

Pro EZLC Chromatogram Modeler Demo



What is the Pro-EZLC Chromatogram Modeler?

- Pro EZLC is an instrument-free, **VIRTUAL LAB DRAWER** for LC method development. It delivers a fast, no-cost starting point.
- Develop and optimize your methods without setting foot in the lab sacrificing valuable instrument uptime:
 - improve data quality,
 - Improve laboratory efficiency,
 - Improve profitability
- Allows Restek to offer an on-demand consultative customer experience with Restek LC columns.

Pro-EZLC Modeler Capabilities

What is the scope/scale of the Pro-EZLC Modeler today?

- Drugs of Abuse Library (DOA), ~ 290 compounds
- Nitrosamines Library, 16 compounds
- 1.8/2.7/5.0 um particle platform (SPP)
- Multiple column dimensions
- Mass Spec detection
- Available in Japanese, Italian, French, English

What will the scope/scale of the Pro-EZLC Modeler be in a year?

- Add PFAS, Pesticides, Mycotoxins, etc.
- Add the FPP particle platform
- Add UV detection
- EZLC is being translated into 8 other languages in total. The last ones should be available in the next 1-2 months (to support our global customers)

Location?



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restek.com/en/

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Pro EZLC

Chromatogram Modeler

Now Available for Drugs of Abuse—Other Compound Libraries Coming Soon!

The new Pro EZLC chromatogram modeler is easy to use and offers powerful LC simulation capabilities. Simply input your compound list to generate an instrument-ready set of conditions. Or refine further to meet specific method requirements by changing the column phase and dimensions, mobile phase, and other optimization parameters.

[Log In to Get Started!](#)

Don't have an account yet? [Click here to register for free!](#)

Works in Your Browser

- Firefox (desktop or Android tablet)
- Chrome (Windows or Mac desktop or Android tablet)
- IE 8 or IE 9 and above (Windows desktop)
- Safari (desktop or iPad)
- Opera (desktop or mobile)



Learn About the New Pro EZLC Modeler

Watch our introductory video to take a quick tour of the Pro EZLC chromatogram modeler and learn how to use this easy-to-use, yet powerful method development tool.

[Learn More](#)

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Generating a Model



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Components

Key

1. Three Important Tabs

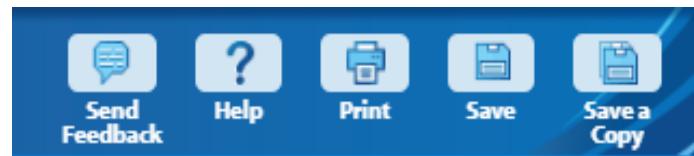
1. Compounds
2. Conditions
3. My EZLC

Pro EZLC Chromatogram

| Compound Name | CAS |
|----------------------------|------------|
| (+)-Ephedrine | 321-98-2 |
| α -Hydroxylprazolam | 37115-43-8 |
| α -Hydroxymidazolam | 59468-90-5 |

2. Five Icons

1. Send Feedback
2. Help
3. Print
4. Save
5. Save a copy



3. Contact Us

1. 4 Ways

Compounds Tab

1. Search for compounds

- a. Scroll (alphabetical)
- b. Typing name into Search bar
- c. Typing CAS Number into Search bar

2. Determine Isobars

- a. Shown by a white checkmark in a blue box

3. Select stationary phase

- a. Raptor Biphenyl
- b. Raptor C18

The screenshot shows the EZLC software interface with the 'Compounds' tab selected. At the top, there are three tabs: 'Compounds' (selected), 'Conditions', and 'My EZLC'. Below the tabs, there are two search/filter fields: 'Compound Class: Drugs of Abuse' and 'Search:'. A list of compounds is displayed in a table with two columns: 'Compound Name' and 'CAS'. The following compounds are listed with their CAS numbers and selection status (checkmark in a blue box):

| Compound Name | CAS |
|-----------------------|-------------|
| Desmethylolanzapine | 161696-76-0 |
| Desomorphine | 427-00-9 |
| Dextromethorphan | 125-71-3 |
| Dextrorphan | 125-73-5 |
| Diazepam | 439-14-5 |
| Diclofenac | 15307-86-5 |
| Didesmethylcitalopram | 62498-69-5 |
| Diethylpropion | 90-84-6 |
| Dihydrocodeine | 125-28-0 |
| Dihydromorphine | 509-60-4 |
| Diphenhydramine | 58-73-1 |
| ... | ... |

At the bottom of the list, there are buttons for 'Select All' and 'Clear' for the selected compounds, and 'Target All' and 'Clear' for the isobars. The 'Phase:' dropdown is set to 'Raptor Biphenyl' and the 'Detector:' dropdown is set to 'MS'. A 'Generate Model' button is located at the bottom right.

