LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121922\
Data File : BF131693.D
Acq On : 19 Dec 2022 17:28
Operator : CG\JU
Sample : N6099-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PURGE-WATER-2

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131693.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.134	3	8	14	rVB	1604989	2034980	59.97%	10.401%
2	2.240	21	26	31	rBV	62438	71337	2.10%	0.365%
3	2.499	61	70	76	rVB	64456	96100	2.83%	0.491%
4	3.352	212	215	225	rBV	32739	65473	1.93%	0.335%
5	5.075	504	508	517	rVB	415186	497680	14.67%	2.544%
6	5.487	573	578	581	rBV	1552596	1409811	41.55%	7.205%
7	6.498	746	750	753	rVB	1111619	935997	27.58%	4.784%
8	6.869	810	813	817	rBV	538965	468241	13.80%	2.393%
9	6.928	820	823	829	rBV	102900	93613	2.76%	0.478%
10	7.222	865	873	881	rBV2	29456	51719	1.52%	0.264%
11	7.445	905	911	914	rVB	1750113	1822710	53.72%	9.316%
12	7.540	920	927	937	rVB	74650	119340	3.52%	0.610%
13	7.898	981	988	994	rVB	83757	108214	3.19%	0.553%
14	8.163	1029	1033	1036	rVB	694577	587482	17.31%	3.003%
15	8.510	1086	1092	1101	rBV	119713	143264	4.22%	0.732%
16	9.245	1211	1217	1220	rBV	4008945	3393171	100.00%	17.342%
17	9.922	1326	1332	1336	rVB	791474	745257	21.96%	3.809%
18	10.722	1463	1468	1471	rBV	2499857	2248645	66.27%	11.493%
19	11.416	1583	1586	1590	rVB	867265	737625	21.74%	3.770%
20	13.016	1853	1858	1861	rBV	3486717	3107966	91.59%	15.884%
21	14.069	2033	2037	2041	rBV	477203	421350	12.42%	2.153%
22	15.568	2287	2292	2300	rBV	326360	406155	11.97%	2.076%

