



# Lifeline:

**S**ocial **O**nline **S**pectrometry



Steve Stein Yuri Mirokhin



Manor Askenazi

# Lifeline-S.O.S: 'Crowd Curation' of Unidentified GC-(EI)MS spectra through Social Online Spectrometry

Manor Askenazi<sup>1</sup>, Yuri Mirokhin<sup>2</sup>, Stephen Stein<sup>2</sup>

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email: [lifeline@biomedical-hosting.net](mailto:lifeline@biomedical-hosting.net) website: <http://lifeline.biomedical-hosting.net> blog: <http://blogline.biomedical-hosting.net>

## Introduction

The physicochemical relationship between molecular structures and their EI-MS spectra is famously both reproducible and opaque (difficult to predict): whereas reproducibility has underpinned the success of mass spectral libraries, opacity has stymied de-novo structure elucidation for decades. Consequently, unmatched spectra are simply ignored by most identification pipelines. In an effort to gather, prioritize and elucidate unidentified EI spectra we are introducing 'Lifeline' -- a feature of the NIST MS Search software enabling users to submit unidentified spectra to the Lifeline-SOS website where they will be scored for quality, classified into broad molecular category and assigned to appropriate spectral clusters. The submitter can then exchange hypotheses with other cluster members as well as annotations for the individual peaks comprising the cluster centroid.

## Methods

In contrast to other online spectral repositories, Lifeline-S.O.S is intended entirely for individual, unidentified spectra. Furthermore, the website emphasizes communication over algorithmic 'cleverness' by seeking to make submitters aware of other researchers which may be stymied by the same unknown spectra. Importantly, the submitters are not required to disclose their identity nor the identity of the lab in which the spectrum was acquired, neither are they required to provide an exhaustive characterization of the sample or experimental context of the originating acquisition. Users will be able to register for alerts regarding their submitted spectrum (such as a matching submission by another user or the posting of a hypothesis/annotation by another cluster-member) and are, of course, encouraged to participate in the cooperative elucidation process...

## Preliminary Results/Abstract

The ability to submit unidentified spectra to the Lifeline-SOS website has been incorporated directly into the latest release (14) of NIST's MS Search software (this feature is currently in alpha and is disabled by default-- if you would like to enable it, please email a request to the following address: [lifeline@biomedical-hosting.net](mailto:lifeline@biomedical-hosting.net)). We expect that a facile submission process with essentially no (compulsory) reporting requirements, will encourage the elicitation of challenging spectra from the user community. Submissions to the Lifeline-SOS site will, following an aggregation and curation process, form the basis for an 'open source' spectral library, similar to NIST's peptide spectral library. Furthermore, the library will serve as the default destination for recurring and unidentified spectra generated by NIST's internal spectral acquisition efforts, e.g. the site has been pre-populated with recurrent unidentified spectra generated from internal metabolic samples. Nevertheless, the project is in its infancy and one of our goals at this juncture is to validate the overall design of the system as well as its underlying principles: Does the system provide sufficient feedback to justify the submission of spectra? Is an emergent community, assembled by a common spectral cluster, more effective at spectral identification than the individual members on their own? Does the promise of cooperative prioritization and elucidation constitute sufficient incentive for the users to curate their submissions with e.g. information regarding the experimental context or the nature of the sample? More generally, will users be willing to communicate unidentified data when not mandated by e.g. the academic publication process?

## Novel Aspect

A website accessible directly through NIST's MS Search software, enabling submitters to communicate, prioritize and ultimately elucidate unidentified GC-(EI)MS spectra.

NIST Standard Reference Data Gateway

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About: Standard Reference Data (SRD)  
Standard Reference Data Act of 1968 (PL 90-396)

The NIST Data Gateway  
NIST Data Gateway provides easy access to many (currently over 80) of the NIST scientific and technical databases. These databases cover a broad range of substances and properties from many different scientific disciplines. The Gateway includes links to free

What's New in NIST Data  
Rate our Products and Services  
NIST-JANAF Thermochemical Tables  
Chem-Blast Gateway for PDB Ligands  
NIST/EPA/NIH Mass Spectral Database NIST 11  
What's New in v.2.0g distributed with NIST 11  
Click here for a list of our distributors.  
NIST Standard Reference Subscription Database 1 NIST X-Ray Photoelectron Spectroscopy Database: Version 4.0  
NIST Standard Reference Subscription Database 2 Web Thermo Tables (WTT) - Lite Edition  
NIST Standard Reference Subscription Database 3 Web Thermo Tables (WTT) - Professional Edition

# S... Name  
4 A Scan 1339 (26.715 min) of JAN21  
5 A Scan 1889 (36.437 min) of JAN25  
6 A Scan 1108 (22.633 min) of JAN26  
7 A Scan 222 (6.972 min) of DEC010  
8 A Scan 815 (17.453 min) of DEC07  
9 A Scan 741 (16.144 min) of DEC10  
10 A Average of 38.980 to 39.086 min  
11 A Scan 1038 (21.397 min) of MAR0

mainib: 147198 total spectra

100  
10  
1  
1000 900 800 700 600 500 400

U... M... R. Mol... Prob... Name  
1 M 987 987 0.98 Ethyl hept  
2 M 490 720 0.98 Ethyl pent  
3 M 567 576 0.25 4,6-Nonan  
4 M 554 615 0.16 1,1,1,5,5,6  
5 M 543 641 0.11 Butanac c  
6 M 504 690 0.02 1,3-Dioxar  
7 M 502 683 0.02 1,3-Dioxar  
8 M 499 683 0.02 1,3-Dioxar

Name: Scan 222 (6.972 min) of DEC010701007.d 9906  
MW: N/A ID#: 625 DB: Text File  
120 m/z Values and Intensities:  
4 32 | 12 5 | 13 20 |  
14 39 | 15 70 | 16 4 |  
17 2 | 18 4 | 19 14 |  
20 4 | 24 2 | 25 9 |  
26 45 | 27 232 | 28 67 |  
29 685 | 30 29 | 31 197 |  
32 5 | 33 7 | 37 3 |

(Text File) Scan 222 (6.972 min) of DEC010701007

Name: Ethyl heptfluorobutanoylacetate  
Formula: C<sub>8</sub>H<sub>7</sub>F<sub>7</sub>O<sub>2</sub>  
MW: 284 CAS#: 336-62-9 NIST#: 135929  
ID#: 26564 DB: mainib  
Other DBs: None  
Contributor: NIST Mass Spectrometry Data Center, 1994  
119 m/z Values and Intensities:  
12 5 | 13 20 | 14 39 |  
15 70 | 16 4 | 17 2 |  
18 4 | 19 14 | 20 4 |  
24 1 | 25 9 | 26 45 |  
27 232 | 28 67 | 29 686 |  
30 29 | 31 197 | 32 5 | 33 7 | 37 3 |

(mainib) Ethyl heptfluorobutanoylacetate

# NIST Spectral Library GC-EI/MS, 1992



Public Law 90-396  
90th Congress, H. R. 6279  
July 11, 1968

## An Act

To provide for the collection, compilation, critical evaluation, publication, and sale of standard reference data.

