

Data Path : Z:\HPCHEM1\BNA G\DATA\BG101817\
 Data File : BG029364.D
 Acq On : 19 Oct 2017 13:17
 Operator : SJ/JU
 Sample : I5901-05
 Misc :
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 S-5-20170692

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-BG101617.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	5.240	326	332	344	rVB	206173	315145	6.19%	1.105%
2	5.716	406	413	424	rVB	1159560	1817544	35.70%	6.371%
3	7.320	678	686	702	rBV	1179888	2135074	41.93%	7.484%
4	7.696	742	750	760	rBV	1142239	1954676	38.39%	6.851%
5	8.166	820	830	838	rBV	233246	391923	7.70%	1.374%
6	8.489	878	885	894	rBV	767525	1369807	26.90%	4.801%
7	9.330	1020	1028	1037	rBV	672876	1179783	23.17%	4.135%
8	10.981	1300	1309	1317	rVB	334345	601486	11.81%	2.108%
9	13.413	1714	1723	1736	rBV	1842557	2887949	56.72%	10.122%
10	14.224	1855	1861	1868	rVB	76346	108977	2.14%	0.382%
11	14.782	1947	1956	1964	rBV2	614884	959311	18.84%	3.362%
12	16.263	2201	2208	2216	rBV	1999475	3146353	61.80%	11.028%
13	17.520	2415	2422	2430	rBV2	875565	1338856	26.30%	4.693%
14	18.390	2564	2570	2581	rBV	297824	424768	8.34%	1.489%
15	19.647	2780	2784	2796	rBV	78081	112635	2.21%	0.395%
16	20.111	2857	2863	2870	rBV	3762841	5091582	100.00%	17.846%
17	21.086	3025	3029	3035	rVB	93578	119007	2.34%	0.417%
18	21.410	3079	3084	3102	rBV	396560	648293	12.73%	2.272%
19	21.668	3119	3128	3134	rBV	47960	151071	2.97%	0.530%
20	21.792	3142	3149	3158	rVB2	1002072	1681594	33.03%	5.894%
21	22.226	3217	3223	3230	rBV2	144770	220681	4.33%	0.773%
22	22.620	3284	3290	3302	rVB4	43262	119796	2.35%	0.420%
23	23.672	3464	3469	3483	rVB4	46405	100890	1.98%	0.354%
24	25.099	3701	3712	3724	rVB3	554877	1653181	32.47%	5.794%

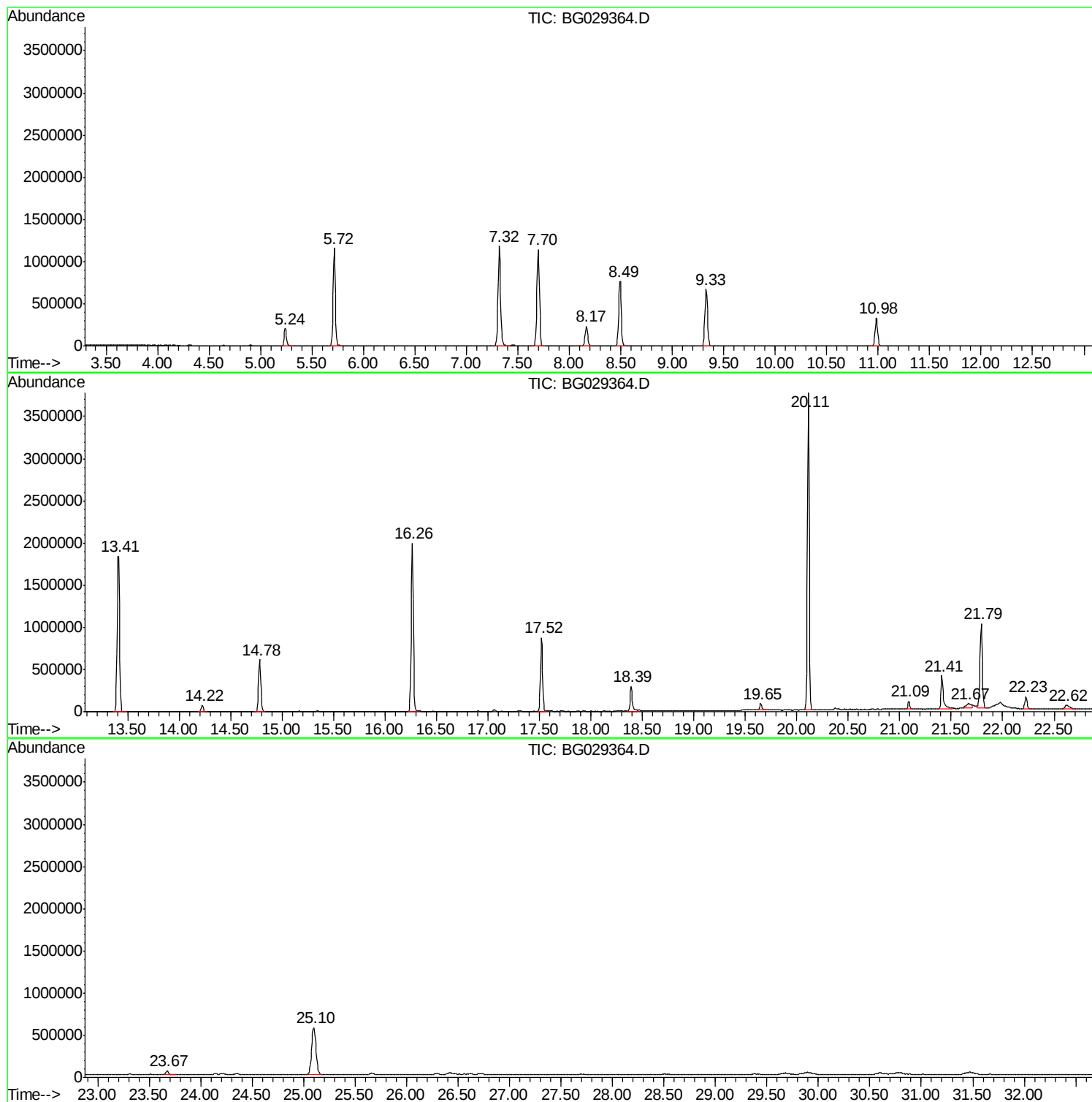