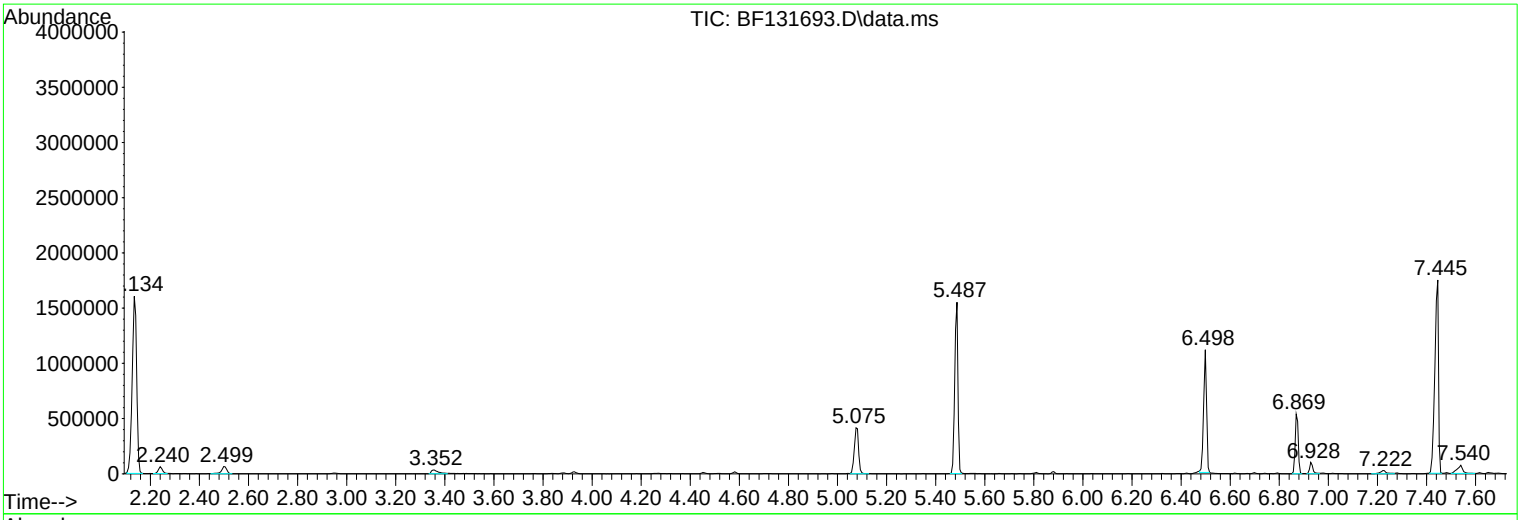
Sum of corrected areas: 19566130

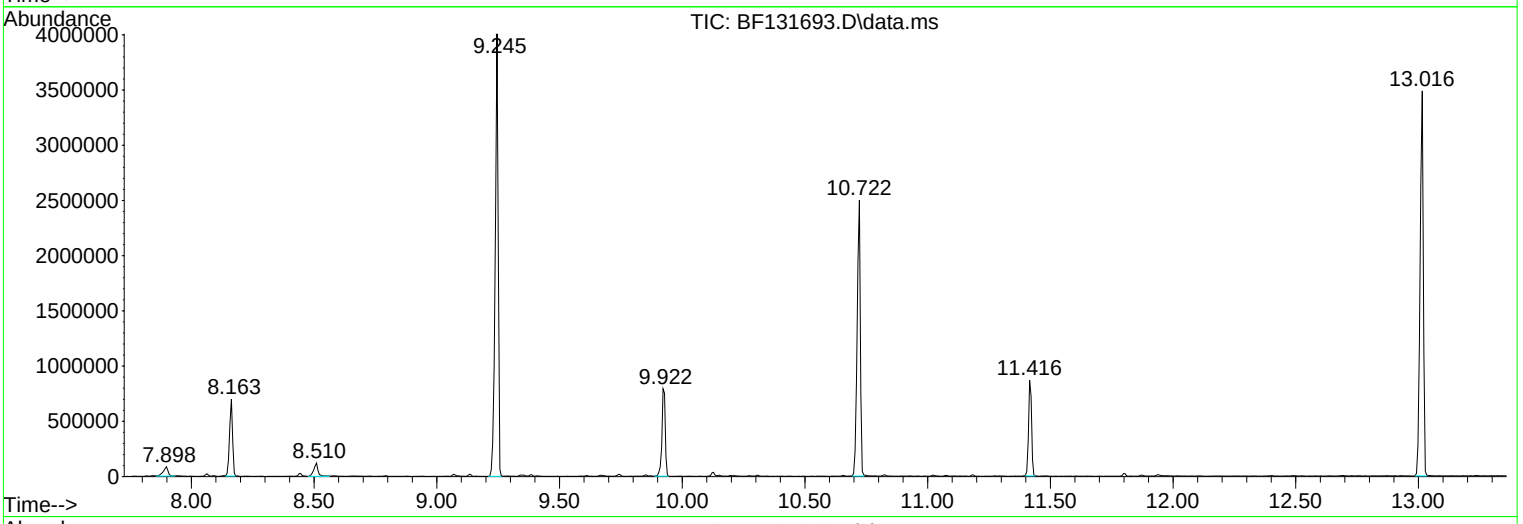
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121922\
Data File : BF131693.D
Acq On : 19 Dec 2022 17:28
Operator : CG\JU
Sample : N6099-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

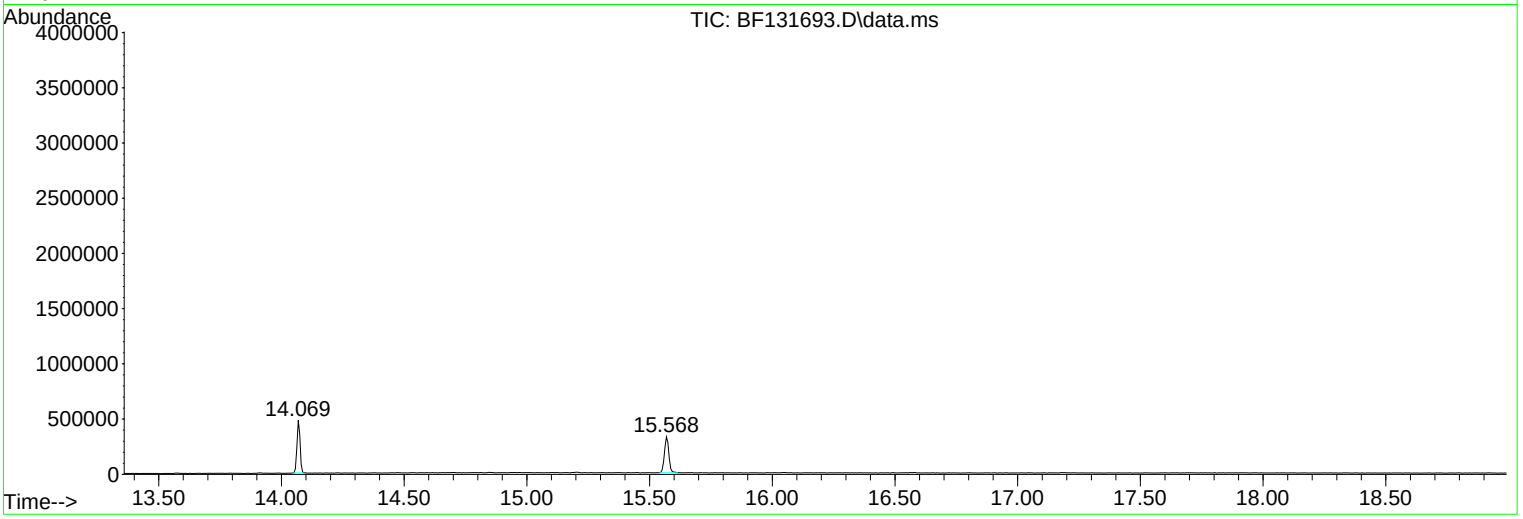
Instrument :
BNA_F
ClientSampleId :
PURGE-WATER-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P







Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121922\
Data File : BF131693.D
Acq On : 19 Dec 2022 17:28
Operator : CG\JU
Sample : N6099-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PURGE-WATER-2

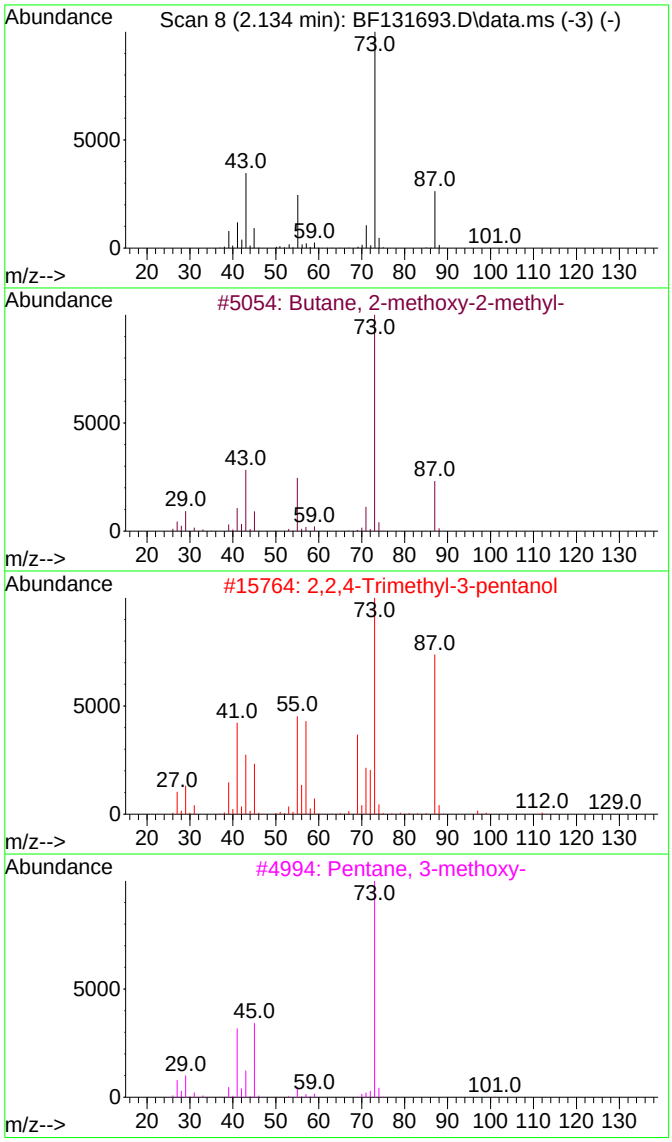
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

