

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041621\
 Data File : BM029521.D
 Acq On : 16 Apr 2021 14:40
 Operator : CG/JU
 Sample : M1982-02
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 WC-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-BM040121.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM029521.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.936	308	311	313	rBV	17467222	15070384	82.62%	20.741%
2	1.954	313	314	316	rBV2	18087283	18240568	100.00%	25.104%
3	1.977	316	318	320	rBV2	12582174	14515570	79.58%	19.978%
4	2.712	438	443	460	rVB	4642230	5204110	28.53%	7.162%
5	2.918	474	478	494	rVB	585430	757781	4.15%	1.043%
6	5.271	872	878	891	rBV	1212505	1684943	9.24%	2.319%
7	6.847	1137	1146	1160	rBV	1206296	1920111	10.53%	2.643%
8	7.671	1280	1286	1296	rBV	342427	536978	2.94%	0.739%
9	8.824	1474	1482	1492	rBV	733888	1192298	6.54%	1.641%
10	10.453	1750	1759	1765	rBV	422768	706272	3.87%	0.972%
11	12.929	2172	2180	2192	rBV	1601270	2302818	12.62%	3.169%
12	14.312	2409	2415	2422	rBV2	593137	877935	4.81%	1.208%
13	15.800	2661	2668	2677	rBV	1309824	1839185	10.08%	2.531%
14	17.053	2875	2881	2886	rBV	727198	1010145	5.54%	1.390%
15	19.111	3224	3231	3240	rBV	223629	342151	1.88%	0.471%
16	19.682	3321	3328	3339	rBV	2614971	3202083	17.55%	4.407%
17	20.958	3541	3545	3552	rBV	379390	501825	2.75%	0.691%
18	21.235	3585	3592	3596	rBV2	879413	1323997	7.26%	1.822%
19	22.782	3850	3855	3859	rBV	187453	359651	1.97%	0.495%
20	23.440	3961	3967	3973	rBV2	610042	1070142	5.87%	1.473%

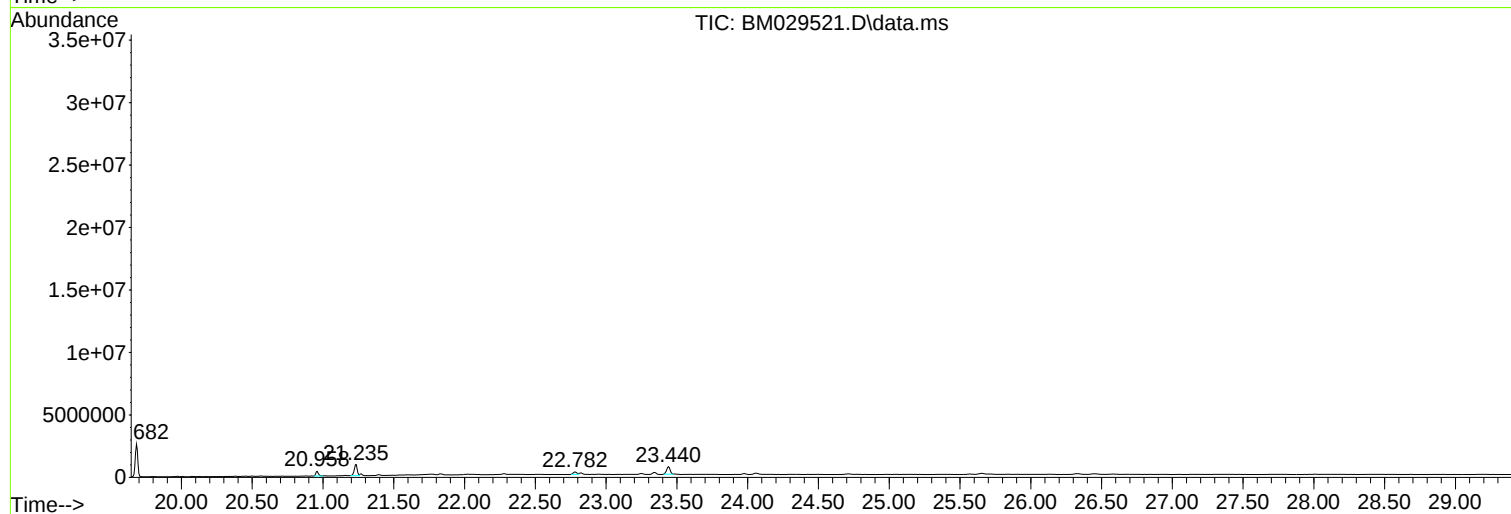
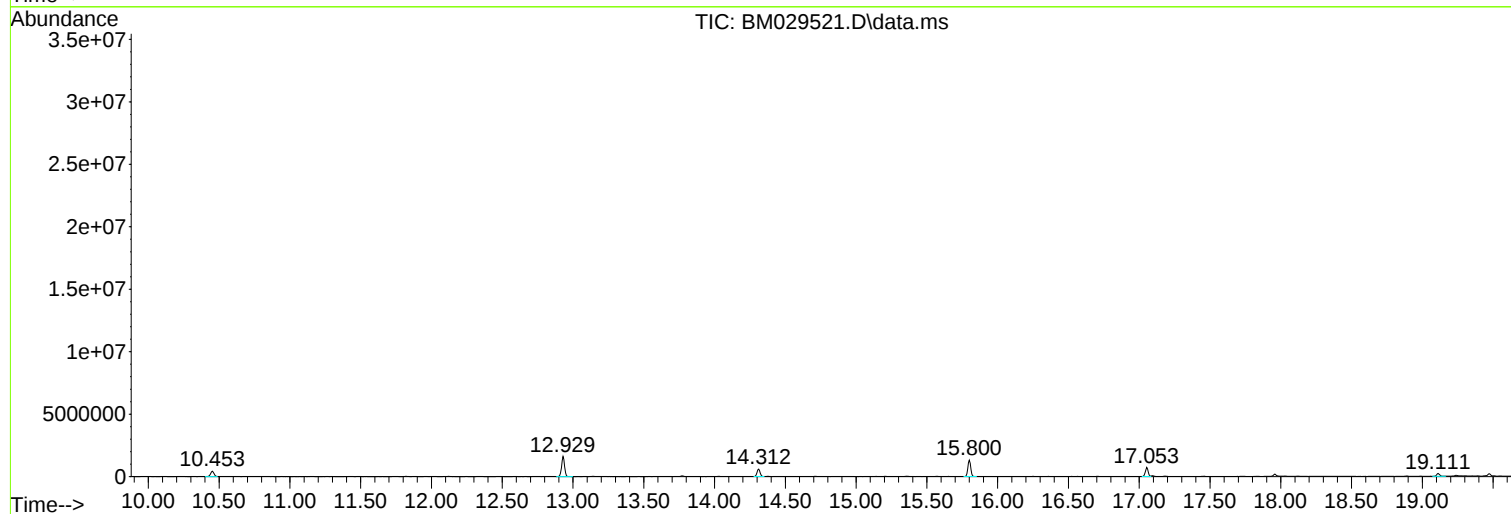
