

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031816\
 Data File : BF085603.D
 Acq On : 20 Mar 2016 7:35
 Operator : UM/SJ
 Sample : H1804-12
 Misc :
 ALS Vial : 61 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TRACK-D-GRID-9A

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_F\METHODS\8270-BF031816.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	2.470	10	16	24	rVB3	16100	59975	1.36%	0.156%
2	2.721	36	38	45	rVB	126358	199442	4.53%	0.517%
3	5.064	241	243	248	rBV2	243935	422877	9.60%	1.097%
4	5.464	275	278	281	rBV	2696641	3264766	74.11%	8.469%
5	6.493	364	368	370	rBV	2854976	3396861	77.11%	8.812%
6	6.630	377	380	382	rBV	2689661	3941780	89.48%	10.226%
7	6.847	397	399	402	rBV	731257	985102	22.36%	2.556%
8	7.007	411	413	416	rBV	2768556	2932822	66.57%	7.608%
9	7.419	446	449	451	rBV	2239451	2441675	55.42%	6.334%
10	8.162	509	514	516	rBV2	1492298	2793512	63.41%	7.247%
11	8.207	516	518	520	rVB	117451	104466	2.37%	0.271%
12	8.847	572	574	576	rBV	318841	265881	6.04%	0.690%
13	8.950	580	583	585	rBV	107455	110807	2.52%	0.287%
14	9.213	603	606	609	rBV	3878056	4405417	100.00%	11.428%
15	9.888	663	665	667	rBV	1403891	1380228	31.33%	3.581%
16	10.093	681	683	685	rBV	103853	86302	1.96%	0.224%
17	10.436	711	713	715	rVB	116989	96190	2.18%	0.250%
18	10.688	731	735	737	rBV2	1966598	2973042	67.49%	7.713%
19	11.373	793	795	796	rBV	1565984	1339837	30.41%	3.476%
20	11.396	796	797	799	rVB	190966	140046	3.18%	0.363%
21	12.094	854	858	864	rBV2	28157	62529	1.42%	0.162%
22	12.779	916	918	921	rBV	649744	569667	12.93%	1.478%
23	12.859	921	925	927	rVB2	75886	88206	2.00%	0.229%
24	12.962	931	934	936	rBV	4108774	4094224	92.94%	10.621%
25	13.488	977	980	982	rBV	315149	324736	7.37%	0.842%
26	13.534	982	984	988	rVB2	40431	70116	1.59%	0.182%
27	14.002	1022	1025	1028	rBV	822247	980547	22.26%	2.544%
28	14.174	1038	1040	1042	rBV	63576	53551	1.22%	0.139%
29	14.780	1090	1093	1095	rBV	41713	49996	1.13%	0.130%
30	15.100	1118	1121	1124	rBV	41800	44720	1.02%	0.116%
