**Table S7. Minimum inhibitory concentrations of QAC analogues measured by the *E. coli* ATCC 25922 assay.**

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| --- | --- | --- | --- | --- | --- |
| **Test No.** | **CAS No.** | **Chemical Name/Abbreviation** | **MICa (mg/L)** | **Predicted label** | **True label** |
| 1 | 2083-68-3 | ATMAC-8 | 250 | 1 | 1 |
| 2 | 2082-84-0 | ATMAC-10 | 125 | 1 | 1 |
| 3 | 1119-94-4 | ATMAC-12 | 62.5 | 1 | 1 |
| 4 | 1119-97-7 | ATMAC-14 | 62.5 | 1 | 1 |
| 5 | 57-09-0 | ATMAC-16 | 62.5 | 1 | 1 |
| 6 | 1120-02-1 | ATMAC-18 | 125 | 1 | 1 |
| 7 | 959-55-7 | BAC-8 | 125 | 1 | 1 |
| 8 | 965-32-2 | BAC-10 | 31 | 1 | 1 |
| 9 | 139-07-1 | BAC-12 | 31 | 1 | 1 |
| 10 | 139-08-2 | BAC-14 | 15.5 | 1 | 1 |
| 11 | 122-18-9 | BAC-16 | 31 | 1 | 1 |
| 12 | 122-19-0 | BAC-18 | 125 | 1 | 1 |
| 13 | 3026-69-5 | DADMAC-8:8 | 31 | 1 | 1 |
| 14 | 2390-68-3 | DADMAC-10:10 | 15.5 | 1 | 1 |
| 15 | 3282-73-3 | DADMAC-12:12 | 125 | 1 | 1 |
| 16 | 68105-02-2 | DADMAC-14:14b | 8000 | 1 | 0 |
| 17 | 70755-47-4 | DADMAC-16:16b | >8000 | 1 | 0 |
| 18 | 3700-67-2 | DADMAC-18:18b | >8000 | 0 | 0 |
| 19 | 121-54-0 | Benzethonium | 31 | 1 | 1 |
| 20 | 104-74-5 | Laurylpyridinium | 15.5 | 1 | 1 |
| 21 | 6004-24-6 | Cetylpyridinium | 31 | 1 | 1 |
| 22 | 124-03-8 | Cetyldimethylethylammonium | 62.5 | 1 | 1 |
| 23 | 538-71-6 | Domiphen | 15.5 | 1 | 1 |
| 24 | 7009-61-2 | Dodecyl(2-hydroxyethyl)-dimethylammonium | 62.5 | 1 | 1 |
| 25 | 22340-01-8 | Dodecyl-bis(2-hydroxyethyl)-methylazanium | 62.5 | 1 | 1 |
| 26 | 86438-79-1 | Lauramidopropyl betaine | 1000 | 1 | 1 |
| 27 |  | DADMAC-10:18 | >8000 | 1 | 0 |
| 28 |  | DADMAC-12:16 | 8000 | 1 | 0 |
| 29 |  | DADMAC-13:15 | >8000 | 1 | 0 |
| 30 |  | Bis(2-hexadecanoyloxyethyl)-dimethylazanium | >8000 | 0 | 0 |

a Minimum inhibitory concentrations (MICs) of QACs against *E. coli* ATCC 25922 were determined using micro broth dilution or agar dilution methods. b The agar dilution method was used for insoluble compounds (*i.e.,* DADMAC-14:14, 16:16, 18:18). Compounds with MICs less than 1 mg/mL were labelled as positive compounds.