LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM120321\
Data File : BM033293.D
Acq On : 03 Dec 2021 19:14
Operator : CG/JU
Sample : M4908-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TW-1

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_M\Methods\8270-BM112421.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM033293.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.555	31	37	48	rVB4	62756	139812	1.19%	0.249%
2	3.666	52	56	62	rBV	103870	144043	1.23%	0.256%
3	4.631	209	220	226	rBV	4674877	6791915	57.90%	12.078%
4	4.678	226	228	233	rVB	88391	117729	1.00%	0.209%
5	4.919	263	269	279	rVB	670091	1008747	8.60%	1.794%
6	5.049	285	291	297	rBV	187425	279269	2.38%	0.497%
7	5.131	299	305	311	rVB	214307	315166	2.69%	0.560%
8	5.519	364	371	382	rVB	1715047	2560428	21.83%	4.553%
9	7.113	635	642	655	rVB	609700	1064404	9.07%	1.893%
10	7.466	695	702	711	rBV	1032167	1686188	14.38%	2.999%
11	7.925	773	780	787	rBV	571476	962414	8.20%	1.712%
12	9.089	970	978	988	rBV	2478236	4248466	36.22%	7.555%
13	10.501	1211	1218	1226	rBV	80956	142888	1.22%	0.254%
14	10.613	1229	1237	1248	rVV	875547	1536168	13.10%	2.732%
15	10.725	1249	1256	1265	rVB	777114	1332840	11.36%	2.370%
16	13.177	1665	1673	1683	rBV	5750197	8434752	71.91%	15.000%
17	14.554	1898	1907	1917	rVB	1106403	1699954	14.49%	3.023%
18	16.036	2153	2159	2172	rBV	3621730	5310287	45.27%	9.444%
19	17.289	2365	2372	2379	rBV	1338051	1974712	16.83%	3.512%
20	18.171	2517	2522	2527	rBV	90384	137200	1.17%	0.244%
21	19.900	2810	2816	2821	rBV	9316599	11729955	100.00%	20.860%
22	21.147	3025	3028	3030	rBV2	126027	139626	1.19%	0.248%
23	21.224	3038	3041	3048	rVB	162858	198739	1.69%	0.353%
24	21.447	3074	3079	3088	rBV	1642036	2155693	18.38%	3.834%
25	23.777	3469	3475	3488	rVB2	1042048	2120474	18.08%	3.771%

