

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG050815\
 Data File : BG017004.D
 Acq On : 9 May 2015 23:51
 Operator : TP/IZ
 Sample : G2104-02
 Misc :
 ALS Vial : 49 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 MW-103

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-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	2.917	34	39	48	rBV	350890	554567	10.67%	1.984%
2	2.993	48	52	63	rVB	693032	884498	17.01%	3.165%
3	4.909	372	378	385	rVB	62121	94016	1.81%	0.336%
4	5.373	451	457	466	rBV	674024	951758	18.30%	3.406%
5	6.959	721	727	735	rBV	541951	851736	16.38%	3.048%
6	7.324	780	789	798	rBV	1202527	1848832	35.56%	6.616%
7	7.788	862	868	875	rVB	326395	519311	9.99%	1.858%
8	8.111	914	923	931	rVB	898505	1455326	27.99%	5.208%
9	8.945	1056	1065	1075	rBV	898012	1480627	28.48%	5.298%
10	10.579	1336	1343	1351	rVB	474905	794348	15.28%	2.843%
11	12.782	1713	1718	1724	rBV	111514	156810	3.02%	0.561%
12	13.052	1756	1764	1771	rBV	2220376	3401018	65.41%	12.170%
13	13.881	1899	1905	1909	rBV	39364	55454	1.07%	0.198%
14	14.427	1990	1998	2005	rBV2	778904	1199133	23.06%	4.291%
15	15.250	2131	2138	2146	rVB	139443	195883	3.77%	0.701%
16	15.784	2225	2229	2236	rVB	47943	65485	1.26%	0.234%
17	15.913	2244	2251	2262	rBV	2010669	2907722	55.92%	10.405%
18	17.171	2456	2465	2472	rBV2	1125950	1577419	30.34%	5.645%
19	18.064	2611	2617	2622	rBV	150120	203935	3.92%	0.730%
20	19.345	2831	2835	2843	rBV2	89556	139555	2.68%	0.499%
21	19.797	2905	2912	2921	rBV	4232992	5199726	100.00%	18.607%
22	21.055	3122	3126	3132	rBV6	77417	104203	2.00%	0.373%
23	21.348	3170	3176	3185	rBV	1280386	1684452	32.40%	6.028%
24	23.640	3557	3566	3577	rBV2	795502	1619282	31.14%	5.795%

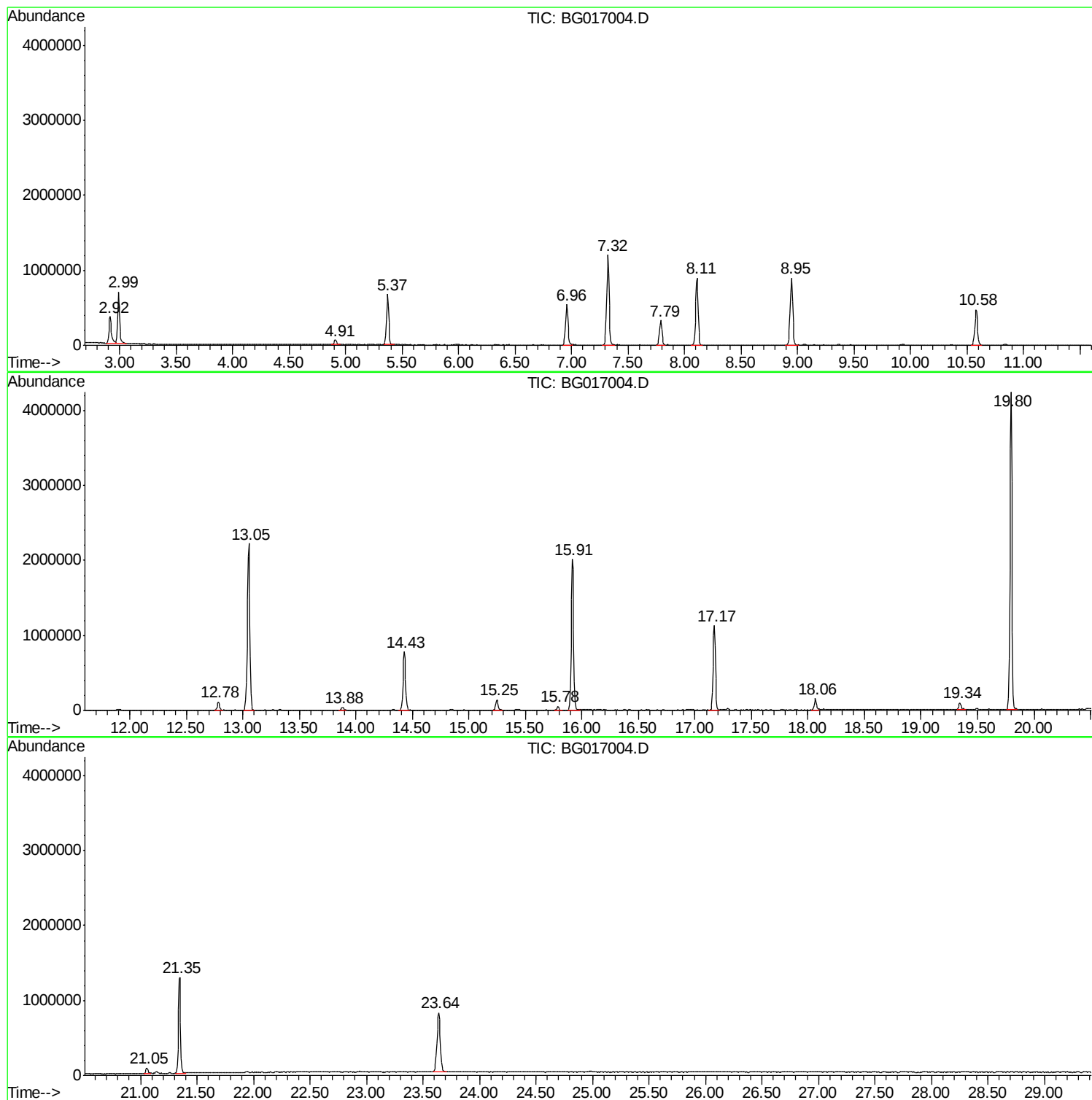
