Supplement of Atmos. Chem. Phys., 20, 9783–9803, 2020
https://doi.org/10.5194/acp-20-9783-2020-supplement
© Author(s) 2020. This work is distributed under
the Creative Commons Attribution 4.0 License.

Atmospheric Chemistry and Physics
Open Access
EGU

*Supplement of*

# Evaluation of the chemical composition of gas- and particle-phase products of aromatic oxidation

**Archit Mehra et al.**

*Correspondence to:* Hugh Coe (hugh.coe@manchester.ac.uk)

The copyright of individual parts of the supplement might differ from the CC BY 4.0 License.

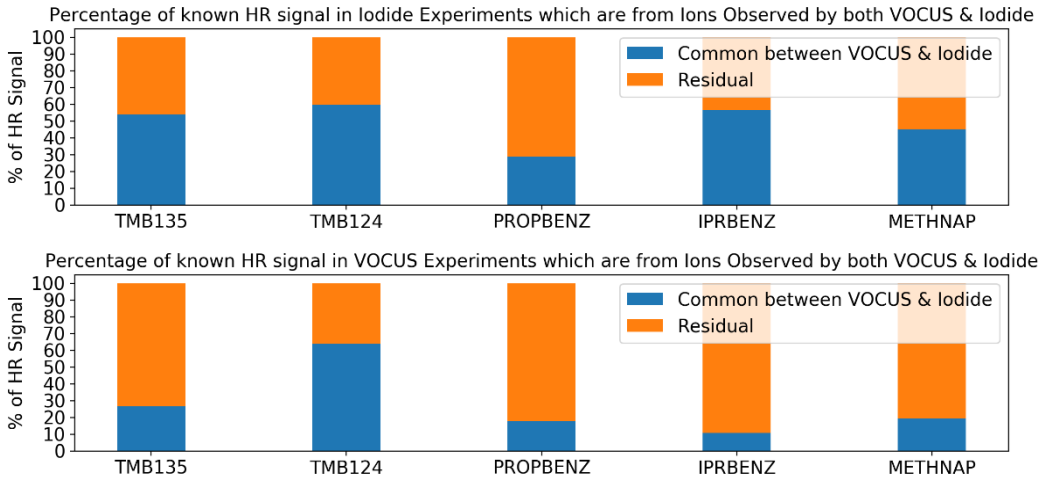


Figure S1 - Signal Contribution of Ions observed by both Vocus & I-CIMS during OH experiments (I-CIMS particle phase) and Vocus (gas phase)

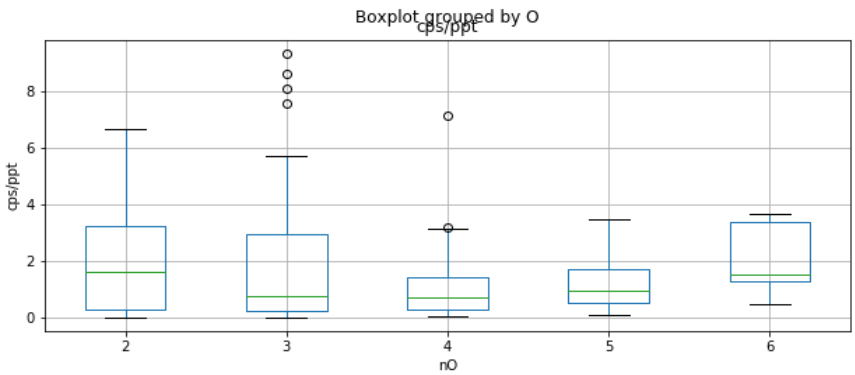


Figure S2 – Derivation of relative sensitivities from measured ion signals common between both iodide and Vocus in the gas phase under low-NOx conditions.

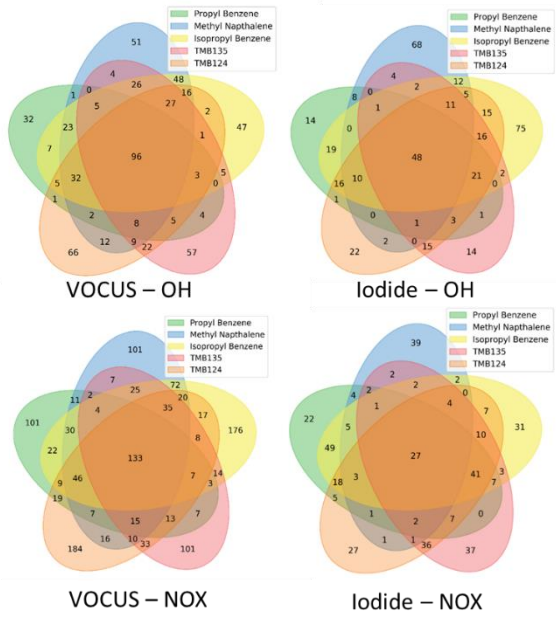


Figure S3- Venn Diagrams showing number of ions overlap in ions observed from all precursors under different conditions

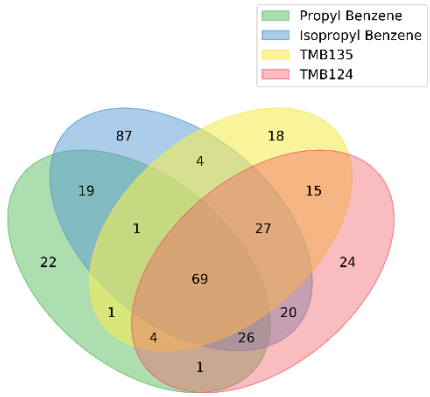


Figure S4- Venn showing overlap in number of ion formulas for $C_9$ –aromatics

Table S1. Comparison with Ions observed from LC-MS by (Sato et al., 2012)

| Ion | I-CIMS | VOCUS |
|---|---|---|
| C3H4O3 | ✓ | ✓ |
| C6H8O3 | ✓ | × |
| C6H10O5 | ✓ | × |
| C8H10O4 | ✓ | × |
| C7H10O5 | ✓ | × |
| C9H12O4 | ✓ | × |
| C8H10O5 | ✓ | × |
| C7H10O7 | ✓ | × |
| C7H12O6 | ✓ | × |
| C9H12O5 | ✓ | × |
| C9H14O5 | ✓ | × |
| C8H12O6 | ✓ | × |
| C9H12O6 | ✓ | × |
| C9H14O6 | ✓ | × |
| C9H12O7 | ✓ | × |
| C9H14O7 | ✓ | × |

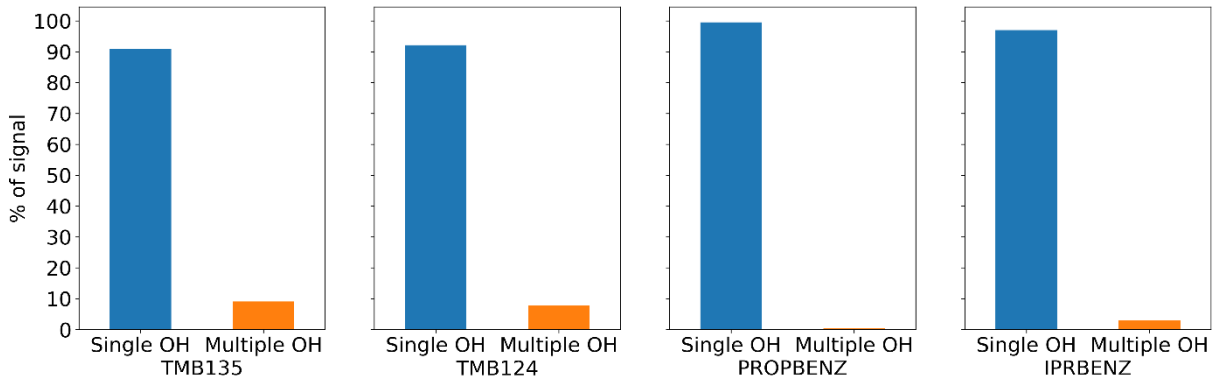


Figure S5– Signal contribution from ions associated with multiple generations of reaction with OH under low-NOx conditions, defined as ions which contain > 4 hydrogen atoms more than the VOC precursor species (14 in all cases)

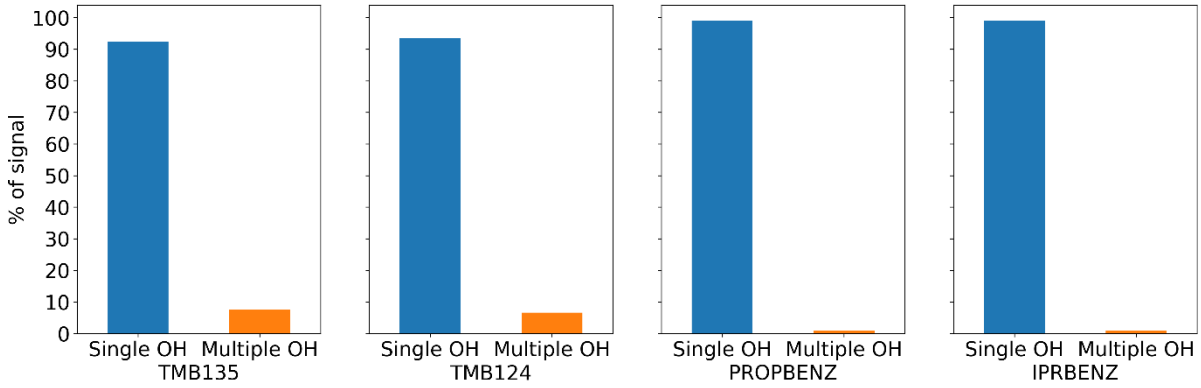


Figure S5 – Signal contribution from ions associated with multiple generations of reaction with OH under med-NOx conditions, defined as ions which contain > 4 hydrogen atoms more than the VOC precursor species (14 in all cases)

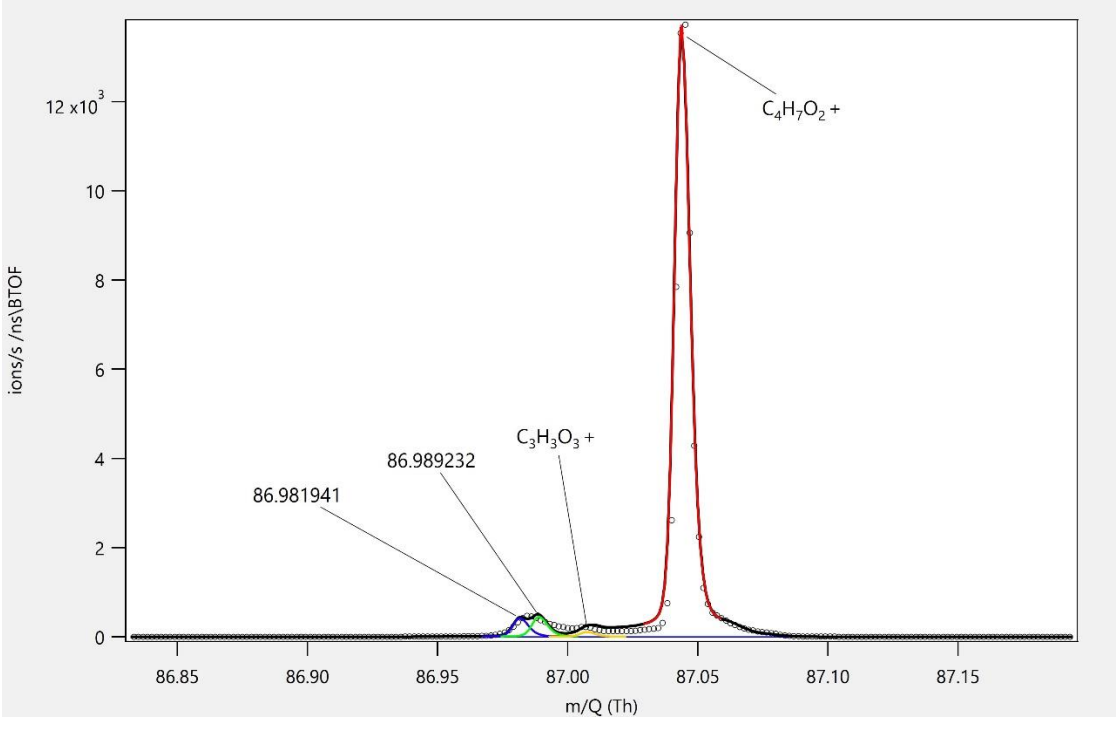


Figure S6 – High resolution peak fit of the ion C4H7O3+ corresponding to C4H6O3 detected by Vocus

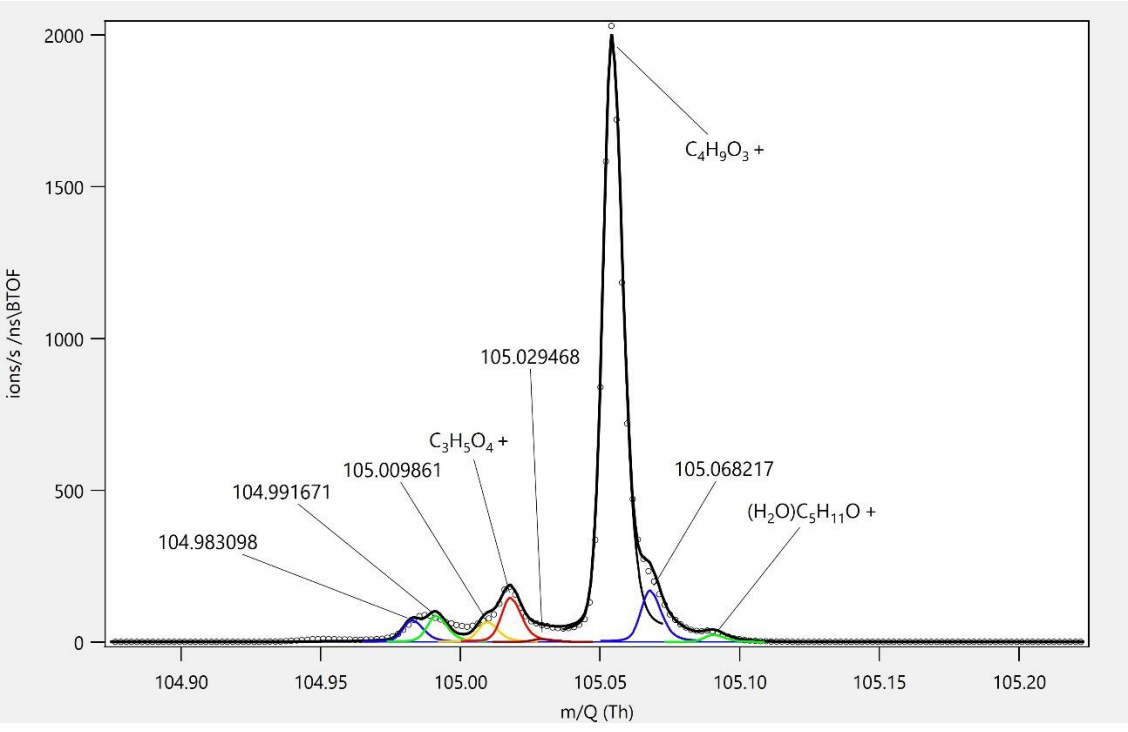


Figure S7– High resolution peak fit of the ion C4H9O3+ corresponding to C4H8O3 detected by Vocus

The structures of the MCM ions described in the tables below can be seen by entering the codes in the tables in the search panel of mcm.york.ac.uk

| 1,2,4-trimethyl benzene: Top 20 ions detected by I-CIMS under low-$NO_x$ conditions | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| **Ion Formula** | **Exact Mass (with adduct)** | **Common to All VOCs** | **Unique to this VOC** | **HOM** | **DBE** | **Classified as Ring Scission** | **Classified as Ring Retaining** | **Signal Contribution (%)** | **Corresponding MCM Ion(s)** |
| C4H4O6 | 274.9058 | TRUE | FALSE | TRUE | 3 | TRUE | FALSE | 6.012896 | MALANHYOOH |
| C5H6O5 | 272.9265 | TRUE | FALSE | FALSE | 3 | TRUE | FALSE | 4.580014 | MMALNHY2OH, C5CO234OOH, C23O3CCO2H |
| C7H10O6 | 316.9528 | FALSE | FALSE | TRUE | 3 | FALSE | FALSE | 3.140251 | |
| C9H14O6 | 344.9841 | TRUE | FALSE | TRUE | 3 | FALSE | FALSE | 2.92903 | TM124OLOOH, TM124MUOOH |
| C9H12O6 | 342.9684 | TRUE | FALSE | TRUE | 4 | FALSE | TRUE | 2.921696 | C7MOCOCO3H |
| C6H8O5 | 286.9422 | FALSE | FALSE | FALSE | 3 | FALSE | FALSE | 2.649253 | EPXM2DCO3H |
| C7H10O5 | 300.9578 | FALSE | FALSE | FALSE | 3 | FALSE | FALSE | 2.5002 | |
| C7H8O6 | 314.9371 | TRUE | FALSE | TRUE | 4 | FALSE | TRUE | 2.398255 | |
| C9H12O7 | 358.9633 | TRUE | FALSE | TRUE | 4 | FALSE | TRUE | 2.333237 | |
| C8H10O6 | 328.9528 | TRUE | FALSE | TRUE | 4 | FALSE | TRUE | 2.324428 | |
| C3H4O5 | 246.9109 | TRUE | FALSE | FALSE | 2 | TRUE | FALSE | 2.269543 | PPACLOOA, HCOCOHCO3H |
| C6H8O6 | 302.9371 | FALSE | FALSE | TRUE | 3 | FALSE | FALSE | 2.13735 | |
| C4H4O4 | 242.916 | TRUE | FALSE | FALSE | 3 | TRUE | FALSE | 2.10775 | C23O3CHO |
| C5H8O5 | 274.9422 | FALSE | FALSE | FALSE | 2 | TRUE | FALSE | 2.092267 | PXYFUOOH, C4MALOHOOH |
| C4H2O4 | 240.9003 | TRUE | FALSE | FALSE | 4 | TRUE | FALSE | 2.04383 | |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| C5H6O6 | 288.9215 | TRUE | FALSE | TRUE | 3 | TRUE | FALSE | 1.988325 | MMALNHYOOH, C23O3CCO3H |
| C3H4O4 | 230.916 | TRUE | FALSE | FALSE | 2 | TRUE | FALSE | 1.956021 | CH3COCO3H |
| C2H2O3 | 200.9054 | FALSE | FALSE | FALSE | 2 | TRUE | FALSE | 1.94557 | GLYOO, GLYOOC, HCOCO2H |
| C8H12O6 | 330.9684 | TRUE | FALSE | TRUE | 3 | FALSE | FALSE | 1.93045 | |
| C4H4O5 | 258.9109 | TRUE | FALSE | FALSE | 3 | TRUE | FALSE | 1.916885 | MALANHY2OH |

