

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG012418\
 Data File : BG032268.D
 Acq On : 24 Jan 2018 19:40
 Operator : SJ/JU
 Sample : J1250-03
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 AB-12(0-2)

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-BG011218.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	3.469	25	31	45	rVB	308694	478442	18.83%	3.595%
2	5.649	394	402	408	rBV3	16035	28237	1.11%	0.212%
3	6.160	481	489	498	rBV	421991	755566	29.73%	5.677%
4	7.835	766	774	789	rBV	451774	849977	33.45%	6.386%
5	8.240	835	843	854	rBV	449741	846261	33.30%	6.358%
6	8.722	917	925	932	rBV	112355	205916	8.10%	1.547%
7	9.063	974	983	992	rBV	347906	660017	25.97%	4.959%
8	9.921	1121	1129	1142	rBV	269629	497178	19.56%	3.736%
9	11.607	1408	1416	1425	rBV	150915	284762	11.21%	2.140%
10	13.986	1813	1821	1833	rBV	845029	1321831	52.01%	9.932%
11	14.780	1951	1956	1963	rBV	87481	137255	5.40%	1.031%
12	15.361	2048	2055	2066	rVB2	272979	463430	18.24%	3.482%
13	16.689	2276	2281	2290	rVB	21266	32348	1.27%	0.243%
14	16.836	2297	2306	2319	rBV	752469	1237097	48.68%	9.295%
15	18.093	2513	2520	2529	rVB	450499	700869	27.58%	5.266%
16	18.910	2654	2659	2670	rBV2	50655	81154	3.19%	0.610%
17	20.291	2889	2894	2899	rBV3	26504	36301	1.43%	0.273%
18	20.631	2946	2952	2961	rBV	1871228	2541360	100.00%	19.095%
19	21.959	3173	3178	3189	rBV2	122009	200104	7.87%	1.503%
20	22.424	3249	3257	3267	rVB2	523411	956871	37.65%	7.189%
21	26.107	3870	3884	3896	rBV2	305210	961785	37.85%	7.226%
22	27.553	4125	4130	4142	rVB2	9972	32562	1.28%	0.245%

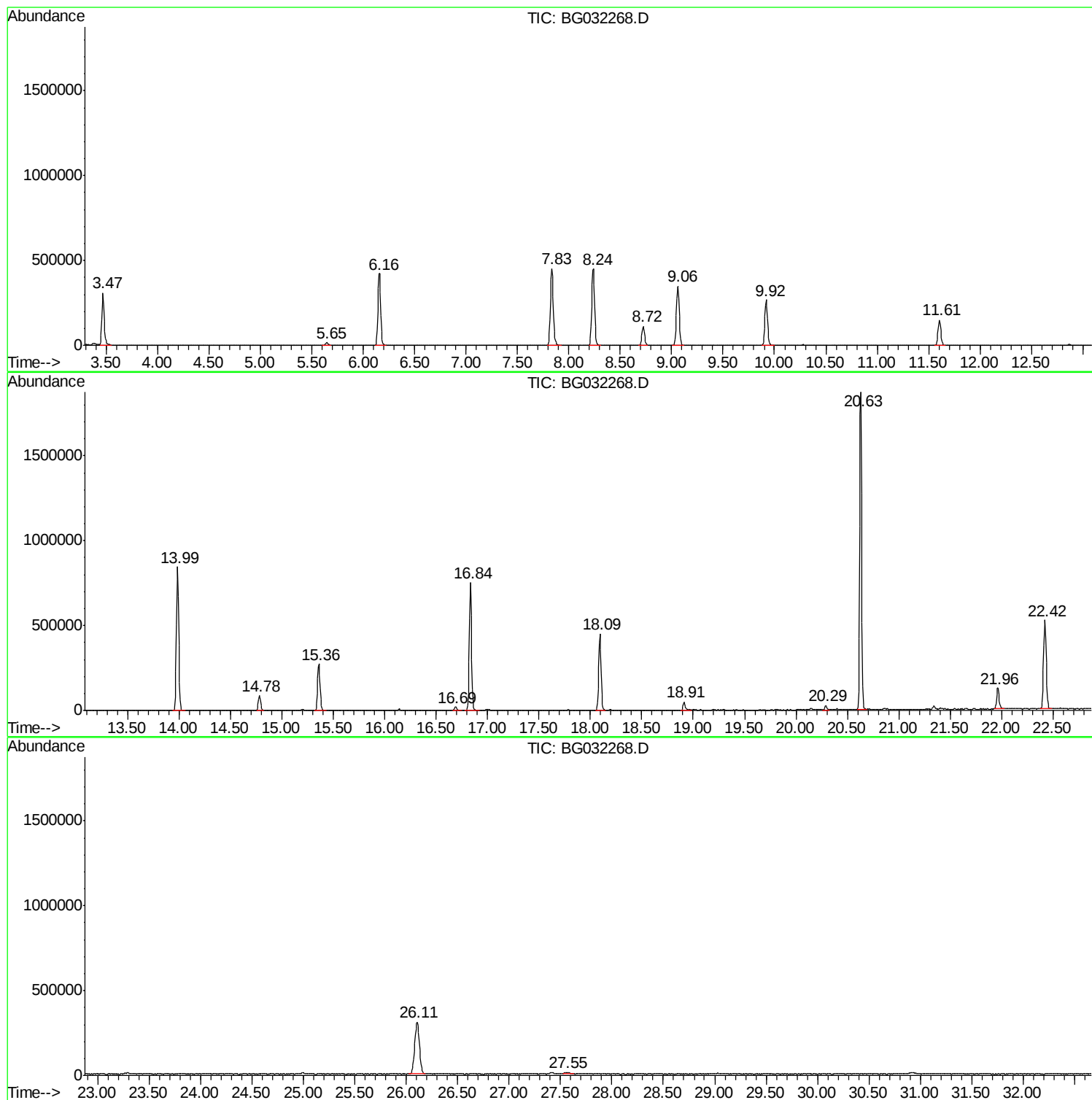
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG011218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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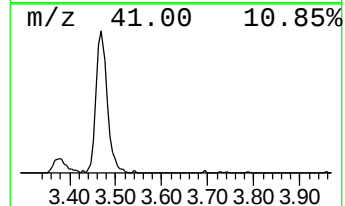
