

Data Path : Z:\HPCHEM1\BNA G\DATA\BG021418\
 Data File : BG032690.D
 Acq On : 14 Feb 2018 20:46
 Operator : SJ/JU
 Sample : J1545-08
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TEST-PIT-2

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-BG021218.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	3.414	16	21	32	rVB	67150	104965	3.33%	0.851%
2	6.099	468	478	493	rBV	284230	543443	17.25%	4.407%
3	7.779	756	764	779	rBV	297778	637775	20.24%	5.173%
4	8.167	821	830	847	rBV	356652	649874	20.63%	5.271%
5	8.661	907	914	928	rBV2	42070	95769	3.04%	0.777%
6	8.990	963	970	982	rBV	307343	588229	18.67%	4.771%
7	9.853	1109	1117	1133	rBV	175578	394793	12.53%	3.202%
8	11.534	1395	1403	1417	rBV	82708	176744	5.61%	1.433%
9	13.919	1802	1809	1823	rBV	871129	1454294	46.16%	11.795%
10	14.718	1940	1945	1952	rBV	53871	89171	2.83%	0.723%
11	15.300	2037	2044	2052	rBV2	174342	329380	10.45%	2.671%
12	16.775	2287	2295	2310	rBV	957072	1634647	51.88%	13.257%
13	18.032	2502	2509	2519	rBV2	299786	526942	16.73%	4.274%
14	18.854	2643	2649	2654	rBV3	37422	61880	1.96%	0.502%
15	20.576	2936	2942	2954	rBV	2239794	3150595	100.00%	25.552%
16	21.898	3161	3167	3176	rBV2	128833	222019	7.05%	1.801%
17	22.350	3237	3244	3255	rBV2	384257	724368	22.99%	5.875%
18	22.497	3264	3269	3276	rVB5	30973	52017	1.65%	0.422%
19	23.179	3380	3385	3395	rBV6	29089	59263	1.88%	0.481%
20	23.960	3512	3518	3524	rVB7	21033	42028	1.33%	0.341%
21	24.877	3666	3674	3679	rBV5	15404	38098	1.21%	0.309%
22	25.981	3850	3862	3877	rBV3	221813	753717	23.92%	6.113%

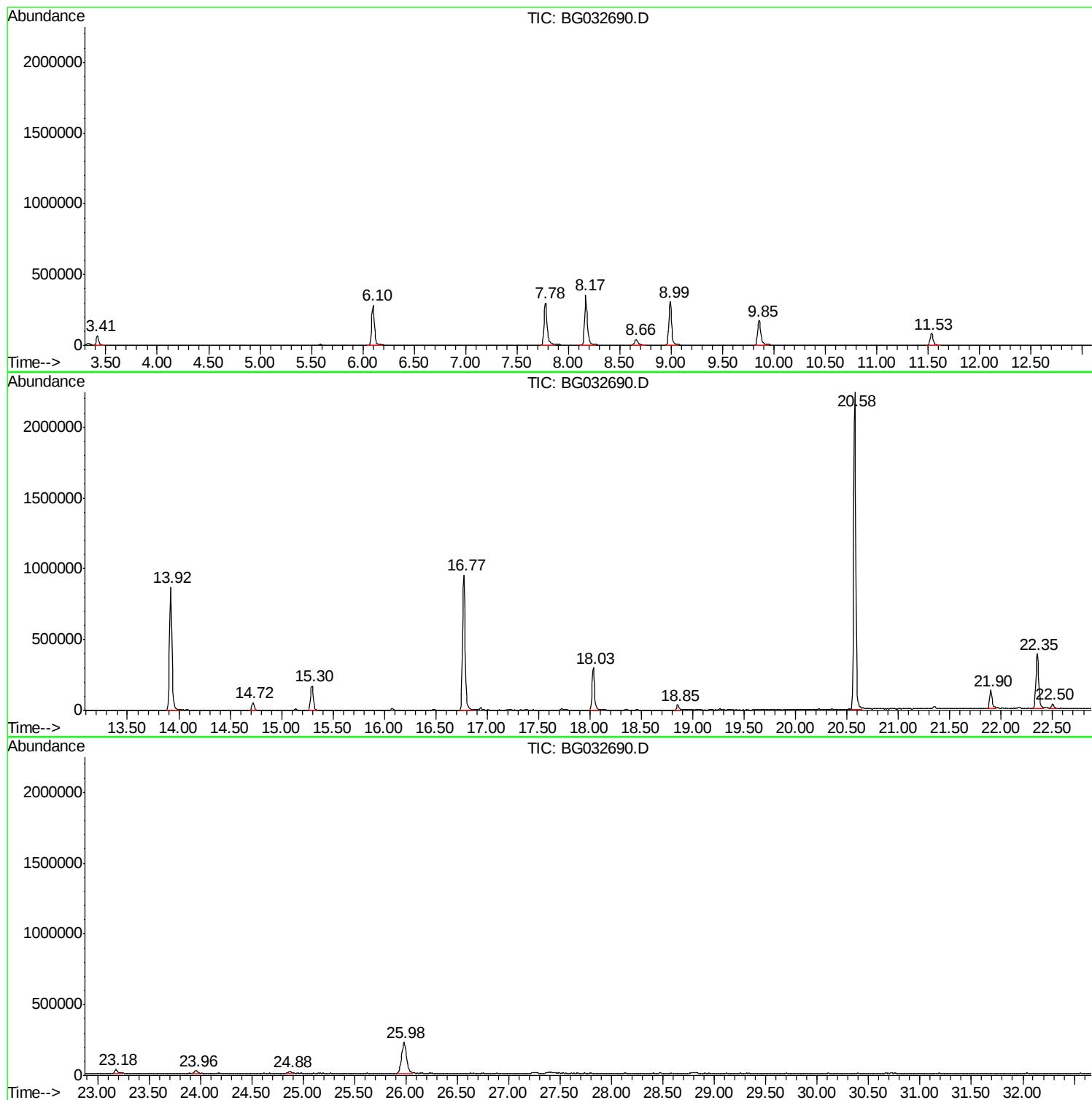
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG021218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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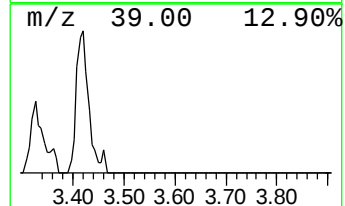
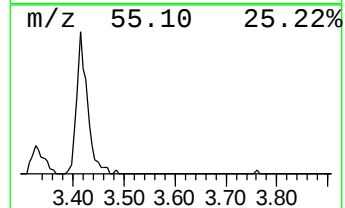
