

Data Path : Z:\HPCHEM1\BNA G\DATA\BG080316\
 Data File : BG023432.D
 Acq On : 3 Aug 2016 19:23
 Operator : UM/SJ
 Sample : H4287-16
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB-62-14.0-15.0

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	2.990	22	26	46	rVB	4411420	6554023	73.40%	11.930%
2	5.181	393	399	410	rVB	551405	842713	9.44%	1.534%
3	5.657	473	480	490	rBV	2086829	3402726	38.11%	6.194%
4	7.272	748	755	769	rBV	2215512	3933499	44.05%	7.160%
5	7.648	812	819	829	rBV	2092351	3606502	40.39%	6.565%
6	8.118	890	899	905	rBV	333300	568408	6.37%	1.035%
7	8.441	943	954	962	rBV	1366764	2472897	27.69%	4.501%
8	9.293	1089	1099	1109	rBV	1313666	2375888	26.61%	4.325%
9	10.950	1373	1381	1388	rBV	480870	869520	9.74%	1.583%
10	13.399	1788	1798	1810	rBV	3316323	5225059	58.51%	9.511%
11	14.222	1932	1938	1944	rBV	1090455	1607955	18.01%	2.927%
12	14.780	2027	2033	2041	rBV3	869102	1403893	15.72%	2.555%
13	16.278	2281	2288	2302	rBV	3597813	5531970	61.95%	10.070%
14	16.466	2316	2320	2330	rBV2	63219	118776	1.33%	0.216%
15	17.541	2495	2503	2513	rBV2	1340376	2070488	23.19%	3.769%
16	17.905	2560	2565	2570	rBV6	48162	97753	1.09%	0.178%
17	18.410	2645	2651	2661	rBV	276829	418249	4.68%	0.761%
18	19.679	2863	2867	2872	rBV2	231096	304104	3.41%	0.554%
19	20.149	2941	2947	2954	rBV	6476389	8929565	100.00%	16.254%
20	21.853	3231	3237	3249	rVB2	1399770	2402380	26.90%	4.373%
21	25.236	3803	3813	3827	rVB2	720164	2200391	24.64%	4.005%

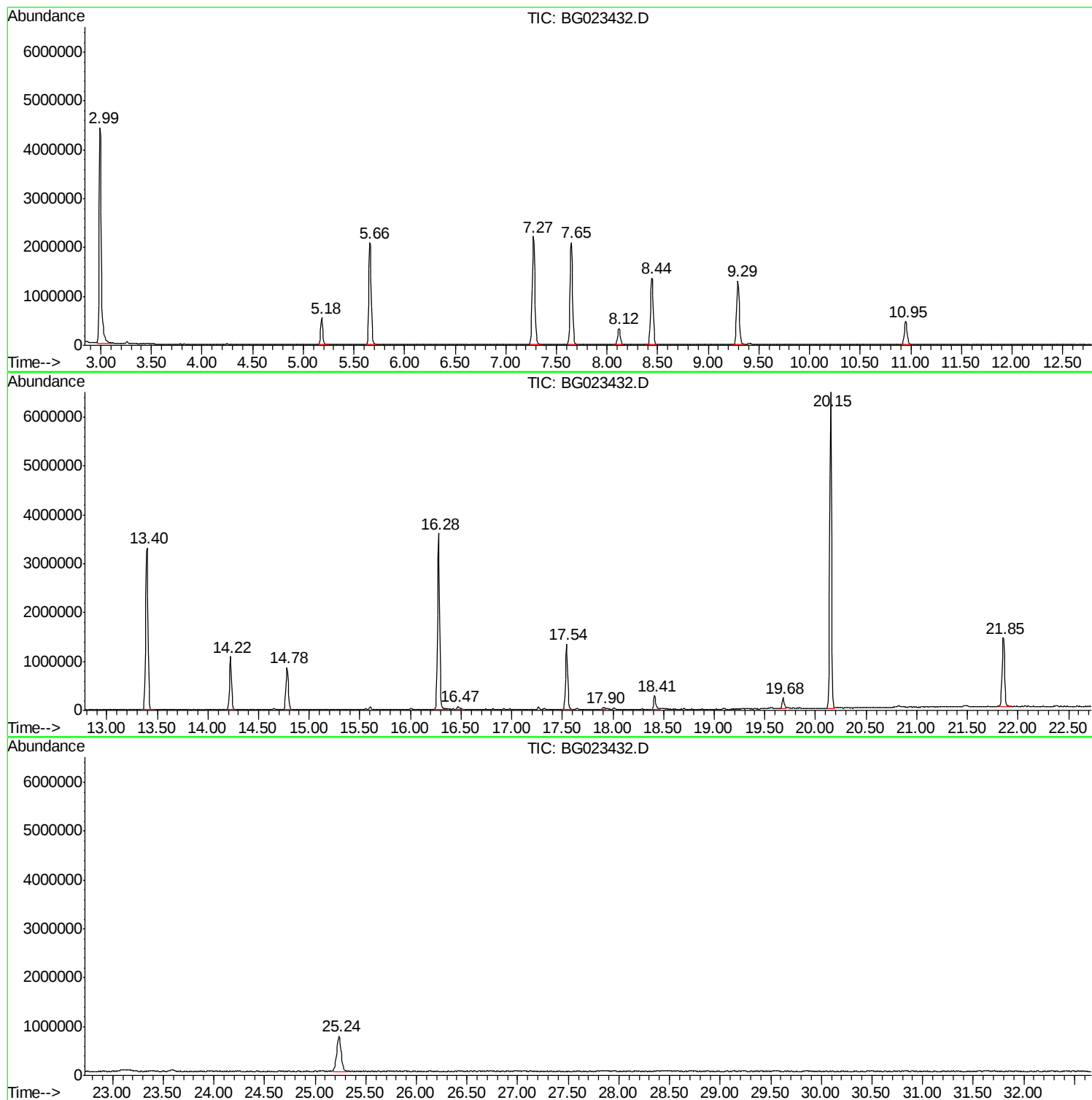
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG080116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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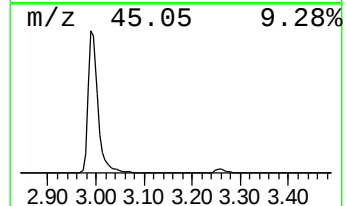
