.38
VL49	V40G2	1.244	23.63
VL50	L17D2	0.975	23.78
VL51	L19D2	0.84	23.92
VL52	L163D2	0.732	24.17
VL53	L80D2	0.961	24.35
VL54	L138D2	1.045	24.52
VL55	L85D1	0.981	24.69
VL56		0.874	24.54
VL57	L85D2	0.877	24.67
VL58	L218D2	0.756	24.84
VL59	L220D1	0.731	24.93
VL60	L163D1	0.62	25.51
VL61	L218D1	0.559	26.07
VL62	L220D2	0.681	26.16
VL63		0.791	26.08
VL64	L17D1	0.834	25.79
VL65	L177D1	0.839	25.97
VL66	L142D1	0.899	26.23
VL67	L144D2	0.942	26.38
VL68		0.962	26.52
VL69	L80D1	0.996	26.52
VL70	L92D1	0.961	26.72
VL71	L118D1	1.005	26.22
VL72	L123D1	1.012	26.09
VL73	L137D2	1.038	25.66
VL74	L138D1	1.039	25.56
VL75		1.006	25.46
VL76	L158D1	0.926	25.78
VL77	L18D1	0.928	25.58
VL78	L115D1	0.816	25.53
VL79		0.935	25.49
VL80	L19D1	0.913	25.44
VL81	L149D1	0.892	25.42
VL82	L79D2	0.866	25.44
VL83	L6D2	0.841	25.42
VL84	L44D2	0.877	25.67
VL85	L54D1	0.996	26.11
VL86	V107G2	0.981	23.81
VL87		0.875	22.94
VL88		0.926	25.78

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