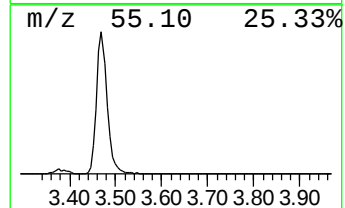
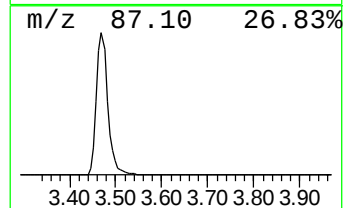
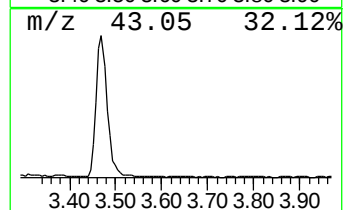
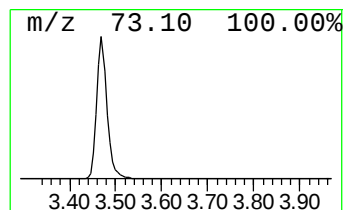
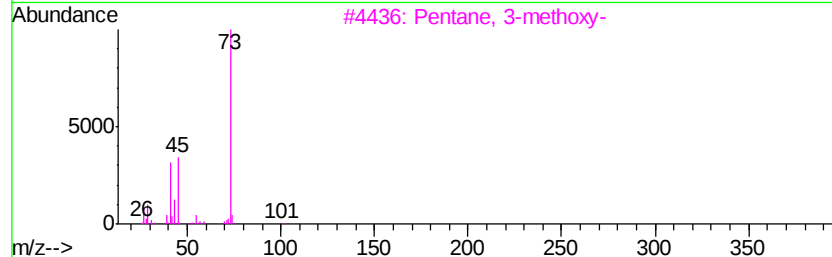
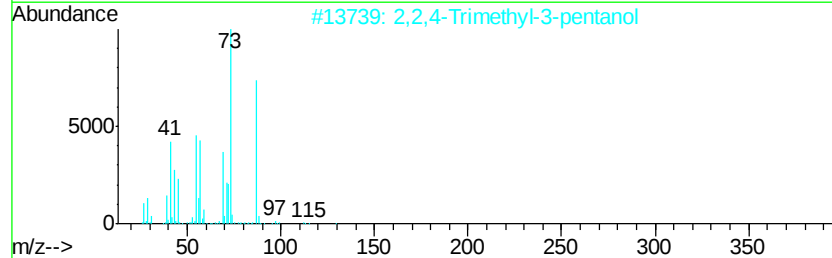
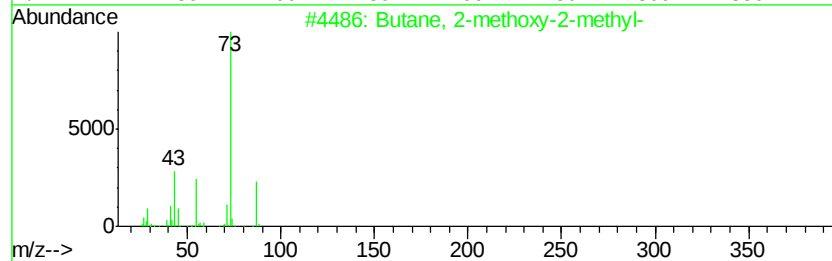
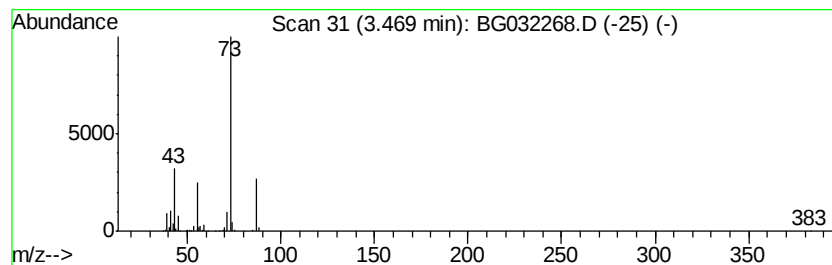
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.47	46.47 ng	478442	1,4-Dichlorobenzene-d4	8.72

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	86
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4			N-Ethylformamide	73	C3H7NO	000627-45-2	9
5			4-Hydroxybutyric acid hydrazide	118	C4H10N2O2	003879-08-1	9



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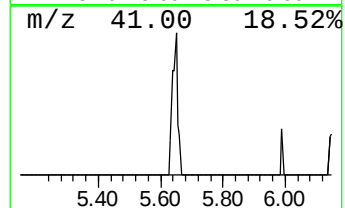
