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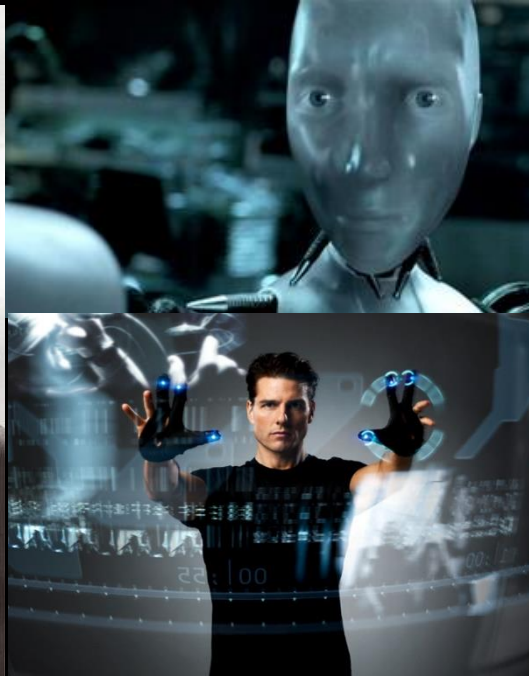
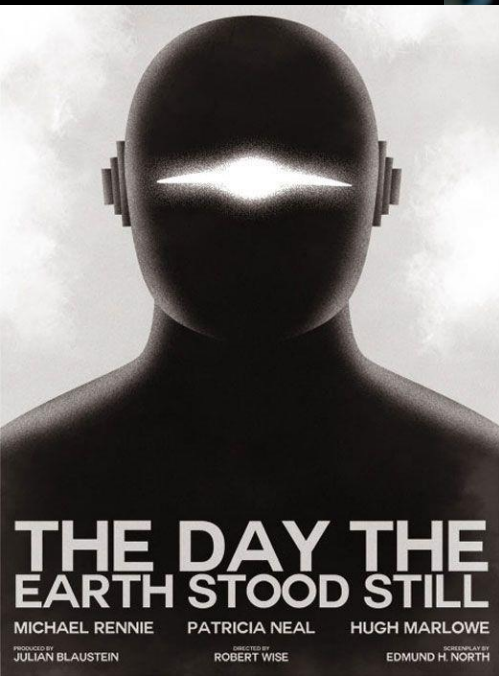
A Vision for the **Future**

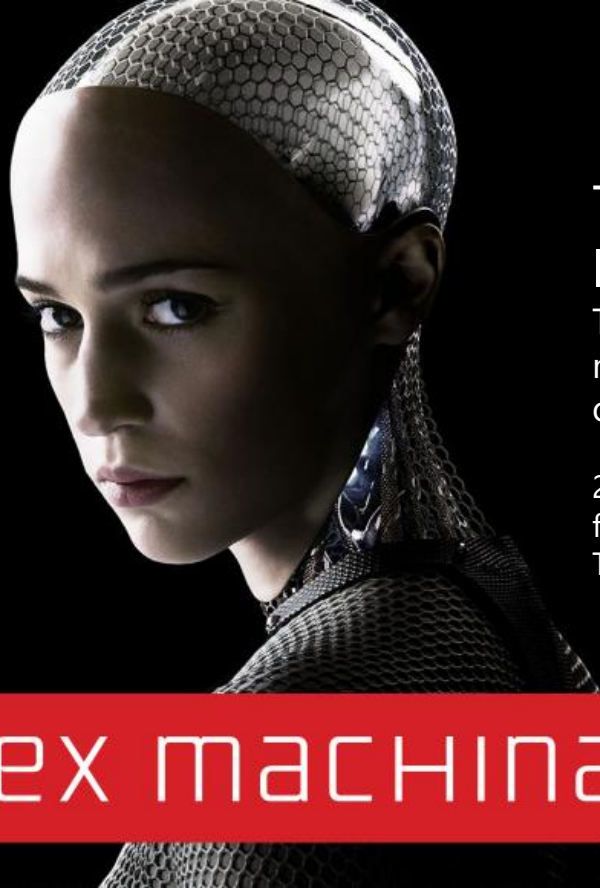
Informatics and decision making (AI?)

Neil Loftus

Shimadzu Corporation

Disclaimer | This is purely a speculative and personal view of what may happen and in no capacity does it reflect the views of Shimadzu Corporation





The story line

Is a conscious android human?

The Turing test, developed by Alan Turing in 1950, is a test of a machine's ability to exhibit intelligent behaviour equivalent to, or indistinguishable from, that of a human.

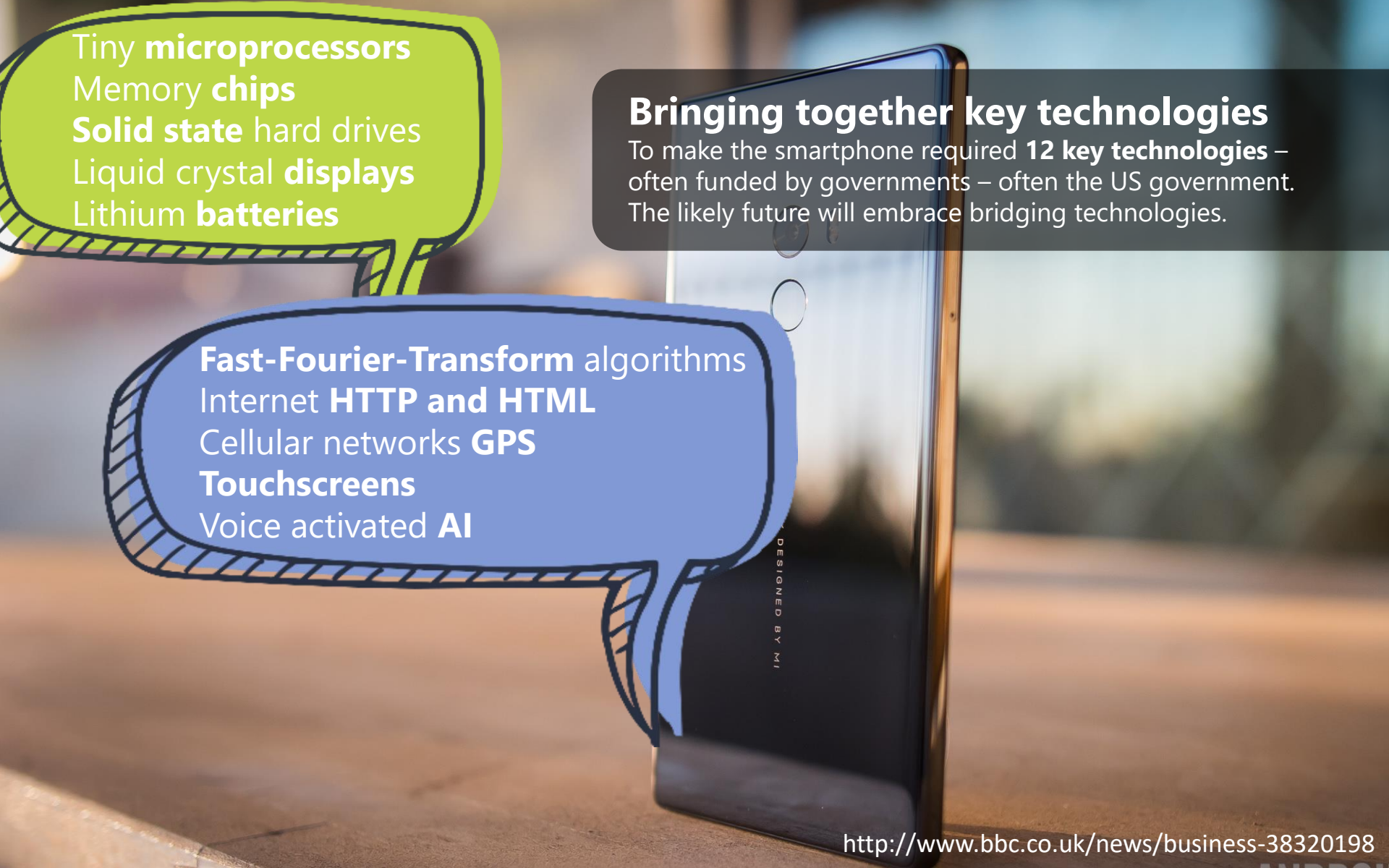
2015 independent science fiction psychological thriller film. The film follows a programmer who is invited by his CEO to administer the Turing test to an intelligent humanoid robot.

