

Supplementary data for the article:

Milenković, I.; Radotić, K.; Trifković, J.; Vujisić, L.; Beškoski, V. P. Screening of Semi-Volatile Compounds in Plants Treated with Coated Cerium Oxide Nanoparticles by Comprehensive Two-Dimensional Gas Chromatography. *Journal of Separation Science* **2021**, *44* (11), 2260–2268. <https://doi.org/10.1002/jssc.202100145>.

Supplementary Table S1. Compounds tentatively identified by software of GCxGC-MS method in methylene chloride extracts of **wheat** shoot; + means presence and - means absence of compounds in the sample

| Compounds | Formula | Order number | RT1 | RT2 | Similarity (%) | Presence | Treatments |
|-----------------------------------|----------------------------------|--------------|--------|------|----------------|----------|--------------------|
| 1,2-dimethyl-benzene | C ₈ H ₁₀ | 1 | 12.769 | 2.64 | 95 | + | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 2,3,4-trimethyl-hexane | C ₉ H ₂₀ | 2 | 12.948 | 1.35 | 85 | - | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| <i>(E)</i> -2,2-dimethyl-3-decene | C ₁₂ H ₂₄ | 3 | 13.650 | 1.44 | 85 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 2,6,6-trimethyl-1-heptene | C ₁₀ H ₂₀ | 4 | 14.350 | 1.50 | 82 | + | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 3-ethyl-2-methyl-1-heptene | C ₁₀ H ₂₀ | 5 | 14.952 | 1.59 | 85 | + | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | - | P-CeO ₂ |
| 2,4,4-trimethyl-1-hexene | C ₉ H ₁₈ | 6 | 15.253 | 1.65 | 86 | + | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| <i>(E)</i> -2-heptenal | C ₇ H ₁₂ O | 7 | 15.653 | 1.65 | 91 | + | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| Benzaldehyde | C ₇ H ₆ O | 8 | 15.664 | 2.31 | 85 | - | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | - | L-CeO ₂ |
| | | | | | | - | P-CeO ₂ |
| 1-methyl-2-propyl-cyclohexane | C ₁₀ H ₂₀ | 9 | 15.953 | 1.68 | 90 | + | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 2-methyl-nonane | C ₁₀ H ₂₂ | 10 | 16.650 | 1.50 | 92 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |

| Compounds | Formula | Order number | RT1 | RT2 | Similarity (%) | Presence | Treatments |
|-------------------------------|---|--------------|--------|------|----------------|----------|--------------------|
| | | | | | | + | P-CeO ₂ |
| Heptanoic acid | C ₇ H ₁₄ O ₂ | 11 | 16.745 | 1.20 | 84 | - | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 3-methyl-nonane | C ₁₀ H ₂₂ | 12 | 16.851 | 1.53 | 90 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| <i>(E,E)</i> -2,4-heptadienal | C ₇ H ₁₀ O | 13 | 17.054 | 1.74 | 91 | + | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 3-methyl-undecane | C ₁₂ H ₂₆ | 14 | 17.150 | 1.44 | 92 | - | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| Octanal | C ₈ H ₁₆ O | 15 | 17.346 | 1.23 | 86 | - | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| Decane | C ₁₀ H ₂₂ | 16 | 17.852 | 1.62 | 94 | - | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 3,3-dimethyl-octane | C ₁₀ H ₂₂ | 17 | 18.251 | 1.53 | 88 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 2,5,6-trimethyl-decane | C ₁₃ H ₂₈ | 18 | 18.451 | 1.56 | 92 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 2-ethyl-1-hexanol | C ₈ H ₁₈ O | 19 | 18.544 | 1.11 | 89 | + | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 2,2,6-trimethyl-cyclohexanone | C ₉ H ₁₆ O | 20 | 18.548 | 1.38 | 86 | - | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | - | G-CeO ₂ |
| | | | | | | - | L-CeO ₂ |
| | | | | | | - | P-CeO ₂ |
| 2,6,7-trimethyl-decane | C ₁₃ H ₂₈ | 21 | 18.651 | 1.53 | 92 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |

| Compounds | Formula | Order number | RT1 | RT2 | Similarity (%) | Presence | Treatments |
|--|-----------------------------------|--------------|--------|------|----------------|----------|--------------------|
| | | | | | | + | L-CeO ₂ |
| | | | | | | - | P-CeO ₂ |
| (S)-1-methyl-4-(1-methylethenyl)-cyclohexene | C ₁₀ H ₁₆ | 22 | 18.667 | 2.40 | 86 | + | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | - | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 4-methyl-decane | C ₁₁ H ₂₄ | 23 | 18.751 | 1.53 | 92 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | - | P-CeO ₂ |
| 1-phenyl-ethanone | C ₈ H ₈ O | 24 | 19.363 | 2.28 | 86 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 2-methyl-benzaldehyde | C ₈ H ₈ O | 25 | 19.460 | 2.10 | 89 | + | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 4-methyl-benzaldehyde | C ₈ H ₈ O | 26 | 19.861 | 2.13 | 96 | + | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 4,6-dimethyl-dodecane | C ₁₄ H ₃₀ | 27 | 19.951 | 1.56 | 93 | - | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| Cyclohexanol | C ₆ H ₁₂ O | 28 | 20.144 | 1.08 | 83 | + | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 1-methyl-4-(1-methylethyl)-benzene | C ₁₀ H ₁₄ | 29 | 20.446 | 1.26 | 80 | - | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | - | L-CeO ₂ |
| | | | | | | - | P-CeO ₂ |
| 1-decanol | C ₁₀ H ₂₂ O | 30 | 20.554 | 1.68 | 84 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | - | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| Nonanal | C ₉ H ₁₈ O | 31 | 20.845 | 1.17 | 95 | + | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 2,6-dimethyl-cyclohexanol | C ₈ H ₁₆ O | 32 | 20.952 | 1.59 | 86 | - | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |

