

Untargeted Screening on the X500R QTOF

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Outline

X500R technology and performance

X500R QTOF Scan modes

Application Examples



X500R Technology and Performance

Super simplified TOF

- At t=0, all ions are accelerated to the detector
- Acceleration is constant energy, all ions achieve the same K.E.
- Since KE=0.5*mass*velocity², velocity is mass dependent, therefore the time to impinge on the detector is mass dependent



lons enter the accelerator





Resolution is a key requirement

- Necessary for mass accuracy, but does not guarantee mass accuracy
- For differentiation of nearby peaks
- Helps with sensitivity in TOF



Causes of resolution loss

- Jitter timing and voltage
- Path-length variation detector, mechanical variation
- Trajectory variation ion position, ion velocity variation



Mass Resolution



ESI QTOF Geometry

| Parameter | Value |
|-------------------------------|----------|
| Liner length | 495mm |
| Mirror Length | 102mm |
| Mirror Stage 1 length | 36mm |
| Mirror Stage 2 length | 66mm |
| Accelerator AC section length | 12mm |
| Accelerator DC section length | 60mm |
| Liner potential | +/-6kV |
| Mirror Plate potential | -/+2.1kV |
| Mirror Grid Potential | 0 |
| Pusher plate potential | -/+1.6kV |
| Beam energy | 22eV |
| Effective flight path length | 2.35m |
| Actual path length | 1.95m |
| | |

Inlet orifice





Space velocity correlation focusing





Correlated position and velocity eliminates turnaround time problem

"Resolution and spectral line shapes in the reflecting time-of-flight mass spectrometer with orthogonally injected ions," V. V. Laiko and A. F. Dodonov, RCMS 8 720-726 (1994).

"Improved resolution and substantially higher sensitivity on a QTOF mass spectrometer," A. Loboda, I. V. Chernushevich, and Nic Bloomfield, 57th ASMS conference 2009.



0.15

0.1

0.05

Z=65

Z=70

Z=75

Z=80 Z=85 Z=65

Z=70

Z=75

Z=80

Z=85

•

.

500

400

300

200

100

0

8

-6

counts



NTOF Analyzer





Mass Resolution – Detector tilter





Resolution Performance, MS mode



Resolution Stability





Mass Accuracy

- Resolution is nothing without mass accuracy¹
- Mass accuracy means confidence in the indicated peak position is accurate and stable.
- A narrow high resolution peak can be an unreliable indicator of peak position.

¹Bob Haufler, NEMC 2016



Mass Accuracy: Thermal effects





The high voltage power supplies are independently thermally stabilized



Mass Accuracy - Statistical



Each sample was acquired every 20 minutes.



Mass Accuracy - Systematic

Linear calibration equation, 2 coefficients: a and t_0 : $mass = [a \cdot (t - t_0)]^2$



GluFib=[Glu1]-fibrinopeptide B



Sensitivity – no beam aperturing





X500R Scan Modes and Data Acquisition

QTOF scan modes

| Mode | Q1 | Collision cell | TOF | Workflow |
|-------------------|---------------------------|----------------|--------------------------------|---|
| TOFMS | Open, all ions pass | Off | All ions detected (precursors) | Targeted, suspect and unknown screening |
| TOFMSMS | Set to target precursor | On | All fragments detected | Targeted, suspect and unknown screening |
| SWATH | Scanning 25 amu window | On | All fragments detected | Suspect and unknown screening |
| MRM ^{HR} | Set to precursor | On | All fragments detected | Targeted quantitation and confirmation |

| IDA | Scan mode | | Time |
|--------|-----------|--|--------------|
| Step 1 | TOFMS | Survey Scan-Obtain precursor ion list | 0.1-0.5 sec |
| Step 2 | TOFMSMS | Obtain fragment MS of 1 st precursor | 0.05-0.1 sec |
| Step 3 | TOFMSMS | Obtain fragment MS of 2 nd precursor | 0.05-0.1 sec |
| Step 4 | TOFMSMS | Obtain fragment MS of 3 rd precursor | 0.05-0.1 sec |
| | | Total | ~1sec |

