

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG081616\
 Data File : BG023734.D
 Acq On : 16 Aug 2016 19:18
 Operator : UM/SJ
 Sample : PB92660BL
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 PB92660BL

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-BG080116.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	2.968	17	22	36	rBV	1277103	1678396	18.27%	3.770%
2	5.159	389	395	406	rBV	614450	925526	10.07%	2.079%
3	5.640	470	477	493	rBV	1820943	2951092	32.12%	6.628%
4	7.262	745	753	762	rBV	1832726	3246014	35.33%	7.290%
5	7.632	808	816	830	rBV	1744806	3102842	33.77%	6.969%
6	8.102	889	896	905	rVB	347607	606715	6.60%	1.363%
7	8.425	942	951	960	rBV	1264336	2253164	24.52%	5.060%
8	9.283	1090	1097	1108	rBV	1118918	2020376	21.99%	4.538%
9	10.939	1371	1379	1391	rBV	475601	870780	9.48%	1.956%
10	13.395	1790	1797	1806	rBV	2855899	4578410	49.83%	10.283%
11	14.781	2026	2033	2043	rVB2	774255	1279806	13.93%	2.874%
12	16.279	2281	2288	2301	rBV	2772280	4552686	49.55%	10.225%
13	17.548	2497	2504	2515	rBV2	1182372	1841254	20.04%	4.135%
14	19.827	2887	2892	2898	rVB	464246	528290	5.75%	1.186%
15	20.156	2942	2948	2955	rBV	6690340	9188761	100.00%	20.637%
16	20.873	3066	3070	3074	rBV	334296	380578	4.14%	0.855%
17	21.866	3233	3239	3249	rVB	1350491	2344058	25.51%	5.265%
18	25.279	3809	3820	3831	rVB2	685717	2176559	23.69%	4.888%

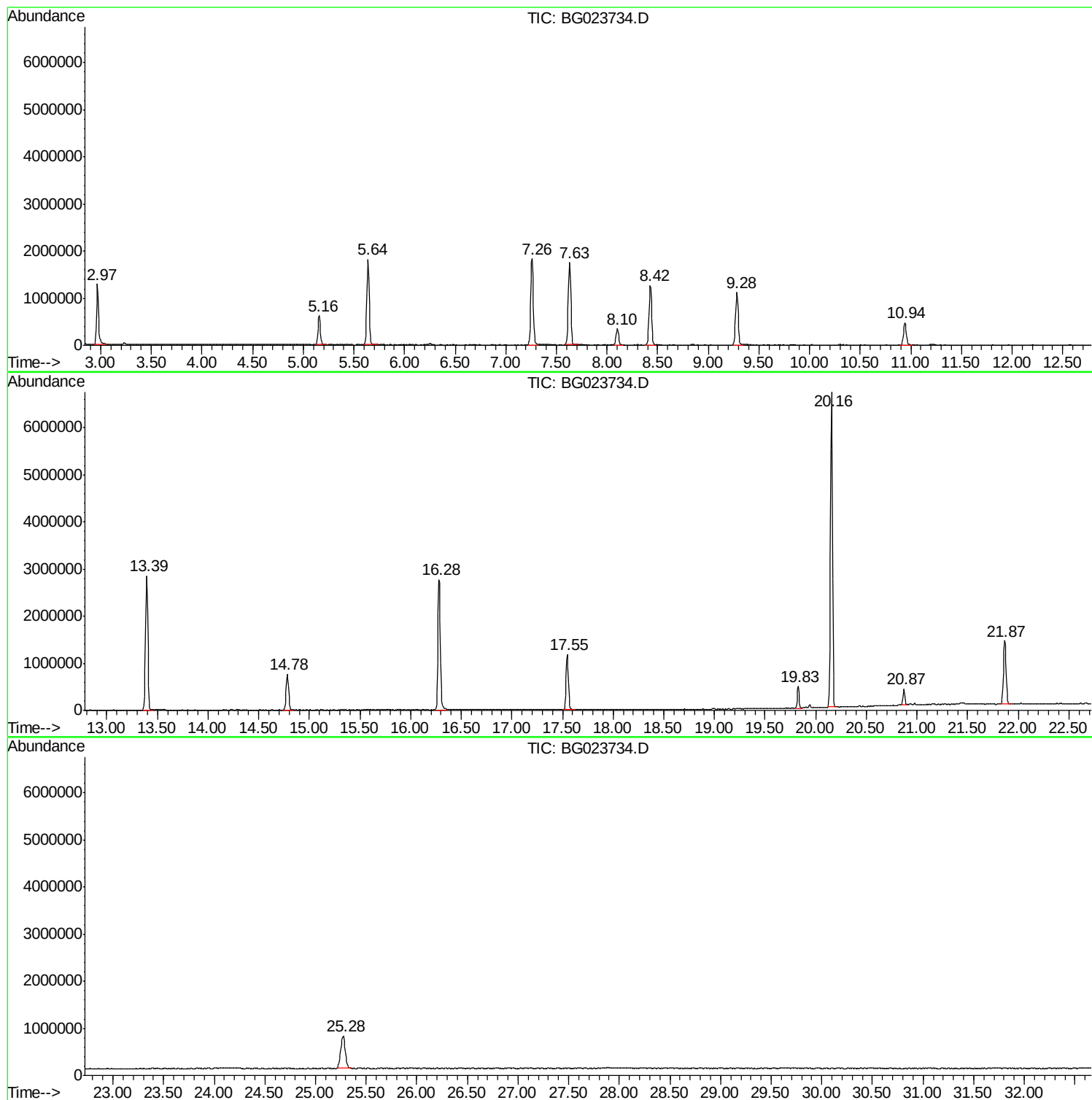
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Quant Method : Z:\HPCHEM1\BNA_G\Methods\8270-BG080116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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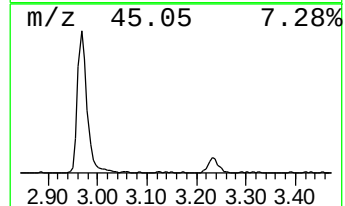
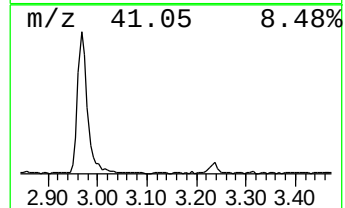
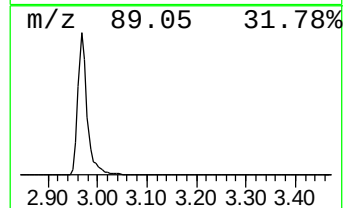
