reQuest

MS Service

sample analysis

request handling

results interpretation

Request Handling

On-line system
Individual accounts
Archiving
Request tracking
Notifications
More secure
One account for many services

Results Interpretation

Unified data format

Data viewer

Useful tools

Detailed analysis

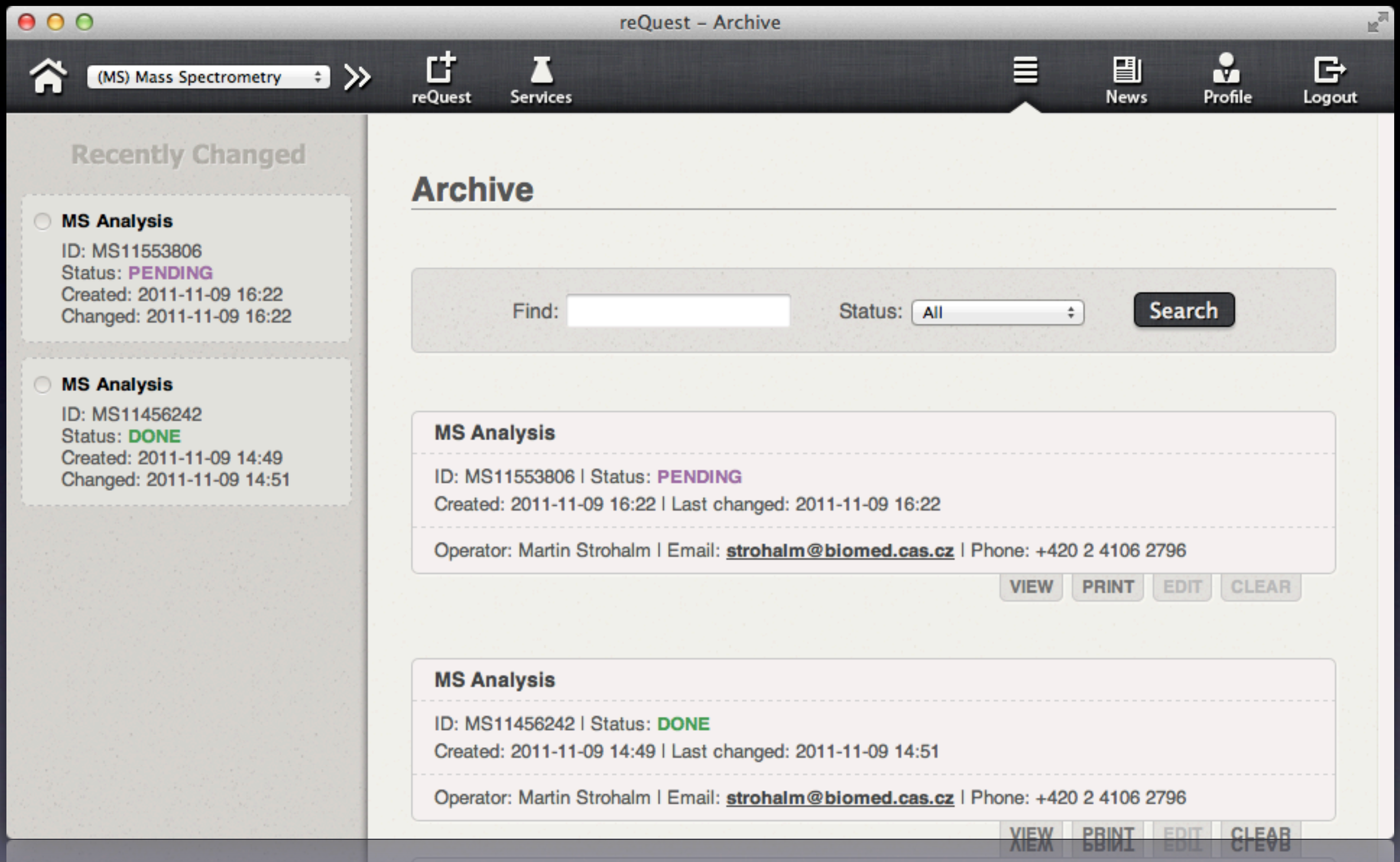
reQuest – Login

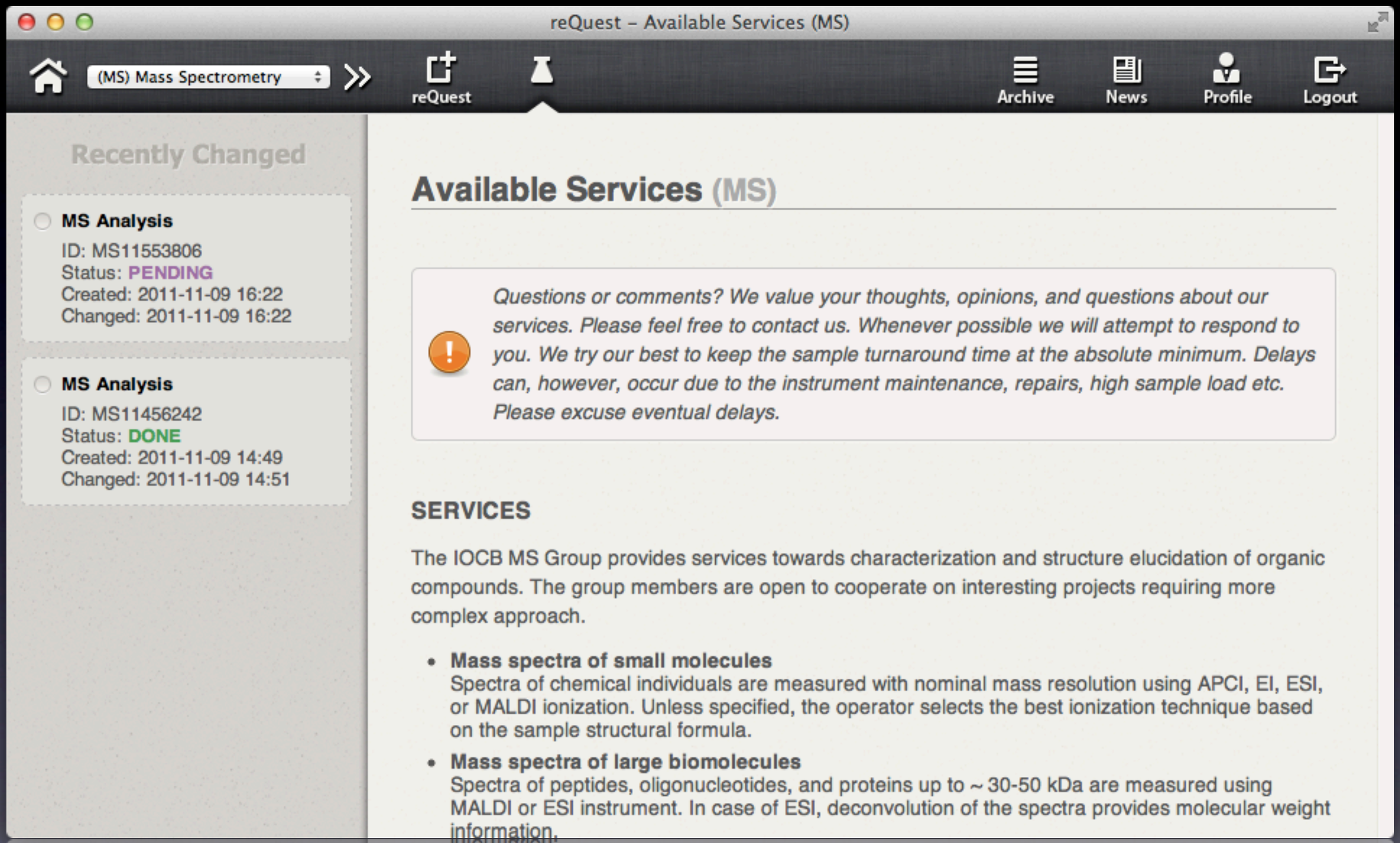
reQuest - Login

E-mail

Login

Not registered? Forgot your password?