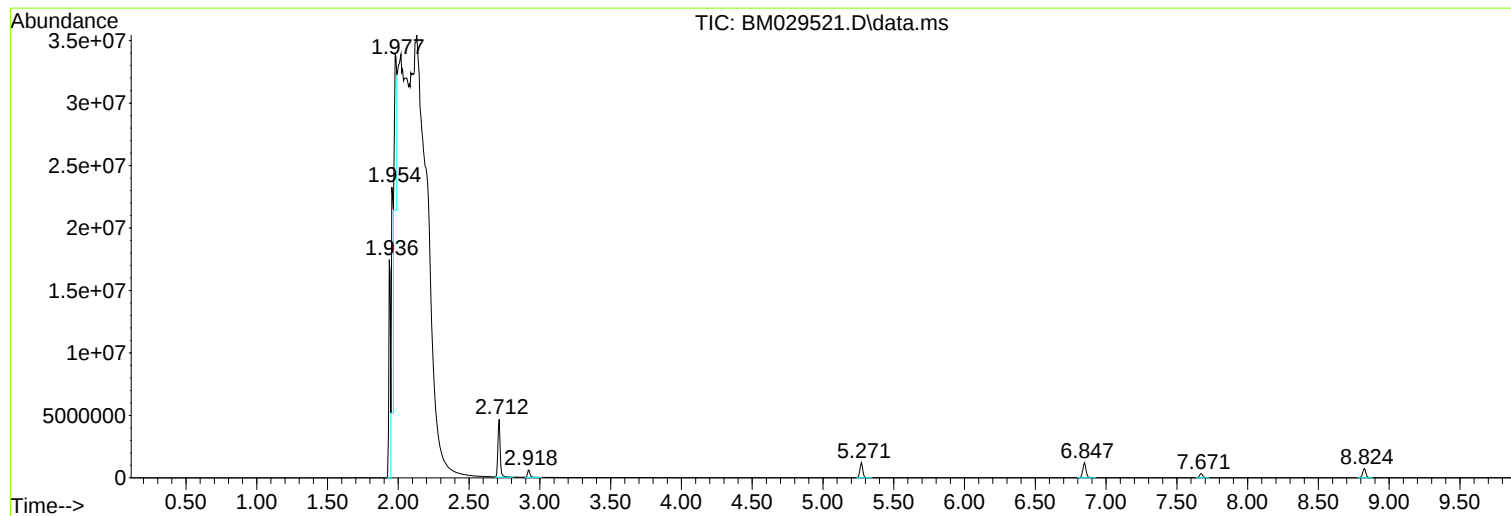
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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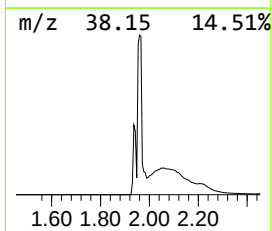
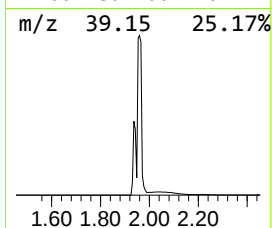
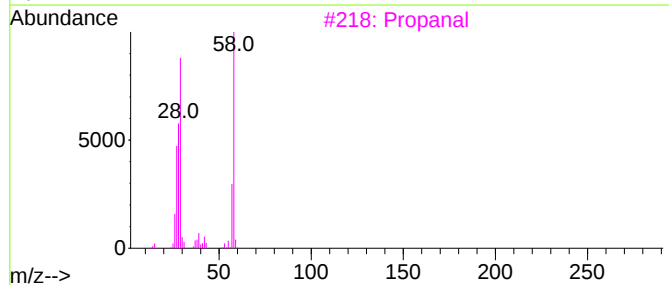
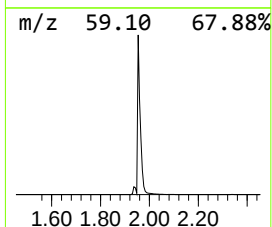
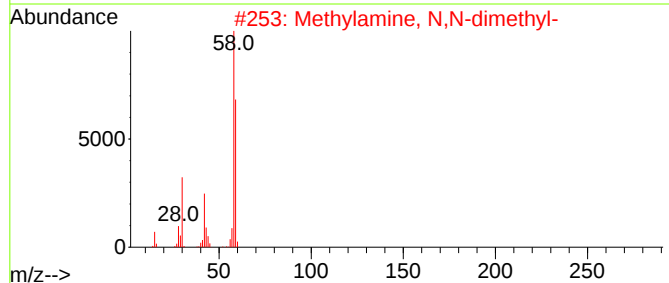
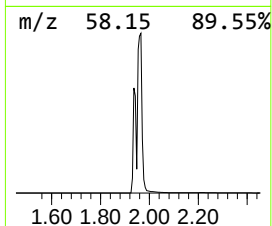
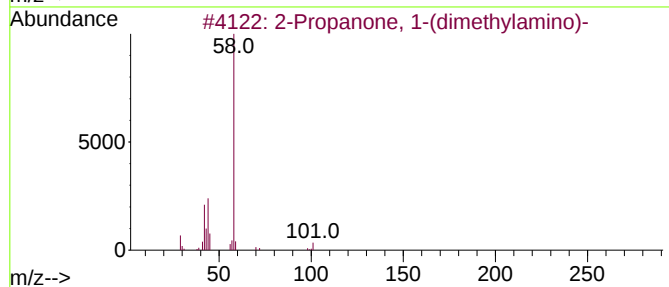
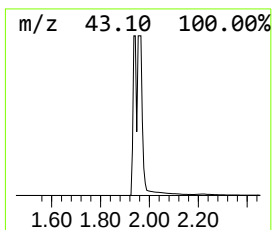
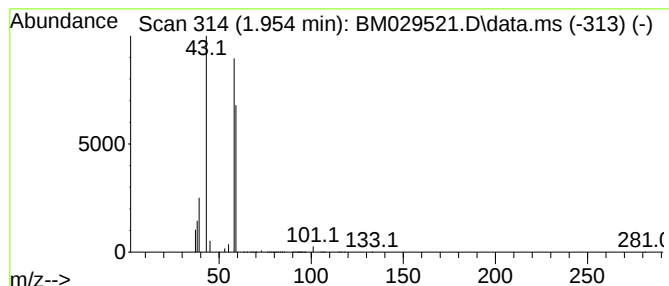
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown1.954 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.954	679.38 ng	18240600	1,4-Dichlorobenzene-d4	7.671

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanone, 1-(dimethylamino)-		101	C5H11NO	015364-56-4	5	