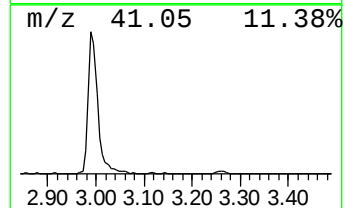
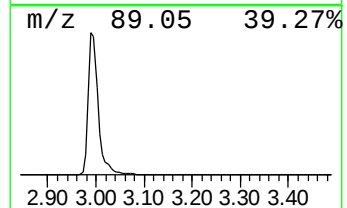
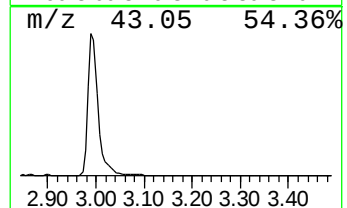
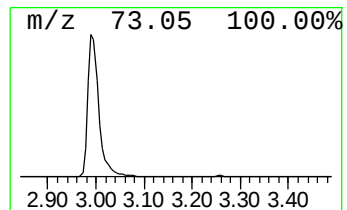
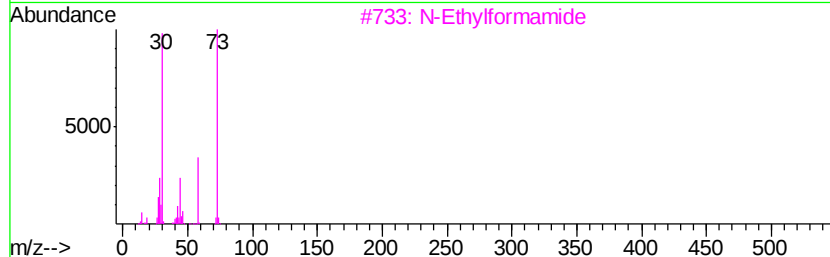
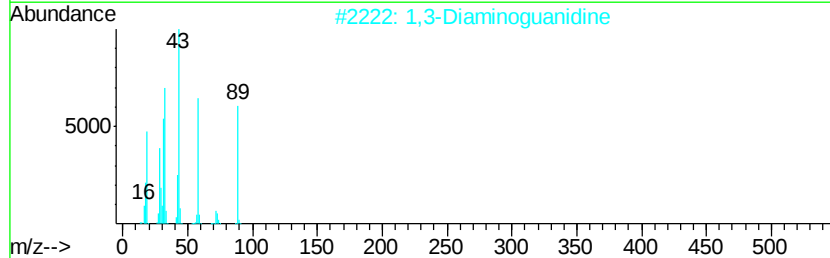
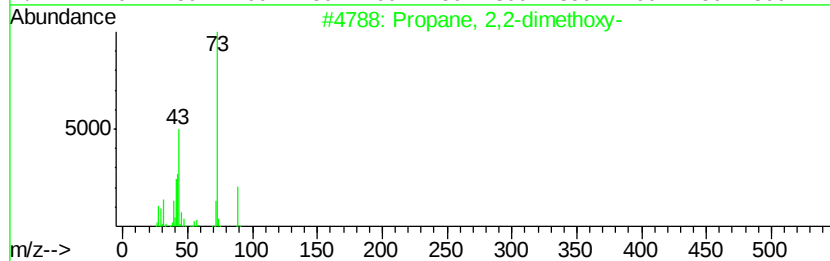
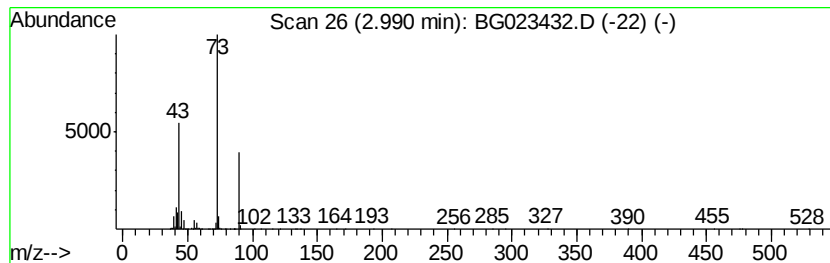
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.99	230.61 ng	6554020	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	64
2		1,3-Diaminoguanidine	89	CH7N5	004364-78-7	28
3		N-Ethylformamide	73	C3H7NO	000627-45-2	9
4		1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
5		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9



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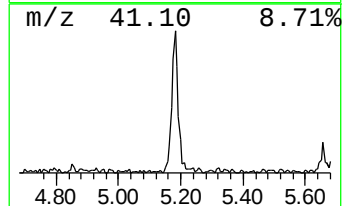
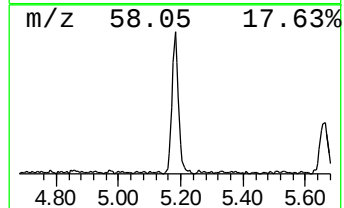
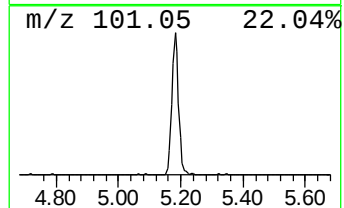