reQuest – Archive
(MS) Mass Spectrometry
reQuest
Services
News
Profile
Logout
Recently Changed
MS Analysis
ID: MS11553806
Status: PENDING
Created: 2011-11-09 16:22
Changed: 2011-11-09 16:22
MS Analysis
ID: MS11456242
Status: DONE
Created: 2011-11-09 14:49
Changed: 2011-11-09 14:51
Archive
Find:
Status: All
Search
MS Analysis
ID: MS11553806 | Status: PENDING
Created: 2011-11-09 16:22 | Last changed: 2011-11-09 16:22
Operator: Martin Strohalm | Email: strohalm@biomed.cas.cz | Phone: +420 2 4106 2796
VIEW
PRINT
EDIT
CLEAR
MS Analysis
ID: MS11456242 | Status: DONE
Created: 2011-11-09 14:49 | Last changed: 2011-11-09 14:51
Operator: Martin Strohalm | Email: strohalm@biomed.cas.cz | Phone: +420 2 4106 2796
VIEW
PRINT
EDIT
CLEAR


reQuest – Available Services (MS)
(MS) Mass Spectrometry
reQuest
Archive
News
Profile
Logout
Recently Changed
MS Analysis
ID: MS11553806
Status: PENDING
Created: 2011-11-09 16:22
Changed: 2011-11-09 16:22
MS Analysis
ID: MS11456242
Status: DONE
Created: 2011-11-09 14:49
Changed: 2011-11-09 14:51
Available Services (MS)
Questions or comments? We value your thoughts, opinions, and questions about our services. Please feel free to contact us. Whenever possible we will attempt to respond to you. We try our best to keep the sample turnaround time at the absolute minimum. Delays can, however, occur due to the instrument maintenance, repairs, high sample load etc. Please excuse eventual delays.
SERVICES
The IOCB MS Group provides services towards characterization and structure elucidation of organic compounds. The group members are open to cooperate on interesting projects requiring more complex approach.
Mass spectra of small molecules
Spectra of chemical individuals are measured with nominal mass resolution using APCI, EI, ESI, or MALDI ionization. Unless specified, the operator selects the best ionization technique based on the sample structural formula.
Mass spectra of large biomolecules
Spectra of peptides, oligonucleotides, and proteins up to ~ 30-50 kDa are measured using MALDI or ESI instrument. In case of ESI, deconvolution of the spectra provides molecular weight information.

SAMPLE SUBMISSION AND REQUIREMENTS

Please submit your samples to the basement of the main building, in front of the room 33. The samples must be labeled and accompanied by a submission form generated from this website. A freezer (-12 °C) is available for unstable samples. In case of toxic or otherwise hazardous samples please contact the laboratory staff. **The samples that are not related to the projects currently running in the IOCB and radioactive samples cannot be accepted!**

- **APCI:** The sample (10 μg - 1.0 mg) should be submitted as the dry solid or the neat liquid in a vial. The sample must be soluble in a suitable solvent compatible with APCI. The best solvents are methanol, acetonitrile, ethanol, 2-propanol, or acetone.
- **EI:** The sample (100 μg - 1.0 mg) should be submitted as the dry solid or the neat liquid in a vial. The samples must have sufficient volatility and thermal stability to evaporate from the sample probe under vacuum. The samples for GC/MS must be free from nonvolatile buffers, strong acid, bases and oxidizing compounds.
- **MALDI:** The sample (10 μg - 1.0 mg) should be submitted as the dry solid or in a solution free from nonvolatile buffers, solvents, and surfactants. Proteomic samples are submitted as gels or tryptic digests.

OVERVIEW OF THE IONIZATION TECHNIQUES

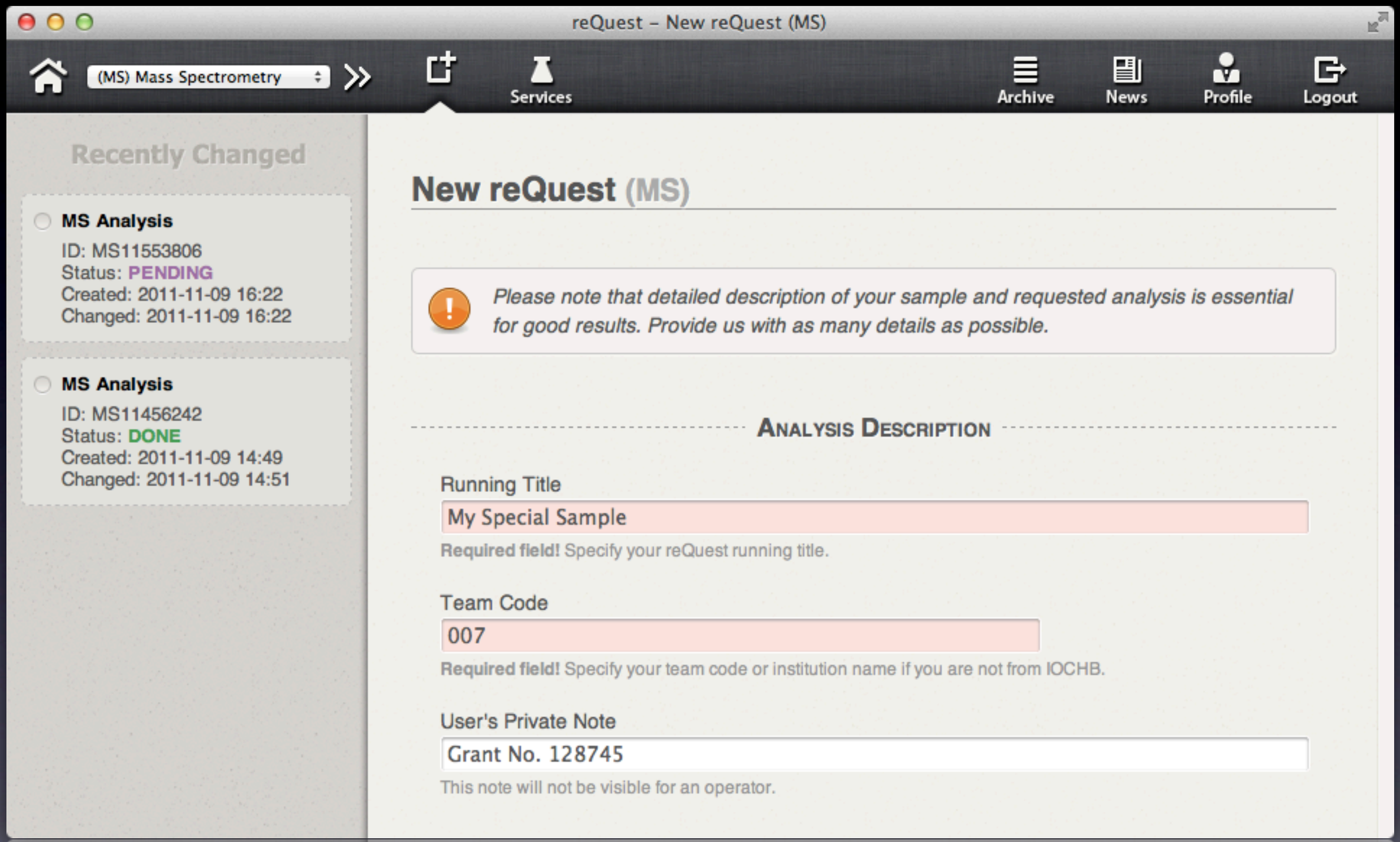
- **Atmospheric Pressure Chemical Ionization (APCI)**
is a soft ionization technique used for organic compounds with medium to high polarity. The dissolved sample is introduced into the APCI source. The solvent is evaporated and the sample passes through a corona discharge where reagent ions are formed from the solvent molecules and the nitrogen gas. These ions react with the analyte. The relative gas phase acidity of the reagent ions and the analyte molecules play important roles in the APCI process. Positive ions are formed by proton addition $[M+H]^+$ and negative ions by proton abstraction $[M-H]^-$. cation or

