**Supplemental Table 2 Volatile Organic Compounds in Acute Kidney Injury**

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| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Signal** | **Volatile Organic Compound** | **CAS-Number** | **Drift-Time [V s cm-2]** | **Retention-Time [s]** | **Peak Area Overlapping** | **Occurrance in n Patients** | **Tending Course during Dialysis** | **VOC Intensity AKI [mV]** | **VOC Intensity Control [mV] §** |
| 1 | Acetone (Monomer) | 67-64-1 | 0.495 | 2.4 | 61% | 19 | constant | 101 (46-165) | 151 (126-221) |
| 2 | Acetone (Dimer) | 67-64-1 | 0.544 | 2.4 | 56% | 20 | constant | 76 (41-205) # | 35 (27-69) |
| 3 | Acetophenone (Monomer) | 98-86-2 | 0.58 | 39.3 | 65% | 19 | decreasing \* | 9 (7-10) # | 5 (4-6) |
| 4 | alpha-Pinene (Dimer) | 80-56-8 | 0.646 | 15.2 | 32% | 15 | constant | 7 (0-15) | 7 (0-11) |
| 5 | Benzaldehyde (Monomer) | 100-52-7 | 0.562 | 20.5 | 59% | 20 | decreasing \* | 12 (9-15) | 14 (11-19) |
| 6 | Butanal (Monomer) | 123-72-8 | 0.579 | 4.5 | 41% | 20 | decreasing \* | 39 (22-72) # | 14 (9-19) |
| 7 | Butanal (Dimer) | 123-72-8 | 0.627 | 4.5 | 41% | 20 | constant | 36 (16-53) # | 9 (7-21) |
| 8 | 2,3-Butandiol (Monomer) | 513-85-9 | 0.571 | 14.7 | 81% | 20 | decreasing \* | 13 (9-18) # | 8 (6-11) |
| 9 | 1-Butanol (Monomer) | 71-36-3 | 0.577 | 4.1 | 43% | 20 | decreasing \* | 39 (27-45) # | 9 (7-14) |
| 10 | 1-Butanol (Dimer) | 71-36-3 | 0.684 | 4.1 | 35% | 17 | decreasing \* | 7 (4-11) # | n.d. |
| 11 | Butanone (Monomer) | 78-93-3 | 0.521 | 4.9 | 64% | 20 | constant | 24 (17-48) # | 11 (8-16) |
| 12 | Butanone (Dimer) | 78-93-3 | 0.608 | 4.9 | 100% | 20 | constant | 21 (13-36) # | 10 (8-13) |
| 13 | (+)Camphene (Monomer) | 79-92-5 | 0.593 | 17.7 | 56% | 19 | decreasing \* | 10 (7-13) | 8 (7-13) |
| 14 | Camphor (Monomer) | 76-22-2 | 0.659 | 66.5 | 30% | 15 | constant | 10 (5-18) | 12 (2-15) |
| 15 | (+)3-Carene (Monomer) | 498-15-7 | 0.594 | 25.0 | 77% | 13 | decreasing \* | 5 (0-8) # | n.d. |
| 16 | Cyclohexanol (Monomer) | 108-93-0 | 0.611 | 10.8 | 100% $ | 20 | decreasing \* | 23 (19-38) # | 12 (10-16) |
| 17 | Cyclohexanone (Monomer) | 108-94-1 | 0.563 | 12.6 | 65% | 20 | constant | 155 (133-201) | 168 (39-128) |
| 18 | Cyclohexanone (Dimer) | 108-94-1 | 0.71 | 12.6 | 44% | 20 | constant | 103 (50-147) # | 53 (25-89) |
| 19 | Dimethyldisulfide (Monomer) | 624-92-0 | 0.493 | 6.6 | 100% | 20 | constant | 251 (186-277) # | 158 (123-230) |
| 20 | 2-Ethyl-1-Hexanol (Monomer) | 104-76-7 | 0.694 | 32.5 | 26% | 20 | constant | 18 (14-24) # | 12 (8-15) |
| 21 | 4-Ethyltoluol | 622-96-8 | 0.596 | 18.9 | 65% | 19 | decreasing \* | 11 (7-16) # | n.d. |
| 22 | Heptanal (Dimer) | 111-71-7 | 0.823 | 12.7 | 29% | 2 | constant | 11 (7-16) # | n.d. |
| 23 | 3-Heptanone (Dimer) | 106-35-4 | 0.775 | 11.9 | 52% | 13 | decreasing \* | 6 (0-8) # | n.d. |
| 24 | 4-Heptanone (Monomer) | 123-19-3 | 0.605 | 11.8 | 28% | 20 | constant | 26 (18-43) # | 19 (10-28) |
| 25 | 1-Hexanol (Monomer) | 111-27-3 | 0.648 | 11.5 | 57% | 20 | decreasing \* | 13 (9-0.20) # | 8 (6-11) |
| 26 | 2-Hexanol | 626-93-7 | 0.63 | 10.8 | 54% | 20 | decreasing \* | 101 (52-172) # | 30 (18-70) |
| 27 | 3-Hydroxy-2-Butanone (Dimer) | 513-86-0 | 0.647 | 6.1 | 100% $ | 20 | decreasing \* | 16 (9-26) # | 8 (7-14) |
| 28 | Isoprene (Monomer) | 78-79-5 | 0.518 | 4.6 | 63% | 20 | constant | 11 (8-14) # | 4 (3-8) |
| 29 | Isoprene (Dimer) | 78-79-5 | 0.595 | 4.6 | 100% $ | 19 | decreasing \* | 26 (18-32) # | 4 (0-6) |
| 30 | Isopropylamine (Monomer) | 75-31-0 | 0.506 | 2.0 | 100% | 17 | constant | 6 (1-8) | 6 (3-12) |
| 31 | S(-)-Limonene (Monomer) | 5989-54-8 | 0.594 | 27.4 | 77% | 15 | decreasing \* | 5 (2-9) # | n.d. |