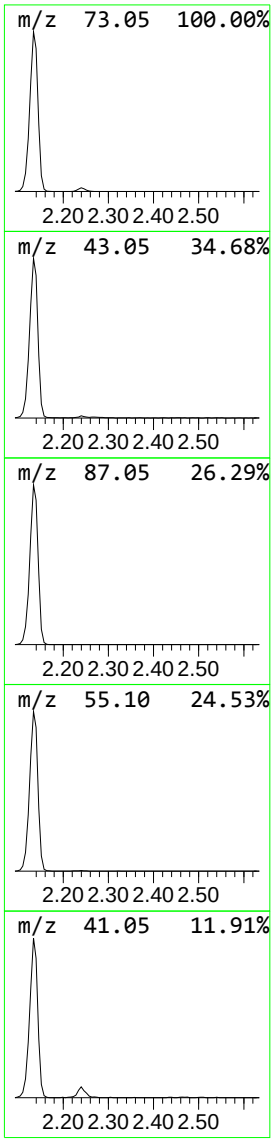
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.134	86.92 ng	2034980	1,4-Dichlorobenzene-d4	6.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





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Data File : BF131693.D
Acq On : 19 Dec 2022 17:28
Operator : CG\JU
Sample : N6099-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PURGE-WATER-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

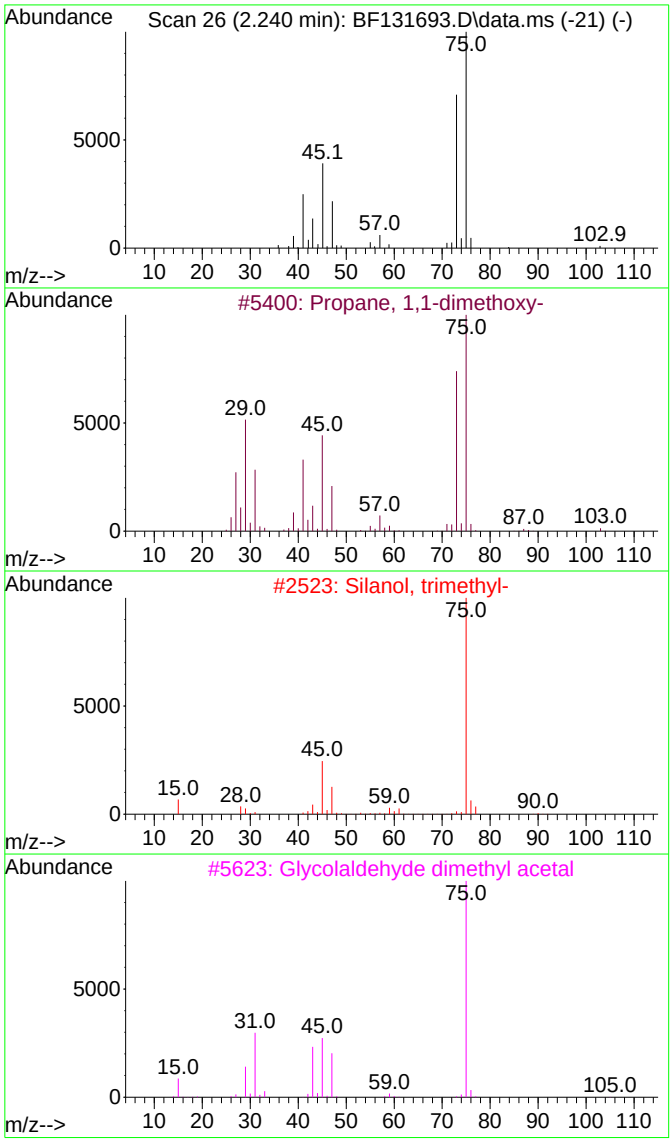
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

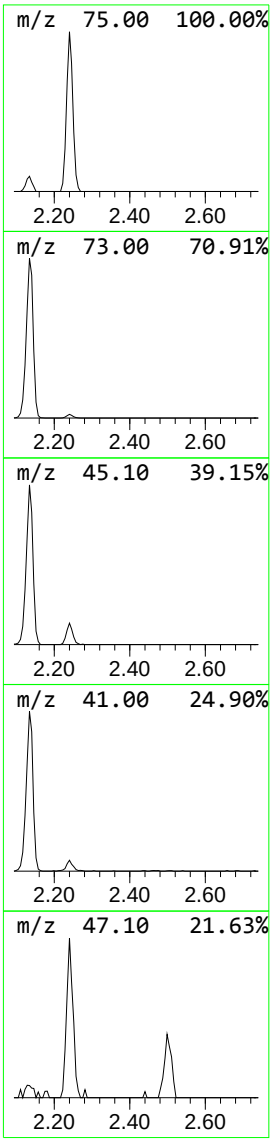
****

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.240	3.05 ng	71337	1,4-Dichlorobenzene-d4	6.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2	Silanol, trimethyl-	90	C3H10OSi	001066-40-6	72
3	Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	72
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	14
5	Thiocyanic acid, methyl ester	73	C2H3NS	000556-64-9	9





