

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062821\
 Data File : BG049123.D
 Acq On : 28 Jun 2021 17:42
 Operator : CG/JU
 Sample : M2827-06
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 ERM-7

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_G\METHODS\8270-BG061121.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG049123.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.152	11	19	28	rBV2	105377	231309	7.34%	2.133%
2	3.229	28	32	44	rVB2	41087	71023	2.25%	0.655%
3	5.185	361	365	373	rVB	18762	32051	1.02%	0.296%
4	5.655	438	445	457	rBV	294532	494571	15.70%	4.562%
5	7.253	710	717	727	rBV	182301	329605	10.46%	3.040%
6	8.099	855	861	869	rBV	99803	177035	5.62%	1.633%
7	9.268	1050	1060	1069	rBV	379647	709448	22.51%	6.543%
8	10.684	1294	1301	1313	rBV2	36857	76404	2.42%	0.705%
9	10.925	1334	1342	1351	rBV	134390	244247	7.75%	2.253%
10	13.364	1748	1757	1767	rBV	992412	1594191	50.59%	14.704%
11	14.744	1985	1992	2001	rVB	233902	371566	11.79%	3.427%
12	16.231	2234	2245	2259	rBV	951858	1626468	51.62%	15.001%
13	17.494	2454	2460	2466	rBV	301988	479961	15.23%	4.427%
14	20.097	2896	2903	2910	rBV	2390356	3151056	100.00%	29.063%
15	21.413	3123	3127	3133	rBV7	23868	55176	1.75%	0.509%
16	21.489	3136	3140	3144	rVB	24691	43367	1.38%	0.400%
17	21.777	3182	3189	3197	rBV2	338517	572039	18.15%	5.276%
18	25.091	3743	3753	3763	rVB2	198138	582687	18.49%	5.374%

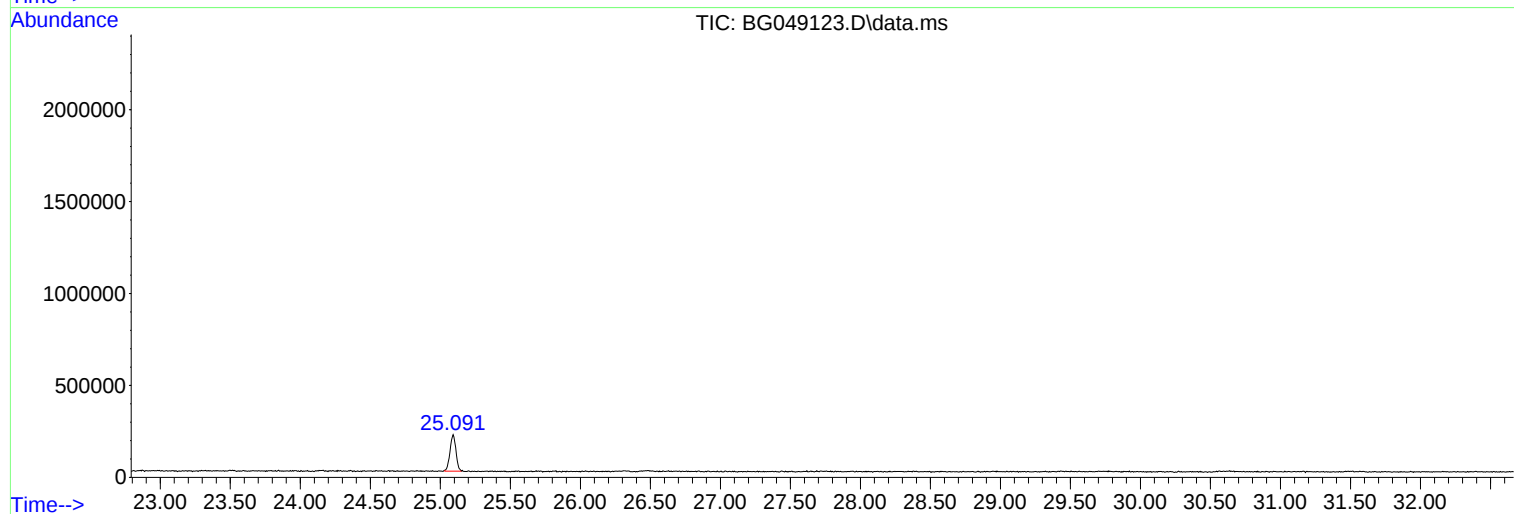
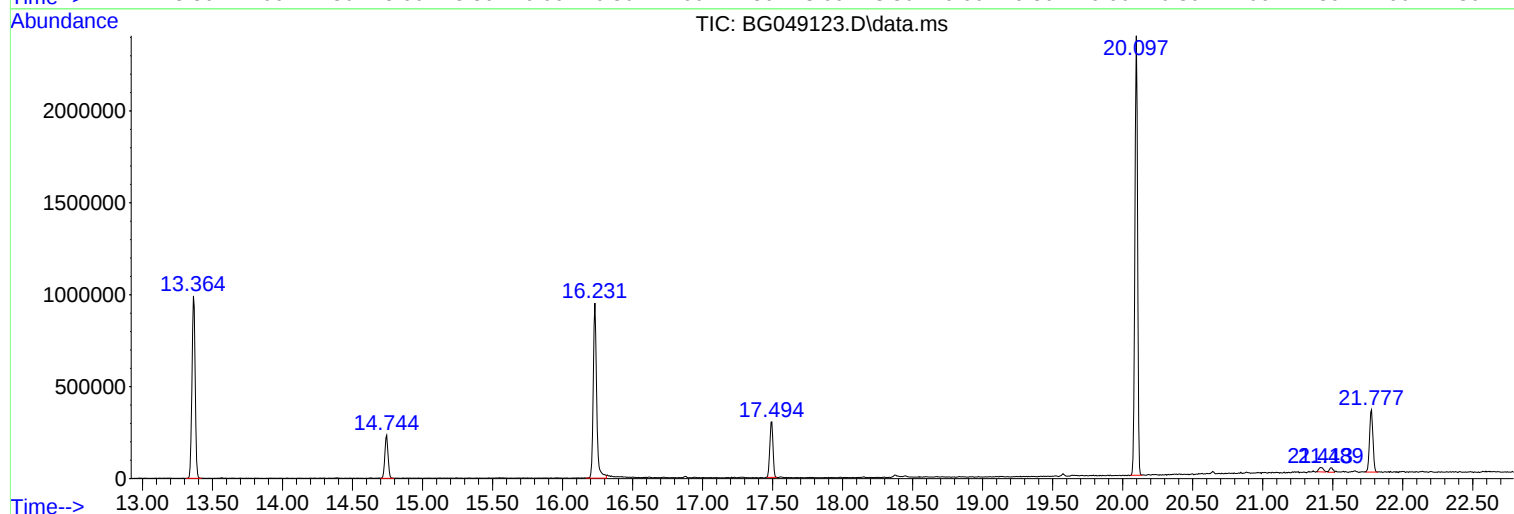
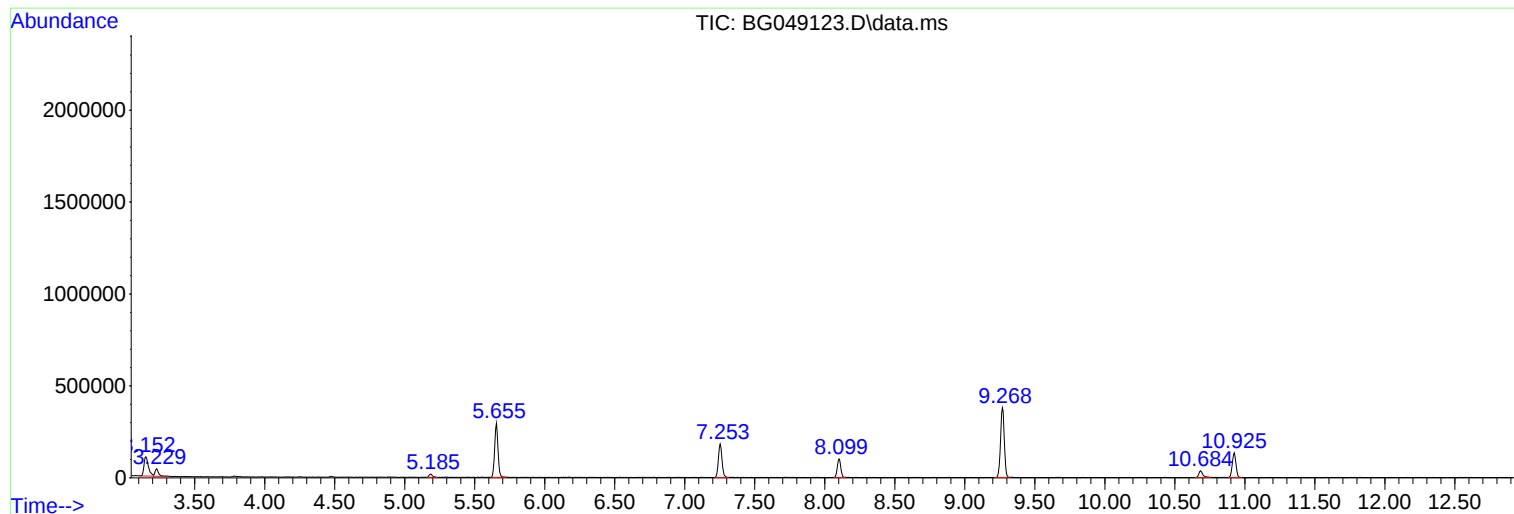