*Be it enacted by the Senate and House of Representatives of the United States of America in Congress assembled,*

### DECLARATION OF POLICY

SECTION 1. The Congress hereby finds and declares that reliable standardized scientific and technical reference data are of vital importance to the progress of the Nation's science and technology. It is therefore the policy of the Congress to make critically evaluated reference data readily available to scientists, engineers, and the general public. It is the purpose of this Act to strengthen and enhance this policy

---

Standard Reference Data Act  
H.R. 6279, 1968



United States Constitution  
Article 1, Section 8, 1787



“מֵאֲזֵנֵי צֶדֶק אֲבִנֵי־צֶדֶק ... יִהְיֶה לָכֶם”

“Just balances, just weights ... shall ye have”



Leviticus, 19:35

NIST Standard Reference Data Gateway

Publications Subject Areas Products/Services NIST Organization News Programs & Projects User Facilities Work with NIST

About: Standard Reference Data (SRD)  
Standard Reference Data Act of 1968 (PL 90-396)

The NIST Data Gateway provides easy access to many (currently over 80) of the NIST scientific and technical databases. These databases cover a broad range of substances and properties from many different scientific disciplines. The Gateway includes links to free

What's New in NIST Data  
Rate our Products and Services  
NIST-JANAF Thermochemical Tables  
Chem-Blast Gateway for PDB Ligands  
NIST/EPA/NIH Mass Spectral Database NIST 11  
What's New in v.2.0g distributed with NIST 11  
Click here for a list of our distributors.  
NIST Standard Reference Subscription Database 1 NIST X-Ray Photoelectron Spectroscopy Database: Version 4.0  
NIST Standard Reference Subscription Database 2 Web Thermo Tables (WTT) - Lite Edition  
NIST Standard Reference Subscription Database 3 Web Thermo Tables (WTT) - Professional Edition

mainlib: 147198 total spectra

Li.	Ma.	R. Mol.	Prob.	Name
1	M	987	98.2	Ethyl hept
2	M	600	720	Ethyl pent
3	M	567	576	4,4-Nonan
4	M	554	615	1,1,1,5,5,6
5	M	543	641	Butanac c
6	M	504	690	1,3-Dioxar
7	M	502	683	1,3-Dioxar
8	M	499	683	1,3-Dioxar

Name: Ethyl heptfluorobutanoylacetate  
Formula: C<sub>8</sub>H<sub>7</sub>F<sub>7</sub>O<sub>2</sub>  
MW: 284 CAS#: 336-62-9 NIST#: 135929  
ID#: 26564 DB: mainlib  
Other DBs: None  
Contributor: NIST  
Center, 1994  
119 m/z Values and Intensities:

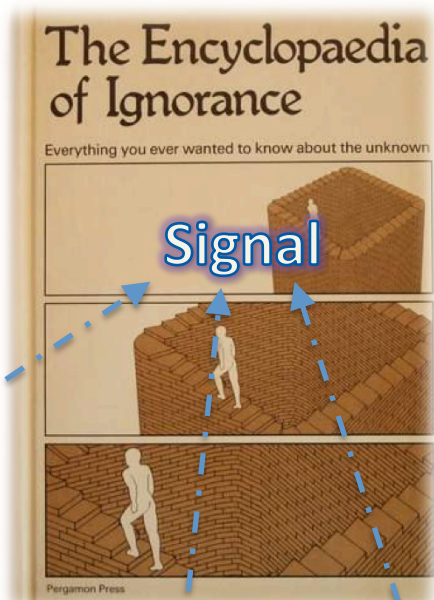
m/z	Value	Intensity
12	5	1
15	70	1
18	4	1
24	1	1
26	45	1
27	232	1
28	684	1

NIST Spectral Library release 14  
276,248 GC-MS Spectra, today

identified

unidentified

reproducible



irreproducible

Noise Noise Noise Noise Noise Noise Noise Noise Noise Noise  
 Noise Noise Noise Noise Noise Noise Noise Noise Noise Noise  
 Noise Noise Noise Noise Noise Noise Noise Noise Noise Noise

(user-submitted spectra will help to "rescue" unidentified signal from noise...)



NIST MS Search 2.2 - [Ident, Presearch Default - InLib = 1525, 100 spectra]

File Search View Tools Options Window Help

1. Scan 222 (6.972 min) of DEC010701007.d

#	Src.	Name
6	A	Scan 1339 (26.715 min) of JAN210401004.d 10167
7	A	Scan 1889 (36.437 min) of JAN250301003.d 10180
8	A	Scan 1108 (22.633 min) of JAN260701007.d 10191
9	A	Scan 222 (6.972 min) of DEC010701007.d 9906
10	A	Scan 815 (17.453 min) of DEC071101011.d 9934

Names Structures Spec List

mainlib; repib; 276259 total spectra

### Match Factor Distribution

Plot/Text of Search Spectrum Plot of Search Spectrum Spec List

### Query Spectrum

Name: Scan 222 (6.972 min) of DEC010701007.d 9906  
 MW: N/A ID#: 16 DB: Text File  
 10 largest peaks:  
 69 999 | 29 685 | 87 437 | 115 370 | 239 260 |  
 43 233 | 27 232 | 31 197 | 42 192 | 41 166 |  
 Synonyms:  
 no synonyms.

### Visual Confirmation

Scan 222 (6.972 min) of DEC010701007.d 9906 Head to Tail MW=367 NMR=367 Ethyl heptafluorobutanoylacetate  
 Difference Head to Tail Side by Side Subtraction 987 987R 98.1P

### Reference Spectrum

Name: Ethyl heptafluorobutanoylacetate  
 Formula: C<sub>8</sub>H<sub>7</sub>F<sub>7</sub>O<sub>3</sub>  
 MW: 284 Exact Mass: 284.028341 CAS#: 336-62-9 NIST#: 135929  
 Other DBs: Fine  
 Contributor: NIST Mass Spectrometry Data Center, 1994  
 InChIKey: CMGCMFZWEPCGSQ-UHFFFAOYSA-N  
 10 largest peaks:  
 69 999 | 29 686 | 87 437 | 115 371 | 239 260 |  
 43 233 | 27 232 | 31 197 | 42 192 | 41 166 |  
 Synonyms:  
 1. Ethyl heptafluorobutyrylacetate  
 2. Ethyl 4,4,5,5,6,6,6-heptafluoro-2-oxobutanoate #

#	Lib.	Match	R.Match	Prob. (%)	RI	Name
1	M	987	987	98.1	-	Ethyl hept...
2	M	597	719	0.98	-	Ethyl pent...
3	M	567	576	0.27	-	4,6-Nonar...
4	M	554	615	0.17	-	1,1,1,5,5,...
5	M	543	641	0.12	-	Butanoic a...
6	M	504	690	0.02	-	1,3-Dioxar...
7	M	502	683	0.02	1...	1,3-Dioxar...
8	M	499	683	0.02	-	1,3-Dioxar...

Names Structures InLib = 1525, Hit List

Lib. Search Other Search Names Compare Librarian MSMS

Ident Ident

(NIST MS Search when things are going well...)



(NIST MS Search when no match is found...)

NIST MS Search 2.2 - [Ident, Presearch Default - InLib = -2433, 100 spectra]

File Search View Tools Options Window Help

1. MYSTERY\_MOL

#	Src.	Name
1	A	MYSTERY_MOL
3	A	Scan 1467 (28.976 min) of JAN3103D1003.d 10149
4	A	Scan 1573 (30.855 min) of JAN3105D1005.d 10156
5	A	Scan 1488 (29.348 min) of JAN2101D1001.d 10164
6	A	Scan 1339 (26.715 min) of JAN2104D1004.d 10167

mainlib; replib; 276259 total spectra

1000 900 800 700 600 500 400 300

(Text File) MYSTERY\_MOL

Plot/Text of Search Spectrum

100 50 0 50 100

43 57 71 85 99 113 141 155

MYSTERY\_MOL

Difference Head to Tail Side by Side

100 50 0 50 100

43 57 71 85 99 155 197 253

(replib) Octadecane, 1-iodo-

Plot/Text of Hit

Name: MYSTERY\_MOL  
MW: N/A ID#: 24 DB: Text File  
10 largest peaks:  
121 57 890 | 99 550 | 43 516 |  
231 317 302 | 466 300 | 141 216 |

533

10 540

Octadecane, 1-iodo-

450 690R 4.28P

Mass: 380.193998 CAS#: 629-93-6 NIST#: 135509 |  
SCA, HODOC, NIH, EINECS, IRDB  
Mass Spectrometry Data Center, 1994  
LVYVOUGB-UHFFFAOYSA-N

10 largest peaks:  
57 999 | 43 849 | 71 631 | 41 566 | 85 430 |  
55 399 | 29 269 | 69 158 | 99 144 | 42 122 |

Synonyms:  
1-Octadecyl iodide  
? Iodo-

Lib. Search Other Search Names Compare Librarian MSMS

Ident Ident

(The user can now provide feedback regarding the failure to identify...)

