

Item name: MD_M POPLAWSKI

Created by: Chemistry, Chemistry

Created on: Sep 07, 2023

Created time: 13:59:44 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_a3 ACN		Unknown	1	2:A,8	3.00	Complete	No Checks Performed

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Created time: 13:59:44 GMT Daylight Time

Component name: MP11B.mol

Component name: MP11B.mol

.	Item name	Sample position	Replicate number	Component name	Identification status	Neutral mass (Da)	Observed neutral mass (Da)
1	int1_a3 ACN	2:A,8	1	MP11B.mol	Identified	756.22705	756.2257

.	Item name	Sample position	Replicate number	Component name	Identification status	Observed m/z	Mass error (mDa)
1	int1_a3 ACN	2:A,8	1	MP11B.mol	Identified	379.1201	-1.3

.	Item name	Sample position	Replicate number	Component name	Identification status	Mass error (ppm)	Expected RT (min)	Observed RT (min)
1	int1_a3 ACN	2:A,8	1	MP11B.mol	Identified	-1.8		1.52

.	Item name	Sample position	Replicate number	Component name	Identification status	Detector counts	Response	Adducts
1	int1_a3 ACN	2:A,8	1	MP11B.mol	Identified	15276	15276	2x(+H)

.	Item name	Sample position	Replicate number	Component name	Identification status	Formula
1	int1_a3 ACN	2:A,8	1	MP11B.mol	Identified	C36[13C]3H35N3O13

Component name: MP11B.mol

.	Item name	Sample position	Replicate number	Component name	Identification status	Neutral mass (Da)	Observed neutral mass (Da)
1	int1_a3 ACN	2:A,8	1	MP11B.mol	Identified	756.22705	756.2272

.	Item name	Sample position	Replicate number	Component name	Identification status	Observed m/z	Mass error (mDa)
1	int1_a3 ACN	2:A,8	1	MP11B.mol	Identified	378.1130	0.1

.	Item name	Sample position	Replicate number	Component name	Identification status	Mass error (ppm)	Expected RT (min)	Observed RT (min)
1	int1_a3 ACN	2:A,8	1	MP11B.mol	Identified	0.2		1.72

.	Item name	Sample position	Replicate number	Component name	Identification status	Detector counts	Response	Adducts
1	int1_a3 ACN	2:A,8	1	MP11B.mol	Identified	20287	14146	2x(-e)

.	Item name	Sample position	Replicate number	Component name	Identification status	Formula
1	int1_a3 ACN	2:A,8	1	MP11B.mol	Identified	C36[13C]3H35N3O13

Item name: int1_a3 ACN

Item name: MD_M POPLAWSKI

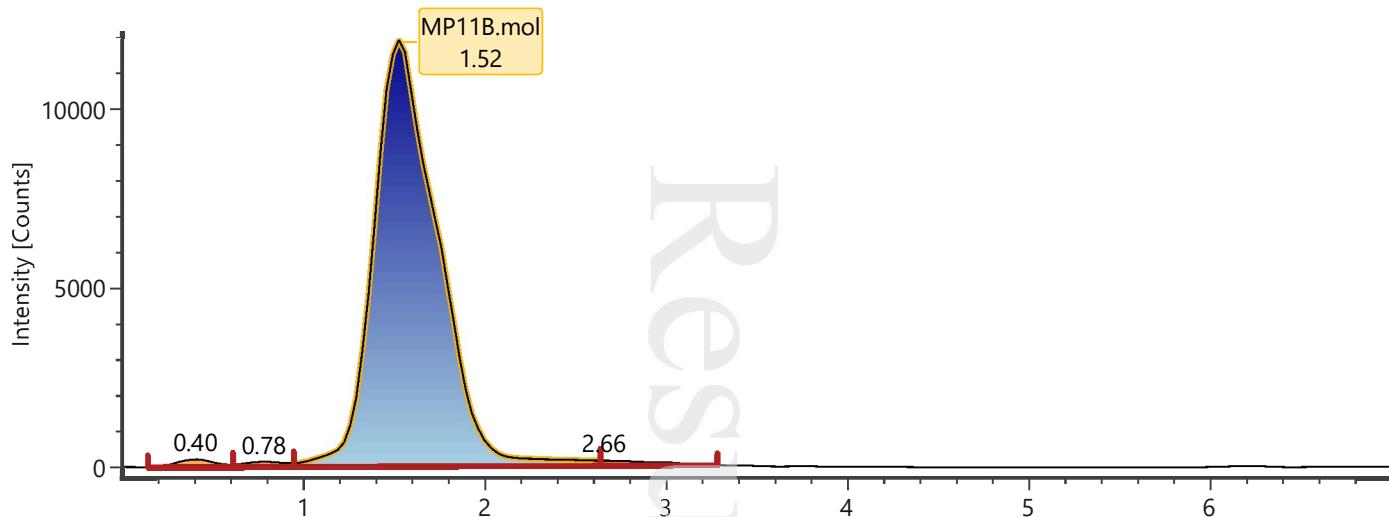
Created by: Chemistry, Chemistry

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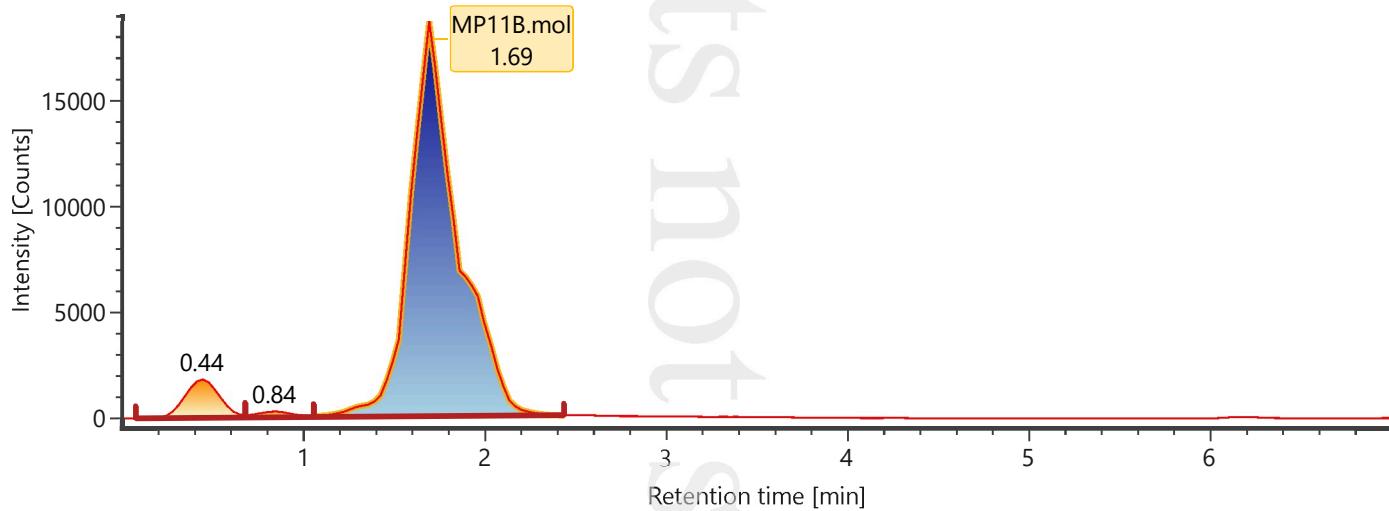
Item name: int1_a3 ACN

Channel name: MP11B.mol [2x(+H)] : (35.9 PPM) 379.1201



Item name: int1_a3 ACN

Channel name: MP11B.mol [2x(-e)] : (35.9 PPM) 378.1130



Item name: MD_M POPLAWSKI

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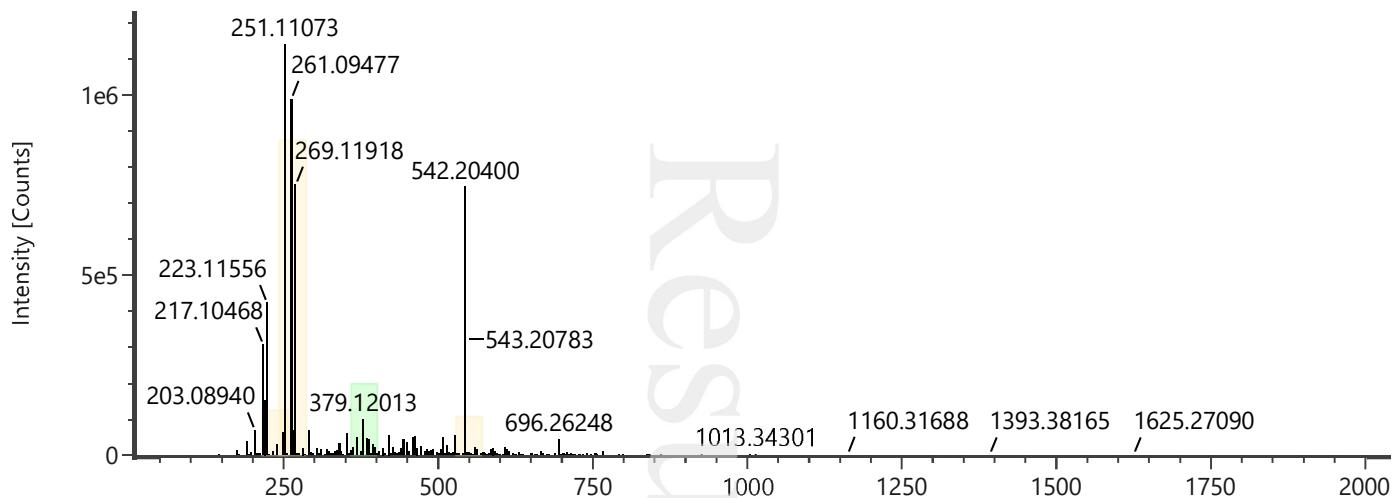
Created on: Sep 07, 2023

Item name: int1_a3 ACN

Created time: 13:59:44 GMT Daylight Time

Item description:

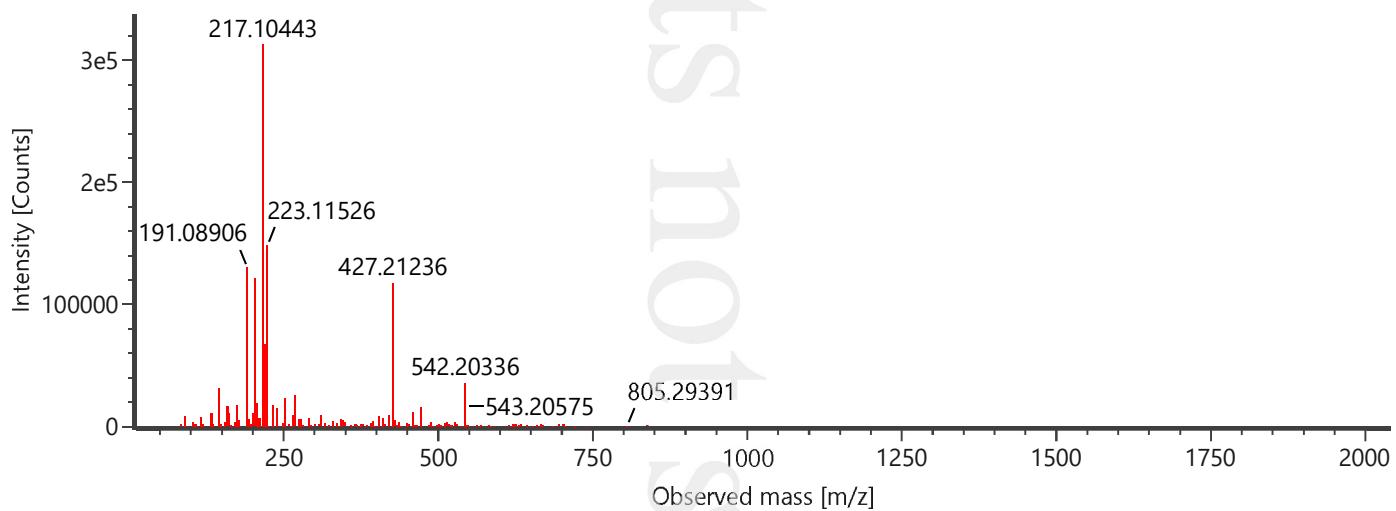
Channel name: Low energy : Time 1.5197 +/- 0.0652 minutes



Item name: int1_a3 ACN

Channel name: High energy : Time 1.5197 +/- 0.0652 minutes

Item description:



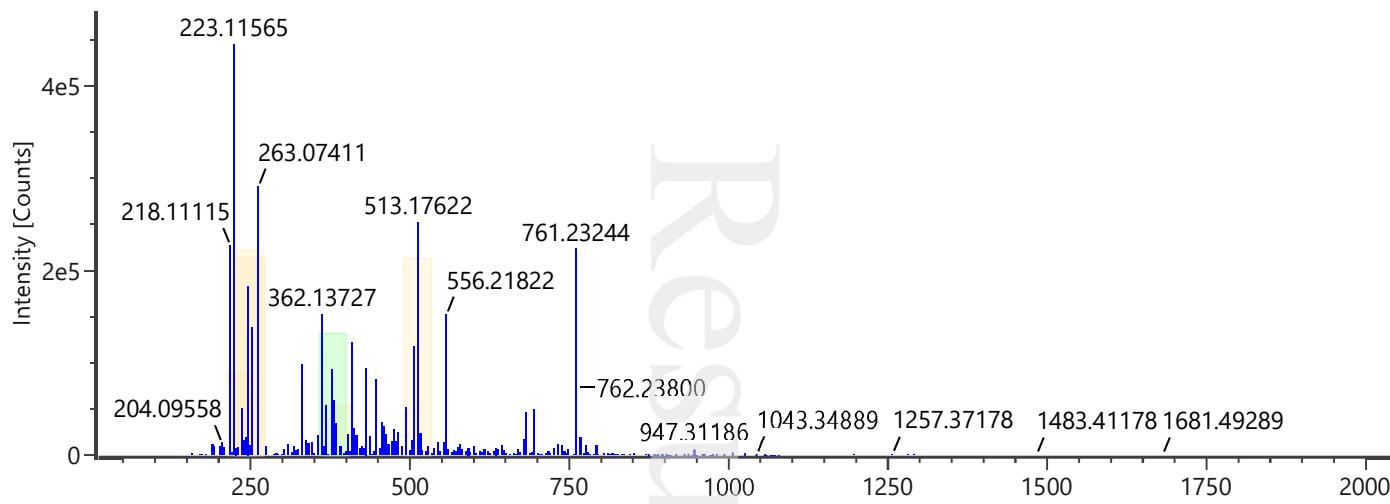
Item name: MD_M POPLAWSKI

Created time: 13:59:44 GMT Daylight Time

Item name: int1_a3 ACN

Channel name: Low energy : Time 1.7152 +/- 0.0652 minutes

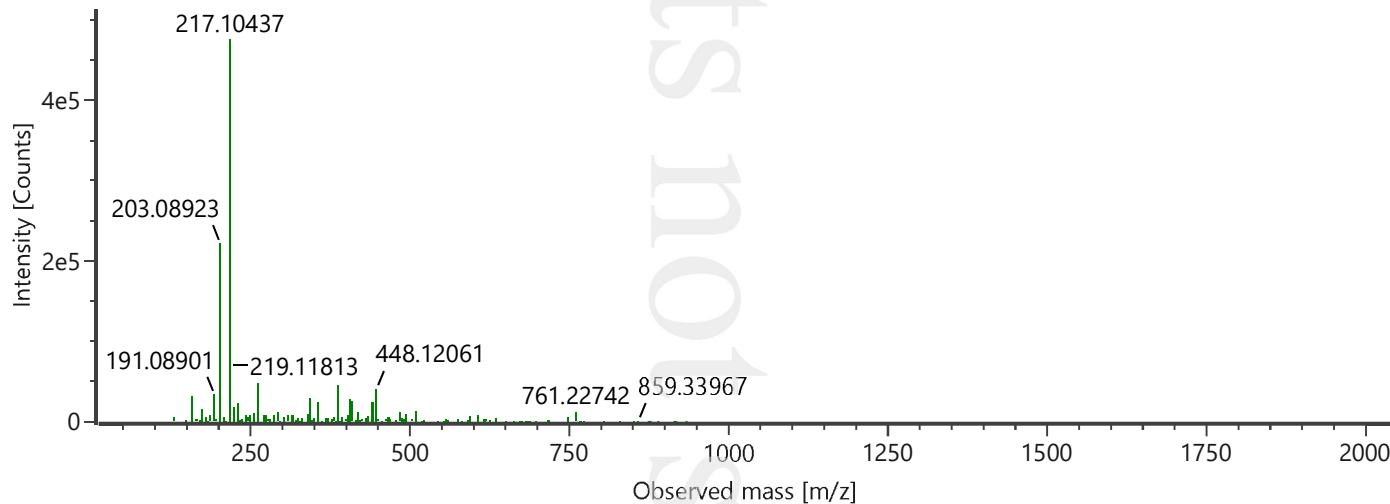
Item description:



Item name: int1_a3 ACN

Channel name: High energy : Time 1.7152 +/- 0.0652 minutes

Item description:



Component name: MP12B.mol

Component name: MP12B.mol

.	Item name	Sample position	Replicate number	Component name	Identification status	Neutral mass (Da)	Observed neutral mass (Da)
1	int1_a3 ACN	2:A,8	1	MP12B.mol	Identified	770.24270	770.2410

.	Item name	Sample position	Replicate number	Component name	Identification status	Observed m/z	Mass error (mDa)
1	int1_a3 ACN	2:A,8	1	MP12B.mol	Identified	385.1199	-1.8

.	Item name	Sample position	Replicate number	Component name	Identification status	Mass error (ppm)	Expected RT (min)	Observed RT (min)
1	int1_a3 ACN	2:A,8	1	MP12B.mol	Identified	-2.3		1.66

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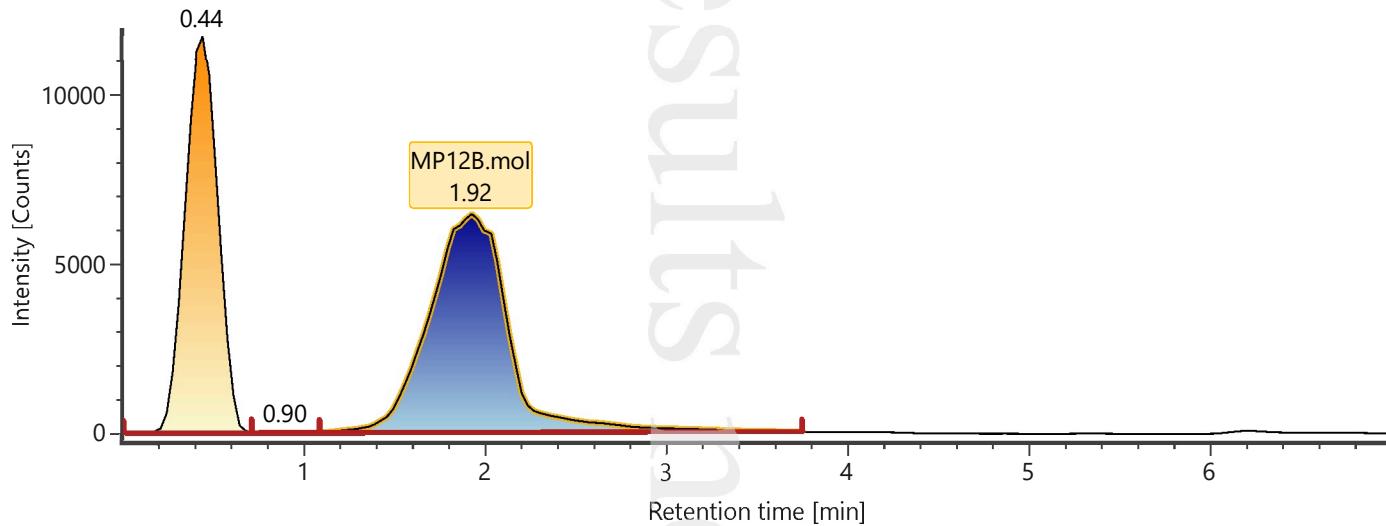
.	Item name	Sample position	Replicate number	Component name	Identification status	Detector counts	Response	Adducts
1	int1_a3 ACN	2:A,8	1	MP12B.mol	Identified	2331	2331	2x(-e)

.	Item name	Sample position	Replicate number	Component name	Identification status	Formula
1	int1_a3 ACN	2:A,8	1	MP12B.mol	Identified	C37[13C]3H37N3O13

Item name: int1_a3 ACN

Item name: int1_a3 ACN

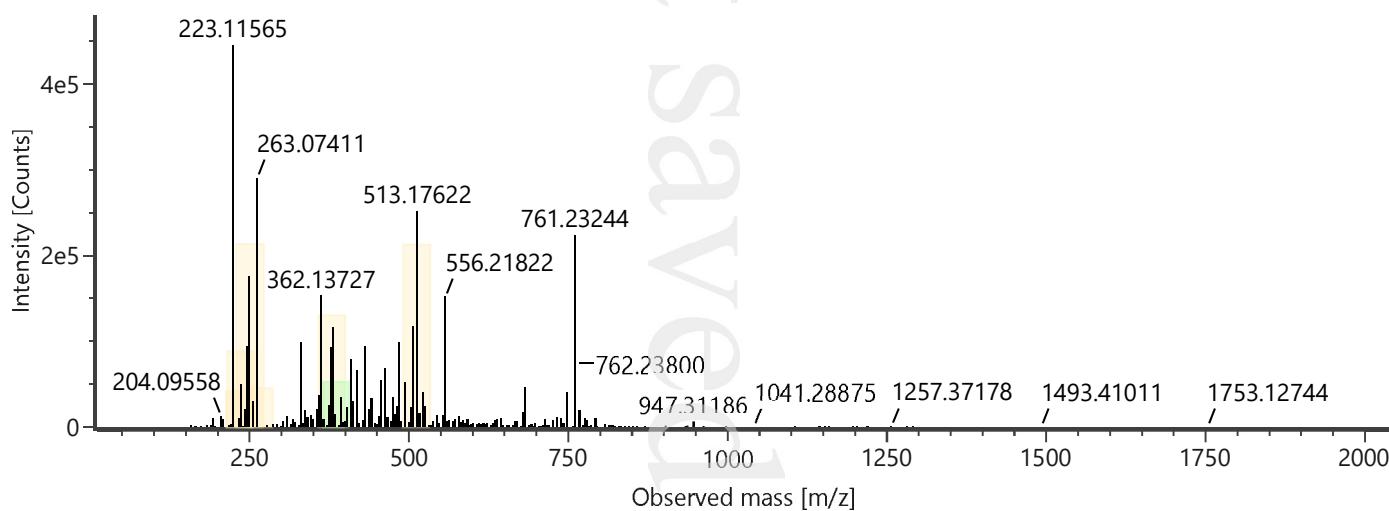
Channel name: MP12B.mol [2x(-e)] : (35.9 PPM) 385.1199



Item name: int1_a3 ACN

Item description:

Channel name: Low energy : Time 1.6646 +/- 0.0652 minutes



Item name: MD_M POPLAWSKI

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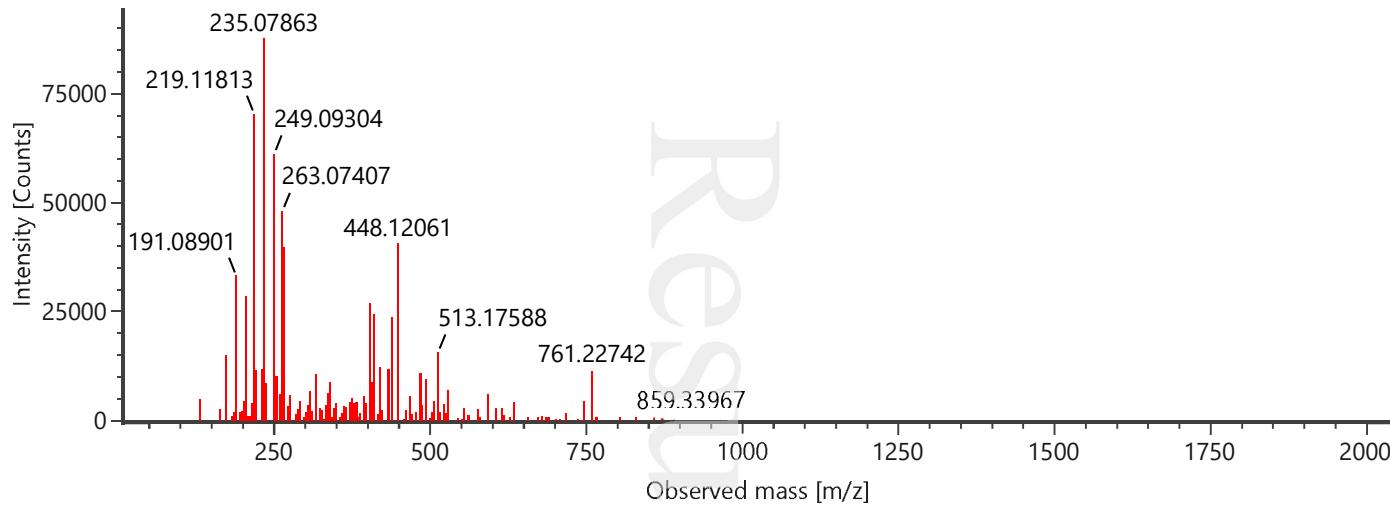
Created on: Sep 07, 2023

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Item name: int1_a3 ACN

Channel name: High energy : Time 1.6646 +/- 0.0652 minutes

Item description:



Component name: MP1B.mol

Component name: MP1B.mol

.	Item name	Sample position	Replicate number	Component name	Identification status	Neutral mass (Da)	Observed neutral mass (Da)
1	int1_a3 ACN	2:A,8	1	MP1B.mol	Identified	266.09838	266.0983

.	Item name	Sample position	Replicate number	Component name	Identification status	Observed m/z	Mass error (mDa)
1	int1_a3 ACN	2:A,8	1	MP1B.mol	Identified	267.1056	0.0

.	Item name	Sample position	Replicate number	Component name	Identification status	Mass error (ppm)	Expected RT (min)	Observed RT (min)
1	int1_a3 ACN	2:A,8	1	MP1B.mol	Identified	-0.1		0.81

.	Item name	Sample position	Replicate number	Component name	Identification status	Detector counts	Response
1	int1_a3 ACN	2:A,8	1	MP1B.mol	Identified	629599	537651

.	Item name	Sample position	Replicate number	Component name	Identification status	Adducts	Formula
1	int1_a3 ACN	2:A,8	1	MP1B.mol	Identified	+H, +Na	C12[13C]H15NO5

