

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG062616\
 Data File : BG022608.D
 Acq On : 26 Jun 2016 13:25
 Operator : UM/SJ
 Sample : H3761-06
 Misc :
 ALS Vial : 63 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 LOCATION-9B-9-11

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-BG062516.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	3.058	32	37	54	rBV	6879990	10639261	100.00%	17.419%
2	5.237	402	408	418	rVB	163835	244492	2.30%	0.400%
3	5.708	478	488	496	rBV	2097632	3418442	32.13%	5.597%
4	7.306	751	760	771	rBV	2303139	4048519	38.05%	6.628%
5	7.688	818	825	834	rVB	2112473	3705099	34.82%	6.066%
6	8.163	899	906	912	rBV	474857	826904	7.77%	1.354%
7	8.487	951	961	973	rBV	1501193	2656428	24.97%	4.349%
8	9.333	1097	1105	1113	rBV	1374479	2471620	23.23%	4.047%
9	10.984	1379	1386	1395	rVB	636430	1161132	10.91%	1.901%
10	13.416	1793	1800	1809	rBV	3227355	5185733	48.74%	8.490%
11	14.239	1934	1940	1947	rBV	501077	735538	6.91%	1.204%
12	14.797	2022	2035	2043	rBV2	1080241	1728328	16.24%	2.830%
13	16.289	2278	2289	2299	rBV	3592015	5660182	53.20%	9.267%
14	16.489	2319	2323	2332	rVB5	69832	117568	1.11%	0.192%
15	17.552	2497	2504	2510	rBV2	1547518	2418488	22.73%	3.960%
16	18.428	2648	2653	2662	rBV2	414252	607695	5.71%	0.995%
17	19.691	2864	2868	2875	rBV4	290933	413118	3.88%	0.676%
18	19.844	2890	2894	2898	rVB3	201301	231080	2.17%	0.378%
19	20.155	2941	2947	2953	rBV	6552298	8519650	80.08%	13.949%
20	20.878	3067	3070	3074	rBV2	150738	189592	1.78%	0.310%
21	21.466	3166	3170	3179	rVB7	151348	271893	2.56%	0.445%
22	21.689	3204	3208	3210	rBV5	80672	127462	1.20%	0.209%
23	21.847	3228	3235	3242	rVB	1708818	2882937	27.10%	4.720%
24	25.208	3797	3807	3820	rVB2	914889	2817862	26.49%	4.613%

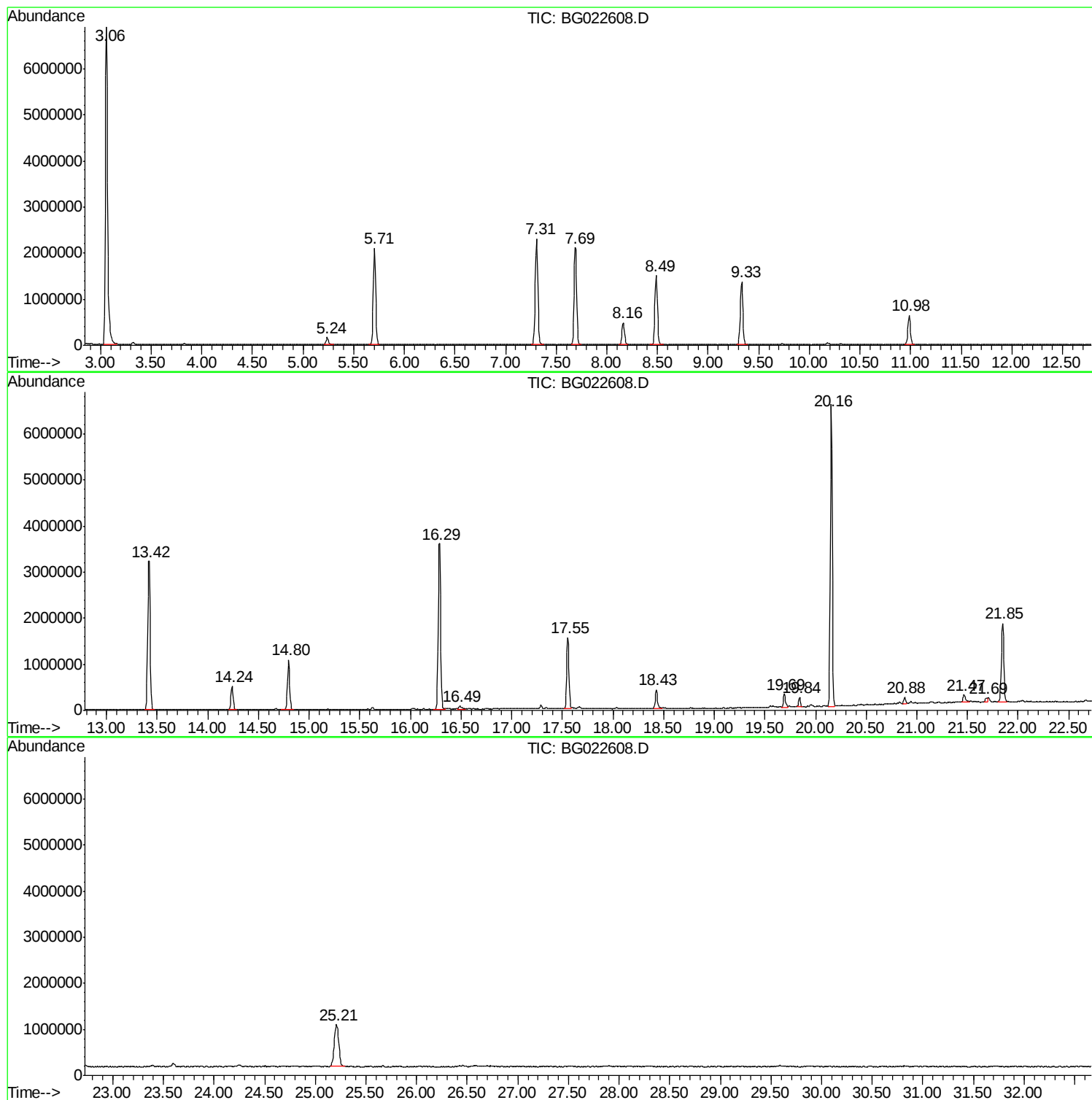