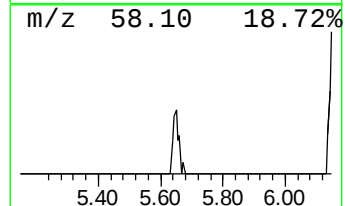
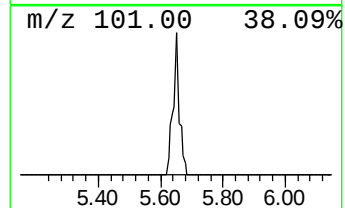
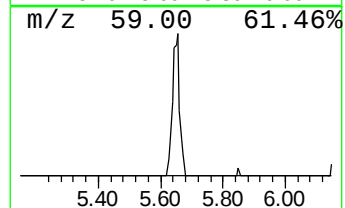
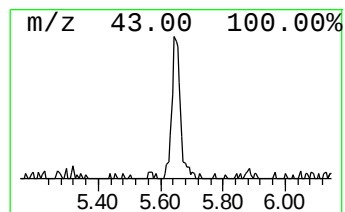
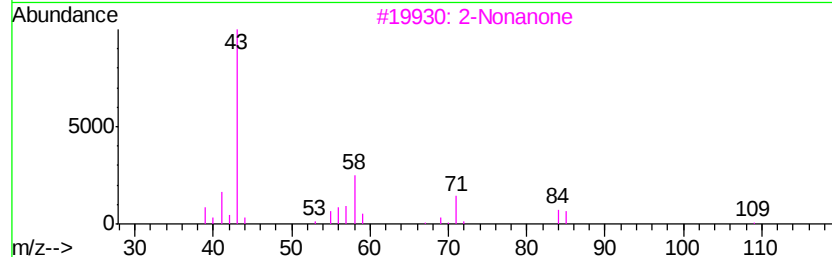
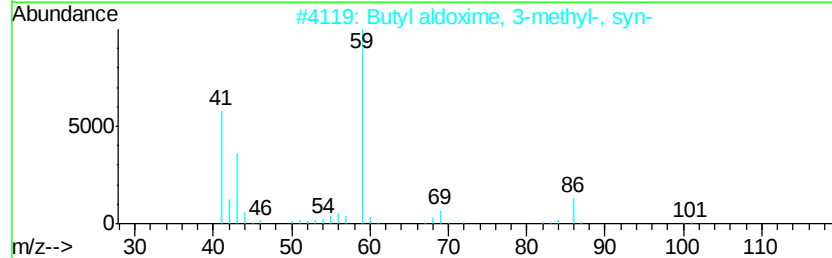
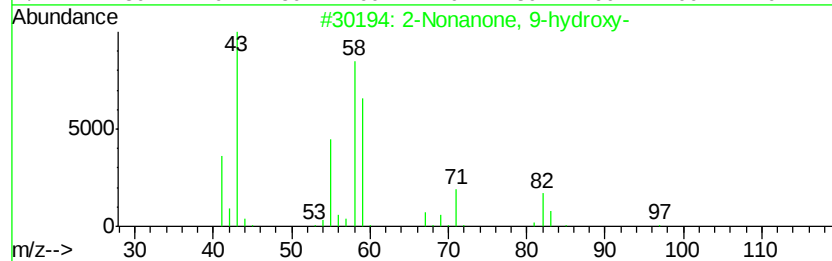
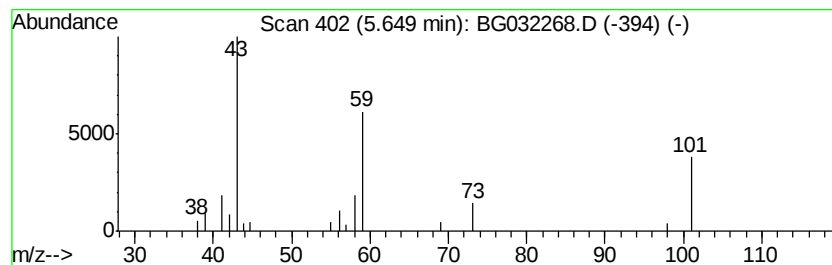
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown5.65 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.65	2.74 ng	28237	1,4-Dichlorobenzene-d4	8.72

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Nonanone, 9-hydroxy-			158	C9H18O2	025368-56-3	23
2	Butyl aldoxime, 3-methyl-, syn-			101	C5H11NO	005780-40-5	10
3	2-Nonanone			142	C9H18O	000821-55-6	10
4	Isobutylamine			73	C4H11N	000078-81-9	9
5	2,3-Butanedione, monooxime			101	C4H7NO2	000057-71-6	9



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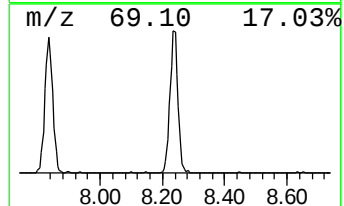