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Data File : BF131693.D
Acq On : 19 Dec 2022 17:28
Operator : CG\JU
Sample : N6099-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PURGE-WATER-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

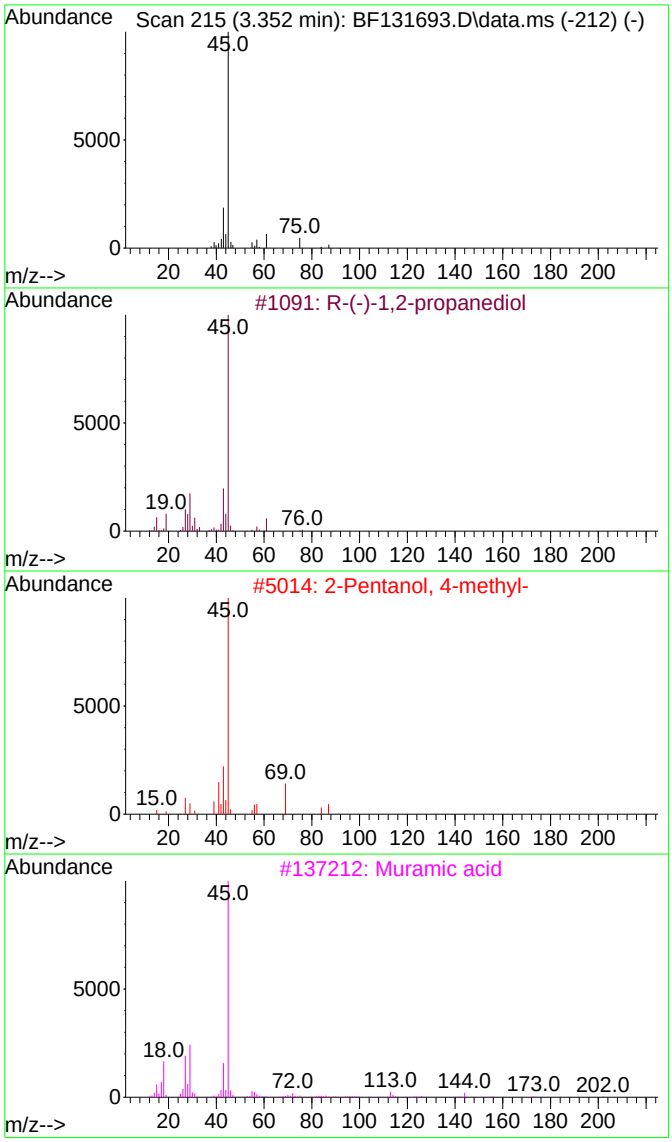
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

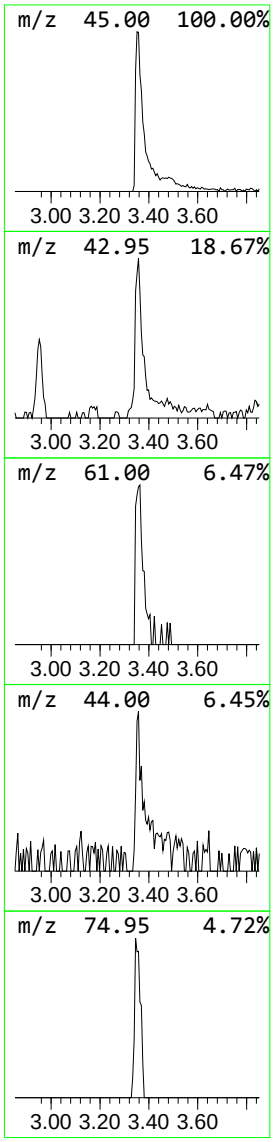
****

Peak Number 4 unknown3.352 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.352	2.80 ng	65473	1,4-Dichlorobenzene-d4	6.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	43
2	2-Pentanol, 4-methyl-	102	C6H14O	000108-11-2	40
3	Muramic acid	251	C9H17NO7	001114-41-6	9
4	2-Hexanol, 3-methyl-	116	C7H16O	002313-65-7	9
5	Propylene Glycol	76	C3H8O2	000057-55-6	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121922\
Data File : BF131693.D
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Operator : CG\JU
Sample : N6099-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PURGE-WATER-2