ex machina

The development of full artificial intelligence could spell the end of the human race
Stephen Hawking

First the machines will do a lot of jobs for us and not be super intelligent....

A few decades after that though the intelligence is strong enough to be a concern
Bill Gates



Tiny **microprocessors**
Memory **chips**
Solid state hard drives
Liquid crystal **displays**
Lithium **batteries**

Bringing together key technologies

To make the smartphone required **12 key technologies** – often funded by governments – often the US government. The likely future will embrace bridging technologies.

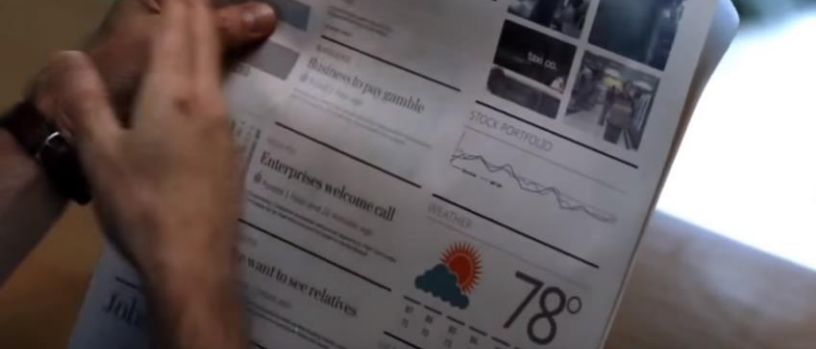
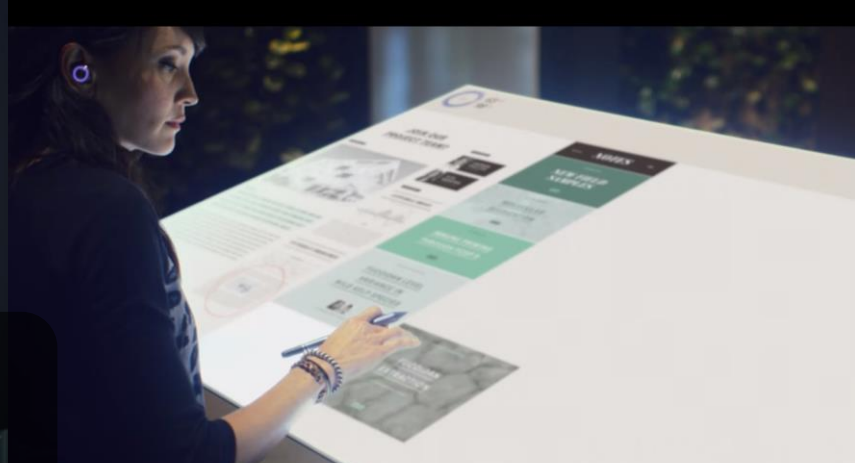
Fast-Fourier-Transform algorithms
Internet **HTTP and HTML**
Cellular networks **GPS**
Touchscreens
Voice activated **AI**

COLLABORATIVE
**BRINGING PEOPLE
TOGETHER**

INTELLIGENT
**LIVING
SMARTER**

NATURAL
**FRICTION FREE
CREATIVITY**

MOBILE
**FLUID
MOBILITY**



Bringing together key technologies
Likely impact of new tools to view data and results.
This is part of the Productivity Future Vision by Microsoft

Informatics in Healthcare Systems

Using AI to help drive higher efficiencies and possibly deliver better decision making
IBM Watson, Google, Microsoft, Phillips

IBM Watson Health

IBM Watson Health Oncology

300 medical journals,
200+ textbooks,
15 million pages of text
Designed to analyse a patient's medical records and help personalised treatment options

Medical data

Expected to double every 73 days by 2020



Study in India; , Watson's treatment recommendations were in agreement with those of physicians;
96% lung cancer, 93% rectal cancer, and 81% colon cancer. Similar rates for colorectal, lung, breast and gastric cancer treatments (Thai-based study).
Additionally, Watson was able to screen breast and lung cancer patients for clinical trial eligibility 78 percent faster than a human, reducing screening time from 110 minutes down to just 24.

Himss[®] 17

CONFERENCE & EXHIBITION | FEB 19–23, 2017
ORLANDO | ORANGE COUNTY CONVENTION CENTER

Healthcare Information and Management Systems Society Convention

Google has been working on deep learning in the healthcare space for some time, and is expanding its reach into the industry by teaming up with FHIR (Fast Health Interoperability Resources; FIRE)
Microsoft Healthcare NExT, 'patient engagement and business intelligence to predictive analytics and genomics'

Informatics in Healthcare Systems

Can we do things better?

Use IoT and AI to help speed decision making, increase efficiencies.

The problem is a global ageing population.

From 2015 to 2030, the U.S. population is projected to grow by nearly

12%



The population of those aged 65 and older is projected to grow by

55%

and as patients age, they require **2 to 3 times** as many services

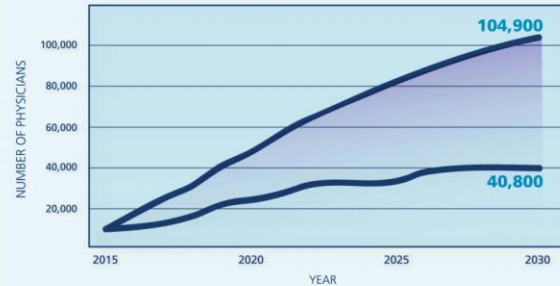
If currently underserved populations access and use health care at the same rate as the rest of the population, the U.S. would have needed

34,800 to 96,800

additional physicians in 2015*



By 2030, the total physician shortage is projected to be between **40,800** and **104,900** doctors



Association of American Medical Colleges

Addressing the shortage will require a multipronged approach, including innovation in delivery; **greater use of technology**; improved, efficient use of all health professionals on the care team

Impact on informatics and AI on routine workflows

Informatics will change how we do our work in the future. Decision making (AI?) tools will enable routine environments to increase productivity and ROI.