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG062516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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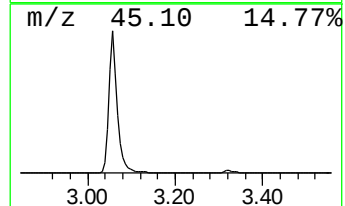
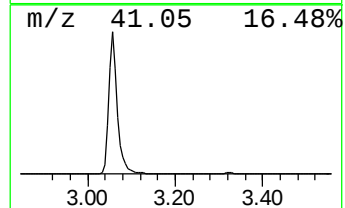
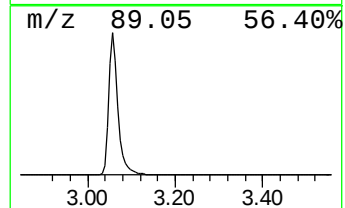
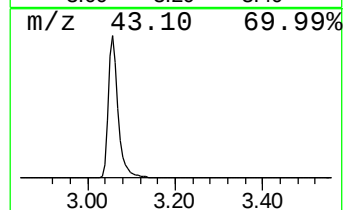
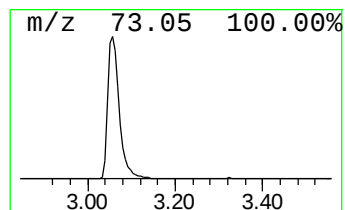
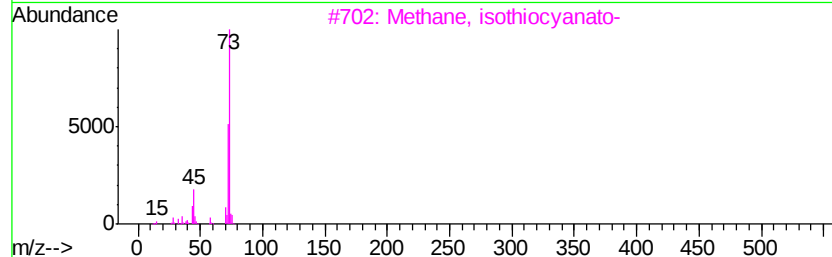
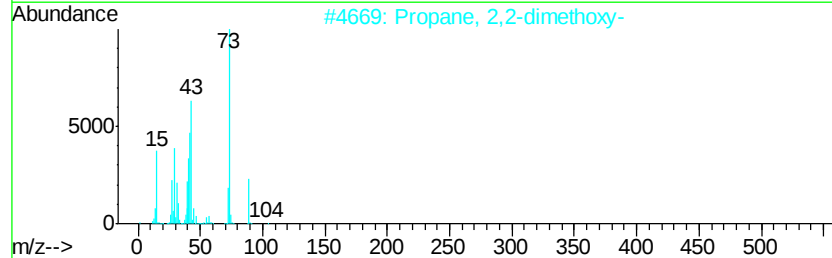
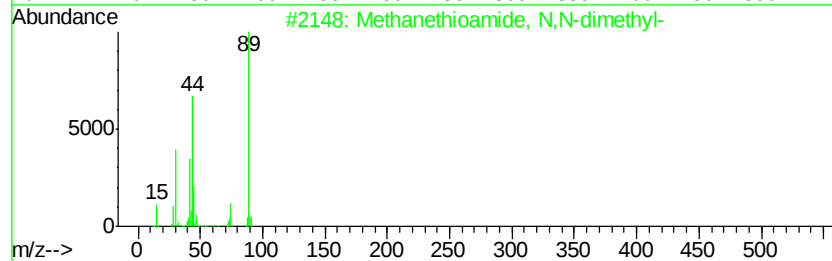
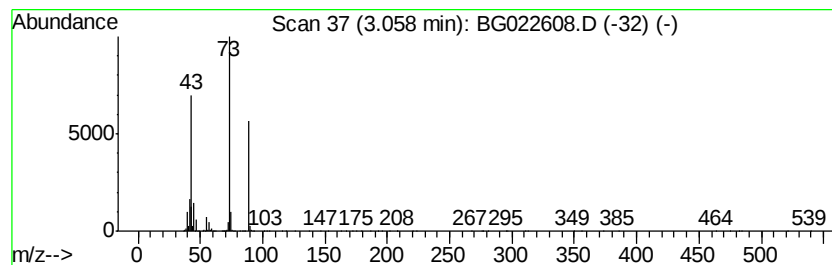
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG062516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown3.06 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.06	257.33 ng	10639300	1,4-Dichlorobenzene-d4	8.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Methanethioamide, N,N-dimethyl-	89	C3H7NS	000758-16-7	47
2		Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	25
3		Methane, isothiocyanato-	73	C2H3NS	000556-61-6	12
