

Data Path : Z:\HPCHEM1\BNA G\DATA\BG110116\
 Data File : BG024626.D
 Acq On : 2 Nov 2016 13:26
 Operator : UM/SJ
 Sample : H5491-06
 Misc :
 ALS Vial : 33 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB-DUP-102816

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-BG102516.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	3.131	44	50	70	rVB	9262547	20237734	100.00%	24.818%
2	5.335	417	425	432	rBV	613058	1015816	5.02%	1.246%
3	5.799	497	504	513	rBV	2799742	4911921	24.27%	6.023%
4	7.409	770	778	790	rBV	2970517	5454713	26.95%	6.689%
5	7.796	836	844	852	rBV	2794854	5164432	25.52%	6.333%
6	8.266	916	924	935	rBV2	460544	873466	4.32%	1.071%
7	8.596	972	980	988	rBV	2061202	3722356	18.39%	4.565%
8	9.442	1116	1124	1134	rBV	1824494	3381436	16.71%	4.147%
9	11.093	1397	1405	1414	rBV2	599075	1123132	5.55%	1.377%
10	13.507	1807	1816	1827	rBV	4138677	6749261	33.35%	8.277%
11	14.324	1947	1955	1961	rBV	1049124	1631694	8.06%	2.001%
12	14.882	2041	2050	2060	rVB2	970487	1590749	7.86%	1.951%
13	16.369	2295	2303	2316	rBV	4190830	6775722	33.48%	8.309%
14	17.626	2510	2517	2524	rBV	1273516	2012441	9.94%	2.468%
15	18.472	2656	2661	2668	rBV2	222947	352757	1.74%	0.433%
16	20.205	2950	2956	2965	rVB	7646491	10387429	51.33%	12.738%
17	21.498	3171	3176	3186	rBV3	229873	467152	2.31%	0.573%
18	21.921	3240	3248	3256	rVB	1555996	2811213	13.89%	3.447%
19	25.352	3818	3832	3848	rVB	946792	2882709	14.24%	3.535%

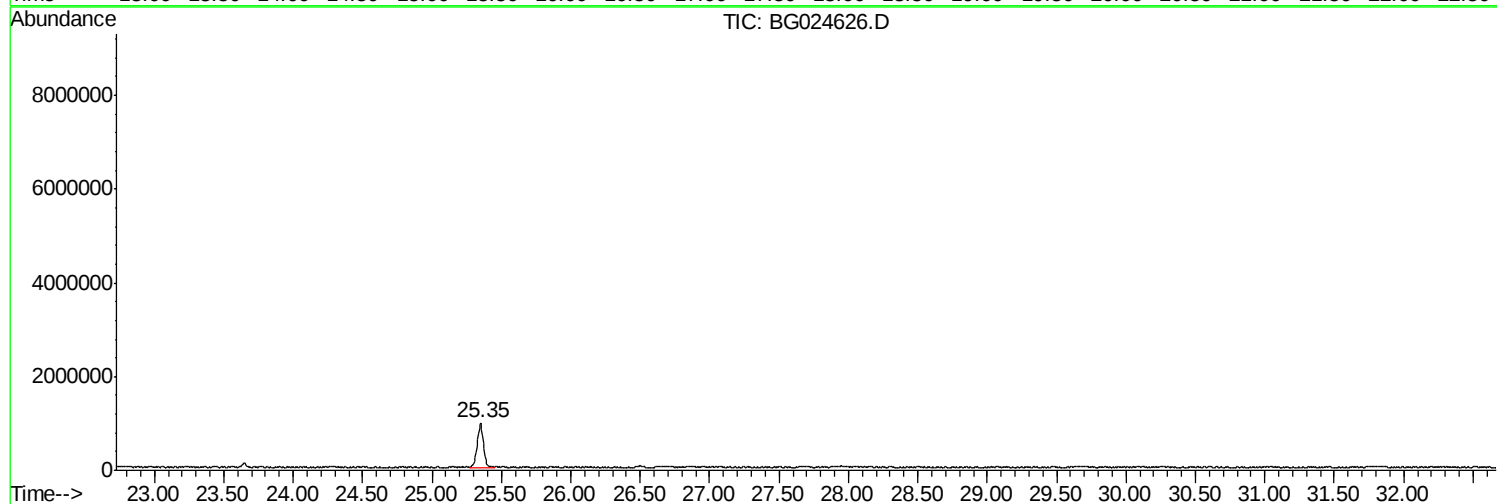
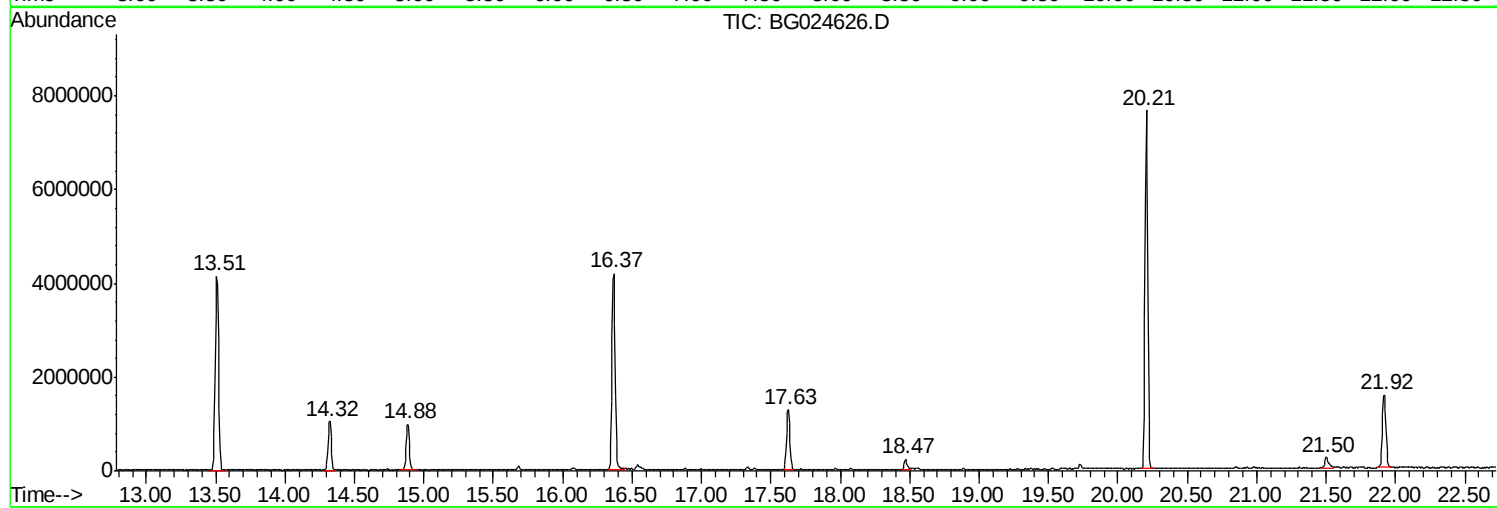
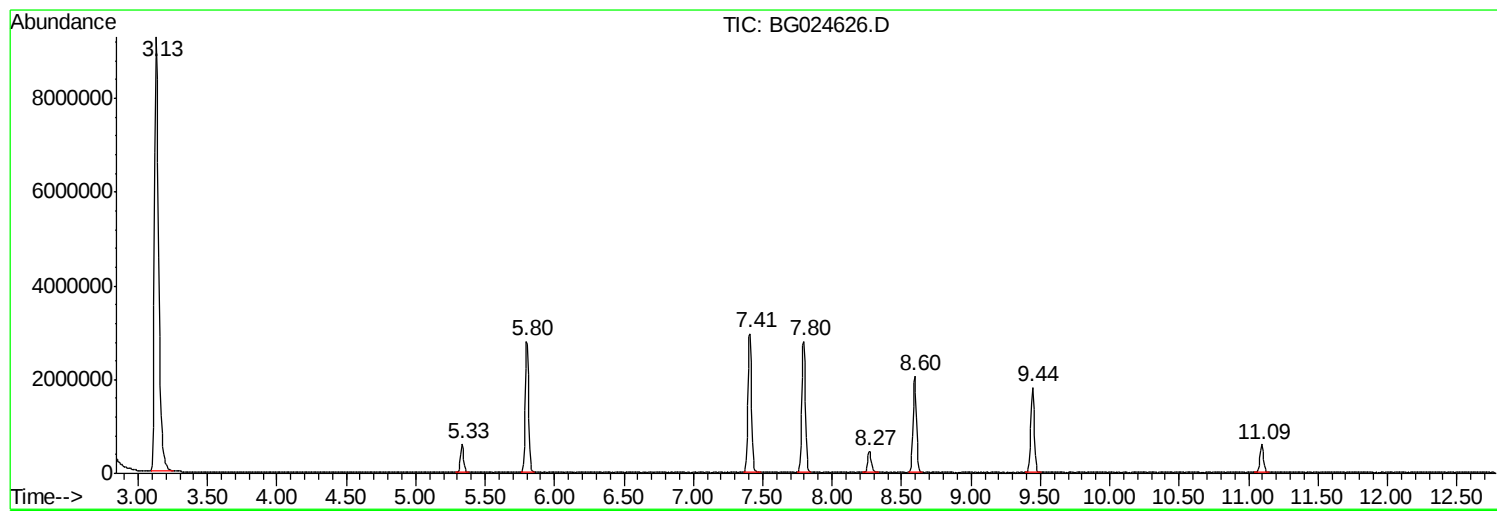
