

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG050815\
 Data File : BG016952.D
 Acq On : 8 May 2015 12:30
 Operator : TP/IZ
 Sample : G2057-04
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 MWJ-2

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_G\METHODS\8270-BG050515.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	2.911	33	38	47	rBV	371240	585784	10.12%	2.122%
2	2.987	47	51	62	rVB	836704	972186	16.79%	3.522%
3	4.908	371	378	384	rBV	60137	94544	1.63%	0.342%
4	5.367	450	456	465	rBV	664708	967790	16.72%	3.506%
5	6.953	719	726	735	rVB	448426	677021	11.70%	2.453%
6	7.323	780	789	799	rBV	1166948	1844804	31.87%	6.683%
7	7.787	862	868	877	rBV	231493	363313	6.28%	1.316%
8	8.111	916	923	930	rBV	977982	1564866	27.03%	5.669%
9	8.951	1058	1066	1075	rBV	914219	1526791	26.38%	5.531%
10	10.584	1337	1344	1352	rVB	326743	531626	9.18%	1.926%
11	13.058	1757	1765	1774	rVB	2220897	3403243	58.79%	12.329%
12	14.433	1993	1999	2006	rBV2	526300	786296	13.58%	2.848%
13	15.919	2245	2252	2264	rBV	2160725	3040920	52.53%	11.016%
14	17.176	2460	2466	2475	rBV2	758291	1056182	18.25%	3.826%
15	18.070	2614	2618	2626	rVB3	81584	115889	2.00%	0.420%
16	19.350	2832	2836	2841	rBV5	60829	82068	1.42%	0.297%
17	19.803	2907	2913	2919	rBV	4753961	5788699	100.00%	20.970%
18	21.072	3125	3129	3136	rBV	1040448	1095400	18.92%	3.968%
19	21.348	3171	3176	3183	rBV	939726	1158423	20.01%	4.197%
20	21.953	3275	3279	3286	rVB	725232	891664	15.40%	3.230%
21	23.651	3561	3568	3575	rVB2	537307	1056761	18.26%	3.828%

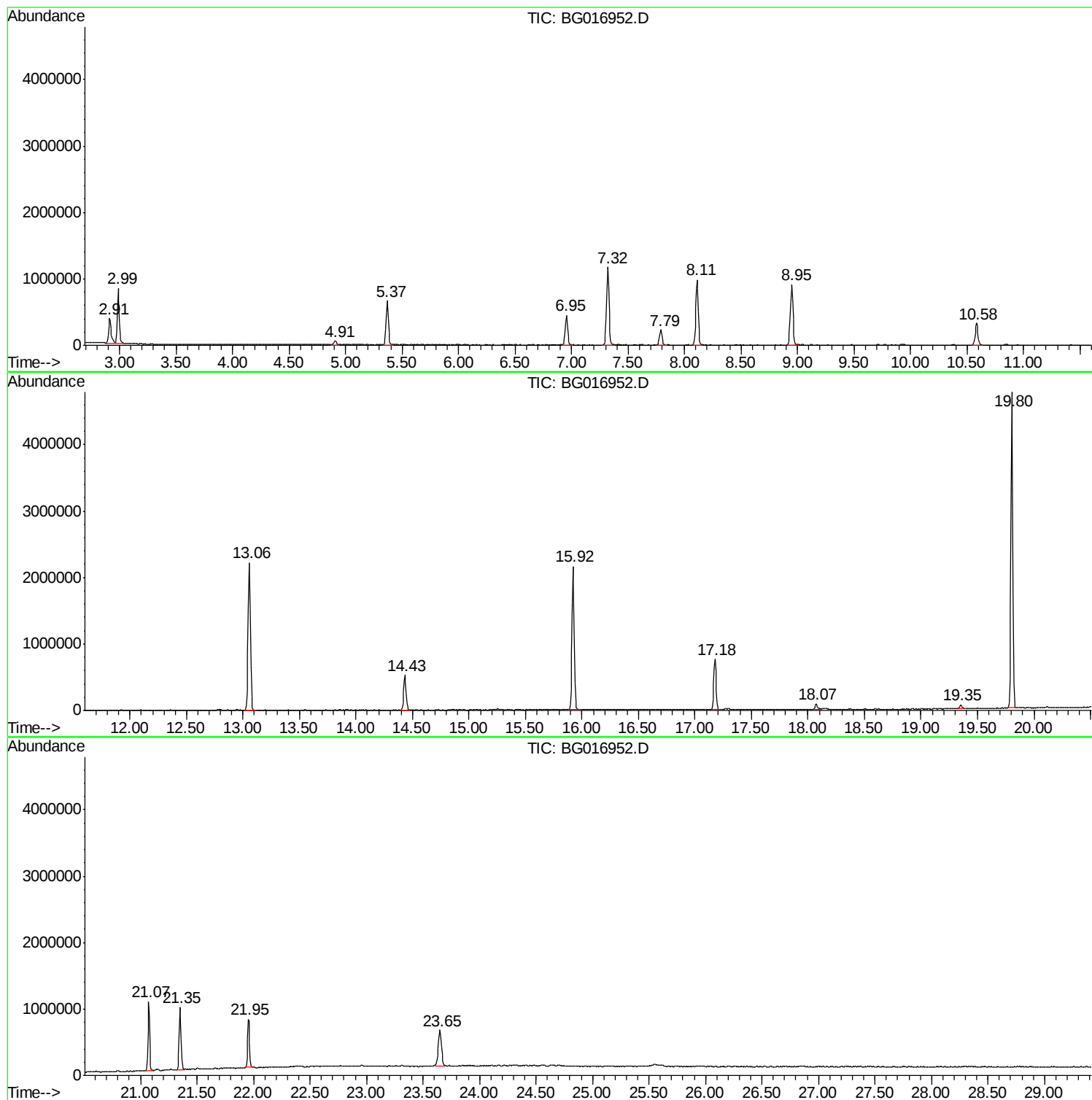
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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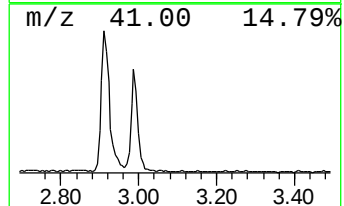