4		Thiazole, tetrahydro-	89	C3H7NS	000504-78-9	9
5		1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9



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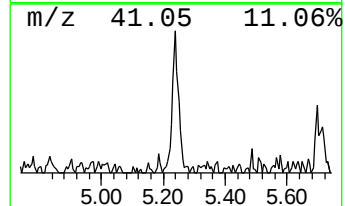
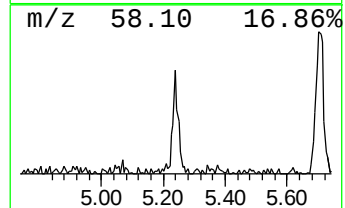
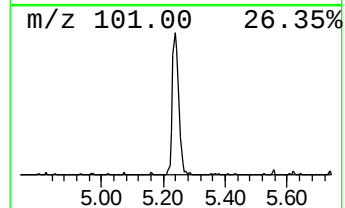
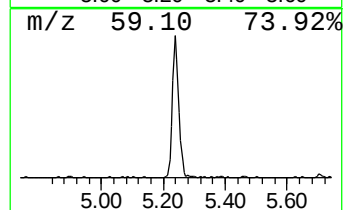
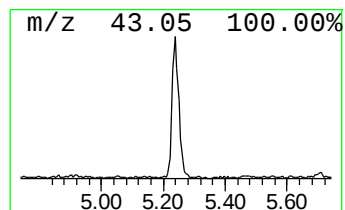
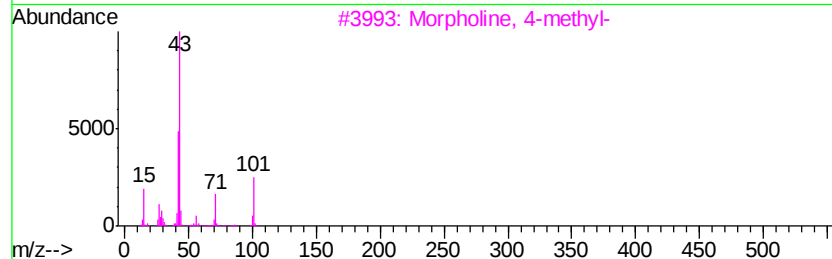
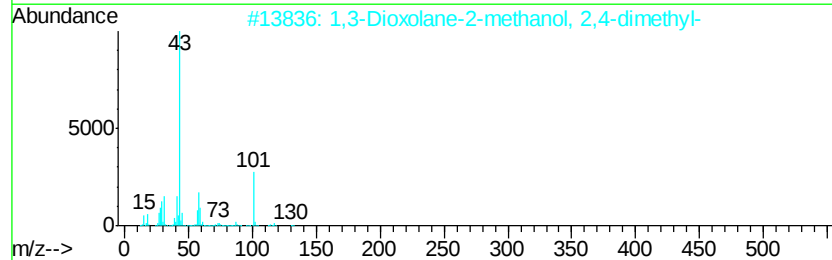
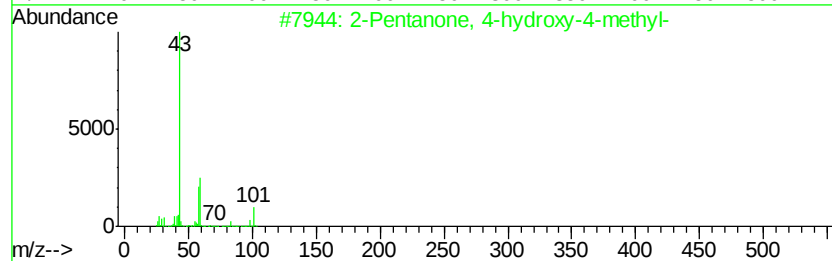
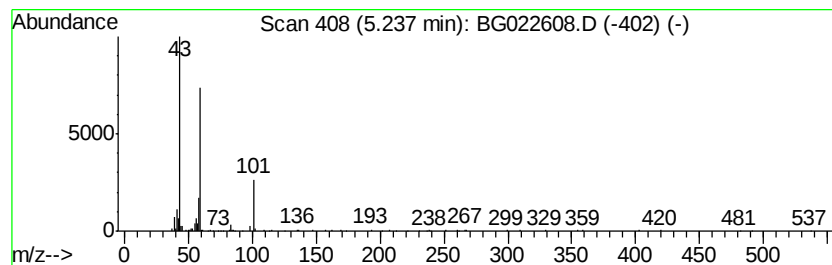
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.24	5.91 ng	244492	1,4-Dichlorobenzene-d4	8.16

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	10
3			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4			Guanidine	59	CH5N3	000113-00-8	9
5			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7N2O2	016504-58-8	9