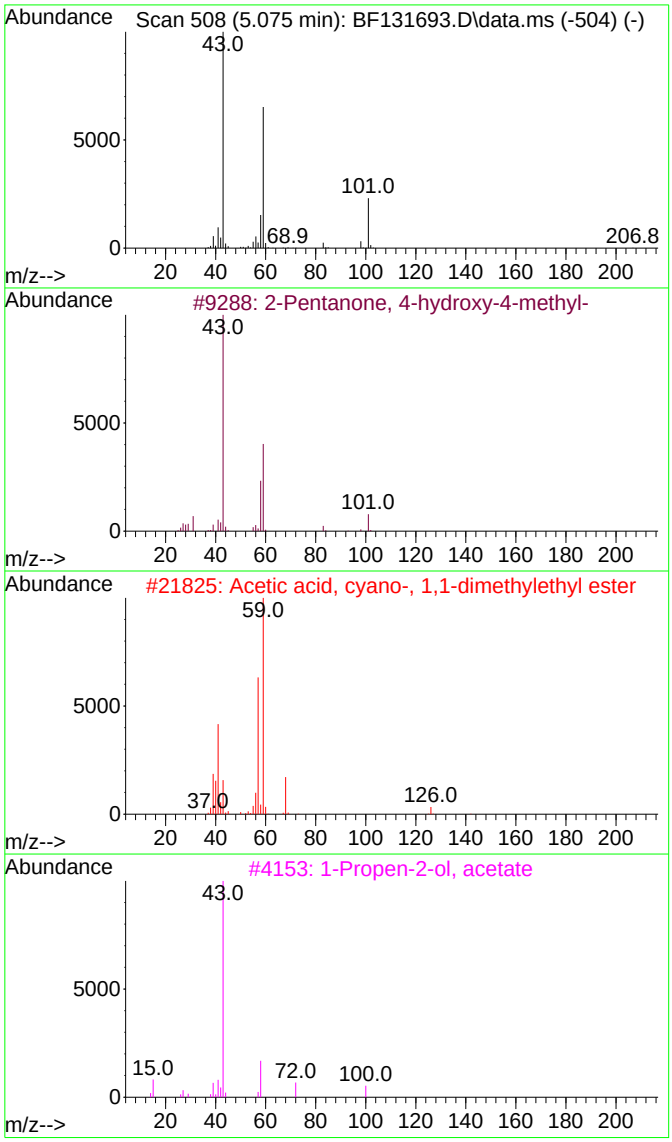
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

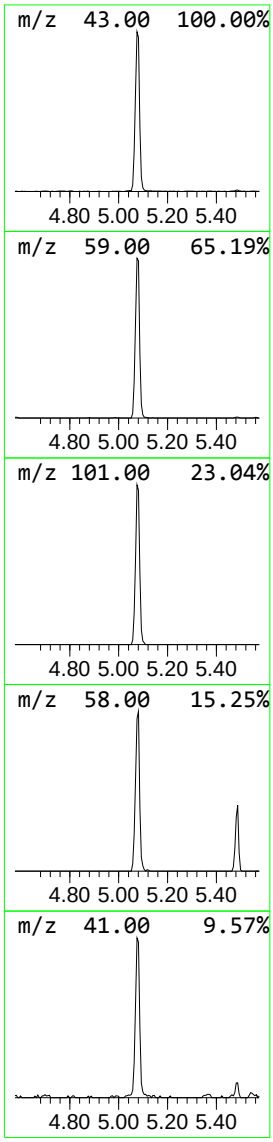
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.075	21.26 ng	497680	1,4-Dichlorobenzene-d4	6.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121922\
Data File : BF131693.D
Acq On : 19 Dec 2022 17:28
Operator : CG\JU
Sample : N6099-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PURGE-WATER-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

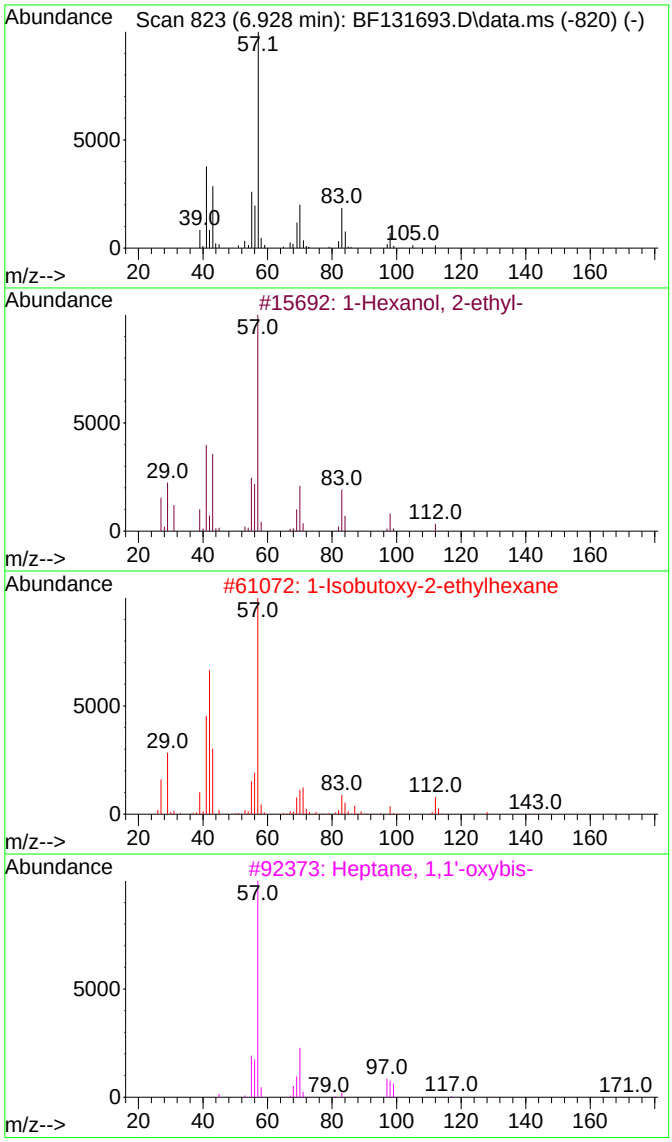
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

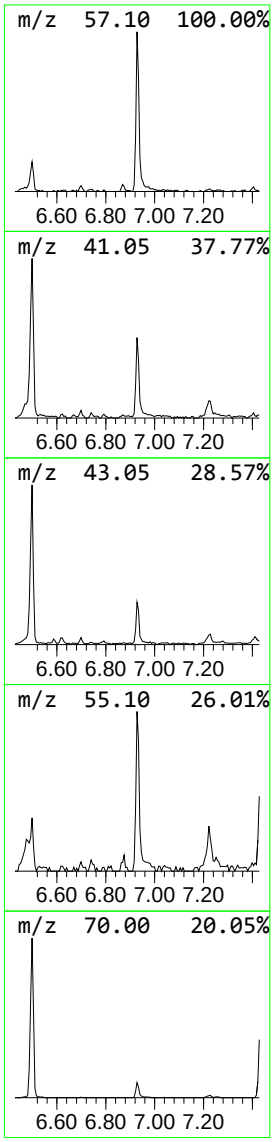
****

Peak Number 6 1-Hexanol, 2-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.928	4.00 ng	93613	1,4-Dichlorobenzene-d4	6.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2	1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	78
3	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	64
4	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	53
5	Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	50