Cycles repeatedly during chromatography



Untargeted Analysis

- Known unknowns (suspect screening) spectra exists in library (MSMS and possibly retention time)
 - Library match
 - Formula finder
 - Isotope pattern
 - MSMS pattern
 - Compare retention time if LC method is standard
 - Obtain standard for confirmation and quantitation
- Unknowns (unknown screening) no spectra exists in library
 - Formula finder
 - Isotope pattern
 - ChemSpider
 - MSMS pattern
 - Obtain standard based on ChemSpider results for confirmation



IDA details - Data Acquisition Setup

| | | | | | | New | ♥ Open | Save | Print | Advanced 🔹 🗙 |
|--|--|---|---|--|-------------------------------|--------------------|--------|-------|--------|------------------|
| 沿 Untitled | | | | | | | | | | |
| Method Overview Device: X500 QTOF Ion Source: TurboSpray | Method duration Estimated cycles: | 5 min | Total scan time: | 1.311 sec | | | | | | Add Experiment 💌 |
| IDA 0 min + 5 min | TOF MS TOF start mass TOF stop mass Accumulation time | 100 Da 1000 Da 0.25 sec | Declustering potential DP spread | 80 V 0 V | Collision energy CE spread | 10 C V 0 C V | | | | |
| | Advanced Experiment Sett Time bins to sum Channel 3 | ings 4 | Channel 1 Channel 4 | ✓✓ | Channel 2 | V | | | | 1 |
| | IDA Criteria All Maximum candidate ions Intensity threshold exceed | 10 Cps | ✓ Dynamic backgroun Exclude former cance For After | id subtraction fidate ions sec ccurrences | Dynamic CE for N Charge state | ts/MS 2 to 4 | | | | |
| | Dynamic accumulatio Candidate mass range t Inclusion List Exclusion List | n e 400 🗘 Da to 1250 🏶 Da | Exclude isotopes +/ Adjust CE when usin Mass Defect Filter Isotopic Matching | - 4 Da | Mass tolerance +/- | 50 🔹 e mDa 🔵 ppm | | | | |
| Data Acquicition | TOF MSMS Precursor ion TOF start mass | 830 🗘 Da 50 🗘 Da | Declustering potential DP spread | 80 ° V 0 ° V | Collision energy CE spread | 35 V 15 V | | Chart | - Fina | Four |
| M | 15 | | | | | | | | | |



IDA Data





IDA Data





Sample - Control Comparison in SCIEX OS Software

Quick example: unknown screening of food dye compounds

| 🗘 - Analytics 🔷 🗠 | | 💄 🕜 Offline 🕴 ? – 🗗 🗴 |
|--|---|---|
| | Project: AS artificial food dyes Projects | Results Reporting Views Process Method X |
| Samples Components and Groups Options * | | Begin by creating a results table or opening an existing one. |
| | Process New Results X 1. Select batch samples to process Available Image: Selected Image: Select batch samples to process Image: Select batch samples to procese samples t | - Select samples |
| | dyes neg 03_yellow 1.wiff2 dyes prec 03_yellow 1.wiff2 equil column.wiff2 C. Select a processing method GUS dyes.qmethod Select a comparison sample for Non-targeted workflow sugar (dyes neg 02_sugar 1.wiff2, 2) Process Cancel [Help] | Select control |
| Data Acquisition Ms | | Start 💌 🖬 Stop Save 🕅 |