Item name: int1_a3 ACN

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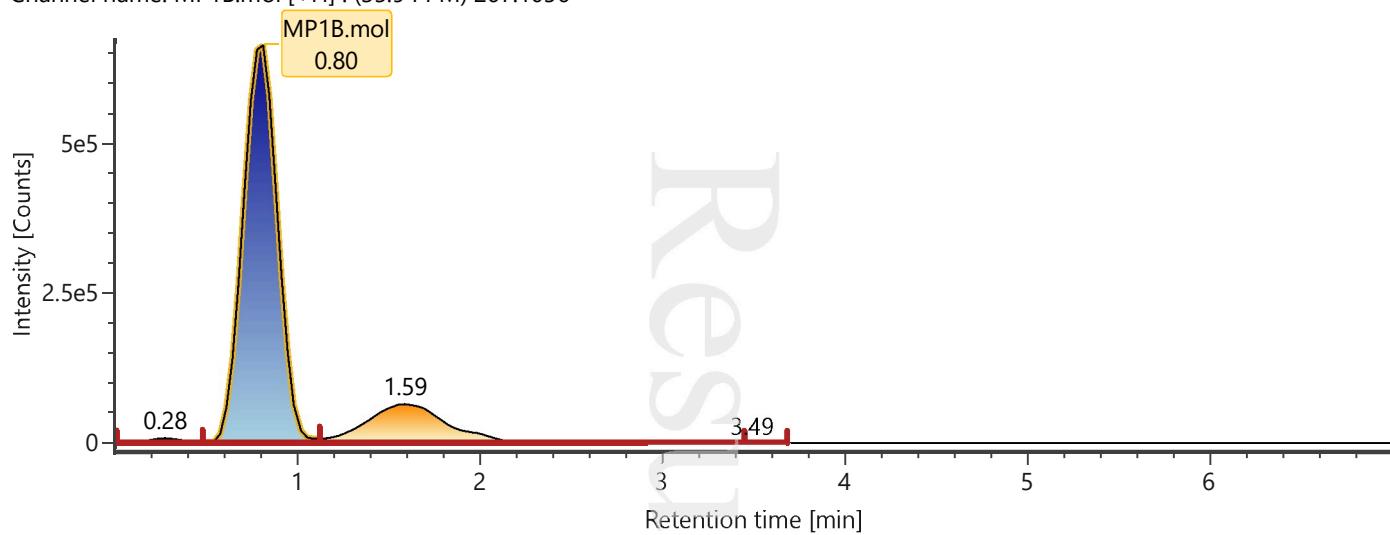
Created by: Chemistry, Chemistry

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Item name: int1_a3 ACN

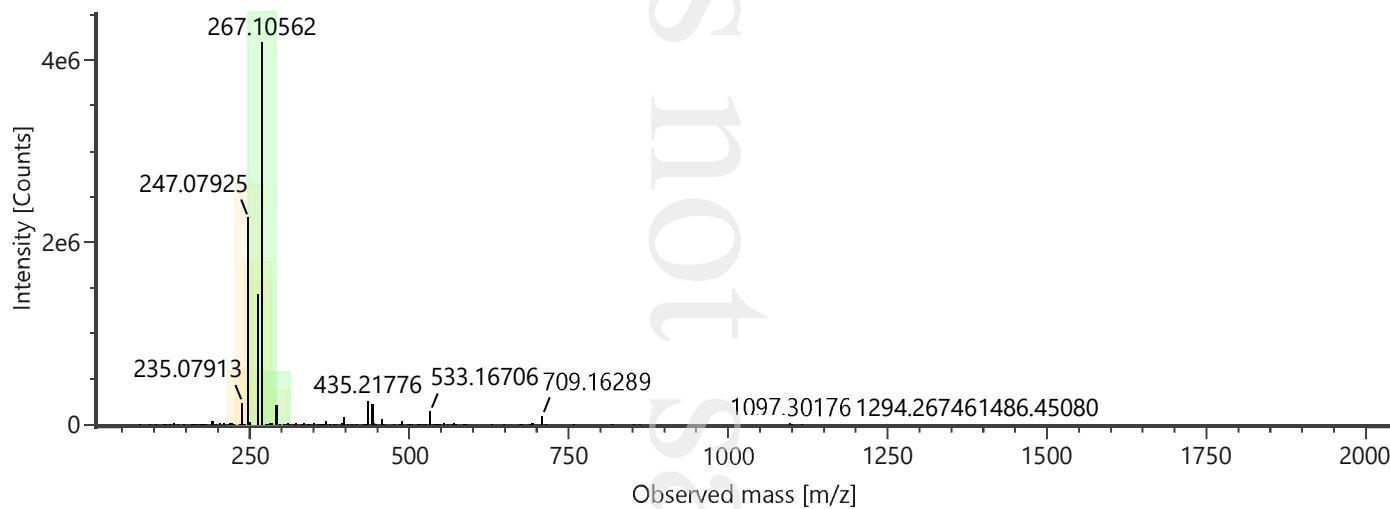
Channel name: MP1B.mol [+H] : (35.9 PPM) 267.1056



Item name: int1_a3 ACN

Item description:

Channel name: Low energy : Time 0.8055 +/- 0.0652 minutes



Item name: MD_M POPLAWSKI

Created by: Chemistry, Chemistry

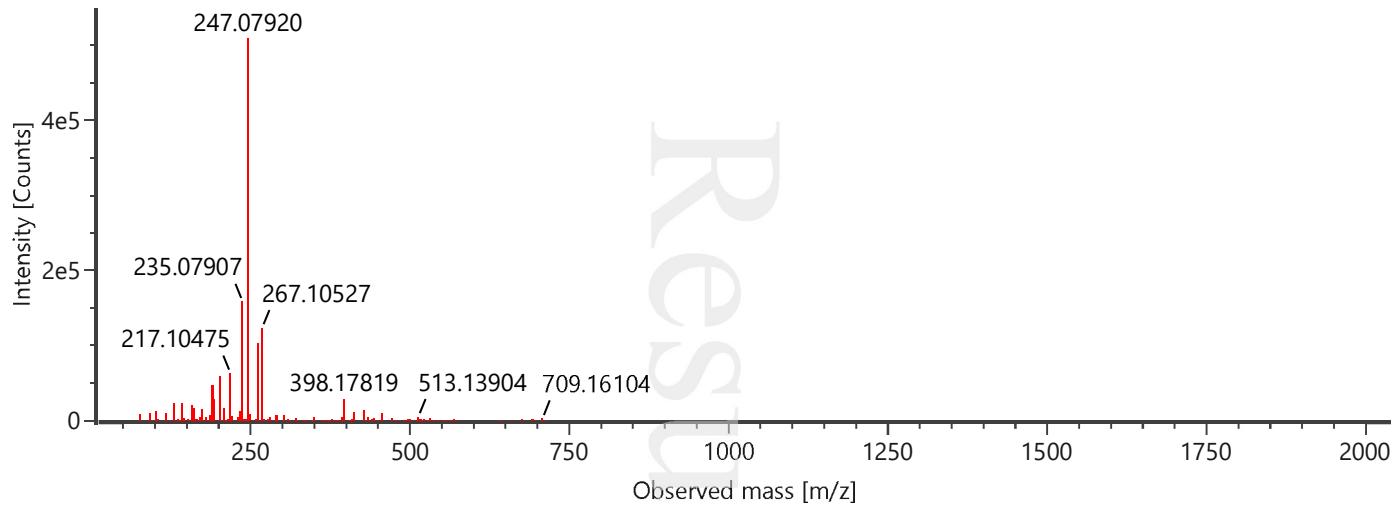
Created on: Sep 07, 2023

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Item name: int1_a3 ACN

Channel name: High energy : Time 0.8055 +/- 0.0652 minutes

Item description:



Component name: MP2B.mol

Component name: MP2B.mol

.	Item name	Sample position	Replicate number	Component name	Identification status	Neutral mass (Da)	Observed neutral mass (Da)
1	int1_a3 ACN	2:A,8	1	MP2B.mol	Identified	264.08273	264.0824

.	Item name	Sample position	Replicate number	Component name	Identification status	Observed m/z	Mass error (mDa)
1	int1_a3 ACN	2:A,8	1	MP2B.mol	Identified	265.0896	-0.4

.	Item name	Sample position	Replicate number	Component name	Identification status	Mass error (ppm)	Expected RT (min)	Observed RT (min)
1	int1_a3 ACN	2:A,8	1	MP2B.mol	Identified	-1.4		0.82

.	Item name	Sample position	Replicate number	Component name	Identification status	Detector counts	Response	Adducts
1	int1_a3 ACN	2:A,8	1	MP2B.mol	Identified	24239	21178	+H

.	Item name	Sample position	Replicate number	Component name	Identification status	Formula
1	int1_a3 ACN	2:A,8	1	MP2B.mol	Identified	C12[13C]H13NO5

Component name: MP2B.mol

.	Item name	Sample position	Replicate number	Component name	Identification status	Neutral mass (Da)	Observed neutral mass (Da)
1	int1_a3 ACN	2:A,8	1	MP2B.mol	Identified	264.08273	264.0818

.	Item name	Sample position	Replicate number	Component name	Identification status	Observed m/z	Mass error (mDa)
1	int1_a3 ACN	2:A,8	1	MP2B.mol	Identified	265.0890	-1.0

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.	Item name	Sample position	Replicate number	Component name	Identification status	Mass error (ppm)	Expected RT (min)	Observed RT (min)
1	int1_a3 ACN	2:A,8	1	MP2B.mol	Identified	-3.7		1.14

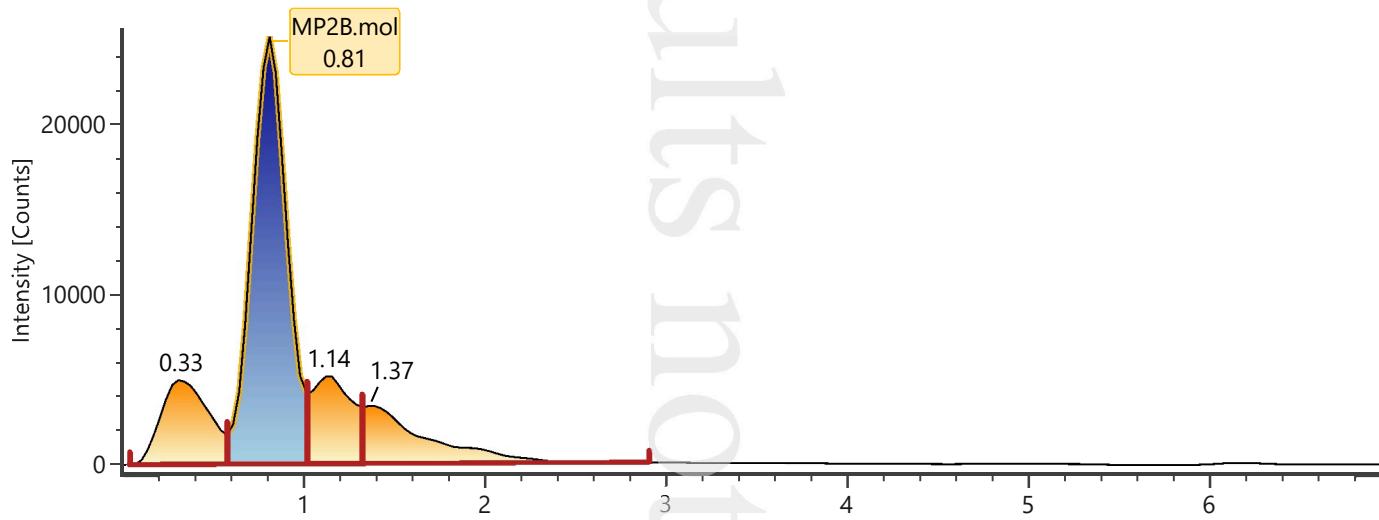
.	Item name	Sample position	Replicate number	Component name	Identification status	Detector counts	Response	Adducts
1	int1_a3 ACN	2:A,8	1	MP2B.mol	Identified	7123	4016	+H

.	Item name	Sample position	Replicate number	Component name	Identification status	Formula
1	int1_a3 ACN	2:A,8	1	MP2B.mol	Identified	C12[13C]H13NO5

Item name: int1_a3 ACN

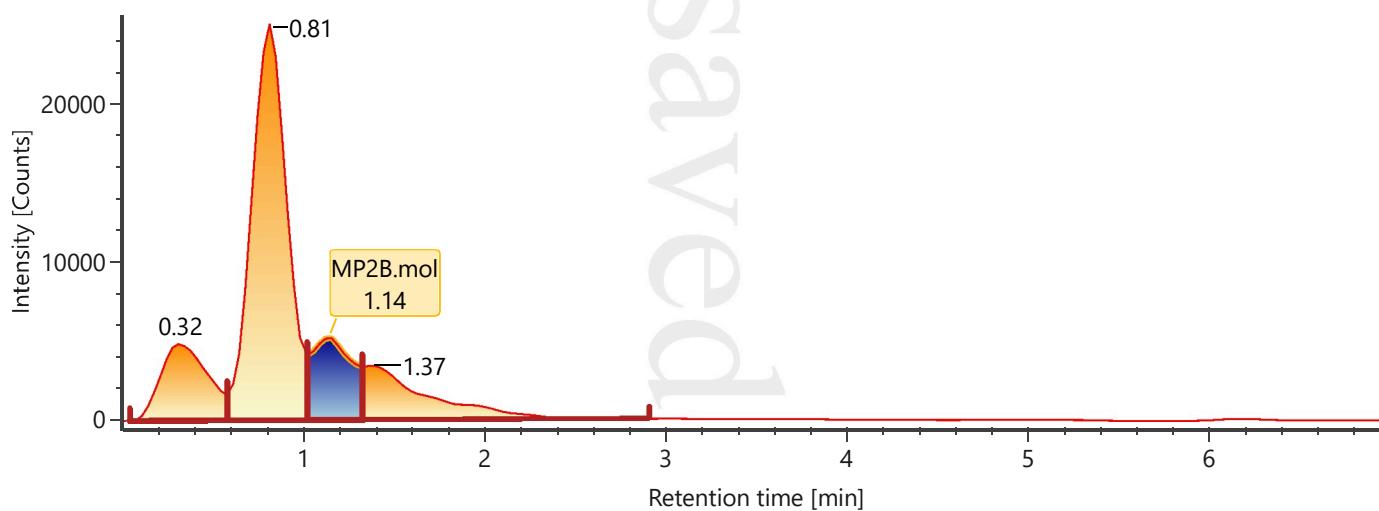
Item name: int1_a3 ACN

Channel name: MP2B.mol [+H] : (35.9 PPM) 265.0896



Item name: int1_a3 ACN

Channel name: MP2B.mol [+H] : (35.9 PPM) 265.0890



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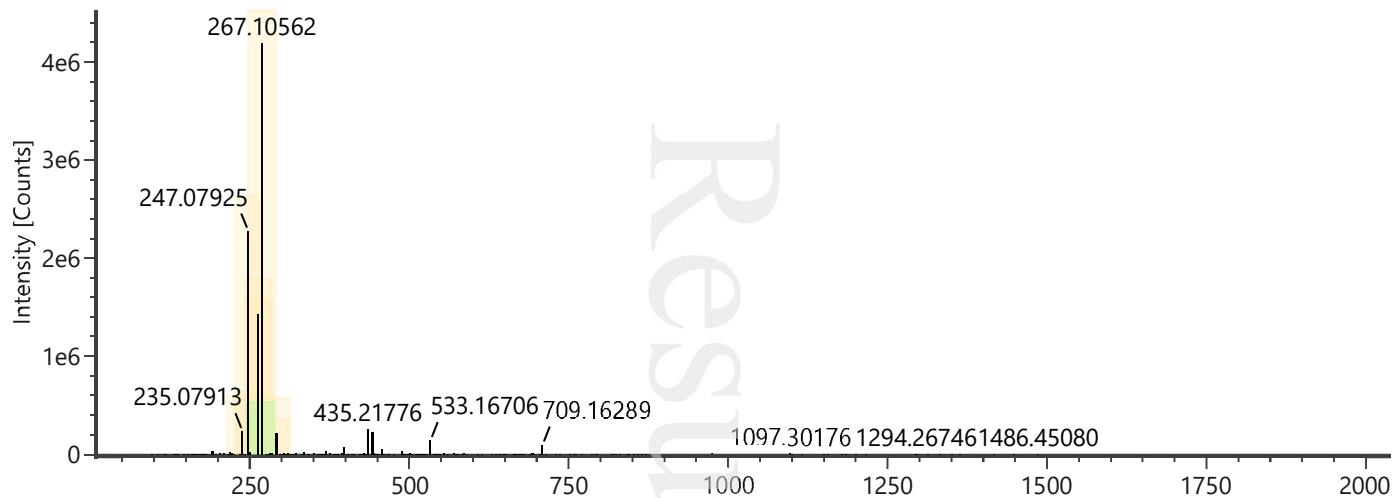
Created on: Sep 07, 2023

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Item name: int1_a3 ACN

Channel name: Low energy : Time 0.8165 +/- 0.0652 minutes

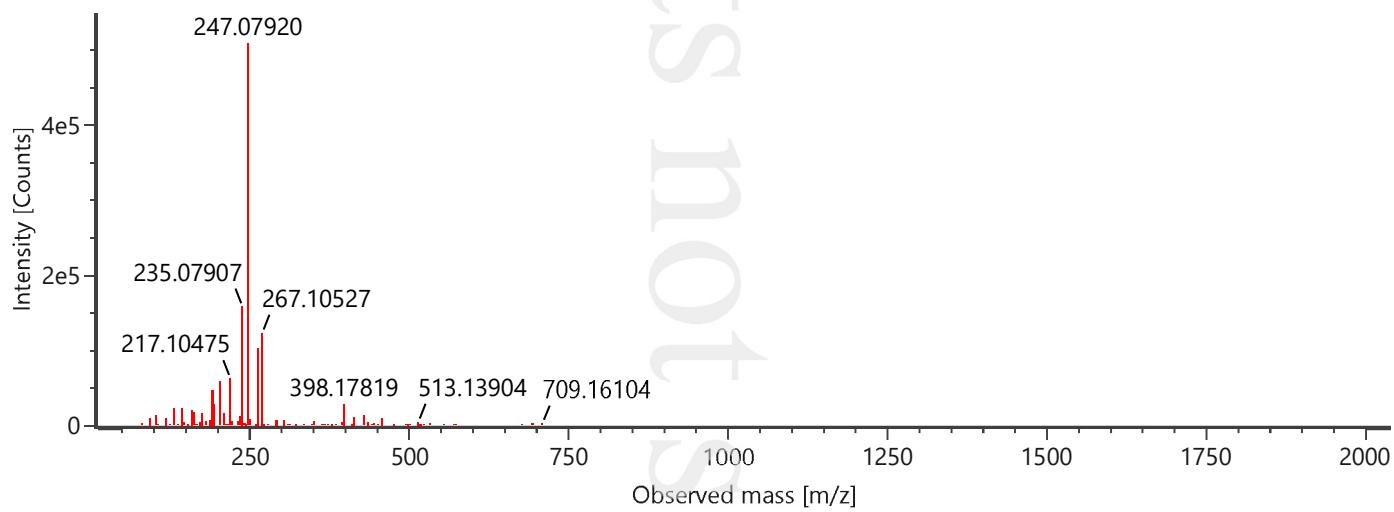
Item description:



Item name: int1_a3 ACN

Channel name: High energy : Time 0.8165 +/- 0.0652 minutes

Item description:



Item name: MD_M POPLAWSKI

Created by: Chemistry, Chemistry

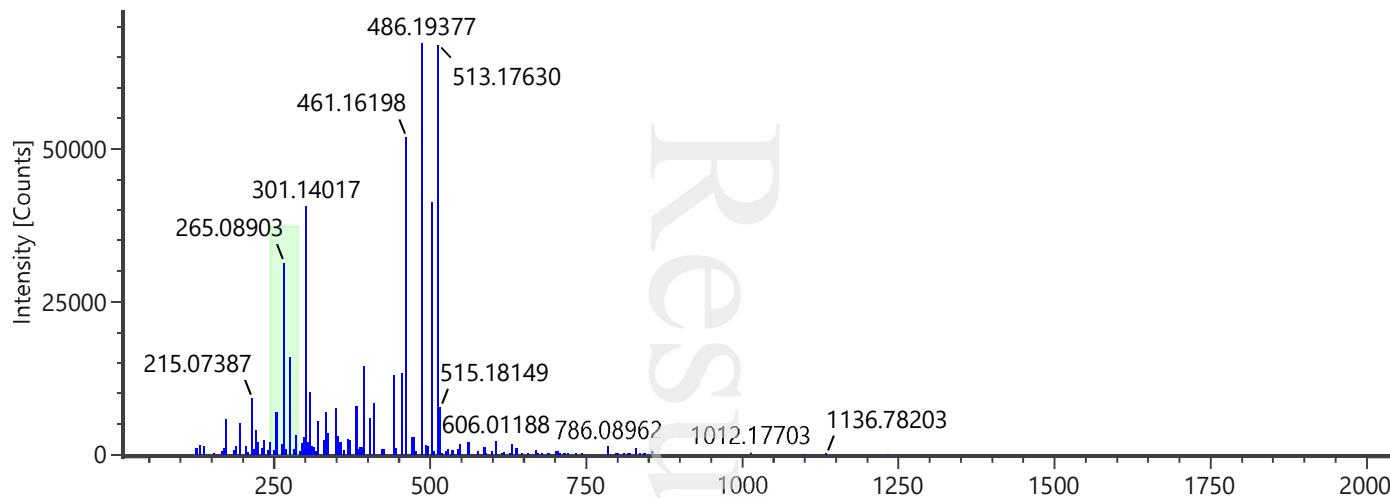
Created on: Sep 07, 2023

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Item name: int1_a3 ACN

Channel name: Low energy : Time 1.1387 +/- 0.0652 minutes

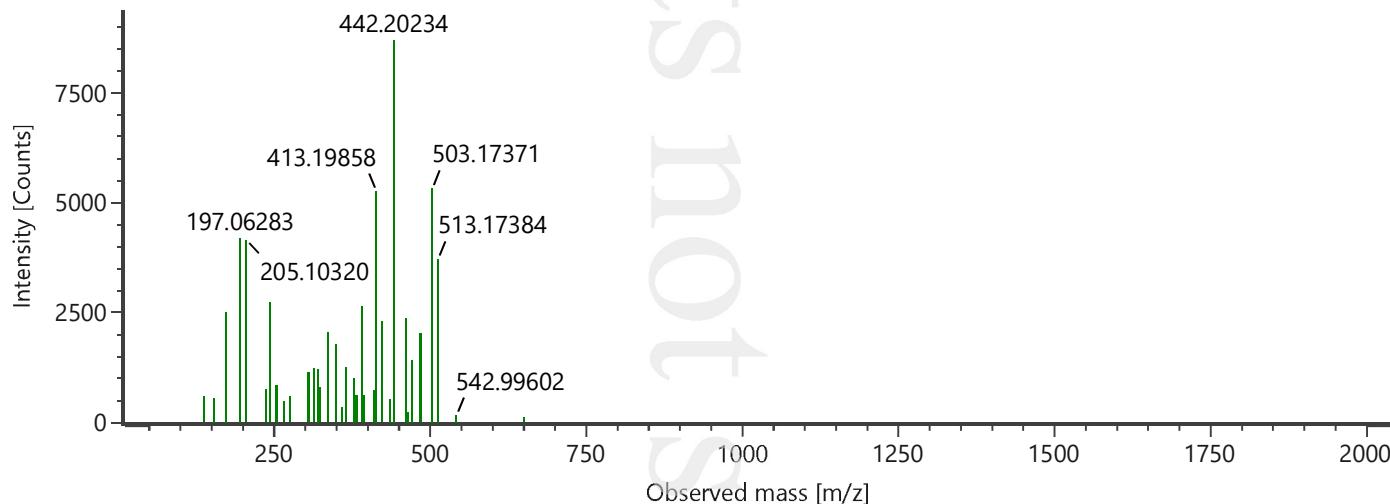
Item description:



Item name: int1_a3 ACN

Channel name: High energy : Time 1.1387 +/- 0.0652 minutes

Item description:



Component name: MP3B.mol

Component name: MP3B.mol

.	Item name	Sample position	Replicate number	Component name	Identification status	Neutral mass (Da)	Observed neutral mass (Da)
1	int1_a3 ACN	2:A,8	1	MP3B.mol	Identified	248.08781	248.0869

.	Item name	Sample position	Replicate number	Component name	Identification status	Observed m/z	Mass error (mDa)
1	int1_a3 ACN	2:A,8	1	MP3B.mol	Identified	249.0942	-0.9

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.	Item name	Sample position	Replicate number	Component name	Identification status	Mass error (ppm)	Expected RT (min)	Observed RT (min)
1	int1_a3 ACN	2:A,8	1	MP3B.mol	Identified	-3.5		0.81

.	Item name	Sample position	Replicate number	Component name	Identification status	Detector counts	Response	Adducts
1	int1_a3 ACN	2:A,8	1	MP3B.mol	Identified	34385	31242	+H, +K

.	Item name	Sample position	Replicate number	Component name	Identification status	Formula
1	int1_a3 ACN	2:A,8	1	MP3B.mol	Identified	C12[13C]H13NO4

Component name: MP3B.mol

.	Item name	Sample position	Replicate number	Component name	Identification status	Neutral mass (Da)	Observed neutral mass (Da)
1	int1_a3 ACN	2:A,8	1	MP3B.mol	Identified	248.08781	248.0867

.	Item name	Sample position	Replicate number	Component name	Identification status	Observed m/z	Mass error (mDa)
1	int1_a3 ACN	2:A,8	1	MP3B.mol	Identified	249.0940	-1.1

.	Item name	Sample position	Replicate number	Component name	Identification status	Mass error (ppm)	Expected RT (min)	Observed RT (min)
1	int1_a3 ACN	2:A,8	1	MP3B.mol	Identified	-4.3		1.69

