# SUPPORTING INFORMATION

# On the characterization of tetrahydrofuran low-temperature oxidation products including keto-hydroperoxides and highly oxygenated organic molecules (HOMs): An experimental study.

Nesrine Belhadj[1,2], Roland Benoit[1], Philippe Dagaut[1, *], Maxence Lailliau[1,2]

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**Table S1**. Analytical conditions.

| APCI source parameters | FIA mode<br>Flow rate: 1-3 µL/min | HPLC, 2 µL of sample<br>Flow rate: 250 µL | HPLC, 0.8 µL of sample<br>Flow rate: 100 µL |
|---|---|---|---|
| Sheat gas flow rate | 9 | 55 | 45 |
| Aux flow rate | 0 | 15 | 5 |
| Sweep gas flow rate | 0 | 0 | 0 |
| Discharge voltage (kV) | 3.77 | 3.88 | 3.8 |
| Discharge current (µA) | 1.2 | 3.8 | 3.0 |
| Capillary temperature (°C) | 274 | 320 | 300 |
| S-lens RF level | 50 | 50 | 50 |
| Vaporizer temperature (°C) | 117 | 150 | 150 |

**Table S2.** Composition of elution solvents used in UHPLC and HPLC analyses.

| Column (oven temperature 40 °C) | Mobile phase - Flow rate | Separated products |
|---|---|---|
| C18 UHPLC column | 100 % Water - 100 ul/min | γ-Butyrolactone (Rt 7.96 min)<br>THF-3-one (Rt 8.44 min)<br>3,4-epoxy-THF (Rt 4.86 min)<br>2,3-DHF (Rt 28.2 min)<br>2,5-DHF (Rt 21.1 min)<br>Cyclopropane carboxaldehyde (Rt 15.30 min)<br>Furan (Rt 7.98 min) |
| Silica HPLC column | 100 % Acetonitrile - 250ul/min | KHPs |
| Hypercarb™ PGC HPLC column | 100 % Acetonitrile – 100 ul/min | KHPs |

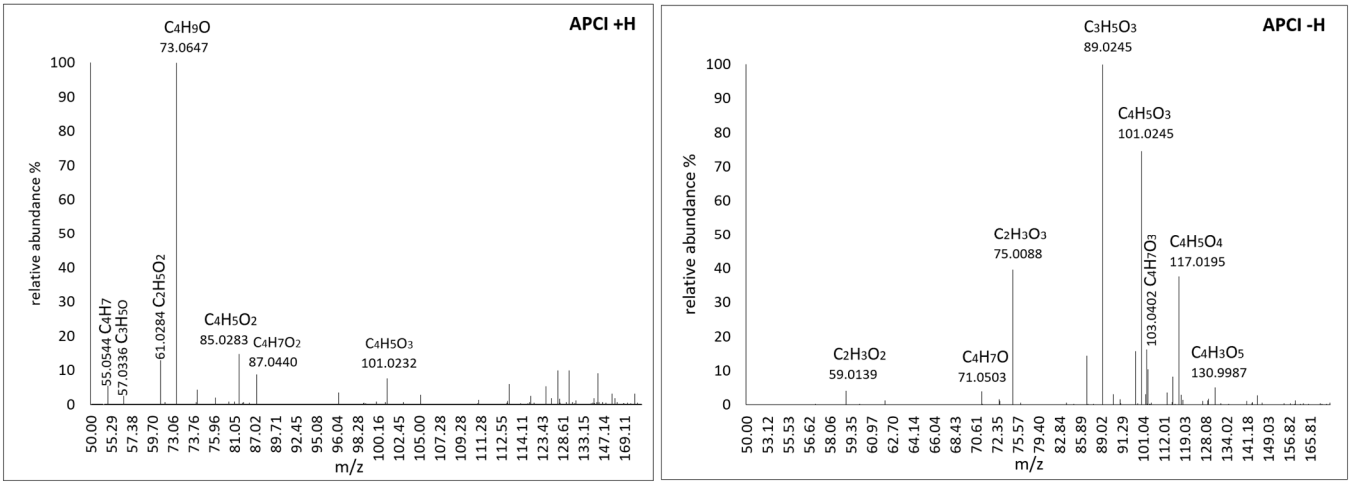
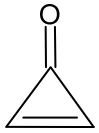
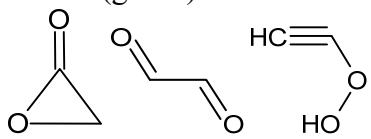
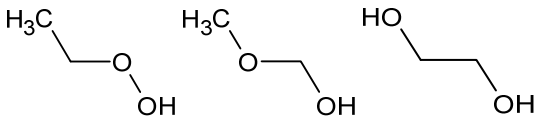
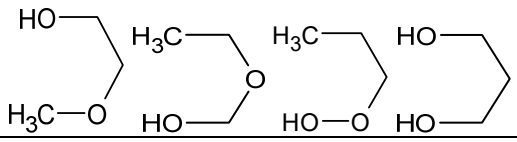
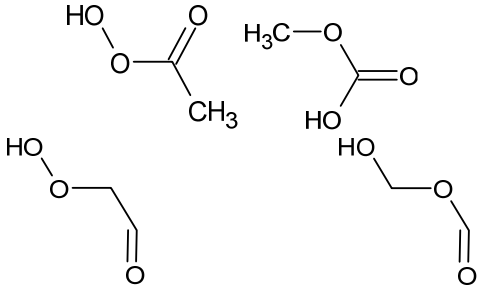
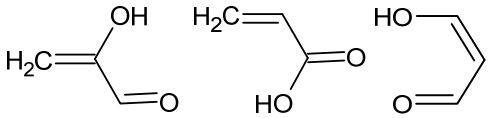
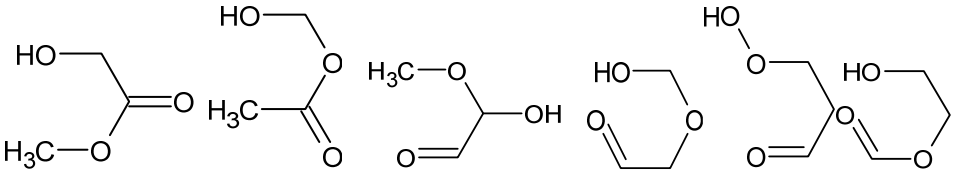
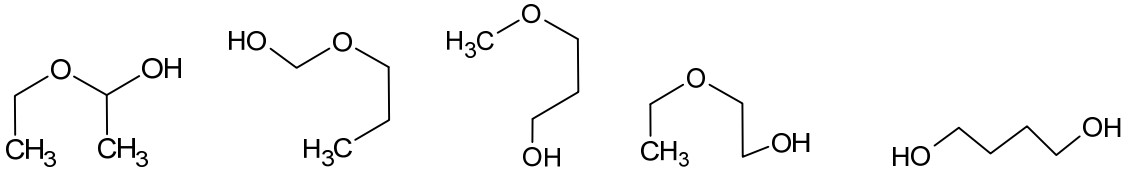
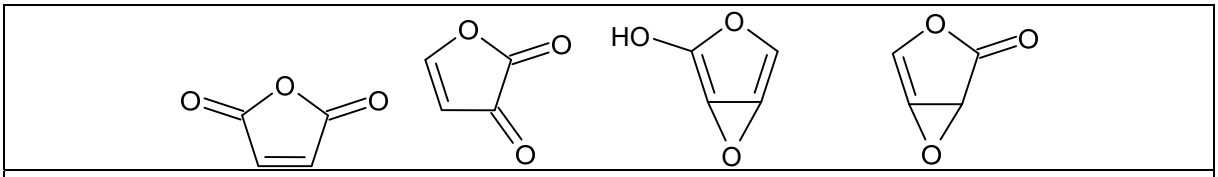