There are still many caveats (peak integration, matrix effects) but change is very likely

Things that are likely to change

Accelerate Sample to Result

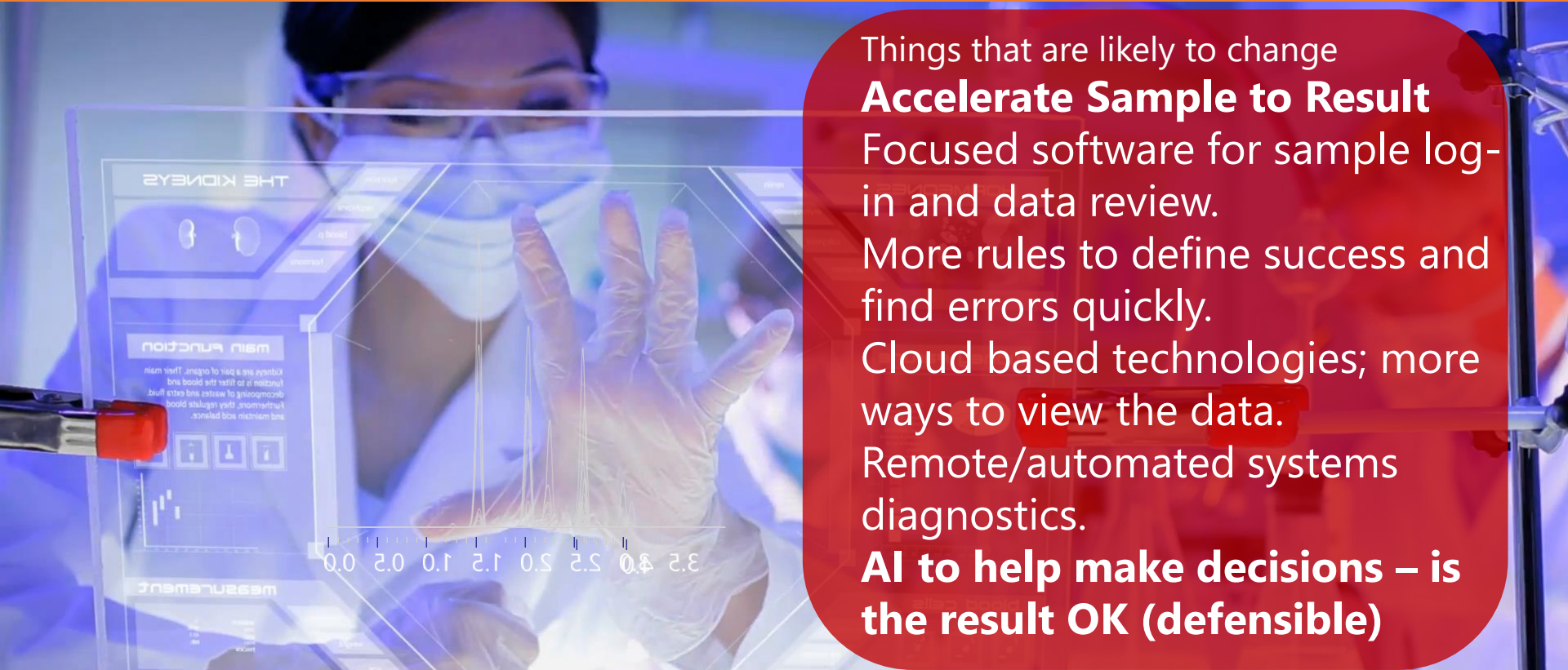
Focused software for sample log-in and data review.

More rules to define success and find errors quickly.

Cloud based technologies; more ways to view the data.

Remote/automated systems diagnostics.

AI to help make decisions – is the result OK (defensible)



Data spaces to review data and make decisions

Information rich environments

LabSolutions Insight Library Screening (Admin) - (Insight_CAO_batch.Icb - Insight_CAO_results.Icm)

Shortcuts

- Open
- Save
- Close
- Compound Details
- All
- Load Flags

File

- View
- Edit
- Report

Sample List

| # | Sample Name |
|----|-------------|
| 1 | 100 |
| 2 | 10 |
| 3 | 200 |
| 4 | 500 |
| 5 | 50 |
| 6 | 5 |
| 7 | 0 |
| 8 | PatientID 1 |
| 9 | PatientID 2 |
| 10 | PatientID 3 |
| 11 | PatientID 4 |
| 12 | PatientID 5 |
| 13 | PatientID 6 |
| 14 | PatientID 7 |
| 15 | PatientID 8 |
| 16 | PatientID 9 |

Compound Results - 500 Ug-L_cao_ABC-MTS-method-U-ISTD_008

| # | Flag ID | Flags | Name | m/z | Found RT | Area | Conc. | Lib. Compound Name | Lib. SI | Lib. RT | Lib. errRT |
|----|---------|-------|---------------------------------|---------------|----------|----------|-------|------------------------------|---------|---------|------------|
| 24 | | | MDMA | 194.10>163.10 | 4.233 | 21785465 | 531 | MDMA | 91 | 4.298 | 0.065 |
| 26 | | | Mephedrone | 178.10>145.15 | 4.419 | 16001392 | 518 | Mephedrone | 93 | 4.491 | 0.072 |
| 81 | | | Methadone | 310.20>265.15 | 8.309 | 59539849 | 505 | Methadone | 91 | 8.374 | 0.065 |
| 15 | | | Methamphetamine | 150.15>91.10 | 3.958 | 66043392 | 490 | Methamphetamine | 93 | 4.017 | 0.059 |
| 13 | | | Methcathinone | 164.10>131.10 | 3.709 | 20531162 | 500 | Methcathinone | 97 | 3.763 | 0.054 |
| 11 | | | Methiopropamine | 156.10>97.10 | 3.673 | 36036800 | 497 | Methiopropamine | 91 | 3.727 | 0.054 |
| 40 | | | Methylphenidate | 234.15>84.10 | 5.195 | 40966354 | 515 | Methylphenidate | 88 | 5.270 | 0.075 |
| 5 | | | Morphine | 286.15>152.10 | 3.399 | 2949415 | 504 | Morphine | 93 | 3.489 | 0.090 |
| 17 | | | Naloxone | 328.15>212.10 | 3.974 | 2860130 | 492 | Naloxone | 94 | 4.130 | 0.156 |
| 19 | | | Naltrexone | 342.15>270.15 | 4.114 | 2534451 | 504 | Naltrexone | 95 | 4.191 | 0.077 |
| 2 | | | Norephedrine | 152.10>115.10 | 3.248 | 4755268 | 480 | Norephedrine | 89 | 3.066 | 0.182 |
| 3 | | | Norpseudoephedrine | 152.10>115.15 | 3.320 | 7997608 | 500 | Norephedrine | 91 | 3.066 | 0.254 |
| 28 | | | Norfenfluramine | 204.10>159.05 | 4.507 | 39003640 | 497 | Norfenfluramine | 95 | 4.564 | 0.057 |
| 23 | | | Oxycodone | 316.15>241.15 | 4.180 | 5961490 | 500 | Oxycodone | 92 | 4.275 | 0.095 |
| 37 | | | M-CPP (meta-Chlorophenylpipe... | 197.10>154.05 | 4.876 | 10011499 | 498 | P-CPP (P-Chlorophenylpipe... | 93 | 4.537 | 0.339 |
| 22 | | | Pholcodine | 399.25>114.10 | 4.357 | 7328692 | 521 | Pholcodine | 92 | 4.238 | 0.119 |
| 20 | | | Ritalinic acid | 220.15>84.10 | 4.209 | 6598459 | 498 | Ritalinic acid | 96 | 4.201 | 0.008 |
| 4 | | | Anhydroecgonine methyl ester | 182.10>91.15 | 3.392 | 15118774 | 531 | Thiocyclam | 59 | 3.371 | 0.021 |

Compound Details - 500 Ug-L_cao_ABC-MTS-method-U-ISTD_008 - MDMA

Q 194.10-163.10 (-) 6.89e6 Product Ion(+)[194.10] mCE: -10.0-35.0-55.0 RT: [4.178 - 4.179]

CN(C)C(C)Cc1ccc2c(c1)OCO2

Shaping data spaces to meet differing needs

Change the user experience to just show results....