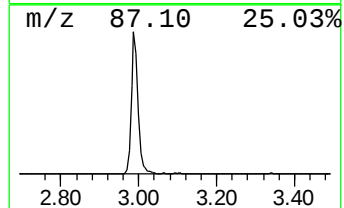
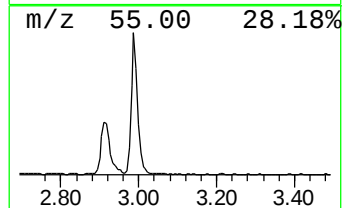
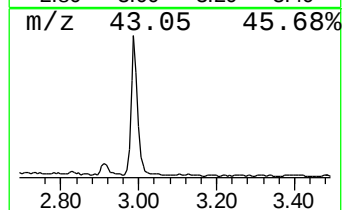
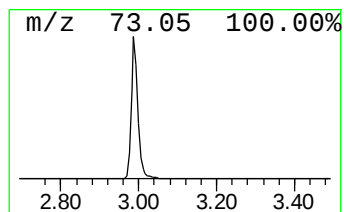
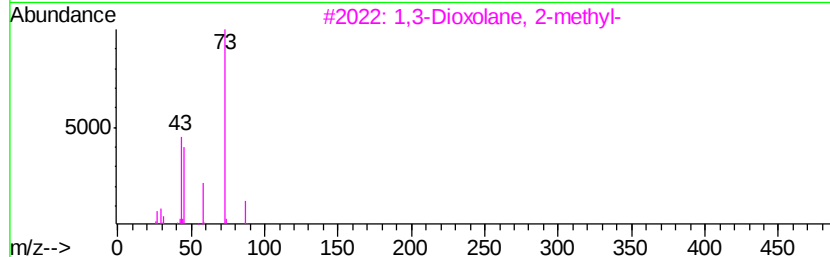
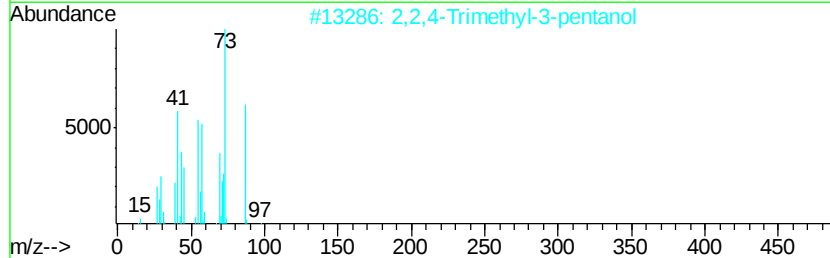
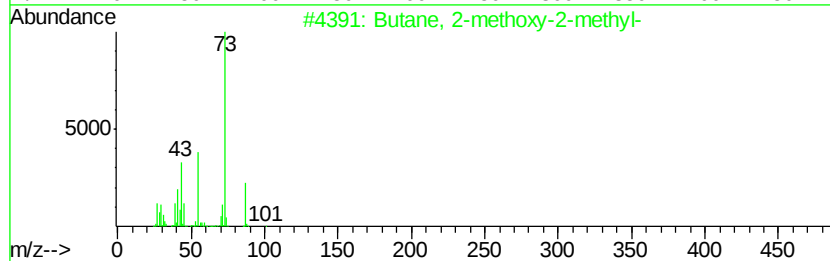
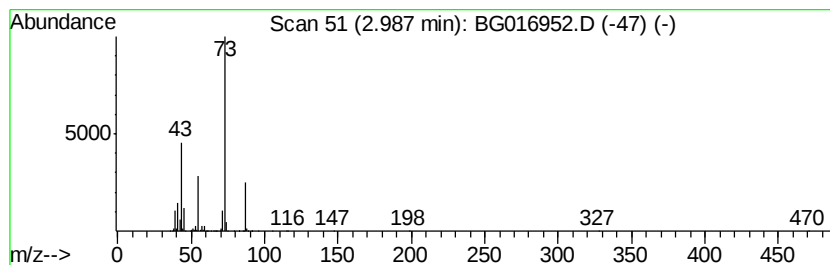
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.99	53.52 ng	972186	1,4-Dichlorobenzene-d4	7.79

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	39	
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25	
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9	
5	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	9	



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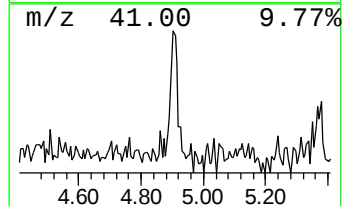
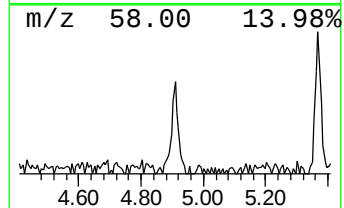
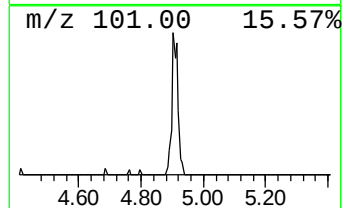