NIST MS Search 2.2 - [Ident, Presearch Default - InLib = -2433, 100 spectra]

File Search View Tools Options Window Help

1. MYSTERY\_MOL

#	Src.	Name
1	A	MYSTERY_MOL
3	A	Scan 1467 (28.976 min) of JAN310301003.d 10149
4	A	Scan 1573 (30.855 min) of JAN310501005.d 10156
5	A	Scan 1488 (29.348 min) of JAN210101001.d 10164
6	A	Scan 1339 (26.715 min) of JAN210401004.d 10171

mainlib; replib; 276259 total spectra

#	Lib.	Match	R.Match	Prob. (%)	RI	Name
1	R	450	690	4.28	2...	Octadecyl iodide
2	M	448	682	3.95	-	Sulfurous acid
3	R	440	673	2.94	1...	Dodecane
4	M	439	662	2.83	-	Pentadecane
5	R	436	689	2.50	1...	Dodecane
6	R	434	683	2.30	2...	Heptacosane
7	M	434	637	2.30	-	3,3-Diethylpentadecane
8	M	433	719	2.22	1...	Decane, 2,2,4,4-tetramethyl-

Plot/Text of Hit / Plot of Hit

Plot of Hit: (replib) Octadecane, 1-iodo-

Plot of Hit: (replib) Octadecane, 1-iodo-

Formula: C<sub>18</sub>H<sub>37</sub>I  
 MW: 380 Exact Mass: 380.193998 CAS#: 629-93-6 NIST#: 135509  
 Other DBs: Fine, TSCA, HODOC, NIH, EINECS, IRDB  
 Contributor: NIST Mass Spectrometry Data Center, 1994  
 InChIKey: ZNJOCVLVYVOUGB-UHFFFAOYSA-N  
 10 largest peaks:  
 57 999 | 43 849 | 71 631 | 41 566 | 85 430 |  
 55 399 | 29 269 | 69 158 | 99 144 | 42 122 |  
 Synonyms:  
 1. Octadecyl iodide  
 2. Stearic iodide

Sending data to external web site

The spectral data may be sent to external web site.

How should the program proceed?

Ask each time  
 Always allow data to be sent  
 Never send data

OK Cancel

Lib. Search Other Search Names Compare Librarian MSMS

For Help, press F1

Ident Ident

(Note: this will involve user-data leaving the lab...)

Browser address bar: <https://lifelin...tgwjcvqdfmzge>


Page title: Lifeline SOS

Navigation: Register Log In Help

Submission ID: **SOS\_202616381** [GROUP\_813985937]

Claim Submission login required

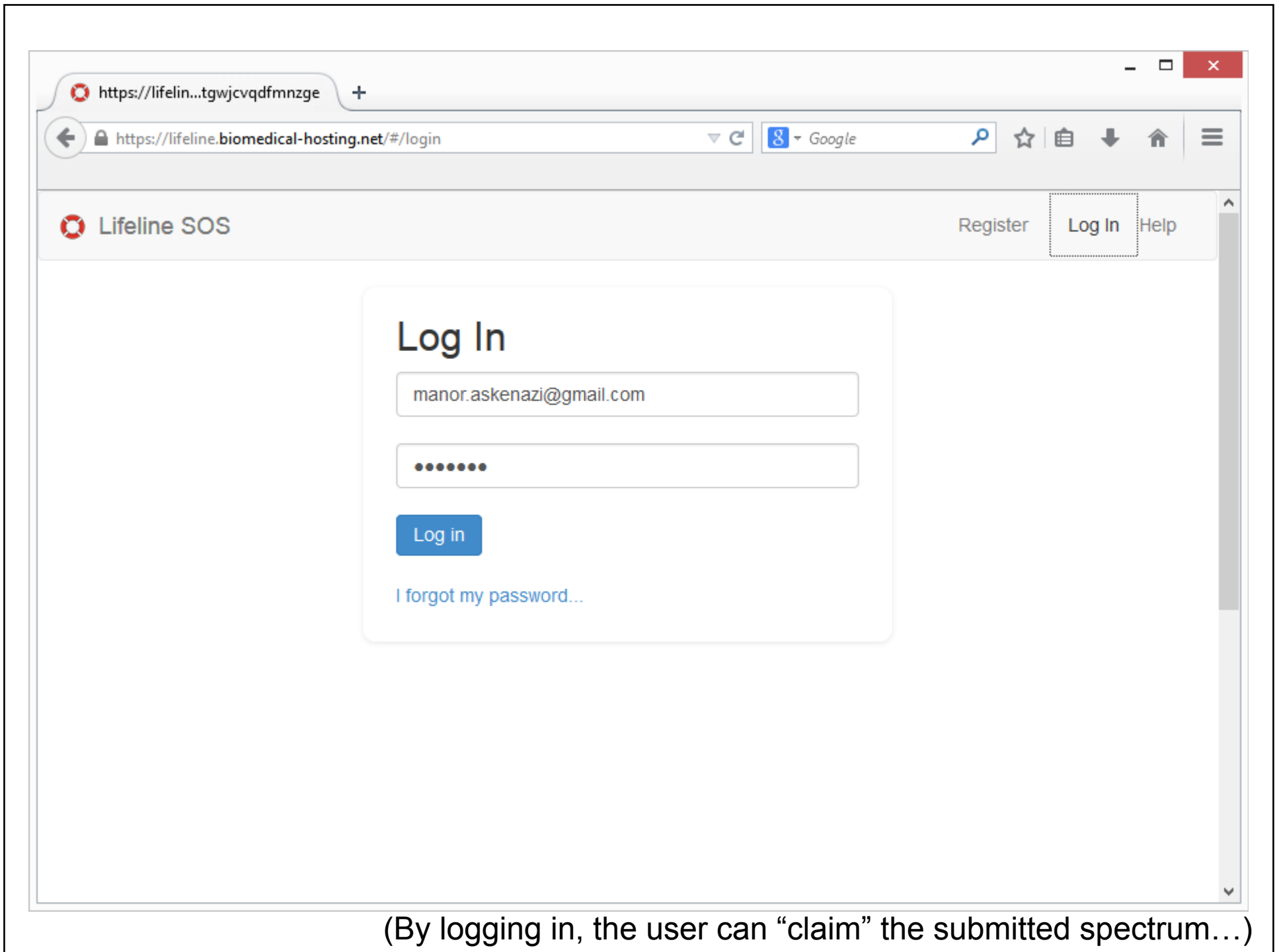
NIST Hits:

CAS	Formula	MF	Name	Prob
 <i>No NIST ID with MF &gt; 500!!!</i>				

ARISTO Categories:

ChEBI_ID	ChEBI_Name	Preci...	score	N	AUC
CHEBI:18310	alkane	0.666	0.775	37	0.967

(By default an accession is provided, but the submission remains anonymous...)



https://lifelin...tgwjcvqdfmzge

https://lifeline.biomedical-hosting.net/#/submission/SOS\_202616381/REC\_slcp

Lifeline SOS manor [Logout](#) [Help](#)

## SOS\_202616381 [GROUP\_813985937]

[Claim Submission](#)

