

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010416\
 Data File : BF084244.D
 Acq On : 4 Jan 2016 17:40
 Operator : UM/SJ
 Sample : PB87615BL
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB87615BL

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:\HPCHEM1\BNA_F\METHODS\8270-BF123115.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	2.201	8	10	32	rVB3	110332	341946	4.52%	0.518%
2	5.104	261	264	271	rVB	1599361	2131365	28.19%	3.227%
3	5.516	297	300	303	rBV	6164874	6643411	87.86%	10.060%
4	6.544	387	390	392	rBV	6739937	7489116	99.04%	11.340%
5	6.670	398	401	403	rBV	6508431	7561513	100.00%	11.450%
6	6.887	418	420	423	rVB	1914894	1773602	23.46%	2.686%
7	7.047	431	434	436	rBV	6026421	5387284	71.25%	8.158%
8	7.459	467	470	472	rBV	4658277	4921571	65.09%	7.452%
9	8.179	530	533	535	rBV	2605855	2478810	32.78%	3.753%
10	9.253	624	627	630	rBV	6225605	7529194	99.57%	11.401%
11	9.939	684	687	689	rBV	1841021	2535018	33.53%	3.839%
12	10.728	753	756	758	rBV	4154824	4924075	65.12%	7.456%
13	11.413	814	816	819	rBV2	2016052	2337152	30.91%	3.539%
14	12.831	938	940	942	rBV	507357	432924	5.73%	0.656%
15	12.911	942	947	949	rVB2	58153	89036	1.18%	0.135%
16	13.002	953	955	958	rBV	5023411	5979817	79.08%	9.055%
17	13.539	1000	1002	1004	rBV	235910	275491	3.64%	0.417%
18	14.054	1044	1047	1049	rBV	1841053	1675896	22.16%	2.538%
19	15.494	1170	1173	1176	rBV	1187113	1533126	20.28%	2.321%

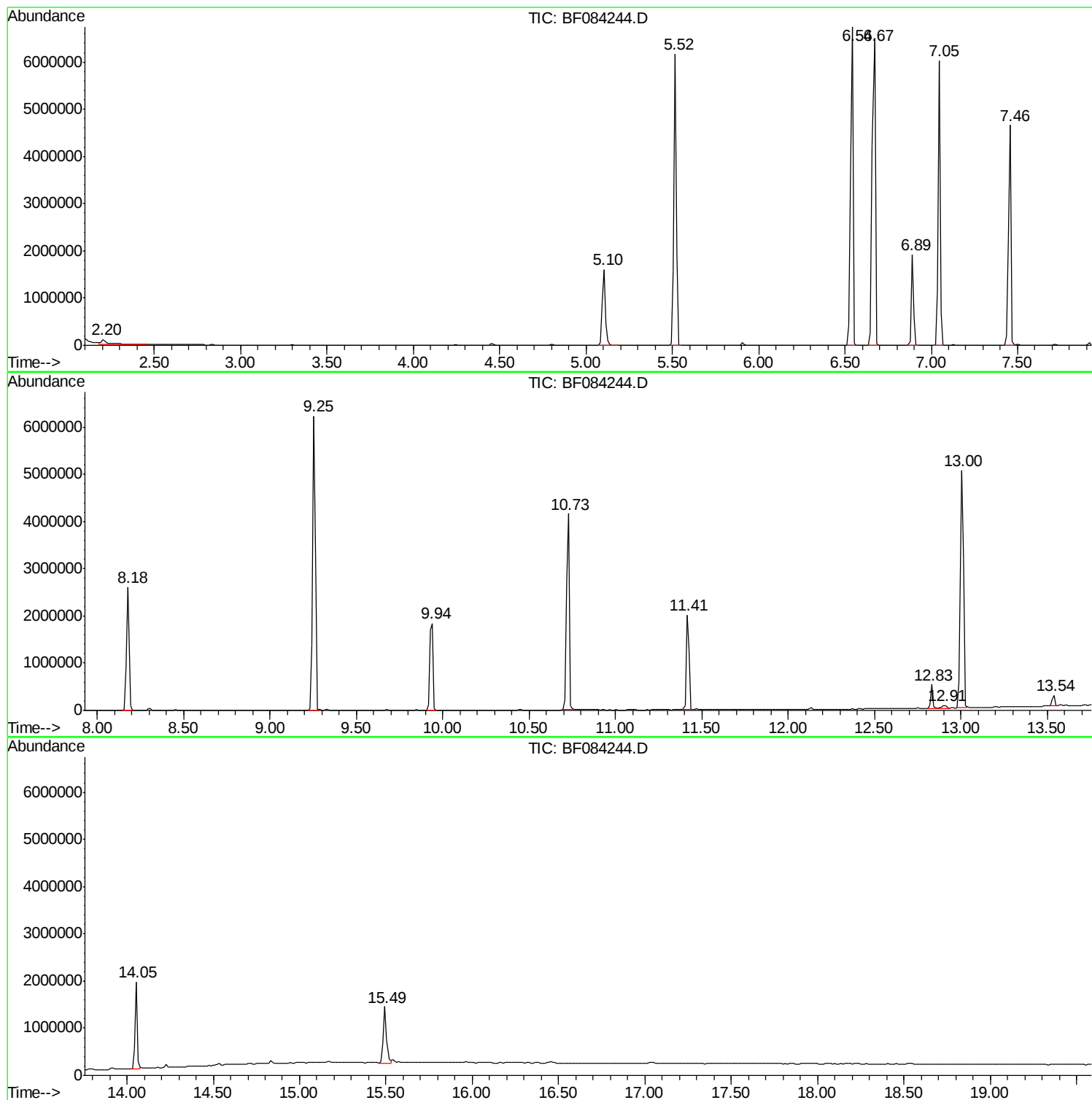
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ClientSampled :
PB87615BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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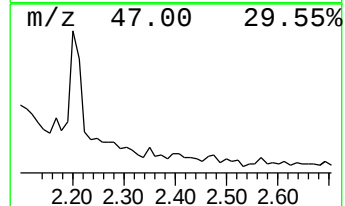
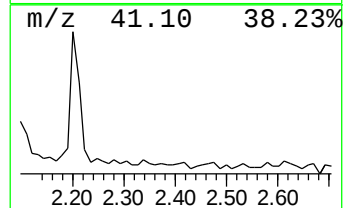