Sum of corrected areas: 56231869

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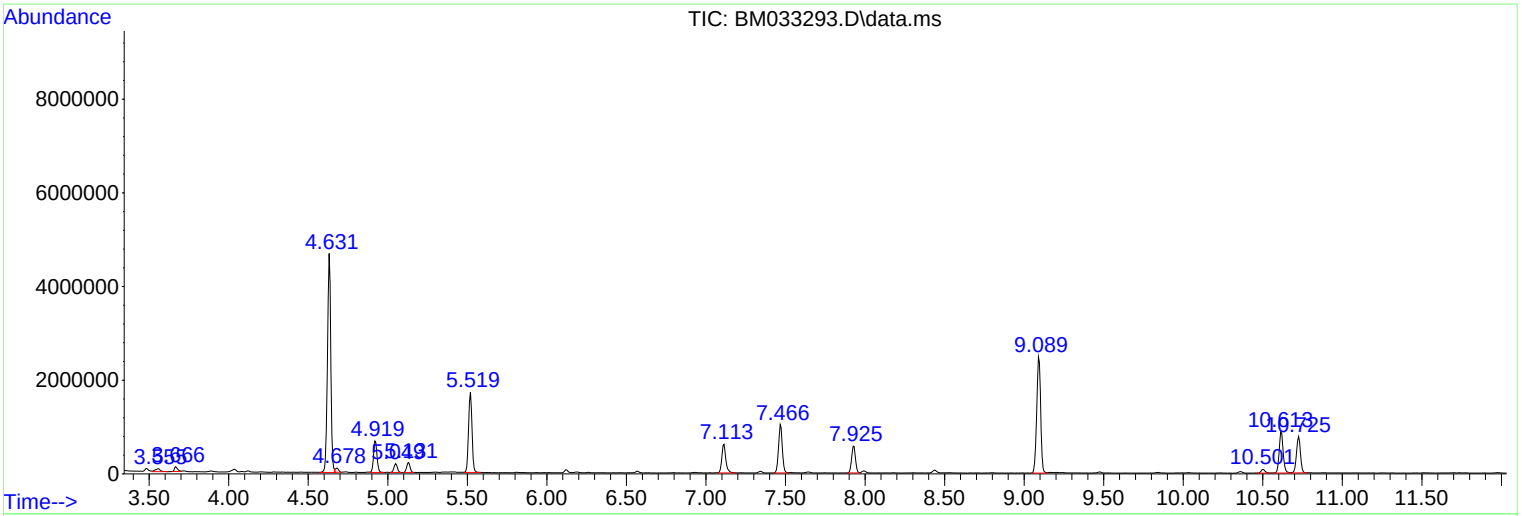
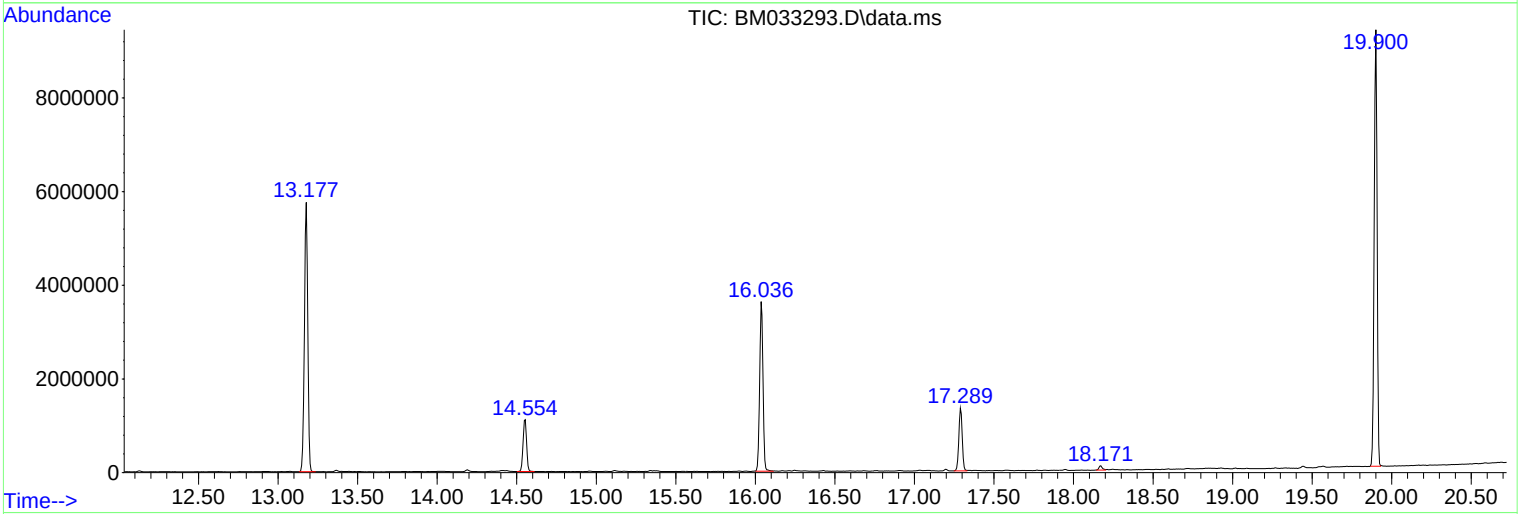
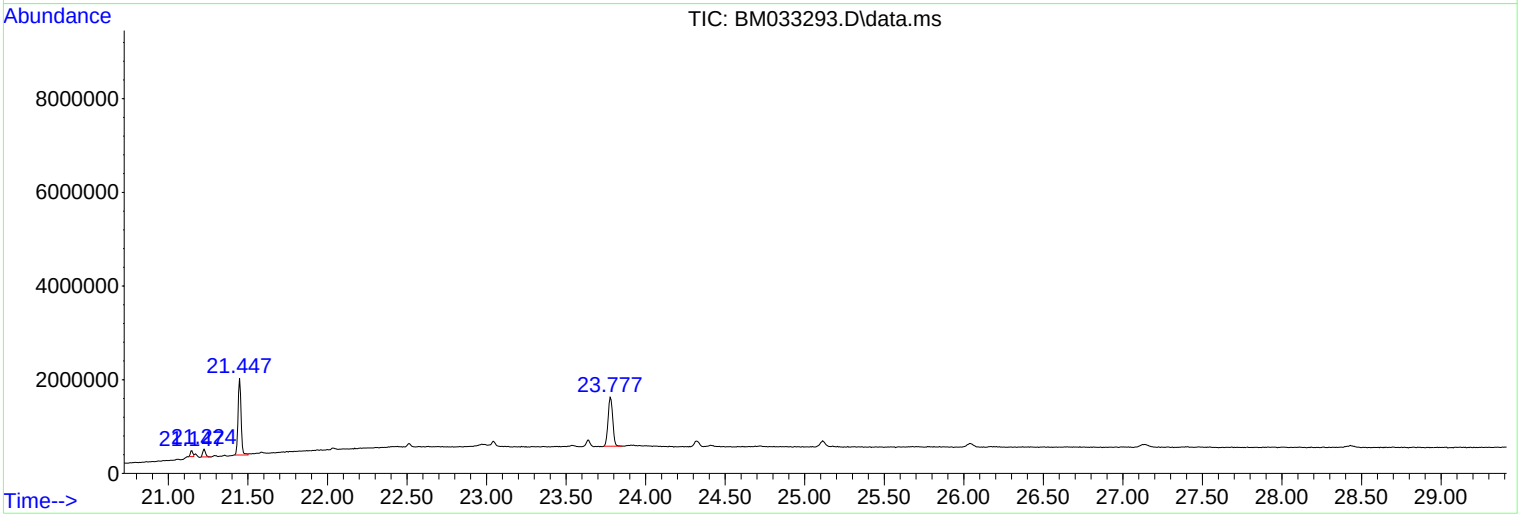
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM112421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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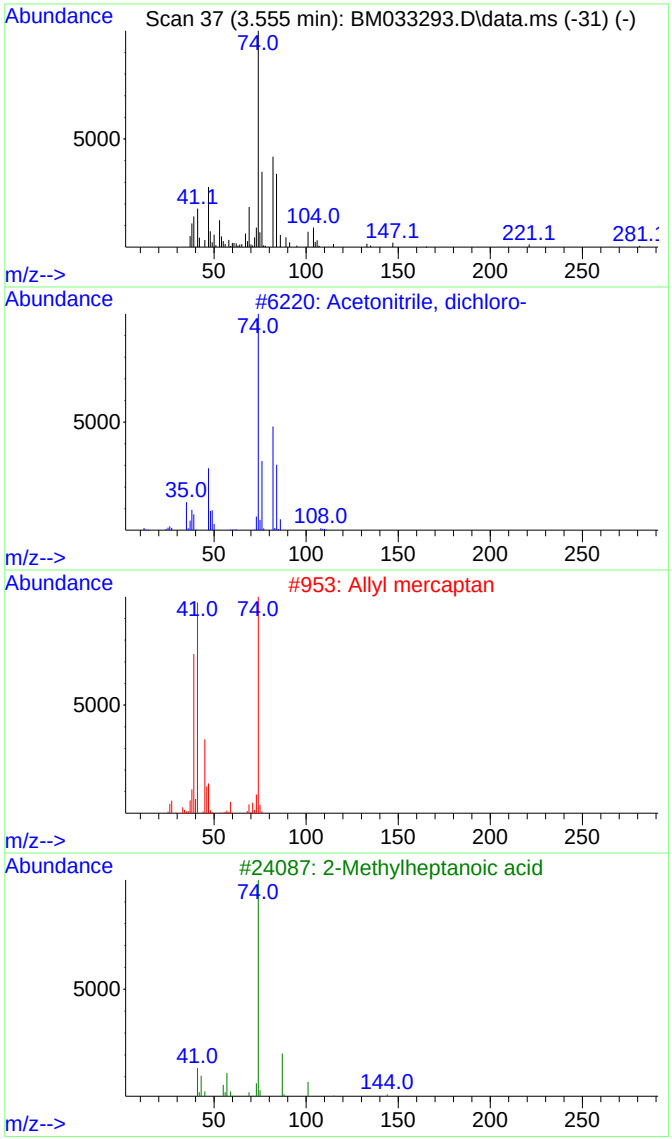
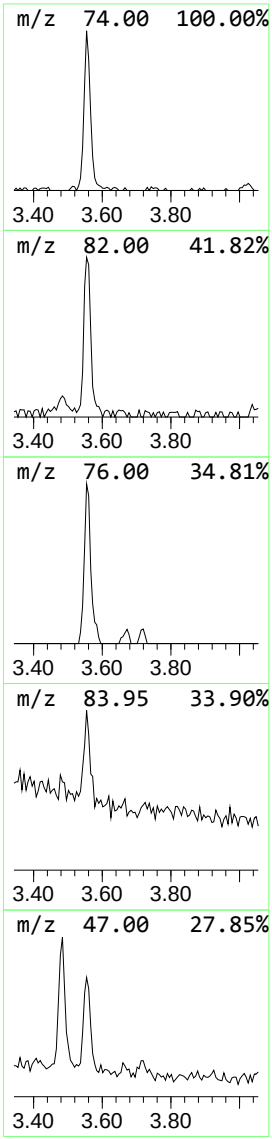
Peak Number 1 Acetonitrile, dichloro- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.555	2.91 ng	139812	1,4-Dichlorobenzene-d4	7.931