**NIST Hits:**

CAS	Formula	MF	Name	Prob

**ARISTO Categories:**

ChEBI_ID	ChEBI_Name	Preci...	score	N	AUC
<a href="#">CHEBI:18310</a>	alkane	0.666	0.775	37	0.967

(By logging in, the user can “claim” the submitted spectrum...)

https://lifelin...tgwjcvqdfmzge +

https://lifeline.biomedical-hosting.net/#/submission/SOS\_202616381/REC\_slcp Google

Lifeline SOS manor Logout Help

## SOS\_202616381 [GROUP\_813985937]

---

### Provenance

**Sample:**

**Treatment:**

**Derivatization:**

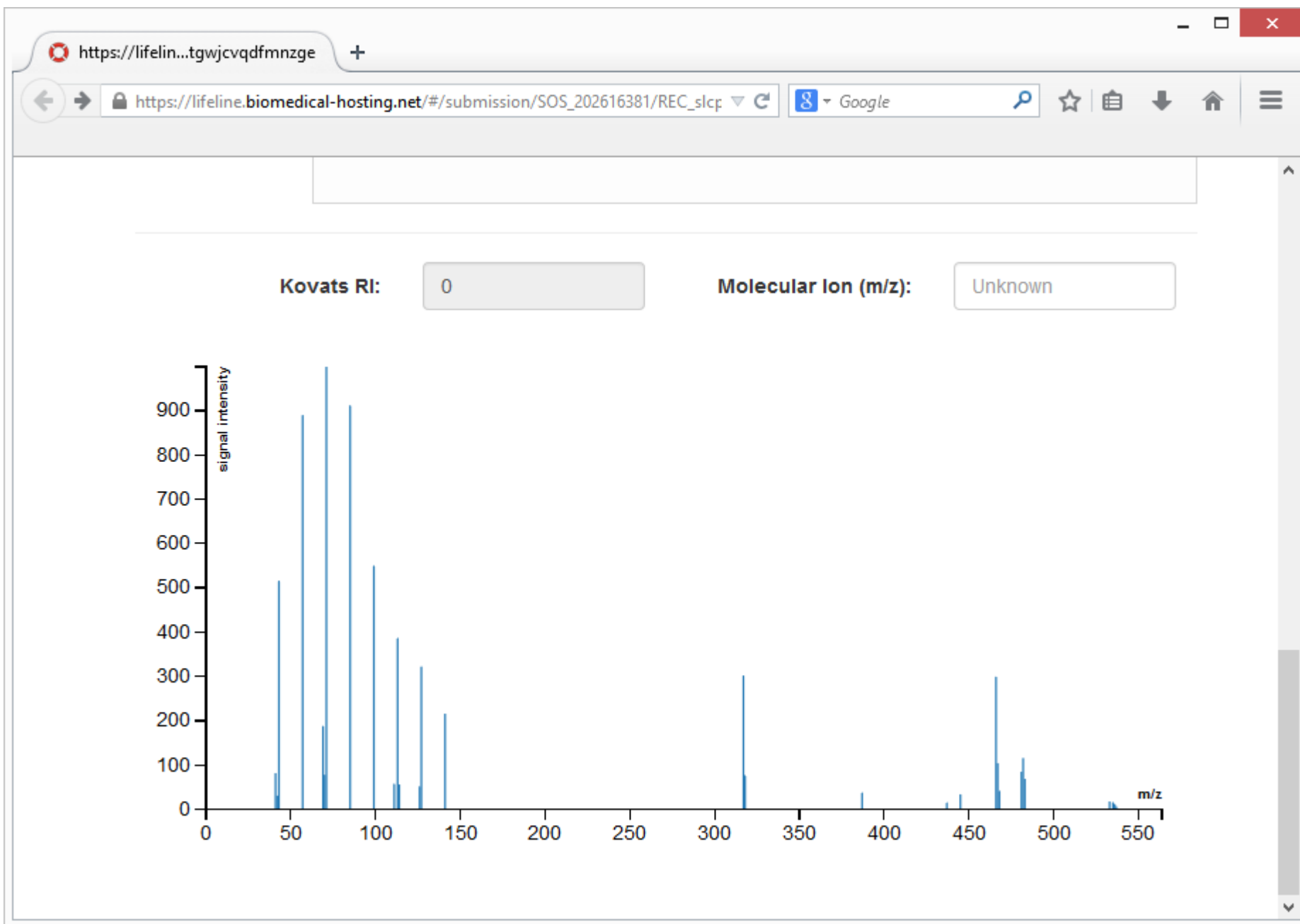
**Instrument:**

**Acquisition:**

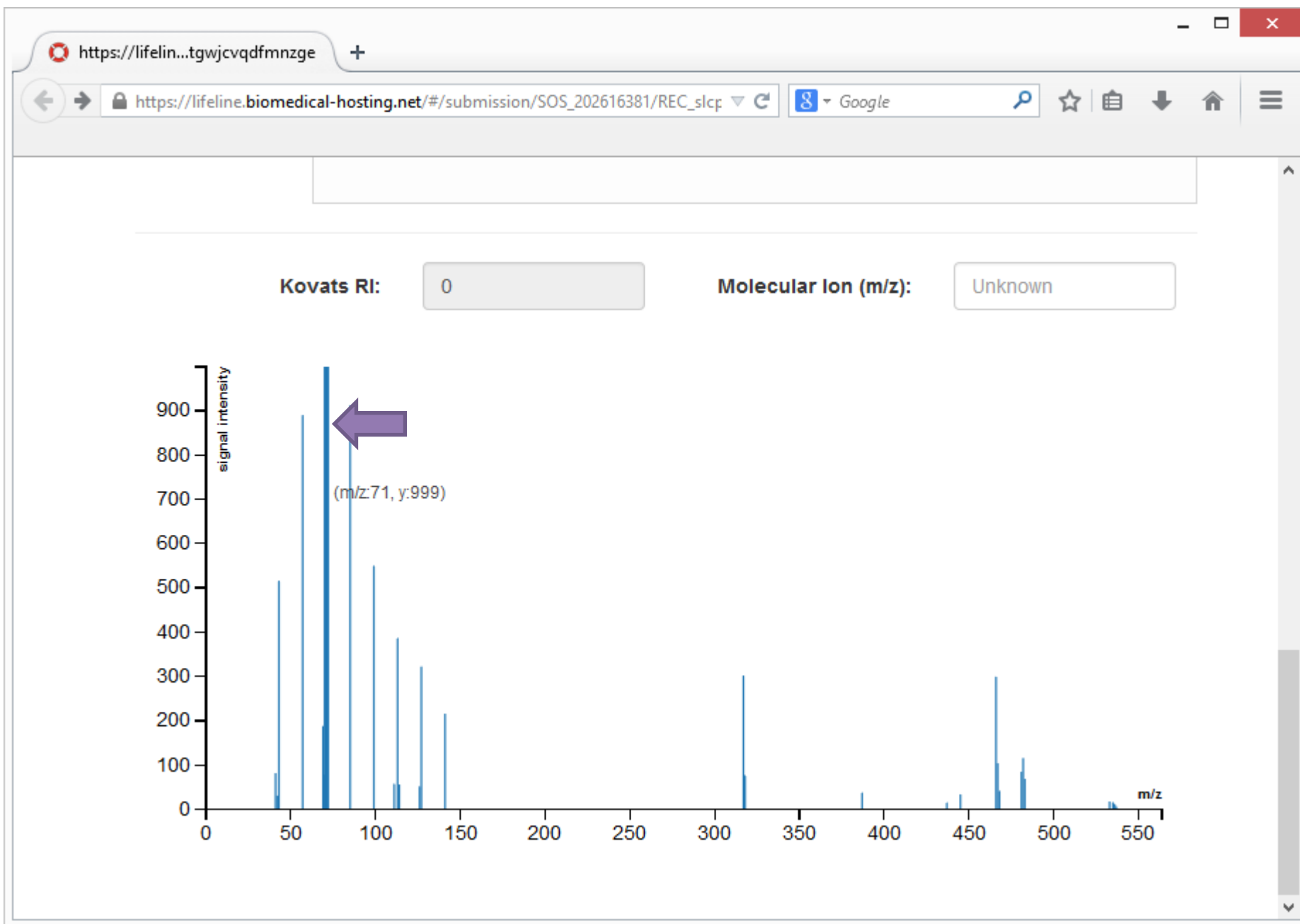
**Comments:**

(S/he is then able to provide meta-data describing the submission...)