LabSolutions Insight Library Screening (Admin) - (Insight_CAO_batch.Icb - Insight_CAO_results.Icm)

Shortcuts

- File
- View
- Edit
- Edit Method
- Integrate Batch
- Integrate Sample
- Integrate Compound
- Integrate Result
- Edit Tables
- Edit Flags
- Select Compounds
- Review
- Report

| Sample List | | | | | Compound Results - 100_ug-L_cao_ABC-MTS-method-U-ISTD_006 | | | | | | | | | | |
|-------------------------------------|-------------|-------------|-------|---------|---|------|---------------------------------|-------|---------------|------|----------------|--------------------|-----------|---------------|--|
| # | Sample Name | Level | Flags | Flag ID | # | Name | Found RT | m/z | Conc. | Mode | R ² | Ref 1 Actual Ratio | Ref 1 m/z | | |
| <input checked="" type="checkbox"/> | | | | | <input checked="" type="checkbox"/> | 3 | Norpseudoephedrine | 3.324 | 152.10>115.15 | 97 | Auto | 0.99987 | 95.94 | 152.10>117.15 | |
| <input checked="" type="checkbox"/> | 1 | 100 | | 4 | <input checked="" type="checkbox"/> | 4 | Anhydroecgonine methyl ester | 3.402 | 182.10>91.15 | 97 | Auto | 0.99264 | 88.09 | 182.10>118.15 | |
| <input checked="" type="checkbox"/> | 2 | 10 | | 2 | <input checked="" type="checkbox"/> | 5 | Morphine | 3.405 | 286.15>152.10 | 102 | Auto | 0.99875 | 71.85 | 286.15>201.10 | |
| <input checked="" type="checkbox"/> | 3 | 200 | | 5 | <input checked="" type="checkbox"/> | 6 | Ephedrine | 3.580 | 166.10>115.15 | 110 | Auto | 0.99714 | 79.11 | 166.10>117.15 | |
| <input checked="" type="checkbox"/> | 4 | 500 | | 6 | <input checked="" type="checkbox"/> | 7 | Pseudoephedrine | 3.580 | 166.10>115.15 | 99 | Auto | 0.99972 | 99.31 | 166.10>91.10 | |
| <input checked="" type="checkbox"/> | 5 | 50 | | 3 | <input checked="" type="checkbox"/> | 8 | Scopolamine | 4.111 | 304.15>138.10 | 0 | Auto | 0.00000 | 0.00 | 304.15>156.15 | |
| <input checked="" type="checkbox"/> | 6 | 5 | | 1 | <input checked="" type="checkbox"/> | 9 | Hydromorphone | 3.617 | 286.15>185.10 | 98 | Auto | 0.99629 | 67.20 | 286.15>157.10 | |
| <input checked="" type="checkbox"/> | 7 | 0 | | 1 | <input checked="" type="checkbox"/> | 10 | Morphine-6-glucuronide | 3.444 | 462.20>286.15 | 0 | Auto | 0.00000 | 0.00 | 462.20>201.10 | |
| <input checked="" type="checkbox"/> | 8 | PatientID 1 | | ---- | <input checked="" type="checkbox"/> | 11 | Methiopropamine | 3.679 | 156.10>97.10 | 103 | Auto | 0.99913 | 64.50 | 156.10>58.10 | |
| <input checked="" type="checkbox"/> | 9 | PatientID 2 | | ---- | <input checked="" type="checkbox"/> | 12 | Amphetamine | 3.699 | 136.10>91.10 | 100 | Auto | 0.99859 | 22.58 | 136.10>119.15 | |
| <input checked="" type="checkbox"/> | 10 | PatientID 3 | | ---- | <input checked="" type="checkbox"/> | 13 | Methcathinone | 3.708 | 164.10>131.10 | 94 | Auto | 0.99971 | 82.35 | 164.10>130.10 | |
| <input checked="" type="checkbox"/> | 11 | PatientID 4 | | ---- | <input checked="" type="checkbox"/> | 14 | Noroxycodone | 3.929 | 302.15>187.10 | 120 | Auto | 0.99086 | 109.20 | 302.15>227.10 | |
| <input checked="" type="checkbox"/> | 12 | PatientID 5 | | ---- | <input checked="" type="checkbox"/> | 15 | Methamphetamine | 3.963 | 150.15>91.10 | 96 | Auto | 0.99838 | 17.30 | 150.15>119.15 | |
| <input checked="" type="checkbox"/> | 13 | PatientID 6 | | ---- | <input checked="" type="checkbox"/> | 16 | MDA | 3.980 | 180.10>163.15 | 112 | Auto | 0.99772 | 66.72 | 180.10>105.15 | |
| <input checked="" type="checkbox"/> | 14 | PatientID 7 | | ---- | <input checked="" type="checkbox"/> | 17 | Naloxone | 3.978 | 328.15>212.10 | 122 | Auto | 0.99285 | 42.28 | 328.15>268.20 | |
| <input checked="" type="checkbox"/> | 15 | PatientID 8 | | ---- | <input checked="" type="checkbox"/> | 18 | Dihydrocodeine | 4.085 | 302.20>199.10 | 109 | Auto | 0.99516 | 76.63 | 302.20>128.05 | |
| <input checked="" type="checkbox"/> | 16 | PatientID 9 | | ---- | <input checked="" type="checkbox"/> | 19 | Naltrexone | 4.114 | 342.15>270.15 | 97 | Auto | 0.99806 | 92.97 | 342.15>267.15 | |
| | | | | | <input checked="" type="checkbox"/> | 20 | Ritalinic acid | 4.208 | 220.15>84.10 | 100 | Auto | 0.99797 | 20.39 | 220.15>56.05 | |
| | | | | | <input checked="" type="checkbox"/> | 21 | Codeine | 4.113 | 300.15>152.10 | 114 | Auto | 0.99572 | 80.54 | 300.15>215.15 | |
| | | | | | <input checked="" type="checkbox"/> | 22 | Pholcodine | 4.474 | 399.25>114.10 | 98 | Auto | 0.99132 | 10.58 | 399.25>70.10 | |
| | | | | | <input checked="" type="checkbox"/> | 23 | Oxycodone | 4.200 | 316.15>241.15 | 107 | Auto | 0.99862 | 80.79 | 316.15>256.15 | |
| | | | | | <input checked="" type="checkbox"/> | 24 | MDMA | 4.235 | 194.10>163.10 | 93 | Auto | 0.99335 | 155.02 | 194.10>105.10 | |
| | | | | | <input checked="" type="checkbox"/> | 25 | 6-MAM | 4.241 | 328.15>165.15 | 96 | Auto | 0.99579 | 66.73 | 328.15>211.15 | |
| | | | | | <input checked="" type="checkbox"/> | 26 | Mephedrone | 4.429 | 178.10>145.15 | 88 | Auto | 0.99676 | 179.41 | 178.10>144.15 | |
| | | | | | <input checked="" type="checkbox"/> | 27 | BDB | 4.447 | 194.10>135.05 | 106 | Auto | 0.99680 | 24.54 | 194.10>177.10 | |
| | | | | | <input checked="" type="checkbox"/> | 28 | Norfenfluramine | 4.512 | 204.10>159.05 | 95 | Auto | 0.99933 | 37.29 | 204.10>109.05 | |
| | | | | | <input checked="" type="checkbox"/> | 29 | MDEA | 4.546 | 208.15>163.10 | 102 | Auto | 0.99872 | 65.28 | 208.15>105.10 | |
| | | | | | <input checked="" type="checkbox"/> | 30 | Tramadol | 4.270 | 264.20>58.05 | 0 | Auto | 0.00000 | 0.00 | 264.20>42.10 | |
| | | | | | <input checked="" type="checkbox"/> | 31 | Benzoylcegonine | 4.635 | 290.15>168.15 | 99 | Auto | 0.99855 | 36.50 | 290.15>77.00 | |
| | | | | | <input checked="" type="checkbox"/> | 32 | Hydrocodone | 4.518 | 300.15>199.15 | 110 | Auto | 0.99438 | 44.29 | 300.15>128.10 | |
| | | | | | <input checked="" type="checkbox"/> | 33 | MBDB | 4.741 | 208.15>135.05 | 97 | Auto | 0.99963 | 28.17 | 208.15>77.05 | |
| | | | | | <input checked="" type="checkbox"/> | 34 | Ethylmorphine | 4.711 | 314.20>152.15 | 109 | Auto | 0.99928 | 96.02 | 314.20>229.15 | |
| | | | | | <input checked="" type="checkbox"/> | 35 | 4-MTA | 4.888 | 182.10>165.15 | 100 | Auto | 0.99801 | 161.85 | 182.10>117.15 | |
| | | | | | <input checked="" type="checkbox"/> | 36 | Ketamine | 5.446 | 238.10>125.00 | 0 | Auto | 0.00000 | 0.00 | 238.10>179.05 | |
| | | | | | <input checked="" type="checkbox"/> | 37 | M-CPP (meta-Chlorophenylpipe... | 4.886 | 197.10>154.05 | 94 | Auto | 0.99911 | 105.08 | 197.10>118.10 | |
| | | | | | <input checked="" type="checkbox"/> | 38 | 2-CB | 5.030 | 230.10>214.95 | 105 | Auto | 0.99949 | 55.76 | 230.10>106.05 | |
| | | | | | <input checked="" type="checkbox"/> | 39 | Niaprazine | 5.268 | 357.20>177.10 | 0 | Auto | 0.00000 | 0.00 | 357.20>149.10 | |
| | | | | | <input checked="" type="checkbox"/> | 40 | Methylphenidate | 5.204 | 234.15>84.10 | 90 | Auto | 0.99772 | 33.62 | 234.15>56.05 | |
| | | | | | <input checked="" type="checkbox"/> | 41 | 7-aminonitrazepam | 5.021 | 252.10>121.10 | 0 | Auto | 0.00000 | 21.56 | 252.10>77.05 | |
| | | | | | <input checked="" type="checkbox"/> | 42 | 7-aminoclonazepam | 5.813 | 286.05>121.10 | 0 | Auto | 0.00000 | 0.00 | 286.05>222.10 | |

