Appendix D

Sequential Assignments

A total of 20 sequence fragments were found; these are presented below, numbered from 0 to 19. Each fragment starts with three summary lines:

- The first line gives the position of the fragment in the assignment list, the score and the "original" score before any penalisations were applied;

- The second line shows the residues putatively found, in single letter code notation;

- The third line shows the penalisation algorithms which were activated by the fragment and the severity of the penalisation applied in each case.

After the summary lines, the results that were chained together to make the fragment are shown, in the order they appear in the fragment. The chemical shift connectivities are always fairly clear; take CB, for example: for a given result, the CB entry in column 4 of the chemical shift table should match fairly closely to the CB in column 3 of the result above.

Putative sequential assignment 0: score=751527, orig_score=7471106, 3 results
Sequence fragment: F87 F88 R89 N90
Penalisations: low_count=0.22 imperfect_connectivity=0.45 excessive_start_pt=1.00

H#1	N#1	CB#1	CB	CA#1	CA	CO	CO#1	Assignment
8.45	127.1	44.3	42.4	55.0	55.0	180.0	176.6	6
8.98	119.4	34.8	44.3	54.4	53.7	176.3	176.3	13
9.09	124.3	31.7	34.8	61.3	54.4	176.3	178.4	14

Putative sequential assignment 1: score=927936, orig_score=5783695, 4 results
Sequence fragment: K97 E98 Y99 T100 A101
Penalisations: low_count=0.29 imperfect_connectivity=0.57 excessive_start_pt=0.98

H#1	N#1	CB#1	CB	CA#1	CA	CO	CO#1	Assignment
8.33	124.6	32.9	30.4	55.0	60.7	172.2	175.0	104
9.09	124.3	31.7	34.8	61.3	54.4	176.3	178.4	14

8.18	110.2	63.8	31.7	60.7	61.3	178.4	175.3	15
7.63	118.8	19.0	63.8	52.5	60.7	175.3	177.7	16

Putative sequential assignment 2: score=994094, orig_score=6196051, 4 results
Sequence fragment: K97 E98 Y99 T100 A101
Penalisations: low_count=0.29 imperfect_connectivity=0.57 excessive_start_pt=0.98

H#1	N#1	CB#1	CB	CA#1	CA	CO	CO#1	Assignment
8.33	124.6	32.9	30.4	55.0	60.7	177.8	176.3	104
9.09	124.3	31.7	34.8	61.3	54.4	176.3	178.4	14
8.18	110.2	63.8	31.7	60.7	61.3	178.4	175.3	15
7.63	118.8	19.0	63.8	52.5	60.7	175.3	177.7	16

Putative sequential assignment 3: score=996048, orig_score=9882089, 3 results
Sequence fragment: K86 F87 F88 R89
Penalisations: low_count=0.22 imperfect_connectivity=0.45 excessive_start_pt=1.00

H#1	N#1	CB#1	CB	CA#1	CA	CO	CO#1	Assignment
8.39	125.6	32.3	32.3	52.5	63.8	175.2	173.5	119
9.25	125.9	43.6	32.3	55.6	52.5	173.2	175.8	62
9.50	122.2	26.0	43.6	50.0	55.6	175.8	176.4	63

Putative sequential assignment 4: score=1141968, orig_score=9049179, 5 results
Sequence fragment: P96 K97 E98 Y99 T100 A101
Penalisations: low_count=0.36 imperfect_connectivity=0.37 excessive_start_pt=0.96

H#1	N#1	CB#1	CB	CA#1	CA	CO	CO#1	Assignment
7.93	120.6	32.3	32.3	58.2	60.1	177.3	178.3	53
7.42	117.6	31.0	32.3	56.3	58.2	178.3	176.6	115
7.22	108.6	31.7	31.7	62.0	55.6	176.4	174.4	81
8.18	110.2	63.8	31.7	60.7	61.3	175.3	175.3	15
7.63	118.8	19.0	63.8	52.5	60.7	175.3	177.7	16

Putative sequential assignment 5: score=1148414, orig_score=5122048, 3 results
Sequence fragment: W111 L112 K113 K114
Penalisations: low_count=0.22

H#1	N#1	CB#1	CB	CA#1	CA	CO	CO#1	Assignment
9.41	130.5	41.8	42.4	57.5	55.6	173.5	173.9	88
8.97	123.4	33.5	41.8	53.7	57.5	173.9	176.6	89
9.95	124.3	38.0	33.5	55.0	53.7	176.6	175.6	90

Putative sequential assignment 6: score=1172831, orig_score=19708368, 5 results
Sequence fragment: D72 L73 A74 Q75 Q76 Y77
Penalisations: low_count=0.36 imperfect_connectivity=0.17 excessive_start_pt=0.99