Table S2. 1,2,4-trimethyl benzene: Top 20 ions detected by I-CIMS under low-NOx conditions

| **1,3,5- trimethyl benzene: Top 20 Ions detected by I-CIMS under low-$NO_x$ Conditions** | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| **Ion Formula** | **Exact Mass (with adduct)** | **Common to All VOCs** | **Unique to this VOC** | **HOM** | **DBE** | **Classified as Ring Scission** | **Classified as Ring Retaining** | **Signal Contribution (%)** | **Corresponding MCM Ion(s)** |
| C2H2O4 | 216.9003 | FALSE | FALSE | FALSE | 2 | TRUE | FALSE | 7.352414 | HCOCO3H |
| C7H10O6 | 316.9528 | FALSE | FALSE | TRUE | 3 | FALSE | FALSE | 5.501754 | |
| C5H6O5 | 272.9265 | TRUE | FALSE | FALSE | 3 | TRUE | FALSE | 4.345837 | C5CO234OOH, MMALNHY2OH |
| C9H12O6 | 342.9684 | TRUE | FALSE | TRUE | 4 | FALSE | TRUE | 4.203891 | |
| C9H14O6 | 344.9841 | TRUE | FALSE | TRUE | 3 | FALSE | FALSE | 4.00152 | TM135MUOOH, TM135OLOOH |
| C8H10O6 | 328.9528 | TRUE | FALSE | TRUE | 4 | FALSE | TRUE | 3.711394 | |
| C7H10O5 | 300.9578 | FALSE | FALSE | FALSE | 3 | FALSE | FALSE | 3.594323 | |
| C8H10O7 | 344.9477 | TRUE | FALSE | TRUE | 4 | FALSE | TRUE | 3.383244 | |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| C7H8O6 | 314.9371 | TRUE | FALSE | TRUE | 4 | FALSE | TRUE | 2.81836 | |
| C9H12O7 | 358.9633 | TRUE | FALSE | TRUE | 4 | FALSE | TRUE | 2.764992 | |
| C4H4O6 | 274.9058 | TRUE | FALSE | TRUE | 3 | TRUE | FALSE | 2.510926 | |
| C6H8O6 | 302.9371 | FALSE | FALSE | TRUE | 3 | FALSE | FALSE | 2.34924 | C5COHOCO3H, C23O3MCO3H |
| C9H14O5 | 328.9891 | TRUE | FALSE | FALSE | 3 | FALSE | FALSE | 2.243439 | TM135MUOH, TM135OLOH, TM135BPOOH |
| C8H12O6 | 330.9684 | TRUE | FALSE | TRUE | 3 | FALSE | FALSE | 2.034618 | |
| C3H4O4 | 230.916 | TRUE | FALSE | FALSE | 2 | TRUE | FALSE | 1.73814 | |
| C6H8O5 | 286.9422 | FALSE | FALSE | FALSE | 3 | FALSE | FALSE | 1.692857 | C23O3MCO2H, EPXMKTCO3H |
| C5H6O6 | 288.9215 | TRUE | FALSE | TRUE | 3 | TRUE | FALSE | 1.666914 | MMALNHYOOH, ACCOCOMOOH |
| C5H8O5 | 274.9422 | FALSE | FALSE | FALSE | 2 | TRUE | FALSE | 1.6258 | C23O3MCOOH |
| C5H6O4 | 256.9316 | TRUE | FALSE | FALSE | 3 | TRUE | FALSE | 1.58486 | ACECOCOCH3 |
| C6H6O6 | 300.9215 | TRUE | FALSE | TRUE | 4 | FALSE | TRUE | 1.439263 | |

Table S3. 1,3,5- trimethyl benzene: Top 20 Ions detected by I-CIMS under low-NOx Conditions

| **Propyl benzene: Top 20 ions detected by I-CIMS under low-$NO_x$ conditions** | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| **Ion Formula** | **Exact Mass (with adduct)** | **Common to All VOCs** | **Unique to this VOC** | **HOM** | **DBE** | **Classified as Ring Scission** | **Classified as Ring Retaining** | **Signal Contribution (%)** | **Corresponding MCM Ion(s)** |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| C2H2O4 | 216.9003 | FALSE | FALSE | FALSE | 2 | TRUE | FALSE | 21.49648 | HCOCO3H |
| C3H4O5 | 246.9109 | TRUE | FALSE | FALSE | 2 | TRUE | FALSE | 12.95699 | HCOCOHCO3H |
| C4H4O6 | 274.9058 | TRUE | FALSE | TRUE | 3 | TRUE | FALSE | 6.708613 | MALANHYOOH |
| C4H4O5 | 258.9109 | TRUE | FALSE | FALSE | 3 | TRUE | FALSE | 5.027733 | BZFUONOOA, CO14O3CO2H, BZFUONOO, MALANHY2OH, EPXDLCO3H |
| C3H4O4 | 230.916 | TRUE | FALSE | FALSE | 2 | TRUE | FALSE | 4.696877 | C3DIALOOH |
| C4H4O4 | 242.916 | TRUE | FALSE | FALSE | 3 | TRUE | FALSE | 3.923437 | HOCOC4DIAL, MALDALCO3H, EPXDLCO2H, CO14O3CHO, BZFUCO |
| C4H2O4 | 240.9003 | TRUE | FALSE | FALSE | 4 | TRUE | FALSE | 3.528494 | CO2C4DIAL |
| C5H6O6 | 288.9215 | TRUE | FALSE | TRUE | 3 | TRUE | FALSE | 2.633203 | |
| C5H6O5 | 272.9265 | TRUE | FALSE | FALSE | 3 | TRUE | FALSE | 2.310703 | |
| C8H4O3 | 274.9211 | FALSE | TRUE | FALSE | 7 | FALSE | TRUE | 2.220923 | |
| C2H4O3 | 202.9211 | TRUE | FALSE | FALSE | 1 | TRUE | FALSE | 2.139349 | HOCH2CO2H, HCOCH2OOH, CH3CO3H |
| C4H6O5 | 260.9265 | TRUE | FALSE | FALSE | 2 | TRUE | FALSE | 1.655772 | MALDIALOOH, BZFUOOH |
| C2H2O3 | 200.9054 | FALSE | FALSE | FALSE | 2 | TRUE | FALSE | 1.547297 | GLYOO, GLYOOA, HCOCO2H |
| C5H4O5 | 270.9109 | FALSE | FALSE | FALSE | 4 | TRUE | FALSE | 1.516128 | |
| C4H6O6 | 276.9215 | TRUE | FALSE | TRUE | 2 | TRUE | FALSE | 1.447665 | |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| C4H2O5 | 256.8952 | FALSE | FALSE | FALSE | 4 | TRUE | FALSE | 1.360946 | MALNHYOHCO |
| C4H6O4 | 244.9316 | TRUE | FALSE | FALSE | 2 | TRUE | FALSE | 1.303606 | CO2C3CO3H, HOHOC4DIAL, BZFUOH |
| C8H4O2 | 258.9262 | FALSE | TRUE | FALSE | 7 | FALSE | TRUE | 1.283982 | |
| C6H6O6 | 300.9215 | TRUE | FALSE | TRUE | 4 | FALSE | TRUE | 1.165822 | |
| C6H4O6 | 298.9058 | TRUE | FALSE | TRUE | 5 | FALSE | TRUE | 0.872085 | |

Table S3. Propyl benzene: Top 20 ions detected by I-CIMS under low-NOx conditions

| **Isopropyl benzene: Top 20 ions detected by I-CIMS under low-$NO_x$ conditions** | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| **Ion Formula** | **Exact Mass (with adduct)** | **Common to All VOCs** | **Unique to this VOC** | **HOM** | **DBE** | **Classified as Ring Scission** | **Classified as Ring Retaining** | **Signal Contribution (%)** | **Corresponding MCM Ion(s)** |
| C3H4O5 | 246.9109 | TRUE | FALSE | FALSE | 2 | TRUE | FALSE | 12.63549 | HCOCOHCO3H |
| C4H4O6 | 274.9058 | TRUE | FALSE | TRUE | 3 | TRUE | FALSE | 7.757967 | MALANHYOOH |
| C4H6O6 | 276.9215 | TRUE | FALSE | TRUE | 2 | TRUE | FALSE | 5.822939 | |
| C3H4O4 | 230.916 | TRUE | FALSE | FALSE | 2 | TRUE | FALSE | 5.748912 | C3DIALOOH |
| C4H4O5 | 258.9109 | TRUE | FALSE | FALSE | 3 | TRUE | FALSE | 3.894225 | CO14O3CO2H, BZFUONOO, MALANHY2OH, BZFUONOOA, EPXDLCO3H |
| C5H6O6 | 288.9215 | TRUE | FALSE | TRUE | 3 | TRUE | FALSE | 3.820777 | |
| C4H6O5 | 260.9265 | TRUE | FALSE | FALSE | 2 | TRUE | FALSE | 3.28047 | MALDIALOOH, BZFUOOH |
| C5H12O4 | 262.9786 | FALSE | FALSE | FALSE | 0 | TRUE | FALSE | 3.124739 | |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| C5H10O4 | 260.9629 | FALSE | FALSE | FALSE | 1 | TRUE | FALSE | 2.841323 | C3M3OHCO3H |
| C4H4O4 | 242.916 | TRUE | FALSE | FALSE | 3 | TRUE | FALSE | 2.689354 | EPXDLCO2H, HOCOC4DIAL, BZFUCO, CO14O3CHO, MALDALCO3H |
| C6H8O6 | 302.9371 | FALSE | FALSE | TRUE | 3 | FALSE | FALSE | 2.603863 | |
| C5H6O5 | 272.9265 | TRUE | FALSE | FALSE | 3 | TRUE | FALSE | 2.496512 | |
| C2H4O3 | 202.9211 | TRUE | FALSE | FALSE | 1 | TRUE | FALSE | 1.93612 | CH3CO3H, HOCH2CO2H, HCOCH2OOH |
| C6H6O6 | 300.9215 | TRUE | FALSE | TRUE | 4 | FALSE | TRUE | 1.842123 | |
| C8H12O6 | 330.9684 | TRUE | FALSE | TRUE | 3 | FALSE | FALSE | 1.635625 | C7MO3OHOOH |
| C5H8O4 | 258.9473 | FALSE | FALSE | FALSE | 2 | TRUE | FALSE | 1.53248 | |
| C9H12O6 | 342.9684 | TRUE | FALSE | TRUE | 4 | FALSE | TRUE | 1.460753 | C8O2OHCO3H, C8OHO2CO3H |
| C8H10O6 | 328.9528 | TRUE | FALSE | TRUE | 4 | FALSE | TRUE | 1.430135 | |
| C7H10O6 | 316.9528 | FALSE | FALSE | TRUE | 3 | FALSE | FALSE | 1.283872 | C61CO3H, IPMLNHYOOH, C62CO3H |
| C5H8O5 | 274.9422 | FALSE | FALSE | FALSE | 2 | TRUE | FALSE | 1.266971 | |

Table S4. Isopropyl benzene: Top 20 ions detected by I-CIMS under low-NOx conditions

| **1-methyl naphthalene: Top 20 ions detected by I-CIMS under low-$NO_x$ conditions** | | | | | | |
|---|---|---|---|---|---|---|
| **Ion Formula** | **Common to All VOCs** | **Unique to this VOC** | **HOM** | **DBE** | **Signal Contribution (%)** | **Exact Mass (with adduct)** |
| C3H4O5 | TRUE | FALSE | FALSE | 2 | 7.847247 | 246.9109 |

| | | | | | | |
|---|---|---|---|---|---|---|
| C4H4O6 | TRUE | FALSE | TRUE | 3 | 7.631276 | 274.9058 |
| C4H4O5 | TRUE | FALSE | FALSE | 3 | 4.773724 | 258.9109 |
| C2H4O3 | TRUE | FALSE | FALSE | 1 | 4.754491 | 202.9211 |
| C4H4O4 | TRUE | FALSE | FALSE | 3 | 4.369071 | 242.916 |
| C3H4O4 | TRUE | FALSE | FALSE | 2 | 4.245468 | 230.916 |
| C4H2O4 | TRUE | FALSE | FALSE | 4 | 4.199632 | 240.9003 |
| C5H4O5 | FALSE | FALSE | FALSE | 4 | 2.565137 | 270.9109 |
| C4H2O5 | FALSE | FALSE | FALSE | 4 | 2.406614 | 256.8952 |
| C5H6O5 | TRUE | FALSE | FALSE | 3 | 2.398728 | 272.9265 |
| C9H6O4 | FALSE | FALSE | FALSE | 7 | 1.637607 | 304.9316 |
| C6H6O5 | TRUE | FALSE | FALSE | 4 | 1.563208 | 284.9265 |
| C6H4O6 | TRUE | FALSE | TRUE | 5 | 1.491724 | 298.9058 |
| C5H6O6 | TRUE | FALSE | TRUE | 3 | 1.429587 | 288.9215 |
| C5H4O4 | TRUE | FALSE | FALSE | 4 | 1.429004 | 254.916 |
| C6H6O6 | TRUE | FALSE | TRUE | 4 | 1.422434 | 300.9215 |
| C5H6O4 | TRUE | FALSE | FALSE | 3 | 1.397616 | 256.9316 |
| C7H6O5 | TRUE | FALSE | FALSE | 5 | 1.156873 | 296.9265 |
| C10H8O4 | FALSE | FALSE | FALSE | 7 | 1.107862 | 318.9473 |
| C3H2O4 | TRUE | FALSE | FALSE | 3 | 1.041955 | 228.9003 |

Table S5. 1-methyl naphthalene: Top 20 ions detected by I-CIMS under low-NOx conditions

| 1,2,4-trimethyl benzene: Top 20 ions detected by under medium-NOx conditions | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| **Ion Formula** | **Exact Mass (with adduct)** | **Common to All VOCs** | **Unique to this VOC** | **HOM** | **DBE** | **Classified as Ring Scission** | **Classified as Ring Retaining** | **Signal Contribution (%)** | **Corresponding MCM Ion(s)** |
| C2H2O4 | 216.9003 | FALSE | FALSE | FALSE | 2 | TRUE | FALSE | 4.57099 | HCOCO3H |
| C9H12O6 | 342.9684 | FALSE | FALSE | TRUE | 4 | FALSE | TRUE | 4.455449 | C7MOCOCO3H |
| C7H10O6 | 316.9528 | TRUE | FALSE | TRUE | 3 | FALSE | FALSE | 4.434045 | |
| C8H10O6 | 328.9528 | TRUE | FALSE | TRUE | 4 | FALSE | TRUE | 4.298127 | |
| C8H10O7 | 344.9477 | TRUE | FALSE | TRUE | 4 | FALSE | TRUE | 3.859657 | |
| C9H14O6 | 344.9841 | FALSE | FALSE | TRUE | 3 | FALSE | FALSE | 3.224949 | TM124OLOOH, TM124MUOOH |
| C7H8O6 | 314.9371 | FALSE | FALSE | TRUE | 4 | FALSE | TRUE | 3.11834 | |
| C5H6O5 | 272.9265 | TRUE | FALSE | FALSE | 3 | TRUE | FALSE | 2.91674 | MMALNHY2OH, C5CO234OOH, C23O3CCO2H |
| C7H10O5 | 300.9578 | FALSE | FALSE | FALSE | 3 | FALSE | FALSE | 2.878091 | |
| C8H12O6 | 330.9684 | FALSE | FALSE | TRUE | 3 | FALSE | FALSE | 2.464581 | |
| C6H8O6 | 302.9371 | FALSE | FALSE | TRUE | 3 | FALSE | FALSE | 2.419906 | |
| C2H2O3 | 200.9054 | FALSE | FALSE | FALSE | 2 | TRUE | FALSE | 2.085772 | GLYOO, GLYOOC, HCOCO2H |
| C10H6NO4 | 330.9347 | FALSE | FALSE | FALSE | 8 | FALSE | TRUE | 2.002643 | |
| C4H4O6 | 274.9058 | FALSE | FALSE | TRUE | 3 | TRUE | FALSE | 1.96203 | MALANHYOOH |
| C6H8O5 | 286.9422 | TRUE | FALSE | FALSE | 3 | FALSE | FALSE | 1.90656 | EPXM2DCO3H |
| C4H4O4 | 242.916 | TRUE | FALSE | FALSE | 3 | TRUE | FALSE | 1.802118 | C23O3CHO |
| C7H8O5 | 298.9422 | FALSE | FALSE | FALSE | 4 | FALSE | TRUE | 1.779689 | C4DBM2CO3H |
| C3H4O4 | 230.916 | TRUE | FALSE | FALSE | 2 | TRUE | FALSE | 1.618456 | CH3COCO3H |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| C6H6O6 | 300.9215 | FALSE | FALSE | TRUE | 4 | FALSE | TRUE | 1.606628 | |
| C8H10NO7 | 358.9507 | FALSE | FALSE | TRUE | 4 | FALSE | TRUE | 1.559239 | TM124NO2O |

