

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG110316\
 Data File : BG024659.D
 Acq On : 3 Nov 2016 23:02
 Operator : UM/SJ
 Sample : H5502-04
 Misc :
 ALS Vial : 29 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB-80-13.5-14.0

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

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

Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.125	44	49	69	rVB	7683831	12776589	100.00%	19.796%
2	5.328	417	424	432	rBV	515657	850076	6.65%	1.317%
3	5.798	496	504	514	rBV	2335060	3946389	30.89%	6.115%
4	7.402	769	777	788	rBV	2418721	4441585	34.76%	6.882%
5	7.790	835	843	854	rBV	2355461	4128232	32.31%	6.396%
6	8.266	916	924	931	rBV	369935	644092	5.04%	0.998%
7	8.595	971	980	989	rBV	1667020	2993588	23.43%	4.638%
8	9.441	1114	1124	1132	rBV	1490956	2743129	21.47%	4.250%
9	11.092	1399	1405	1414	rVB	486095	899226	7.04%	1.393%
10	13.507	1806	1816	1823	rBV	3481865	5694702	44.57%	8.823%
11	14.318	1947	1954	1960	rBV	557648	851630	6.67%	1.320%
12	14.882	2042	2050	2057	rBV2	824611	1312381	10.27%	2.033%
13	16.362	2295	2302	2313	rBV	3697913	5936094	46.46%	9.197%
14	17.626	2509	2517	2524	rBV	1123388	1822352	14.26%	2.824%
15	18.466	2655	2660	2667	rBV3	182666	284948	2.23%	0.442%
16	20.205	2950	2956	2962	rBV	7362882	9878486	77.32%	15.306%
17	21.497	3171	3176	3188	rBV	280430	542219	4.24%	0.840%
18	21.920	3238	3248	3255	rBV	1342222	2436921	19.07%	3.776%
19	25.346	3820	3831	3845	rVB2	758257	2357884	18.45%	3.653%

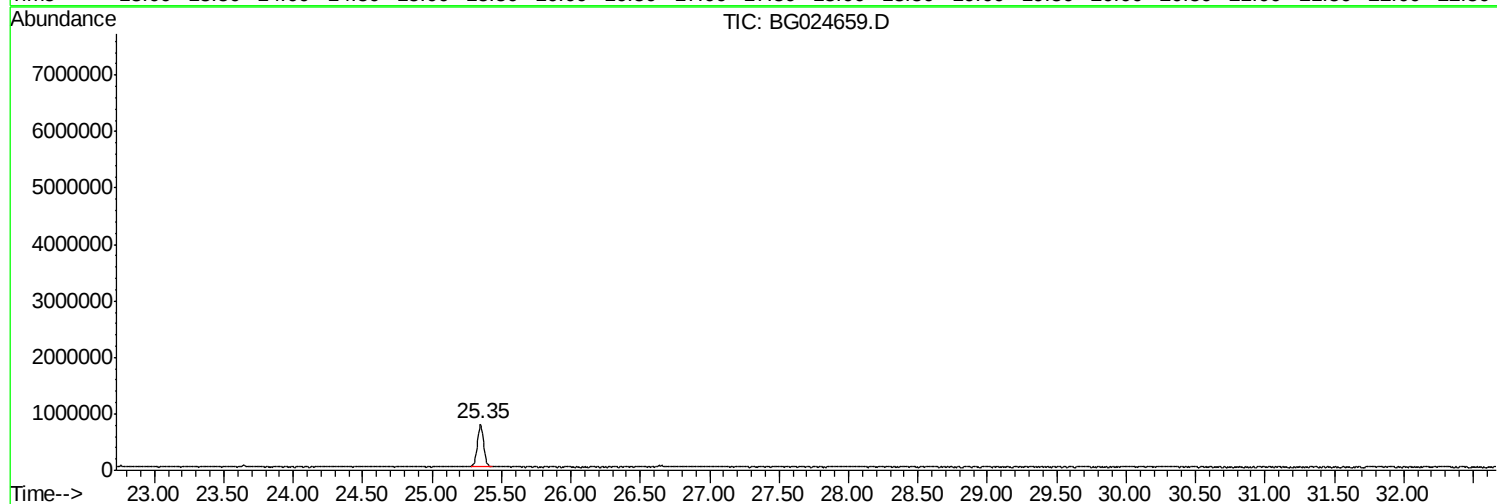
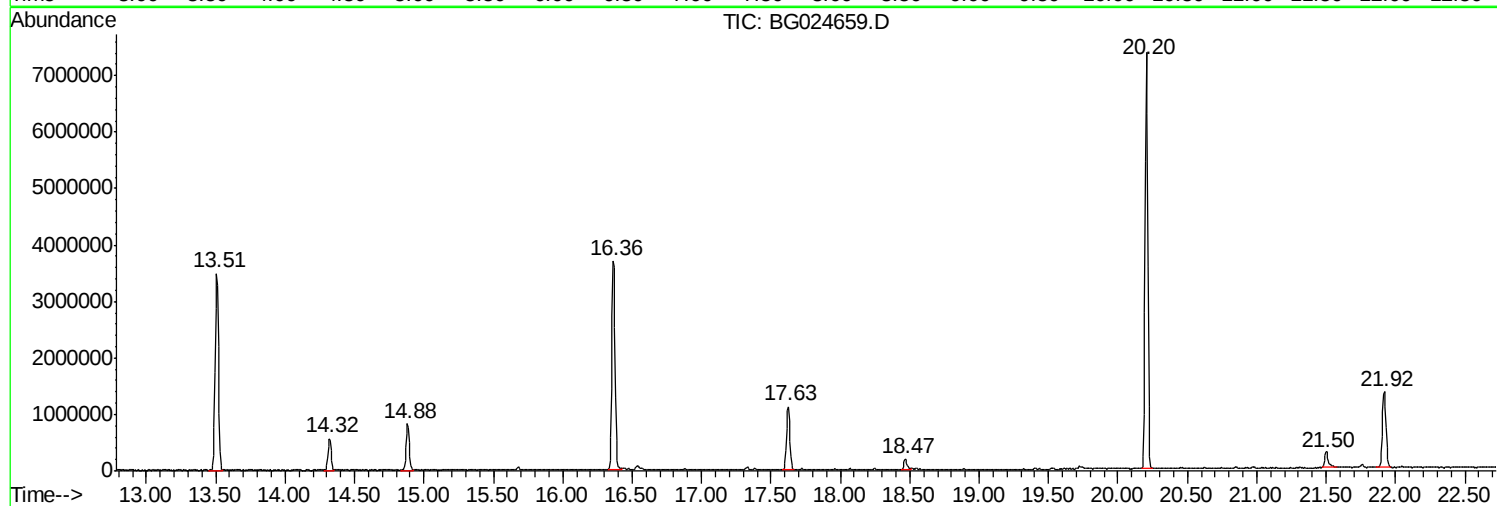