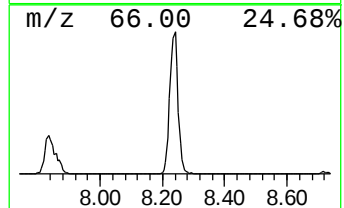
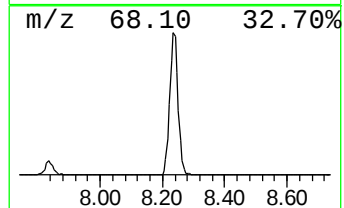
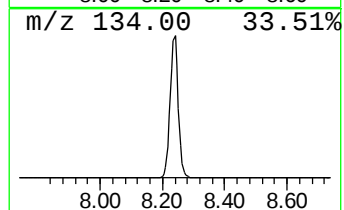
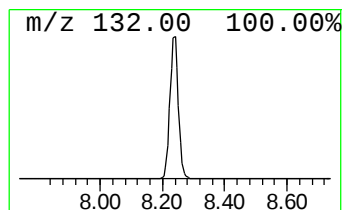
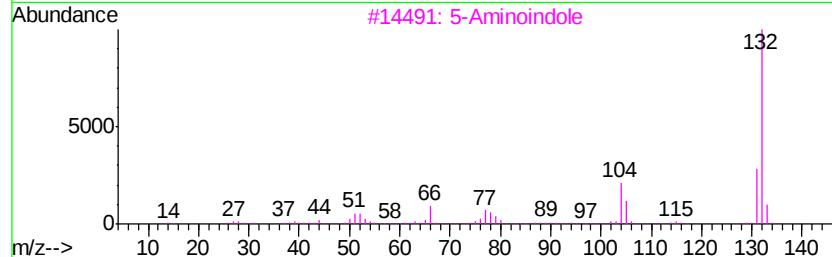
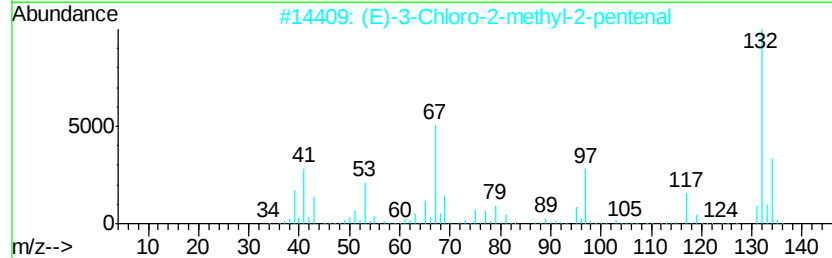
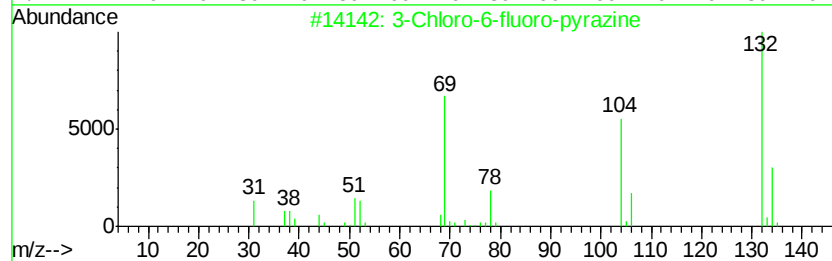
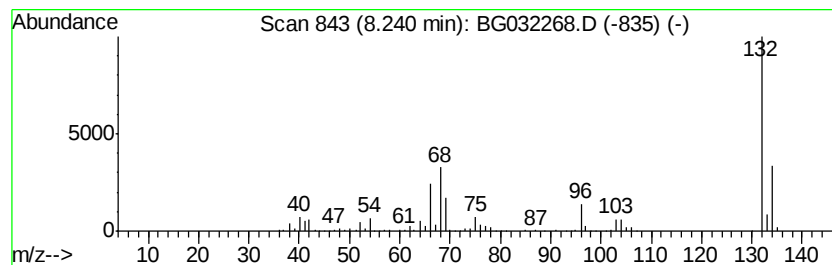
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Peak Number 3 unknown8.24 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.24	82.19 ng	846261	1,4-Dichlorobenzene-d4	8.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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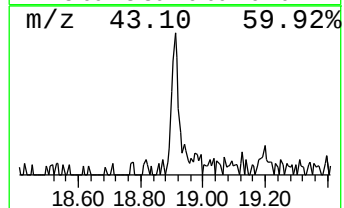
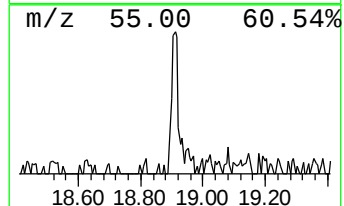
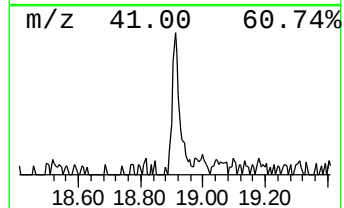
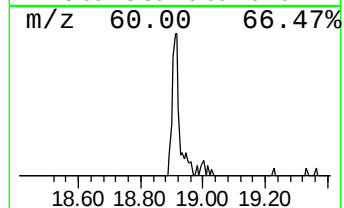
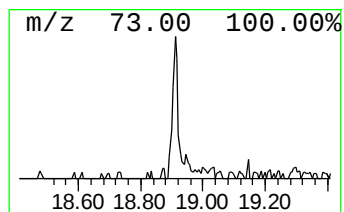
