1.1 Summary tables for MC1037

Table 2: Summary table for MC1037 (1 of 2): Shifts, splitting, COSY, HSQC and HMBC

Amino acid	Atom name	C	H	Multip.	COSY	HSQC	HSQC_+/-	HMBC
Leu1	1		-		-	-		-
	2	50.1	4.50	dd (12.8)	1.13, 1.80, 7.14	50.1	+	-
	2-NH		7.14	br d (13.8)	4.50	-		-
	3	39.4	1.80	dd (14.3)	1.13, 1.44, 4.50	39.4	-	-
			1.13	br Weak s/m	1.80, 4.50	39.4		-
	4	24.5	1.44	m	0.78, 1.80	24.5	+	-
	5a	23.1	0.78	d (7.2)	1.44	23.1	+	-
	5b	21.0	0.78	d (7.0)	1.44	21.0	+	-
Leu2	1		-		-	-	0	-
	2	53.5	4.00	m	1.49, 1.74, 7.64	53.5	+	-
	2-NH		7.64	d (6.2)	4.00	-		-
	3	39.2	1.74	m	1.49, 4.00	39.2	-	-
			1.49	m	1.66, 1.74, 4.00	39.2		-
	4	24.2	1.66	m	0.80, 0.86, 1.49	24.2	+	-
	5a	23.0	0.86	d (6.8)	1.66	23.0	+	21.0, 39.2
	5b	21.0	0.80	d (6.8)	1.66	21.0	+	39.2
Me-Asp3	1		-		-	-	0	-
	2	55.4	4.12	m	7.87	-	?	-
	2-NH		7.87	d (10.7)	4.12	-		-
	3	39.4	3.12	m	0.89	39.4	?	-
	3-Me	15.1	0.89	d (7.8)	3.12	15.1	+	178.4, 39.4, 55.4
	4	178.4	-		-	-		-
Arg4	1		-		-	-	0	-
	2	51.6	4.13	td (10.1, 3.6)	1.30, 1.97, 8.83	51.6	+	-
	2-NH		8.83	d (10.5)	4.13	-		-

	3	28.4	1.97		1.30, 1.37, 4.13	28.4	-	-
			1.30		-	28.4		-
	4	25.9	1.37		1.97, 3.01	25.9	-	-
			1.30		1.97, 3.01, 4.13	25.9		-
	5	40.5	3.01		1.30, 1.37, 7.37	40.5	-	-
	5-NH		7.37		3.01	-		128.1
Adda5	1	173.8	-		-	-	0	-
	2	43.1	2.78	br dd (?, ?)	0.92, 4.35	43.1	+	-
	2-Me	16.0	0.92	d (7.2)	2.78	16.0	+	173.8, 43.1, 54.4
	3	54.4	4.35	ddd (?, ?, ?)	2.78, 5.32, 7.75	54.4	+	-
	3-NH		7.75	br d (?)	4.35	-		-
	4	126.3	5.32	dd (16.4, 8.3)	4.35, 6.09	126.3	+	132.0
	5	135.4	6.09	d (16.4)	5.32	135.4	+	12.5, 135.3, 54.4
	6	132.0	-		-	-	0	-
	6-Me	12.5	1.55	d (1.0)	5.45	12.5	+	132.0
	7	135.3	5.45	dd (10.8, 1.0)	1.55, 2.56	135.3	+	12.5, 135.4
	8	35.4	2.56	ddd (10.8, 7.0, 5.4)	0.98, 3.25, 5.45	35.4	+	-
	8-Me	15.8	0.98	d (7.0)	2.56	15.8	+	135.3, 35.4, 85.8
	9	85.8	3.25	ddd (7.2, 5.4, 5.4)	2.56, 2.68, 2.74	85.8	+	139.2, 15.8, 57.4
	9-OMe	57.4	-	s	-	-	+	-
	10	37.0	2.74	dd (14.0, 5.4)	3.25	37.0	-	129.3, 139.2, 35.4, 85.8
			2.68	dd (14.0, 7.2)	3.25	37.0		129.3, 139.2, 35.4, 85.8
	11	139.2	-		-	-	0	-
	12	129.3	7.19	dd (8.3, 1.2)	-	129.3	+	125.9, 129.3, 37.0
	13	128.1	7.27	dd (8.3, 7.3)	-	128.1	+	128.1, 139.2
	14	125.9	7.18	dt (7.3, 1.2)	-	125.9	+	-
Glu6	1		-		-	-	0	-
	2	52.8	4.35		1.88, 9.28	52.8	+	-
	2-NH		9.28		4.35	-		-
	3		1.88		2.21, 4.35	-	-	-
	4	31.3	2.21		1.88	31.3	-	-