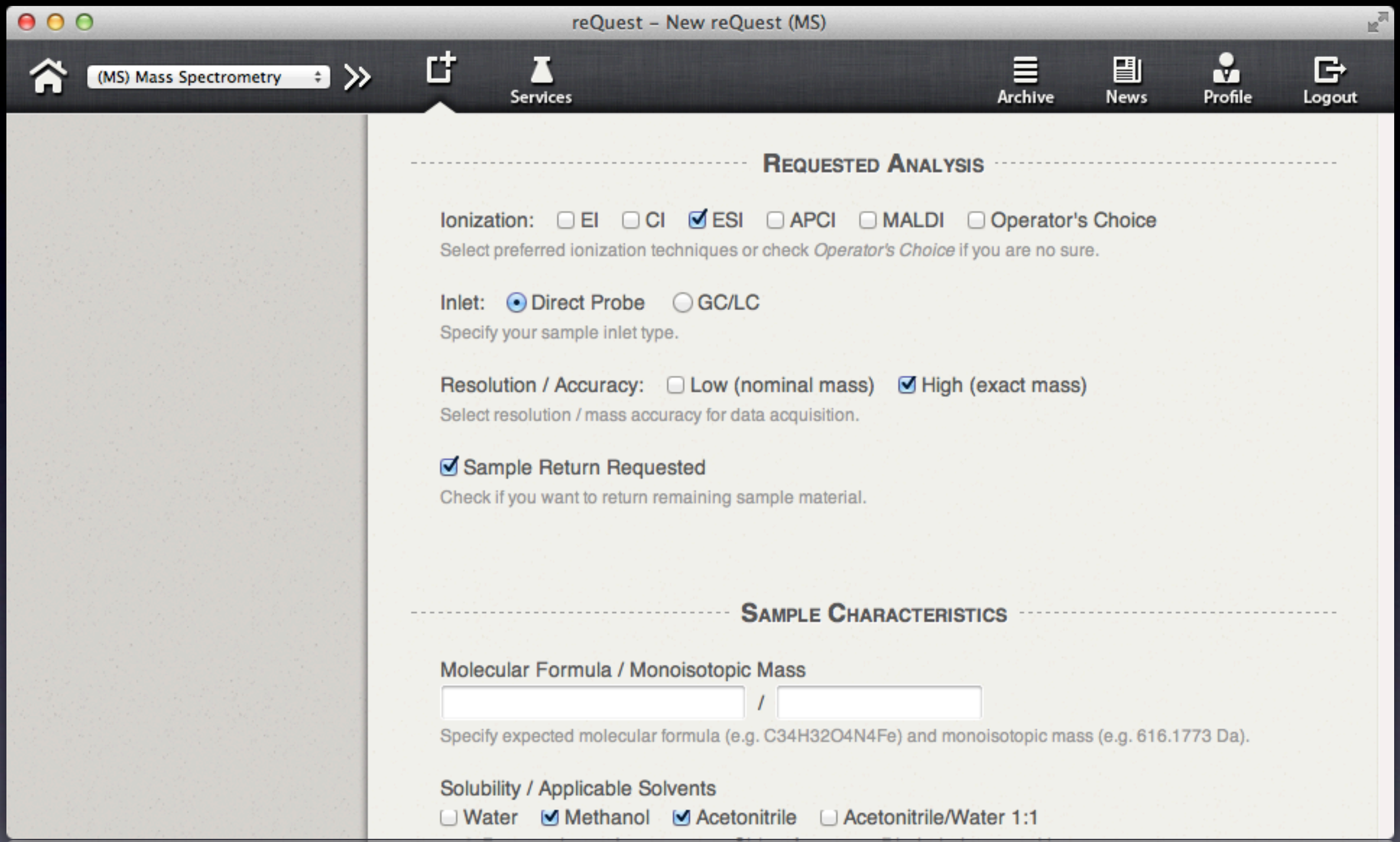
in solution is passed through a capillary held at high potential (a few kV). The liquid at the tip of the capillary blows apart into a cloud of tiny, highly charged droplets, which further repeatedly shrink and blow to eventually form the ions. For small molecules either $[M+H]^+$ or $[M-H]^-$ ions are formed. Because of alkali metal impurities, $[M+Na]^+$ ions are observed. Molecules with higher masses usually produce a series of multiply charged ions. No or few fragments are usually observed. The molecular weight range is up to ~200 000 u.

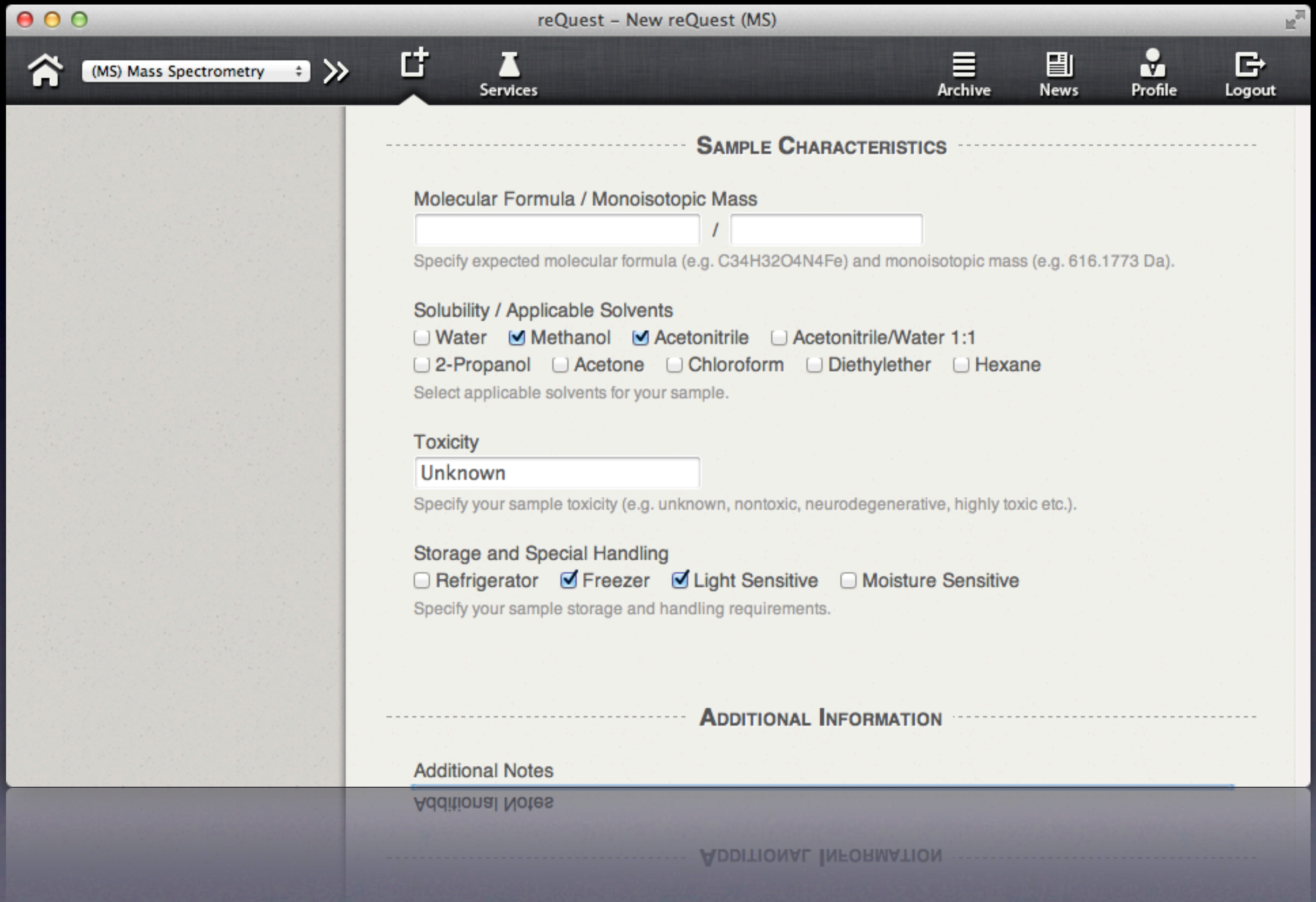
- **Matrix-Assisted Laser Desorption/Ionisation (MALDI)**
  is a soft ionization technique suitable for a wide range of biologically important molecules as well as for other compounds, such as synthetic polymers, large organic molecules, or organometallic complexes. Most often MALDI is used for analyzing proteins or protein digests.The sample is mixed with a matrix solution and allowed to co-crystallize on a target plate. Laser (usually nitrogen laser 337 nm) is fired at the target, and the absorbed laser energy desorbs the sample and matrix from the surface. The matrix also serves as a proton donor and acceptor, acting to ionize the analyte. A voltage is applied to the target plate to accelerate the analyte ions towards a mass analyzer. The choice of matrix is crucial for successful MALDI analysis. The analyte molecules are usually ionized by a simple protonation or cationization leading to the formation of $[M+H]^+$, $[M+Na]^+$ etc. in positive ion mode or by deprotonation in negative ion mode ($[M-H]^-$). MALDI has tendency to produce singly-charged ions even with very large molecules, however, some multiply charged species, or singly charged dimers and trimers can also be formed. The molecular weight range is up to ~500 000 u.

