**SUPPLEMENTARY MATERIAL**

# Essential oils biofilm modulation activity chemical and machine learning analysis. Application on *Staphylococcus aureus* isolates from cystic fibrosis patients.

**Rosanna Papa[1,§], Stefania Garzoli[2,§], Gianluca Vrenna[3], Manuela Sabatino[4,5], Michela Relucenti[6], Orlando Donfrancesco[7], Ersilia Vita Fiscarelli[8], Marco Artini[9], Laura Selan[10,*] and Rino Ragno[11,12,*]**

**Rosanna Papa[1,§], Stefania Garzoli[2,§], Gianluca Vrenna[3], Manuela Sabatino[4,5], Michela Relucenti[6], Orlando Donfrancesco[7], Ersilia Vita Fiscarelli[8], Marco Artini[9], Laura Selan[10,*] and Rino Ragno[11,12,*]**

1 Department of Public Health and Infectious Diseases, Sapienza University, p.le Aldo Moro 5, 00185 Rome, Italy; rosanna.papa@uniroma1.it
2 Department of Drug Chemistry and Technology, Sapienza University, p.le Aldo Moro 5, 00185 Rome, Italy; stefania.garzoli@uniroma1.it
3 Department of Public Health and Infectious Diseases, Sapienza University, p.le Aldo Moro 5, 00185 Rome, Italy; gianluca.vrenna@uniroma1.it
4 Department of Drug Chemistry and Technology, Sapienza University, p.le Aldo Moro 5, 00185 Rome, Italy; manuela.sabatino@uniroma1.it
5 Rome Center for Molecular Design, Department of Drug Chemistry and Technology, Sapienza University, p.le Aldo Moro 5, 00185 Rome, Italy; manuela.sabatino@uniroma1.it
6 Department of Anatomy, Histology, Forensic Medicine and Orthopaedics, Sapienza University of Rome, via Alfonso Borelli 50, Rome, 00161, Italy; michela.relucenti@uniroma1.it
7 Department of Anatomy, Histology, Forensic Medicine and Orthopaedics, Sapienza University of Rome, via Alfonso Borelli 50, Rome, 00161, Italy; orlando.donfrancesco@uniroma1.it
8 Paediatric and Laboratory Department. Children's Hospital and Institure Research Bambino Gesù, Italy; evita.fiscarelli@opbg.net
9 Department of Public Health and Infectious Diseases, Sapienza University, p.le Aldo Moro 5, 00185 Rome, Italy; marco.artini@uniroma1.it
10 Department of Public Health and Infectious Diseases, Sapienza University, p.le Aldo Moro 5, 00185 Rome, Italy; laura.selan@uniroma1.it
11 Department of Drug Chemistry and Technology, Sapienza University, p.le Aldo Moro 5, 00185 Rome, Italy; rino.ragno@uniroma1.it
12 Rome Center for Molecular Design, Department of Drug Chemistry and Technology, Sapienza University, p.le Aldo Moro 5, 00185 Rome, Italy; rino.ragno@uniroma1.it

**Table SM1.** Qualitative descriptors used for the unsupervised Machine Learning clusterization of *S. aureus* strains.

| **Descriptor Name** | **Parameter** |
|---|---|
| Type of sample | Esp: sputum; AT: hypopharyngeal suction |
| Methicillin profile | MRSA e MSSA |
| Phenotype | Small colony variant, normal |
| Quinolones Sensitivity | Resistant or Susceptible |
| Trimethoprim/Sulfamethoxazole Sensitivity | Resistant or Susceptible |
| Erythromycin Sensitivity | Resistant or Susceptible |
| Clindamycin Sensitivity | Resistant or Susceptible |
| Linezolid Sensitivity | Resistant or Susceptible |
| Inducible Clindamycin resistance ability | Positive or negative |
| Fungal Co-infection | *Scedosporium prolificans* |
| *P. aeruginosa* co-infection | Positive or negative |
| *cftr* gene mutation | 621+1G>T/R553X |
| | F508del/F508del |
| | L636P/P499A |
| Biofilm formation | Strong, moderate or weak |

**Table SM2.** Phenotypical and genotypical characterization of 3 representative strains of *S. aureus.*

| ID pt | ID | SAM | Date | Str | Ph | QUIN | B | ER | CLI | LIN | RCLI | CF | CPA | GENOTYPE |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 4 | 4S | AT | 2/20/2009 | MRSA | - | S | S | Nt | S | S | P | | | 621+1G>T/R553X |
| 5 | 5S | ESP | 11/13/2009 | MRSA | - | R | S | Nt | R | S | N | Sp | | F508del/F508del |
| 19 | 19S | ESP | 6/15/2017 | MSSA | - | S | S | R | R | S | P | | X | L636P/P499A |

The 3 *Staphylococcus aureus* clinical isolates and their characterization by several properties. **ID pt:** Patient Identification; **ID**: Strain Code; **SAM**: Sample; **Date**: Date of collection; **Str**: Strain; **Ph**: Phenotype; **QUIN**: Quinolones; **B**: Trimethoprim/Sulfamethoxazole; **ER**: Erythromycin; **CLI**: Clindamycin; **LIN**: Linezolid; **RCLI**: Inducible Clindamycin resistance; **CF**: Fungal Co-infection; **CPA**: *P. aeruginosa* co-infection; **GEN**: Pts Genotype; **Esp**: Sputum; **AT**: Hypopharyngeal Suction; **MRSA**: Methicillin Resistant *S. aureus*; **MSSA**: Methicillin Sensitive *S. aureus*;; **R**: Resistant; **S**: Susceptible; **N**: Negative; **Nt**: Non tested; Sp*: Scedosporium prolificans.*

**Table SM3**. SEM $OsO_4$-RR-TA-IL protocol and operating conditions for observation.

| **Steps** | **$OsO_4$-RR-TA-IL Protocol** |
|---|---|
| **Fixation** | Glutharaldehyde 2,5% in PB 0.1 M pH 7.4 at least 48 h |
| **Washing** | 10 min x2 times in PB 0.1 M pH 7.4 |
| **Postfixation** | $OsO_4$ 2%+RR 0.2% 1:1 solution, 1 h |
| **Washing** | 10 min -2 times in $H_20$ |
| **Impregnation** | Tannic Acid 1% in d $H_20$ 30 min |
| **Washing** | 10 min -2 times in $H_20$ |
| **Dehydration** | None |
| **Drying** | None |
| **Pt Sputter coating** | Replaced by IL |
| **Operating conditions** | 15-20 kV, high vacuum |

**Table SM4**. ID and plant name of essential oils used in the investigation.

| EO ID | EO Name | EO ID | EO Name |
|---|---|---|---|
| EO1 | Chamomile Morocco | EO32 | Birch |
| EO2 | Sage Sclarea | EO33 | Fennel |
| EO3 | Salvia Officinalis | EO34 | Cedar Fruit |
| EO4 | Red Thyme | EO35 | Lemon |
| EO5 | Tea Tree Oil | EO36 | Roman Chamomile |
| EO6 | Melissa Oiio Essential | EO37 | Savory |
| EO7 | Pinus Mugo | EO38 | Rosemary |
| EO8 | Geranium Bourbon | EO39 | Ceylon Cinnamon Peel |
| EO9 | Oregano | EO40 | Eucaliptus Globulus |
| EO10 | Ylang Ylang | EO41 | Sweet Orange |
| EO11 | Coriander | EO42 | Niaouly |
| EO12 | Lavandula Angustifoglia | EO43 | Artemisia |
| EO13 | Myrtle | EO44 | Cajeput |
| EO14 | Garlic | EO45 | Black Pepper |
| EO15 | Cardamom | EO46 | White Thyme |
| EO16 | Mandarin | EO47 | Marjoram |
| EO17 | Hyssop | EO48 | Cloves |
| EO18 | Grapefruit | EO49 | Cypress |
| EO19 | Cymbopogon | EO50 | Nutmeg Natural |
| EO20 | Pinus Sibirica | EO51 | Peppermint |
| EO21 | Camphor | EO52 | Verbena officinalis |
| EO22 | Cadè | EO53 | Basil |
| EO23 | Cedar Leaves | EO54 | Cymbopogon martinii |
| EO24 | Ginger | EO55 | Laurel |
| EO25 | Cumin | EO56 | Anise |
| EO26 | Patchouli | EO57 | Incense |
| EO27 | Bitter Orange | EO58 | Mentha Suaveolens |
| EO28 | Eucalyptus | EO59 | Coridotthymus Capitatus |
| EO29 | Pinus Silvester | EO60 | Thymus Vulgaris |
| EO30 | Bergamot | EO61 | Origanum Hirtum |
| EO31 | Juniper | | |

**Table SM5**. Antimicrobial activity of EOs listed in Table S4**Errore. L'origine riferimento non è stata trovata.** on representative clinical strains and reference strains of *S. aureus* [19].

| EOs ID | 6538P | 25923 | 4S | 5S | 19S |
|---|---|---|---|---|---|
| 1 | Antibacterial | Antibacterial | Antibacterial | Inactive | Inactive |
| 2 | Inactive | Inactive | Inactive | Inactive | Inactive |
| 3 | Inactive | Inactive | Inactive | Inactive | Inactive |
| 4 | Antibacterial | Antibacterial | Antibacterial | Antibacterial | Antibacterial |
| 5 | Inactive | Inactive | Inactive | Inactive | Inactive |
| 6 | Inactive | Antibacterial | Antibacterial | Antibacterial | Antibacterial |
| 7 | Inactive | Inactive | Inactive | Inactive | Inactive |
| 8 | Inactive | Inactive | Inactive | Inactive | Inactive |
| 9 | Antibacterial | Antibacterial | Antibacterial | Antibacterial | Antibacterial |
| 10 | Inactive | Inactive | Inactive | Inactive | Inactive |
| 11 | Inactive | Inactive | Inactive | Inactive | Inactive |
| 12 | Inactive | Inactive | Inactive | Inactive | Inactive |
| 13 | Inactive | Inactive | Inactive | Inactive | Inactive |
| 14 | Antibacterial | Antibacterial | Antibacterial | Antibacterial | Antibacterial |
| 15 | Inactive | Inactive | Inactive | Inactive | Inactive |
| 16 | Inactive | Inactive | Inactive | Inactive | Inactive |
| 17 | Inactive | Inactive | Inactive | Inactive | Inactive |
| 18 | Inactive | Inactive | Inactive | Inactive | Inactive |
| 19 | Inactive | Inactive | Inactive | Inactive | Inactive |
| 20 | Inactive | Inactive | Inactive | Inactive | Inactive |
| 21 | Inactive | Inactive | Inactive | Inactive | Inactive |
| 22 | Antibacterial | Antibacterial | Antibacterial | Antibacterial | Antibacterial |
| 23 | Inactive | Inactive | Inactive | Inactive | Inactive |
| 24 | Inactive | Inactive | Inactive | Inactive | Inactive |
| 25 | Inactive | Inactive | Inactive | Inactive | Inactive |
| 26 | Inactive | Inactive | Inactive | Inactive | Inactive |
| 27 | Inactive | Inactive | Inactive | Inactive | Inactive |
| 28 | Inactive | Inactive | Inactive | Inactive | Inactive |
| 29 | Inactive | Inactive | Inactive | Inactive | Inactive |
| 30 | Inactive | Inactive | Inactive | Inactive | Inactive |
| 31 | Inactive | Inactive | Inactive | Inactive | Inactive |
| 32 | Antibacterial | Antibacterial | Antibacterial | Antibacterial | Antibacterial |
| 33 | Inactive | Inactive | Inactive | Inactive | Inactive |
| 34 | Inactive | Inactive | Inactive | Inactive | Inactive |
| 35 | Inactive | Inactive | Inactive | Inactive | Inactive |
| 36 | Inactive | Inactive | Inactive | Inactive | Inactive |
| 37 | Antibacterial | Antibacterial | Antibacterial | Antibacterial | Antibacterial |
| 38 | Inactive | Inactive | Inactive | Inactive | Inactive |
| 39 | Antibacterial | Antibacterial | Antibacterial | Antibacterial | Antibacterial |
| 40 | Inactive | Inactive | Inactive | Inactive | Inactive |
| 41 | Inactive | Inactive | Inactive | Inactive | Inactive |
| 42 | Inactive | Inactive | Inactive | Inactive | Inactive |
| 43 | Inactive | Inactive | Inactive | Inactive | Inactive |
| 44 | Inactive | Inactive | Inactive | Inactive | Inactive |
| 45 | Inactive | Inactive | Inactive | Inactive | Inactive |
| 46 | Antibacterial | Antibacterial | Antibacterial | Antibacterial | Antibacterial |
| 47 | Inactive | Inactive | Inactive | Inactive | Inactive |
| 48 | Antibacterial | Antibacterial | Antibacterial | Antibacterial | Antibacterial |
| 49 | Inactive | Inactive | Inactive | Inactive | Inactive |
| 50 | Inactive | Inactive | Inactive | Inactive | Inactive |
| 51 | Inactive | Inactive | Inactive | Inactive | Inactive |
| 52 | Inactive | Inactive | Inactive | Antibacterial | Antibacterial |
| 53 | Inactive | Inactive | Inactive | Inactive | Inactive |
| 54 | Antibacterial | Inactive | Inactive | Inactive | Antibacterial |
| 55 | Inactive | Inactive | Inactive | Inactive | Inactive |
| 56 | Inactive | Inactive | Inactive | Inactive | Inactive |
| 57 | Inactive | Inactive | Inactive | Inactive | Inactive |
| 58 | Inactive | Inactive | Inactive | Inactive | Inactive |
| 59 | Antibacterial | Antibacterial | Antibacterial | Antibacterial | Antibacterial |

| | | | | | |
|---|---|---|---|---|---|
| 60 | Inactive | Inactive | Inactive | Antibacterial | Antibacterial |
| 61 | Antibacterial | Inactive | Inactive | Antibacterial | Inactive |

**Table SM6.** Percentage of bacterial biofilm formation in the presence of each EO listed in Table S4 at concentration 1.00% v/v relative to untreated bacteria. Bacterial strains: *S. aureus* ATCC 6538P and *S. aureus* ATCC 25923, *S. aureus* 4S, *S. aureus* 5S and *S. aureus* 19S. Each data point is composed of 4 independent experiments, each performed with at least three replicates. The mean values are listed along with the calculated standard deviations (SD).