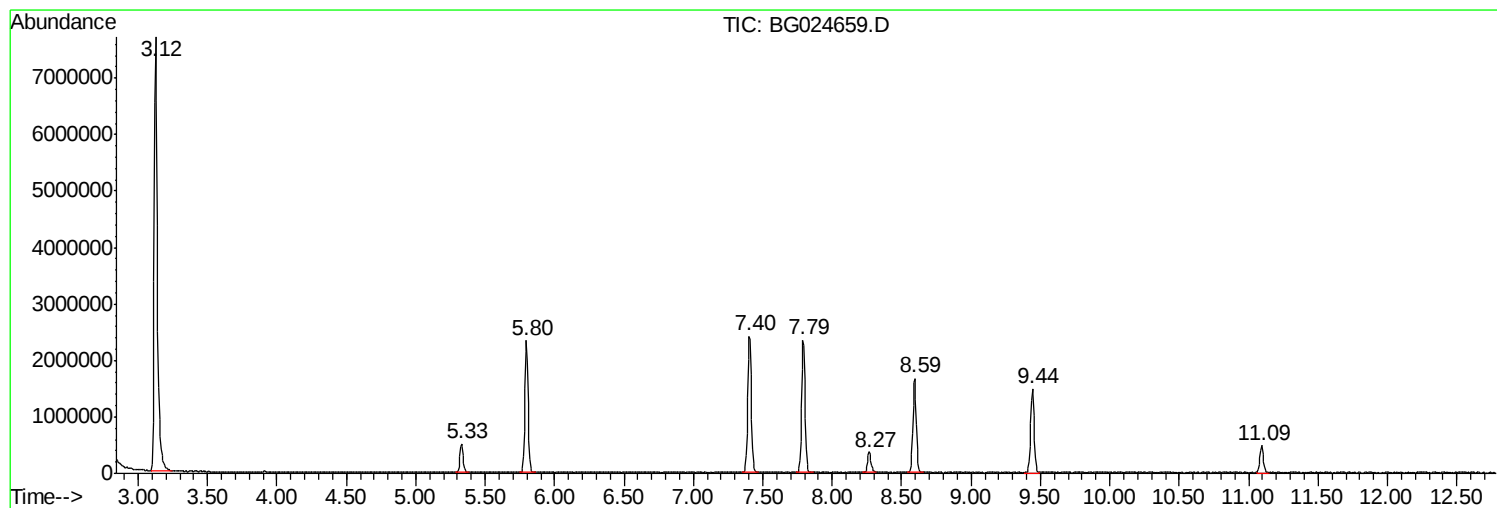
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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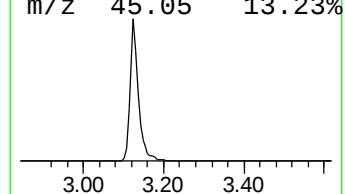
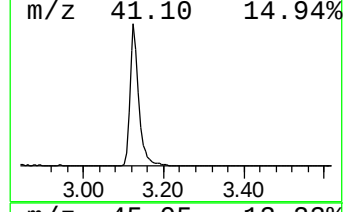
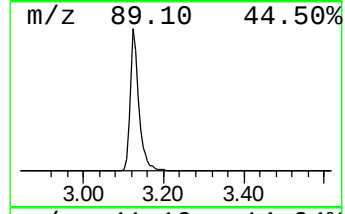
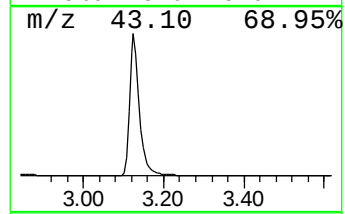
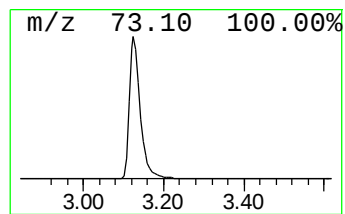
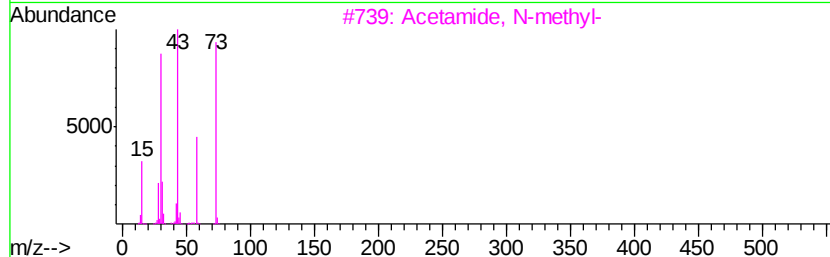
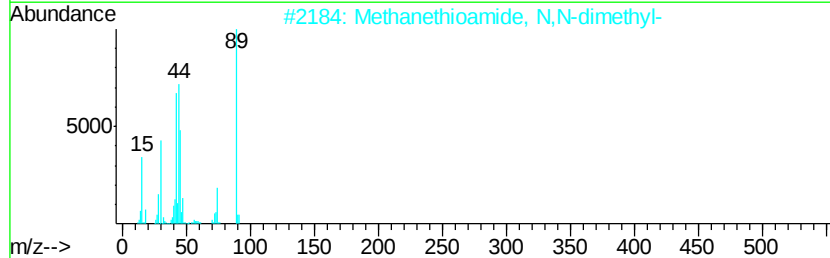
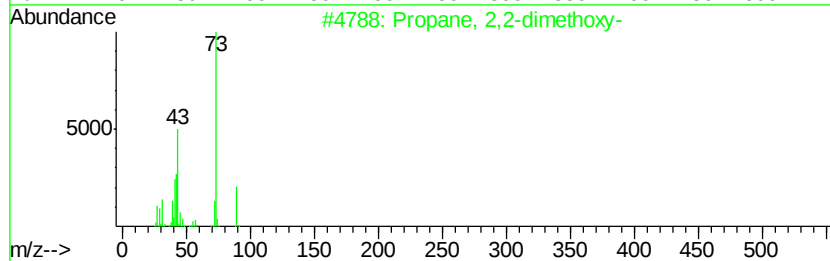
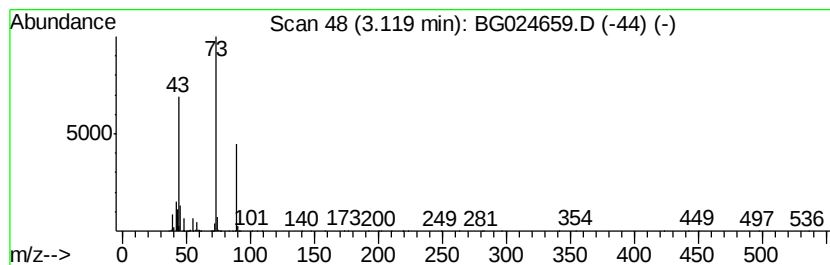
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown3.12 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.12	396.73 ng	12776600	1,4-Dichlorobenzene-d4	8.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	40
2		Methanethioamide, N,N-dimethyl-	89	C3H7NS	000758-16-7	40