31	15.431	1147	1150	1158	rBV	636204	822906	18.68%	2.135%
32	16.357	1227	1231	1235	rBV	24479	45645	1.04%	0.118%

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Misc :
ALS Vial : 61 Sample Multiplier: 1

Instrument :
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ClientSampleId :
TRACK-D-GRID-9A

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-BF031816.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

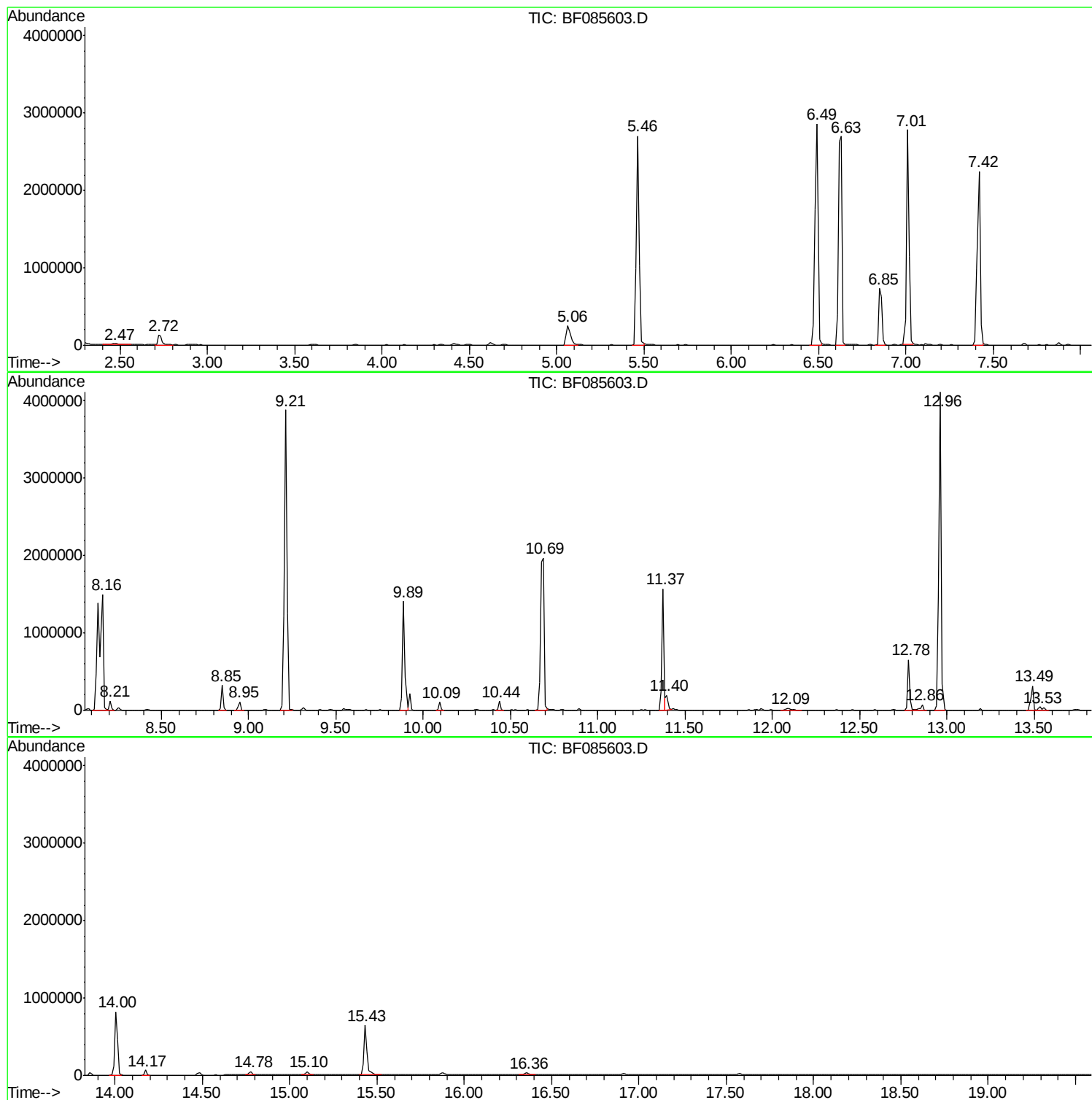
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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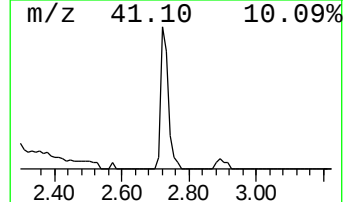
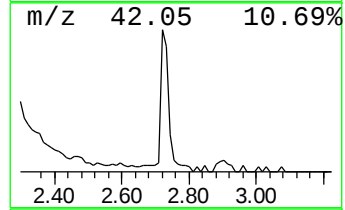
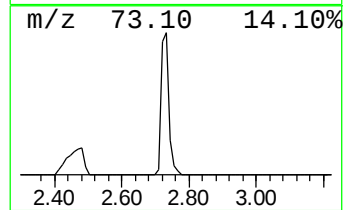
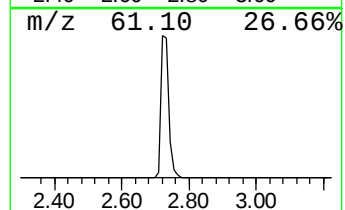
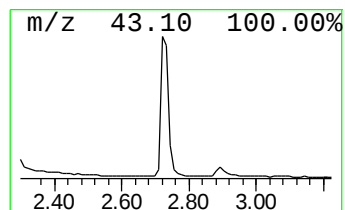
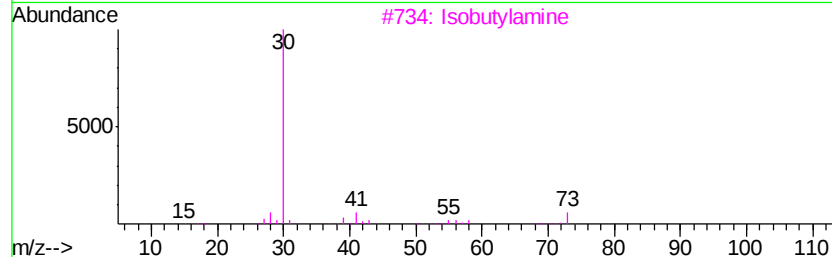
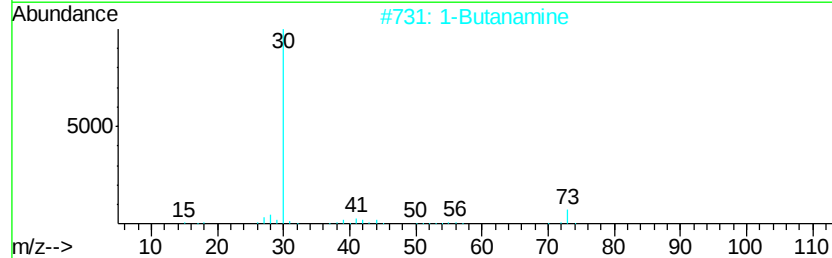
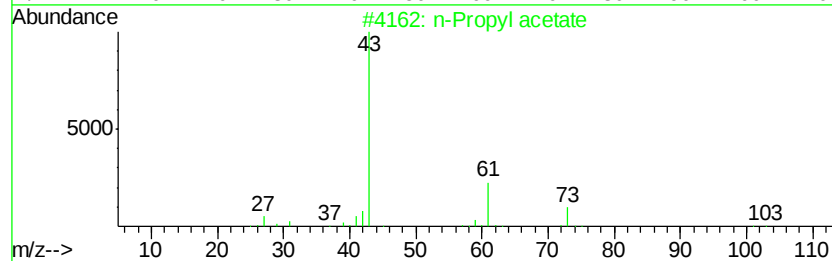
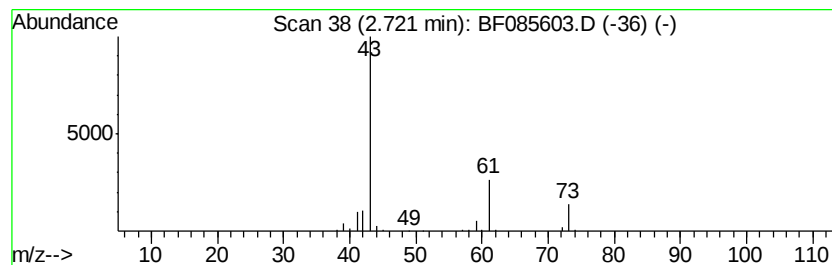