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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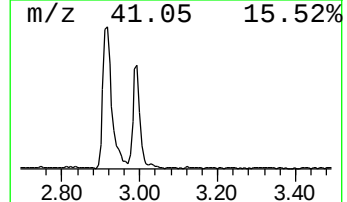
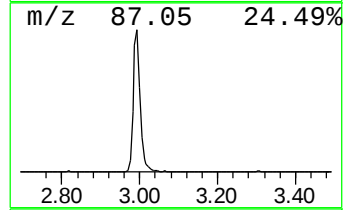
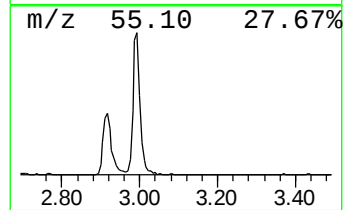
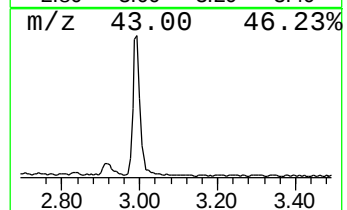
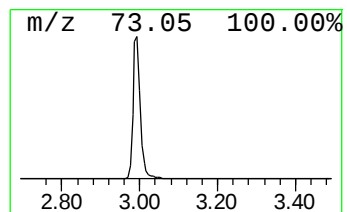
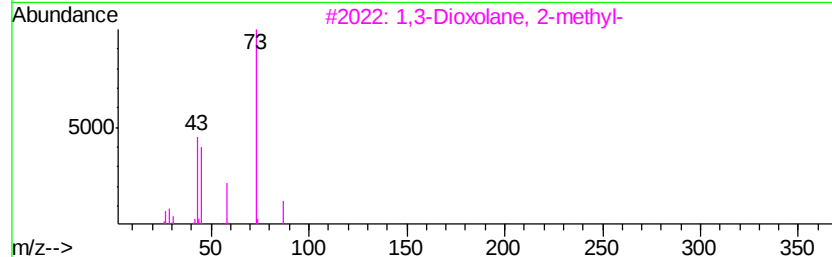
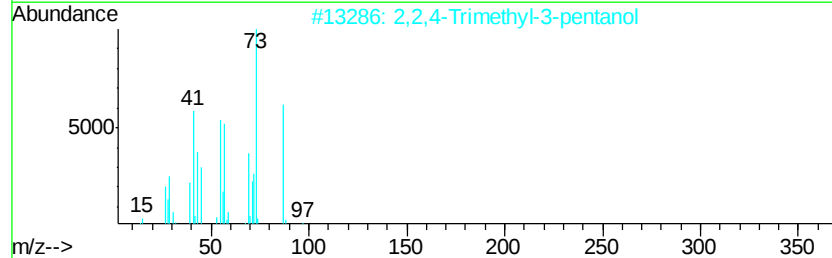
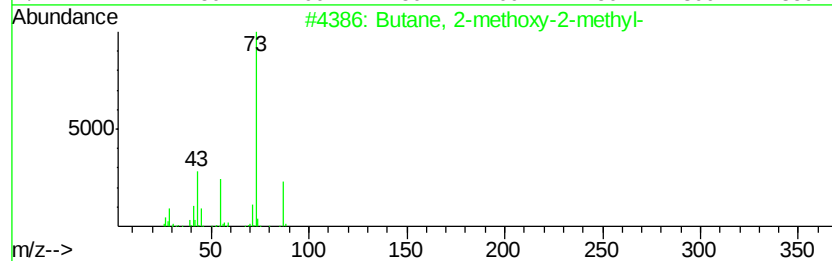
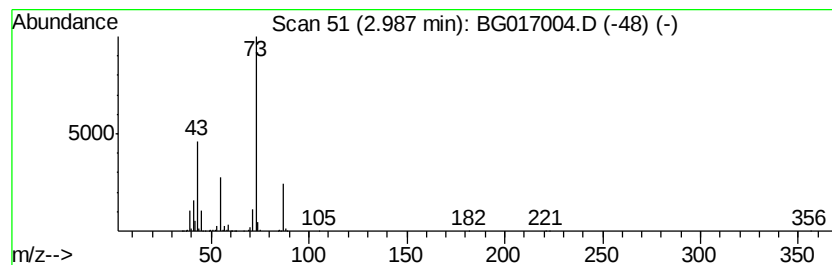
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	34.06 ng	884498	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	36
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	28
4			N-Ethylformamide	73	C3H7NO	000627-45-2	9
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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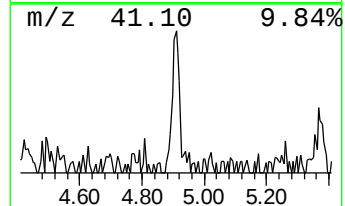
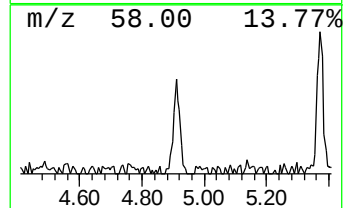