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetonitrile, dichloro-	109	C2HCl2N	003018-12-0	86
2	Allyl mercaptan	74	C3H6S	000870-23-5	17
3	2-Methylheptanoic acid	144	C8H16O2	001188-02-9	17
4	Benzo[d]isothiazol-3(2H)-one, 4,...	273	C7H3N3O7S	321372-60-5	12
5	Diethanolamine	105	C4H11NO2	000111-42-2	10





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Data File : BM033293.D
Acq On : 03 Dec 2021 19:14
Operator : CG/JU
Sample : M4908-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM112421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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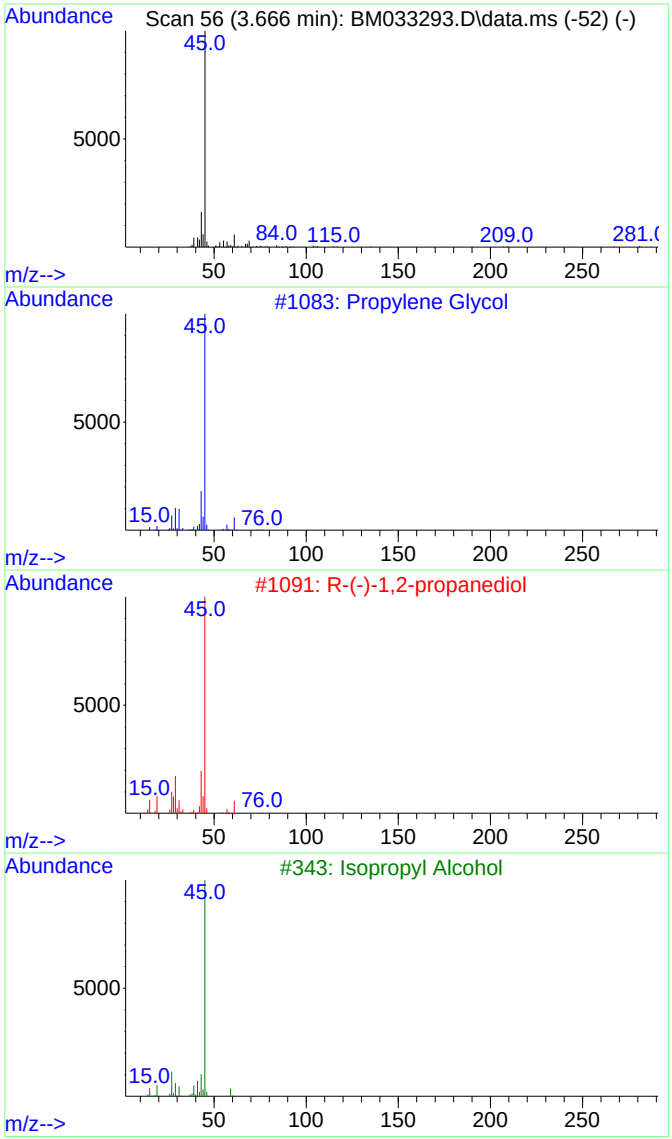
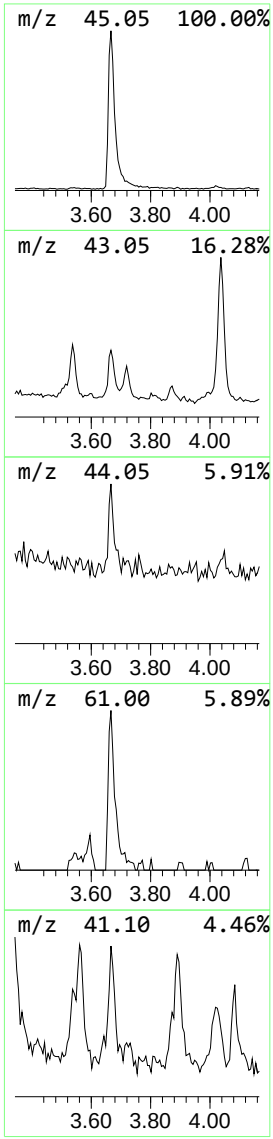
Peak Number 2 Propylene Glycol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.666	2.99 ng	144043	1,4-Dichlorobenzene-d4	7.931