			2.31		-	31.3		-
	5	175.1	-		-	-	0	-
Mdha7	1	163.0	-		-	-	0	-
	2	144.8	-		-	-	0	-
	2-N-Me	37.3	3.12	s	-	37.3	+	144.8, 175.1
	3	113.9	5.81		-	113.9	-	163.0
			5.39		-	113.9		144.8, 163.0

Table 3: Summary table for MC1037 (2 of 2): TOCSY and ROESY

Amino acid	Atom name	C	H	TOCSY	ROESY
Leu1	1		-	-	-
	2	50.1	4.50	0.78, 1.13, 1.44, 1.80, 7.14	1.13, 1.44, 1.80, 7.14, 7.64
	2-NH		7.14	0.78, 1.13, 1.44, 1.80, 4.50	1.13, 1.44, 3.12, 4.13, 4.50, 7.64, 7.87
	3	39.4	1.80	1.13, 1.44, 4.50, 7.14	1.13, 4.50
			1.13	1.80, 4.50, 7.14	1.80, 4.50, 7.14
	4	24.5	1.44	0.78, 1.80, 4.50, 7.14	4.50, 7.14
	5a	23.1	0.78	1.44, 4.50, 7.14	-
	5b	21.0	0.78	1.44, 4.50, 7.14	-
Leu2	1		-	-	-
	2	53.5	4.00	0.80, 0.86, 1.49, 1.66, 1.74, 7.64	0.80, 1.49, 7.64, 7.87
	2-NH		7.64	0.80, 0.86, 1.49, 1.66, 1.74, 4.00	1.66, 1.74, 4.00, 4.50, 7.14, 7.87
	3	39.2	1.74	0.80, 0.86, 1.49, 4.00, 7.64	0.86, 1.49, 4.35, 7.64, 7.87
			1.49	0.80, 0.86, 1.66, 1.74, 4.00, 7.64	1.74, 4.00, 7.87
	4	24.2	1.66	0.80, 0.86, 1.49, 4.00, 7.64	7.64
	5a	23.0	0.86	1.49, 1.66, 1.74, 4.00, 7.64	1.74
	5b	21.0	0.80	1.49, 1.66, 1.74, 4.00, 7.64	4.00, 5.81
Me-Asp3	1		-	-	-
	2	55.4	4.12	0.89, 3.12, 7.87	0.89, 3.12, 7.87
	2-NH		7.87	0.89, 3.12, 4.12	0.89, 1.49, 1.74, 1.88, 4.00, 4.12, 7.14, 7.64
	3	39.4	3.12	0.89, 4.12, 7.87	0.89, 4.12, 7.14, 7.37, 8.83
	3-Me	15.1	0.89	3.12, 4.12, 7.87	3.12, 4.12, 7.87, 8.83
	4	178.4	-	-	-
Arg4	1		-	-	-
	2	51.6	4.13	1.30, 1.37, 1.97, 3.01, 7.37, 8.83	1.30, 1.37, 1.97, 2.31, 7.14, 7.75, 8.83
	2-NH		8.83	1.30, 1.37, 1.97, 3.01, 4.13	0.89, 1.30, 1.37, 3.12, 4.13, 6.09, 7.75
	3	28.4	1.97	1.30, 1.37, 3.01, 4.13, 7.37, 8.83	3.01, 4.13, 7.37
			1.30	-	-
	4	25.9	1.37	1.97, 3.01, 4.13, 7.37, 8.83	3.01, 4.13, 8.83
			1.30	1.97, 3.01, 4.13, 7.37, 8.83	3.01, 4.13, 8.83
	5	40.5	3.01	1.30, 1.37, 1.97, 4.13, 7.37, 8.83	1.30, 1.37, 1.97, 7.19, 7.27, 7.37