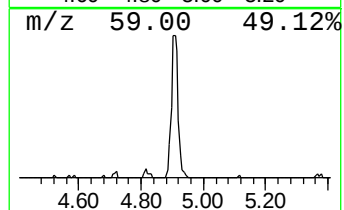
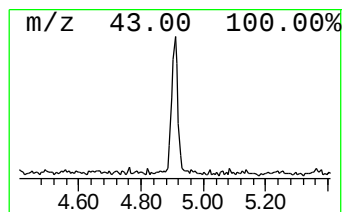
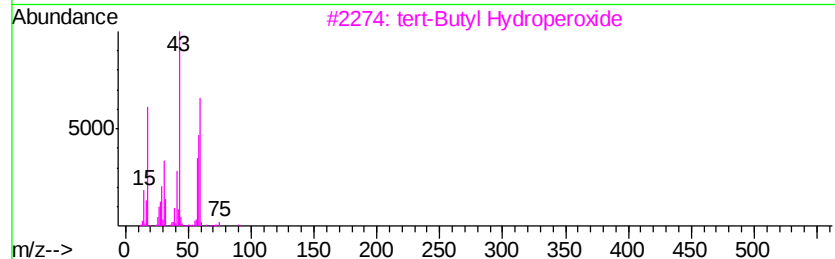
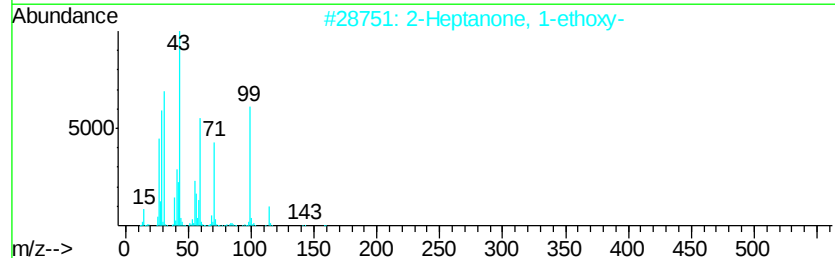
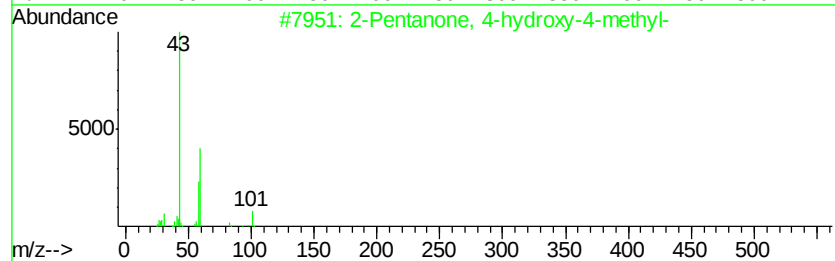
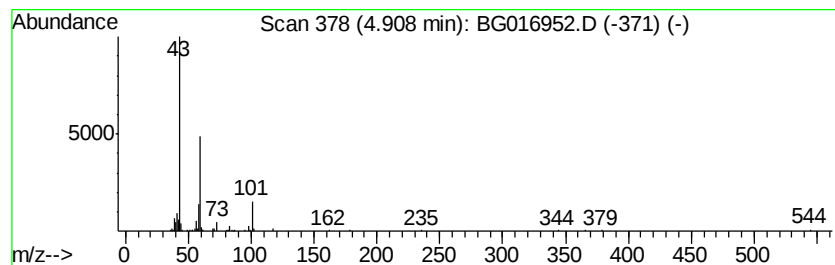
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.91	5.20 ng	94544	1,4-Dichlorobenzene-d4	7.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
2		2-Heptanone, 1-ethoxy-	158	C9H18O2	051149-70-3	36
3		tert-Butyl Hydroperoxide	90	C4H10O2	000075-91-2	28
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
5		1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	10



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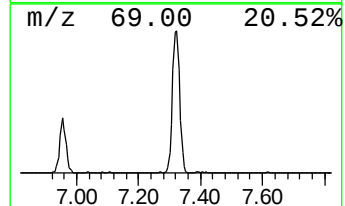
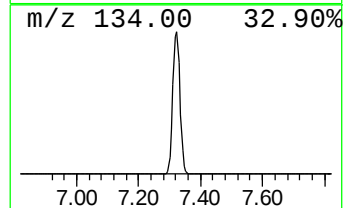
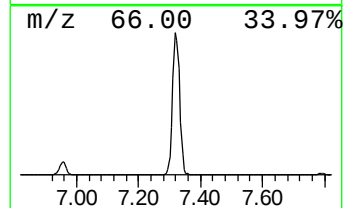
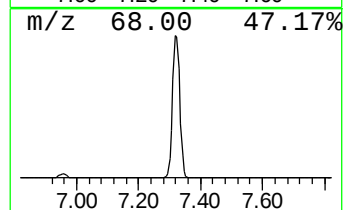
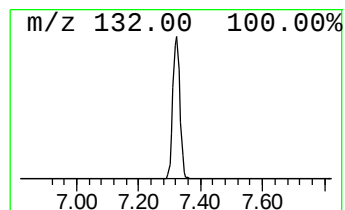