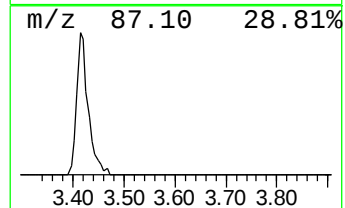
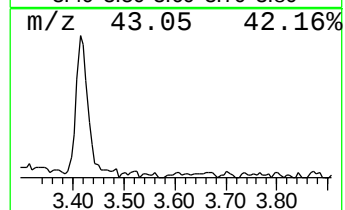
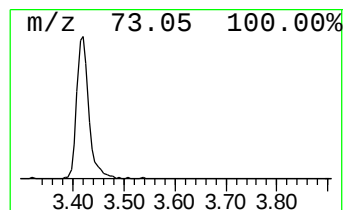
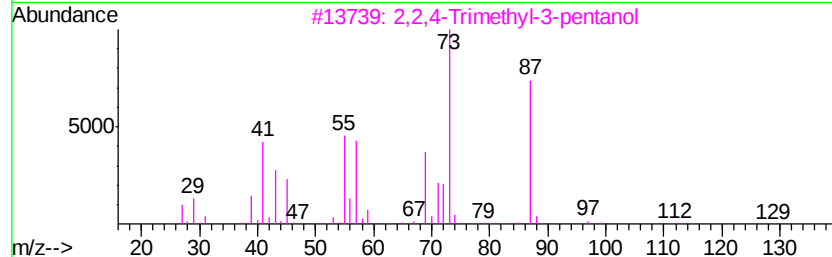
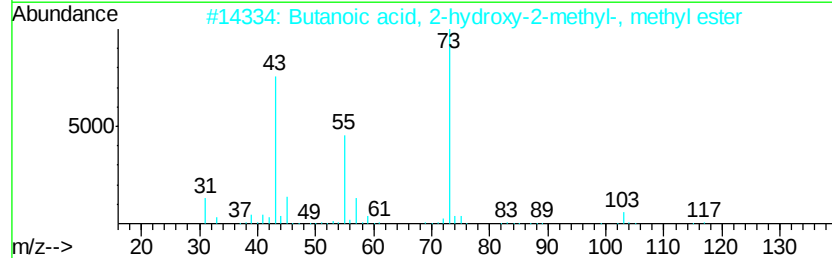
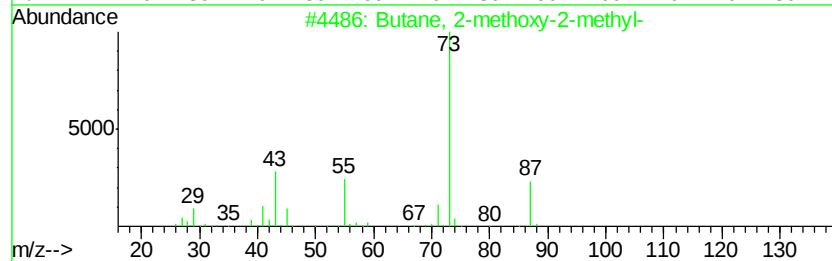
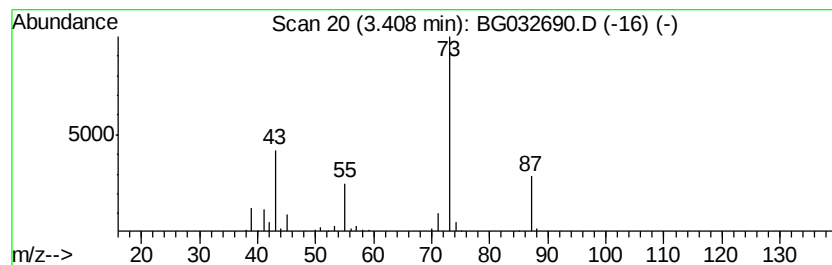
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG021218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.41	21.92 ng	104965	1,4-Dichlorobenzene-d4	8.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	74
2		Butanoic acid, 2-hydroxy-2-methyl...	132	C6H12O3	032793-34-3	38
3		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	33
4		3-Hexanol, 2,4-dimethyl-	130	C8H18O	013432-25-2	33
5		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	16



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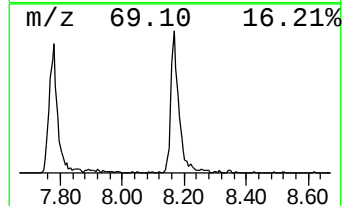
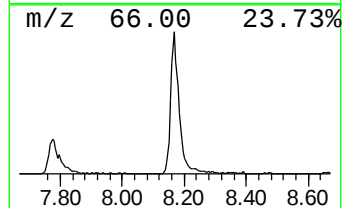