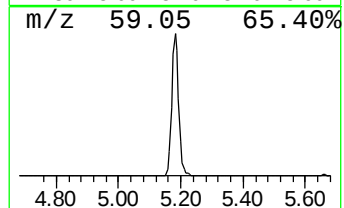
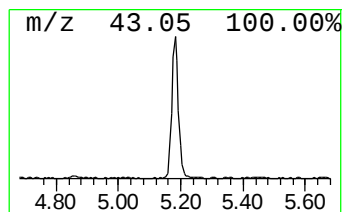
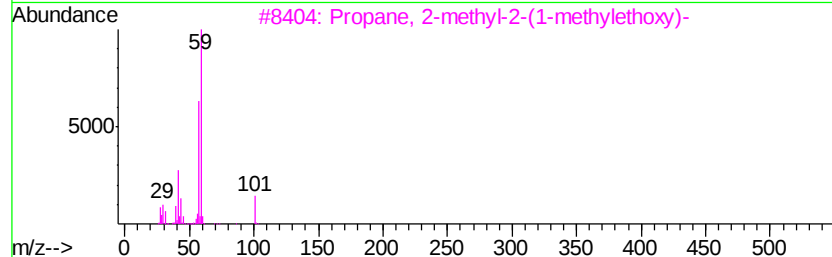
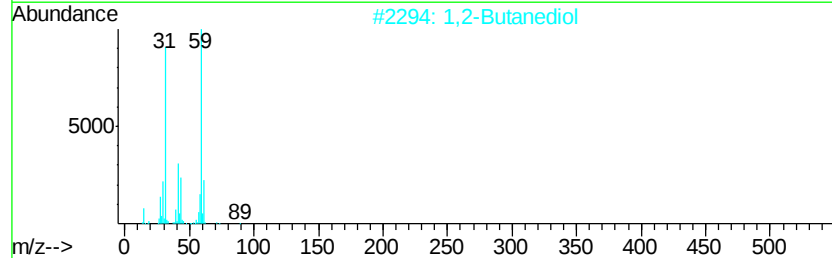
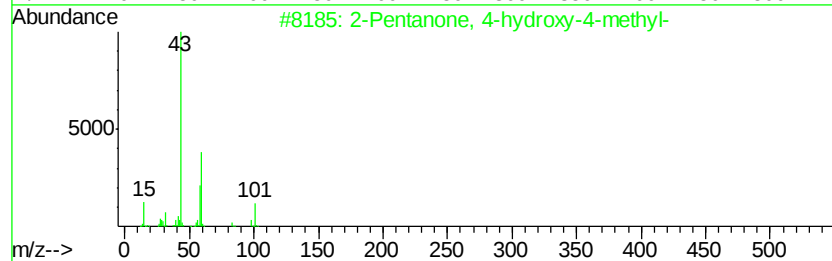
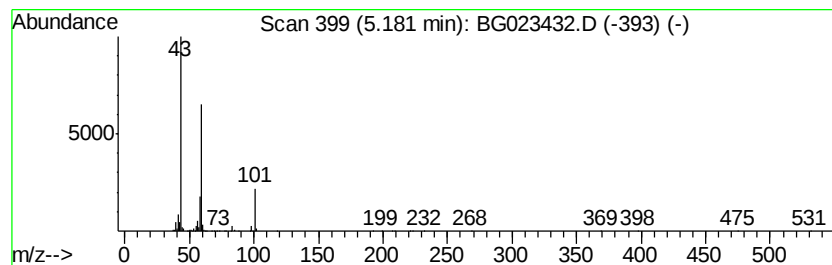
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.18	29.65 ng	842713	1,4-Dichlorobenzene-d4	8.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2		1,2-Butanediol	90	C4H10O2	000584-03-2	25
3		Propane, 2-methyl-2-(1-methylethyl)-	116	C7H16O	017348-59-3	23
4		Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	23
5		Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	17



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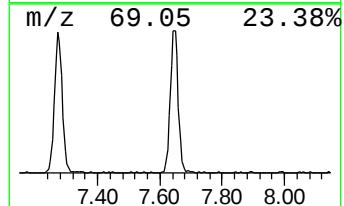
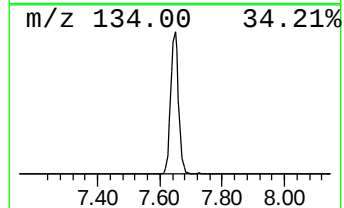
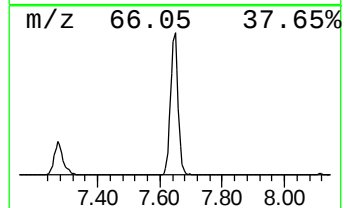
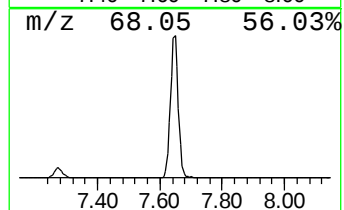