| Compounds | Formula | Order number | RT1 | RT2 | Similarity (%) | Presence | Treatments |
|-----------------------------|---|--------------|--------|------|----------------|----------|--------------------|
| | | | | | | + | L-CeO ₂ |
| | | | | | | - | P-CeO ₂ |
| 4,5-dimethyl-nonane | C ₁₁ H ₂₄ | 33 | 21.352 | 1.62 | 93 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 2-ethyl-hexanoic acid | C ₈ H ₁₆ O ₂ | 34 | 21.443 | 1.08 | 82 | + | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 2,6,11-trimethyl-dodecane | C ₁₅ H ₃₂ | 35 | 21.552 | 1.59 | 91 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 1,2,3,4-tetramethyl-benzene | C ₁₀ H ₁₄ | 36 | 21.647 | 1.32 | 91 | - | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | - | L-CeO ₂ |
| | | | | | | - | P-CeO ₂ |
| Dodecane | C ₁₂ H ₂₆ | 37 | 21.752 | 1.62 | 87 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | - | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| Hexadecane | C ₁₆ H ₃₄ | 38 | 22.153 | 1.65 | 85 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | - | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 1-phenyl-1-propanone | C ₉ H ₁₀ O | 39 | 22.559 | 2.04 | 85 | - | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| Octanoic acid | C ₈ H ₁₆ O ₂ | 40 | 22.945 | 1.20 | 88 | - | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 3,5-dimethyl-benzaldehyde | C ₉ H ₁₀ O | 41 | 22.958 | 1.92 | 81 | + | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | - | P-CeO ₂ |
| 1-(4-methylphenyl)-ethanone | C ₉ H ₁₀ O | 42 | 23.160 | 2.10 | 94 | - | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 2-methyl-undecane | C ₁₂ H ₂₆ | 43 | 23.254 | 1.71 | 91 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | - | G-CeO ₂ |

| Compounds | Formula | Order number | RT1 | RT2 | Similarity (%) | Presence | Treatments |
|--|---|--------------|--------|------|----------------|----------|--------------------|
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| Naphthalene | C ₁₀ H ₈ | 44 | 23.460 | 2.10 | 95 | + | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| Tetradecane | C ₁₄ H ₃₀ | 45 | 23.653 | 1.65 | 86 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | - | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| Decanal | C ₁₀ H ₂₀ O | 46 | 23.945 | 1.17 | 95 | + | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 1,2,3,4,5-pentamethylbenzene | C ₁₁ H ₁₆ | 47 | 24.047 | 1.32 | 88 | - | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | - | P-CeO ₂ |
| 2,4-dimethylbenzaldehyde | C ₉ H ₁₀ O | 48 | 24.160 | 2.13 | 96 | + | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 2-phenoxyethanol | C ₈ H ₁₀ O ₂ | 49 | 24.165 | 2.37 | 92 | + | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| Benzothiazole | C ₇ H ₅ NS | 50 | 24.374 | 2.88 | 91 | + | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 2,6,6-trimethyl-1-cyclohexene-1-carboxaldehyde | C ₁₀ H ₁₆ O | 51 | 24.453 | 1.65 | 91 | + | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| (E)-2-decenal | C ₁₀ H ₁₈ O | 52 | 25.547 | 1.32 | 88 | + | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| α, α - dimethylbenzenemethanol | C ₉ H ₁₂ O | 53 | 25.562 | 2.19 | 80 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | - | L-CeO ₂ |
| | | | | | | - | P-CeO ₂ |
| 2,6,6-trimethyl-1-cyclohexene-1-acetaldehyde | C ₁₁ H ₁₈ O | 54 | 25.650 | 1.50 | 94 | + | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |

| Compounds | Formula | Order number | RT1 | RT2 | Similarity (%) | Presence | Treatments |
|---|---|--------------|--------|------|----------------|----------|--------------------|
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| Nonanoic acid | C ₉ H ₁₈ O ₂ | 55 | 25.746 | 1.23 | 91 | + | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| Methyl-1,2-benzenecarboxylate | C ₉ H ₈ O ₄ | 56 | 26.380 | 3.30 | 92 | + | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 3-(1,1-dimethylethyl)-phenol | C ₁₀ H ₁₆ O | 57 | 26.455 | 1.80 | 91 | + | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 2,3,5,8-tetramethyl-decane | C ₁₄ H ₃₀ | 58 | 26.755 | 1.74 | 81 | - | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 1-methyl-naphthalene | C ₁₁ H ₁₀ | 59 | 26.759 | 2.04 | 89 | - | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| Undecanal | C ₁₁ H ₂₂ O | 60 | 26.945 | 1.20 | 92 | + | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| (E,E)-2,4-decadienal | C ₁₀ H ₁₆ O | 61 | 27.051 | 1.53 | 87 | - | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 2-methyl-naphthalene | C ₁₁ H ₁₀ | 62 | 27.162 | 2.19 | 83 | - | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 1,2,3-propanetriol triacetate | C ₉ H ₁₄ O ₆ | 63 | 27.459 | 1.98 | 95 | + | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 2-dodecenal | C ₁₂ H ₂₂ O | 64 | 28.448 | 1.35 | 87 | + | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 1,2-dihydro-1,1,6-trimethyl-naphthalene | C ₁₃ H ₁₆ | 65 | 28.453 | 1.65 | 88 | + | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |