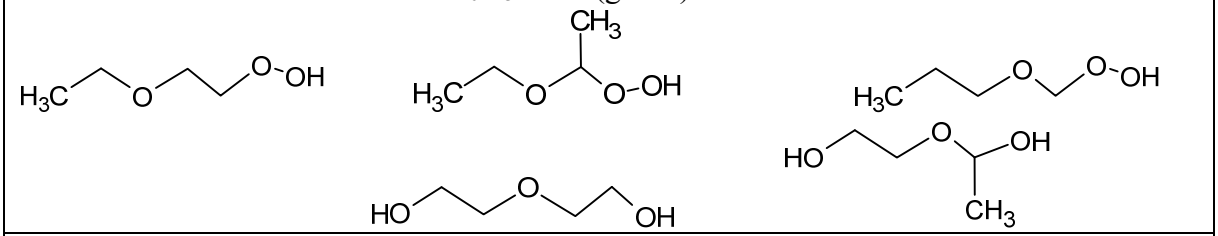

**Figure S1.** Mass spectra obtained by FIA, APCI (+) and (-) for the sample taken at 600 K

**Table S3.** Potential isomers for the newly detected species

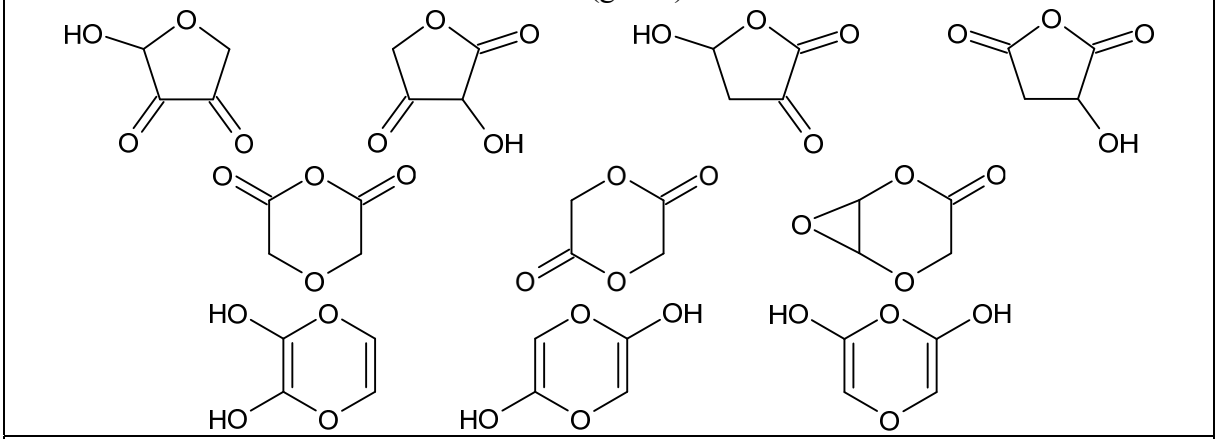
| | |
|---|---|
| **$C_3H_2O$**<br>M (g/mol) 54.0105<br>  | **$C_2H_2O_2$**<br>M (g/mol) 58.0054<br>  |
| **$C_2H_6O_2$**<br>M (g/mol) 62.0367<br>  | **$C_3H_8O_2$**<br>M (g/mol) 76.0524<br>  |
| **$C_2H_4O_3$**<br>M (g/mol) 76.0160<br>  | **$C_3H_4O_2$**<br>M (g/mol) 72.0211<br>  |
| **$C_3H_6O_3$**<br>M (g/mol) 90.0316<br>  | |
| **$C_4H_2O_2$** M (g/mol) 82.0054<br> | |
| **$C_4H_{10}O_2$** M (g/mol) 90.0680<br>  | |
| **$C_7H_8$** M (g/mol) 92.0620<br> | |
| **$C_4H_2O_3$** M (g/mol) 98.0003 | |