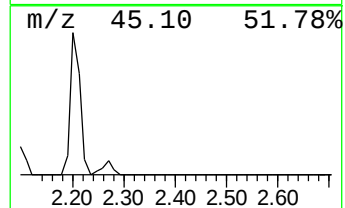
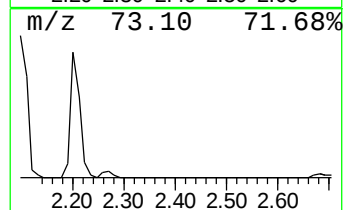
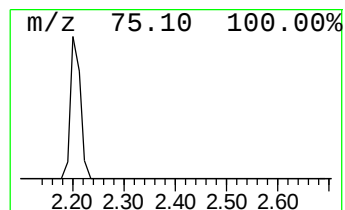
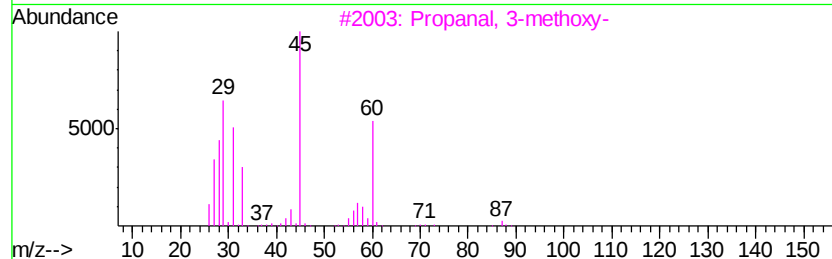
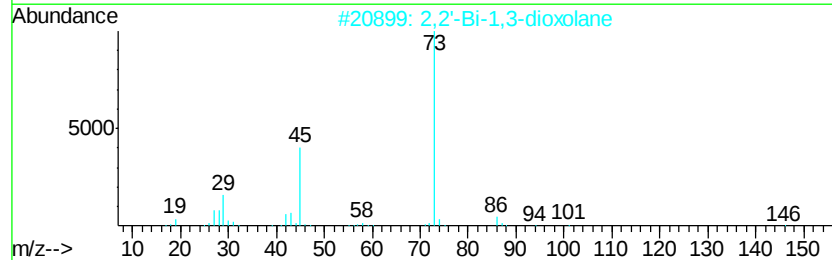
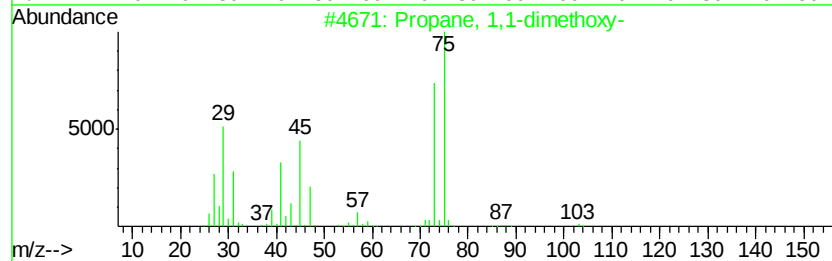
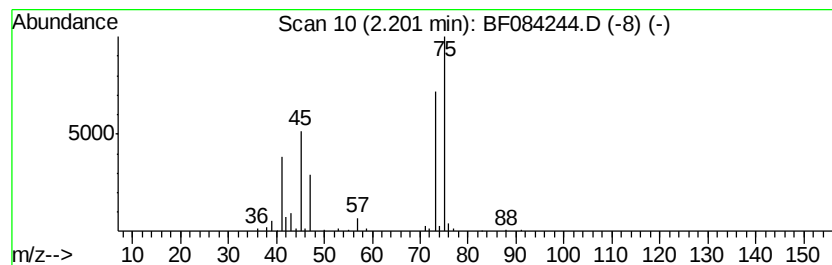
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Propane, 1,1-dimethoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.20	3.86 ng	341946	1,4-Dichlorobenzene-d4	6.89

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	64	
2	2,2'-Bi-1,3-dioxolane	146	C6H10O4	006705-89-1	22	
3	Propanal, 3-methoxy-	88	C4H8O2	002806-84-0	9	
4	Butane, 1-methoxy-	88	C5H12O	000628-28-4	9	
5	1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	9	



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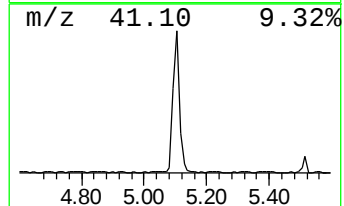
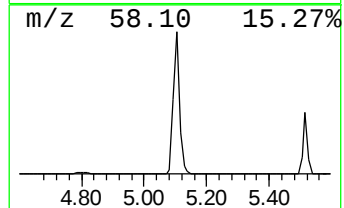
