

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG090616\
 Data File : BG023948.D
 Acq On : 6 Sep 2016 14:59
 Operator : UM/SJ
 Sample : PB93238BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 PB93238BL

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-BG083116.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	2.944	13	18	35	rVB	5389253	8727489	100.00%	25.769%
2	5.159	390	395	405	rVB	176766	270860	3.10%	0.800%
3	5.641	471	477	492	rVB	953282	1542090	17.67%	4.553%
4	7.262	746	753	764	rBV	956743	1715052	19.65%	5.064%
5	7.626	807	815	829	rBV	938004	1629977	18.68%	4.813%
6	8.090	886	894	902	rVB	274750	463437	5.31%	1.368%
7	8.413	942	949	961	rBV	720571	1238700	14.19%	3.657%
8	9.271	1088	1095	1105	rBV	602842	1095017	12.55%	3.233%
9	10.922	1368	1376	1384	rBV	352398	647646	7.42%	1.912%
10	13.365	1782	1792	1803	rBV	1601475	2523993	28.92%	7.452%
11	14.752	2022	2028	2037	rVB2	605793	979595	11.22%	2.892%
12	16.256	2276	2284	2297	rBV	1707314	2673648	30.63%	7.894%
13	17.519	2493	2499	2506	rBV2	834806	1345898	15.42%	3.974%
14	18.388	2642	2647	2656	rBV2	286487	463737	5.31%	1.369%
15	19.657	2858	2863	2875	rBV	462149	827160	9.48%	2.442%
16	20.121	2936	2942	2948	rBV	3547667	4493062	51.48%	13.266%
17	21.531	3178	3182	3187	rBV2	53229	88037	1.01%	0.260%
18	21.825	3226	3232	3243	rVB2	933696	1619027	18.55%	4.780%
19	25.191	3795	3805	3823	rVB	486981	1524274	17.47%	4.501%

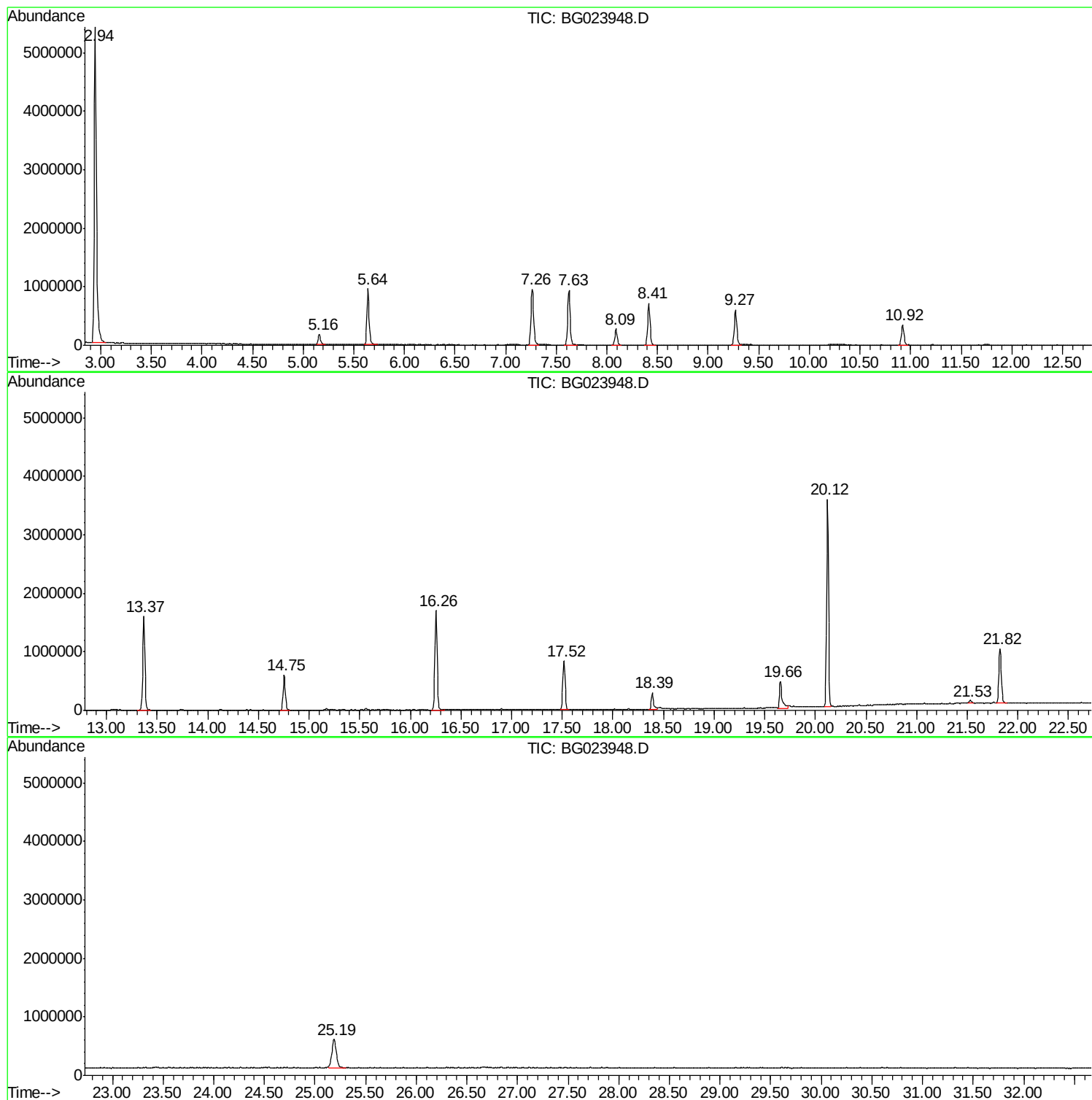
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG083116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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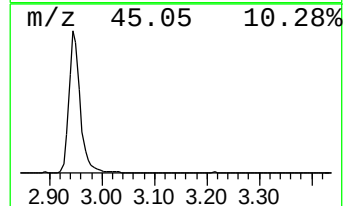
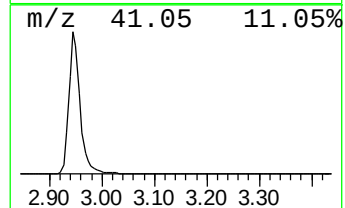