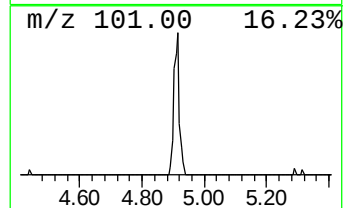
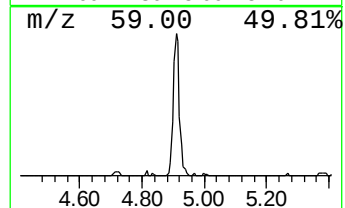
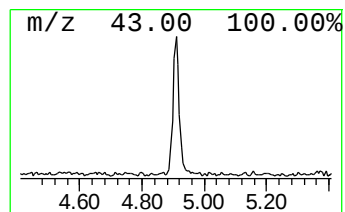
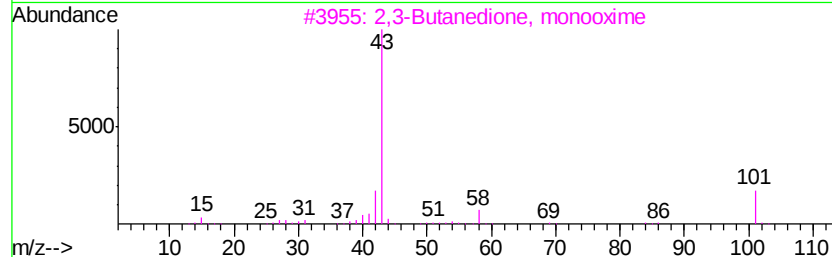
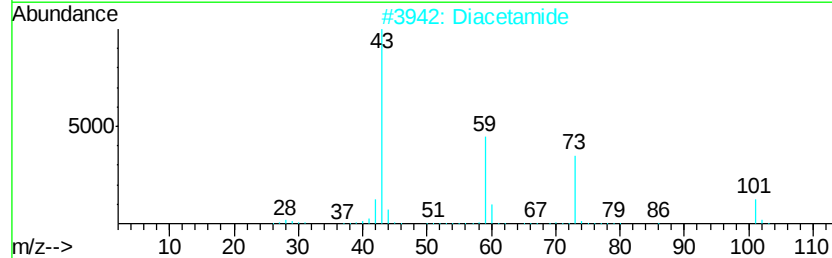
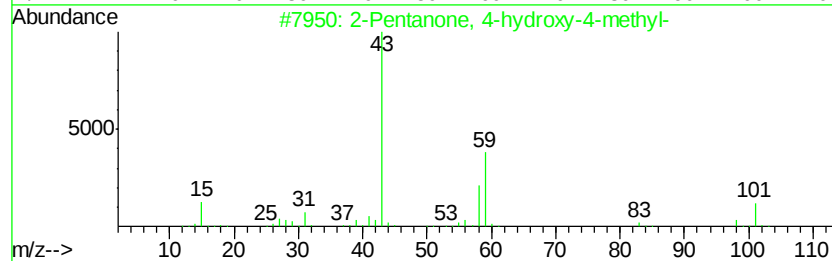
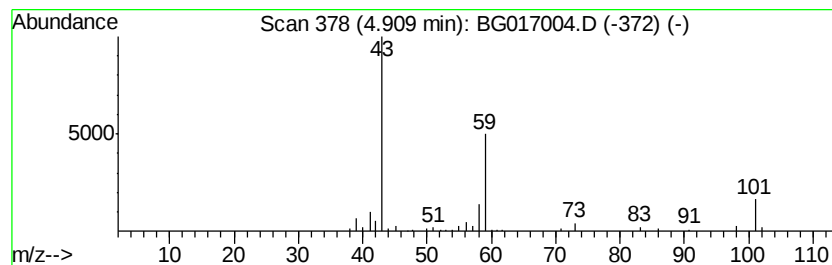
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown4.91 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.91	3.62 ng	94016	1,4-Dichlorobenzene-d4	7.79

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2			Diacetamide	101	C4H7NO2	000625-77-4	36
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
5			2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9



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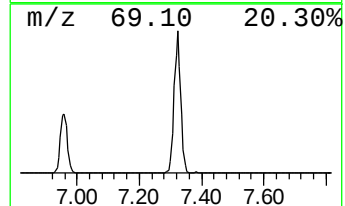
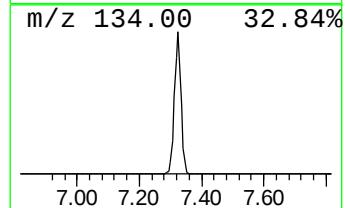
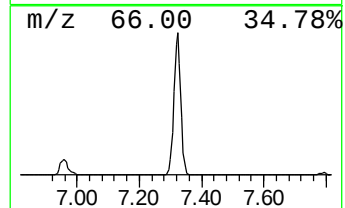
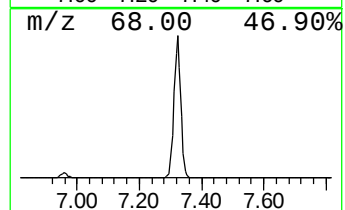