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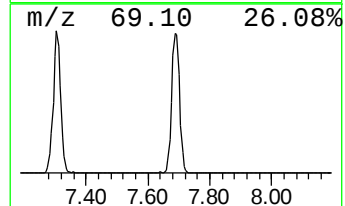
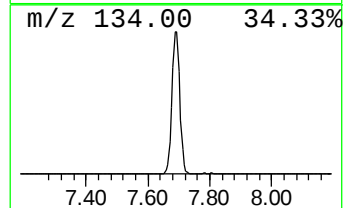
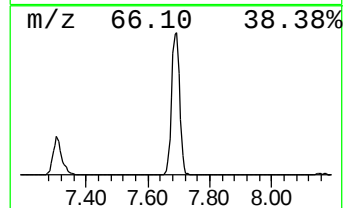
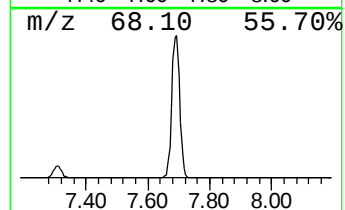
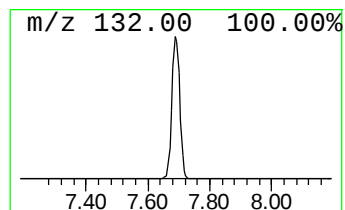
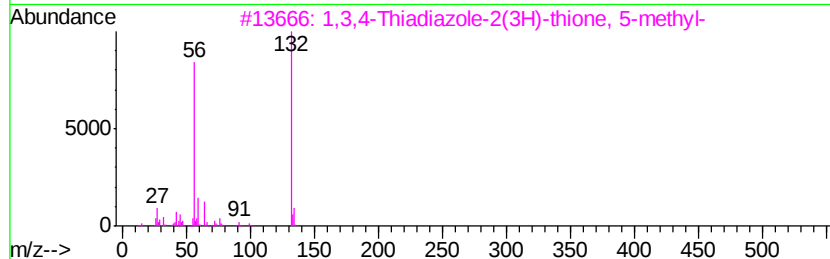
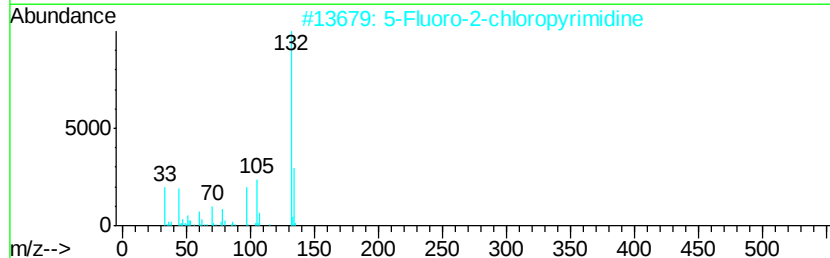
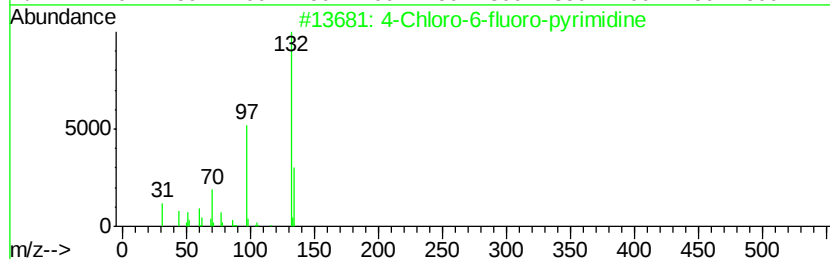
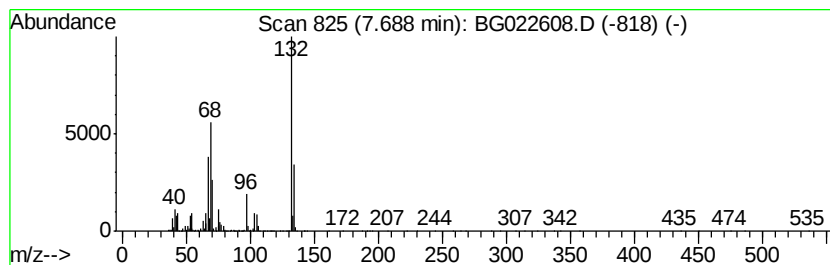
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Peak Number 3 unknown7.69 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.69	89.61 ng	3705100	1,4-Dichlorobenzene-d4	8.16

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		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	14
4		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	10
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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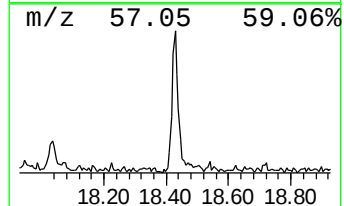