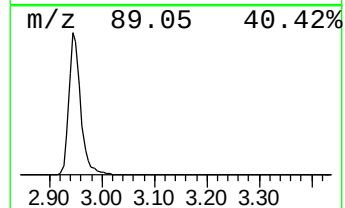
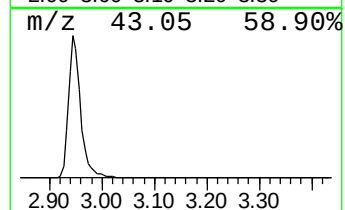
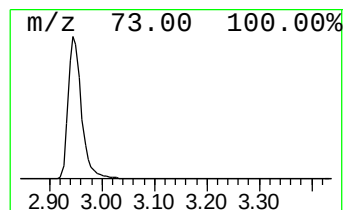
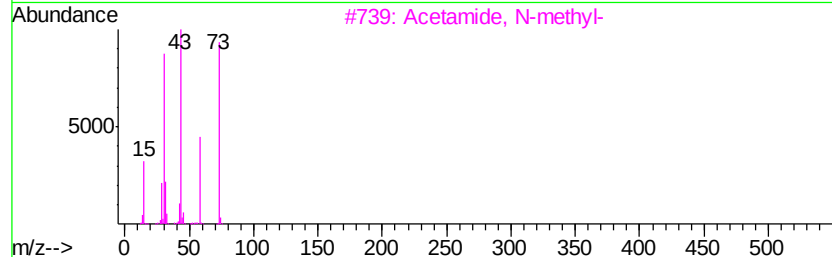
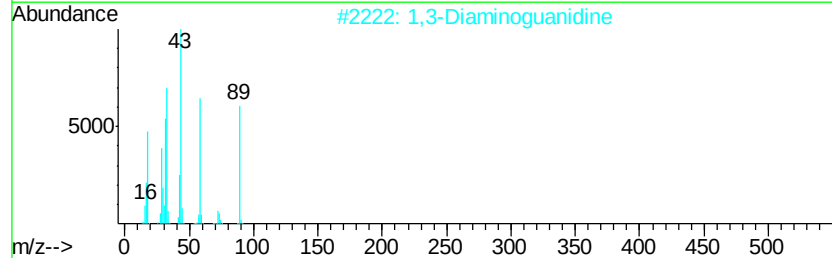
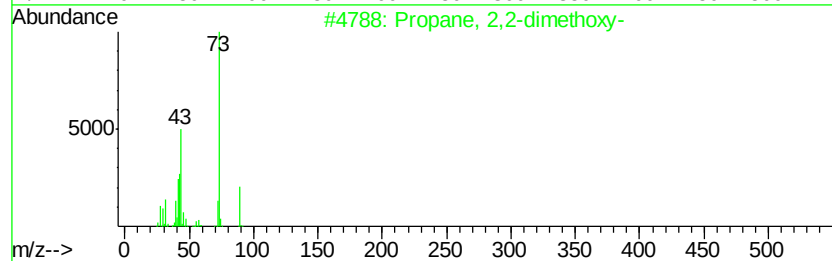
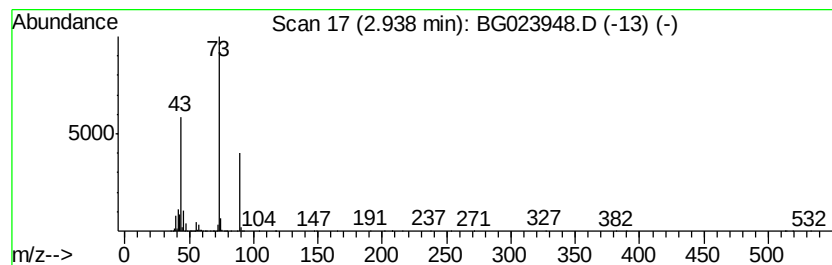
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG083116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown2.94 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.94	376.64 ng	8727490	1,4-Dichlorobenzene-d4	8.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	38
2		1,3-Diaminoguanidine	89	CH7N5	004364-78-7	25
3		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	12
4		Methane, isothiocyanato-	73	C2H3NS	000556-61-6	10
5		N-Ethylformamide	73	C3H7NO	000627-45-2	9



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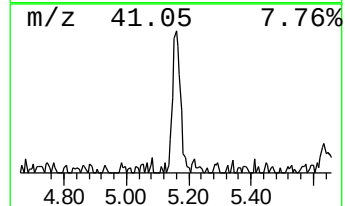
