

Supplementary Material

Red Analytical Performance Index (RAPI) and software: the missing tool for assessing methods in terms of analytical performance

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Table S1. The details of assessment performed using the RAPI tool.

| Method description (Analyte, sample type, instrumental technique) | Repeatability | Intermediate precision | Reproducibility | Trueness | Recovery & matrix effect | LOQ (% of expected mean analyte concentration in the matrix) | Working range | Simplified linearity estimation | Ruggedness/robustness | Selectivity | Total Points | Ref. * |
|--|---------------------------------------|--|---------------------------|--|--|--|--|--------------------------------------|---------------------------------|---------------------------------|--------------|---------------|
| Triazines/Fruit juice/HPLC-DAD | c≤0.000001% RSD<8% Points: 10.0 | c≤0.000001% RSD<16% Points: 10.0 | Not tested Points: 0.0 | c≤0.000001% Bias<20% Points: 7.5 | c≤0.000001% >80, <110; acceptable ME Points: 7.5 | LOQ<10% Points: 5.0 | Wider than 100× LOQ Points: 10.0 | R ² >0.99 Points: 10.0 | Not demonstrated Points: 0.0 | Not demonstrated Points: 0.0 | 60.0 | ³³ |
| Triazines/Water/HP LC-DAD | c≤0.000001% RSD<8% Points: 10.0 | c≤0.000001% RSD<16% Points: 10.0 | Not tested Points: 0.0 | c≤0.000001% Bias<20% Points: 7.5 | c≤0.000001% >80, <110; acceptable ME Points: 7.5 | LOQ<25% Points: 2.5 | Wider than 100× LOQ Points: 10.0 | R ² >0.99 Points: 10.0 | Not demonstrated Points: 0.0 | Not demonstrated Points: 0.0 | 57.5 | ³⁴ |
| Triazines/Herbal | c≤0.00001% | c≤0.00001% | Not tested | c≤0.00001% | c≤0.00001% | LOQ<25% | Wider | R ² >0.99 | Not | Not | 52.5 | ³⁵ |

| Method description (Analyte, sample type, instrumental technique) | Repeatability | Intermediate precision | Reproducibility | Trueness | Recovery & matrix effect | LOQ (% of expected mean analyte concentration in the matrix) | Working range | Simplified linearity estimation | Ruggedness/robustness | Selectivity | Total Points | Ref. * |
|--|--|---------------------------------------|---------------------------|--------------------------------------|---|--|--------------------------------------|--------------------------------------|--|--|--------------|---------------|
| infusion/HPLC-DAD | RSD<11.3% Points: 7.5 | RSD<11.3% Points: 10.0 | Points: 0.0 | Bias<10% Points: 7.5 | >80, <110; acceptable ME Points: 5.0 | Points: 2.5 | than 100× LOQ Points: 10.0 | Points: 10.0 | demonstrated Points: 0.0 | demonstrated Points: 0.0 | | |
| Histidine/Urine/HP LC-PCD-FLD | c≤0.0001% RSD<4.0% Points: 10.0 | c≤0.0001% RSD<8.0% Points: 10.0 | Not tested Points: 0.0 | c≤0.0001% Bias<20% Points: 5.0 | c≤0.0001% >90, <107; acceptable ME Points: 7.5 | LOQ<1% Points: 10.0 | Wider than 30× LOQ Points: 7.5 | R ² >0.99 Points: 10.0 | Demonstrated for 5 or more factors Points: 10.0 | Demonstrated for 5 or more potential interferences Points: 10.0 | 80.0 | ³⁶ |
| Histidine/Urine/Smartphone | c≤0.001% RSD<8.475% Points: 5.0 | c≤0.001% RSD<11.3% Points: 5.0 | Not tested Points: 0.0 | c≤0.001% Bias<40% Points: 2.5 | c≤0.001% >60, <115; ME study optional Points: 2.5 | LOQ<1% Points: 10.0 | Wider than 5× LOQ Points: 2.5 | R ² >0.99 Points: 10.0 | Not demonstrated Points: 0.0 | Demonstrated for 5 or more potential interferences Points: 10.0 | 47.5 | ³⁷ |
| Histidine/Fish samples/HPLC-PCD-FLD | c≤0.001% RSD<2.825% Points: 10.0 | c≤0.001% RSD<5.7% Points: 10.0 | Not tested Points: 0.0 | c≤0.001% Bias<20% Points: 5.0 | c≤0.001% >80, <110; ME study optional Points: 5.0 | LOQ<1% Points: 10.0 | Wider than 30× LOQ Points: 7.5 | R ² >0.99 Points: 10.0 | Demonstrated for 5 or more factors Points: 10.0 | Demonstrated for 5 or more potential interferences Points: 10.0 | 77.5 | ³⁸ |
| Parabens/Urine/HP LC-DAD | c≤0.0001% RSD<16% | c≤0.0001% RSD<20% | Not tested Points: 0.0 | c≤0.0001% Bias<20% | c≤0.0001% >80, <110; | LOQ<25% Points: 2.5 | Wider than 100× | R ² >0.99 Points: | Demonstrated for 5 or more | Not demonstrated | 47.5 | ³⁹ |

