

Data Path : Z:\HPCHEM1\BNA G\DATA\BG080316\
 Data File : BG023433.D
 Acq On : 3 Aug 2016 20:03
 Operator : UM/SJ
 Sample : H4287-20
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB-63-14.0-15.0

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-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	2.992	21	26	41	rVB	3234124	4576575	44.27%	7.712%
2	5.183	392	399	407	rBV	586379	912121	8.82%	1.537%
3	5.659	473	480	495	rBV	2245590	3596535	34.79%	6.060%
4	7.275	747	755	769	rBV	2373184	4229046	40.91%	7.126%
5	7.645	810	818	828	rBV	2189999	3890406	37.63%	6.555%
6	8.115	891	898	906	rBV	354596	626411	6.06%	1.056%
7	8.444	945	954	962	rBV	1474962	2608855	25.24%	4.396%
8	9.296	1091	1099	1107	rBV	1413313	2527594	24.45%	4.259%
9	10.952	1371	1381	1389	rBV	548531	976225	9.44%	1.645%
10	13.396	1787	1797	1808	rBV	3749739	5880279	56.88%	9.908%
11	14.224	1931	1938	1945	rBV	1381907	2020405	19.54%	3.404%
12	14.782	2026	2033	2043	rVB2	960483	1548556	14.98%	2.609%
13	16.280	2281	2288	2302	rBV	3987618	6260771	60.56%	10.549%
14	16.468	2316	2320	2328	rBV2	91562	154467	1.49%	0.260%
15	17.543	2495	2503	2513	rBV	1439733	2297004	22.22%	3.870%
16	18.413	2646	2651	2662	rBV2	489399	741728	7.18%	1.250%
17	19.681	2862	2867	2880	rBV2	376801	562612	5.44%	0.948%
18	19.828	2888	2892	2899	rBV2	95032	125066	1.21%	0.211%
19	20.151	2941	2947	2954	rBV	7556119	10337348	100.00%	17.418%
20	20.827	3055	3062	3066	rBV2	140315	222853	2.16%	0.376%
21	21.467	3166	3171	3177	rBV9	51070	132386	1.28%	0.223%
22	21.855	3230	3237	3246	rBV2	1567560	2648157	25.62%	4.462%
23	25.233	3801	3812	3826	rBV2	851343	2471642	23.91%	4.165%

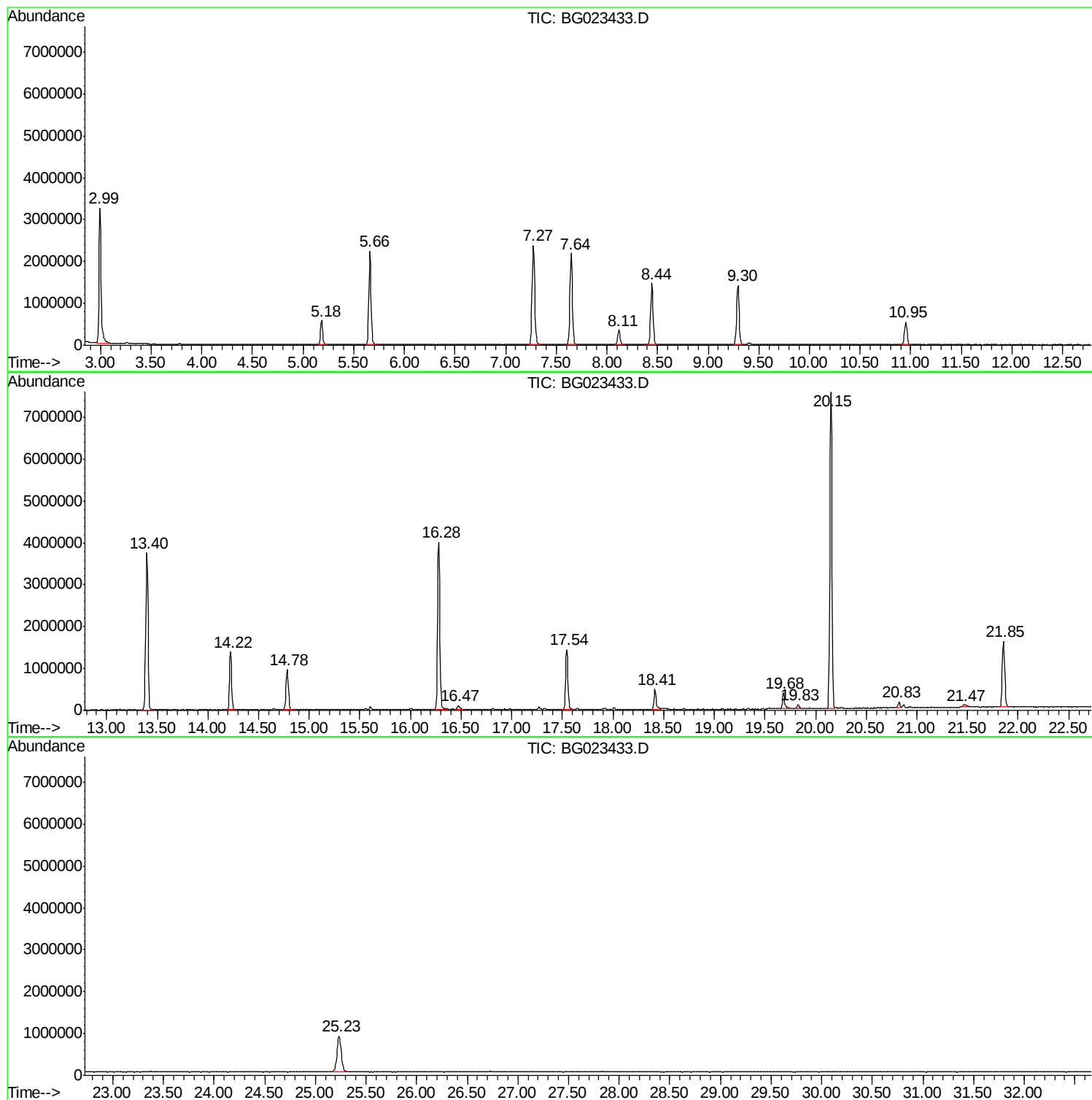
