

**SUPPORTIVE INFORMATION for Identification of Novel Classes of Protein Kinase Inhibitors Using Combinatorial Peptide Chemistry Based on Functional Genomics Knowledge**

Thomas J. Lukas, Salida Mirzoeva, Urszula Slomczynska, and D. Martin Watterson

**Table 1.**  
Amino acid ratios of the pools 1a - 1r from first peptide combinatorial library.

| Amino acid | Pool 1a | Pool 1b | Pool 1c | Pool 1d | Pool 1e | Pool 1f | Pool 1g | Pool 1h | Pool 1i |
|------------|---------|---------|---------|---------|---------|---------|---------|---------|---------|
| D          | 4.1     | 11.7    | 3.4     | 2.1     | 0.5     | 3.2     | 2.6     | 0.5     | 3.5     |
| E          | 4.2     | 3.2     | 19.7    | 2.9     | 3.5     | 3.7     | 3.3     | 5.0     | 4.1     |
| S          | 2.2     | 1.6     | 2.1     | 1.8     | 2.0     | 1.9     | 1.7     | 2.5     | 2.2     |
| G          | 1.7     | 1.5     | 1.6     | 1.6     | 15.0    | 1.7     | 1.4     | 2.0     | 2.6     |
| H          | 2.8     | 2.1     | 2.1     | 2.1     | 2.3     | 14.5    | 1.9     | 3.2     | 1.9     |
| R          | 49.3    | 44.8    | 41.7    | 42.7    | 43.1    | 42.0    | 42.7    | 64.6    | 41.4    |
| T          | 2.4     | 2.1     | 2.0     | 2.3     | 2.2     | 1.8     | 1.9     | 2.8     | 2.3     |
| A          | 20.7    | 2.5     | 2.6     | 2.7     | 2.7     | 2.6     | 2.6     | 3.9     | 2.8     |
| P          | 2.5     | 3.4     | 2.3     | 2.0     | 2.2     | 2.1     | 1.9     | 2.8     | 2.0     |
| Y          | 2.5     | 2.0     | 1.9     | 2.2     | 2.0     | 2.0     | 1.8     | 2.8     | 2.1     |
| V          | 5.3     | 4.2     | 4.1     | 4.3     | 4.8     | 4.6     | 4.1     | 6.2     | 4.7     |
| M          | 1.5     | 2.3     | 1.5     | 2.4     | 1.8     | 1.2     | 1.6     | 2.5     | 1.8     |
| I          | 1.7     | 1.3     | 1.5     | 1.3     | 1.7     | 1.5     | 17.0    | 2.2     | 1.7     |
| L          | 1.5     | 1.1     | 1.3     | 1.1     | 1.3     | 1.3     | 1.1     | 1.9     | 15.4    |
| F          | 1.6     | 1.3     | 1.3     | 16.9    | 1.5     | 1.4     | 1.4     | 2.0     | 1.4     |
| K          | 34.7    | 53.8    | 49.9    | 50.6    | 52.4    | 50.2    | 52.1    | 34.0    | 49.0    |

**Table 1 (continued)**  
**Amino acid ratios of the pools 1a - 1r from first peptide combinatorial library.**

| Amino acid | Pool 1j | Pool 1k | Pool 1l | Pool 1m | Pool 1n | Pool 1o | Pool 1p | Pool 1q | Pool 1r |
|------------|---------|---------|---------|---------|---------|---------|---------|---------|---------|
| D          | 2.2     | 14.1    | 2.1     | 3.1     | 2.1     | 2.2     | 2.1     | 2.1     | 2.3     |
| E          | 3.0     | 3.8     | 2.5     | 19.5    | 2.8     | 3.1     | 3.1     | 2.8     | 2.2     |
| S          | 1.7     | 2.0     | 1.7     | 1.7     | 14.4    | 2.0     | 1.7     | 1.5     | 2.0     |
| G          | 2.2     | 1.6     | 1.8     | 1.6     | 1.7     | 2.0     | 1.8     | 1.4     | 1.7     |
| H          | 1.8     | 2.1     | 1.7     | 1.8     | 1.8     | 2.1     | 2.1     | 1.9     | 2.1     |
| R          | 43.0    | 46.9    | 43.3    | 41.7    | 45.1    | 43.6    | 43.9    | 39.3    | 53.4    |
| T          | 2.2     | 2.2     | 2.0     | 1.9     | 2.1     | 16.1    | 2.6     | 1.8     | 2.3     |
| A          | 2.9     | 2.8     | 2.4     | 2.5     | 2.6     | 2.6     | 3.3     | 2.4     | 3.1     |
| P          | 2.0     | 2.8     | 18.7    | 1.8     | 1.7     | 2.0     | 1.9     | 1.6     | 1.8     |
| Y          | 2.4     | 2.3     | 1.9     | 1.8     | 1.9     | 2.1     | 18.1    | 1.8     | 2.1     |
| V          | 4.3     | 4.9     | 4.3     | 4.7     | 4.5     | 4.3     | 4.4     | 31.0    | 4.9     |
| M          | 18.2    | 2.3     | 2.4     | 1.9     | 2.4     | 2.4     | 2.4     | 2.2     | 2.7     |
| I          | 1.5     | 1.6     | 1.3     | 1.5     | 1.3     | 1.4     | 1.5     | 1.1     | 1.4     |
| L          | 1.1     | 1.4     | 1.1     | 1.2     | 1.2     | 1.2     | 1.2     | 1.0     | 1.3     |
| F          | 1.2     | 1.5     | 1.2     | 1.4     | 1.5     | 1.4     | 1.3     | 1.2     | 1.4     |
| K          | 49.0    | 56.6    | 50.6    | 50.9    | 52.0    | 50.8    | 47.5    | 46.0    | 54.3    |