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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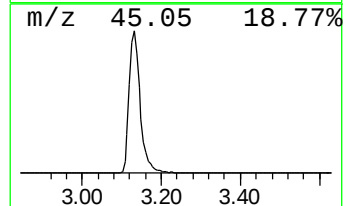
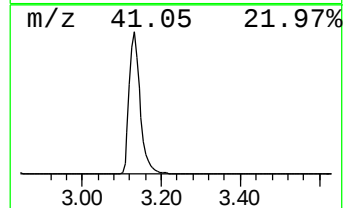
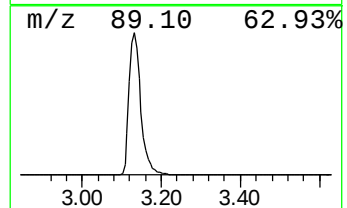
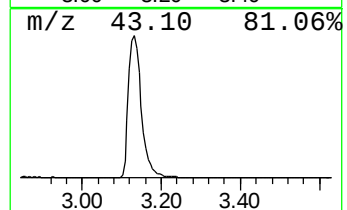
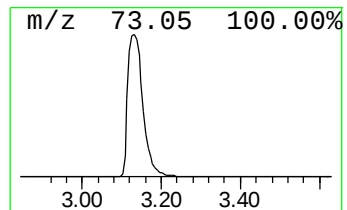
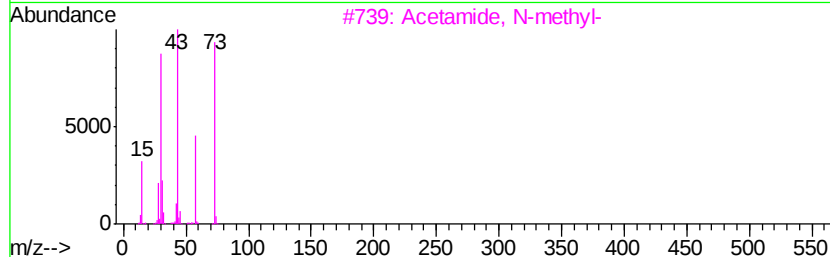
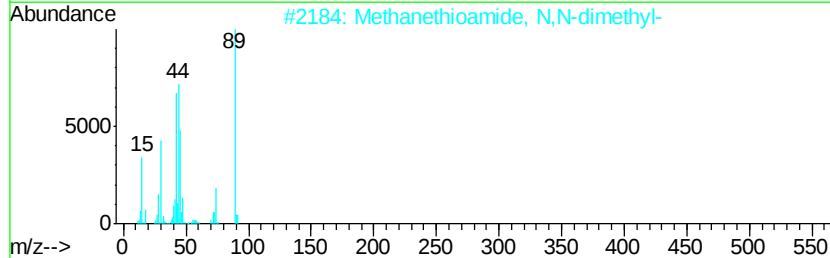
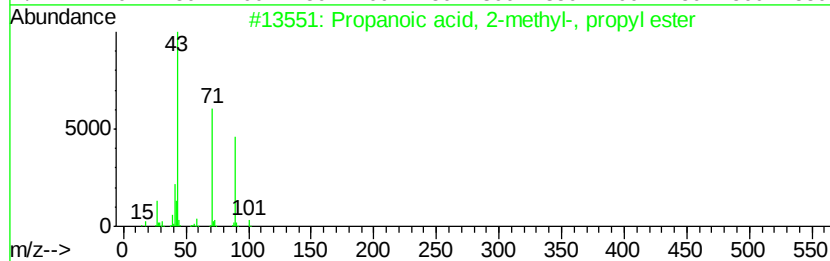
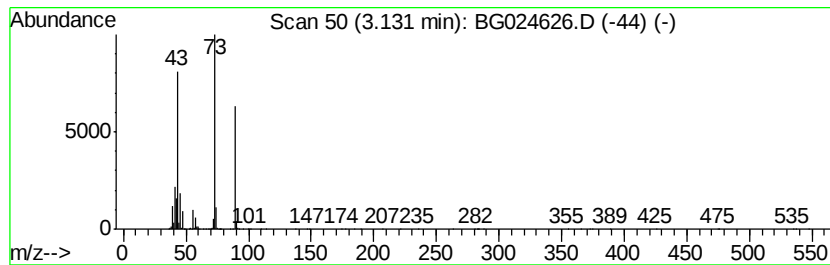
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown3.13 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.13	463.39 ng	20237700	1,4-Dichlorobenzene-d4	8.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propanoic acid, 2-methyl-, propyl...	130	C7H14O2	000644-49-5	47
2		Methanethioamide, N,N-dimethyl-	89	C3H7NS	000758-16-7	37