Unknown Screening in SCIEX OS Software





Results Review and Filtering in SCIEX OS Software

Table is Filtered by Formula Finding Results and Sorted by Area

| 🗘 - Analytics 🔷 🖄 | - | | | | | | | | | | | | | | - | 9 | 🕜 Offlir | ie ? | - 8 × |
|-------------------------------|------------|-----------------------|---------------------------|--------------|------------------|--------------|------------|------------------|------------------|-------------------------|--------------|------------------------|--------------------------------|---------------|-------------|-------------|-----------------------------|-------------------|--------------|
| | | | | | | | | | P | oject: AS artificial fo | od dyes | rojects 🔹 Resu | ılts | 👻 Repo | rting | ♥ Vie | ews | Process Metho | od 👻 🗙 |
| Samples Components and Groups | [MQ4] Pea | k Review (Untitled) | | | | | | | | | | | | | | | | | |
| Options 👻 | 0 | | | | | | | | (Charles and the | THE | | | *a 🗾 di | CH / | | | | | |
| R 10000x | | | r | | _ | | - | | Sample | Type • Aco | eptance 👻 | % ♣ /az | C III | | <u> </u> | | | Aore 👻 | |
| Y 10000x | Index | Sample Name | Component Name | Area | Retention | Found | Used | Library Confi | Form | Library Hit | Library | Formula Finder Results | Area | Formula | Non-Tar | | | | Â |
| BI 10000x | | | | 10000 | Time | At Mass | 10000 | | C | | Score | | Ratio of | . Finder Sc | . Peak | | | | |
| Br 10000x | ♦ 400 | R 10000x | 834.6480 / 5.02 | 4.051e6 | 5.03 | 834.6481 | | • | 1 | No Match | 0.0 | C20H8I4O5 | N/A | 94.470 | | | | | |
| El sugar | 384 | R 10000x | 708.7515 / 4.91 | 2.790e5 | 4.91 | 708.7515 | V | • | ~ | No Match | 0.0 | C20H9I3O5 | N/A | 93.441 | V | | | | |
| u suga | 86 | R 10000x | 206.9994 / 2.76 | 5.477e4 | 2.77 | 206.9994 | V | • | ~ | No Match | 0.0 | C10H5N2NaS | N/A | 73.708 | V | | | | |
| | 37 | R 10000x | 170.9994 / 2.76 | 5.225e4 | 2.77 | 170.9995 | V | • | ~ | No Match | 0.0 | C7H5N2NaS | N/A | 74.458 | V | | | | E. |
| | 402 | R 10000x | 890.6733 / 5.47 | 4.678e4 | 5.48 | 890.6733 | V | • | ~ | No Match | 0.0 | C25H14I3Na3S4 | N/A | 99.445 | V | - | | | |
| | 313 | R 10000x | 407.0012 / 2.76 | 2.964e4 | 2.77 | 407.0014 | 1 | • | ~ | No Match | 0.0 | C16H12N2O7S2 | N/A | 96.180 | 1 | | | | |
| | 373 | R 10000x | 582.8543 / 4.87 | 1.664e4 | 4.87 | 582.8546 | | | ~ | No Match | 0.0 | C22H3INa2O9 | N/A | 92.544 | V | _ | | | |
| | 73 | R 10000x | 197.9867 / 0.53 | 1.225e4 | 0.55 | 197.9865 | V | • | | No Match | 0.0 | C3H4N3Na3O3 | N/A | 63.922 | V | - | | | |
| | 401 | R 10000x | 848.6628 / 5.64 | 1.205e4 | 5.64 | 848.6629 | | • | ~ | No Match | 0.0 | C15H20I4Na2S3 | N/A | 98.088 | | _ | | | |
| | 403 | R 10000x | 908.6835 / 5.36 | 1.143e4 | 5.36 | 908.6836 | | • | ~ | No Match | 0.0 | C24H4I3N4Na3O7 | N/A | 96.518 | | _ | | | |
| | 85 | R 10000x | 206.9994 / 3.31 | 1.14/e3 | 3.32 | 205.9988 | | - | ~ | No Acquired MS | N/A | C3H3N6Na3O | N/A | 94.883 | V | - | | | |