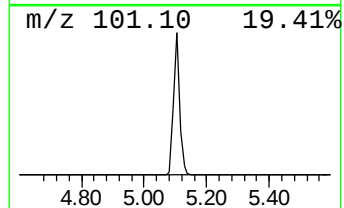
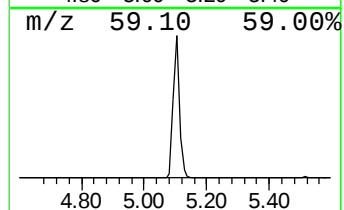
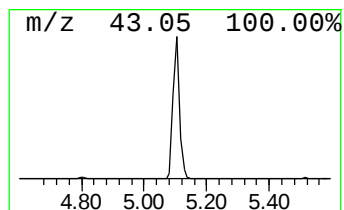
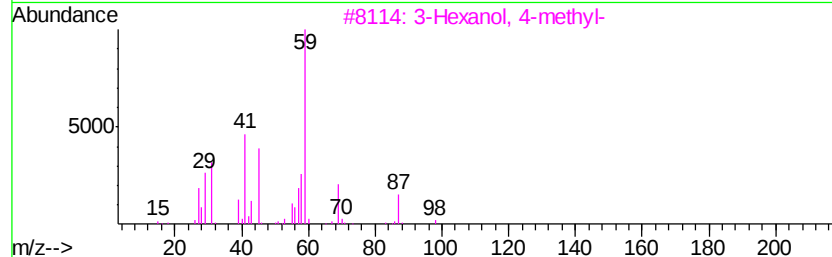
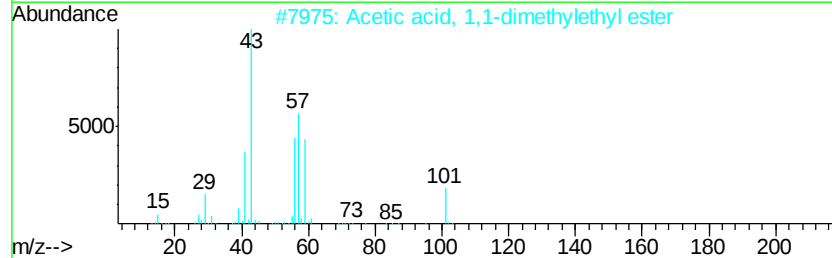
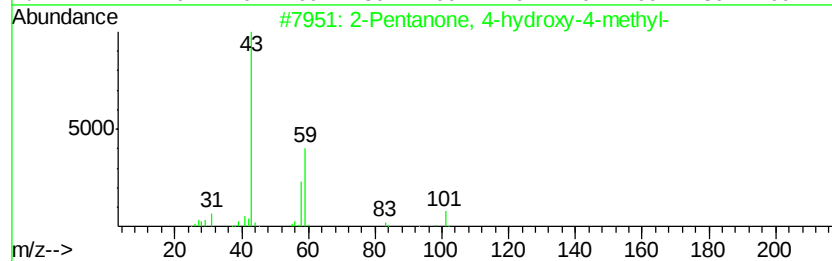
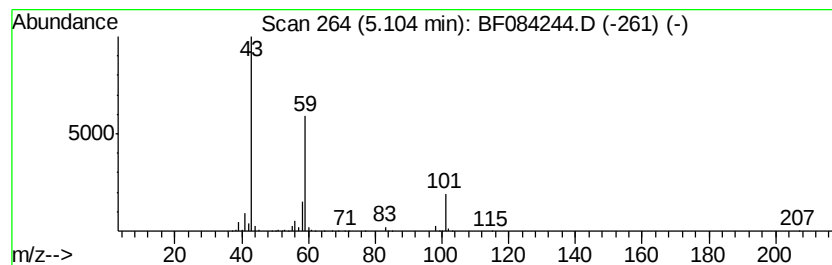
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	24.03 ng	2131370	1,4-Dichlorobenzene-d4	6.89

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, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39	
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28	
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23	
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9	



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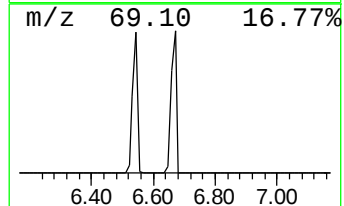
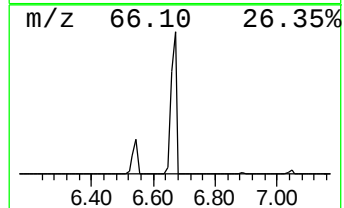
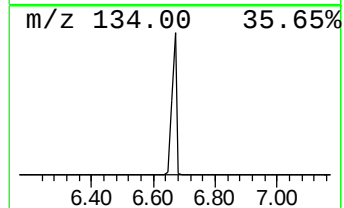
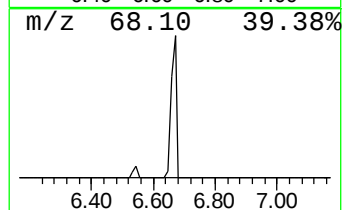