SOFTWARE DOWNLOADS

Please **download** and unzip the latest version (1.0) of the MSreView software to be able to view and analyze measeured data. If you are an experienced MS user, you can download a more advanced mMass software directly from **project website**.


reQuest – New reQuest (MS)
(MS) Mass Spectrometry
Services
Archive
News
Profile
Logout
Recently Changed
MS Analysis
ID: MS11553806
Status: PENDING
Created: 2011-11-09 16:22
Changed: 2011-11-09 16:22
MS Analysis
ID: MS11456242
Status: DONE
Created: 2011-11-09 14:49
Changed: 2011-11-09 14:51
New reQuest (MS)
Please note that detailed description of your sample and requested analysis is essential for good results. Provide us with as many details as possible.
Analysis Description
Running Title
My Special Sample
Required field! Specify your reQuest running title.
Team Code
007
Required field! Specify your team code or institution name if you are not from IOCHB.
User's Private Note
Grant No. 128745
This note will not be visible for an operator.


reQuest – New reQuest (MS)
(MS) Mass Spectrometry
Services
Archive
News
Profile
Logout
Requested Analysis
Ionization: EI CI ESI APCI MALDI Operator's Choice
Select preferred ionization techniques or check Operator's Choice if you are no sure.
Inlet: Direct Probe GC/LC
Specify your sample inlet type.
Resolution / Accuracy: Low (nominal mass) High (exact mass)
Select resolution / mass accuracy for data acquisition.
Sample Return Requested
Check if you want to return remaining sample material.
Sample Characteristics
Molecular Formula / Monoisotopic Mass
/
Specify expected molecular formula (e.g. C34H32O4N4Fe) and monoisotopic mass (e.g. 616.1773 Da).
Solubility / Applicable Solvents
Water Methanol Acetonitrile Acetonitrile/Water 1:1


reQuest – New reQuest (MS)
(MS) Mass Spectrometry
Services
Archive
News
Profile
Logout
Sample Characteristics
Molecular Formula / Monoisotopic Mass
/
Specify expected molecular formula (e.g. C34H32O4N4Fe) and monoisotopic mass (e.g. 616.1773 Da).
Solubility / Applicable Solvents
Water
Methanol
Acetonitrile
Acetonitrile/Water 1:1
2-Propanol
Acetone
Chloroform
Diethylether
Hexane
Select applicable solvents for your sample.
Toxicity
Unknown
Specify your sample toxicity (e.g. unknown, nontoxic, neurodegenerative, highly toxic etc.).
Storage and Special Handling
Refrigerator
Freezer
Light Sensitive
Moisture Sensitive
Specify your sample storage and handling requirements.
Additional Information
Additional Notes

reQuest – New reQuest (MS)

(MS) Mass Spectrometry

Services | Archive | News | Profile | Logout

Additional Information

Additional Notes

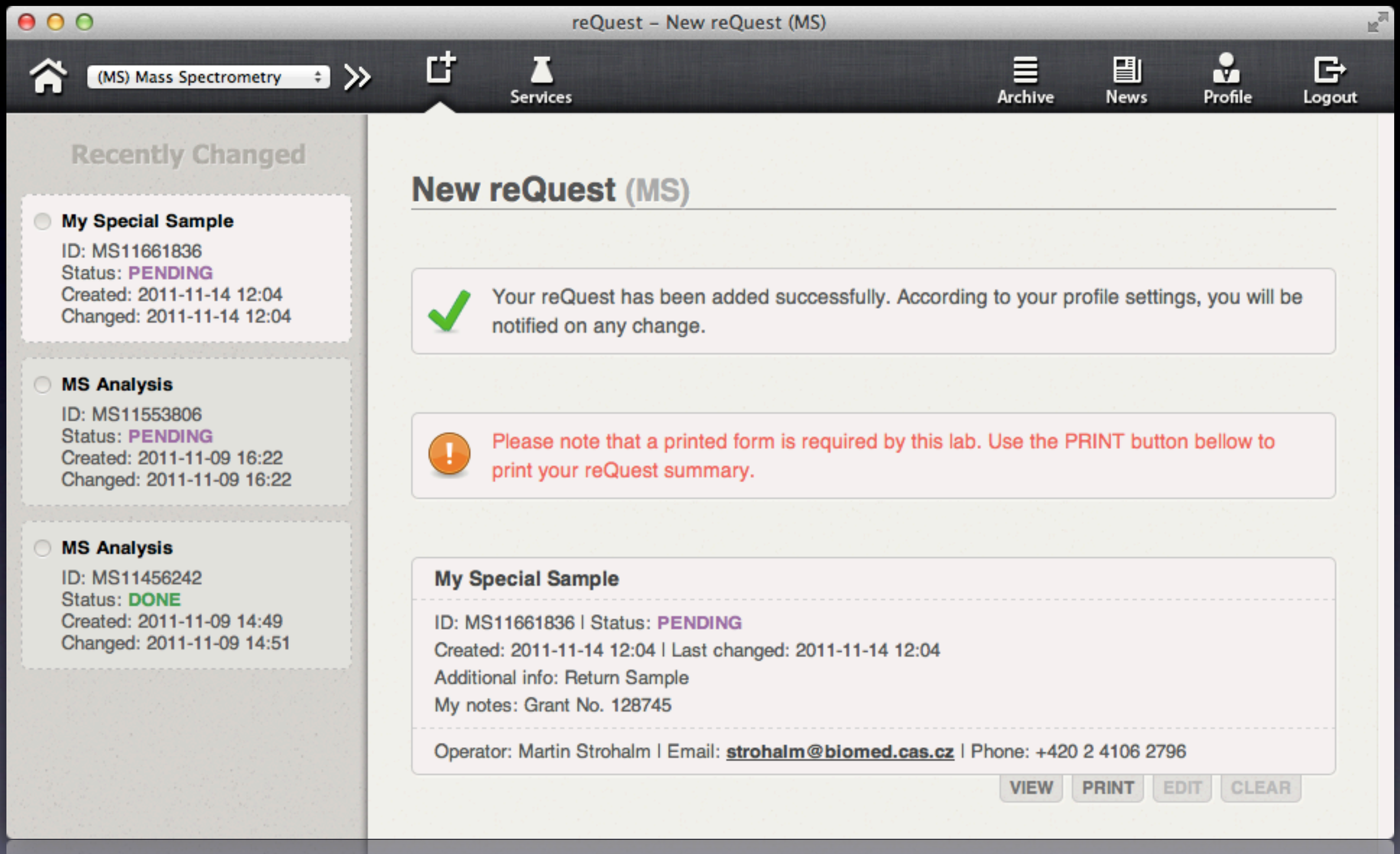
Explosive, handle with care!

