

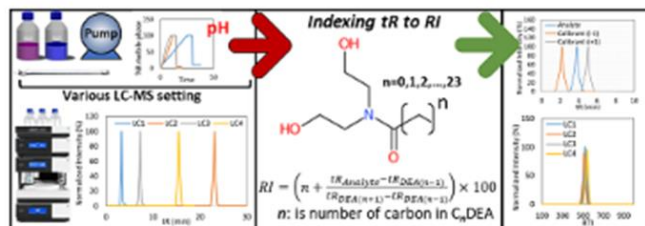
Three tabs of the app

About Prediction of RI RI bank

Citation:

R. Aalizadeh, V. Nikolopoulou and N. S. Thomaidis,

Development of Liquid Chromatographic Retention Index based on Cocamide Diethanolamine Homologous Series (C(n)-DEA), Analytical Chemistry, Submitted, 2022



[Download manual](#)

Are you interested to purchase RI mix?

Contact information:

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C(n=0-23)-DEA Calibrant for LC

Serial No.: #CA0110

For Research Use Only
For Qualitative Analysis

CAS No. 68603-42-9
EC No. 111-42-2

Mild skin irritation. It can be absorbed through skin.
Skin and respiratory protection is necessary.

Appearance at 20°C: Yellowish viscous liquid
Density at 20°C: 0.9986 g/cm³
Solvent: Acetonitrile
Active ingredients: Cocamide DEA
Storage: <8°C
Concentration: Averaged 8.5 mgL⁻¹
Quantity: 1 ml

C(n=0-23)-DEA Calibrant for LC

Serial No.: #CW0110

For Research Use Only
For Qualitative Analysis

CAS No. 68603-42-9
EC No. 111-42-2

Mild skin irritation. It can be absorbed through skin.
Skin and respiratory protection is necessary.

Appearance at 20°C: Yellowish viscous liquid
Density at 20°C: 0.9986 g/cm³
Solvent: Milli-Q water
Active ingredients: Cocamide DEA
Storage: <8°C
Concentration: Averaged 8.5 mgL⁻¹
Quantity: 1 ml

C(n=0-23)-DEA Calibrant for LC

Serial No.: #CM0110

For Research Use Only
For Qualitative Analysis

CAS No. 68603-42-9
EC No. 111-42-2

Mild skin irritation. It can be absorbed through skin.
Skin and respiratory protection is necessary.

Appearance at 20°C: Yellowish viscous liquid
Density at 20°C: 0.9986 g/cm³
Solvent: Methanol
Active ingredients: Cocamide DEA
Storage: <8°C
Concentration: Averaged 8.5 mgL⁻¹
Quantity: 1 ml



CDEA RI standards can be obtained from University of Athens

pH of mobile phase:

☒ pH >= 6

☐ pH <= 4

Choose relevant pH value

Download CDEA RI calibrants Template

See the template file required for RI CDEA calibrant

Upload the tR data of CDEA calibrant...

Browse...

Template_calibrants.csv

Upload complete

Upload the RI CDEA calibrant file (*.csv)

Insert SMILES and tR here...

```
c1ccc(c(c1)CC(=O)OCC(=O)O)Nc2c(cccc2Cl)Cl 9.2
COC1=C(OC)C=C(C(C2=C(N)N=C(N)N=C2)=O)C=C1OC 5.49
CCCCCCCCn1c(=O)c(c(s1)Cl)Cl 12.49
```

Insert SMILES and tR data of suspects

Note:

1) Space separated between SMILES & tR

2) Tab separated between entries

3) Do not leave any line empty

Input is less than 1000 entries. Acceptable

Example: SMILES tR

c1ccc(c(c1)CC(=O)OCC(=O)O)Nc2c(cccc2Cl)Cl 9.2

COC1=C(OC)C=C(C(C2=C(N)N=C(N)N=C2)=O)C=C1OC 5.49

CCCCCCCCn1c(=O)c(c(s1)Cl)Cl 12.49

Submit the calculation

Perform steps 2-5, press this button to run the calculation

Show 10 entries

Search:

ID	SMILES	tR	Exp RI	Pred RI	Probability Level 1	Probability Level 2	pH chemical Space	RI reliability	AD model
All	All	All	All	All	All	All	All	All	All
1	c1ccc(c(c1)CC(=O)OCC(=O)O)Nc2c(cccc2Cl)Cl	9.2	811.54	886.772	0.963	0.037	0	Level 1 (RI may not be affected by pH)	Within the Chemical Space Domain
2	COC1=C(OC)C=C(C(C2=C(N)N=C(N)N=C2)=O)C=C1OC	5.49	502.46	539.825	0.958	0.042	0	Level 1 (RI may not be affected by pH)	Within the Chemical Space Domain
3	CCCCCCCCn1c(=O)c(c(s1)Cl)Cl	12.49	1222.03	1168.218	0.871	0.129	0	Level 1 (RI may not be affected by pH)	Within the Chemical Space Domain

Showing 1 to 3 of 3 entries

Previous

1

Next

Download the list

Download Results

The results are depicted after steps 2-6

Interface for Experimental RIs

[About](#)
[Prediction of RI](#)
[RI bank](#)

Enter the m/z value (Da) here:

Enter mass accuracy (Da):

Ion Type:

Search Database

Show 10 entries

Search:

ID	name	SMILES	InChikey	Comment	Experimental RI	Probability Level 1	Probability Level 2	pH chemical Space	RI reliability	AD model
D00209	Atrazine	CCNc1nc(nc(n1)Cl)NC(C)C	MXWJVTOOROXGIU-UHFFFAOYSA-N	pH < 4	714.02	1	0	0	Level 1 (RI may not be affected by pH)	Analyte may not be appropriate for LC
D02346	Atrazine	CCNc1nc(nc(n1)Cl)NC(C)C	MXWJVTOOROXGIU-UHFFFAOYSA-N	pH > 6	706.96	1	0	0	Level 1 (RI may not be affected by pH)	Analyte may not be appropriate for LC

Showing 1 to 2 of 2 entries

Download the list

- 1
- 2 Insert m/z of analyte of interest
- 3 Insert mass accuracy
- 4 Insert the adduct form
- 5 Search database for experimental RI values

- 6 Download Results

The results are depicted after steps 2-5



National and Kapodistrian
UNIVERSITY OF ATHENS

This app is written by Dr. Reza Aalizadeh (2022)

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Laboratory of Analytical Chemistry

National and Kapodistrian University of Athens

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