| Method description (Analyte, sample type, instrumental technique) | Repeatability | Intermediate precision | Reproducibility | Trueness | Recovery & matrix effect | LOQ (% of expected mean analyte concentration in the matrix) | Working range | Simplified linearity estimation | Ruggedness/robustness | Selectivity | Total Points | Ref. * |
|--|---|--------------------------------------|---------------------------|---|---|--|--|--|--|--|--------------|---------------|
| | Points: 2.5 | Points: 2.5 | | Points: 5.0 | acceptable ME Points: 5.0 | | LOQ Points: 10.0 | 10.0 Points: 10.0 | factors Points: 10.0 | ated Points: 0.0 | | |
| Parabens/Urine/HP LC-DAD | c≤0.001% RSD≥11.3% Points: 0.0 | c≤0.001% RSD<14.1% Points: 2.5 | Not tested Points: 0.0 | c≤0.001% Bias<20% Points: 5.0 | c≤0.0001% >80, <110; acceptable ME Points: 5.0 | LOQ<25% Points: 2.5 | Wider than 100× LOQ Points: 10.0 | R ² >0.97 Points: 10.0 Points: 7.5 | Demonstrated for 5 or more factors Points: 10.0 | Not demonstrated Points: 0.0 | 42.5 | ⁴⁰ |
| Parabens/Breast tissue/HPLC-DAD | c≤0.00001% RSD<11.3% Points: 7.5 | c≤0.00001% RSD<7% Points: 7.5 | Not tested Points: 0.0 | c≤0.00001% Bias<20% Points: 5.0 | c≤0.0001% >80, <110; acceptable ME Points: 5.0 | LOQ≥25% Points: 0.0 | Wider than 100× LOQ Points: 10.0 | R ² >0.99 Points: 10.0 Points: 10.0 | Not demonstrated Points: 0.0 | Not demonstrated Points: 0.0 | 45.0 | ⁴¹ |
| Lead/Water/FAAS | c≤0.00001% RSD<5.65% Points: 10.0 | Not tested Points: 0.0 | Not tested Points: 0.0 | c≤0.00001% Bias<10%, confirmed with CRMs Points: 10.0 | c≤0.0001% >90, <107; acceptable ME Points: 7.5 | LOQ<10% Points: 5.0 | Wider than 30× LOQ Points: 7.5 | R ² >0.99 Points: 10.0 Points: 10.0 | Not demonstrated Points: 0.0 | Demonstrated for 5 or more potential interferences Points: 10.0 | 60.0 | ⁴² |
| Lead/Water/FAAS | c≤0.00001% RSD<5.65% Points: 10.0 | Not tested Points: 0.0 | Not tested Points: 0.0 | c≤0.00001% Bias<10%, confirmed with CRMs Points: 10.0 | c≤0.0001% >95, <105; weak ME Points: 10.0 | LOQ<1% Points: 10.0 | Wider than 30× LOQ Points: 7.5 | R ² >0.99 Points: 10.0 Points: 10.0 | Not demonstrated Points: 0.0 | Demonstrated for 5 or more potential interferences Points: 10.0 | 67.5 | ⁴³ |
| Lead/Water/FAAS | c≤0.00001% | Not tested | Not tested | c≤0.00001% | c≤0.0001% | LOQ≥25% | Wider | R ² >0.99 | Not | Demonstr | 60.0 | ⁴⁴ |

| Method description (Analyte, sample type, instrumental technique) | Repeatability | Intermediate precision | Reproducibility | Trueness | Recovery & matrix effect | LOQ (% of expected mean analyte concentration in the matrix) | Working range | Simplified linearity estimation | Ruggedness/robustness | Selectivity | Total Points | Ref. * |
|--|---------------------------|------------------------|-----------------|---|------------------------------------|--|----------------------------------|---------------------------------|-----------------------------|--|--------------|--------|
| | RSD<5.65% Points: 10.0 | Points: 0.0 | Points: 0.0 | Bias<10%, confirmed with CRMs Points: 10.0 | >95, <105; weak ME Points: 10.0 | Points: 0.0 | than 100× LOQ Points: 10.0 | Points: 10.0 Points: 10.0 | demonstrated Points: 0.0 | ated for 5 or more potential interferences Points: 10.0 | | |

* see the main document for the literature references