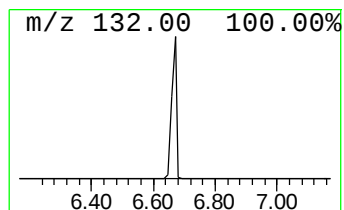
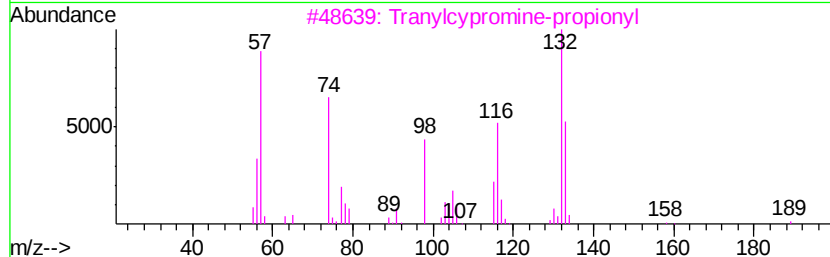
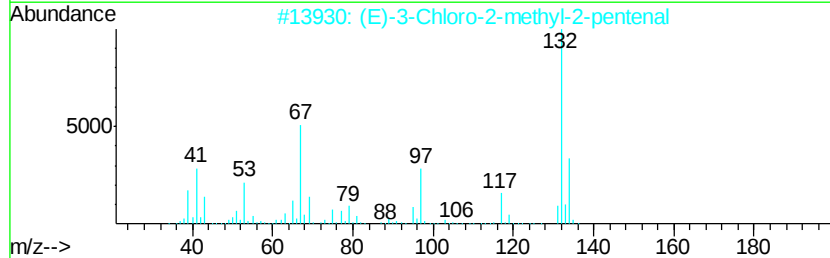
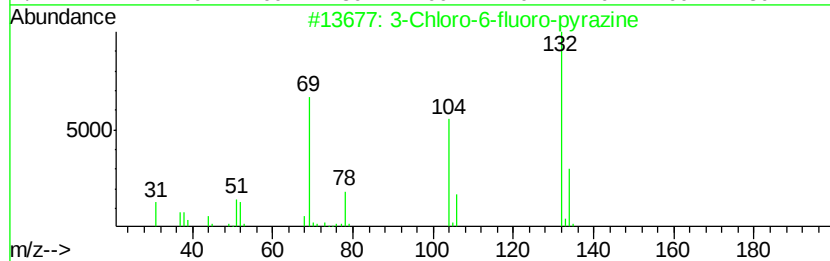
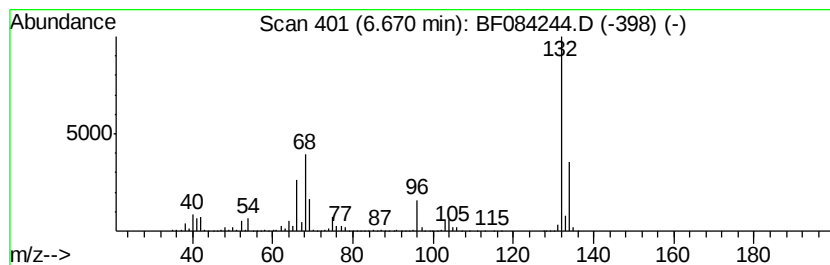
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Peak Number 3 unknown6.67 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.67	85.27 ng	7561510	1,4-Dichlorobenzene-d4	6.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9
5		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9



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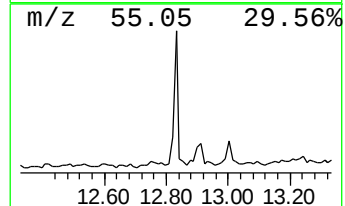
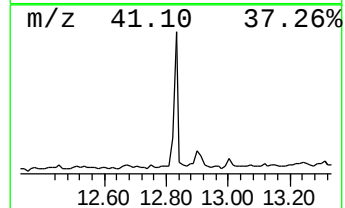
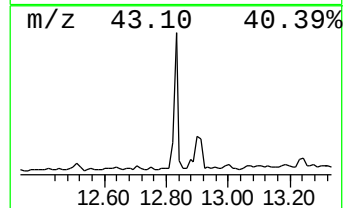
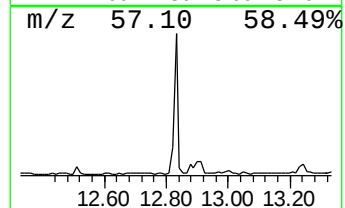
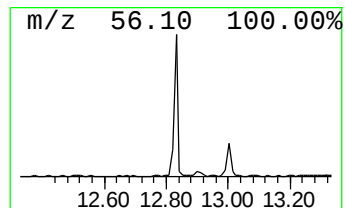
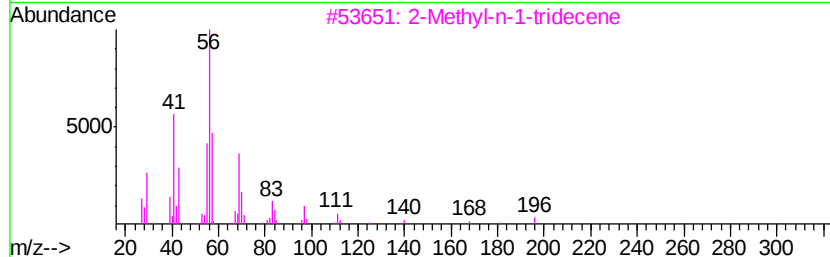
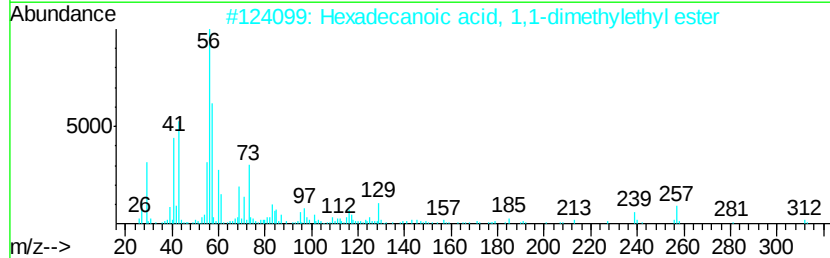