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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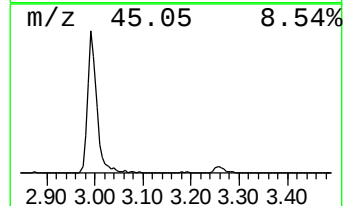
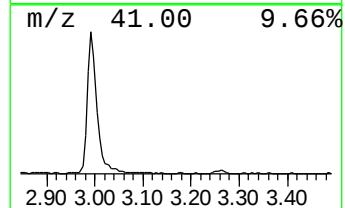
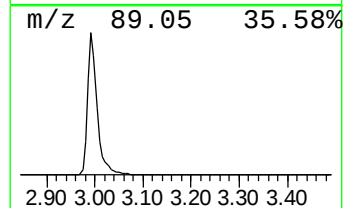
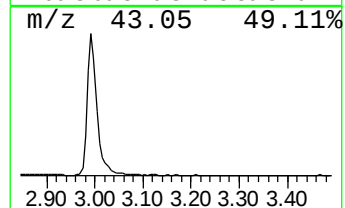
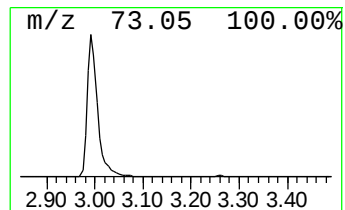
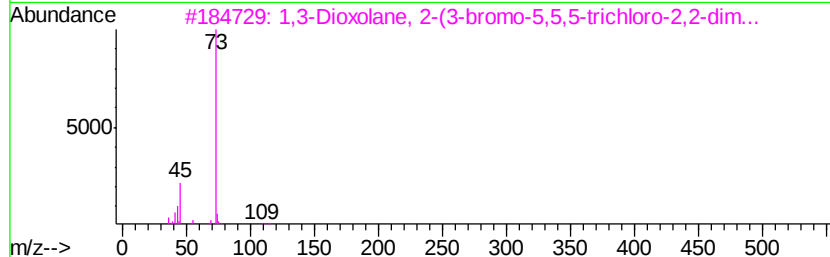
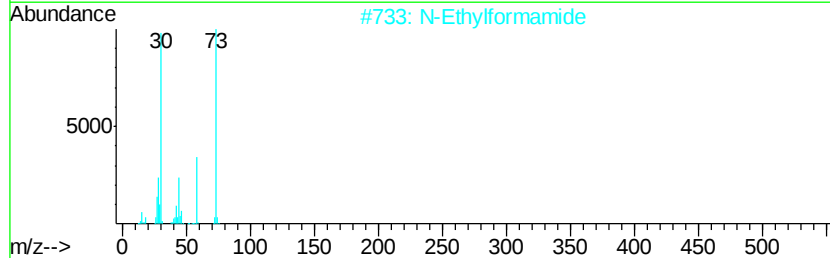
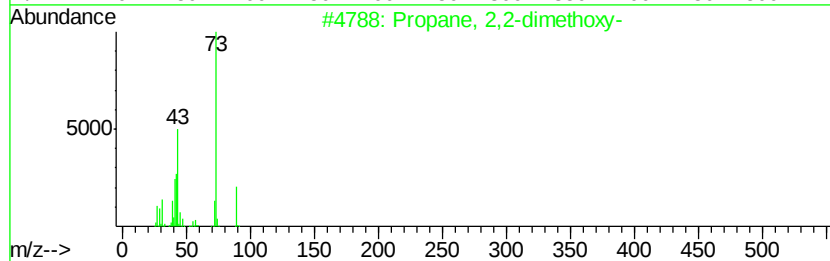
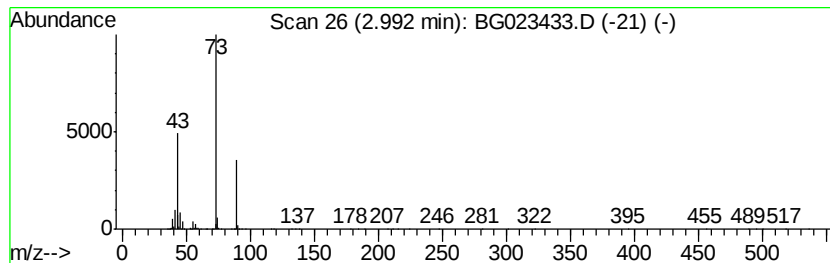
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG080116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown2.99 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.99	146.12 ng	4576580	1,4-Dichlorobenzene-d4	8.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	38
2		N-Ethylformamide	73	C3H7NO	000627-45-2	9
3		1,3-Dioxolane, 2-(3-bromo-5,5,5-...	352	C10H16BrCl3O2	1000115-31-4	9
4		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