2	Methylamine, N,N-dimethyl-		59	C3H9N	000075-50-3	5	
3	Propanal		58	C3H6O	000123-38-6	4	
4	Guanidine		59	CH5N3	000113-00-8	4	
5	2-Hexanol, methyl ether		116	C7H16O	1000333-92-0	4	



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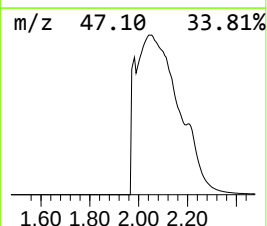
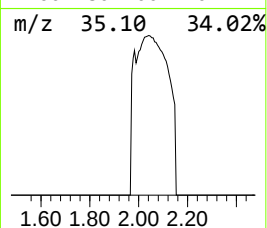
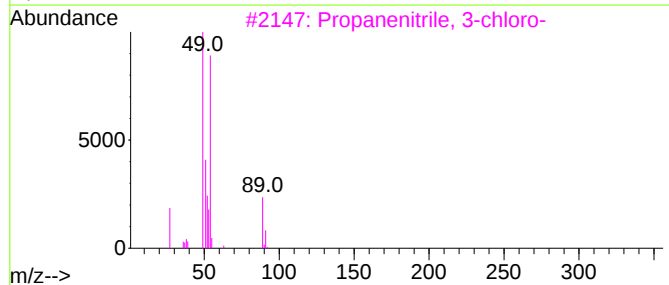
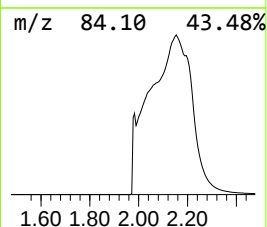
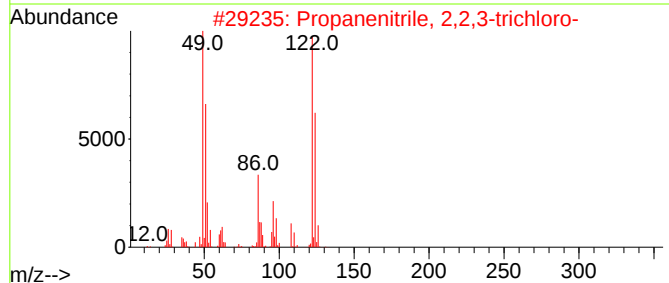
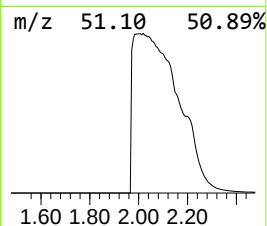
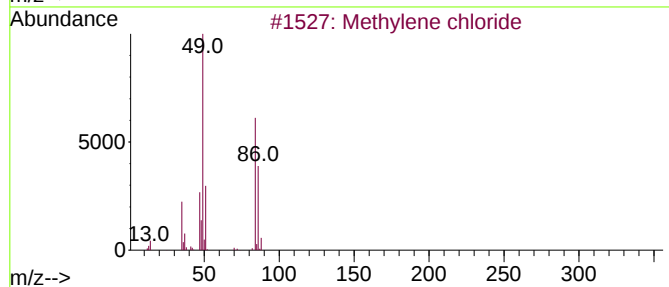
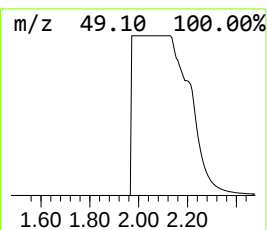
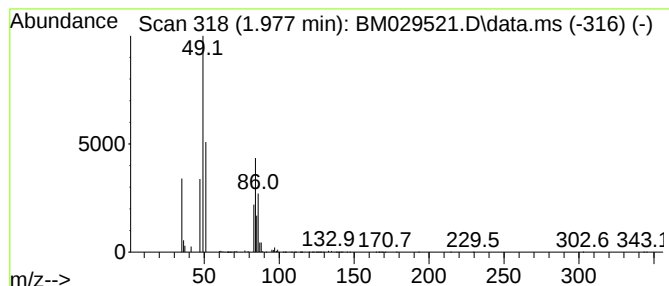
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 Methylene chloride Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.977	540.64 ng	14515600	1,4-Dichlorobenzene-d4	7.671