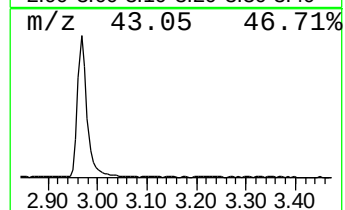
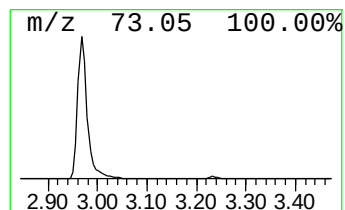
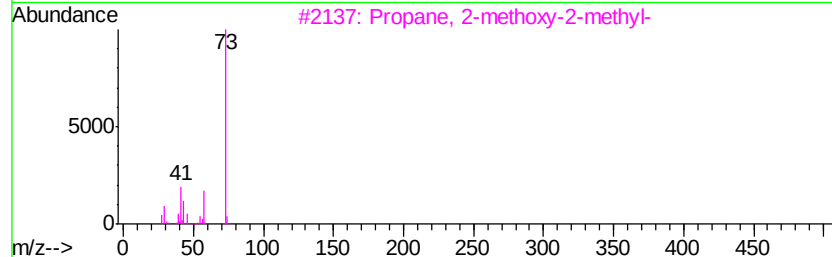
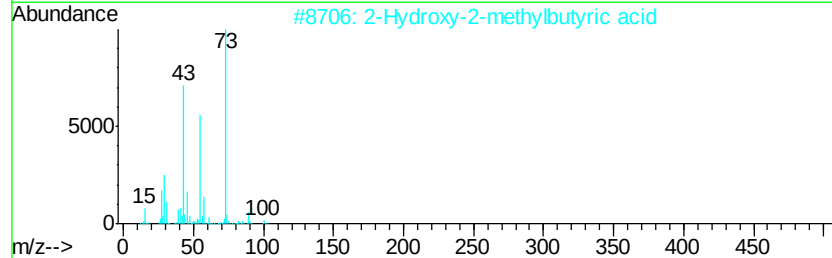
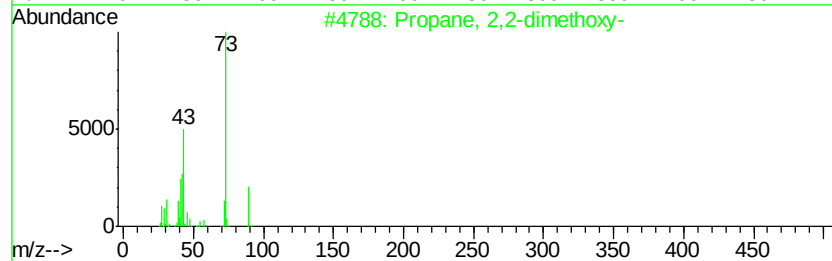
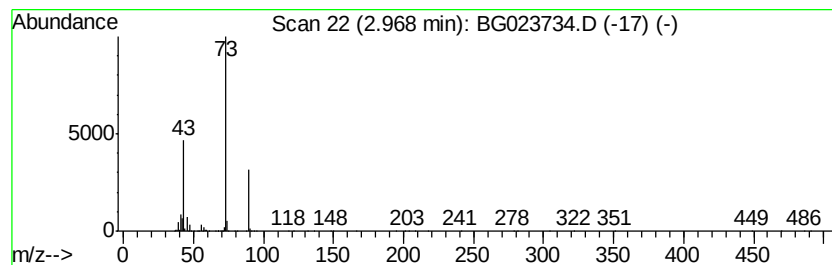
Quant Method : Z:\HPCHEM1\BNA_G\Methods\8270-BG080116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown2.97 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.97	55.33 ng	1678400	1,4-Dichlorobenzene-d4	8.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	45
2		2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9
3		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
4		Methane, isothiocyanato-	73	C2H3NS	000556-61-6	7
5		N-Ethylformamide	73	C3H7NO	000627-45-2	5



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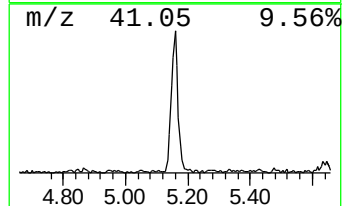