3		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	32
4		Thiazole, tetrahydro-	89	C3H7NS	000504-78-9	9
5		1-Propanol, 2-methyl-2-nitro-	119	C4H9NO3	000076-39-1	9



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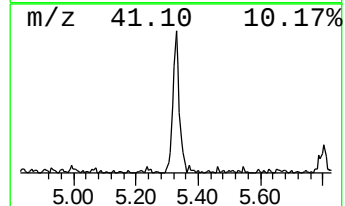
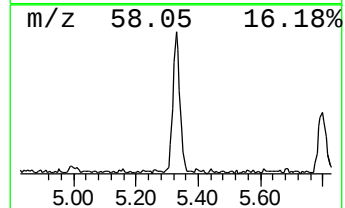
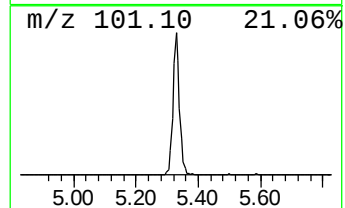
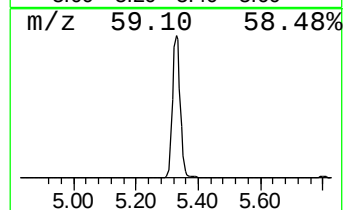
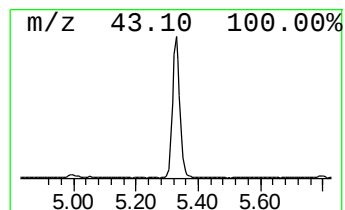
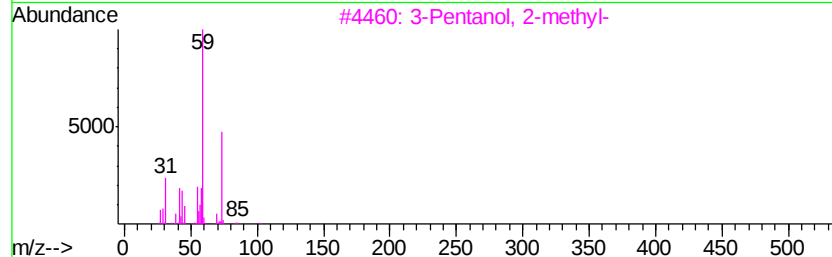
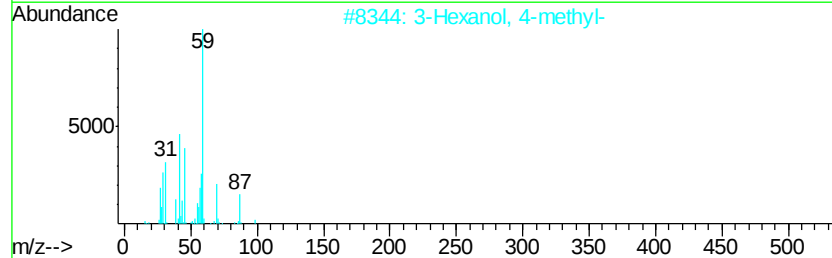
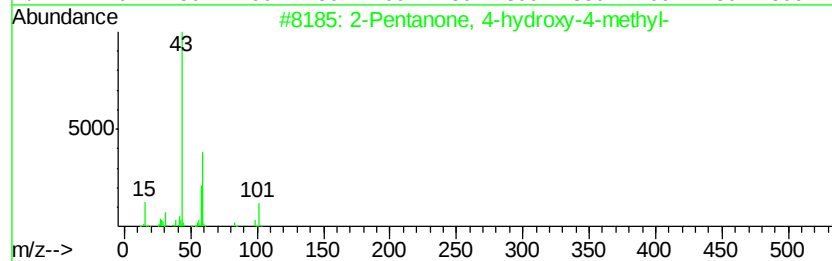
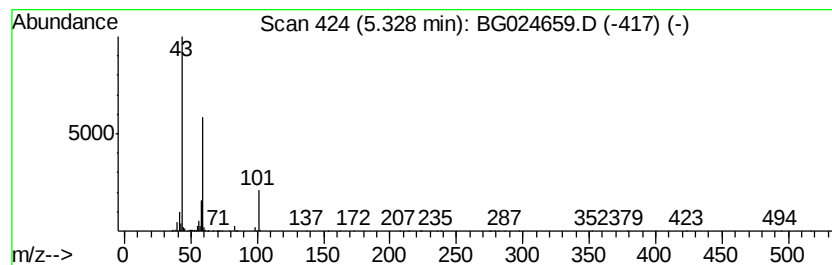
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.33	26.40 ng	850076	1,4-Dichlorobenzene-d4	8.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
3		3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	25