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**Table 2.**  
Amino acid ratios of the pools 2a - 2r from second peptide combinatorial library.

| Amino acid | Pool 2a | Pool 2b | Pool 2c | Pool 2d | Pool 2e | Pool 2f | Pool 2g | Pool 2h | Pool 2i |
|------------|---------|---------|---------|---------|---------|---------|---------|---------|---------|
| D          | 1.4     | 17.8    | 2.3     | 1.1     | 1.1     | 1.9     | 1.2     | 0.9     | 1.3     |
| E          | 1.8     | 2.0     | 20.6    | 1.1     | 1.5     | 1.8     | 1.4     | 1.1     | 1.6     |
| S          | 1.0     | 0.8     | 0.9     | 1.3     | 0.7     | 0.9     | 0.9     | 1.1     | 1.3     |
| G          | 1.1     | 1.0     | 0.9     | 0.9     | 17.6    | 1.5     | 0.9     | 1.1     | 1.2     |
| H          | 1.9     | 1.8     | 1.7     | 1.5     | 2.2     | 17.9    | 1.8     | 1.9     | 1.8     |
| R          | 46.4    | 52.9    | 50.9    | 55.0    | 52.8    | 52.7    | 53.1    | 54.1    | 53.0    |
| T          | 1.1     | 1.1     | 1.7     | 1.0     | 1.0     | 1.1     | 1.0     | 1.2     | 1.4     |
| A          | 20.5    | 1.5     | 1.4     | 1.0     | 1.3     | 1.3     | 1.3     | 1.5     | 1.6     |
| P          | 1.0     | 0.9     | 0.8     | 0.7     | 0.9     | 0.8     | 0.9     | 1.0     | 1.0     |
| Y          | 19.2    | 17.7    | 17.4    | 18.2    | 18.0    | 17.4    | 17.9    | 17.9    | 17.7    |
| V          | 1.2     | 1.0     | 1.0     | 0.9     | 1.1     | 0.9     | 1.0     | 1.2     | 1.0     |
| M          | 0.8     | 0.8     | 0.8     | 0.6     | 0.8     | 0.8     | 0.7     | 0.7     | 0.7     |
| I          | 1.0     | 0.9     | 0.9     | 0.7     | 0.9     | 0.9     | 17.2    | 1.0     | 1.2     |
| L          | 1.0     | 0.8     | 0.9     | 0.6     | 0.8     | 0.9     | 0.8     | 0.9     | 17.4    |
| F          | 0.6     | 0.5     | 0.5     | 18.6    | 0.5     | 0.5     | 0.5     | 0.5     | 0.6     |
| K          | 55.9    | 52.4    | 51.4    | 53.7    | 54.7    | 54.7    | 55.4    | 69.9    | 53.3    |

Table 2 (continued).  
Amino acid ratios of the pools 2a - 2r from second peptide combinatorial library.

| Amino acid | Pool 2j | Pool 2k | Pool 2l | Pool 2m | Pool 2n | Pool 2o | Pool 2p | Pool 2q | Pool 2r |
|------------|---------|---------|---------|---------|---------|---------|---------|---------|---------|
| D          | 1.4     | 16.4    | 0.8     | 1.1     | 0.8     | 1.0     | 0.4     | 1.1     | 1.3     |
| E          | 1.9     | 2.0     | 1.0     | 21.0    | 1.1     | 1.3     | 1.1     | 1.4     | 1.6     |
| S          | 1.6     | 0.9     | 1.1     | 0.9     | 15.9    | 1.0     | 1.0     | 1.4     | 1.5     |
| G          | 1.9     | 0.9     | 1.1     | 1.0     | 1.2     | 1.1     | 0.9     | 1.1     | 1.3     |
| H          | 1.8     | 1.8     | 1.7     | 1.9     | 1.7     | 1.7     | 1.6     | 2.0     | 1.9     |
| R          | 52.4    | 53.8    | 54.0    | 52.3    | 54.4    | 53.6    | 53.7    | 53.4    | 59.7    |
| T          | 1.7     | 1.2     | 1.4     | 1.1     | 1.3     | 17.7    | 1.2     | 1.2     | 1.4     |
| A          | 1.6     | 1.9     | 1.3     | 1.4     | 1.4     | 1.4     | 1.4     | 1.3     | 1.5     |
| P          | 1.6     | 0.9     | 18.0    | 0.8     | 0.9     | 1.0     | 0.9     | 1.2     | 1.2     |
| Y          | 17.4    | 17.9    | 17.4    | 17.5    | 18.5    | 17.5    | 35.5    | 18.0    | 20.4    |
| V          | 1.4     | 1.1     | 1.2     | 1.1     | 1.2     | 1.4     | 1.2     | 19.6    | 1.4     |
| M          | 16.6    | 0.7     | 0.7     | 0.9     | 0.7     | 1.1     | 0.7     | 0.7     | 0.9     |
| I          | 1.2     | 1.0     | 1.0     | 0.9     | 0.9     | 1.0     | 1.0     | 0.9     | 0.9     |
| L          | 1.3     | 1.0     | 0.9     | 0.9     | 0.9     | 1.0     | 0.9     | 0.8     | 1.0     |
| F          | 0.6     | 0.5     | 0.5     | 0.5     | 0.5     | 0.5     | 0.5     | 0.5     | 0.5     |
| K          | 51.7    | 54.0    | 53.9    | 52.8    | 54.5    | 53.8    | 53.9    | 51.4    | 59.5    |