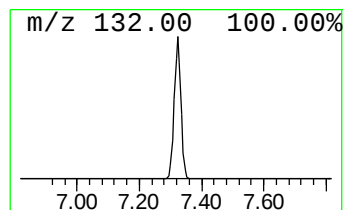
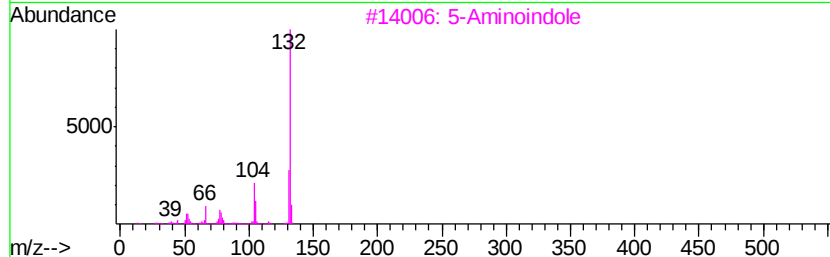
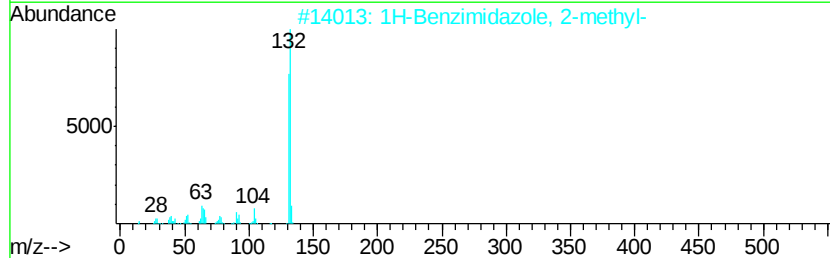
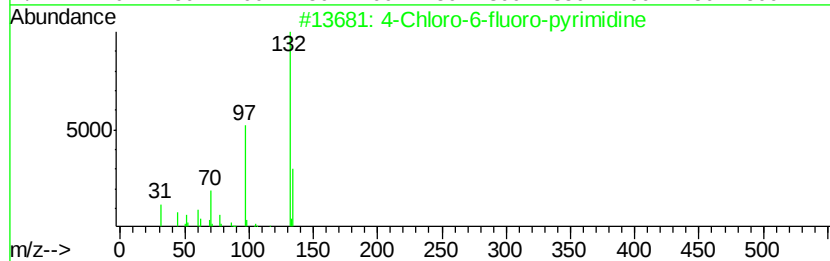
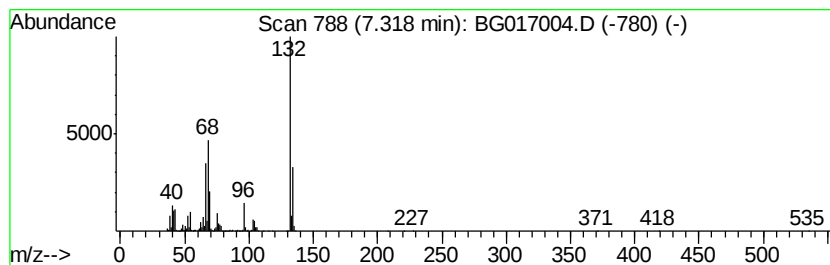
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 4 unknown7.32 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.32	71.20 ng	1848830	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		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3		5-Aminoindole	132	C8H8N2	005192-03-0	22
4		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	16



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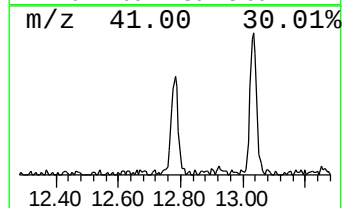
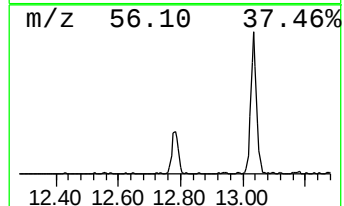
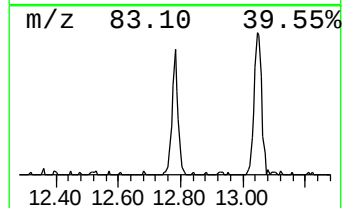
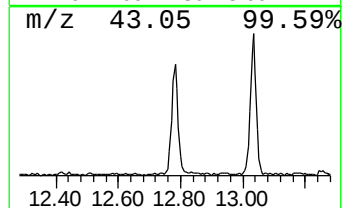
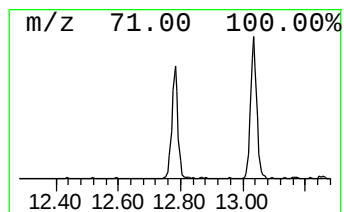
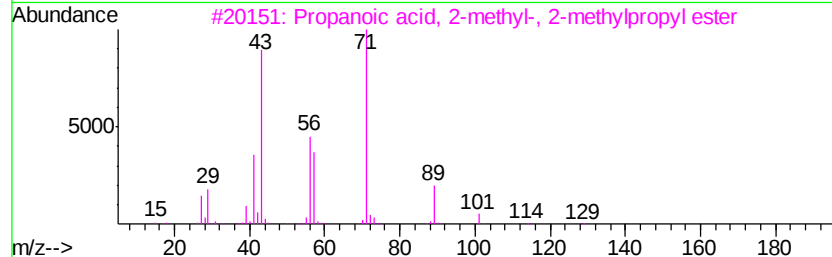