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	78
2	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	72
3	Isopropyl Alcohol	60	C3H8O	000067-63-0	56
4	(2R,4R)-(-)-Pentanediol	104	C5H12O2	042075-32-1	50
5	2-Hexanol, (R)-	102	C6H14O	026549-24-6	40





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Acq On : 03 Dec 2021 19:14
Operator : CG/JU
Sample : M4908-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TW-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM112421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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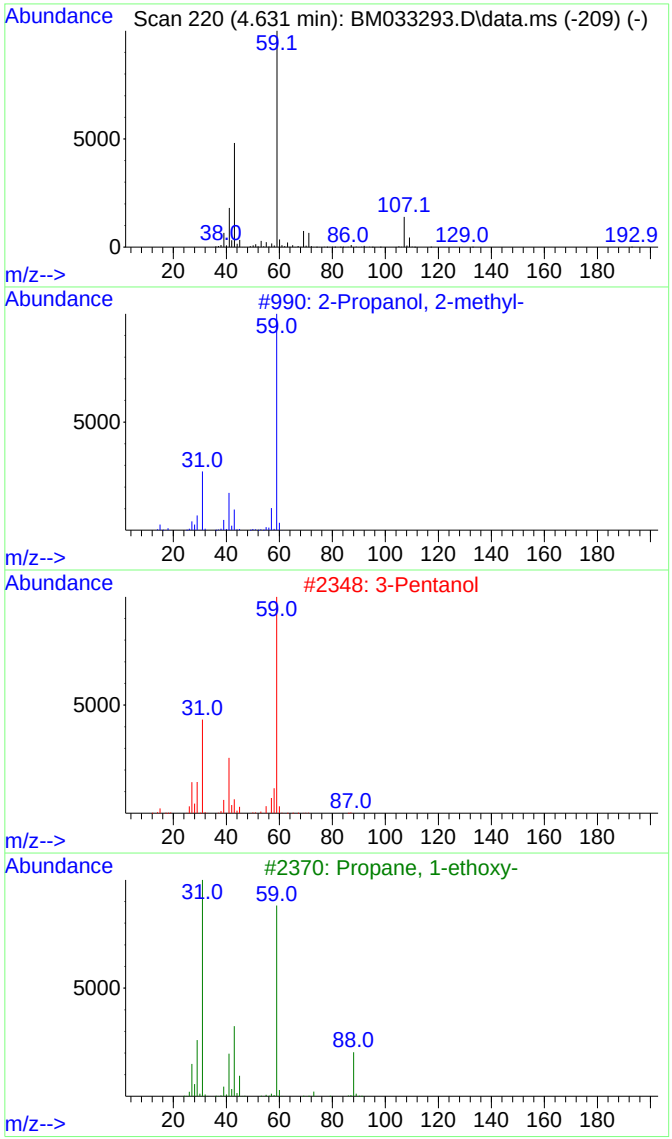
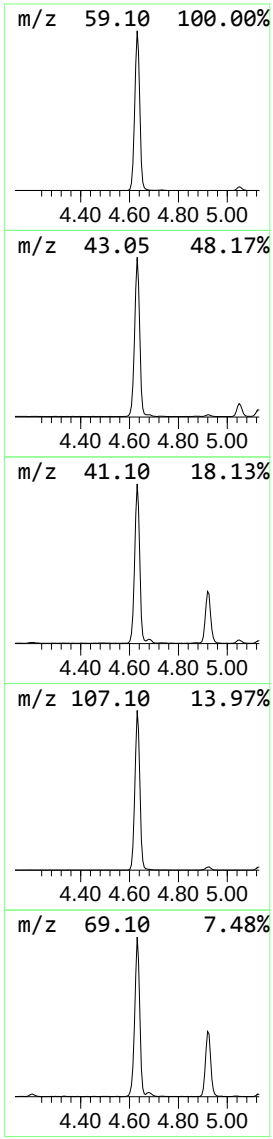
Peak Number 3 2-Propanol, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.631	141.14 ng	6791920	1,4-Dichlorobenzene-d4	7.931

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	50
2	3-Pentanol	88	C5H12O	000584-02-1	42
3	Propane, 1-ethoxy-	88	C5H12O	000628-32-0	36
4	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	33
5	2,4-Dimethyl-2,4-pentanediol	132	C7H16O2	024892-49-7	9





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Operator : CG/JU
Sample : M4908-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TW-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM112421.M
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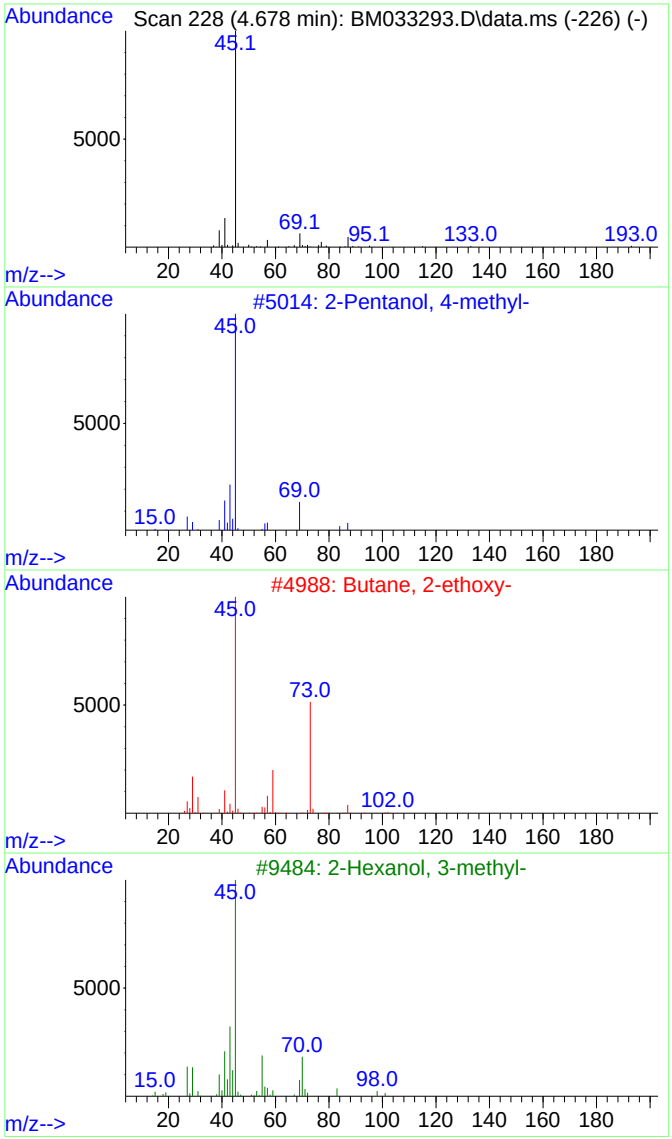
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