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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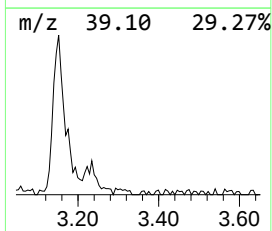
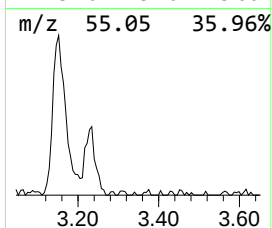
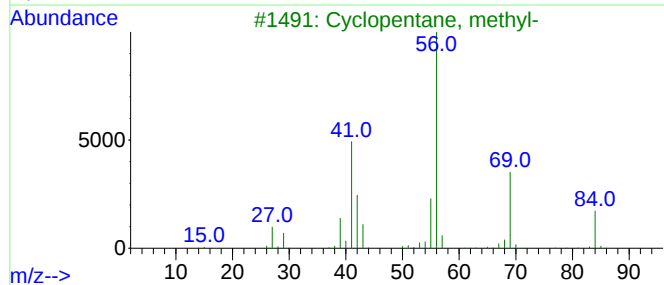
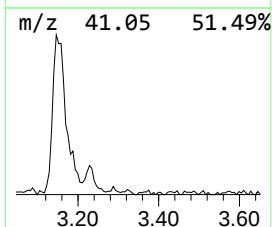
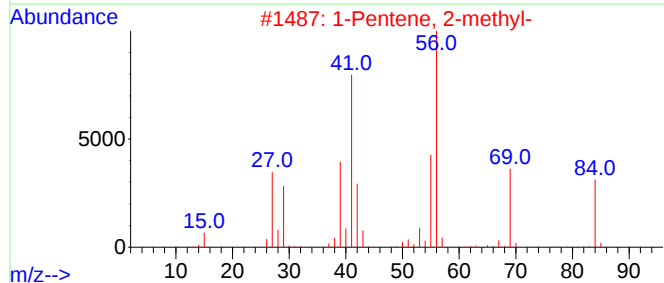
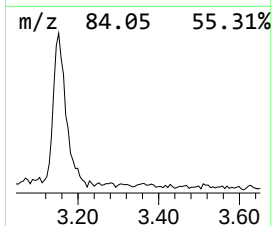
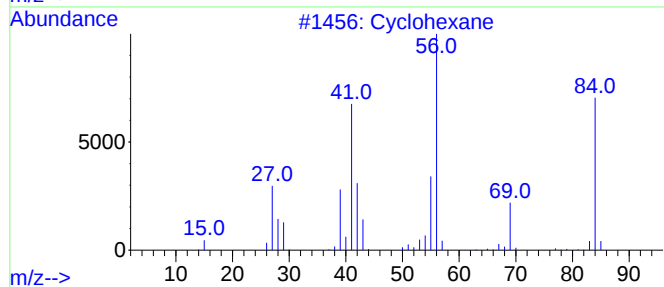
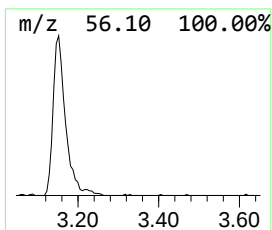
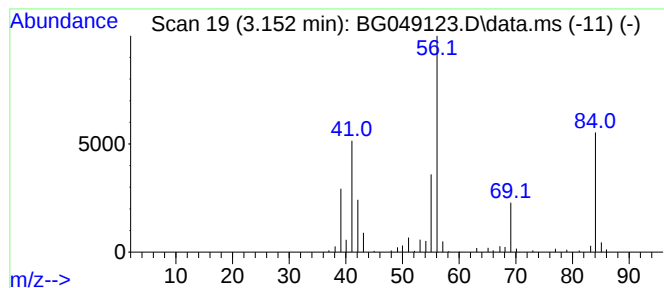
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Cyclohexane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.152	26.13 ng	231309	1,4-Dichlorobenzene-d4	8.099

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane	84	C6H12	000110-82-7	91
2			1-Pentene, 2-methyl-	84	C6H12	000763-29-1	78
3			Cyclopentane, methyl-	84	C6H12	000096-37-7	78