4		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	17
5		4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	9



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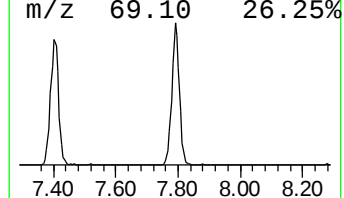
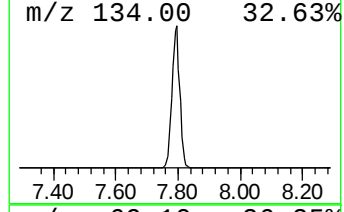
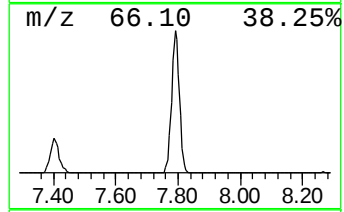
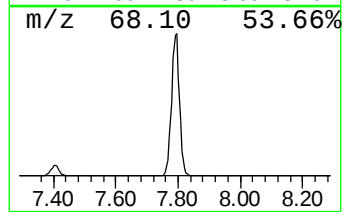
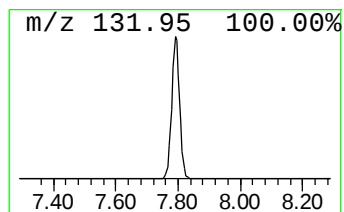
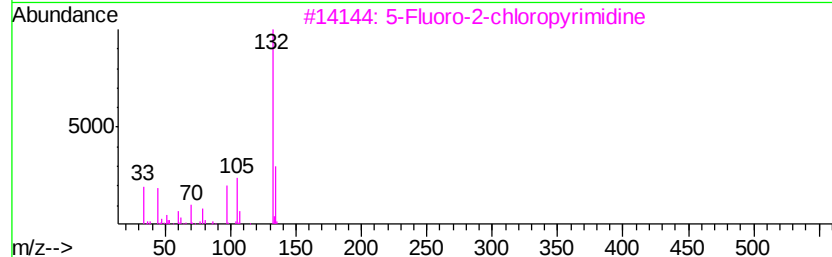
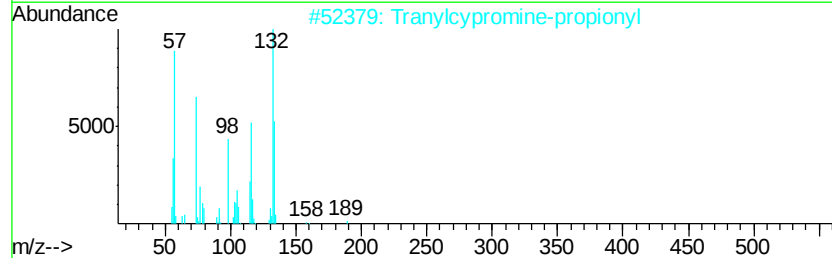
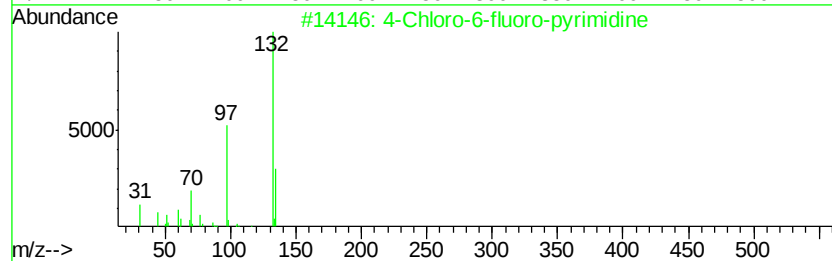
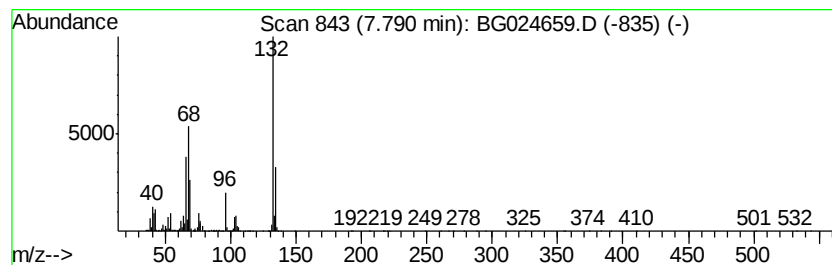
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Peak Number 3 unknown7.79 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.79	128.19 ng	4128230	1,4-Dichlorobenzene-d4	8.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	10