| EOs ID | ***S. aureus* strains** | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | **6538P** | | **25923** | | **4S** | | **5S** | | **19S** | |
| | Mean | SD | Mean | SD | Mean | SD | Mean | SD | Mean | SD |
| **1** | NA | NA | NA | NA | NA | NA | 97.73 | 13.59 | 77.65 | 23.82 |
| **2** | 17.65 | 8.04 | 109.52 | 18.54 | 108.40 | 28.53 | 100.49 | 11.14 | 87.76 | 12.18 |
| **3** | 5.98 | 0.93 | 86.15 | 3.94 | 34.27 | 6.15 | 74.62 | 4.28 | 11.65 | 0.32 |
| **4** | NA | NA | NA | NA | NA | NA | NA | NA | NA | NA |
| **5** | 46.75 | 8.05 | 116.19 | 4.66 | 34.88 | 12.10 | 74.41 | 14.37 | 74.84 | 15.74 |
| **6** | 20.86 | 1.29 | NA | NA | NA | NA | NA | NA | NA | NA |
| **7** | 27.32 | 2.56 | 102.06 | 6.62 | 62.83 | 5.78 | 101.88 | 10.02 | 68.40 | 7.16 |
| **8** | 66.27 | 8.13 | 64.83 | 9.79 | 81.04 | 6.94 | 120.85 | 15.29 | 67.67 | 7.40 |
| **9** | NA | NA | NA | NA | NA | NA | NA | NA | NA | NA |
| **10** | 36.33 | 5.92 | 80.39 | 5.60 | 54.27 | 14.79 | 61.74 | 8.16 | 78.10 | 21.33 |
| **11** | 5.64 | 1.11 | 58.98 | 3.56 | 49.26 | 11.24 | 63.88 | 6.90 | 23.88 | 8.33 |
| **12** | 41.65 | 13.47 | 98.21 | 8.46 | 70.87 | 1.31 | 69.10 | 4.08 | 82.61 | 5.72 |
| **13** | 7.15 | 0.71 | 81.27 | 3.62 | 70.78 | 15.26 | 74.28 | 15.89 | 30.87 | 7.36 |
| **14** | NA | NA | NA | NA | NA | NA | NA | NA | NA | NA |
| **15** | 16.85 | 10.62 | 81.81 | 5.31 | 49.82 | 9.40 | 58.81 | 8.11 | 41.19 | 18.08 |
| **16** | 47.48 | 8.77 | 217.49 | 11.25 | 52.61 | 9.15 | 91.81 | 12.97 | 75.44 | 21.36 |
| **17** | 14.36 | 7.84 | 80.85 | 15.12 | 75.61 | 6.26 | 72.99 | 5.51 | 82.05 | 4.28 |
| **18** | 64.47 | 3.83 | 141.11 | 19.59 | 39.23 | 5.34 | 62.52 | 11.97 | 82.69 | 14.52 |
| **19** | 35.75 | 3.12 | 32.51 | 4.45 | 54.17 | 8.33 | 60.48 | 7.59 | 81.17 | 9.64 |
| **20** | 55.81 | 2.55 | 211.67 | 18.55 | 57.18 | 5.82 | 91.18 | 13.41 | 114.73 | 16.47 |
| **21** | 57.92 | 13.33 | 141.14 | 7.78 | 65.74 | 6.01 | 205.38 | 19.38 | 100.03 | 17.48 |
| **22** | NA | NA | NA | NA | NA | NA | NA | NA | NA | NA |
| **23** | 168.07 | 4.85 | 94.70 | 2.24 | 80.65 | 8.23 | 66.17 | 3.83 | 93.75 | 17.00 |
| **24** | 16.56 | 2.71 | 72.53 | 3.06 | 36.19 | 6.34 | 31.72 | 1.88 | 53.00 | 10.41 |
| **25** | 7.56 | 0.88 | 29.76 | 8.43 | 99.13 | 19.23 | 57.63 | 9.26 | 25.33 | 2.29 |
| **26** | 7.52 | 0.62 | 346.73 | 6.35 | 14.97 | 1.11 | 48.41 | 1.21 | 38.46 | 7.32 |
| **27** | 13.46 | 0.75 | 57.88 | 12.91 | 28.18 | 8.35 | 32.42 | 12.80 | 55.90 | 0.76 |
| **28** | 172.60 | 0.40 | 76.21 | 2.15 | 106.80 | 17.54 | 78.15 | 4.99 | 108.47 | 14.10 |
| **29** | 48.04 | 2.37 | 89.89 | 9.17 | 57.81 | 1.70 | 100.87 | 5.18 | 66.71 | 2.83 |
| **30** | 41.27 | 8.28 | 97.98 | 16.34 | 70.67 | 16.35 | 200.34 | 22.82 | 78.20 | 8.21 |
| **31** | 69.71 | 19.66 | 58.36 | 4.05 | 79.57 | 15.17 | 157.62 | 11.98 | 97.02 | 14.90 |
| **32** | NA | NA | NA | NA | NA | NA | NA | NA | NA | NA |
| **33** | 148.88 | 15.05 | 64.11 | 4.79 | 70.65 | 3.93 | 189.08 | 15.76 | 135.61 | 21.86 |
| **34** | 24.79 | 5.08 | 162.31 | 15.36 | 28.14 | 7.18 | 33.96 | 5.09 | 36.67 | 3.26 |
| **35** | 48.04 | 9.26 | 89.89 | 4.29 | 57.81 | 4.54 | 100.87 | 10.06 | 66.71 | 3.70 |
| **36** | 50.48 | 4.74 | 157.31 | 13.26 | 30.91 | 1.86 | 38.94 | 7.99 | 40.88 | 9.48 |
| **37** | NA | NA | NA | NA | NA | NA | NA | NA | NA | NA |
| **38** | 5.60 | 1.09 | 46.71 | 20.34 | 28.68 | 11.30 | 68.31 | 15.42 | 12.83 | 3.37 |
| **39** | NA | NA | NA | NA | NA | NA | NA | NA | NA | NA |
| **40** | 48.25 | 5.73 | 119.87 | 13.19 | 65.10 | 5.60 | 17.,39 | 10.08 | 70.58 | 4.20 |
| **41** | 30.60 | 8.35 | 61.90 | 9.02 | 89.66 | 15.45 | 36.25 | 10.47 | 119.29 | 12.75 |
| **42** | 55.30 | 10.99 | 80.86 | 2.09 | 89.41 | 9.31 | 143.41 | 5.50 | 74.34 | 6.19 |
| **43** | 30.45 | 6.28 | 56.99 | 5.90 | 108.71 | 14.92 | 75.51 | 2.46 | 96.23 | 14.76 |
| **44** | 45.77 | 14.40 | 50.08 | 16.13 | 64.64 | 17.02 | 60.51 | 4.58 | 96.96 | 16.93 |
| **45** | 4.72 | 0.69 | 36.24 | 15.21 | 34.85 | 15.73 | 32.23 | 13.35 | 17.07 | 5.52 |
| **46** | NA | NA | NA | NA | NA | NA | NA | NA | NA | NA |
| **47** | 10.08 | 1.37 | 46.59 | 14.20 | 40.78 | 19.99 | 38.46 | 15.12 | 18.04 | 3.72 |
| **48** | NA | NA | NA | NA | NA | NA | NA | NA | NA | NA |
| **49** | 267.37 | 3.58 | 31.48 | 12.65 | 79.44 | 13.07 | 101.06 | 5.93 | 143.09 | 9.16 |
| **50** | 84.44 | 12.16 | 53.16 | 9.38 | 90.01 | 13.94 | 64.02 | 21.78 | 64.63 | 7.54 |
| **51** | 21.14 | 12.27 | 49.12 | 6.98 | 90.36 | 18.14 | 62.49 | 8.98 | 63.16 | 5.22 |
| **52** | 16.21 | 8.11 | 59.86 | 7.09 | 55.13 | 2.49 | NA | NA | NA | NA |
| **53** | 32.05 | 6.30 | 36.17 | 2.71 | 61.13 | 3.99 | 42.67 | 2.42 | 69.56 | 7.91 |
| **54** | NA | NA | 27.97 | 1.38 | 47.85 | 8.09 | 25.21 | 0.96 | NA | NA |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| **55** | 145.12 | 17.00 | 33.92 | 3.39 | 58.11 | 5.39 | 71.55 | 9.00 | 93.09 | 21.61 |
| **56** | 127.30 | 11.50 | 65.23 | 2.99 | 90.94 | 10.39 | 75.24 | 14.78 | 123.07 | 17.95 |
| **57** | 7.65 | 1.61 | 65.02 | 4.20 | 57.74 | 7.35 | 92.57 | 15.58 | 82.20 | 5.83 |
| **58** | 4.46 | 0.69 | 22.83 | 12.78 | 25.10 | 7.09 | 38.38 | 13.46 | 13.51 | 1.38 |
| **59** | NA | NA | NA | NA | NA | NA | NA | NA | NA | NA |
| **60** | 6.59 | 0.76 | 61.09 | 4.39 | 52.16 | 3.77 | NA | NA | NA | NA |
| **61** | NA | NA | 38.42 | 2.13 | 83.56 | 14.98 | NA | NA | 121.45 | 9.14 |
| **# Values** | 48 | | 49 | | 49 | | 47 | | 47 | 48 |
| **median** | 131.5 | | 79.23 | | 96.95 | | 119.34 | | 99.94 | 131.5 |
| **Median Corr** | 31.13 | | 65.02 | | 65.1 | | 74.93 | | 82.05 | 31.13 |

**Table SM7.** Percentage of bacterial biofilm formation in the presence of each EO listed in Table S4 at concentration 0.05% v/v relative to untreated bacteria. Bacterial strains: *S. aureus* ATCC 6538P and *S. aureus* ATCC 25923, *S. aureus* 4S, *S. aureus* 5S and *S. aureus* 19S. Each data point is composed of 4 independent experiments, each performed with at least three replicates. The mean values are listed along with the calculated standard deviations (SD).