Conditions Tab

1. Column

- a. Available Dimensions – (12)

2. Volume Effects

- a. Dwell Volume (0-2 mL)
- b. Extra-Column Volume (0 – 150 μ L)

3. Mobile Phase

- a. Mobile Phase A – Water
- b. Mobile Phase B – Methanol or Acetonitrile
- c. Temperature – (30 – 60 °C)

4. Gradient Program

- a. Initial Isocratic Hold
- b. # of Gradient Steps – (3)
- c. Final Isocratic Hold
- d. Re-equilibration Time
- e. Target Resolution
- f. Optimize Gradient Slope

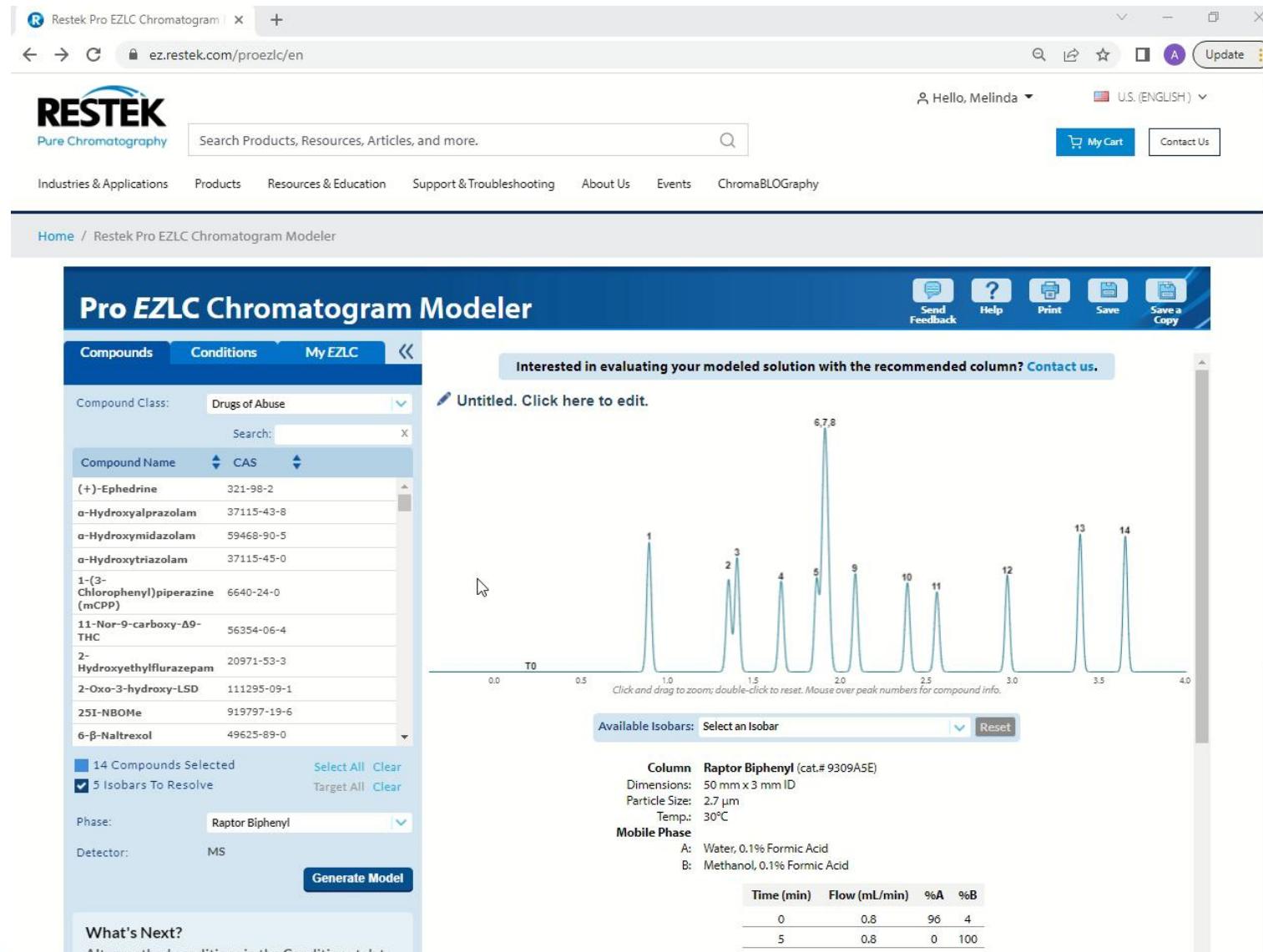
5. Results

- a. Undo/Redo

When altering values, check that the back pressure does not exceed the LC instrument's maximum pressure. Resolution may vary with injection amount/technique/instrument.

| Compounds | Conditions | My EZLC |
|---|-------------------------------------|----------------------------------|
| Column | | |
| Length | 50.00 | mm |
| Inner Diameter | 3.00 | mm |
| Particle Size | 2.70 | μ m |
| Available Columns | 50, 3.00, 2.70 | <input type="button" value="▼"/> |
| Volume Effects | | |
| Dwell Volume | 0.25 | mL |
| Extra-Column Volume | 25.00 | μ L |
| Mobile Phase | | |
| Eluent A | Water | 0.1% Formic Acid |
| Eluent B | Methanol | 0.1% Formic Acid |
| Temperature | 30.00 | °C |
| Back Pressure | psi | 2862 psi |
| Gradient Program | | |
| <input type="checkbox"/> Add Start Isocratic Hold | Time (min) | Flow (mL/min) |
| <input checked="" type="checkbox"/> 1 # of Gradient Steps | 0 | 4 0.8 |
| <input type="checkbox"/> Add Final Isocratic Hold | 5 | 100 0.8 |