3		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	25
4		1-Hepten-4-ol	114	C7H14O	003521-91-3	23
5		Thiazole, tetrahydro-	89	C3H7NS	000504-78-9	9



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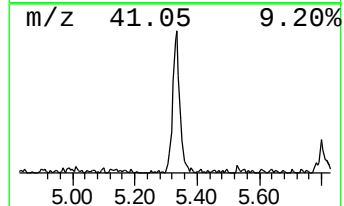
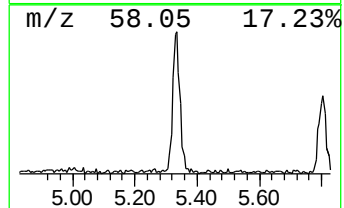
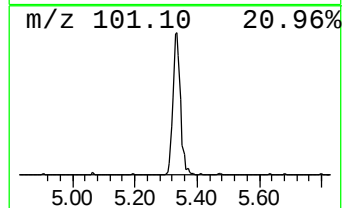
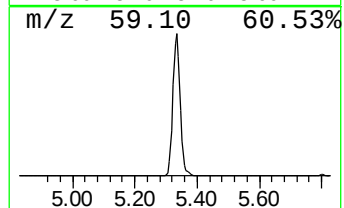
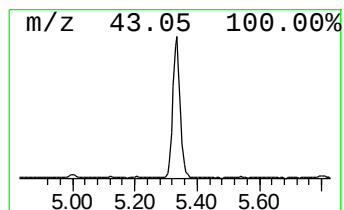
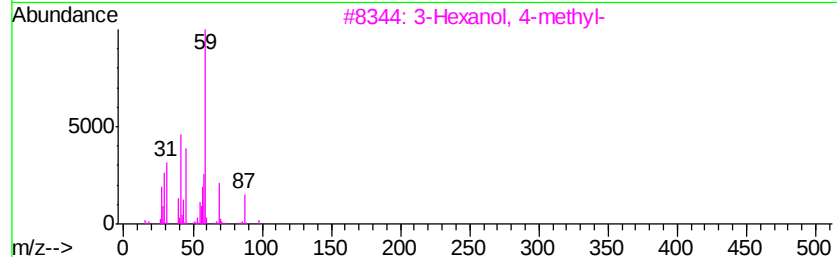
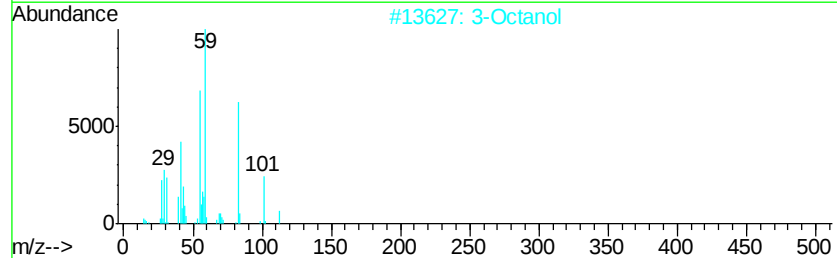
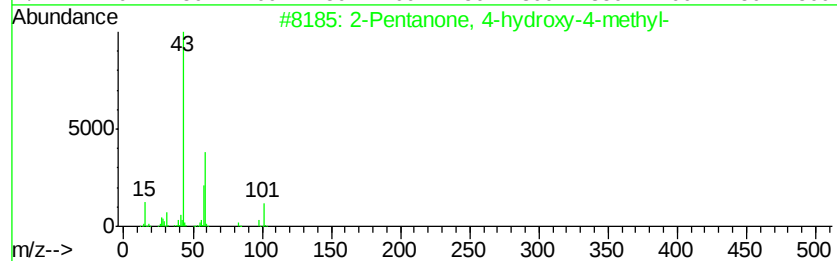
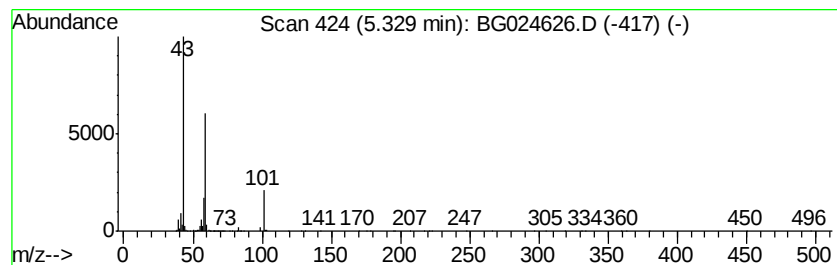
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.33	23.26 ng	1015820	1,4-Dichlorobenzene-d4	8.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2		3-Octanol	130	C8H18O	000589-98-0	33
