

Item name: MD_M POPLAWSKI

Created by: Chemistry, Chemistry

Created on: Sep 07, 2023

Created time: 13:57:06 GMT Daylight Time

Analysis Information

| | | | |
|----------------|---|------------------------------------|---|
| Item name: | MD_M POPLAWSKI | Analysis Method Item name: | OPENACCess-120-40-2PLUS |
| Version: | 1 | Analysis Method Version: | 1 |
| Modified date: | Sep 06, 2023 14:41:56 GMT Daylight Time | Sample Set Created date: | Sep 06, 2023 14:31:58 GMT Daylight Time |
| Modified by: | Chemistry, Chemistry | Sample Set Instrument system name: | Vion full System |
| Folder: | Company/OpenAccess/M Spec | | |

Analysis injection list

| . | Item name | Item description | Sample type | Replicate number | Sample position | Injection volume (µL) | Acquisition status | Limit status |
|---|-------------|------------------|-------------|------------------|-----------------|-----------------------|--------------------|---------------------|
| 1 | int1_a2 ACN | | Unknown | 1 | 2:A,7 | 3.00 | Complete | No Checks Performed |

Item name: MD_M POPLAWSKI

Created by: Chemistry, Chemistry

Created on: Sep 07, 2023

Created time: 13:57:06 GMT Daylight Time

Component name: MP1.mol

Component name: MP1.mol

| . | Item name | Sample position | Replicate number | Component name | Identification status | Neutral mass (Da) | Observed neutral mass (Da) |
|---|-------------|-----------------|------------------|----------------|-----------------------|-------------------|----------------------------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP1.mol | Identified | 267.10758 | 267.1080 |

| . | Item name | Sample position | Replicate number | Component name | Identification status | Observed m/z | Mass error (mDa) |
|---|-------------|-----------------|------------------|----------------|-----------------------|--------------|------------------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP1.mol | Identified | 268.1153 | 0.4 |

| . | Item name | Sample position | Replicate number | Component name | Identification status | Mass error (ppm) | Expected RT (min) | Observed RT (min) |
|---|-------------|-----------------|------------------|----------------|-----------------------|------------------|-------------------|-------------------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP1.mol | Identified | 1.5 | | 0.79 |

| . | Item name | Sample position | Replicate number | Component name | Identification status | Detector counts | Response |
|---|-------------|-----------------|------------------|----------------|-----------------------|-----------------|----------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP1.mol | Identified | 504731 | 418187 |

| . | Item name | Sample position | Replicate number | Component name | Identification status | Adducts |
|---|-------------|-----------------|------------------|----------------|-----------------------|-------------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP1.mol | Identified | +H, +Na, -e |

Component name: MP1.mol

| . | Item name | Sample position | Replicate number | Component name | Identification status | Neutral mass (Da) | Observed neutral mass (Da) |
|---|-------------|-----------------|------------------|----------------|-----------------------|-------------------|----------------------------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP1.mol | Identified | 267.10758 | 267.1086 |

| . | Item name | Sample position | Replicate number | Component name | Identification status | Observed m/z | Mass error (mDa) |
|---|-------------|-----------------|------------------|----------------|-----------------------|--------------|------------------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP1.mol | Identified | 268.1159 | 1.0 |

| . | Item name | Sample position | Replicate number | Component name | Identification status | Mass error (ppm) | Expected RT (min) | Observed RT (min) |
|---|-------------|-----------------|------------------|----------------|-----------------------|------------------|-------------------|-------------------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP1.mol | Identified | 3.8 | | 0.41 |

| . | Item name | Sample position | Replicate number | Component name | Identification status | Detector counts | Response | Adducts |
|---|-------------|-----------------|------------------|----------------|-----------------------|-----------------|----------|---------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP1.mol | Identified | 27722 | 23449 | +H |

Component name: MP1.mol

| . | Item name | Sample position | Replicate number | Component name | Identification status | Neutral mass (Da) | Observed neutral mass (Da) |
|---|-------------|-----------------|------------------|----------------|-----------------------|-------------------|----------------------------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP1.mol | Identified | 267.10758 | 267.1076 |

| . | Item name | Sample position | Replicate number | Component name | Identification status | Observed m/z | Mass error (mDa) |
|---|-------------|-----------------|------------------|----------------|-----------------------|--------------|------------------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP1.mol | Identified | 268.1148 | 0.0 |

| . | Item name | Sample position | Replicate number | Component name | Identification status | Mass error (ppm) | Expected RT (min) | Observed RT (min) |
|---|-------------|-----------------|------------------|----------------|-----------------------|------------------|-------------------|-------------------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP1.mol | Identified | -0.1 | | 1.70 |

Item name: MD_M POPLAWSKI

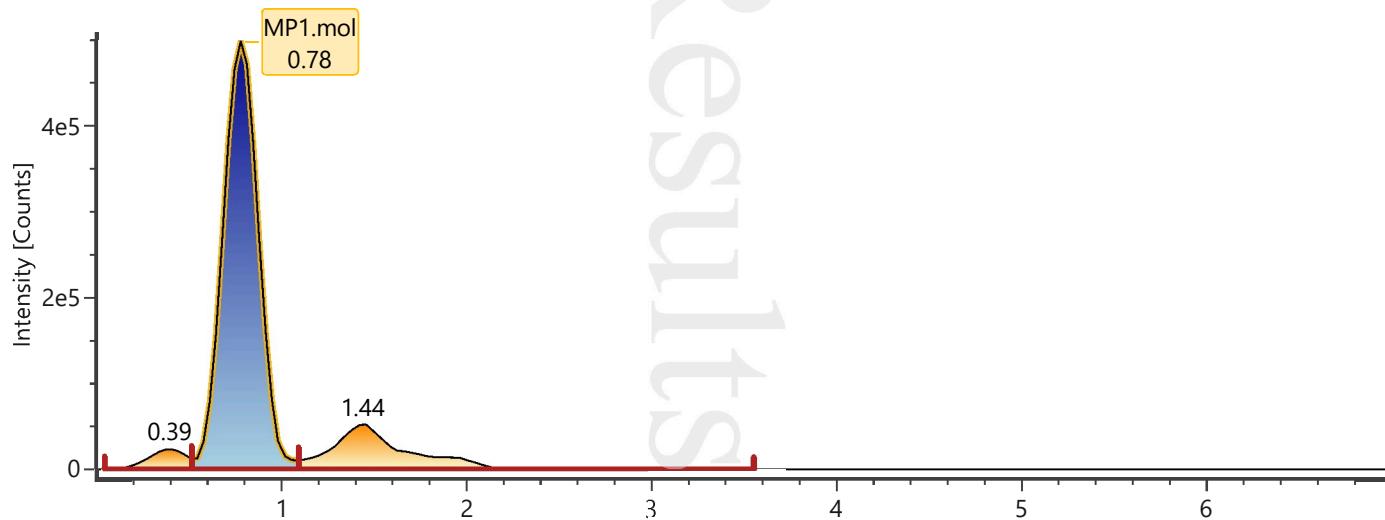
Created time: 13:57:06 GMT Daylight Time

| . | Item name | Sample position | Replicate number | Component name | Identification status | Detector counts | Response | Adducts |
|---|-------------|-----------------|------------------|----------------|-----------------------|-----------------|----------|---------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP1.mol | Identified | 20510 | 19406 | +H |

Item name: int1_a2 ACN

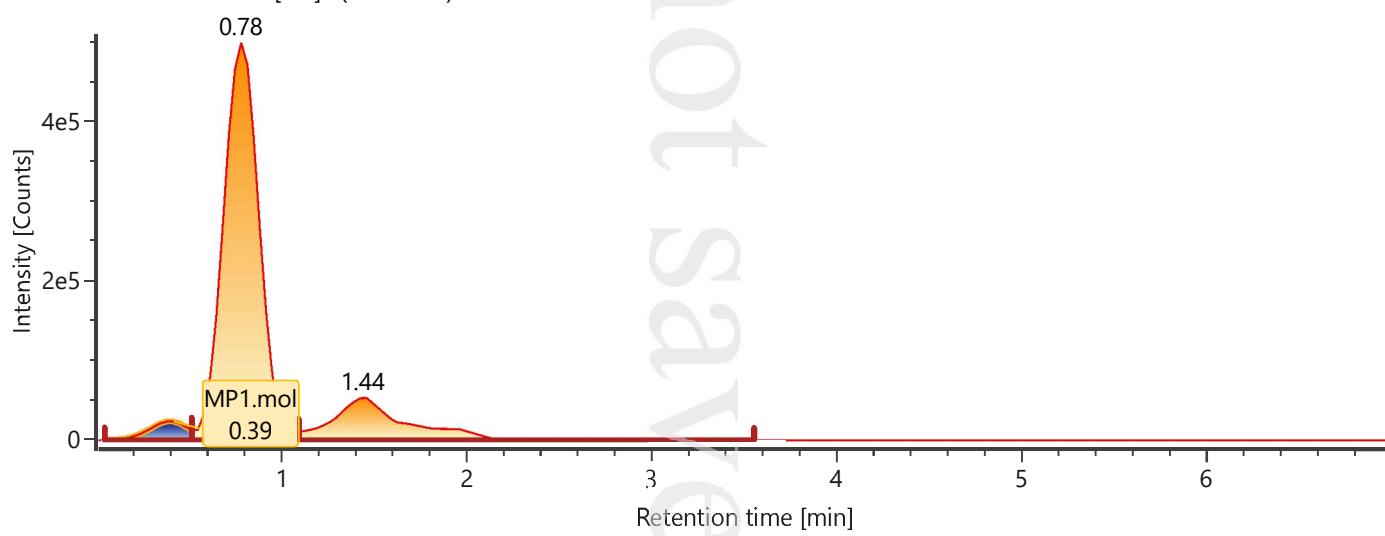
Item name: int1_a2 ACN

Channel name: MP1.mol [+H] : (35.9 PPM) 268.1153



Item name: int1_a2 ACN

Channel name: MP1.mol [+H] : (35.9 PPM) 268.1159

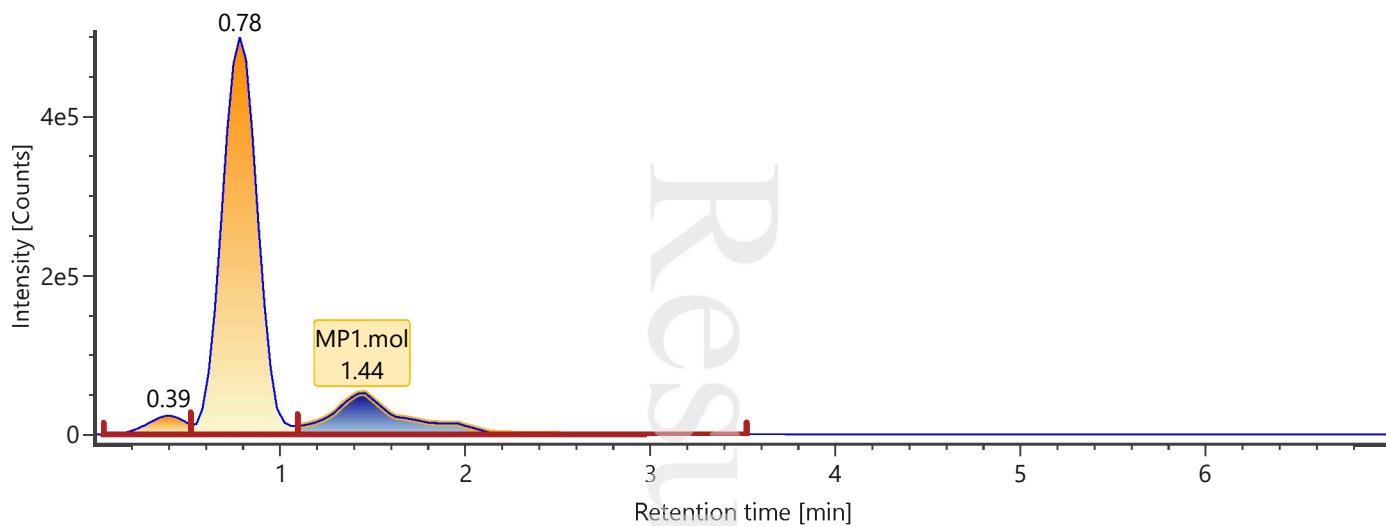


Item name: MD_M POPLAWSKI

Created time: 13:57:06 GMT Daylight Time

Item name: int1_a2 ACN

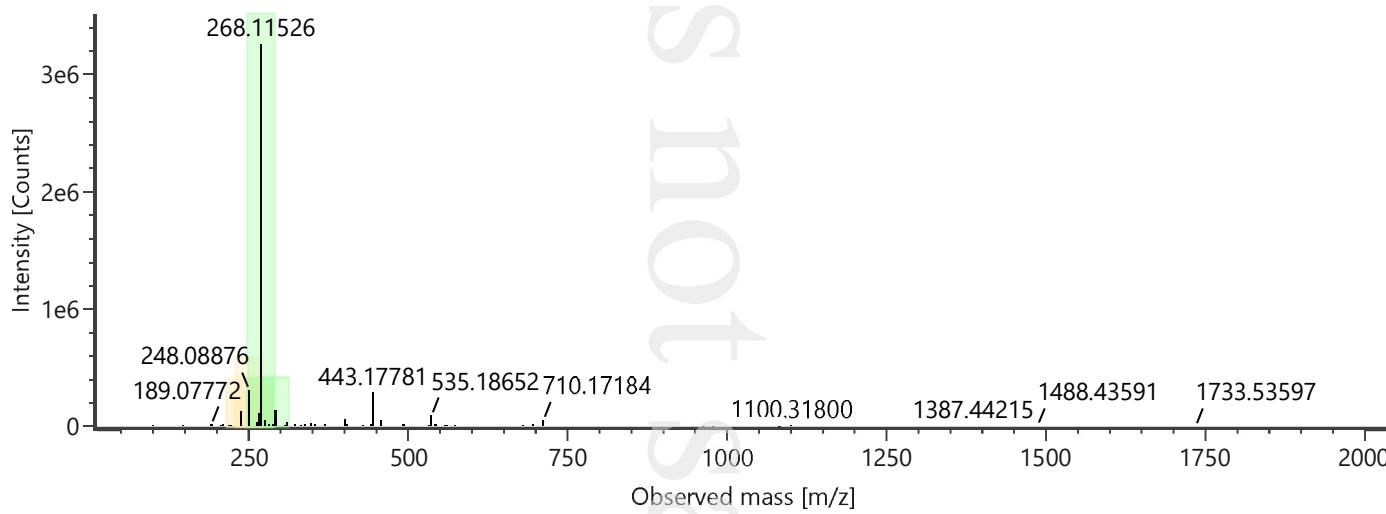
Channel name: MP1.mol [+H] : (35.9 PPM) 268.1148



Item name: int1_a2 ACN

Item description:

Channel name: Low energy : Time 0.7882 +/- 0.0588 minutes



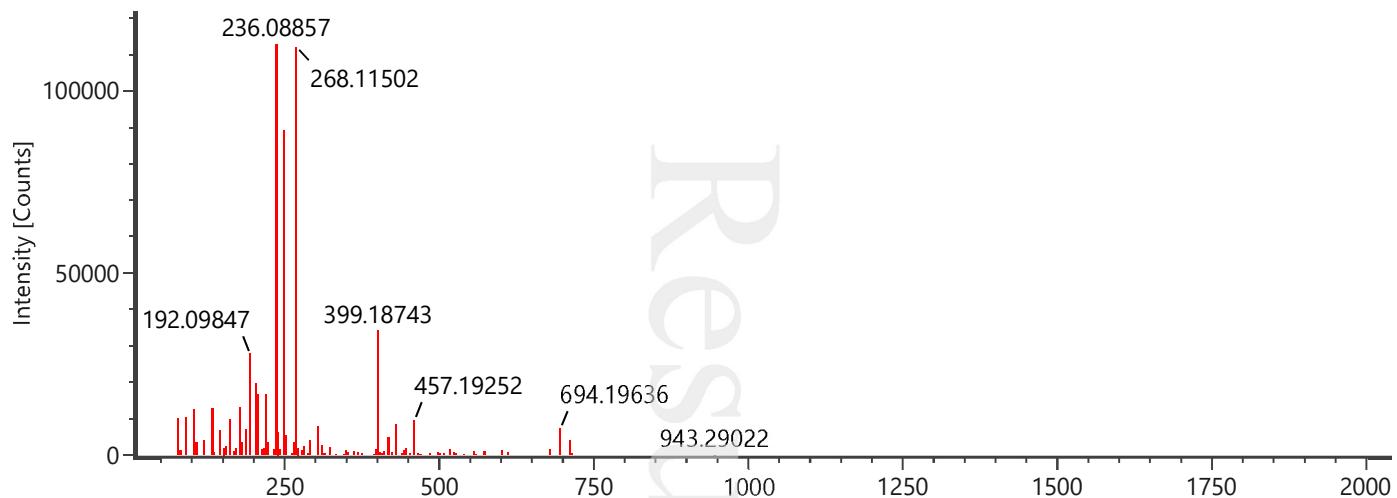
Item name: MD_M POPLAWSKI

Created time: 13:57:06 GMT Daylight Time

Item name: int1_a2 ACN

Channel name: High energy : Time 0.7882 +/- 0.0588 minutes

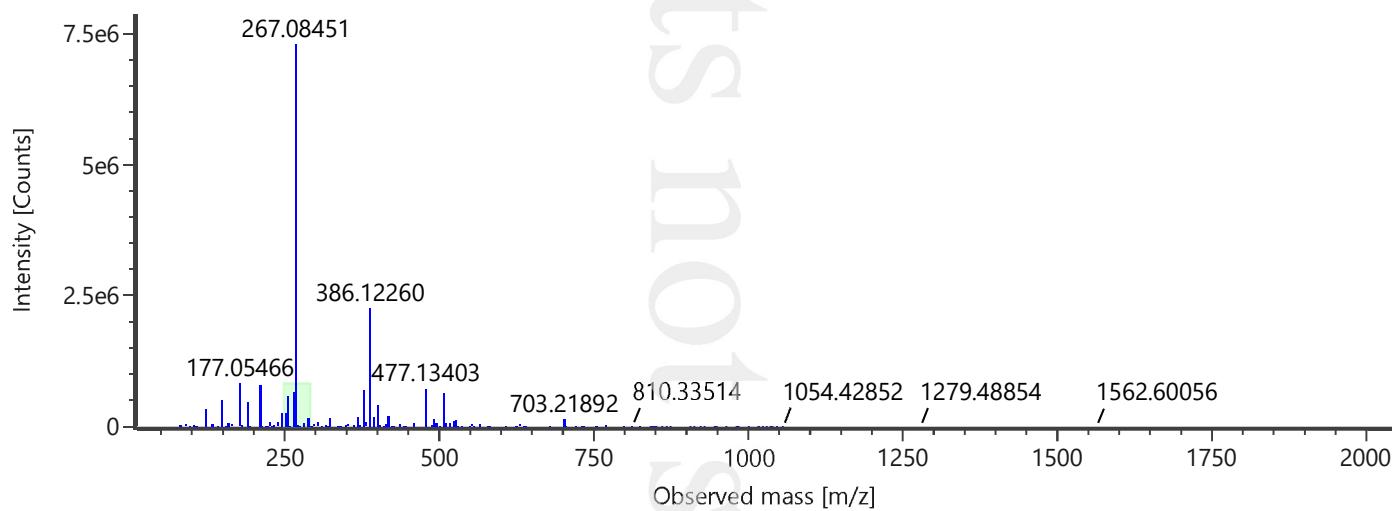
Item description:



Item name: int1_a2 ACN

Channel name: Low energy : Time 0.4127 +/- 0.0588 minutes

Item description:



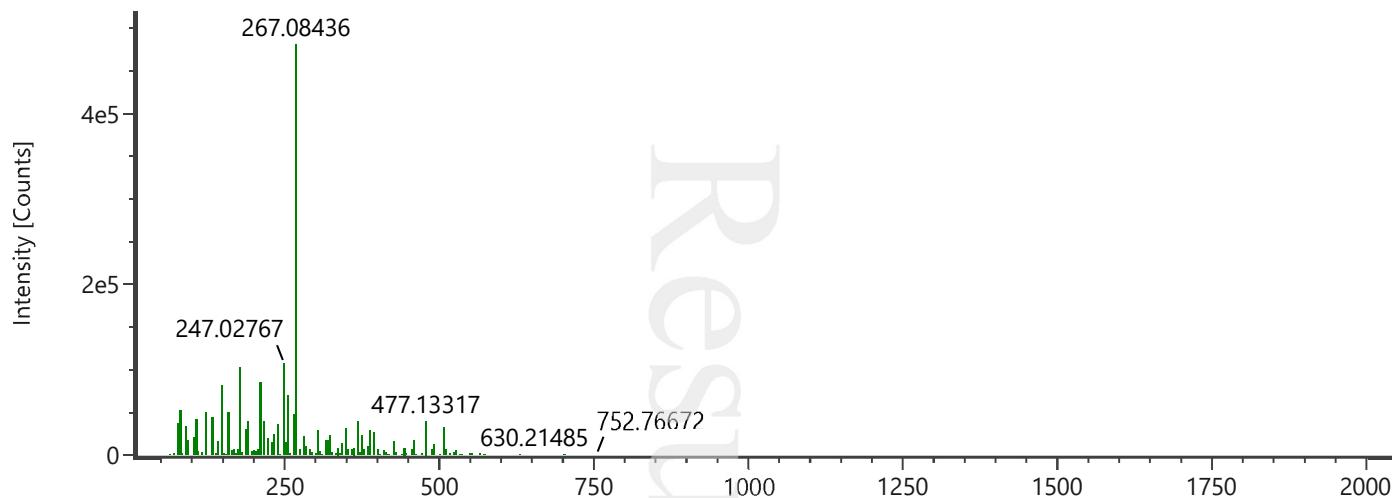
Item name: MD_M POPLAWSKI

Created time: 13:57:06 GMT Daylight Time

Item name: int1_a2 ACN

Channel name: High energy : Time 0.4127 +/- 0.0588 minutes

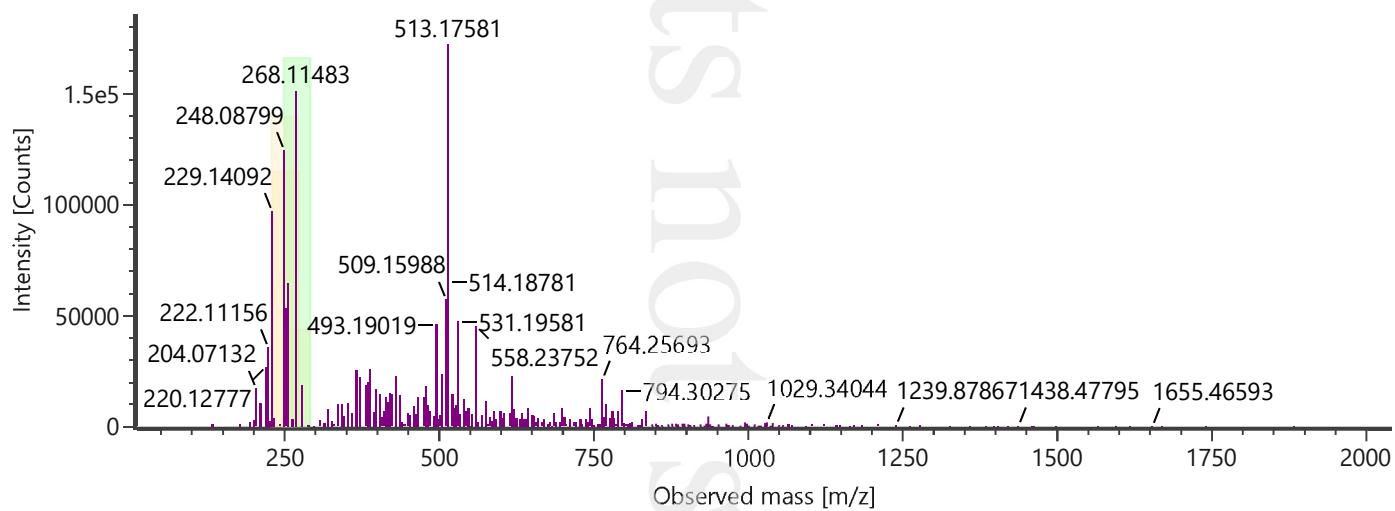
Item description:



Item name: int1_a2 ACN

Channel name: Low energy : Time 1.6957 +/- 0.0588 minutes

Item description:



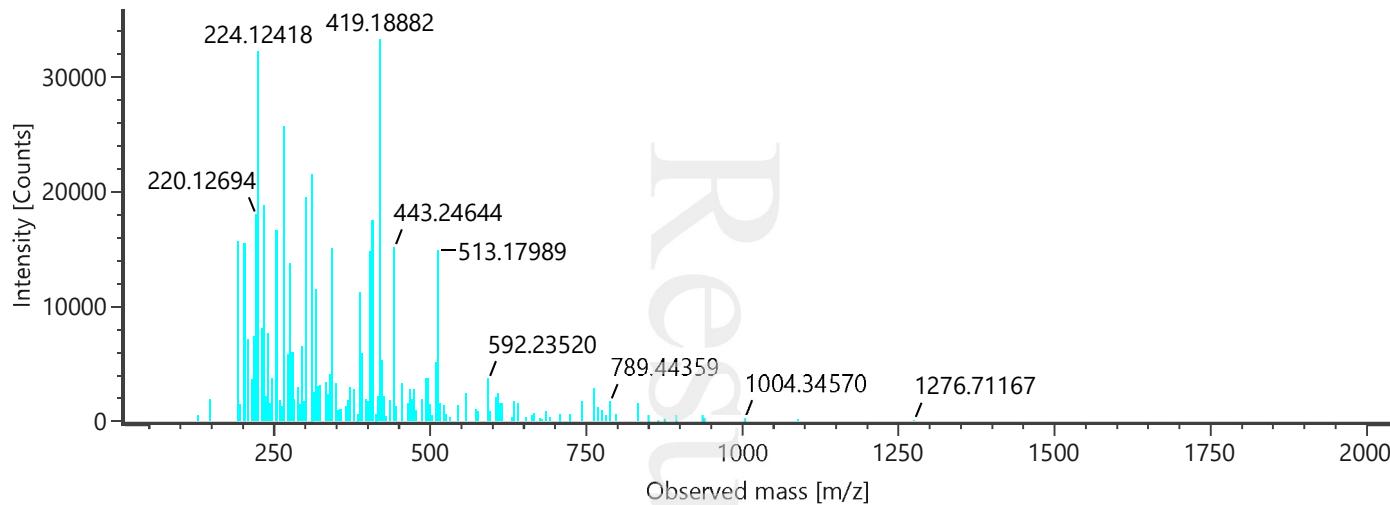
Item name: MD_M POPLAWSKI

Created time: 13:57:06 GMT Daylight Time

Item name: int1_a2 ACN

Channel name: High energy : Time 1.6957 +/- 0.0588 minutes

Item description:



Component name: MP10.mol

Component name: MP10.mol

| . | Item name | Sample position | Replicate number | Component name | Identification status | Neutral mass (Da) | Observed neutral mass (Da) |
|---|-------------|-----------------|------------------|----------------|-----------------------|-------------------|----------------------------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP10.mol | Identified | 759.25465 | 759.2539 |

| . | Item name | Sample position | Replicate number | Component name | Identification status | Observed m/z | Mass error (mDa) |
|---|-------------|-----------------|------------------|----------------|-----------------------|--------------|------------------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP10.mol | Identified | 380.6342 | -0.7 |

| . | Item name | Sample position | Replicate number | Component name | Identification status | Mass error (ppm) | Expected RT (min) | Observed RT (min) |
|---|-------------|-----------------|------------------|----------------|-----------------------|------------------|-------------------|-------------------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP10.mol | Identified | -0.9 | | 1.50 |

| . | Item name | Sample position | Replicate number | Component name | Identification status | Detector counts | Response | Adducts |
|---|-------------|-----------------|------------------|----------------|-----------------------|-----------------|----------|---------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP10.mol | Identified | 16332 | 16332 | 2x(+H) |

Item name: int1_a2 ACN

Item name: MD_M POPLAWSKI

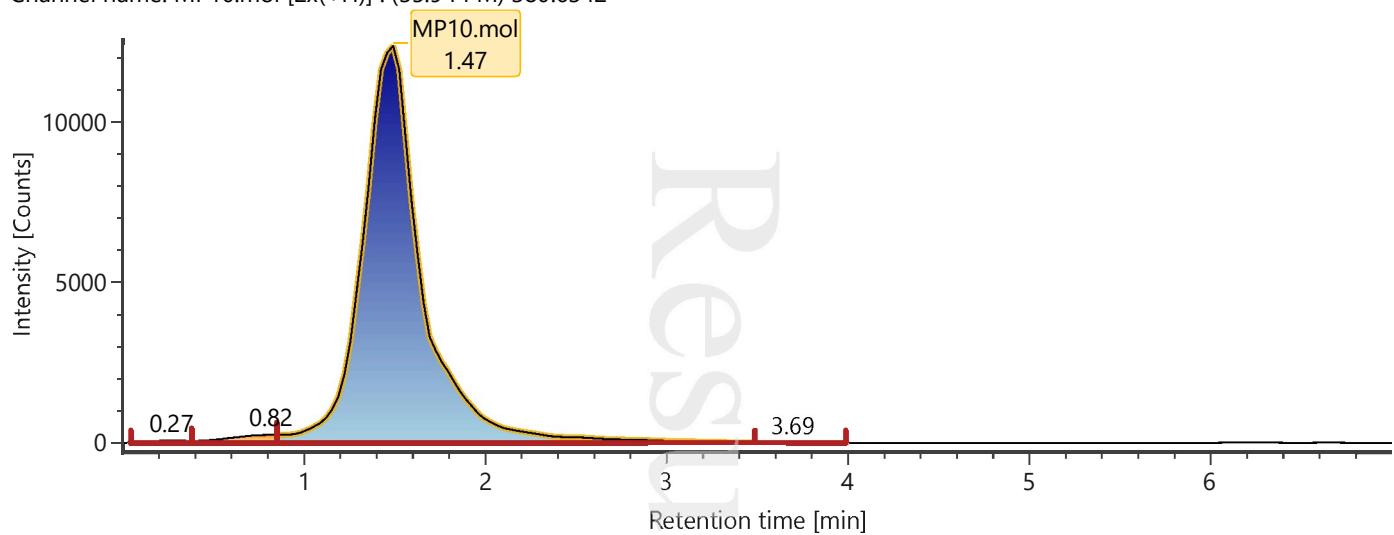
Created by: Chemistry, Chemistry

Created on: Sep 07, 2023

Created time: 13:57:06 GMT Daylight Time

Item name: int1_a2 ACN

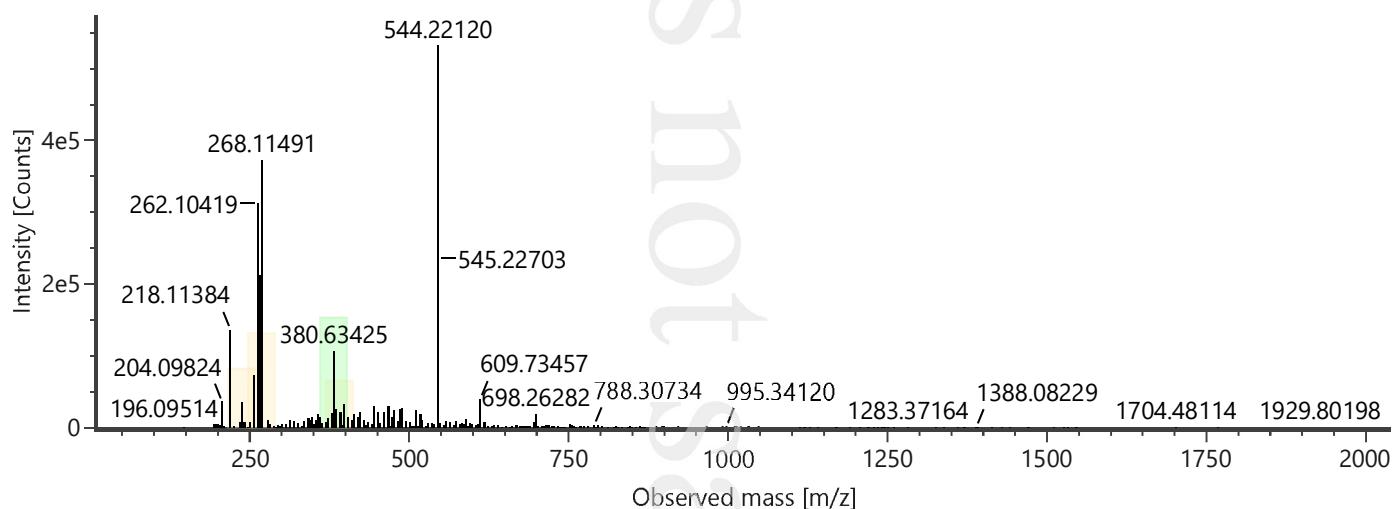
Channel name: MP10.mol [2x(+H)] : (35.9 PPM) 380.6342



Item name: int1_a2 ACN

Item description:

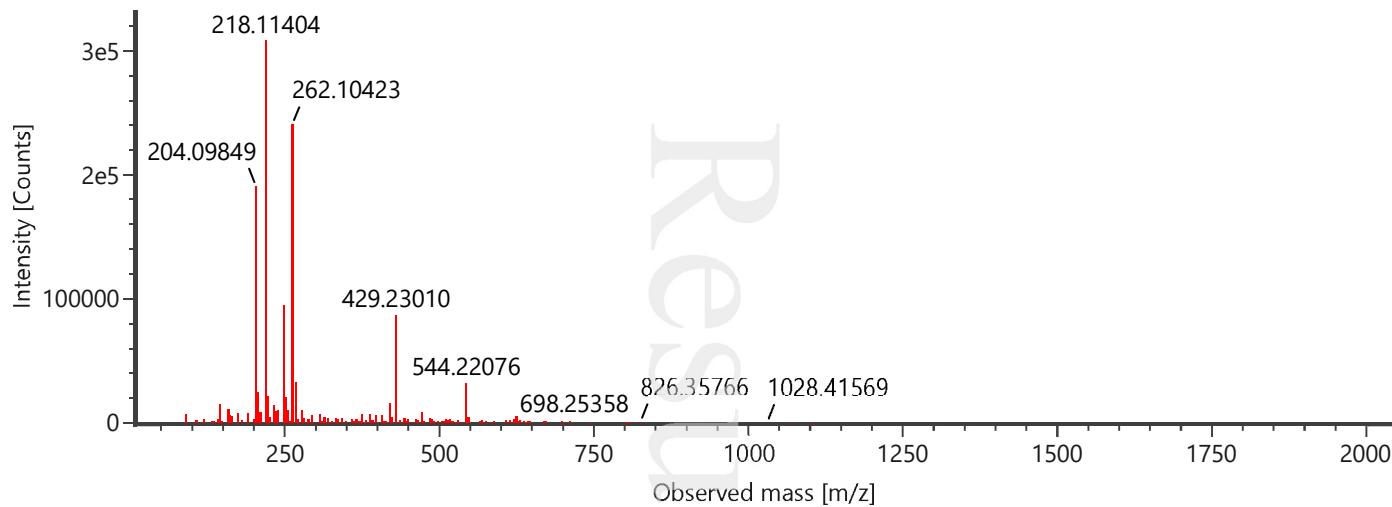
Channel name: Low energy : Time 1.5009 +/- 0.0588 minutes



Item name: int1_a2 ACN

Channel name: High energy : Time 1.5009 +/- 0.0588 minutes

Item description:



Component name: MP11.mol

Component name: MP11.mol

| . | Item name | Sample position | Replicate number | Component name | Identification status | Neutral mass (Da) | Observed neutral mass (Da) |
|---|-------------|-----------------|------------------|----------------|-----------------------|-------------------|----------------------------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP11.mol | Identified | 773.27030 | 773.2670 |

| . | Item name | Sample position | Replicate number | Component name | Identification status | Observed m/z | Mass error (mDa) |
|---|-------------|-----------------|------------------|----------------|-----------------------|--------------|------------------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP11.mol | Identified | 796.2562 | -3.3 |

| . | Item name | Sample position | Replicate number | Component name | Identification status | Mass error (ppm) | Expected RT (min) | Observed RT (min) |
|---|-------------|-----------------|------------------|----------------|-----------------------|------------------|-------------------|-------------------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP11.mol | Identified | -4.2 | | 0.70 |

| . | Item name | Sample position | Replicate number | Component name | Identification status | Detector counts | Response | Adducts |
|---|-------------|-----------------|------------------|----------------|-----------------------|-----------------|----------|---------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP11.mol | Identified | 2761 | 2036 | +Na |

Component name: MP11.mol

| . | Item name | Sample position | Replicate number | Component name | Identification status | Neutral mass (Da) | Observed neutral mass (Da) |
|---|-------------|-----------------|------------------|----------------|-----------------------|-------------------|----------------------------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP11.mol | Identified | 773.27030 | 773.2679 |

| . | Item name | Sample position | Replicate number | Component name | Identification status | Observed m/z | Mass error (mDa) |
|---|-------------|-----------------|------------------|----------------|-----------------------|--------------|------------------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP11.mol | Identified | 387.6412 | -2.4 |

| . | Item name | Sample position | Replicate number | Component name | Identification status | Mass error (ppm) | Expected RT (min) | Observed RT (min) |
|---|-------------|-----------------|------------------|----------------|-----------------------|------------------|-------------------|-------------------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP11.mol | Identified | -3.1 | | 1.42 |

Item name: MD_M POPLAWSKI

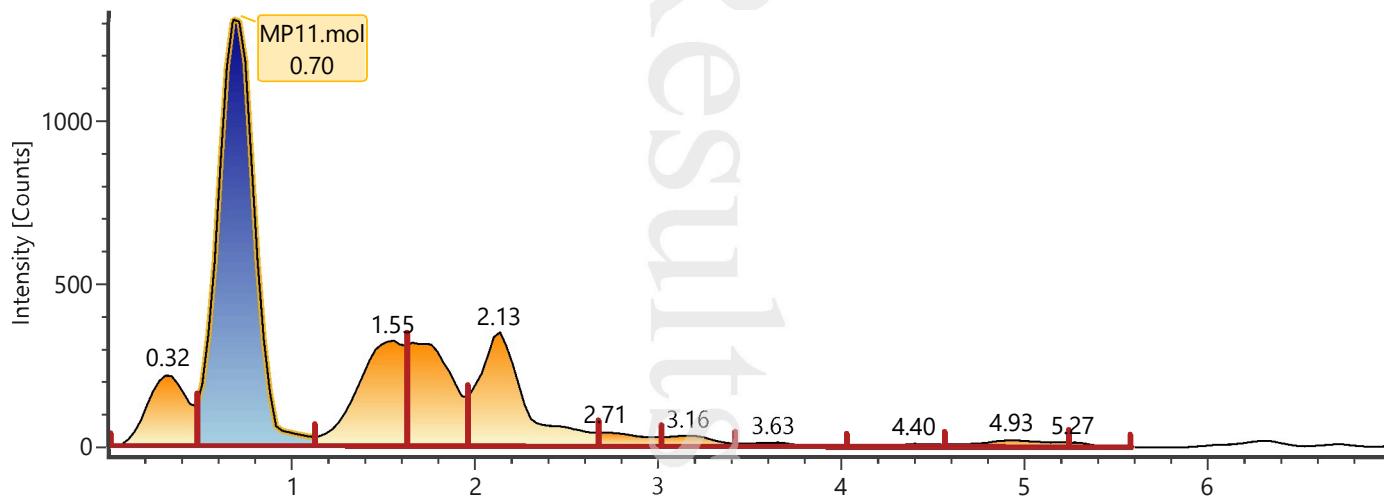
Created time: 13:57:06 GMT Daylight Time

| . | Item name | Sample position | Replicate number | Component name | Identification status | Detector counts | Response | Adducts |
|---|-------------|-----------------|------------------|----------------|-----------------------|-----------------|----------|---------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP11.mol | Identified | 10556 | 3340 | 2x(+H) |