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methylene chloride	84	CH2Cl2	000075-09-2	86
2			Propanenitrile, 2,2,3-trichloro-	157	C3H2Cl3N	000813-74-1	9
3			Propanenitrile, 3-chloro-	89	C3H4ClN	000542-76-7	9
4			Dichloroacetaldehyde	112	C2H2Cl2O	000079-02-7	9
5			Chloromethanesulfonyl chloride	148	CH2Cl2O2S	003518-65-8	4



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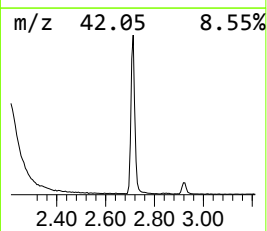
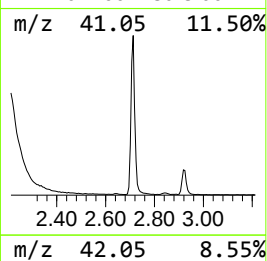
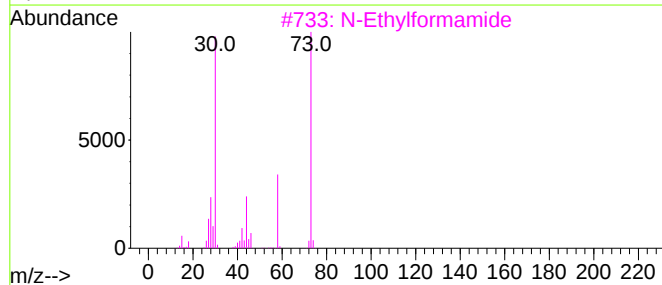
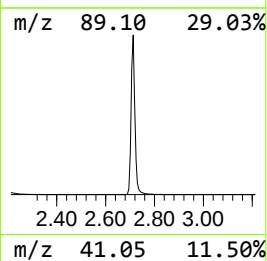
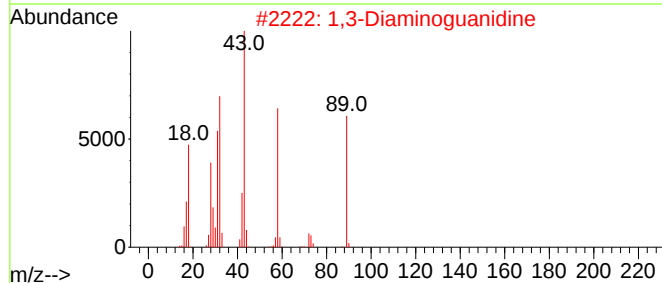
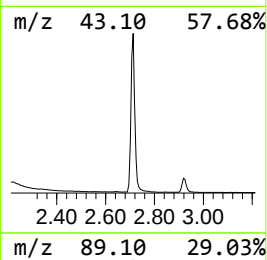
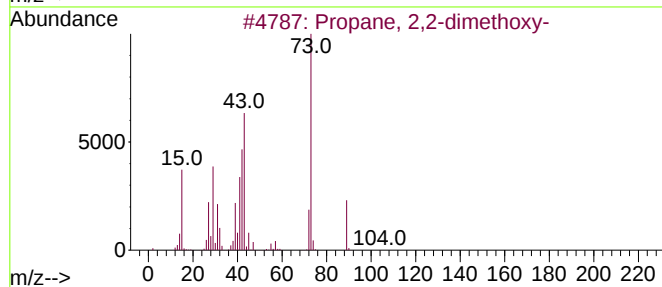
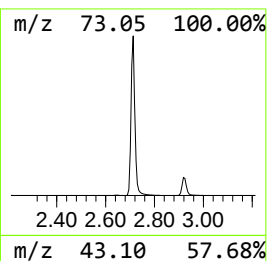
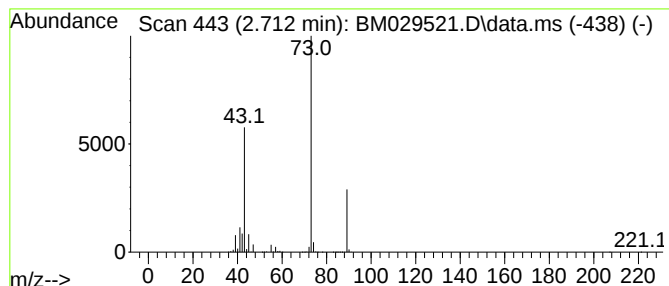
