

Data Path : Z:\HPCHEM1\BNA G\DATA\BG070816\
 Data File : BG022930.D
 Acq On : 8 Jul 2016 14:04
 Operator : UM/SJ
 Sample : H3876-07
 Misc :
 ALS Vial : 30 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 4-A-LOCATION-4-0-5FT

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-BG070816.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	3.039	31	34	44	rVB	192452	257753	3.84%	0.646%
2	5.225	400	406	411	rBV	88365	133054	1.98%	0.333%
3	5.695	478	486	498	rBV	1319320	2229396	33.21%	5.588%
4	7.305	752	760	771	rBV	1663186	2911347	43.36%	7.297%
5	7.681	817	824	832	rBV	1448089	2526708	37.64%	6.333%
6	8.151	894	904	916	rVB	393684	708027	10.55%	1.775%
7	8.480	952	960	971	rVB	922717	1658187	24.70%	4.156%
8	9.326	1095	1104	1112	rBV	1046626	1876470	27.95%	4.703%
9	10.983	1378	1386	1393	rBV	598886	1096357	16.33%	2.748%
10	13.415	1791	1800	1808	rBV	2580476	4015300	59.81%	10.064%
11	14.238	1934	1940	1946	rBV	405231	592028	8.82%	1.484%
12	14.796	2028	2035	2048	rVB2	1151430	1877372	27.96%	4.705%
13	15.619	2170	2175	2181	rBV2	55537	77322	1.15%	0.194%
14	16.289	2282	2289	2300	rBV	2642984	4099806	61.07%	10.275%
15	16.482	2318	2322	2326	rBV2	62114	86327	1.29%	0.216%
16	17.282	2453	2458	2461	rBV2	84503	101643	1.51%	0.255%
17	17.552	2497	2504	2513	rBV2	1524279	2443519	36.40%	6.124%
18	18.421	2647	2652	2659	rBV2	245814	346485	5.16%	0.868%
19	19.685	2864	2867	2873	rBV6	65468	92732	1.38%	0.232%
20	20.155	2941	2947	2953	rBV	5164260	6713601	100.00%	16.826%
21	21.453	3163	3168	3180	rBV	288843	483642	7.20%	1.212%
22	21.847	3228	3235	3246	rVB2	1669245	2816389	41.95%	7.059%
23	24.209	3632	3637	3642	rBV9	41339	90036	1.34%	0.226%
24	25.208	3796	3807	3820	rVB	893049	2665801	39.71%	6.681%

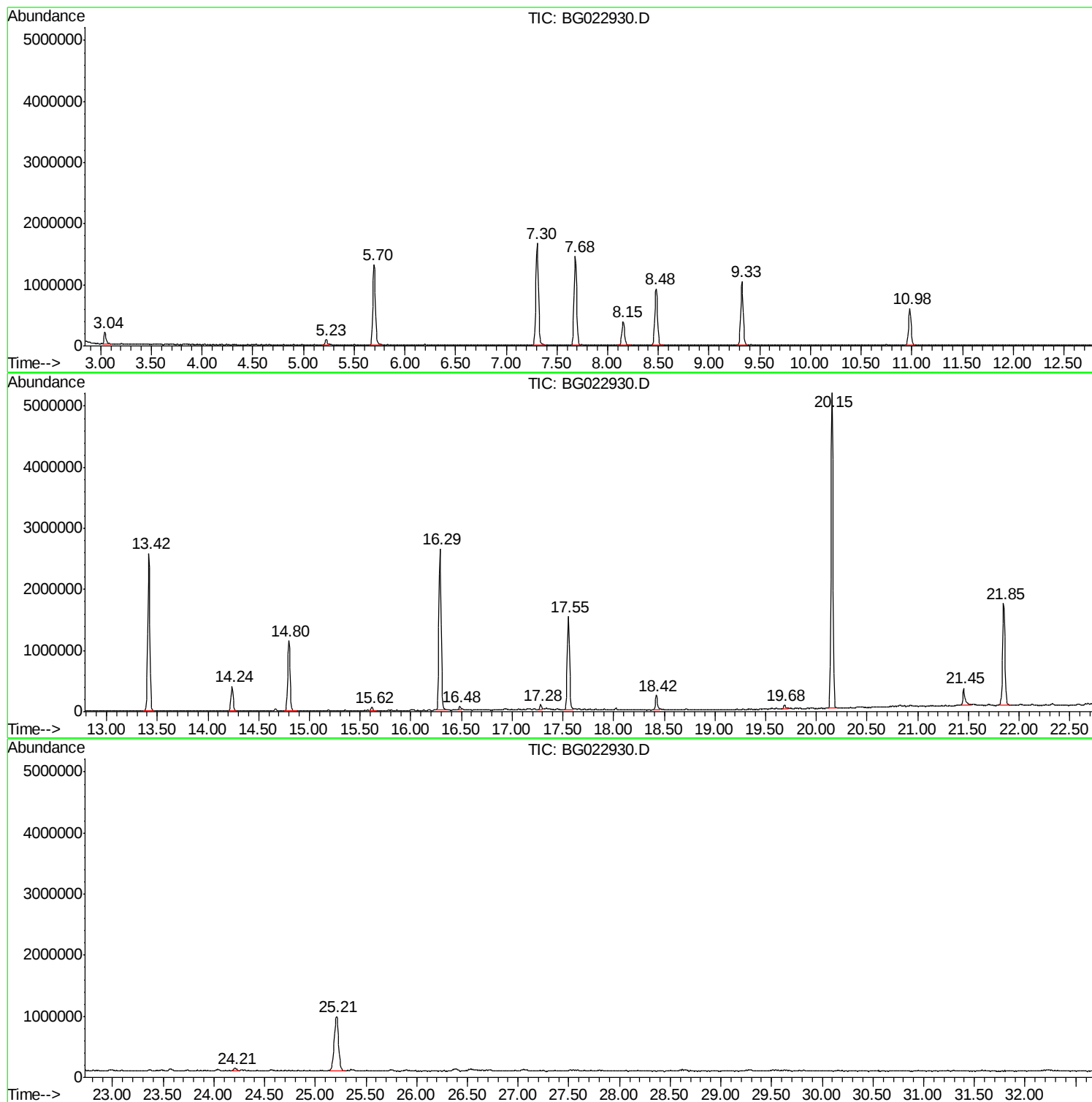