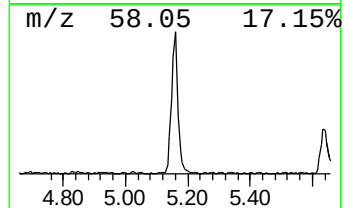
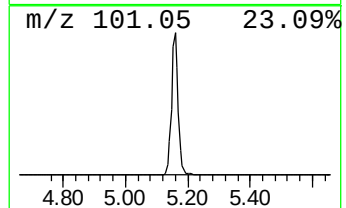
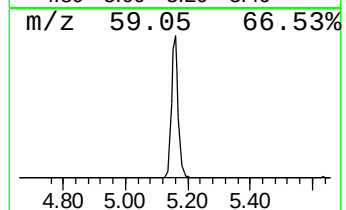
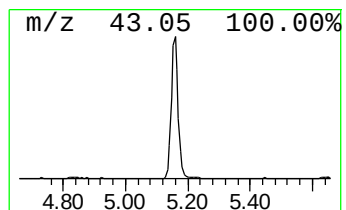
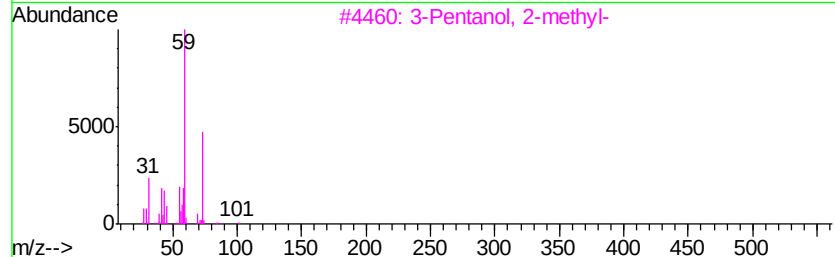
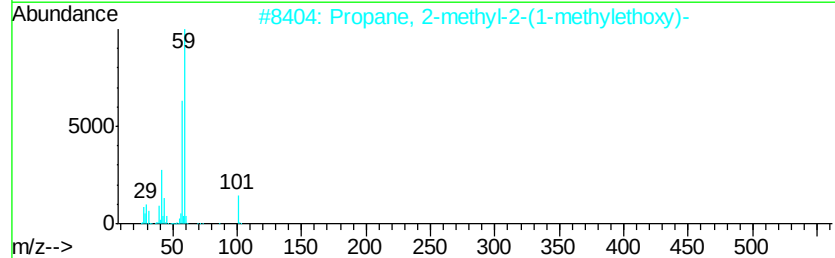
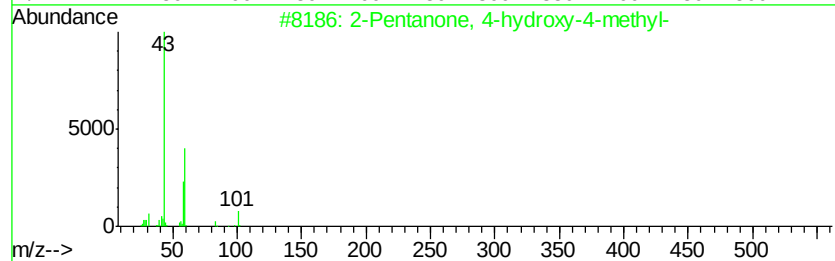
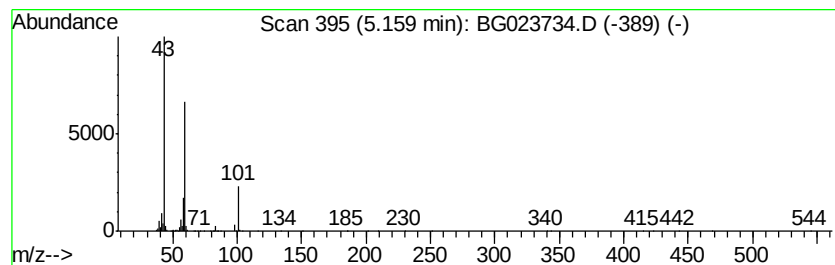
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.16	30.51 ng	925526	1,4-Dichlorobenzene-d4	8.10

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2		000123-42-2	56
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O		017348-59-3	53
3	3-Pentanol, 2-methyl-	102	C6H14O		000565-67-3	47
4	Pentane, 2-methoxy-	102	C6H14O		006795-88-6	9
5	Acetone	58	C3H6O		000067-64-1	9



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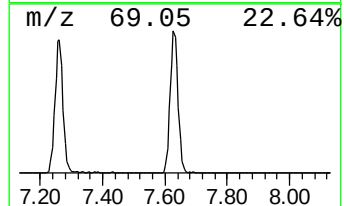
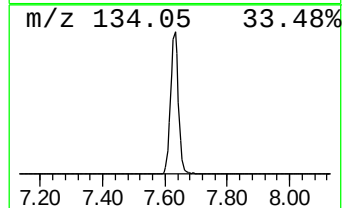
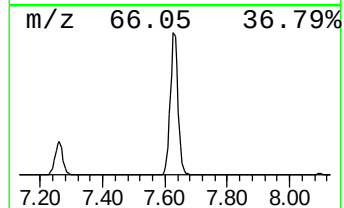