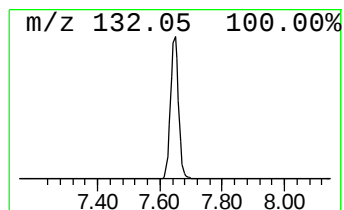
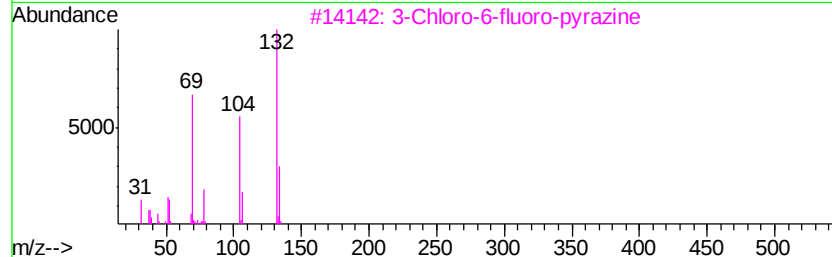
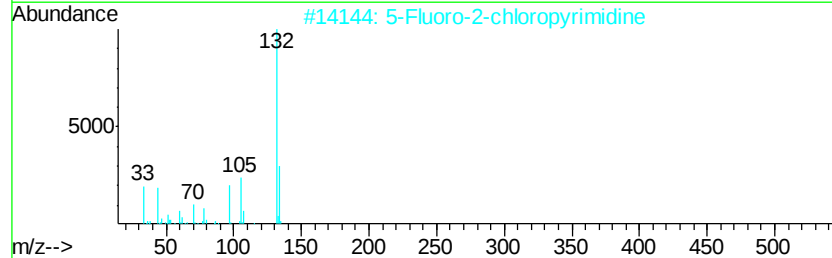
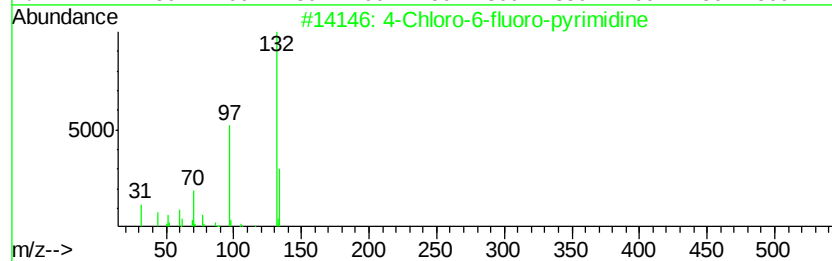
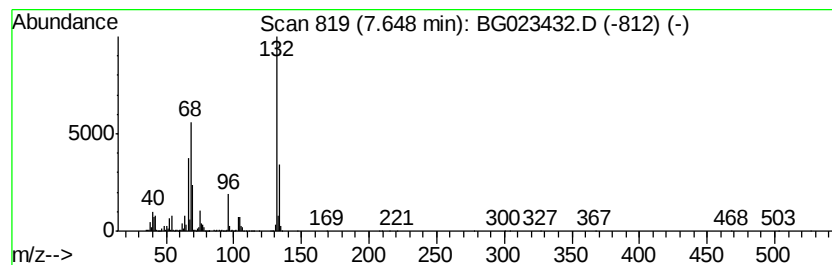
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Peak Number 3 unknown7.65 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.65	126.90 ng	3606500	1,4-Dichlorobenzene-d4	8.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	27
3		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
4		5-Aminoindole	132	C8H8N2	005192-03-0	22
5		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22



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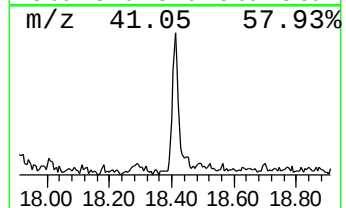
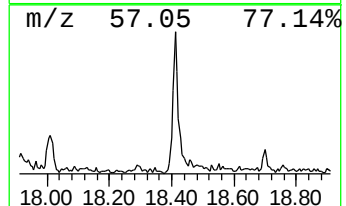
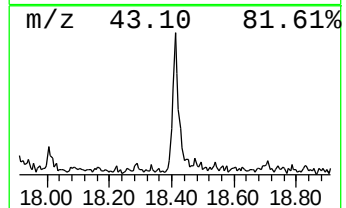
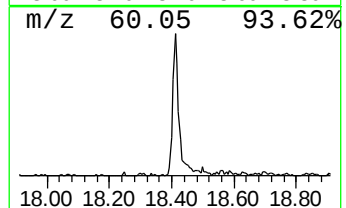
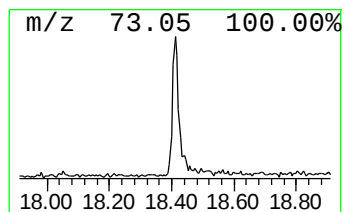