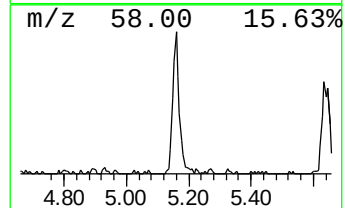
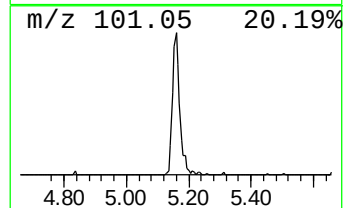
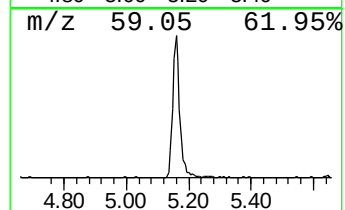
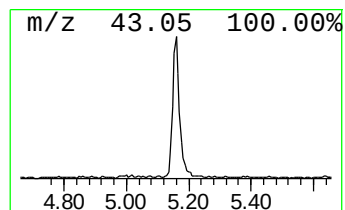
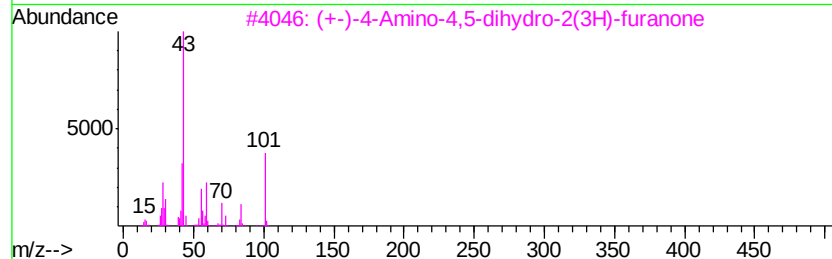
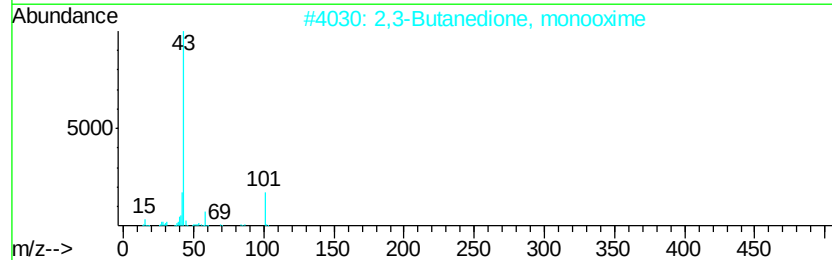
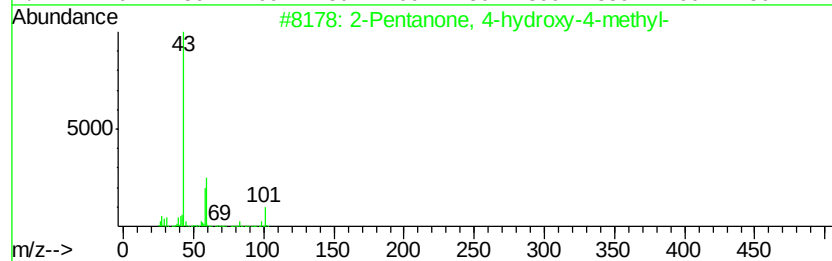
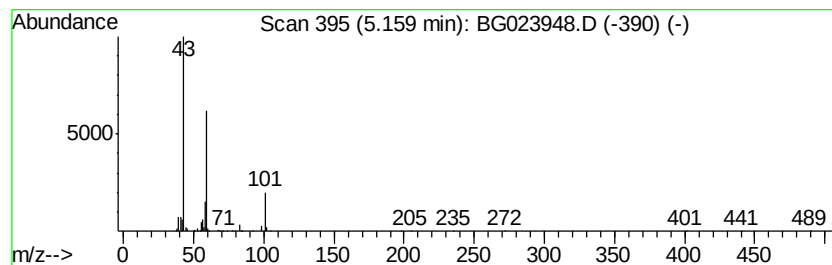
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown5.16 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.16	11.69 ng	270860	1,4-Dichlorobenzene-d4	8.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
3	(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
4	Guanidine	59	CH5N3	000113-00-8	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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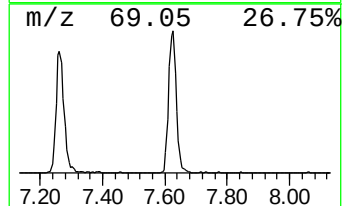
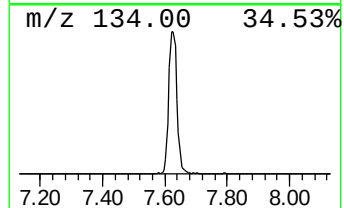