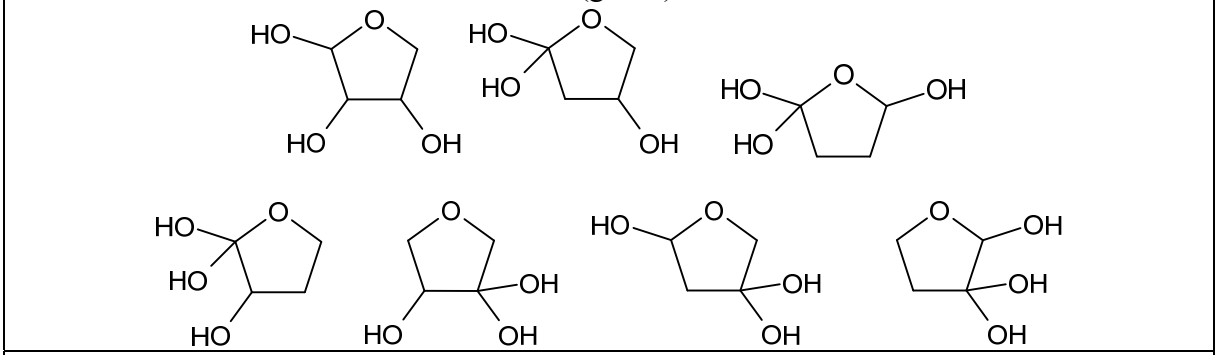
**$C_4H_{10}O_3$** M (g/mol) 106.0629



**$C_4H_4O_4$** M (g/mol) 116.0109



**$C_4H_8O_4$** M (g/mol) 120.0422



**$C_4H_6O_5$** M (g/mol) 134.0215

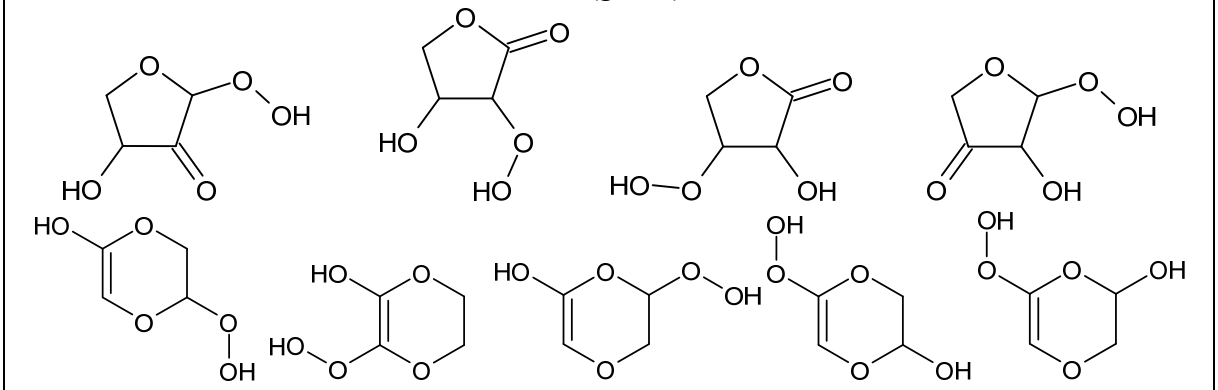


**Table S4.** MS/MS analyses of KHPs

| Retention time (min) | Fragment and relative intensities | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | 52.0182 | 55.0178 $C_3H_3O$ | 57.0335 $C_3H_5O$ | 73.0282 $C_3H_5O_2$ | 79.0288 | 84.0204 | 85.0281 $C_4H_5O_2$ | 91.0540 $C_7H_7$ | 101.0230 $C_4H_5O_3$ | 119.0338 $C_4H_7O_4$ |
| 4.28 | 12% | 100% | 16% | 25% | 43% | 21% | 27% | 20% | 15% | 6% |
| 4.49 | 25% | 90% | 12% | 35% | 100% | 19% | 21% | 46% | 23% | 4% |
| 4.53 | 26% | 92% | 12% | 30% | 100% | 19% | 21% | 51% | 23% | 5% |
| 5.06 | 24% | 62% | 2% | 28% | 100% | 1% | 2% | 50% | 26% | 2% |
| 5.20 | 23% | 34% | 2% | 35% | 100% | 2% | 2% | 50% | 64% | 3% |