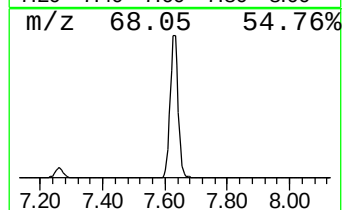
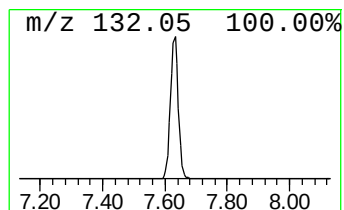
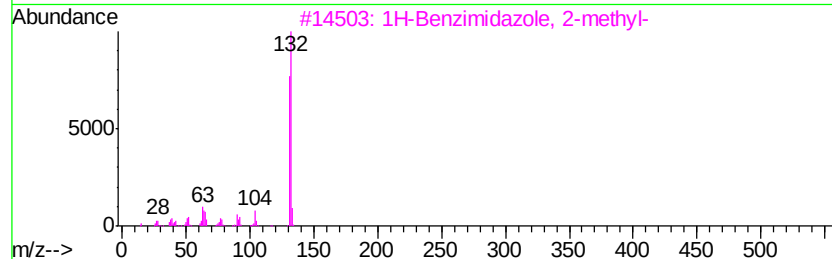
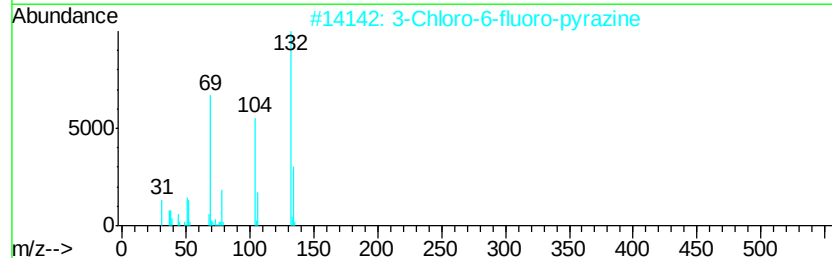
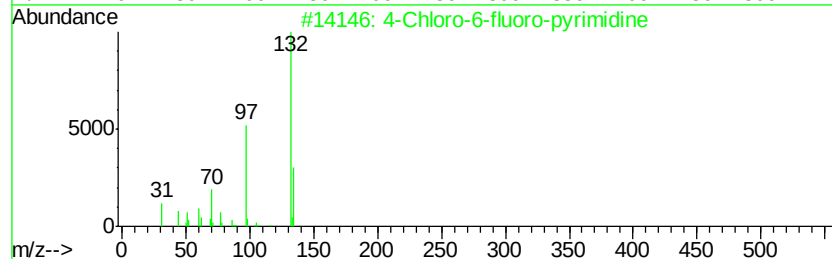
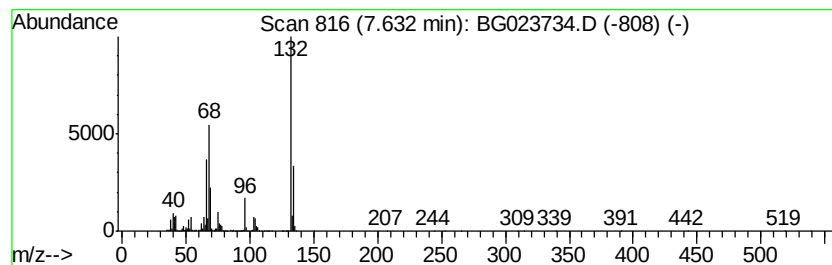
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Peak Number 3 unknown7.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.63	102.28 ng	3102840	1,4-Dichlorobenzene-d4	8.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	13
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12



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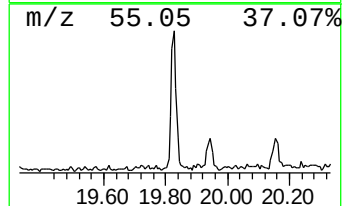
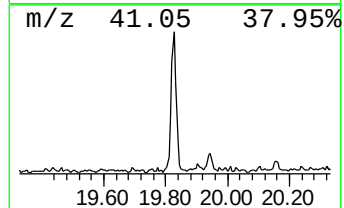
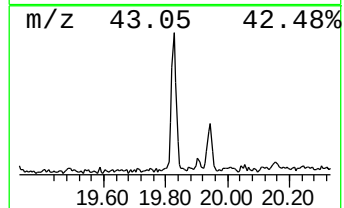
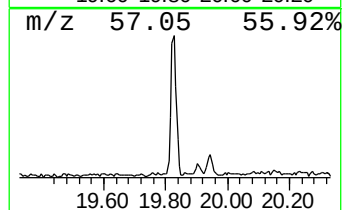
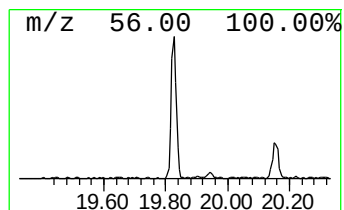
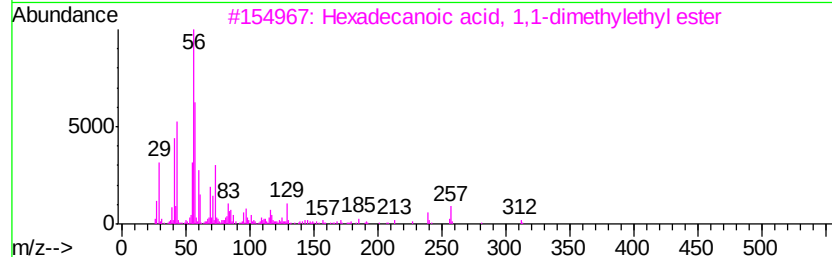