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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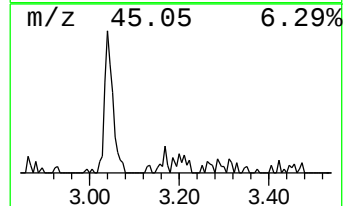
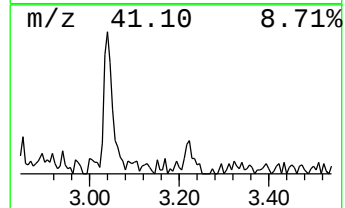
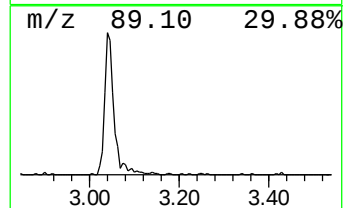
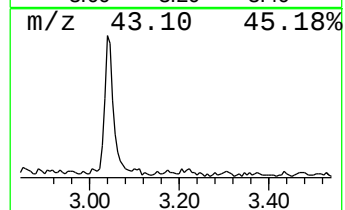
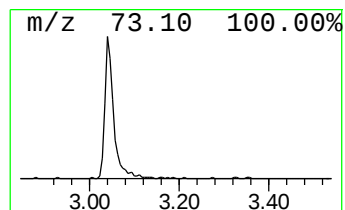
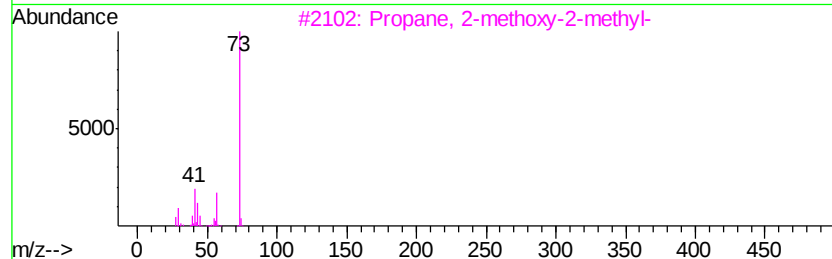
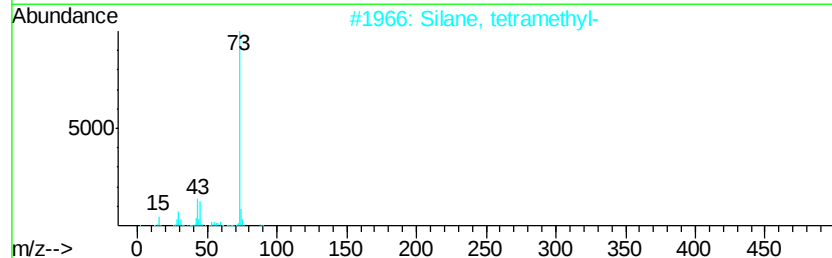
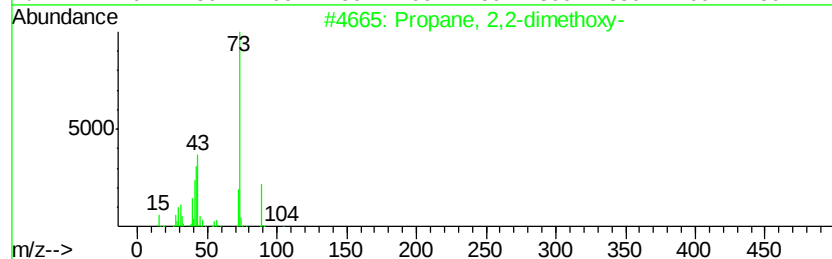
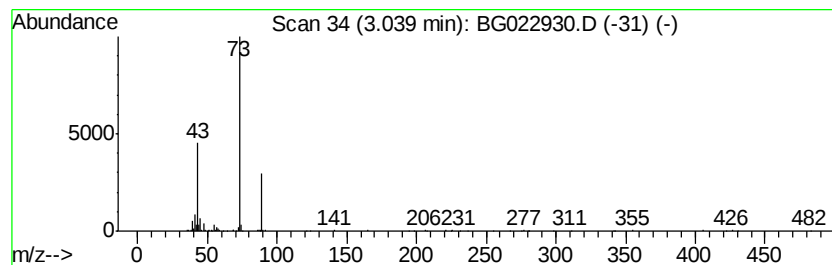
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown3.04 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.04	7.28 ng	257753	1,4-Dichlorobenzene-d4	8.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	36
2		Silane, tetramethyl-	88	C4H12Si	000075-76-3	14
3		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
4		2,2'-Trimethylenebis-1,3-dioxolane	188	C9H16O4	006543-04-0	9
5		1,3-Dioxolane, 2-pentadecyl-	284	C18H36O2	004360-57-0	9