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Peak Number 4 Propane, 2,2-dimethoxy- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.712	193.83 ng	5204110	1,4-Dichlorobenzene-d4	7.671

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	50
2			1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
3			N-Ethylformamide	73	C3H7NO	000627-45-2	9
4			1-Hexen-4-ol, 1-chloro-3,5-dimet...	162	C8H15ClO	100244-09-5	9
5			2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9



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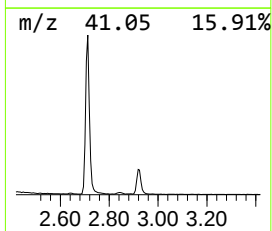
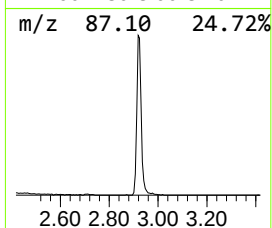
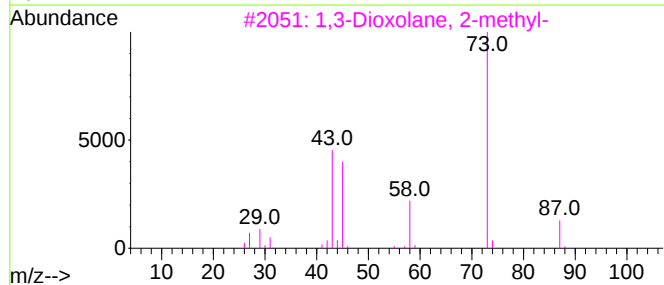
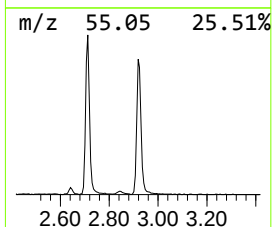
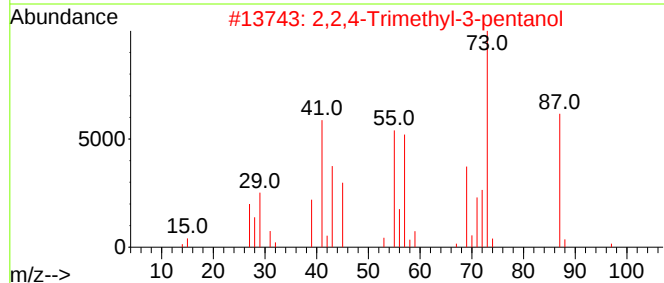
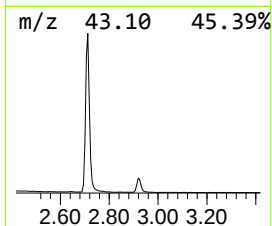
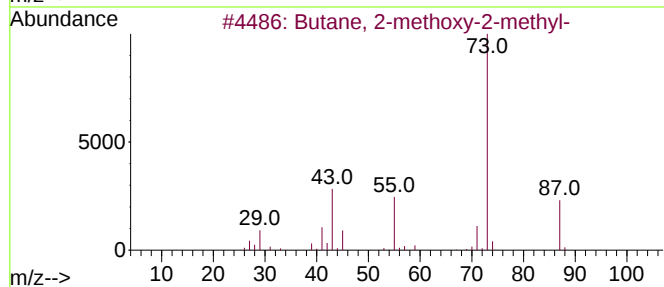
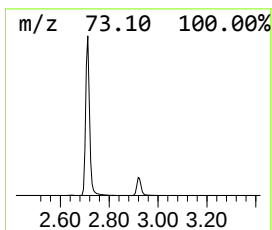