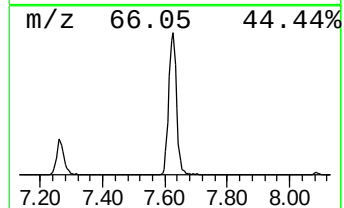
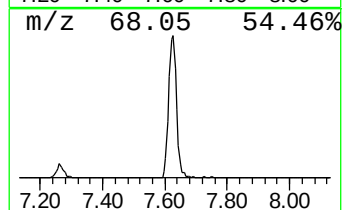
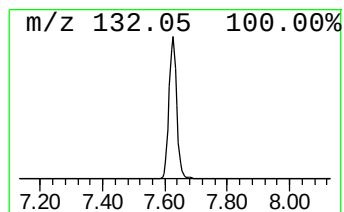
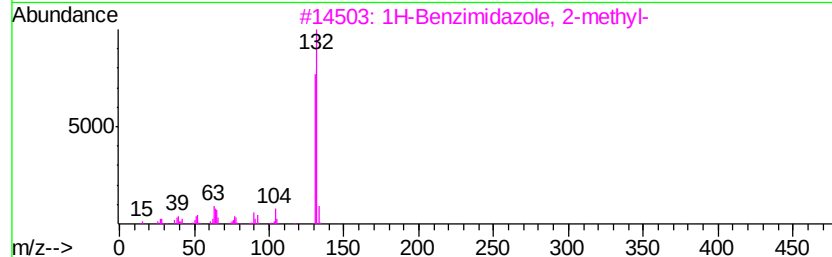
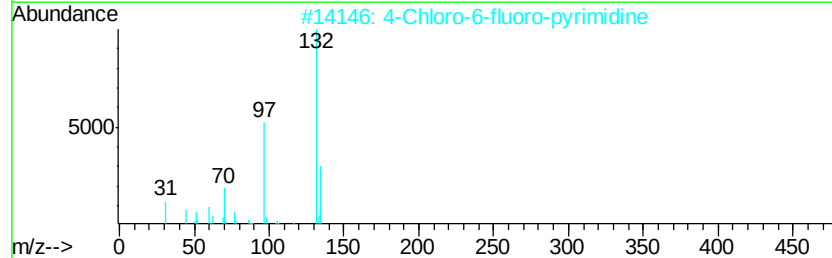
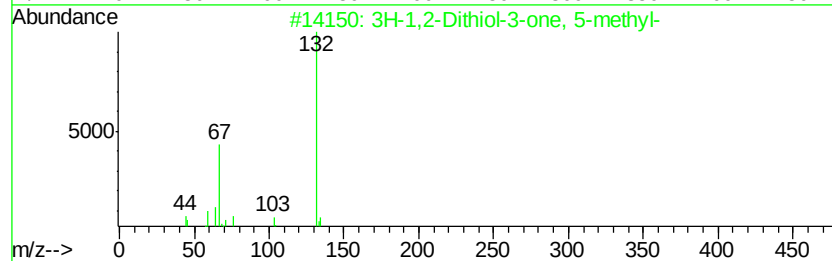
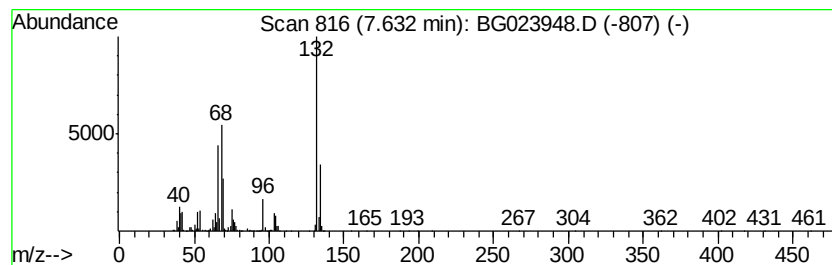
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Peak Number 3 unknown7.63 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.63	70.34 ng	1629980	1,4-Dichlorobenzene-d4	8.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	14
2		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	14
4		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	10
5		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10



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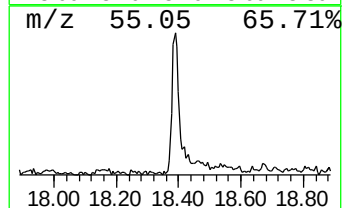
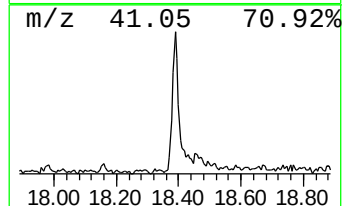