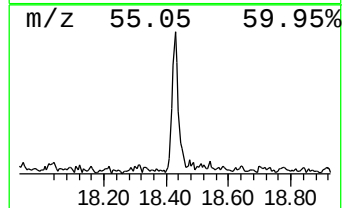
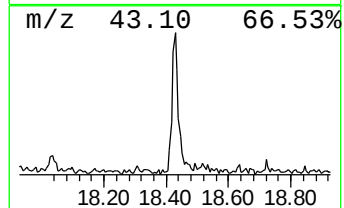
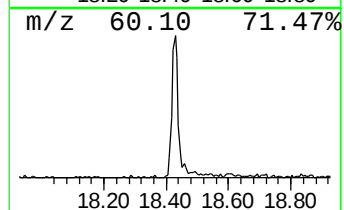
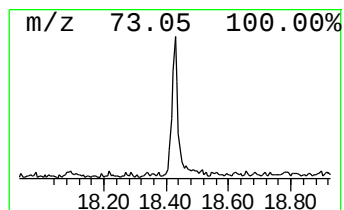
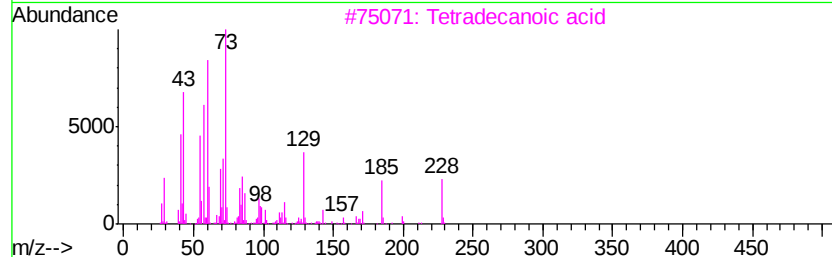
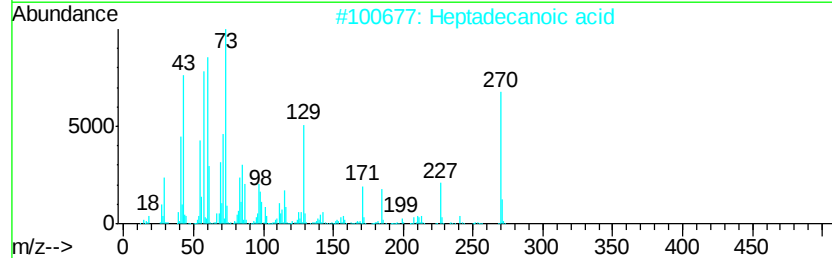
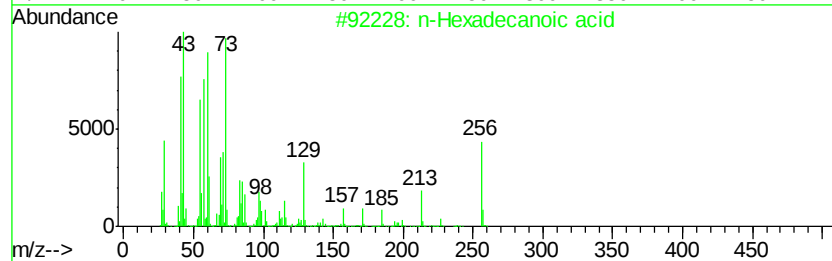
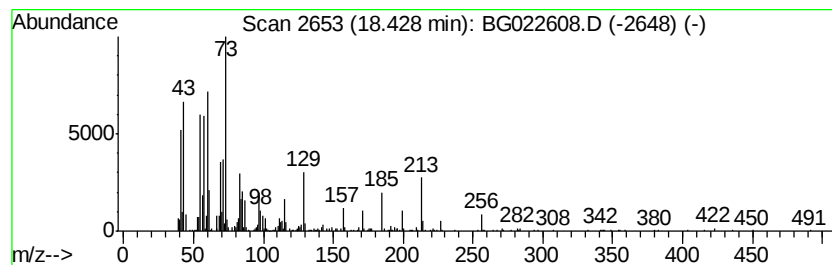
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.43	5.03 ng	607695	Phenanthrene-d10	17.55

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2		Heptadecanoic acid	270	C17H34O2	000506-12-7	93
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4		Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	64
5		Octadecanoic acid	284	C18H36O2	000057-11-4	64



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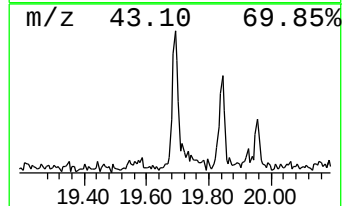
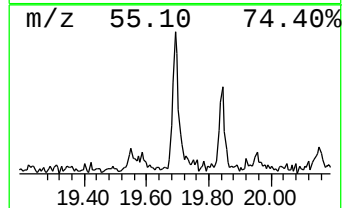
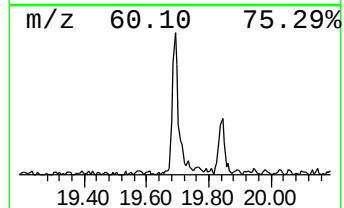
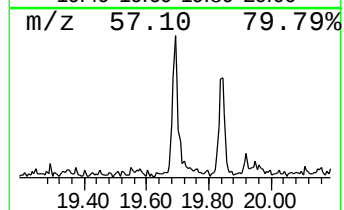