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Sample : N6099-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PURGE-WATER-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

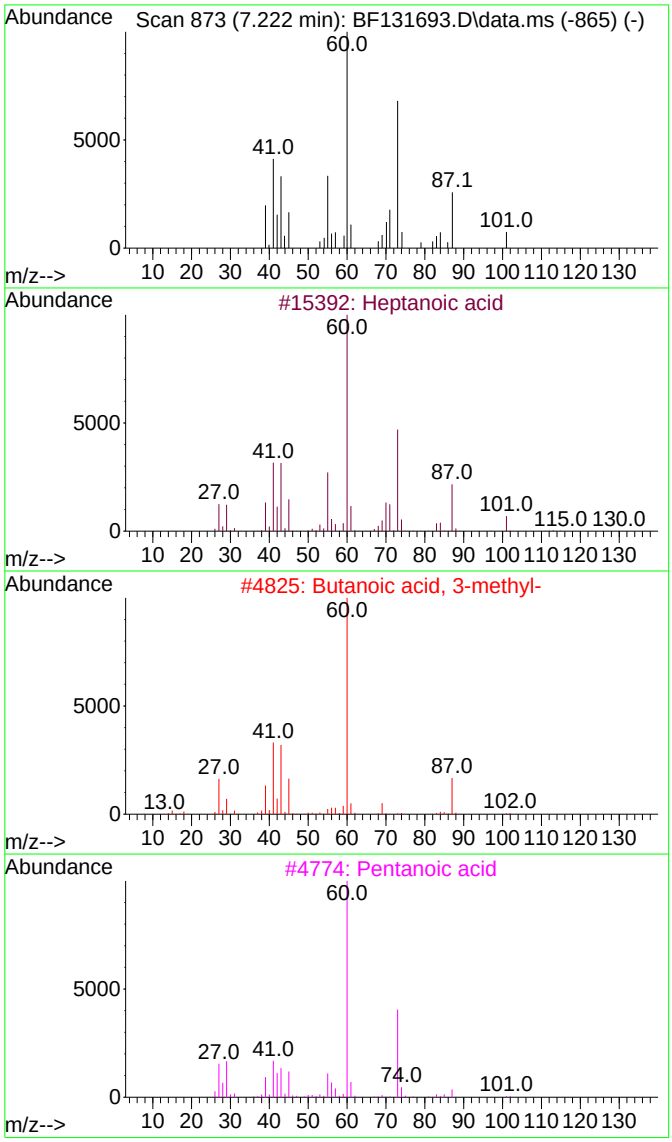
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

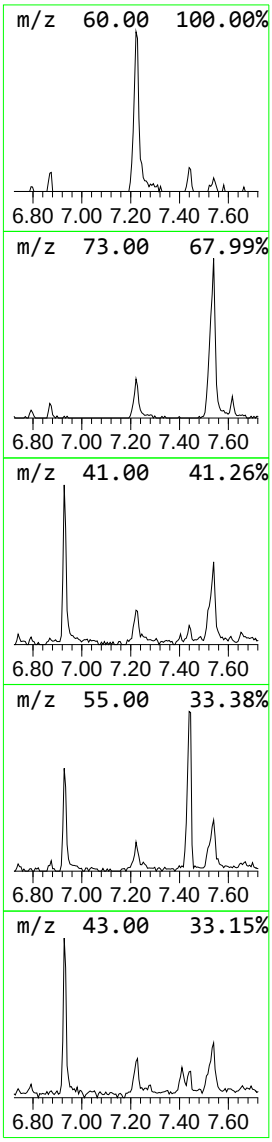
****

Peak Number 7 Heptanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.222	2.21 ng	51719	1,4-Dichlorobenzene-d4	6.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptanoic acid	130	C7H14O2	000111-14-8	90
2	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	59
3	Pentanoic acid	102	C5H10O2	000109-52-4	53
4	Hexanoic acid	116	C6H12O2	000142-62-1	50
5	Pentanoic acid, 3-methyl-	116	C6H12O2	000105-43-1	50





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Instrument :
BNA_F
ClientSampleId :
PURGE-WATER-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

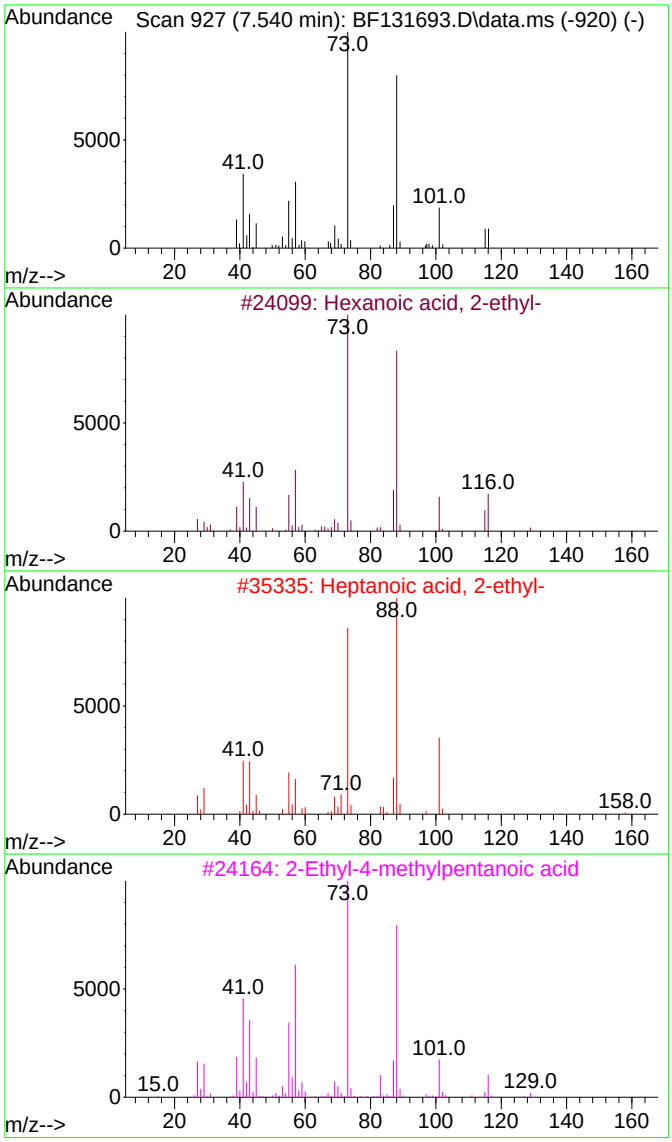
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