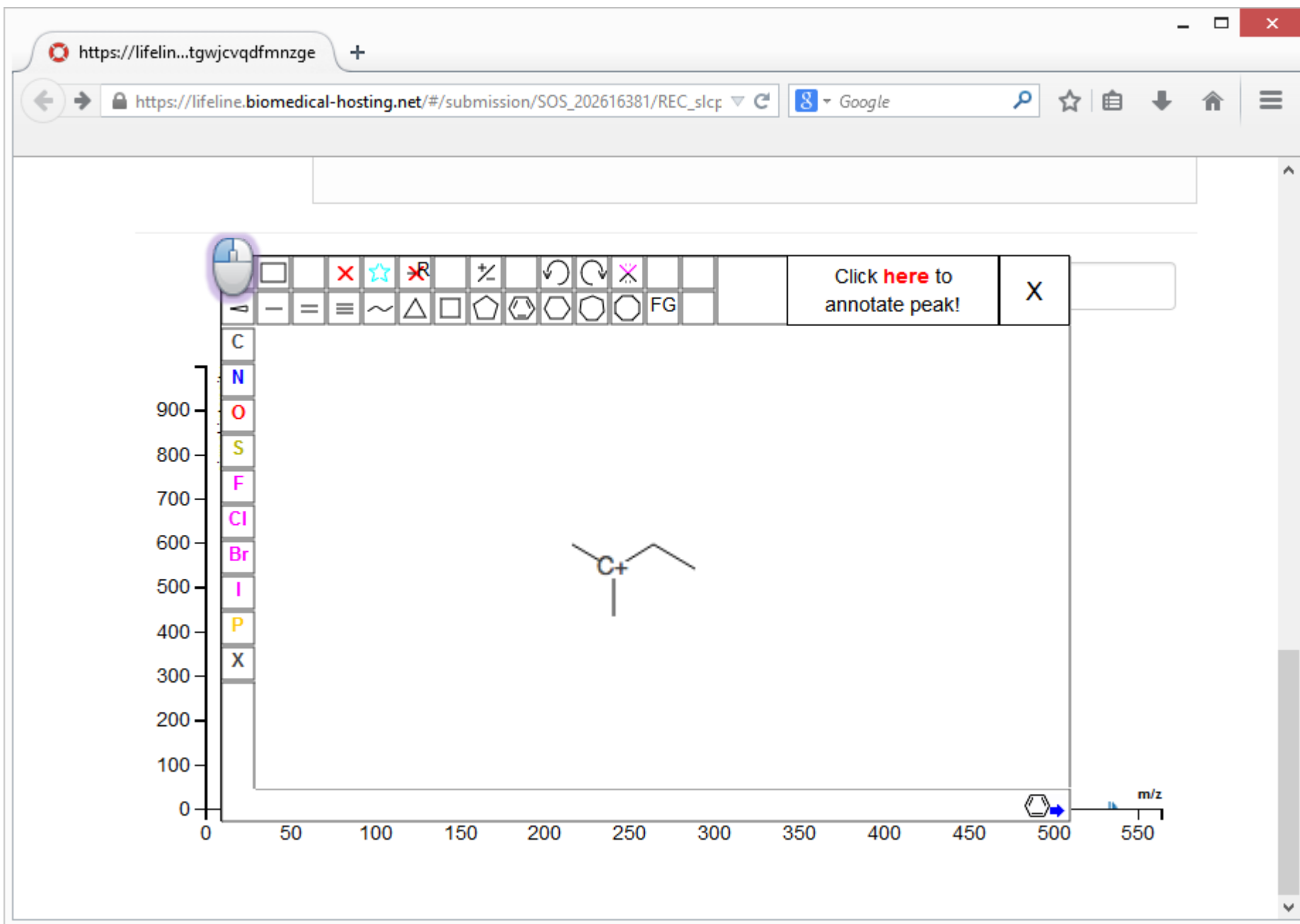




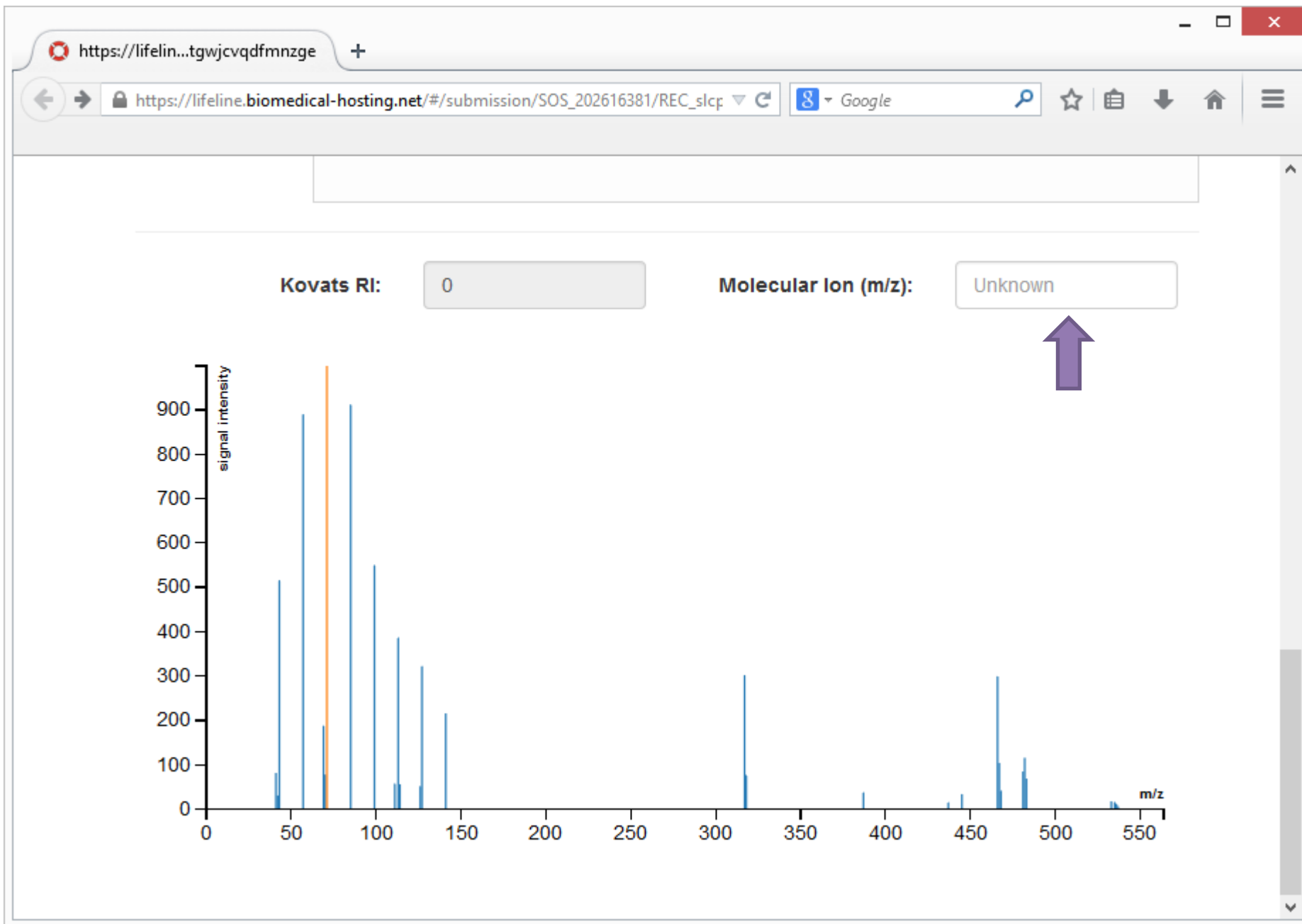
(Visually inspect the resulting spectral submission...)