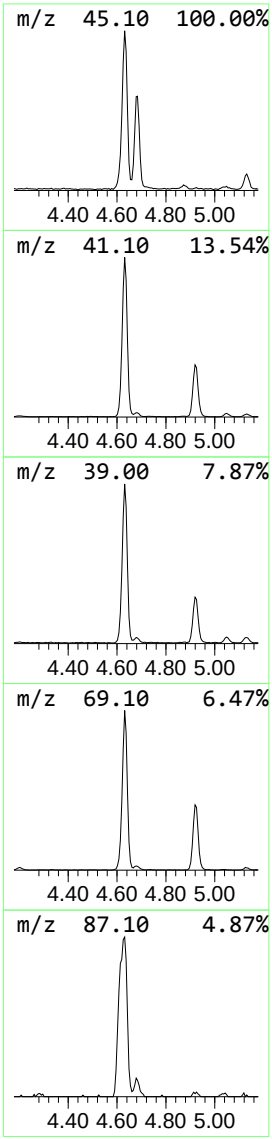
****

Peak Number 4 unknown4.678 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.678	2.45 ng	117729	1,4-Dichlorobenzene-d4	7.931

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanol, 4-methyl-	102	C6H14O	000108-11-2	9
2	Butane, 2-ethoxy-	102	C6H14O	002679-87-0	9
3	2-Hexanol, 3-methyl-	116	C7H16O	002313-65-7	9
4	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	7
5	1-Butene, 4-methoxy	86	C5H10O	004696-30-4	5





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Operator : CG/JU
Sample : M4908-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TW-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM112421.M
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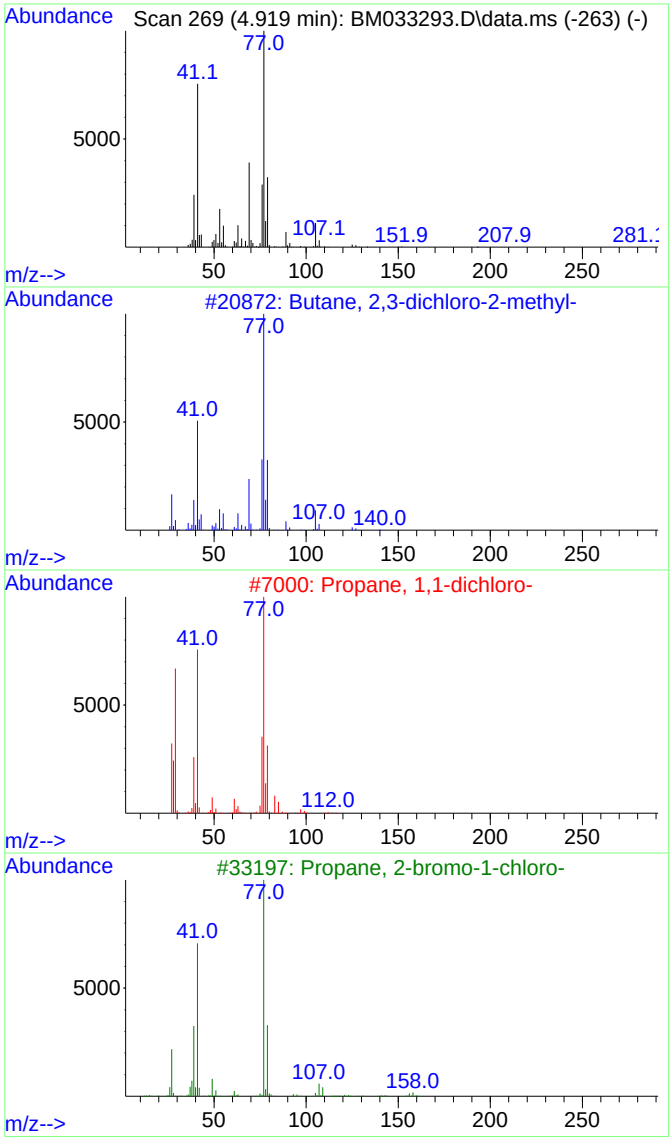
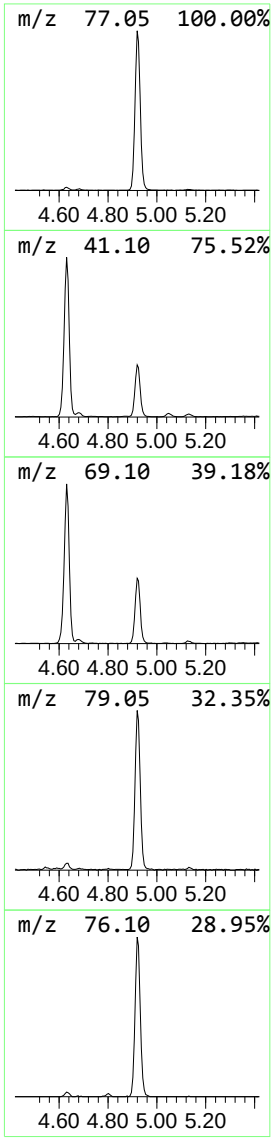
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Butane, 2,3-dichloro-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.919	20.96 ng	1008750	1,4-Dichlorobenzene-d4	7.931