4			1-Hexene	84	C6H12	000592-41-6	53
5			Cyclobutane, ethyl-	84	C6H12	004806-61-5	47



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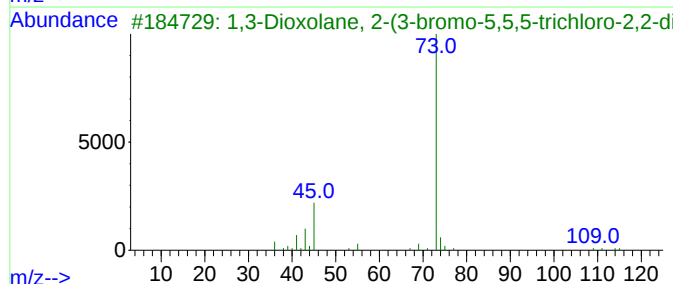
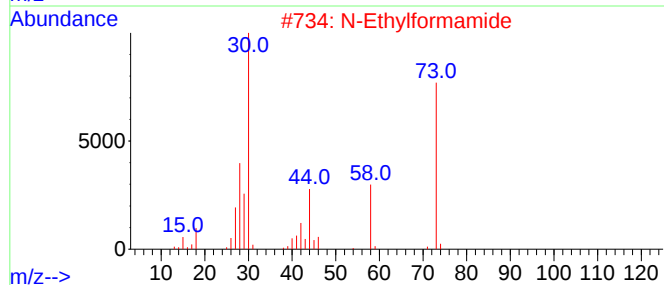
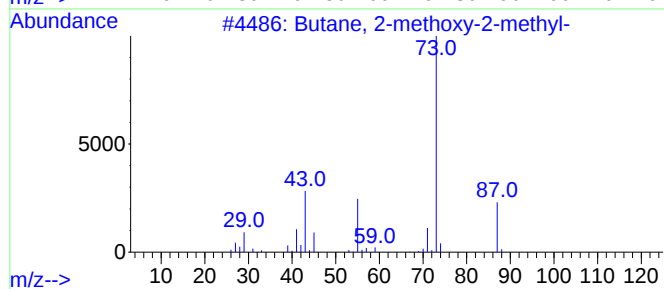
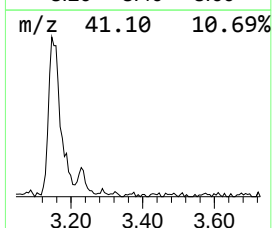
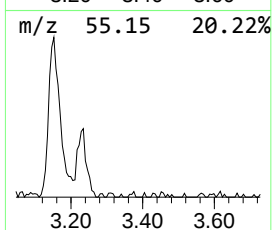
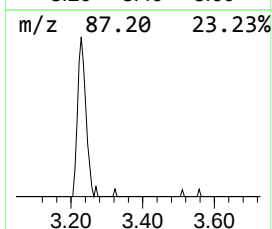
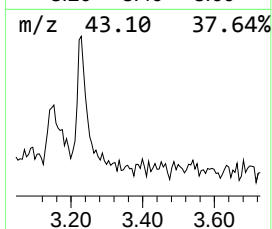
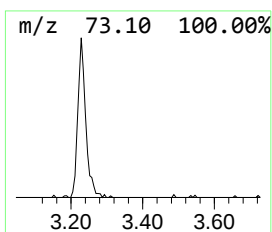
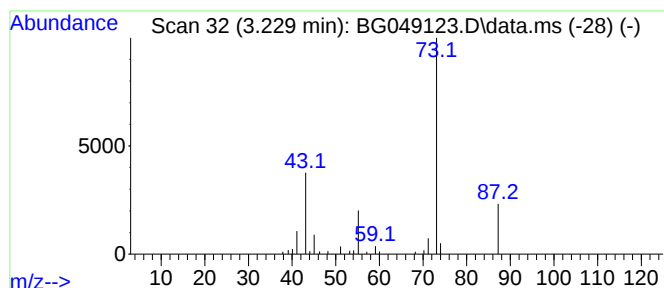
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TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown3.229 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.229	8.02 ng	71023	1,4-Dichlorobenzene-d4	8.099