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
5		Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	17



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Instrument :
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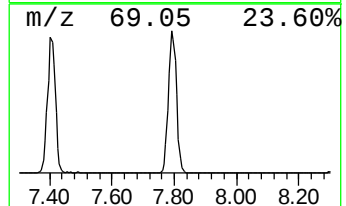
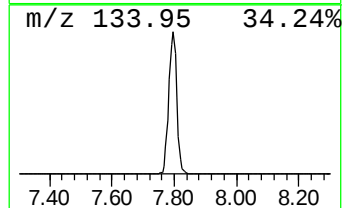
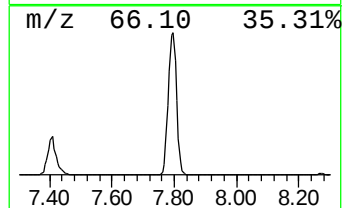
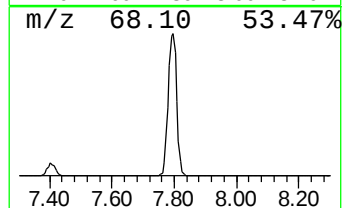
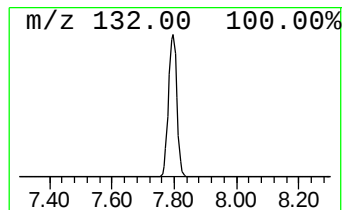
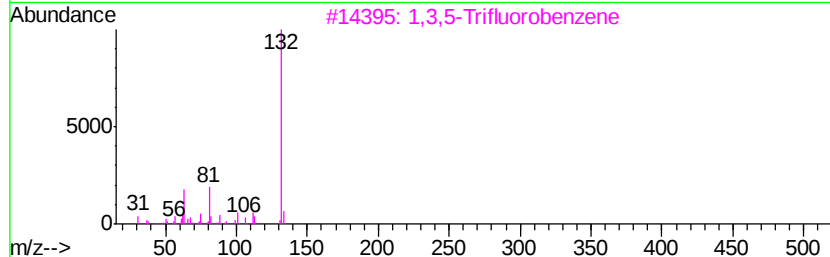
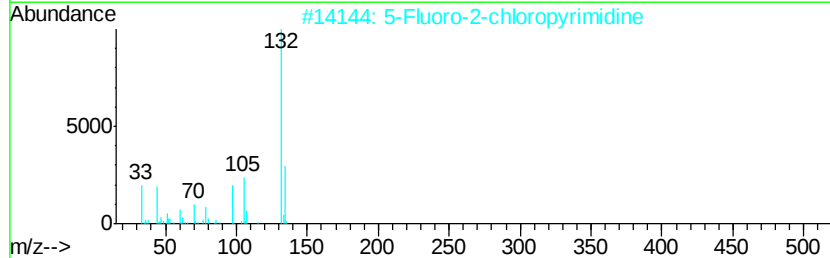
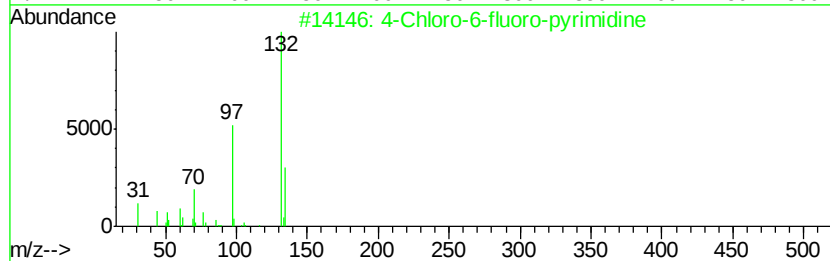
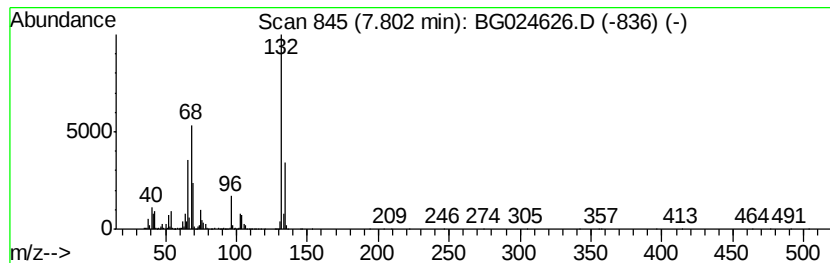
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Peak Number 3 unknown7.80 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.80	118.25 ng	5164430	1,4-Dichlorobenzene-d4	8.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	14