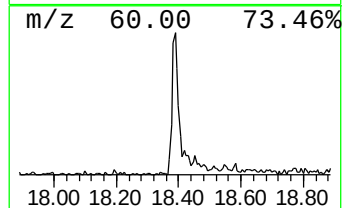
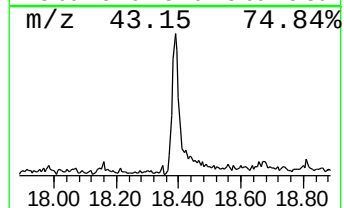
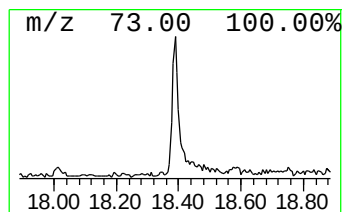
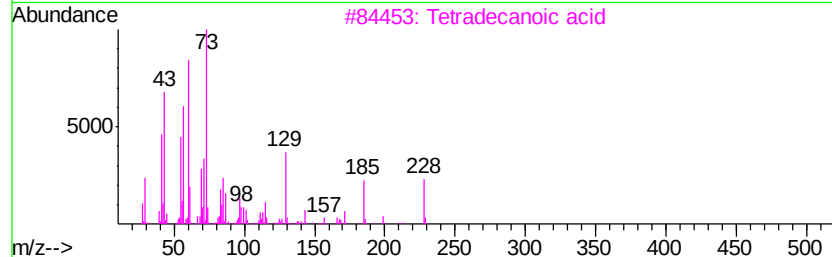
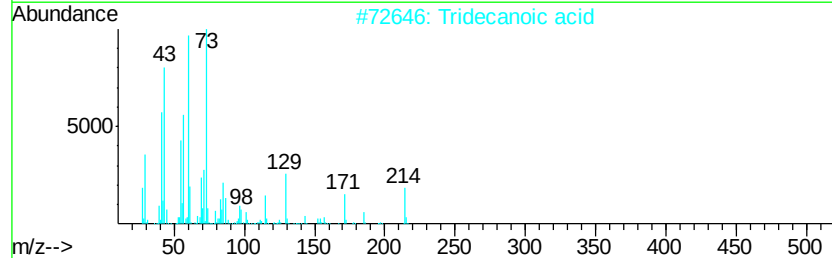
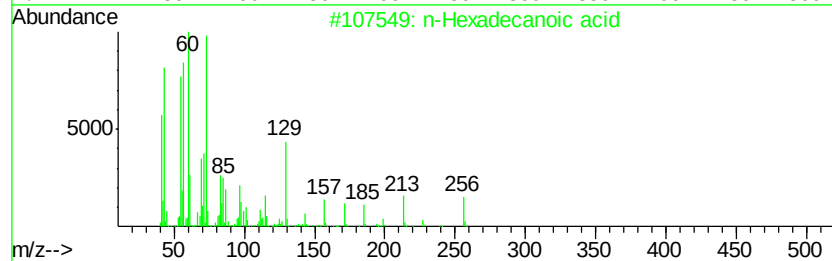
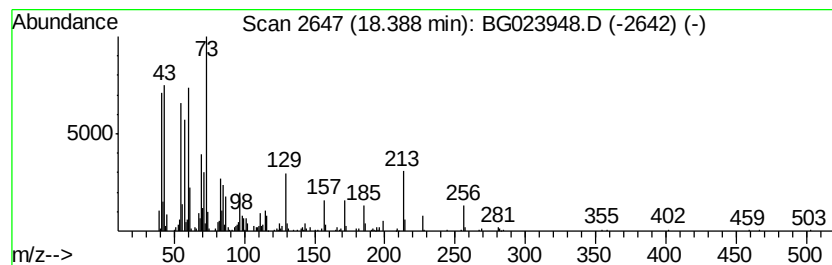
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TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.39	6.89 ng	463737	Phenanthrene-d10	17.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	89
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	59
4	Undecanoic acid	186	C11H22O2	000112-37-8	50
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	50



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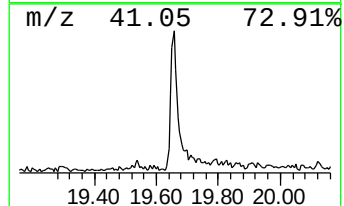
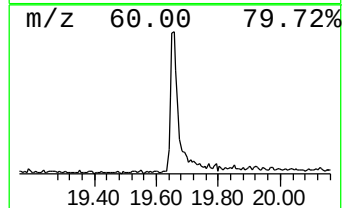
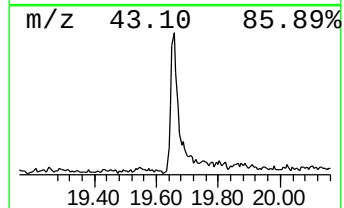
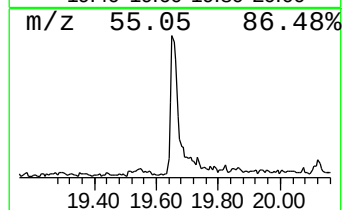
