*Table S1. Temperature program*

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **All analytes except ethanol** | | | | |
|  | *Rate*  *(°C/min)* | *Value*  *(°C)* | *Hold time*  *(min)* | *Run time*  *(min)* |
| *(Initial)* | - | 30 | 5 | 5 |
| *Ramp 1* | 20 | 100 | 0 | 8.5 |
| *Ramp 2* | 35 | 200 | 0 | 11.4 |
| **Ethanol** | | | | |
|  | *Rate*  *(°C/min)* | *Value*  *(°C)* | *Hold time*  *(min)* | *Run time*  *(min)* |
| *(Initial)* | - | 70 | 4 | 4 |
| *Ramp 1* | 40 | 150 | 0 | 6 |

*Table S2. Instrument and analysis parameters*

|  |  |
| --- | --- |
| ***All analytes except ethanol*** | |
| **Instrument** | |
| **Parameter** | **Operating conditions** |
| **Headspace sampler** | |
| Vial pressurization gas: | Helium |
| Oven temperature: | 90°C |
| Loop temperature: | 115°C |
| Transfer line temperature: | 120°C |
| Vial equilibration: | 10 min |
| Injection duration: | 0.10 min |
| GC Cycle time: | 25 min |
| **GC** | |
| Inlet: | 200°C, 75:1 split ratio in split mode |
| Helium carrier gas flow rate: | 2.5 mL/min, constant flow mode |
| **FID** | |
| Heater: | 280°C |
| H2 Flow: | 40 mL/min |
| Air Flow | 450 mL/min |
| Makeup Flow | 50 mL/min |
| Run time: | 11.4 min |
| ***Ethanol*** | |
| **Instrument** | |
| **Parameter** | **Operating conditions** |
| **Automatic liquid sampler** | |
| Injection volume: | 1 μL |
| **GC**- Inlet | |
| Heater: | 250°C |
| Preasure: | 15.554 psi |
| Total flow: | 54.838 mL/min |
| Septum purge flow | 3 mL/min |
| Split: | 40:1 |
| Split flow: | 50.574 mL/min |
| **FID** | |
| Heater: | 270°C |
| H2 Fuel flow: | 30 mL/min |
| Air Flow: | 400 mL/min |
| Makeup Flow (N2): | 50 mL/min |

*Table S3. AMPHORA chemical testing limits for the substances of interest*

|  |  |  |
| --- | --- | --- |
| **Substance** | **Maximum limit**  **g/hL pure alcohol (p.a.)** | **Maximum limit**  **mg/L p.a.** |
| methanol | 1 000 | 10 000 |
| ethyl acetate | 1 000 | 10 000 |
| acetaldehyde | 50 | 500 |
| higher alcohols (sum) | 1 000 | 10 000 |

*Table S4. Toxicological thresholds used for the calculation of margin of exposure of ethanol and other aliphatic alcohols*

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Alcohol** | **Type of toxicological threshold** | **Experimental animal** | **Value of toxicological threshold**  **[mg/kg bw/day]** | **Reference** |
| **methanol** | BMDL05a | rat | 43.1 | EPA IRIS, 2013 |
| NOAELb | rat | 500 | EFSA FEEDAP, 2013 |
| **ethanol** | BMDL1.5 | mice | 440 | Lachenmeier et al.,  2011, U. S. EPA, 2004 |
| NOAEL | rat | 1730 | EFSA FEEDAP, 2013 |
| **1-propanol** | NOAEL | rat | 296 | Lachenmeier et al., 2008 |
| **1-butanol** | BMDL10 | rat | 26.1 | Sitarek et al., 1994,  EPA IRIS, 2011 |
| NOAEL | rat | 125 | EPA IRIS, 1991 |
| **2-butanol** | NOAEL | rat | 347 | Lachenmeier et al., 2008 |
| **isobutanol** | NOAEL | rat | 316 | EPA IRIS, 1986 |
| **isoamyl alcohol** | NOAEL | rat | 206 | Lachenmeier et al., 2008 |
| **acetaldehyde** | NOEL | rat | 125 | SCCS, 2012 |
| **ethyl acetate** | NOEL | rat | 900 | EPA IRIS, 1987 |

**a BMDLx:**lower bound of the benchmark dose confidence interval where the change in response is likely to be smaller than x%.

**b NOAEL:** no observed adverse effect level

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*Figure S1. Chromatograms of a) calibration solution b) fruit spirit sample*

1- acetaldehyde (Rt 2.381 min), 2- ethylacetate (Rt 4.548 min), 3- methanol (Rt 4.952 min), 4- methyl isobutil ketone (Rt 7.192, the internal standard), 5- n-propanol (Rt 7.900min), 6- isobutanol (Rt 8.752 min), 7- n-butanol (Rt 9.394 min), 8- isoamyl alcohol (10.018), 9- n-amyl alcohol (Rt 10.417 min)