One click to show flagged compounds

Or change the view to show any outliers or problems....

LabSolutions Insight Library Screening (Admin) - (Insight_CAO_batch.Icb - Insight_CAO_results.Icm)

Shortcuts

- File
- View
- Compound
- Review only
- Compound Details
- Calibration Curve
- Library Hits
- Survey
- QC Chart
- Settings

Edit

Review

Report

Sample List

| # | Sample Name | Level | Flags | Flag ID |
|--|-------------|-------|-------|---------|
| <input checked="" type="checkbox"/> | | | | |
| <input checked="" type="checkbox"/> 8 | PatientID 1 | ---- | F | >R |
| <input checked="" type="checkbox"/> 9 | PatientID 2 | ---- | F | >R |
| <input checked="" type="checkbox"/> 10 | PatientID 3 | ---- | F | >R |
| <input checked="" type="checkbox"/> 11 | PatientID 4 | ---- | F | >R |
| <input checked="" type="checkbox"/> 12 | PatientID 5 | ---- | F | >R |
| <input checked="" type="checkbox"/> 13 | PatientID 6 | ---- | F | >R |
| <input checked="" type="checkbox"/> 14 | PatientID 7 | ---- | F | >R |
| <input checked="" type="checkbox"/> 15 | PatientID 8 | ---- | F | >R |
| <input checked="" type="checkbox"/> 16 | PatientID 9 | ---- | F | >R |

Compound Results - Archive10_PatientID5

| # | Name | Found RT | m/z | Co... | Mode | R ² | Ref 1 Actual Ratio | Ref 1 m/z | Re |
|--|----------------------|----------|---------------|-------|------|----------------|--------------------|---------------|----|
| <input checked="" type="checkbox"/> | | | | | | | | | |
| <input checked="" type="checkbox"/> 31 | Benzoylcgonine | 4.635 | 290.15>168.15 | 622 | Auto | 0.99855 | 32.84 | 290.15>77.00 | |
| <input checked="" type="checkbox"/> 1 | Ecgonine methylester | 1.042 | 200.15>82.05 | 118 | Auto | 0.99967 | 13.49 | 200.15>150.10 | |
| <input checked="" type="checkbox"/> 12 | Amphetamine | 3.692 | 136.10>91.10 | 49 | Auto | 0.99859 | 22.71 | 136.10>119.15 | |
| <input checked="" type="checkbox"/> 44 | Cocaine | 5.515 | 304.15>182.15 | 15 | Auto | 0.99973 | 23.54 | 304.15>82.05 | |

One click to map a compound in different patients

The user experience can be simply changed to meet individual needs...