| **EOs ID** | ***S. aureus* strains** | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | **6538P** | | **25923** | | **4S** | | **5S** | | **19S** | |
| | Mean | SD | Mean | SD | Mean | SD | Mean | SD | Mean | SD |
| **1** | 135.03 | 11.02 | 80.21 | 9.52 | 102.47 | 11.03 | 111.15 | 4.45 | 77.13 | 6.88 |
| **2** | 113.75 | 14.12 | 97.93 | 7.03 | 105.31 | 13.17 | 110.31 | 14.98 | 89.80 | 10.10 |
| **3** | 70.40 | 19.49 | 81.04 | 2.80 | 110.08 | 14.32 | 136.43 | 15.04 | 126.19 | 14.83 |
| **4** | 28.24 | 3.91 | 34.89 | 2.16 | 81.10 | 2.17 | 117.42 | 17.82 | 95.52 | 15.10 |
| **5** | 59.07 | 14.39 | 67.59 | 17.86 | 95.10 | 1.49 | 140.99 | 13.57 | 99.94 | 11.11 |
| **6** | 37.77 | 12.45 | 74.20 | 3.22 | 81.27 | 8.09 | 126.40 | 15.52 | 95.33 | 18.47 |
| **7** | 87.94 | 19.53 | 79.23 | 9.62 | 77.49 | 6.27 | 143.71 | 15.68 | 97.43 | 12.13 |
| **8** | 66.08 | 13.13 | 72.43 | 8.82 | 78.73 | 4.75 | 107.67 | 11.14 | 98.57 | 19.25 |
| **9** | 18.83 | 0.65 | 16.38 | 3.87 | 58.07 | 1.72 | 71.29 | 11.15 | 84.88 | 18.57 |
| **10** | 144.14 | 14.55 | 86.60 | 11.64 | 86.42 | 1.47 | 90.25 | 14.19 | 82.50 | 7.32 |
| **11** | 141.67 | 9.05 | 64.94 | 2.74 | 79.95 | 5.83 | 126.16 | 7.63 | 76.85 | 13.42 |
| **12** | 132.58 | 9.58 | 68.17 | 4.45 | 83.30 | 1.33 | 121.08 | 6.29 | 111.25 | 14.09 |
| **13** | 98.21 | 2.02 | 76.85 | 4.48 | 93.50 | 12.90 | 135.45 | 11.52 | 97.52 | 7.47 |
| **14** | 126.24 | 13.22 | 51.11 | 6.95 | 95.28 | 14.29 | 144.57 | 15.18 | 106.08 | 24.37 |
| **15** | 131.50 | 10.11 | 59.06 | 6.96 | 104.54 | 8.71 | 131.08 | 2.31 | 91.93 | 4.54 |
| **16** | 159.66 | 5.62 | 74.07 | 20.36 | 86.79 | 3.93 | 161.38 | 12.34 | 91.74 | 9.16 |
| **17** | 113.90 | 1.05 | 73.84 | 16.70 | 89.48 | 1.03 | 147.96 | 3.46 | 82.87 | 16.12 |
| **18** | 103.23 | 11.41 | 61.92 | 14.20 | 74.27 | 8.90 | 171.62 | 17.51 | 85.13 | 14.70 |
| **19** | 169.86 | 19.53 | 90.88 | 16.47 | 77.24 | 2.57 | 93.30 | 10.33 | 90.10 | 7.63 |
| **20** | 158.00 | 20.95 | 69.83 | 14.43 | 92.21 | 11.34 | 143.89 | 10.27 | 95.57 | 4.89 |
| **21** | 171.07 | 14.48 | 77.25 | 2.80 | 80.76 | 11.71 | 140.55 | 4.61 | 116.49 | 8.30 |
| **22** | 84.73 | 7.49 | 95.99 | 10.66 | 84.98 | 2.54 | 133.61 | 7.27 | 159.18 | 35.47 |
| **23** | 171.77 | 12.76 | 76.56 | 7.94 | 82.22 | 9.80 | 162.48 | 8.19 | 100.53 | 14.59 |
| **24** | 165.90 | 12.16 | 72.29 | 15.22 | 94.10 | 6.28 | 128.64 | 19.79 | 94.47 | 3.20 |
| **25** | 150.26 | 19.92 | 71.32 | 2.78 | 96.95 | 6.06 | 140.68 | 11.70 | 94.58 | 6.34 |
| **26** | 136.17 | 12.17 | 79.89 | 1.58 | 82.27 | 14.13 | 101.60 | 4.06 | 137.50 | 19.22 |
| **27** | 138.63 | 15.76 | 103.92 | 16.36 | 102.83 | 0.38 | 144.65 | 14.62 | 105.29 | 18.64 |
| **28** | 140.48 | 16.89 | 83.31 | 9.58 | 97.12 | 13.05 | 134.48 | 17.79 | 97.23 | 11.69 |
| **29** | 148.46 | 14.81 | 80.68 | 2.68 | 104.29 | 12.40 | 130.03 | 9.65 | 90.49 | 16.19 |
| **30** | 140.50 | 15.82 | 85.28 | 8.93 | 115.31 | 16.19 | 122.47 | 10.01 | 112.01 | 12.93 |
| **31** | 128.06 | 14.42 | 56.04 | 18.66 | 125.86 | 16.83 | 90.33 | 8.43 | 108.56 | 10.54 |
| **32** | 98.75 | 10.33 | 79.98 | 9.82 | 76.00 | 2.61 | 105.70 | 13.39 | 120.50 | 19.14 |
| **33** | 137.24 | 18.95 | 76.93 | 5.45 | 97.87 | 9.90 | 119.77 | 14.80 | 98.36 | 16.51 |
| **34** | 135.25 | 12.55 | 76.57 | 4.70 | 93.34 | 16.50 | 127.73 | 5.18 | 95.91 | 2.92 |
| **35** | 133.13 | 9.83 | 80.49 | 3.49 | 98.54 | 2.07 | 112.77 | 15.39 | 106.28 | 13.47 |
| **36** | 129.54 | 13.57 | 85.70 | 3.65 | 88.63 | 10.48 | 114.68 | 2.28 | 101.05 | 13.11 |
| **37** | 26.61 | 3.16 | 33.89 | 6.75 | 122.88 | 10.70 | 91.74 | 9.11 | 77.76 | 10.48 |
| **38** | 98.62 | 19.73 | 116.68 | 14.38 | 91.26 | 14.85 | 107.57 | 6.29 | 148.92 | 13.50 |
| **39** | 14.45 | 1.69 | 41.84 | 3.24 | 98.42 | 6.48 | 149.59 | 15.40 | 150.48 | 24.73 |
| **40** | 153.87 | 18.24 | 103.74 | 4.23 | 126.13 | 28.79 | 128.35 | 16.55 | 146.65 | 19.76 |
| **41** | 182.91 | 14.78 | 127.44 | 20.69 | 119.87 | 8.82 | 73.91 | 11.42 | 135.03 | 11.86 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| **42** | 177.84 | 20.39 | 105.17 | 2.23 | 122.90 | 16.76 | 110.24 | 10.13 | 145.96 | 20.05 |
| **43** | 174.00 | 13.00 | 110.57 | 8.41 | 128.05 | 9.27 | 119.34 | 4.01 | 127.73 | 1.51 |
| **44** | 189.15 | 24.74 | 108.57 | 3.89 | 124.22 | 18.79 | 120.79 | 15.69 | 122.34 | 14.38 |
| **45** | 145.90 | 19.48 | 97.22 | 16.93 | 41.70 | 2.56 | 107.36 | 5.15 | 145.20 | 16.41 |
| **46** | 25.73 | 1.69 | 34.16 | 8.41 | 128.20 | 25.48 | 85.26 | 1.41 | 84.31 | 7.72 |
| **47** | 56.40 | 14.16 | 86.49 | 2.41 | 102.25 | 30.06 | 107.60 | 5.72 | 107.55 | 18.55 |
| **48** | 25.00 | 1.90 | 93.20 | 5.18 | 122.70 | 15.89 | 88.74 | 9.47 | 109.67 | 15.14 |
| **49** | 120.18 | 17.90 | 102.73 | 11.27 | 144.27 | 15.25 | 104.41 | 11.66 | 111.80 | 6.01 |
| **50** | 124.03 | 19.29 | 156.94 | 13.36 | 123.96 | 10.85 | 96.21 | 9.63 | 120.98 | 13.59 |
| **51** | 137.65 | 19.52 | 114.17 | 10.27 | 111.24 | 9.19 | 111.93 | 9.90 | 115.81 | 12.05 |
| **52** | 58.72 | 12.64 | 99.47 | 7.92 | 116.11 | 11.62 | 122.86 | 11.56 | 108.43 | 13.30 |
| **53** | 164.31 | 10.61 | 107.73 | 4.89 | 122.89 | 9.81 | 126.40 | 14.00 | 107.99 | 11.05 |
| **54** | 164.94 | 14.00 | 135.94 | 3.80 | 34.63 | 3.03 | 86.44 | 4.76 | 118.41 | 16.60 |
| **55** | 187.74 | 1.20 | 75.60 | 11.45 | 109.22 | 14.62 | 87.41 | 4.94 | 87.14 | 6.01 |
| **56** | 200.70 | 18.95 | 69.44 | 3.95 | 108.19 | 13.04 | 112.60 | 5.56 | 87.13 | 5.59 |
| **57** | 80.55 | 3.07 | 89.36 | 4.48 | 111.99 | 16.37 | 71.90 | 10.05 | 100.00 | 15.62 |
| **58** | 90.44 | 12.94 | 76.02 | 2.07 | 120.73 | 16.97 | 175.17 | 12.19 | 91.59 | 4.81 |
| **59** | 29.84 | 0.98 | 22.55 | 1.88 | 50.81 | 7.98 | 66.17 | 7.97 | 99.43 | 4.14 |
| **60** | 35.99 | 3.23 | 36.93 | 3.93 | 75.54 | 7.20 | 91.75 | 11.03 | 96.80 | 9.34 |
| **61** | 31.13 | 2.82 | 29.41 | 2.63 | 72.04 | 12.05 | 94.06 | 19.81 | 94.35 | 9.03 |
| **Median** | 131.5 | | 79.23 | | 96.95 | | 119.34 | | 99.94 | 131.5 |

**Table SM8**. Occurrences of the EOs' chemical components. Only the most frequent compounds are listed.

| Component | #[a] | Component | #[a] | Component | #[a] |
|---|---|---|---|---|---|
| limonene | 51 | p-cymen-8-ol | 10 | linalyl anthranilate | 6 |
| α-pinene | 47 | terpinolene | 9 | calamenene | 6 |
| β-caryophyllene | 39 | α-citral | 9 | β-phellandrene | 6 |
| β-myrcene | 36 | β-bisabolene | 9 | 3-carene | 6 |
| linalool | 35 | carvacrol | 8 | α-cadinol | 6 |
| eucalyptol | 33 | α-muurolene | 8 | spathulenol | 6 |
| β-pinene | 30 | γ-muurolene | 8 | germacrene d | 6 |
| o-cymene | 29 | carvone | 8 | α-phellandrene | 5 |
| α-terpineol | 28 | bornyl acetate | 8 | nerol acetate | 5 |
| caryophyllene oxide | 27 | eugenol | 7 | myrtenol | 5 |
| terpinen-4-ol | 26 | thymol | 7 | cis-β-farnesene | 5 |
| sabinene | 22 | α-bergamotene | 7 | γ-cadinene | 5 |
| γ-terpinene | 21 | geranyl acetate | 7 | estragole | 5 |
| borneol | 16 | camphor | 7 | cis-β-terpineol | 5 |
| humulene | 16 | pinocarveol | 7 | cis-verbenol | 5 |
| δ-cadinene | 13 | α-terpinene | 7 | elemol | 4 |
| camphene | 13 | α-terpineol acetate | 7 | α-cubebene | 4 |
| cis-geraniol | 12 | 1-octen-3-ol | 6 | cis-carveol | 4 |
| p-cymene | 11 | β-elemene | 6 | β-citral | 4 |
| α-copaene | 11 | humulene epoxide 2 | 6 | methyl thymyl ether | 4 |

**Table SM9**. Description of the datasets used to develop the classification models for the biofilm data.

| #[a] | Strain | Threshold[b] | A[a] | | B | | C | |
|---|---|---|---|---|---|---|---|---|
| | | | Biofilm Modulation at 0.05 % v/v[c] | | Biofilm Modulation at 1.00 % v/v[d] | | Biofilm Modulation at 1.00 % v/v Corr[e] | |
| | | | Negative | Positive | Negative | Positive | Negative | Positive |
| **1** | 6538P | | 10 | 51 | 26 | 22 | 34 | 27 |
| **2** | 25923 | | 7 | 54 | 9 | 40 | 14 | 47 |
| **3** | 4S | 40% | 1 | 60 | 11 | 38 | 11 | 50 |
| **4** | 5S | | 0 | 61 | 9 | 38 | 9 | 52 |
| **5** | 19S | | 0 | 61 | 10 | 37 | 10 | 51 |
| **6** | 6538P | | 15 | 46 | 41 | 7 | 49 | 12 |
| **7** | 25923 | | 33 | 28 | 27 | 22 | 36 | 25 |
| **8** | 4S | 80% | 12 | 49 | 37 | 12 | 40 | 21 |
| **9** | 5S | | 4 | 57 | 31 | 16 | 33 | 28 |
| **10** | 19S | | 3 | 58 | 28 | 19 | 29 | 32 |
| **11** | 6538P | | 22 | 39 | 42 | 6 | 52 | 9 |
| **12** | 25923 | | 49 | 12 | 38 | 11 | 50 | 11 |
| **13** | 4S | 100% | 35 | 26 | 46 | 3 | 54 | 7 |
| **14** | 5S | | 15 | 46 | 35 | 12 | 42 | 19 |
| **15** | 19S | | 32 | 29 | 39 | 8 | 46 | 15 |
| **16** | 6538P | | 25 | 36 | 42 | 6 | 52 | 9 |
| **17** | 25923 | | 58 | 3 | 42 | 7 | 54 | 7 |
| **18** | 4S | 120% | 49 | 12 | 49 | 0 | 58 | 3 |
| **19** | 5S | | 32 | 29 | 40 | 7 | 49 | 12 |
| **20** | 19S | | 48 | 13 | 43 | 4 | 54 | 7 |
| **21** | 6538P | | 31 | 30 | 24 | 24 | 31 | 30 |
| **22** | 25923 | | 31 | 30 | 25 | 24 | 31 | 30 |
| **23** | 4S | median | 31 | 30 | 25 | 24 | 31 | 30 |
| **24** | 5S | | 31 | 30 | 24 | 23 | 31 | 30 |
| **25** | 19S | | 31 | 30 | 24 | 23 | 31 | 30 |

a) dataset numbers and letters used for the dataset combination: 1A, 2A….1B, 2B….1C,2C…25C;
b) Threshold used to binarize data;
c) column indicating the number of samples showing biofilm growth modulation, negative or positive at the selected threshold at 0.05% v/v concentration;
d) column indicating the number of samples showing biofilm growth modulation, negative or positive at the selected threshold 1.00% v/v concentration;
e) column indicating the number of samples showing biofilm growth modulation, negative or positive at the selected threshold at 1.00% v/v concentration implemented with data at 0.05% v/v for missing values.

**Table SM10.** Description of the datasets used to develop the classification models for the antimicrobial data.

| #[a] | Strain | D[b] | |
|---|---|---|---|
| | | **Actives** | **Inactives** |
| **1** | 6538P | 13 | 48 |
| **2** | 25923 | 12 | 49 |
| **3** | 4S | 12 | 49 |
| **4** | 5S | 14 | 47 |
| **5** | 19S | 14 | 47 |

a) dataset number used for the combination;
b) column indicating the number of samples as active or inactives.

**Table SM11**. List of hyperparameters setting used for the models' random search optimization.

| Algorithm | Parameters | Settings | Total Combinations |
|---|---|---|---|
| RF | class_weight | list_weight | 133970183 |
| | n_estimators | from 1 to 200, step 1 | |
| | max_depth | from 1 to 200, step 1 | |
| | min_samples_leaf | from 1 to 200, step 1 | |
| GB | n_estimators | from 1 to 200, step 1 | 7880599 |
| | max_depth | from 1 to 200, step 1 | |
| | min_samples_leaf | from 1 to 200, step 1 | |
| LR | class_weight | list_weight | 50745 |
| | C | from 1 to 200, step 1 | |
| | penalty | l1, l2, elasticnet | |
| | solver | newton-cg, lbfgs, liblinear, sag, saga | |
| | max_iter | 10000 | |
| SV | class_weight | list_weight | 13532 |
| | C | from 1 to 200, step 1 | |
| | kernel | linear, poly, rbf, sigmoid | |
| | probability | True | |
| DT | class_weight | list_weight | 2176000 |
| | criterion | gini, entropy | |
| | splitter | best, random | |
| | max_depth | from 1 to 21, step 1 | |
| | min_samples_split | from 1 to 21, step 1 | |
| | min_samples_leaf | from 1 to 21, step 1 | |
| | max_features | auto, sqrt, log2, None | |
| KNN | n_neighbors | from 1 to 31, step 1 | 57600 |
| | weights | uniform, distance | |
| | algorithm | auto, ball_tree, kd_tree, brute | |
| | leaf_size | from 1 to 31, step 1 | |
| | metric | minkowski, euclidean, manhattan, chebyshev | |
| | metric_params | None | |
| | p | 1, 2 | |