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 n-Propyl acetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
2.72	4.05 ng	199442	1,4-Dichlorobenzene-d4	6.86	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate	102	C5H10O2	000109-60-4	83
2	1-Butanamine	73	C4H11N	000109-73-9	7
3	Isobutylamine	73	C4H11N	000078-81-9	5
4	Pentane	72	C5H12	000109-66-0	5
5	Butane, 2-methyl-	72	C5H12	000078-78-4	4



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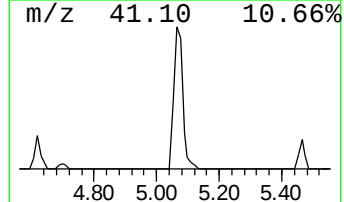
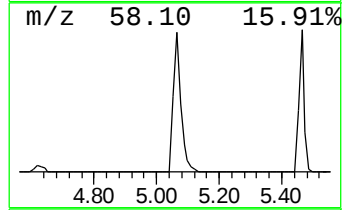
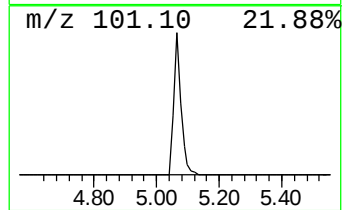
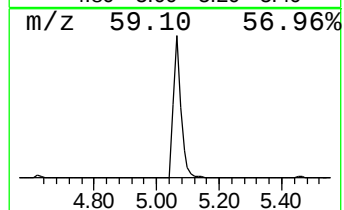
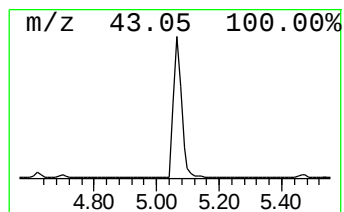
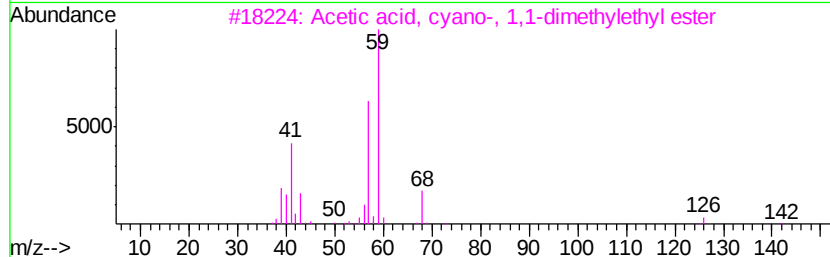
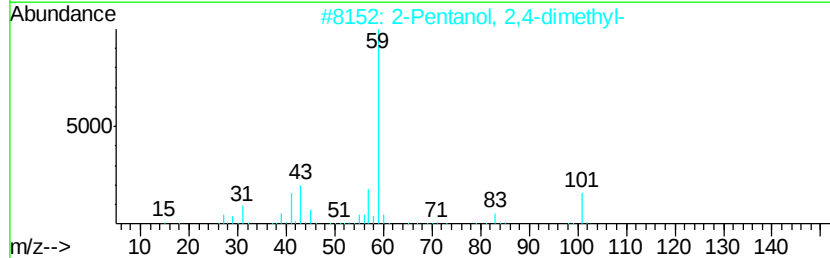
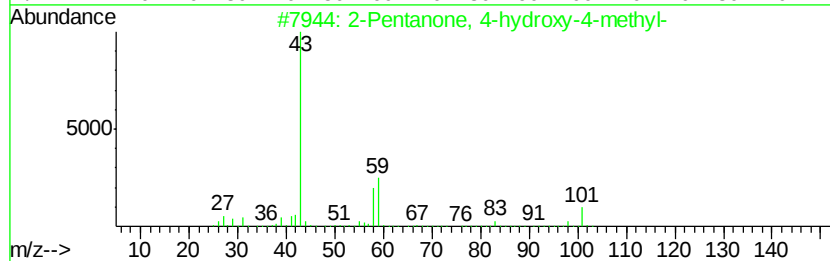
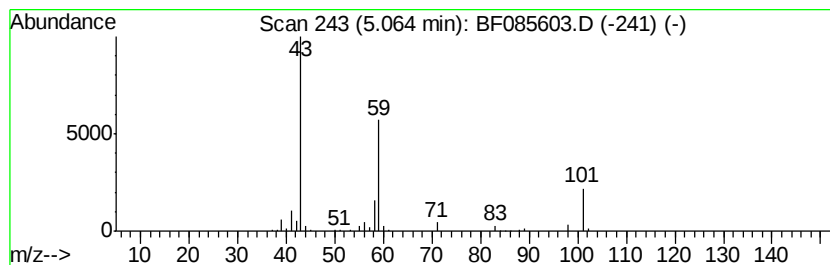
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.06	8.59 ng	422877	1,4-Dichlorobenzene-d4	6.86

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	40