5		1-Hexen-4-ol, 1-chloro-3,5-dimet...	162	C8H15ClO	100244-09-5	9



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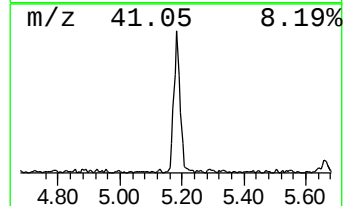
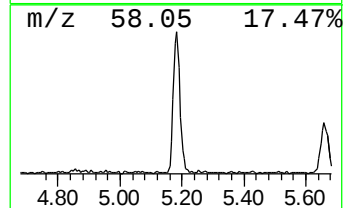
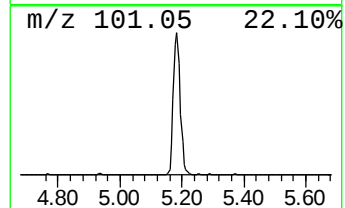
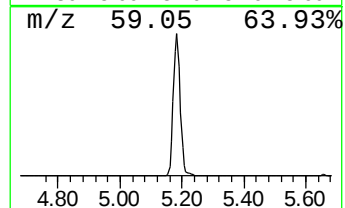
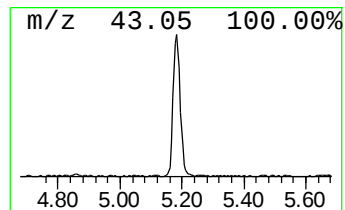
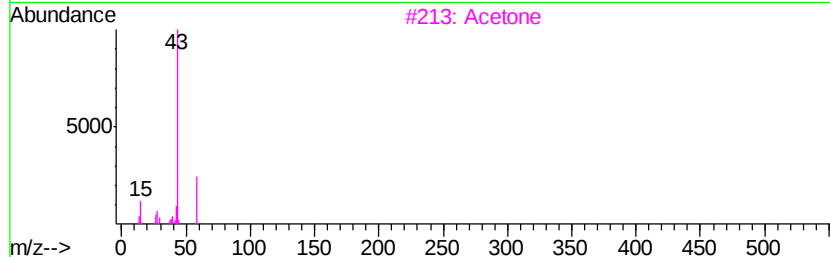
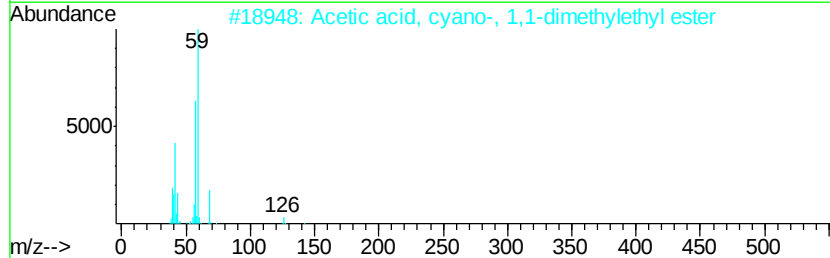
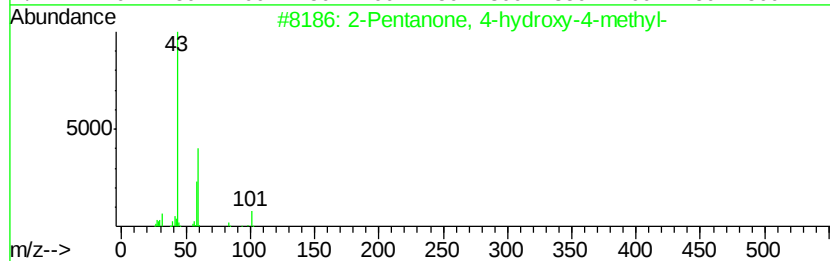
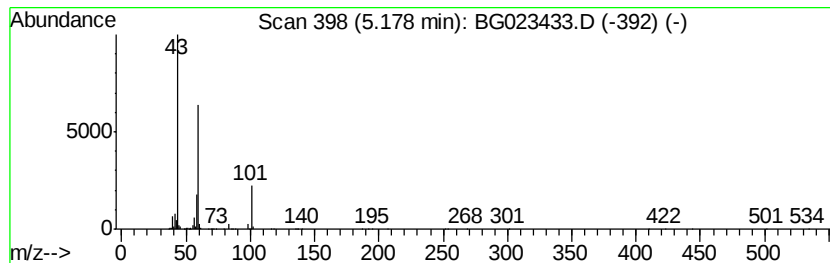
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.18	29.12 ng	912121	1,4-Dichlorobenzene-d4	8.12

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53	
2	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17	
3	Acetone	58	C3H6O	000067-64-1	9	
4	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	9	
5	2-Hexanol, 2,3-dimethyl-	130	C8H18O	019550-03-9	9	