3		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	10
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
5		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	10



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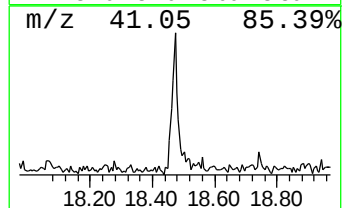
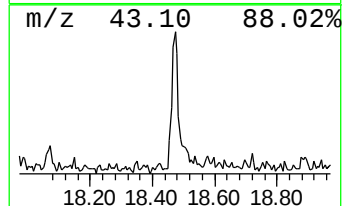
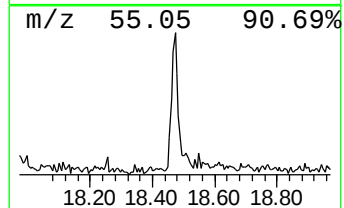
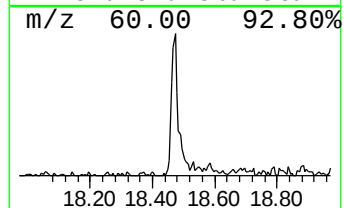
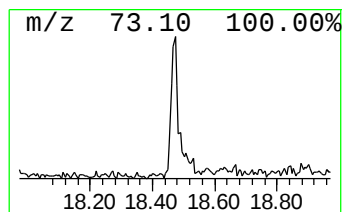
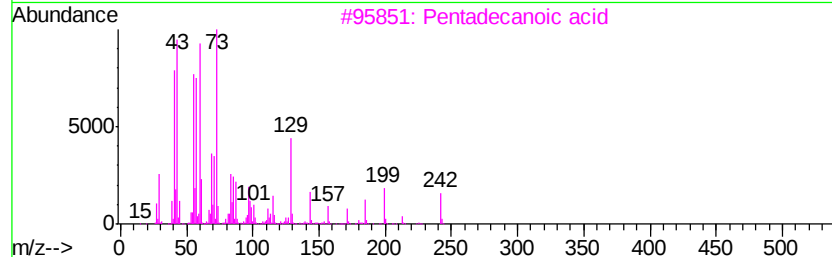
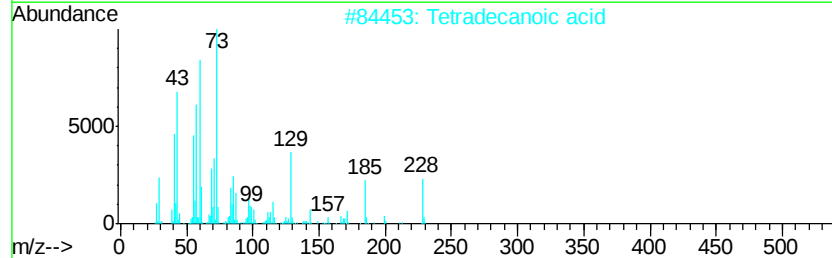
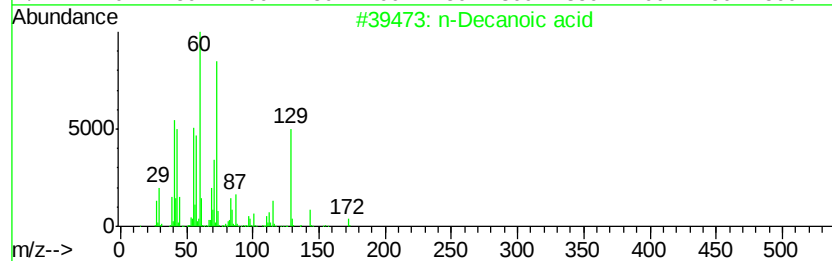
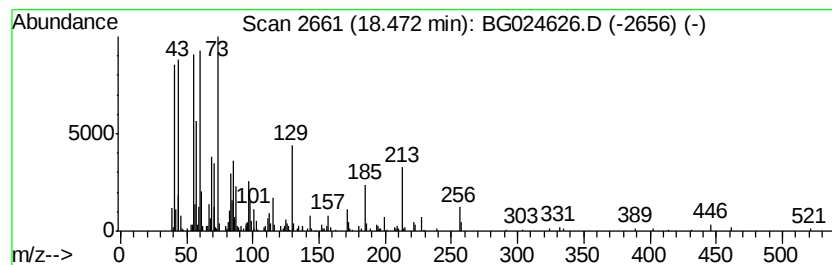
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Peak Number 5 n-Decanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.47	3.51 ng	352757	Phenanthrene-d10	17.63