Formation of fragments

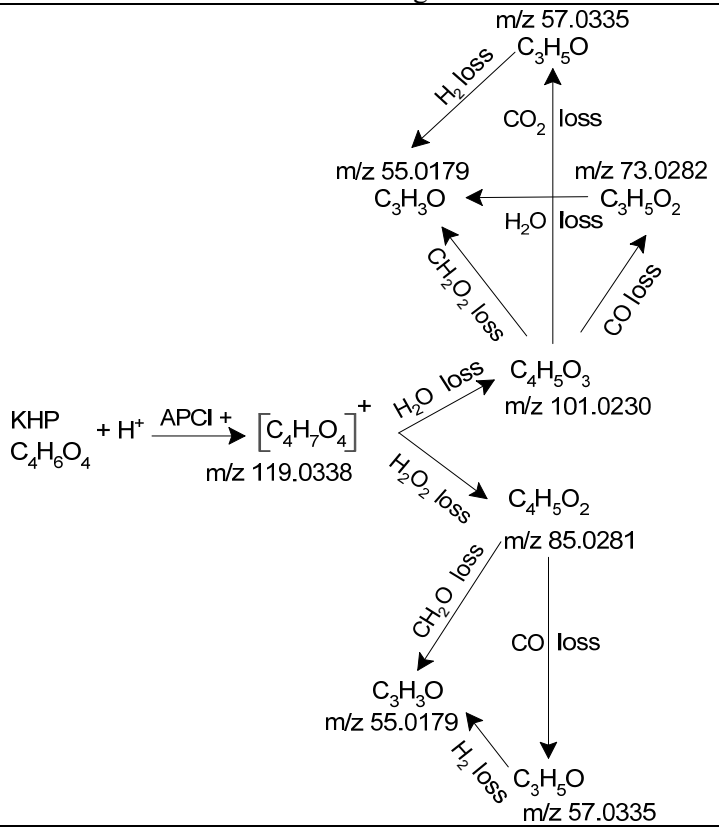


Table S5. MS/MS data for KHPs

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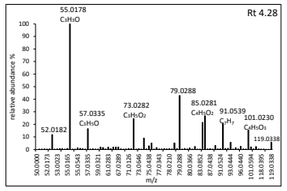
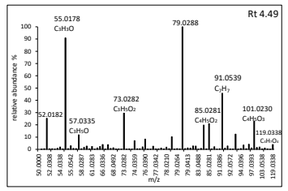
[2] Université d'Orléans, Avenue du Parc Floral, 45067 Orléans Cedex 2, France

KHPs MSMS spectra (HCD 10 eV)

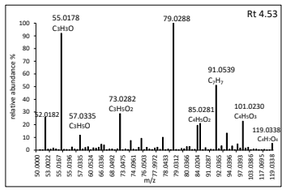
| m/z | Relative | Composition |
|---|---|---|
| 50.0000 | 0 | |
| 50.0151 | 0.26807528 | |
| 51.0104 | 0.22176224 | |
| 51.0231 | 0.32761263 | $C_4H_3$ |
| 52.0173 | 0.20591452 | |
| 52.0176 | 0.30405733 | |
| 52.0183 | 11.7914295 | |
| 52.0308 | 0.19585776 | |
| 53.0023 | 0.35717075 | $C_3HO$ |
| 53.9975 | 0.64314608 | |
| 54.0339 | 0.64783875 | |
| 55.0071 | 0.22789489 | |
| 55.0165 | 0.75342044 | |
| 55.0178 | 100 | $C_3H_5O$ |
| 55.0201 | 0.20172841 | |
| 55.0223 | 0.25325143 | |
| 55.0543 | 1.24553647 | $C_4H_7$ |
| 56.0212 | 0.81060757 | |
| 56.0256 | 0.67237062 | |
| 56.0494 | 0.23724682 | |
| 57.0335 | 16.4831504 | $C_3H_5O$ |
| 57.0345 | 0.23569155 | |
| 58.0286 | 0.48193574 | |
| 58.0368 | 0.24889916 | |
| 59.0321 | 0.2694279 | |
| 59.0491 | 1.93719012 | $C_3H_7O$ |
| 60.0443 | 1.44970638 | |
| 60.0524 | 0.31504221 | |
| 61.0283 | 1.82625409 | $C_3H_5O_2$ |
| 65.0384 | 0.51221216 | $C_5H_5$ |
| 66.0210 | 1.82501123 | |
| 66.0336 | 1.91593898 | |
| 67.0289 | 1.8400532 | |
| 68.0241 | 0.41331495 | |
| 68.0493 | 0.28365609 | |
| 69.0207 | 0.31927486 | |
| 71.0261 | 0.72388819 | $C_3H_7O_2$ |
| 72.0441 | 0.41539913 | |
| 73.0282 | 24.5139734 | $C_3H_5O_2$ |
| 73.0475 | 0.23408881 | |
| 73.0646 | 0.55601123 | $C_4H_9O$ |
| 74.0315 | 0.22653486 | |
| 74.0360 | 8.97590598 | |
| 74.0961 | 0.30932009 | |
| 75.0438 | 2.78311207 | $C_3H_7O_2$ |
| 76.0390 | 5.02508667 | |
| 76.0503 | 0.23773429 | |
| 77.0131 | 1.45709545 | |
| 77.0343 | 0.29116262 | |
| 77.0594 | 0.32687616 | $C_4H_9O_2$ |
| 77.9972 | 0.63008548 | |
| 78.0085 | 0.3481307 | |
| 78.0210 | 0.60230573 | |
| 78.0292 | 0.3102829 | |
| 78.0335 | 5.05958438 | |
| 79.0279 | 0.63822814 | |
| 79.0288 | 42.9576349 | |
| 79.0387 | 0.22999213 | $C_3H_7O_3$ |
| 79.0414 | 0.73039137 | |
| 79.0540 | 0.29554122 | $C_6H_7$ |
| 80.0366 | 1.18779286 | |
| 80.2646 | 0.19521216 | |
| 83.0125 | 2.26620905 | $C_4H_5O_2$ |
| 83.0489 | 0.23817921 | $C_5H_7O$ |
| 83.0852 | 0.22441344 | $C_6H_{11}$ |
| 84.0203 | 21.5421171 | |
| 85.0281 | 26.7579461 | $C_4H_5O_2$ |
| 86.0314 | 0.31378073 | |
| 87.0438 | 0.55459223 | $C_4H_7O_2$ |
| 89.0230 | 0.20852313 | $C_4H_9O_3$ |
| 89.0594 | 3.16584304 | $C_4H_9O_2$ |
| 91.0386 | 0.31285103 | $C_4H_5O_3$ |
| 91.0524 | 0.39784062 | |
| 91.0539 | 20.4618205 | $C_7H_7$ |
| 92.0366 | 0.73138756 | |
| 92.0492 | 0.86105046 | |
| 93.0444 | 5.66819545 | |
| 94.0396 | 0.25619176 | |
| 95.0237 | 1.41217291 | |
| 96.0314 | 0.34734902 | |
| 96.0440 | 2.45077655 | |
| 97.0393 | 0.34738312 | |
| 100.6905 | 0.19850678 | |
| 101.0230 | 15.4787125 | $C_4H_5O_3$ |
| 101.0594 | 1.98790934 | $C_4H_9O_2$ |
| 102.0264 | 0.34490347 | |
| 102.0308 | 2.17911075 | |
| 110.0597 | 0.31556618 | |
| 118.0395 | 0.19716948 | |
| 118.0521 | 0.23360027 | |
| 118.0700 | 0.01444546 | |
| 119.0122 | 0.02051246 | |
| 119.0338 | 5.73254783 | $C_4H_7O_4$ |