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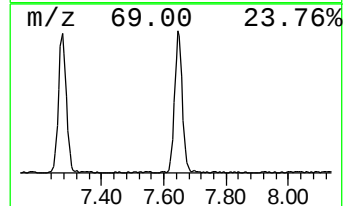
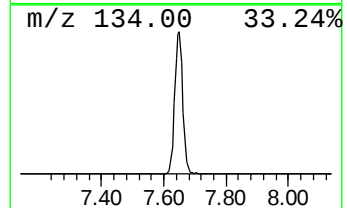
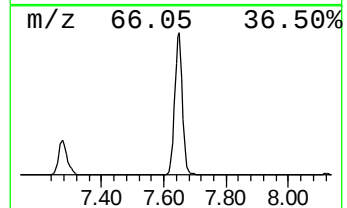
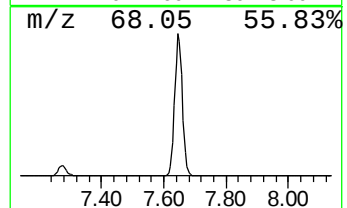
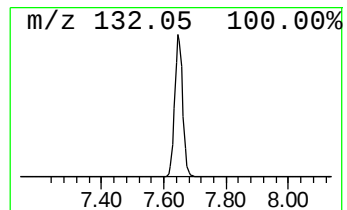
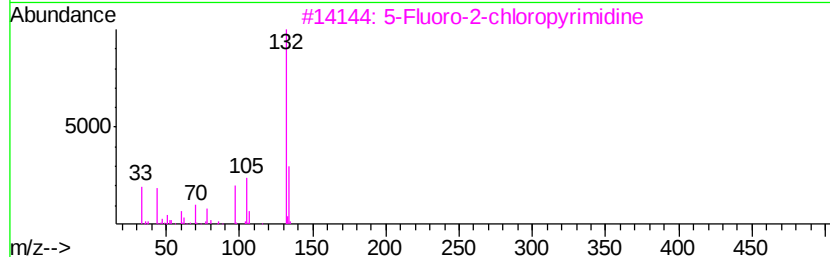
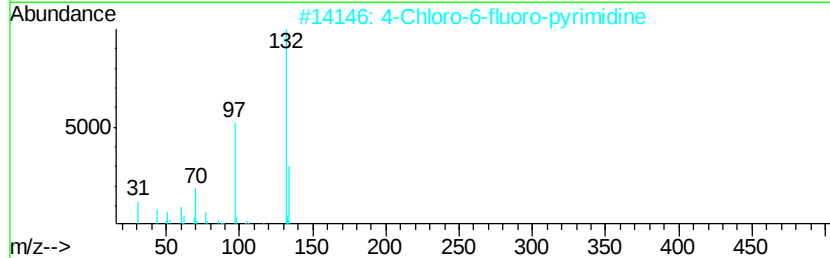
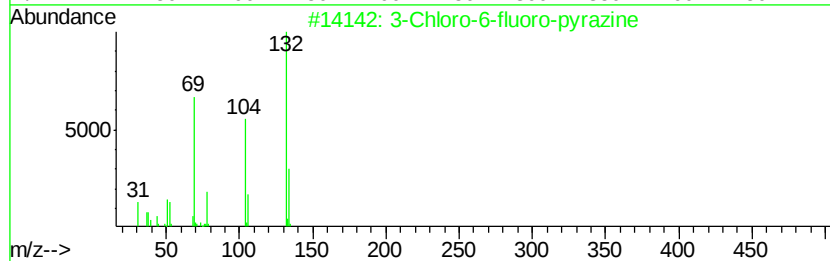
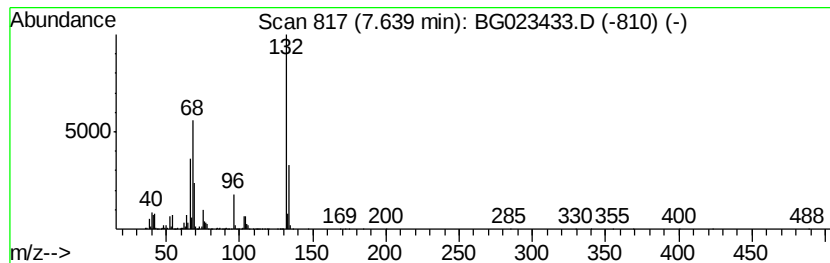
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Peak Number 3 unknown7.64 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.64	124.21 ng	3890410	1,4-Dichlorobenzene-d4	8.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4		2-Cyclohexen-1-one	96	C6H8O	000930-68-7	11
5		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10



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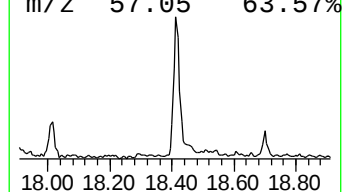