LabSolutions Insight Library Screening (Admin) - (Insight_CAO_batch.lcb - Insight_CAO_results.lcm)

Shortcuts

- File
- View
- Compound
- Outliers or Review
- Compound Details
- Calibration Curve
- Library Hits
- Survey
- QC Chart
- Settings

Sample List

| # | Sample Name |
|----|-------------|
| 8 | PatientID 1 |
| 9 | PatientID 2 |
| 10 | PatientID 3 |
| 11 | PatientID 4 |

Compound Results - Archive10_PatientID5

| # | Flag ID | Flags | Name | m/z | Found RT | Area | Co... | Lib. Compound Name | Lib. SI | Lib. RT | Lib |
|----|---------|-------|----------------------|---------------|----------|----------|-------|----------------------|---------|---------|-----|
| 31 | >R | F | Benzoylecgonine | 290.15>168.15 | 4.635 | 40750917 | 622 | Benzoylecgonine | 95 | 4.634 | |
| 1 | >R | F | Ecgonine methylester | 200.15>82.05 | 1.042 | 1555797 | 118 | Ecgonine methylester | 69 | 1.044 | |
| 12 | >R | F | Amphetamine | 136.10>91.10 | 3.692 | 3066953 | 49 | Phenylpropylamine | 67 | 3.614 | |
| 44 | >R | F | Cocaine | 304.15>182.15 | 5.515 | 1455517 | 15 | Cocaine | 82 | 5.590 | |

Survey

Zoom Show selected compound only

#31 Benzoylecgonine

Archive10_PatientID5 RT=4.635 1.08e7

Archive11_PatientID6 RT=4.636 1.28e6

Archive13_PatientID8 RT=4.637 2.64e6

Archive15_PatientID2 RT=4.631 2.89e6

Archive16_PatientID7 RT=4.635 1.31e6

Archive9_patientID4 RT=4.633 3.20e6

Compound Details Survey

Touchscreen sample login

To help multi-discipline users it makes a difference to change their experience and adapt to workflows. In this case it is delivering software for clinical environments.

The screenshot displays the 'Open Solution Connect' software interface. On the left is a data table with columns: Status, Batch #, Tray, Vial, Accession #, Method, Data File, Dilution Factor, and Injection Volume. The table lists 46 rows of data, all with a 'Queued' status. At the bottom of the table are three icons: a download arrow, a trash can, and a pencil. To the right of the table is a 12x12 grid for sample login. The grid is divided into four 6x6 quadrants. The top-left quadrant shows numbers 2, 4, and 6. The top-right quadrant shows numbers 1, 3, and 5. The bottom-left quadrant shows numbers 1 through 12 in a 3x4 grid. The bottom-right quadrant shows numbers 1 through 12 in a 3x4 grid. The grid cells are represented by small circles, some of which are filled with green or black to indicate sample placement.

| Status | Batch # | Tray | Vial | Accession # | Method | Data File | Dilution Factor | Injection Volume |
|--------|---------|------|------|-------------|--------------------|-----------|-----------------|------------------|
| Queued | 1 | 1 | 1 | 1312050001 | New MethodSDFGSDFG | | 1 | 1.000 |
| Queued | 1 | 1 | 2 | 1312050002 | New MethodSDFGSDFG | | 1 | 1.000 |
| Queued | 1 | 1 | 3 | 1312050003 | New MethodSDFGSDFG | | 1 | 1.000 |
| Queued | 1 | 1 | 4 | 1312050004 | New MethodSDFGSDFG | | 1 | 1.000 |
| Queued | 1 | 1 | 5 | 1312050005 | New MethodSDFGSDFG | | 1 | 1.000 |
| Queued | 1 | 1 | 6 | 1312050006 | New MethodSDFGSDFG | | 1 | 1.000 |
| Queued | 1 | 1 | 7 | 1312050007 | New MethodSDFGSDFG | | 1 | 1.000 |
| Queued | 1 | 1 | 8 | 1312050008 | New MethodSDFGSDFG | | 1 | 1.000 |
| Queued | 1 | 1 | 9 | 1312050009 | New MethodSDFGSDFG | | 1 | 1.000 |
| Queued | 1 | 1 | 10 | 1312050010 | New MethodSDFGSDFG | | 1 | 1.000 |
| Queued | 1 | 1 | 11 | 1312050011 | New MethodSDFGSDFG | | 1 | 1.000 |
| Queued | 1 | 1 | 12 | 1312050012 | New MethodSDFGSDFG | | 1 | 1.000 |
| Queued | 1 | 1 | 13 | 1312050013 | New MethodSDFGSDFG | | 1 | 1.000 |
| Queued | 1 | 1 | 14 | 1312050014 | New MethodSDFGSDFG | | 1 | 1.000 |
| Queued | 1 | 1 | 15 | 1312050015 | New MethodSDFGSDFG | | 1 | 1.000 |
| Queued | 1 | 1 | 16 | 1312050016 | New MethodSDFGSDFG | | 1 | 1.000 |
| Queued | 1 | 1 | 17 | 1312050017 | New MethodSDFGSDFG | | 1 | 1.000 |
| Queued | 1 | 1 | 18 | 1312050018 | New MethodSDFGSDFG | | 1 | 1.000 |
| Queued | 1 | 1 | 19 | 1312050019 | New MethodSDFGSDFG | | 1 | 1.000 |
| Queued | 1 | 1 | 20 | 1312050020 | New MethodSDFGSDFG | | 1 | 1.000 |
| Queued | 1 | 1 | 21 | 1312050021 | New MethodSDFGSDFG | | 1 | 1.000 |
| Queued | 1 | 1 | 22 | 1312050022 | New MethodSDFGSDFG | | 1 | 1.000 |
| Queued | 1 | 1 | 23 | 1312050023 | New MethodSDFGSDFG | | 1 | 1.000 |
| Queued | 1 | 1 | 24 | 1312050024 | New MethodSDFGSDFG | | 1 | 1.000 |
| Queued | 1 | 1 | 25 | 1312050025 | New MethodSDFGSDFG | | 1 | 1.000 |
| Queued | 1 | 1 | 26 | 1312050026 | New MethodSDFGSDFG | | 1 | 1.000 |
| Queued | 1 | 1 | 27 | 1312050027 | New MethodSDFGSDFG | | 1 | 1.000 |
| Queued | 1 | 1 | 28 | 1312050028 | New MethodSDFGSDFG | | 1 | 1.000 |
| Queued | 1 | 1 | 29 | 1312050029 | New MethodSDFGSDFG | | 1 | 1.000 |
| Queued | 1 | 1 | 30 | 1312050030 | New MethodSDFGSDFG | | 1 | 1.000 |
| Queued | 1 | 1 | 31 | 1312050031 | New MethodSDFGSDFG | | 1 | 1.000 |
| Queued | 1 | 1 | 32 | 1312050032 | New MethodSDFGSDFG | | 1 | 1.000 |
| Queued | 1 | 1 | 33 | 1312050033 | New MethodSDFGSDFG | | 1 | 1.000 |
| Queued | 1 | 1 | 34 | 1312050034 | New MethodSDFGSDFG | | 1 | 1.000 |
| Queued | 1 | 1 | 35 | 1312050035 | New MethodSDFGSDFG | | 1 | 1.000 |
| Queued | 1 | 1 | 36 | 1312050036 | New MethodSDFGSDFG | | 1 | 1.000 |
| Queued | 1 | 1 | 37 | 1312050037 | New MethodSDFGSDFG | | 1 | 1.000 |
| Queued | 1 | 1 | 38 | 1312050038 | New MethodSDFGSDFG | | 1 | 1.000 |
| Queued | 1 | 1 | 39 | 1312050039 | New MethodSDFGSDFG | | 1 | 1.000 |
| Queued | 1 | 1 | 40 | 1312050040 | New MethodSDFGSDFG | | 1 | 1.000 |
| Queued | 1 | 1 | 41 | 1312050041 | New MethodSDFGSDFG | | 1 | 1.000 |
| Queued | 1 | 1 | 42 | 1312050042 | New MethodSDFGSDFG | | 1 | 1.000 |
| Queued | 1 | 1 | 43 | 1312050043 | New MethodSDFGSDFG | | 1 | 1.000 |
| Queued | 1 | 1 | 44 | 1312050044 | New MethodSDFGSDFG | | 1 | 1.000 |
| Queued | 1 | 1 | 45 | 1312050045 | New MethodSDFGSDFG | | 1 | 1.000 |
| Queued | 1 | 1 | 46 | 1312050046 | New MethodSDFGSDFG | | 1 | 1.000 |