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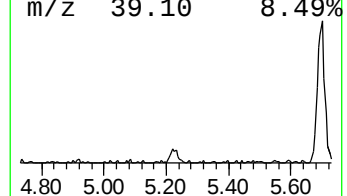
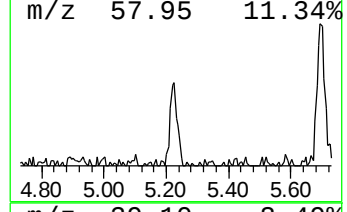
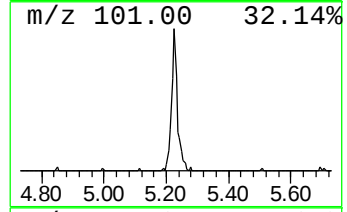
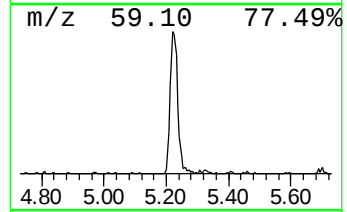
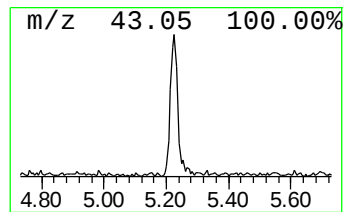
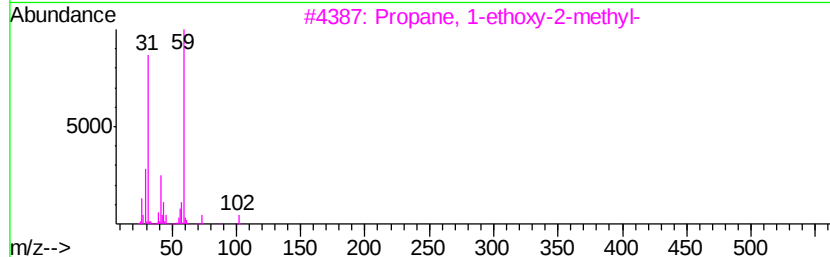
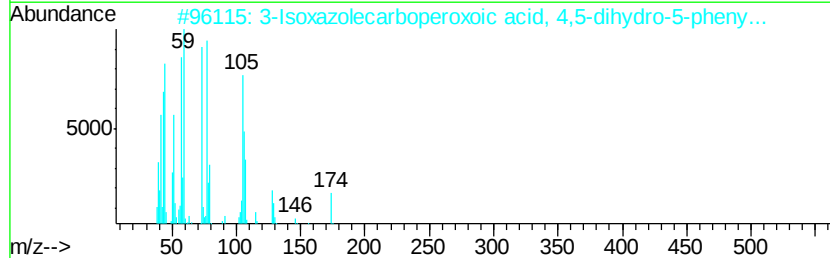
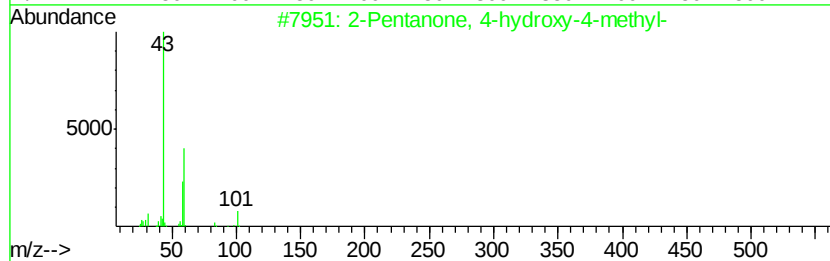
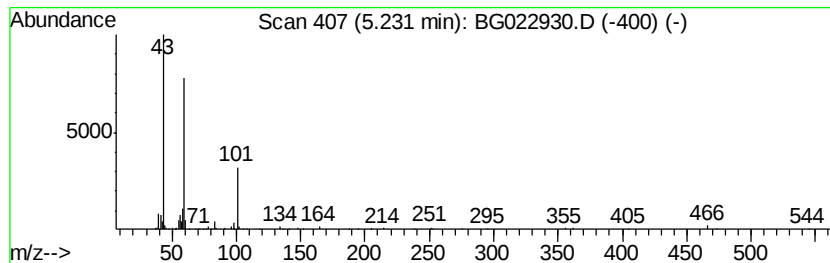
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.23	3.76 ng	133054	1,4-Dichlorobenzene-d4	8.15

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
2			3-Isoxazolecarboxylic acid, 4...	263	C14H17NO4	035145-84-7	37
3			Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	35
4			Guanidine	59	CH5N3	000113-00-8	35
5			5-Ethyl-3-methylhept-1-en-4-ol	156	C10H20O	286424-80-4	34



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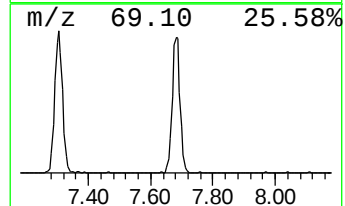