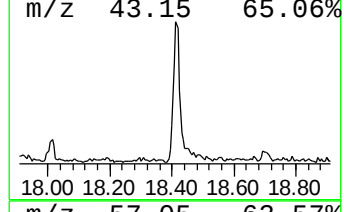
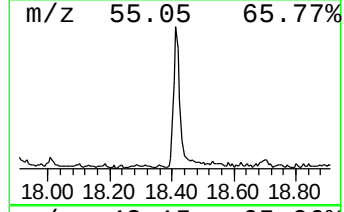
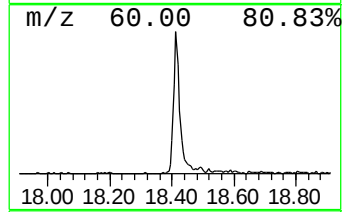
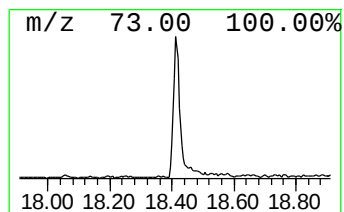
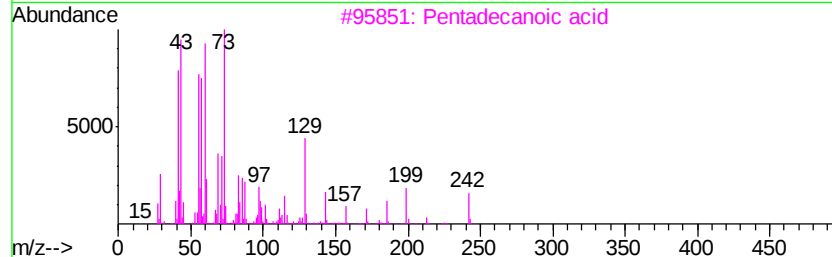
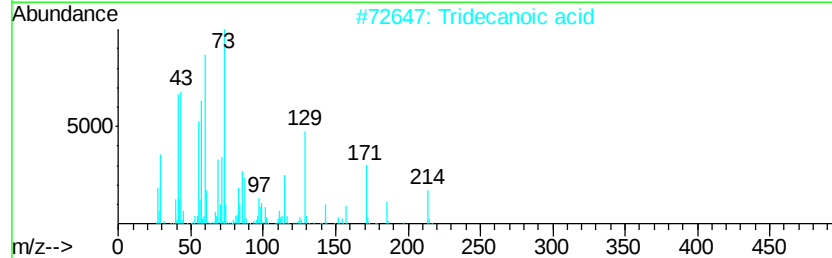
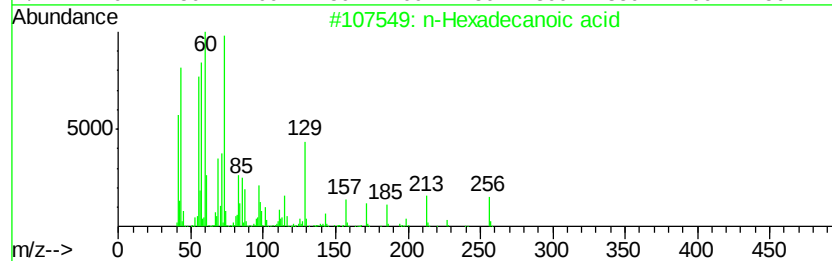
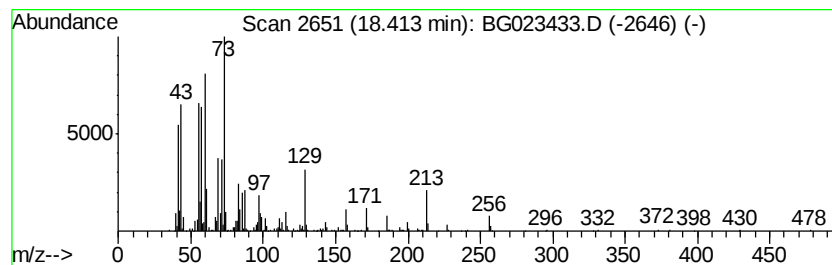
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.41	6.46 ng	741728	Phenanthrene-d10	17.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2		Tridecanoic acid	214	C13H26O2	000638-53-9	91
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5		Dodecanoic acid	200	C12H24O2	000143-07-7	64



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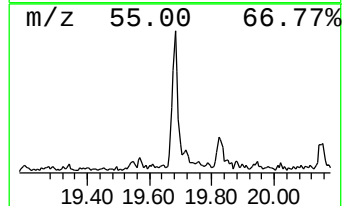
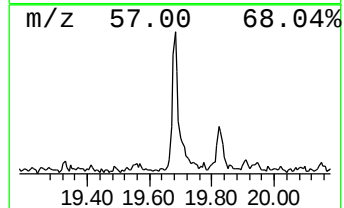
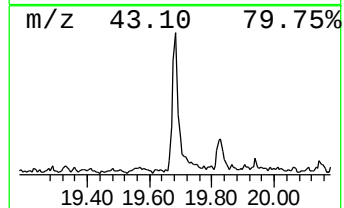
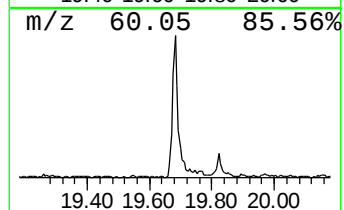