Sample log-in software designed for each need
Clinical context
Touch screen
Bi-directional communication with LIS

Designed to make things better, easier and help improve the productivity of the clinical lab

Changing sample management experiences

By developing automated sample preparation tools in the clinical toxicology domain it's also important to design the sample login software for the lab environment

Shimadzu Clinical Laboratory Automation Module

SHIMADZU 2017/03/24 16:49:31

Start Pause Alarm Stop KIT Status Print Scrn Error LabSol Log-In/Quit

PC: Analyzing
UNIT: Starting up
LabSol: Ready User Level: 6 Help

| Request KIT | Step | Time |
|-------------|------|------|
| | | |

PID
Rack
Request No.
End Time

- Analyzing Unit
- LabSolutionsLCMS
Waiting Req. 7

Filtration Pressure

| Vacuum | Port 1 | Port 2 |
|------------|-----------|-----------|
| -52.29 kPa | -0.45 kPa | -0.72 kPa |

Vial Set

| Rest | Required |
|------|----------|
| 16 | 14 |

Temperature(°C)

| Cooler | Heater |
|--------|--------|
| 9 | 25.6 |

- Washing Water Level
- Degas Pump Press.
- Waste Tank Level
- Waste Box Full
- Water Pump Press.

LC

| LC Pump A | Oven Temp. |
|-----------|------------|
| 1.5 MPa | 23.1 °C |

| LC Pump B | LC Pump C |
|-----------|-----------|
| 1.5 MPa | --- |

MS

| Nebulizer Gas Flow | IG Vacuum |
|--------------------|-------------|
| 2.7 L/min | 1.8e-003 Pa |

| Drying Gas Flow | PG Vacuum |
|-----------------|-------------|
| 15.0 L/min | 1.0e+002 Pa |

| DL Temp. | Heating Gas Flow |
|----------|------------------|
| 250 °C | --- |

| Heat Block Temp. | Interface |
|------------------|-----------|
| 400 °C | --- |

Analyzing starting up

Request KIT: 10, 7, 6, 5, 3, 2, 1

Unit Status
Request
Reagent
Calibration
Control
Maintenance
To Setting

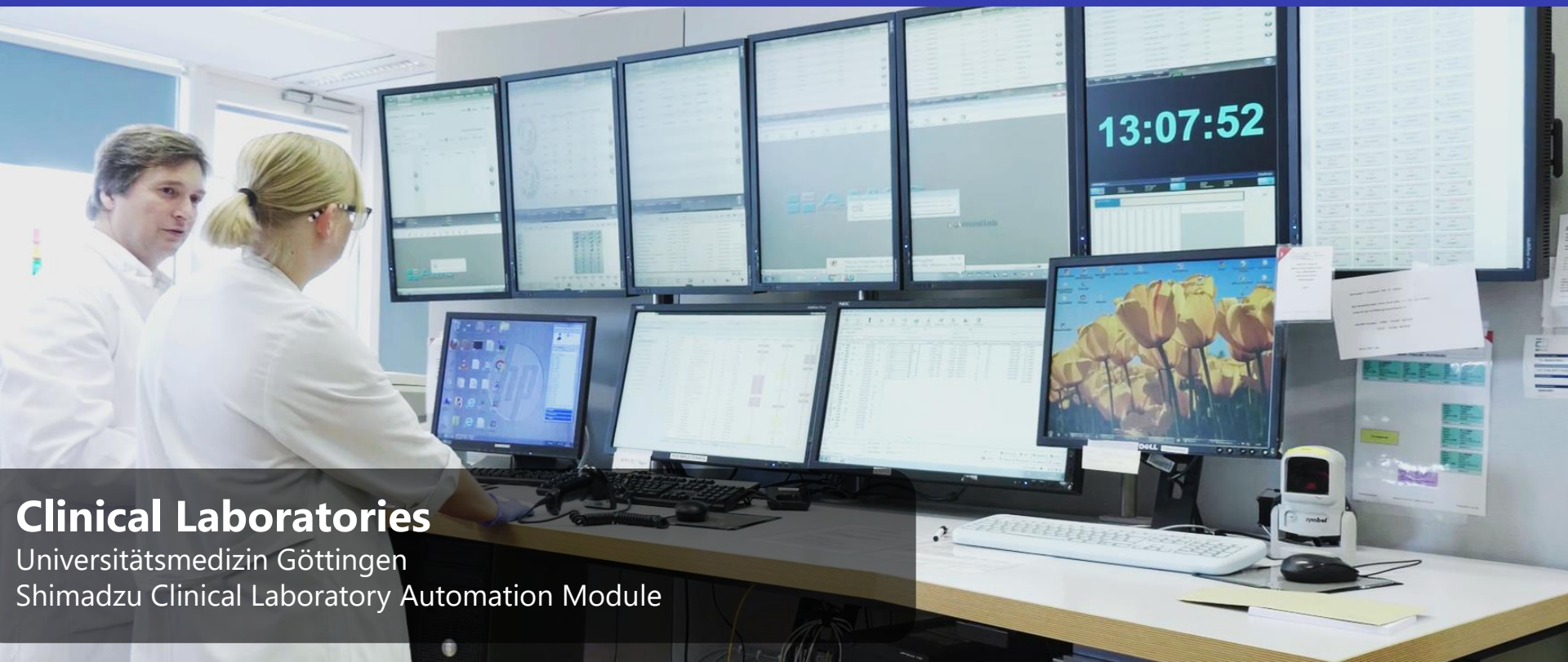
LC Stop
MS Stop
Reconnected Unit
Update

Waiting Busy Complete Error Data Alarm
No request Next BCR Barcode OK No Read

Checking data quality, enhancing automation

In routine LC-MS/MS analysis labs reviewing results and checking data quality are critical components in the workflow.

Creating data spaces to review the analysis, check the data quickly will drive future software designs working with new visualization technologies.



Clinical Laboratories

Universitätsmedizin Göttingen

Shimadzu Clinical Laboratory Automation Module

Faster data acquisition, higher data quality, better identification

Trend towards faster data acquisition, higher quality MS/MS

Key driver 'Driving higher sensitivity but also higher data quality'



High data density

Enables a higher number of compounds in a test panel. Better identification power (libraries; full scan or MRM)

Do more with faster data acquisition instruments

Using high speed data acquisition systems methods can be changed to deliver high sensitivity but also better identification. Driving informatic workflows.

Key driver 'Library searchable identification, reducing false positive and false negative reporting'.