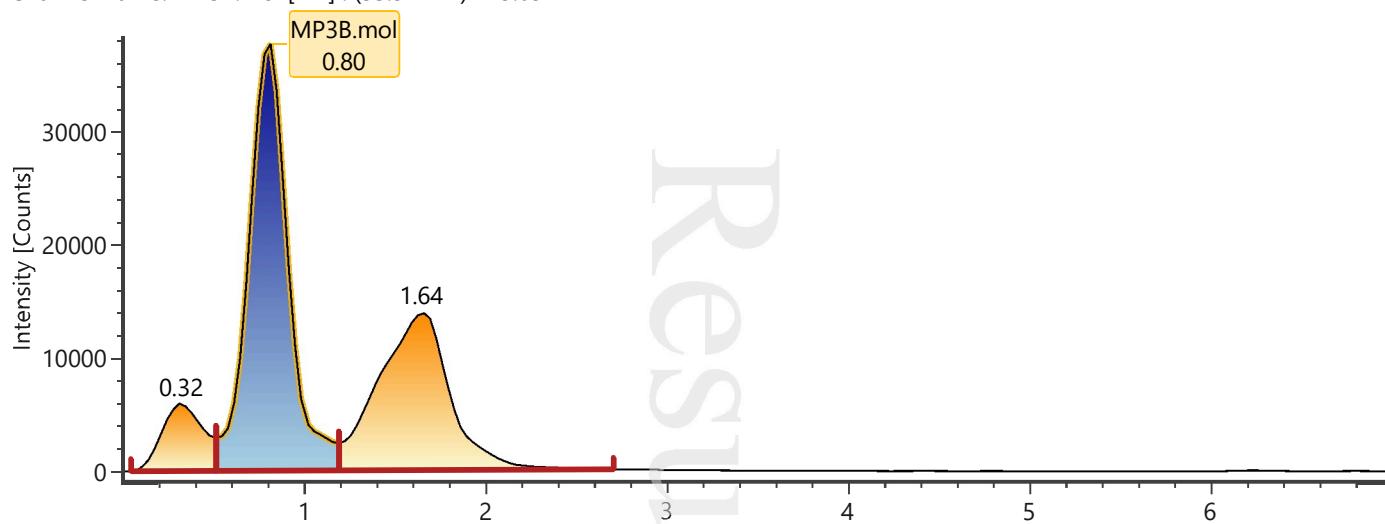
.	Item name	Sample position	Replicate number	Component name	Identification status	Detector counts	Response	Adducts
1	int1_a3 ACN	2:A,8	1	MP3B.mol	Identified	23012	21706	+H

.	Item name	Sample position	Replicate number	Component name	Identification status	Formula
1	int1_a3 ACN	2:A,8	1	MP3B.mol	Identified	C12[13C]H13NO4

Item name: int1_a3 ACN

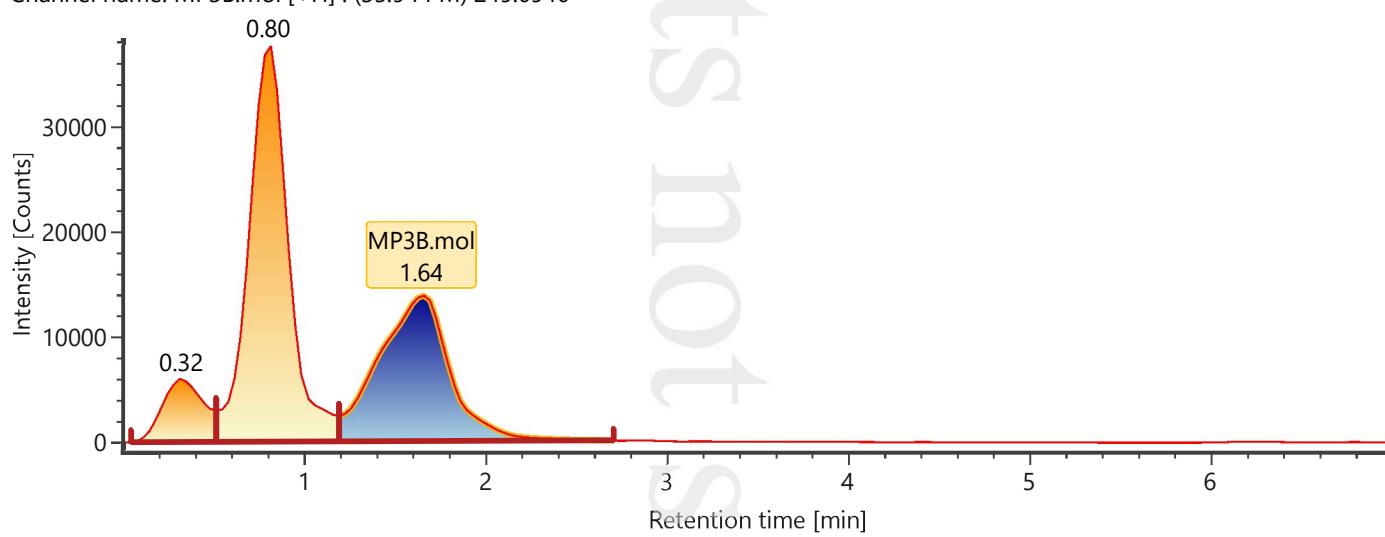
Item name: int1_a3 ACN

Channel name: MP3B.mol [+H] : (35.9 PPM) 249.0942



Item name: int1_a3 ACN

Channel name: MP3B.mol [+H] : (35.9 PPM) 249.0940



Item name: MD_M POPLAWSKI

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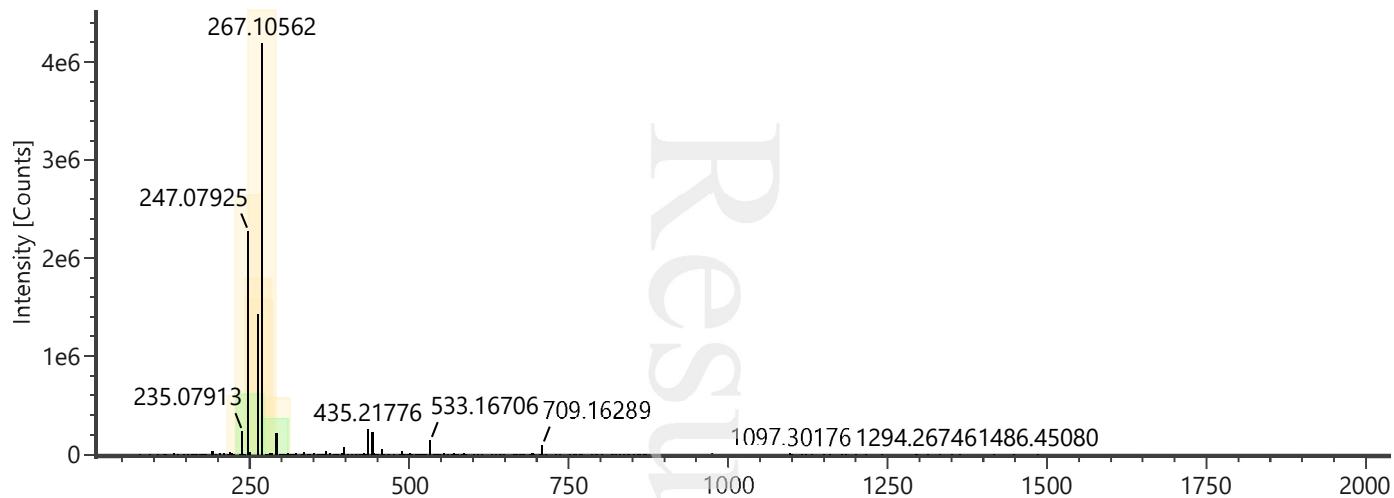
Created on: Sep 07, 2023

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Item name: int1_a3 ACN

Channel name: Low energy : Time 0.8095 +/- 0.0652 minutes

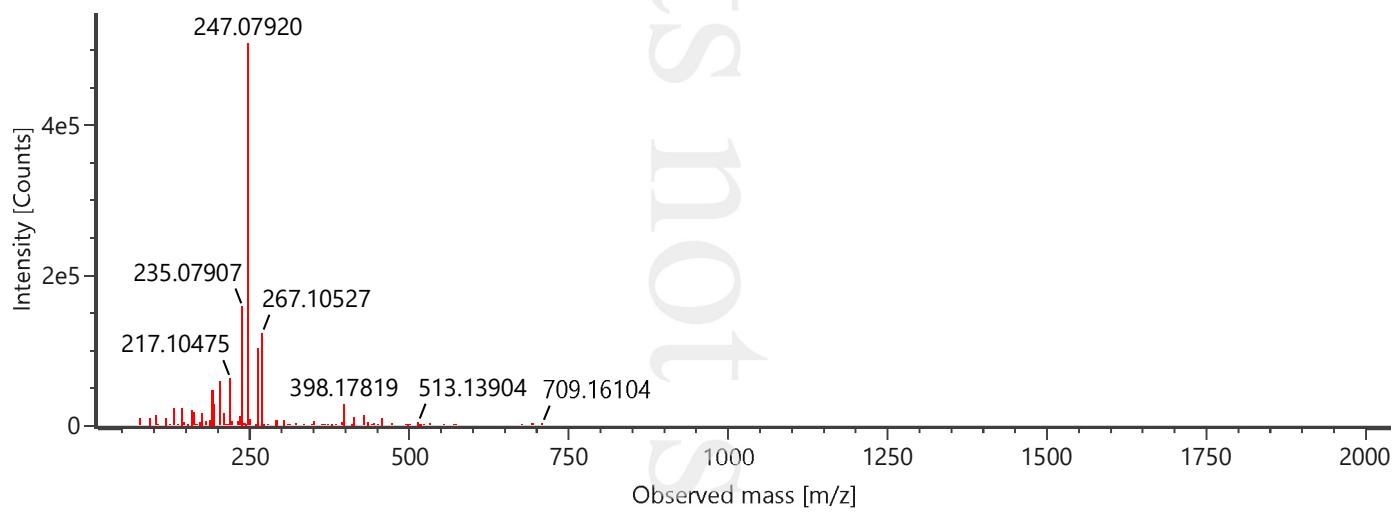
Item description:



Item name: int1_a3 ACN

Channel name: High energy : Time 0.8095 +/- 0.0652 minutes

Item description:



Item name: MD_M POPLAWSKI

Created by: Chemistry, Chemistry

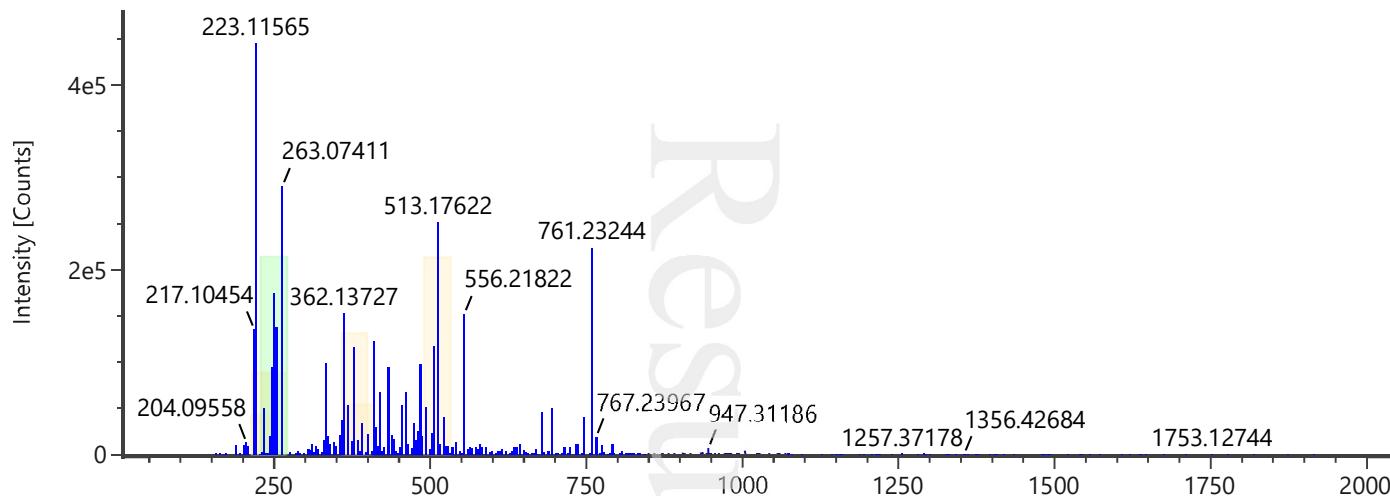
Created on: Sep 07, 2023

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Item name: int1_a3 ACN

Channel name: Low energy : Time 1.6856 +/- 0.0652 minutes

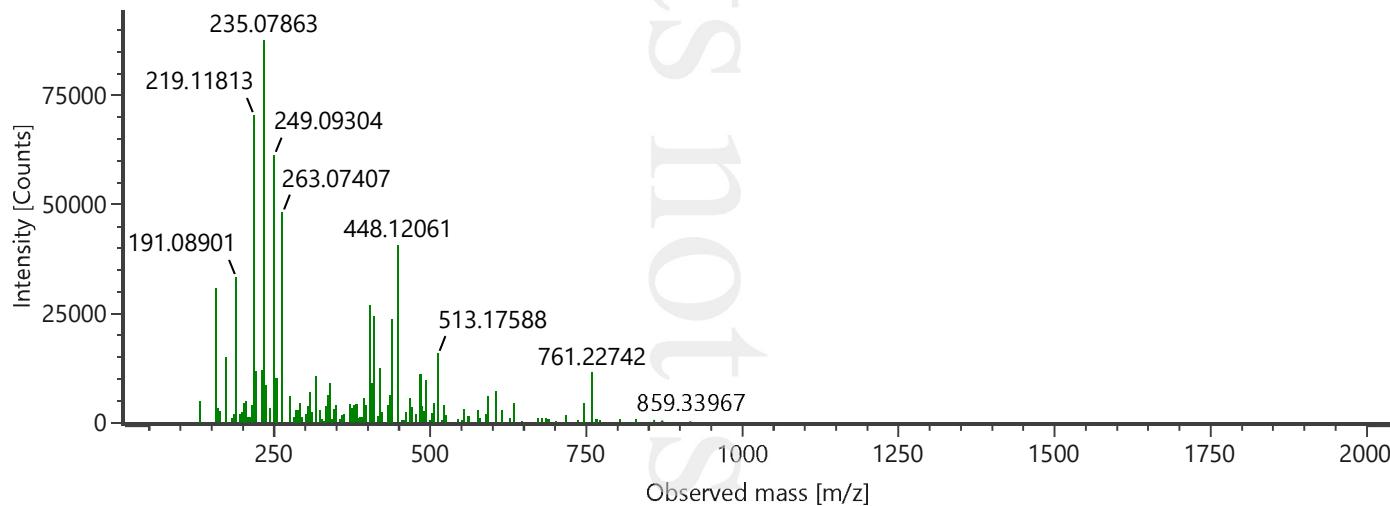
Item description:



Item name: int1_a3 ACN

Channel name: High energy : Time 1.6856 +/- 0.0652 minutes

Item description:



Component name: MP4B.mol

Component name: MP4B.mol

.	Item name	Sample position	Replicate number	Component name	Identification status	Neutral mass (Da)	Observed neutral mass (Da)
1	int1_a3 ACN	2:A,8	1	MP4B.mol	Identified	247.07999	247.0793

.	Item name	Sample position	Replicate number	Component name	Identification status	Observed m/z	Mass error (mDa)
1	int1_a3 ACN	2:A,8	1	MP4B.mol	Identified	247.0788	-0.7

Item name: MD_M POPLAWSKI

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.	Item name	Sample position	Replicate number	Component name	Identification status	Mass error (ppm)	Expected RT (min)	Observed RT (min)
1	int1_a3 ACN	2:A,8	1	MP4B.mol	Identified	-2.7		1.77

.	Item name	Sample position	Replicate number	Component name	Identification status	Detector counts	Response	Adducts
1	int1_a3 ACN	2:A,8	1	MP4B.mol	Identified	28635	22611	-e

.	Item name	Sample position	Replicate number	Component name	Identification status	Formula
1	int1_a3 ACN	2:A,8	1	MP4B.mol	Identified	C12[13C]H12NO4

Component name: MP4B.mol

.	Item name	Sample position	Replicate number	Component name	Identification status	Neutral mass (Da)	Observed neutral mass (Da)
1	int1_a3 ACN	2:A,8	1	MP4B.mol	Identified	247.07999	247.0798

.	Item name	Sample position	Replicate number	Component name	Identification status	Observed m/z	Mass error (mDa)
1	int1_a3 ACN	2:A,8	1	MP4B.mol	Identified	247.0793	-0.2

.	Item name	Sample position	Replicate number	Component name	Identification status	Mass error (ppm)	Expected RT (min)	Observed RT (min)
1	int1_a3 ACN	2:A,8	1	MP4B.mol	Identified	-0.7		0.86

.	Item name	Sample position	Replicate number	Component name	Identification status	Detector counts	Response
1	int1_a3 ACN	2:A,8	1	MP4B.mol	Identified	305208	280252

.	Item name	Sample position	Replicate number	Component name	Identification status	Adducts	Formula
1	int1_a3 ACN	2:A,8	1	MP4B.mol	Identified	-e	C12[13C]H12NO4

Component name: MP4B.mol

.	Item name	Sample position	Replicate number	Component name	Identification status	Neutral mass (Da)	Observed neutral mass (Da)
1	int1_a3 ACN	2:A,8	1	MP4B.mol	Identified	247.07999	247.0797

.	Item name	Sample position	Replicate number	Component name	Identification status	Observed m/z	Mass error (mDa)
1	int1_a3 ACN	2:A,8	1	MP4B.mol	Identified	247.0792	-0.3

.	Item name	Sample position	Replicate number	Component name	Identification status	Mass error (ppm)	Expected RT (min)	Observed RT (min)
1	int1_a3 ACN	2:A,8	1	MP4B.mol	Identified	-1.1		1.40

.	Item name	Sample position	Replicate number	Component name	Identification status	Detector counts	Response
1	int1_a3 ACN	2:A,8	1	MP4B.mol	Identified	195545	174222

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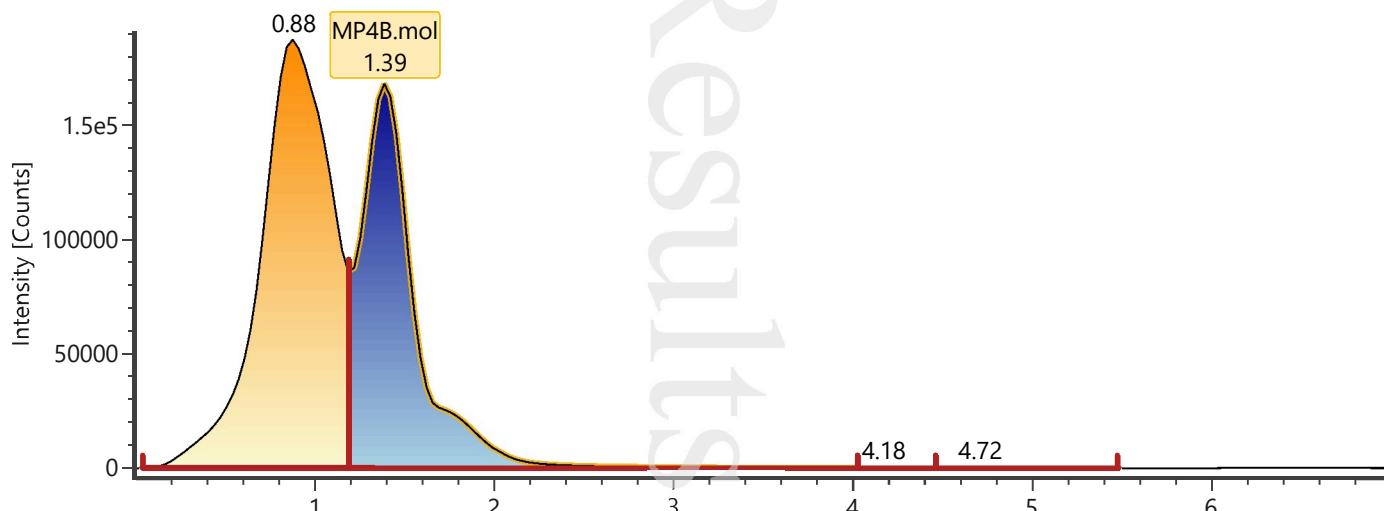
Created time: 13:59:44 GMT Daylight Time

.	Item name	Sample position	Replicate number	Component name	Identification status	Adducts	Formula
1	int1_a3 ACN	2:A,8	1	MP4B.mol	Identified	-e	C12[13C]H12NO4

Item name: int1_a3 ACN

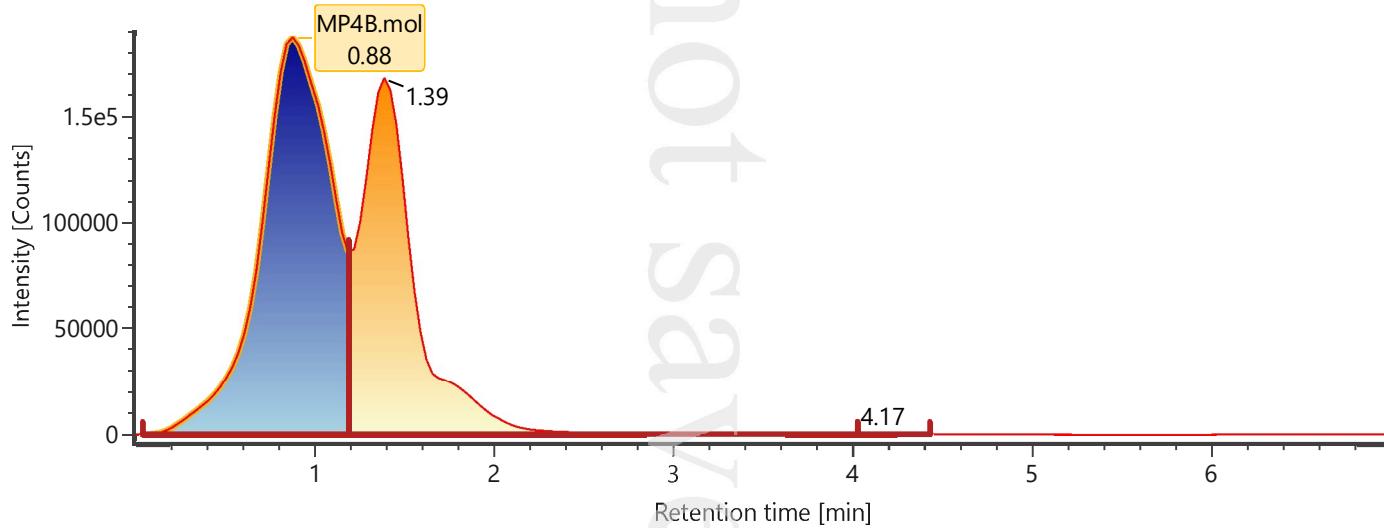
Item name: int1_a3 ACN

Channel name: MP4B.mol [-e] : (35.9 PPM) 247.0788



Item name: int1_a3 ACN

Channel name: MP4B.mol [-e] : (35.9 PPM) 247.0793



Item name: MD_M POPLAWSKI

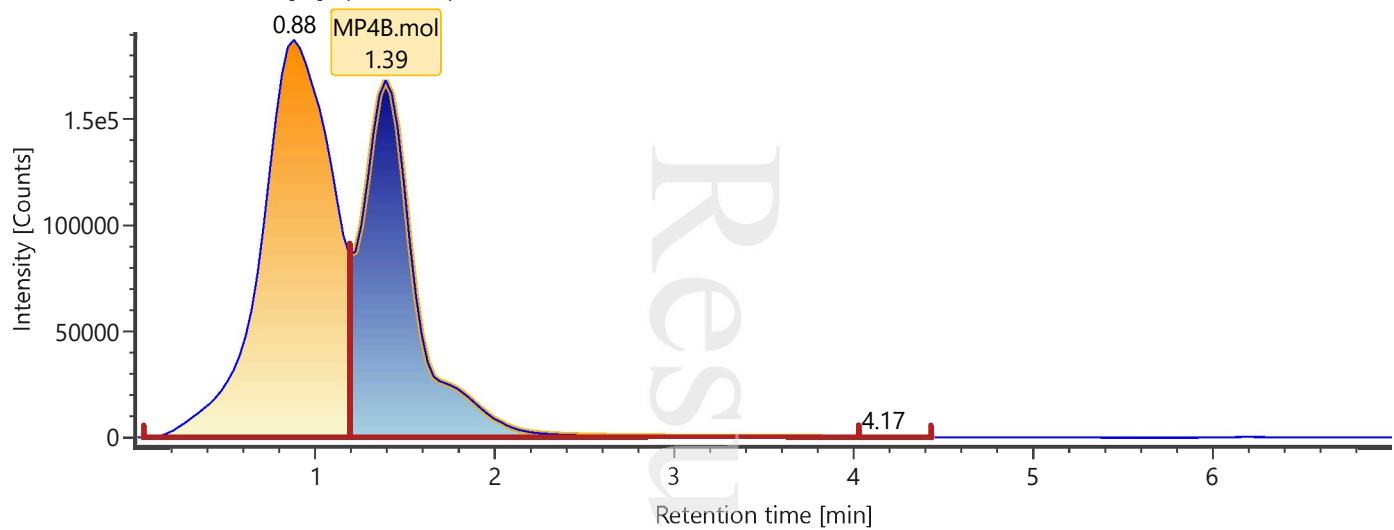
Created by: Chemistry, Chemistry

Created on: Sep 07, 2023

Created time: 13:59:44 GMT Daylight Time

Item name: int1_a3 ACN

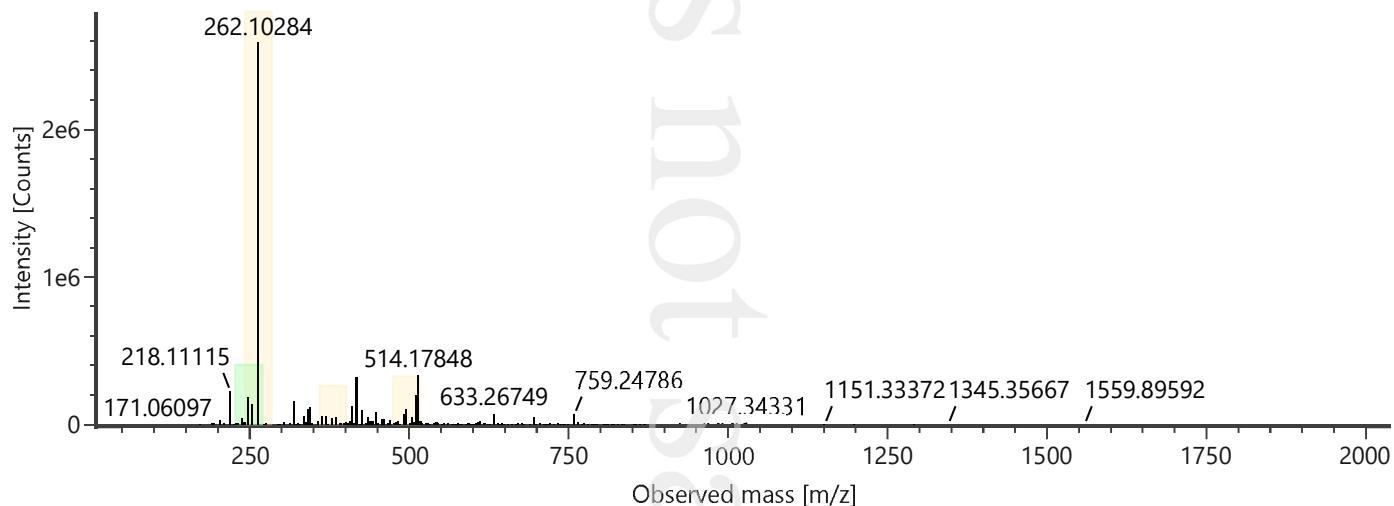
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Item name: int1_a3 ACN