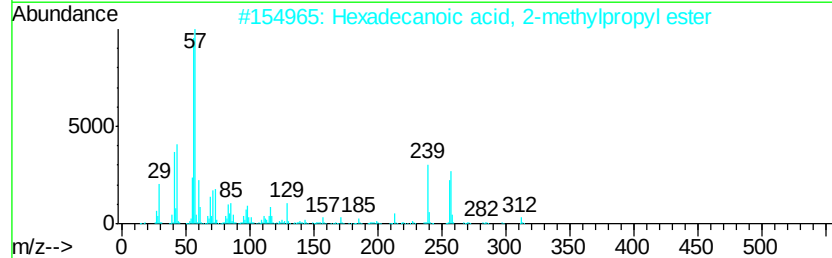
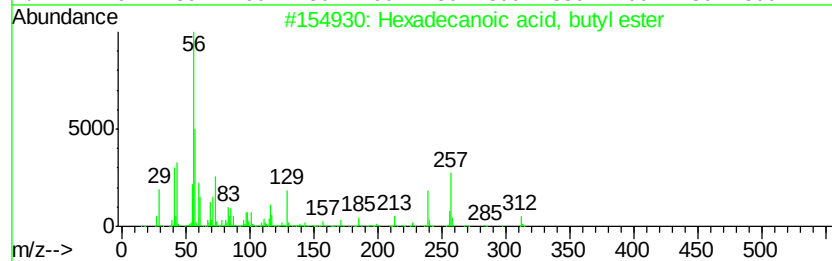
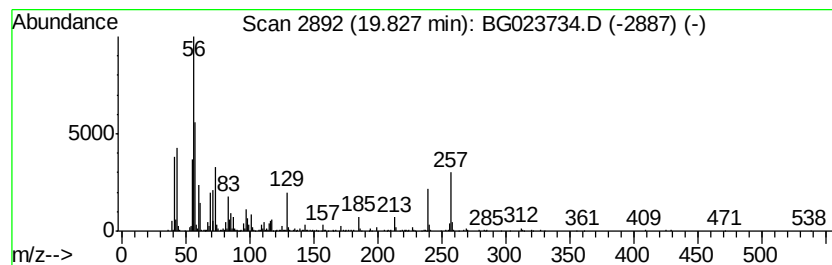
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.83	4.51 ng	528290	Chrysene-d12	21.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2		Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	55
3		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	46
4		2-Butyl-1-decene	196	C14H28	051655-65-3	27
5		1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	27



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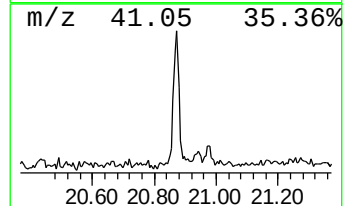
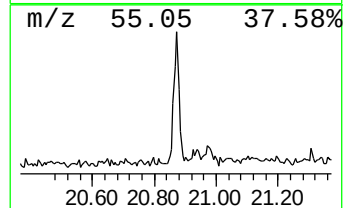
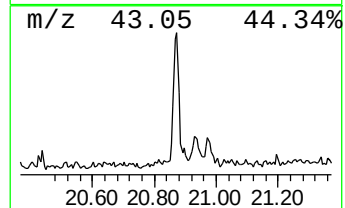
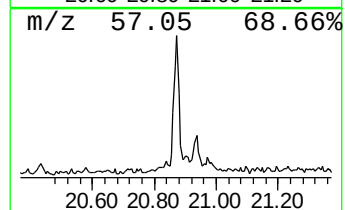
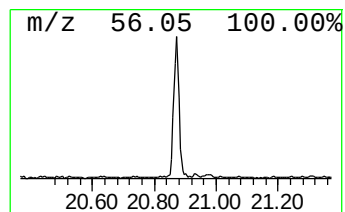
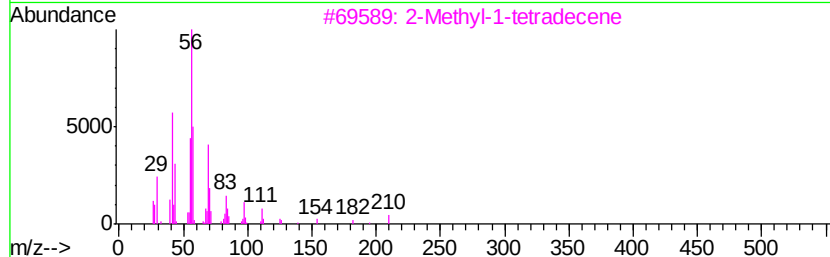
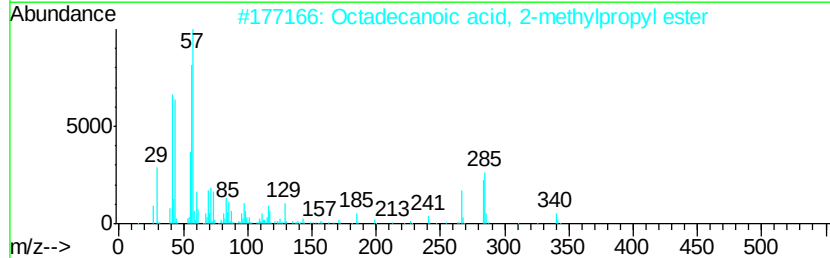
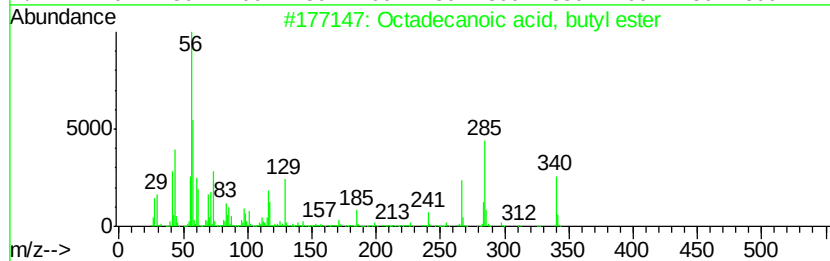