Item name: int1_a2 ACN

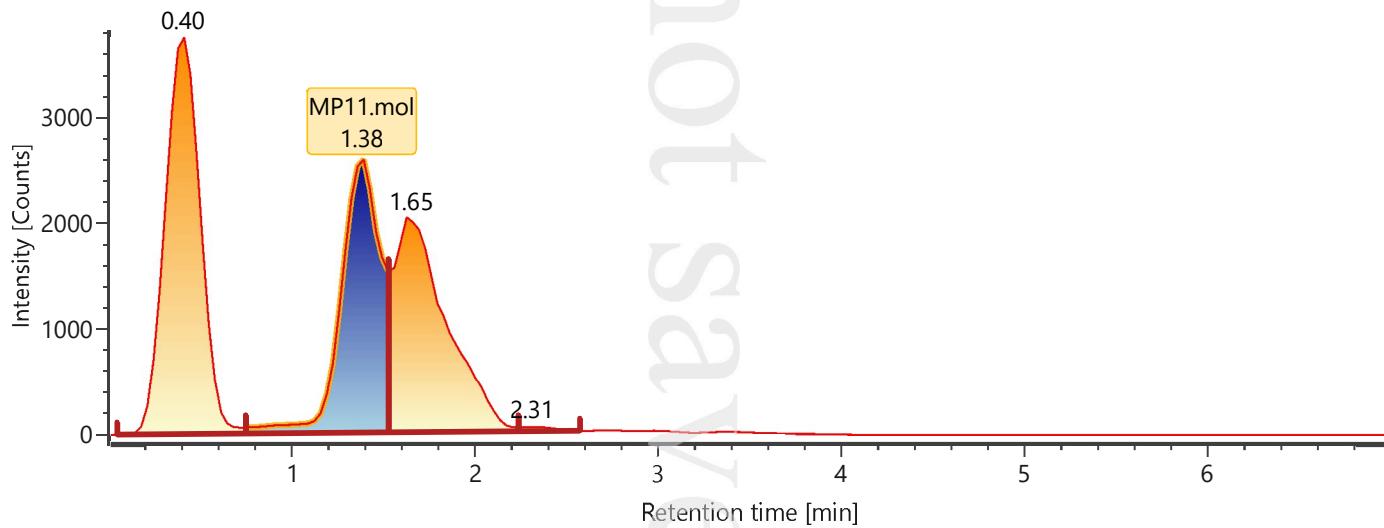
Item name: int1_a2 ACN

Channel name: MP11.mol [+Na] : (35.9 PPM) 796.2562



Item name: int1_a2 ACN

Channel name: MP11.mol [2x(+H)] : (35.9 PPM) 387.6412



Item name: MD_M POPLAWSKI

Created by: Chemistry, Chemistry

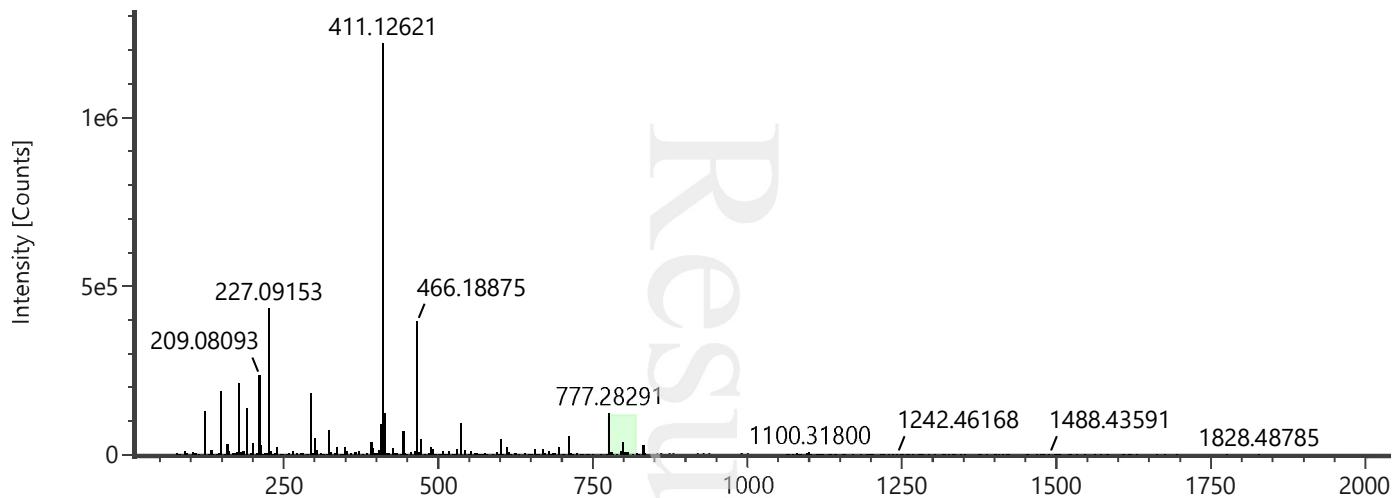
Created on: Sep 07, 2023

Created time: 13:57:06 GMT Daylight Time

Item name: int1_a2 ACN

Channel name: Low energy : Time 0.7040 +/- 0.0588 minutes

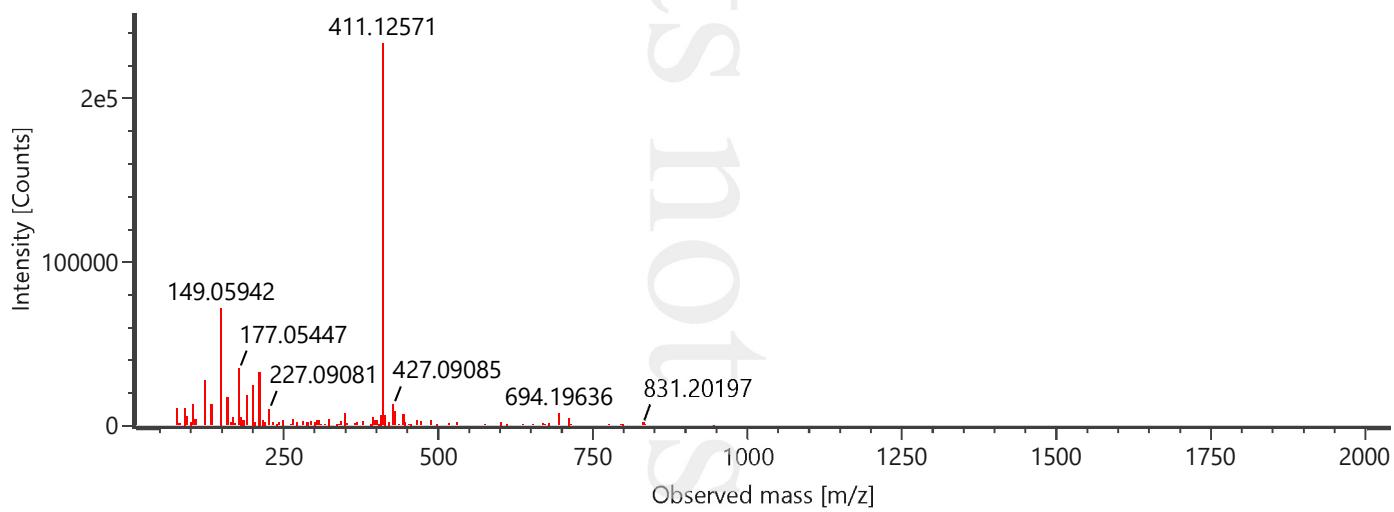
Item description:



Item name: int1_a2 ACN

Channel name: High energy : Time 0.7040 +/- 0.0588 minutes

Item description:



Item name: MD_M POPLAWSKI

Created by: Chemistry, Chemistry

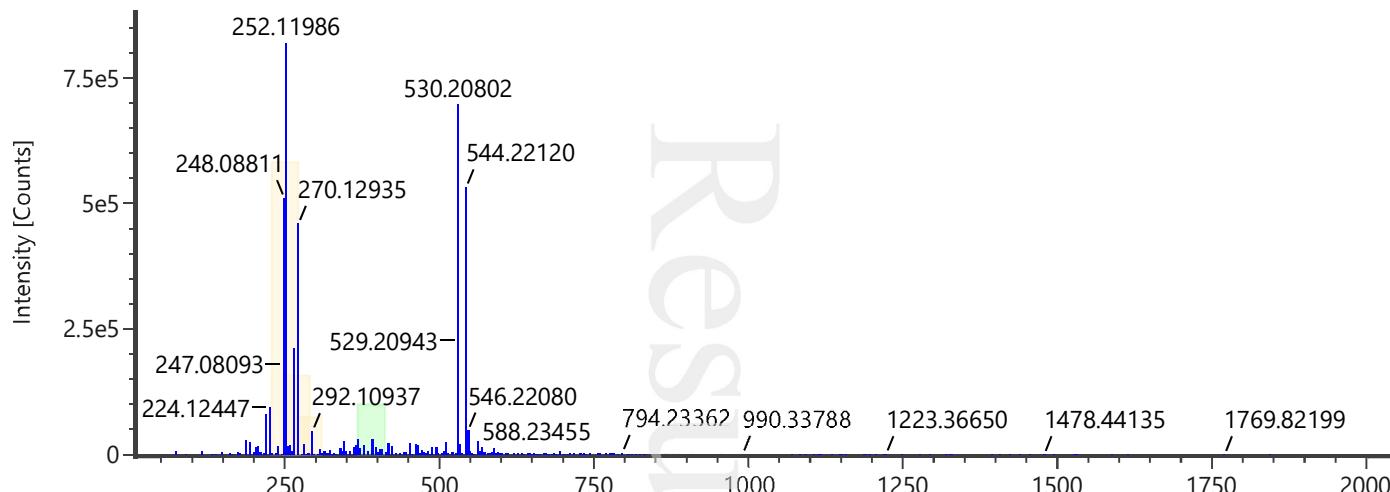
Created on: Sep 07, 2023

Created time: 13:57:06 GMT Daylight Time

Item name: int1_a2 ACN

Channel name: Low energy : Time 1.4240 +/- 0.0588 minutes

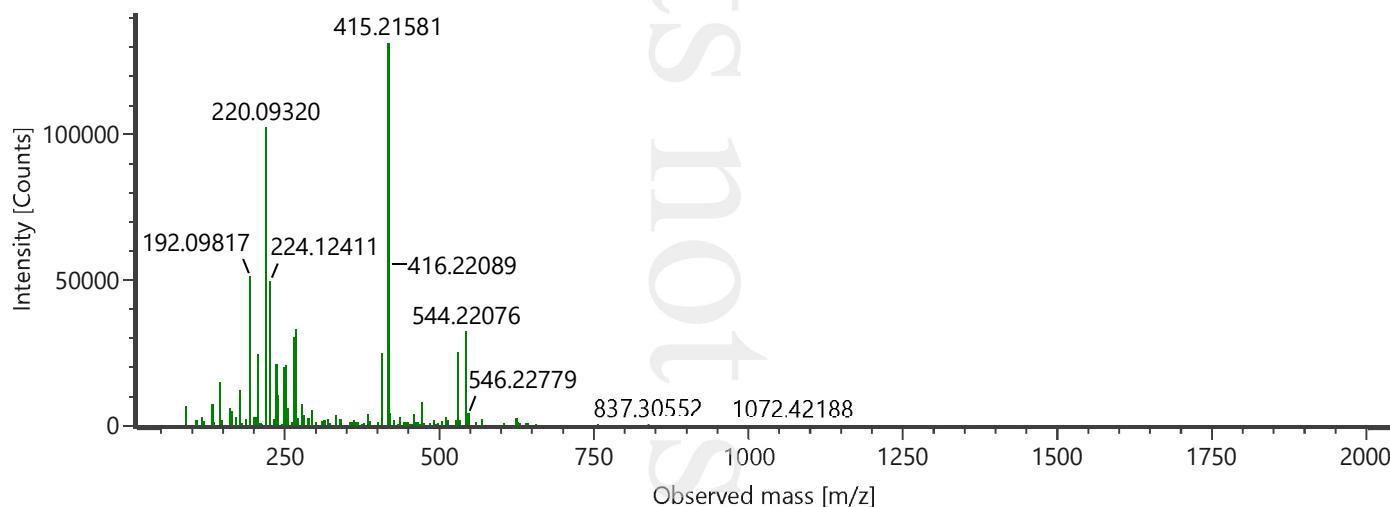
Item description:



Item name: int1_a2 ACN

Channel name: High energy : Time 1.4240 +/- 0.0588 minutes

Item description:



Component name: MP2.mol

Component name: MP2.mol

| . | Item name | Sample position | Replicate number | Component name | Identification status | Neutral mass (Da) | Observed neutral mass (Da) |
|---|-------------|-----------------|------------------|----------------|-----------------------|-------------------|----------------------------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP2.mol | Identified | 265.09193 | 265.0927 |

| . | Item name | Sample position | Replicate number | Component name | Identification status | Observed m/z | Mass error (mDa) |
|---|-------------|-----------------|------------------|----------------|-----------------------|--------------|------------------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP2.mol | Identified | 266.0999 | 0.7 |

Item name: MD_M POPLAWSKI

Created time: 13:57:06 GMT Daylight Time

| . | Item name | Sample position | Replicate number | Component name | Identification status | Mass error (ppm) | Expected RT (min) | Observed RT (min) |
|---|-------------|-----------------|------------------|----------------|-----------------------|------------------|-------------------|-------------------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP2.mol | Identified | 2.8 | | 0.27 |

| . | Item name | Sample position | Replicate number | Component name | Identification status | Detector counts | Response | Adducts |
|---|-------------|-----------------|------------------|----------------|-----------------------|-----------------|----------|---------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP2.mol | Identified | 4861 | 4486 | +H, -e |

Component name: MP2.mol

| . | Item name | Sample position | Replicate number | Component name | Identification status | Neutral mass (Da) | Observed neutral mass (Da) |
|---|-------------|-----------------|------------------|----------------|-----------------------|-------------------|----------------------------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP2.mol | Identified | 265.09193 | 265.0925 |

| . | Item name | Sample position | Replicate number | Component name | Identification status | Observed m/z | Mass error (mDa) |
|---|-------------|-----------------|------------------|----------------|-----------------------|--------------|------------------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP2.mol | Identified | 266.0998 | 0.6 |

| . | Item name | Sample position | Replicate number | Component name | Identification status | Mass error (ppm) | Expected RT (min) | Observed RT (min) |
|---|-------------|-----------------|------------------|----------------|-----------------------|------------------|-------------------|-------------------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP2.mol | Identified | 2.2 | | 1.65 |

| . | Item name | Sample position | Replicate number | Component name | Identification status | Detector counts | Response | Adducts |
|---|-------------|-----------------|------------------|----------------|-----------------------|-----------------|----------|---------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP2.mol | Identified | 6820 | 3143 | +H |

Component name: MP2.mol

| . | Item name | Sample position | Replicate number | Component name | Identification status | Neutral mass (Da) | Observed neutral mass (Da) |
|---|-------------|-----------------|------------------|----------------|-----------------------|-------------------|----------------------------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP2.mol | Identified | 265.09193 | 265.0923 |

| . | Item name | Sample position | Replicate number | Component name | Identification status | Observed m/z | Mass error (mDa) |
|---|-------------|-----------------|------------------|----------------|-----------------------|--------------|------------------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP2.mol | Identified | 266.0996 | 0.4 |

| . | Item name | Sample position | Replicate number | Component name | Identification status | Mass error (ppm) | Expected RT (min) | Observed RT (min) |
|---|-------------|-----------------|------------------|----------------|-----------------------|------------------|-------------------|-------------------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP2.mol | Identified | 1.6 | | 1.45 |

| . | Item name | Sample position | Replicate number | Component name | Identification status | Detector counts | Response | Adducts |
|---|-------------|-----------------|------------------|----------------|-----------------------|-----------------|----------|---------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP2.mol | Identified | 19037 | 7806 | +H, +Na |

Component name: MP2.mol

| . | Item name | Sample position | Replicate number | Component name | Identification status | Neutral mass (Da) | Observed neutral mass (Da) |
|---|-------------|-----------------|------------------|----------------|-----------------------|-------------------|----------------------------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP2.mol | Identified | 265.09193 | 265.0922 |

| . | Item name | Sample position | Replicate number | Component name | Identification status | Observed m/z | Mass error (mDa) |
|---|-------------|-----------------|------------------|----------------|-----------------------|--------------|------------------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP2.mol | Identified | 266.0995 | 0.3 |

Item name: MD_M POPLAWSKI

Created time: 13:57:06 GMT Daylight Time

| . | Item name | Sample position | Replicate number | Component name | Identification status | Mass error (ppm) | Expected RT (min) | Observed RT (min) |
|---|-------------|-----------------|------------------|----------------|-----------------------|------------------|-------------------|-------------------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP2.mol | Identified | 1.0 | | 1.13 |

| . | Item name | Sample position | Replicate number | Component name | Identification status | Detector counts | Response | Adducts |
|---|-------------|-----------------|------------------|----------------|-----------------------|-----------------|----------|---------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP2.mol | Identified | 27492 | 17848 | +H, +Na |

Component name: MP2.mol

| . | Item name | Sample position | Replicate number | Component name | Identification status | Neutral mass (Da) | Observed neutral mass (Da) |
|---|-------------|-----------------|------------------|----------------|-----------------------|-------------------|----------------------------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP2.mol | Identified | 265.09193 | 265.0927 |

| . | Item name | Sample position | Replicate number | Component name | Identification status | Observed m/z | Mass error (mDa) |
|---|-------------|-----------------|------------------|----------------|-----------------------|--------------|------------------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP2.mol | Identified | 266.0999 | 0.7 |

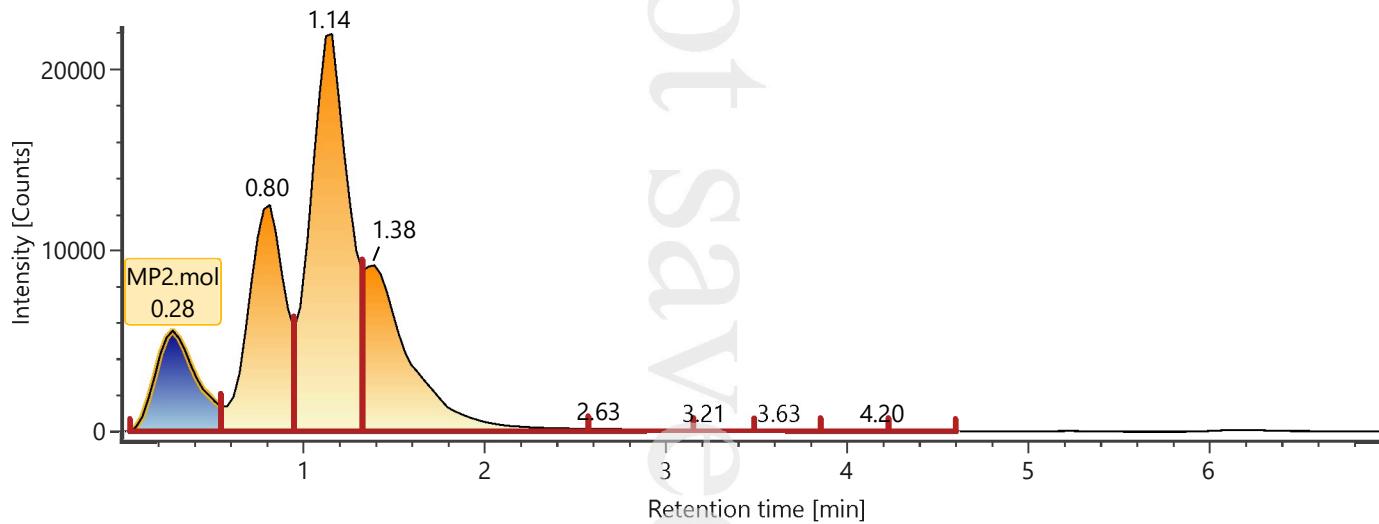
| . | Item name | Sample position | Replicate number | Component name | Identification status | Mass error (ppm) | Expected RT (min) | Observed RT (min) |
|---|-------------|-----------------|------------------|----------------|-----------------------|------------------|-------------------|-------------------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP2.mol | Identified | 2.7 | | 0.80 |

| . | Item name | Sample position | Replicate number | Component name | Identification status | Detector counts | Response | Adducts |
|---|-------------|-----------------|------------------|----------------|-----------------------|-----------------|----------|---------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP2.mol | Identified | 11066 | 10301 | +H, -e |