Item description:

Channel name: Low energy : Time 1.7684 +/- 0.0652 minutes



Item name: MD_M POPLAWSKI

Created by: Chemistry, Chemistry

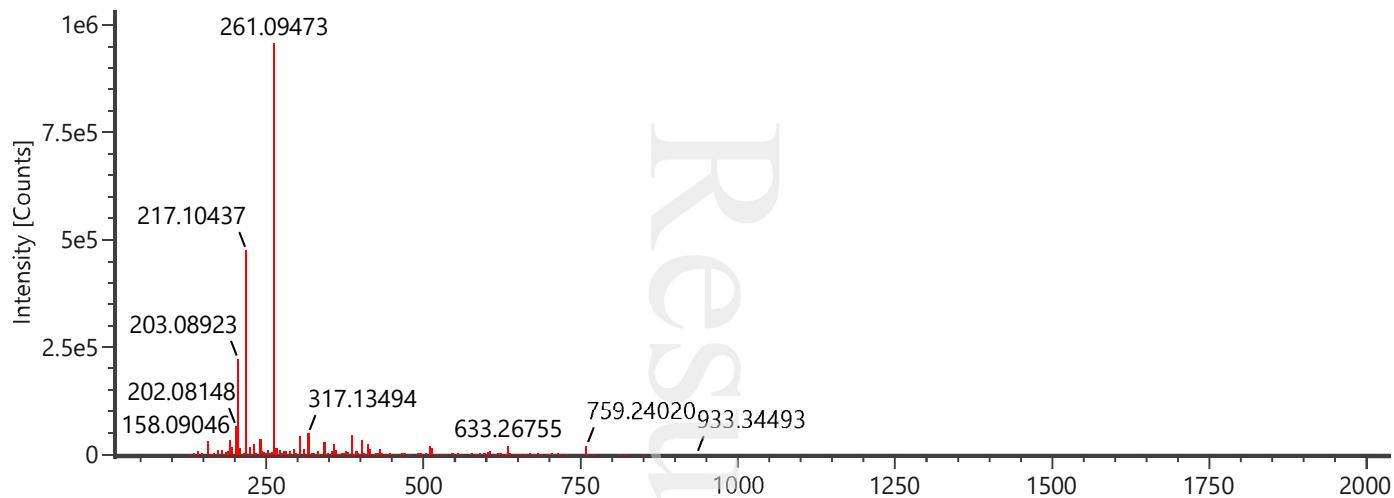
Created on: Sep 07, 2023

Created time: 13:59:44 GMT Daylight Time

Item name: int1_a3 ACN

Channel name: High energy : Time 1.7684 +/- 0.0652 minutes

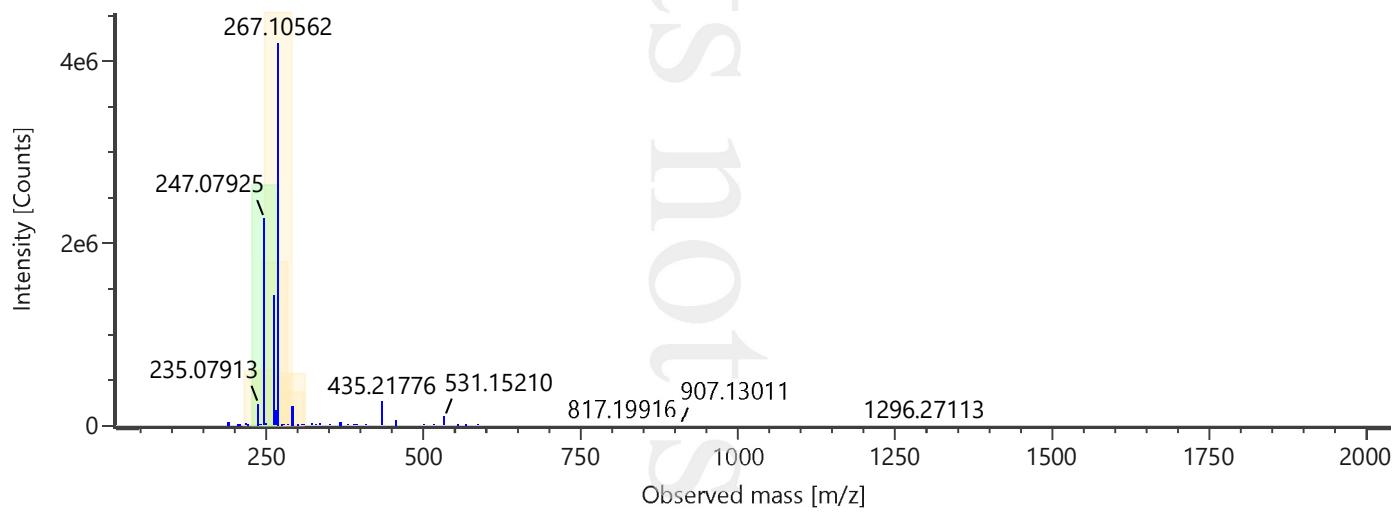
Item description:



Item name: int1_a3 ACN

Channel name: Low energy : Time 0.8598 +/- 0.0652 minutes

Item description:



Item name: MD_M POPLAWSKI

Created by: Chemistry, Chemistry

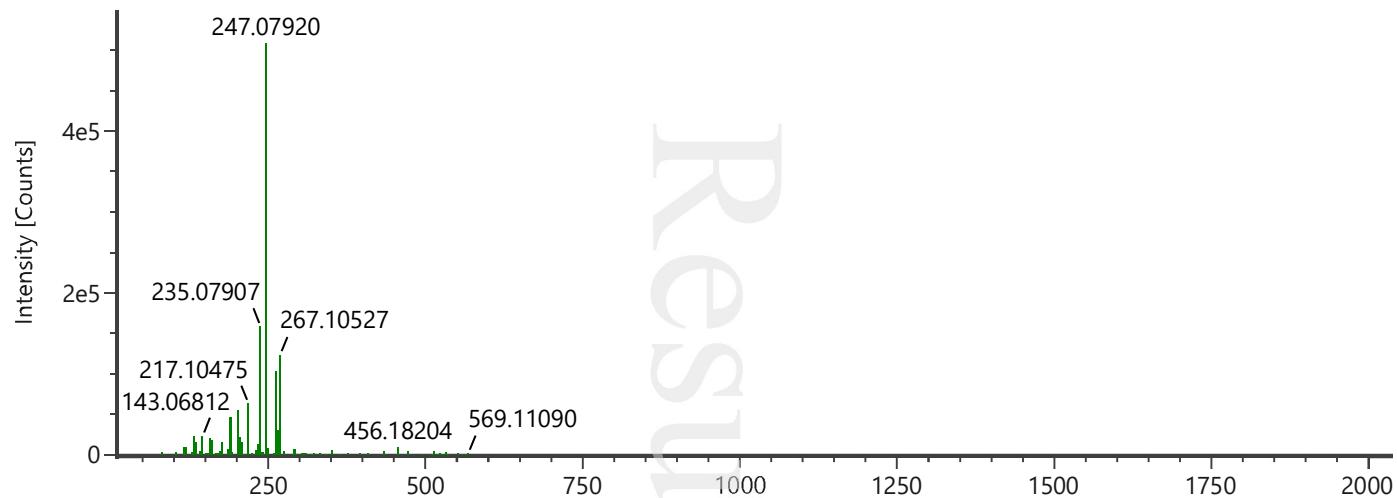
Created on: Sep 07, 2023

Created time: 13:59:44 GMT Daylight Time

Item name: int1_a3 ACN

Channel name: High energy : Time 0.8598 +/- 0.0652 minutes

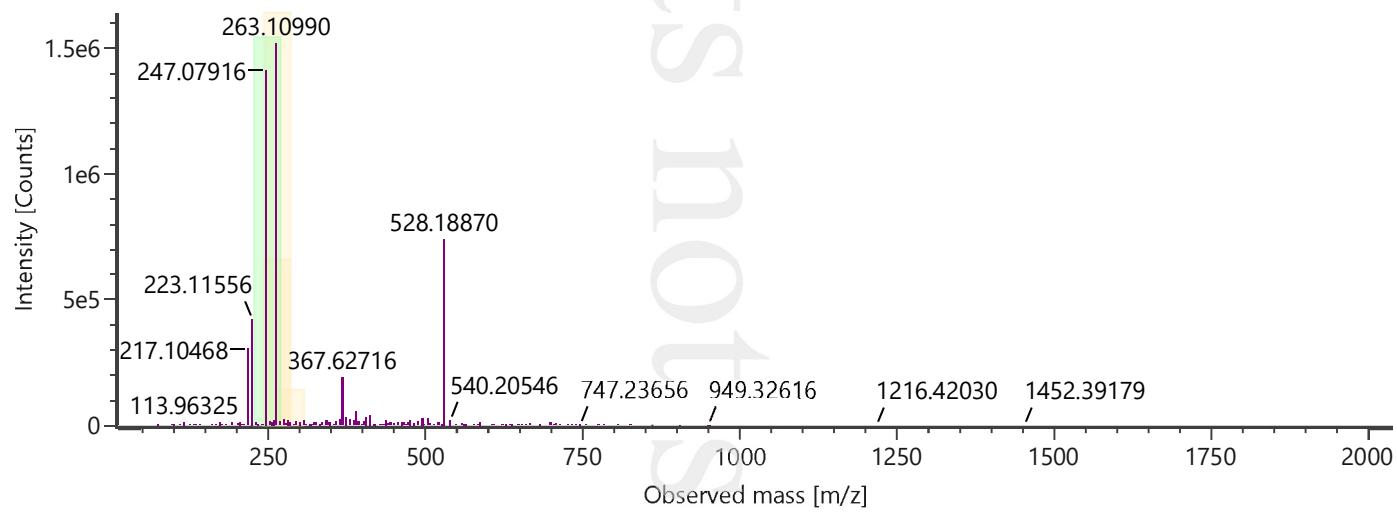
Item description:



Item name: int1_a3 ACN

Channel name: Low energy : Time 1.4035 +/- 0.0652 minutes

Item description:



Item name: MD_M POPLAWSKI

Created by: Chemistry, Chemistry

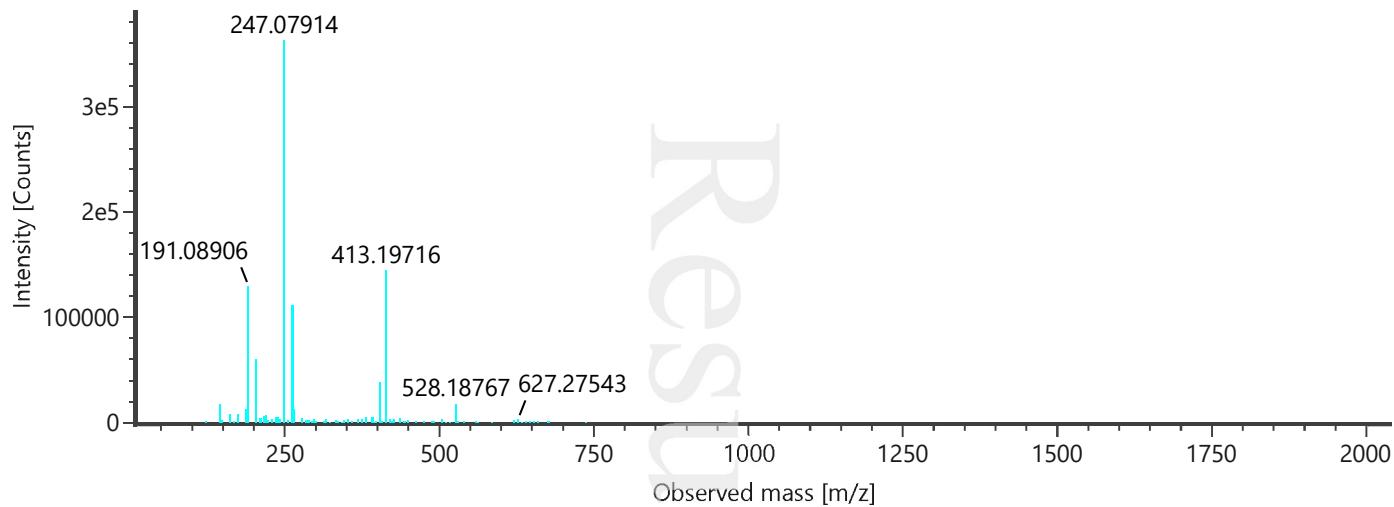
Created on: Sep 07, 2023

Created time: 13:59:44 GMT Daylight Time

Item name: int1_a3 ACN

Channel name: High energy : Time 1.4035 +/- 0.0652 minutes

Item description:



Component name: MP5B.mol

Component name: MP5B.mol

.	Item name	Sample position	Replicate number	Component name	Identification status	Neutral mass (Da)	Observed neutral mass (Da)
1	int1_a3 ACN	2:A,8	1	MP5B.mol	Identified	234.07216	234.0714

.	Item name	Sample position	Replicate number	Component name	Identification status	Observed m/z	Mass error (mDa)
1	int1_a3 ACN	2:A,8	1	MP5B.mol	Identified	235.0787	-0.7

.	Item name	Sample position	Replicate number	Component name	Identification status	Mass error (ppm)	Expected RT (min)	Observed RT (min)
1	int1_a3 ACN	2:A,8	1	MP5B.mol	Identified	-3.1		1.51

.	Item name	Sample position	Replicate number	Component name	Identification status	Detector counts	Response	Adducts
1	int1_a3 ACN	2:A,8	1	MP5B.mol	Identified	4071	2921	+H

.	Item name	Sample position	Replicate number	Component name	Identification status	Formula
1	int1_a3 ACN	2:A,8	1	MP5B.mol	Identified	C11[13C]H11NO4

Component name: MP5B.mol

.	Item name	Sample position	Replicate number	Component name	Identification status	Neutral mass (Da)	Observed neutral mass (Da)
1	int1_a3 ACN	2:A,8	1	MP5B.mol	Identified	234.07216	234.0712

.	Item name	Sample position	Replicate number	Component name	Identification status	Observed m/z	Mass error (mDa)
1	int1_a3 ACN	2:A,8	1	MP5B.mol	Identified	235.0785	-0.9

Item name: MD_M POPLAWSKI

Created time: 13:59:44 GMT Daylight Time

.	Item name	Sample position	Replicate number	Component name	Identification status	Mass error (ppm)	Expected RT (min)	Observed RT (min)
1	int1_a3 ACN	2:A,8	1	MP5B.mol	Identified	-4.0		0.31

.	Item name	Sample position	Replicate number	Component name	Identification status	Detector counts	Response	Adducts
1	int1_a3 ACN	2:A,8	1	MP5B.mol	Identified	6541	6341	+H, -e

.	Item name	Sample position	Replicate number	Component name	Identification status	Formula
1	int1_a3 ACN	2:A,8	1	MP5B.mol	Identified	C11[13C]H11NO4

Component name: MP5B.mol

.	Item name	Sample position	Replicate number	Component name	Identification status	Neutral mass (Da)	Observed neutral mass (Da)
1	int1_a3 ACN	2:A,8	1	MP5B.mol	Identified	234.07216	234.0712

.	Item name	Sample position	Replicate number	Component name	Identification status	Observed m/z	Mass error (mDa)
1	int1_a3 ACN	2:A,8	1	MP5B.mol	Identified	235.0785	-0.9

.	Item name	Sample position	Replicate number	Component name	Identification status	Mass error (ppm)	Expected RT (min)	Observed RT (min)
1	int1_a3 ACN	2:A,8	1	MP5B.mol	Identified	-4.0		1.67

.	Item name	Sample position	Replicate number	Component name	Identification status	Detector counts	Response	Adducts
1	int1_a3 ACN	2:A,8	1	MP5B.mol	Identified	6371	5996	+H, -e

.	Item name	Sample position	Replicate number	Component name	Identification status	Formula
1	int1_a3 ACN	2:A,8	1	MP5B.mol	Identified	C11[13C]H11NO4

Component name: MP5B.mol

.	Item name	Sample position	Replicate number	Component name	Identification status	Neutral mass (Da)	Observed neutral mass (Da)
1	int1_a3 ACN	2:A,8	1	MP5B.mol	Identified	234.07216	234.0719

.	Item name	Sample position	Replicate number	Component name	Identification status	Observed m/z	Mass error (mDa)
1	int1_a3 ACN	2:A,8	1	MP5B.mol	Identified	235.0791	-0.3

.	Item name	Sample position	Replicate number	Component name	Identification status	Mass error (ppm)	Expected RT (min)	Observed RT (min)
1	int1_a3 ACN	2:A,8	1	MP5B.mol	Identified	-1.3		0.81

.	Item name	Sample position	Replicate number	Component name	Identification status	Detector counts	Response	Adducts
1	int1_a3 ACN	2:A,8	1	MP5B.mol	Identified	30111	28278	+H

Item name: MD_M POPLAWSKI

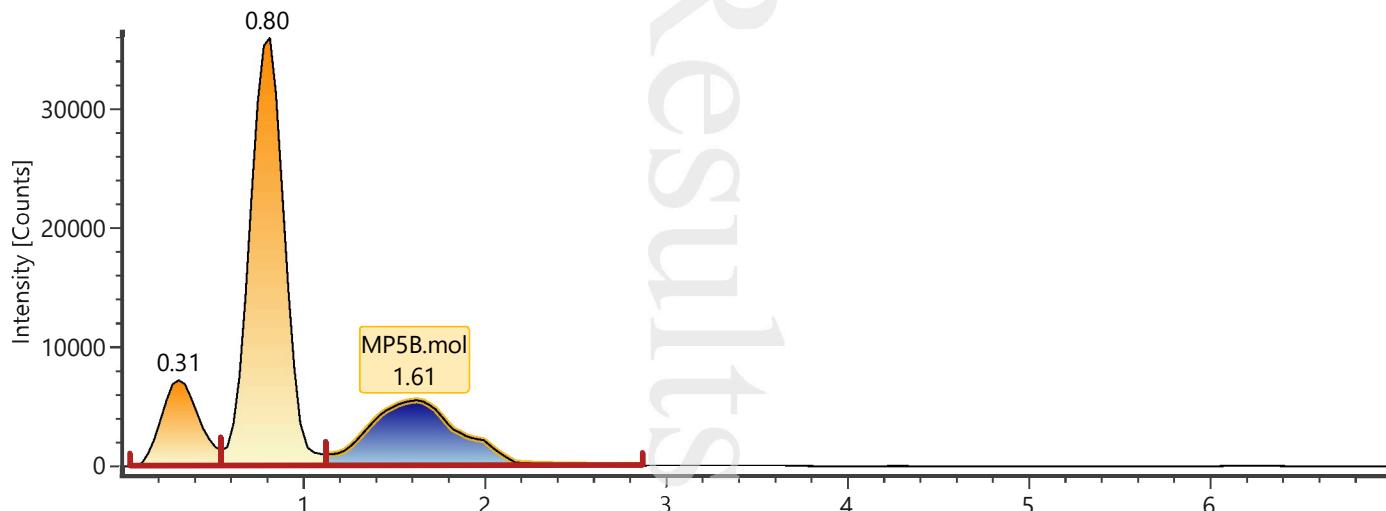
Created time: 13:59:44 GMT Daylight Time

.	Item name	Sample position	Replicate number	Component name	Identification status	Formula
1	int1_a3 ACN	2:A,8	1	MP5B.mol	Identified	C11[13C]H11NO4

Item name: int1_a3 ACN

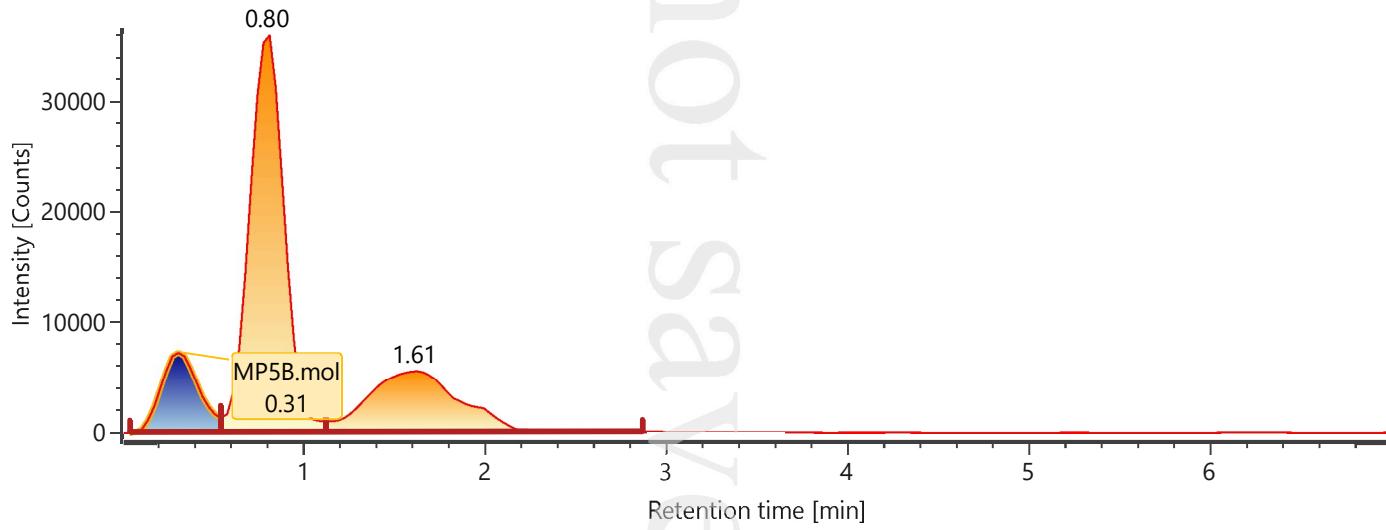
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Channel name: MP5B.mol [+H] : (35.9 PPM) 235.0787