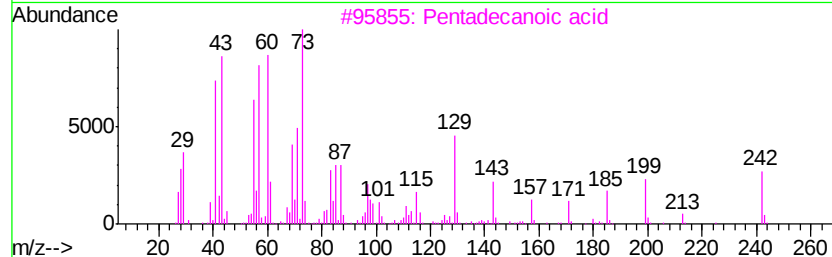
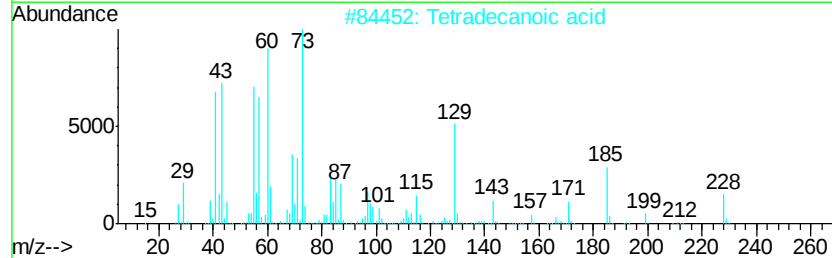
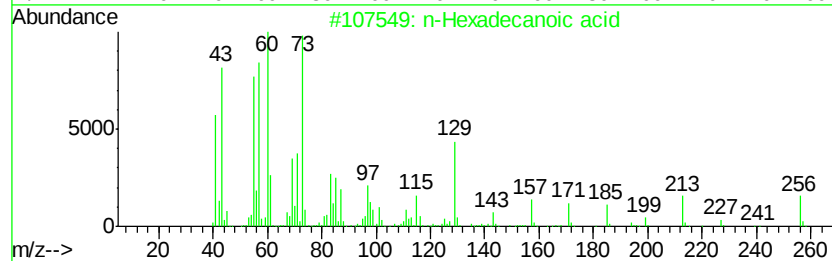
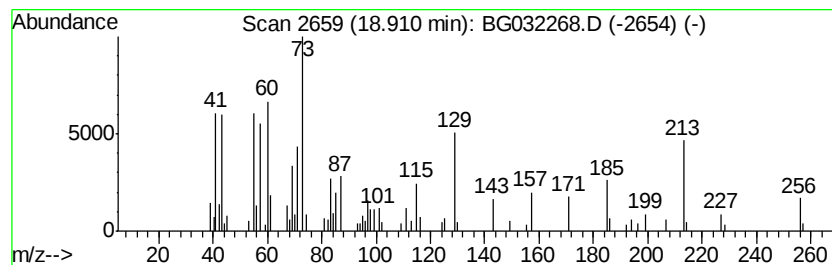
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.91	2.32 ng	81154	Phenanthrene-d10		18.09	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	92
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	53
4		Tridecanoic acid	214	C13H26O2	000638-53-9	49
5		Undecanoic acid	186	C11H22O2	000112-37-8	46



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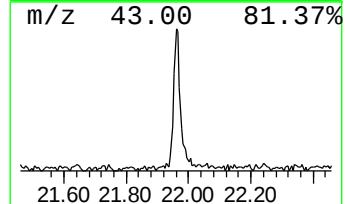
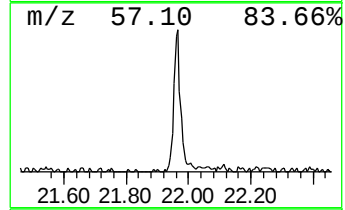
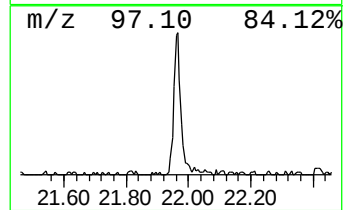
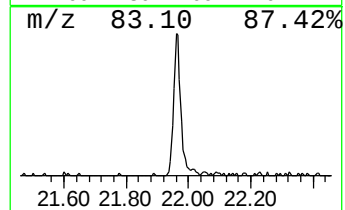
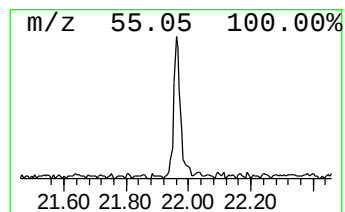
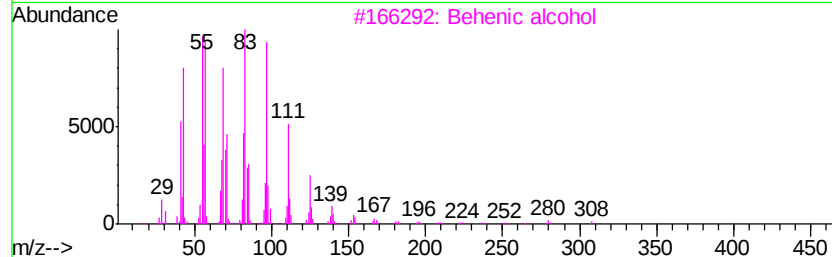
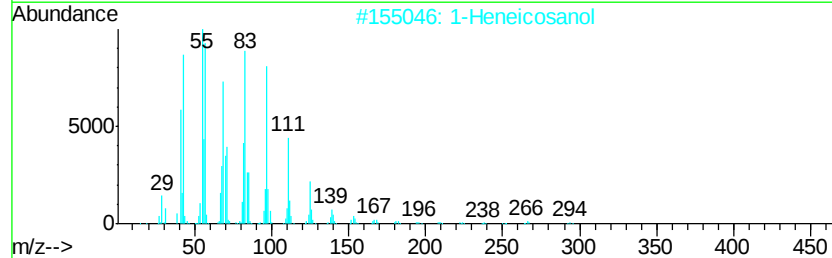