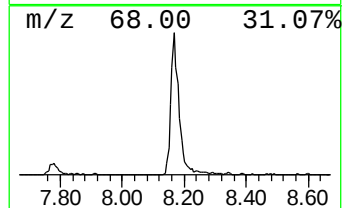
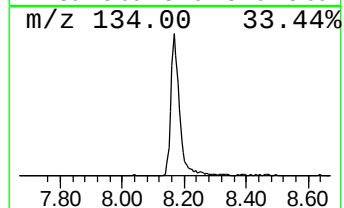
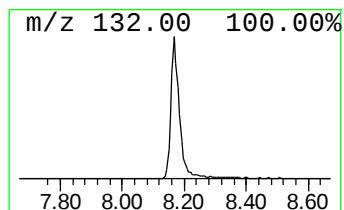
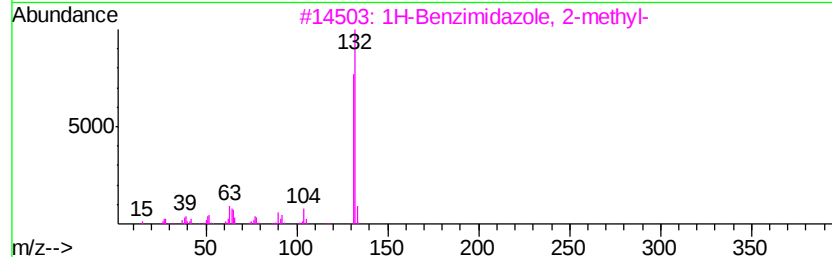
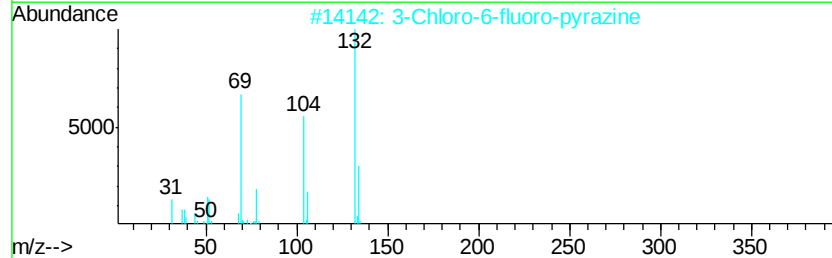
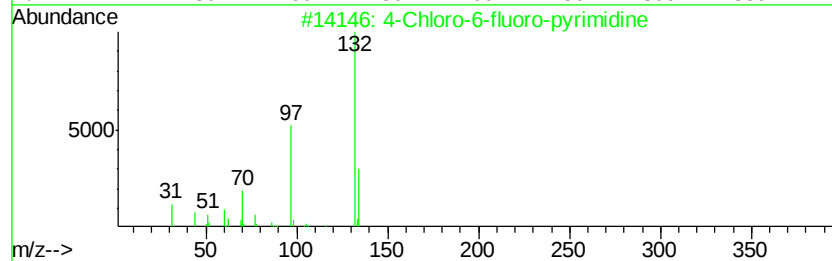
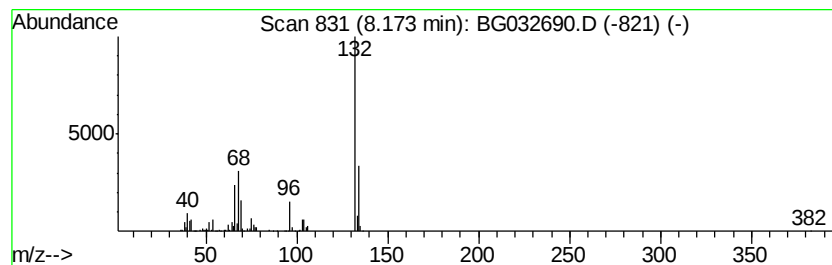
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Peak Number 2 unknown8.17 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.17	135.72 ng	649874	1,4-Dichlorobenzene-d4	8.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	35
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	27
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	25
5		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10



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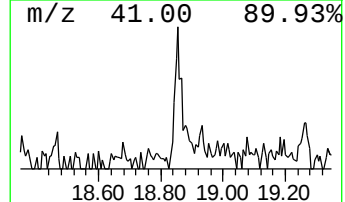
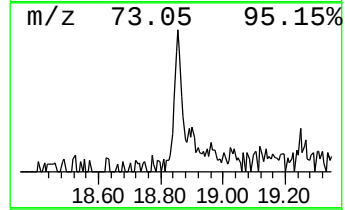
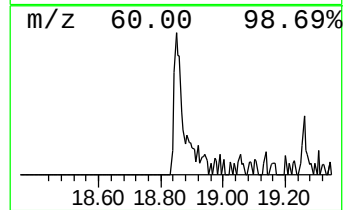
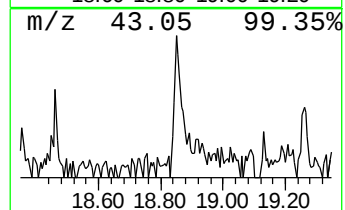