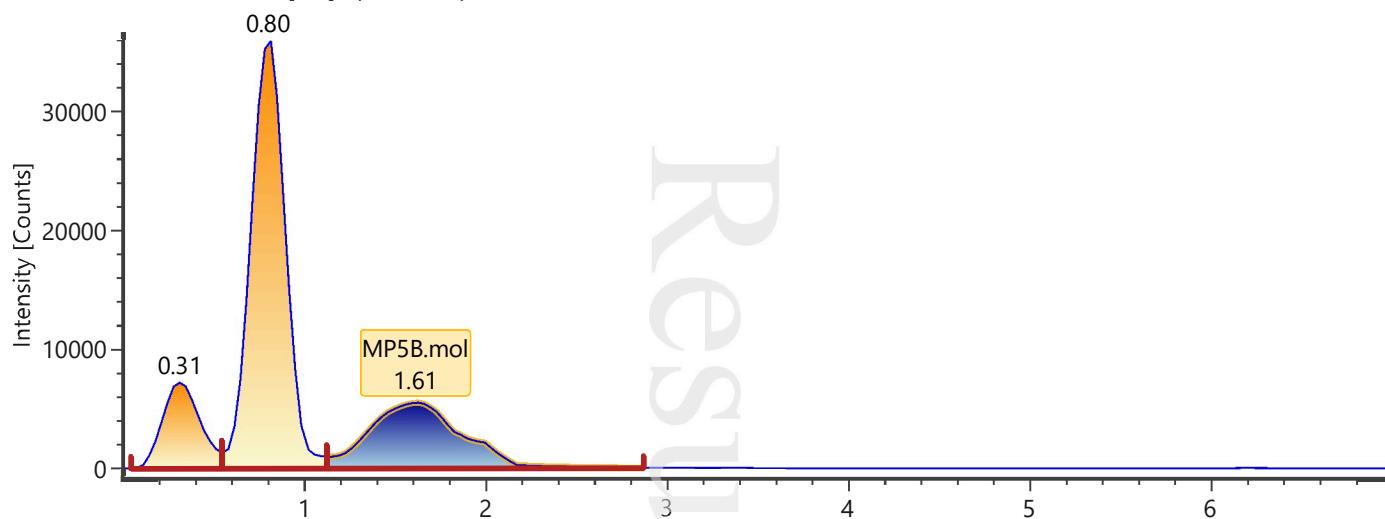
Item name: int1_a3 ACN

Channel name: MP5B.mol [+H] : (35.9 PPM) 235.0785



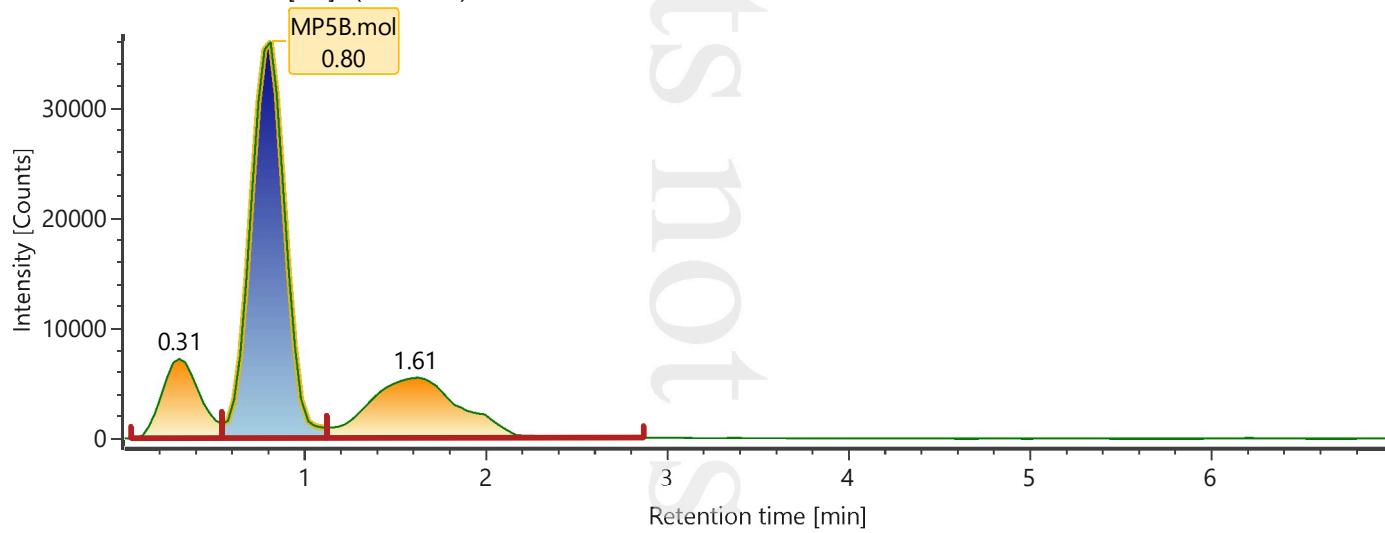
Item name: int1_a3 ACN

Channel name: MP5B.mol [+H] : (35.9 PPM) 235.0785



Item name: int1_a3 ACN

Channel name: MP5B.mol [+H] : (35.9 PPM) 235.0791



Item name: MD_M POPLAWSKI

Created by: Chemistry, Chemistry

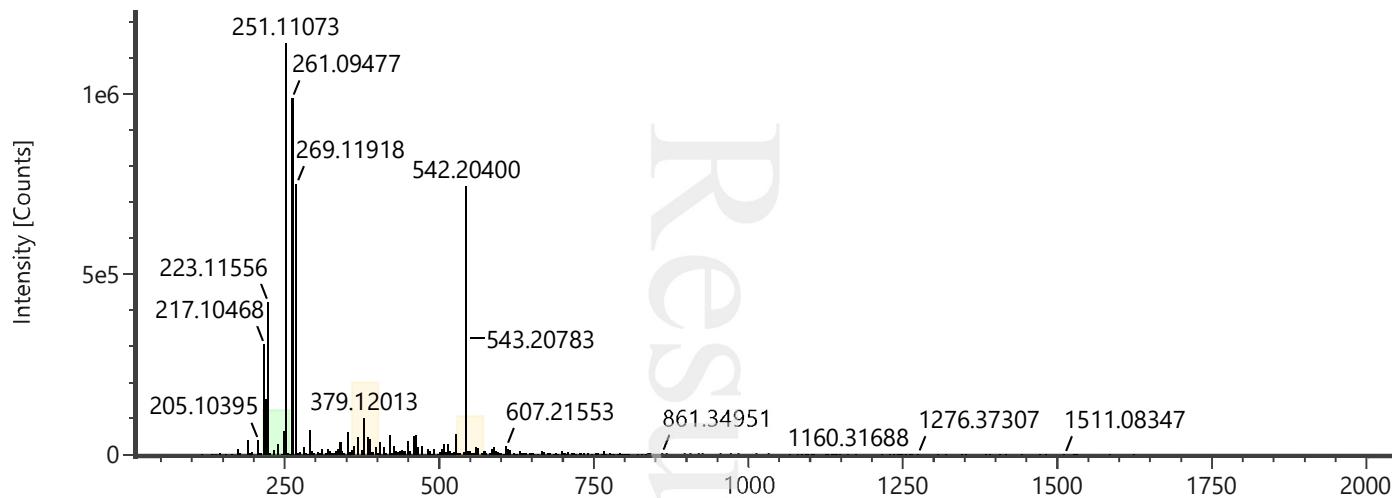
Created on: Sep 07, 2023

Created time: 13:59:44 GMT Daylight Time

Item name: int1_a3 ACN

Channel name: Low energy : Time 1.5085 +/- 0.0652 minutes

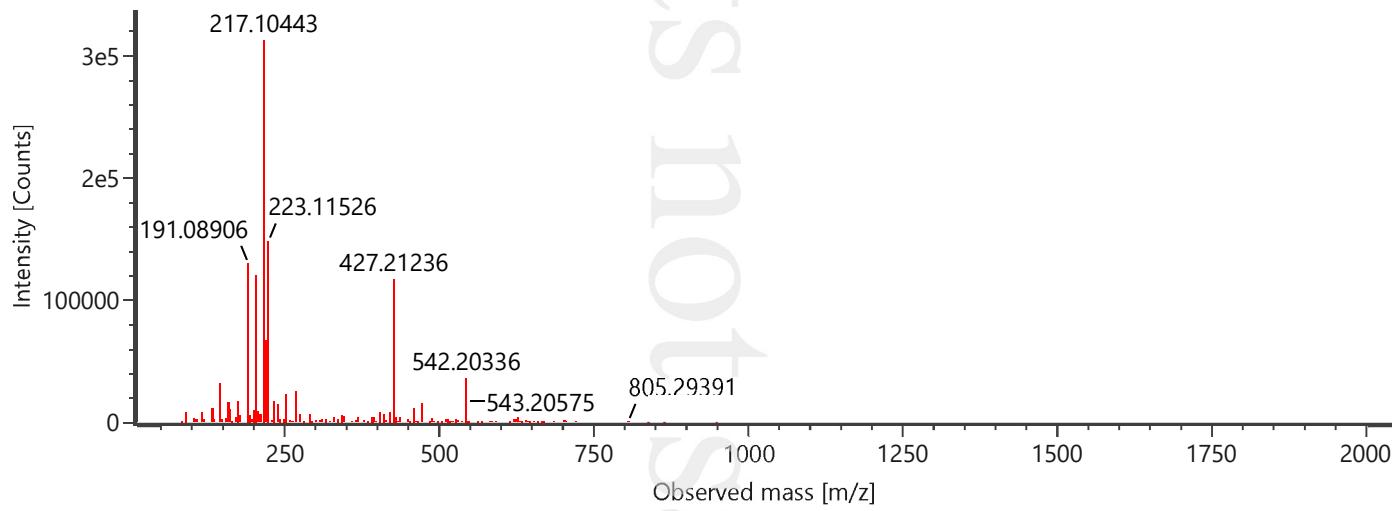
Item description:



Item name: int1_a3 ACN

Channel name: High energy : Time 1.5085 +/- 0.0652 minutes

Item description:



Item name: MD_M POPLAWSKI

Created by: Chemistry, Chemistry

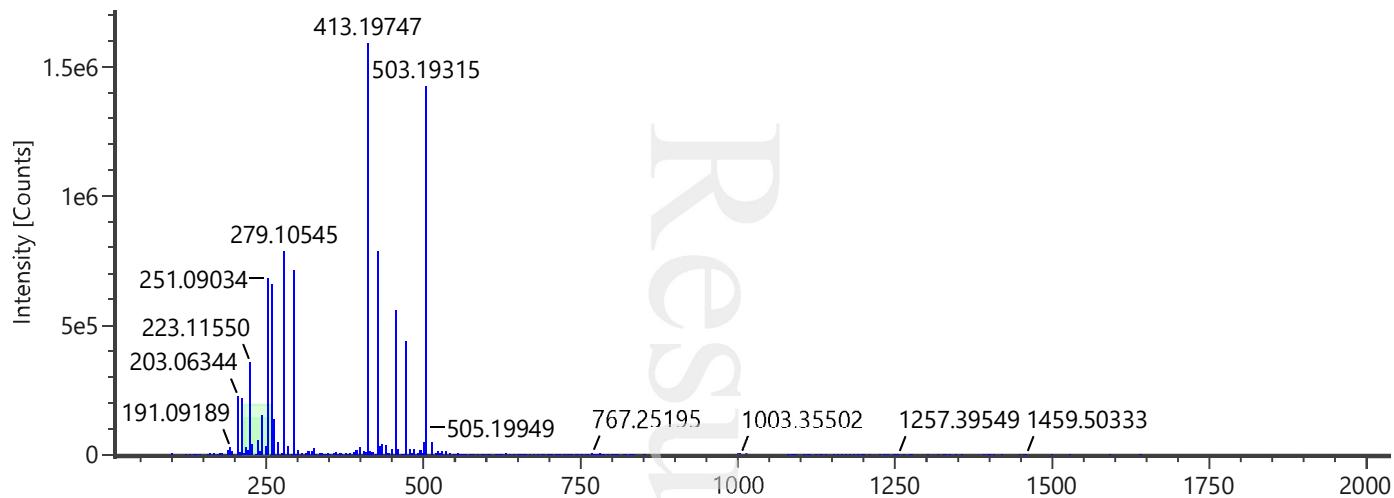
Created on: Sep 07, 2023

Created time: 13:59:44 GMT Daylight Time

Item name: int1_a3 ACN

Channel name: Low energy : Time 0.3106 +/- 0.0652 minutes

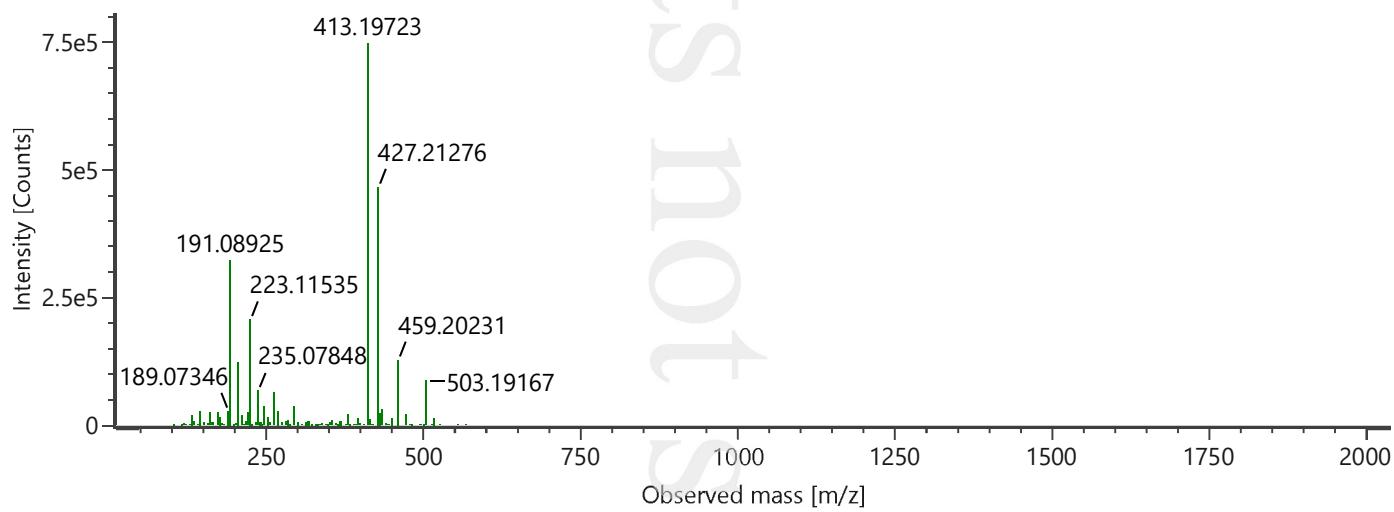
Item description:



Item name: int1_a3 ACN

Channel name: High energy : Time 0.3106 +/- 0.0652 minutes

Item description:



Item name: MD_M POPLAWSKI

Created by: Chemistry, Chemistry

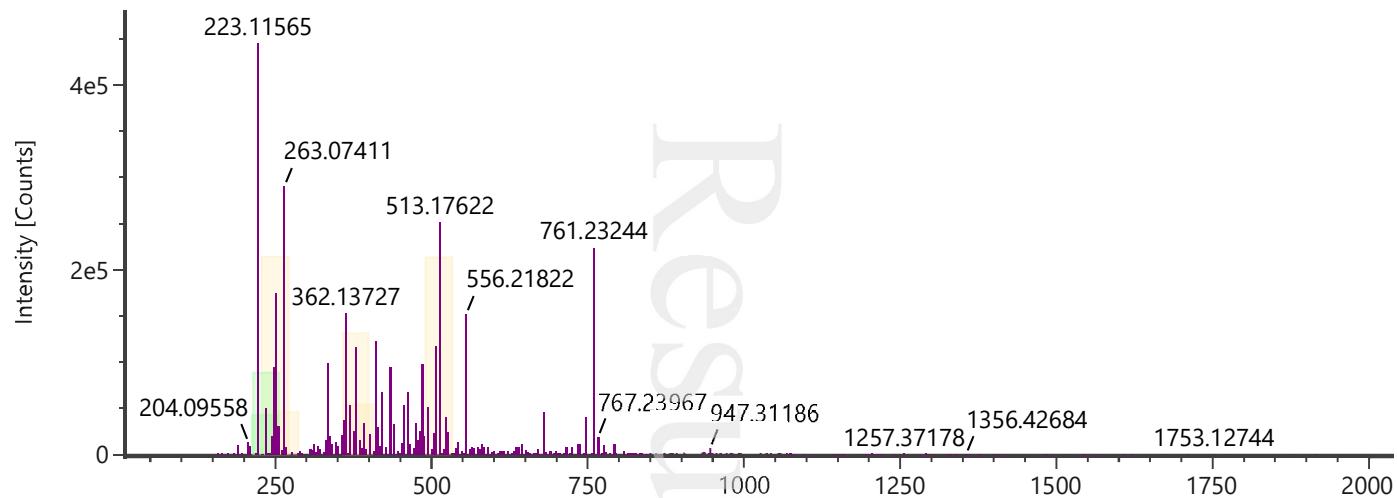
Created on: Sep 07, 2023

Created time: 13:59:44 GMT Daylight Time

Item name: int1_a3 ACN

Channel name: Low energy : Time 1.6694 +/- 0.0652 minutes

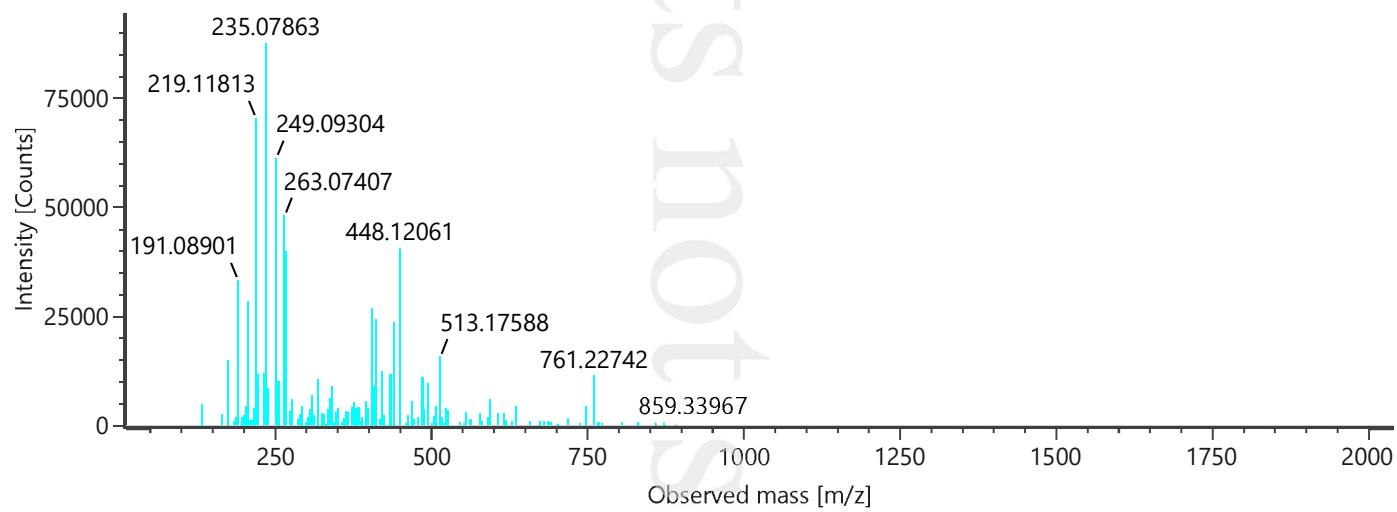
Item description:



Item name: int1_a3 ACN

Channel name: High energy : Time 1.6694 +/- 0.0652 minutes

Item description:



Item name: MD_M POPLAWSKI

Created by: Chemistry, Chemistry

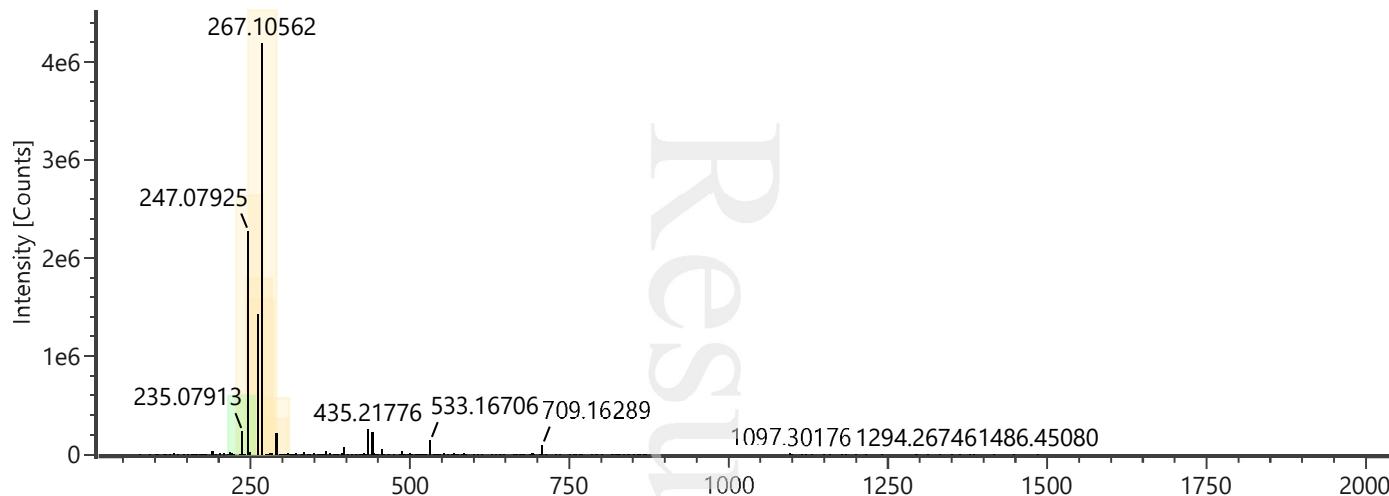
Created on: Sep 07, 2023

Created time: 13:59:44 GMT Daylight Time

Item name: int1_a3 ACN

Channel name: Low energy : Time 0.8061 +/- 0.0652 minutes

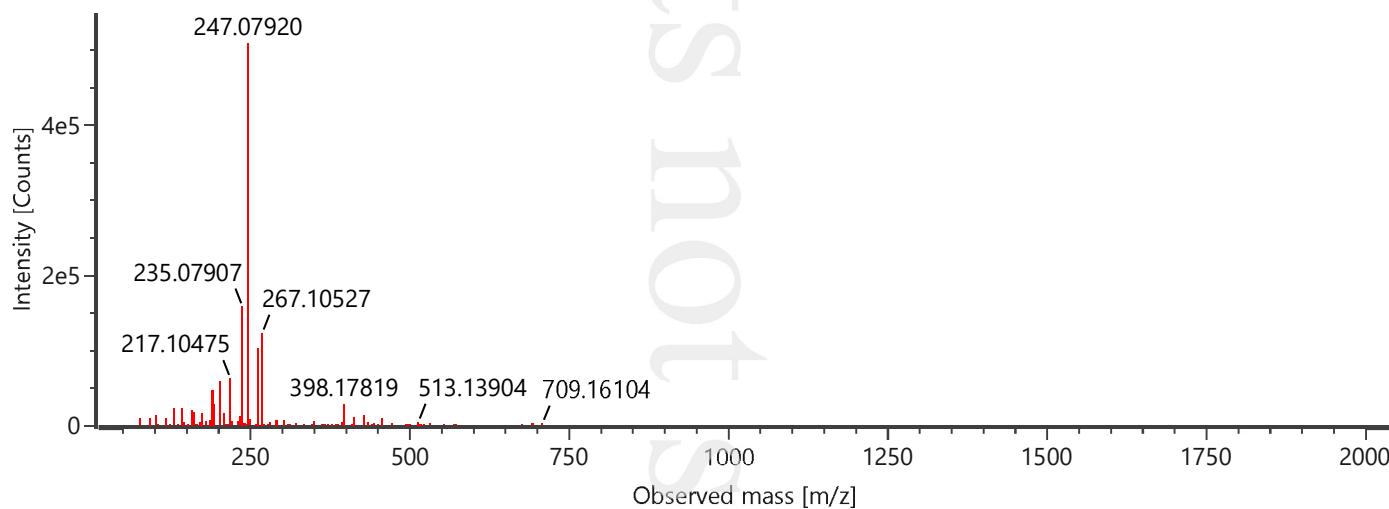
Item description:



Item name: int1_a3 ACN

Channel name: High energy : Time 0.8061 +/- 0.0652 minutes

Item description:



Component name: MP6B.mol

Component name: MP6B.mol

.	Item name	Sample position	Replicate number	Component name	Identification status	Neutral mass (Da)	Observed neutral mass (Da)
1	int1_a3 ACN	2:A,8	1	MP6B.mol	Identified	262.10346	262.1030

.	Item name	Sample position	Replicate number	Component name	Identification status	Observed m/z	Mass error (mDa)
1	int1_a3 ACN	2:A,8	1	MP6B.mol	Identified	262.1025	-0.4

Item name: MD_M POPLAWSKI

Created time: 13:59:44 GMT Daylight Time

.	Item name	Sample position	Replicate number	Component name	Identification status	Mass error (ppm)	Expected RT (min)	Observed RT (min)
1	int1_a3 ACN	2:A,8	1	MP6B.mol	Identified	-1.6		0.50

.	Item name	Sample position	Replicate number	Component name	Identification status	Detector counts	Response	Adducts
1	int1_a3 ACN	2:A,8	1	MP6B.mol	Identified	56420	56420	-e

.	Item name	Sample position	Replicate number	Component name	Identification status	Formula
1	int1_a3 ACN	2:A,8	1	MP6B.mol	Identified	C13[13C]H15NO4

Component name: MP6B.mol

.	Item name	Sample position	Replicate number	Component name	Identification status	Neutral mass (Da)	Observed neutral mass (Da)
1	int1_a3 ACN	2:A,8	1	MP6B.mol	Identified	262.10346	262.1026

.	Item name	Sample position	Replicate number	Component name	Identification status	Observed m/z	Mass error (mDa)
1	int1_a3 ACN	2:A,8	1	MP6B.mol	Identified	263.1099	-0.8

.	Item name	Sample position	Replicate number	Component name	Identification status	Mass error (ppm)	Expected RT (min)	Observed RT (min)
1	int1_a3 ACN	2:A,8	1	MP6B.mol	Identified	-3.2		1.42

.	Item name	Sample position	Replicate number	Component name	Identification status	Detector counts	Response
1	int1_a3 ACN	2:A,8	1	MP6B.mol	Identified	278796	193146

.	Item name	Sample position	Replicate number	Component name	Identification status	Adducts	Formula
1	int1_a3 ACN	2:A,8	1	MP6B.mol	Identified	+H, +Na, -e	C13[13C]H15NO4

Component name: MP6B.mol

.	Item name	Sample position	Replicate number	Component name	Identification status	Neutral mass (Da)	Observed neutral mass (Da)
1	int1_a3 ACN	2:A,8	1	MP6B.mol	Identified	262.10346	262.1032

.	Item name	Sample position	Replicate number	Component name	Identification status	Observed m/z	Mass error (mDa)
1	int1_a3 ACN	2:A,8	1	MP6B.mol	Identified	262.1026	-0.3

.	Item name	Sample position	Replicate number	Component name	Identification status	Mass error (ppm)	Expected RT (min)	Observed RT (min)
1	int1_a3 ACN	2:A,8	1	MP6B.mol	Identified	-1.0		0.85

.	Item name	Sample position	Replicate number	Component name	Identification status	Detector counts	Response
1	int1_a3 ACN	2:A,8	1	MP6B.mol	Identified	181524	181524

Item name: MD_M POPLAWSKI

Created time: 13:59:44 GMT Daylight Time

.	Item name	Sample position	Replicate number	Component name	Identification status	Adducts	Formula
1	int1_a3 ACN	2:A,8	1	MP6B.mol	Identified	-e	C13[13C]H15NO4

Component name: MP6B.mol

.	Item name	Sample position	Replicate number	Component name	Identification status	Neutral mass (Da)	Observed neutral mass (Da)
1	int1_a3 ACN	2:A,8	1	MP6B.mol	Identified	262.10346	262.1023

.	Item name	Sample position	Replicate number	Component name	Identification status	Observed m/z	Mass error (mDa)
1	int1_a3 ACN	2:A,8	1	MP6B.mol	Identified	263.1096	-1.1

.	Item name	Sample position	Replicate number	Component name	Identification status	Mass error (ppm)	Expected RT (min)	Observed RT (min)
1	int1_a3 ACN	2:A,8	1	MP6B.mol	Identified	-4.3		0.78

.	Item name	Sample position	Replicate number	Component name	Identification status	Detector counts	Response
1	int1_a3 ACN	2:A,8	1	MP6B.mol	Identified	169844	154511

.	Item name	Sample position	Replicate number	Component name	Identification status	Adducts	Formula
1	int1_a3 ACN	2:A,8	1	MP6B.mol	Identified	+H	C13[13C]H15NO4

Component name: MP6B.mol

.	Item name	Sample position	Replicate number	Component name	Identification status	Neutral mass (Da)	Observed neutral mass (Da)
1	int1_a3 ACN	2:A,8	1	MP6B.mol	Identified	262.10346	262.1025

.	Item name	Sample position	Replicate number	Component name	Identification status	Observed m/z	Mass error (mDa)
1	int1_a3 ACN	2:A,8	1	MP6B.mol	Identified	263.1098	-0.9

.	Item name	Sample position	Replicate number	Component name	Identification status	Mass error (ppm)	Expected RT (min)	Observed RT (min)
1	int1_a3 ACN	2:A,8	1	MP6B.mol	Identified	-3.6		1.58

.	Item name	Sample position	Replicate number	Component name	Identification status	Detector counts	Response
1	int1_a3 ACN	2:A,8	1	MP6B.mol	Identified	108005	98474

.	Item name	Sample position	Replicate number	Component name	Identification status	Adducts	Formula
1	int1_a3 ACN	2:A,8	1	MP6B.mol	Identified	+H	C13[13C]H15NO4

Component name: MP6B.mol

.	Item name	Sample position	Replicate number	Component name	Identification status	Neutral mass (Da)	Observed neutral mass (Da)
1	int1_a3 ACN	2:A,8	1	MP6B.mol	Identified	262.10346	262.1034

Item name: MD_M POPLAWSKI

Created time: 13:59:44 GMT Daylight Time

.	Item name	Sample position	Replicate number	Component name	Identification status	Observed m/z	Mass error (mDa)
1	int1_a3 ACN	2:A,8	1	MP6B.mol	Identified	262.1028	-0.1