| Compounds | Formula | Order number | RT1 | RT2 | Similarity (%) | Presence | Treatments |
|--|--|--------------|--------|------|----------------|----------|--------------------|
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 1,2,3,4-tetrahydro-1,1,6-trimethylnaphthalene | C ₁₃ H ₁₈ | 66 | 28.551 | 1.56 | 94 | + | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 4-hydroxy-3-methoxybenzaldehyde | C ₈ H ₈ O ₃ | 67 | 28.875 | 2.97 | 85 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | - | P-CeO ₂ |
| 2-ethylnaphthalene | C ₁₂ H ₁₀ | 68 | 28.962 | 2.19 | 90 | + | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| Dodecanal | C ₁₂ H ₂₄ O | 69 | 29.646 | 1.23 | 96 | + | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 1,6-dimethylnaphthalene | C ₁₂ H ₁₂ | 70 | 29.759 | 1.98 | 95 | + | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 1,8-dimethylnaphthalene | C ₁₂ H ₁₂ | 71 | 30.160 | 2.07 | 86 | + | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| (1R,2S,7S,9S)-3,3,7-trimethyl-8-methylidenebicyclo[5.4.0.0 ^{2,9}]undecan | C ₁₅ H ₂₄ | 72 | 30.347 | 1.26 | 92 | - | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 1-(2,4-dimethylphenyl)-1-propanone | C ₁₁ H ₁₄ O | 73 | 30.374 | 2.88 | 81 | - | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 6,10-dimethyl-5,9-undecadien-2-one | C ₁₃ H ₂₂ O | 74 | 30.749 | 1.41 | 89 | + | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 1-hexadecanol | C ₁₆ H ₃₄ O | 75 | 31.142 | 0.96 | 88 | - | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | - | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 1-dodecanol | C ₁₂ H ₂₆ O | 76 | 31.645 | 1.17 | 96 | + | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |

| Compounds | Formula | Order number | RT1 | RT2 | Similarity (%) | Presence | Treatments |
|---|--|--------------|--------|------|----------------|----------|--------------------|
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 4-(2,6,6-trimethyl-1-cyclohexen-2-yl)-3-buten-2-one | C ₁₃ H ₂₀ O | 77 | 31.753 | 1.62 | 93 | + | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 10-methyl-8-tetradecenyl acetate | C ₁₇ H ₃₂ O ₂ | 78 | 31.967 | 2.46 | 81 | + | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | - | P-CeO ₂ |
| Tridecanal | C ₁₃ H ₂₆ O | 79 | 32.246 | 1.23 | 92 | - | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | - | L-CeO ₂ |
| | | | | | | - | P-CeO ₂ |
| 2,4-bis(1,1-dimethylethyl)-phenol | C ₁₆ H ₂₆ O | 80 | 32.251 | 1.53 | 93 | + | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 3,7,11-trimethyl-2,6,10-dodecatrien-1-ol | C ₁₅ H ₂₆ O | 81 | 32.650 | 1.44 | 86 | + | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 2-methyl-1-pentadecene | C ₁₆ H ₃₂ | 82 | 33.044 | 1.11 | 81 | + | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| Diethyl-1,2-benzenedicarboxylate | C ₁₂ H ₁₄ O ₄ | 83 | 33.767 | 2.46 | 89 | + | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-3-buten-2-one | C ₁₃ H ₂₀ O | 84 | 34.555 | 1.77 | 82 | - | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | - | G-CeO ₂ |
| | | | | | | - | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| Tetradecanal | C ₁₄ H ₂₈ O | 85 | 34.647 | 1.26 | 95 | + | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| Isopropyl dodecanoate | C ₁₅ H ₃₀ O ₂ | 86 | 35.045 | 1.14 | 91 | + | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| Methyl-(3-oxo-2-pentyl-, cyclopentyl)acetate | C ₁₃ H ₂₂ O ₃ | 87 | 35.357 | 1.89 | 91 | + | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |

| Compounds | Formula | Order number | RT1 | RT2 | Similarity (%) | Presence | Treatments |
|--|--|--------------|--------|------|----------------|----------|--------------------|
| e | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 2-tetradecanol | C ₁₄ H ₃₀ O | 88 | 36.043 | 1.02 | 84 | + | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | - | G-CeO ₂ |
| | | | | | | - | L-CeO ₂ |
| | | | | | | - | P-CeO ₂ |
| 1-(4-isopropylphenyl)-2-methylpropyl acetate | C ₁₅ H ₂₂ O ₂ | 89 | 36.153 | 1.62 | 86 | + | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| <i>n</i> -hexyl salicylate | C ₁₃ H ₁₈ O ₃ | 90 | 36.154 | 1.71 | 89 | + | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 1-tetradecanol | C ₁₄ H ₃₀ O | 91 | 36.447 | 1.26 | 90 | + | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 13-tetradecenal | C ₁₄ H ₂₆ O | 92 | 36.549 | 1.38 | 87 | + | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| Pentadecanal | C ₁₅ H ₃₀ O | 93 | 36.947 | 1.29 | 95 | + | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 2,6-di- <i>t</i> -butyl-4-hydroxymethylene-2,3,5,6-tetrahydrocyclohexanone | C ₁₅ H ₂₂ O ₂ | 94 | 37.860 | 2.04 | 85 | + | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 2,3,6-trimethyl-1,4-naphthalenedione | C ₁₃ H ₁₂ O ₂ | 95 | 37.871 | 2.67 | 80 | - | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| Pentyl benzoate | C ₁₂ H ₁₆ O ₂ | 96 | 38.553 | 1.65 | 81 | + | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 2-methyl-2-phenyl-tridecane | C ₂₀ H ₃₄ | 97 | 38.661 | 2.10 | 84 | + | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| Hexadecanal | C ₁₆ H ₃₂ O | 98 | 39.048 | 1.32 | 94 | + | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |

| Compounds | Formula | Order number | RT1 | RT2 | Similarity (%) | Presence | Treatments |
|--|--|--------------|--------|------|----------------|----------|--------------------|
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| N,N-diethyl-1-dodecaneamine | C ₁₄ H ₃₁ N | 99 | 39.450 | 1.44 | 89 | + | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| bis(2-methylpropyl)-1,2-benzenedicarboxylate | C ₁₆ H ₂₂ O ₄ | 100 | 39.762 | 2.16 | 96 | + | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| Heptyl benzoate | C ₁₄ H ₂₀ O ₂ | 101 | 39.955 | 1.77 | 82 | + | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| Tridecyl benzoate | C ₂₀ H ₃₂ O ₂ | 102 | 40.455 | 1.77 | 87 | + | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| <i>n</i> -hexadecanoic acid | C ₁₆ H ₃₂ O ₂ | 103 | 41.849 | 1.41 | 92 | + | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| cis,cis,cis-7,10,13-hexadecatrienal | C ₁₆ H ₂₆ O | 104 | 42.454 | 1.65 | 91 | + | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| Ethyl heptadecanoate | C ₁₉ H ₃₈ O ₂ | 105 | 42.547 | 1.29 | 83 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| (Z)-9-Octadecenal | C ₁₈ H ₃₄ O | 106 | 42.550 | 1.47 | 92 | + | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| Heptadecanal | C ₁₇ H ₃₄ O | 107 | 43.049 | 1.38 | 94 | + | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | - | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 2-methyltetracosane | C ₂₅ H ₅₂ | 108 | 56.669 | 2.58 | 86 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | - | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |

Supplementary Table S2. Compounds tentatively identified by software of GCxGC-MS method in methylene chloride extracts of **pea** shoot; + means presence and - means absence of compounds in the sample

| Compounds | Formula | Order number | RT1 | RT2 | Similarity (%) | Presence | Treatments |
|---------------------------------|---|--------------|--------|------|----------------|----------|--------------------|
| 1,2-dimethylbenzene | C ₈ H ₁₀ | 1 | 12.769 | 2.64 | 92 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | - | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 2,3,4-trimethylhexane | C ₉ H ₂₀ | 2 | 12.948 | 1.35 | 80 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | - | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | - | P-CeO ₂ |
| (1,2-dimethylbutyl)-cyclohexane | C ₁₂ H ₂₄ | 3 | 14.054 | 1.77 | 84 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | - | G-CeO ₂ |
| | | | | | | - | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| Cyclopentane-1,2-diol | C ₅ H ₁₀ O ₂ | 4 | 14.858 | 1.95 | 85 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| (E)-2-heptenal | C ₇ H ₁₂ O | 5 | 15.651 | 1.56 | 86 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | - | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| Benzaldehyde | C ₇ H ₆ O | 6 | 15.664 | 2.31 | 82 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 3,7-dimethyl-1-octen | C ₁₀ H ₂₀ | 7 | 15.961 | 2.16 | 88 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| (E,E)-2,4-heptadienal | C ₇ H ₁₀ O | 8 | 17.054 | 1.74 | 88 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | - | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| Octanal | C ₈ H ₁₆ O | 9 | 17.346 | 1.23 | 82 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 2-ethyl-1-hexanol | C ₈ H ₁₈ O | 10 | 18.544 | 1.11 | 82 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | - | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |

| Compounds | Formula | Order number | RT1 | RT2 | Similarity (%) | Presence | Treatments |
|------------------------------------|-----------------------------------|--------------|--------|------|----------------|----------|--------------------|
| 3,7-dimethyl-2,6-octadien-1-ol | C ₁₀ H ₁₈ O | 11 | 19.147 | 1.32 | 81 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 2-methyl-benzaldehyde | C ₈ H ₈ O | 12 | 19.460 | 2.10 | 88 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | - | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 4-methyl-phenol | C ₇ H ₈ O | 13 | 19.856 | 1.83 | 90 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 4-methyl-benzaldehyde | C ₈ H ₈ O | 14 | 19.861 | 2.13 | 96 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| Cyclohexanol | C ₆ H ₁₂ O | 15 | 20.144 | 1.08 | 82 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 4,5-dimethyl-1-hexene | C ₈ H ₁₆ | 16 | 20.246 | 1.23 | 82 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 1-methyl-4-(1-methylethyl)-benzene | C ₁₀ H ₁₄ | 17 | 20.446 | 1.26 | 81 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| Nonanal | C ₉ H ₁₈ O | 18 | 20.845 | 1.17 | 95 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 1,2,3,4-tetramethyl-benzene | C ₁₀ H ₁₄ | 19 | 21.647 | 1.32 | 92 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | - | P-CeO ₂ |
| 1-methyl-2-phenylcyclopropane | C ₁₀ H ₁₂ | 20 | 22.151 | 1.53 | 80 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | - | P-CeO ₂ |
| 1-ethyl-2,3-dimethyl-benzene | C ₁₀ H ₁₄ | 21 | 22.649 | 1.41 | 89 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | - | P-CeO ₂ |