**Table SM12.** Random forest models MCC and ROC AUC values.

| #[a] | Strain | T[b] | A[a] | | | B | | | C | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | Biofilm 0.05 % v/v[c] | | | Biofilm 1.00 % v/v[d] | | | Biofilm 1.00 % v/v Corr[e] | | |
| | | | L[f] | MCC | AUC | L | MCC | AUC | L | MCC | AUC |
| **1** | 6538P | 40% | 1 | 0.67 | 0.87 | 1 | 0.67 | 0.87 | 2 | 0.33 | 0.58 |
| **2** | 25923 | | 1 | 0.83 | 0.92 | 1 | 0.83 | 0.92 | 4 | 0.19 | 0.85 |
| **3** | 4S | | -[g] | - | - | - | - | - | 2 | 0.27 | 0.49 |
| **4** | 5S | | - | - | - | - | - | - | 1 | 0.00[h] | 0.00 |
| **5** | 19S | | - | - | - | - | - | - | 4 | 0.15 | 0.51 |
| **6** | 6538P | 80% | 3 | 0.68 | 0.82 | 3 | 0.68 | 0.82 | 1 | 0.50 | 0.72 |
| **7** | 25923 | | 4 | 0.33 | 0.61 | 4 | 0.33 | 0.61 | 4 | 0.38 | 0.62 |
| **8** | 4S | | 1 | 0.14 | 0.69 | 1 | 0.14 | 0.69 | 1 | 0.00 | 0.00 |
| **9** | 5S | | - | - | - | - | - | - | 2 | 0.19 | 0.36 |
| **10** | 19S | | - | - | - | - | - | - | 1 | 0.18 | 0.27 |
| **11** | 6538P | 100% | 4 | 0.53 | 0.78 | 4 | 0.53 | 0.78 | 1 | 0.55 | 0.62 |
| **12** | 25923 | | 1 | 0.26 | 0.50 | 1 | 0.26 | 0.50 | 1 | 0.20 | 0.59 |
| **13** | 4S | | 3 | 0.16 | 0.51 | 3 | 0.16 | 0.51 | - | - | - |
| **14** | 5S | | 1 | 0.46 | 0.66 | 1 | 0.46 | 0.66 | 2 | 0.12 | 0.47 |
| **15** | 19S | | 2 | 0.41 | 0.72 | 2 | 0.41 | 0.72 | 1 | 0.33 | 0.56 |
| **16** | 6538P | 120% | 1 | 0.37 | 0.69 | 1 | 0.37 | 0.69 | 1 | 0.55 | 0.65 |
| **17** | 25923 | | - | - | - | - | - | - | 1 | 0.00 | 0.00 |
| **18** | 4S | | 1 | 0.26 | 0.39 | 1 | 0.26 | 0.39 | - | - | - |
| **19** | 5S | | 3 | 0.10 | 0.39 | 3 | 0.10 | 0.39 | 1 | 0.00 | 0.00 |
| **20** | 19S | | 3 | 0.25 | 0.65 | 3 | 0.25 | 0.65 | - | - | - |
| **21** | 6538P | median | 2 | 0.32 | 0.66 | 2 | 0.32 | 0.66 | 1 | 0.17 | 0.55 |
| **22** | 25923 | | 4 | 0.44 | 0.61 | 4 | 0.44 | 0.61 | 4 | 0.32 | 0.70 |
| **23** | 4S | | 1 | 0.19 | 0.62 | 1 | 0.19 | 0.62 | 2 | 0.14 | 0.49 |
| **24** | 5S | | 3 | 0.29 | 0.45 | 3 | 0.29 | 0.45 | 1 | 0.13 | 0.49 |
| **25** | 19S | | 2 | 0.28 | 0.68 | 2 | 0.28 | 0.68 | 1 | 0.00 | 0.00 |

a) dataset numbers and letters used for the dataset combination: 1A, 2A….1B, 2B….1C,2C…25C;
b) Threshold used to binarize data;
c) column indicating the MCC and ROC AUC values for datasets compiled with biofilm formation at 0.05% v/v concentration;
d) column indicating the MCC and ROC AUC values for datasets compiled with biofilm formation at 1.00% v/v concentration;
e) column indicating the MCC and ROC AUC values for datasets compiled with biofilm formation at 1.00% v/v concentration implemented with data at 0.05% v/v for missing values.
f) optimal nlevel value
g) a dash indicates too unbalanced dataset and no model was elaborated
h) 0.00 indicates the model was characterized with MCC negative values

**Table SM13**. Gradient bosting models MCC and ROC AUC values.

| #[a] | Strain | T[b] | A[a] | | | B | | | C | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | Biofilm 0.05 % v/v[c] | | | Biofilm 1.00 % v/v[d] | | | Biofilm 1.00 % v/v Corr[e] | | |
| | | | L[f] | MCC | AUC | L | MCC | AUC | L | MCC | AUC |
| **1** | 6538P | 40% | 4 | 0.88 | 0.93 | 4 | 0.88 | 0.93 | 1 | 0.24 | 0.66 |
| **2** | 25923 | | 1 | 1.00 | 1.00 | 1 | 1.00 | 1.00 | 4 | 0.22 | 0.76 |
| **3** | 4S | | -[g] | - | - | - | - | - | 2 | 0.07 | 0.63 |
| **4** | 5S | | - | - | - | - | - | - | 3 | 0.25 | 0.67 |
| **5** | 19S | | - | - | - | - | - | - | 1 | 0.15 | 0.69 |
| **6** | 6538P | 80% | 2 | 0.75 | 0.89 | 2 | 0.75 | 0.89 | 1 | 0.52 | 0.81 |
| **7** | 25923 | | 2 | 0.35 | 0.69 | 2 | 0.35 | 0.69 | 1 | 0.29 | 0.60 |
| **8** | 4S | | 4 | 0.25 | 0.64 | 4 | 0.25 | 0.64 | 1 | 0.00[h] | 0.00 |
| **9** | 5S | | - | - | - | - | - | - | 4 | 0.36 | 0.72 |
| **10** | 19S | | - | - | - | - | - | - | 2 | 0.32 | 0.58 |
| **11** | 6538P | 100% | 1 | 0.53 | 0.84 | 1 | 0.53 | 0.84 | 1 | 0.57 | 0.68 |
| **12** | 25923 | | 2 | 0.48 | 0.77 | 2 | 0.48 | 0.77 | 1 | 0.41 | 0.61 |
| **13** | 4S | | 2 | 0.32 | 0.59 | 2 | 0.32 | 0.59 | - | - | - |
| **14** | 5S | | 4 | 0.63 | 0.71 | 4 | 0.63 | 0.71 | 4 | 0.11 | 0.66 |
| **15** | 19S | | 1 | 0.38 | 0.67 | 1 | 0.38 | 0.67 | 3 | 0.58 | 0.82 |
| **16** | 6538P | 120% | 3 | 0.45 | 0.72 | 3 | 0.45 | 0.72 | 1 | 0.34 | 0.63 |
| **17** | 25923 | | - | - | - | - | - | - | 4 | 0.21 | 0.39 |
| **18** | 4S | | 3 | 0.15 | 0.32 | 3 | 0.15 | 0.32 | - | - | - |
| **19** | 5S | | 1 | 0.00 | 0.00 | 1 | 0.00 | 0.00 | 1 | 0.30 | 0.44 |
| **20** | 19S | | 4 | 0.45 | 0.67 | 4 | 0.45 | 0.67 | - | - | - |
| **21** | 6538P | median | 2 | 0.32 | 0.69 | 2 | 0.32 | 0.69 | 4 | 0.13 | 0.51 |
| **22** | 25923 | | 2 | 0.18 | 0.64 | 2 | 0.18 | 0.64 | 1 | 0.31 | 0.66 |
| **23** | 4S | | 1 | 0.55 | 0.73 | 1 | 0.55 | 0.73 | 2 | 0.18 | 0.54 |
| **24** | 5S | | 1 | 0.00 | 0.00 | 1 | 0.00 | 0.00 | 1 | 0.28 | 0.61 |
| **25** | 19S | | 2 | 0.38 | 0.72 | 2 | 0.38 | 0.72 | 1 | 0.00 | 0.00 |

a) dataset numbers and letters used for the dataset combination: 1A, 2A….1B, 2B….1C,2C…25C;
b) Threshold used to binarize data;
c) column indicating the MCC and ROC AUC values for datasets compiled with biofilm formation at 0.05% v/v concentration;
d) column indicating the MCC and ROC AUC values for datasets compiled with biofilm formation at 1.00% v/v concentration;
e) column indicating the MCC and ROC AUC values for datasets compiled with biofilm formation at 1.00% v/v concentration implemented with data at 0.05% v/v for missing values.
f) optimal nlevel value
g) a dash indicates too unbalanced dataset and no model was elaborated
h) 0.00 indicates the model was characterized with MCC negative values

**Table SM14.** Logistic regression models MCC and ROC AUC values.

| #[a] | Strain | T[b] | A[a] | | | B | | | C | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | Biofilm 0.05 % v/v[c] | | | Biofilm 1.00 % v/v[d] | | | Biofilm 1.00 % v/v Corr[e] | | |
| | | | L[f] | MCC | AUC | L | MCC | AUC | L | MCC | AUC |
| **1** | 6538P | 40% | 1 | 0.83 | 0.97 | 1 | 0.83 | 0.97 | 1 | 0.28 | 0.65 |
| **2** | 25923 | | 3 | 1.00 | 1.00 | 3 | 1.00 | 1.00 | 4 | 0.14 | 0.58 |
| **3** | 4S | | -[g] | - | - | - | - | - | 2 | 0.09 | 0.52 |
| **4** | 5S | | - | - | - | - | - | - | 1 | 0.13 | 0.58 |
| **5** | 19S | | - | - | - | - | - | - | 1 | 0.00[h] | 0.00 |
| **6** | 6538P | 80% | 2 | 0.73 | 0.91 | 2 | 0.73 | 0.91 | 1 | 0.73 | 0.84 |
| **7** | 25923 | | 4 | 0.18 | 0.42 | 4 | 0.18 | 0.42 | 4 | 0.33 | 0.65 |
| **8** | 4S | | 1 | 0.36 | 0.71 | 1 | 0.36 | 0.71 | 4 | 0.06 | 0.52 |
| **9** | 5S | | - | - | - | - | - | - | 4 | 0.26 | 0.45 |
| **10** | 19S | | - | - | - | - | - | - | 1 | 0.26 | 0.45 |
| **11** | 6538P | 100% | 2 | 0.52 | 0.77 | 2 | 0.52 | 0.77 | 1 | 0.43 | 0.84 |
| **12** | 25923 | | 1 | 0.27 | 0.65 | 1 | 0.27 | 0.65 | 1 | 0.38 | 0.68 |
| **13** | 4S | | 4 | 0.06 | 0.50 | 4 | 0.06 | 0.50 | - | - | - |
| **14** | 5S | | 4 | 0.57 | 0.70 | 4 | 0.57 | 0.70 | 2 | 0.25 | 0.49 |
| **15** | 19S | | 3 | 0.46 | 0.69 | 3 | 0.46 | 0.69 | 1 | 0.33 | 0.51 |
| **16** | 6538P | 120% | 2 | 0.41 | 0.61 | 2 | 0.41 | 0.61 | 1 | 0.43 | 0.86 |
| **17** | 25923 | | - | - | - | - | - | - | 1 | 0.35 | 0.54 |
| **18** | 4S | | 1 | 0.08 | 0.44 | 1 | 0.08 | 0.44 | - | - | - |
| **19** | 5S | | 4 | 0.18 | 0.44 | 4 | 0.18 | 0.44 | 1 | 0.28 | 0.55 |
| **20** | 19S | | 2 | 0.50 | 0.78 | 2 | 0.50 | 0.78 | - | - | - |
| **21** | 6538P | median | 2 | 0.28 | 0.66 | 2 | 0.28 | 0.66 | 4 | 0.35 | 0.57 |
| **22** | 25923 | | 3 | 0.27 | 0.48 | 3 | 0.27 | 0.48 | 1 | 0.36 | 0.74 |
| **23** | 4S | | 4 | 0.20 | 0.59 | 4 | 0.20 | 0.59 | 1 | 0.11 | 0.48 |
| **24** | 5S | | 3 | 0.35 | 0.47 | 3 | 0.35 | 0.47 | 2 | 0.20 | 0.54 |
| **25** | 19S | | 2 | 0.35 | 0.65 | 2 | 0.35 | 0.65 | 1 | 0.06 | 0.47 |

a) dataset numbers and letters used for the dataset combination: 1A, 2A….1B, 2B….1C,2C…25C;
b) Threshold used to binarize data;
c) column indicating the MCC and ROC AUC values for datasets compiled with biofilm formation at 0.05% v/v concentration;
d) column indicating the MCC and ROC AUC values for datasets compiled with biofilm formation at 1.00% v/v concentration;
e) column indicating the MCC and ROC AUC values for datasets compiled with biofilm formation at 1.00% v/v concentration implemented with data at 0.05% v/v for missing values.
f) optimal nlevel value
g) a dash indicates too unbalanced dataset and no model was elaborated
h) 0.00 indicates the model was characterized with MCC negative values

**Table SM15.** Support vector machine models MCC and ROC AUC values.

| #[a] | Strain | T[b] | A[a] | | | B | | | C | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | Biofilm 0.05 % v/v[c] | | | Biofilm 1.00 % v/v[d] | | | Biofilm 1.00 % v/v Corr[e] | | |
| | | | L[f] | MCC | AUC | L | MCC | AUC | L | MCC | AUC |
| **1** | 6538P | 40% | 2 | 0.94 | 0.98 | 2 | 0.94 | 0.98 | 2 | 0.33 | 0.25 |
| **2** | 25923 | | 1 | 1.00 | 1.00 | 1 | 1.00 | 1.00 | 3 | 0.05 | 0.17 |
| **3** | 4S | | -[g] | - | - | - | - | - | 3 | 0.33 | 0.51 |
| **4** | 5S | | - | - | - | - | - | - | 1 | 0.24 | 0.00 |
| **5** | 19S | | - | - | - | - | - | - | 4 | 0.28 | 0.43 |
| **6** | 6538P | 80% | 1 | 0.82 | 0.90 | 1 | 0.82 | 0.90 | 1 | 0.63 | 0.80 |
| **7** | 25923 | | 2 | 0.34 | 0.60 | 2 | 0.34 | 0.60 | 4 | 0.25 | 0.55 |
| **8** | 4S | | 4 | 0.39 | 0.67 | 4 | 0.39 | 0.67 | 4 | 0.18 | 0.13 |
| **9** | 5S | | - | - | - | - | - | - | 3 | 0.33 | 0.35 |
| **10** | 19S | | - | - | - | - | - | - | 4 | 0.23 | 0.06 |
| **11** | 6538P | 100% | 3 | 0.64 | 0.76 | 3 | 0.64 | 0.76 | 1 | 0.57 | 0.63 |
| **12** | 25923 | | 2 | 0.48 | 0.62 | 2 | 0.48 | 0.62 | 4 | 0.27 | 0.33 |
| **13** | 4S | | 2 | 0.09 | 0.10 | 2 | 0.09 | 0.10 | - | - | - |
| **14** | 5S | | 3 | 0.63 | 0.58 | 3 | 0.63 | 0.58 | 1 | 0.31 | 0.28 |
| **15** | 19S | | 4 | 0.27 | 0.24 | 4 | 0.27 | 0.24 | 1 | 0.47 | 0.03 |
| **16** | 6538P | 120% | 3 | 0.52 | 0.76 | 3 | 0.52 | 0.76 | 1 | 0.57 | 0.54 |
| **17** | 25923 | | - | - | - | - | - | - | 1 | 0.09 | 0.22 |
| **18** | 4S | | 3 | 0.24 | 0.22 | 3 | 0.24 | 0.22 | - | - | - |
| **19** | 5S | | 2 | 0.21 | 0.39 | 2 | 0.21 | 0.39 | 3 | 0.33 | 0.48 |
| **20** | 19S | | 4 | 0.46 | 0.49 | 4 | 0.46 | 0.49 | - | - | - |
| **21** | 6538P | median | 3 | 0.48 | 0.66 | 3 | 0.48 | 0.66 | 2 | 0.30 | 0.35 |
| **22** | 25923 | | 2 | 0.35 | 0.38 | 2 | 0.35 | 0.38 | 4 | 0.34 | 0.51 |
| **23** | 4S | | 3 | 0.25 | 0.55 | 3 | 0.25 | 0.55 | 2 | 0.24 | 0.21 |
| **24** | 5S | | 3 | 0.26 | 0.44 | 3 | 0.26 | 0.44 | 4 | 0.25 | 0.45 |
| **25** | 19S | | 4 | 0.32 | 0.39 | 4 | 0.32 | 0.39 | 1 | 0.15 | 0.42 |

a) dataset numbers and letters used for the dataset combination: 1A, 2A….1B, 2B….1C,2C…25C;
b) Threshold used to binarize data;
c) column indicating the MCC and ROC AUC values for datasets compiled with biofilm formation at 0.05% v/v concentration;
d) column indicating the MCC and ROC AUC values for datasets compiled with biofilm formation at 1.00% v/v concentration;
e) column indicating the MCC and ROC AUC values for datasets compiled with biofilm formation at 1.00% v/v concentration implemented with data at 0.05% v/v for missing values.
f) optimal nlevel value
g) a dash indicates too unbalanced dataset and no model was elaborated