4		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	10
5		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10



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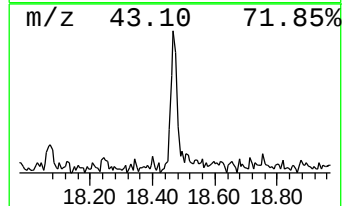
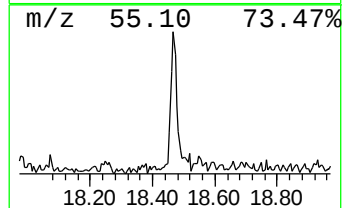
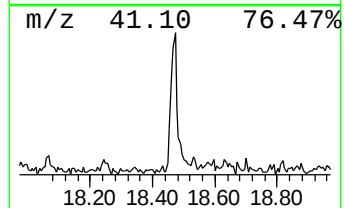
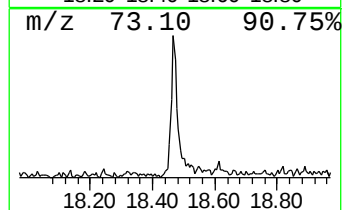
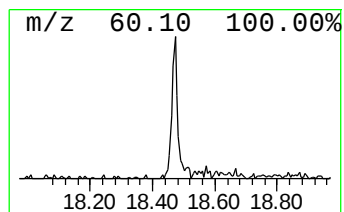
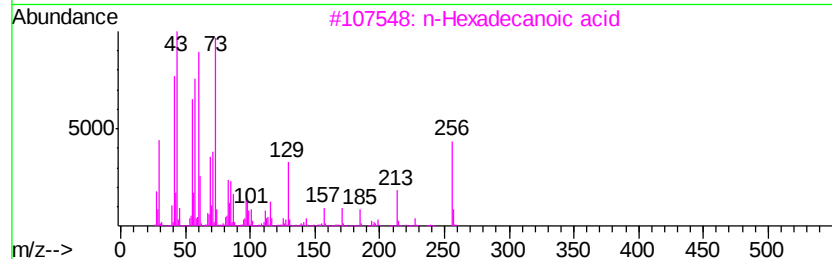
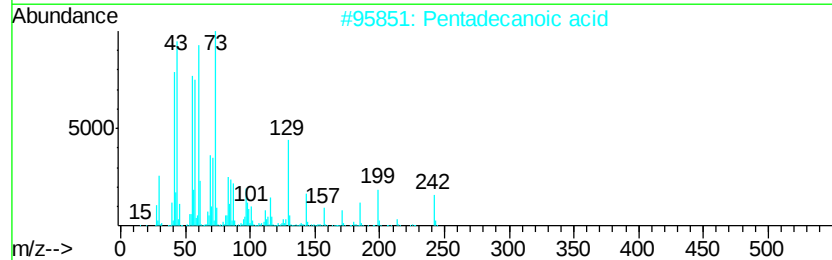
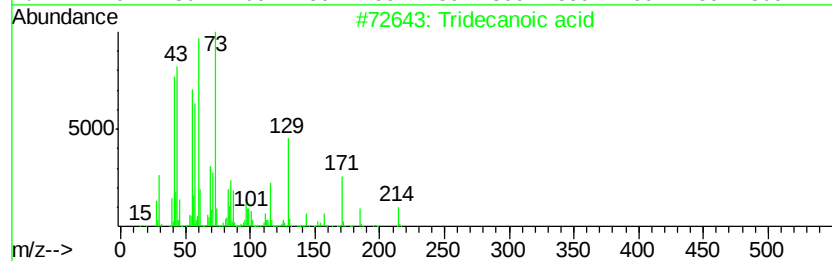
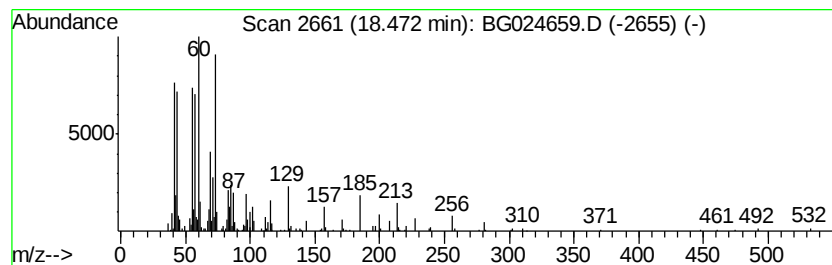
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Peak Number 5 Tridecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.47	3.13 ng	284948	Phenanthrene-d10	17.63