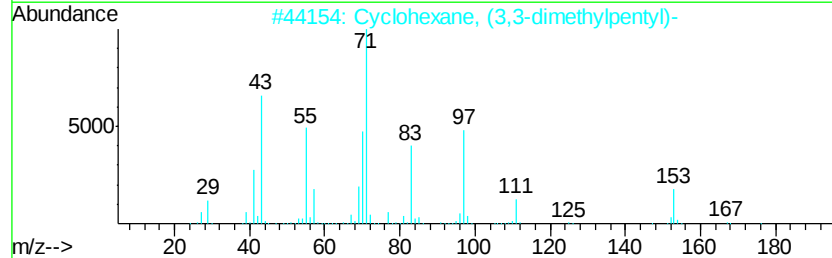
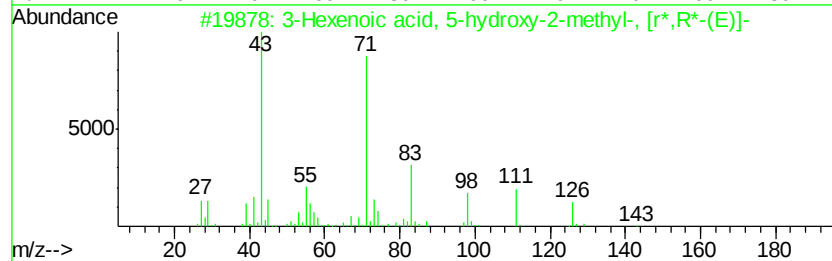
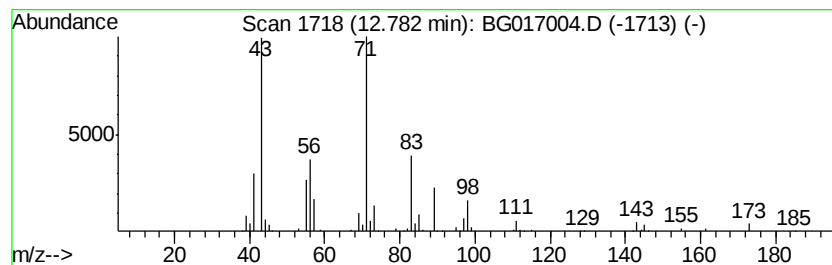
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Peak Number 6 3-Hexenoic acid, 5-hydroxy-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.		
12.78	2.62 ng	156810	Acenaphthene-d10	14.43		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Hexenoic acid, 5-hydroxy-2-met...	144	C7H12O3	110678-36-9	53
2		Cyclohexane, (3,3-dimethylpentyl)-	182	C13H26	061142-22-1	38
3		Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	38
4		Propanoic acid, 2-methyl-, 1-(1,...	286	C16H30O4	074381-40-1	38
5		Propanoic acid, 2-methyl-, 2,2-d...	216	C12H24O3	074367-33-2	38



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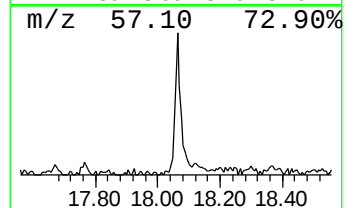
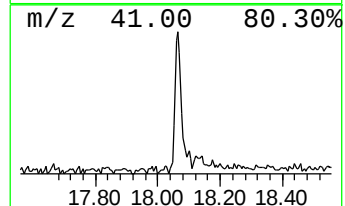
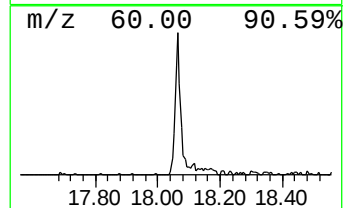