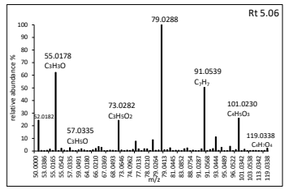

| m/z | Relative | Composition |
|---|---|---|
| 50.0000 | 0 | |
| 50.0152 | 0.2908455 | |
| 51.0230 | 0.54519898 | $C_4H_3$ |
| 52.0182 | 25.273922 | |
| 52.0308 | 0.49620067 | |
| 53.0022 | 0.57531441 | $C_3HO$ |
| 53.0386 | 0.29147593 | $C_4H_5$ |
| 53.9975 | 0.90690987 | |
| 54.0338 | 1.94909074 | |
| 55.0165 | 0.48932082 | |
| 55.0178 | 90.8501886 | $C_3H_5O$ |
| 55.0192 | 0.66493148 | |
| 55.0542 | 2.89009671 | $C_4H_7$ |
| 56.0212 | 0.80486309 | |
| 56.0256 | 0.63533602 | |
| 57.0335 | 11.8851778 | $C_3H_5O$ |
| 58.0287 | 0.56714568 | |
| 59.0490 | 1.66840061 | $C_3H_7O$ |
| 60.0443 | 2.64154709 | |
| 60.0524 | 0.50129219 | |
| 61.0283 | 2.32934643 | $C_3H_5O_2$ |
| 65.0257 | 0.3728344 | |
| 65.0384 | 1.14292068 | $C_5H_5$ |
| 66.0210 | 2.36494956 | |
| 66.0336 | 3.95666258 | |
| 66.0345 | 0.34084054 | |
| 67.0288 | 3.8711526 | |
| 68.0241 | 0.78857607 | |
| 68.0492 | 1.24040633 | |
| 69.0207 | 0.33767554 | |
| 71.0125 | 0.460135 | $C_3H_3O_2$ |
| 71.0488 | 0.34326643 | $C_4H_7O$ |
| 73.0282 | 29.5608941 | $C_3H_5O_2$ |
| 73.0475 | 0.31962447 | |
| 73.0646 | 0.47917994 | $C_4H_9O$ |
| 74.0315 | 0.33655038 | |
| 74.0359 | 7.08835434 | |
| 74.0962 | 0.53470052 | |
| 75.0324 | 0.49375744 | |
| 75.0438 | 2.03036361 | $C_3H_7O_2$ |
| 76.0390 | 8.35256847 | |
| 76.0402 | 0.35457899 | |
| 76.0502 | 0.31260411 | |
| 77.0131 | 2.50947565 | |
| 77.0342 | 0.40291567 | |
| 77.0594 | 0.40432375 | $C_4H_9O_2$ |
| 77.9972 | 1.03434108 | |
| 78.0084 | 0.32054588 | |
| 78.0210 | 1.82353733 | |
| 78.0291 | 0.58996775 | |
| 78.0336 | 10.2612693 | |
| 78.0628 | 0.322404 | |
| 79.0264 | 0.62657681 | |
| 79.0269 | 0.47739477 | |
| 79.0288 | 100 | |
| 79.0312 | 0.69085717 | |
| 79.0413 | 1.12823981 | |
| 79.0539 | 0.96107884 | $C_6H_7$ |
| 80.0366 | 2.77085767 | |
| 83.0124 | 2.64332066 | $C_4H_5O_2$ |
| 83.0488 | 0.36291597 | $C_5H_7O$ |
| 83.0852 | 0.71644359 | $C_6H_{11}$ |
| 84.0204 | 19.8072347 | |
| 84.0216 | 0.43882639 | |
| 85.0281 | 20.9945809 | $C_4H_5O_2$ |
| 86.0314 | 0.44992709 | |
| 89.0593 | 2.09504018 | $C_4H_9O_2$ |
| 91.0288 | 0.36227027 | |
| 91.0386 | 0.57024534 | $C_4H_5O_3$ |
| 91.0539 | 45.8093584 | $C_7H_7$ |
| 92.0366 | 0.93880218 | |
| 92.0491 | 2.79941775 | |
| 92.0572 | 0.48979033 | |
| 93.0429 | 0.30903488 | |
| 93.0444 | 12.4142387 | |
| 93.0459 | 0.35159502 | |
| 94.0396 | 0.60963371 | |
| 95.0236 | 3.47958668 | |
| 96.0314 | 0.49751687 | |
| 96.0440 | 4.14239408 | |
| 97.0393 | 1.15300147 | |
| 101.0229 | 22.9550316 | $C_4H_5O_3$ |
| 101.0593 | 1.54897859 | $C_4H_9O_2$ |
| 102.0307 | 1.95578105 | |
| 103.0538 | 0.40535279 | $C_4H_7$ |
| 110.0597 | 1.07126717 | |
| 111.0549 | 0.45209789 | |
| 118.0700 | 0.00523214 | |
| 119.0338 | 3.93901202 | $C_4H_7O_4$ |

