|                    | β             | α             | <b>g</b> 3    | g <sub>2</sub> | <b>g</b> 1    | Σ  |
|--------------------|---------------|---------------|---------------|----------------|---------------|----|
| CHARMM<br>36       | M             |               | M             |                | М             | 3  |
| CHARMM<br>36-UA    | M             | F             | M             | M              | M<br>F        | 6  |
| MacRog             | <b>M</b><br>F | F             | M<br>F        |                | M<br>F        | 8  |
| Hög-<br>berg08     |               | <b>M</b><br>F | M<br><b>F</b> | M              | F             | 8  |
| GAFFlipid          | <b>M</b><br>F | F             | M<br>F        | М              | M<br>F        | 9  |
| Lipid14            | M<br>F        | M             | M<br><b>F</b> | M              | M<br>F        | 11 |
| Chiu               | <b>M</b><br>F | M<br>F        | M<br><b>F</b> | М              | <b>M</b><br>F | 11 |
| Ulm-<br>schneiders | M             | F             | <b>M</b><br>F | M              | M<br>F        | 12 |
| Slipid             | F             | F             | M<br>F        | M              | M             | 13 |
| Poger              | м<br><b>F</b> | M<br>F        | M<br>F        | M              | M             | 13 |
| Tjörn-<br>hammar14 | M             | М             | M<br>F        | M              | M<br>F        | 15 |
| Berger             | <b>M</b><br>F | M<br>F        | M<br><b>F</b> | M              | M<br>F        | 15 |
| Kukol              | <b>F</b>      | <b>M</b><br>F | M<br>F        | M              | <b>M</b><br>F | 16 |