| Compounds | Formula | Order number | RT1 | RT2 | Similarity (%) | Presence | Treatments |
|--|--|--------------|--------|------|----------------|----------|--------------------|
| Octanoic acid | C ₈ H ₁₆ O ₂ | 22 | 22.945 | 1.20 | 89 | + | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| Naphthalene | C ₁₀ H ₈ | 23 | 23.460 | 2.10 | 94 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| Decanal | C ₁₀ H ₂₀ O | 24 | 23.945 | 1.17 | 94 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 1,2,3,4,5-pentamethylbenzene | C ₁₁ H ₁₆ | 25 | 24.047 | 1.32 | 83 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | - | P-CeO ₂ |
| 2,4-dimethylbenzaldehyde | C ₉ H ₁₀ O | 26 | 24.160 | 2.13 | 96 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| Benzothiazole | C ₇ H ₅ NS | 27 | 24.374 | 2.88 | 87 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 2,6,6-trimethyl-1-cyclohexene-1-carboxaldehyde | C ₁₀ H ₁₆ O | 28 | 24.453 | 1.65 | 87 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | - | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| <i>(E)</i> -2-decenal | C ₁₀ H ₁₈ O | 29 | 25.547 | 1.32 | 90 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| Nonanoic acid | C ₉ H ₁₈ O ₂ | 30 | 25.746 | 1.23 | 85 | + | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 2-hydroxy-iso-butyrophenone | C ₁₀ H ₁₂ O ₂ | 31 | 26.061 | 2.13 | 92 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| Methyl-1,2-benzenecarboxylate | C ₉ H ₇ O ₄ | 32 | 26.380 | 3.30 | 93 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |

| Compounds | Formula | Order number | RT1 | RT2 | Similarity (%) | Presence | Treatments |
|---|--|--------------|--------|------|----------------|----------|--------------------|
| 3-(1,1-dimethylethyl)-phenol | C ₁₀ H ₁₆ O | 33 | 26.455 | 1.80 | 88 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 1-methyl-naphthalene | C ₁₁ H ₁₀ | 34 | 26.759 | 2.04 | 88 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| Undecanal | C ₁₁ H ₂₂ O | 35 | 26.945 | 1.20 | 93 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| <i>(E,E)</i> -2,4-decadienal | C ₁₀ H ₁₆ O | 36 | 27.051 | 1.53 | 89 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 1,2,3-propanetriol triacetate | C ₉ H ₁₄ O ₆ | 37 | 27.459 | 1.98 | 94 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 2-dodecenal | C ₁₂ H ₂₂ O | 38 | 28.448 | 1.35 | 89 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 1,2,3,4-tetrahydro-1,1,6-trimethyl-naphthalene | C ₁₃ H ₁₈ | 39 | 28.551 | 1.56 | 92 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 3-hydroxy-2,4,4-trimethylpentyl-2-methyl-, propanoate | C ₁₂ H ₂₄ O ₃ | 40 | 28.848 | 1.38 | 91 | + | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 2-ethenyl-naphthalene | C ₁₂ H ₁₀ | 41 | 28.962 | 2.19 | 89 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| Dodecanal | C ₁₂ H ₂₄ O | 42 | 29.646 | 1.23 | 97 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 1,6-dimethyl-naphthalene | C ₁₂ H ₁₂ | 43 | 29.759 | 1.98 | 92 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |

| Compounds | Formula | Order number | RT1 | RT2 | Similarity (%) | Presence | Treatments |
|---|--|--------------|--------|------|----------------|----------|--------------------|
| 1,8-dimethylnaphthalene | C ₁₂ H ₁₂ | 44 | 30.160 | 2.07 | 81 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| (1 <i>R</i> ,2 <i>S</i> ,7 <i>S</i> ,9 <i>S</i>)-3,3,7-trimethyl-8-methylidenetricyclo[5.4.0.0 ^{2,9}]undecan | C ₁₅ H ₂₄ | 45 | 30.347 | 1.26 | 91 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | - | P-CeO ₂ |
| 6,10-dimethyl-5,9-undecadien-2-one | C ₁₃ H ₂₂ O | 46 | 30.749 | 1.41 | 87 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 2,6-di-butyl-2,5-cyclohexadiene-1,4-dione | C ₁₄ H ₂₀ O ₂ | 47 | 31.250 | 1.44 | 82 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-3-buten-2-one | C ₁₃ H ₂₀ O | 48 | 31.753 | 1.62 | 91 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| Tridecanal | C ₁₃ H ₂₆ O | 49 | 32.246 | 1.23 | 91 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 2,4-bis(1,1-dimethylethyl)phenol | C ₁₆ H ₂₆ O | 50 | 32.251 | 1.53 | 91 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| <i>o</i> -hydroxybiphenyl | C ₁₂ H ₁₀ O | 51 | 32.269 | 2.58 | 95 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| cis-hexahydro-8a-methyl-, 1,8(2 <i>H</i> ,5 <i>H</i>)-naphthalenedione | C ₁₁ H ₁₆ O ₂ | 52 | 32.359 | 1.98 | 81 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| (R)-5,6,7,7A-tetrahydro-4,4,7A-trimethyl-2(4 <i>H</i>)-benzofuranone | C ₁₁ H ₁₆ O ₂ | 53 | 32.471 | 2.70 | 89 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 3,7,11-trimethyl-2,6,10-dodecatrien-1-ol | C ₁₅ H ₂₆ O | 54 | 32.650 | 1.44 | 84 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |

| Compounds | Formula | Order number | RT1 | RT2 | Similarity (%) | Presence | Treatments |
|--|--|--------------|--------|------|----------------|----------|--------------------|
| 2-methyl-1-pentadecene | C ₁₆ H ₃₂ | 55 | 33.044 | 1.11 | 81 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | - | P-CeO ₂ |
| Diethyl-1,2-benzenedicarboxylate | C ₁₂ H ₁₄ O ₄ | 56 | 33.767 | 2.46 | 89 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| Isobutyl-2,2,4-trimethyl-3-carboxyisopropyl-pentanoate | C ₁₆ H ₃₀ O ₄ | 57 | 34.447 | 1.26 | 90 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| Tetradecanal | C ₁₄ H ₂₈ O | 58 | 34.647 | 1.26 | 93 | - | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| Isopropyl dodecanoate | C ₁₅ H ₃₀ O ₂ | 59 | 35.045 | 1.14 | 88 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | - | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| Methyl-(3-oxo-2-pentyl-, cyclopentyl)acetate | C ₁₃ H ₂₂ O ₃ | 60 | 35.357 | 1.89 | 89 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| n-hexyl salicylate | C ₁₃ H ₁₈ O ₃ | 61 | 36.154 | 1.71 | 84 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | - | P-CeO ₂ |
| 1-tetradecanol | C ₁₄ H ₃₀ O | 62 | 36.447 | 1.26 | 88 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 13-tetradecenal | C ₁₄ H ₂₆ O | 63 | 36.549 | 1.38 | 88 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| Pentadecanal | C ₁₅ H ₃₀ O | 64 | 36.947 | 1.29 | 93 | + | Control |
| | | | | | | + | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| Triethyl- <i>O</i> -acetyl citrate | C ₁₄ H ₂₂ O ₈ | 65 | 37.259 | 2.04 | 87 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | - | P-CeO ₂ |

| Compounds | Formula | Order number | RT1 | RT2 | Similarity (%) | Presence | Treatments |
|---|--|--------------|--------|------|----------------|----------|--------------------|
| (6 <i>S</i> -cis)-5,6,7,7 <i>A</i> -tetrahydro-6-hydroxy-4,4,7 <i>A</i> -trimethyl-, 2(4 <i>H</i>)-benzofuranone | C ₁₁ H ₁₆ O ₃ | 66 | 37.486 | 3.63 | 85 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| Docosanoic acid | C ₂₂ H ₄₄ O ₂ | 67 | 37.849 | 1.35 | 82 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | - | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 2-methyl-2-phenyl-tridecane | C ₂₀ H ₃₄ | 68 | 38.661 | 2.10 | 80 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 6,10,14-trimethyl-2-pentadecanone | C ₁₈ H ₃₆ O | 69 | 38.748 | 1.32 | 84 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | - | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| Hexadecanal | C ₁₆ H ₃₂ O | 70 | 39.048 | 1.32 | 90 | + | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | - | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| <i>N,N</i> -diethyl-1-dodecaneamine | C ₁₄ H ₃₁ N | 71 | 39.450 | 1.44 | 89 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| bis(2-methylpropyl)-1,2-benzenedicarboxylate | C ₁₆ H ₂₂ O ₄ | 72 | 39.762 | 2.16 | 94 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| Heptyl benzoate | C ₁₄ H ₂₀ O ₂ | 73 | 39.955 | 1.77 | 82 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| 3,7,11,15-tetramethyl-1-hexadecen-3-ol | C ₂₀ H ₄₀ O | 74 | 41.846 | 1.2 | 90 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | - | G-CeO ₂ |
| | | | | | | - | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| <i>n</i> -hexadecanoic acid | C ₁₆ H ₃₂ O ₂ | 75 | 41.849 | 1.41 | 92 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | - | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |
| <i>Z,E</i> -3,13-octadecadien-1-ol | C ₁₈ H ₃₄ O | 76 | 42.452 | 1.56 | 84 | - | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | - | G-CeO ₂ |
| | | | | | | - | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |

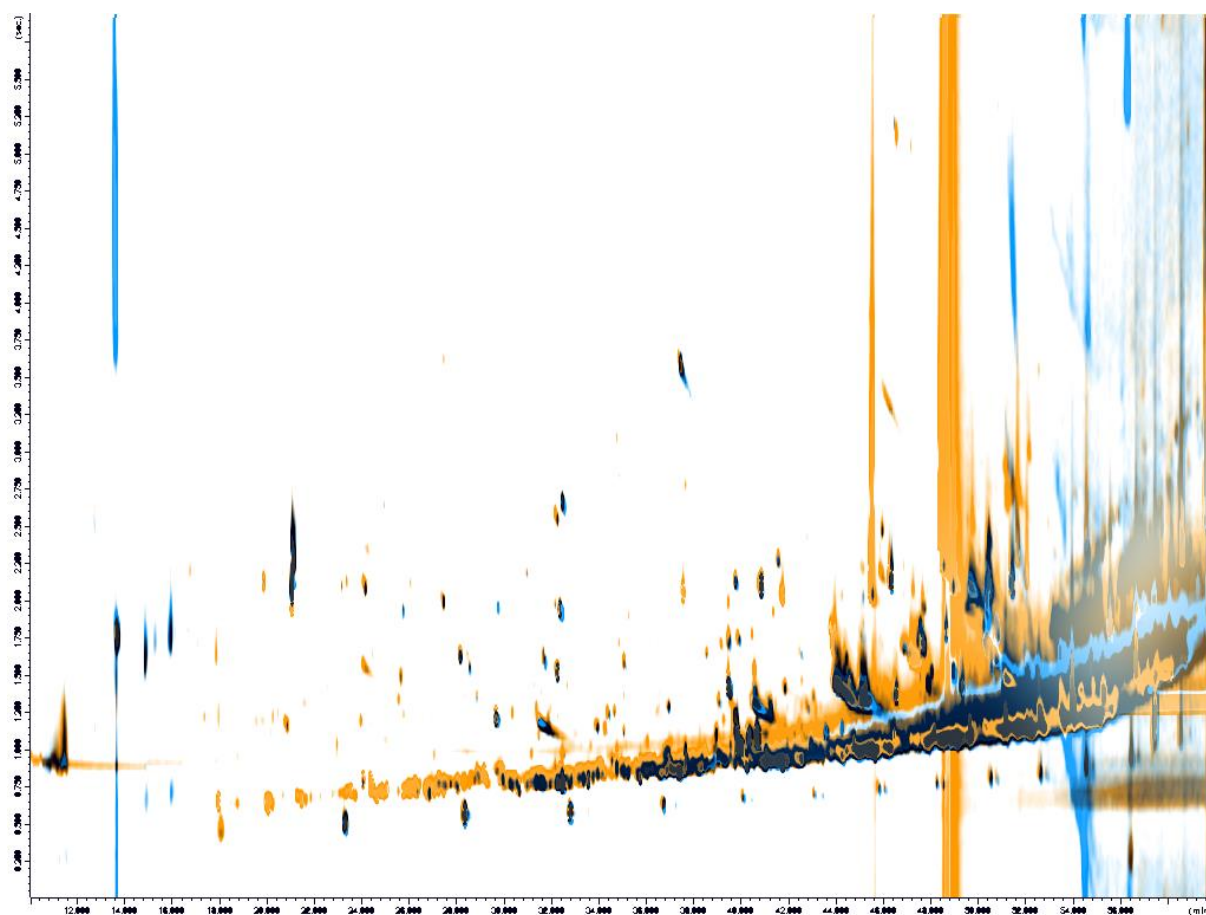
| Compounds | Formula | Order number | RT1 | RT2 | Similarity (%) | Presence | Treatments |
|--------------|-----------------------------------|--------------|--------|------|----------------|----------|--------------------|
| Heptadecanal | C ₁₇ H ₃₄ O | 77 | 43.049 | 1.38 | 93 | + | Control |
| | | | | | | - | nCeO ₂ |
| | | | | | | + | G-CeO ₂ |
| | | | | | | + | L-CeO ₂ |
| | | | | | | + | P-CeO ₂ |

Supplementary Table S3. Nonlinear principal component analysis; Component Loadings for wheat and pea samples

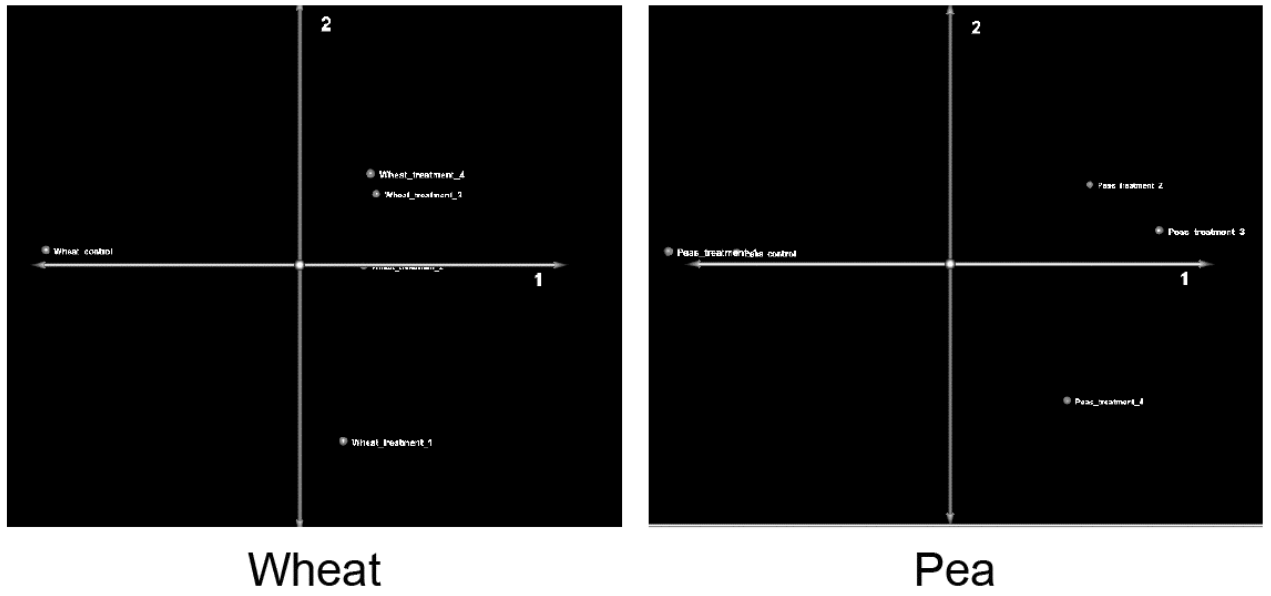
| Wheat | | | Pea | | |
|-------|-----------|--------|-----|-----------|--------|
| | Dimension | | | Dimension | |
| | 1 | 2 | | 1 | 2 |
| V2 | 0.956 | -0.245 | V3 | 0.401 | 0.812 |
| V11 | 0.956 | -0.245 | V74 | 0.401 | 0.812 |
| V14 | 0.956 | -0.245 | V76 | 0.401 | 0.812 |
| V15 | 0.956 | -0.245 | V1 | 0.719 | 0.588 |
| V16 | 0.956 | -0.245 | V5 | 0.719 | 0.588 |
| V27 | 0.956 | -0.245 | V8 | 0.719 | 0.588 |
| V39 | 0.956 | -0.245 | V10 | 0.719 | 0.588 |
| V40 | 0.956 | -0.245 | V12 | 0.719 | 0.588 |
| V42 | 0.956 | -0.245 | V28 | 0.719 | 0.588 |
| V58 | 0.956 | -0.245 | V59 | 0.719 | 0.588 |
| V59 | 0.956 | -0.245 | V67 | 0.719 | 0.588 |
| V61 | 0.956 | -0.245 | V69 | 0.719 | 0.588 |
| V62 | 0.956 | -0.245 | V75 | 0.719 | 0.588 |
| V72 | 0.956 | -0.245 | V19 | 0.668 | -0.696 |
| V73 | 0.956 | -0.245 | V20 | 0.668 | -0.696 |
| V95 | 0.956 | -0.245 | V21 | 0.668 | -0.696 |
| V3 | 0.811 | 0.409 | V25 | 0.668 | -0.696 |
| V10 | 0.811 | 0.409 | V45 | 0.668 | -0.696 |
| V12 | 0.811 | 0.409 | V55 | 0.668 | -0.696 |
| V17 | 0.811 | 0.409 | V61 | 0.668 | -0.696 |
| V18 | 0.811 | 0.409 | V65 | 0.668 | -0.696 |
| V24 | 0.811 | 0.409 | V22 | 0.626 | 0.021 |
| V33 | 0.811 | 0.409 | V30 | 0.626 | 0.021 |
| V35 | 0.811 | 0.409 | V77 | 0.626 | 0.021 |
| V105 | 0.811 | 0.409 | V4 | 0.996 | -0.033 |
| V8 | 0.198 | -0.958 | V6 | 0.996 | -0.033 |
| V29 | 0.198 | -0.958 | V7 | 0.996 | -0.033 |
| V36 | 0.198 | -0.958 | V9 | 0.996 | -0.033 |
| V21 | 0.540 | -0.052 | V11 | 0.996 | -0.033 |
| V23 | 0.540 | -0.052 | V13 | 0.996 | -0.033 |
| V67 | 0.540 | -0.052 | V14 | 0.996 | -0.033 |