Item name: int1_a2 ACN

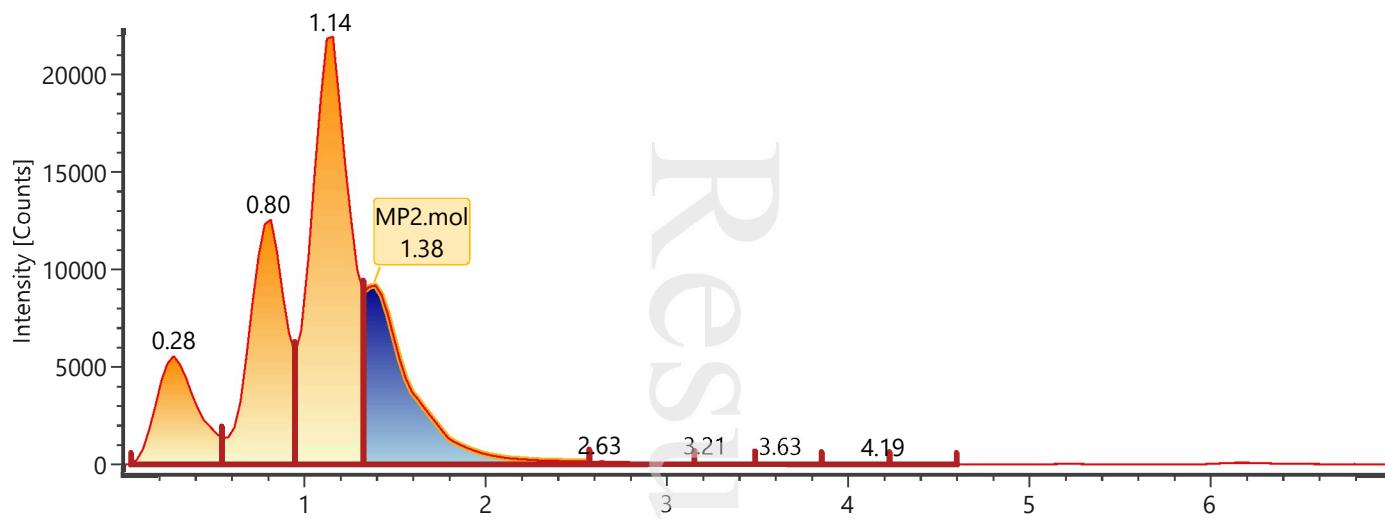
Item name: int1_a2 ACN

Channel name: MP2.mol [+H] : (35.9 PPM) 266.0999



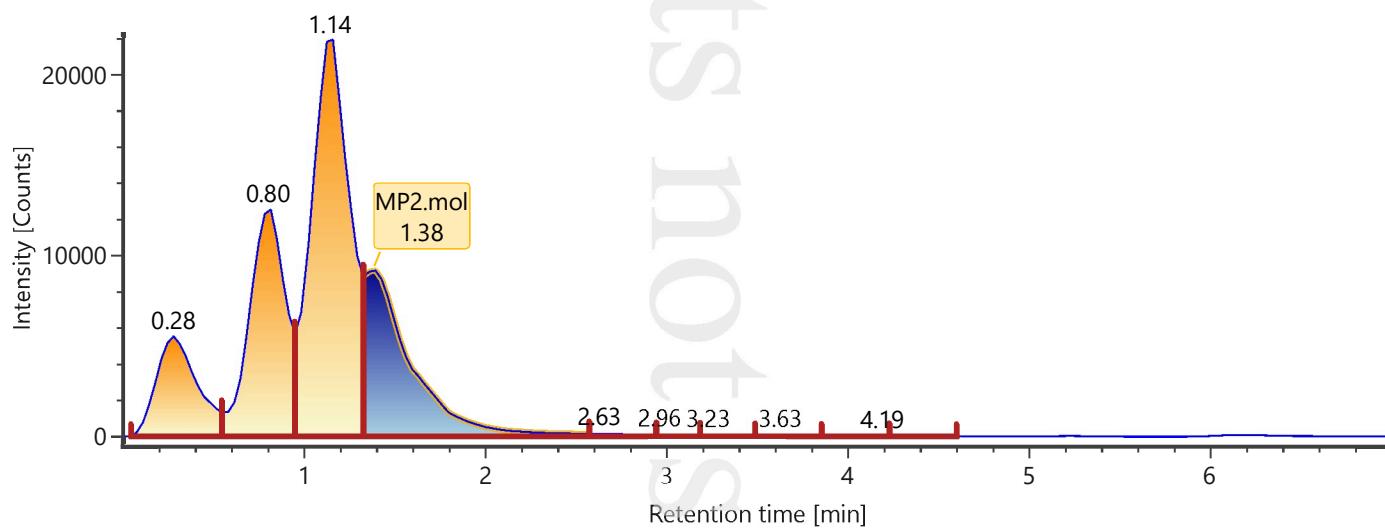
Item name: int1_a2 ACN

Channel name: MP2.mol [+H] : (35.9 PPM) 266.0998



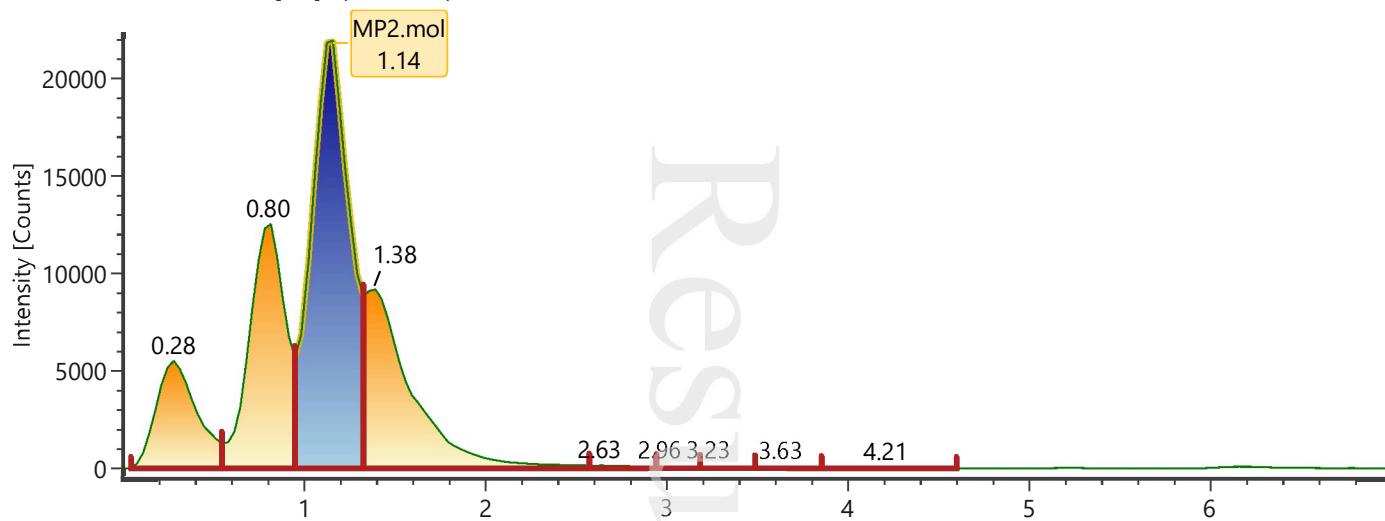
Item name: int1_a2 ACN

Channel name: MP2.mol [+H] : (35.9 PPM) 266.0996



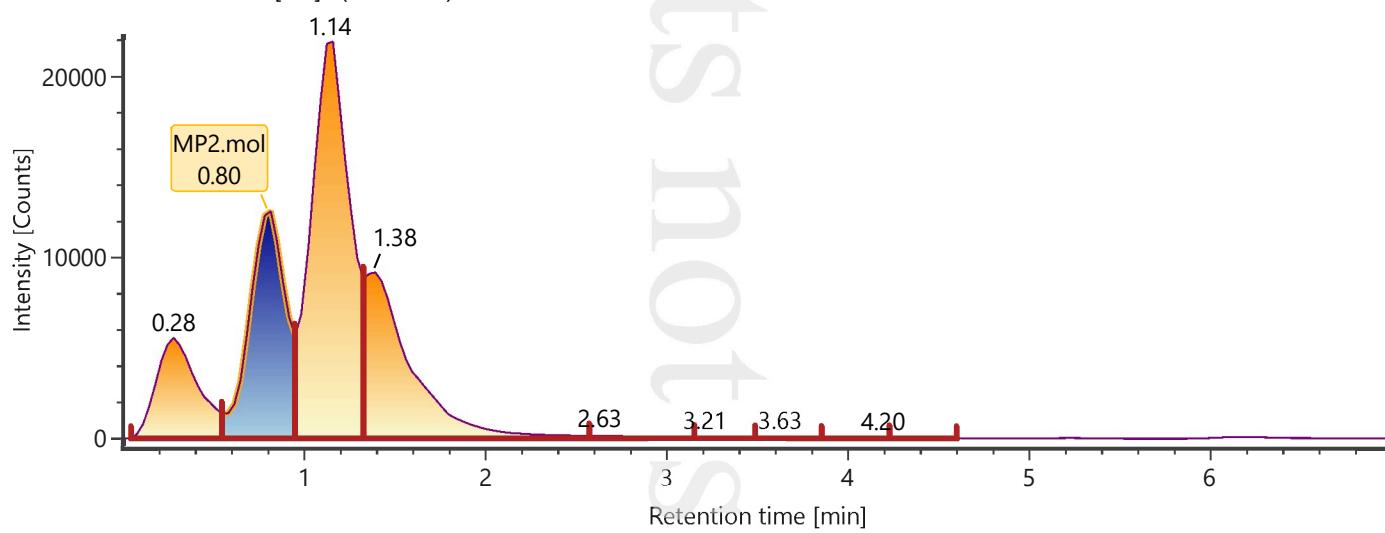
Item name: int1_a2 ACN

Channel name: MP2.mol [+H] : (35.9 PPM) 266.0995



Item name: int1_a2 ACN

Channel name: MP2.mol [+H] : (35.9 PPM) 266.0999



Item name: MD_M POPLAWSKI

Created by: Chemistry, Chemistry

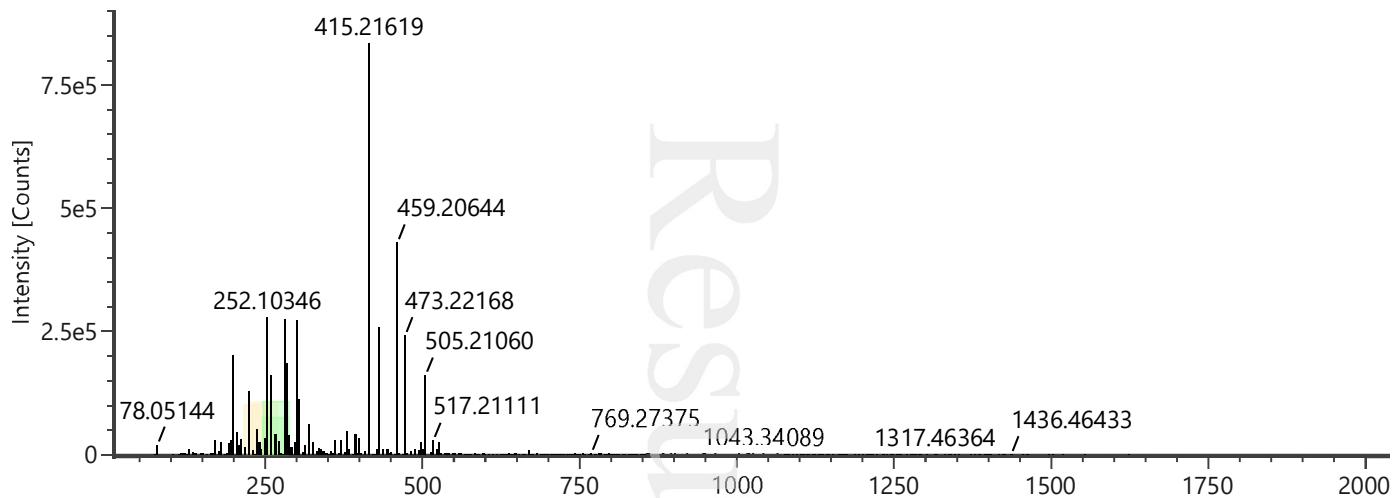
Created on: Sep 07, 2023

Created time: 13:57:06 GMT Daylight Time

Item name: int1_a2 ACN

Channel name: Low energy : Time 0.2684 +/- 0.0588 minutes

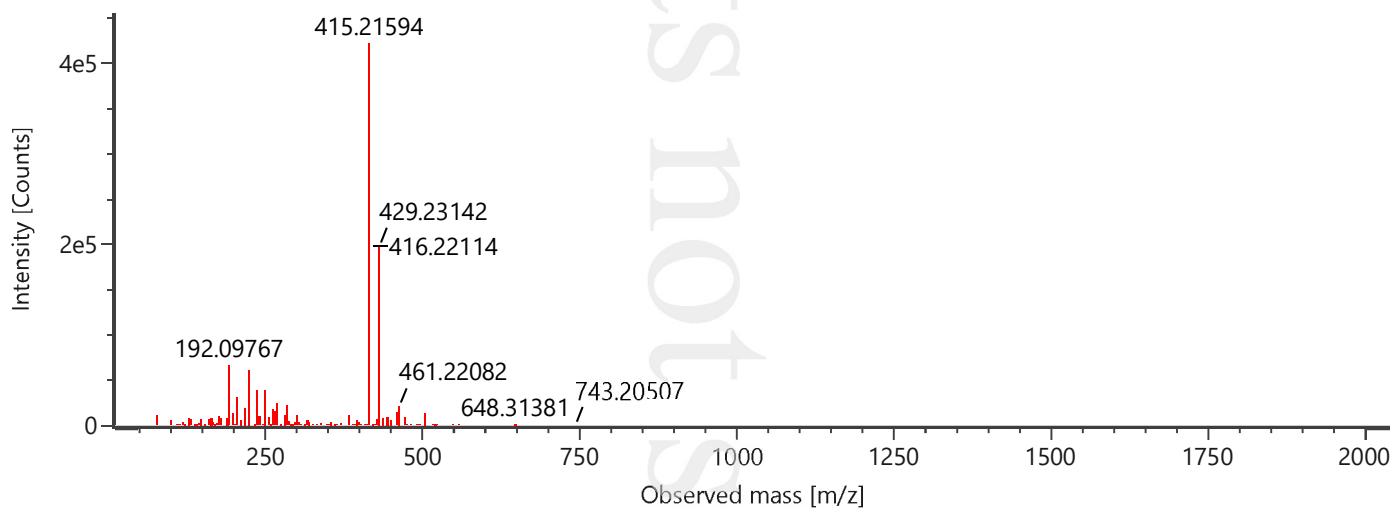
Item description:



Item name: int1_a2 ACN

Channel name: High energy : Time 0.2684 +/- 0.0588 minutes

Item description:



Item name: MD_M POPLAWSKI

Created by: Chemistry, Chemistry

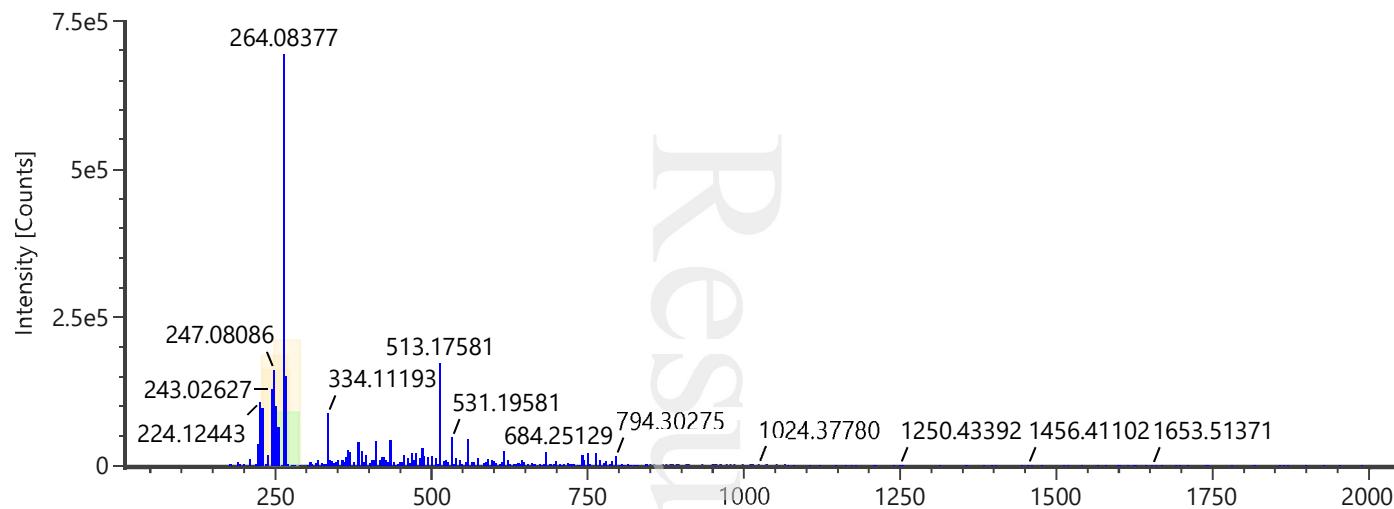
Created on: Sep 07, 2023

Created time: 13:57:06 GMT Daylight Time

Item name: int1_a2 ACN

Channel name: Low energy : Time 1.6502 +/- 0.0588 minutes

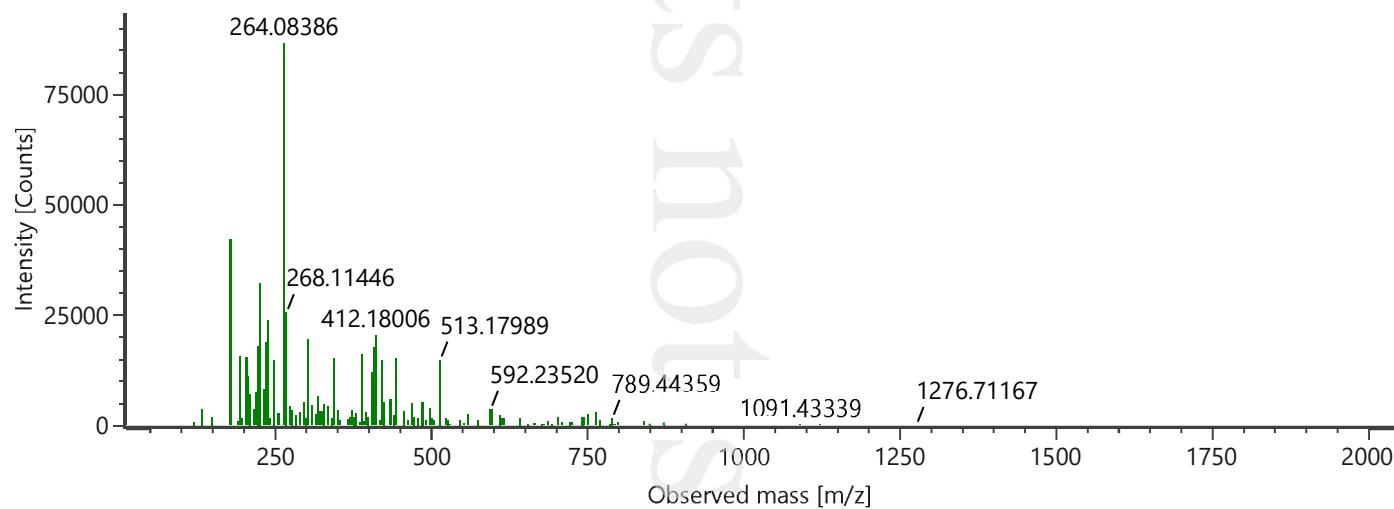
Item description:



Item name: int1_a2 ACN

Channel name: High energy : Time 1.6502 +/- 0.0588 minutes

Item description:



Item name: MD_M POPLAWSKI

Created by: Chemistry, Chemistry

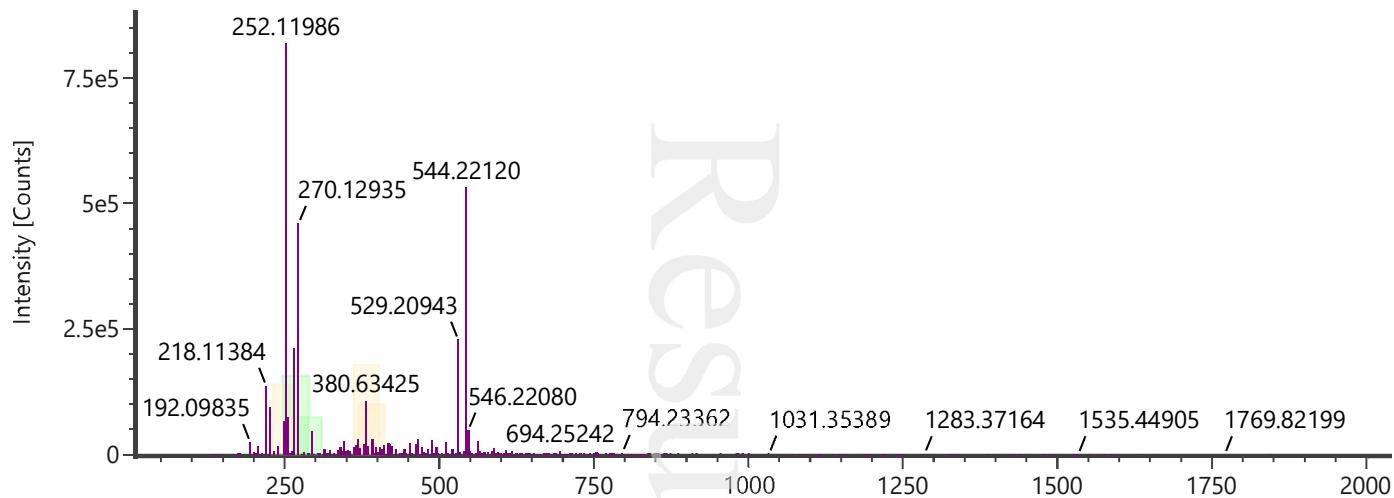
Created on: Sep 07, 2023

Created time: 13:57:06 GMT Daylight Time

Item name: int1_a2 ACN

Channel name: Low energy : Time 1.4548 +/- 0.0588 minutes

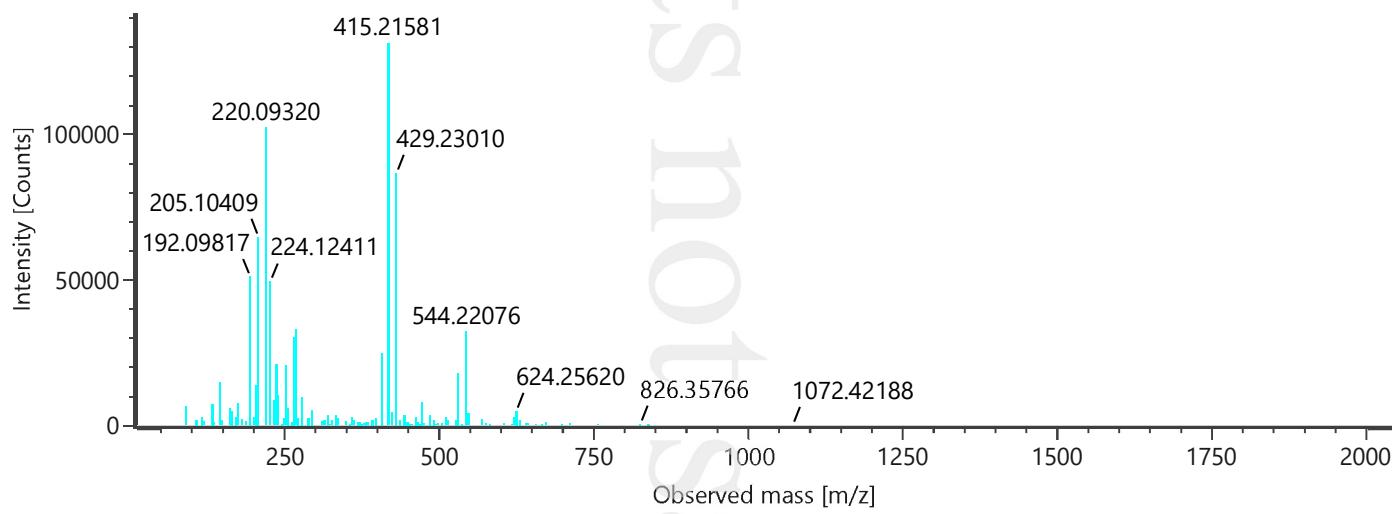
Item description:



Item name: int1_a2 ACN

Channel name: High energy : Time 1.4548 +/- 0.0588 minutes

Item description:



Item name: MD_M POPLAWSKI

Created by: Chemistry, Chemistry

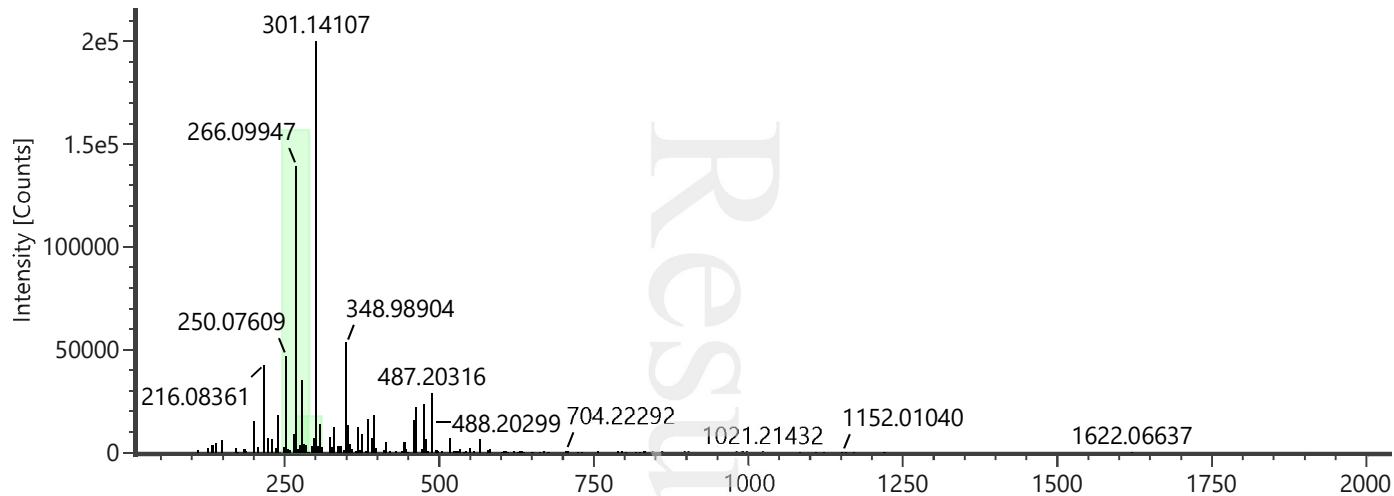
Created on: Sep 07, 2023

Created time: 13:57:06 GMT Daylight Time

Item name: int1_a2 ACN

Channel name: Low energy : Time 1.1322 +/- 0.0588 minutes

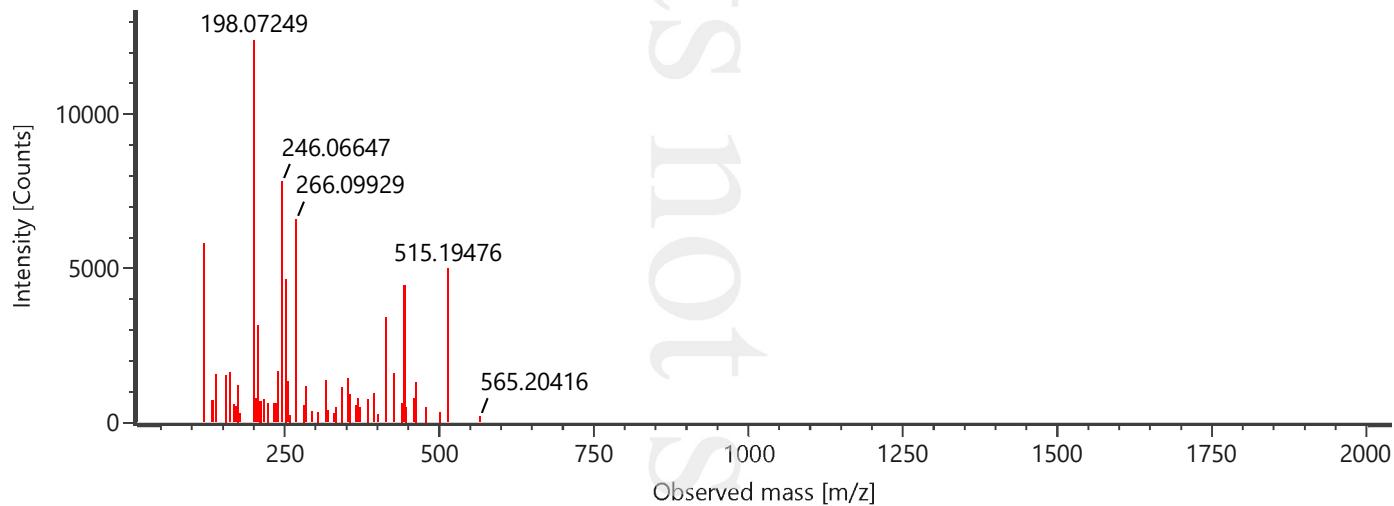
Item description:



Item name: int1_a2 ACN

Channel name: High energy : Time 1.1322 +/- 0.0588 minutes

Item description:



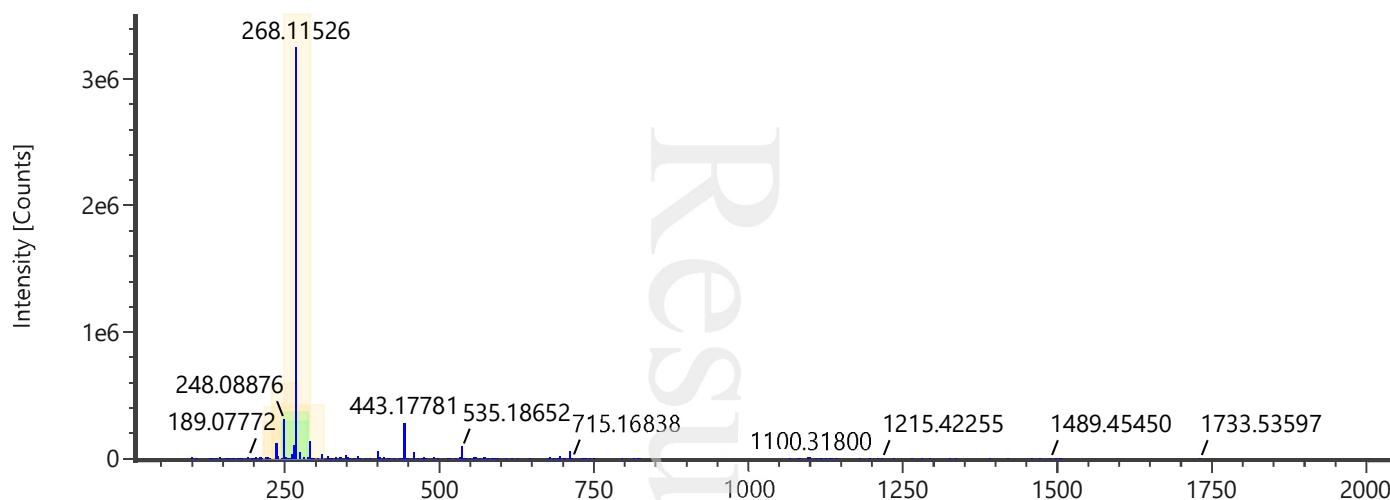
Item name: MD_M POPLAWSKI

Created time: 13:57:06 GMT Daylight Time

Item name: int1_a2 ACN

Channel name: Low energy : Time 0.8043 +/- 0.0588 minutes

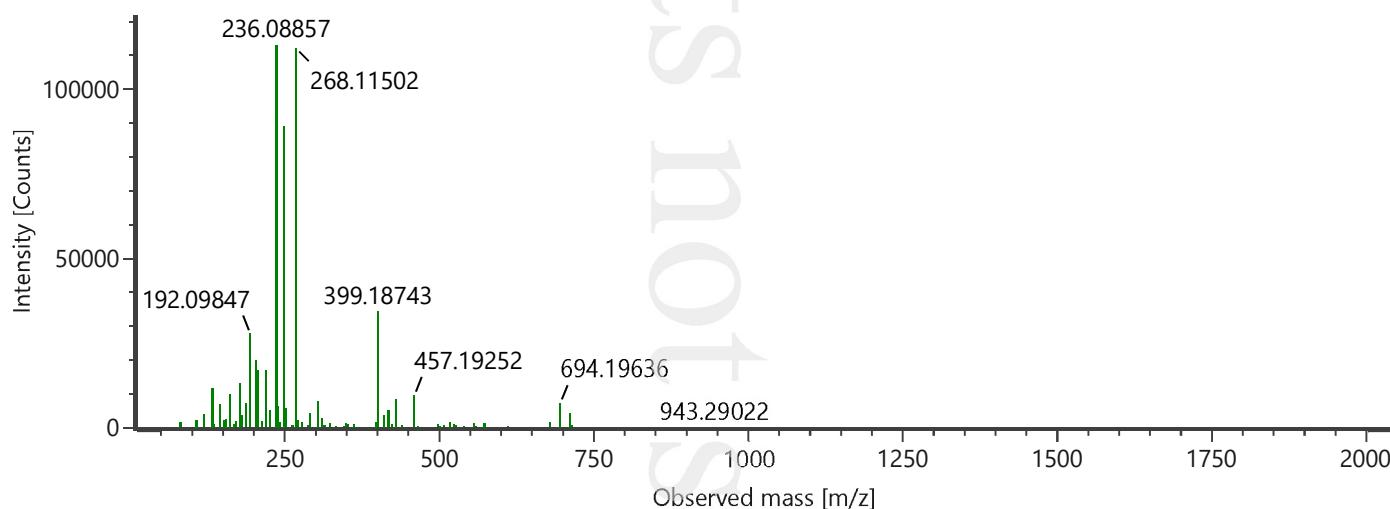
Item description:



Item name: int1_a2 ACN

Channel name: High energy : Time 0.8043 +/- 0.0588 minutes

Item description:



Component name: MP3.mol

Component name: MP3.mol

| . | Item name | Sample position | Replicate number | Component name | Identification status | Neutral mass (Da) | Observed neutral mass (Da) |
|---|-------------|-----------------|------------------|----------------|-----------------------|-------------------|----------------------------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP3.mol | Identified | 249.09701 | 249.0968 |

| . | Item name | Sample position | Replicate number | Component name | Identification status | Observed m/z | Mass error (mDa) |
|---|-------------|-----------------|------------------|----------------|-----------------------|--------------|------------------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP3.mol | Identified | 250.1041 | -0.2 |

Item name: MD_M POPLAWSKI

Created time: 13:57:06 GMT Daylight Time

| . | Item name | Sample position | Replicate number | Component name | Identification status | Mass error (ppm) | Expected RT (min) | Observed RT (min) |
|---|-------------|-----------------|------------------|----------------|-----------------------|------------------|-------------------|-------------------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP3.mol | Identified | -0.9 | | 0.79 |

| . | Item name | Sample position | Replicate number | Component name | Identification status | Detector counts | Response | Adducts |
|---|-------------|-----------------|------------------|----------------|-----------------------|-----------------|----------|---------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP3.mol | Identified | 19765 | 17906 | +H |

Component name: MP3.mol

| . | Item name | Sample position | Replicate number | Component name | Identification status | Neutral mass (Da) | Observed neutral mass (Da) |
|---|-------------|-----------------|------------------|----------------|-----------------------|-------------------|----------------------------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP3.mol | Identified | 249.09701 | 249.0962 |

| . | Item name | Sample position | Replicate number | Component name | Identification status | Observed m/z | Mass error (mDa) |
|---|-------------|-----------------|------------------|----------------|-----------------------|--------------|------------------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP3.mol | Identified | 250.1034 | -0.8 |

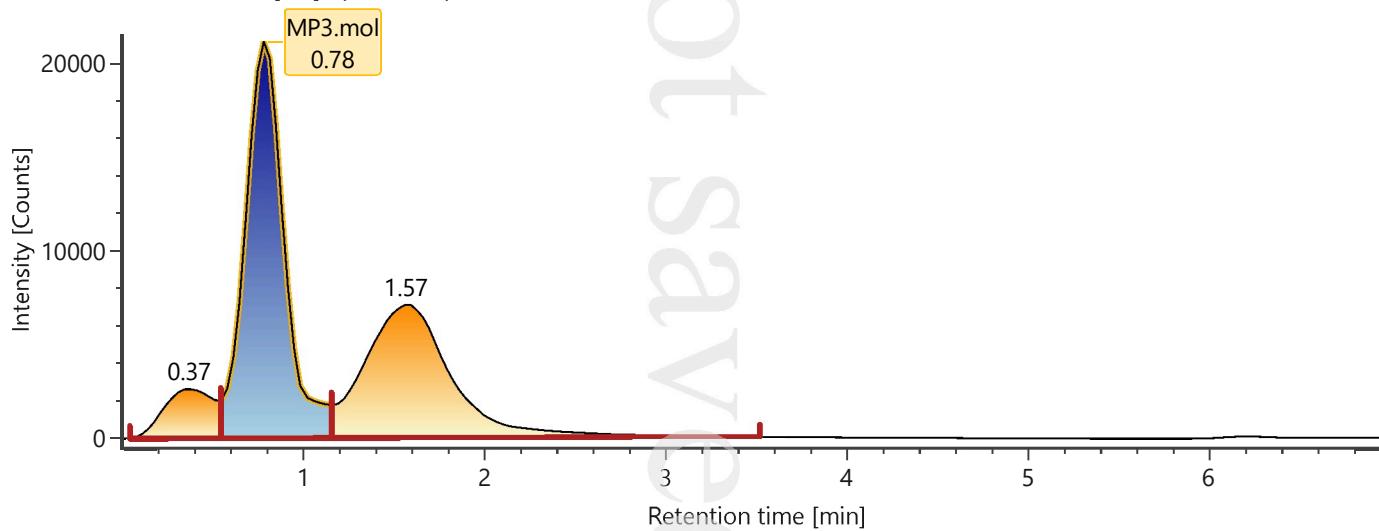
| . | Item name | Sample position | Replicate number | Component name | Identification status | Mass error (ppm) | Expected RT (min) | Observed RT (min) |
|---|-------------|-----------------|------------------|----------------|-----------------------|------------------|-------------------|-------------------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP3.mol | Identified | -3.4 | | 1.64 |

| . | Item name | Sample position | Replicate number | Component name | Identification status | Detector counts | Response | Adducts |
|---|-------------|-----------------|------------------|----------------|-----------------------|-----------------|----------|---------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP3.mol | Identified | 13101 | 12427 | +H |

Item name: int1_a2 ACN

Item name: int1_a2 ACN

Channel name: MP3.mol [+H] : (35.9 PPM) 250.1041



Item name: MD_M POPLAWSKI

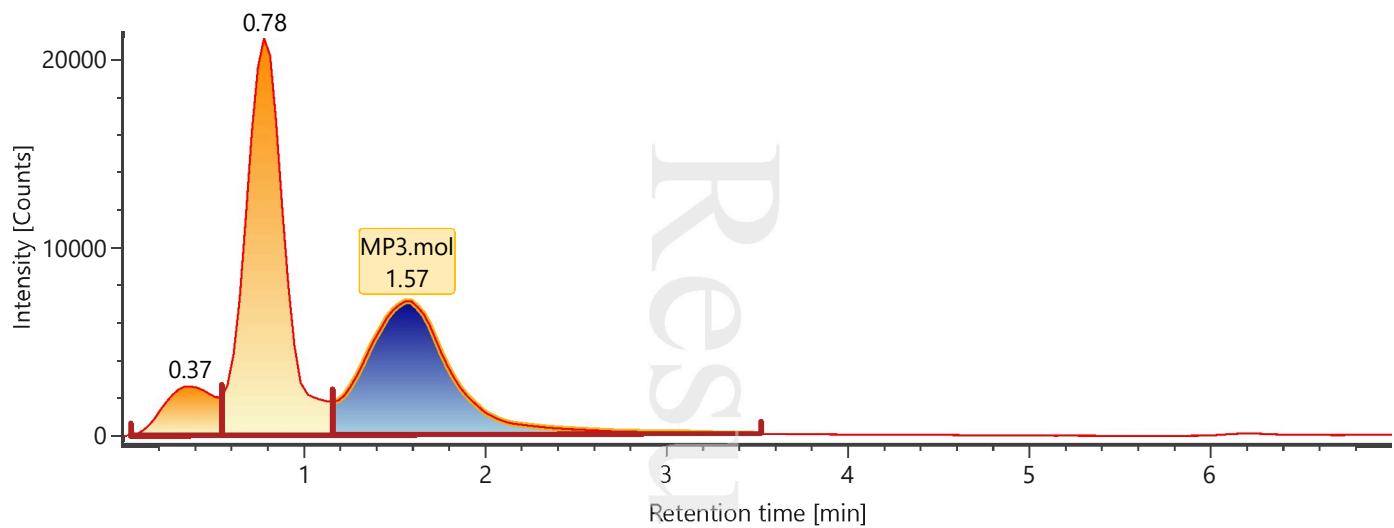
Created by: Chemistry, Chemistry

Created on: Sep 07, 2023

Created time: 13:57:06 GMT Daylight Time

Item name: int1_a2 ACN

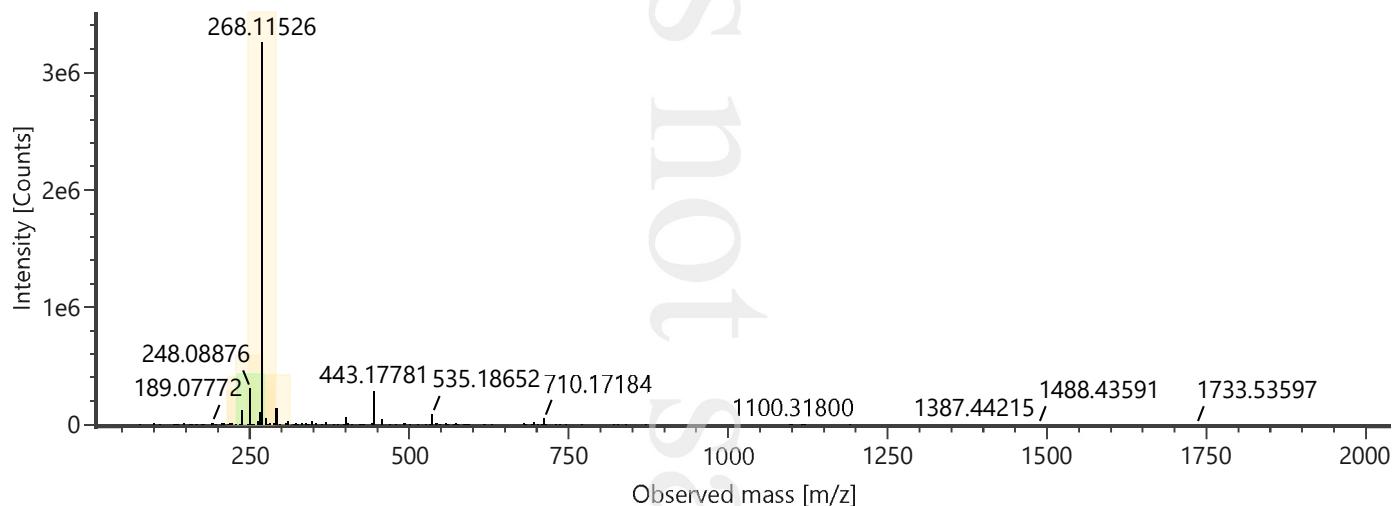
Channel name: MP3.mol [+H] : (35.9 PPM) 250.1034



Item name: int1_a2 ACN

Item description:

Channel name: Low energy : Time 0.7904 +/- 0.0588 minutes



Item name: MD_M POPLAWSKI

Created by: Chemistry, Chemistry

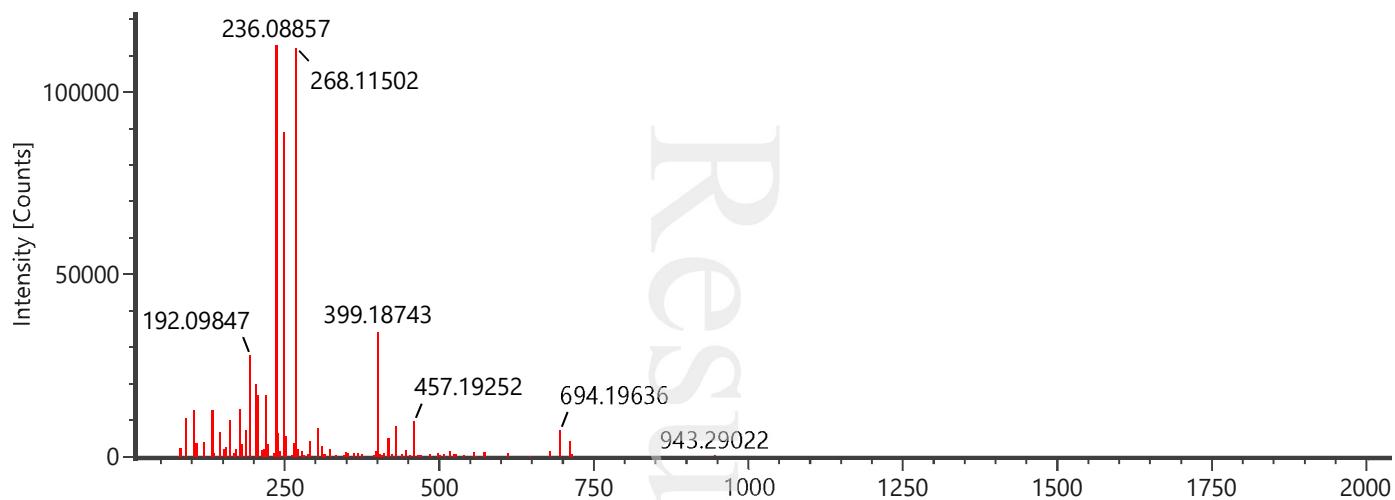
Created on: Sep 07, 2023

Created time: 13:57:06 GMT Daylight Time

Item name: int1_a2 ACN

Channel name: High energy : Time 0.7904 +/- 0.0588 minutes

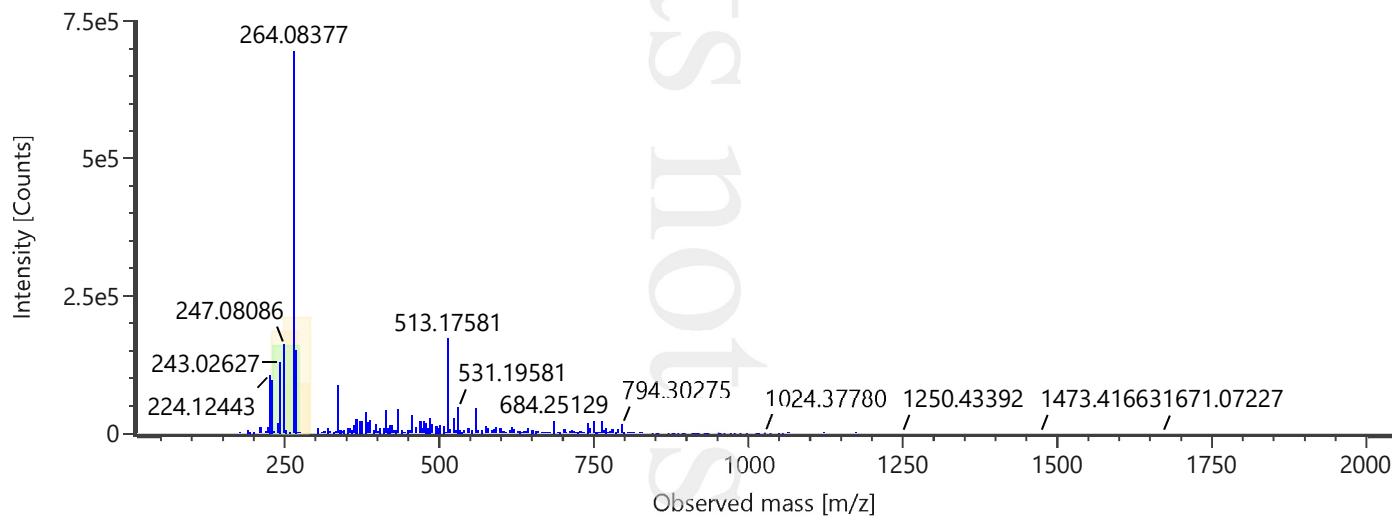
Item description:



Item name: int1_a2 ACN

Channel name: Low energy : Time 1.6422 +/- 0.0588 minutes

Item description:



Item name: MD_M POPLAWSKI

Created by: Chemistry, Chemistry

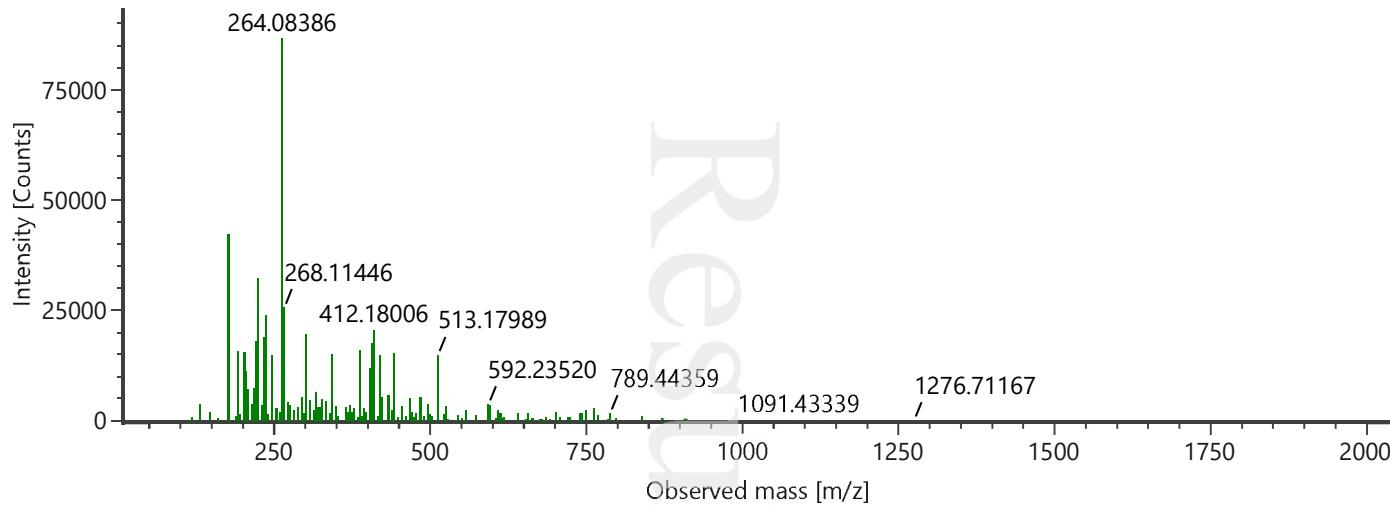
Created on: Sep 07, 2023

Created time: 13:57:06 GMT Daylight Time

Item name: int1_a2 ACN

Channel name: High energy : Time 1.6422 +/- 0.0588 minutes

Item description:



Component name: MP4.mol

Component name: MP4.mol

| . | Item name | Sample position | Replicate number | Component name | Identification status | Neutral mass (Da) | Observed neutral mass (Da) |
|---|-------------|-----------------|------------------|----------------|-----------------------|-------------------|----------------------------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP4.mol | Identified | 248.08919 | 248.0886 |

| . | Item name | Sample position | Replicate number | Component name | Identification status | Observed m/z | Mass error (mDa) |
|---|-------------|-----------------|------------------|----------------|-----------------------|--------------|------------------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP4.mol | Identified | 248.0880 | -0.6 |

| . | Item name | Sample position | Replicate number | Component name | Identification status | Mass error (ppm) | Expected RT (min) | Observed RT (min) |
|---|-------------|-----------------|------------------|----------------|-----------------------|------------------|-------------------|-------------------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP4.mol | Identified | -2.4 | | 0.28 |

| . | Item name | Sample position | Replicate number | Component name | Identification status | Detector counts | Response | Adducts |
|---|-------------|-----------------|------------------|----------------|-----------------------|-----------------|----------|---------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP4.mol | Identified | 4148 | 4148 | -e |

Component name: MP4.mol

| . | Item name | Sample position | Replicate number | Component name | Identification status | Neutral mass (Da) | Observed neutral mass (Da) |
|---|-------------|-----------------|------------------|----------------|-----------------------|-------------------|----------------------------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP4.mol | Identified | 248.08919 | 248.0885 |

| . | Item name | Sample position | Replicate number | Component name | Identification status | Observed m/z | Mass error (mDa) |
|---|-------------|-----------------|------------------|----------------|-----------------------|--------------|------------------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP4.mol | Identified | 248.0880 | -0.6 |

| . | Item name | Sample position | Replicate number | Component name | Identification status | Mass error (ppm) | Expected RT (min) | Observed RT (min) |
|---|-------------|-----------------|------------------|----------------|-----------------------|------------------|-------------------|-------------------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP4.mol | Identified | -2.6 | | 1.69 |

Item name: MD_M POPLAWSKI

Created time: 13:57:06 GMT Daylight Time

| . | Item name | Sample position | Replicate number | Component name | Identification status | Detector counts | Response | Adducts |
|---|-------------|-----------------|------------------|----------------|-----------------------|-----------------|----------|---------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP4.mol | Identified | 15395 | 15395 | -e |

Component name: MP4.mol

| . | Item name | Sample position | Replicate number | Component name | Identification status | Neutral mass (Da) | Observed neutral mass (Da) |
|---|-------------|-----------------|------------------|----------------|-----------------------|-------------------|----------------------------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP4.mol | Identified | 248.08919 | 248.0893 |

| . | Item name | Sample position | Replicate number | Component name | Identification status | Observed m/z | Mass error (mDa) |
|---|-------------|-----------------|------------------|----------------|-----------------------|--------------|------------------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP4.mol | Identified | 248.0888 | 0.1 |

| . | Item name | Sample position | Replicate number | Component name | Identification status | Mass error (ppm) | Expected RT (min) | Observed RT (min) |
|---|-------------|-----------------|------------------|----------------|-----------------------|------------------|-------------------|-------------------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP4.mol | Identified | 0.5 | | 0.82 |

| . | Item name | Sample position | Replicate number | Component name | Identification status | Detector counts | Response | Adducts |
|---|-------------|-----------------|------------------|----------------|-----------------------|-----------------|----------|---------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP4.mol | Identified | 41436 | 37995 | -e |

Component name: MP4.mol

| . | Item name | Sample position | Replicate number | Component name | Identification status | Neutral mass (Da) | Observed neutral mass (Da) |
|---|-------------|-----------------|------------------|----------------|-----------------------|-------------------|----------------------------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP4.mol | Identified | 248.08919 | 248.0887 |

| . | Item name | Sample position | Replicate number | Component name | Identification status | Observed m/z | Mass error (mDa) |
|---|-------------|-----------------|------------------|----------------|-----------------------|--------------|------------------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP4.mol | Identified | 248.0881 | -0.5 |

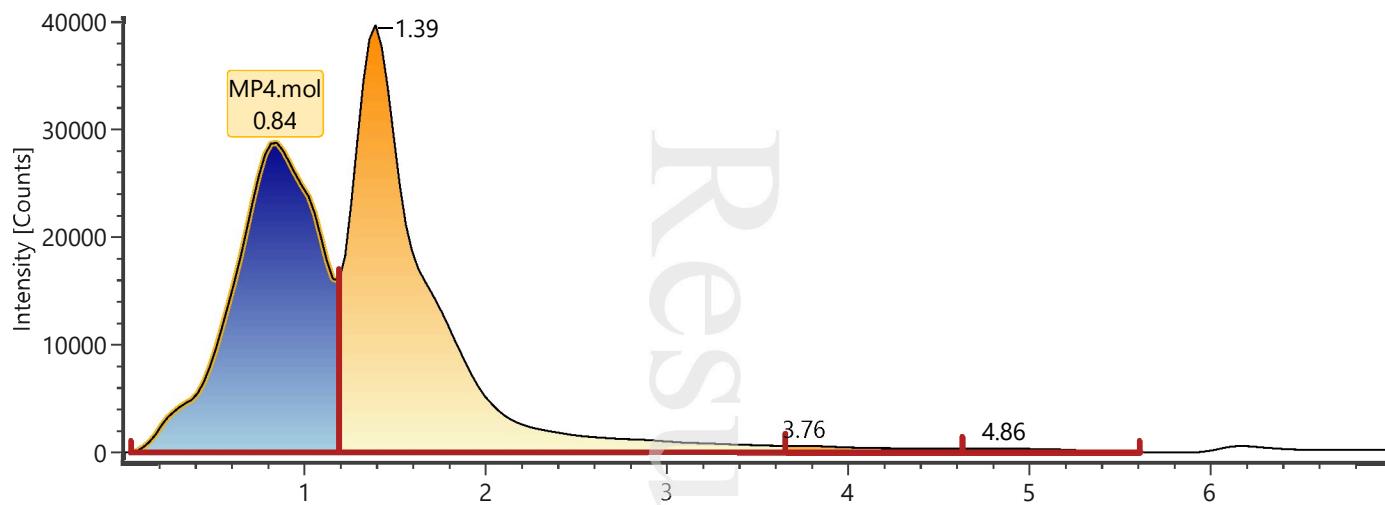
| . | Item name | Sample position | Replicate number | Component name | Identification status | Mass error (ppm) | Expected RT (min) | Observed RT (min) |
|---|-------------|-----------------|------------------|----------------|-----------------------|------------------|-------------------|-------------------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP4.mol | Identified | -2.1 | | 1.39 |

| . | Item name | Sample position | Replicate number | Component name | Identification status | Detector counts | Response | Adducts |
|---|-------------|-----------------|------------------|----------------|-----------------------|-----------------|----------|---------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP4.mol | Identified | 71486 | 63150 | -e |

Item name: int1_a2 ACN

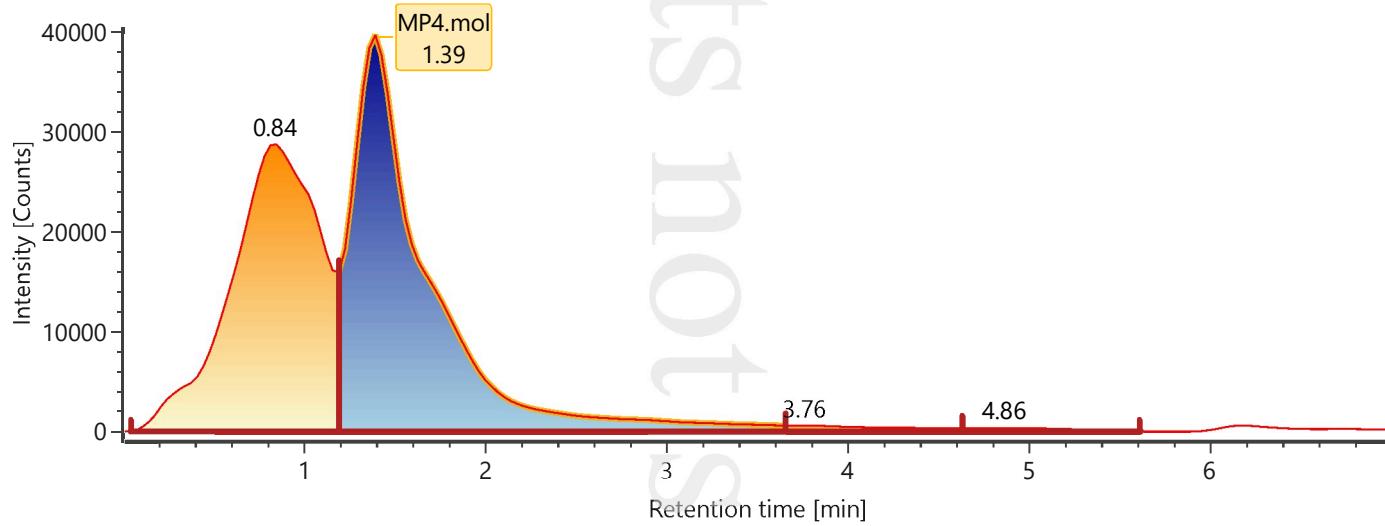
Item name: int1_a2 ACN

Channel name: MP4.mol [-e] : (35.9 PPM) 248.0880



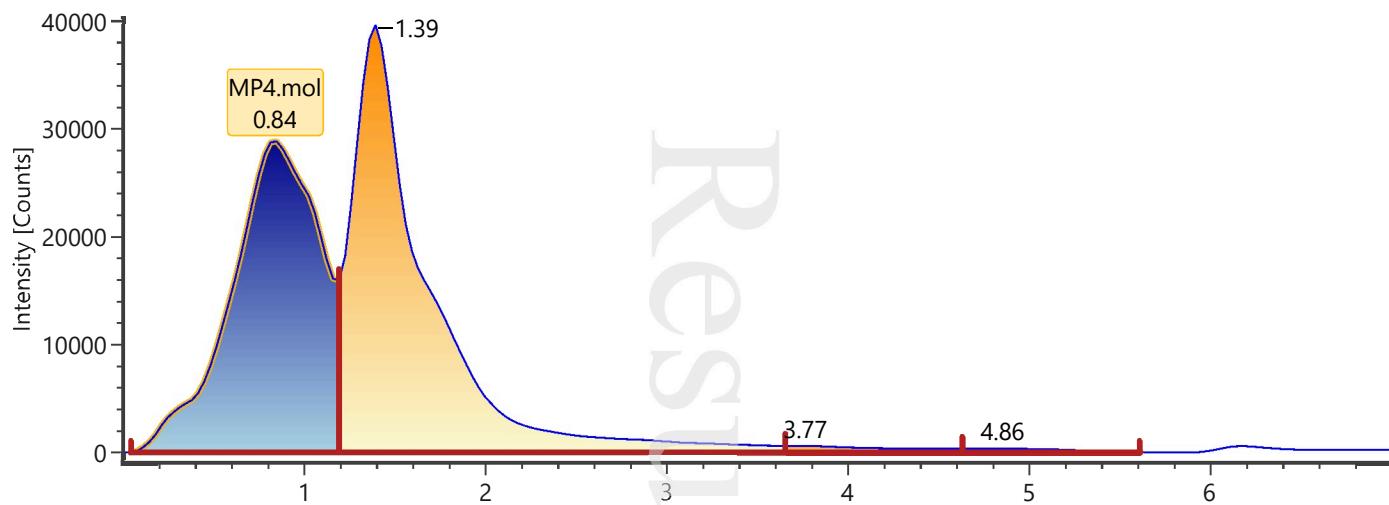
Item name: int1_a2 ACN

Channel name: MP4.mol [-e] : (35.9 PPM) 248.0880



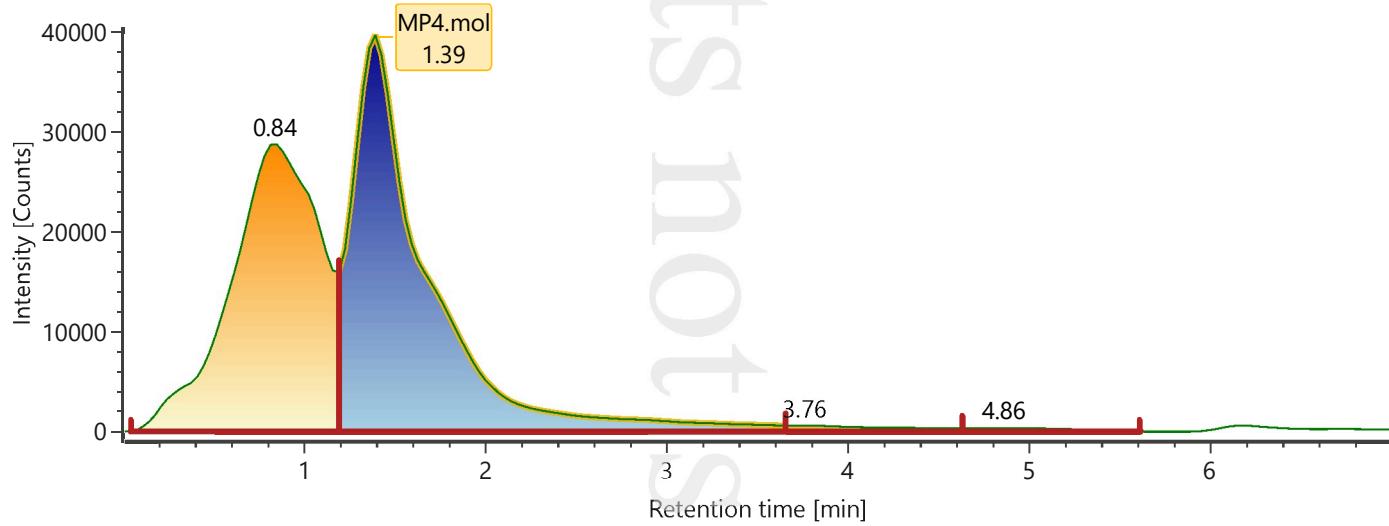
Item name: int1_a2 ACN

Channel name: MP4.mol [-e] : (35.9 PPM) 248.0888



Item name: int1_a2 ACN

Channel name: MP4.mol [-e] : (35.9 PPM) 248.0881



Item name: MD_M POPLAWSKI

Created by: Chemistry, Chemistry

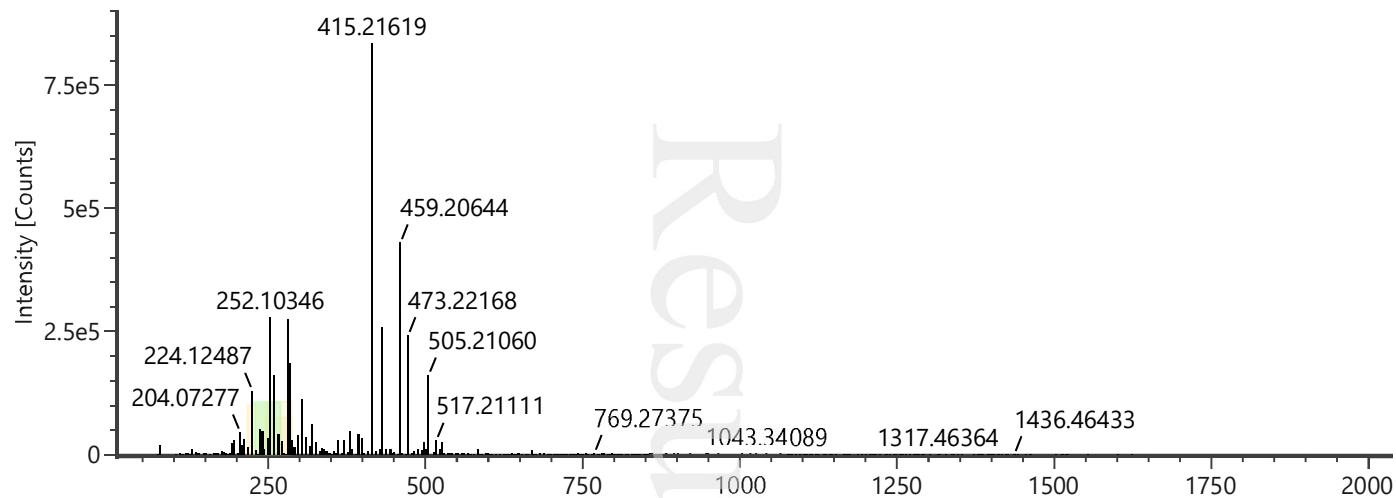
Created on: Sep 07, 2023

Created time: 13:57:06 GMT Daylight Time

Item name: int1_a2 ACN

Channel name: Low energy : Time 0.2818 +/- 0.0588 minutes

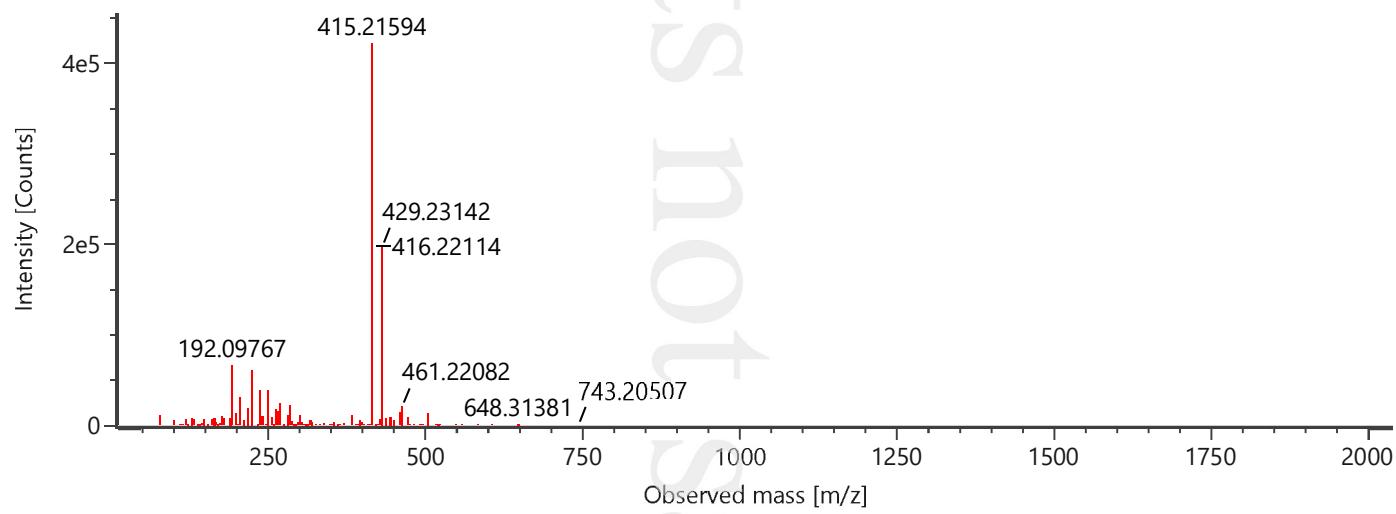
Item description:



Item name: int1_a2 ACN

Channel name: High energy : Time 0.2818 +/- 0.0588 minutes

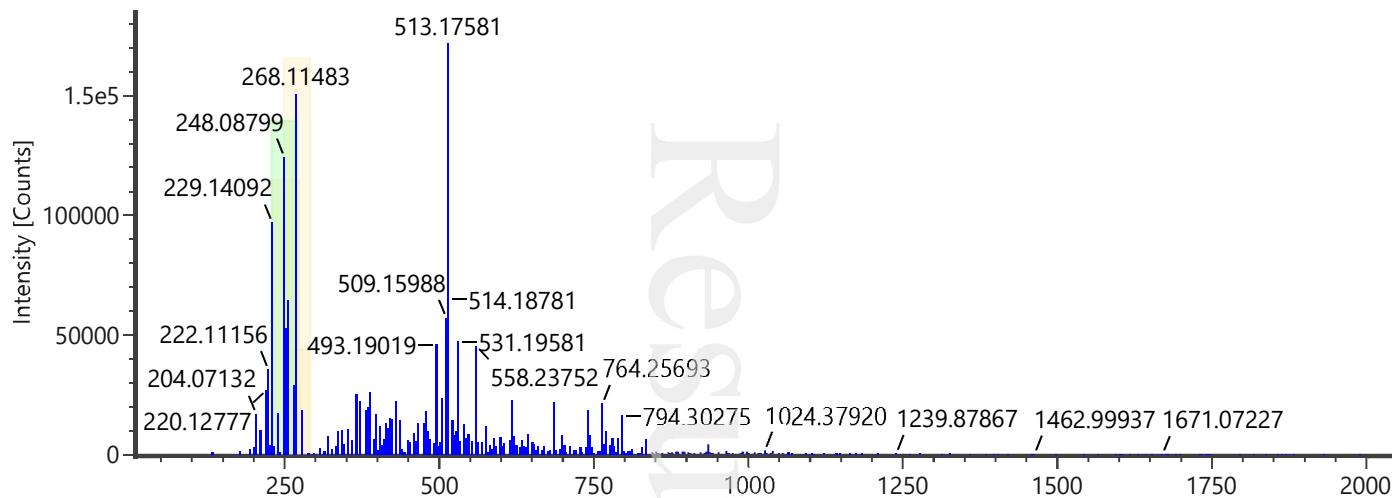
Item description:



Item name: int1_a2 ACN

Channel name: Low energy : Time 1.6908 +/- 0.0588 minutes

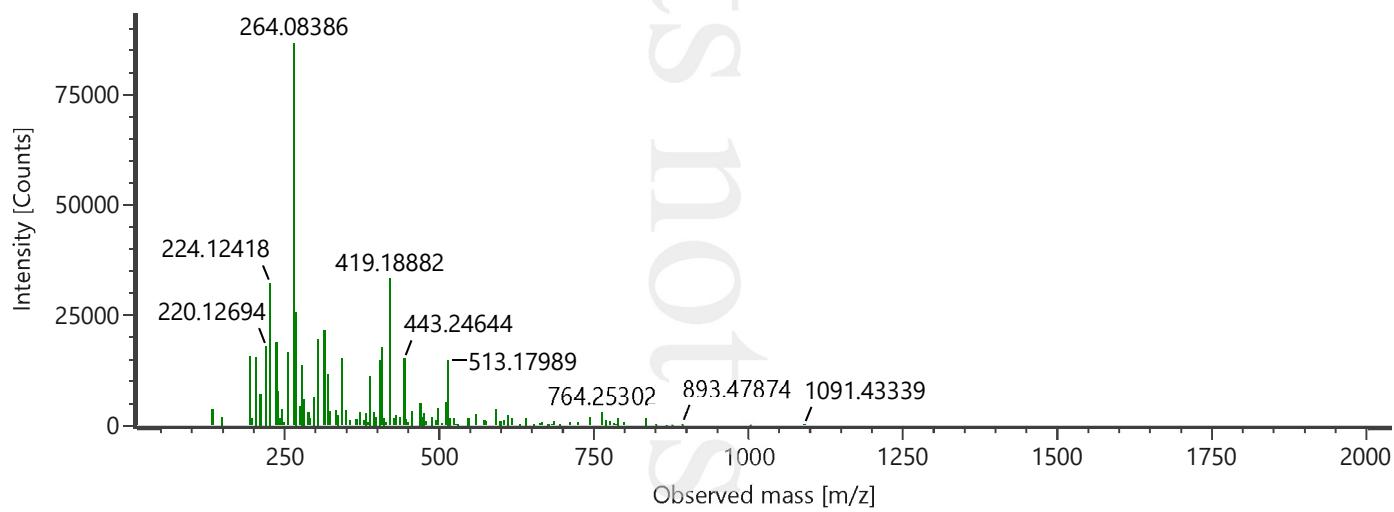
Item description:



Item name: int1_a2 ACN

Channel name: High energy : Time 1.6908 +/- 0.0588 minutes

Item description:



Item name: MD_M POPLAWSKI

Created by: Chemistry, Chemistry

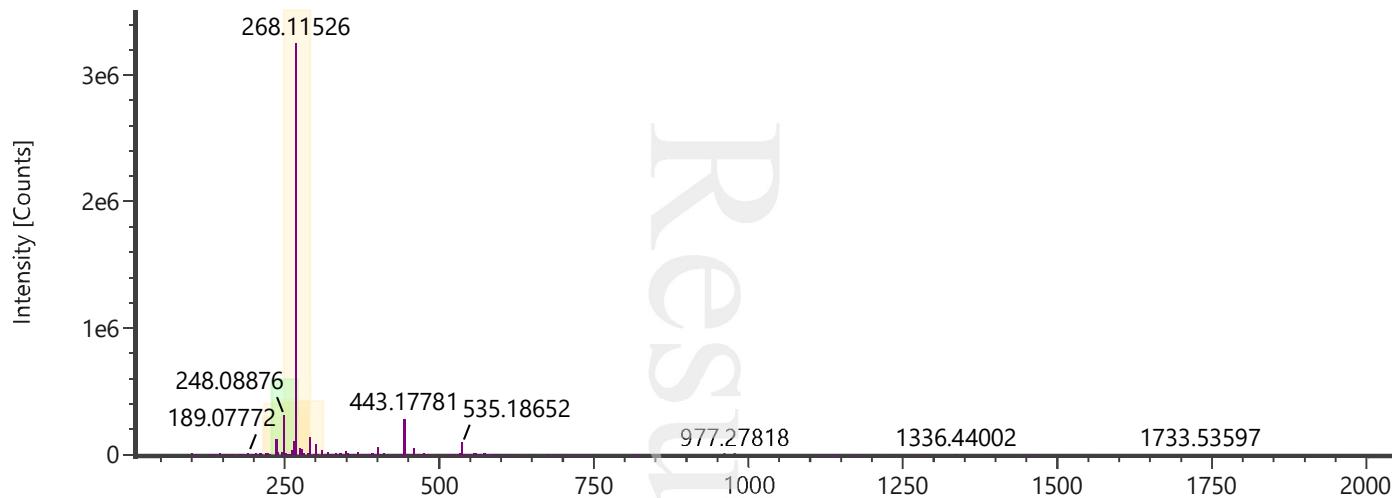
Created on: Sep 07, 2023

Created time: 13:57:06 GMT Daylight Time

Item name: int1_a2 ACN

Channel name: Low energy : Time 0.8187 +/- 0.0588 minutes

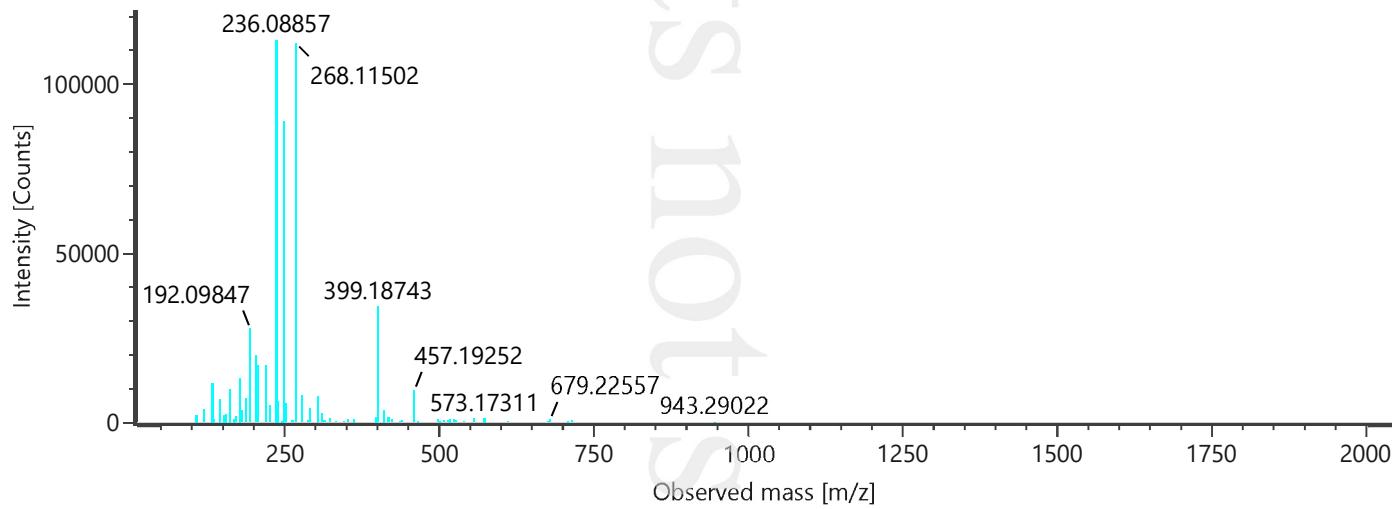
Item description:



Item name: int1_a2 ACN

Channel name: High energy : Time 0.8187 +/- 0.0588 minutes

Item description:



Item name: MD_M POPLAWSKI

Created by: Chemistry, Chemistry

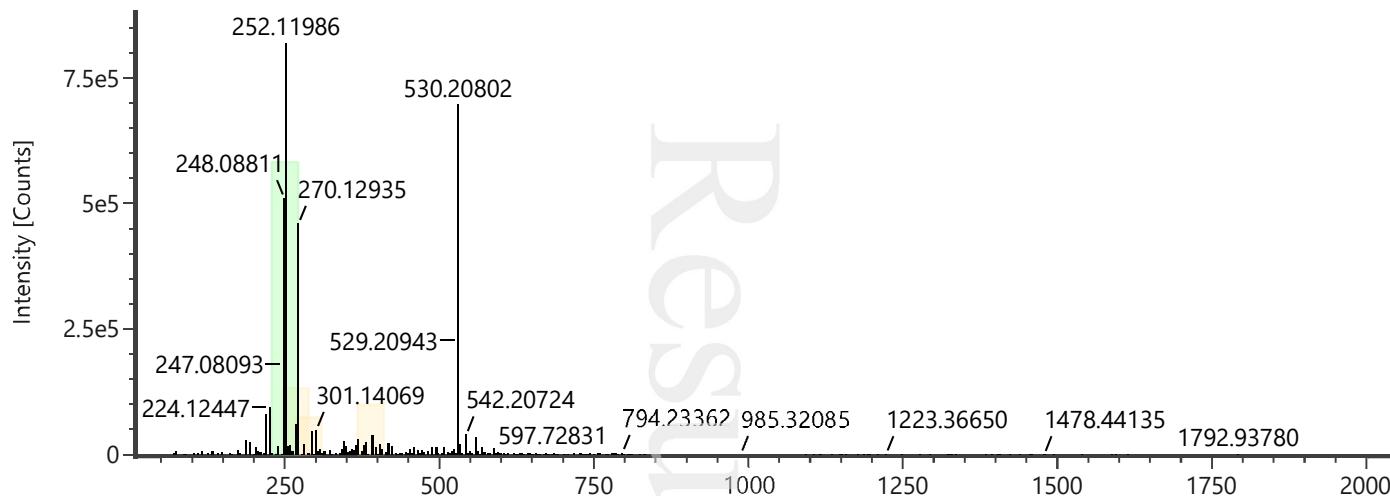
Created on: Sep 07, 2023

Created time: 13:57:06 GMT Daylight Time

Item name: int1_a2 ACN

Channel name: Low energy : Time 1.3922 +/- 0.0588 minutes

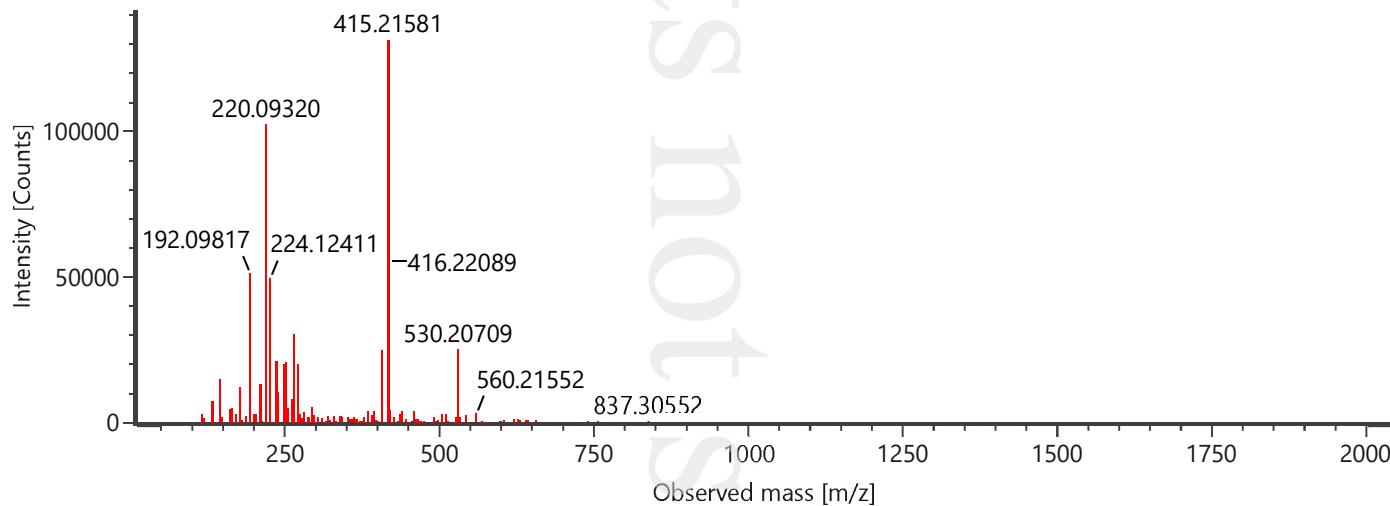
Item description:



Item name: int1_a2 ACN

Channel name: High energy : Time 1.3922 +/- 0.0588 minutes

Item description:



Component name: MP5.mol

Component name: MP5.mol

| . | Item name | Sample position | Replicate number | Component name | Identification status | Neutral mass (Da) | Observed neutral mass (Da) |
|---|-------------|-----------------|------------------|----------------|-----------------------|-------------------|----------------------------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP5.mol | Identified | 235.08136 | 235.0815 |

| . | Item name | Sample position | Replicate number | Component name | Identification status | Observed m/z | Mass error (mDa) |
|---|-------------|-----------------|------------------|----------------|-----------------------|--------------|------------------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP5.mol | Identified | 236.0888 | 0.2 |

Item name: MD_M POPLAWSKI

Created time: 13:57:06 GMT Daylight Time

| . | Item name | Sample position | Replicate number | Component name | Identification status | Mass error (ppm) | Expected RT (min) | Observed RT (min) |
|---|-------------|-----------------|------------------|----------------|-----------------------|------------------|-------------------|-------------------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP5.mol | Identified | 0.8 | | 0.79 |

| . | Item name | Sample position | Replicate number | Component name | Identification status | Detector counts | Response | Adducts |
|---|-------------|-----------------|------------------|----------------|-----------------------|-----------------|----------|---------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP5.mol | Identified | 15305 | 14560 | +H, -e |

Component name: MP5.mol

| . | Item name | Sample position | Replicate number | Component name | Identification status | Neutral mass (Da) | Observed neutral mass (Da) |
|---|-------------|-----------------|------------------|----------------|-----------------------|-------------------|----------------------------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP5.mol | Identified | 235.08136 | 235.0811 |

| . | Item name | Sample position | Replicate number | Component name | Identification status | Observed m/z | Mass error (mDa) |
|---|-------------|-----------------|------------------|----------------|-----------------------|--------------|------------------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP5.mol | Identified | 236.0884 | -0.2 |

| . | Item name | Sample position | Replicate number | Component name | Identification status | Mass error (ppm) | Expected RT (min) | Observed RT (min) |
|---|-------------|-----------------|------------------|----------------|-----------------------|------------------|-------------------|-------------------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP5.mol | Identified | -1.0 | | 1.53 |

| . | Item name | Sample position | Replicate number | Component name | Identification status | Detector counts | Response | Adducts |
|---|-------------|-----------------|------------------|----------------|-----------------------|-----------------|----------|---------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP5.mol | Identified | 4230 | 4230 | +H |

Component name: MP5.mol

| . | Item name | Sample position | Replicate number | Component name | Identification status | Neutral mass (Da) | Observed neutral mass (Da) |
|---|-------------|-----------------|------------------|----------------|-----------------------|-------------------|----------------------------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP5.mol | Identified | 235.08136 | 235.0812 |

| . | Item name | Sample position | Replicate number | Component name | Identification status | Observed m/z | Mass error (mDa) |
|---|-------------|-----------------|------------------|----------------|-----------------------|--------------|------------------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP5.mol | Identified | 236.0885 | -0.2 |

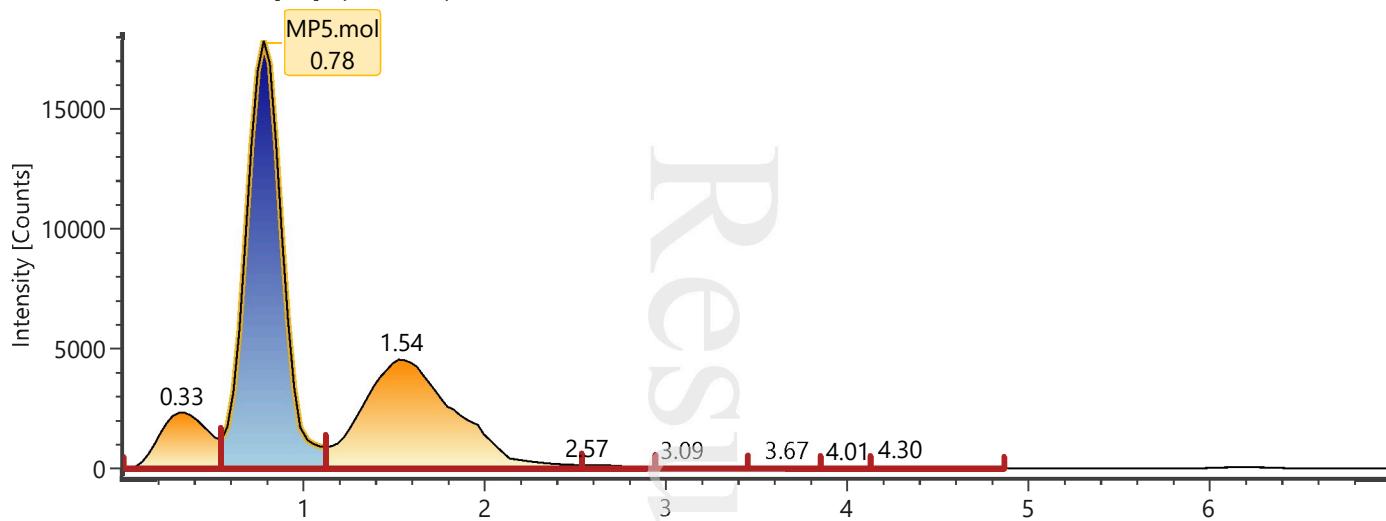
| . | Item name | Sample position | Replicate number | Component name | Identification status | Mass error (ppm) | Expected RT (min) | Observed RT (min) |
|---|-------------|-----------------|------------------|----------------|-----------------------|------------------|-------------------|-------------------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP5.mol | Identified | -0.8 | | 0.29 |

| . | Item name | Sample position | Replicate number | Component name | Identification status | Detector counts | Response | Adducts |
|---|-------------|-----------------|------------------|----------------|-----------------------|-----------------|----------|---------|
| 1 | int1_a2 ACN | 2:A,7 | 1 | MP5.mol | Identified | 3955 | 3206 | +H |

