

**Table 2** Amino Acid Sequence of OC-17 as taken from ref. 28

| Amino Acid    | Abbr. | Sequence Position | Amino Acid    | Abbr. | Sequence Position | Amino Acid    | Abbr. | Sequence Position |
|---------------|-------|-------------------|---------------|-------|-------------------|---------------|-------|-------------------|
| Aspartic Acid | ASP   | 1                 | Alanine       | ALA   | 49                | Arginine      | ARG   | 97                |
| Proline       | PRO   | 2                 | Glutamic Acid | GLU   | 50                | Phenylalanine | PHE   | 98                |
| Aspartic Acid | ASP   | 3                 | Leucine       | LEU   | 51                | Alanine       | ALA   | 99                |
| Glycine       | GLY   | 4                 | Arginine      | ARG   | 52                | Serine        | SER   | 100               |
| Cysteine      | CYS   | 5                 | Leucine       | LEU   | 53                | Tryptophan    | TRP   | 101               |
| Glycine       | GLY   | 6                 | Leucine       | LEU   | 54                | Histidine     | HIE   | 102               |
| Proline       | PRO   | 7                 | Alanine       | ALA   | 55                | Arginine      | ARG   | 103               |
| Glycine       | GLY   | 8                 | Glutamic Acid | GLU   | 56                | Threonine     | THR   | 104               |
| Tryptophan    | TRP   | 9                 | Leucine       | LEU   | 57                | Alanine       | ALA   | 105               |
| Valine        | VAL   | 10                | Leucine       | LEU   | 58                | Lysine        | LYS   | 106               |
| Proline       | PRO   | 11                | Asparagine    | ASN   | 59                | Alanine       | ALA   | 107               |
| Threonine     | THR   | 12                | Alanine       | ALA   | 60                | Arginine      | ARG   | 108               |
| Proline       | PRO   | 13                | Serine        | SER   | 61                | Arginine      | ARG   | 109               |
| Glycine       | GLY   | 14                | Arginine      | ARG   | 62                | Glycine       | GLY   | 110               |
| Glycine       | GLY   | 15                | Glycine       | GLY   | 63                | Glycine       | GLY   | 111               |
| Cysteine      | CYS   | 16                | Glycine       | GLY   | 64                | Arginine      | ARG   | 112               |
| Leucine       | LEU   | 17                | Aspartic Acid | ASP   | 65                | Cysteine      | CYS   | 113               |
| Glycine       | GLY   | 18                | Glycine       | GLY   | 66                | Alanine       | ALA   | 114               |
| Phenylalanine | PHE   | 19                | Serine        | SER   | 67                | Alanine       | ALA   | 115               |
| Phenylalanine | PHE   | 20                | Glycine       | GLY   | 68                | Leucine       | LEU   | 116               |
| Serine        | SER   | 21                | Glutamic Acid | GLU   | 69                | Arginine      | ARG   | 117               |
| Arginine      | ARG   | 22                | Glycine       | GLY   | 70                | Aspartic Acid | ASP   | 118               |
| Glutamic Acid | GLU   | 23                | Alanine       | ALA   | 71                | Glutamic Acid | GLU   | 119               |
| Leucine       | LEU   | 24                | Aspartic Acid | ASP   | 72                | Glutamic Acid | GLU   | 120               |
| Serine        | SER   | 25                | Glycine       | GLY   | 73                | Alanine       | ALA   | 121               |
| Tryptophan    | TRP   | 26                | Arginine      | ARG   | 74                | Phenylalanine | PHE   | 122               |
| Serine        | SER   | 27                | Valine        | VAL   | 75                | Threonine     | THR   | 123               |
| Arginine      | ARG   | 28                | Tryptophan    | TRP   | 76                | Serine        | SER   | 124               |
| Alanine       | ALA   | 29                | Isoleucine    | ILE   | 77                | Tryptophan    | TRP   | 125               |
| Glutamic Acid | GLU   | 30                | Glycine       | GLY   | 78                | Alanine       | ALA   | 126               |
| Serine        | SER   | 31                | Leucine       | LEU   | 79                | Alanine       | ALA   | 127               |
| Phenylalanine | PHE   | 32                | Histidine     | HIE   | 80                | Arginine      | ARG   | 128               |
| Cysteine      | CYS   | 33                | Arginine      | ARG   | 81                | Proline       | PRO   | 129               |
| Arginine      | ARG   | 34                | Proline       | PRO   | 82                | Cysteine      | CYS   | 130               |
| Arginine      | ARG   | 35                | Alanine       | ALA   | 83                | Threonine     | THR   | 131               |
| Tryptophan    | TRP   | 36                | Glycine       | GLY   | 84                | Glutamic Acid | GLU   | 132               |
| Glycine       | GLY   | 37                | Serine        | SER   | 85                | Arginine      | ARG   | 133               |
| Proline       | PRO   | 38                | Arginine      | ARG   | 86                | Asparagine    | ASN   | 134               |
| Glycine       | GLY   | 39                | Serine        | SER   | 87                | Alanine       | ALA   | 135               |
| Serine        | SER   | 40                | Tryptophan    | TRP   | 88                | Phenylalanine | PHE   | 136               |
| Histidine     | HIE   | 41                | Arginine      | ARG   | 89                | Valine        | VAL   | 137               |
| Leucine       | LEU   | 42                | Tryptophan    | TRP   | 90                | Cysteine      | CYS   | 138               |
| Alanine       | ALA   | 43                | Serine        | SER   | 91                | Lysine        | LYS   | 139               |
| Alanine       | ALA   | 44                | Aspartic Acid | ASP   | 92                | Alanine       | ALA   | 140               |
| Valine        | VAL   | 45                | Glycine       | GLY   | 93                | Alanine       | ALA   | 141               |
| Arginine      | ARG   | 46                | Threonine     | THR   | 94                | Alanine       | ALA   | 142               |
| Serine        | SER   | 47                | Alanine       | ALA   | 95                |               |       |                   |
| Alanine       | ALA   | 48                | Proline       | PRO   | 96                |               |       |                   |

**Table 1** Average number of H-bonds for water molecules within the first two layers on the vicinal surfaces.

| Surface | Layer | H-bonds with layer |            |             | total      |
|---------|-------|--------------------|------------|-------------|------------|
|         |       | 1st                | 2nd        | bulk        |            |
| 31.8    | 1st   | 0.05±0.007         | 0.80±0.022 | 0.009±0.005 | 0.86±0.024 |
| 31.8    | 2nd   | 0.41±0.013         | 0.01±0.005 | 0.35±0.017  | 0.77±0.029 |
| 31.16   | 1st   | 0.25±0.047         | 0.86±0.017 | 0.01±0.004  | 1.12±0.043 |
| 31.16   | 2nd   | 0.47±0.017         | 0.01±0.004 | 0.37±0.017  | 0.86±0.026 |