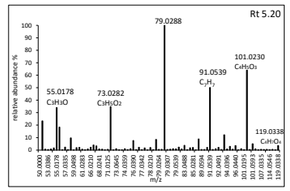



| m/z | Relative | Composition |
|---|---|---|
| 50.0000 | 0 | |
| 50.0152 | 0.35632561 | |
| 51.0230 | 0.31034797 | $C_4H_3$ |
| 52.0182 | 25.8120912 | |
| 53.0022 | 0.63453267 | $C_3HO$ |
| 53.9975 | 0.70867415 | |
| 54.0338 | 1.61128809 | |
| 55.0164 | 0.85720519 | |
| 55.0167 | 0.41965429 | |
| 55.0178 | 92.0366037 | $C_3H_5O$ |
| 55.0189 | 0.55814912 | |
| 55.0193 | 0.4858956 | |
| 55.0196 | 0.41006018 | |
| 55.0542 | 2.43615483 | $C_4H_7$ |
| 56.0212 | 0.80881221 | |
| 56.0256 | 0.51572318 | |
| 57.0335 | 11.7464012 | $C_3H_5O$ |
| 58.0287 | 0.80886375 | |
| 59.0490 | 2.04329729 | $C_3H_7O$ |
| 60.0443 | 2.66928544 | |
| 60.0524 | 0.37281499 | |
| 61.0283 | 1.76773009 | $C_3H_5O_2$ |
| 65.0384 | 1.441024 | $C_5H_5$ |
| 66.0210 | 2.2387532 | |
| 66.0336 | 4.56367847 | |
| 67.0288 | 3.90954692 | |
| 68.0128 | 0.32887209 | |
| 68.0241 | 0.79234948 | |
| 68.0492 | 0.91584419 | |
| 69.0207 | 0.32258845 | |
| 71.0125 | 0.97822548 | $C_3H_3O_2$ |
| 73.0282 | 28.6756045 | $C_3H_5O_2$ |
| 73.0475 | 0.32583476 | |
| 73.0645 | 0.79070156 | $C_4H_9O$ |
| 74.0315 | 0.51366429 | |
| 74.0359 | 7.48528263 | |
| 74.0961 | 0.71220053 | |
| 75.0324 | 0.40880606 | |
| 75.0438 | 2.11020957 | $C_3H_7O_2$ |
| 76.0390 | 9.23161695 | |
| 76.0503 | 0.43584515 | |
| 77.0131 | 2.09400576 | |
| 77.0343 | 0.86276324 | |
| 77.0594 | 0.52705423 | $C_4H_9O_2$ |
| 77.9972 | 1.57304371 | |
| 78.0210 | 2.26586365 | |
| 78.0291 | 0.55800316 | |
| 78.0336 | 10.1096808 | |
| 78.0433 | 0.41893762 | |
| 79.0264 | 0.81201652 | |
| 79.0269 | 0.34895941 | |
| 79.0288 | 100 | |
| 79.0312 | 0.47779584 | |
| 79.0318 | 0.35753663 | |
| 79.0413 | 1.24732143 | |
| 79.0539 | 0.97843447 | $C_6H_7$ |
| 80.0366 | 2.71616932 | |
| 83.0124 | 2.80264531 | $C_4H_5O_2$ |
| 83.0488 | 0.44799172 | $C_5H_7O$ |
| 83.0852 | 0.56361455 | $C_6H_{11}$ |
| 84.0204 | 19.4863488 | |
| 85.0281 | 21.0781252 | $C_4H_5O_2$ |
| 86.0315 | 0.33507471 | |
| 89.0593 | 1.93756889 | $C_4H_9O_2$ |
| 91.0287 | 0.40240204 | |
| 91.0387 | 0.71105652 | $C_4H_5O_3$ |
| 91.0509 | 0.4745804 | |
| 91.0539 | 51.063067 | $C_7H_7$ |
| 92.0365 | 1.07267007 | |
| 92.0491 | 3.37952972 | |
| 92.0572 | 0.45566886 | |
| 93.0444 | 13.414437 | |
| 94.0396 | 0.70571733 | |
| 95.0236 | 3.22327783 | |
| 96.0314 | 0.36115544 | |
| 96.0440 | 4.86961343 | |
| 97.0393 | 1.57535369 | |
| 101.0229 | 22.7380903 | $C_4H_5O_3$ |
| 101.0593 | 1.64714932 | $C_4H_9O_2$ |
| 102.0308 | 2.18987323 | |
| 103.0386 | 0.40967639 | $C_4H_7O_3$ |
| 110.0596 | 0.85113219 | |
| 111.0549 | 0.77454402 | |
| 113.0342 | 0.3816311 | |
| 117.0695 | 0.33349152 | $C_8H_9$ |
| 118.0396 | 0.56608248 | |
| 118.0520 | 0.01200145 | |
| 118.0523 | 0.29462848 | |
| 119.0338 | 5.2790844 | $C_4H_7O_4$ |