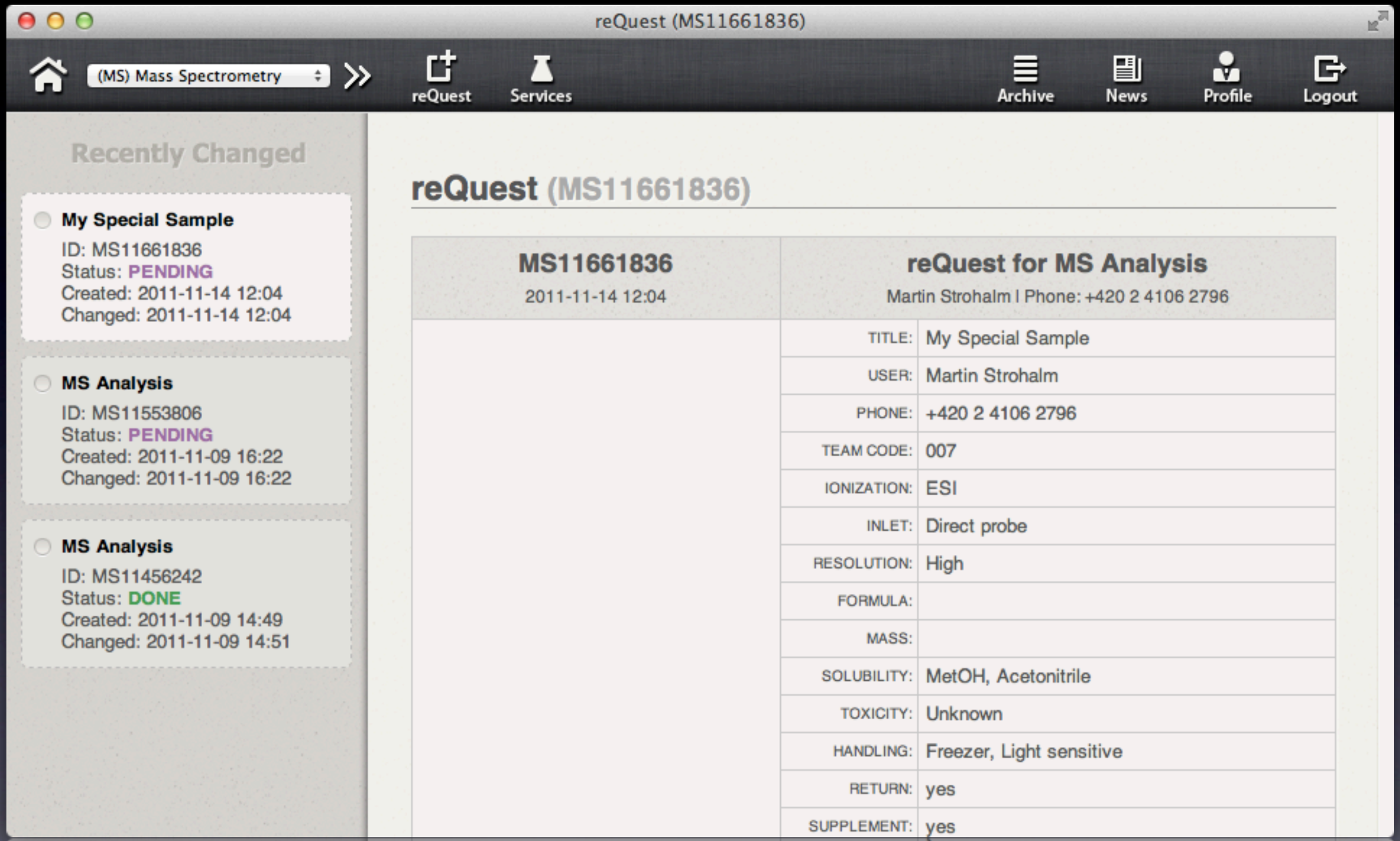
Specify any additional notes for your sample.

Supplemental File Choose File supplement.pdf Delete Only

You can attach any supplemental file (**2 MB max**). Any previously uploaded file will be overwritten.

Submit reQuest


reQuest – New reQuest (MS)
(MS) Mass Spectrometry
Services
Archive
News
Profile
Logout
Recently Changed
My Special Sample
ID: MS11661836
Status: PENDING
Created: 2011-11-14 12:04
Changed: 2011-11-14 12:04
MS Analysis
ID: MS11553806
Status: PENDING
Created: 2011-11-09 16:22
Changed: 2011-11-09 16:22
MS Analysis
ID: MS11456242
Status: DONE
Created: 2011-11-09 14:49
Changed: 2011-11-09 14:51
New reQuest (MS)
Your reQuest has been added successfully. According to your profile settings, you will be notified on any change.
Please note that a printed form is required by this lab. Use the PRINT button bellow to print your reQuest summary.
My Special Sample
ID: MS11661836 | Status: PENDING
Created: 2011-11-14 12:04 | Last changed: 2011-11-14 12:04
Additional info: Return Sample
My notes: Grant No. 128745
Operator: Martin Strohalm | Email: strohalm@biomed.cas.cz | Phone: +420 2 4106 2796
VIEW
PRINT
EDIT
CLEAR


reQuest (MS11661836)
(MS) Mass Spectrometry
reQuest
Services
Archive
News
Profile
Logout
Recently Changed
My Special Sample
ID: MS11661836
Status: PENDING
Created: 2011-11-14 12:04
Changed: 2011-11-14 12:04
MS Analysis
ID: MS11553806
Status: PENDING
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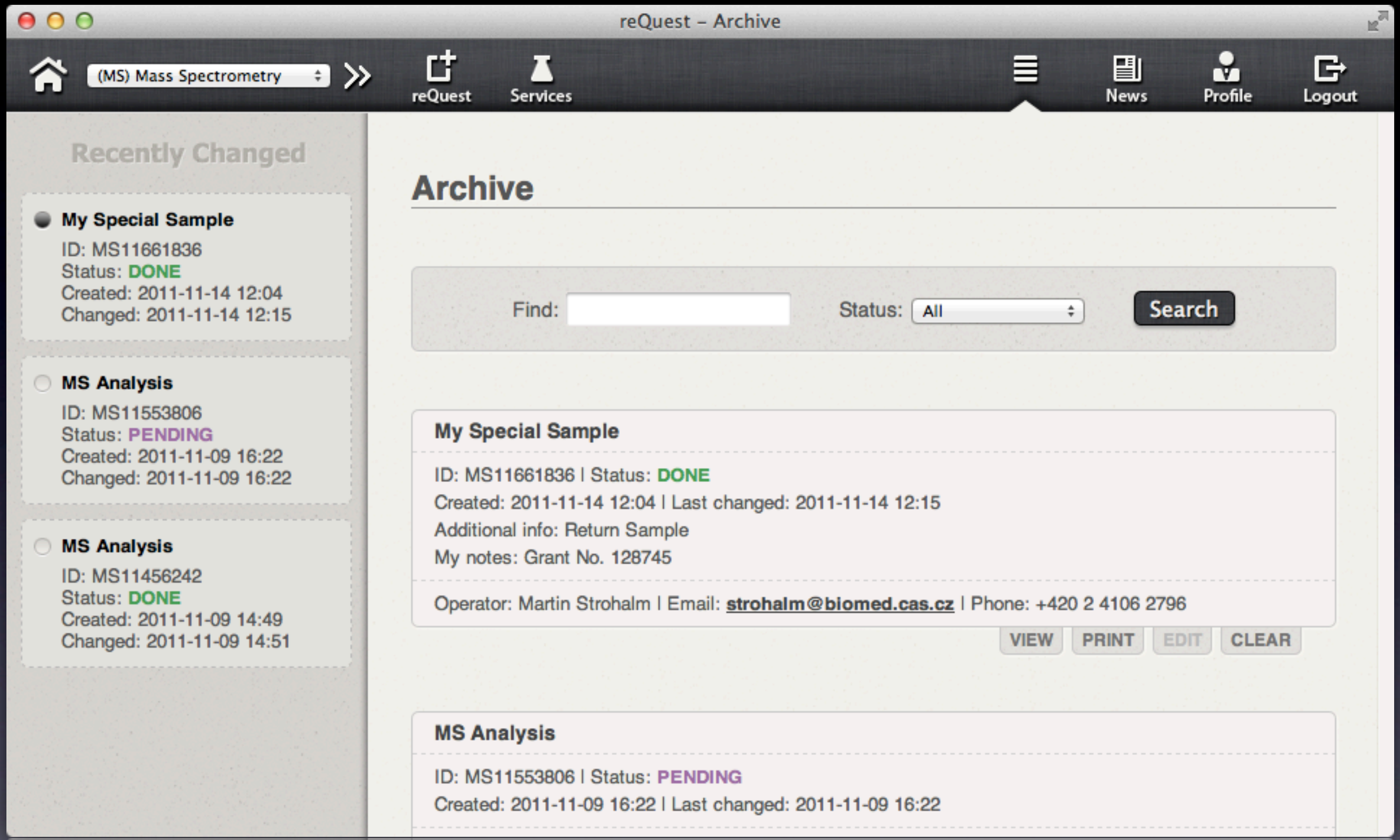
Changed: 2011-11-09 16:22
MS Analysis
ID: MS11456242
Status: DONE
Created: 2011-11-09 14:49
Changed: 2011-11-09 14:51
reQuest (MS11661836)
MS11661836
2011-11-14 12:04
reQuest for MS Analysis
Martin Strohalm | Phone: +420 2 4106 2796
TITLE: My Special Sample
USER: Martin Strohalm
PHONE: +420 2 4106 2796
TEAM CODE: 007
IONIZATION: ESI
INLET: Direct probe
RESOLUTION: High
FORMULA:
MASS:
SOLUBILITY: MetOH, Acetonitrile
TOXICITY: Unknown
HANDLING: Freezer, Light sensitive
RETURN: yes
SUPPLEMENT: yes