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,3-dichloro-2-methyl-	140	C5H10Cl2	000507-45-9	90
2	Propane, 1,1-dichloro-	112	C3H6Cl2	000078-99-9	42
3	Propane, 2-bromo-1-chloro-	156	C3H6BrCl	003017-95-6	25
4	2-Chlorobutan-1-ol	108	C4H9ClO	108269-46-1	10
5	1-Propene, 1-chloro-	76	C3H5Cl	000590-21-6	9





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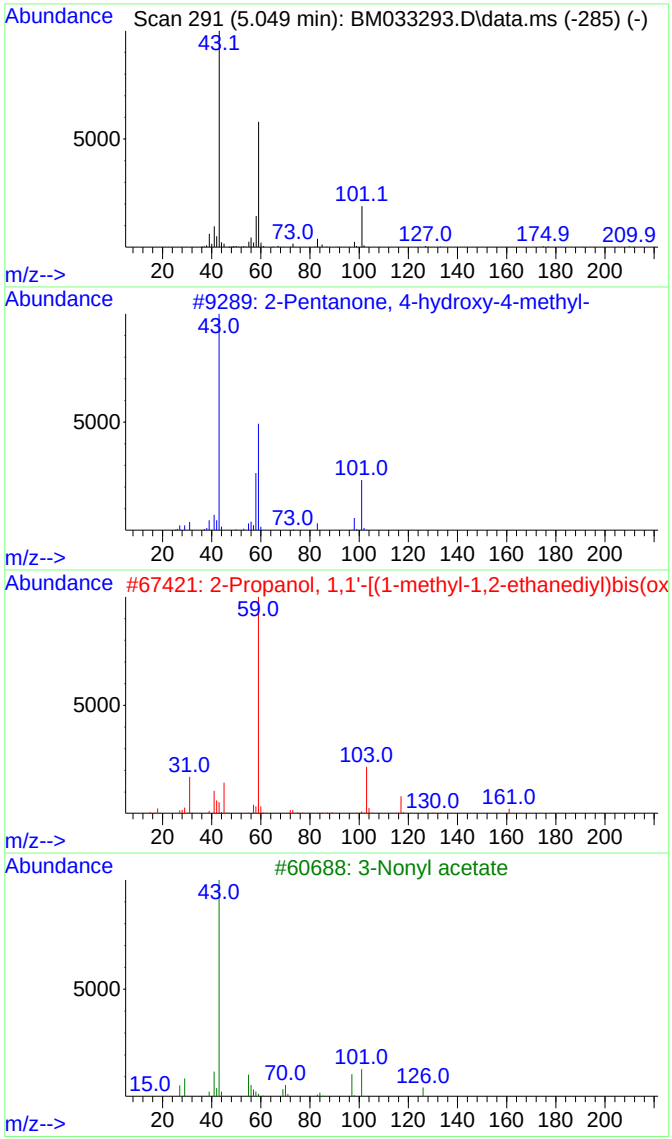
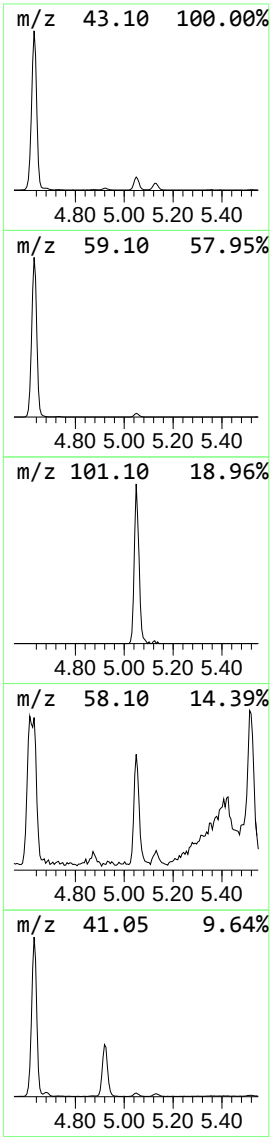
****
Peak Number 6 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.049	5.80 ng	279269	1,4-Dichlorobenzene-d4	7.931

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	2-Propanol, 1,1'-[(1-methyl-1,2-...	192	C9H20O4	001638-16-0	23
3	3-Nonyl acetate	186	C11H22O2	1010429-16-2	17
4	4-Methoxy-1-pentene	100	C6H12O	098386-09-5	17
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10