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tridecanoic acid	214	C13H26O2	000638-53-9	87
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	62
3		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	60
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	49
5		l-(+)-Ascorbic acid 2,6-dihexade...	652	C38H68O8	028474-90-0	49



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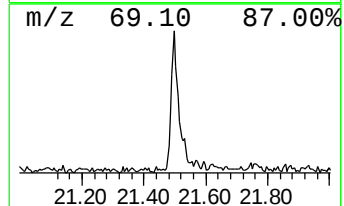
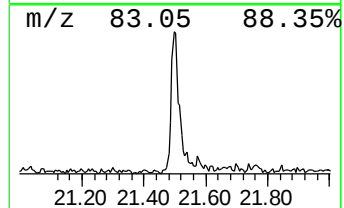
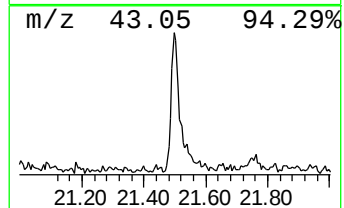
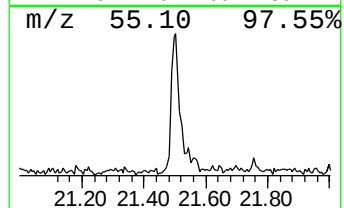
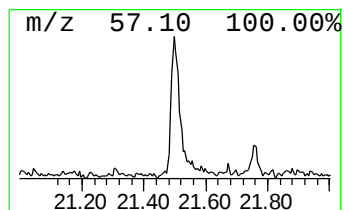
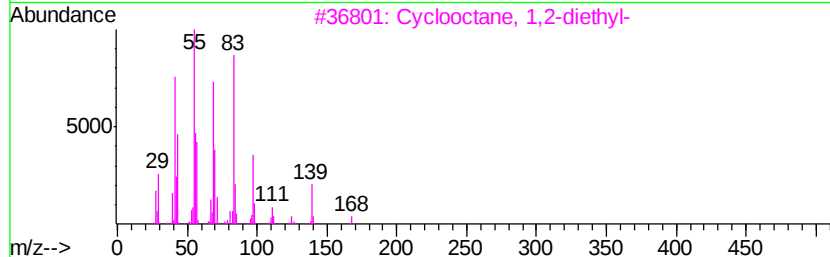
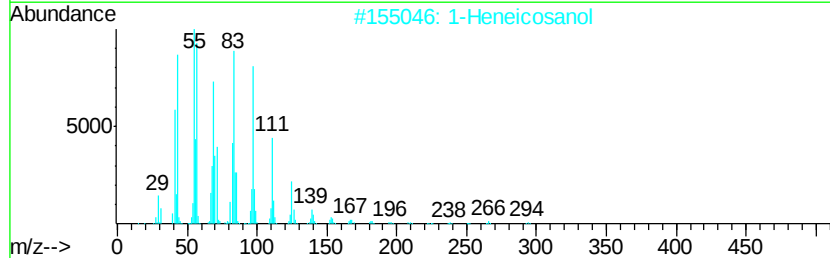
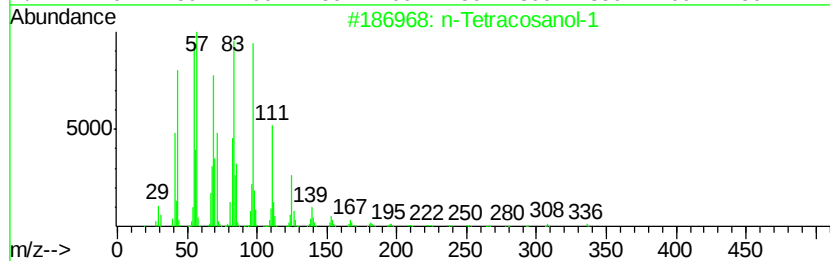
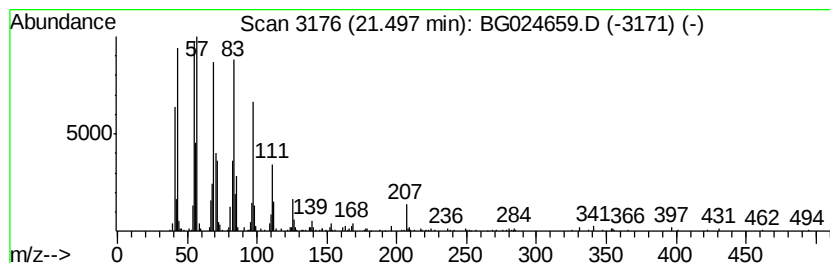
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 n-Tetracosanol-1 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.50	4.45 ng	542219	Chrysene-d12	21.92	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	90
2	1-Heneicosanol	312	C21H44O	015594-90-8	86
3	Cyclooctane, 1,2-diethyl-	168	C12H24	023609-46-3	81
4	Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	74
5	E-7-Octadecene	252	C18H36	1000130-92-0	64



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TIC Library : C:\DATABASE\NIST11.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown3.12	3.12	396.7	ng	12776600	1	8.27	644092	20.0
2-Pentanone, 4-hy...	5.33	26.4	ng	850076	1	8.27	644092	20.0
unknown7.79	7.79	128.2	ng	4128230	1	8.27	644092	20.0
Tridecanoic acid	18.47	3.1	ng	284948	4	17.63	1822350	20.0
n-Tetracosanol-1	21.50	4.5	ng	542219	5	21.92	2436920	20.0