| | | |
|------|--------|--------|
| V32 | 0.510 | -0.662 |
| V47 | 0.510 | -0.662 |
| V30 | 0.583 | 0.757 |
| V37 | 0.583 | 0.757 |
| V38 | 0.583 | 0.757 |
| V43 | 0.583 | 0.757 |
| V45 | 0.583 | 0.757 |
| V108 | 0.583 | 0.757 |
| V41 | -0.331 | -0.565 |
| V78 | -0.327 | -0.548 |
| V22 | -0.198 | 0.958 |
| V20 | -0.037 | -0.746 |
| V5 | -0.240 | 0.148 |
| V53 | 0.279 | -0.426 |
| V75 | 0.553 | 0.148 |
| V79 | 0.198 | -0.958 |
| V84 | 0.240 | -0.148 |
| V87 | -0.944 | 0.273 |
| V88 | -0.956 | 0.245 |

| | | |
|-----|-------|--------|
| V15 | 0.996 | -0.033 |
| V16 | 0.996 | -0.033 |
| V17 | 0.996 | -0.033 |
| V18 | 0.996 | -0.033 |
| V23 | 0.996 | -0.033 |
| V24 | 0.996 | -0.033 |
| V26 | 0.996 | -0.033 |
| V27 | 0.996 | -0.033 |
| V29 | 0.996 | -0.033 |
| V31 | 0.996 | -0.033 |
| V32 | 0.996 | -0.033 |
| V33 | 0.996 | -0.033 |
| V34 | 0.996 | -0.033 |
| V35 | 0.996 | -0.033 |
| V36 | 0.996 | -0.033 |
| V37 | 0.996 | -0.033 |
| V38 | 0.996 | -0.033 |
| V39 | 0.996 | -0.033 |
| V41 | 0.996 | -0.033 |
| V42 | 0.996 | -0.033 |
| V43 | 0.996 | -0.033 |
| V44 | 0.996 | -0.033 |
| V46 | 0.996 | -0.033 |
| V47 | 0.996 | -0.033 |
| V48 | 0.996 | -0.033 |
| V49 | 0.996 | -0.033 |
| V50 | 0.996 | -0.033 |
| V51 | 0.996 | -0.033 |
| V52 | 0.996 | -0.033 |
| V53 | 0.996 | -0.033 |
| V54 | 0.996 | -0.033 |
| V56 | 0.996 | -0.033 |
| V57 | 0.996 | -0.033 |
| V60 | 0.996 | -0.033 |
| V62 | 0.996 | -0.033 |
| V63 | 0.996 | -0.033 |
| V66 | 0.996 | -0.033 |
| V68 | 0.996 | -0.033 |
| V71 | 0.996 | -0.033 |
| V72 | 0.996 | -0.033 |
| V73 | 0.996 | -0.033 |
| V2 | 0.479 | -0.092 |
| V58 | 0.594 | -0.061 |



Supplementary Figure S1. Pair-wise image warping illustrated for wheat control and $n\text{CeO}_2$ treated sample by using a dual-channel image (one image is false-colored in orange, the second one in blue) (The reader is referred to the Web version of the article for the interpretation of the references to color in this figure legend).



Supplementary Figure S2. Score plot of a linear principal component model for wheat, *i.e.* pea samples (treatment 1: CeO₂, treatment 2: G-CeO₂, treatment 3: L-CeO₂, and treatment 4: P-CeO₂).