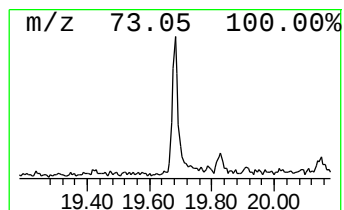
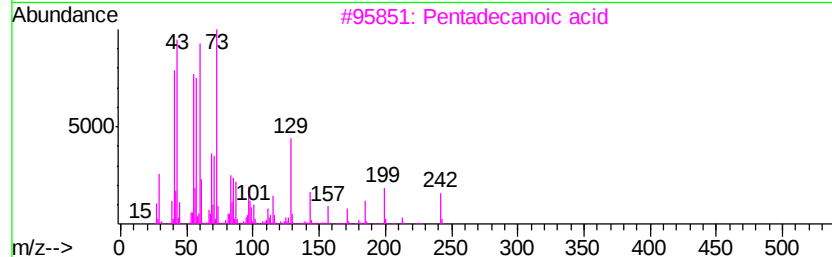
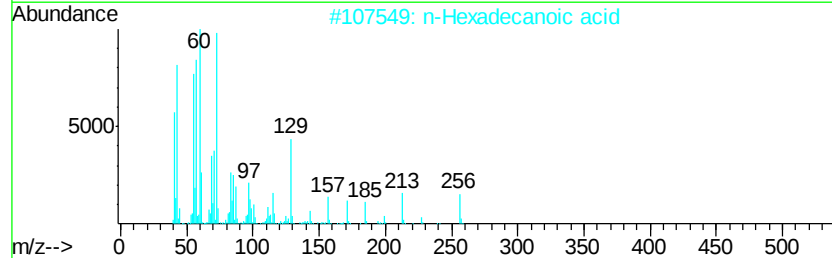
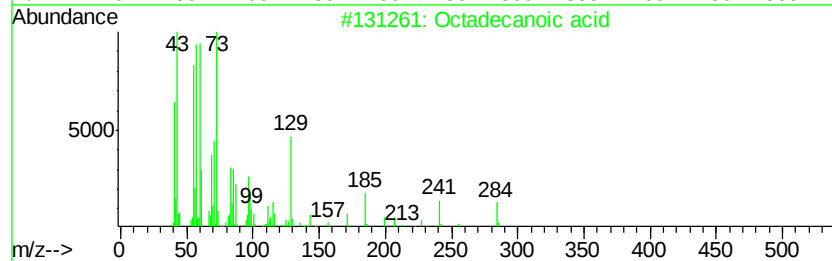
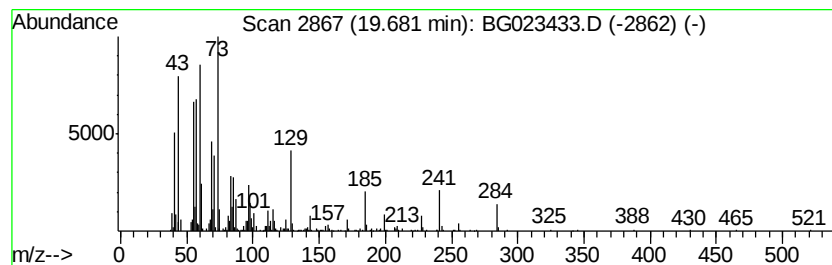
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.68	4.90 ng	562612	Phenanthrene-d10	17.54

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	98
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	86
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5		n-Decanoic acid	172	C10H20O2	000334-48-5	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown2.99	2.99	146.1	ng	4576580	1	8.12	626411	20.0
2-Pentanone, 4-hy...	5.18	29.1	ng	912121	1	8.12	626411	20.0
unknown7.64	7.64	124.2	ng	3890410	1	8.12	626411	20.0
n-Hexadecanoic acid	18.41	6.5	ng	741728	4	17.54	2297000	20.0
Octadecanoic acid	19.68	4.9	ng	562612	4	17.54	2297000	20.0