

Chemical shifts for Kalata B8

Chemical shift	Atom	Residue
7.587	HN	1
4.952	HA	1
3.629	HB2	1
2.311	HB3	1
8.410	HN	2
3.804	HA1	2
3.533	HA2	2
4.483	HA	3
2.560	HB2	3
2.402	HB3	3
1.952	HG2	3
1.798	HG3	3
8.581	HN	4
4.388	HA	4
4.270	HB	4
1.201	QG2	4
8.297	HN	5
4.971	HA	5
2.865	HB2	5
2.343	HB3	5
8.837	HN	6
3.843	HA	6
1.585	QB	6
1.459	HG	6
0.807	QQD	6
7.994	HN	7
4.382	HA	7
1.629	HB2	7
1.560	HB3	7
1.419	HG	7
0.765	QD1	7
0.689	QD2	7
7.673	HN	8
4.143	HA1	8
3.736	HA2	8
7.355	HN	9
4.325	HA	9
3.538	HB	9
0.557	QG2	9
8.690	HN	10
4.300	HA	10
2.548	HB2	10
2.944	HB3	10
8.699	HN	11
4.209	HA	11
2.983	HB2	11

2.694	HB3	11
6.596	QE	11
6.955	QD	11
7.956	HN	12
4.167	HA	12
4.006	HB	12
1.172	QG2	12
8.452	HN	13
3.728	HA	13
3.835	HB	13
1.059	QG2	13
8.790	HN	14
4.018	HA1	14
3.505	HA2	14
7.602	HN	15
4.883	HA	15
3.281	HB2	15
2.479	HB3	15
9.369	HN	16
4.356	HA	16
3.917	HB	16
0.953	QG2	16
8.669	HN	17
4.355	HA	17
2.791	HB2	17
2.552	HB3	17
8.624	HN	18
4.559	HA	18
3.408	HB2	18
2.870	HB3	18
7.120	HD21	18
7.412	HD22	18
8.256	HN	19
3.820	HA	19
1.465	QB	19
0.324	QG	19
1.253	HD2	19
0.784	HD3	19
2.589	QE	19
7.324	QZ	19
7.410	HN	20
4.402	HA	20
3.226	HB2	20
2.576	HB3	20
6.645	QE	20
6.897	QD	20
8.095	HN	21
3.635	HA	21
2.143	QB	21
1.496	HG2	21

1.434	HG3	21
3.054	QD	21
6.735	HE	21
7.666	HN	22
4.050	HA	22
1.681	HB	22
0.712	QG1	22
0.677	QG2	22
0.674	QQG	22
8.209	HN	23
4.928	HA	23
3.110	HB2	23
2.602	HB3	23
9.492	HN	24
4.725	HA	24
3.735	HB	24
0.885	QG2	24
8.450	HN	25
4.540	HA	25
1.650	QB	25
1.194	HG2	25
1.057	HG3	25
1.483	HD2	25
1.440	HD3	25
1.456	QD	25
2.754	QE	25
7.416	QZ	25
9.485	HN	26
4.199	HA	26
2.908	HB2	26
2.622	HB3	26
8.575	HN	27
4.021	HA1	27
3.530	HA2	27
7.746	HN	28
4.692	HA	28
3.753	HB2	28
3.648	HB3	28
8.202	HN	29
4.186	HA	29
2.154	HB	29
0.803	QG1	29
0.751	QG2	29
8.134	HN	30
3.956	HA	30
1.440	QB	30
1.362	HG	30
0.751	QD1	30
0.708	QD2	30
0.708	QQD	30

8.257	HN	31
4.412	HA	31
2.719	QB	31