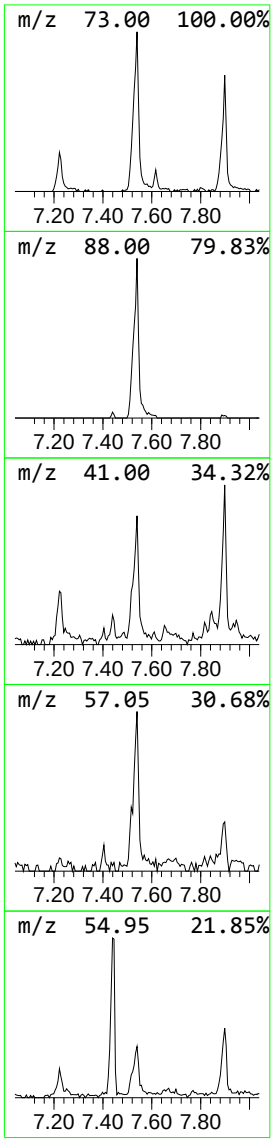
****

Peak Number 8 Hexanoic acid, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.540	4.06 ng	119340	Naphthalene-d8	8.163

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	83
2	Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	64
3	2-Ethyl-4-methylpentanoic acid	144	C8H16O2	000108-81-6	59
4	Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	45
5	Methyl-4-deoxy-2,3-di-O-methyl.b...	218	C9H14O6	1000312-09-9	40





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BNA_F
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

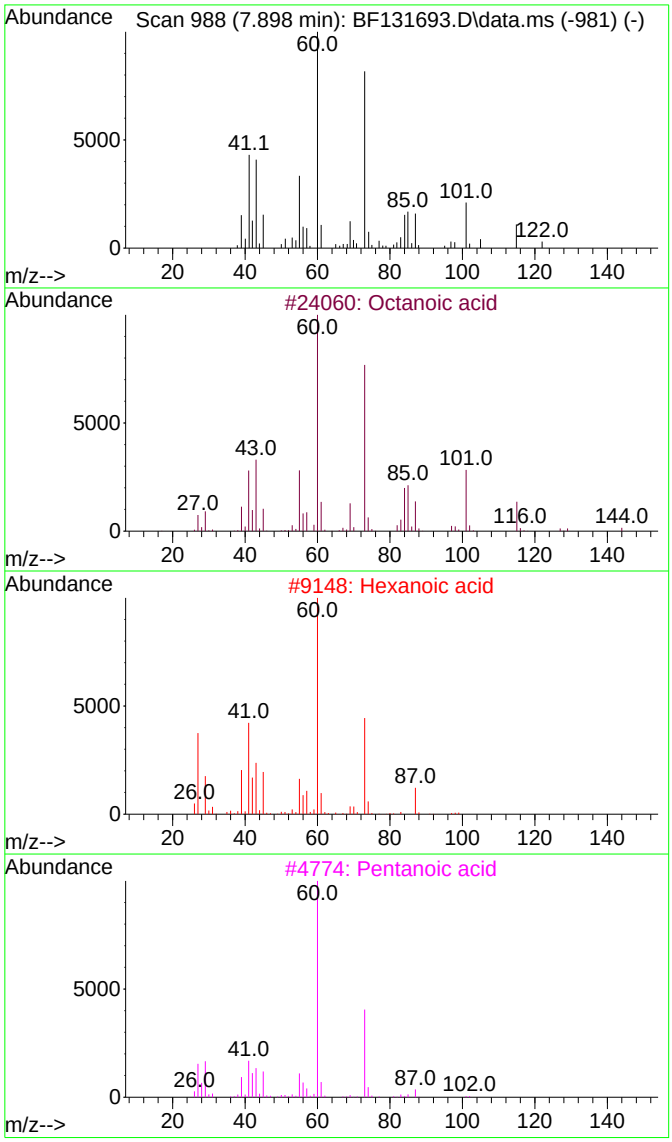
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

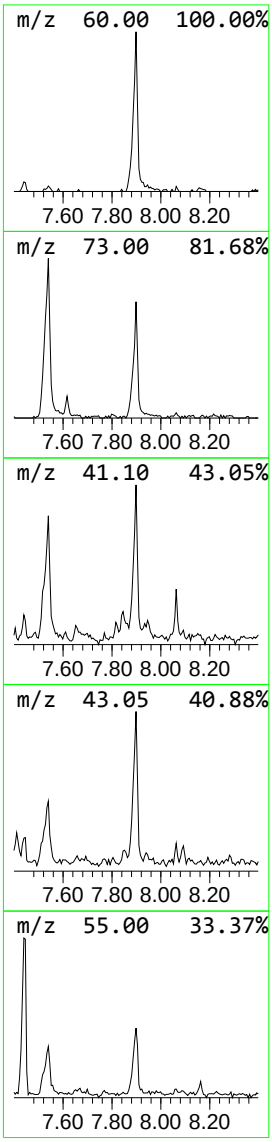
****

Peak Number 9 Octanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.898	3.68 ng	108214	Naphthalene-d8	8.163