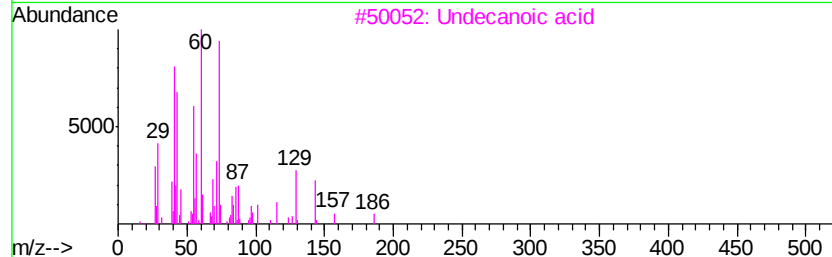
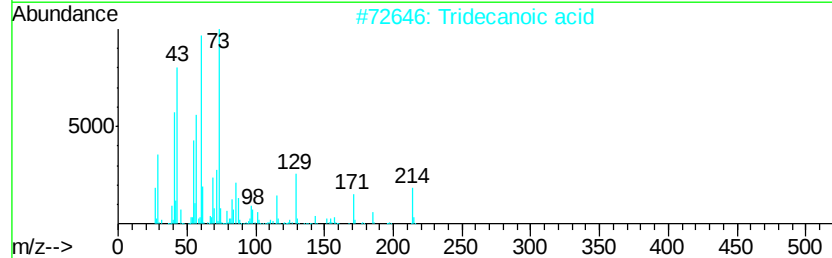
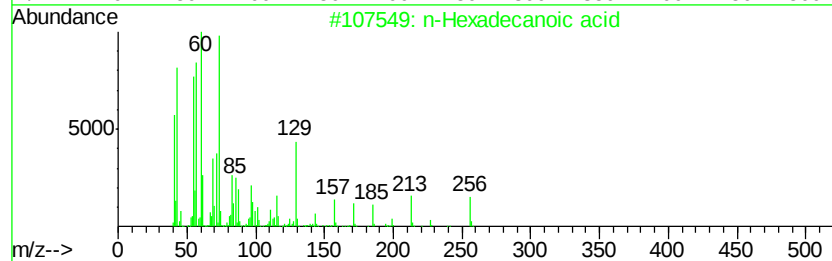
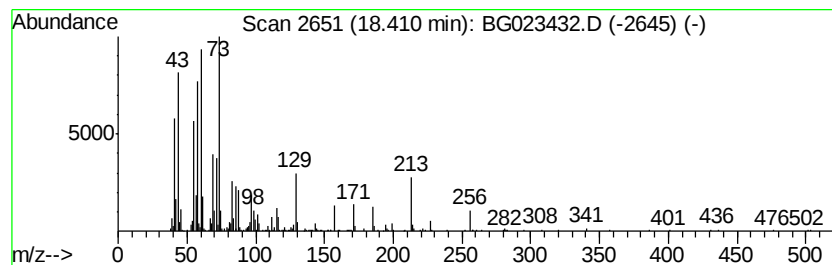
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.41	4.04 ng	418249	Phenanthrene-d10	17.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
2	Tridecanoic acid	214	C13H26O2	000638-53-9	76
3	Undecanoic acid	186	C11H22O2	000112-37-8	64
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	62



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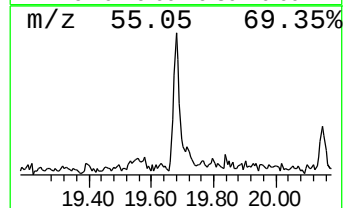
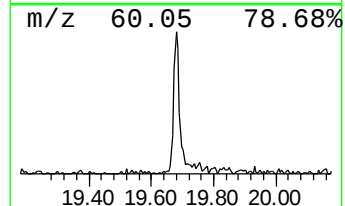
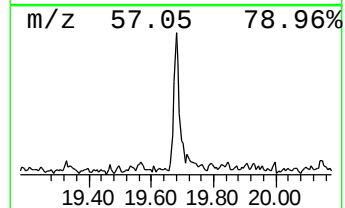
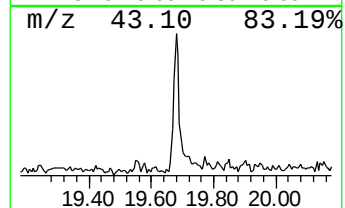
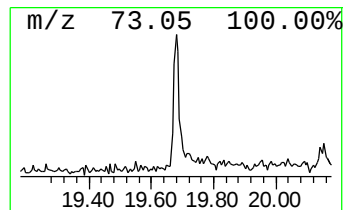
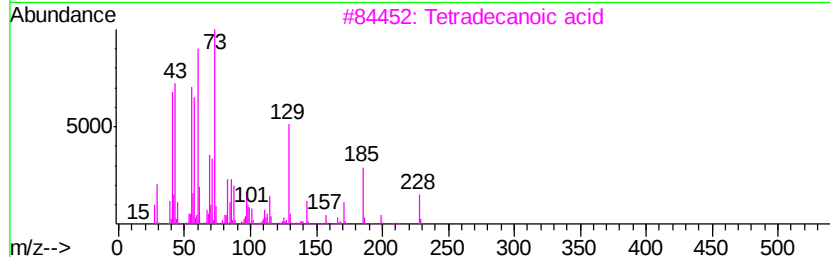
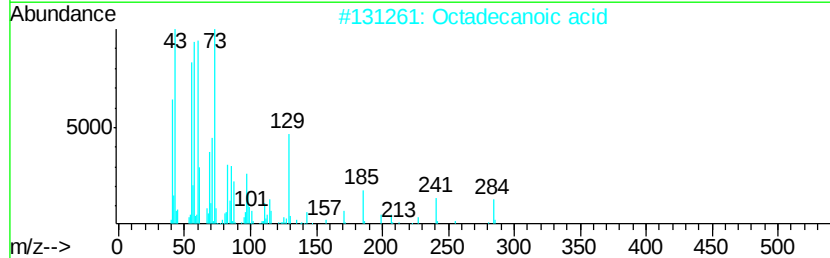
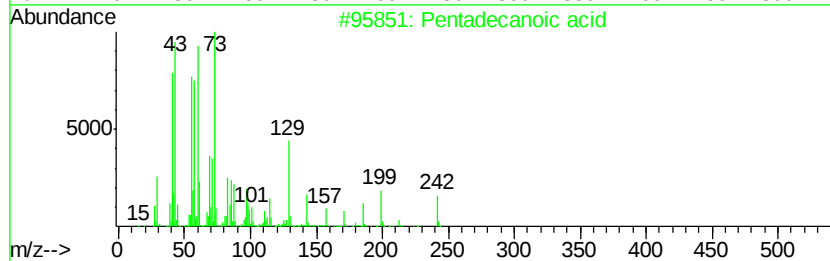