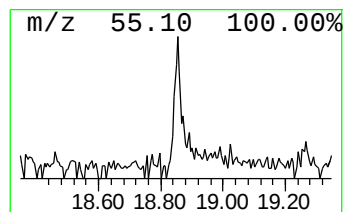
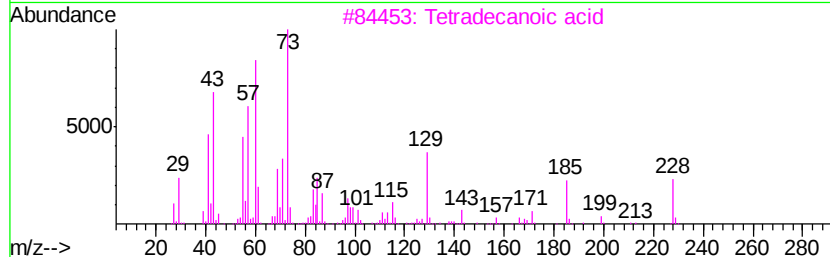
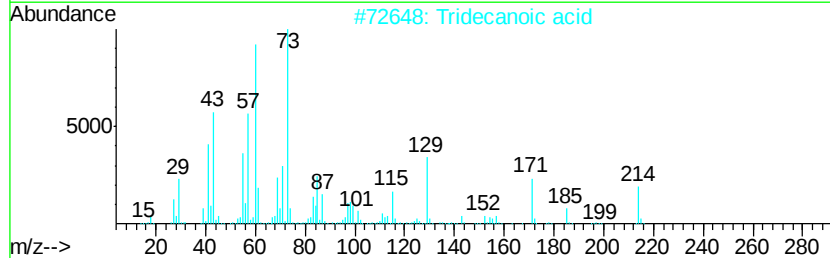
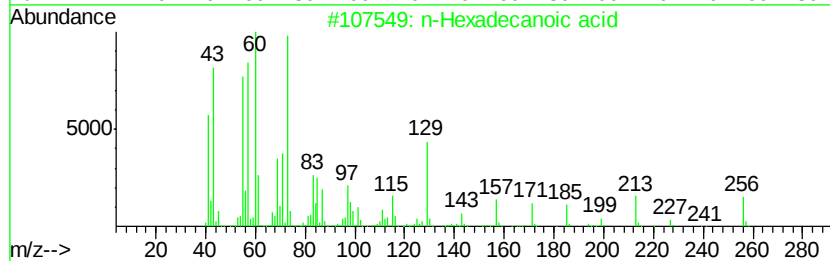
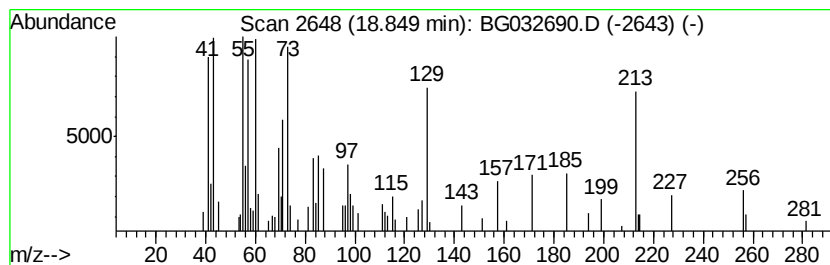
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.85	2.35 ng	61880	Phenanthrene-d10	18.03	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	92
2	Tridecanoic acid	214	C13H26O2	000638-53-9	42
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	27
4	1-Phenazinecarboxylic acid, 6-[1...	506	C31H42N2O4	120464-92-8	27
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	22



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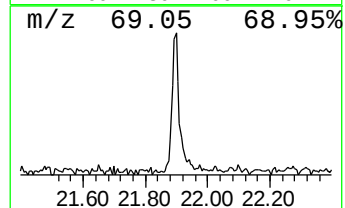
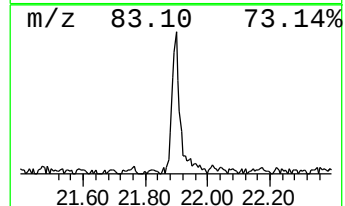
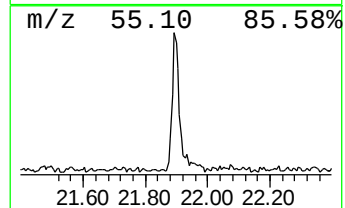
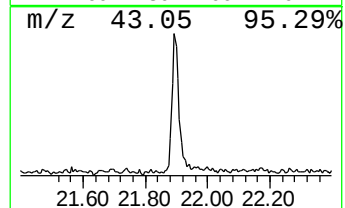
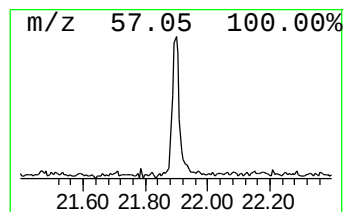
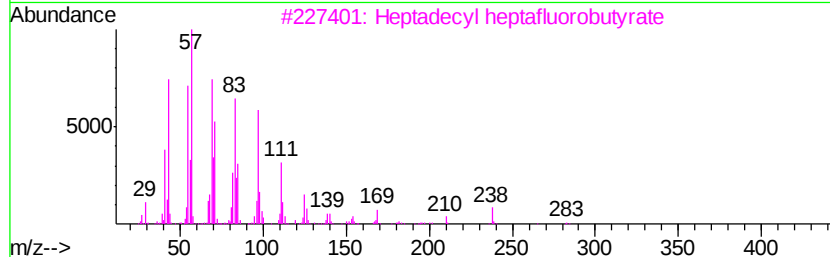