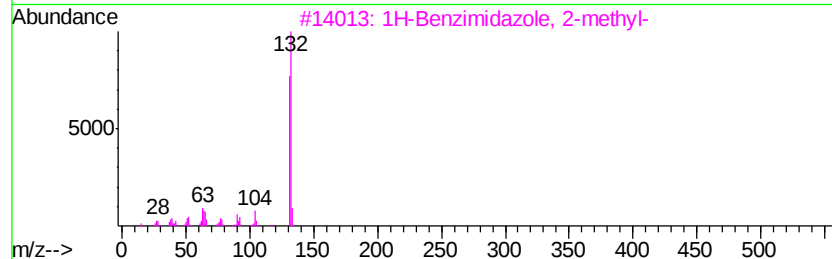
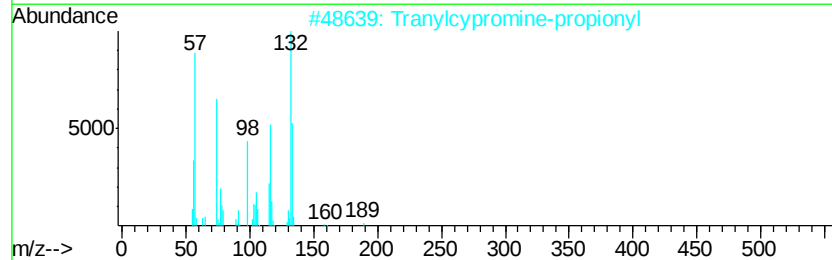
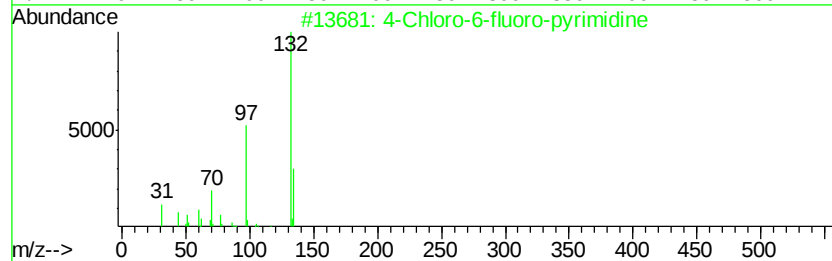
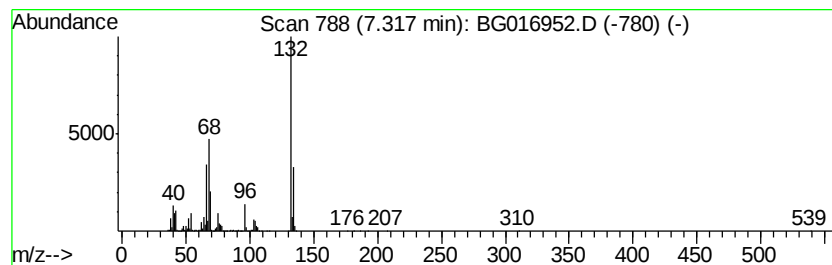
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 4 unknown7.32 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.32	101.56 ng	1844800	1,4-Dichlorobenzene-d4	7.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5		Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	12



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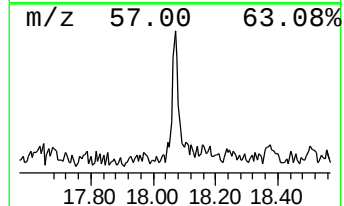
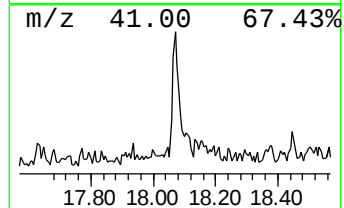
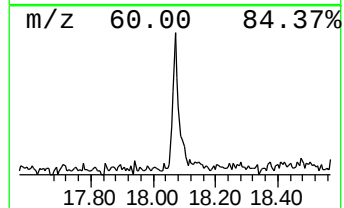
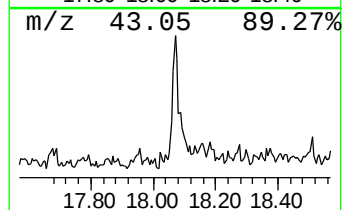
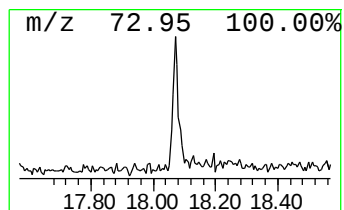
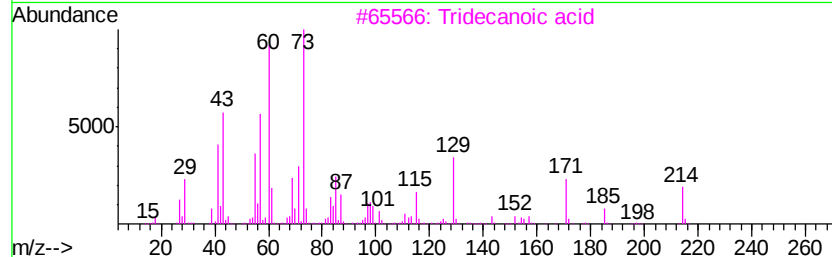
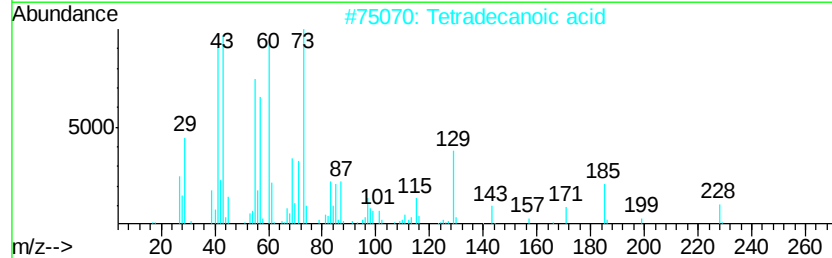
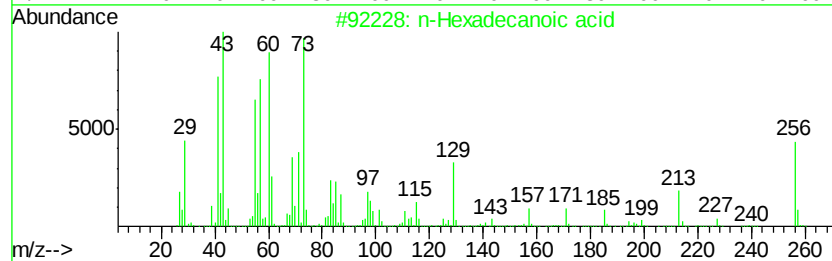