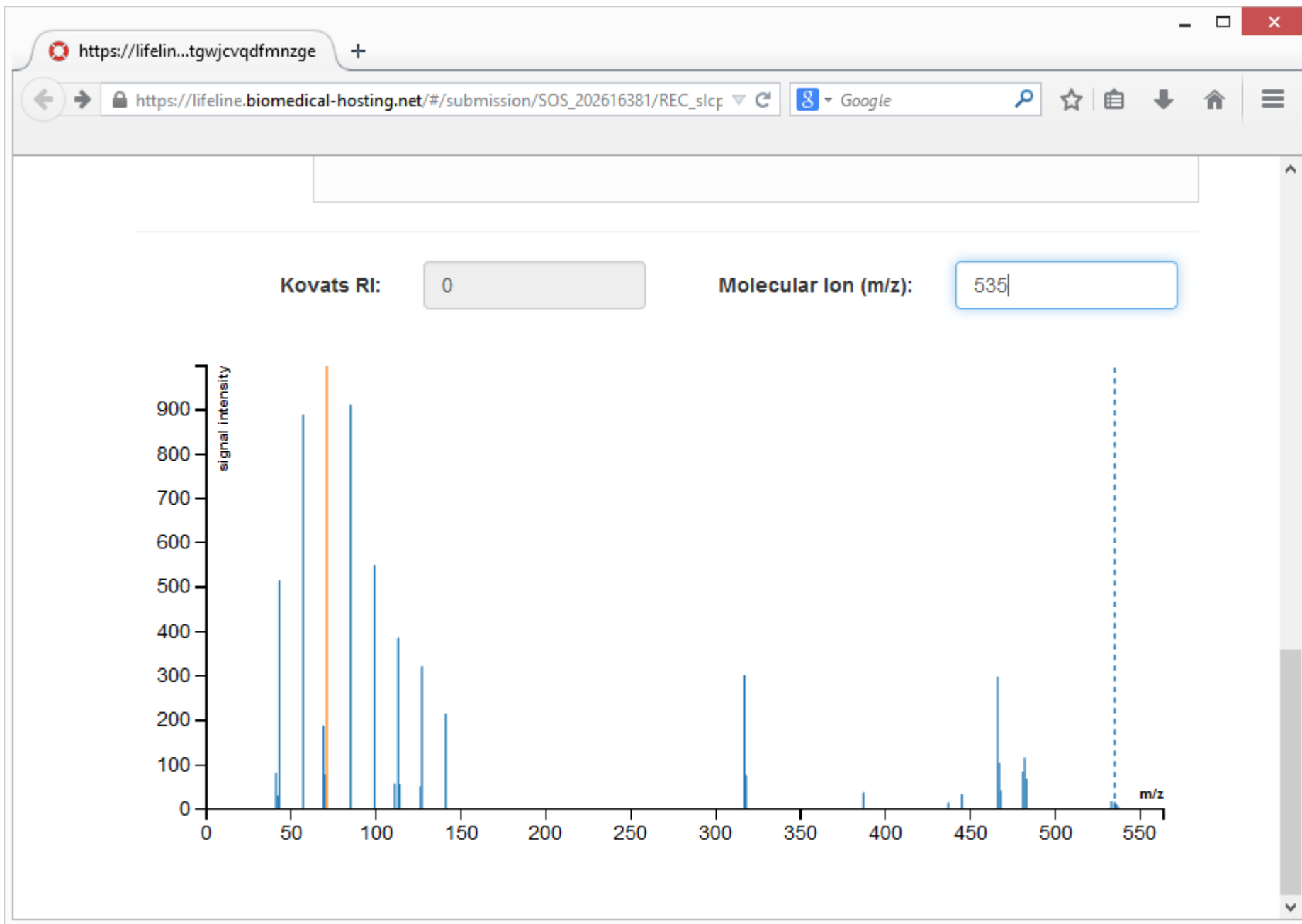
(Provide structural peak annotation...)



(Provide structural peak annotation...)



(And suggest the mass of the Molecular Ion...)



(And suggest the mass of the Molecular Ion...)

https://lifelin...n/SOS\_202616381

https://lifeline.biomedical-hosting.net/#/submission/SOS\_202616381

Google

NIST Hits:

CAS	Formula	MF	Name	Prob
-----	---------	----	------	------

ARISTO Categories:

ChEBI_ID	ChEBI_Name	Preci...	score	N	AUC
<a href="#">CHEBI:18310</a>	alkane	0.666	0.775	37	0.967

Kovats RI:

0

Molecular Ion (m/z):