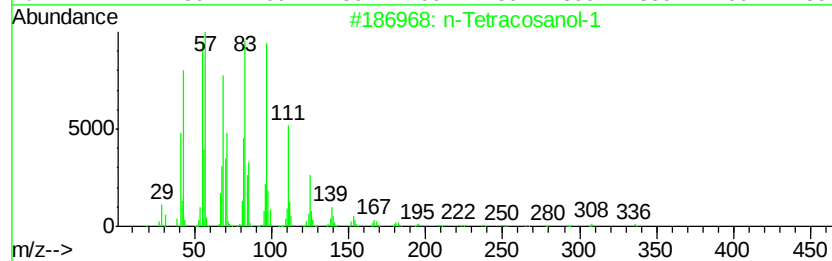
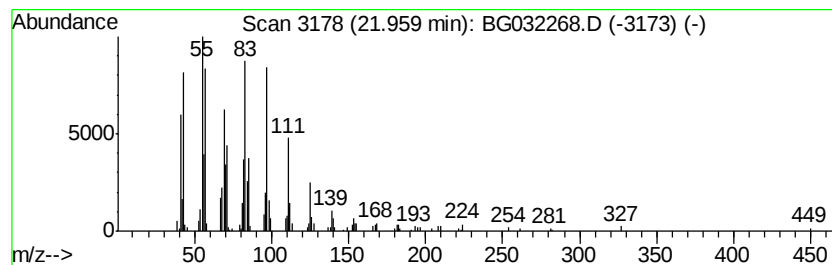
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Peak Number 6 n-Tetracosanol-1 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.		
21.96	4.18 ng	200104	Chrysene-d12	22.42		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Tetracosanol-1	354	C24H50O	000506-51-4	95
2		1-Heneicosanol	312	C21H44O	015594-90-8	94
3		Behenic alcohol	326	C22H46O	000661-19-8	94
4		Octacosanol	410	C28H58O	000557-61-9	94
5		Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	93



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	3.47	46.5	ng	478442	1	8.72	205916	20.0
unknown5.65	5.65	2.7	ng	28237	1	8.72	205916	20.0
unknown8.24	8.24	82.2	ng	846261	1	8.72	205916	20.0
n-Hexadecanoic acid	18.91	2.3	ng	81154	4	18.09	700869	20.0
n-Tetracosanol-1	21.96	4.2	ng	200104	5	22.42	956871	20.0