

Supplementary materials

The application of citronella oil and citronellol as antibacterial ingredients in chitosan coatings for titanium surfaces

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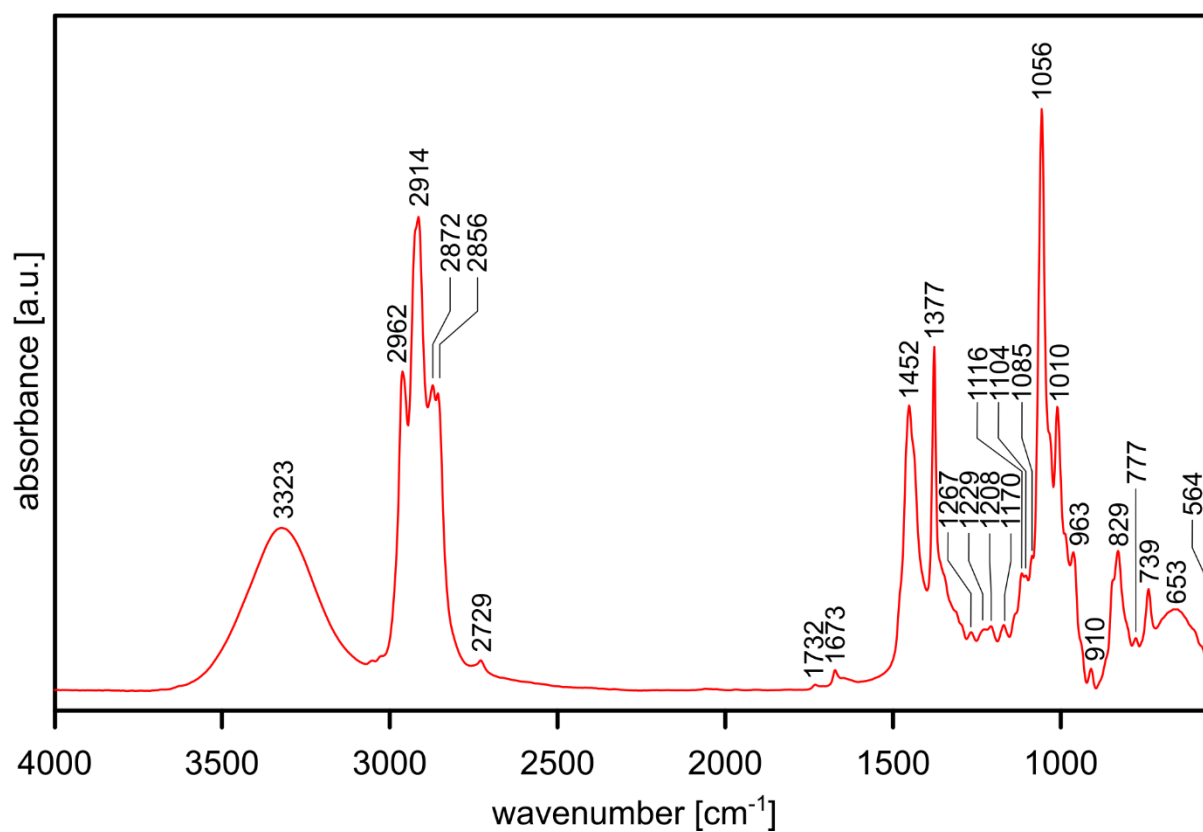