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4			4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	17
5			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	16



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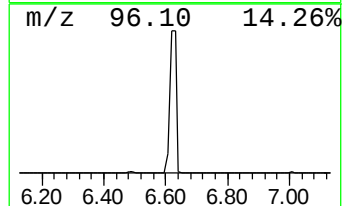
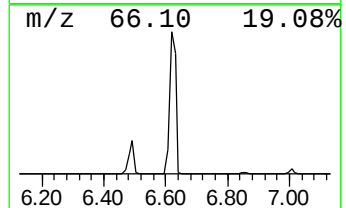
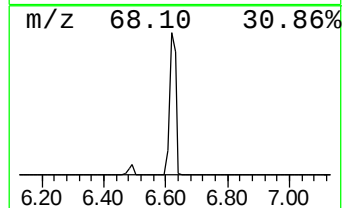
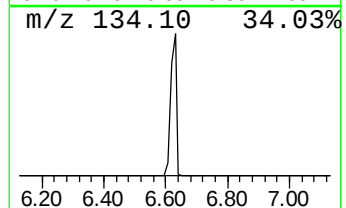
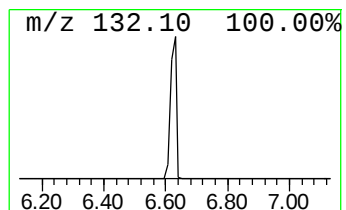
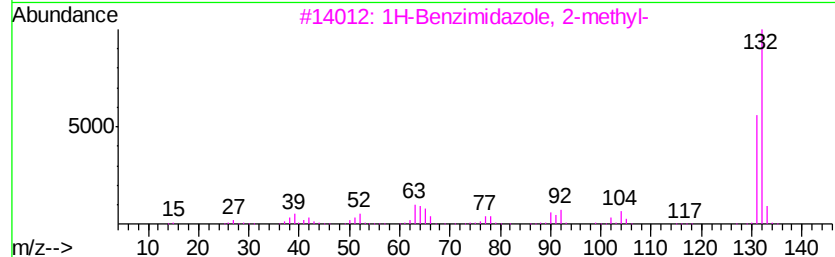
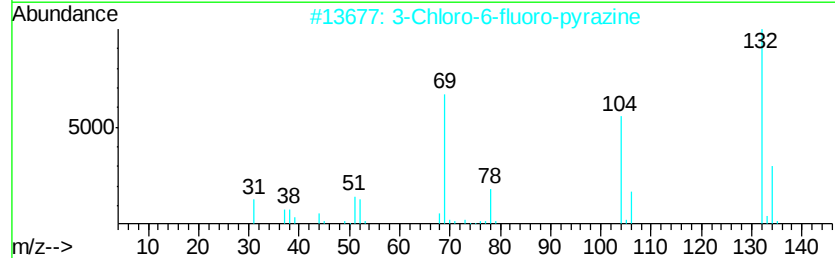
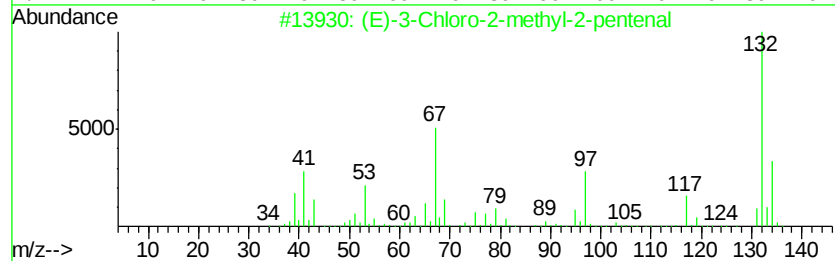
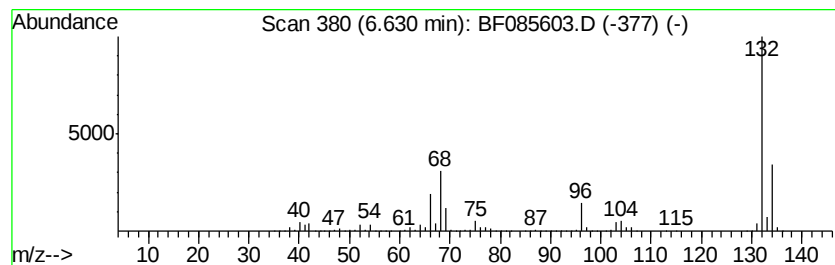
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	80.03 ng	3941780	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9
4		Xenon	132	Xe	007440-63-3	9
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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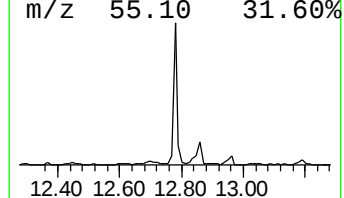
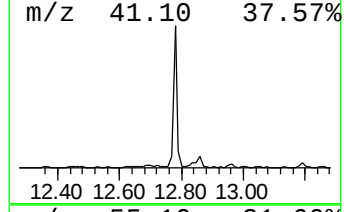
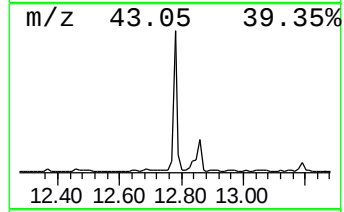