H#1	N#1	CB#1	CB	CA#1	CA	CO	CO#1	Assignment
7.93	120.6	41.8	32.3	55.6	60.1	177.3	175.9	53
8.46	127.4	17.8	41.8	55.0	55.0	175.8	178.0	2
8.22	117.9	28.5	18.4	59.4	55.6	177.7	180.1	75
8.13	122.8	27.9	27.9	59.4	59.4	180.0	177.3	76
7.12	114.2	38.0	27.9	59.4	59.4	177.3	175.0	77

Putative sequential assignment 7: score=1173032, orig_score=8950720, 5 results
Sequence fragment: H38 C39 K40 A41 L42 A43
Penalisations: low_count=0.36 imperfect_connectivity=0.37

H#1	N#1	CB#1	CB	CA#1	CA	CO	CO#1	Assignment
7.95	120.3	41.8	43.0	58.8	60.1	175.5	179.5	53
7.77	120.9	32.3	41.8	59.4	58.8	178.9	180.5	54
8.03	124.0	17.8	32.3	55.6	59.4	180.5	179.4	49
7.63	119.1	42.4	19.0	57.5	55.6	179.5	177.7	21
7.18	117.6	17.8	42.4	53.7	57.5	177.7	179.1	22

Putative sequential assignment 8: score=1359777, orig_score=10775141, 5 results
Sequence fragment: P96 K97 E98 Y99 T100 A101
Penalisations: low_count=0.36 imperfect_connectivity=0.37 excessive_start_pt=0.96

H#1	N#1	CB#1	CB	CA#1	CA	CO	CO#1	Assignment
8.71	124.0	30.4	32.3	57.5	63.2	176.9	175.5	4
8.37	121.6	33.5	31.0	55.6	57.5	175.5	175.8	5
9.09	124.3	31.7	34.8	61.3	54.4	176.3	178.4	14
8.18	110.2	63.8	31.7	60.7	61.3	178.4	175.3	15
7.63	118.8	19.0	63.8	52.5	60.7	175.3	177.7	16

Putative sequential assignment 9: score=1727581, orig_score=13182157, 5 results
Sequence fragment: R103 E104 A105 D106 D107 I108
Penalisations: low_count=0.36 imperfect_connectivity=0.37

H#1	N#1	CB#1	CB	CA#1	CA	CO	CO#1	Assignment
7.22	108.6	31.0	31.0	61.3	56.9	180.3	177.5	116
7.93	120.3	18.4	32.3	55.6	60.1	178.1	179.4	74
8.22	117.9	28.5	18.4	59.4	55.6	179.4	180.0	75

H#1	N#1	CB#1	CB	CA#1	CA	CO	CO#1	Assignment
8.13	122.8	27.9	27.9	59.4	59.4	180.0	177.3	76
7.12	114.2	38.0	27.9	59.4	59.4	177.3	175.0	77

Putative sequential assignment 10: score=2276766, orig_score=23438426, 7 results
Sequence fragment: A20 L21 A22 A23 H24 K25 Y26 L27
Penalisations: low_count=0.52 imperfect_connectivity=0.19 excessive_start_pt=0.98

H#1	N#1	CB#1	CB	CA#1	CA	CO	CO#1	Assignment
7.62	119.1	42.4	19.0	53.1	55.6	179.5	176.9	33
8.46	127.1	18.4	41.8	51.2	55.0	177.5	177.0	56
7.75	129.9	20.3	19.7	54.4	52.5	176.4	182.6	120
8.22	117.9	28.5	18.4	59.4	55.6	182.6	179.4	75
8.13	122.8	27.9	27.9	59.4	59.4	180.0	177.3	76
7.12	114.2	38.0	27.9	59.4	59.4	177.3	175.0	77
7.60	109.5	48.1	38.0	59.4	59.4	175.0	175.0	78

Putative sequential assignment 11: score=2365037, orig_score=24347140, 7 results
Sequence fragment: A20 L21 A22 A23 H24 K25 Y26 L27
Penalisations: low_count=0.52 imperfect_connectivity=0.19 excessive_start_pt=0.98

H#1	N#1	CB#1	CB	CA#1	CA	CO	CO#1	Assignment
7.63	119.1	42.4	19.0	53.1	55.6	177.8	179.7	21
8.46	127.1	18.4	41.8	51.2	55.0	180.0	178.6	48
7.75	129.9	20.3	19.7	54.4	52.5	178.7	180.3	120
8.22	117.9	28.5	18.4	59.4	55.6	179.4	180.0	75
8.13	122.8	27.9	27.9	59.4	59.4	180.0	177.3	76
7.12	114.2	38.0	27.9	59.4	59.4	177.3	175.0	77
7.60	109.5	48.1	38.0	59.4	59.4	175.0	175.0	78