Item name: int1_a2 ACN

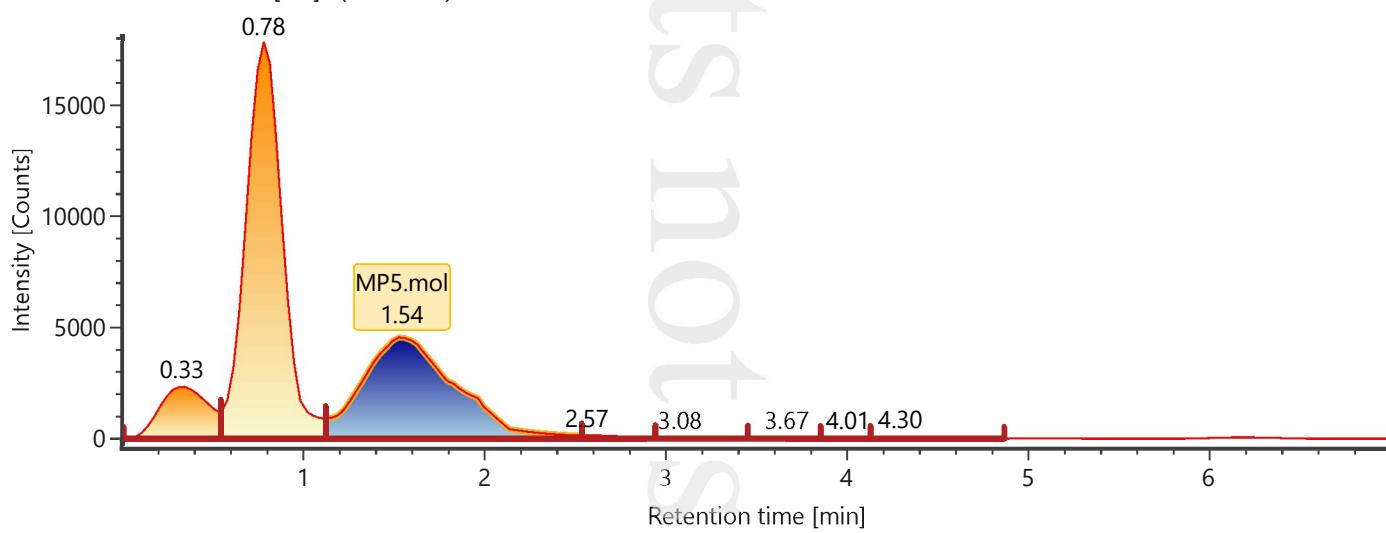
Item name: int1_a2 ACN

Channel name: MP5.mol [+H] : (35.9 PPM) 236.0888



Item name: int1_a2 ACN

Channel name: MP5.mol [+H] : (35.9 PPM) 236.0884



Item name: MD_M POPLAWSKI

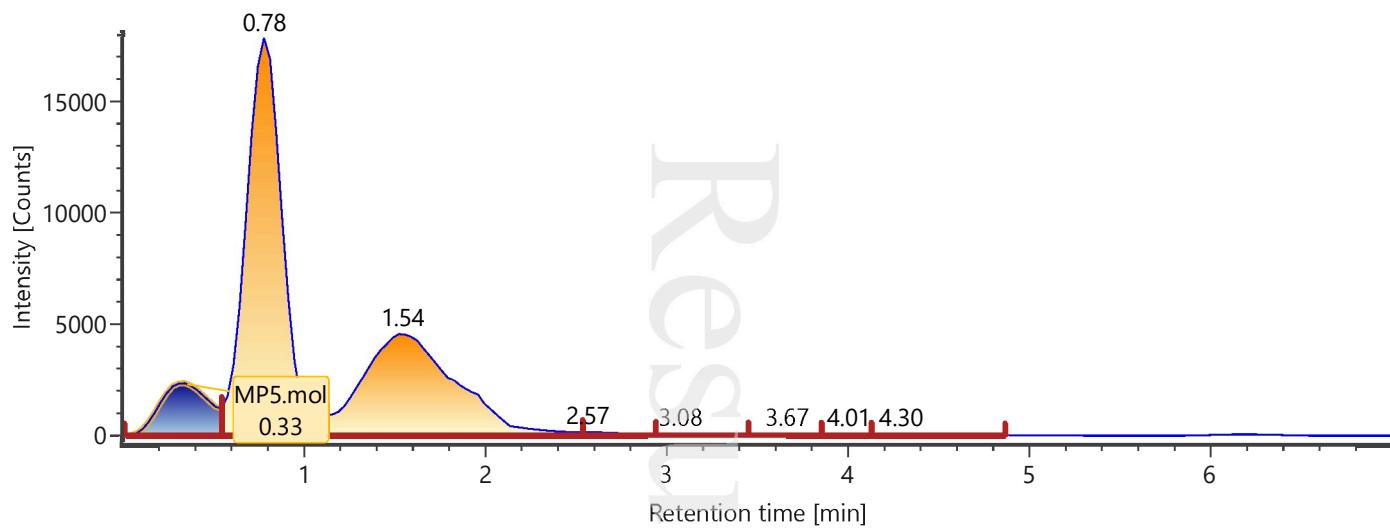
Created by: Chemistry, Chemistry

Created on: Sep 07, 2023

Created time: 13:57:06 GMT Daylight Time

Item name: int1_a2 ACN

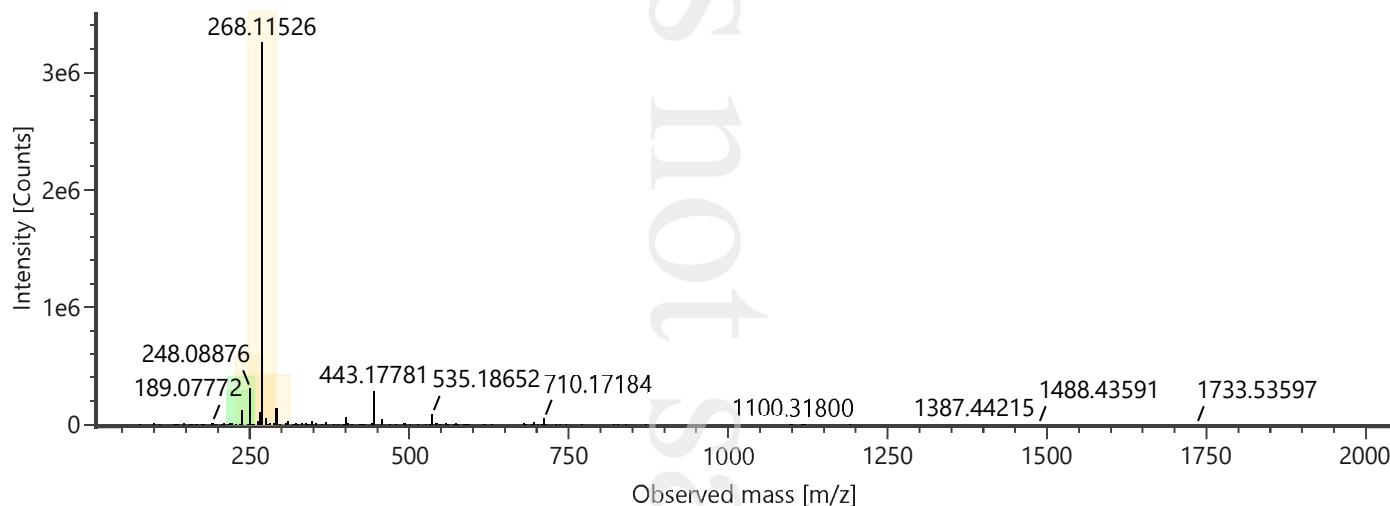
Channel name: MP5.mol [+H] : (35.9 PPM) 236.0885



Item name: int1_a2 ACN

Item description:

Channel name: Low energy : Time 0.7891 +/- 0.0588 minutes



Item name: MD_M POPLAWSKI

Created by: Chemistry, Chemistry

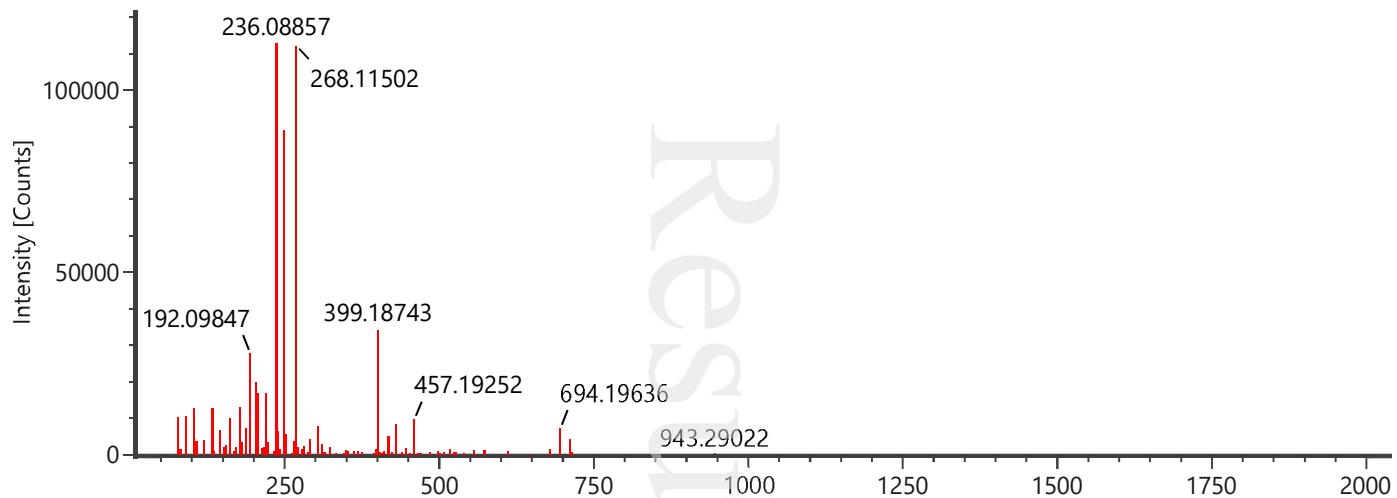
Created on: Sep 07, 2023

Created time: 13:57:06 GMT Daylight Time

Item name: int1_a2 ACN

Channel name: High energy : Time 0.7891 +/- 0.0588 minutes

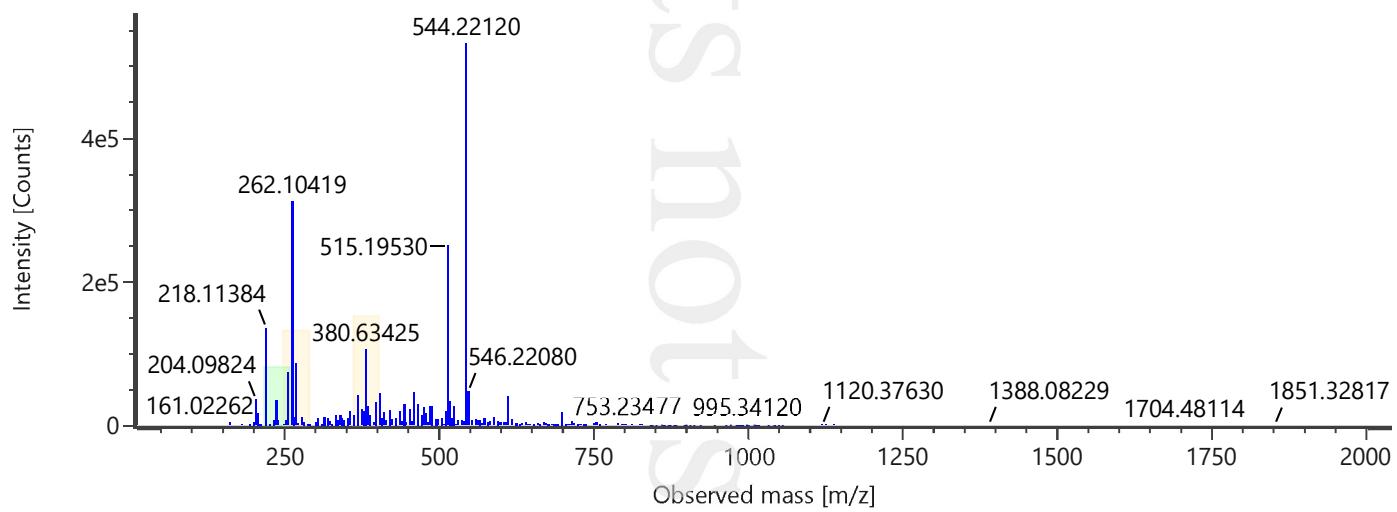
Item description:



Item name: int1_a2 ACN

Channel name: Low energy : Time 1.5309 +/- 0.0588 minutes

Item description:



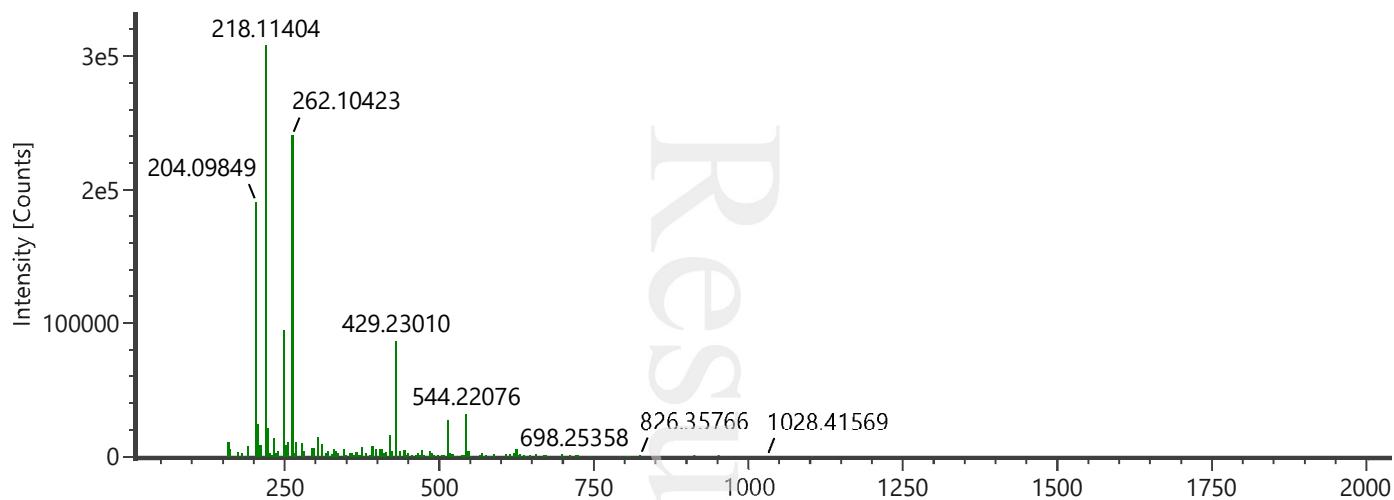
Item name: MD_M POPLAWSKI

Created time: 13:57:06 GMT Daylight Time

Item name: int1_a2 ACN

Channel name: High energy : Time 1.5309 +/- 0.0588 minutes

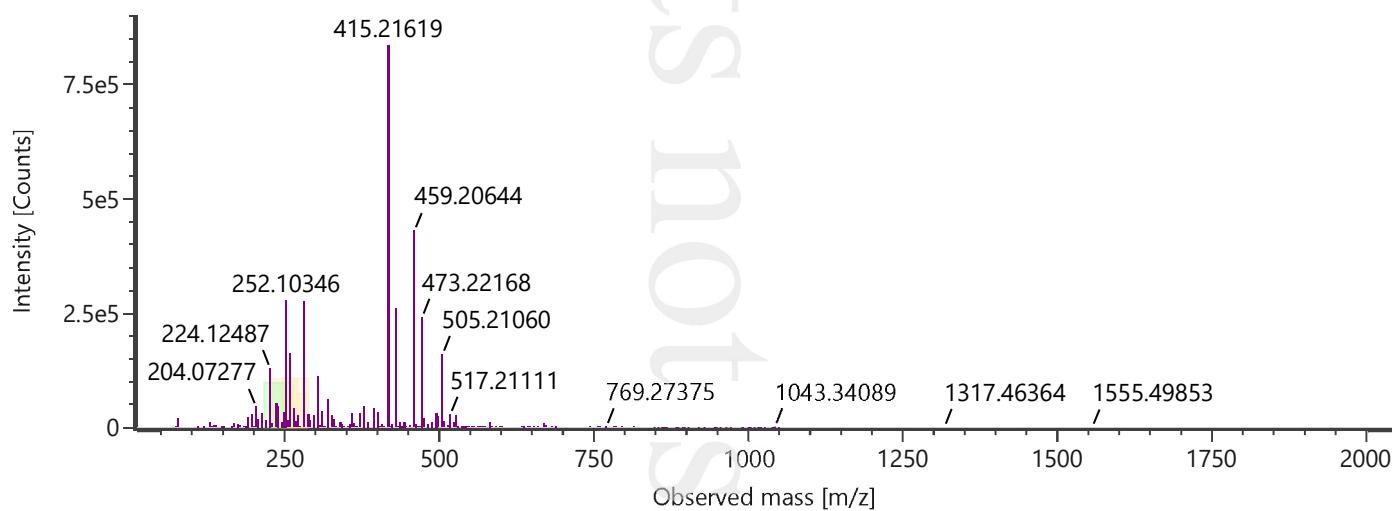
Item description:



Item name: int1_a2 ACN

Channel name: Low energy : Time 0.2852 +/- 0.0588 minutes

Item description:



Item name: MD_M POPLAWSKI

Created by: Chemistry, Chemistry

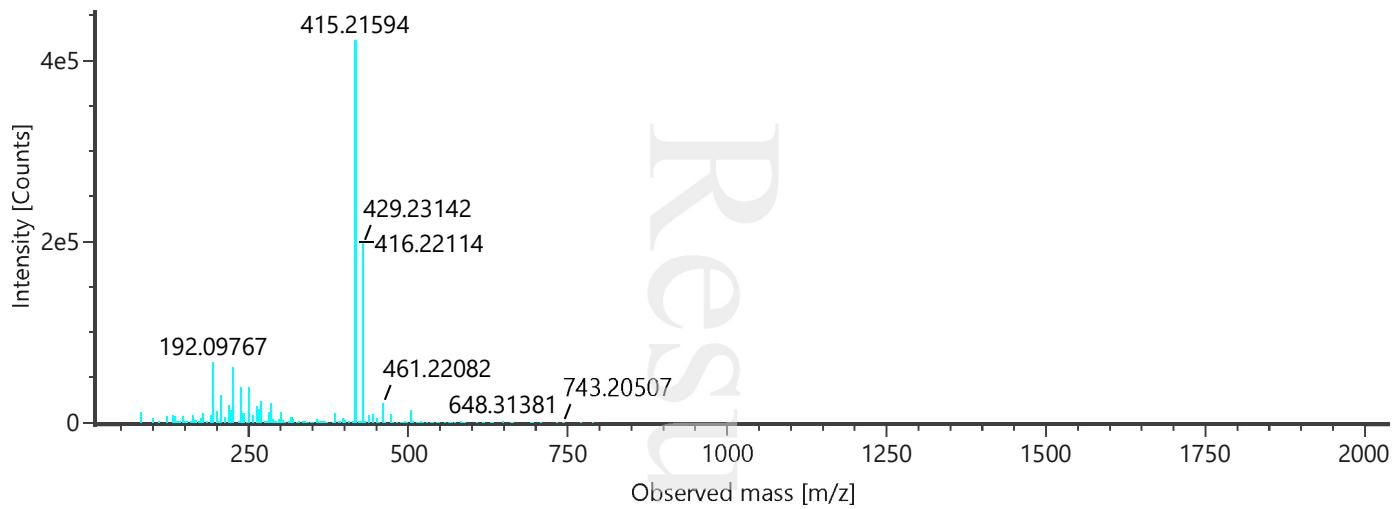
Created on: Sep 07, 2023

Created time: 13:57:06 GMT Daylight Time

Item name: int1_a2 ACN

Channel name: High energy : Time 0.2852 +/- 0.0588 minutes

Item description:



Item name: MD_M POPLAWSKI

Created by: Chemistry, Chemistry

Created on: Sep 07, 2023

Created time: 13:57:06 GMT Daylight Time

Report Log

Template Report

Report Template "Untitled" has not been saved.

Results not saved