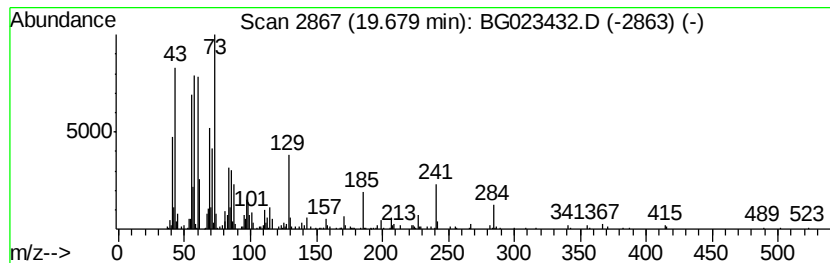
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Pentadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.68	2.94 ng	304104	Phenanthrene-d10	17.54

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	93	
2	Octadecanoic acid	284	C18H36O2	000057-11-4	92	
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	81	
4	Undecanoic acid	186	C11H22O2	000112-37-8	59	
5	Tridecanoic acid	214	C13H26O2	000638-53-9	53	



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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
Propane, 2,2-dime...	2.99	230.6	ng	6554020	1	8.12	568408	20.0
2-Pentanone, 4-hy...	5.18	29.6	ng	842713	1	8.12	568408	20.0
unknown7.65	7.65	126.9	ng	3606500	1	8.12	568408	20.0
n-Hexadecanoic acid	18.41	4.0	ng	418249	4	17.54	2070490	20.0
Pentadecanoic acid	19.68	2.9	ng	304104	4	17.54	2070490	20.0