Putative sequential assignment 12: score=2450798, orig_score=29343635, 9 results
Sequence fragment: A18 E19 A20 L21 A22 A23 H24 K25 Y26 L27
Penalisations: low_count=0.70 imperfect_connectivity=0.12 excessive_start_pt=1.00

H#1	N#1	CB#1	CB	CA#1	CA	CO	CO#1	Assignment
7.93	120.6	32.3	17.8	64.5	56.3	177.3	171.4	3
8.39	125.6	19.0	32.3	52.5	63.8	171.9	177.5	119
7.77	129.9	37.3	18.4	54.4	52.5	176.4	176.4	120
8.78	131.1	20.9	38.6	53.7	52.5	175.8	177.0	67
7.98	130.5	20.3	19.7	54.4	53.7	176.3	182.5	120
8.22	117.9	28.5	18.4	59.4	55.6	182.6	179.4	75
8.13	122.8	27.9	27.9	59.4	59.4	180.0	177.3	76
7.12	114.2	38.0	27.9	59.4	59.4	177.3	175.0	77
7.60	109.5	48.1	38.0	59.4	59.4	175.0	175.0	78

Putative sequential assignment 13: score=2622021, orig_score=33540128, 10 results
Sequence fragment: F17 A18 E19 A20 L21 A22 A23 H24 K25 Y26 L27
Penalisations: low_count=0.79 imperfect_connectivity=0.10 excessive_start_pt=0.99

H#1	N#1	CB#1	CB	CA#1	CA	CO	CO#1	Assignment
7.54	121.2	17.8	32.3	55.0	60.1	176.7	179.2	41
7.93	120.6	32.3	17.8	64.5	56.3	178.3	176.1	115
8.39	125.6	19.0	32.3	52.5	63.8	176.9	176.4	119
7.77	129.9	37.3	18.4	54.4	52.5	176.4	176.4	120
8.78	131.1	20.9	38.6	53.7	52.5	175.8	177.0	67
7.63	119.1	19.0	19.0	57.5	55.6	177.8	179.7	21
8.22	117.9	28.5	18.4	59.4	55.6	179.4	180.0	75
8.13	122.8	27.9	27.9	59.4	59.4	180.0	177.3	76
7.12	114.2	38.0	27.9	59.4	59.4	177.3	175.0	77
7.60	109.5	48.1	38.0	59.4	59.4	175.0	175.0	78

Putative sequential assignment 14: score=2689324, orig_score=19340730, 9 results
Sequence fragment: D7 H8 V9 L10 V11 L12 R13 K14 S15 N16
Penalisations: low_count=0.70 imperfect_connectivity=0.21 excessive_start_pt=0.97

H#1	N#1	CB#1	CB	CA#1	CA	CO	CO#1	Assignment
7.93	120.6	32.3	32.3	64.5	60.7	175.0	176.3	53
8.39	125.6	32.3	32.3	52.5	63.8	176.9	176.4	119
9.95	124.3	38.0	33.5	55.0	53.7	176.6	175.6	90
7.98	124.9	32.9	39.9	53.1	53.1	175.0	173.2	17
9.25	125.9	43.6	32.3	55.6	52.5	173.2	175.8	62
8.98	119.4	34.8	44.3	54.4	53.7	176.3	176.3	13
9.09	124.3	31.7	34.8	61.3	54.4	176.3	178.4	14
8.18	110.2	63.8	31.7	60.7	61.3	178.4	175.3	15
7.63	118.8	39.9	63.8	52.5	60.7	175.3	177.7	16

Putative sequential assignment 15: score=2914289, orig_score=23394866, 11 results
Sequence fragment: D66 A67 T68 E69 E70 S71 D72 L73 A74 Q75 Q76 Y77
Penalisations: low_count=0.89 imperfect_connectivity=0.14 excessive_start_pt=0.99

H#1	N#1	CB#1	CB	CA#1	CA	CO	CO#1	Assignment
8.38	125.3	19.0	32.3	52.5	63.8	171.0	174.2	119
8.66	110.5	68.9	20.9	64.5	53.7	174.7	175.9	68
6.92	123.4	31.0	68.9	57.5	63.8	175.8	177.2	69
8.33	121.2	27.2	31.7	53.1	57.5	177.3	176.9	70
7.54	116.9	63.2	27.2	62.0	53.1	176.9	177.5	71
8.51	122.5	39.9	63.2	58.8	62.0	177.5	179.1	72
7.85	122.2	43.6	40.5	58.2	58.2	178.9	178.0	73
7.95	120.0	18.4	43.6	55.6	58.2	176.7	181.5	74
8.22	117.9	28.5	18.4	59.4	55.6	181.1	179.2	75

8.13	122.8	27.9	27.9	59.4	59.4	180.0	177.3	76
7.12	114.2	38.0	27.9	59.4	59.4	177.3	175.0	77