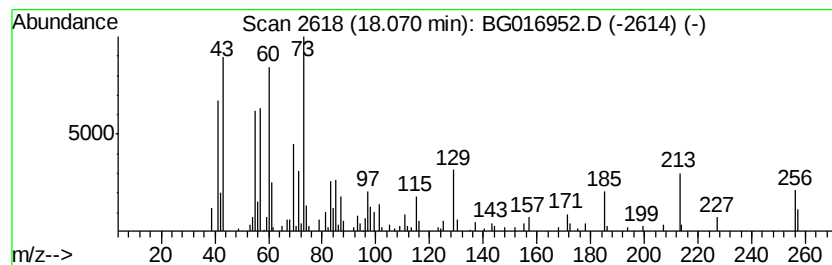
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.07	2.19 ng	115889	Phenanthrene-d10	17.18
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		n-Hexadecanoic acid	256 C16H32O2	000057-10-3 99
2		Tetradecanoic acid	228 C14H28O2	000544-63-8 70
3		Tridecanoic acid	214 C13H26O2	000638-53-9 58
4		Pentadecanoic acid	242 C15H30O2	001002-84-2 50
5		Dodecanoic acid	200 C12H24O2	000143-07-7 49



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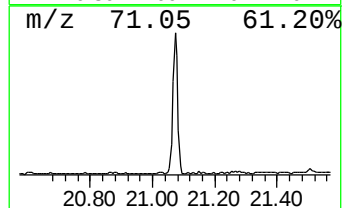
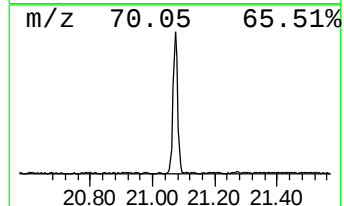
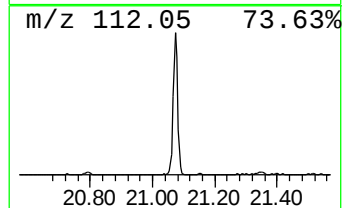
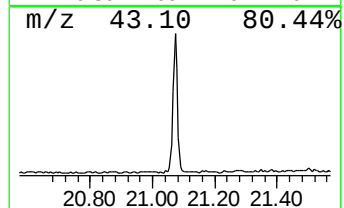
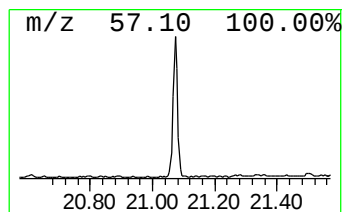
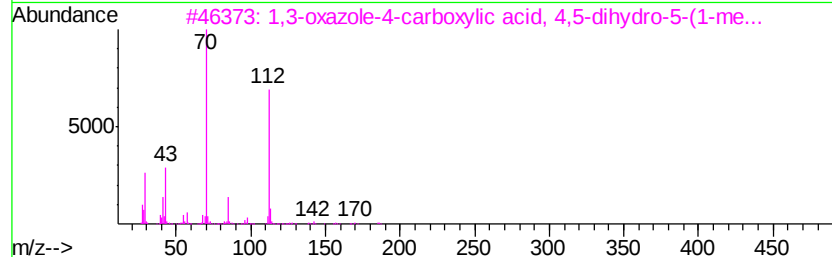
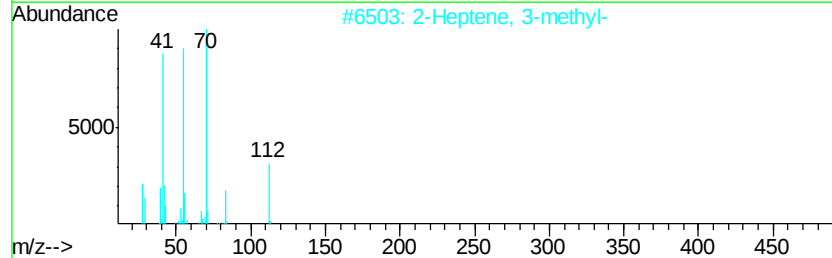
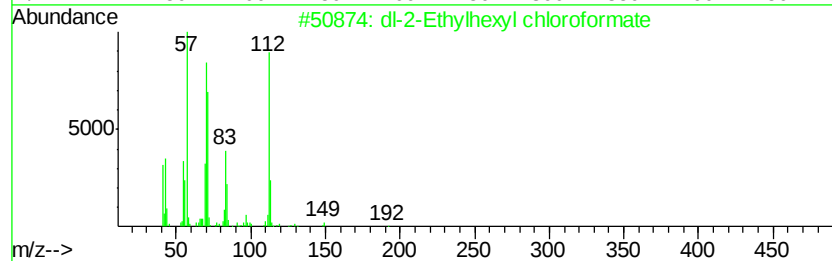
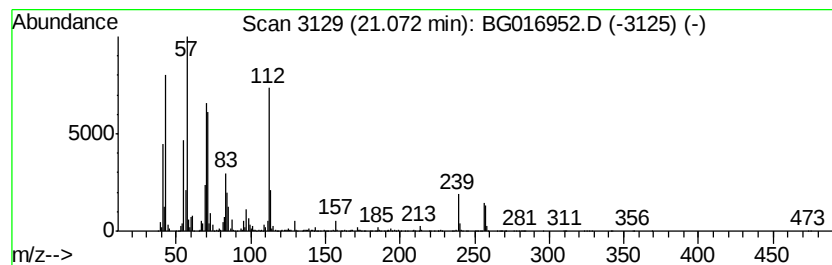
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 7 dl-2-Ethylhexyl chloroformate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.07	18.91 ng	1095400	Chrysene-d12	21.35	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	dl-2-Ethylhexyl chloroformate	192	C9H17ClO2	024468-13-1	93
2	2-Heptene, 3-methyl-	112	C8H16	003404-75-9	43
3	1,3-oxazole-4-carboxylic acid, 4...	185	C9H15N03	1000197-69-0	38
4	3-Methylpyridazin-5-one	112	C5H8N2O	1000130-58-4	35
5	Lauric acid, 2-methylbutyl ester	270	C17H34O2	093815-53-3	25



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.99	53.5	ng	972186	1	7.79	363313	20.0
2-Pentanone, 4-hy...	4.91	5.2	ng	94544	1	7.79	363313	20.0
unknown7.32	7.32	101.6	ng	1844800	1	7.79	363313	20.0
n-Hexadecanoic acid	18.07	2.2	ng	115889	4	17.18	1056180	20.0
dl-2-Ethylhexyl c...	21.07	18.9	ng	1095400	5	21.35	1158420	20.0