| <input type="checkbox"/> Add Re-equilibration Time | | |
| Target Resolution | 1.50 | |
| <input type="button" value="Optimize Gradient Slope"/> | | |
| Results | | |
| Gradient Time + Delay / Run Time | 5.52 / 5.52 min | |
| T0 | 0.21 min | |
| Isobaric Compounds Separated | 12 | |
| Critical Pair | 2,4 | |
| Critical Pair Resolution | 4.85 (3.80 - 5.90) Rs | |
| <input type="button" value="Undo"/> | <input type="button" value="Redo"/> | |

Optimizing A Model



Saving a Model

Restek Pro EZLC Chromatogram | x +

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Pro EZLC Chromatogram Modeler

Compounds Conditions My EZLC Column

Length 50.00 mm
Inner Diameter 3.00 mm
Particle Size 2.70 μ m
Available Columns 50, 3.00, 2.70

Volume Effects

Dwell Volume 0.25 mL
Extra-Column Volume 25.00 μ L

Mobile Phase

Eluent A Water, 0.1% Formic Acid
Eluent B Methanol, 0.1% Formic Acid
Temperature 30.00 °C
Back Pressure 2862 psi

Gradient Program

Add Start Isocratic Hold Time (min) %B Flow (mL/min)
1 # of Gradient Steps 0 4 0.8
Add Final Isocratic Hold 2.2 100 0.8
Add Re-equilibration Time
Target Resolution 1.50
Optimize Gradient Slope

Results

Gradient Time + Delay / Run Time 2.72 / 2.72 min
T0 0.21 min
Isobaric Compounds Separated 12
Critical Pair 2.4
Critical Pair Resolution 3.04 (2.03 - 4.06) Rs

Send Feedback Help Print Save Save a Copy

Interested in evaluating your modeled solution with the recommended column? [Contact us.](#)

Untitled. Click here to edit.