reQuest – Archive
(MS) Mass Spectrometry
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Services
News
Profile
Logout
Recently Changed
My Special Sample
ID: MS11661836
Status: DONE
Created: 2011-11-14 12:04
Changed: 2011-11-14 12:15
MS Analysis
ID: MS11553806
Status: PENDING
Created: 2011-11-09 16:22
Changed: 2011-11-09 16:22
MS Analysis
ID: MS11456242
Status: DONE
Created: 2011-11-09 14:49
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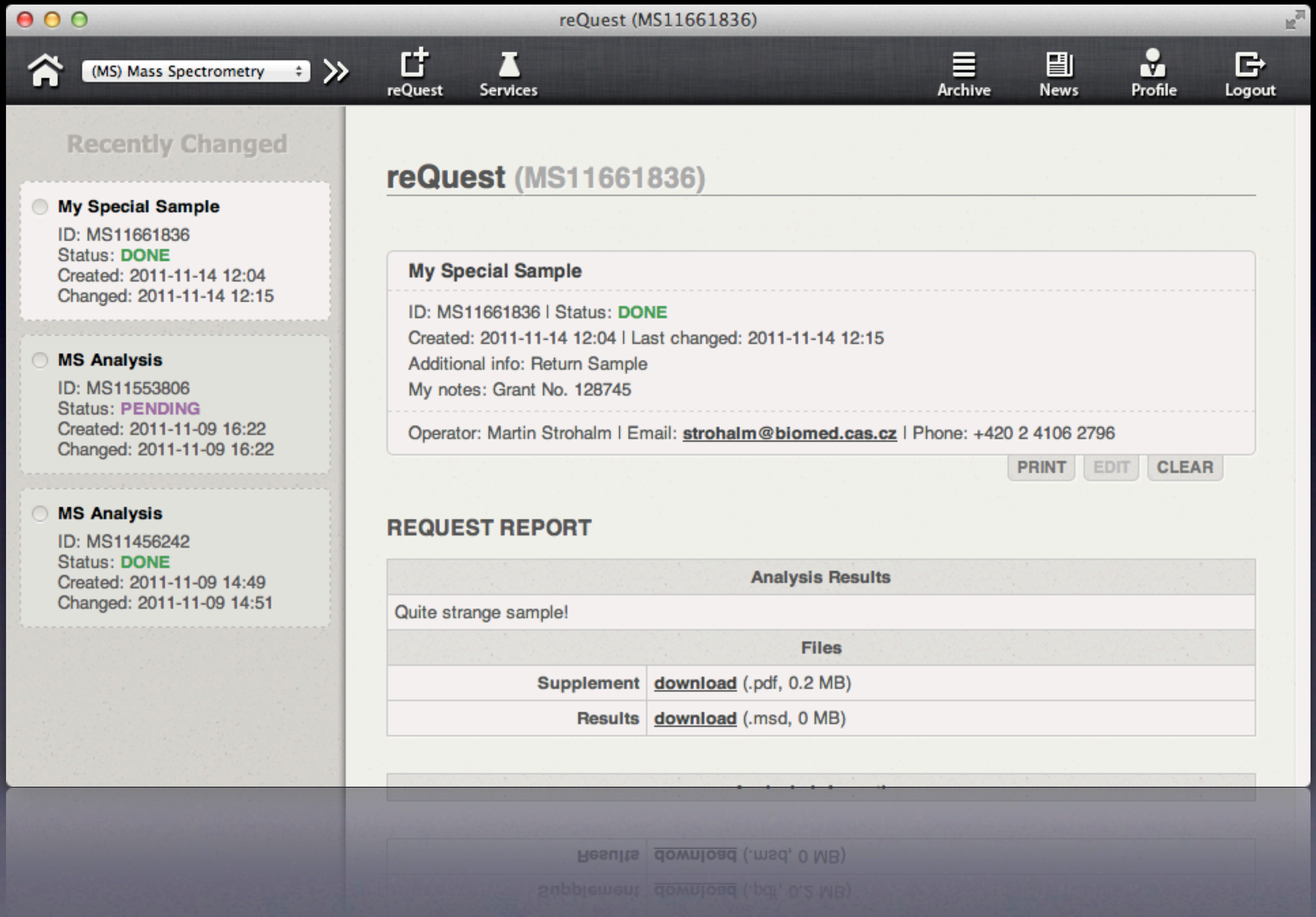
Archive
Find:
Status: All
Search
My Special Sample
ID: MS11661836 | Status: DONE
Created: 2011-11-14 12:04 | Last changed: 2011-11-14 12:15
Additional info: Return Sample
My notes: Grant No. 128745
Operator: Martin Strohalm | Email: strohalm@biomed.cas.cz | Phone: +420 2 4106 2796
VIEW
PRINT
EDIT
CLEAR
MS Analysis
ID: MS11553806 | Status: PENDING
Created: 2011-11-09 16:22 | Last changed: 2011-11-09 16:22


reQuest (MS11661836)
(MS) Mass Spectrometry
reQuest
Services
Archive
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Profile
Logout
Recently Changed
My Special Sample
ID: MS11661836
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reQuest (MS11661836)
My Special Sample
ID: MS11661836 | Status: DONE
Created: 2011-11-14 12:04 | Last changed: 2011-11-14 12:15
Additional info: Return Sample
My notes: Grant No. 128745
Operator: Martin Strohalm | Email: strohalm@biomed.cas.cz | Phone: +420 2 4106 2796
PRINT
EDIT
CLEAR
REQUEST REPORT
Analysis Results
Quite strange sample!
Files
Supplement
download (.pdf, 0.2 MB)
Results
download (.msd, 0 MB)

reQuest (MS11661836)

(MS) Mass Spectrometry

reQuest | Services | Archive | News | Profile | Logout

Recently Changed

My Special Sample
ID: MS11661836
Status: DONE
Created: 2011-11-14 12:04
Changed: 2011-11-14 12:15

MS Analysis
ID: MS11553806
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Additional info: Return Sample
My notes: Grant No. 128745

Operator: Martin Strohalm | Email: strohalm@biomed.cas.cz | Phone: +420 2 4106 2796