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Sample : M4908-01
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ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM112421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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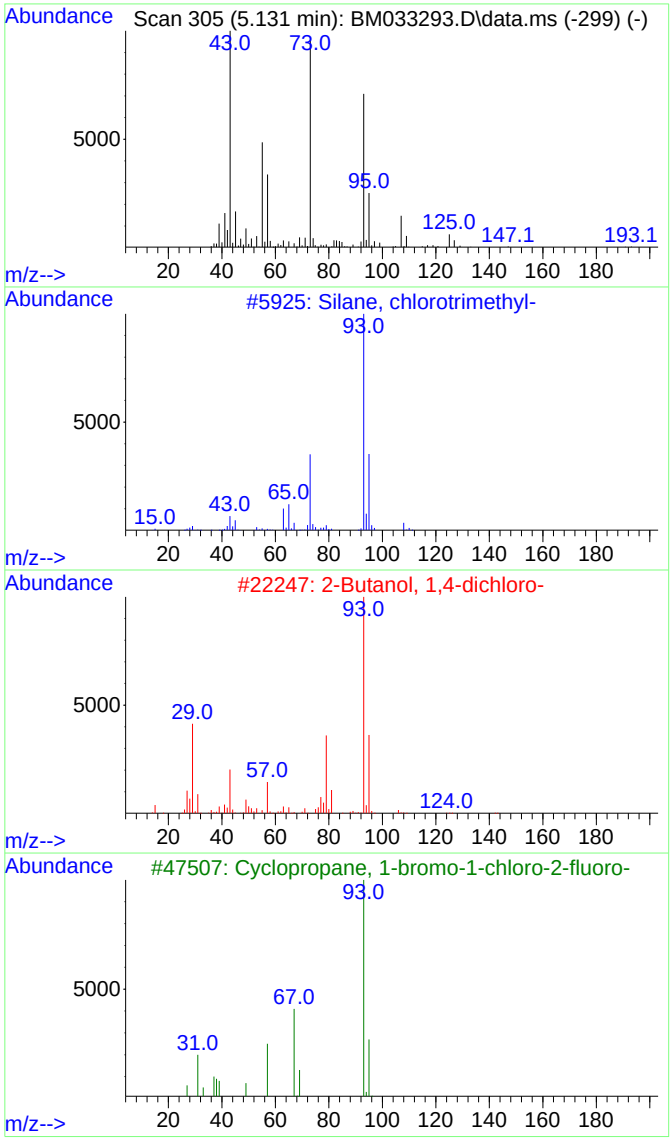
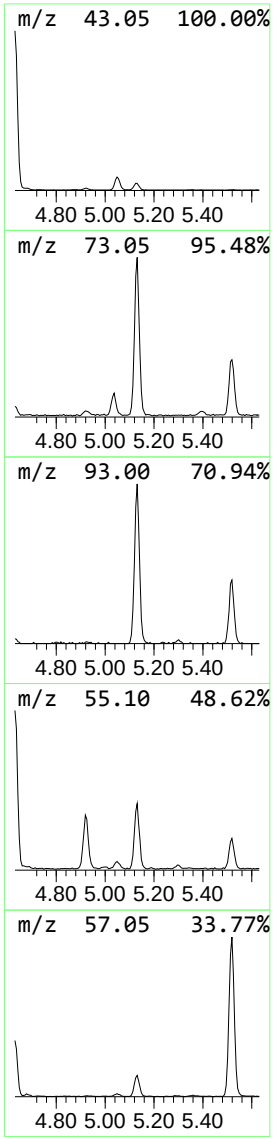
Peak Number 7 unknown5.131 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.131	6.55 ng	315166	1,4-Dichlorobenzene-d4	7.931

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Silane, chlorotrimethyl-	108	C3H9ClSi	000075-77-4	33
2	2-Butanol, 1,4-dichloro-	142	C4H8Cl2O	002419-74-1	25
3	Cyclopropane, 1-bromo-1-chloro-2...	172	C3H3BrClF	024071-59-8	23
4	Methylthio(methylthio-methyl)sul...	172	C3H8O2S3	058000-45-6	17
5	Pyridine, 2-nonyl-	205	C14H23N	010523-35-0	10





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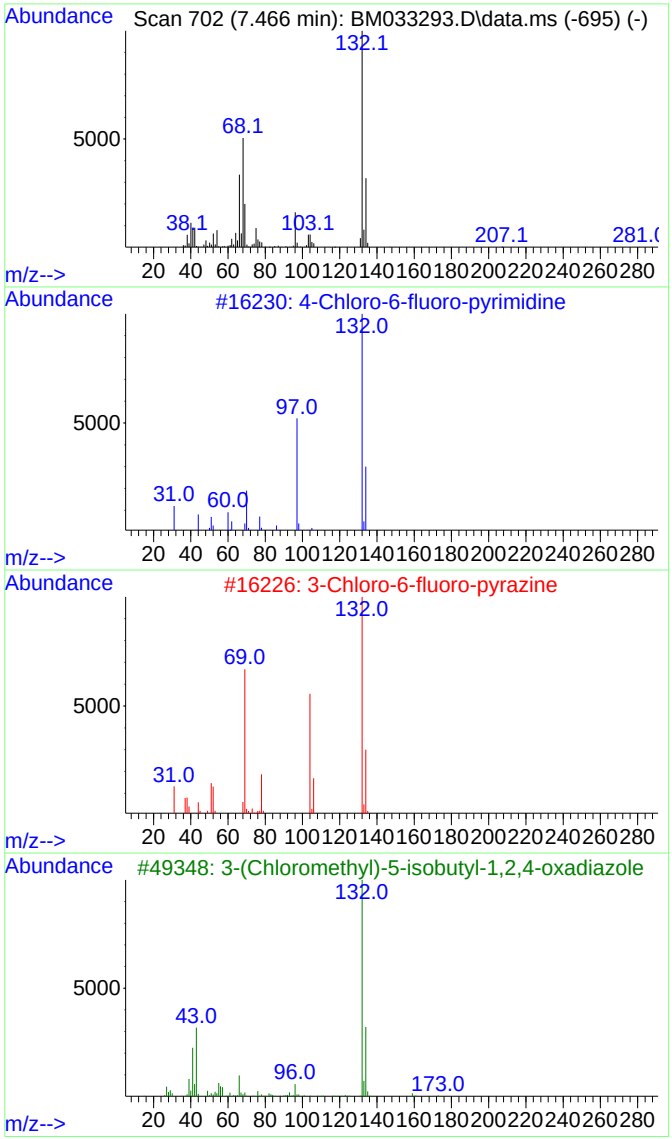
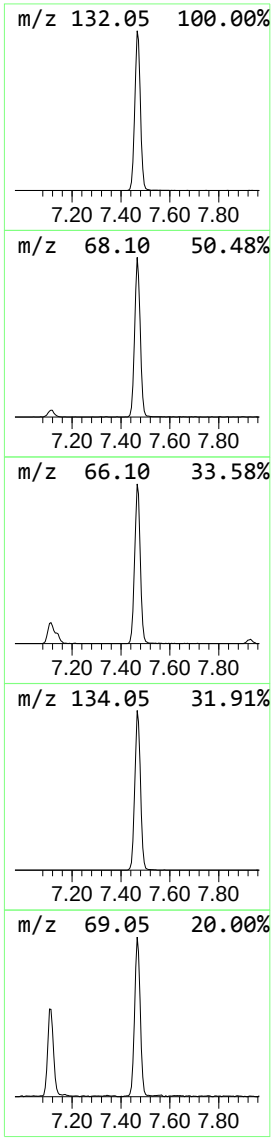
Peak Number 8 unknown7.466 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.466	35.04 ng	1686190	1,4-Dichlorobenzene-d4	7.931