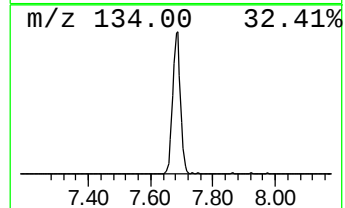
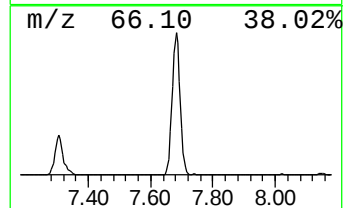
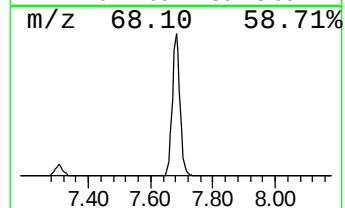
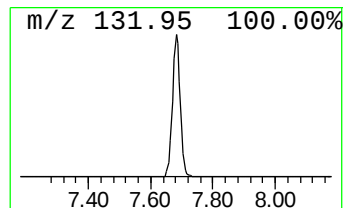
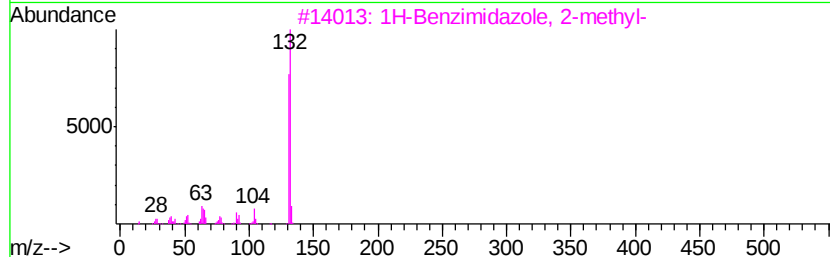
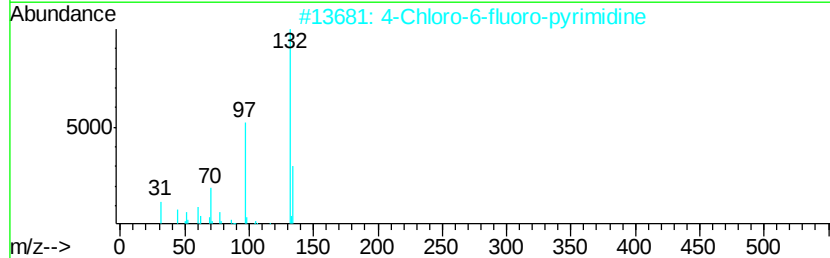
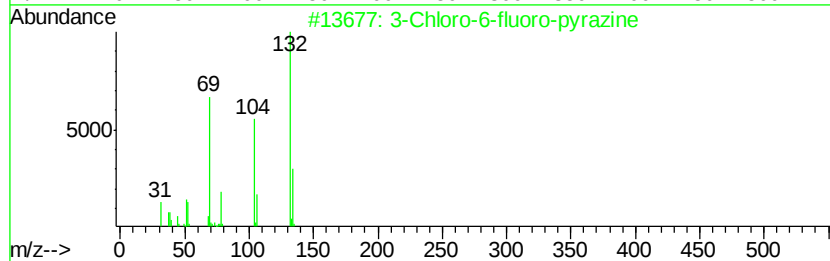
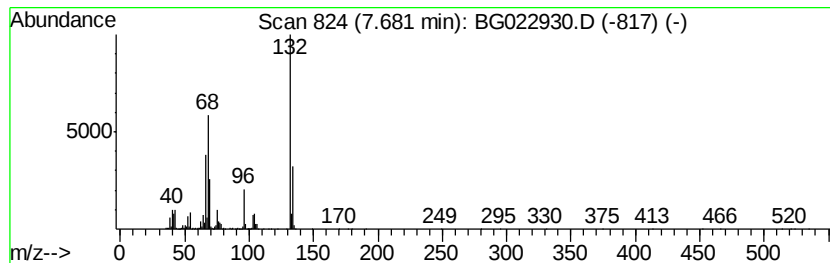
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Peak Number 3 unknown7.68 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.68	71.37 ng	2526710	1,4-Dichlorobenzene-d4	8.15

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		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	22
5		5-Aminoindole	132	C8H8N2	005192-03-0	10



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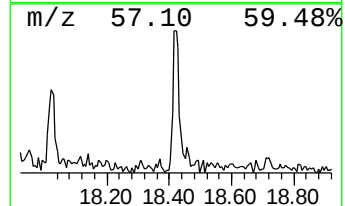
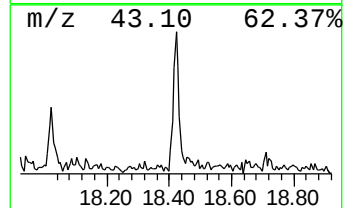
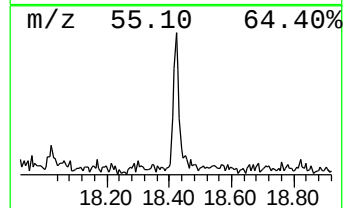
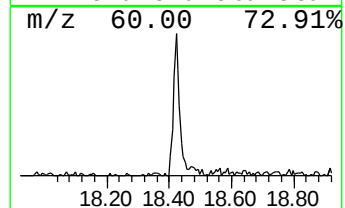