| | 10 | R 10000x | 155.9883 / 0.53 | 9.352e2 | 0.55 | 155.9882 | | | | No Acquired MS | N/A | C/H4NNa5 | N/A | 53,499 | | - | | | |
| | 240 | R 10000x | 341.1090 / 2.67 | 6.620+2 | 2.20 | 200.0022 | | - | ~ | No Acquired MS | N/A | CI2HIDN8NaU3 | N/A | 91.040 | | -6 | | | |
| | | R 10000X | 200.00207 3.31 | 0.02062 | 5.52 | 200.0033 | nim | - | | No Acquired Mis | N/A | CSHONSINASOS | N/A | 00.110 | 1000 | - | | | * |
| | ΛA | Manual Integr | ation 🔝 | | | | | | | | | | | | View | v | • Optio | ns 🔹 🗖 | \mathbb{Z} |
| | sugar - 83 | 34.6480 / 5.02 (Unkn | own) 834.6380 neg 0 | 2_sugar 1.wi | iff2), (sample I | ndex: 2) | 100 | ^{0%}] | | | _ | | _ 1 | 00%] | | | | | |
| Control — | Area: N/A | , Height N/A, KI: N/ | 4 min | | XIC |) u | 50 | 0% | | | | TOF-MS | of 1.0 | 50% - | | | | MS/MS | 3 |
| Control | | 1 2 | 3 4 🕈 | 6 7 | 8 9 | ~ % | | 19/ | | | | |)% | 0% | | | | | |
| | | | Time, mi | n | | | | //0 | 0.1 0 | .2 0.3 0.4 | 0.5 0.6 | 0.7 0.8 0.9 | | 0.0 | 1 0.2 | 0.3 0. | .4 0.5 0.6 | 0.7 0.8 0. | 9 |
| | Peak D | etails | | | | - * | Formula | Finder Re | sults — | | | | Library | Search Result | 5 | | | | - @ |
| | Precurso | or m/z Retention Tin | ne (min) Ion Ratio | | | | Name | e Form | ula Se | ore m/z (Da) | Error (ppm) |) Error MSMS (ppm) | I Nan | ne CAS# | Formula | MW (Da | a) Fit Rev. | Fit Purity CE (| aV) |
| | 834.648 | N/A | N/A | | | | | | | | | | | | | | | | |
| | R 10000 | . 934 6490 / 5 03 // | lalua ana) 834 63 - a a a | 04 and 1 | (D) (an angle Ia | days 20 Cara | 3 | | 04 | | (100 1000) | 6 | 5. U | | 04 and 1 | :#2 TDA | TOT MEMO (EO | 1000\ 6 m E 020 m | A |
| | Area: 4.05 | 51e6, Height: 1.163e6 | i, RT: 5.03 min | 04_red 1.wi | | uex: 2) Spe | 1009 | muyes n %₁ | leg 04_re | 0 1.WIT2 (OF MS) | (100 - 1000) | | Precursor: 8 | 34.6 Da, +1 | 04_red 1.wi | 102IDA | TOP INSINS (50 | | |
| Sample – | | | 5.0 | 03 | | / | | | | 834. | 6481 835.6 | | | | | | | 662.7452 | 2 |
| e ampre | | 1 2 | 3 4 🕈 | 6 7 | 8 9 | - 1 | 05 | 832 | 833 | 834 835 | 836 | 837 838 | U | 100 | 200 3 | 300 4 | 00 500 | 600 700 80 | 00 |
| | 1 | | Time, mir | ı | | | | | | Mass/C | harge, Da | | | | | Mas | ss/Charge, Da | - | |
| | Peak D | etails | 10 March 15 March 19 | | | | Formula Fi | inder Resi | ults | | 152 Za a | <u> </u> | Library Se | earch Results | | - 19-27-18- | V 19455 - 485 - 4 85 | | G |
| | Precurso | or m/z Retention Tin | ne (min) Ion Ratio | | | | Name | Formu | ıla Sc | ore m/z (Da) | Error (ppm) | Error MSMS (ppm) | Name | e CAS# I | Formula | MW (Da) | Fit Rev. F | it Purity CE (eV |) |
| | 834.048 | 5.03 | N/A | | | | | C20H8I4 | 405 94. | a 834.64781 C | 1.3 | 1 | | | | | | | |
| | <u> </u> | | | | | | _ | _ | _ | | | | | | | _ | | | |
| Data Acquisition | | | | | | _ | | | _ | | | | _ | | Start | | Stop | Save | |
| MS | | | | | | | | | | | | | | | Stdit | | 100 | Sauce | |

