**Table S1.** Basic information of the experimental strains

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Species | Strains | Source | Label | Number of spectra for training and validation | Number of spectra for prediction | |
| *Enterococcus faecalis* | 23658 | Reference strain | A | 3000  3000 | | 500 |
| 140623 | Reference strain | 500 |
| *Staphylococcus aureus* | LHL40230 | Isolated strain | B | 300 | | 50 |
| LHL38966 | Isolated strain | 300 | | 50 |
| LHL39092 | Isolated strain | 300 | | 50 |
| LHL39727 | Isolated strain | 300 | | 50 |
| LHL38648 | Isolated strain | 300 | | 50 |
| LHL38766 | Isolated strain | 300 | | 50 |
| LHL39689 | Isolated strain | 300 | | 50 |
| LHL38133 | Isolated strain | 300 | | 50 |
| LHL39536 | Isolated strain | 300 | | 50 |
| LHL39312 | Isolated strain | 300 | | 50 |
| LHL39289 | Isolated strain | 300 | | 50 |
| LHL39210 | Isolated strain | 300 | | 50 |
| LHL37386 | Isolated strain | 300 | | 50 |
| LHL37022 | Isolated strain | 300 | | 50 |
| LHL37415 | Isolated strain | 300 | | 50 |
| LHL38825 | Isolated strain | 300 | | 50 |
| CICC23656 | Reference strain | 300 | | 50 |
| ATCC6538 | Reference strain | 300 | | 50 |
| CMCC26003 | Reference strain | 300 | | 50 |
| YS4 | Isolated strain | 300 | | 50 |
| *Staphylococcus capitis* | CICC21723 | Reference strain | C | 6000 | | 1000 |
| *Staphylococcus sciuri* | CICC23471 | Reference strain | D | 6000 | | 1000 |
| *Staphylococcus vitulinus* | CICC10850 | Reference strain | E | 6000 | | 1000 |
| *Staphylococcus xylosus* | CICC22112 | Reference strain | F | 6000 | | 1000 |
| *Staphylococcus epidermidis* | CMCC26069 | Reference strain | G | 3000 | | 500 |
| YS5 | Isolated strain | 3000 | | 500 |
| *Staphylococcus simulans* | YS1 | Isolated strain | H | 6000 | | 1000 |
| *Staphylococcus haemolyticus* | YS2 | Isolated strain | I | 6000 | | 1000 |
| *Staphylococcus hominis* | YS3 | Isolated strain | J | 6000 | | 1000 |
| *Salmonella* | LHL37207 | Isolated strain | K | 1200 | | 200 |
| LHL40665 | Isolated strain | 1200 | | 200 |
| LHL1 | Isolated strain | 1200 | | 200 |
| LHL2 | Isolated strain | 1200 | | 200 |
| LHL3 | Isolated strain | 1200 | | 200 |
| *Kocuria rhizophila* | CMCC28001 | Reference strain | L | 6000 | | 1000 |
| *Staphylococcus lentus* | CICC21602 | Reference strain | M | 6000 | | 1000 |
| *Escherichia coli* | KW03004 | Isolated strain | N | 300 | | 50 |
| KW03005 | Isolated strain | 300 | | 50 |
| KW03006 | Isolated strain | 300 | | 50 |
| KW03007 | Isolated strain | 300 | | 50 |
| KW03008 | Isolated strain | 300 | | 50 |
| KW03010 | Isolated strain | 300 | | 50 |
| KW03011 | Isolated strain | 300 | | 50 |
| KW03012 | Isolated strain | 300 | | 50 |
| KW03013 | Isolated strain | 300 | | 50 |
| KW03021 | Isolated strain | 300 | | 50 |
| KW03025 | Isolated strain | 300 | | 50 |
| KW03038 | Isolated strain | 300 | | 50 |
| KW03076 | Isolated strain | 300 | | 50 |
| CMCC44102 | Reference strain | 300 | | 50 |
| CMCC44113 | Reference strain | 300 | | 50 |
| CMCC44829 | Reference strain | 300 | | 50 |
| LHL40179 | Isolated strain | 300 | | 50 |
| LHL40245 | Isolated strain | 300 | | 50 |
| LHL40505 | Isolated strain | 300 | | 50 |
| LHL40540 | Isolated strain | 300 | | 50 |