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3	3-(Chloromethyl)-5-isobutyl-1,2,...	174	C7H11ClN2O	189130-85-6	25
4	5-Aminoindole	132	C8H8N2	005192-03-0	22
5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22





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Operator : CG/JU
Sample : M4908-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TW-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM112421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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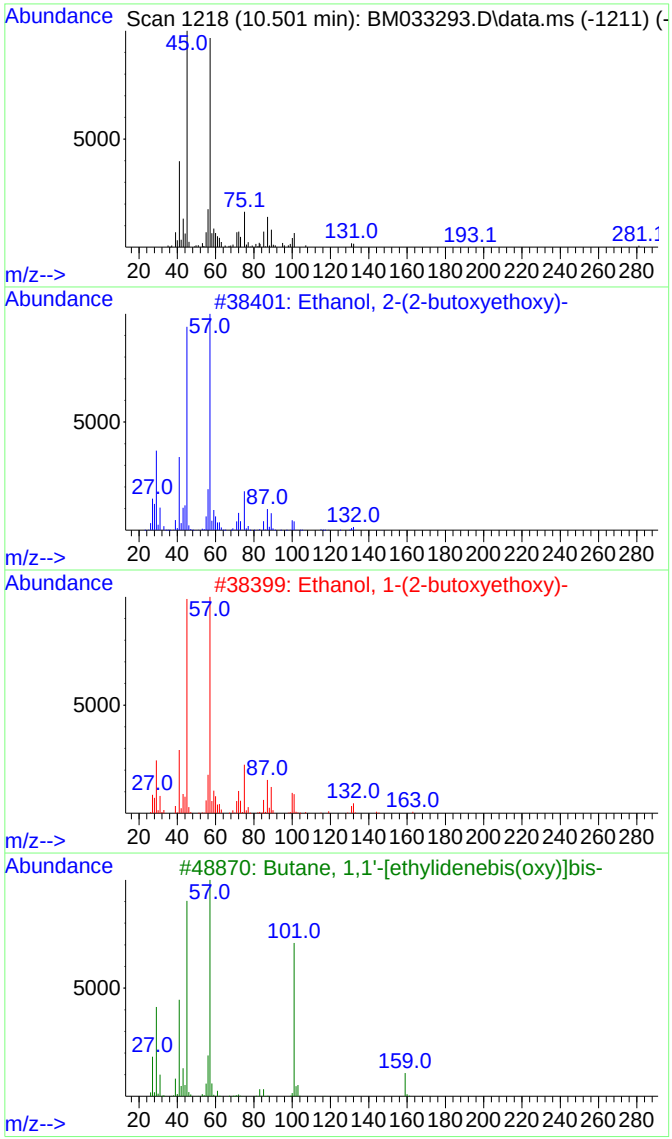
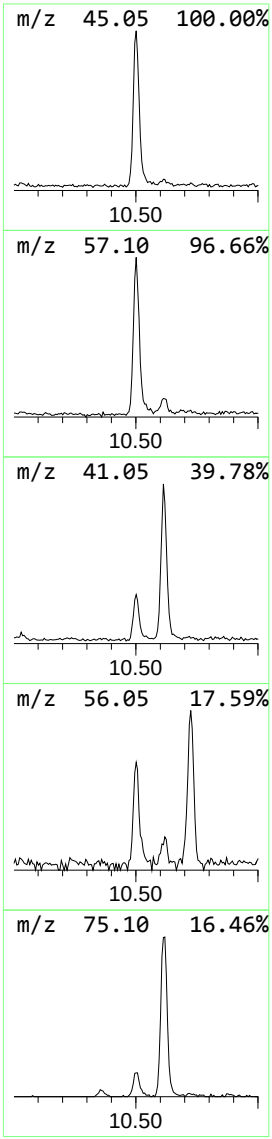
Peak Number 9 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.501	2.14 ng	142888	Naphthalene-d8	10.725

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	90
3	Butane, 1,1'-[ethylidenebis(oxy)...	174	C10H22O2	000871-22-7	53
4	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53
5	Methoxyacetic acid, 2-butyl ester	146	C7H14O3	070159-90-9	53





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM120321\
Data File : BM033293.D
Acq On : 03 Dec 2021 19:14
Operator : CG/JU
Sample : M4908-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TW-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM112421.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
Acetonitrile, d...	3.555	2.9	ng	139812	1	7.931	962414	20.0
Propylene Glycol	3.666	3.0	ng	144043	1	7.931	962414	20.0
2-Propanol, 2-m...	4.631	141.1	ng	6791920	1	7.931	962414	20.0
unknown4.678	4.678	2.5	ng	117729	1	7.931	962414	20.0
Butane, 2,3-dic...	4.919	21.0	ng	1008750	1	7.931	962414	20.0
2-Pentanone, 4-...	5.049	5.8	ng	279269	1	7.931	962414	20.0
unknown5.131	5.131	6.5	ng	315166	1	7.931	962414	20.0
unknown7.466	7.466	35.0	ng	1686190	1	7.931	962414	20.0
Ethanol, 2-(2-b...	10.501	2.1	ng	142888	2	10.725	1332840	20.0