Table S6. 1,2,4-trimethyl benzene: Top 20 ions detected by under medium-NOx conditions

| **1,3,5-trimethyl benzene: Top 20 ions detected by I-CIMS under medium-$NO_x$ conditions** | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| **Ion Formula** | **Exact Mass (with adduct)** | **Common to All VOCs** | **Unique to this VOC** | **HOM** | **DBE** | **Classified as Ring Scission** | **Classified as Ring Retaining** | **Signal Contribution (%)** | **Corresponding MCM Ion(s)** |
| C7H10O6 | 316.9528 | TRUE | FALSE | TRUE | 3 | FALSE | FALSE | 6.747114 | |
| C9H12O6 | 342.9684 | FALSE | FALSE | TRUE | 4 | FALSE | TRUE | 5.299848 | |
| C8H10O7 | 344.9477 | TRUE | FALSE | TRUE | 4 | FALSE | TRUE | 4.306614 | |
| C8H10O6 | 328.9528 | TRUE | FALSE | TRUE | 4 | FALSE | TRUE | 3.982593 | |
| C2H2O4 | 216.9003 | FALSE | FALSE | FALSE | 2 | TRUE | FALSE | 3.706818 | HCOCO3H |
| C7H10O5 | 300.9578 | FALSE | FALSE | FALSE | 3 | FALSE | FALSE | 3.593619 | |
| C9H12O7 | 358.9633 | FALSE | FALSE | TRUE | 4 | FALSE | TRUE | 3.512631 | |
| C5H6O5 | 272.9265 | TRUE | FALSE | FALSE | 3 | TRUE | FALSE | 3.267785 | C5CO234OOH, MMALNHY2OH |
| C9H14O6 | 344.9841 | FALSE | FALSE | TRUE | 3 | FALSE | FALSE | 3.163163 | TM135MUOOH, TM135OLOOH |
| C10H6NO3 | 314.9398 | FALSE | FALSE | FALSE | 8 | FALSE | TRUE | 2.436078 | |
| C6H8O6 | 302.9371 | FALSE | FALSE | TRUE | 3 | FALSE | FALSE | 2.423461 | C5COHOCO3H, C23O3MCO3H |
| C8H12O6 | 330.9684 | FALSE | FALSE | TRUE | 3 | FALSE | FALSE | 2.129311 | |
| C7H8O7 | 330.932 | FALSE | TRUE | TRUE | 4 | FALSE | TRUE | 1.929702 | |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| C9H14O5 | 328.9891 | FALSE | FALSE | FALSE | 3 | FALSE | FALSE | 1.919614 | TM135MUOH, TM135OLOH, TM135BPOOH |
| C6H6O6 | 300.9215 | FALSE | FALSE | TRUE | 4 | FALSE | TRUE | 1.867648 | |
| C4H4O6 | 274.9058 | FALSE | FALSE | TRUE | 3 | TRUE | FALSE | 1.808459 | |
| C5H6O6 | 288.9215 | FALSE | FALSE | TRUE | 3 | TRUE | FALSE | 1.700825 | MMALNHYOOH, ACCOCOMOOH |
| C8H8O7 | 342.932 | TRUE | FALSE | TRUE | 5 | FALSE | TRUE | 1.635219 | |
| C3H4O4 | 230.916 | TRUE | FALSE | FALSE | 2 | TRUE | FALSE | 1.571756 | |
| C8H10O8 | 360.9426 | FALSE | FALSE | TRUE | 4 | FALSE | TRUE | 1.491458 | |

Table S7. 1,3,5-trimethyl benzene: Top 20 ions detected by I-CIMS under medium-NOx conditions

| **Propyl benzene: Top 20 ions detected by I-CIMS under medium-$NO_x$ conditions** | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| **Ion Formula** | **Exact Mass (with adduct)** | **Common to All VOCs** | **Unique to this VOC** | **HOM** | **DBE** | **Classified as Ring Scission** | **Classified as Ring Retaining** | **Signal Contribution (%)** | **Corresponding MCM Ion(s)** |
| C2H2O4 | 216.9003 | FALSE | FALSE | FALSE | 2 | TRUE | FALSE | 19.32162 | HCOCO3H |
| C3H4O5 | 246.9109 | TRUE | FALSE | FALSE | 2 | TRUE | FALSE | 9.252501 | HCOCOHCO3H |
| C4H4O6 | 274.9058 | FALSE | FALSE | TRUE | 3 | TRUE | FALSE | 7.26004 | MALANHYOOH |
| C4H4O5 | 258.9109 | TRUE | FALSE | FALSE | 3 | TRUE | FALSE | 5.580908 | BZFUONOOA, CO14O3CO2H, BZFUONOO, MALANHY2OH, EPXDLCO3H |
| C4H4O4 | 242.916 | TRUE | FALSE | FALSE | 3 | TRUE | FALSE | 4.434534 | HOCOC4DIAL, MALDALCO3H, |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | EPXDLCO2H, CO14O3CHO, BZFUCO |
| C3H4O4 | 230.916 | TRUE | FALSE | FALSE | 2 | TRUE | FALSE | 4.405548 | C3DIALOOH |
| C4H2O4 | 240.9003 | TRUE | FALSE | FALSE | 4 | TRUE | FALSE | 3.178436 | CO2C4DIAL |
| C5H6O6 | 288.9215 | FALSE | FALSE | TRUE | 3 | TRUE | FALSE | 2.967571 | |
| C5H6O5 | 272.9265 | TRUE | FALSE | FALSE | 3 | TRUE | FALSE | 2.769482 | |
| C2H4O3 | 202.9211 | TRUE | FALSE | FALSE | 1 | TRUE | FALSE | 2.695386 | HOCH2CO2H, HCOCH2OOH, CH3CO3H |
| C2H2O3 | 200.9054 | FALSE | FALSE | FALSE | 2 | TRUE | FALSE | 2.408014 | GLYOO, GLYOOA, HCOCO2H |
| C5H4O5 | 270.9109 | FALSE | FALSE | FALSE | 4 | TRUE | FALSE | 2.183965 | |
| C4H6O5 | 260.9265 | TRUE | FALSE | FALSE | 2 | TRUE | FALSE | 1.896644 | MALDIALOOH, BZFUOOH |
| C6H6O6 | 300.9215 | FALSE | FALSE | TRUE | 4 | FALSE | TRUE | 1.758648 | |
| C4H2O5 | 256.8952 | TRUE | FALSE | FALSE | 4 | TRUE | FALSE | 1.477842 | MALNHYOHCO |
| C4H6O6 | 276.9215 | FALSE | FALSE | TRUE | 2 | TRUE | FALSE | 1.453477 | |
| C4H6O4 | 244.9316 | TRUE | FALSE | FALSE | 2 | TRUE | FALSE | 1.218929 | CO2C3CO3H, HOHOC4DIAL, BZFUOH |
| C6H4O6 | 298.9058 | TRUE | FALSE | TRUE | 5 | FALSE | TRUE | 1.189767 | |
| C6H8O6 | 302.9371 | FALSE | FALSE | TRUE | 3 | FALSE | FALSE | 1.131341 | |
| C3H2O4 | 228.9003 | TRUE | FALSE | FALSE | 3 | TRUE | FALSE | 1.001921 | |

Table S8. Propyl benzene: Top 20 ions detected by I-CIMS under medium-NOx conditions

| Isopropyl benzene: Top 20 I-CIMS Ions under Medium-NOx Conditions | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| **Ion Formula** | **Exact Mass (with adduct)** | **Common to All VOCs** | **Unique to this VOC** | **HOM** | **DBE** | **Classified as Ring Scission** | **Classified as Ring Retaining** | **Signal Contribution (%)** | **Corresponding MCM Ion(s)** |
| C3H6O3 | 216.9367 | FALSE | FALSE | FALSE | 1 | TRUE | FALSE | 23.70164 | PROPALOOH, HYPERACET, PERPROACID, HOC2H4CO2H |
| C4H4O4 | 242.916 | TRUE | FALSE | FALSE | 3 | TRUE | FALSE | 5.522321 | EPXDLCO2H, HOCOC4DIAL, BZFUCO, CO14O3CHO, MALDALCO3H |
| C5H6O6 | 288.9215 | FALSE | FALSE | TRUE | 3 | TRUE | FALSE | 5.39958 | |
| C4H4O5 | 258.9109 | TRUE | FALSE | FALSE | 3 | TRUE | FALSE | 4.456028 | CO14O3CO2H, BZFUONOO, MALANHY2OH, BZFUONOOA, EPXDLCO3H |
| C3H4O5 | 246.9109 | TRUE | FALSE | FALSE | 2 | TRUE | FALSE | 3.534205 | HCOCOHCO3H |
| C4H4O6 | 274.9058 | FALSE | FALSE | TRUE | 3 | TRUE | FALSE | 2.994197 | MALANHYOOH |
| C6H6O6 | 300.9215 | FALSE | FALSE | TRUE | 4 | FALSE | TRUE | 2.899814 | |
| C5H6O5 | 272.9265 | TRUE | FALSE | FALSE | 3 | TRUE | FALSE | 2.558614 | |
| C4H6O6 | 276.9215 | FALSE | FALSE | TRUE | 2 | TRUE | FALSE | 2.543821 | |
| C5H4O5 | 270.9109 | FALSE | FALSE | FALSE | 4 | TRUE | FALSE | 2.180888 | |
| C3H4O4 | 230.916 | TRUE | FALSE | FALSE | 2 | TRUE | FALSE | 1.951163 | C3DIALOOH |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| C4H6O5 | 260.9265 | TRUE | FALSE | FALSE | 2 | TRUE | FALSE | 1.934661 | MALDIALOOH, BZFUOOH |
| C6H8O6 | 302.9371 | FALSE | FALSE | TRUE | 3 | FALSE | FALSE | 1.657392 | |
| C4H2O5 | 256.8952 | TRUE | FALSE | FALSE | 4 | TRUE | FALSE | 1.588134 | MALNHYOHCO |
| C6H6O7 | 316.9164 | FALSE | FALSE | TRUE | 4 | FALSE | TRUE | 1.523712 | |
| C8H10O6 | 328.9528 | TRUE | FALSE | TRUE | 4 | FALSE | TRUE | 1.39343 | |
| C5H4O6 | 286.9058 | TRUE | FALSE | TRUE | 4 | TRUE | FALSE | 1.341136 | |
| C6H6O5 | 284.9265 | TRUE | FALSE | FALSE | 4 | FALSE | TRUE | 1.256508 | |
| C8H10O7 | 344.9477 | TRUE | FALSE | TRUE | 4 | FALSE | TRUE | 1.248085 | |
| C9H12O7 | 358.9633 | FALSE | FALSE | TRUE | 4 | FALSE | TRUE | 1.18151 | |

Table S9. Isopropyl benzene: Top 20 I-CIMS Ions under Medium-NOx Conditions

| **1-methyl naphthalene: Top 20 ions detected by I-CIMS under medium-$NO_x$ conditions** | | | | | | |
|---|---|---|---|---|---|---|
| **Ion Formula** | **Common to All VOCs** | **Unique to this VOC** | **HOM** | **DBE** | **Signal Contribution (%)** | **Exact Mass (with adduct)** |
| C4H2O4 | TRUE | FALSE | FALSE | 4 | 6.126329 | 240.9003 |
| C4H4O5 | TRUE | FALSE | FALSE | 3 | 5.949903 | 258.9109 |
| C7H2NO3 | FALSE | TRUE | FALSE | 7 | 5.495028 | 274.9085 |
| C4H4O4 | TRUE | FALSE | FALSE | 3 | 4.963095 | 242.916 |
| C2H4O3 | TRUE | FALSE | FALSE | 1 | 4.409859 | 202.9211 |
| C3H4O4 | TRUE | FALSE | FALSE | 2 | 3.809387 | 230.916 |
| C3H4O5 | TRUE | FALSE | FALSE | 2 | 3.717899 | 246.9109 |
| C8H2NO2 | FALSE | TRUE | FALSE | 8 | 3.510183 | 270.9136 |
| C3H2O5 | FALSE | FALSE | FALSE | 3 | 3.477236 | 244.8952 |
| C3H2O4 | TRUE | FALSE | FALSE | 3 | 2.753131 | 228.9003 |
| C5H6O5 | TRUE | FALSE | FALSE | 3 | 2.392786 | 272.9265 |

| | | | | | | |
|---|---|---|---|---|---|---|
| C9H6O4 | FALSE | TRUE | FALSE | 7 | 2.182095 | 304.9316 |
| C4H2O5 | TRUE | FALSE | FALSE | 4 | 2.10023 | 256.8952 |
| C8H4NO3 | FALSE | TRUE | FALSE | 7 | 1.994792 | 288.9241 |
| C9H4NO3 | FALSE | TRUE | FALSE | 8 | 1.951284 | 300.9241 |
| C6H6O5 | TRUE | FALSE | FALSE | 4 | 1.913073 | 284.9265 |
| C5H4O4 | TRUE | FALSE | FALSE | 4 | 1.708749 | 254.916 |
| C6H4O5 | TRUE | FALSE | FALSE | 5 | 1.559751 | 282.9109 |
| C6H4O6 | TRUE | FALSE | TRUE | 5 | 1.550059 | 298.9058 |
| C5H4O6 | TRUE | FALSE | TRUE | 4 | 1.308137 | 286.9058 |

Table S10. 1-methyl naphthalene: Top 20 ions detected by I-CIMS under medium-NOx conditions

| **1,2,4-trimethyl benzene: Top 20 ions detected by Vocus under low-$NO_x$ conditions** | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| **Ion Formula** | **Exact Mass (with adduct)** | **Common to All VOCs** | **Unique to this VOC** | **HOM** | **DBE** | **Classified as Ring Scission** | **Classified as Ring Retaining** | **Signal Contribution (%)** | **Corresponding MCM Ion(s)** |
| C4H6O2 | 87.04406 | TRUE | FALSE | FALSE | 2 | TRUE | FALSE | 36.86747 | BIACET |
| C4H8O3 | 105.0546 | TRUE | FALSE | FALSE | 1 | TRUE | FALSE | 6.011468 | MEKBOOH |
| C2H8O4 | 97.04953 | TRUE | FALSE | FALSE | -1 | TRUE | FALSE | 4.284034 | |
| C3H6O2 | 75.04406 | TRUE | FALSE | FALSE | 1 | TRUE | FALSE | 3.961608 | ACETOL |
| C3H8O2 | 77.05971 | TRUE | FALSE | FALSE | 0 | TRUE | FALSE | 3.355556 | |
| C2H4O3 | 77.02332 | FALSE | FALSE | FALSE | 1 | TRUE | FALSE | 2.072851 | HOCH2CO2H, HCOCH2OOH, CH3CO3H |
| C5H8O2 | 101.0597 | TRUE | FALSE | FALSE | 2 | TRUE | FALSE | 1.711721 | |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| C4H6O3 | 103.039 | TRUE | FALSE | FALSE | 2 | TRUE | FALSE | 1.608876 | BIACETOH, MEK2OO, CO2H3CHO, MEK2OOC, MEK2OOA, C3MDIALOH |
| C5H6O3 | 115.039 | TRUE | FALSE | FALSE | 3 | TRUE | FALSE | 1.549366 | C5CO234, C5CO14OH, MC3ODBCO2H |
| C6H8O2 | 113.0597 | TRUE | FALSE | FALSE | 3 | FALSE | FALSE | 1.514183 | TMB1FUONE, C4DBDIKET, MC5DICARB |
| C4H4O3 | 101.0233 | TRUE | FALSE | FALSE | 3 | TRUE | FALSE | 1.200937 | CO23C3CHO |
| C6H8O3 | 129.0546 | TRUE | FALSE | FALSE | 3 | FALSE | FALSE | 1.040435 | EPXM2C4DAL, C5DBCOCO2H, C3M2COCO2H, C5CODBCO2H |
| C8H10O3 | 155.0703 | TRUE | FALSE | FALSE | 4 | FALSE | TRUE | 0.996789 | |
| C6H6O3 | 127.039 | TRUE | FALSE | FALSE | 4 | FALSE | TRUE | 0.995358 | |
| C8H6O4 | 167.0339 | TRUE | FALSE | FALSE | 6 | FALSE | TRUE | 0.964009 | |
| C5H6O2 | 99.04406 | TRUE | FALSE | FALSE | 3 | TRUE | FALSE | 0.947526 | C4MDIAL, PXYFUONE |
| C6H8O1 | 97.06479 | FALSE | FALSE | FALSE | 3 | FALSE | FALSE | 0.899348 | |
| C6H8O4 | 145.0495 | TRUE | FALSE | FALSE | 3 | FALSE | FALSE | 0.882797 | C5OCO3M, EPXM2DCO2H, C5DBCOCO3H, DMKCOOH |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| C8H4O3 | 149.0233 | TRUE | FALSE | FALSE | 7 | FALSE | TRUE | 0.859661 | |
| C2H6O4 | 95.03389 | TRUE | FALSE | FALSE | 0 | TRUE | FALSE | 0.831874 | |

Table S11. 1,2,4-trimethyl benzene: Top 20 ions detected by Vocus under low-NOx conditions

| **1,3,5-trimethyl benzene: Top 20 ions detected by Vocus under low-$NO_x$ conditions** | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| **Ion Formula** | **Exact Mass (with adduct)** | **Common to All VOCs** | **Unique to this VOC** | **HOM** | **DBE** | **Classified as Ring Scission** | **Classified as Ring Retaining** | **Signal Contribution (%)** | **Corresponding MCM Ion(s)** |
| C4H6O2 | 87.04406 | TRUE | FALSE | FALSE | 2 | TRUE | FALSE | 20.05423 | |
| C3H6O2 | 75.04406 | TRUE | FALSE | FALSE | 1 | TRUE | FALSE | 10.5303 | |
| C2H8O4 | 97.04953 | TRUE | FALSE | FALSE | -1 | TRUE | FALSE | 6.721699 | |
| C3H8O2 | 77.05971 | TRUE | FALSE | FALSE | 0 | TRUE | FALSE | 5.023779 | |
| C2H4O3 | 77.02332 | FALSE | FALSE | FALSE | 1 | TRUE | FALSE | 3.667135 | HOCH2CO2H, HCOCH2OOH, CH3CO3H |
| C4H8O3 | 105.0546 | TRUE | FALSE | FALSE | 1 | TRUE | FALSE | 3.451569 | |
| C5H6O3 | 115.039 | TRUE | FALSE | FALSE | 3 | TRUE | FALSE | 3.266301 | C5CO234 |
| C4H6O3 | 103.039 | TRUE | FALSE | FALSE | 2 | TRUE | FALSE | 3.206798 | C3MDIALOH |
| C6H8O3 | 129.0546 | TRUE | FALSE | FALSE | 3 | FALSE | FALSE | 2.669817 | EPXMALKT, C5CODBCO2H |
| C6H8O2 | 113.0597 | TRUE | FALSE | FALSE | 3 | FALSE | FALSE | 2.66317 | MXYFUONE, C5MDICARB |
| C5H8O2 | 101.0597 | TRUE | FALSE | FALSE | 2 | TRUE | FALSE | 2.318317 | |
| C6H8O1 | 97.06479 | FALSE | FALSE | FALSE | 3 | FALSE | FALSE | 1.844767 | |
| C2H6O4 | 95.03389 | TRUE | FALSE | FALSE | 0 | TRUE | FALSE | 1.370254 | |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| C6H8O4 | 145.0495 | TRUE | FALSE | FALSE | 3 | FALSE | FALSE | 1.293725 | C5CODBCO3H, C6CO3MOH, C23O3MCHO, EPXMKTCO2H |
| C6H6O1 | 95.04914 | FALSE | FALSE | FALSE | 4 | FALSE | TRUE | 1.178453 | |
| C6H6O3 | 127.039 | TRUE | FALSE | FALSE | 4 | FALSE | TRUE | 1.083227 | |
| C4H4O2 | 85.02841 | TRUE | FALSE | FALSE | 3 | TRUE | FALSE | 1.061629 | |
| C9H10O2 | 151.0754 | FALSE | FALSE | FALSE | 5 | FALSE | TRUE | 1.056132 | TMBCO2H |
| C5H6O4 | 131.0339 | TRUE | FALSE | FALSE | 3 | TRUE | FALSE | 0.931806 | ACECOCOCH3 |
| C8H10O3 | 155.0703 | TRUE | FALSE | FALSE | 4 | FALSE | TRUE | 0.852728 | C7M3CO |