535

signal intensity

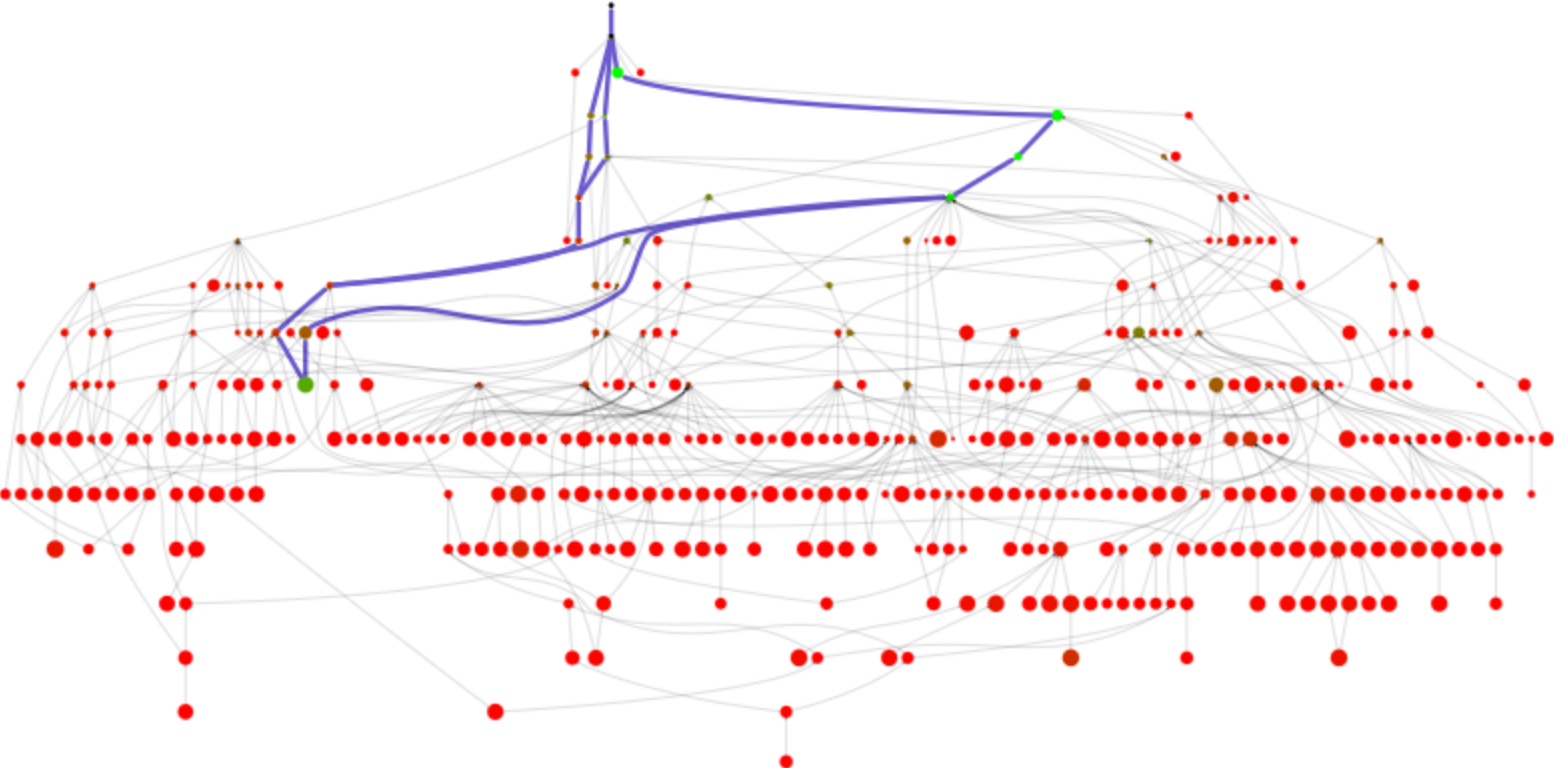
900

800

(ARISTO is run on behalf of the user...)

El by ChEBI

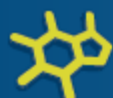
www.ionspectra.org/aristo/report/



Download data as tab delimited file  Filtered

score	ChEBI	N	AUC	Est. Precision
0.775	<a href="#">alkane</a>	37	0.967	0.666

(Yielding a ChEBI Ontology-based annotation...)



- ▣ ChEBI Home
  - ▣ Advanced Search
  - ⌵ Browse
  - ▣ Submit
  - ▣ Download
  - ⌵ Documentation
  - ⌵ Developer Resources
  - ⌵ Tools
  - ▣ Preferences
  - ▣ Contact ChEBI
- 
- ▣ Printer Friendly View

EBI &gt; Databases &gt; Small Molecules &gt; ChEBI &gt; Main

alkane (CHEBI:18310)

Search ChEBI here!

Search ChEBI

Search for  ★★ ★ only All in ChEBI

Main

ChEBI Ontology

Automatic Xrefs

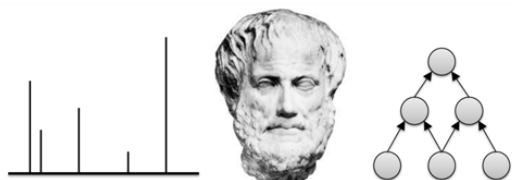
ChEBI Name **alkane**ChEBI ID **CHEBI:18310**Definition An acyclic branched or unbranched hydrocarbon having the general formula  $C_nH_{2n+2}$ , and therefore consisting entirely of hydrogen atoms and saturated carbon atoms.Stars **★★★★** This entity has been manually annotated by the ChEBI Team.Secondary ChEBI IDs CHEBI:13435, CHEBI:22317, CHEBI:2576ChEBI Ontology

Outgoing

alkane (CHEBI:18310) **is a** aliphatic compound (CHEBI:33653)alkane (CHEBI:18310) **is a** hydrocarbon (CHEBI:24632)2,2,4,6,6-pentamethylheptane (CHEBI:77509) **is a** alkane (CHEBI:18310)2,4,6,10-tetramethylpentadecane (CHEBI:77510) **is a** alkane (CHEBI:18310)2,5-dimethylundecane (CHEBI:77445) **is a** alkane (CHEBI:18310)4-methylheptane (CHEBI:77446) **is a** alkane (CHEBI:18310)

(Yielding a ChEBI Ontology-based annotation...)





Automatic Reduction of Ion Spectra To Ontology

*Nucleic Acids Research*, 2011, Vol. 39, Web Server issue W505–W510  
doi:10.1093/nar/gkr403

## ARISTO: ontological classification of small molecules by electron ionization-mass spectrometry

Manor Askenazi<sup>1,2,\*</sup> and Michal Linial<sup>1</sup>

<sup>1</sup>Sudarsky Center for Computational Biology, Department of Biological Chemistry, Hebrew University of Jerusalem, Israel and <sup>2</sup>Blais Proteomics Center, Dana-Farber Cancer Institute, Boston, MA, USA

Received February 15, 2011; Revised May 2, 2011; Accepted May 5, 2011

Download data as tab delimited file  Filtered

score	ChEBI	N	AUC	Est. Precision
0.775	<a href="#">alkane</a>	37	0.967	0.666

(Yielding a ChEBI Ontology-based annotation...)

https://lifelin...tgwjcvqdfmzge +

https://lifeline.biomedical-hosting.net/#/submission/SOS\_202616381/REC\_slcp

Lifeline SOS manor Logout Help

**SOS\_202616381** [\[GROUP\\_813985937\]](#)

### Provenance

**Sample:** Sample source...

**Treatment:** Sample processing (excludes derivatization)

**Derivatization:** Derivatization applied...

**Instrument:** Instrumentation used...

**Acquisition:**

**Comments:** Any other useful meta-data?


https://lifeline.biomedical-hosting.net/#/group/GROUP\_813985937

(Every submission is associated with a Spectral Cluster...)


https://lifelin...tgwjcvqdfmzge +

https://lifeline.biomedical-hosting.net/#/submission/SOS\_202616381/REC\_slcp Google