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octanoic acid	144	C8H16O2	000124-07-2	90
2	Hexanoic acid	116	C6H12O2	000142-62-1	53
3	Pentanoic acid	102	C5H10O2	000109-52-4	52
4	3-Methyl-hexanoic acid	130	C7H14O2	1000365-65-4	43
5	Propanedioic acid, propyl-	146	C6H10O4	000616-62-6	38





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Operator : CG\JU
Sample : N6099-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PURGE-WATER-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

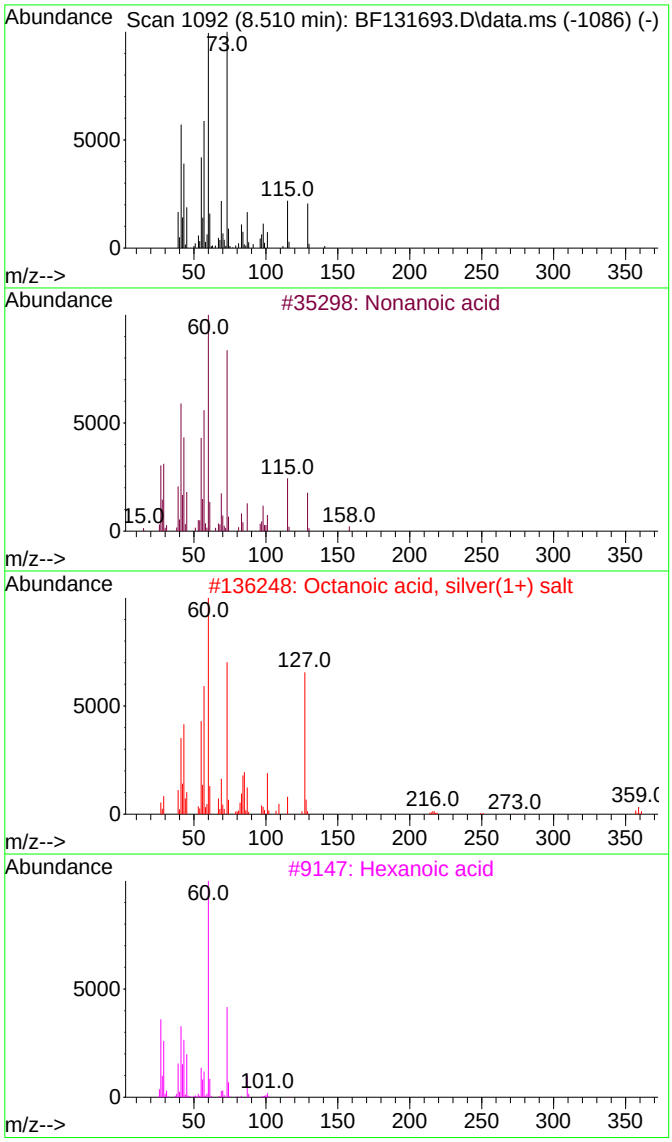
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

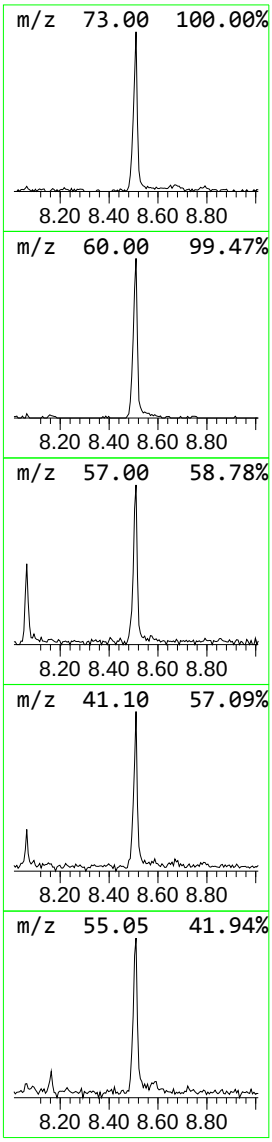
****

Peak Number 10 Nonanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.510	4.88 ng	143264	Naphthalene-d8	8.163

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonanoic acid	158	C9H18O2	000112-05-0	91
2	Octanoic acid, silver(1+) salt	250	C8H15AgO2	024927-67-1	50
3	Hexanoic acid	116	C6H12O2	000142-62-1	47
4	Heptanoic acid	130	C7H14O2	000111-14-8	43
5	Pentanoic acid, 3-methyl-	116	C6H12O2	000105-43-1	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121922\
Data File : BF131693.D
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Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PURGE-WATER-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.134	86.9	ng	2034980	1	6.869	468241	20.0
Propane, 1,1-di...	2.240	3.0	ng	71337	1	6.869	468241	20.0
unknown3.352	3.352	2.8	ng	65473	1	6.869	468241	20.0
2-Pentanone, 4-...	5.075	21.3	ng	497680	1	6.869	468241	20.0
1-Hexanol, 2-et...	6.928	4.0	ng	93613	1	6.869	468241	20.0
Heptanoic acid	7.222	2.2	ng	51719	1	6.869	468241	20.0
Hexanoic acid, ...	7.540	4.1	ng	119340	2	8.163	587482	20.0
Octanoic acid	7.898	3.7	ng	108214	2	8.163	587482	20.0
Nonanoic acid	8.510	4.9	ng	143264	2	8.163	587482	20.0