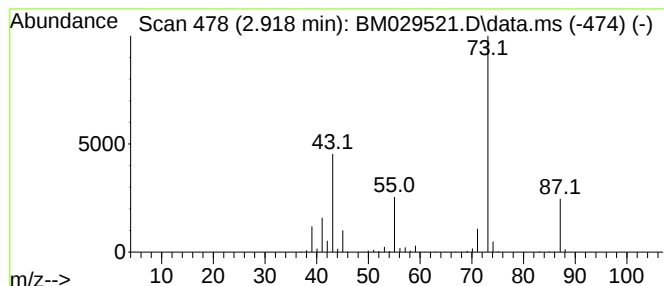
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Peak Number 5 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.918	28.22 ng	757781	1,4-Dichlorobenzene-d4	7.671

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	38
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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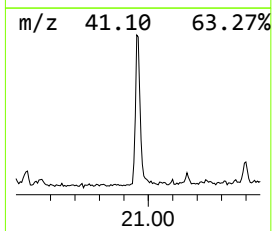
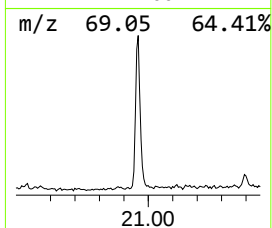
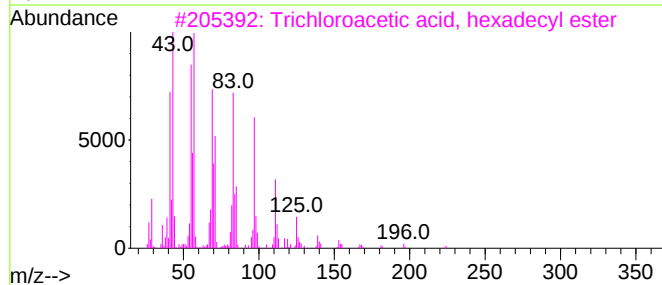
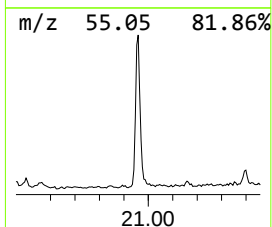
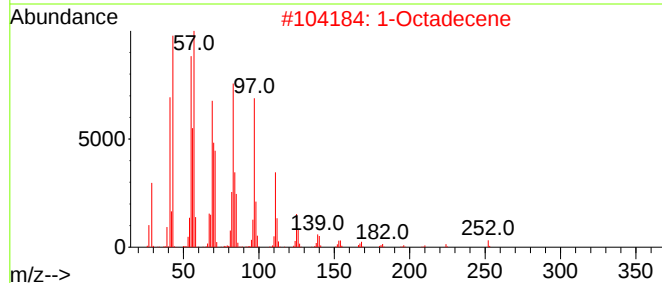
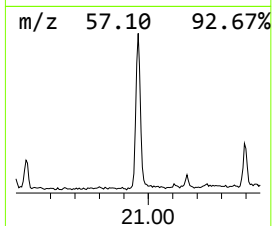
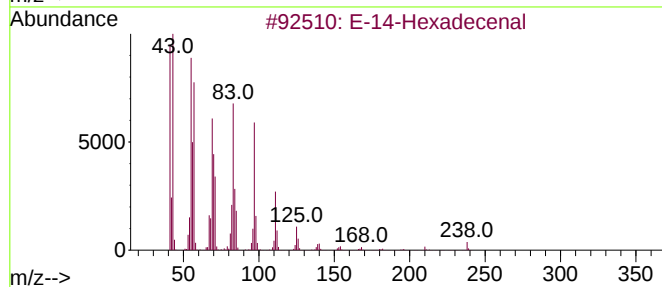
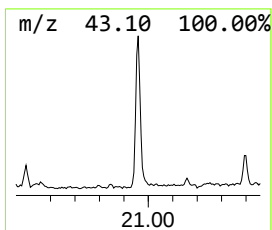
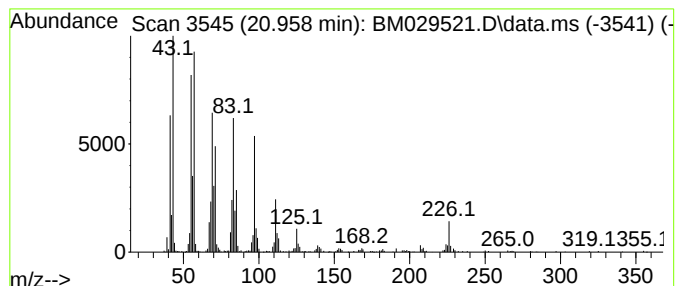
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Peak Number 6 E-14-Hexadecenal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.958	7.58 ng	501825	Chrysene-d12	21.235

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			E-14-Hexadecenal	238	C16H30O	330207-53-9	97
2			1-Octadecene	252	C18H36	000112-88-9	96
3			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	93
4			Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	90
5			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	90



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown1.954	1.954	679.4	ng	18240600	1	7.671	536978	20.0
Methylene chloride	1.977	540.6	ng	14515600	1	7.671	536978	20.0
Propane, 2,2-di...	2.712	193.8	ng	5204110	1	7.671	536978	20.0
Butane, 2-metho...	2.918	28.2	ng	757781	1	7.671	536978	20.0
E-14-Hexadecenal	20.958	7.6	ng	501825	5	21.235	1324000	20.0