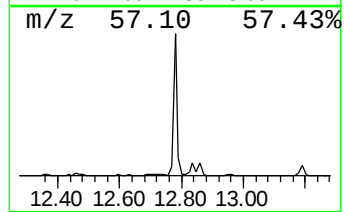
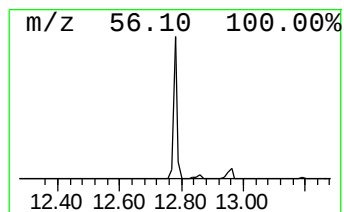
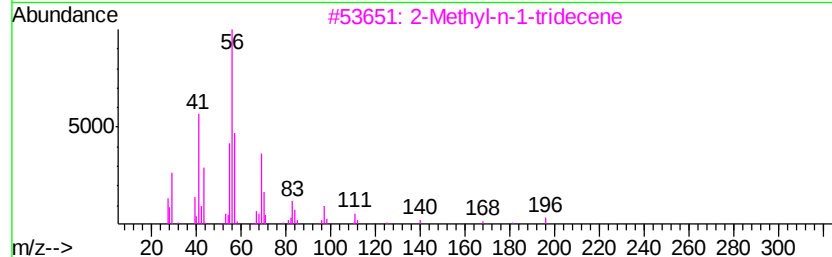
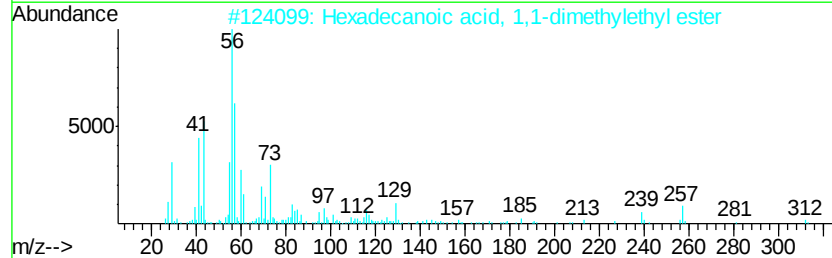
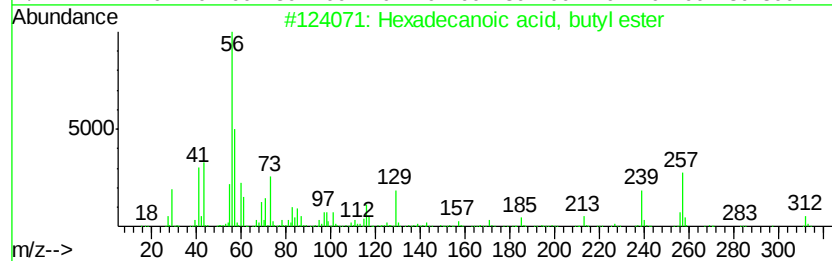
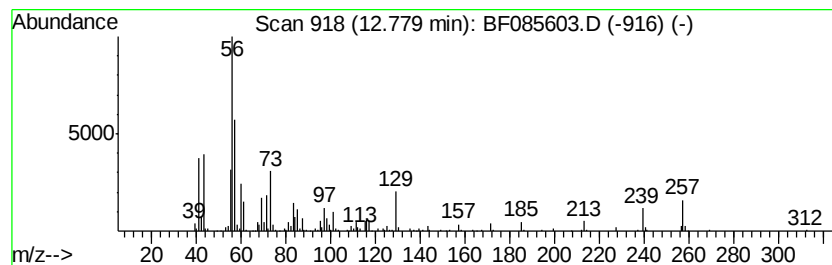
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Hexadecanoic acid, butyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.78	11.62 ng	569667	Chrysene-d12	14.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	95
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	87
3		2-Methyl-n-1-tridecene	196	C14H28	018094-01-4	35
4		Pentadecane, 8-methylene-	224	C16H32	055668-09-2	32
5		Cyclohexanol, 4-amino-, trans-	115	C6H13NO	027489-62-9	30



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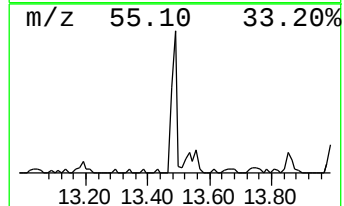
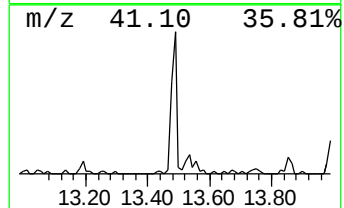
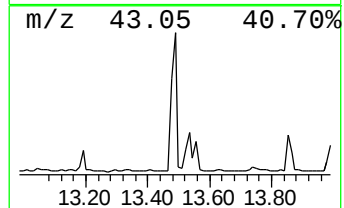
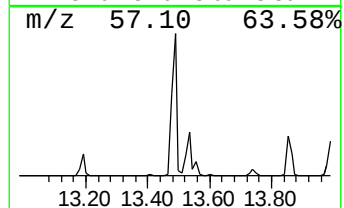
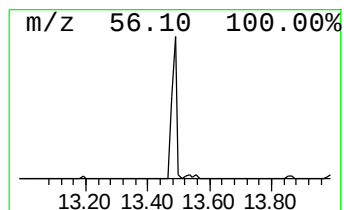
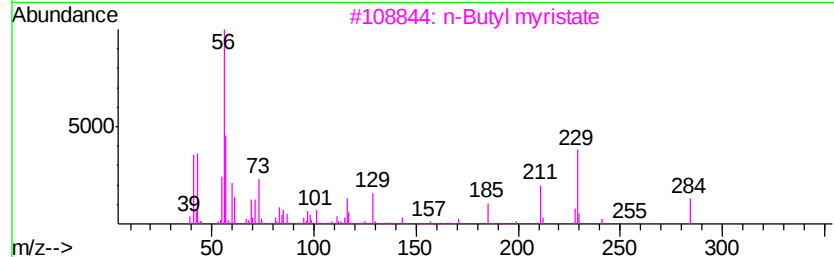