| m/z | Relative | Composition |
|---|---|---|
| 50.0000 | 0 | |
| 52.0182 | 24.4190514 | |
| 53.0023 | 0.4629099 | $C_3HO$ |
| 53.0386 | 0.30741074 | $C_4H_5$ |
| 53.9975 | 0.6175893 | |
| 54.0338 | 1.56916405 | |
| 55.0165 | 0.46808908 | |
| 55.0178 | 62.3404596 | $C_3H_5O$ |
| 55.0193 | 0.3691769 | |
| 55.0542 | 2.13301608 | $C_4H_7$ |
| 56.0212 | 0.69007338 | |
| 56.0495 | 0.21612927 | |
| 57.0335 | 2.61162206 | $C_3H_5O$ |
| 58.0287 | 0.51087258 | |
| 59.0320 | 0.21551721 | |
| 59.0491 | 0.96867325 | $C_3H_7O$ |
| 60.0443 | 1.80607965 | |
| 61.0283 | 0.85075974 | $C_3H_5O_2$ |
| 64.0180 | 0.28474193 | |
| 65.0258 | 0.24158149 | |
| 65.0384 | 1.0495502 | $C_5H_5$ |
| 66.0210 | 2.00160828 | |
| 66.0336 | 3.54249477 | |
| 67.0288 | 3.00323231 | |
| 67.0369 | 0.26421966 | |
| 68.0129 | 0.27323227 | |
| 68.0241 | 0.67878479 | |
| 68.0493 | 0.62961095 | |
| 69.0207 | 0.31441806 | |
| 73.0282 | 24.3112556 | $C_3H_5O_2$ |
| 73.0646 | 0.81797296 | $C_4H_9O$ |
| 74.0315 | 0.28498934 | |
| 74.0360 | 0.74296666 | |
| 74.0962 | 0.4591748 | |
| 75.0438 | 1.3431678 | $C_3H_7O_2$ |
| 76.0390 | 7.74200281 | |
| 77.0131 | 1.74636844 | |
| 77.0343 | 0.41301717 | |
| 77.9972 | 1.82383734 | |
| 78.0210 | 1.71124973 | |
| 78.0291 | 0.52897589 | |
| 78.0336 | 8.95007686 | |
| 79.0264 | 0.63397322 | |
| 79.0269 | 0.78430056 | |
| 79.0288 | 100 | |
| 79.0413 | 0.96334549 | |
| 79.0539 | 0.97406437 | $C_6H_7$ |
| 80.0366 | 2.55290535 | |
| 81.0445 | 0.27538096 | |
| 83.0124 | 0.61213585 | $C_4H_5O_2$ |
| 83.0488 | 0.61460879 | $C_5H_7O$ |
| 83.0852 | 0.3637532 | $C_6H_{11}$ |
| 84.0203 | 1.86114611 | |
| 85.0281 | 2.43786417 | $C_4H_5O_2$ |
| 88.0754 | 0.23509342 | |
| 89.0594 | 0.72100697 | $C_4H_9O_2$ |
| 89.0787 | 0.31804646 | |
| 91.0287 | 0.28748374 | |
| 91.0387 | 1.67725463 | $C_4H_5O_3$ |
| 91.0539 | 50.5120106 | $C_7H_7$ |
| 91.0568 | 0.26571143 | |
| 92.0366 | 1.24476364 | |
| 92.0491 | 1.9415118 | |
| 93.0444 | 11.227288 | |
| 94.0396 | 0.51110152 | |
| 95.0236 | 2.93596679 | |
| 95.0489 | 0.22747053 | $C_6H_7O$ |
| 96.0314 | 0.36961734 | |
| 96.0440 | 3.80656139 | |
| 96.0522 | 0.27313347 | |
| 97.0393 | 1.21457873 | |
| 101.0230 | 26.0614097 | $C_4H_5O_3$ |
| 101.0342 | 0.22654171 | |
| 101.0593 | 1.39164781 | $C_4H_9O_2$ |
| 102.0263 | 0.29147253 | |
| 103.0538 | 0.3801334 | $C_4H_7$ |
| 110.0597 | 0.49724907 | |
| 111.0549 | 0.52440471 | |
| 113.0342 | 0.26792108 | |
| 117.0695 | 0.26351453 | $C_8H_9$ |
| 118.0396 | 0.52972214 | |
| 119.0338 | 2.26781436 | $C_4H_7O_4$ |