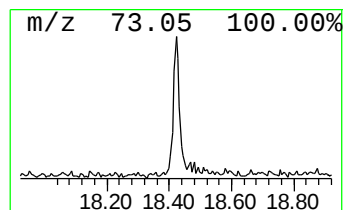
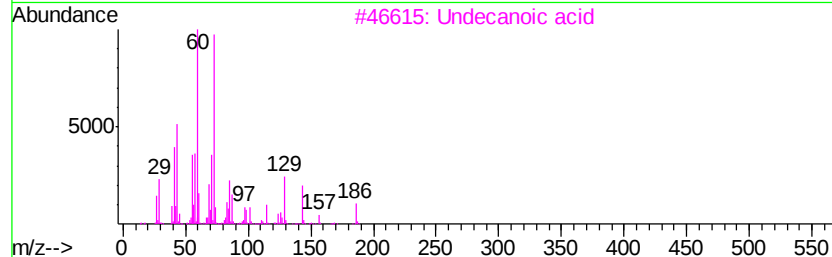
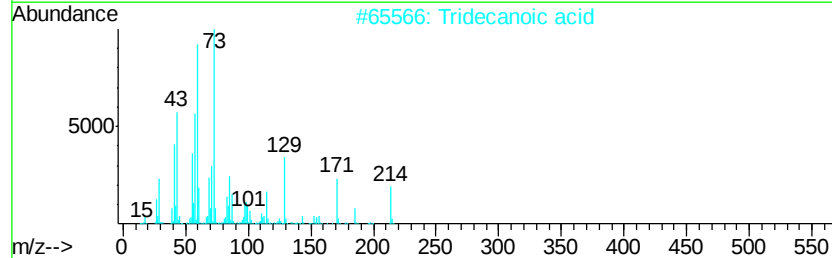
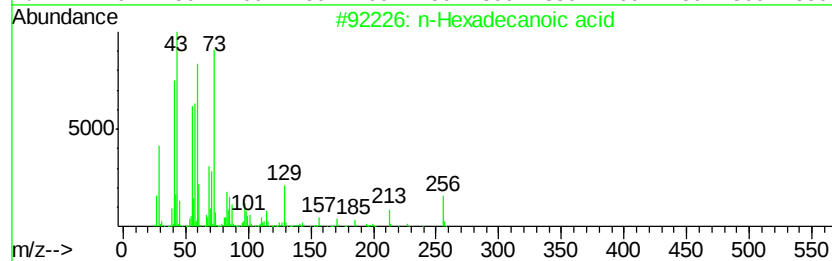
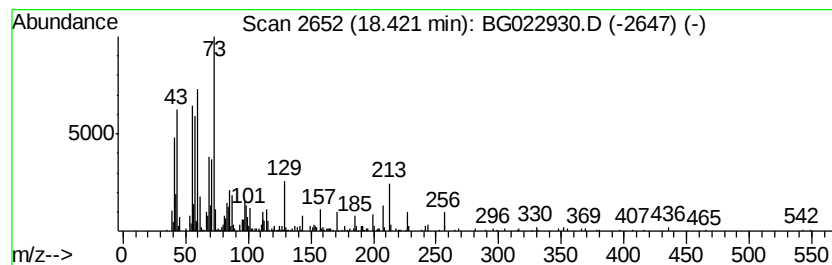
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.42	2.84 ng	346485	Phenanthrene-d10	17.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Tridecanoic acid	214	C13H26O2	000638-53-9	52
3	Undecanoic acid	186	C11H22O2	000112-37-8	50
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	49
5	l-(+)-Ascorbic acid 2,6-dihexade...	652	C38H68O8	028474-90-0	49



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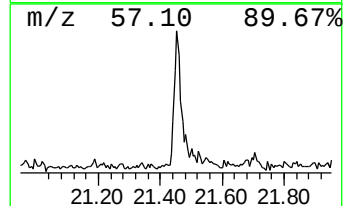
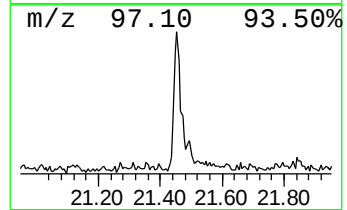
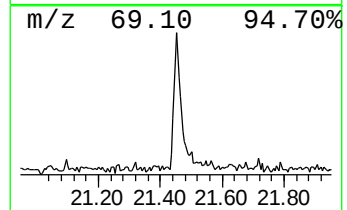
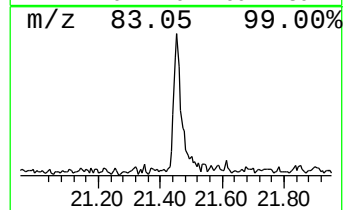
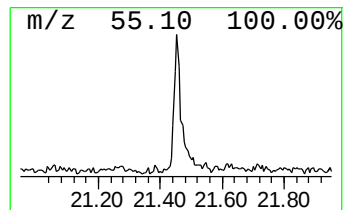
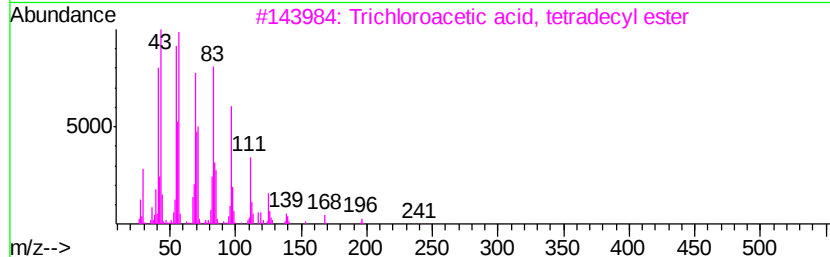
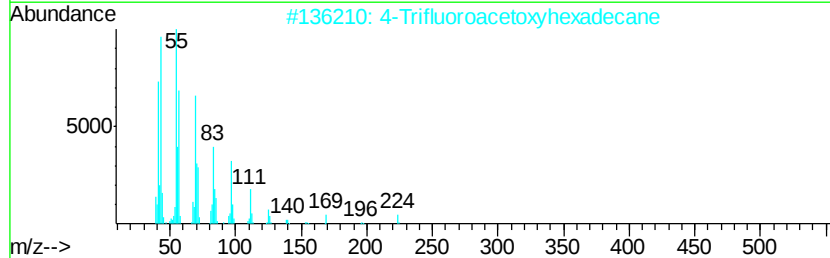