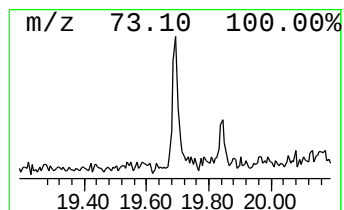
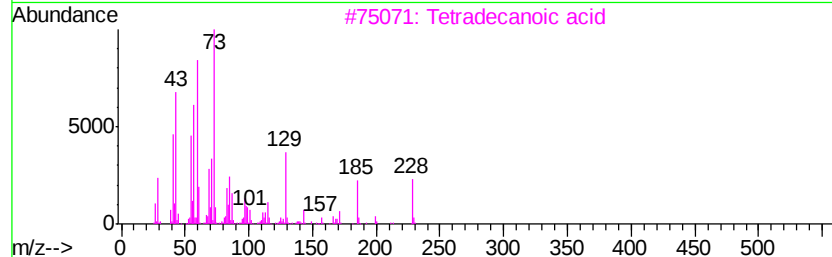
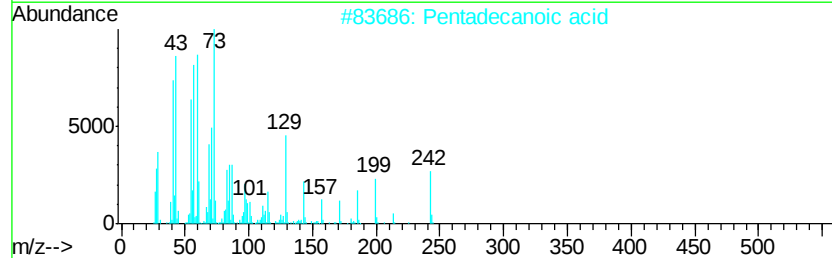
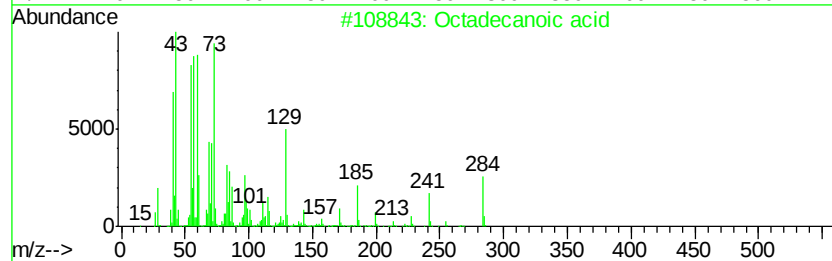
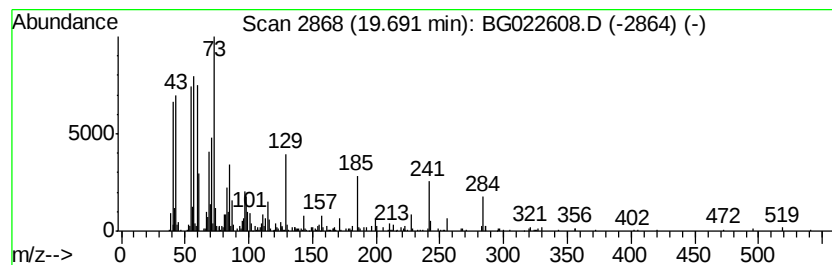
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 6 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.69	3.42 ng	413118	Phenanthrene-d10	17.55

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	98
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	59
4		Lactose	342	C12H22O11	000063-42-3	47
5		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	42



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown3.06	3.06	257.3	ng	10639300	1	8.16	826904	20.0
2-Pentanone, 4-hy...	5.24	5.9	ng	244492	1	8.16	826904	20.0
unknown7.69	7.69	89.6	ng	3705100	1	8.16	826904	20.0
n-Hexadecanoic acid	18.43	5.0	ng	607695	4	17.55	2418490	20.0
Octadecanoic acid	19.69	3.4	ng	413118	4	17.55	2418490	20.0