**Table SM16.** Decision trees models MCC and ROC AUC values.

| #[a] | Strain | T[b] | A[a] | | | B | | | C | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | Biofilm 0.05 % v/v[c] | | | Biofilm 1.00 % v/v[d] | | | Biofilm 1.00 % v/v Corr[e] | | |
| | | | L[f] | MCC | AUC | L | MCC | AUC | L | MCC | AUC |
| **1** | 6538P | 40% | 2 | 0.83 | 0.92 | 2 | 0.83 | 0.92 | 4 | 0.42 | 0.41 |
| **2** | 25923 | | 2 | 0.93 | 0.98 | 2 | 0.93 | 0.98 | 4 | 0.54 | 0.69 |
| **3** | 4S | | -[g] | - | - | - | - | - | 2 | 0.38 | 0.48 |
| **4** | 5S | | - | - | - | - | - | - | 3 | 0.42 | 0.65 |
| **5** | 19S | | - | - | - | - | - | - | 4 | 0.31 | 0.55 |
| **6** | 6538P | 80% | 2 | 0.80 | 0.89 | 2 | 0.80 | 0.89 | 2 | 0.62 | 0.77 |
| **7** | 25923 | | 4 | 0.61 | 0.78 | 4 | 0.61 | 0.78 | 4 | 0.52 | 0.77 |
| **8** | 4S | | 1 | 0.44 | 0.62 | 1 | 0.44 | 0.62 | 2 | 0.05 | 0.36 |
| **9** | 5S | | - | - | - | - | - | - | 4 | 0.47 | 0.50 |
| **10** | 19S | | - | - | - | - | - | - | 2 | 0.42 | 0.64 |
| **11** | 6538P | 100% | 2 | 0.60 | 0.79 | 2 | 0.60 | 0.79 | 4 | 0.57 | 0.84 |
| **12** | 25923 | | 1 | 0.39 | 0.62 | 1 | 0.39 | 0.62 | 1 | 0.55 | 0.37 |
| **13** | 4S | | 2 | 0.24 | 0.50 | 2 | 0.24 | 0.50 | - | - | - |
| **14** | 5S | | 4 | 0.68 | 0.74 | 4 | 0.68 | 0.74 | 4 | 0.45 | 0.56 |
| **15** | 19S | | 1 | 0.44 | 0.67 | 1 | 0.44 | 0.67 | 3 | 0.61 | 0.80 |
| **16** | 6538P | 120% | 4 | 0.51 | 0.46 | 4 | 0.51 | 0.46 | 4 | 0.74 | 0.83 |
| **17** | 25923 | | - | - | - | - | - | - | 1 | 0.38 | 0.41 |
| **18** | 4S | | 2 | 0.11 | 0.48 | 2 | 0.11 | 0.48 | - | - | - |
| **19** | 5S | | 3 | 0.36 | 0.48 | 3 | 0.36 | 0.48 | 2 | 0.35 | 0.35 |
| **20** | 19S | | 3 | 0.41 | 0.72 | 3 | 0.41 | 0.72 | - | - | - |
| **21** | 6538P | median | 1 | 0.36 | 0.56 | 1 | 0.36 | 0.56 | 4 | 0.37 | 0.45 |
| **22** | 25923 | | 1 | 0.29 | 0.53 | 1 | 0.29 | 0.53 | 1 | 0.51 | 0.61 |
| **23** | 4S | | 1 | 0.55 | 0.76 | 1 | 0.55 | 0.76 | 2 | 0.39 | 0.54 |
| **24** | 5S | | 3 | 0.38 | 0.41 | 3 | 0.38 | 0.41 | 2 | 0.36 | 0.56 |
| **25** | 19S | | 2 | 0.43 | 0.73 | 2 | 0.43 | 0.73 | 4 | 0.08 | 0.38 |

a) dataset numbers and letters used for the dataset combination: 1A, 2A….1B, 2B….1C,2C…25C;
b) Threshold used to binarize data;
c) column indicating the MCC and ROC AUC values for datasets compiled with biofilm formation at 0.05% v/v concentration;
d) column indicating the MCC and ROC AUC values for datasets compiled with biofilm formation at 1.00% v/v concentration;
e) column indicating the MCC and ROC AUC values for datasets compiled with biofilm formation at 1.00% v/v concentration implemented with data at 0.05% v/v for missing values.
f) optimal nlevel value
g) a dash indicates too unbalanced dataset and no model was elaborated

**Table SM17**. KNN models MCC and ROC AUC values.

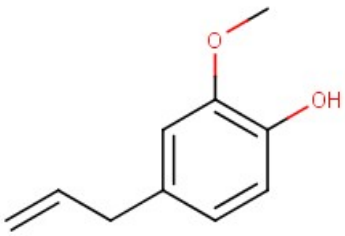
| #[a] | Strain | T[b] | A[a] | | | B | | | C | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | Biofilm 0.05 % v/v[c] | | | Biofilm 1.00 % v/v[d] | | | Biofilm 1.00 % v/v Corr[e] | | |
| | | | L[f] | MCC | AUC | L | MCC | AUC | L | MCC | AUC |
| **1** | 6538P | 40% | 4 | 0.88 | 0.93 | 4 | 0.88 | 0.93 | 3 | 0.41 | 0.70 |
| **2** | 25923 | | 1 | 1.00 | 1.00 | 1 | 1.00 | 1.00 | 4 | 0.26 | 0.62 |
| **3** | 4S | | - | - | - | - | - | - | 1 | 0.38 | 0.39 |
| **4** | 5S | | - | - | - | - | - | - | 4 | 0.18 | 0.57 |
| **5** | 19S | | - | - | - | - | - | - | 4 | 0.29 | 0.70 |
| **6** | 6538P | 80% | 1 | 0.77 | 0.88 | 1 | 0.77 | 0.88 | 1 | 0.29 | 0.71 |
| **7** | 25923 | | 3 | 0.27 | 0.58 | 3 | 0.27 | 0.58 | 3 | 0.13 | 0.58 |
| **8** | 4S | | 1 | 0.39 | 0.76 | 1 | 0.39 | 0.76 | 1 | 0.17 | 0.52 |
| **9** | 5S | | - | - | - | - | - | - | 3 | 0.11 | 0.39 |
| **10** | 19S | | - | - | - | - | - | - | 1 | 0.16 | 0.39 |
| **11** | 6538P | 100% | 1 | 0.61 | 0.79 | 1 | 0.61 | 0.79 | 1 | 0.39 | 0.54 |
| **12** | 25923 | | 2 | 0.42 | 0.68 | 2 | 0.42 | 0.68 | 1 | 0.10 | 0.49 |
| **13** | 4S | | 3 | 0.23 | 0.40 | 3 | 0.23 | 0.40 | - | - | - |
| **14** | 5S | | 4 | 0.52 | 0.77 | 4 | 0.52 | 0.77 | 3 | 0.23 | 0.62 |
| **15** | 19S | | 3 | 0.39 | 0.62 | 3 | 0.39 | 0.62 | 1 | 0.25 | 0.55 |
| **16** | 6538P | 120% | 1 | 0.59 | 0.76 | 1 | 0.59 | 0.76 | 1 | 0.39 | 0.58 |
| **17** | 25923 | | - | - | - | - | - | - | 1 | 0.21 | 0.53 |
| **18** | 4S | | 2 | 0.27 | 0.35 | 2 | 0.27 | 0.35 | - | - | - |
| **19** | 5S | | 2 | 0.31 | 0.56 | 2 | 0.31 | 0.56 | 1 | 0.20 | 0.57 |
| **20** | 19S | | 2 | 0.37 | 0.67 | 2 | 0.37 | 0.67 | - | - | - |
| **21** | 6538P | median | 1 | 0.44 | 0.68 | 1 | 0.44 | 0.68 | 3 | 0.38 | 0.64 |
| **22** | 25923 | | 1 | 0.21 | 0.57 | 1 | 0.21 | 0.57 | 3 | 0.31 | 0.56 |
| **23** | 4S | | 3 | 0.31 | 0.56 | 3 | 0.31 | 0.56 | 4 | 0.20 | 0.40 |
| **24** | 5S | | 2 | 0.35 | 0.52 | 2 | 0.35 | 0.52 | 2 | 0.28 | 0.64 |
| **25** | 19S | | 3 | 0.35 | 0.56 | 3 | 0.35 | 0.56 | 1 | 0.00 | 0.00 |

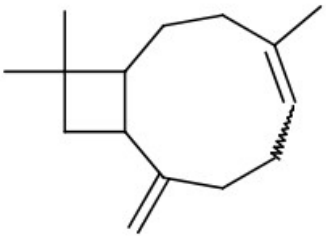
a) dataset numbers and letters used for the dataset combination: 1A, 2A….1B, 2B….1C,2C…25C;
b) Threshold used to binarize data;
c) column indicating the MCC and ROC AUC values for datasets compiled with biofilm formation at 0.05% v/v concentration;
d) column indicating the MCC and ROC AUC values for datasets compiled with biofilm formation at 1.00% v/v concentration;
e) column indicating the MCC and ROC AUC values for datasets compiled with biofilm formation at 1.00% v/v concentration implemented with data at 0.05% v/v for missing values.
f) optimal nlevel value
g) a dash indicates too unbalanced dataset and no model was elaborated

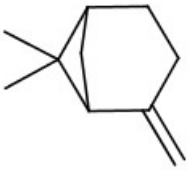
**Table SM18**. RF, GB, LR, SV, DT and KNN ML learning algorithms MCC and ROC AUC values for the antimicrobial dataset.

| #[a] | Strain[b] | RF[c] | | | GB[c] | | | LR[c] | | | SV[c] | | | DT[c] | | | KNN[c] | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | L[d] | MCC[e] | AUC[f] | L | MCC | AUC | L | MCC | AUC | L | MCC | AUC | L | MCC | AUC | L | MCC | AUC |
| **1D** | 6538P | 1 | 0.44 | 0.80 | 4 | 0.57 | 0.86 | 1 | 0.44 | 0.80 | 4 | 0.69 | 0.85 | 1 | 0.63 | 0.88 | 3 | 0.65 | 0.84 |
| **2D** | 25923 | 1 | 0.46 | 0.82 | 2 | 0.54 | 0.82 | 1 | 0.46 | 0.82 | 4 | 0.72 | 0.86 | 3 | 0.60 | 0.82 | 2 | 0.63 | 0.86 |
| **3D** | 4S | 4 | 0.47 | 0.80 | 2 | 0.54 | 0.84 | 4 | 0.47 | 0.80 | 4 | 0.72 | 0.87 | 3 | 0.66 | 0.80 | 2 | 0.67 | 0.87 |
| **4D** | 5S | 4 | 0.71 | 0.89 | 4 | 0.76 | 0.87 | 4 | 0.71 | 0.89 | 2 | 0.95 | 0.99 | 2 | 0.71 | 0.83 | 2 | 0.87 | 0.93 |
| **5D** | 19S | 4 | 0.65 | 0.85 | 3 | 0.71 | 0.77 | 4 | 0.65 | 0.85 | 4 | 0.81 | 0.93 | 2 | 0.71 | 0.87 | 2 | 0.76 | 0.91 |

a) Dataset combination defined similarly as from tables 12-17; b) *S aureus* strain code; c) Machine learning agorithm as defined in Material and Methods; ; d) Matthew correlation coefficient; e) ROC AUC values.

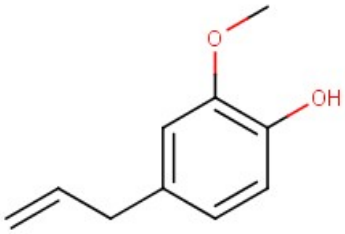


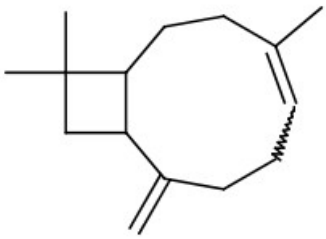





eugenol β-caryophyllene □-pinene

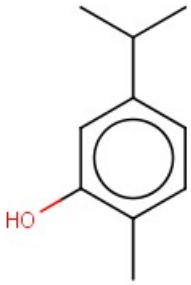
**Figure SM1**. Chemical structure of compounds mostly predicted as reducer of biofilm production (main text Table 3).



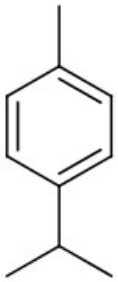



eugenol β-caryophyllene

**Figure SM2.** Chemical structure of compounds predicted to have both ability to reduce biofilm production and as antibacterial (main text Table 3).