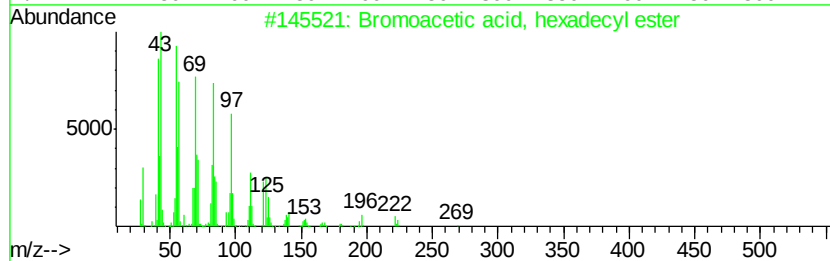
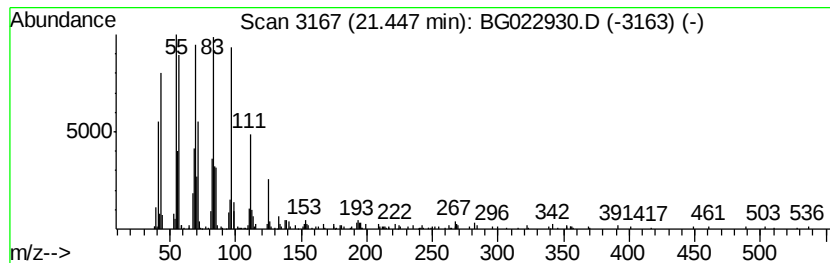
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 6 Bromoacetic acid, hexadecyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.45	3.43 ng	483642	Chrysene-d12	21.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	91
2		4-Trifluoroacetoxyhexadecane	338	C18H33F3O2	1000215-97-5	91
3		Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91
4		1-Heneicosyl formate	340	C22H44O2	077899-03-7	87
5		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	87



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown3.04	3.04	7.3	ng	257753	1	8.15	708027	20.0
2-Pentanone, 4-hy...	5.23	3.8	ng	133054	1	8.15	708027	20.0
unknown7.68	7.68	71.4	ng	2526710	1	8.15	708027	20.0
n-Hexadecanoic acid	18.42	2.8	ng	346485	4	17.56	2443520	20.0
Bromoacetic acid,...	21.45	3.4	ng	483642	5	21.85	2816390	20.0