Sample was diluted with water/sugar solution (10.000x)

to simulate dissolved cake icing



Review of Formula Finding Results in SCIEX OS Software

Evaluation of TOF-MS and MS/MS Error and ChemSpider Hit Count

| 🗘 - Analytics 🔷 🖄 | b. | | | | | | | | | | | | | | | 9 | 🕜 Offlir | ie | ? = @ > |
|-------------------------------|--|---|--------------------------|--------------------|----------------------------|-------------|-----------|------------------|---------------|-------------------------|---------------------|------------------------|----------|---------------------------------------|---------|---------|----------|-------------|--------------|
| | | | | | | | | | Pr | oject: AS artificial fo | od dyes Pr | rojects 🔹 Resu | ilts | * Repo | rting | 👻 Vi | ews | Process Met | hod 🔹 🗙 |
| Samples Components and Groups | [MQ4] Peak | k Review (Untitled) | | | | | | | | | | | | | | | | | |
| Options 👻 | 0 | | | | | | | | Connella | Terror and Arrest | | | "o | | | | | | |
| R 10000x | | | | 1 | - | | r - 1 | | aampie | туре 🗸 🛛 Ассе | eptance 🔹 | | | • • • • • • • • • • • • • • • • • • • | | 1 Kal 🖬 | | iore 🔹 | |
| Y 10000x | Index | Sample Name | Component Name | Area | Retention | Found | Used | Library Confi | Form Confi | Library Hit | Library | Formula Finder Results | Area | Formula | Non-Tar | | | | Â |
| BI 10000× | | | | 1.000 | lime | At Mass | | | | | Score | | Ratio of | Finder Sc | Peak | | | | |
| Br 10000x | ▶ 400 | R 10000x | 834.6480 / 5.02 | 4.051e6 | 5.03 | 834,6481 | | ٠ | 11 A | No Match | 0.0 | C20H8I4O5 | N/A | 94.470 | | | | | |
| E sugar | 384 | R 10000x | 708.7515 / 4.91 | 2.790e5 | 4.91 | 708.7515 | V | • | ~ | No Match | 0.0 | C20H9I3O5 | N/A | 93.441 | V | | | | |
| | 86 | R 10000x | 206.9994 / 2.76 | 5.477e4 | 2.77 | 206.9994 | V | • | ~ | No Match | 0.0 | C10H5N2NaS | N/A | 73.708 | V | | | | - |
| | 37 | R 10000x | 170.9994 / 2.76 | 5.225e4 | 2.77 | 170.9995 | | • | ~ | No Match | 0.0 | C7H5N2NaS | N/A | 74.458 | V | - | | | |
| | 402 | R 10000x | 890.6733 / 5.47 | 4.678e4 | 5.48 | 890.6733 | V | • | ~ | No Match | 0.0 | C25H14I3Na3S4 | N/A | 99.445 | V | | | | |
| | 313 | R 10000x | 407.0012 / 2.76 | 2.964e4 | 2.77 | 407.0014 | V | • | ~ | No Match | 0.0 | C16H12N2O7S2 | N/A | 96.180 | V | - | | | |
| | 373 | R 10000x | 582.8543 / 4.87 | 1.664e4 | 4.87 | 582.8546 | V | • | ~ | No Match | 0.0 | C22H3INa2O9 | N/A | 92.544 | V | - | | | |
| | /3 | R 10000x | 197.986770.53 | 1.225e4 | 0.55 | 197.9865 | | • | - | No Match | 0.0 | C3H4N3Na3O3 | N/A | 63.922 | V | | | | |
| | 401 | R 10000x | 848.6628 / 5.64 | 1.205e4 | 5.64 | 848.6629 | | • | ~ | No Match | 0.0 | C15H20I4Na2S3 | N/A | 98.088 | | | | | |
| | 403 | R 10000x | 908.6835 / 5.36 | 1.143e4 | 5.36 | 908.6836 | | • | ~ | No Match | 0.0 | C24H4I3N4Na3O/ | N/A | 96.518 | | - | | | |
| | 85 | R 10000x | 206.9994 / 3.31 | 1.14/e3 | 3.32 | 206.9988 | | - | ~ | No Acquired MS | N/A | C3H3N6Na3O | N/A | 94.883 | | - | | | |
| | 10 | R 10000x | 155.9883 / 0.53 | 9.352e2 | 0.55 | 155.9882 | | - | A | No Acquired MS | N/A | C/H4NNa5 | N/A | 53,499 | | - | | | |
| | 240 | R 10000x | 341.1090/2.0/ | 6.620+2 | 2.20 | 200.0022 | | - | ~ | No Acquired MS | N/A | CI2HIDN8NaU3 | N/A | 91.040 | | -0. | | | |
| | | R 10000X | 200.002073.31 | 0.02062 | 5.52 | 200.0033 | 1000 | - | | No Acquired Mis | N/A | CSHONSINASUS | N/A | 00.110 | 1000 | - | | | • |
| | ΛA | Manual Integr | ation | | | | | | | | | | | | View | v | • Optio | ns 🔹 🗖 | \mathbb{X} |
| | Spectrum 10 (38: 2 30) (38: 2 30) (39: 2 30) | from dyes neg 04_re 00% 80% 60% 40% | d 1.wiff2 (sample 2) - R | 10000x, Exp | riment 1, -IDA | TOF MS (100 | 0 - 1000) | from 5.02 | 21 to 5.04 | 48 min 834.6481 | | | | ink | to | Ch | | Spide | or |
| | % Int | 20% - | | | | | | | | | 8 | 335.6514 | 836. | 6542 | ιΟ | U | Iem, | Spide | |
| Formula | ▲ Formula | 832.0 | 832.5 | 833.0 | 833.5 | | 834.0 | | 834.5 | 835.0 Mass/ | 835. /Charge, Da | 5 836.0 | 836.5 | 837 | .0 | 837.5 | 838.0 | 838.5 | |
| | | Name | Formula S | icore m/z | (Da) Error | (ppm) Er | ror MSM | IS (ppm) | Hit C | punt | | | | | | | | | 6 |
| | | | C20H8I4O5 94 | 1.5 834.6 | 4781 0.3 | 1 | | 41.4 | 5 | | | | | | | | | | |
| with 5 Hits | | N | C8H11I4N4Na3O6 94 | .4 834.6 | 478 0.3 | 1 | | | 0 | | | | | | | | | | |
| | | N | C15HI3N6Na2O7S 93 | 1.7 834.6 | 4844 0.5 | 1 | | | 0 | | | | | | | | | | |
| | | | C21H12I4S2 93 | 1.6 834.6 | 4868 0.7 | 0.5 | | | 0 | | | | | | | | | | |
| | | | C1/H10/MN/M32OS 02 | 834.6 1.8 834.6 | 4775 0.4 <u>477 0.4</u> | 1.2 | | | 0 | | | | | | | | | | v |
| | L | | | | | | | | | | | | | | | | | | |
| Data Acquisition Ms | | | | | | | | | | | | | | | Start | v | Stop | Save | A |



