TABLE 1. Summary of volatile organic compounds with significantly different abundance in Parkinson’s disease and control groups.

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| --- | --- | --- |
| **Volatile organic compound** | **FDR** | **Increased in** |
| **PD vs primary controls** |
| ***1,3-ditert-butylbenzene\**** | **1.80E-24** | **PD** |
| Phenol | 6.46E-09 | Control |
| 5-methylheptan-2-one | 6.73E-06 | Control |
| Acetic acid | 0.001 | Control |
| *Propanoic acid\** | 0.001 | Control |
| *Pentanoic acid\** | 0.001 | Control |
| *Heptan-2-one\** | 0.001 | Control |
| 1H-indole | 0.001 | Control |
| **1-methyl-4-propan-2-ylcyclohexa-1,4-diene (γ-terpinene)** | **0.001** | **PD** |
| *Butanoic acid\** | 0.001 | Control |
| **Butan-2-one** | **0.001** | **PD** |
| ***2,6,6-trimethylbicyclo[3.1.1]hept-2-ene (α-pinene)\**** | **0.002** | **PD** |
| Heptanal | 0.009 | Control |
| **1-methyl-2-(1-methylethyl)-benzene (O-Cymene)** | **0.014** | **PD** |
| 2-phenylacetaldehyde | 0.015 | Control |
| 2-methylbutanoic acid | 0.02 | Control |
| **Cyclohexene, 1-methyl-4-(1-methylethenyl)-, (R)- (D-Limonene)** | **0.02** | **PD** |
| 2-Methylphenol | 0.024 | Control |
| **PD vs secondary controls** |
| ***1,3-ditert-butylbenzene\**** | **7.12E-21** | **PD** |
| **2-methylpropanal** | **2.17E-06** | **PD** |
| **Octane** | 0.001 | Control |
| *Butanoic acid\** | 0.001 | Control |
| *Propanoic acid\** | 0.001 | Control |
| **3-methylsulfanylpropanal** | **0.002** | **PD** |
| **Hexanal** | **0.01** | **PD** |
| ***2,6,6-trimethylbicyclo[3.1.1]hept-2-ene (α-pinene)\**** | **0.017** | **PD** |
| *Pentanoic acid\** | 0.023 | Control |
| **3-methylbutanal** | **0.023** | **PD** |
| *Heptan-2-one\** | 0.026 | Control |
| Nonan-2-one | 0.041 | Control |

\*represents volatile organic compounds common to both comparisons. Compounds increased in PD are in bold. Data shown adjusted for multiple comparisons using false discovery rate (FDR).