MRM Spectrum Mode

11 MRM's acquired for
chlortetracycline at 10pg/uL

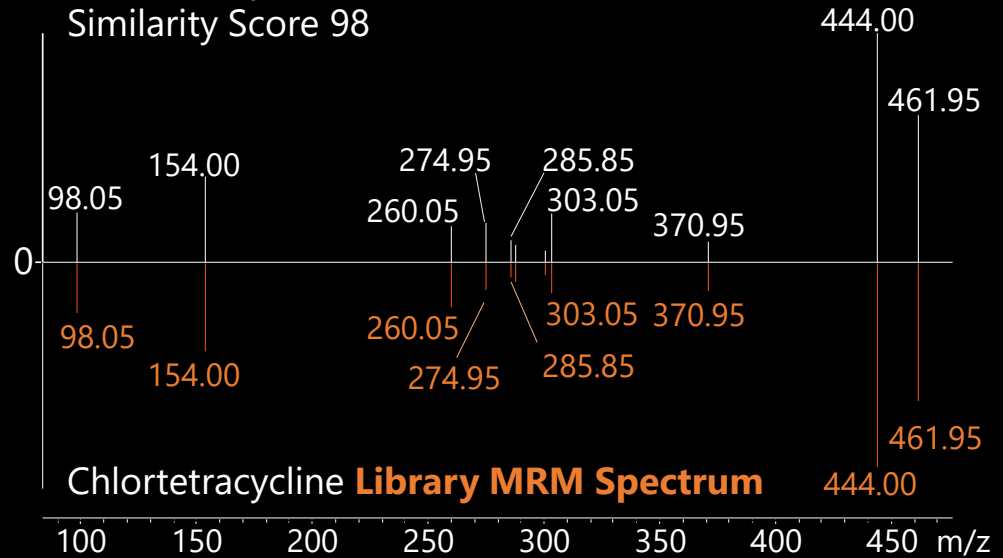
- 1:479.10>444.00 (+) CE: -23V
- 2:479.10>461.95 (+) CE: -35V
- 3:479.10>154.00 (+) CE: -34V
- 4:479.10>98.05(+) CE: -45V
- 5:479.10>260.05(+) CE: -60V
- 6:479.10>303.05(+) CE: -37V
- 7:479.10>300.80(+) CE: -45V
- 8:479.10>287.90(+) CE: -53V
- 9:479.10>274.95(+) CE: -44V
- 10:479.10>370.95(+) CE: -31V
- 11:479.10>285.85(+) CE: -56V



6.50 6.75 7.00 7.25 7.50 min

Chlortetracycline Acquired MRM Spectrum

Similarity Score 98



How will informatics change knowledge, let's look at metabolomics....

1600 publications (search term metabolomics+biomarker from 2000)

No clinically approved metabolite biomarkers have emerged with failure in validation phases often being a reason.



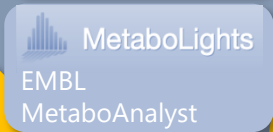
MetabolomeXchange

NIH
Public repository



408
MetabolomeXchange
July 17

50k
Jobs per month



275
MetabolomeXchange
July 17

Metabolomics Databases

- Glycan Mass Spectral Database (GMDB)
- Human Metabolome Database (HMDB)
- LIPID MAPS Structure Database (LMSD)
- LIPID MAPS Proteome Database (LMPD)
- MassBank
- Metlin
- MetabolomeXchange
- Metabolights
- Metabolomics Workbench
- mzCloud
- Metabolome Express
- XCMS

Connecting software tools and instruments

Key words; vendor neutrality, open source but also remote service centres, remote diagnostic tools

Bringing together business models and good ideas, delivering better science



Shimadzu LabSolutions DB/CS
Driver support for other instrument providers





The **BIG** Picture

For **routine method** analysis

Likely direction to lower cost platforms by adding focused software tools for sample log-in and data review (review by exception)

Decision making software will play an increasing role in automating data review

Remote centers

24/7 service, enhanced reliability metrics

Finding unknown components in complex samples

Component detection

Better ID

Correlating structures with fragmentation patterns.

More connections

Allowing greater vendor neutrality

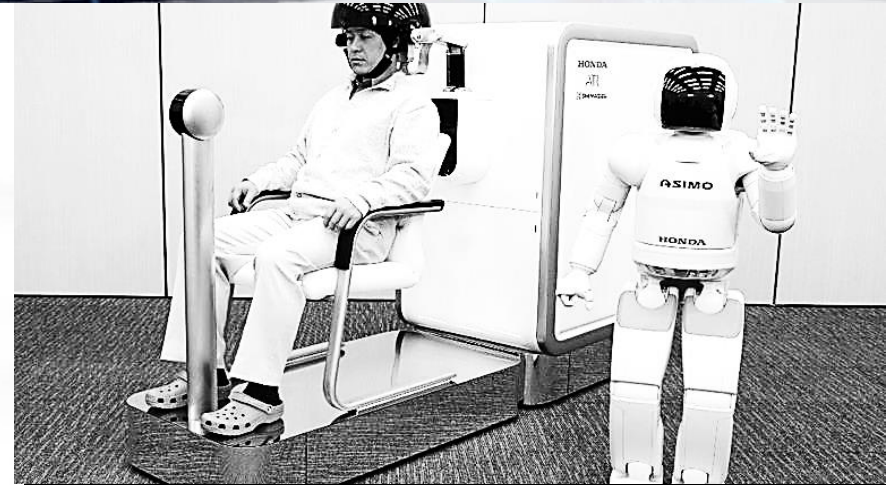
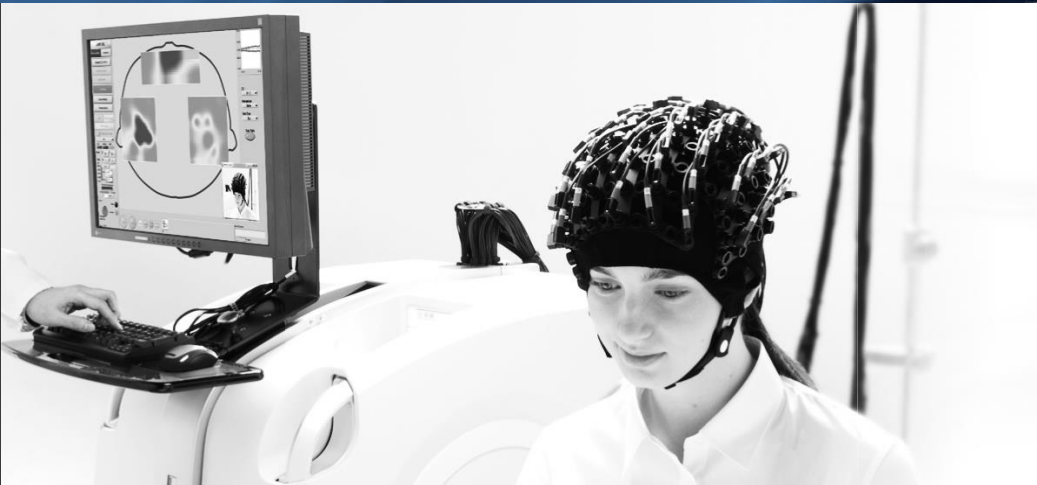
Support for knowledge not just information

BIG Data

It will have an impact

Next-Generation optical brain-function imaging

fNIRS – functional Near-Infrared Spectroscopy Systems LABNIRS and LIGHTNIRS



What can we do now? One example, Shimadzu LabNIRS | Machine brain interface
In vivo optical imaging using functional near-infrared spectroscopy (fNIRS) to map blood flows, add in EEG and you can extend the capability of measuring cortical currents with high spatio-temporal resolution



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