| 32 | S(-)-Limonene (Dimer) | 5989-54-8 | 0.642 | 27.4 | 32% | 20 | constant | 38 (22-96) # | 35 (27-46) |
| 33 | Methanol | 67-56-1 | 0.478 | 3.5 | 43% | 20 | constant | 94 (88-101) | 104 (96-111) |
| 34 | 3-Methyl-1-Butanol (Dimer) | 123-51-3 | 0.742 | 15.0 | 16% | 19 | decreasing \* | 18 (11-28) # | 7 (3-11) |
| 35 | 3-Methylbutanal | 590-86-3 | 0.593 | 3.6 | 100% $ | 19 | decreasing \* | 20 (14-26) # | n.d. |
| 36 | 2-Methylfuran (Dimer) | 534-22-5 | 0.644 | 4.0 | 46% | 20 | decreasing \* | 25 (19-30) # | 19 (15-23) |
| 37 | 2-Methylpentane | 107-83-5 | 0.511 | 5.9 | 47% | 20 | decreasing \* | 19 (11-31) # | 6 (4-19) |
| 38 | 1-Octanol | 111-87-5 | 0.718 | 48.0 | 18% | 18 | constant | 5 (4-7) # | 4 (2-7) |
| 39 | Pentanal (Dimer) | 110-62-3 | 0.694 | 5.0 | 88% | 15 | decreasing \* | 5 (0-9) # | n.d. |
| 40 | 3-Pentanone (Monomer) | 96-22-0 | 0.546 | 7.4 | 71% | 20 | constant | 384 (181-640) # | 73 (49-163) |
| 41 | 3-Pentanone (Dimer) | 96-22-0 | 0.663 | 7.4 | 64% | 20 | decreasing \* | 21 (12-30) # | 9 (7-12) |
| 42 | 1-Propanol (Dimer) | 71-23-8 | 0.617 | 2.2 | 58% | 20 | decreasing \* | 14 (11-21) # | 8 (7-10) |
| 43 | Propofol | 2078-54-8 | 0.672 | 452.4 | 41% | 19 | constant | 31 (24-54) # | 16 (0-35) |
| 44 | o-Xylol | 95-47-6 | 0.521 | 12.4 | 67% | 19 | decreasing \* | 6 (4-10) # | 5 (2-9) |
| 45 | unknown 1 | - | 0.533 | 7.5 | - | 20 | decreasing \* | 41 (29-53) # | 19 (14-59) |
| 46 | unknown 2 | - | 0.547 | 48.4 | - | 19 | decreasing \* | 7 (5-11) # | 0 (0-8) |
| 47 | unknown 3 | - | 0.516 | 22.5 | - | 17 | decreasing \* | 6 (4-8) # | 5 (3-7) |
| 48 | unknown 4 | - | 0.577 | 23.5 | - | 19 | decreasing \* | 7 (6-11) # | 4 (0-7) |
| 49 | unknown 5 | - | 0.529 | 2.6 | - | 20 | decreasing \* | 22 (14-35) # | 19 (8-32) |
| 50 | unknown 6 | - | 0.669 | 23.8 | - | 10 | constant | 0 (0-8) | 5 (0-9) |
| 51 | unknown 7 | - | 0.605 | 6.7 | - | 20 | constant | 20 (14-33) # | 12 (8-14) |
| 52 | unknown 8 | - | 0.447 | 5.5 | - | 20 | constant | 26 (23-31) | 30 (25-34) |
| 53 | unknown 9 | - | 0.492 | 15.1 | - | 20 | constant | 51 (27-94) | 37 (16-130) |
| 54 | unknown 10 | - | 0.444 | 2.0 | - | 20 | constant | 29 (27-35) | 34 (13-39) |
| 55 | unknown 11 | - | 0.638 | 6.2 | - | 20 | decreasing \* | 19 (9-30) # | 8 (7-10) |
| 56 | unknown 12 | - | 0.482 | 30.0 | - | 15 | constant | 6 (0-13) | 7 (0-29) |
| 57 | unknown 13 | - | 0.680 | 6.9 | - | 20 | decreasing \* | 9 (6-15) | 14 (12-17) |
| 58 | unknown 14 | - | 0.697 | 10.8 | - | 19 | decreasing \* | 8 (6-13) # | 5 (4-9) |
| 59 | unknown 15 | - | 0.712 | 7.4 | - | 17 | decreasing \* | 10 (5-15) # | 0 (0-6) |
| 60 | unknown 16 | - | 0.511 | 15.4 | - | 13 | decreasing \* | 5 (0-11) | 4 (0-12) |

Volatile organic compounds in expired air of ventilated patients with acute kidney injury before initiation of hemodialysis. Retention and drift times are given for the IMS chromatogram. Peak area overlapping describes the relative agreement of the chromatogram with the reference chromatogram of the database. Unknown volatiles were designated only by unique peak numbers.\* p<0.05, significant decreasing intensities during hemodialysis treatment compared to baseline values (ANOVA); # p<0.05, significant higher intensities in expired air of patients with acute renal failure compared to control group with normal renal function (Mann-Whitney Rank Sum Test), all data shown as median (25%-75% percentiles); § data obtained from (14). $ Volatile compound was verified by pure substance measurement. CAS-Number = Chemical Abstracts Service Number; VOC = Volatile Organic Compound; n.d. = not detectable.