Review of ChemSpider Results in SCIEX OS Software

Automatic In-silico Fragmentation of Structure Found in ChemSpider



Tentative identification of Erythrosine in **RED** food color



Examples

Three Isomers Analysis by MRM^{HR}

3 compounds with same formula but separated by LC conditions

| 38 | 1039 | Methabenzthiazuron | Bayern-LC-Mix | 18691-97-9 | C10H11N3OS | 222.06956 | 220.05501 |
|------|-------------|---|---------------------------|------------------------|------------------------|------------------------|-----------------------|
| 66 | 2618 | Benfuracarb (Carbofuran) | Bayern-LC-Mix | 1563-66-2 | C12H15NO3 | 222.11247 | 220.09792 |
| 391 | 978 | Acetamiprid | SuMS-Mix 1 | 135410-20-7 | C10H11CIN4 | 223.0745 | 221.05995 |
| 42 | 1219 | Monocrotophos | SuMS-Mix 1 | 6923-22-4 | C7H14NO5P | 224.06824 | 222.05368 |
| 445 | 909 | Mepanipyrim | SuMS-Mix 2 | 110235-47-7 | C14H13N3 | 224.11822 | 222.10367 |
| 338 | 493 | Mevinphos | Bayern-LC-Mix | 7786-34-7 | C7H13O6P | 225.05225 | 223.0377 |
| 447 | 473 | Methiocarb | SuMS-Mix 2 | 2032-65-7 | C11H15NO2S | 226.08963 | 224.07507 |
| 351 | 949 | Cyprodinil | Bayern-GC-Mix | 121552-61-2 | C14H15N3 | 226.13387 | 224.11932 |
| 196 | 609 | Prometon | Bayern-LC-Mix | 1610-18-0 | C10H19N5O | 226.16624 | 224.15168 |
| 198 | 1118 | Terbumeton | Bayern-GC-Mix | 33693-04-8 | C10H19N5O | 226.16624 | 224.15168 |
| 1106 | 2211 | Metyrapone | SuMS-Mix 3 | 54-36-4 | C14H14N2O | 227.11789 | 225.10334 |
| 195 | 151 | Ametryn | Bayern-GC-Mix | 834-12-8 | C9H17N5S | 228.12774 | 226.11319 |
| 41 | 490 | Metoxuron | Bayern-LC-Mix | 19937-59-8 | C10H13CIN2O2 | 229.07383 | 227.05928 |
| 24 | 332 | Dimethoate | Bavern-GC-Mix | 60-51-5 | C5H12NO3PS2 | 230.0069 | 227.99235 |
| | 6: 3 | Propazine | Bayern-GC-Mix | 139-40-2 | C9H16CIN5 | 230.1167 | 228.10215 |
| 53 | 123 | Sebuthylazine | Bayern-GC-Mix | 7286-69-3 | C9H16CIN5 | 230.1167 | 228.10215 |
| 58 | 65 | terbuthylazine | Bayern-GC-Mix | 5915-41-3 | C9H16CIN5 | 230.1167 | 228.10215 |
| 407 | 2748 | Oxydemeton-methyl (Demeton-S-methyl) | Sums-mix 2 | 919-86-8 | C6H15O3PS2 | 231.0273 | 229.01275 |
| 176 | 1116 | Asulam | SuMS-Mix 1 | 3337-71-1 | C8H10N2O4S | 231.04341 | 229.02885 |
| 132 | 516 | Naproxen | Arzneimittel-Mix1 | 22204-53-1 | C14H14O3 | 231.10157 | 229.08702 |
| 378 | 617 | Propyphenazone | Arzneimittel-Mix1 | 479-92-5 | C14H18N2O | 231.14919 | 229.13464 |
| 591 | 765 | N-Formyl-4-aminoantipyrin | Arzneimittel-Mix1 | 1672-58-8 | C12H13N3O2 | 232.10805 | 230.0935 |
| 25 | 855 | Diuron | Bayern-LC-Mix | 330-54-1 | C9H10Cl2N2O | 233.02429 | 231.00974 |
| 264 | 1619 | Fluometuron | SuMS-Mix 1 | 2164-17-2 | C10H11F3N2O | 233.08962 | 231.07507 |
| 001 | | | | | | | |
| 331 | 842 | Sulbactam | SuMS-Mix 3 | 68373-14-8 | C8H11NO5S | 234.04307 | 232.02852 |
| 840 | 842 3121 | Sulbactam Methylphenidate hydrochloride C II (Ritalin) in Lösung | SuMS-Mix 3 Für AZM-Std | 68373-14-8 298-59-9 | C8H11NO5S C14H19NO2 | 234.04307 234.14886 | 232.02852 232.1343 |