Table S12. 1,3,5-trimethyl benzene: Top 20 ions detected by Vocus under low-NOx conditions

| **Propyl benzene: Top 20 ions detected by Vocus under low-$NO_x$ conditions** | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| **Ion Formula** | **Exact Mass (with adduct)** | **Common to All VOCs** | **Unique to this VOC** | **HOM** | **DBE** | **Classified as Ring Scission** | **Classified as Ring Retaining** | **Signal Contribution (%)** | **Corresponding MCM Ion(s)** |
| C9H10O1 | 135.0804 | FALSE | FALSE | FALSE | 5 | FALSE | TRUE | 17.93436 | |
| C3H8O2 | 77.05971 | TRUE | FALSE | FALSE | 0 | TRUE | FALSE | 9.708987 | NC3H7OOH, HOC3H6OH, PROPGLY, IC3H7OOH |
| C3H6O2 | 75.04406 | TRUE | FALSE | FALSE | 1 | TRUE | FALSE | 8.724536 | PROPACID, ACETOL, CH3CHOHCHO, HOC2H4CHO |
| C7H6O1 | 107.0491 | FALSE | FALSE | FALSE | 5 | FALSE | TRUE | 7.945055 | |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| C4H10O3 | 107.0703 | TRUE | FALSE | FALSE | 0 | TRUE | FALSE | 5.750638 | |
| C3H8O3 | 93.05462 | TRUE | FALSE | FALSE | 0 | TRUE | FALSE | 5.045235 | IPROPOLO2H, HO1C3OOH, HYPROPO2H |
| C7H8O2 | 125.0597 | TRUE | FALSE | FALSE | 4 | FALSE | TRUE | 3.710935 | |
| C6H6O1 | 95.04914 | FALSE | FALSE | FALSE | 4 | FALSE | TRUE | 3.044274 | |
| C4H6O2 | 87.04406 | TRUE | FALSE | FALSE | 2 | TRUE | FALSE | 2.966568 | CO2C3CHO |
| C4H8O2 | 89.05971 | TRUE | FALSE | FALSE | 1 | TRUE | FALSE | 2.492485 | BUTACID, HO2C3CHO |
| C2H8O4 | 97.04953 | TRUE | FALSE | FALSE | -1 | TRUE | FALSE | 2.312975 | |
| C4H10O2 | 91.07536 | TRUE | FALSE | FALSE | 0 | TRUE | FALSE | 1.956998 | |
| C3H4O4 | 105.0182 | FALSE | FALSE | FALSE | 2 | TRUE | FALSE | 1.233683 | C3DIALOOH |
| C4H8O3 | 105.0546 | TRUE | FALSE | FALSE | 1 | TRUE | FALSE | 1.171317 | PERBUACID, BUTALO2H, HO2C3CO2H |
| C3H2O3 | 87.00767 | FALSE | FALSE | FALSE | 3 | TRUE | FALSE | 1.141834 | C33CO |
| C3H4O3 | 89.02332 | TRUE | FALSE | FALSE | 2 | TRUE | FALSE | 1.07 | C32OH13CO |
| C4H4O3 | 101.0233 | TRUE | FALSE | FALSE | 3 | TRUE | FALSE | 1.064566 | MALDALCO2H, EPXC4DIAL |
| C3H6O3 | 91.03897 | TRUE | FALSE | FALSE | 1 | TRUE | FALSE | 0.978132 | HOC2H4CO2H, PERPROACID, HYPERACET |
| C4H6O3 | 103.039 | TRUE | FALSE | FALSE | 2 | TRUE | FALSE | 0.862132 | |
| C2H10O3 | 83.07027 | TRUE | FALSE | FALSE | -2 | TRUE | FALSE | 0.83743 | |

Table S13. Propyl benzene: Top 20 ions detected by Vocus under low-NOx conditions

| Isopropyl benzene: Top 20 ions detected by Vocus under low-$NO_x$ conditions | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| **Ion Formula** | **Exact Mass (with adduct)** | **Common to All VOCs** | **Unique to this VOC** | **HOM** | **DBE** | **Classified as Ring Scission** | **Classified as Ring Retaining** | **Signal Contribution (%)** | **Corresponding MCM Ion(s)** |
| C3H8O2 | 77.05971 | TRUE | FALSE | FALSE | 0 | TRUE | FALSE | 66.76889 | NC3H7OOH, PROPGLY, IC3H7OOH, HOC3H6OH |
| C3H6O2 | 75.04406 | TRUE | FALSE | FALSE | 1 | TRUE | FALSE | 5.926456 | PROPACID, CH3CHOHCHO, ACETOL, HOC2H4CHO |
| C2H8O4 | 97.04953 | TRUE | FALSE | FALSE | -1 | TRUE | FALSE | 2.323228 | |
| C4H8O2 | 89.05971 | TRUE | FALSE | FALSE | 1 | TRUE | FALSE | 1.77461 | HOIPRCHO, IBUTALOH, BUTACID, IBUTACID, HO2C3CHO |
| C4H6O2 | 87.04406 | TRUE | FALSE | FALSE | 2 | TRUE | FALSE | 1.429481 | IBUTDIAL, CO2C3CHO |
| C4H6O3 | 103.039 | TRUE | FALSE | FALSE | 2 | TRUE | FALSE | 1.079561 | PRPAL2CO2H |
| C4H10O3 | 107.0703 | TRUE | FALSE | FALSE | 0 | TRUE | FALSE | 0.920301 | |
| C4H8O3 | 105.0546 | TRUE | FALSE | FALSE | 1 | TRUE | FALSE | 0.903628 | IPRHOCO2H, HO2C3CO2H, IBUTALO2H, PERBUACID, PERIBUACID, |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | BUTALO2H, HOIPRCO2H, IBUTALBO2H |
| C8H10O2 | 139.0754 | TRUE | FALSE | FALSE | 4 | FALSE | TRUE | 0.833782 | |
| C6H6O4 | 143.0339 | FALSE | FALSE | FALSE | 4 | FALSE | TRUE | 0.745205 | |
| C3H4O4 | 105.0182 | FALSE | FALSE | FALSE | 2 | TRUE | FALSE | 0.737379 | C3DIALOOH |
| C6H6O1 | 95.04914 | FALSE | FALSE | FALSE | 4 | FALSE | TRUE | 0.671568 | |
| C5H8O2 | 101.0597 | TRUE | FALSE | FALSE | 2 | TRUE | FALSE | 0.647038 | IPRGLYOX |
| C3H4O3 | 89.02332 | TRUE | FALSE | FALSE | 2 | TRUE | FALSE | 0.626329 | C32OH13CO |
| C6H4O3 | 125.0233 | TRUE | FALSE | FALSE | 5 | FALSE | TRUE | 0.623331 | |
| C3H6O4 | 107.0339 | TRUE | FALSE | FALSE | 1 | TRUE | FALSE | 0.580875 | IPROPOLPER, HOC2H4CO3H |
| C3H8O3 | 93.05462 | TRUE | FALSE | FALSE | 0 | TRUE | FALSE | 0.492228 | HO1C3OOH, HYPROPO2H, IPROPOLO2H |
| C5H6O3 | 115.039 | TRUE | FALSE | FALSE | 3 | TRUE | FALSE | 0.464824 | |
| C5H6O2 | 99.04406 | TRUE | FALSE | FALSE | 3 | TRUE | FALSE | 0.435992 | |
| C6H6O3 | 127.039 | TRUE | FALSE | FALSE | 4 | FALSE | TRUE | 0.429587 | |

Table S14. Isopropyl benzene: Top 20 ions detected by Vocus under low-NOx conditions

| **1-methyl naphthalene: Top 20 Vocus Ions under Low-NOx conditions** | | | | | | |
|---|---|---|---|---|---|---|
| **Ion Formula** | **Common to All VOCs** | **Unique to this VOC** | **HOM** | **DBE** | **Signal Contribution (%)** | **Exact Mass (with adduct)** |
| C3H8O2 | TRUE | FALSE | FALSE | 0 | 38.49449 | 77.05971 |
| C8H6O4 | TRUE | FALSE | FALSE | 6 | 5.206569 | 167.0339 |
| C3H6O2 | TRUE | FALSE | FALSE | 1 | 3.603318 | 75.04406 |
| C3H4O3 | TRUE | FALSE | FALSE | 2 | 2.707882 | 89.02332 |

| | | | | | | |
|---|---|---|---|---|---|---|
| C6H4O3 | TRUE | FALSE | FALSE | 5 | 2.679679 | 125.0233 |
| C3H4O4 | FALSE | FALSE | FALSE | 2 | 2.334667 | 105.0182 |
| C2H8O4 | TRUE | FALSE | FALSE | -1 | 2.144438 | 97.04953 |
| C8H4O3 | TRUE | FALSE | FALSE | 7 | 1.764107 | 149.0233 |
| C6H6O3 | TRUE | FALSE | FALSE | 4 | 1.683379 | 127.039 |
| C3H6O4 | TRUE | FALSE | FALSE | 1 | 1.608593 | 107.0339 |
| C6H6O1 | FALSE | FALSE | FALSE | 4 | 1.364991 | 95.04914 |
| C5H4O2 | TRUE | FALSE | FALSE | 4 | 1.299702 | 97.02841 |
| C9H8O4 | FALSE | FALSE | FALSE | 6 | 1.24875 | 181.0495 |
| C4H6O3 | TRUE | FALSE | FALSE | 2 | 1.200943 | 103.039 |
| C4H6O2 | TRUE | FALSE | FALSE | 2 | 1.080589 | 87.04406 |
| C5H6O2 | TRUE | FALSE | FALSE | 3 | 1.004867 | 99.04406 |
| C5H8O5 | TRUE | FALSE | FALSE | 2 | 0.951157 | 149.0445 |
| C5H8O2 | TRUE | FALSE | FALSE | 2 | 0.900235 | 101.0597 |
| C3H6O3 | TRUE | FALSE | FALSE | 1 | 0.744321 | 91.03897 |
| C3H2O3 | FALSE | FALSE | FALSE | 3 | 0.74301 | 87.00767 |

Table S15. 1-methyl naphthalene: Top 20 Vocus Ions under Low-NOx conditions

| **1,2,4-trimethyl benzene: Top 20 ions detected by Vocus under medium-$NO_x$ conditions** | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| **Ion Formula** | **Exact Mass (with adduct)** | **Common to All VOCs** | **Unique to this VOC** | **HOM** | **DBE** | **Classified as Ring Scission** | **Classified as Ring Retaining** | **Signal Contribution (%)** | **Corresponding MCM Ion(s)** |
| C4H6O2 | 87.04406 | TRUE | FALSE | FALSE | 2 | TRUE | FALSE | 31.68284 | BIACET |
| C2H8O4 | 97.04953 | FALSE | TRUE | FALSE | -1 | TRUE | FALSE | 6.552441 | |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| C2H4O3 | 77.02332 | FALSE | FALSE | FALSE | 1 | TRUE | FALSE | 5.425794 | HOCH2CO2H, HCOCH2OOH, CH3CO3H |
| C4H8O3 | 105.0546 | TRUE | FALSE | FALSE | 1 | TRUE | FALSE | 5.351598 | MEKBOOH |
| C3H6O2 | 75.04406 | TRUE | FALSE | FALSE | 1 | TRUE | FALSE | 4.770131 | ACETOL |
| C3H8O2 | 77.05971 | TRUE | FALSE | FALSE | 0 | TRUE | FALSE | 3.354085 | |
| C4H6O3 | 103.039 | TRUE | FALSE | FALSE | 2 | TRUE | FALSE | 2.711248 | BIACETOH, MEK2OO, CO2H3CHO, MEK2OOC, MEK2OOA, C3MDIALOH |
| C2H6O4 | 95.03389 | TRUE | FALSE | FALSE | 0 | TRUE | FALSE | 2.482865 | |
| C5H8O2 | 101.0597 | TRUE | FALSE | FALSE | 2 | TRUE | FALSE | 1.719972 | |
| C5H6O3 | 115.039 | TRUE | FALSE | FALSE | 3 | TRUE | FALSE | 1.631809 | C5CO234, C5CO14OH, MC3ODBCO2H |
| C6H8O2 | 113.0597 | TRUE | FALSE | FALSE | 3 | FALSE | FALSE | 1.330846 | TMB1FUONE, C4DBDIKET, MC5DICARB |
| C5H6O2 | 99.04406 | TRUE | FALSE | FALSE | 3 | TRUE | FALSE | 1.055239 | C4MDIAL, PXYFUONE |
| C6H8O4 | 145.0495 | TRUE | FALSE | FALSE | 3 | FALSE | FALSE | 0.982059 | C5OCO3M, EPXM2DCO2H, C5DBCOCO3H, DMKCOOH |
| C8H10O3 | 155.0703 | TRUE | FALSE | FALSE | 4 | FALSE | TRUE | 0.975248 | |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| C4H4O3 | 101.0233 | TRUE | FALSE | FALSE | 3 | TRUE | FALSE | 0.974501 | CO23C3CHO |
| C6H8O3 | 129.0546 | TRUE | FALSE | FALSE | 3 | FALSE | FALSE | 0.967168 | EPXM2C4DAL, C5DBCOCO2H, C3M2COCO2H, C5CODBCO2H |
| C6H6O3 | 127.039 | TRUE | FALSE | FALSE | 4 | FALSE | TRUE | 0.833534 | |
| C4H4O2 | 85.02841 | TRUE | FALSE | FALSE | 3 | TRUE | FALSE | 0.763029 | |
| C6H8O1 | 97.06479 | FALSE | FALSE | FALSE | 3 | FALSE | FALSE | 0.732771 | |
| C3H4O3 | 89.02332 | TRUE | FALSE | FALSE | 2 | TRUE | FALSE | 0.651496 | MGLOO, CH3COCO2H, MGLYOO, MGLOOB, MGLOOC, MGLYOOA |

Table S16. 1,2,4-trimethyl benzene: Top 20 ions detected by Vocus under medium-NOx conditions

| **1,3,5-trimethyl benzene: Top 20 ions detected by Vocus under medium-$NO_x$ conditions** | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| **Ion Formula** | **Exact Mass (with adduct)** | **Common to All VOCs** | **Unique to this VOC** | **HOM** | **DBE** | **Classified as Ring Scission** | **Classified as Ring Retaining** | **Signal Contribution (%)** | **Corresponding MCM Ion(s)** |
| C4H6O2 | 87.04406 | TRUE | FALSE | FALSE | 2 | TRUE | FALSE | 13.84322 | |
| C3H6O2 | 75.04406 | TRUE | FALSE | FALSE | 1 | TRUE | FALSE | 9.577703 | |
| C2H4O3 | 77.02332 | FALSE | FALSE | FALSE | 1 | TRUE | FALSE | 6.655196 | HOCH2CO2H, HCOCH2OOH, CH3CO3H |
| C5H6O3 | 115.039 | TRUE | FALSE | FALSE | 3 | TRUE | FALSE | 4.254671 | C5CO234 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| C4H6O3 | 103.039 | TRUE | FALSE | FALSE | 2 | TRUE | FALSE | 3.900905 | C3MDIALOH |
| C6H8O3 | 129.0546 | TRUE | FALSE | FALSE | 3 | FALSE | FALSE | 3.821282 | EPXMALKT, C5CODBCO2H |
| C6H8O2 | 113.0597 | TRUE | FALSE | FALSE | 3 | FALSE | FALSE | 3.711534 | MXYFUONE, C5MDICARB |
| C5H8O2 | 101.0597 | TRUE | FALSE | FALSE | 2 | TRUE | FALSE | 2.666999 | |
| C3H8O2 | 77.05971 | TRUE | FALSE | FALSE | 0 | TRUE | FALSE | 2.502063 | |
| C2H6O4 | 95.03389 | TRUE | FALSE | FALSE | 0 | TRUE | FALSE | 2.40255 | |
| C6H8O1 | 97.06479 | FALSE | FALSE | FALSE | 3 | FALSE | FALSE | 2.267597 | |
| C4H8O3 | 105.0546 | TRUE | FALSE | FALSE | 1 | TRUE | FALSE | 2.240999 | |
| C6H8O4 | 145.0495 | TRUE | FALSE | FALSE | 3 | FALSE | FALSE | 1.991909 | C5CODBCO3H, C6CO3MOH, C23O3MCHO, EPXMKTCO2H |
| C4H4O2 | 85.02841 | TRUE | FALSE | FALSE | 3 | TRUE | FALSE | 1.618734 | |
| C9H10O2 | 151.0754 | TRUE | FALSE | FALSE | 5 | FALSE | TRUE | 1.568081 | TMBCO2H |
| C8H10O3 | 155.0703 | TRUE | FALSE | FALSE | 4 | FALSE | TRUE | 1.530006 | C7M3CO |
| C6H10O4 | 147.0652 | TRUE | FALSE | FALSE | 2 | FALSE | FALSE | 1.140713 | MXYFUOH, C6CO2M2OH |
| C6H6O2 | 111.0441 | FALSE | FALSE | FALSE | 4 | FALSE | TRUE | 1.130971 | |
| C6H6O3 | 127.039 | TRUE | FALSE | FALSE | 4 | FALSE | TRUE | 1.112758 | |
| C5H6O4 | 131.0339 | TRUE | FALSE | FALSE | 3 | TRUE | FALSE | 1.066246 | ACECOCOCH3 |