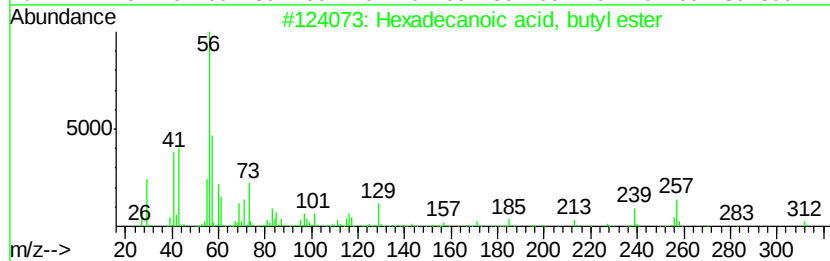
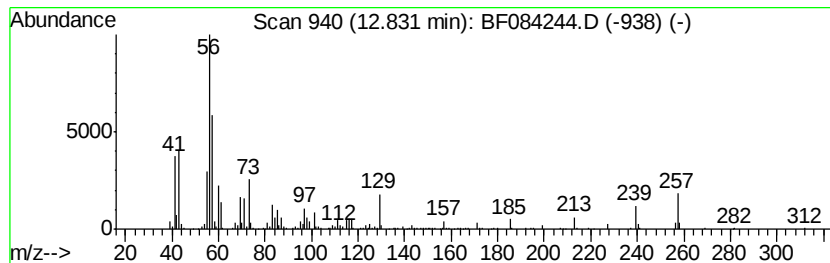
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Peak Number 5 Hexadecanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.83	5.17 ng	432924	Chrysene-d12	14.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	40
3		2-Methyl-n-1-tridecene	196	C14H28	018094-01-4	38
4		Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	38
5		Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	38



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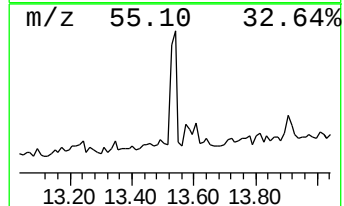
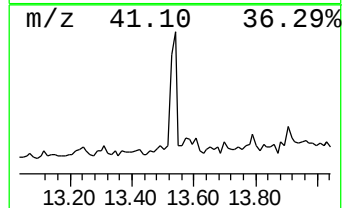
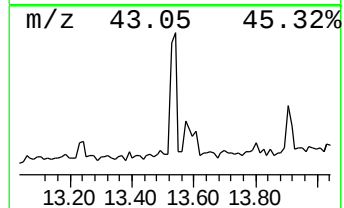
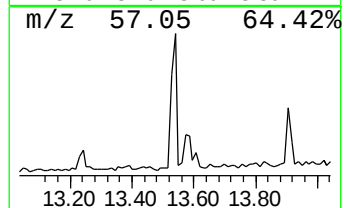
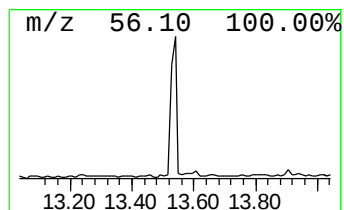
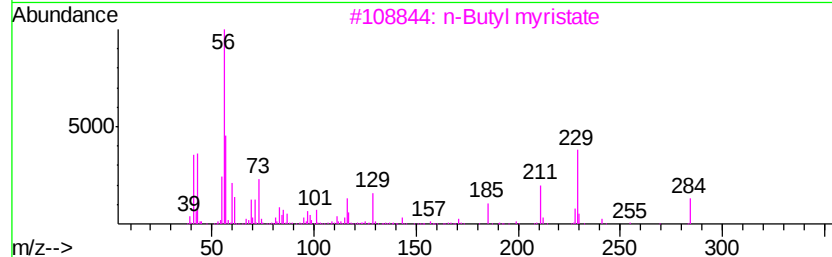
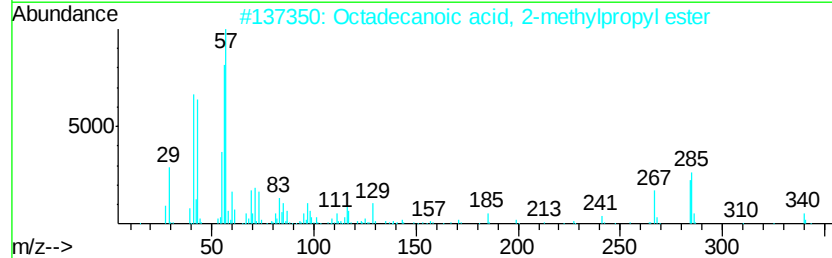
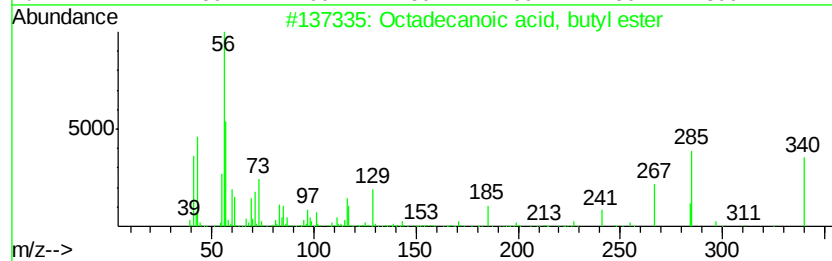