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	33
2			N-Ethylformamide	73	C3H7NO	000627-45-2	9
3			1,3-Dioxolane, 2-(3-bromo-5,5,5-...	352	C10H16BrCl3O2	1000115-31-4	9
4			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	4
5			2-(2-Bromoethyl)-1,3-dioxolane	180	C5H9BrO2	018742-02-4	4



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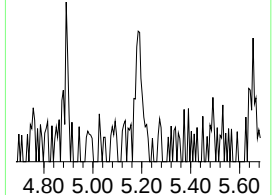
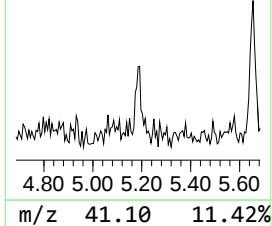
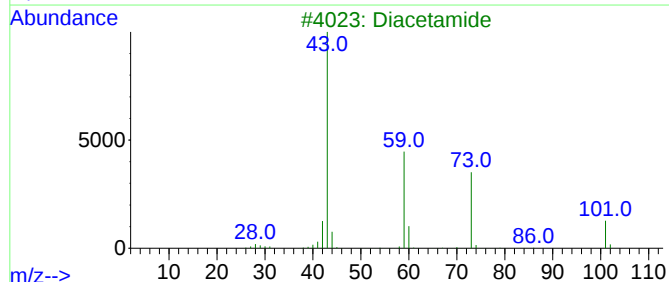
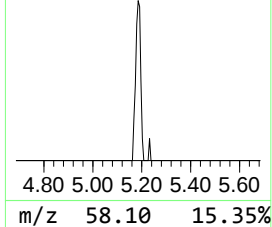
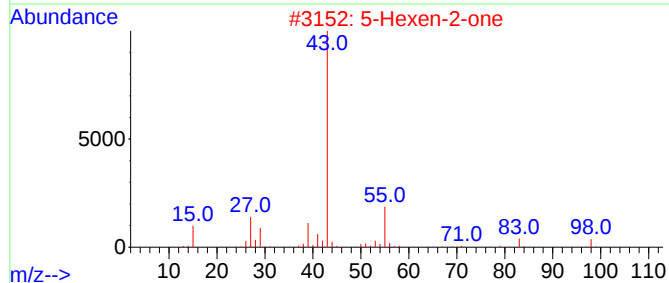
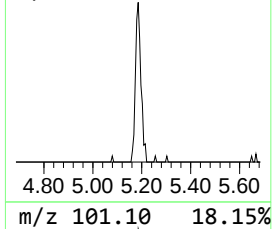
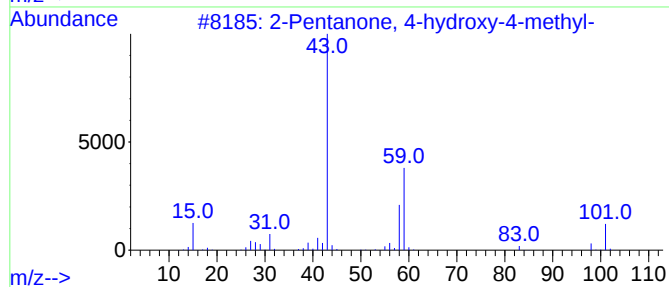
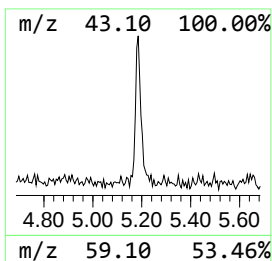
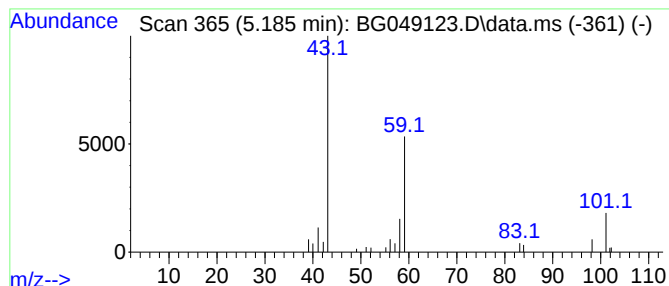
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