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Decanoic acid	172	C10H20O2	000334-48-5	90
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	80
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	72
4		Dodecanoic acid	200	C12H24O2	000143-07-7	64
5		Tridecanoic acid	214	C13H26O2	000638-53-9	59



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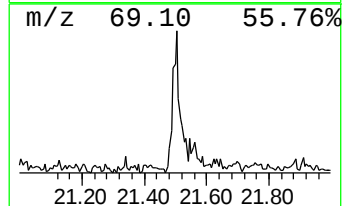
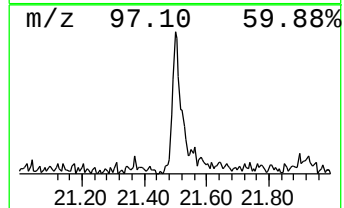
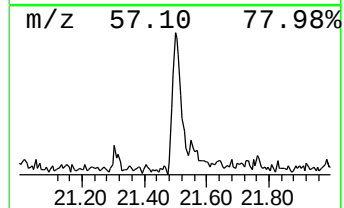
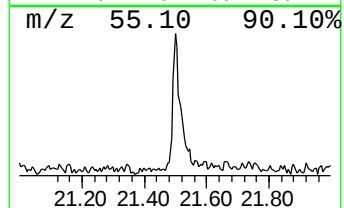
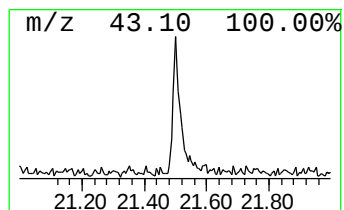
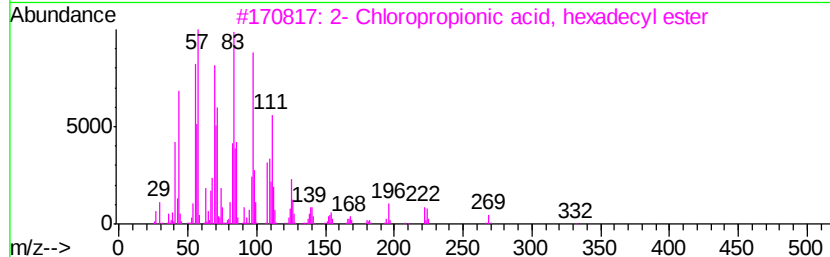
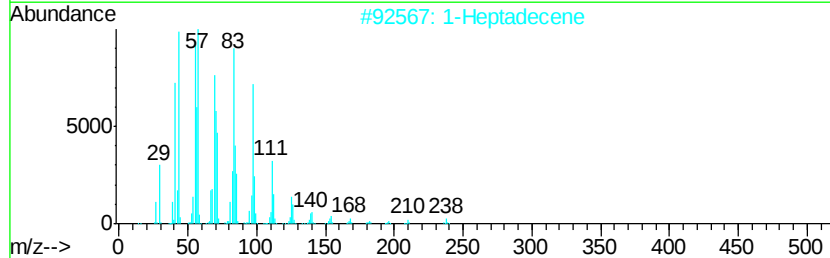
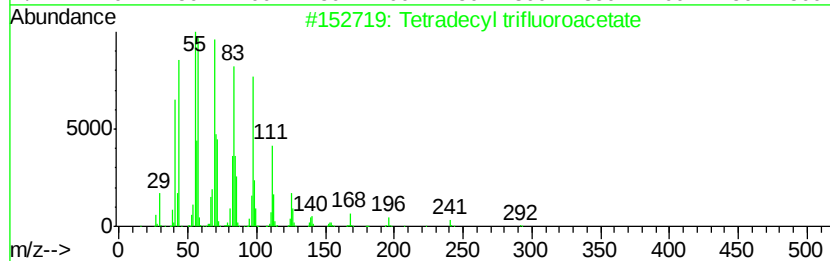
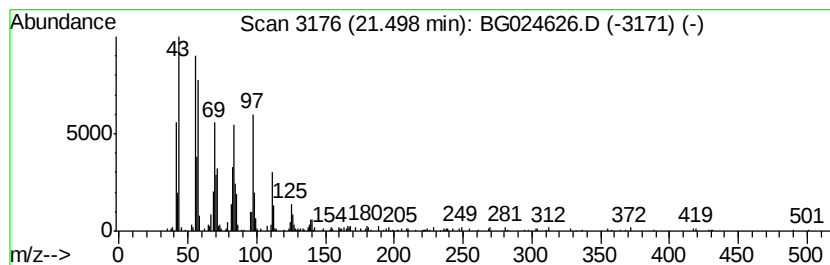
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Peak Number 6 Tetradecyl trifluoroacetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.50	3.32 ng	467152	Chrysene-d12	21.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	94
2		1-Heptadecene	238	C17H34	006765-39-5	93
3		2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	93
4		Acetic acid, chloro-, octadecyl ...	346	C20H39ClO2	005348-82-3	91
5		n-Pentadecanol	228	C15H32O	000629-76-5	91



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown3.13	3.13	463.4	ng	20237700	1	8.27	873466	20.0
2-Pentanone, 4-hy...	5.33	23.3	ng	1015820	1	8.27	873466	20.0
unknown7.80	7.80	118.3	ng	5164430	1	8.27	873466	20.0
n-Decanoic acid	18.47	3.5	ng	352757	4	17.63	2012440	20.0
Tetradecyl triflu...	21.50	3.3	ng	467152	5	21.92	2811210	20.0