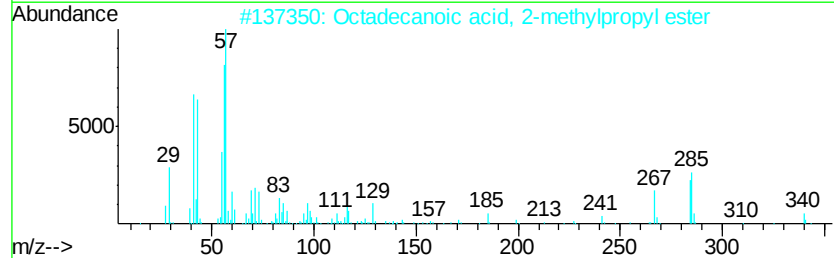
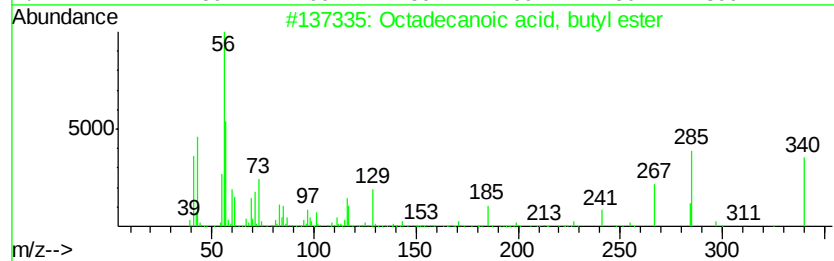
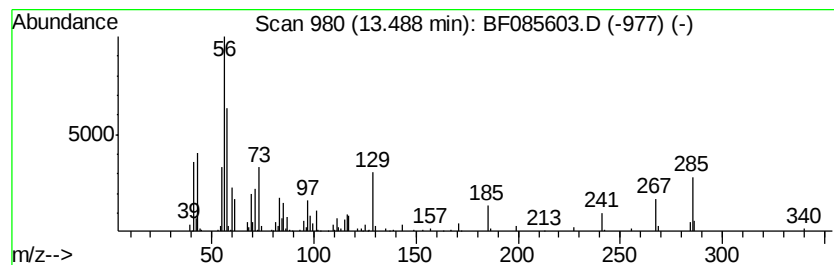
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 6 Octadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.49	6.62 ng	324736	Chrysene-d12	14.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	94
2		Octadecanoic acid, 2-methylpropy...	340	C22H44O2	000646-13-9	72
3		n-Butyl myristate	284	C18H36O2	000110-36-1	58
4		Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	32
5		1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	27



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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
n-Propyl acetate	2.72	4.0	ng	199442	1	6.86	985102	20.0
2-Pentanone, 4-hy...	5.06	8.6	ng	422877	1	6.86	985102	20.0
unknown6.63	6.63	80.0	ng	3941780	1	6.86	985102	20.0
Hexadecanoic acid...	12.78	11.6	ng	569667	5	14.00	980547	20.0
Octadecanoic acid...	13.49	6.6	ng	324736	5	14.00	980547	20.0