PRINT EDIT CLEAR

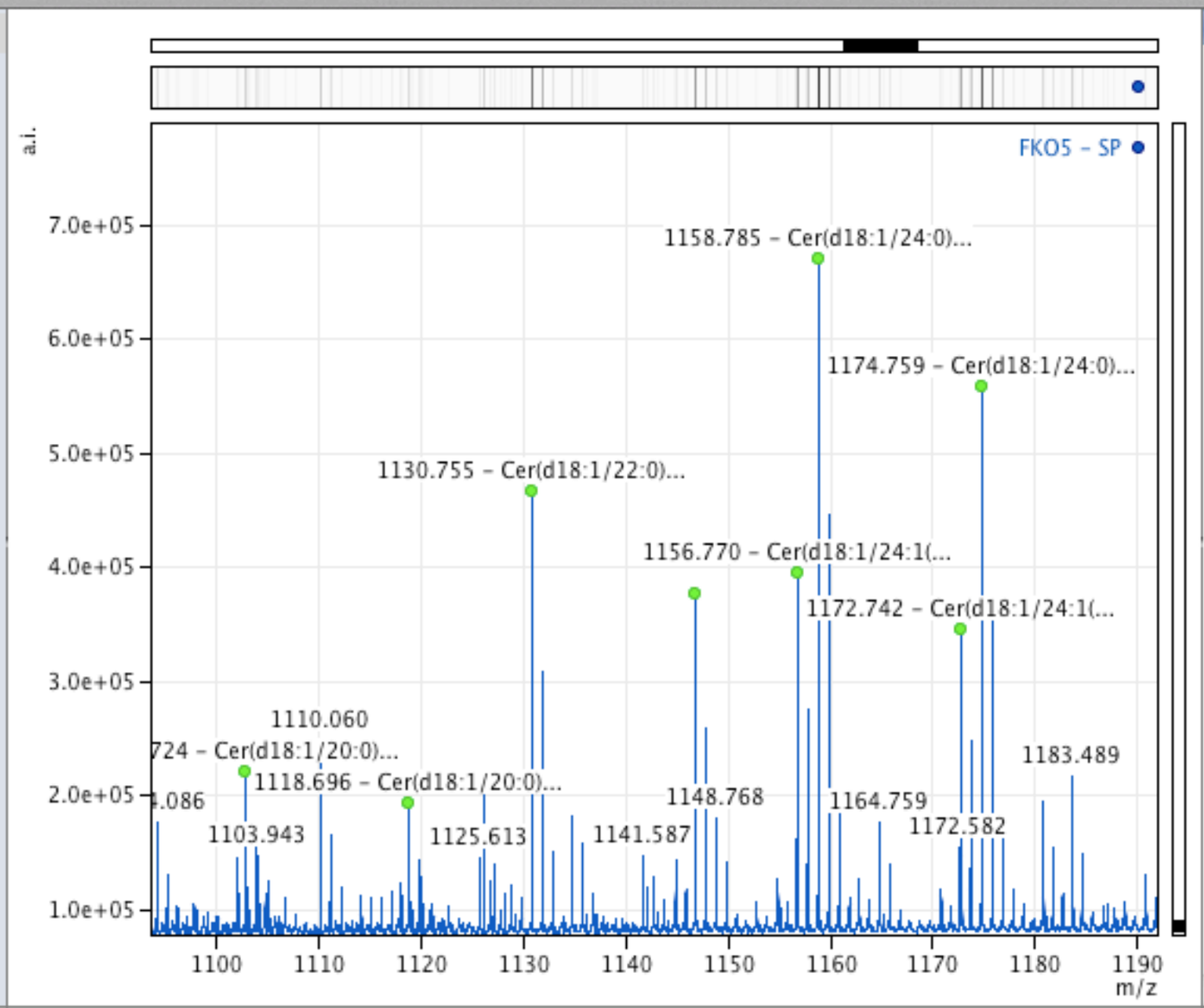
REQUEST REPORT

Analysis Information	
Ionization	ESI
Inlet	Direct probe
Resolution	High
Solubility	MetOH, Acetonitrile
Toxicity	Unknown
Handling	Freezer, Light sensitive

MSreView – FKO5 – SP

Masscalc Compounds Differences Compare Notes Report Export

FKO5 – SP



m/z	int.
238.162	75701
240.207	64368
241.175	76379
241.191	48828
246.500	51081
249.988	468220
251.845	240664
252.184	70820
252.195	1634324
252.530	582544
252.865	74805
252.868	403097
256.505	177494
256.839	64438
257.170	109110
257.855	466729
259.549	95905
260.196	496348
260.531	186911
260.552	61259
260.868	435473
261.203	150000
261.540	127783
265.521	351039
265.856	130011

Peaks: 728

MSreView – FKO5 – SP

Masscalc | Compounds | Differences | Compare | Notes | Report | Export

FKO5 – SP

Compounds Search

Formula: C58H109NO18 Tolerance: 2.0 Da ppm Search Annotate

Mass: Mo Av Max z: 1 M* Adducts: Na K Li NH4 -H2O ACN MeOH

formula	m/z	z	adduct	error
C58H109NO18	1108.772	1		
C58H109NO18(K)(H-1)	1146.728	1	K	-0.7
C58H109NO18(Na)(H-1)	1130.754	1	Na	1.0

m/z	int.
238.162	75701
0.207	64368
1.175	76379
1.191	48828
6.500	51081
9.988	468220
1.845	240664
2.184	70820
2.195	1634324
2.530	582544
2.865	74805
2.868	403097
6.505	177494
6.839	64438
7.170	109110
7.855	466729
9.549	95905
0.196	496348
0.531	186911
0.552	61259
0.868	435473
1.203	150000
261.540	127783
265.521	351039
265.856	130011

1.0e+05

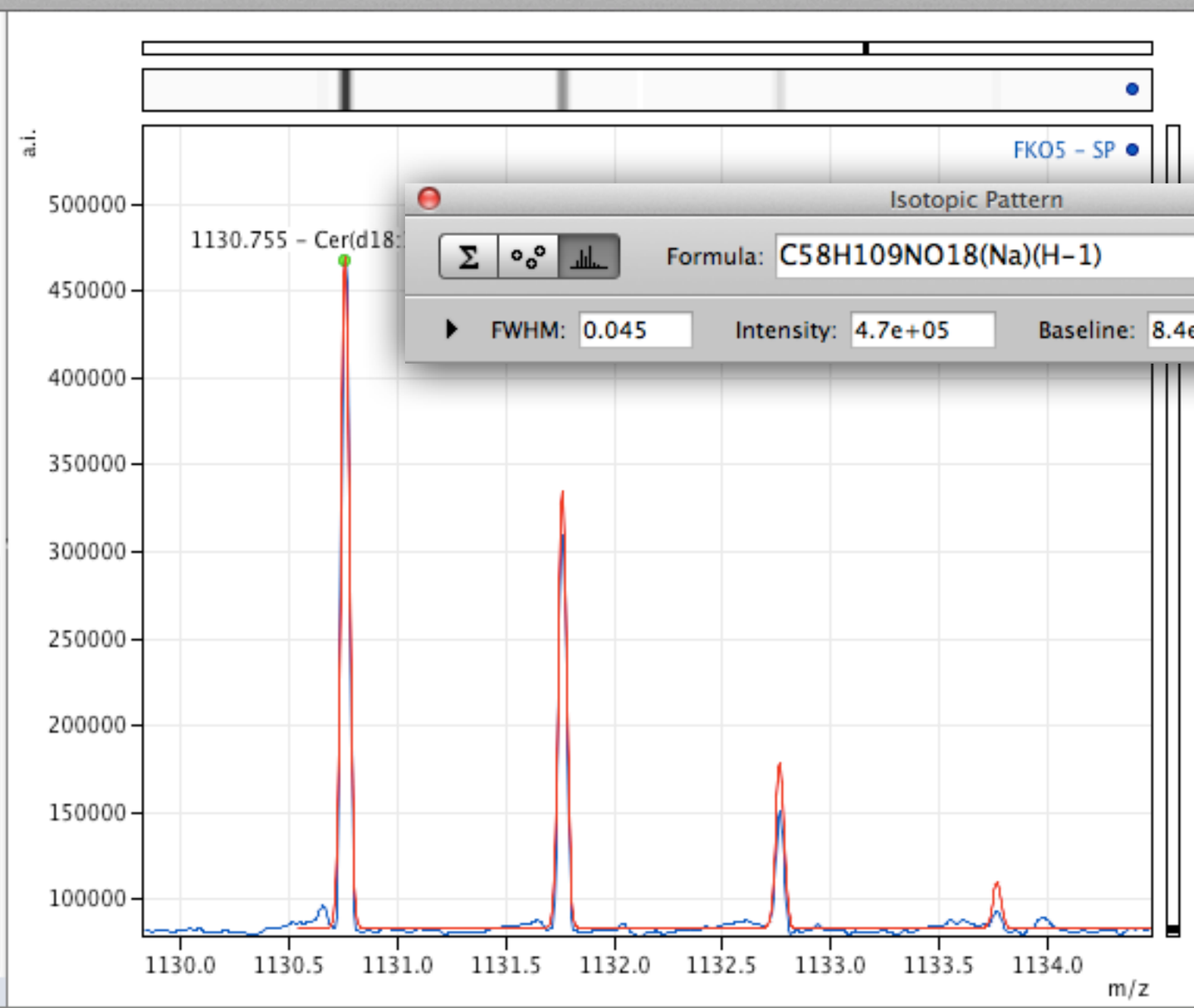
1100 1110 1120 1130 1140 1150 1160 1170 1180 1190 m/z