| m/z | Relative | Composition |
|---|---|---|
| 50.0000 | 0 | |
| 52.0182 | 23.3651922 | |
| 53.0022 | 0.65186616 | $C_3HO$ |
| 53.0386 | 0.4825759 | $C_4H_5$ |
| 53.9975 | 0.831286 | |
| 54.0338 | 1.71654348 | |
| 55.0178 | 33.9640134 | $C_3H_5O$ |
| 55.0542 | 18.4165461 | $C_4H_7$ |
| 56.0212 | 0.40821247 | |
| 57.0335 | 2.30952594 | $C_3H_5O$ |
| 58.0287 | 0.33618962 | |
| 59.0490 | 9.70387441 | $C_3H_7O$ |
| 59.0498 | 0.25376603 | |
| 60.0205 | 1.94650292 | |
| 60.0443 | 2.19024289 | |
| 61.0283 | 0.71159629 | $C_3H_5O_2$ |
| 65.0258 | 0.29193094 | |
| 65.0383 | 0.95196642 | $C_5H_5$ |
| 66.0210 | 2.29867969 | |
| 66.0336 | 3.98181785 | |
| 67.0288 | 3.31481544 | |
| 68.0241 | 0.94837137 | |
| 68.0492 | 0.68397287 | |
| 69.0207 | 0.32779268 | |
| 71.0125 | 0.55408006 | $C_3H_3O_2$ |
| 73.0281 | 34.7949424 | $C_3H_5O_2$ |
| 73.0303 | 0.30321821 | |
| 73.0645 | 1.0592833 | $C_4H_9O$ |
| 74.0234 | 0.29904368 | |
| 74.0314 | 0.26934554 | |
| 74.0359 | 1.06531925 | |
| 74.0961 | 0.34391196 | |
| 75.0438 | 1.15018688 | $C_3H_7O_2$ |
| 76.0390 | 7.68705562 | |
| 76.0503 | 0.42024663 | |
| 77.0131 | 2.29958826 | |
| 77.0342 | 0.97481479 | |
| 77.9972 | 1.78447126 | |
| 78.0084 | 0.26521493 | |
| 78.0210 | 2.03911359 | |
| 78.0291 | 0.39388304 | |
| 78.0336 | 8.47680477 | |
| 79.0264 | 0.59304377 | |
| 79.0269 | 0.56628396 | |
| 79.0288 | 100 | |
| 79.0307 | 0.43763524 | |
| 79.0312 | 0.64997722 | |
| 79.0413 | 1.06761872 | |
| 79.0539 | 0.89134733 | $C_6H_7$ |
| 80.0365 | 2.33477204 | |
| 83.0124 | 0.84340328 | $C_4H_5O_2$ |
| 83.0488 | 3.81554341 | $C_5H_7O$ |
| 83.0852 | 0.35026929 | $C_6H_{11}$ |
| 84.0202 | 1.8308492 | |
| 85.0281 | 2.09250783 | $C_4H_5O_2$ |
| 88.0753 | 0.24905201 | |
| 89.0230 | 8.89417301 | $C_4H_9O_3$ |
| 89.0594 | 0.52953941 | $C_4H_9O_2$ |
| 91.0287 | 0.44252423 | |
| 91.0386 | 2.1014669 | $C_4H_5O_3$ |
| 91.0539 | 50.1428006 | $C_7H_7$ |
| 91.0568 | 0.45960535 | |
| 92.0365 | 1.11415297 | |
| 92.0491 | 2.14055319 | |
| 92.0572 | 0.44741849 | |
| 93.0444 | 12.272456 | |
| 94.0396 | 0.75481709 | |
| 95.0236 | 2.98906004 | |
| 96.0314 | 0.6579585 | |
| 96.0440 | 3.59886403 | |
| 96.0520 | 0.26957086 | |
| 97.0393 | 1.1560328 | |
| 101.0195 | 0.33929241 | |
| 101.0229 | 64.0199995 | $C_4H_5O_3$ |
| 101.0264 | 0.48374133 | |
| 101.0593 | 5.03905478 | $C_4H_9O_2$ |
| 102.0262 | 0.99843062 | |
| 103.0539 | 0.40155231 | $C_4H_7$ |
| 107.0335 | 0.64095308 | $C_3H_3O_4$ |
| 110.0596 | 0.48967729 | |
| 111.0549 | 0.54722846 | |
| 114.0546 | 0.38971328 | |
| 118.0395 | 0.57071731 | |
| 118.0521 | 0.31998547 | |
| 119.0338 | 3.59332734 | $C_4H_7O_4$ |