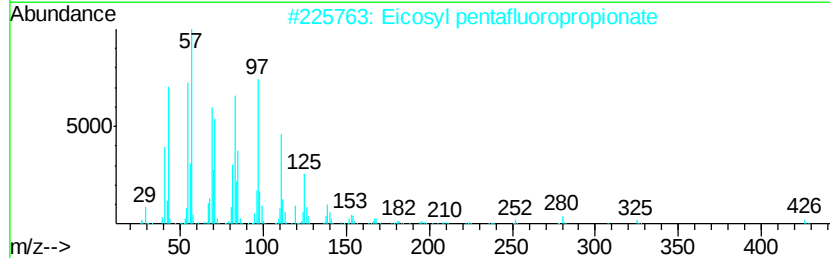
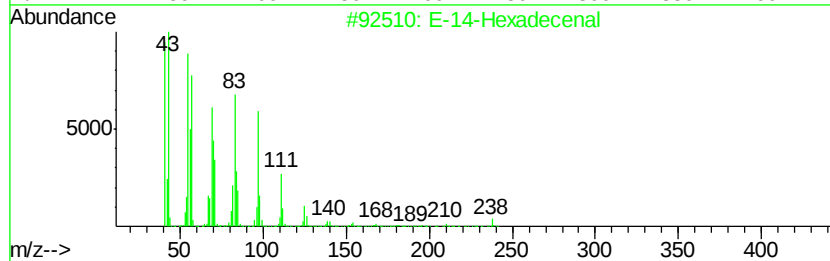
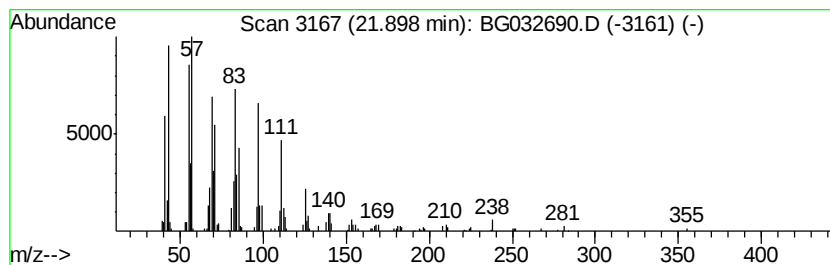
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Peak Number 5 E-14-Hexadecenal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.90	6.13 ng	222019	Chrysene-d12	22.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	E-14-Hexadecenal	238	C16H30O	330207-53-9	94
2		Eicosyl pentafluoropropionate	444	C23H41F5O2	1000351-80-8	93
3		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
4		Triacontyl trifluoroacetate	534	C32H61F3O2	1000351-75-7	90
5		Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	90



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	3.41	21.9	ng	104965	1	8.66	95769	20.0
unknown8.17	8.17	135.7	ng	649874	1	8.66	95769	20.0
n-Hexadecanoic acid	18.85	2.4	ng	61880	4	18.03	526942	20.0
E-14-Hexadecenal	21.90	6.1	ng	222019	5	22.35	724368	20.0