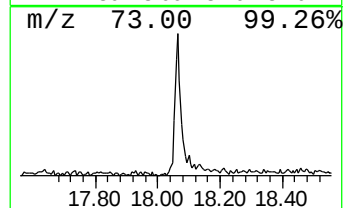
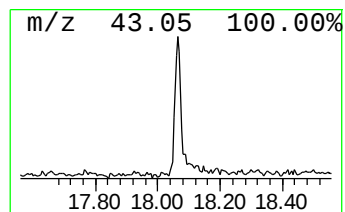
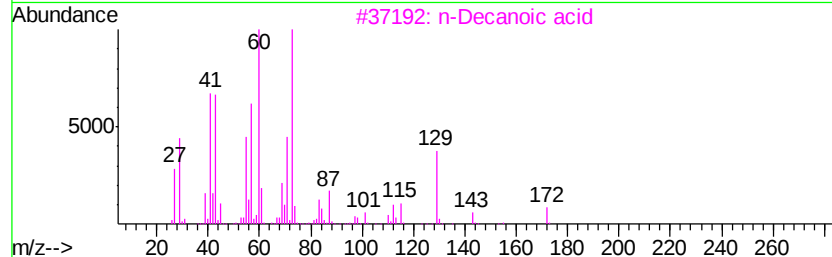
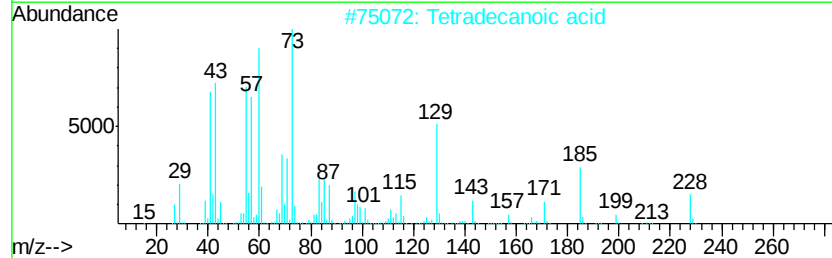
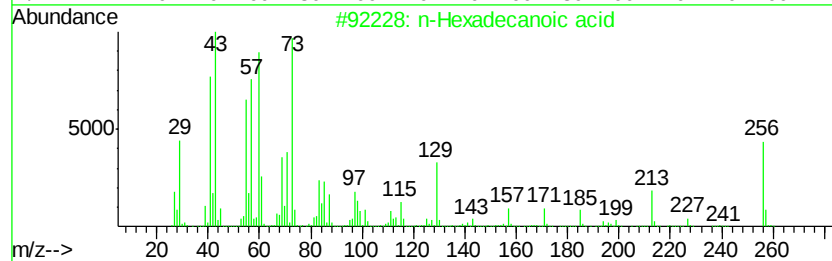
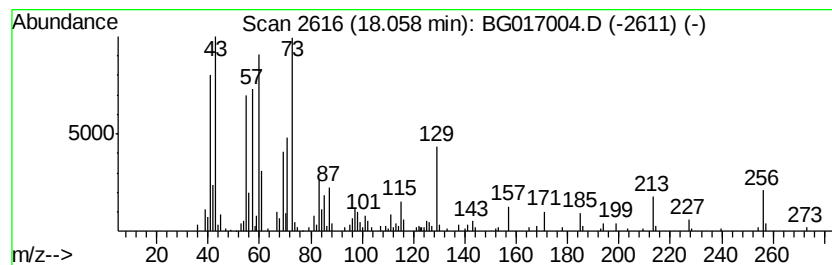
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 7 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.06	2.59 ng	203935	Phenanthrene-d10	17.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	68
3		n-Decanoic acid	172	C10H20O2	000334-48-5	60
4		Tridecanoic acid	214	C13H26O2	000638-53-9	58
5		Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.99	34.1	ng	884498	1	7.79	519311	20.0
unknown4.91	4.91	3.6	ng	94016	1	7.79	519311	20.0
unknown7.32	7.32	71.2	ng	1848830	1	7.79	519311	20.0
3-Hexenoic acid, ...	12.78	2.6	ng	156810	3	14.43	1199130	20.0
n-Hexadecanoic acid	18.06	2.6	ng	203935	4	17.17	1577420	20.0