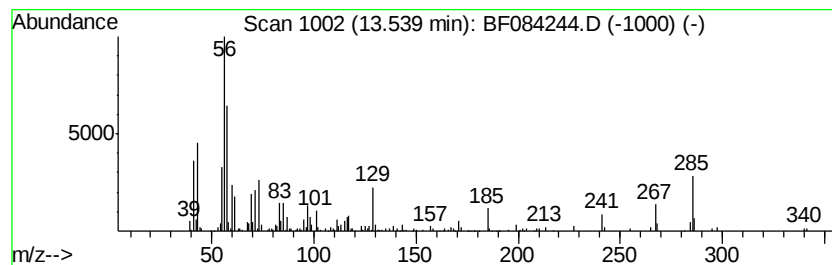
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Octadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.54	3.29 ng	275491	Chrysene-d12	14.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	87
2		Octadecanoic acid, 2-methylpropyl ester	340	C22H44O2	000646-13-9	72
3		n-Butyl myristate	284	C18H36O2	000110-36-1	68
4		1,3-Pentanediol, 2,2,4-trimethyl-	146	C8H18O2	000144-19-4	38
5		1-Undecene, 2-methyl-	168	C12H24	018516-37-5	30



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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 1,1-dime...	2.20	3.9	ng	341946	1	6.89	1773600	20.0
2-Pentanone, 4-hy...	5.10	24.0	ng	2131370	1	6.89	1773600	20.0
unknown6.67	6.67	85.3	ng	7561510	1	6.89	1773600	20.0
Hexadecanoic acid...	12.83	5.2	ng	432924	5	14.05	1675900	20.0
Octadecanoic acid...	13.54	3.3	ng	275491	5	14.05	1675900	20.0