Table S17. 1,3,5-trimethyl benzene: Top 20 ions detected by Vocus under medium-NOx conditions

| Propyl benzene: Top 20 ions detected by Vocus under medium-$NO_x$ conditions | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| **Ion Formula** | **Exact Mass (with adduct)** | **Common to All VOCs** | **Unique to this VOC** | **HOM** | **DBE** | **Classified as Ring Scission** | **Classified as Ring Retaining** | **Signal Contribution (%)** | **Corresponding MCM Ion(s)** |
| C9H10O1 | 135.0804 | FALSE | FALSE | FALSE | 5 | FALSE | TRUE | 14.90927 | |
| C7H6O1 | 107.0491 | FALSE | FALSE | FALSE | 5 | FALSE | TRUE | 10.3082 | |
| C3H6O2 | 75.04406 | TRUE | FALSE | FALSE | 1 | TRUE | FALSE | 6.818748 | PROPACID, ACETOL, CH3CHOHCHO, HOC2H4CHO |
| C4H10O3 | 107.0703 | TRUE | FALSE | FALSE | 0 | TRUE | FALSE | 6.422779 | |
| C3H8O2 | 77.05971 | TRUE | FALSE | FALSE | 0 | TRUE | FALSE | 6.002502 | NC3H7OOH, HOC3H6OH, PROPGLY, IC3H7OOH |
| C7H8O2 | 125.0597 | TRUE | FALSE | FALSE | 4 | FALSE | TRUE | 5.176596 | |
| C3H8O3 | 93.05462 | TRUE | FALSE | FALSE | 0 | TRUE | FALSE | 4.905477 | IPROPOLO2H, HO1C3OOH, HYPROPO2H |
| C6H6O1 | 95.04914 | FALSE | FALSE | FALSE | 4 | FALSE | TRUE | 3.362889 | |
| C7H4O1 | 105.0335 | FALSE | FALSE | FALSE | 6 | FALSE | TRUE | 2.911002 | |
| C4H6O2 | 87.04406 | TRUE | FALSE | FALSE | 2 | TRUE | FALSE | 2.61802 | CO2C3CHO |
| C2H4O3 | 77.02332 | FALSE | FALSE | FALSE | 1 | TRUE | FALSE | 2.389549 | HOCH2CO2H, HCOCH2OOH, CH3CO3H |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| C4H8O2 | 89.05971 | TRUE | FALSE | FALSE | 1 | TRUE | FALSE | 2.041239 | BUTACID, HO2C3CHO |
| C4H8O3 | 105.0546 | TRUE | FALSE | FALSE | 1 | TRUE | FALSE | 1.78207 | PERBUACID, BUTALO2H, HO2C3CO2H |
| C3H6O3 | 91.03897 | TRUE | FALSE | FALSE | 1 | TRUE | FALSE | 1.64673 | HOC2H4CO2H, PERPROACID, HYPERACET |
| C7H6O3 | 139.039 | TRUE | FALSE | FALSE | 5 | FALSE | TRUE | 1.644625 | C6H5CO3H |
| C4H10O2 | 91.07536 | TRUE | FALSE | FALSE | 0 | TRUE | FALSE | 1.375682 | |
| C3H4O3 | 89.02332 | TRUE | FALSE | FALSE | 2 | TRUE | FALSE | 1.284849 | C32OH13CO |
| C2H6O4 | 95.03389 | TRUE | FALSE | FALSE | 0 | TRUE | FALSE | 1.273289 | |
| C3H4O4 | 105.0182 | FALSE | FALSE | FALSE | 2 | TRUE | FALSE | 1.217835 | C3DIALOOH |
| C7H8O3 | 141.0546 | TRUE | FALSE | FALSE | 4 | FALSE | TRUE | 1.07062 | PMALANHY |

Table S18. Propyl benzene: Top 20 ions detected by Vocus under medium-NOx conditions

| **Isopropyl benzene: Top 20 ions detected by Vocus under medium-$NO_x$ conditions** | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| **Ion Formula** | **Exact Mass (with adduct)** | **Common to All VOCs** | **Unique to this VOC** | **HOM** | **DBE** | **Classified as Ring Scission** | **Classified as Ring Retaining** | **Signal Contribution (%)** | **Corresponding MCM Ion(s)** |
| C3H8O2 | 77.05971 | TRUE | FALSE | FALSE | 0 | TRUE | FALSE | 46.11367 | NC3H7OOH, PROPGLY, IC3H7OOH, HOC3H6OH |
| C3H6O2 | 75.04406 | TRUE | FALSE | FALSE | 1 | TRUE | FALSE | 15.24104 | PROPACID, CH3CHOHCHO, |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | ACETOL, HOC2H4CHO |
| C4H6O2 | 87.04406 | TRUE | FALSE | FALSE | 2 | TRUE | FALSE | 2.730163 | IBUTDIAL, CO2C3CHO |
| C4H6O3 | 103.039 | TRUE | FALSE | FALSE | 2 | TRUE | FALSE | 2.397467 | PRPAL2CO2H |
| C4H8O2 | 89.05971 | TRUE | FALSE | FALSE | 1 | TRUE | FALSE | 1.888148 | HOIPRCHO, IBUTALOH, BUTACID, IBUTACID, HO2C3CHO |
| C6H6O1 | 95.04914 | FALSE | FALSE | FALSE | 4 | FALSE | TRUE | 1.844616 | |
| C4H8O3 | 105.0546 | TRUE | FALSE | FALSE | 1 | TRUE | FALSE | 1.812185 | IPRHOCO2H, HO2C3CO2H, IBUTALO2H, PERBUACID, PERIBUACID, BUTALO2H, HOIPRCO2H, IBUTALBO2H |
| C4H10O3 | 107.0703 | TRUE | FALSE | FALSE | 0 | TRUE | FALSE | 1.517179 | |
| C5H8O2 | 101.0597 | TRUE | FALSE | FALSE | 2 | TRUE | FALSE | 1.435523 | IPRGLYOX |
| C8H10O2 | 139.0754 | TRUE | FALSE | FALSE | 4 | FALSE | TRUE | 1.398999 | |
| C2H3N1O3 | 90.01857 | FALSE | FALSE | FALSE | 2 | TRUE | FALSE | 1.171302 | |
| C5H6O3 | 115.039 | TRUE | FALSE | FALSE | 3 | TRUE | FALSE | 1.097173 | |
| C3H4O3 | 89.02332 | TRUE | FALSE | FALSE | 2 | TRUE | FALSE | 0.929696 | C32OH13CO |
| C3H4O4 | 105.0182 | FALSE | FALSE | FALSE | 2 | TRUE | FALSE | 0.845416 | C3DIALOOH |
| C5H6O2 | 99.04406 | TRUE | FALSE | FALSE | 3 | TRUE | FALSE | 0.807644 | |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| C9H10O1 | 135.0804 | FALSE | FALSE | FALSE | 5 | FALSE | TRUE | 0.770437 | |
| C2H6O4 | 95.03389 | TRUE | FALSE | FALSE | 0 | TRUE | FALSE | 0.655641 | |
| C5H6O1 | 83.04914 | FALSE | FALSE | FALSE | 3 | TRUE | FALSE | 0.583242 | |
| C3H6O3 | 91.03897 | TRUE | FALSE | FALSE | 1 | TRUE | FALSE | 0.538058 | PROPALOOH, HYPERACET, PERPROACID, HOC2H4CO2H |
| C8H8O2 | 137.0597 | TRUE | FALSE | FALSE | 5 | FALSE | TRUE | 0.526159 | PHCOMEOH |

Table S19. Isopropyl benzene: Top 20 ions detected by Vocus under medium-NOx conditions

| **1-methyl naphthalene: Top 20 ions detected by Vocus under medium-$NO_x$ conditions** | | | | | | |
|---|---|---|---|---|---|---|
| **Ion Formula** | **Common to All VOCs** | **Unique to this VOC** | **HOM** | **DBE** | **Signal Contribution (%)** | **Exact Mass (with adduct)** |
| C3H8O2 | TRUE | FALSE | FALSE | 0 | 14.83332 | 77.05971 |
| C8H6O4 | FALSE | FALSE | FALSE | 6 | 8.602579 | 167.0339 |
| C2H3N1O3 | FALSE | FALSE | FALSE | 2 | 7.186787 | 90.01857 |
| C3H6O2 | TRUE | FALSE | FALSE | 1 | 5.831916 | 75.04406 |
| C8H4O3 | FALSE | FALSE | FALSE | 7 | 4.694622 | 149.0233 |
| C3H4O3 | TRUE | FALSE | FALSE | 2 | 2.837655 | 89.02332 |
| C2H5N1O4 | FALSE | FALSE | FALSE | 1 | 2.71726 | 108.0291 |
| C6H4O3 | TRUE | FALSE | FALSE | 5 | 2.585931 | 125.0233 |
| C9H8O4 | FALSE | FALSE | FALSE | 6 | 2.413681 | 181.0495 |
| C3H4O4 | FALSE | FALSE | FALSE | 2 | 2.084004 | 105.0182 |
| C4H6O2 | TRUE | FALSE | FALSE | 2 | 1.722465 | 87.04406 |
| C4H6O3 | TRUE | FALSE | FALSE | 2 | 1.670649 | 103.039 |
| C9H6O3 | FALSE | FALSE | FALSE | 7 | 1.651424 | 163.039 |

| | | | | | | |
|---|---|---|---|---|---|---|
| C6H6O3 | TRUE | FALSE | FALSE | 4 | 1.430152 | 127.039 |
| C5H4O2 | TRUE | FALSE | FALSE | 4 | 1.427493 | 97.02841 |
| C5H8O2 | TRUE | FALSE | FALSE | 2 | 1.24446 | 101.0597 |
| C5H6O2 | TRUE | FALSE | FALSE | 3 | 1.1377 | 99.04406 |
| C3H6O4 | TRUE | FALSE | FALSE | 1 | 1.095035 | 107.0339 |
| C2H4N2O2 | FALSE | FALSE | FALSE | 2 | 0.958981 | 89.03455 |
| C3H2O3 | FALSE | FALSE | FALSE | 3 | 0.932904 | 87.00767 |

Table S20. 1-methyl naphthalene: Top 20 ions detected by Vocus under medium-NOx conditions

| **MCM Ions not detected by I-CIMS for 1,2,4-trimethyl benzene under low-NOx conditions** | | **MCM Ions not detected by I-CIMS for 1,2,4-trimethyl benzene under medium-NOx conditions** | |
|---|---|---|---|
| **Formula** | **Corresponding MCM Ion(s)** | **Formula** | **Corresponding MCM Ion(s)** |
| CH2O | HCHO | CH2O | HCHO |
| CH3O | CH3O | CH3O | CH3O |
| CH4O | CH3OH | CH4O | CH3OH |
| C2H4O | CH3CHO | C2H4O | CH3CHO |
| CH3O2 | CH3O2 | CH3O2 | CH3O2 |
| CH4O2 | CH3OOH | CH4O2 | CH3OOH |
| C2HO2 | HCOCO | C2HO2 | HCOCO |
| C2H2O2 | GLYOX | C2H2O2 | GLYOX |
| C3H6O | CH3COCH3 | C3H6O | CH3COCH3 |
| C2H3O2 | HCOCH2O | C2H3O2 | HCOCH2O |
| C2H4O2 | HOCH2CHO;CH3CO2H | C2H4O2 | HOCH2CHO;CH3CO2H |
| C3H4O2 | MGLYOX | C3H4O2 | MGLYOX |

| | | | |
|---|---|---|---|
| C3H6O2 | ACETOL | C3H6O2 | ACETOL |
| C2HO4 | HCOCO3 | C4H8O2 | BUT2OLO |
| C2H2O4 | HCOCO3H | C2HO4 | HCOCO3 |
| C3H6O3 | HYPERACET | C5H6O2 | C4MDIAL;PXYFUONE |
| C5H6O2 | C4MDIAL;PXYFUONE | C3H3O4 | CH3COCO3 |
| C3H3O4 | CH3COCO3 | C2H2O5 | PPGAOOB |
| C2H2O5 | PPGAOOB | C6H8O2 | TMB1FUONE;C4DBDIKET;MC5 DICARB |
| C6H8O2 | TMB1FUONE;C4DBDIKET;M C5DICARB | C9H12 | TM124B |
| C9H12 | TM124B | C8H9O | DM124O |
| C8H9O | DM124O | C4H3O5 | MALANHYO |
| C4H3O5 | MALANHYO | C9H10O | TM124BCHO |
| C9H10O | TM124BCHO | C9H11O | TM124BO;TM124O |
| C9H11O | TM124BO;TM124O | C9H12O | TM124OL;TM124BOH |
| C9H12O | TM124OL;TM124BOH | C2H3NO6 | PHAN |
| C5H5O5 | C5CO234O2;MMALANHYO | C4H3O6 | MALANHYO2 |
| C4H3O6 | MALANHYO2 | C7H11O4 | C7BDCO |
| C5H5O6 | MMALANHYO2;C23O3CCO3 | C5H5O6 | MMALANHYO2;C23O3CCO3 |
| C7H7O5 | C4DBM2CO3 | C9H11O3 | T124CAT1O2 |
| | | C8H11O4 | C7CO2M5O2 |
| | | C7H12O5 | C7BDCOOH |
| | | C4H5NO7 | C4PAN6;CHOMOHPAN |

| | | | |
|---|---|---|---|
| | | C9H10NO3 | NT124L1O |
| | | C7H7NO7 | C4DBM2PAN |
| | | C9H11N2O11 | T124NNCTO2 |
| | | C9H12N2O11 | T124NNCOOH |
| | | C9H10N3O11 | NDNT124LO |
| | | C9H10N3O12 | NDNT124LO2 |
| | | C9H11N3O12 | NDNT124OOH |

Table S21. MCM Ions not detected by I-CIMS for 1,2,4-trimethyl benzene

| **MCM Ions not detected by I-CIMS for 1,3,5-trimethyl benzene under low-NOx conditions** | | **MCM Ions not detected by I-CIMS for 1,3,5-trimethyl benzene under medium-NOx conditions** | |
|---|---|---|---|
| **Formula** | **Corresponding MCM Ion(s)** | **Formula** | **Corresponding MCM Ion(s)** |
| CH2O | HCHO | CH2O | HCHO |
| CH3O | CH3O | CH3O | CH3O |
| CH4O | CH3OH | CH4O | CH3OH |
| C2H4O | CH3CHO | C2H4O | CH3CHO |
| CH3O2 | CH3O2 | CH3O2 | CH3O2 |
| CH4O2 | CH3OOH | CH4O2 | CH3OOH |
| C2HO2 | HCOCO | C2HO2 | HCOCO |
| C2H2O2 | GLYOX | C2H2O2 | GLYOX |
| C2H3O2 | HCOCH2O | C2H3O2 | HCOCH2O |
| C2H4O2 | HOCH2CHO;CH3CO2H | C2H4O2 | HOCH2CHO;CH3CO2H |
| C3H4O2 | MGLYOX | C3H4O2 | MGLYOX |
| C9H12 | TM135B | C9H12 | TM135B |
| C8H9O | DMPHO | C8H9O | DMPHO |

| | | | |
|---|---|---|---|
| C9H10O | TMBCHO | C9H10O | TMBCHO |
| C9H11O | TM135O;TMBO | C9H11O | TM135O;TMBO |
| C9H12O | TMBOH;TM135BZOL | C9H12O | TMBOH;TM135BZOL |
| C9H13O4 | TM135BPRO | C6H9O5 | MXYFUO2;C5MCO2OHO2 |
| C9H14O4 | TM135BP2OH | C9H9NO5 | TMBPAN |
| C9H11O5 | TM135MUCO3 | | |
| C9H13O5 | TM135BPRO2;TM135OLO;TM135MUCO | | |
| C9H13O6 | TM135OLO2;TM135MUCO2 | | |

Table S22. MCM Ions not detected by I-CIMS for 1,3,5-trimethyl benzene

| **MCM Ions not detected by I-CIMS for propyl benzene under low-NOx conditions** | | **MCM Ions not detected by I-CIMS for propyl benzene under medium-NOx conditions** | |
|---|---|---|---|
| **Formula** | **Corresponding MCM Ion(s)** | **Formula** | **Corresponding MCM Ion(s)** |
| C2H4 | C2H4 | C2H4 | C2H4 |
| CH2O | HCHO | CH2O | HCHO |
| CH3O | CH3O | CH3O | CH3O |
| CH4O | CH3OH | CH4O | CH3OH |
| C2H4O | CH3CHO | C2H4O | CH3CHO |
| C2H5O | C2H5O | C2H5O | C2H5O |
| CH2O2 | HCOOH;CH2OOA;CH2OO | CH2O2 | HCOOH;CH2OOA;CH2OO |
| C2H6O | C2H5OH | C2H6O | C2H5OH |
| CH3O2 | CH3O2 | CH3O2 | CH3O2 |
| CH4O2 | CH3OOH | CH4O2 | CH3OOH |
| C2HO2 | HCOCO | C2HO2 | HCOCO |

| | | | |
|---|---|---|---|
| C2H2O2 | GLYOX | C2H2O2 | GLYOX |
| C3H6O | CH3COCH3;C2H5CHO | C3H6O | CH3COCH3;C2H5CHO |
| C2H3O2 | HCOCH2O | C2H3O2 | HCOCH2O |
| C3H7O | NC3H7O;IC3H7O | C3H7O | NC3H7O;IC3H7O |
| C2H4O2 | CH3CO2H;HOCH2CHO | C2H4O2 | CH3CO2H;HOCH2CHO |
| C3H8O | IPROPOL;NPROPOL | C3H8O | IPROPOL;NPROPOL |
| C2H5O2 | C2H5O2;HOCH2CH2O | C2H5O2 | C2H5O2;HOCH2CH2O |
| C2H6O2 | ETHGLY;C2H5OOH | C2H6O2 | ETHGLY;C2H5OOH |
| C3H4O2 | MGLYOX | C3H4O2 | MGLYOX |
| C4H8O | C3H7CHO | C4H8O | C3H7CHO |
| C3H5O2 | CH3COCH2O | C3H6O2 | PROPACID;ACETOL;CH3CHOH CHO;HOC2H4CHO |
| C3H6O2 | PROPACID;ACETOL;CH3CHO HCHO;HOC2H4CHO | C3H7O2 | HO1C3O;HYPROPO;IPROPOLO ;NC3H7O2;IC3H7O2 |
| C3H8O2 | NC3H7OOH;HOC3H6OH;PRO PGLY;IC3H7OOH | C3H8O2 | NC3H7OOH;HOC3H6OH;PROP GLY;IC3H7OOH |
| C2H5O3 | HOCH2CH2O2 | CH3NO3 | CH3NO3 |
| C2H6O3 | HYETHO2H | C4H6O2 | CO2C3CHO |
| C4H6O2 | CO2C3CHO | C4H7O2 | BUTALO |
| C3H3O3 | C3DIALO | C4H8O2 | BUTACID;HO2C3CHO |
| C2HO4 | HCOCO3 | C2HO4 | HCOCO3 |
| C3H6O3 | HOC2H4CO2H;PERPROACID; HYPERACET | C3H6O3 | HOC2H4CO2H;PERPROACID;H YPERACET |