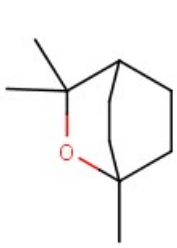




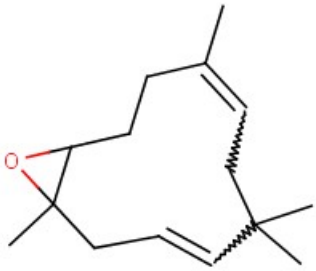



carvacrol □-citral p-cymene 1-octen-3-ol

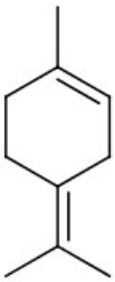
**Figure SM3.** Chemical structure of compounds predicted to increase antibacterial potency (main text Table 3).



eucalyptol

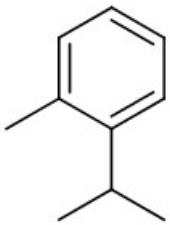


humulene epoxide 2

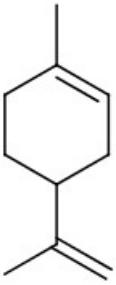


terpinolene

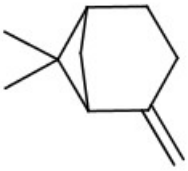
**Figure SM4.** Example of chemical structure of compounds predicted to have the ability to likely modulate the inducing of biofilm production or counteracting biofilm inhibition (main text Table 3).



o-cymene

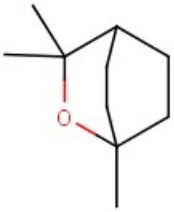


limonene

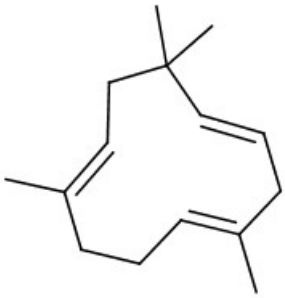


□-pinene

**Figure SM5.** Chemical structure of compounds predicted not to have fixed behavior on different *S. aureus* bacterial strains (main text Table 3).



eucalyptol



humulene

**Figure SM6.** Chemical structure of compounds predicted to have ability to induce biofilm production and antisynergistic antibacterial activity (main text Table 3).

**Table SM18**. Compositions of the 61 essential oils used in the study

| | EO1 |
|---|---|
| .τ.-muurolol | 2.1 |
| artemisia alcohol | 1.3 |
| borneol | 1.2 |
| borneol, butyrate | 4.3 |
| β-caryophyllene | 1.0 |
| caryophyllene oxide | 1.3 |
| cis-3-pinanone | 0.3 |
| cis-β-farnesene | 5.2 |
| eucalyptol | 2.0 |
| germacrene d | 4.5 |
| isobornyl 3-methylbutanoate | 3.1 |
| limonene | 6.7 |
| linalool | 0.3 |
| myrtenol | 0.4 |
| o-cymene | 0.2 |
| pinocarveol | 7.4 |
| sativene | 0.9 |
| spathulenol | 4.0 |
| terpinen-4-ol | 0.4 |
| trans-2,7-dimethyl-4,6-octadien-2-ol | 33.2 |
| yomogi alcohol | 1.3 |
| α-pinene | 14.4 |
| β-myrcene | 1.4 |
| δ-cadinene | 0.5 |
| δ-elemene | 1.7 |
| τ-cadinol | 0.5 |

| | EO2 |
|---|---|
| β-caryophyllene | 2.0 |
| caryophyllene oxide | 2.3 |
| cis-geraniol | 1.7 |
| geranyl acetate | 3.5 |
| linalool | 19.9 |
| linalyl anthranilate | 60.0 |
| nerol acetate | 2.2 |
| trans-linalool oxide | 2.1 |
| α-bergamotene | 0.8 |
| α-copaene | 0.6 |
| α-terpineol | 3.8 |
| β-bisabolene | 0.7 |
| β-myrcene | 0.3 |

| | EO3 |
|---|---|
| alcanfor | 21.3 |
| borneol | 4.6 |
| bornyl acetate | 2.6 |
| camphene | 3.5 |
| β-caryophyllene | 6.8 |
| caryophyllene oxide | 0.3 |
| chrysanthone | 25.1 |
| eucalyptol | 11.7 |
| humulene | 7.5 |
| humulene epoxide 2 | 0.3 |
| limonene | 1.3 |
| o-cymene | 1.3 |
| terpinen-4-ol | 0.6 |
| thujone | 7.8 |
| viridiflorol | 0.2 |
| α-pinene | 3.0 |
| β-pinene | 1.4 |
| γ-terpinene | 0.5 |

| | EO4 |
|---|---|
| borneol | 1.5 |
| carvacrol | 7.2 |
| β-caryophyllene | 2.3 |
| caryophyllene oxide | 0.6 |
| eucalyptol | 0.3 |
| limonene | 0.3 |
| linalool | 5.2 |
| methyl thymyl ether | 0.2 |
| p-cymene | 10.5 |
| terpinen-4-ol | 1.8 |
| thymol | 66.3 |
| α-citral | 0.1 |
| α-pinene | 0.4 |
| α-terpinene | 0.4 |
| α-terpineol | 0.2 |
| β-myrcene | 0.5 |
| γ-terpinene | 2.3 |

| | EO5 |
|---|---|
| eucalyptol | 14.9 |
| globulol | 0.4 |
| limonene | 2.0 |
| linalool, oxide | 0.2 |
| longifolene | 0.2 |
| o-cymene | 3.5 |
| terpinen-4-ol | 37.5 |
| terpinolene | 1.7 |
| viridiflorene | 1.1 |
| α-gurjunene | 0.2 |
| α-pinene | 11.1 |
| α-terpinene | 4.6 |
| α-terpineol | 8.1 |
| β-myrcene | 0.2 |
| β-pinene | 2.5 |
| γ-terpinene | 11.8 |

| | EO6 |
|---|---|
| 6-methyl-5-hepten-2-one | 0.3 |
| β-caryophyllene | 31.4 |
| caryophyllene oxide | 5.5 |
| cis-geraniol | 2.5 |
| citronellal | 26.3 |
| eucalyptol | 0.7 |
| humulene epoxide 2 | 0.9 |
| limonene | 1.6 |
| linalool | 0.8 |
| α-citral | 28.2 |
| α-copaene | 0.7 |
| γ-cadinene | 0.6 |
| δ-cadinene | 0.5 |

| | EO7 |
|---|---|
| 3-carene | 10.8 |
| bornyl acetate | 13.4 |
| calamenene | 0.7 |
| carvone | 0.3 |
| β-caryophyllene | 21.4 |
| cis-verbenol | 0.5 |
| crypton | 3.7 |
| cumaldehyde | 0.5 |
| humulene | 1.2 |
| isopinocarveol | 0.5 |
| limonene | 10.9 |
| linalool | 0.2 |
| o-cymene | 2.1 |
| p-cymen-8-ol | 0.8 |
| trans-2-caren-4-ol | 0.6 |
| α-copaene | 0.9 |
| α-muurolene | 1.1 |
| α-pinene | 12.5 |
| α-terpineol | 0.4 |
| β-cubebene | 1.2 |
| β-phellandrene | 7.0 |
| β-pinene | 7.6 |
| δ-cadinene | 1.6 |

| | EO8 |
|---|---|
| 1-indanone | 3.8 |
| 2,6-dimethyl-2,6-octadiene | 0.6 |
| 2-pentadecanone, 6,10,14-trimethyl | 0.4 |
| acetic acid | 5.0 |
| cis-geraniol | 12.9 |
| citronellol | 26.3 |
| citronellyl butyrate | 1.5 |
| citronellyl formate | 8.0 |
| geraniol formate | 3.8 |
| geranyl isobutyrate | 1.2 |
| geranyl propionate | 0.8 |
| heptanoic acid | 1.2 |
| hexanoic acid | 0.6 |
| isomenthone | 4.6 |
| limonene | 8.4 |
| linalool | 9.6 |
| linalyl anthranilate | 6.8 |
| o-cymene | 1.3 |
| rose oxide | 0.9 |
| α-pinene | 0.5 |
| β-myrcene | 0.4 |
| β-pinene | 1.2 |

| | EO9 |
|---|---|
| borneol | 0.4 |
| carvacrol | 76.5 |
| β-caryophyllene | 6.7 |
| caryophyllene oxide | 2.3 |
| eucalyptol | 0.4 |
| limonene | 0.5 |
| linalool | 2.4 |
| p-cymene | 6.8 |
| terpinen-4-ol | 0.5 |
| α-pinene | 0.4 |
| α-terpinene | 0.3 |
| β-myrcene | 0.8 |
| γ-terpinene | 1.9 |

| | EO10 |
|---|---|
| acetic acid, cinnamyl ester | 1.0 |
| calamenene | 0.3 |
| β-caryophyllene | 15.5 |
| cis-geraniol | 1.5 |
| cis-β-farnesene | 13.9 |
| eucalyptol | 0.2 |
| eugenol | 0.6 |
| farnesol | 2.6 |
| farnesyl acetate | 3.5 |
| geranyl acetate | 12.2 |
| germacrene d | 18.2 |
| humulene | 4.3 |
| linalool | 10.4 |
| methyl benzoate | 2.1 |
| p-methylanisole | 3.3 |
| α-cadinol | 1.1 |
| α-copaene | 1.2 |
| β-elemene | 0.5 |
| β-ylangene | 0.5 |
| γ-cadinene | 1.0 |
| γ-muurolene | 1.8 |
| δ-cadinene | 3.8 |
| τ-cadinol | 0.6 |

| | EO11 |
|---|---|
| 3,7-octadiene-2,6-diol, 2,6-dimethyl- | 0.2 |
| benzyl benzoate | 6.4 |
| camphene | 0.4 |
| camphor | 5.7 |
| cis-geraniol | 1.7 |
| eucalyptol | 0.4 |
| geranyl acetate | 5.2 |
| limonene | 1.7 |
| linalool | 66.7 |
| o-cymene | 2.5 |
| salicyclic acid, benzyl ester | 2.2 |
| terpinen-4-ol | 0.2 |
| trans-linalool oxide | 0.6 |
| α-pinene | 3.4 |
| α-terpineol | 0.8 |
| β-myrcene | 0.5 |
| β-pinene | 0.3 |
| γ-terpinene | 0.9 |

| | EO12 |
|---|---|
| 1-octen-3-ol | 0.3 |
| 3-octanol | 0.3 |
| 3-octanone | 0.9 |
| borneol | 1.4 |
| butanoic acid, hexyl ester | 0.5 |
| β-caryophyllene | 2.7 |
| cis-geraniol | 0.4 |
| cis-β-farnesene | 1.9 |
| cis-β-ocimene | 1.0 |
| eucalyptol | 2.4 |
| lavandulyl acetate | 4.3 |
| limonene | 0.5 |
| linalool | 34.7 |
| linalyl acetate | 41.4 |
| terpinen-4-ol | 3.8 |
| α-pinene | 0.2 |
| α-terpineol | 1.3 |
| β-myrcene | 0.7 |
| β-ocimene | 1.3 |

| | EO13 |
|---|---|
| 1,4-dihydroxy-p-menth-2-ene | 0.3 |
| 3-carene | 0.2 |
| β-caryophyllene | 2.2 |
| cis-geraniol | 0.7 |
| eucalyptol | 40.8 |
| geranyl acetate | 9.7 |
| humulene | 0.5 |
| isobutyl 2-methylbutyrate | 0.5 |
| isobutyl isobutyrate | 0.3 |
| limonene | 7.1 |
| linalool | 3.7 |
| linalyl anthranilate | 1.2 |
| methyleugenol | 2.0 |
| o-cymene | 5.3 |
| p-cymen-8-ol | 0.7 |
| pinocarveol | 0.2 |
| terpinen-4-ol | 0.6 |
| α-pinene | 17.4 |
| α-terpineol | 3.9 |
| α-terpineol acetate | 1.9 |
| β-myrcene | 0.2 |
| β-pinene | 0.2 |
| γ-elemene | 0.2 |

| | EO14 |
|---|---|
| 1,2-dithiolane | 0.5 |
| 1,2-dithiolane, 1,1-dioxide | 2.8 |
| 3-vinyl-1,2-dithiacyclohex-4-ene | 2.6 |
| diallyl disulphide | 57.6 |
| diallyl sulfide | 3.8 |
| dimethyl trisulfide | 0.5 |
| disulfide, methyl 2-propenyl | 2.7 |
| eucalyptol | 0.3 |
| limonene | 0.5 |
| trans-3,5-diethyl-1,2,4-trithiolane | 0.3 |
| trisulfide, di-2-propenyl | 2.1 |
| trisulfide, methyl 2-propenyl | 26.1 |

| | EO15 |
|---|---|
| cis-geraniol | 1.1 |
| cis-β-terpineol | 0.7 |
| eucalyptol | 34.7 |
| limonene | 2.0 |
| linalool | 5.0 |
| linalyl anthranilate | 8.2 |
| nerolidol | 1.3 |
| o-cymene | 0.4 |
| sabinene | 0.3 |
| α-pinene | 1.3 |
| α-terpineol | 1.9 |
| α-terpineol acetate | 41.8 |
| β-myrcene | 1.1 |
| β-pinene | 0.3 |

| | EO16 |
|---|---|
| limonene | 66.7 |
| o-cymene | 7.6 |
| sabinene | 0.2 |
| terpinolene | 0.9 |
| α-pinene | 2.4 |
| α-terpineol | 0.3 |
| β-myrcene | 1.6 |
| β-pinene | 1.3 |
| γ-terpinene | 19.0 |

| | EO17 |
|---|---|
| 4-methoxycinnamaldehyde | 1.1 |
| borneol | 1.1 |
| β-caryophyllene | 1.3 |
| caryophyllene oxide | 0.6 |
| cis-3-pinanone | 34.1 |
| dhs activator | 0.6 |
| elemol | 1.1 |
| estragole | 0.2 |
| eucalyptol | 0.6 |
| limonene | 1.4 |
| linalool | 18.0 |
| myrtenal | 0.5 |
| myrtenol | 1.0 |
| o-cymene | 0.5 |
| pinocarveol | 0.3 |
| sabinene | 0.6 |
| spathulenol | 1.1 |
| terpinen-4-ol | 0.9 |
| trans-pinocamphone | 18.9 |
| α-pinene | 8.6 |
| α-terpineol | 0.8 |
| β-myrcene | 0.3 |
| β-pinene | 6.4 |

| | EO18 |
|---|---|
| p-mentha-2,8-dien-1-ol | 1.9 |
| carveol | 1.9 |
| carvone | 4.7 |
| caryophyllene oxide | 0.4 |
| cis-carveol | 3.3 |
| cis-limonene oxide | 3.5 |
| limonene | 78.2 |
| limonene-1,2-diol | 0.7 |
| o-cymene | 0.3 |
| trans-limonene oxide | 2.4 |
| trans-p-mentha-2,8-dienol | 2.1 |
| α-pinene | 0.4 |
| β-myrcene | 0.3 |