5.185	3.62 ng	32051	1,4-Dichlorobenzene-d4		8.099	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	45
2	5-Hexen-2-one		98	C6H10O	000109-49-9	9
3	Diacetamide		101	C4H7NO2	000625-77-4	9
4	Propane, 1-ethoxy-2-methyl-		102	C6H14O	000627-02-1	9
5	1,2-Butanediol		90	C4H10O2	000584-03-2	9



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ClientSampleId :
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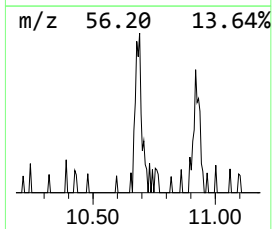
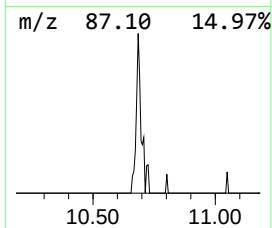
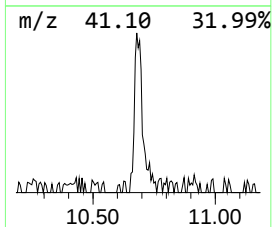
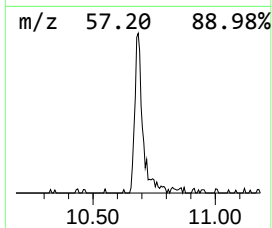
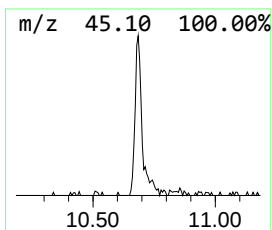
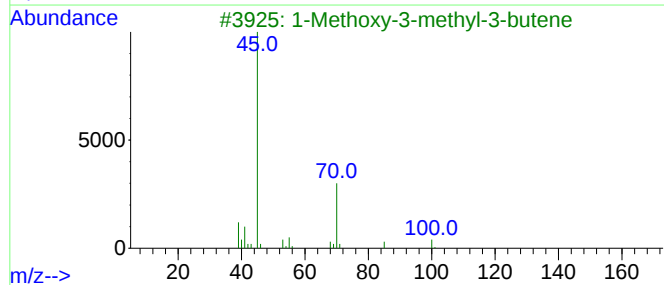
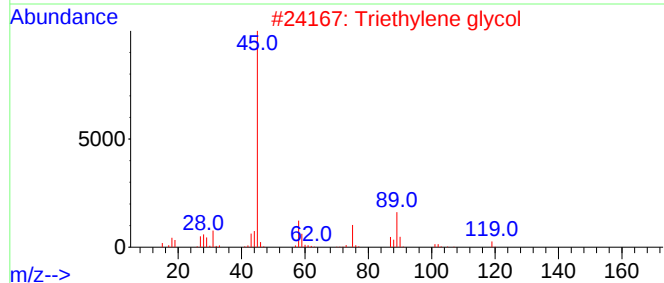
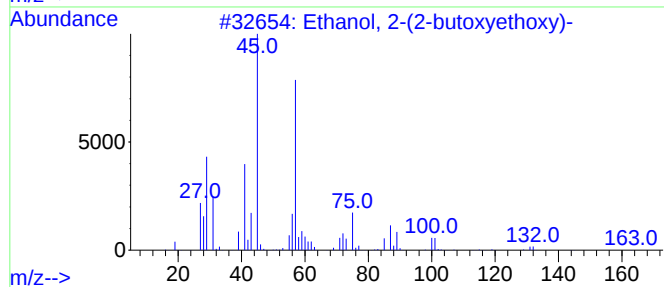
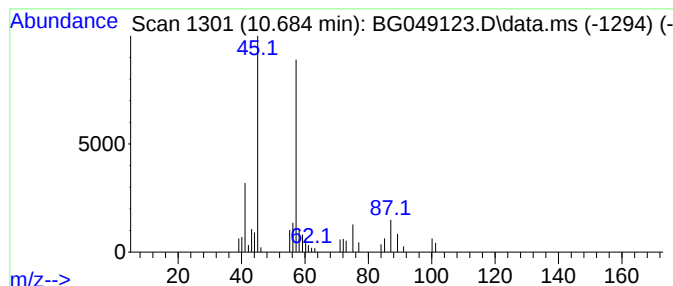
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Peak Number 4 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.685	6.26 ng	76404	Naphthalene-d8	10.925

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	78
2			Triethylene glycol	150	C6H14O4	000112-27-6	50
3			1-Methoxy-3-methyl-3-butene	100	C6H12O	034752-58-4	47
4			Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	43
5			Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	42



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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Cyclohexane	3.152	26.1	ng	231309	1	8.099	177035	20.0
unknown3.229	3.229	8.0	ng	71023	1	8.099	177035	20.0
2-Pentanone, 4-...	5.185	3.6	ng	32051	1	8.099	177035	20.0
Ethanol, 2-(2-b...	10.685	6.3	ng	76404	2	10.925	244247	20.0