| | | | |
|---|---|---|---|
| C3H7O3 | HYPROPO2;HO1C3O2;IPROPOLO2 | C2H5NO3 | C2H5NO3 |
| C6H5O | C6H5O | C3H7O3 | HYPROPO2;HO1C3O2;IPROPOLO2 |
| C5H8O2 | PGLYOX | CH3NO4 | CH3O2NO2 |
| C3H3O4 | C3DIALO2 | C4H3O3 | MALDIALCO2 |
| C4H8O3 | PERBUACID;BUTALO2H;HO2C3CO2H | C5H8O2 | PGLYOX |
| C5H8O3 | PGLYOXOH;PGLOO;PGLOOB;PGLOOA | C3H3O4 | C3DIALO2 |
| C5H9O3 | C4CHOAO2 | C4H8O3 | PERBUACID;BUTALO2H;HO2C3CO2H |
| C5H10O3 | C4CHOAOOH | C2H3NO4 | NO3CH2CHO |
| C3H3O5 | HCOCOHCO3 | C3H7NO3 | IC3H7NO3;NC3H7NO3 |
| C4H8O4 | HO2C3CO3H | C2H4NO4 | ETHENO3O |
| C9H12 | PBENZ | C6H5O2 | C6H5O2 |
| C7H6O2 | PHCOOH | C5H8O3 | PGLYOXOH;PGLOO;PGLOOB;PGLOOA |
| C5H9O4 | C4OHCO3 | C5H10O3 | C4CHOAOOH |
| C5H10O4 | C4OHCO3H | C3H3O5 | HCOCOHCO3 |
| C9H10O | PHCOET | C4H8O4 | HO2C3CO3H |
| C9H11O | PHC3O;PBENZO | C9H12 | PBENZ |
| C9H12O | PHC3OH;PBENZOL | C3H7NO4 | HO1C3NO3;PROLNO3;PROPOLNO3 |

| | | | |
|---|---|---|---|
| C9H8O2 | PHCOCOME | C7H6O2 | PHCOOH |
| C9H11O2 | PHC3O2;PBENZO2;PCATEC1O | C4H7NO4 | BUTALNO3 |
| C8H10O3 | C8CO2DBAL | C5H10O4 | C4OHCO3H |
| C6H10O5 | C5O5OHCO3H | C9H10O | PHCOET |
| C9H7O3 | PHCOCOCO | C9H11O | PHC3O;PBENZO |
| C9H9O3 | PHCOETO2 | C9H12O | PHC3OH;PBENZOL |
| C9H13O4 | PBZBIPERO;PPRBQO | C2H3NO6 | PHAN;NO3CH2CO3H |
| C9H14O4 | PPRBQOH;PBZBPER2OH | C9H8O2 | PHCOCOME |
| C8H11O6 | C8CO3OHO2 | C9H10O2 | PPRBQONE;PHCOETOH |
| | | C9H11O2 | PHC3O2;PBENZO2;PCATEC1O |
| | | C8H10O3 | C8CO2DBAL |
| | | C8H11O3 | C815CO2O |
| | | C4H3NO6 | NBZFUONE;MALDIALPAN |
| | | C9H7O3 | PHCOCOCO |
| | | C3H3NO7 | HCOCOHPAN |
| | | C9H9O3 | PHCOETO2 |
| | | C4H5NO7 | NBZFUOOH |
| | | C5H9NO6 | C4OHPAN |
| | | C9H10NO3 | NPBNZ1O |
| | | C2H2N2O8 | NO3CH2PAN |
| | | C9H13O4 | PBZBIPERO;PPRBQO |
| | | C7H8NO5 | NC4PDCO2 |

| | | | |
|---|---|---|---|
| | | C9H14O4 | PPRBQOH;PBZBPER2OH |
| | | C8H11O5 | C8CO3OHO |
| | | C7H9NO6 | NPBFUONE;C7DCPAN |
| | | C7H10NO6 | NPBFUO |
| | | C8H9NO7 | C8CO2DBPAN |
| | | C9H13NO9 | PNCATECOOH |
| | | C9H11N2O10 | PNNCATECO;DNPBNZLO2 |
| | | C6H5N3O12 | NDNPHENOOH |
| | | C9H11N2O11 | PNNCATECO2 |
| | | C9H10N3O11 | NDNPBNZLO |
| | | C9H10N3O12 | NDNPBNZLO2 |
| | | C9H11N3O12 | NDNPBZLOOH |

Table S23. MCM Ions not detected by I-CIMS for propyl benzene

| **MCM Ions not detected by I-CIMS for isopropyl benzene under low-NOx conditions** | | **MCM Ions not detected by I-CIMS for isopropyl benzene under medium-NOx conditions** | |
|---|---|---|---|
| **Formula** | **Corresponding MCM Ion(s)** | **Formula** | **Corresponding MCM Ion(s)** |
| C2H4 | C2H4 | C2H4 | C2H4 |
| CH2O | HCHO | CH2O | HCHO |
| CH3O | CH3O | CH3O | CH3O |
| CH4O | CH3OH | CH4O | CH3OH |
| C2H4O | CH3CHO | C2H4O | CH3CHO |
| C2H5O | C2H5O | C2H5O | C2H5O |
| CH2O2 | CH2OOA;HCOOH;CH2OO | CH2O2 | CH2OOA;HCOOH;CH2OO |
| C2H6O | C2H5OH | C2H6O | C2H5OH |

| | | | |
|---|---|---|---|
| CH3O2 | CH3O2 | CH3O2 | CH3O2 |
| CH4O2 | CH3OOH | CH4O2 | CH3OOH |
| C2HO2 | HCOCO | C2HO2 | HCOCO |
| C2H2O2 | GLYOX | C2H2O2 | GLYOX |
| C3H6O | CH3COCH3;C2H5CHO | C3H6O | CH3COCH3;C2H5CHO |
| C2H3O2 | HCOCH2O | C2H3O2 | HCOCH2O |
| C3H7O | NC3H7O;IC3H7O | C3H7O | NC3H7O;IC3H7O |
| C2H4O2 | HOCH2CHO;CH3CO2H | C2H4O2 | HOCH2CHO;CH3CO2H |
| C3H8O | IPROPOL;NPROPOL | C3H8O | IPROPOL;NPROPOL |
| C2H5O2 | HOCH2CH2O;C2H5O2 | C2H5O2 | HOCH2CH2O;C2H5O2 |
| C2H6O2 | ETHGLY;C2H5OOH | C2H6O2 | ETHGLY;C2H5OOH |
| C3H4O2 | MGLYOX | C3H4O2 | MGLYOX |
| C4H8O | C3H7CHO;IPRCHO | C4H8O | C3H7CHO;IPRCHO |
| C3H5O2 | PROPALO;CH3COCH2O | C3H5O2 | PROPALO;CH3COCH2O |
| C3H6O2 | PROPACID;CH3CHOHCHO;ACETOL;HOC2H4CHO | C3H6O2 | PROPACID;CH3CHOHCHO;ACETOL;HOC2H4CHO |
| C3H7O2 | HO1C3O;IC3H7O2;HYPROPO;IPROPOLO;NC3H7O2 | C3H7O2 | HO1C3O;IC3H7O2;HYPROPO;IPROPOLO;NC3H7O2 |
| C3H8O2 | NC3H7OOH;PROPGLY;IC3H7OOH;HOC3H6OH | C3H8O2 | NC3H7OOH;PROPGLY;IC3H7OOH;HOC3H6OH |
| C4H6O2 | IBUTDIAL;CO2C3CHO | CH3NO3 | CH3NO3 |
| C4H8O2 | HOIPRCHO;IBUTALOH;BUTACID;IBUTACID;HO2C3CHO | C4H4O2 | MALDIAL;BZFUONE |
| C2HO4 | HCOCO3 | C4H6O2 | IBUTDIAL;CO2C3CHO |
| C2H2O4 | HCOCO3H | C3H3O3 | C3DIALO |
| C3H6O3 | PROPALOOH;HYPERACET;PERPROACID;HOC2H4CO2H | C4H8O2 | HOIPRCHO;IBUTALOH;BUTACID;IBUTACID;HO2C3CHO |

| | | | |
|---|---|---|---|
| C6H5O | C6H5O | C2HO4 | HCOCO3 |
| C5H10O2 | C3M3OH2CHO | C2H2O4 | HCOCO3H |
| C3H3O5 | HCOCOHCO3 | C2H5NO3 | C2H5NO3 |
| C8H8O | PHCOME | CH3NO4 | CH3O2NO2 |
| C9H12 | IPBENZ | C5H8O2 | IPRGLYOX |
| C8H6O2 | PHGLYOX | C5H10O2 | C3M3OH2CHO |
| C8H7O2 | PHCOMEO | C4H7O3 | BUTALO2;IBUTALCO2;IPRCO3;C3H7CO3;IBUTALBO2 |
| C9H11O | IPBENZO;PHIC3O | C2H3NO4 | NO3CH2CHO |
| C8H8O2 | PHCOMEOH | C3H7NO3 | NC3H7NO3;IC3H7NO3 |
| C9H12O | PHIC3OH;IPBENZOL | C5H8O3 | IPGLYOXOH |
| C7H6O3 | C6H5CO3H | C5H9O3 | IC4CHOAO2;IPGLOOB;IPGLOO |
| C8H7O3 | PHCOMEO2 | C5H10O3 | IC4CHOAOOH |
| C9H12O2 | IPCATECHOL;PHIC3OOH;IPBENZOOH | C4H8O4 | HOIPRCO3H;IPRHOCO3H;HO2C3CO3H |
| | | C8H8O | PHCOME |
| | | C9H12 | IPBENZ |
| | | C3H7NO4 | HO1C3NO3;PROLNO3;PROPOLNO3 |
| | | C7H10O2 | IPBFUONE;IC7DICARB |
| | | C6H10O3 | C5MO132OH |
| | | C4H7NO4 | IBUALANO3;BUTALNO3 |
| | | C8H6O2 | PHGLYOX |
| | | C8H7O2 | PHCOMEO |
| | | C2H3NO6 | PHAN;NO3CH2CO3H |
| | | C4H2NO5 | NC4DCO2 |

| | | | |
|---|---|---|---|
| | | C9H10O2 | IPRBQONE |
| | | C8H7O3 | PHCOMEO2 |
| | | C8H10O3 | C7MCO2DBAL |
| | | C6H10O5 | C4MOHOCO3H |
| | | C3H3NO7 | HCOCOHPAN |
| | | C7H5NO5 | PBZN |
| | | C7H10NO6 | NIPBFUO |

Table S24. MCM Ions not detected by I-CIMS for isopropyl benzene

| **MCM Ions not detected by Vocus for 1,3,5-trimethyl benzene under low-NOx conditions** | | **MCM Ions not detected by Vocus for 1,3,5-trimethyl benzene under medium-NOx conditions** | |
|---|---|---|---|
| **Formula** | **Corresponding MCM Ion(s)** | **Formula** | **Corresponding MCM Ion(s)** |
| CH2O | HCHO | CH2O | HCHO |
| CH3O | CH3O | CH3O | CH3O |
| CH4O | CH3OH | CH4O | CH3OH |
| C2H4O | CH3CHO | C2H4O | CH3CHO |
| CH3O2 | CH3O2 | CH3O2 | CH3O2 |
| CH4O2 | CH3OOH | CH4O2 | CH3OOH |
| C2HO2 | HCOCO | C2HO2 | HCOCO |
| C2H2O2 | GLYOX | C2H2O2 | GLYOX |
| C2H3O2 | HCOCH2O | C2H3O2 | HCOCH2O |
| C2H4O2 | HOCH2CHO;CH3CO2H | C2H4O2 | HOCH2CHO;CH3CO2H |
| C3H4O2 | MGLYOX | C3H4O2 | MGLYOX |
| C2H2O3 | HCOCO2H | C2H2O3 | HCOCO2H |
| C2HO4 | HCOCO3 | CH3NO3 | CH3NO3 |

| | | | |
|---|---|---|---|
| C2H2O4 | HCOCO3H | C2HO4 | HCOCO3 |
| C2H3O4 | HOCH2CO3 | C2H2O4 | HCOCO3H |
| C2H4O4 | HOCH2CO3H | C2H3O4 | HOCH2CO3 |
| C4H5O3 | C3MDIALO | CH3NO4 | CH3O2NO2 |
| C5H7O3 | CO24C53O | C5H8O3 | C5CO243OH |
| C5H8O3 | C5CO243OH | C4H5O4 | C3MDIALO2 |
| C4H5O4 | C3MDIALO2 | C4H6O4 | C3MDIALOOH |
| C4H6O4 | C3MDIALOOH | C9H12 | TM135B |
| C9H12 | TM135B | C2H3NO5 | PAN |
| C8H9O | DMPHO | C8H9O | DMPHO |
| C6H7O3 | C4MCODBCO2 | C6H7O3 | C4MCODBCO2 |
| C5H5O4 | C5CO234O | C5H5O4 | C5CO234O |
| C5H7O4 | CO24C53O2;C23O3MO | C5H7O4 | CO24C53O2;C23O3MO |
| C4H5O5 | CHOMOHCO3;CO2H3CO3 | C4H5O5 | CHOMOHCO3;CO2H3CO3 |
| C9H10O | TMBCHO | C9H10O | TMBCHO |
| C9H11O | TM135O;TMBO | C9H11O | TM135O;TMBO |
| C9H12O | TMBOH;TM135BZOL | C9H12O | TMBOH;TM135BZOL |
| C8H9O2 | DMPHO2 | C2H3NO6 | PHAN |
| C5H5O5 | ACCOCOMEO;C5CO234O2;MMALANHYO | C8H9O2 | DMPHO2 |
| C6H9O4 | MXYFUO;C5MCO2OHO | C5H5O5 | ACCOCOMEO;C5CO234O2;MMALANHYO |
| C5H6O5 | C5CO234OOH;MMALNHY2OH | C6H9O4 | MXYFUO;C5MCO2OHO |

| | | | |
|---|---|---|---|
| C5H7O5 | C23O3MO2 | C5H7O5 | C23O3MO2 |
| C9H11O2 | TMBO2 | C9H11O2 | TMBO2 |
| C8H11O3 | C7M2CO5O | C8H11O3 | C7M2CO5O |
| C6H7O5 | EPXMKTCO3 | C6H7O5 | EPXMKTCO3 |
| C5H5O6 | MMALANHYO2;ACCOCOMEO2 | C5H5O6 | MMALANHYO2;ACCOCOMEO2 |
| C6H9O5 | MXYFUO2;C5MCO2OHO2 | C6H9O5 | MXYFUO2;C5MCO2OHO2 |
| C5H6O6 | MMALNHYOOH;ACCOCOMOOH | C5H6O6 | MMALNHYOOH;ACCOCOMOOH |
| C8H11O4 | C7M2CO5O2 | C8H9NO3 | DMPHOHNO2 |
| C6H7O6 | C23O3MCO3;C4COMOHCO3 | C8H11O4 | C7M2CO5O2 |
| C9H13O4 | TM135BPRO | C6H8O6 | C5COHOCO3H;C23O3MCO3H |
| C9H11O5 | TM135MUCO3 | C4H5NO7 | C4PAN6;CHOMOHPAN |
| C9H13O5 | TM135BPRO2;TM135OLO;TM135MUCO | C9H11NO3 | TMBNO3 |
| C9H13O6 | TM135OLO2;TM135MUCO2 | C9H13O4 | TM135BPRO |
| | | C6H7NO6 | C4MCODBPAN |
| | | C6H8NO6 | NMXYFUO |
| | | C9H11O5 | TM135MUCO3 |
| | | C9H13O5 | TM135BPRO2;TM135OLO;TM135MUCO |
| | | C6H7NO7 | EPXMKTPAN |
| | | C6H8NO7 | NMXYFUO2 |

| | | | |
|---|---|---|---|
| | | C6H9NO7 | NMXYFUOOH |
| | | C9H9NO5 | TMBPAN |
| | | C9H13O6 | TM135OLO2;TM135MUCO2 |
| | | C6H7NO8 | C23O3MCPAN;C4COMOHPAN |
| | | C9H13NO6 | TM135BPNO3 |
| | | C8H10NO7 | MXYOHNO2O |
| | | C9H11NO7 | TM135MUPAN |
| | | C9H12NO7 | NTM135OLO |
| | | C9H13NO7 | NTM135OLOH;TM135MUNO3 |
| | | C8H10NO8 | MXYOHNO2O2 |
| | | C8H11NO8 | MXOHNO2OOH |
| | | C9H12NO8 | NTM135OLO2 |
| | | C9H13NO8 | NTM135LOOH |