Peaks: 728

MSreView – FKO5 – SP

Masscalc | Compounds | Differences | Compare | Notes | Report | Export

827.699 (-0.001 Da)
829.716 (0.0 Da) LMS
832.662 (-0.002 Da)
833.65 (-0.001 Da) LI
835.666 (-0.0 Da) LM
837.683 (0.001 Da) L
839.64 (-0.0 Da) LMS
849.624 (-0.001 Da)
851.64 (-0.001 Da) LI
853.656 (-0.0 Da) LM
884.607 (-0.0 Da) LM
994.717 (0.0 Da) LMS
996.732 (-0.001 Da)
1046.661 (0.001 Da)
1062.632 (-0.002 Da
1102.724 (0.001 Da)
1118.696 (-0.0 Da) C
1130.755 (0.001 Da)
1146.727 (-0.001 Da
1156.77 (0.0 Da) Cert
1158.785 (0.0 Da) Ce
1172.742 (-0.001 Da
1174.759 (-0.0 Da) C



Isotopic Pattern

Formula: C58H109NO18(Na)(H-1) Save

FWHM: 0.045 Intensity: 4.7e+05 Baseline: 8.4e+04 Shift: 0

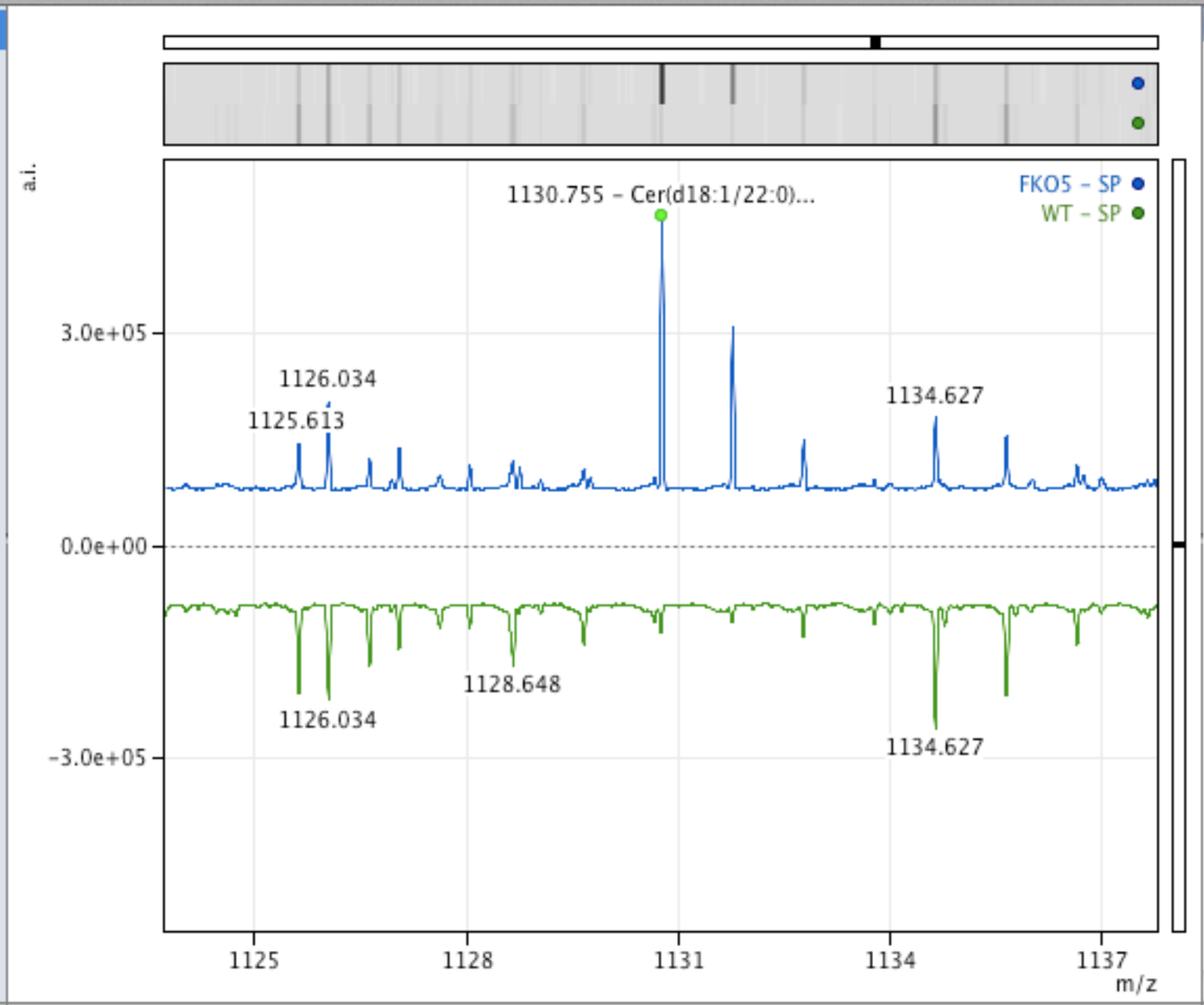
m/z	int.
238.162	75701
240.207	64368
241.175	76379
252.195	1634324
252.530	582544
252.865	74805
252.868	403097
256.505	177494
256.839	64438
257.170	109110
257.855	466729
259.549	95905
260.196	496348
260.531	186911
260.552	61259
260.868	435473
261.203	150000
261.540	127783
265.521	351039

Peaks: 728

MSreView – FKO5 – SP

Masscalc Compounds Differences Compare Notes Report Export

- FKO5 – SP
- *WT – SP
- *Sample 3



m/z	int.
238.162	75701
240.207	64368
241.175	76379
241.191	48828
246.500	51081
249.988	468220
251.845	240664
252.184	70820
252.195	1634324
252.530	582544
252.865	74805
252.868	403097
256.505	177494
256.839	64438
257.170	109110
257.855	466729
259.549	95905
260.196	496348
260.531	186911
260.552	61259
260.868	435473
261.203	150000
261.540	127783
265.521	351039
265.856	130011

Peaks: 728

MSreView – FKO5 – SP

Masscalc | Compounds | Differences | Compare | Notes | Report | Export

Compare Peak Lists

Compare: Peak Lists Tolerance: 1 Da ppm Compare

m/z	*	*	m/z	*	*
1130.755	*		1065.685		*
1134.627	*		1069.575		*
1141.587	*		1084.644		*
1146.727	*		1094.087		*
1148.768	*		1110.059		*
1156.607	*		1125.613		*
1156.770	*		1126.034		*
1158.785	*		1128.648		*
1164.759	*		1134.627		*
1172.582	*		1141.588		*
1172.742	*		1156.607		*
1174.759	*		1172.582		*
1180.734	*		1183.489		*
1183.489	*		1329.571		*
1318.748	*		1349.738		*
1329.571	*		1406.144		*
1349.738	*		1421.737		*
1406.143	*		1428.129		*
1407.758	*		1437.148		*
1421.736	*		1459.129		*

*	m/z	error	a/b	b/a
	1156.607	-0.1	0.48	2.10

int.
75701
64368
76379
48828
51081
468220
240664
70820
1634324
582544
74805
403097
177494
64438
109110
466729
95905
496348
186911
61259
435473
150000
127783
351039
130011

1125 1128 1131 1134 1137 m/z

Peaks: 728

www.mMass.org

Open Source Mass Spectrometry Tool

request.uochb.cas.cz

request@bymartin.cz