Sebuthylazine – MSMS Spectra







Propazine 139-40-2 C9H16CIN5 229.7127

100.0 0.0



Suspect screening: water samples

- Cocaine human metabolite: Benzoylecgonine
- Caffeine
- Sildenafil (viagra)

Water samples from lakes, rivers, drinking water and a few other sources around the world.

Benzoylecgonine in Different Water Samples



BE and other drug metabolites are detected in rivers in major cities, © 2015 AB Sciex concentration can be used to estimate consumption.

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Caffeine in Different Water Samples

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© 2015 AB Sciex human activity, i.e. artificial sweetener SCIEX

Sildenafil in Different Water Samples



Concentration of sildenafil detected were very low (<10 ppt), one exception! SCIEX

Data of Holy Water (Direct Injection 100 µL)

| Compound | µg/L | LOQ (µg/L) |
|---|-------|------------|
| Acetaminophen | 9.1 | 0.010 |
| Benzoylecgonine (metabolite of cocaine) | 0.47 | 0.001 |
| Caffeine | 38 | 0.010 |
| Carbamazepine | 0.21 | < 0.001 |
| Codeine | 0.050 | 0.001 |
| Dextromethorphan | 0.021 | 0.001 |
| Diazepam | 0.003 | 0.001 |
| EDDP (metabolite of methadone) | 0.001 | 0.001 |
| Erythromycin | 1.7 | 0.050 |
| Morphine | 0.15 | 0.005 |
| Sildenafil | 0.015 | 0.005 |
| Thiabendazole | 0.016 | < 0.001 |



Summary

- The X500R technology and performance
 - Technology to achieve high mass resolution (>30,000 resolution)
 - N-geometry.
 - Detector tilter.
 - Space-velocity correlation focusing.
 - Technology to achieve high mass accuracy(<1ppm accuracy for m/z>50amu)
 - Thermal stabilization.
 - Simplified accelerator with no puller.

X500R scan modes

- IDA for suspect and untargeted screening.
- SWATH for suspect and untargeted screening.
- MRM^{HR} for targeted quantification and confirmation.

Application examples

- Unknown food dye compound
- MRM^{HR} identification of identical m/z isomers
- Detection of human activity compounds in various water samples



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