| | EO19 |
|---|---|
| .τ.-muurolol | 0.2 |
| β-caryophyllene | 0.2 |
| citronellal | 38.8 |
| citronellol | 19.0 |
| citronellyl acetate | 2.9 |
| elemol | 2.5 |
| eugenol | 0.9 |
| geraniol | 24.8 |
| germacrene D | 0.7 |
| germacrene-D-4-ol | 0.3 |
| isopulegol | 0.7 |
| linalool | 0.4 |
| α-cadinol | 0.4 |
| α-citral | 2.0 |
| β-citral | 1.2 |
| β-elemene | 0.9 |
| β-myrcene | 3.0 |
| γ-muurolene | 0.3 |
| δ-cadinene | 0.9 |

| | EO20 |
|---|---|
| borneol | 2.7 |
| bornyl acetate | 55.0 |
| camphene | 18.1 |
| camphor | 0.4 |
| β-caryophyllene | 0.9 |
| caryophyllene oxide | 1.3 |
| crypton | 0.6 |
| humulene | 0.5 |
| humulene epoxide 2 | 0.6 |
| limonene | 3.9 |
| o-cymene | 0.4 |
| p-cymen-7-ol | 0.2 |
| p-cymen-8-ol | 0.7 |
| santene | 1.0 |
| tricyclene | 1.5 |
| α-bisabolol | 0.4 |
| α-pinene | 8.4 |
| α-terpineol | 0.4 |
| β-bisabolene | 0.2 |
| β-phellandrene | 1.1 |
| β-pinene | 1.6 |

| | EO21 |
|---|---|
| 1,4-dihydroxy-p-menth-2-ene | 0.5 |
| camphene | 0.4 |
| estragole | 0.3 |
| eucalyptol | 57.0 |
| limonene | 22.8 |
| m-cymene | 13.4 |
| palmitic acid | 1.6 |
| sabinene | 0.6 |
| α-pinene | 0.4 |
| β-pinene | 3.1 |

| | EO22 |
|---|---|
| 2,2,7,7-tetramethyltricyclo[6.2.1.0~1,6~]undeca-3,5,9-triene | 2.4 |
| 2-methoxy-4-propylphenol | 3.0 |
| 2-methoxy-phenol | 4.2 |
| 2-methyl-phenol | 1.3 |
| 3-methyl-1,2-cyclopentanedione | 1.2 |
| 4-ethyl-2-methoxyphenol | 7.3 |
| 8,14-cedranoxide | 0.3 |
| calamenene | 17.4 |
| β-caryophyllene | 1.0 |
| cedrene | 8.8 |
| cedrol | 0.5 |
| creosol | 9.3 |
| cubenol | 2.7 |
| humulene | 1.6 |
| isoeugenol | 1.9 |
| isoledene | 3.7 |
| m-cresol | 1.4 |
| phenol | 1.0 |
| α-cadinol | 0.5 |
| α-calacorene | 6.3 |
| α-curcumene | 1.1 |
| α-muurolene | 4.6 |
| δ-cadinene | 18.6 |

| | EO23 |
|---|---|
| bornyl acetate | 0.6 |
| camphene | 0.3 |
| camphor | 3.8 |
| chrysanthone | 88.5 |
| eucalyptol | 0.3 |
| fenchone | 2.7 |
| limonene | 0.3 |
| sabinene | 0.3 |
| terpinen-4-ol | 0.7 |
| thujone | 1.8 |
| α-pinene | 0.4 |
| β-myrcene | 0.3 |

| | EO24 |
|---|---|
| 6-methyl-5-hepten-2-one | 0.6 |
| borneol | 1.1 |
| camphene | 5.7 |
| cis-geraniol | 0.4 |
| elemol | 0.5 |
| eucalyptol | 7.0 |
| limonene | 1.1 |
| linalool | 0.3 |
| nerolidol | 0.6 |
| zingiberene | 29.9 |
| α-bergamotene | 0.4 |
| α-copaene | 0.6 |
| α-curcumene | 31.6 |
| α-farnesene | 4.3 |
| α-pinene | 1.7 |
| α-terpineol | 0.7 |
| β-bisabolene | 10.6 |
| β-elemene | 1.2 |
| β-eudesmol | 0.3 |
| β-myrcene | 0.6 |
| γ-muurolene | 0.7 |

| | EO25 |
|---|---|
| 2-caren-10-ol | 28.1 |
| carotol | 1.3 |
| carvacrol | 0.3 |
| β-caryophyllene | 0.7 |
| caryophyllene oxide | 0.5 |
| cis-β-farnesene | 0.9 |
| cumaldehyde | 37.9 |
| limonene | 0.3 |
| p-cymen-7-ol | 0.5 |
| p-cymen-8-ol | 0.2 |
| p-cymene | 7.6 |
| sabinene | 0.2 |
| α-phellandrene | 1.0 |
| α-pinene | 0.3 |
| β-myrcene | 0.4 |
| β-phellandrene | 0.3 |
| β-pinene | 5.6 |
| γ-terpinene | 13.9 |

| | EO26 |
|---|---|
| β-caryophyllene | 3.2 |
| caryophyllene oxide | 0.6 |
| globulol | 1.1 |
| ledene oxide-(I) | 0.4 |
| patchouli alcohol | 45.4 |
| seychellene | 6.8 |
| α-guaiene | 15.3 |
| α-panasinsene | 0.3 |
| α-patchoulene | 5.9 |
| β-guaiene | 19.0 |
| β-patchoulene | 2.1 |

| | EO27 |
|---|---|
| decanal | 0.3 |
| limonene | 95.1 |
| linalool | 0.4 |
| linalyl acetate | 0.6 |
| sabinene | 0.2 |
| α-pinene | 0.5 |
| β-pinene | 2.7 |
| γ-terpinene | 0.1 |

| | EO28 |
|---|---|
| carvone | 0.3 |
| eucalyptol | 83.9 |
| limonene | 6.1 |
| p-cymene | 8.1 |
| α-pinene | 1.1 |
| β-myrcene | 0.3 |
| β-pinene | 0.2 |

| | EO29 |
|---|---|
| 3-carene | 16.6 |
| bornyl acetate | 1.4 |
| camphene | 0.9 |
| β-caryophyllene | 16.7 |
| caryophyllene oxide | 3.5 |
| cis-verbenol | 0.2 |
| humulene | 1.2 |
| humulene epoxide 2 | 0.3 |
| limonene | 11.2 |
| longifolene | 2.0 |
| myrtenol | 0.2 |
| o-cymene | 0.5 |
| p-cymen-8-ol | 1.6 |
| pinocarveol | 0.4 |
| terpinolene | 2.0 |
| α-cubebene | 0.5 |
| α-pinene | 22.8 |
| α-terpineol | 0.9 |
| β-pinene | 17.1 |

| | EO30 |
|---|---|
| carvone | 0.4 |
| cis-carveol | 0.3 |
| limonene | 26.1 |
| limonene oxide, cis- | 0.3 |
| linalool | 13.8 |
| linalyl anthranilate | 45.3 |
| nerol acetate | 0.7 |
| o-cymene | 6.5 |
| sabinene | 0.5 |
| α-pinene | 0.7 |
| β-bisabolene | 0.2 |
| β-myrcene | 0.7 |
| β-pinene | 4.6 |

| | EO31 |
|---|---|
| (E)-β-farnesene | 0.6 |
| 4-epi-cubebol | 1.1 |
| β-caryophyllene | 13.7 |
| caryophyllene oxide | 2.9 |
| humulene | 3.6 |
| limonene | 7.5 |
| o-cymene | 3.0 |
| p-cymen-8-ol | 0.6 |
| sabinene | 5.9 |
| spathulenol | 0.8 |
| terpinen-4-ol | 6.3 |
| terpinolene | 0.9 |
| trans-calamenene | 0.9 |
| α-cadinol | 0.4 |
| α-copaene | 1.0 |
| α-cubebene | 0.9 |
| α-muurolene | 0.8 |
| α-pinene | 27.1 |
| α-terpineol | 0.6 |
| β-elemene | 3.6 |
| β-myrcene | 9.3 |
| β-pinene | 3.6 |
| γ-elemene | 2.0 |
| γ-muurolene | 1.5 |
| γ-terpinene | 1.0 |
| δ-cadinene | 0.4 |

| | EO32 |
|---|---|
| 1,8-dimethylnaphthalene | 4.6 |
| 2,2,7,7-tetramethyltricyclo[6.2.1.0~1,6~]undeca-3,5,9-triene | 1.7 |
| 2-methoxy-4-propylphenol | 2.7 |
| 2-methoxy-phenol | 6.6 |
| 2-methyl-phenol | 1.2 |
| 3-methyl-1,2-cyclopentanedione | 0.8 |
| 4-epi-cubebol | 2.8 |
| benzocycloheptatriene | 0.9 |
| cadalene | 5.5 |
| cadina-1(2),4-diene | 2.7 |
| calamenene | 18.1 |
| cedrene | 8.2 |
| creosol | 7.2 |
| dihydrocurcumene | 3.4 |
| isoeugenol | 1.6 |
| m-cresol | 1.3 |
| α-cadinol | 0.6 |
| α-calacorene | 5.8 |
| α-muurolene | 4.4 |
| β-cadinene | 0.7 |
| δ-cadinene | 18.5 |
| δ-cadinol | 0.8 |

| | EO33 |
|---|---|
| anethole | 78.1 |
| camphor | 0.2 |
| estragole | 2.2 |
| fenchone | 3.4 |
| limonene | 3.4 |
| o-cymene | 0.4 |
| p-acetonylanisole | 4.7 |
| p-anisaldehyde | 6.3 |
| α-bergamotene | 0.1 |
| α-pinene | 1.0 |
| β-myrcene | 0.2 |

| | EO34 |
|---|---|
| carveol | 0.4 |
| carvone | 1.4 |
| β-caryophyllene | 0.2 |
| caryophyllene oxide | 0.4 |
| cis-p-mentha-2,8-dien-1-ol | 0.4 |
| geranic acid | 1.0 |
| limonene | 32.2 |
| limonene oxide, cis- | 0.7 |
| limonene oxide, trans- | 0.5 |
| linalool | 6.4 |
| linalyl anthranilate | 25.0 |
| nerol acetate | 1.6 |
| o-cymene | 17.4 |
| sabinene | 0.2 |
| trans-p-mentha-2,8-dienol | 0.4 |
| α-bergamotene | 0.3 |
| α-citral | 4.8 |
| α-pinene | 0.4 |
| β-bisabolene | 0.5 |
| β-citral | 2.1 |
| β-myrcene | 0.4 |
| β-pinene | 3.2 |

| | EO35 |
|---|---|
| carveol | 0.3 |
| caryophyllene oxide | 0.4 |
| cis-geraniol | 2.2 |
| cis-p-mentha-2,8-dien-1-ol | 0.4 |
| geranic acid | 1.6 |
| geranyl acetate | 1.0 |
| limonene | 59.2 |
| limonene glycol | 2.9 |
| limonene oxide, trans- | 0.7 |
| myrtenal | 0.2 |
| nerol acetate | 0.9 |
| o-cymene | 7.9 |
| sabinene | 1.0 |
| α-citral | 7.8 |
| α-pinene | 1.1 |
| β-citral | 3.3 |
| β-myrcene | 0.7 |
| β-pinene | 7.2 |
| γ-terpinene | 1.1 |

| | EO36 |
|---|---|
| artemisia alcohol | 1.7 |
| borneol | 0.8 |
| borneol, butyrate | 1.7 |
| bornyl acetate | 1.0 |
| camphene | 0.4 |
| β-caryophyllene | 6.0 |
| caryophyllene oxide | 0.7 |
| cis-3-pinanone | 0.3 |
| eucalyptol | 2.5 |
| germacrene d | 1.8 |
| limonene | 7.3 |
| o-cymene | 0.2 |
| pinocarveol | 4.8 |
| pinocarvone | 0.3 |
| sabinene | 0.4 |
| sativene | 0.7 |
| spathulenol | 1.3 |
| terpinen-4-ol | 0.3 |
| terpinolene | 0.2 |
| trans-2,7-dimethyl-4,6-octadien-2-ol | 49.3 |
| yomogi alcohol | 1.3 |
| α-pinene | 18.9 |
| β-myrcene | 1.7 |
| δ-elemene | 1.5 |

| | EO37 |
|---|---|
| 1-octen-3-ol | 0.9 |
| borneol | 1.0 |
| carvacrol | 71.5 |
| carvacrol acetate | 0.3 |
| β-caryophyllene | 5.0 |
| caryophyllene oxide | 1.0 |
| eucalyptol | 0.4 |
| limonene | 0.2 |
| linalool | 1.5 |
| p-cymene | 5.6 |
| spathulenol | 0.3 |
| terpinen-4-ol | 1.1 |
| thymol | 1.6 |
| α-pinene | 0.3 |
| α-terpinene | 0.5 |
| α-terpineol | 0.2 |
| β-bisabolene | 4.1 |
| β-myrcene | 0.3 |
| γ-cadinene | 0.4 |
| γ-muurolene | 0.6 |
| γ-terpinene | 2.3 |
| δ-cadinene | 0.8 |

| | EO38 |
|---|---|
| borneol | 1.3 |
| bornyl acetate | 0.4 |
| camphene | 0.8 |
| camphor | 21.4 |
| β-caryophyllene | 6.2 |
| eucalyptol | 53.2 |
| eugenol | 0.7 |
| limonene | 1.7 |
| o-cymene | 0.4 |
| terpinen-4-ol | 0.4 |
| α-pinene | 6.7 |
| α-terpineol | 1.2 |
| β-myrcene | 0.3 |
| β-pinene | 5.3 |

| | EO39 |
|---|---|
| 2-methoxycinnamaldehyde | 0.2 |
| acetic acid, cinnamyl ester | 2.6 |
| acetyleugenol | 1.3 |
| β-caryophyllene | 4.0 |
| caryophyllene oxide | 0.2 |
| eugenol | 34.6 |
| humulene | 0.6 |
| limonene | 0.2 |
| linalool | 3.2 |
| o-cymene | 0.7 |
| tetradecanal | 0.5 |
| trans-3-phenyl-2-propenal | 49.1 |
| α-copaene | 0.5 |
| α-phellandrene | 0.3 |
| α-pinene | 0.2 |
| α-terpineol | 0.3 |
| β-isosafrole | 0.9 |
| β-phellandrene | 0.5 |