Table S25. MCM Ions not detected by Vocus for 1,3,5-trimethyl benzene

| **MCM Ions not detected by Vocus for 1,2,4-trimethyl benzene under low-NOx conditions** | | **MCM Ions not detected by Vocus for 1,2,4-trimethyl benzene under medium-NOx conditions** | |
|---|---|---|---|
| **Formula** | **Corresponding MCM Ion(s)** | **Formula** | **Corresponding MCM Ion(s)** |
| CH2O | HCHO | CH2O | HCHO |
| CH3O | CH3O | CH3O | CH3O |
| CH4O | CH3OH | CH4O | CH3OH |
| C2H4O | CH3CHO | C2H4O | CH3CHO |
| CH3O2 | CH3O2 | CH3O2 | CH3O2 |

| | | | |
|---|---|---|---|
| CH4O2 | CH3OOH | CH4O2 | CH3OOH |
| C2HO2 | HCOCO | C2HO2 | HCOCO |
| C2H2O2 | GLYOX | C2H2O2 | GLYOX |
| C3H6O | CH3COCH3 | C3H6O | CH3COCH3 |
| C2H3O2 | HCOCH2O | C2H3O2 | HCOCH2O |
| C2H4O2 | HOCH2CHO;CH3CO2H | C2H4O2 | HOCH2CHO;CH3CO2H |
| C3H4O2 | MGLYOX | C3H4O2 | MGLYOX |
| C3H5O2 | CH3COCH2O | C3H5O2 | CH3COCH2O |
| C2H2O3 | GLYOO;GLYOOC;HCOCO2H | C2H2O3 | GLYOO;GLYOOC;HCOCO2H |
| C2H3O3 | HCOCH2O2;CH3CO3 | CH3NO3 | CH3NO3 |
| C4H7O2 | MEKBO | C4H7O2 | MEKBO |
| C2HO4 | HCOCO3 | C2HO4 | HCOCO3 |
| C3H5O3 | CH3COCH2O2 | C2H2O4 | HCOCO3H |
| C2H2O4 | HCOCO3H | C2H3O4 | HOCH2CO3 |
| C2H3O4 | HOCH2CO3 | CH3NO4 | CH3O2NO2 |
| C4H5O3 | BIACETO;C3MDIALO | C3H3O4 | CH3COCO3 |
| C3H3O4 | CH3COCO3 | C4H7O3 | MEKBO2 |
| C4H7O3 | MEKBO2 | C2H2O5 | PPGAOOB |
| C2H2O5 | PPGAOOB | C5H7O3 | C4MCO2O |
| C5H7O3 | C4MCO2O | C4H4O4 | C23O3CHO |
| C4H4O4 | C23O3CHO | C5H8O3 | C4MCO2OH;C5CO243OH |
| C5H8O3 | C4MCO2OH;C5CO243OH | C4H5O4 | BIACETO2;MCOCOMOXO;C3MDIALO2 |

| | | | |
|---|---|---|---|
| C4H5O4 | BIACETO2;MCOCOMOXO;C3MDIALO2 | C4H6O4 | C3MDIALOOH;BIACETOOH |
| C4H6O4 | C3MDIALOOH;BIACETOOH | C3H3O5 | HCOCOHCO3 |
| C3H3O5 | HCOCOHCO3 | C3H4O5 | PPACLOOA;HCOCOHCO3H |
| C3H4O5 | PPACLOOA;HCOCOHCO3H | C9H12 | TM124B |
| C9H12 | TM124B | C2H3NO5 | PAN |
| C8H9O | DM124O | C8H9O | DM124O |
| C6H7O3 | MC4CODBCO2;C4MCODBCO2 | C6H7O3 | MC4CODBCO2;C4MCODBCO2 |
| C5H5O4 | MC3CODBCO3;C5CO14O2;C5CO234O;C3MCODBCO3 | C4H2O5 | MALNHYOHCO |
| C4H2O5 | MALNHYOHCO | C4H3O5 | MALANHYO |
| C4H3O5 | MALANHYO | C5H7O4 | PXYFUO;C4M2ALOHO;C4MCO2O2 |
| C5H7O4 | PXYFUO;C4M2ALOHO;C4MCO2O2 | C4H5O5 | MCOCOMOXO2;CHOMOHCO3;CO2H3CO3 |
| C4H5O5 | MCOCOMOXO2;CHOMOHCO3;CO2H3CO3 | C9H10O | TM124BCHO |
| C4H6O5 | MCOCOMOOOH;CO2H3CO3H;CHOMOHCO3H | C9H11O | TM124BO;TM124O |
| C9H10O | TM124BCHO | C9H12O | TM124OL;TM124BOH |
| C9H11O | TM124BO;TM124O | C2H3NO6 | PHAN |
| C9H12O | TM124OL;TM124BOH | C6H7O4 | MC4CODBCO3;C62O |
| C8H9O2 | DM124O2 | C5H5O5 | C5CO234O2;MMALANHYO |

| | | | |
|---|---|---|---|
| C6H7O4 | MC4CODBCO3;C62O | C6H9O4 | TMB1FUO;DMKOHO;MC5CO2OHO |
| C5H5O5 | C5CO234O2;MMALANHYO | C4H3O6 | MALANHYO2 |
| C6H9O4 | TMB1FUO;DMKOHO;MC5CO2OHO | C5H7O5 | PXYFUO2;C4M2ALOHO2 |
| C4H3O6 | MALANHYO2 | C4H4O6 | MALANHYOOH |
| C5H7O5 | PXYFUO2;C4M2ALOHO2 | C3H3NO6 | CH3COPAN |
| C4H4O6 | MALANHYOOH | C9H11O2 | T124CAT1O;TM124BO2;TM124O2 |
| C9H11O2 | T124CAT1O;TM124BO2;TM124O2 | C8H11O3 | C7CO2M5O |
| C8H11O3 | C7CO2M5O | C6H7O5 | EPXM2DLCO3 |
| C6H7O5 | EPXM2DLCO3 | C7H11O4 | C7BDCO |
| C7H11O4 | C7BDCO | C5H5O6 | MMALANHYO2;C23O3CCO3 |
| C5H5O6 | MMALANHYO2;C23O3CCO3 | C6H9O5 | DMKOHO2;TMB1FUO2;MC5CO2OHO2 |
| C6H9O5 | DMKOHO2;TMB1FUO2;MC5CO2OHO2 | C5H6O6 | MMALNHYOOH;C23O3CCO3H |
| C5H6O6 | MMALNHYOOH;C23O3CCO3H | C5H7O6 | C534O;C535O |
| C5H7O6 | C534O;C535O | C3H3NO7 | HCOCOHPAN |
| C9H9O3 | TM124BCO3 | C8H9NO3 | DM124OHNO2 |
| C9H11O3 | T124CAT1O2 | C9H11O3 | T124CAT1O2 |
| C7H7O5 | C4DBM2CO3 | C7H7O5 | C4DBM2CO3 |

| | | | |
|---|---|---|---|
| C8H11O4 | C7CO2M5O2 | C8H11O4 | C7CO2M5O2 |
| C7H11O5 | C7BDCO2 | C6H7NO5 | NC5MDCO2H |
| C5H7O7 | C534O2;C535O2 | C5H5NO6 | C3MCODBPAN;C5COO2NO2; MC3CODBPAN |
| C5H8O7 | C535OOH;C534OOH | C7H11O5 | C7BDCO2 |
| C9H11O4 | TM124QO | C5H6NO6 | NPXYFUO |
| C9H13O4 | TM124BPRO | C4H5NO7 | C4PAN6;CHOMOHPAN |
| C9H11O5 | TM124MUCO3;TM124QO2 | C5H7O7 | C534O2;C535O2 |
| C9H13O5 | TM124BPRO2;TM124OLO;TM 124MUCO | C5H8O7 | C535OOH;C534OOH |
| C9H11O6 | C7MOHCOCO3 | C9H10NO3 | NT124L1O |
| C9H13O6 | TM124OLO2;TM124MUCO2 | C9H11NO3 | TM124BNO3;TM124OHNO2 |
| | | C9H11O4 | TM124QO |
| | | C9H13O4 | TM124BPRO |
| | | C6H7NO6 | MC4CODBPAN |
| | | C6H8NO6 | NTMB1FUO |
| | | C5H6NO7 | NPXYFUO2 |
| | | C5H7NO7 | NPXYFUOOH |
| | | C9H10NO4 | NT124L1O2 |
| | | C9H11NO4 | NT124L1OOH;T124NCATEC |
| | | C9H11O5 | TM124MUCO3;TM124QO2 |
| | | C9H13O5 | TM124BPRO2;TM124OLO;TM 124MUCO |

| | | | |
|---|---|---|---|
| | | C6H7NO7 | EPXM2DLPAN |
| | | C6H8NO7 | NTMB1FUO2 |
| | | C5H5NO8 | C23O3CPAN |
| | | C6H9NO7 | NTMB1FUOOH |
| | | C9H9NO5 | TM124BPAN |
| | | C9H11O6 | C7MOHCOCO3 |
| | | C7H7NO7 | C4DBM2PAN |
| | | C9H13O6 | TM124OLO2;TM124MUCO2 |
| | | C9H10N2O5 | DNT124BOL |
| | | C9H10NO6 | NTM124QO |
| | | C9H13NO6 | TM124BPNO3 |
| | | C8H10NO7 | TM124NO2O |
| | | C9H10NO7 | NTM124QO2 |
| | | C9H11NO7 | NTM124QOOH;TM124MUPAN |
| | | C9H12NO7 | NTM124OLO |
| | | C9H13NO7 | TM124MUNO3;NTM124OLOH |
| | | C8H10NO8 | TM124NO2O2 |
| | | C8H11NO8 | TM124NOOH |
| | | C9H11NO8 | C7MOHCOPAN |
| | | C9H12NO8 | T124NCATO;NTM124OLO2 |
| | | C9H13NO8 | NTM124LOOH |

| | | | |
|---|---|---|---|
| | | C9H12NO9 | T124NCATO2 |
| | | C9H13NO9 | T124NCTOOH |
| | | C9H11N2O9 | DNT124LO |
| | | C9H11N2O10 | T124NNCTO;DNT124LO2 |
| | | C9H12N2O10 | DNT124LOOH |
| | | C9H11N2O11 | T124NNCTO2 |
| | | C9H12N2O11 | T124NNCOOH |
| | | C9H10N3O11 | NDNT124LO |
| | | C9H10N3O12 | NDNT124LO2 |
| | | C9H11N3O12 | NDNT124OOH |
| | | | |
| | | | |
| | | | |
| | | | |
| | | | |
| | | | |
| | | | |
| | | | |
| | | | |
| | | | |

Table S26. MCM Ions not detected by Vocus for 1,2,4-trimethyl benzene

| MCM Ions not detected by Vocus for propylbenzene under low-NOx conditions | | MCM Ions not detected by Vocus for propylbenzene under medium-NOx conditions | |
|---|---|---|---|
| **Formula** | **Corresponding MCM Ion(s)** | **Formula** | **Corresponding MCM Ion(s)** |
| C2H4 | C2H4 | C2H4 | C2H4 |
| CH2O | HCHO | CH2O | HCHO |
| CH3O | CH3O | CH3O | CH3O |
| CH4O | CH3OH | CH4O | CH3OH |
| C2H4O | CH3CHO | C2H4O | CH3CHO |
| C2H5O | C2H5O | C2H5O | C2H5O |
| CH2O2 | HCOOH;CH2OOA;CH2OO | CH2O2 | HCOOH;CH2OOA;CH2OO |
| C2H6O | C2H5OH | C2H6O | C2H5OH |
| CH3O2 | CH3O2 | CH3O2 | CH3O2 |
| CH4O2 | CH3OOH | CH4O2 | CH3OOH |
| C2HO2 | HCOCO | C2HO2 | HCOCO |
| C2H2O2 | GLYOX | C2H2O2 | GLYOX |
| C3H6O | CH3COCH3;C2H5CHO | C3H6O | CH3COCH3;C2H5CHO |
| C2H3O2 | HCOCH2O | C2H3O2 | HCOCH2O |
| C3H7O | NC3H7O;IC3H7O | C3H7O | NC3H7O;IC3H7O |
| C2H4O2 | CH3CO2H;HOCH2CHO | C2H4O2 | CH3CO2H;HOCH2CHO |
| C3H8O | IPROPOL;NPROPOL | C3H8O | IPROPOL;NPROPOL |
| C2H5O2 | C2H5O2;HOCH2CH2O | C2H5O2 | C2H5O2;HOCH2CH2O |
| C2H6O2 | ETHGLY;C2H5OOH | C2H6O2 | ETHGLY;C2H5OOH |
| C3H4O2 | MGLYOX | C3H4O2 | MGLYOX |
| C4H8O | C3H7CHO | C4H8O | C3H7CHO |

| | | | |
|---|---|---|---|
| C3H5O2 | CH3COCH2O | C3H5O2 | CH3COCH2O |
| C2H2O3 | GLYOO;GLYOOA;HCOCO2H | C2H2O3 | GLYOO;GLYOOA;HCOCO2H |
| C2H3O3 | HCOCH2O2;CH3CO3 | C3H7O2 | HO1C3O;HYPROPO;IPROPOLO;NC3H7O2;IC3H7O2 |
| C3H7O2 | HO1C3O;HYPROPO;IPROPOLO;NC3H7O2;IC3H7O2 | CH3NO3 | CH3NO3 |
| C2H4O3 | HOCH2CO2H;HCOCH2OOH;CH3CO3H | C2H6O3 | HYETHO2H |
| C2H5O3 | HOCH2CH2O2 | C4H7O2 | BUTALO |
| C2H6O3 | HYETHO2H | C2HO4 | HCOCO3 |
| C4H7O2 | BUTALO | C2H2O4 | HCOCO3H |
| C2HO4 | HCOCO3 | C2H3O4 | HOCH2CO3 |
| C3H5O3 | C2H5CO3;CH3COCH2O2 | C2H5NO3 | C2H5NO3 |
| C2H2O4 | HCOCO3H | C2H4O4 | HOCH2CO3H |
| C2H3O4 | HOCH2CO3 | CH3NO4 | CH3O2NO2 |
| C3H7O3 | HYPROPO2;HO1C3O2;IPROPOLO2 | C6H5O | C6H5O |
| C2H4O4 | HOCH2CO3H | C5H9O2 | C4CHO2O |
| C6H5O | C6H5O | C3H3O4 | C3DIALO2 |
| C4H3O3 | MALDIALCO2 | C4H7O3 | BUTALO2;C3H7CO3 |
| C5H9O2 | C4CHO2O | C2H3NO4 | NO3CH2CHO |
| C3H3O4 | C3DIALO2 | C3H5O4 | CH3CHOHCO3;HOC2H4CO3 |
| C4H7O3 | BUTALO2;C3H7CO3 | C3H7NO3 | IC3H7NO3;NC3H7NO3 |

| | | | |
|---|---|---|---|
| C3H5O4 | CH3CHOHCO3;HOC2H4CO3 | C2H4NO4 | ETHENO3O |
| C6H5O2 | C6H5O2 | C2H5NO4 | ETHOHNO3 |
| C4H3O4 | MALDIALCO3 | C4H3O4 | MALDIALCO3 |
| C4H4O4 | HOCOC4DIAL;MALDALCO3H;EPXDLCO2H;CO14O3CHO;BZFUCO | C4H4O4 | HOCOC4DIAL;MALDALCO3H;EPXDLCO2H;CO14O3CHO;BZFUCO |
| C5H8O3 | PGLYOXOH;PGLOO;PGLOOB;PGLOOA | C5H8O3 | PGLYOXOH;PGLOO;PGLOOB;PGLOOA |
| C4H5O4 | BZFUO;CO2C3CO3;MALDIALO | C4H5O4 | BZFUO;CO2C3CO3;MALDIALO |
| C5H9O3 | C4CHOAO2 | C5H9O3 | C4CHOAO2 |
| C4H6O4 | CO2C3CO3H;HOHOC4DIAL;BZFUOH | C4H6O4 | CO2C3CO3H;HOHOC4DIAL;BZFUOH |
| C5H10O3 | C4CHOAOOH | C5H10O3 | C4CHOAOOH |
| C3H3O5 | HCOCOHCO3 | C3H3O5 | HCOCOHCO3 |
| C4H7O4 | HO2C3CO3 | C4H7O4 | HO2C3CO3 |
| C3H4O5 | HCOCOHCO3H | C3H4O5 | HCOCOHCO3H |
| C4H8O4 | HO2C3CO3H | C4H8O4 | HO2C3CO3H |
| C9H12 | PBENZ | C9H12 | PBENZ |
| C7H6O2 | PHCOOH | C2H3NO5 | NO3CH2CO2H;PAN |
| C4H2O5 | MALNHYOHCO | C3H7NO4 | HO1C3NO3;PROLNO3;PROPOLNO3 |
| C4H3O5 | EPXDLCO3;MALANHYO | C2H4NO5 | ETHENO3O2 |
| C4H5O5 | BZFUO2;MALDIALO2 | C7H6O2 | PHCOOH |

| | | | |
|---|---|---|---|
| C5H9O4 | C4OHCO3 | C2H5NO5 | ETHO2HNO3 |
| C4H6O5 | MALDIALOOH;BZFUOOH | C4H2O5 | MALNHYOHCO |
| C5H10O4 | C4OHCO3H | C4H3O5 | EPXDLCO3;MALANHYO |
| C9H10O | PHCOET | C4H5O5 | BZFUO2;MALDIALO2 |
| C9H11O | PHC3O;PBENZO | C4H7NO4 | BUTALNO3 |
| C9H12O | PHC3OH;PBENZOL | C5H9O4 | C4OHCO3 |
| C7H5O3 | C6H5CO3 | C4H6O5 | MALDIALOOH;BZFUOOH |
| C7H9O3 | C7DCCO2 | C5H10O4 | C4OHCO3H |
| C4H3O6 | MALANHYO2 | C9H10O | PHCOET |
| C4H4O6 | MALANHYOOH | C3H5NO5 | PPN |
| C9H9O2 | PHCOETO | C9H11O | PHC3O;PBENZO |
| C9H11O2 | PHC3O2;PBENZO2;PCATEC1O | C2H2NO6 | NO3CH2CO3 |
| C8H11O3 | C815CO2O | C9H12O | PHC3OH;PBENZOL |
| C7H9O4 | C7DCCO3 | C2H3NO6 | PHAN;NO3CH2CO3H |
| C7H11O4 | C7DCO;PBFUO | C6H4NO3 | NPHEN1O |
| C6H9O5 | C5O45OHCO3 | C6H5NO3 | HOC6H4NO2 |
| C9H7O3 | PHCOCOCO | C7H9O3 | C7DCCO2 |
| C9H9O3 | PHCOETO2 | C4H2NO5 | NC4DCO2 |
| C9H11O3 | PCATEC1O2 | C4H3NO5 | NC4DCO2H |
| C8H11O4 | C815CO2O2 | C4H3O6 | MALANHYO2 |
| C7H9O5 | PMALANHYO | C4H4O6 | MALANHYOOH |
| C7H11O5 | C7DCO2;PBFUO2 | C4H7NO5 | PBN |
| C7H12O5 | C7DCOOH;PBFUOOH | C3H5NO6 | IPROPOLPAN;C3PAN1 |

| | | | |
|---|---|---|---|
| C9H7O4 | PHCOCOCO2 | C9H11O2 | PHC3O2;PBENZO2;PCATEC1O |
| C9H10O4 | C6PRCO4DB | C6H4NO4 | NPHEN1O2 |
| C8H9O5 | C8CO2DBCO3 | C6H5NO4 | NPHEN1OOH |
| C9H13O4 | PBZBIPERO;PPRBQO | C8H11O3 | C815CO2O |
| C8H10O5 | C8CO2DCO3H | C7H9O4 | C7DCCO3 |
| C8H11O5 | C8CO3OHO | C7H11O4 | C7DCO;PBFUO |
| C7H9O6 | C61CO3;PMALANHYO2 | C4H3NO6 | NBZFUONE;MALDIALPAN |
| C9H11O5 | PBZMUCCO3 | C6H9O5 | C5O45OHCO3 |
| C9H13O5 | PBENZOLO;PPRBQO2;PBZBIPERO2;PBZMUCO | C4H4NO6 | NBZFUO |
| C8H11O6 | C8CO3OHO2 | C4H5NO6 | CO2C3PAN |
| C8H12O6 | C83COOHOOH | C9H7O3 | PHCOCOCO |
| C9H11O6 | C8OHCO2CO3 | C3H3NO7 | HCOCOHPAN |
| C9H12O6 | C8OHO2CO3H | C4H7NO6 | C4PAN3 |
| C9H13O6 | PBZMUCO2;PBENZOLO2 | C9H9O3 | PHCOETO2 |
| C9H14O6 | PBZMUCOOH;PBENZOLOOH | C9H11O3 | PCATEC1O2 |
| | | C8H11O4 | C815CO2O2 |
| | | C7H11O5 | C7DCO2;PBFUO2 |
| | | C4H3NO7 | EPXDLPAN |
| | | C4H4NO7 | NBZFUO2 |
| | | C4H5NO7 | NBZFUOOH |
| | | C9H7O4 | PHCOCOCO2 |
| | | C5H9NO6 | C4OHPAN |