Lifeline SOS manor Logout Help



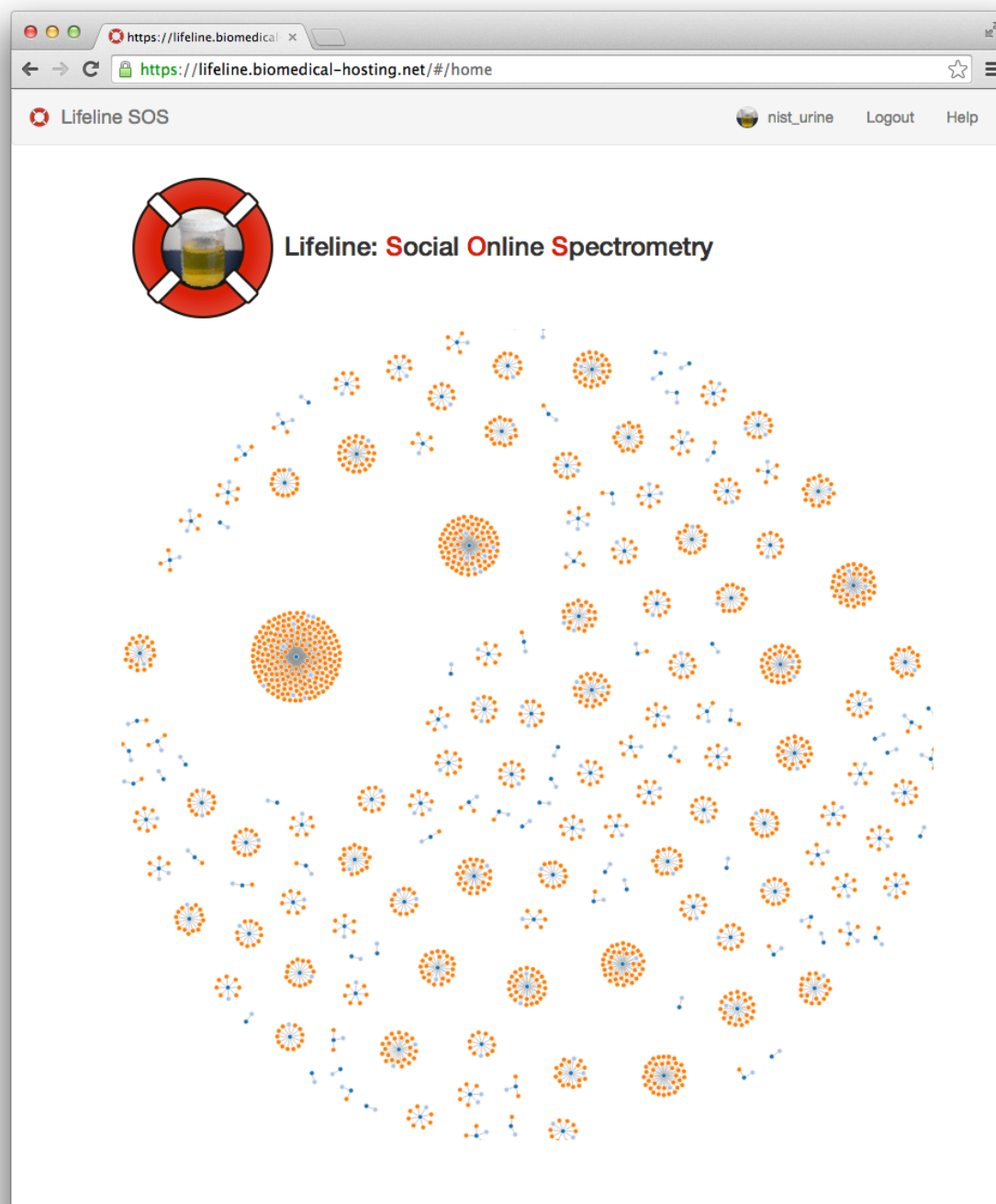
# Lifeline: Social Online Spectrometry



- My spectra!
- Spectral Cluster (Group)
- Someone else's submissions...

https://lifeline.biomedical-hosting.net/#/group/GROUP\_813985937

(The user's homepage shows his/her spectra in context...)



(Bulk loading of spectra is possible, but only through administration tools...)

https://lifelin...tgwjcvqdfmzge +

https://lifeline.biomedical-hosting.net/#/group/GROUP\_813985937

Lifeline SOS manor Logout Help

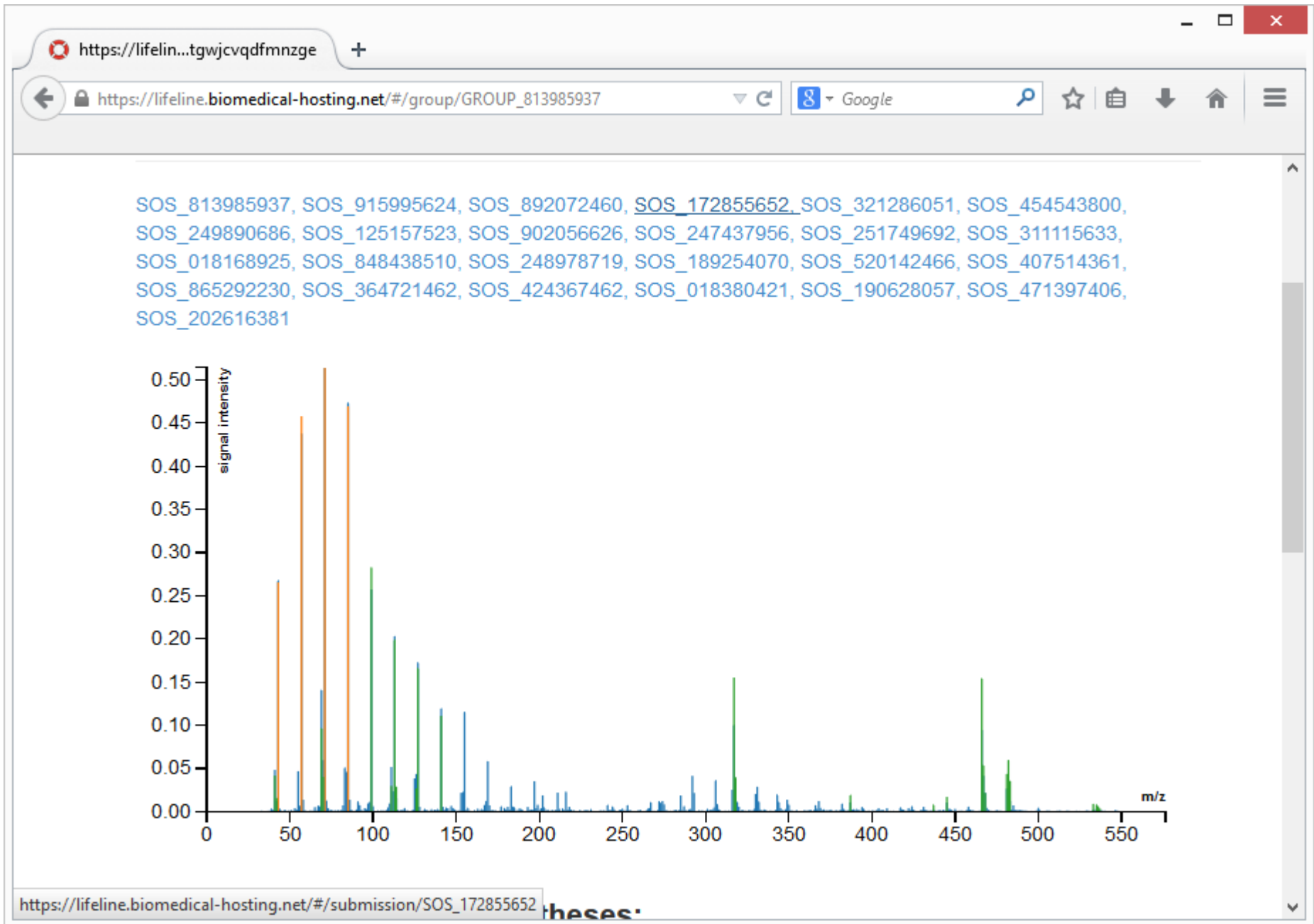
## GROUP\_813985937 (25 spectra)

**Best NIST ID:** MF=615 Eicosane, 2-methyl- [C21H44, CAS# 1560845] **Source Spectrum:** [SOS\\_892072460](#)

[SOS\\_813985937](#), [SOS\\_915995624](#), [SOS\\_892072460](#), [SOS\\_172855652](#), [SOS\\_321286051](#), [SOS\\_454543800](#), [SOS\\_249890686](#), [SOS\\_125157523](#), [SOS\\_902056626](#), [SOS\\_247437956](#), [SOS\\_251749692](#), [SOS\\_311115633](#), [SOS\\_018168925](#), [SOS\\_848438510](#), [SOS\\_248978719](#), [SOS\\_189254070](#), [SOS\\_520142466](#), [SOS\\_407514361](#), [SOS\\_865292230](#), [SOS\\_364721462](#), [SOS\\_424367462](#), [SOS\\_018380421](#), [SOS\\_190628057](#), [SOS\\_471397406](#), [SOS\\_202616381](#)

m/z	Signal Intensity
125	0.43
251	0.47
311	0.50
312	0.47
313	0.25
314	0.20

(The Group Page shows the average spectrum as well as all participating submissions)



(Individual spectra can be visualized as overlays on top of the consensus spectrum)

https://lifelin...tgwjcvqdfmzge +

https://lifeline.biomedical-hosting.net/#/group/GROUP\_813985937

**Comments/Thoughts/Hypotheses:**

I don't think we have any particular reason to believe that the molecular ion is at 535...

posted by manor ([delete](#))

Comment/Thought/Hypothesis

Post

Users can communicate indirectly through the comments section of the Group Page)

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“ לְכוּ-נָא וְנִזְכָּחָה ”

“Come now, and let us reason together”

Isaiah, 1:18