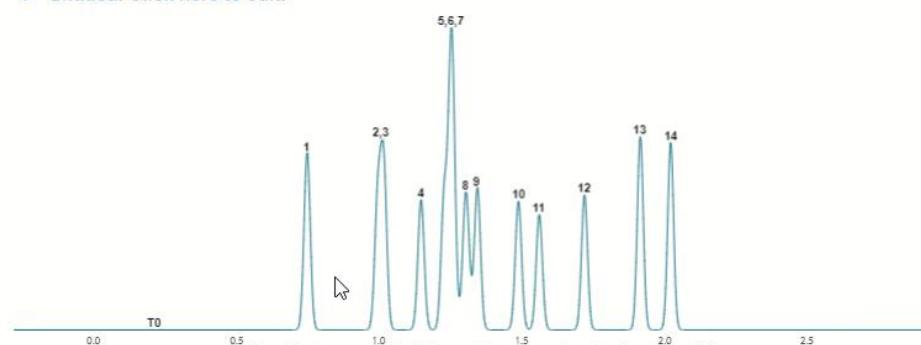
Click and drag to zoom; double-click to reset. Mouse over peak numbers for compound info.

Available Isobars: Select an Isobar Reset

Column: Raptor Biphenyl (cat.# 9309A5E)
Dimensions: 50 mm x 3 mm ID
Particle Size: 2.7 μ m
Temp: 30°C
Mobile Phase
A: Water, 0.1% Formic Acid
B: Methanol, 0.1% Formic Acid

| Time (min) | Flow (mL/min) | %A | %B |
|------------|---------------|----|-----|
| 0 | 0.8 | 96 | 4 |
| 2.2 | 0.8 | 0 | 100 |

Detector: MS
Notes: T0: 0.21 min
Dwell Volume: 0.25 mL
Extra-Column Volume: 25 μ L
Back Pressure: 2862 psi



My EZLC Tab

Saved Models

| Compounds | Conditions | My EZLC |
|---|------------|-------------------|
| Saved Models | | |
| EZLC Training | | X |
| Raptor Biphenyl | | |
| N-Desmethyltapentadol, Dihydrocodeine, Dextromethorphan, O-Desmethyl-cis-tramadol, Methylone... | | |
| | 5-12-2022 | |
| Launch Compounds Optimized | | X |
| Raptor Biphenyl | | |
| Phentermine, N-Desmethyltapentadol, Dihydrocodeine, Dextromethorphan, Pentazocine... | | |
| | 23-09-2022 | |
| Biphenyl 50x3.0 76 compounds | | X |
| Raptor Biphenyl | | |
| 6-Acetylmorphine, 7-Aminoclonazepam, 7-Hydroxyquetiapine, Alprazolam, Amitriptyline... | | |
| | 1-09-2022 | |
| C 18 100x 3 for launch | | X |
| Raptor C18 | | |
| Phentermine, N-Desmethyltapentadol, Dihydrocodeine, Dextromethorphan, Pentazocine... | | |
| | 29-07-2022 | |

Contact Us

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a. Load photo

2. Send Us a Photo

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3. Tell Us About Your Concerns

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Concerns

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EZLC Training

Click and drag to zoom; double-click to reset. Mouse over peak numbers for compound info.

Available Isobars: Select an Isobar | Reset

Column: Raptor Biphenyl (cat.# 9309A5E)
Dimensions: 50 mm x 3 mm ID
Particle Size: 2.7 μ m
Temp.: 30°C

Mobile Phase:
A: Water, 0.1% Formic Acid
B: Methanol, 0.1% Formic Acid

| Time (min) | Flow (mL/min) | %A | %B |
|------------|---------------|----|-----|
| 0 | 0.8 | 96 | 4 |
| 2.2 | 0.8 | 0 | 100 |

Detector Notes:
MS
T0: 0.21 min
Dwell Volume: 0.25 mL
Extra-Column Volume: 25 μ L
Back Pressure: 2862 psi

What's Next?
Alter method conditions in the Conditions tab to see how changes affect the separation.

Need more help?
If you need further assistance, feel free to [send this compound list](#) and any questions you may have to Restek Technical Service.

Looking for other compounds?
Tell us what compound libraries you think Restek should focus on next.

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unds? Tell us what compound libraries you think Restek

>Contact us.