| | | | |
|---|---|---|---|
| | | C9H10NO3 | NPBNZ1O |
| | | C9H11NO3 | PHC3NO3;PBNZOHNO2 |
| | | C2H2N2O8 | NO3CH2PAN |
| | | C7H5NO5 | PBZN |
| | | C6H4N2O5 | DNPHEN |
| | | C8H9O5 | C8CO2DBCO3 |
| | | C9H13O4 | PBZBIPERO;PPRBQO |
| | | C7H8NO5 | NC4PDCO2 |
| | | C7H9NO5 | NC4PDCO2H |
| | | C8H11O5 | C8CO3OHO |
| | | C7H9O6 | C61CO3;PMALANHYO2 |
| | | C9H10NO4 | NPBNZ1O2 |
| | | C9H11NO4 | PNCATECH;NPBNZ1OOH |
| | | C9H11O5 | PBZMUCCO3 |
| | | C9H13O5 | PBENZOLO;PPRBQO2;PBZBIPERO2;PBZMUCO |
| | | C7H9NO6 | NPBFUONE;C7DCPAN |
| | | C8H11O6 | C8CO3OHO2 |
| | | C7H10NO6 | NPBFUO |
| | | C6H9NO7 | C5O45OHPAN |
| | | C9H11O6 | C8OHCO2CO3 |
| | | C9H13O6 | PBZMUCO2;PBENZOLO2 |
| | | C7H10NO7 | NPBFUO2 |

| | | | |
|---|---|---|---|
| | | C7H11NO7 | NPBFUOOH |
| | | C9H10N2O5 | DNPBNZOL |
| | | C9H10NO6 | NPPRBQO |
| | | C8H9NO7 | C8CO2DBPAN |
| | | C9H13NO6 | PBZBPERNO3 |
| | | C7H9NO8 | C61CPAN |
| | | C9H10NO7 | NPPRBQO2 |
| | | C9H11NO7 | NPPRBQOOH;PBZMUCPAN |
| | | C9H12NO7 | NPBNZOLO |
| | | C9H13NO7 | PBZMUCNO3;NPBNZOLOH |
| | | C6H5N2O9 | DNPHENO |
| | | C9H11NO8 | C8OHCO2PAN |
| | | C9H12NO8 | NPBNZOLO2;PNCATECO |
| | | C9H13NO8 | NPBNZOLOOH |
| | | C6H5N2O10 | DNPHENO2 |
| | | C6H6N2O10 | DNPHENOOH |
| | | C9H12NO9 | PNCATECO2 |
| | | C9H13NO9 | PNCATECOOH |
| | | C9H11N2O9 | DNPBNZLO |
| | | C6H4N3O11 | NDNPHENO |
| | | C9H11N2O10 | PNNCATECO;DNPBNZLO2 |
| | | C9H12N2O10 | DNPBNZLOOH |
| | | C6H4N3O12 | NDNPHENO2 |

| | | | |
|---|---|---|---|
| | | C6H5N3O12 | NDNPHENOOH |
| | | C9H11N2O11 | PNNCATECO2 |
| | | C9H12N2O11 | PNNCATCOOH |
| | | C9H10N3O11 | NDNPBNZLO |
| | | C9H10N3O12 | NDNPBNZLO2 |
| | | C9H11N3O12 | NDNPBZLOOH |
| | | | |

Table S27. MCM Ions not detected by Vocus for propylbenzene

| **MCM Ions not detected by Vocus for isopropylbenzene under low-NOx conditions** | | **MCM Ions not detected by Vocus for isopropylbenzene under medium-NOx conditions** | |
|---|---|---|---|
| **Formula** | **Corresponding MCM Ion(s)** | **Formula** | **Corresponding MCM Ion(s)** |
| C2H4 | C2H4 | C2H4 | C2H4 |
| CH2O | HCHO | CH2O | HCHO |
| CH3O | CH3O | CH3O | CH3O |
| CH4O | CH3OH | CH4O | CH3OH |
| C2H4O | CH3CHO | C2H4O | CH3CHO |
| C2H5O | C2H5O | C2H5O | C2H5O |
| CH2O2 | CH2OOA;HCOOH;CH2OO | CH2O2 | CH2OOA;HCOOH;CH2OO |
| C2H6O | C2H5OH | C2H6O | C2H5OH |
| CH3O2 | CH3O2 | CH3O2 | CH3O2 |
| CH4O2 | CH3OOH | CH4O2 | CH3OOH |
| C2HO2 | HCOCO | C2HO2 | HCOCO |
| C2H2O2 | GLYOX | C2H2O2 | GLYOX |

| | | | |
|---|---|---|---|
| C3H6O | CH3COCH3;C2H5CHO | C3H6O | CH3COCH3;C2H5CHO |
| C2H3O2 | HCOCH2O | C2H3O2 | HCOCH2O |
| C3H7O | NC3H7O;IC3H7O | C3H7O | NC3H7O;IC3H7O |
| C2H4O2 | HOCH2CHO;CH3CO2H | C2H4O2 | HOCH2CHO;CH3CO2H |
| C3H8O | IPROPOL;NPROPOL | C3H8O | IPROPOL;NPROPOL |
| C2H5O2 | HOCH2CH2O;C2H5O2 | C2H5O2 | HOCH2CH2O;C2H5O2 |
| C2H6O2 | ETHGLY;C2H5OOH | C2H6O2 | ETHGLY;C2H5OOH |
| C3H4O2 | MGLYOX | C3H4O2 | MGLYOX |
| C4H8O | C3H7CHO;IPRCHO | C4H8O | C3H7CHO;IPRCHO |
| C3H5O2 | PROPALO;CH3COCH2O | C3H5O2 | PROPALO;CH3COCH2O |
| C2H2O3 | HCOCO2H;GLYOO;GLYOOA | C2H2O3 | HCOCO2H;GLYOO;GLYOOA |
| C2H3O3 | HCOCH2O2;CH3CO3 | C2H3O3 | HCOCH2O2;CH3CO3 |
| C3H7O2 | HO1C3O;IC3H7O2;HYPROPO;IPROPOLO;NC3H7O2 | C3H7O2 | HO1C3O;IC3H7O2;HYPROPO;IPROPOLO;NC3H7O2 |
| C2H4O3 | CH3CO3H;HOCH2CO2H;HCOCH2OOH | C2H4O3 | CH3CO3H;HOCH2CO2H;HCOCH2OOH |
| C2H5O3 | HOCH2CH2O2 | CH3NO3 | CH3NO3 |
| C2H6O3 | HYETHO2H | C2H5O3 | HOCH2CH2O2 |
| C3H3O3 | C3DIALO | C2H6O3 | HYETHO2H |
| C4H7O2 | BUTALO;IBUTALBO;M2PROPAL2O | C4H7O2 | BUTALO;IBUTALBO;M2PROPAL2O |
| C2HO4 | HCOCO3 | C2HO4 | HCOCO3 |

| | | | |
|---|---|---|---|
| C3H5O3 | PROPALO2;CH3COCH2O2;C2H5CO3 | C3H5O3 | PROPALO2;CH3COCH2O2;C2H5CO3 |
| C2H2O4 | HCOCO3H | C2H2O4 | HCOCO3H |
| C2H3O4 | HOCH2CO3 | C2H3O4 | HOCH2CO3 |
| C3H7O3 | HO1C3O2;IPROPOLO2;HYPROPO2 | C2H5NO3 | C2H5NO3 |
| C2H4O4 | HOCH2CO3H | C2H4O4 | HOCH2CO3H |
| C6H5O | C6H5O | CH3NO4 | CH3O2NO2 |
| C4H2O3 | MALANHY | C6H5O | C6H5O |
| C4H3O3 | MALDIALCO2 | C4H2O3 | MALANHY |
| C5H9O2 | M3BUTAL2O | C4H3O3 | MALDIALCO2 |
| C3H3O4 | C3DIALO2 | C5H9O2 | M3BUTAL2O |
| C4H7O3 | BUTALO2;IBUTALCO2;IPRCO3;C3H7CO3;IBUTALBO2 | C3H3O4 | C3DIALO2 |
| C3H5O4 | CH3CHOHCO3;HOC2H4CO3 | C4H7O3 | BUTALO2;IBUTALCO2;IPRCO3;C3H7CO3;IBUTALBO2 |
| C6H5O2 | C6H5O2 | C2H3NO4 | NO3CH2CHO |
| C4H2O4 | CO2C4DIAL | C3H5O4 | CH3CHOHCO3;HOC2H4CO3 |
| C4H3O4 | MALDIALCO3 | C3H7NO3 | NC3H7NO3;IC3H7NO3 |
| C4H4O4 | EPXDLCO2H;HOCOC4DIAL;BZFUCO;CO14O3CHO;MALDALCO3H | C2H4NO4 | ETHENO3O |
| C5H8O3 | IPGLYOXOH | C2H5NO4 | ETHOHNO3 |

| | | | |
|---|---|---|---|
| C4H5O4 | BZFUO;MALDIALO;IBUDIALCO3;CO2C3CO3 | C6H5O2 | C6H5O2 |
| C5H9O3 | IC4CHOAO2;IPGLOOB;IPGLOO | C6H6O2 | C6H5OOH |
| C4H6O4 | HOHOC4DIAL;BZFUOH;PRPAL2CO3H;CO2C3CO3H | C4H2O4 | CO2C4DIAL |
| C5H10O3 | IC4CHOAOOH | C4H3O4 | MALDIALCO3 |
| C3H3O5 | HCOCOHCO3 | C4H4O4 | EPXDLCO2H;HOCOC4DIAL;BZFUCO;CO14O3CHO;MALDALCO3H |
| C4H7O4 | IPRHOCO3;HOIPRCO3;HO2C3CO3 | C5H8O3 | IPGLYOXOH |
| C3H4O5 | HCOCOHCO3H | C4H5O4 | BZFUO;MALDIALO;IBUDIALCO3;CO2C3CO3 |
| C4H8O4 | HOIPRCO3H;IPRHOCO3H;HO2C3CO3H | C5H9O3 | IC4CHOAO2;IPGLOOB;IPGLOO |
| C8H8O | PHCOME | C4H6O4 | HOHOC4DIAL;BZFUOH;PRPAL2CO3H;CO2C3CO3H |
| C9H12 | IPBENZ | C5H10O3 | IC4CHOAOOH |
| C7H6O2 | PHCOOH | C3H3O5 | HCOCOHCO3 |
| C4H2O5 | MALNHYOHCO | C4H7O4 | IPRHOCO3;HOIPRCO3;HO2C3CO3 |
| C4H3O5 | MALANHYO;EPXDLCO3 | C3H4O5 | HCOCOHCO3H |

| | | | |
|---|---|---|---|
| C4H5O5 | BZFUO2;MALDIALO2 | C4H8O4 | HOIPRCO3H;IPRHOCO3H;HO2C3CO3H |
| C5H9O4 | C3M3OH2CO3 | C8H8O | PHCOME |
| C8H6O2 | PHGLYOX | C9H12 | IPBENZ |
| C8H7O2 | PHCOMEO | C2H3NO5 | PAN;NO3CH2CO2H |
| C9H11O | IPBENZO;PHIC3O | C3H7NO4 | HO1C3NO3;PROLNO3;PROPOLNO3 |
| C9H12O | PHIC3OH;IPBENZOL | C2H4NO5 | ETHENO3O2 |
| C7H5O3 | C6H5CO3 | C7H6O2 | PHCOOH |
| C7H9O3 | IC7DCCO2 | C2H5NO5 | ETHO2HNO3 |
| C4H3O6 | MALANHYO2 | C4H2O5 | MALNHYOHCO |
| C4H4O6 | MALANHYOOH | C4H3O5 | MALANHYO;EPXDLCO3 |
| C8H7O3 | PHCOMEO2 | C4H5O5 | BZFUO2;MALDIALO2 |
| C9H11O2 | PHIC3O2;IPCATEC1O;IPBENZO2 | C4H7NO4 | IBUALANO3;BUTALNO3 |
| C8H11O3 | C7M15CO2O | C5H9O4 | C3M3OH2CO3 |
| C7H9O4 | IC7DCCO3 | C8H6O2 | PHGLYOX |
| C7H11O4 | IC7DCO;IPBFUO | C3H5NO5 | PPN |
| C6H9O5 | C4MOHOCO3 | C9H11O | IPBENZO;PHIC3O |
| C9H11O3 | IPCATEC1O2 | C2H2NO6 | NO3CH2CO3 |
| C8H11O4 | C7M15CO2O2 | C9H12O | PHIC3OH;IPBENZOL |
| C7H9O5 | IPMALANHYO | C2H3NO6 | PHAN;NO3CH2CO3H |
| C7H11O5 | IC7DCO2;IPBFUO2 | C6H4NO3 | NPHEN1O |

| | | | |
|---|---|---|---|
| C9H10O4 | C6IPRCO4DB;IPRBQCO | C6H5NO3 | HOC6H4NO2 |
| C9H11O4 | IPRBQO | C7H9O3 | IC7DCCO2 |
| C8H9O5 | C8DBCO2CO3;C8CO2DBCO3 | C4H2NO5 | NC4DCO2 |
| C9H13O4 | IPBZBIPRO | C4H3NO5 | NC4DCO2H |
| C8H11O5 | C7MCO3OHO | C4H3O6 | MALANHYO2 |
| C7H9O6 | C61CO3;C62CO3;IPMALNHYO2 | C4H4O6 | MALANHYOOH |
| C9H11O5 | IPRBQO2;IPBZMUCCO3 | C4H7NO5 | PIPN;PBN |
| C9H13O5 | IPBZBIPRO2;IPBZMUCO;IPBENZOLO | C3H5NO6 | C3PAN1;IPROPOLPAN |
| C8H11O6 | C7MCO3OHO2 | C8H7O3 | PHCOMEO2 |
| C9H11O6 | C8CO2OHCO3;C8OHCO2CO3 | C9H11O2 | PHIC3O2;IPCATEC1O;IPBENZO2 |
| C9H12O6 | C8O2OHCO3H;C8OHO2CO3H | C6H4NO4 | NPHEN1O2 |
| C9H13O6 | IPBZMUCO2;IPBENZOLO2 | C6H5NO4 | NPHEN1OOH |
| | | C8H11O3 | C7M15CO2O |
| | | C7H9O4 | IC7DCCO3 |
| | | C7H11O4 | IC7DCO;IPBFUO |
| | | C4H3NO6 | NBZFUONE;MALDIALPAN |
| | | C6H9O5 | C4MOHOCO3 |
| | | C4H4NO6 | NBZFUO |
| | | C4H5NO6 | CO2C3PAN;IBUDIALPAN |
| | | C3H3NO7 | HCOCOHPAN |

| | | | |
|---|---|---|---|
| | | C4H7NO6 | C4PAN4;C4PAN5;C4PAN3 |
| | | C9H11O3 | IPCATEC1O2 |
| | | C8H11O4 | C7M15CO2O2 |
| | | C7H9O5 | IPMALANHYO |
| | | C7H11O5 | IC7DCO2;IPBFUO2 |
| | | C4H3NO7 | EPXDLPAN |
| | | C4H4NO7 | NBZFUO2 |
| | | C4H5NO7 | NBZFUOOH |
| | | C5H9NO6 | C3M3OH2PAN |
| | | C9H10NO3 | NIPBNZ1O |
| | | C9H11NO3 | IPBNZOHNO2;PHIC3NO3 |
| | | C2H2N2O8 | NO3CH2PAN |
| | | C9H10O4 | C6IPRCO4DB;IPRBQCO |
| | | C7H5NO5 | PBZN |
| | | C6H4N2O5 | DNPHEN |
| | | C8H9O5 | C8DBCO2CO3;C8CO2DBCO3 |
| | | C9H13O4 | IPBZBIPRO |
| | | C7H8NO5 | NC4IPDCO2 |
| | | C7H9NO5 | NC4IPDCO2H |
| | | C8H11O5 | C7MCO3OHO |
| | | C7H9O6 | C61CO3;C62CO3;IPMALNHYO2 |
| | | C9H10NO4 | NIPBNZ1O2 |

| | | | |
|---|---|---|---|
| | | C9H11NO4 | NIPBNZ1OOH;IPNCATECH |
| | | C9H11O5 | IPRBQO2;IPBZMUCCO3 |
| | | C9H13O5 | IPBZBIPRO2;IPBZMUCO;IPBENZOLO |
| | | C7H9NO6 | IC7DCPAN;NIPBFUONE |
| | | C8H11O6 | C7MCO3OHO2 |
| | | C7H10NO6 | NIPBFUO |
| | | C6H9NO7 | C4MOHOPAN |
| | | C9H11O6 | C8CO2OHCO3;C8OHCO2CO3 |
| | | C9H12O6 | C8O2OHCO3H;C8OHO2CO3H |
| | | C9H13O6 | IPBZMUCO2;IPBENZOLO2 |
| | | C7H10NO7 | NIPBFUO2 |
| | | C7H11NO7 | NIPBFUOOH |
| | | C9H10N2O5 | DNIPBNZOL |
| | | C9H10NO6 | NIPRBQO |
| | | C8H9NO7 | C8CO2DBPAN;C8DBCO2PAN |
| | | C9H13NO6 | IPBZBPRNO3 |
| | | C7H9NO8 | C62CPAN;C61CPAN |
| | | C9H10NO7 | NIPRBQO2 |
| | | C9H11NO7 | IPBZMUCPAN;NIPRBQOOH |
| | | C9H12NO7 | NIPBNZOLO |
| | | C9H13NO7 | NIPBNZOLOH;IPBZMUCNO3 |
| | | C6H5N2O9 | DNPHENO |

| | | | |
|---|---|---|---|
| | | C9H11NO8 | C8CO2OHPAN;C8OHCO2PAN |
| | | C9H12NO8 | IPNCATECO;NIPBNZOLO2 |
| | | C9H13NO8 | NIPBZOLOOH |
| | | C6H5N2O10 | DNPHENO2 |
| | | C6H6N2O10 | DNPHENOOH |
| | | C9H12NO9 | IPNCATECO2 |
| | | C9H13NO9 | IPNCATCOOH |
| | | C9H11N2O9 | DNIPBNZLO |
| | | C6H4N3O11 | NDNPHENO |
| | | C9H11N2O10 | DNIPBNZLO2;IPNNCATCO |
| | | C9H12N2O10 | DNIPBZLOOH |
| | | C6H4N3O12 | NDNPHENO2 |
| | | C6H5N3O12 | NDNPHENOOH |
| | | C9H11N2O11 | IPNNCATCO2 |
| | | C9H12N2O11 | IPNNCATOOH |
| | | C9H10N3O11 | NDNIPBZLO |
| | | C9H10N3O12 | NDNIPBZLO2 |
| | | C9H11N3O12 | NDNIPBLOOH |

Table S28. MCM Ions not detected by Vocus for isopropylbenzene