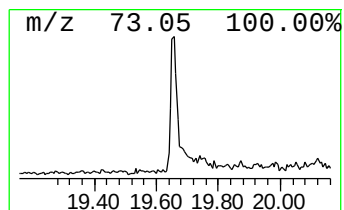
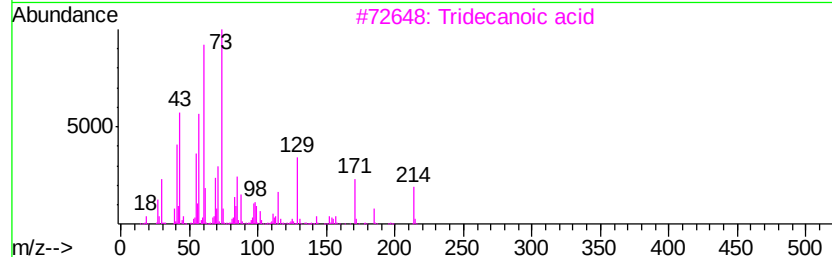
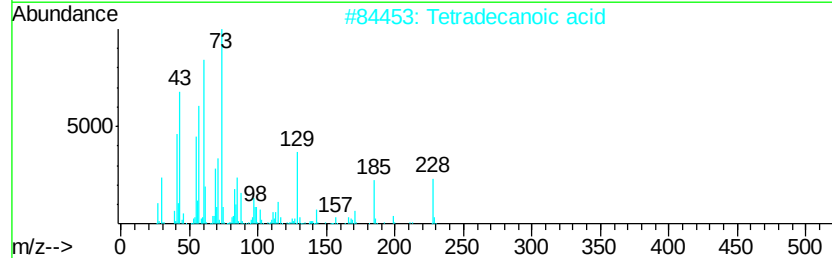
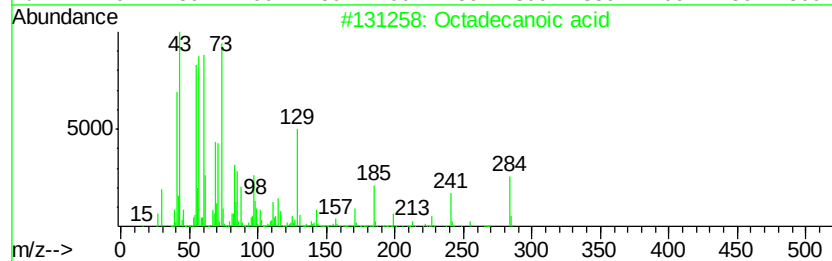
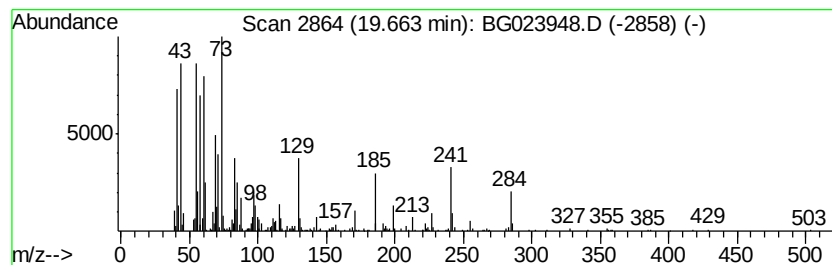
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.66	12.29 ng	827160	Phenanthrene-d10	17.52

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
3		Tridecanoic acid	214	C13H26O2	000638-53-9	58
4		n-Decanoic acid	172	C10H20O2	000334-48-5	58
5		Pentadecanoic acid	242	C15H30O2	001002-84-2	52



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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unknown5.16	5.16	11.7	ng	270860	1	8.09	463437	20.0
unknown7.63	7.63	70.3	ng	1629980	1	8.09	463437	20.0
n-Hexadecanoic acid	18.39	6.9	ng	463737	4	17.52	1345900	20.0
Octadecanoic acid	19.66	12.3	ng	827160	4	17.52	1345900	20.0