Figure S1. FT-IR spectrum for citronellol

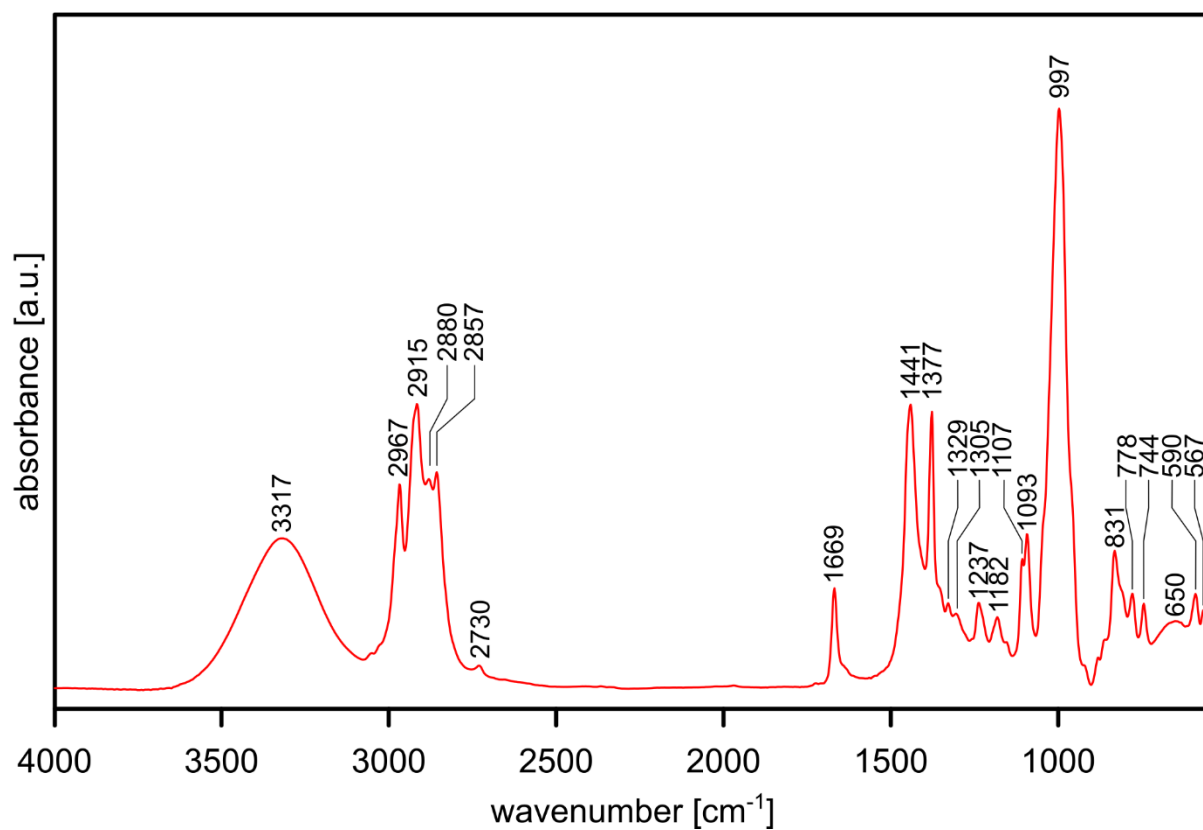


Figure S2. FT-IR spectrum for geraniol

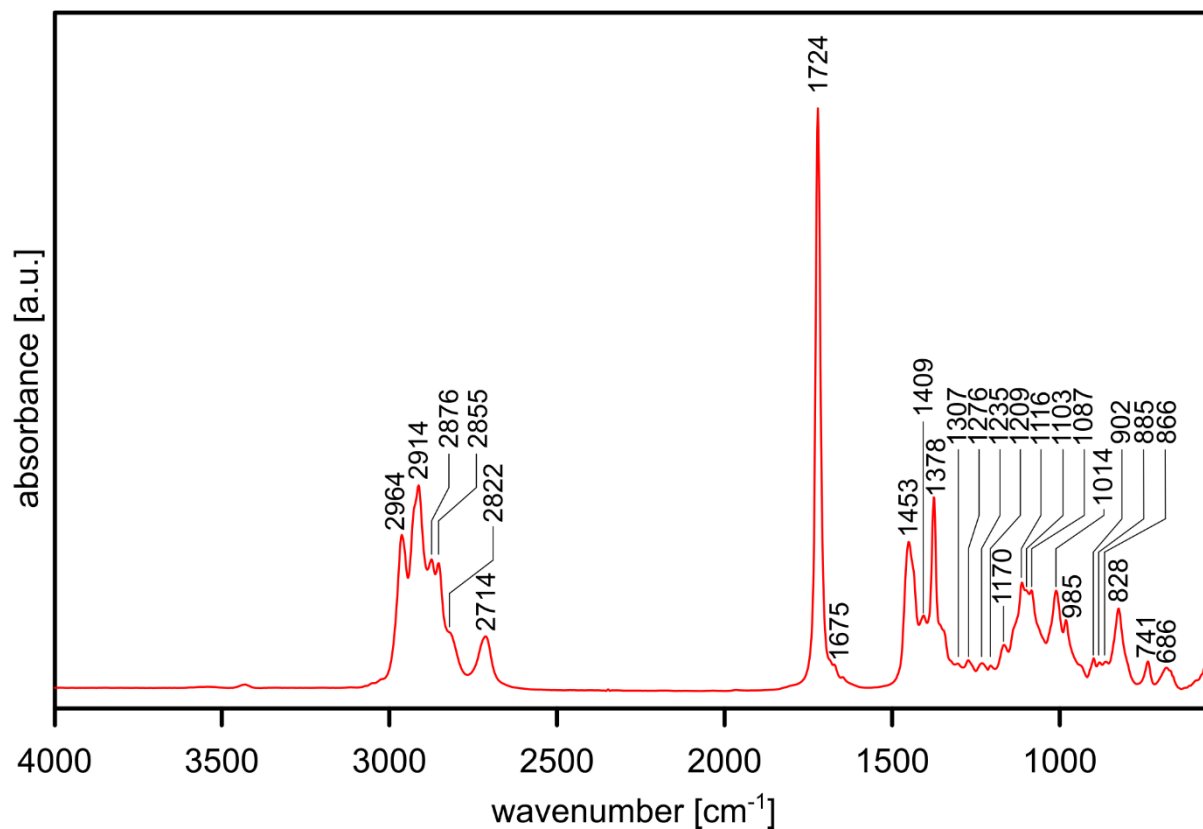


Figure S3. FT-IR spectrum for citronellal

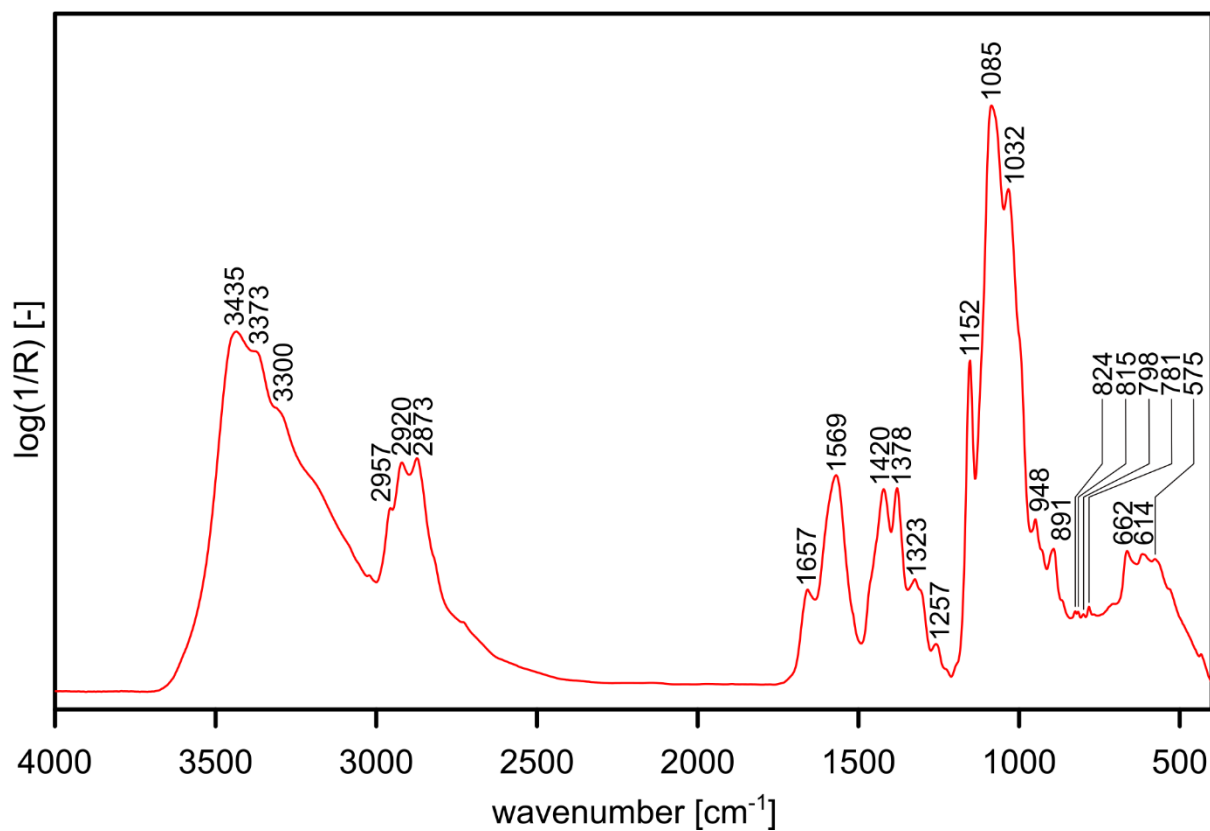


Figure S4. FT-IR spectrum for chitosan coating

Table S1. Detailed FT-IR spectrum analysis for citronellol, abbreviations explained under the table

band position [cm ⁻¹] and characteristics	type of vibration
3323 m, br	ν O-H
2962 s	ν_{as} C-H in -CH ₃
2914 vs	ν_{as} C-H in -CH ₂ -
2872 s	ν_s C-H in -CH ₃
2856 s	ν_s C-H in -CH ₂ -
2729 w	impurity: ν C-H in -CHO
1732 w	impurity: ν C=O in -CHO
1673 w	ν C=C
1452 s	in-plane δ_{as} C-H in -CH
1377 s	in-plane δ_s C-H in -C=C-CH
1267 w	in-plane δ O-H
1229 w	ν C-C
1208 w	ν C-C
1170 w	ν C-C
1116 m	δ C-H in -CH
1104 m	δ C-H in -CH
1085 m	δ C-H in -CH
1056 vs	ν C-O
1010 s	δ C-H in -CH
963 m	out-of-plane δ O-H
910 w	out-of-plane δ C-H in -C=C-CH
829 m	δ C-H in -C=C-CH
777 w	δ C-H in -C-C-OH
739 m	δ C-C
653 m, br	out-of-plane δ O-H
564 w	δ C-O

Abbreviations: bands intensity: vs - very strong, s - strong, m - medium, w - weak; bands shape: br - broad; type of vibration: ν - stretching, δ - bending, s - symmetric, as - asymmetric.