| | EO40 |
|---|---|
| carvone | 0.5 |
| cis-carveol | 0.2 |
| eucalyptol | 85.9 |
| limonene | 4.5 |
| o-cymene | 8.3 |
| α-pinene | 0.6 |

| | EO41 |
|---|---|
| carvone | 0.8 |
| cis-carveol | 0.5 |
| cis-p-mentha-2,8-dien-1-ol | 0.3 |
| limonene | 95.0 |
| linalool | 0.8 |
| sabinene | 0.2 |
| trans-p-mentha-2,8-dienol | 0.3 |
| α-pinene | 0.4 |
| β-myrcene | 1.7 |

| | EO42 |
|---|---|
| β-caryophyllene | 1.8 |
| eucalyptol | 66.0 |
| ledol | 5.4 |
| limonene | 5.9 |
| linalool | 0.2 |
| o-cymene | 1.5 |
| terpinen-4-ol | 0.9 |
| terpinolene | 0.4 |
| α-pinene | 5.3 |
| α-terpineol | 8.3 |
| α-terpineol acetate | 1.4 |
| β-myrcene | 0.7 |
| β-pinene | 1.5 |
| γ-terpinene | 0.8 |

| | EO43 |
|---|---|
| artemisia alcohol | 2.0 |
| borneol | 0.9 |
| camphene | 3.0 |
| camphor | 27.0 |
| cumaldehyde | 0.4 |
| eucalyptol | 2.0 |
| germacrene D | 0.3 |
| myrtenol | 0.3 |
| o-cymene | 1.2 |
| pinocarveol | 0.7 |
| sabinene | 0.9 |
| santolina triene | 2.2 |
| terpinen-4-ol | 2.5 |
| thujone | 44.6 |
| yomogi alcohol | 1.6 |
| α-pinene | 0.2 |
| β-thujone | 9.9 |
| γ-terpinene | 0.3 |

| | EO44 |
|---|---|
| β-caryophyllene | 9.1 |
| cis-β-terpineol | 0.7 |
| eucalyptol | 52.7 |
| limonene | 3.6 |
| linalool | 2.2 |
| p-cymene | 18.4 |
| p-menth-3-en-1-ol | 0.3 |
| terpinolene | 0.5 |
| α-pinene | 1.5 |
| α-terpineol | 7.6 |
| α-terpineol acetate | 1.2 |
| β-myrcene | 0.6 |
| β-pinene | 0.8 |
| γ-terpinene | 0.9 |

| | EO45 |
|---|---|
| 3-carene | 5.9 |
| calamenene | 0.3 |
| β-caryophyllene | 33.6 |
| caryophyllene oxide | 9.7 |
| humulene | 2.4 |
| humulene epoxide 2 | 0.5 |
| limonene | 11.1 |
| linalool | 0.6 |
| p-cymene | 1.1 |
| sabinene | 7.2 |
| spathulenol | 0.4 |
| terpinen-4-ol | 0.4 |
| α-bergamotene | 0.1 |
| α-copaene | 5.4 |
| α-muurolene | 0.4 |
| α-pinene | 6.9 |
| β-bisabolene | 2.0 |
| β-cubebene | 0.7 |
| β-elemene | 0.7 |
| β-pinene | 6.3 |
| β-selinene | 0.5 |
| γ-muurolene | 0.2 |
| δ-cadinene | 0.9 |
| δ-elemene | 2.7 |

| | EO46 |
|---|---|
| 1-octen-3-ol | 0.5 |
| borneol | 2.2 |
| camphene | 1.0 |
| camphor | 2.4 |
| carvacrol | 6.6 |
| β-caryophyllene | 2.4 |
| caryophyllene oxide | 0.7 |
| cis-β-terpineol | 0.2 |
| eucalyptol | 1.2 |
| limonene | 0.5 |
| linalool | 7.5 |
| methyl thymyl ether | 0.4 |
| p-cymene | 18.2 |
| terpinen-4-ol | 3.0 |
| thymol | 44.4 |
| α-pinene | 1.3 |
| α-terpinene | 0.6 |
| α-terpineol | 0.2 |
| β-myrcene | 1.1 |
| β-pinene | 0.3 |
| γ-terpinene | 5.2 |

| | EO47 |
|---|---|
| 1,4-dihydroxy-p-menth-2-ene | 0.8 |
| β-caryophyllene | 0.6 |
| caryophyllene oxide | 1.0 |
| cis-sabinene hydrate | 2.9 |
| cis-β-terpineol | 15.4 |
| eucalyptol | 1.0 |
| limonene | 0.8 |
| linalol oxide | 0.5 |
| linalool | 40.7 |
| o-cymene | 8.5 |
| p-cymen-8-ol | 0.6 |
| sabinene | 2.6 |
| terpinen-4-ol | 23.2 |
| α-pinene | 0.4 |
| α-terpineol | 0.4 |
| β-myrcene | 0.5 |

| | EO48 |
|---|---|
| acetyleugenol | 9.9 |
| β-caryophyllene | 8.8 |
| eugenol | 80.1 |
| humulene | 1.0 |
| methylsalicylate | 0.2 |

| | EO49 |
|---|---|
| 3-carene | 29.3 |
| camphene | 0.6 |
| cedrene | 0.5 |
| cedrol | 4.7 |
| cis-verbenol | 0.3 |
| eucalyptol | 0.5 |
| limonene | 4.0 |
| linalool | 0.7 |
| o-cymene | 1.4 |
| p-cymen-8-ol | 1.2 |
| sabinene | 0.7 |
| terpinen-4-ol | 1.5 |
| terpinolene | 0.7 |
| trans-2-caren-4-ol | 0.4 |
| verbenone | 0.3 |
| α-pinene | 47.7 |
| α-terpineol | 0.4 |
| α-terpineol acetate | 3.8 |
| β-pinene | 1.3 |

| | EO50 |
|---|---|
| eucalyptol | 2.9 |
| eugenol | 2.2 |
| geranyl acetate | 0.2 |
| isoeugenol | 0.3 |
| limonene | 7.8 |
| linalool | 0.5 |
| methyleugenol | 0.3 |
| myristicin | 21.9 |
| o-cymene | 1.6 |
| sabinene | 13.9 |
| terpinen-4-ol | 16.6 |
| terpinolene | 0.7 |
| α-copaene | 0.3 |
| α-phellandrene | 0.8 |
| α-pinene | 12.0 |
| α-terpinene | 0.6 |
| α-terpineol | 0.7 |
| α-terpineol acetate | 0.1 |
| β-isosafrole | 1.5 |
| β-pinene | 11.1 |
| γ-terpinene | 3.8 |

| | EO51 |
|---|---|
| β-caryophyllene | 0.2 |
| eucalyptol | 0.9 |
| isomenthone | 10.0 |
| isopulegol | 0.9 |
| levomenthol | 0.4 |
| limonene | 0.5 |
| menthol | 57.4 |
| menthol, acetate | 5.0 |
| menthone | 23.2 |
| piperitenone | 0.7 |
| pulegone | 0.4 |
| α-terpineol | 0.3 |

| | EO52 |
|---|---|
| 6-methyl-5-hepten-2-one | 1.3 |
| β-caryophyllene | 0.7 |
| cis-geraniol | 0.6 |
| cis-verbenol | 0.3 |
| citronellal | 8.0 |
| citronellyl formate | 1.1 |
| elemol | 0.5 |
| eucalyptol | 0.6 |
| geranic acid | 0.7 |
| geraniol | 5.6 |
| limonene | 9.5 |
| linalool | 1.3 |
| sabinene | 0.5 |
| terpinen-4-ol | 0.2 |
| α-citral | 33.7 |
| α-copaene | 0.1 |
| α-pinene | 1.6 |
| β-citral | 30.9 |
| β-myrcene | 0.4 |
| β-pinene | 2.1 |
| δ-cadinene | 0.2 |

| | EO53 |
|---|---|
| β-caryophyllene | 0.3 |
| caryophyllene oxide | 0.3 |
| cis-α-bisabolene | 2.1 |
| cis-β-farnesene | 0.3 |
| estragole | 75.2 |
| levomenthol | 0.4 |
| linalool | 19.7 |
| α-bergamotene | 0.9 |
| α-citral | 0.7 |

| | EO54 |
|---|---|
| carvone | 0.6 |
| β-caryophyllene | 1.8 |
| cis-geraniol | 76.5 |
| cis-β-ocimene | 0.3 |
| farnesol | 0.7 |
| geranyl acetate | 13.0 |
| humulene | 0.2 |
| linalool | 4.1 |
| nerol acetate | 1.0 |
| α-citral | 0.7 |
| β-ocimene | 1.1 |

| | EO55 |
|---|---|
| eucalyptol | 53.9 |
| eugenol | 1.9 |
| limonene | 2.0 |
| linalool | 3.0 |
| methyleugenol | 4.2 |
| myrtenol | 0.3 |
| o-cymene | 2.4 |
| sabinene | 3.2 |
| terpinen-4-ol | 3.0 |
| α-pinene | 3.2 |
| α-terpineol acetate | 18.8 |
| β-pinene | 2.3 |
| γ-terpinene | 1.8 |

| | EO56 |
|---|---|
| anethole | 88.5 |
| β-caryophyllene | 0.4 |
| estragole | 3.8 |
| isohomogenol | 0.2 |
| limonene | 1.6 |
| linalool | 0.9 |
| nerolidol | 0.3 |
| p-acetonylanisole | 0.9 |
| p-anisaldehyde | 2.1 |
| terpinen-4-ol | 0.3 |
| α-bergamotene | 0.5 |
| α-pinene | 0.3 |
| α-terpineol | 0.2 |

| | EO57 |
|---|---|
| 3-carene | 0.5 |
| 4-epi-cubebol | 1.7 |
| acetic acid | 0.7 |
| bornyl acetate | 1.0 |
| β-caryophyllene | 9.1 |
| caryophyllene oxide | 3.0 |
| cis-verbenol | 1.8 |
| humulene | 2.0 |
| humulene epoxide 2 | 1.1 |
| limonene | 20.3 |
| myrtenyl acetate | 0.3 |
| o-cymene | 3.7 |
| p-cymen-8-ol | 0.2 |
| pinocarveol | 0.9 |
| sabinene | 2.8 |
| terpinen-4-ol | 0.6 |
| viridiflorol | 0.5 |
| α-copaene | 2.3 |
| α-cubebene | 0.4 |
| α-muurolene | 0.4 |
| α-phellandrene | 2.0 |
| α-pinene | 27.0 |
| α-selinene | 1.1 |
| α-terpineol | 0.5 |
| β-elemene | 4.0 |
| β-eudesmol | 0.3 |
| β-myrcene | 3.0 |
| β-phellandrene | 1.0 |
| β-pinene | 1.0 |
| β-selinene | 1.6 |
| γ-eudesmol | 0.5 |
| δ-cadinene | 2.1 |
| τ-cadinol | 2.3 |

| | EO58 |
|---|---|
| .τ.-muurolol | 0.1 |
| calamenene | 0.7 |
| β-caryophyllene | 7.3 |
| caryophyllene oxide | 0.2 |
| cinerolon | 4.6 |
| cubenol | 0.2 |
| cyclohexanone, 2-(1-methylethylidene)- | 1.0 |
| epi-bicyclosesquiphellandrene | 0.9 |
| germacrene D | 5.2 |
| humulene | 1.1 |
| jasmone | 0.6 |
| limonene | 8.8 |
| myrtenal | 0.3 |
| pulegone | 59.8 |
| sabinene | 0.6 |
| terpinen-4-ol | 0.7 |
| thymol | 1.2 |
| α-cadinol | 0.2 |
| α-cubebene | 0.5 |
| α-gurjunene | 0.4 |
| α-muurolene | 0.2 |
| α-pinene | 1.0 |
| β-ocimene | 0.1 |
| β-pinene | 3.8 |
| γ-cadinene | 0.2 |
| γ-terpinene | 0.1 |

| | EO59 |
|---|---|
| 1-octen-3-ol | 0.7 |
| borneol | 0.6 |
| carvacrol | 61.0 |
| β-caryophyllene | 13.6 |
| caryophyllene oxide | 1.4 |
| cis-β-terpineol | 0.2 |
| humulene | 0.6 |
| limonene | 0.3 |
| linalool | 1.8 |
| p-cymene | 7.1 |
| thymol | 0.5 |
| α-citral | 0.2 |
| α-terpinene | 1.5 |
| α-thujene | 1.0 |
| β-bisabolene | 1.6 |
| β-myrcene | 1.6 |
| β-phellandrene | 0.3 |
| γ-terpinene | 6.0 |

| | EO60 |
|---|---|
| 1-octen-3-ol | 0.6 |
| borneol | 2.5 |
| camphene | 0.6 |
| carvacrol | 0.7 |
| β-caryophyllene | 3.4 |
| caryophyllene oxide | 1.8 |
| eucalyptol | 0.9 |
| isothymol methyl ether | 6.0 |
| limonene | 0.4 |
| linalool | 3.7 |
| methyl thymyl ether | 10.7 |
| p-cymene | 30.5 |
| thymol | 34.1 |
| α-pinene | 0.9 |
| α-terpineol | 0.3 |
| β-myrcene | 1.0 |
| γ-muurolene | 0.3 |
| γ-terpinene | 1.8 |

| | EO61 |
|---|---|
| 1-octen-3-ol | 0.5 |
| alcanfor | 0.3 |
| borneol | 0.3 |
| carvacrol | 0.8 |
| β-caryophyllene | 2.9 |
| caryophyllene oxide | 0.6 |
| eucalyptol | 0.5 |
| humulene | 0.3 |
| isothymol methyl ether | 7.4 |
| limonene | 0.4 |
| methyl thymyl ether | 4.9 |
| p-cymen-8-ol | 0.1 |
| p-cymene | 18.5 |
| thymol | 34.7 |
| thymol acetate | 0.3 |
| α-muurolene | 0.2 |
| α-phellandrene | 0.2 |
| α-terpineol | 0.2 |
| α-thujene | 1.1 |
| β-bisabolene | 5.0 |
| β-bourbonene | 0.4 |
| β-myrcene | 1.3 |
| γ-cadinene | 0.4 |
| γ-muurolene | 0.6 |
| γ-terpinene | 17.1 |
| δ-cadinene | 0.7 |