Putative sequential assignment 16: score=3070475, orig_score=23594481, 5 results
Sequence fragment: A22 A23 H24 K25 Y26 L27
Penalisations: low_count=0.36 imperfect_connectivity=0.37 excessive_start_pt=0.99

H#1	N#1	CB#1	CB	CA#1	CA	CO	CO#1	Assignment
7.75	129.9	20.3	19.7	54.4	52.5	176.4	176.4	120
8.22	117.9	28.5	18.4	59.4	55.6	177.7	180.1	75
8.13	122.8	27.9	27.9	59.4	59.4	180.0	177.3	76
7.12	114.2	38.0	27.9	59.4	59.4	177.3	175.0	77
7.60	109.5	48.1	38.0	59.4	59.4	175.0	175.0	78

Putative sequential assignment 17: score=5791958, orig_score=30537464, 11 results
Sequence fragment: D66 A67 T68 E69 E70 S71 D72 L73 A74 Q75 Q76 Y77
Penalisations: low_count=0.89 imperfect_connectivity=0.21 excessive_start_pt=0.99

H#1	N#1	CB#1	CB	CA#1	CA	CO	CO#1	Assignment
8.39	125.6	19.0	32.3	52.5	63.8	169.9	177.5	119
8.65	110.5	68.9	20.9	64.5	53.7	176.9	175.8	68
6.92	123.4	31.0	68.9	57.5	63.8	175.8	177.2	69
7.22	108.6	31.0	31.0	61.3	56.9	178.4	174.9	116
8.18	110.2	63.8	31.7	60.7	61.3	175.3	175.3	15
7.63	118.8	39.9	63.8	57.5	60.7	175.3	179.7	21
7.85	122.2	43.6	40.5	58.2	58.2	178.9	178.0	73
7.97	120.0	18.4	43.6	55.6	58.2	178.0	179.4	74
8.22	117.9	28.5	18.4	59.4	55.6	179.4	180.0	75
8.13	122.8	27.9	27.9	59.4	59.4	180.0	177.3	76
7.12	114.2	38.0	27.9	59.4	59.4	177.3	175.0	77

Putative sequential assignment 18: score=6140603, orig_score=27673616, 12 results
Sequence fragment: H8 V9 L10 V11 L12 R13 K14 S15 N16 F17 A18 E19 A20
Penalisations: imperfect_connectivity=0.26 excessive_start_pt=0.86

H#1	N#1	CB#1	CB	CA#1	CA	CO	CO#1	Assignment
8.39	125.6	32.3	32.3	52.5	63.8	176.9	176.4	119
9.95	124.3	38.0	33.5	55.0	53.7	176.6	175.6	90
7.98	124.9	32.9	39.9	53.1	53.1	175.0	173.2	17
9.25	125.9	43.6	32.3	55.6	52.5	173.2	175.8	62
9.00	119.1	34.8	44.3	54.4	53.7	174.4	176.3	13
9.09	124.3	31.7	34.8	61.3	54.4	176.3	178.4	14
8.18	110.2	63.8	31.7	60.7	61.3	178.4	175.3	15
7.63	118.8	39.9	63.8	57.5	60.7	175.3	179.7	21

7.85	122.2	43.6	40.5	58.2	58.2	178.9	178.0	73
7.97	120.0	18.4	43.6	55.6	58.2	178.0	179.4	74
8.22	117.9	28.5	18.4	59.4	55.6	179.4	180.0	75
7.83	124.6	19.0	29.1	55.6	60.1	178.7	179.7	20

Putative sequential assignment 19: score=6988331, orig_score=28390857, 12 results
Sequence fragment: V11 L12 R13 K14 S15 N16 F17 A18 E19 A20 L21 A22 A23
Penalisations: imperfect_connectivity=0.26 excessive_start_pt=0.96

H#1	N#1	CB#1	CB	CA#1	CA	CO	CO#1	Assignment
7.22	108.6	43.6	31.7	55.6	55.6	174.9	176.4	81
8.98	119.4	34.8	44.3	54.4	53.7	176.3	176.3	13
9.09	124.3	31.7	34.8	61.3	54.4	176.3	178.4	14
8.18	110.2	63.8	31.7	60.7	61.3	178.4	175.3	15
7.63	118.8	39.9	63.8	57.5	60.7	175.3	179.7	21
7.85	122.2	43.6	40.5	58.2	58.2	178.9	178.0	73
7.97	120.0	18.4	43.6	55.6	58.2	178.0	179.4	74
8.22	117.9	28.5	18.4	59.4	55.6	179.4	180.0	75
7.83	124.6	19.0	29.1	55.6	60.1	178.7	179.7	20
8.92	115.1	40.5	19.7	58.2	57.5	179.2	178.3	106
7.18	117.6	17.8	42.4	53.7	57.5	177.7	179.1	22
7.75	129.9	20.3	19.7	54.4	52.5	178.7	172.8	120