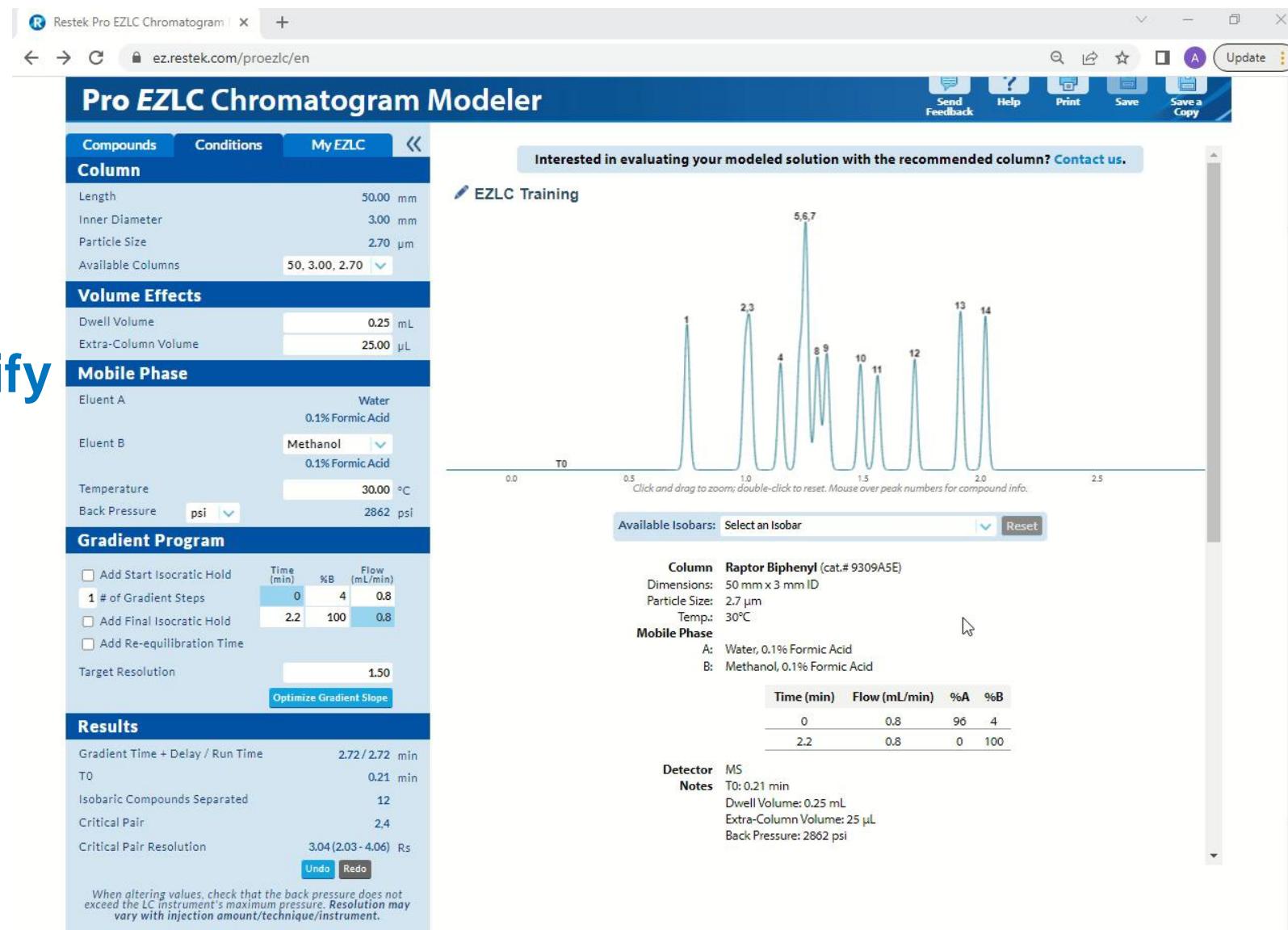
Cool Features

Model View

Zoom

Hovering over peaks to identify
Undo/Redo

View compound structures



Disadvantages

- 1. You cannot simulate matrix effects**
- 2. You cannot simulate differences in concentration**
- 3. You can only simulate known (measured by us) compounds...**

What do you wish for next?

1. You cannot simulate matrix effects
2. You cannot simulate differences in concentration
3. You can only simulate known (measured by us) compounds...

→ **Which libraries would you be interested in next?**

→ **please FILL OUT our SURVEY!**

Beer, Beer, Alt...

When? TODAY, 4.30 pm

Where? Restek Booth No. 8

How? The RESTEK beer coaster is your invitation. ☺