.	Item name	Sample position	Replicate number	Component name	Identification status	Mass error (ppm)	Expected RT (min)	Observed RT (min)
1	int1_a3 ACN	2:A,8	1	MP6B.mol	Identified	-0.3		1.82

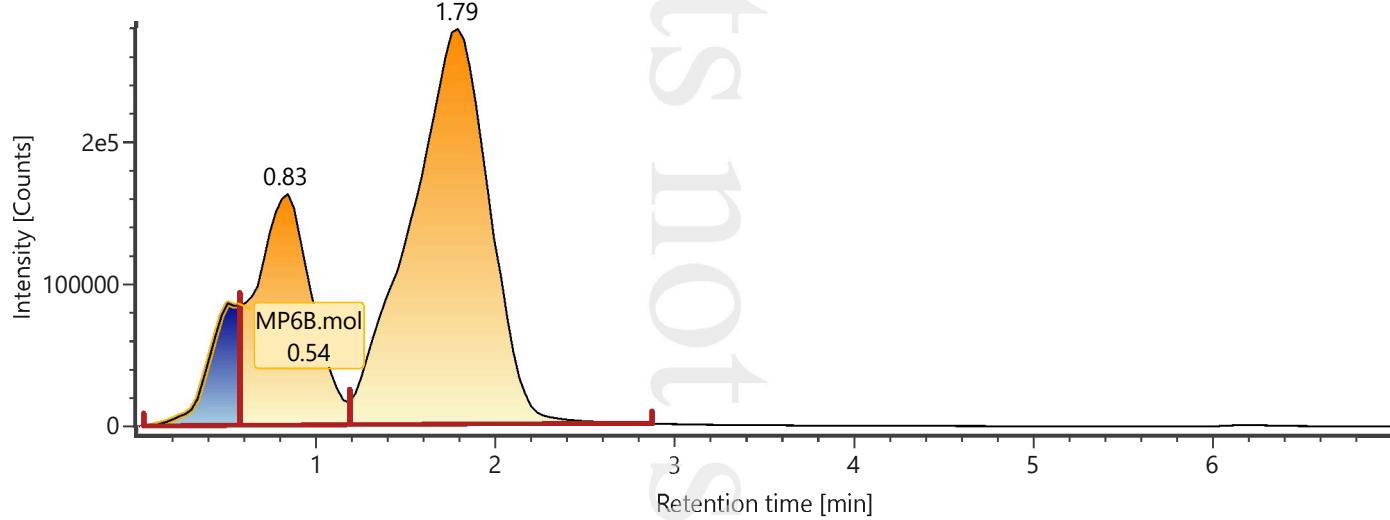
.	Item name	Sample position	Replicate number	Component name	Identification status	Detector counts	Response
1	int1_a3 ACN	2:A,8	1	MP6B.mol	Identified	508331	328849

.	Item name	Sample position	Replicate number	Component name	Identification status	Adducts	Formula
1	int1_a3 ACN	2:A,8	1	MP6B.mol	Identified	-e, +Na	C13[13C]H15NO4

Item name: int1_a3 ACN

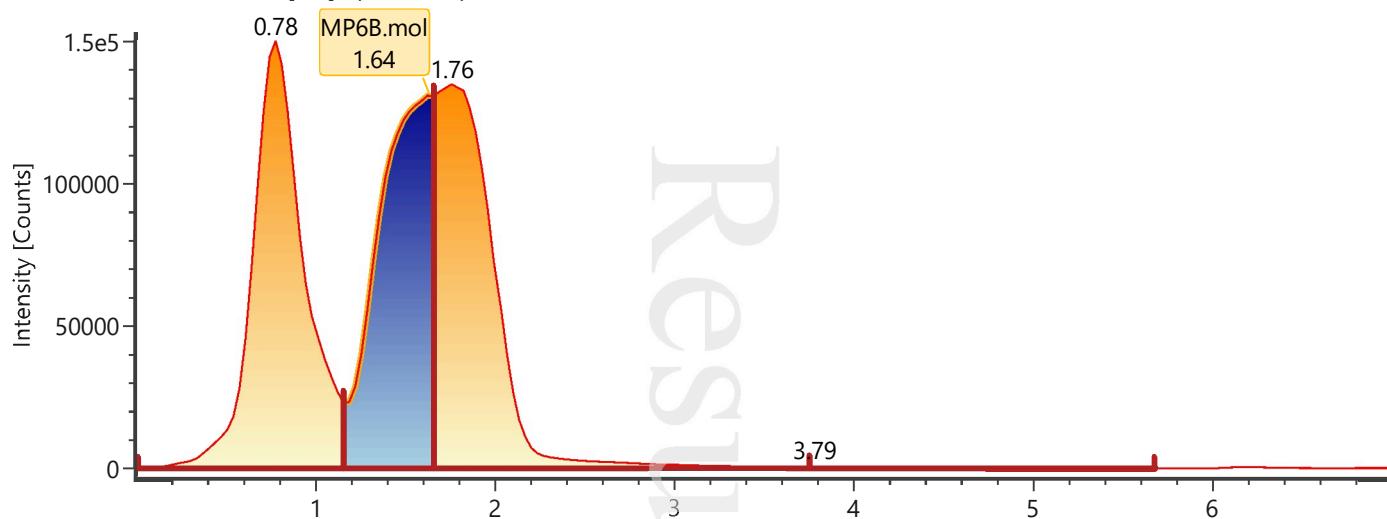
Item name: int1_a3 ACN

Channel name: MP6B.mol [-e] : (35.9 PPM) 262.1025



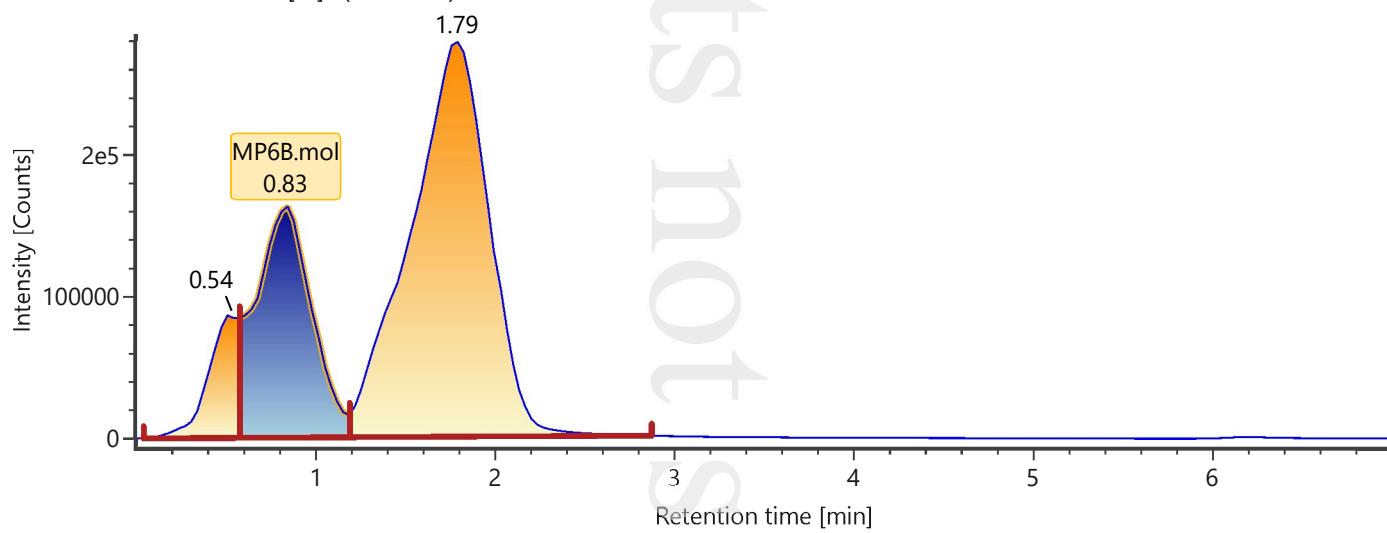
Item name: int1_a3 ACN

Channel name: MP6B.mol [+H] : (35.9 PPM) 263.1099



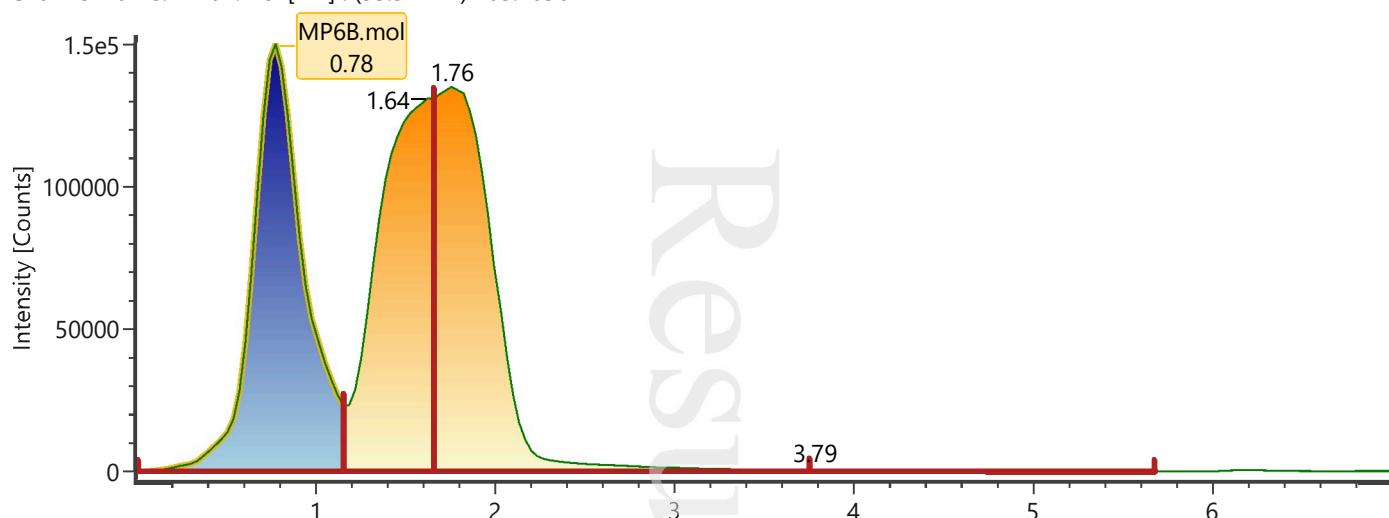
Item name: int1_a3 ACN

Channel name: MP6B.mol [-e] : (35.9 PPM) 262.1026



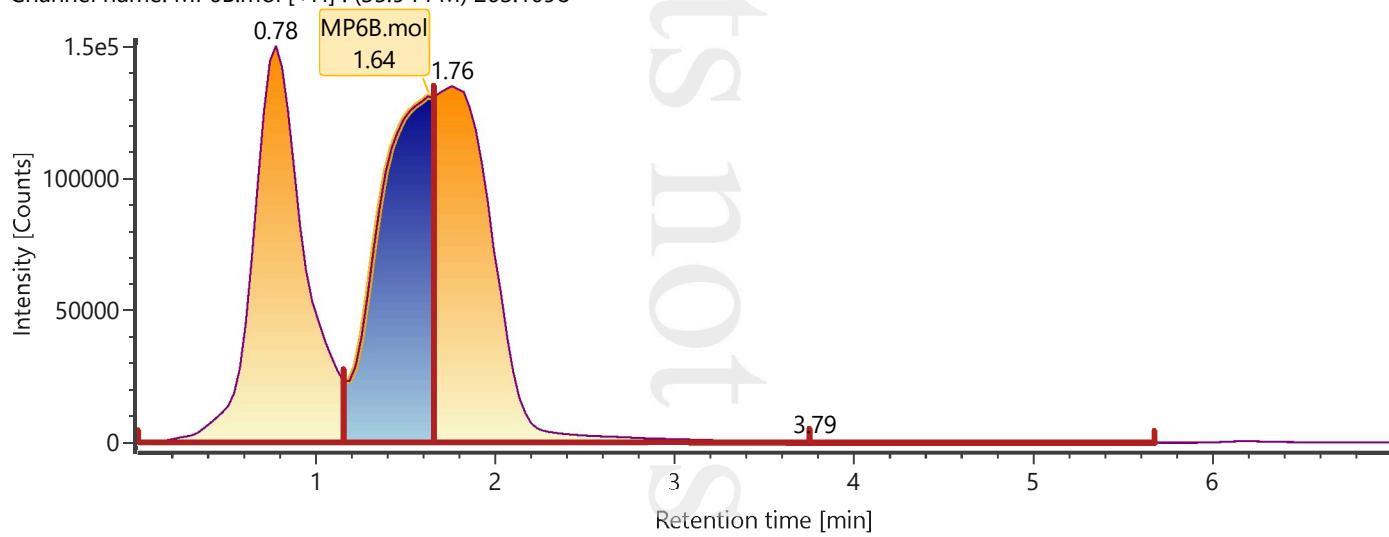
Item name: int1_a3 ACN

Channel name: MP6B.mol [+H] : (35.9 PPM) 263.1096



Item name: int1_a3 ACN

Channel name: MP6B.mol [+H] : (35.9 PPM) 263.1098



Item name: MD_M POPLAWSKI

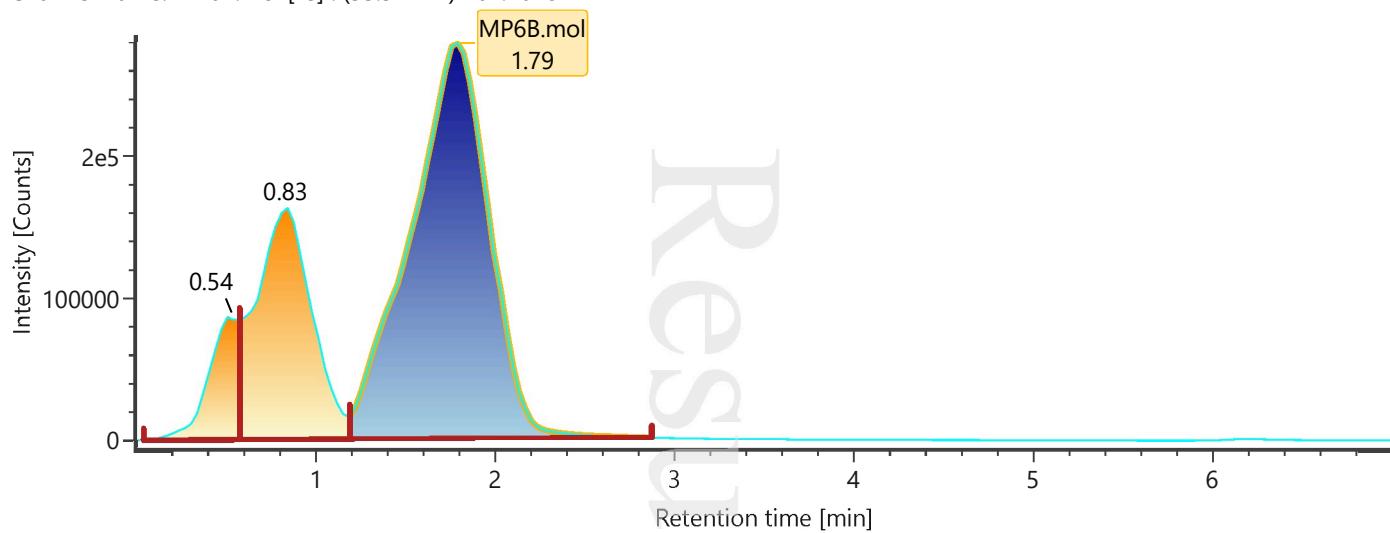
Created by: Chemistry, Chemistry

Created on: Sep 07, 2023

Created time: 13:59:44 GMT Daylight Time

Item name: int1_a3 ACN

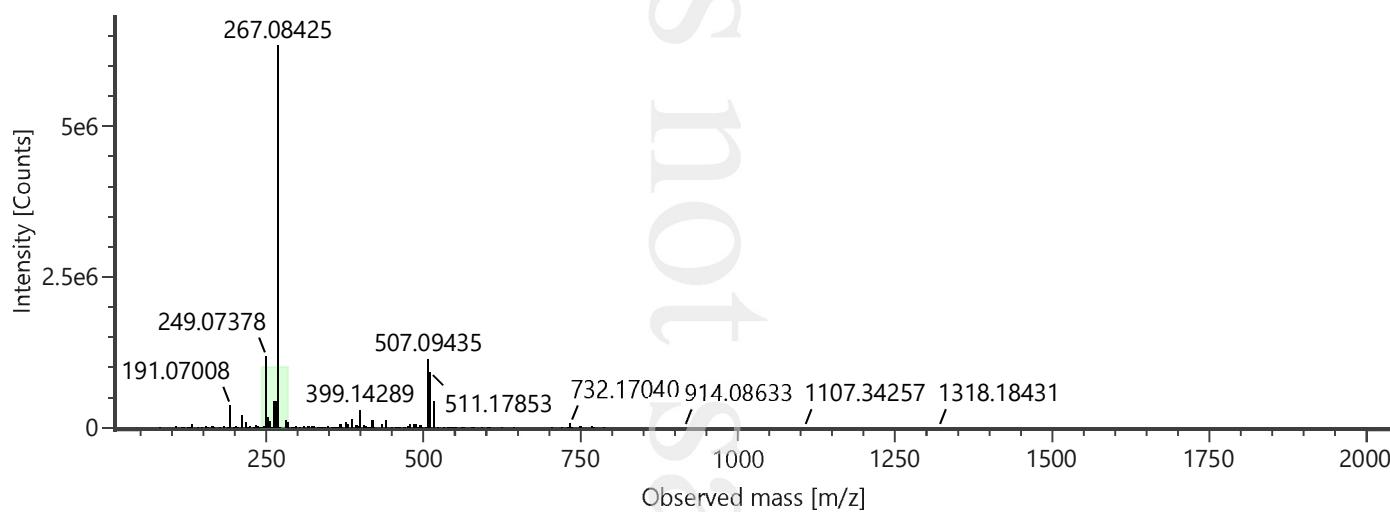
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Item name: int1_a3 ACN

Item description:

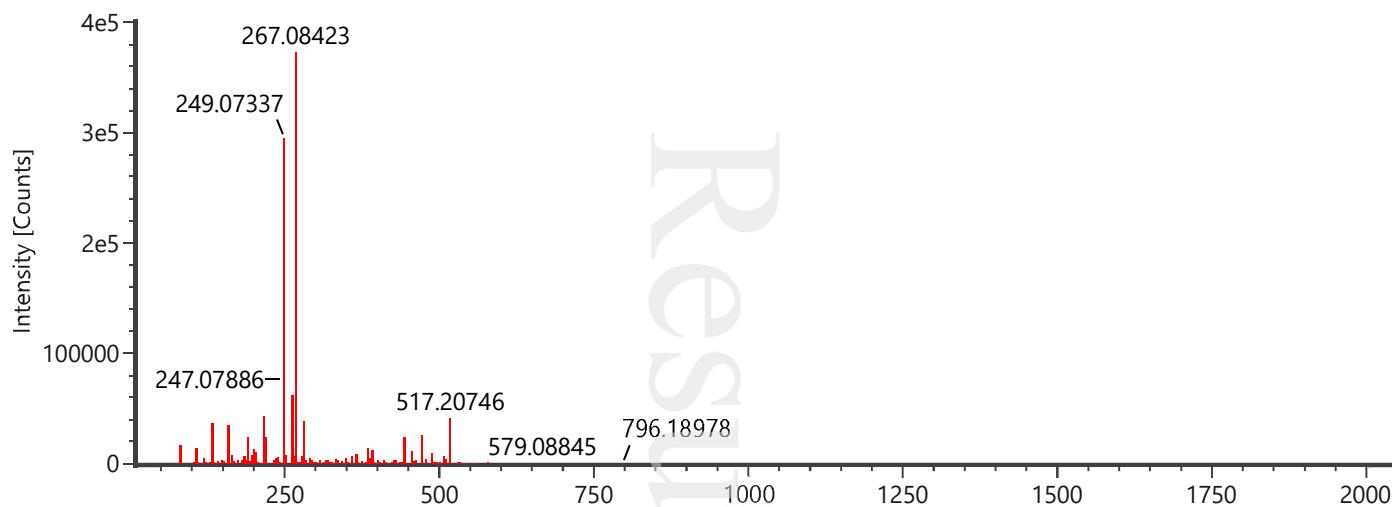
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Item name: int1_a3 ACN

Channel name: High energy : Time 0.5019 +/- 0.0652 minutes

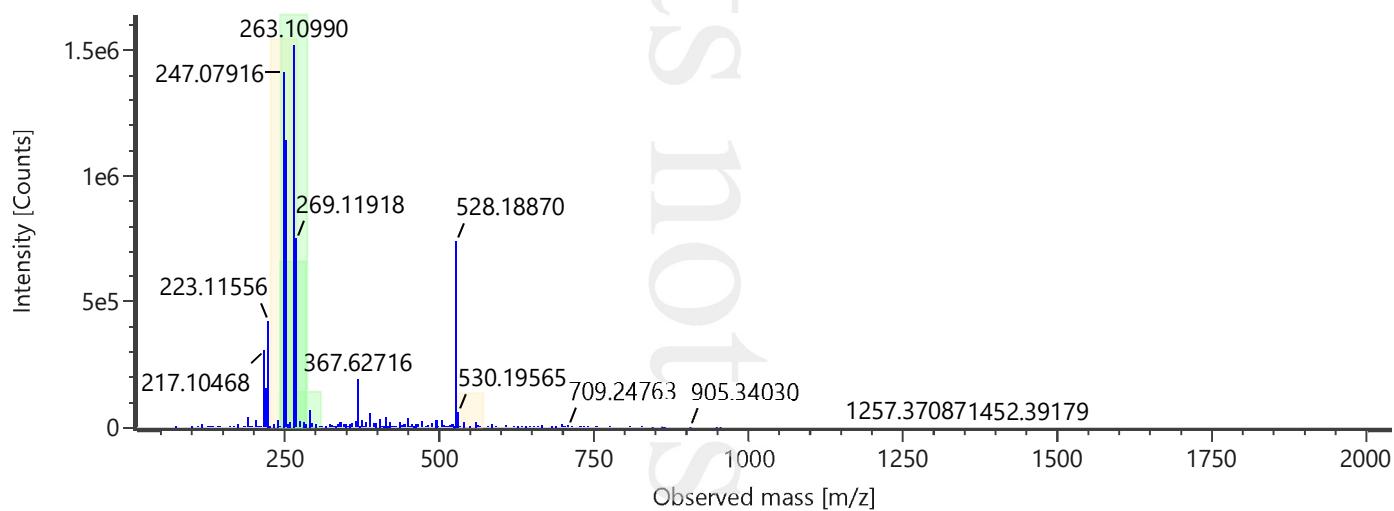
Item description:



Item name: int1_a3 ACN

Channel name: Low energy : Time 1.4210 +/- 0.0652 minutes

Item description:



Item name: MD_M POPLAWSKI

Created by: Chemistry, Chemistry

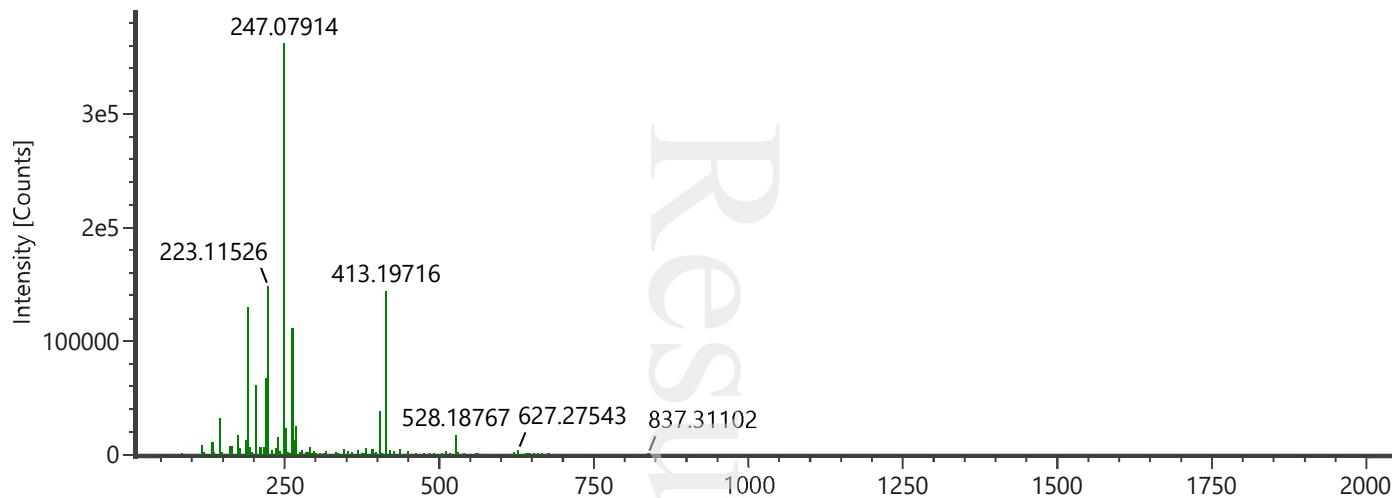
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Created time: 13:59:44 GMT Daylight Time

Item name: int1_a3 ACN

Channel name: High energy : Time 1.4210 +/- 0.0652 minutes

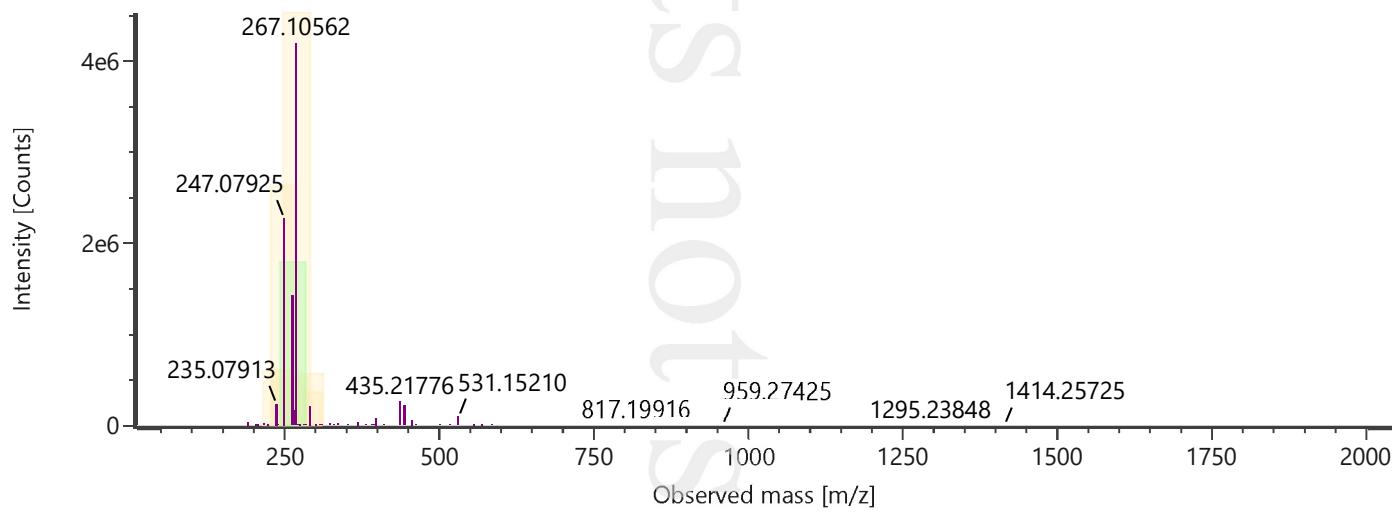
Item description:



Item name: int1_a3 ACN

Channel name: Low energy : Time 0.8481 +/- 0.0652 minutes

Item description:



Item name: MD_M POPLAWSKI

Created by: Chemistry, Chemistry

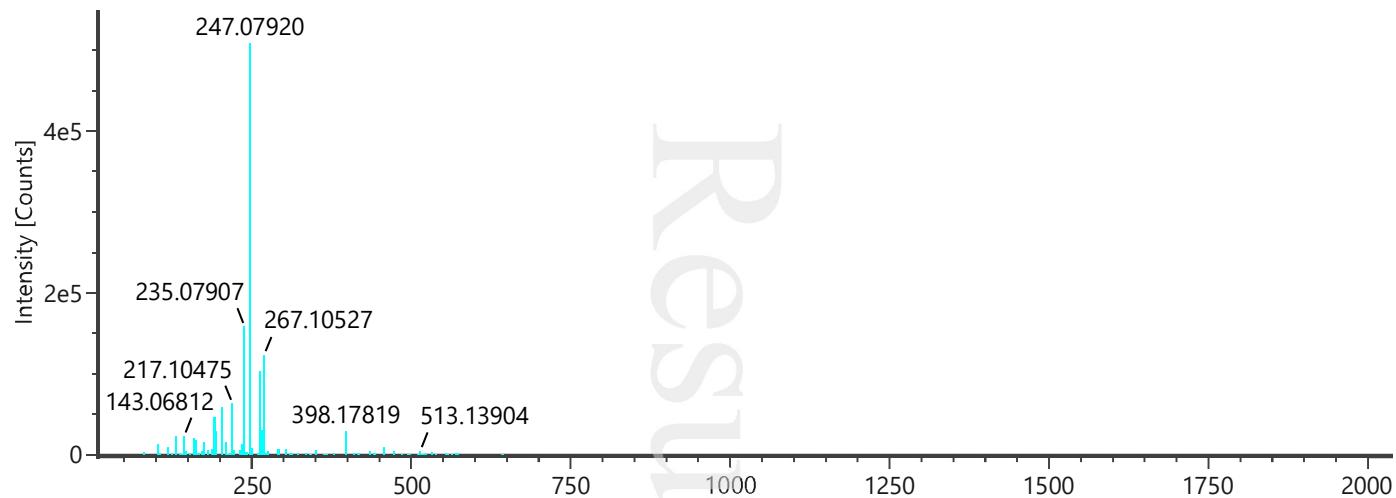
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Item name: int1_a3 ACN

Channel name: High energy : Time 0.8481 +/- 0.0652 minutes

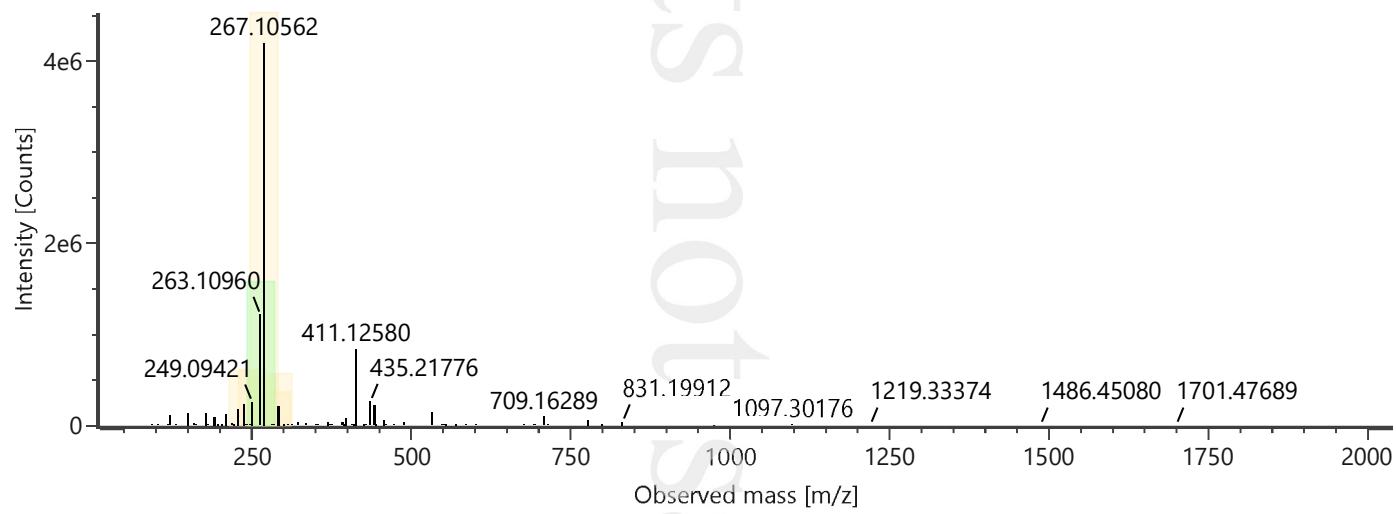
Item description:



Item name: int1_a3 ACN

Channel name: Low energy : Time 0.7752 +/- 0.0652 minutes

Item description:



Item name: MD_M POPLAWSKI

Created by: Chemistry, Chemistry

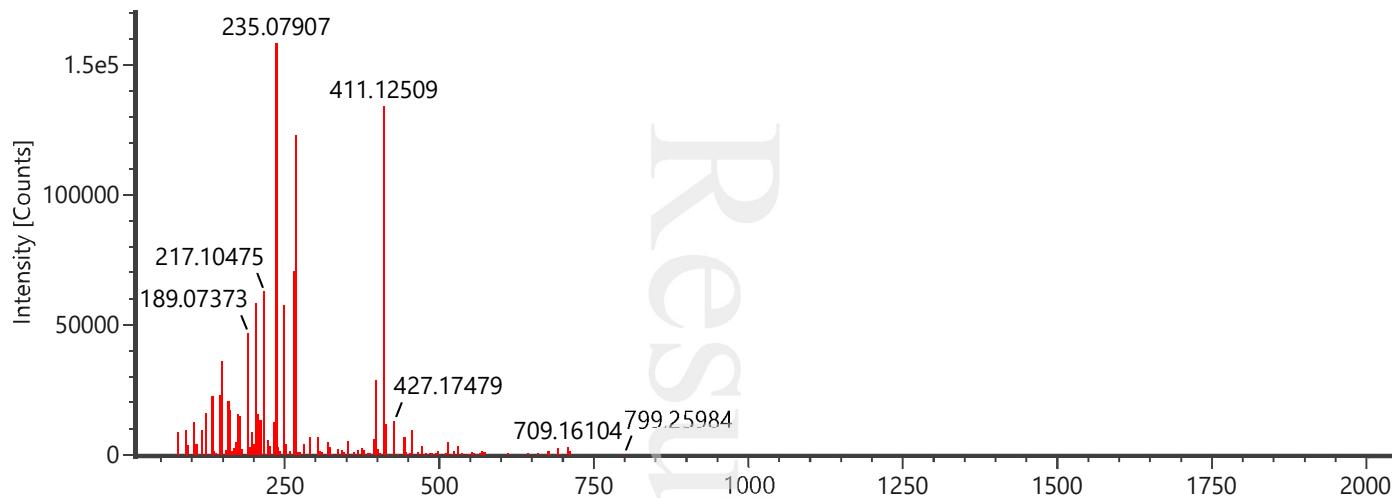
Created on: Sep 07, 2023

Created time: 13:59:44 GMT Daylight Time

Item name: int1_a3 ACN

Channel name: High energy : Time 0.7752 +/- 0.0652 minutes

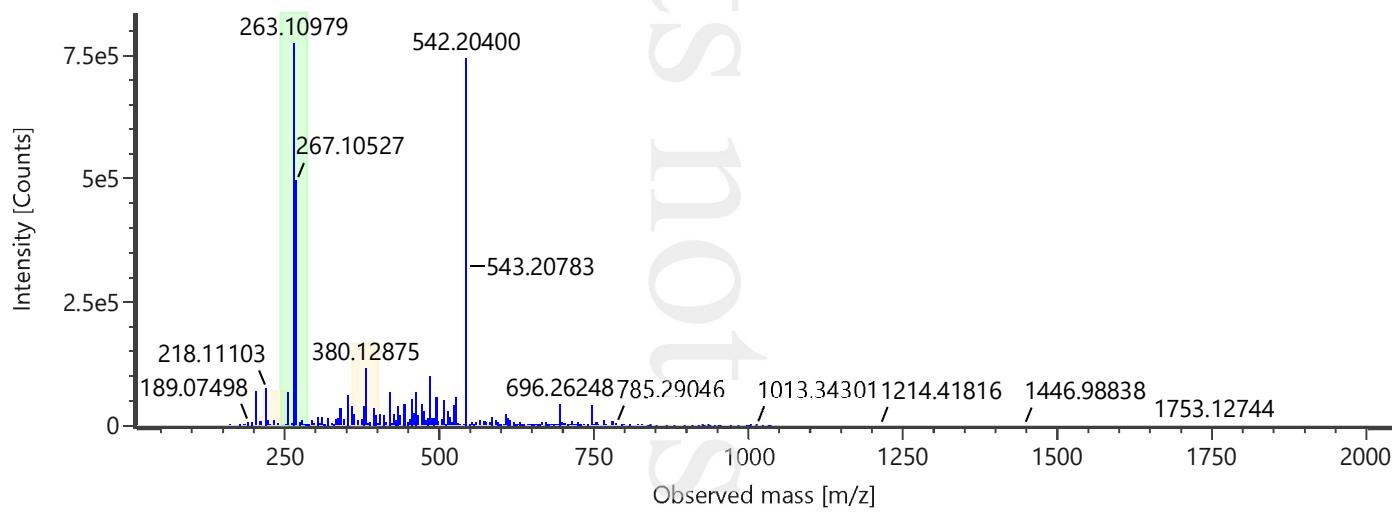
Item description:



Item name: int1_a3 ACN

Channel name: Low energy : Time 1.5801 +/- 0.0652 minutes

Item description:



Item name: MD_M POPLAWSKI

Created by: Chemistry, Chemistry

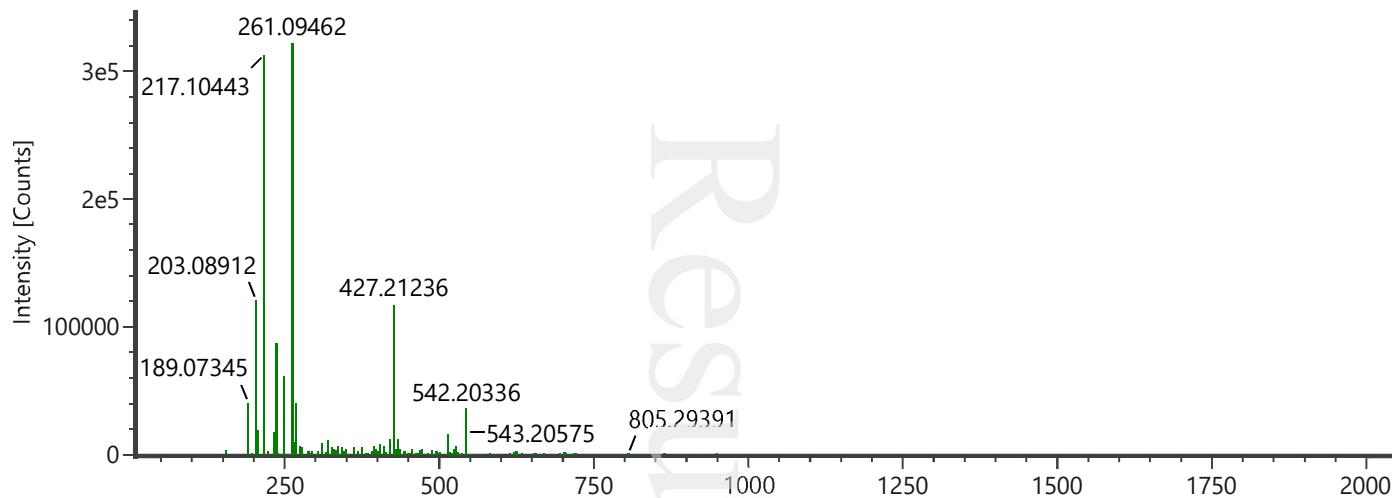
Created on: Sep 07, 2023

Created time: 13:59:44 GMT Daylight Time

Item name: int1_a3 ACN

Channel name: High energy : Time 1.5801 +/- 0.0652 minutes

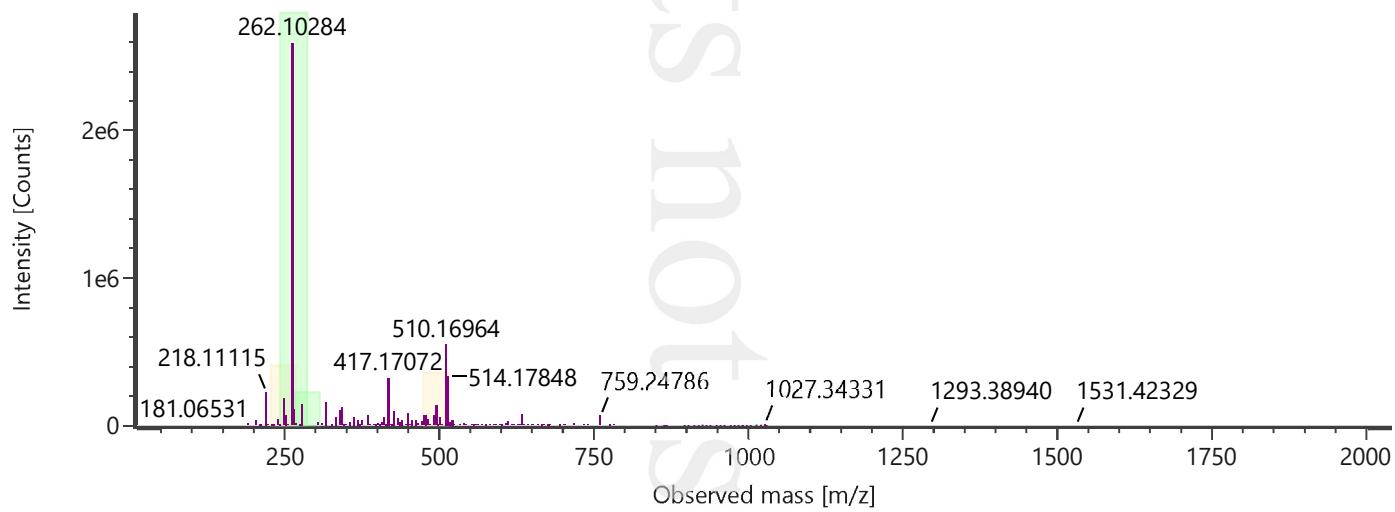
Item description:



Item name: int1_a3 ACN

Channel name: Low energy : Time 1.8162 +/- 0.0652 minutes

Item description:



Item name: MD_M POPLAWSKI

Created by: Chemistry, Chemistry

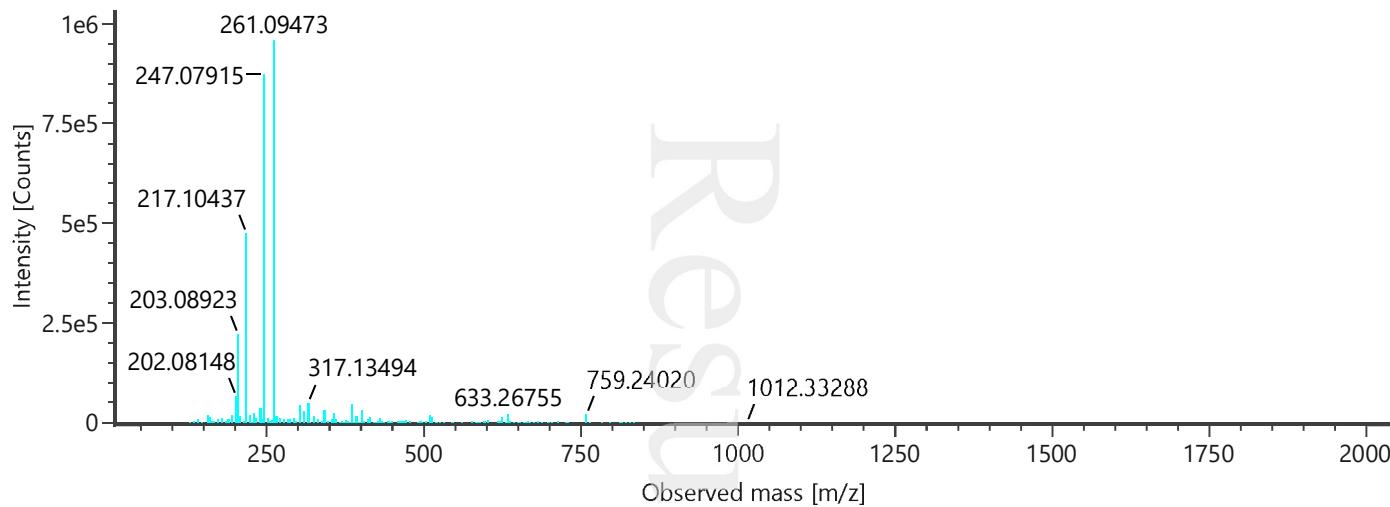
Created on: Sep 07, 2023

Created time: 13:59:44 GMT Daylight Time

Item name: int1_a3 ACN

Channel name: High energy : Time 1.8162 +/- 0.0652 minutes

Item description:



Component name: MP7B.mol

Component name: MP7B.mol

.	Item name	Sample position	Replicate number	Component name	Identification status	Neutral mass (Da)	Observed neutral mass (Da)
1	int1_a3 ACN	2:A,8	1	MP7B.mol	Identified	510.15489	510.1595

.	Item name	Sample position	Replicate number	Component name	Identification status	Observed m/z	Mass error (mDa)
1	int1_a3 ACN	2:A,8	1	MP7B.mol	Identified	549.1227	4.6

.	Item name	Sample position	Replicate number	Component name	Identification status	Mass error (ppm)	Expected RT (min)	Observed RT (min)
1	int1_a3 ACN	2:A,8	1	MP7B.mol	Identified	8.4		1.48

.	Item name	Sample position	Replicate number	Component name	Identification status	Detector counts	Response	Adducts
1	int1_a3 ACN	2:A,8	1	MP7B.mol	Identified	1099	1099	+K

.	Item name	Sample position	Replicate number	Component name	Identification status	Formula
1	int1_a3 ACN	2:A,8	1	MP7B.mol	Identified	C24[13C]2H24N2O9

Component name: MP7B.mol

.	Item name	Sample position	Replicate number	Component name	Identification status	Neutral mass (Da)	Observed neutral mass (Da)
1	int1_a3 ACN	2:A,8	1	MP7B.mol	Identified	510.15489	510.1512

.	Item name	Sample position	Replicate number	Component name	Identification status	Observed m/z	Mass error (mDa)
1	int1_a3 ACN	2:A,8	1	MP7B.mol	Identified	256.0829	-3.7

Item name: MD_M POPLAWSKI

Created by: Chemistry, Chemistry

Created on: Sep 07, 2023

Created time: 13:59:44 GMT Daylight Time

.	Item name	Sample position	Replicate number	Component name	Identification status	Mass error (ppm)	Expected RT (min)	Observed RT (min)
1	int1_a3 ACN	2:A,8	1	MP7B.mol	Identified	-7.3		0.42

.	Item name	Sample position	Replicate number	Component name	Identification status	Detector counts	Response	Adducts
1	int1_a3 ACN	2:A,8	1	MP7B.mol	Identified	1348	1348	2x(+H)

.	Item name	Sample position	Replicate number	Component name	Identification status	Formula
1	int1_a3 ACN	2:A,8	1	MP7B.mol	Identified	C24[13C]2H24N2O9

Component name: MP7B.mol

.	Item name	Sample position	Replicate number	Component name	Identification status	Neutral mass (Da)	Observed neutral mass (Da)
1	int1_a3 ACN	2:A,8	1	MP7B.mol	Identified	510.15489	510.1548

.	Item name	Sample position	Replicate number	Component name	Identification status	Observed m/z	Mass error (mDa)
1	int1_a3 ACN	2:A,8	1	MP7B.mol	Identified	511.1621	-0.1

.	Item name	Sample position	Replicate number	Component name	Identification status	Mass error (ppm)	Expected RT (min)	Observed RT (min)
1	int1_a3 ACN	2:A,8	1	MP7B.mol	Identified	-0.2		1.70

.	Item name	Sample position	Replicate number	Component name	Identification status	Detector counts	Response	Adducts
1	int1_a3 ACN	2:A,8	1	MP7B.mol	Identified	34048	30907	+H

.	Item name	Sample position	Replicate number	Component name	Identification status	Formula
1	int1_a3 ACN	2:A,8	1	MP7B.mol	Identified	C24[13C]2H24N2O9