Table S2. Detailed FT-IR spectrum analysis for geraniol, abbreviations explained under the table

band position [cm ⁻¹] and characteristics	type of vibration
3317 m	ν O-H
2967 m	ν_{as} C-H in -CH ₃
2915 s	ν_{as} C-H in -CH ₂ -
2880 m	ν_s C-H in -CH ₃
2857 m	ν_s C-H in -CH ₂ -
2730 w	impurity: ν C-H in -CHO
1669 m	ν C=C
1441 s	in-plane δ_{as} C-H in -CH
1377 s	in-plane δ_s C-H in -C=C-CH
1329 w	in-plane δ O-H
1305 w	in-plane δ C-H in -C=C-CH
1237 w	ν C-C
1182 w	ν C-C
1107 m	δ C-H in -CH
1093 m	ν C-O
997 vs	out-of-plane δ O-H
831 m	δ C-H in -C=C-CH
778 w	δ C-H in -C-C-OH
744 w	δ C-C
650 w, br	out-of-plane δ O-H
590 w	in-plane δ C=C
567 w	δ C-O

Abbreviations: bands intensity: vs - very strong, s - strong, m - medium, w - weak; bands shape: br - broad; type of vibration: ν - stretching, δ - bending, s - symmetric, as - asymmetric.

Table S3. Detailed FT-IR spectrum analysis for citronellal, abbreviations explained under the table

band position [cm ⁻¹] and characteristics	type of vibration
2964 s	ν_{as} C-H in -CH ₃
2914 s	ν_{as} C-H in -CH ₂ -
2876 s	ν_s C-H in -CH ₃
2855 s	ν_s C-H in -CH ₂ -
2822 m, sh	ν C-H in -CHO
2714 m	ν C-H in -CHO
1724 vs	ν C=O in -CHO
1675 w	ν C=C
1453 s	in-plane δ_{as} C-H in -CH
1409 m	in-plane δ_s C-H in -CH
1378 s	in-plane δ_s C-H in -C=C-CH
1307 w	δ C-H in -C-CHO
1276 w	ν C-C
1235 w	ν C-C
1209 w	ν C-C
1170 w	ν C-C
1116 m	δ C-H in -CH
1103 m	δ C-H in -CH
1087 m	δ C-H in -CH
1014 m	δ C-H in -CH
985 m	δ C-H in -CH
902 w	out-of-plane δ C-H in -C=C-CH
885 w	ν C-C
866 w	ν C-C
828 m	δ C-H in -C=C-CH
741 w	δ C-C
686 w	δ C-C in -C-C-CHO

Abbreviations: bands intensity: vs - very strong, s - strong, m - medium, w - weak; bands shape: br - broad; type of vibration: ν - stretching, δ - bending, s - symmetric, as - asymmetric.

Table S4. Detailed FT-IR spectrum analysis for chitosan coating, abbreviations explained under the table

band position [cm ⁻¹] and characteristics	type of vibration
3435 s, br	ν O-H
3373 s, br	ν N-H in -NH ₂
3300 s, br	ν N-H in CH ₃ CONH-
2957 m	ν C-H
2920 m	ν C-H
2873 m	ν C-H
1657 m	ν C=O in CH ₃ CONH-
1569 m	δ N-H
1420 m	δ C-H in (ring)-CH ₂ OH
1378 m	δ C-H in ring
1323 m	ν C-N
1257 w	ν C-C in ring
1152 s	ν C-O in (ring)-OH
1085 vs	ν C-O-C in ring
1032 s	ν C-O-C between rings
948 m	ν C-C
891 w	ν C-C
824 w	δ C-H
815 w	δ C-H
798 w	δ C-H
781 w	δ C-H
662 m	δ N-H in -NH ₂
614 m	δ N-H in CH ₃ CONH-
575 m	δ C=O in CH ₃ CONH-

Abbreviations: bands intensity: vs - very strong, s - strong, m - medium, w - weak; bands shape: br - broad; type of vibration: ν - stretching, δ - bending, s - symmetric, as - asymmetric.