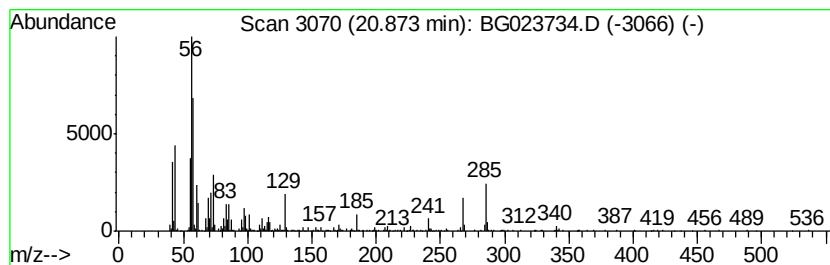
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Peak Number 6 Octadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.87	3.25 ng	380578	Chrysene-d12	21.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	83
2		Octadecanoic acid, 2-methylpropy...	340	C22H44O2	000646-13-9	35
3		2-Methyl-1-tetradecene	210	C15H30	052254-38-3	35
4		1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	27
5		1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	27



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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2-Pentanone, 4-hy...	5.16	30.5	ng	925526	1	8.10	606715	20.0
unknown7.63	7.63	102.3	ng	3102840	1	8.10	606715	20.0
Hexadecanoic acid...	19.83	4.5	ng	528290	5	21.87	2344060	20.0
Octadecanoic acid...	20.87	3.3	ng	380578	5	21.87	2344060	20.0