Item name: int1_a3 ACN

Item name: MD_M POPLAWSKI

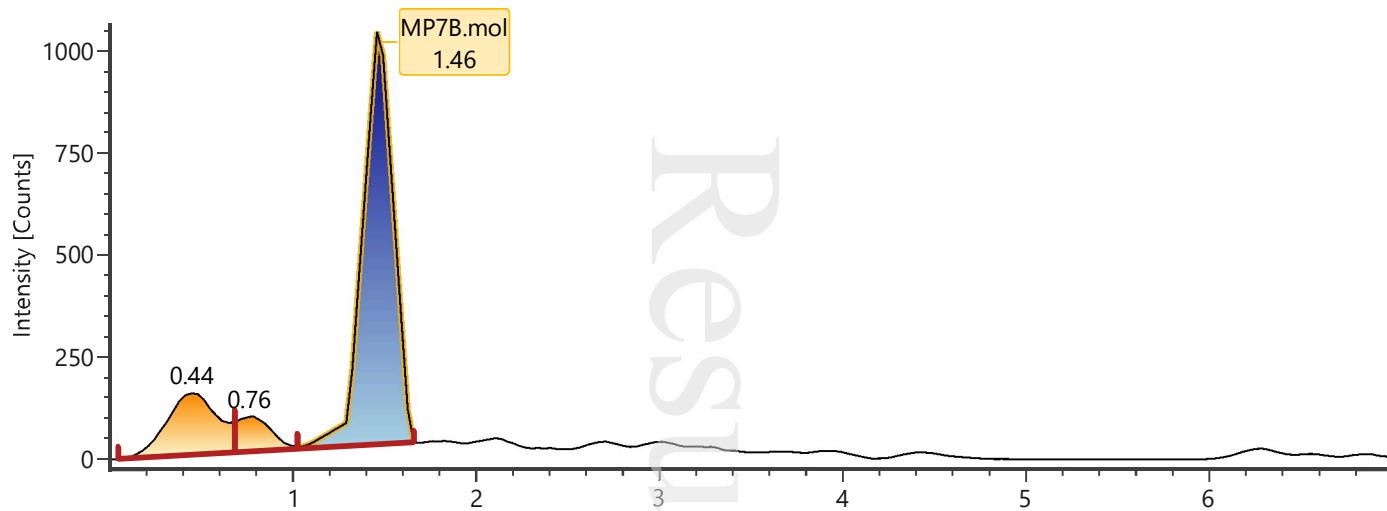
Created by: Chemistry, Chemistry

Created on: Sep 07, 2023

Created time: 13:59:44 GMT Daylight Time

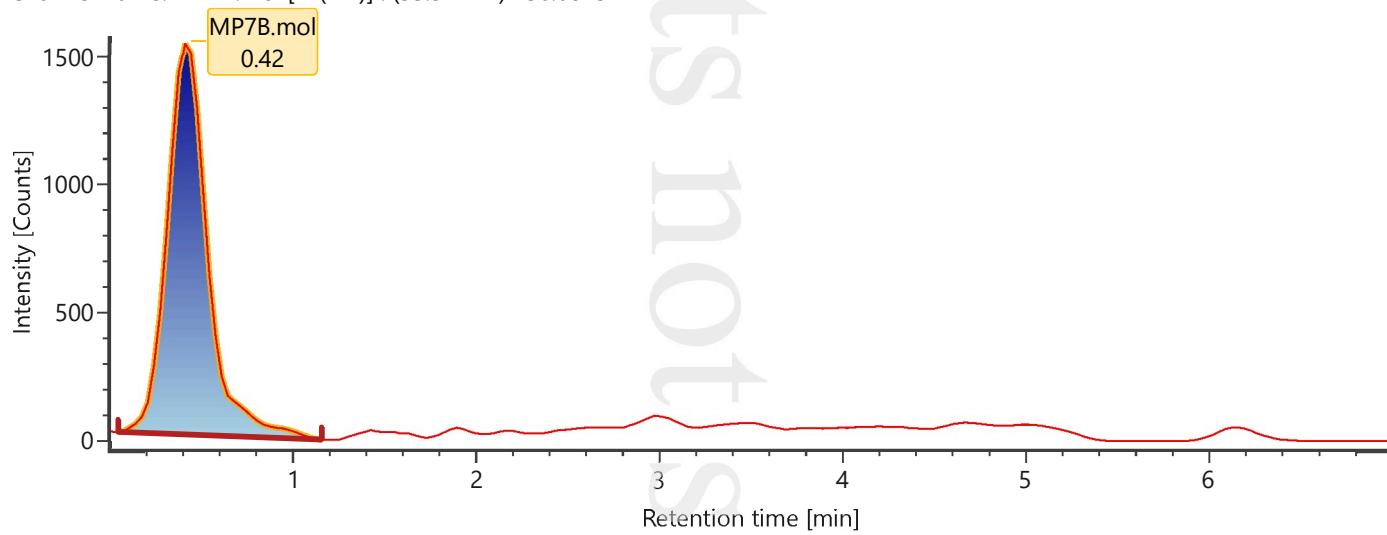
Item name: int1_a3 ACN

Channel name: MP7B.mol [+K] : (35.9 PPM) 549.1227



Item name: int1_a3 ACN

Channel name: MP7B.mol [2x(+H)] : (35.9 PPM) 256.0829



Item name: MD_M POPLAWSKI

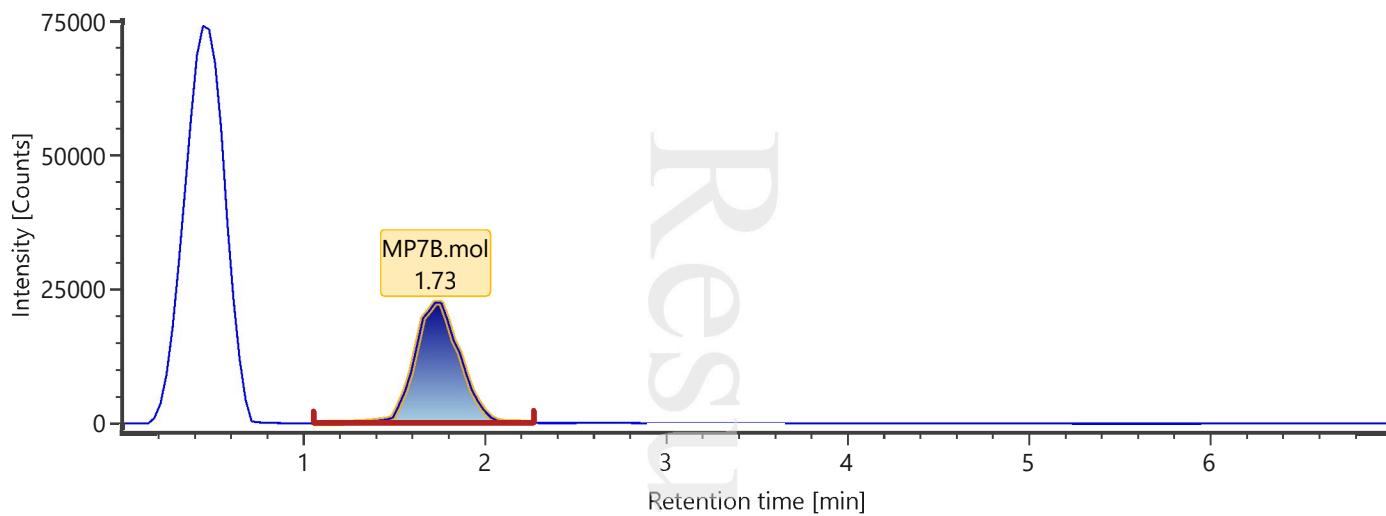
Created by: Chemistry, Chemistry

Created on: Sep 07, 2023

Created time: 13:59:44 GMT Daylight Time

Item name: int1_a3 ACN

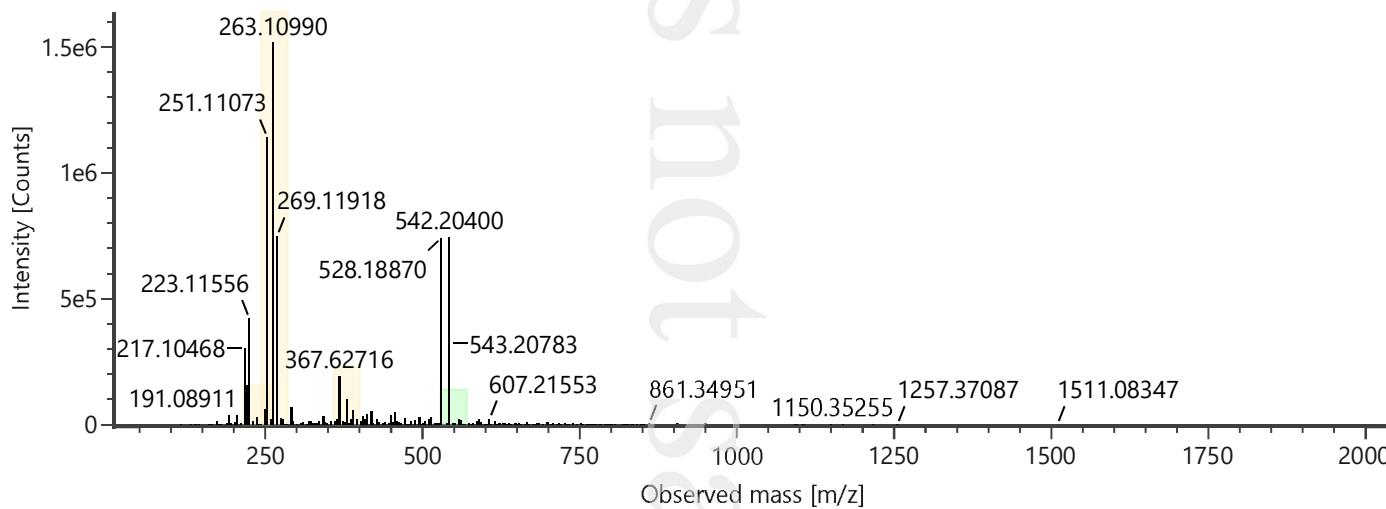
Channel name: MP7B.mol [+H] : (35.9 PPM) 511.1621



Item name: int1_a3 ACN

Item description:

Channel name: Low energy : Time 1.4765 +/- 0.0652 minutes



Item name: MD_M POPLAWSKI

Created by: Chemistry, Chemistry

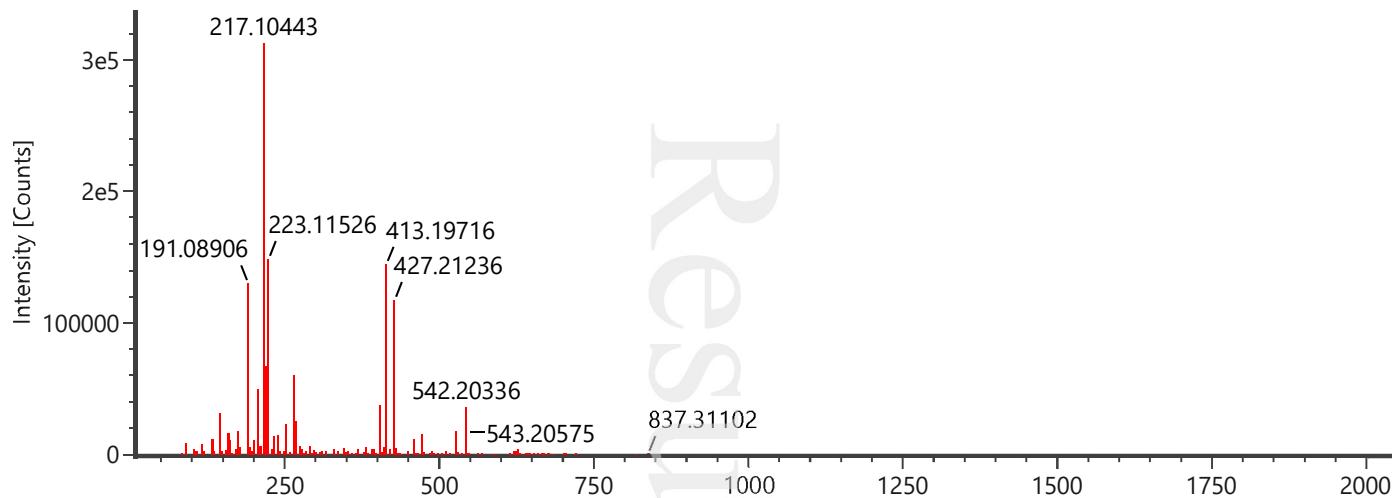
Created on: Sep 07, 2023

Created time: 13:59:44 GMT Daylight Time

Item name: int1_a3 ACN

Channel name: High energy : Time 1.4765 +/- 0.0652 minutes

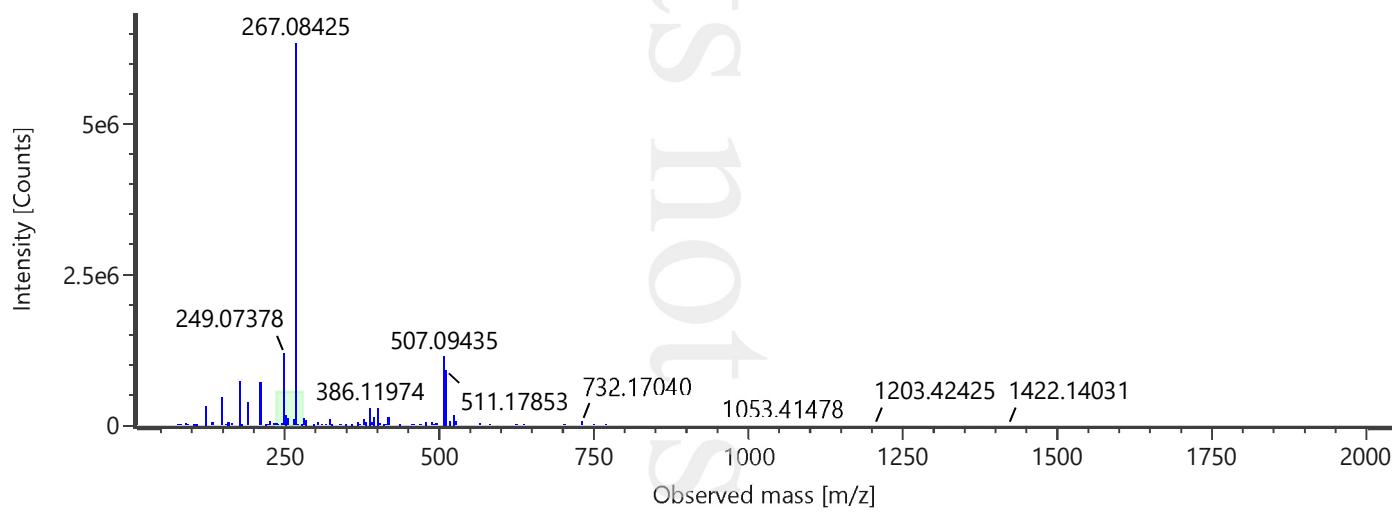
Item description:



Item name: int1_a3 ACN

Channel name: Low energy : Time 0.4222 +/- 0.0652 minutes

Item description:



Item name: MD_M POPLAWSKI

Created by: Chemistry, Chemistry

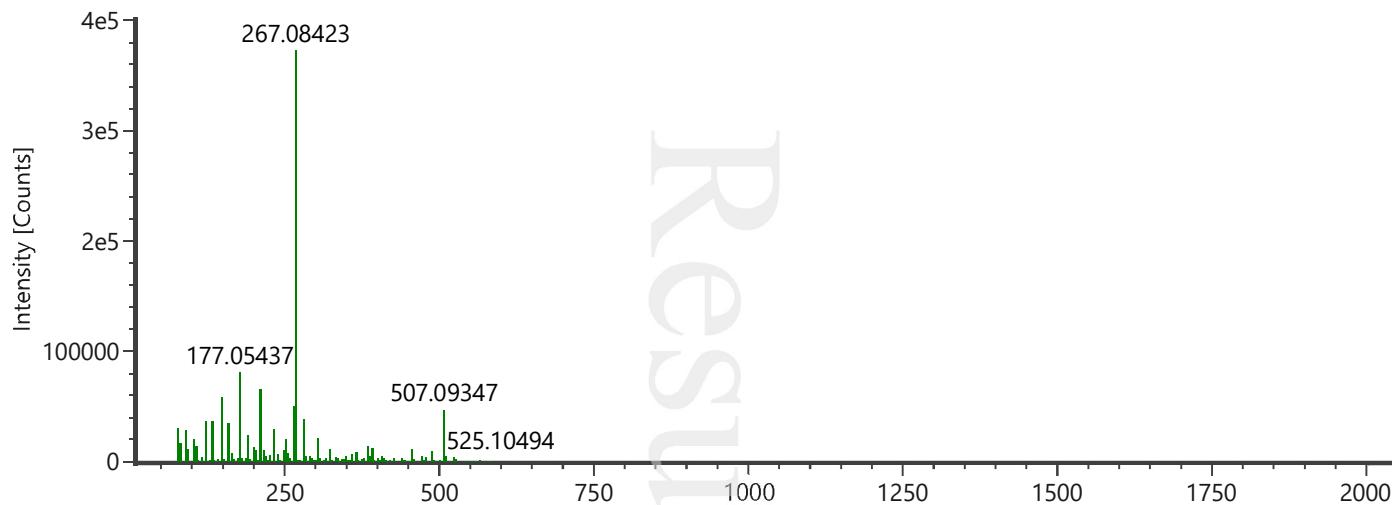
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Created time: 13:59:44 GMT Daylight Time

Item name: int1_a3 ACN

Channel name: High energy : Time 0.4222 +/- 0.0652 minutes

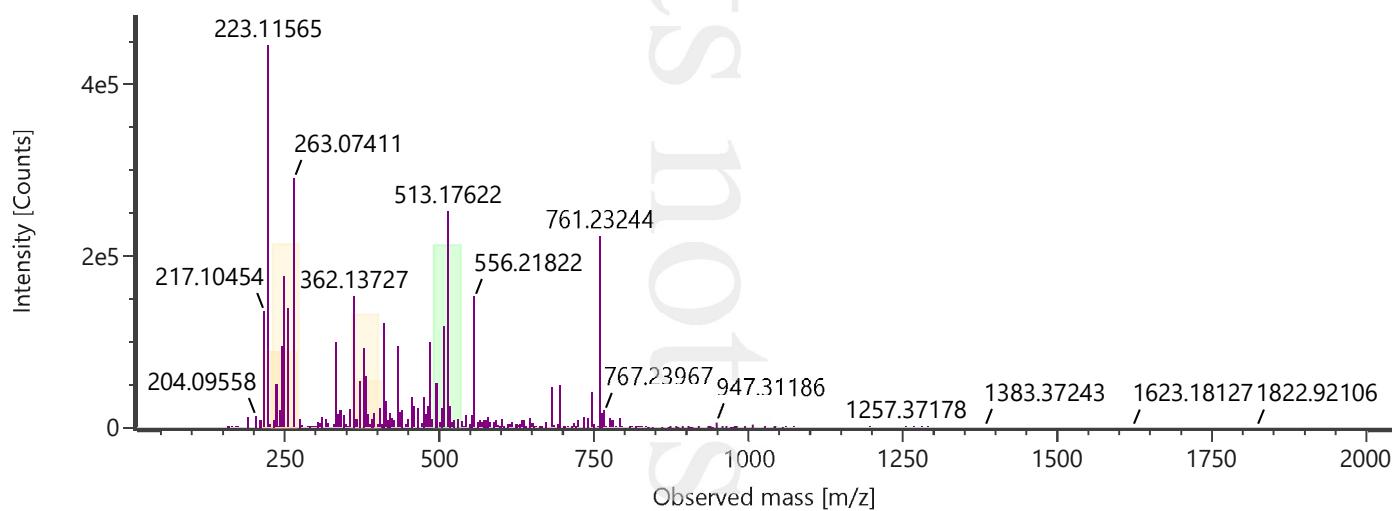
Item description:



Item name: int1_a3 ACN

Channel name: Low energy : Time 1.7005 +/- 0.0652 minutes

Item description:



Item name: MD_M POPLAWSKI

Created by: Chemistry, Chemistry

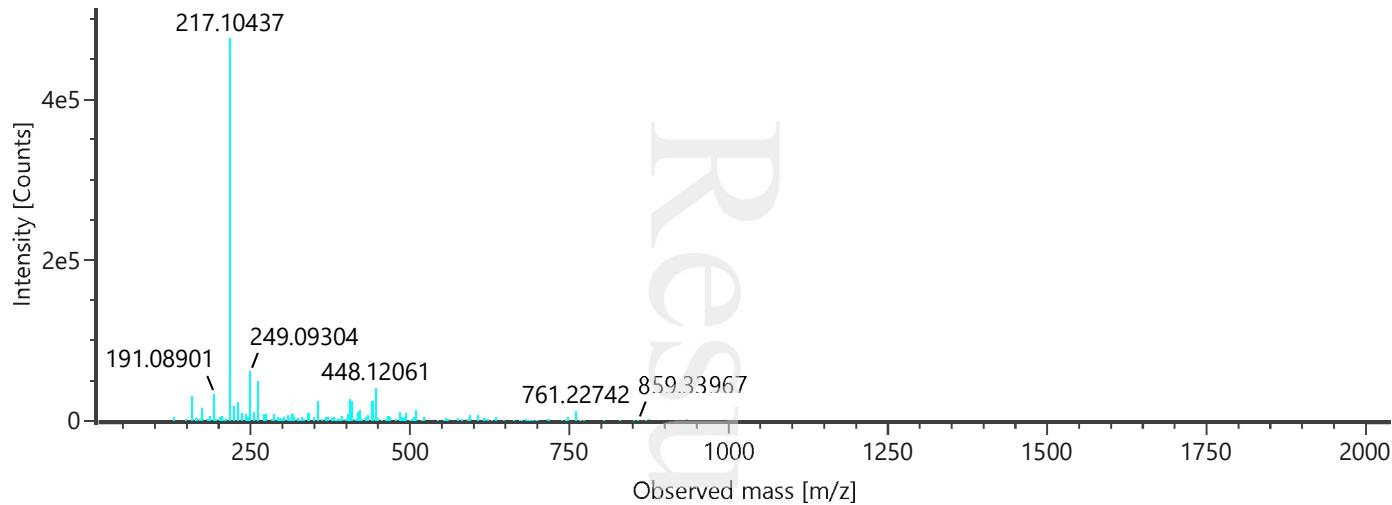
Created on: Sep 07, 2023

Created time: 13:59:44 GMT Daylight Time

Item name: int1_a3 ACN

Channel name: High energy : Time 1.7005 +/- 0.0652 minutes

Item description:



Component name: MP8B.mol

Component name: MP8B.mol

.	Item name	Sample position	Replicate number	Component name	Identification status	Neutral mass (Da)	Observed neutral mass (Da)
1	int1_a3 ACN	2:A,8	1	MP8B.mol	Identified	494.15998	494.1597

.	Item name	Sample position	Replicate number	Component name	Identification status	Observed m/z	Mass error (mDa)
1	int1_a3 ACN	2:A,8	1	MP8B.mol	Identified	494.1592	-0.2

.	Item name	Sample position	Replicate number	Component name	Identification status	Mass error (ppm)	Expected RT (min)	Observed RT (min)
1	int1_a3 ACN	2:A,8	1	MP8B.mol	Identified	-0.5		1.84

.	Item name	Sample position	Replicate number	Component name	Identification status	Detector counts	Response	Adducts
1	int1_a3 ACN	2:A,8	1	MP8B.mol	Identified	41917	23295	-e, +K

.	Item name	Sample position	Replicate number	Component name	Identification status	Formula
1	int1_a3 ACN	2:A,8	1	MP8B.mol	Identified	C24[13C]2H24N2O8

Item name: int1_a3 ACN

Item name: MD_M POPLAWSKI

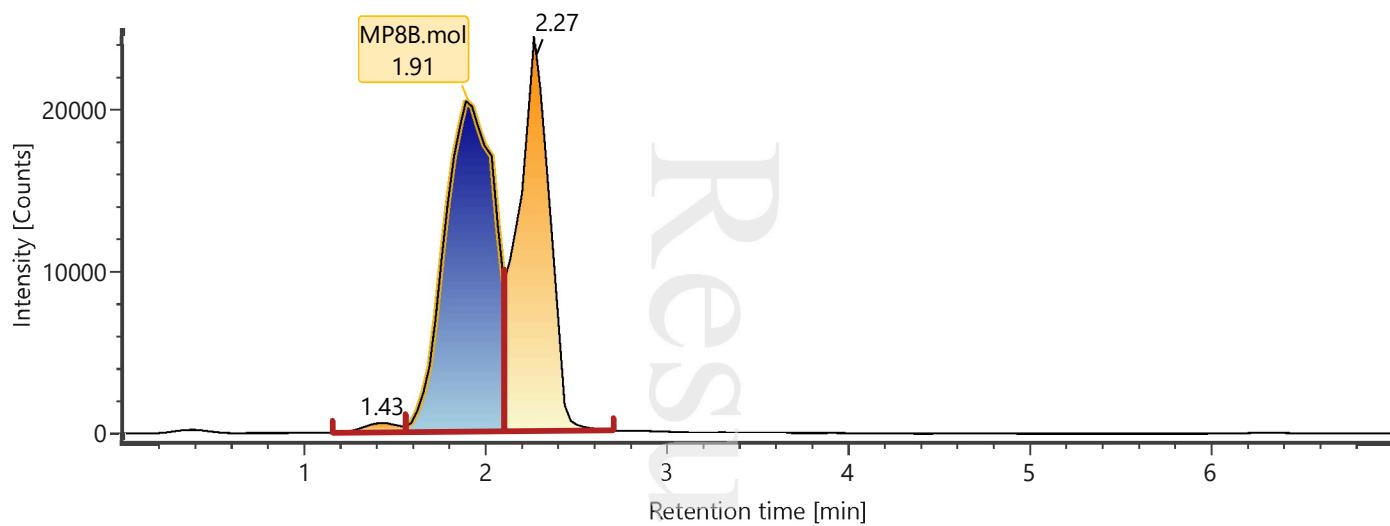
Created by: Chemistry, Chemistry

Created on: Sep 07, 2023

Created time: 13:59:44 GMT Daylight Time

Item name: int1_a3 ACN

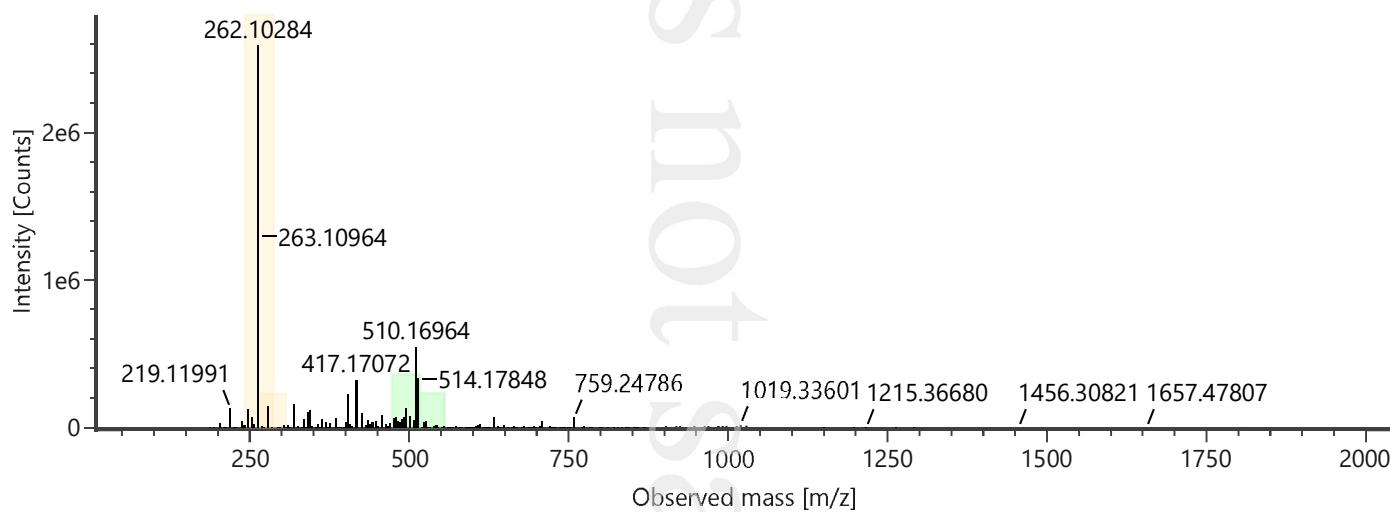
Channel name: MP8B.mol [-e] : (35.9 PPM) 494.1592



Item name: int1_a3 ACN

Item description:

Channel name: Low energy : Time 1.8424 +/- 0.0652 minutes



Item name: MD_M POPLAWSKI

Created by: Chemistry, Chemistry

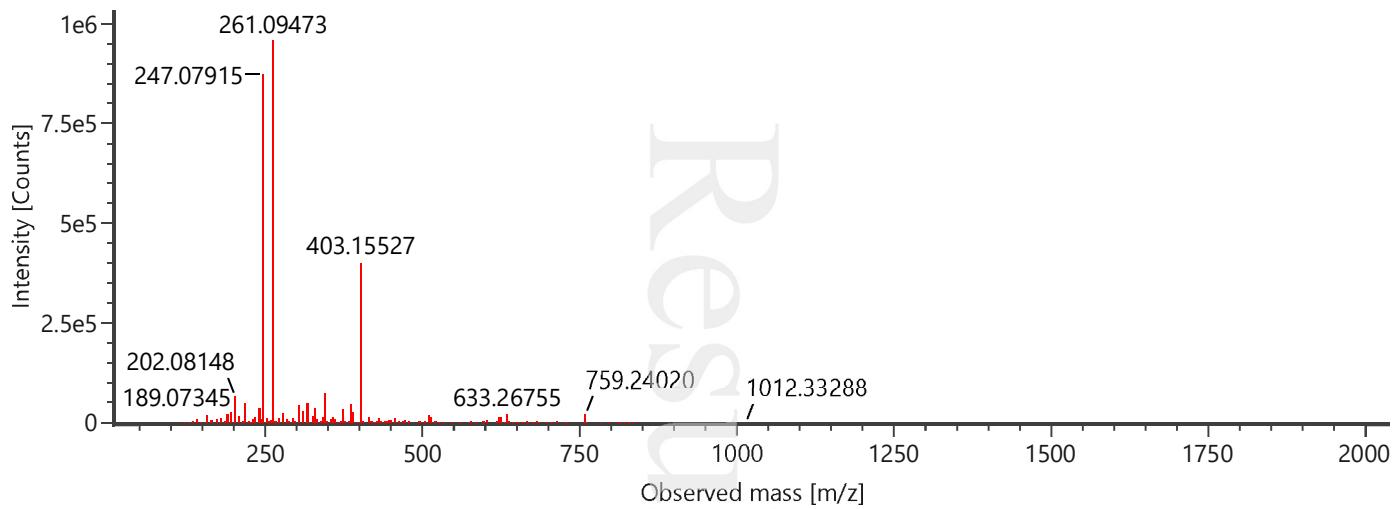
Created on: Sep 07, 2023

Created time: 13:59:44 GMT Daylight Time

Item name: int1_a3 ACN

Channel name: High energy : Time 1.8424 +/- 0.0652 minutes

Item description:



Item name: MD_M POPLAWSKI

Created by: Chemistry, Chemistry

Created on: Sep 07, 2023

Created time: 13:59:44 GMT Daylight Time

Report Log

Template Report

Report Template "Untitled" has not been saved.

Results not saved