	5-NH		7.37	1.30, 1.37, 1.97, 3.01, 4.13	1.97, 3.01, 3.12
Adda5	1	173.8	-	-	-
	2	43.1	2.78	0.92, 4.35, 5.32, 6.09, 7.75	0.92, 4.35, 5.32, 6.09, 7.75, 9.28
	2-Me	16.0	0.92	2.78, 4.35, 5.32, 6.09, 7.75	2.78, 4.35, 5.32, 6.09
	3	54.4	4.35	0.92, 2.78, 5.32, 6.09, 7.75	0.92, 1.55, 2.78, 5.32, 5.45, 6.09, 7.75
	3-NH		7.75	0.92, 2.78, 4.35, 5.32, 6.09	2.78, 4.13, 4.35, 5.32, 6.09, 8.83
	4	126.3	5.32	0.92, 2.78, 4.35, 6.09, 7.75	0.92, 1.55, 2.78, 4.35, 6.09, 7.75
	5	135.4	6.09	0.92, 2.78, 4.35, 5.32, 7.75	0.92, 1.55, 2.78, 4.35, 5.32, 5.45, 7.75, 8.83
	6	132.0	-	-	-
	6-Me	12.5	1.55	5.45	4.35, 5.32, 5.45, 6.09
	7	135.3	5.45	1.55, 2.56, 2.68, 2.74, 3.25	0.98, 1.55, 2.56, 2.68, 2.74, 3.25, 4.35, 6.09
	8	35.4	2.56	0.98, 2.68, 2.74, 3.25, 5.45	5.45, 7.19
	8-Me	15.8	0.98	2.56, 2.68, 2.74, 3.25	2.68, 2.74, 3.25, 5.45
	9	85.8	3.25	0.98, 2.56, 2.68, 2.74, 5.45, 5.56	0.98, 5.45, 7.19
	9-OMe	57.4	-	-	-
	10	37.0	2.74	0.98, 2.56, 2.68, 3.25, 5.45	0.98, 5.45, 7.19, 7.27
			2.68	0.98, 2.56, 2.74, 3.25, 5.45	0.98, 5.45, 7.19
	11	139.2	-	-	-
	12	129.3	7.19	-	2.56, 2.68, 2.74, 3.01, 3.19, 3.25
	13	128.1	7.27	-	2.74, 3.01, 3.19
	14	125.9	7.18	-	-
Glu6	1		-	-	-
	2	52.8	4.35	1.88, 2.21, 2.31, 9.28	1.74, 1.88, 2.21, 2.31, 9.28
	2-NH		9.28	1.88, 2.21, 2.31, 4.35	2.78, 4.35
	3		1.88	2.21, 2.31, 4.35, 9.28	4.35, 7.87
	4	31.3	2.21	1.88, 4.35, 9.28	3.12, 4.35
			2.31	1.88, 4.35, 9.28	3.12, 4.13, 4.35
	5	175.1	-	-	-
Mdha7	1	163.0	-	-	-
	2	144.8	-	-	-
	2-N-Me	37.3	3.12	-	2.21, 2.31, 5.39, 5.81

	3	113.9	5.81	5.39	0.80, 3.12, 5.39
			5.39	5.81	3.12, 5.81