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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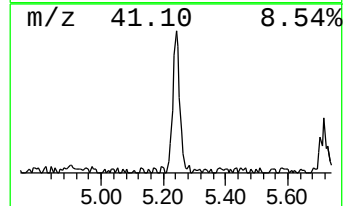
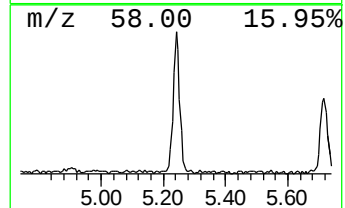
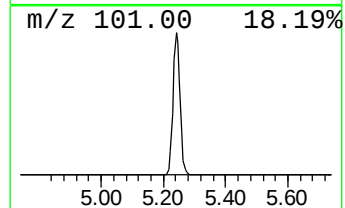
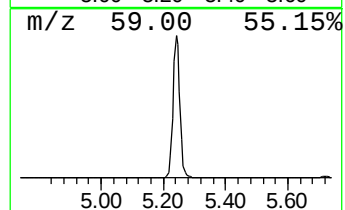
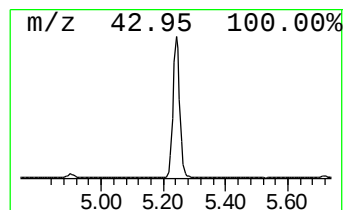
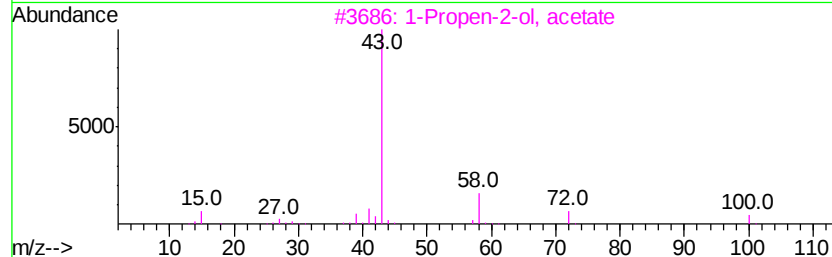
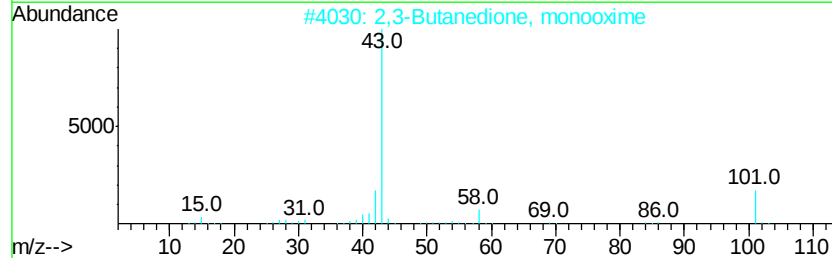
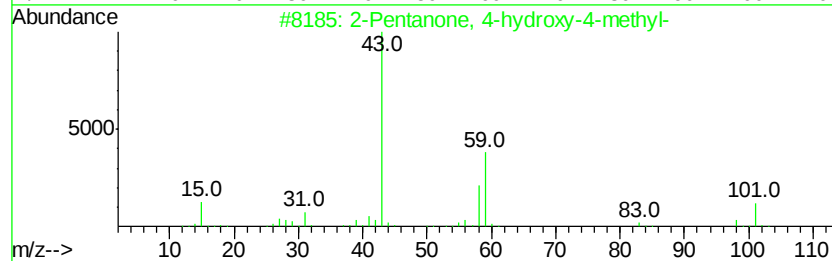
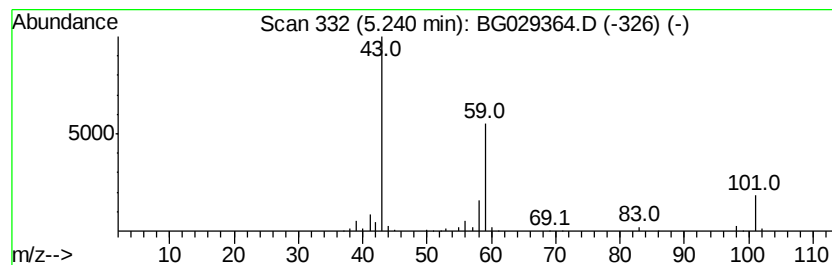
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG101617.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.24	16.08 ng	315145	1,4-Dichlorobenzene-d4	8.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10
3		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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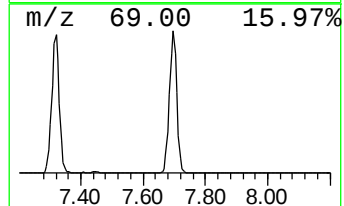
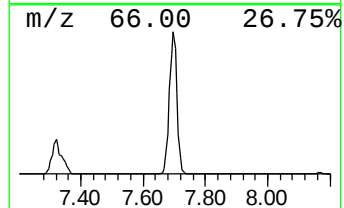
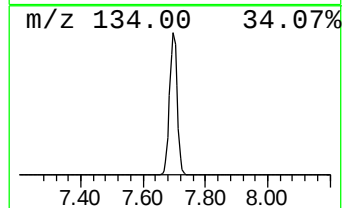
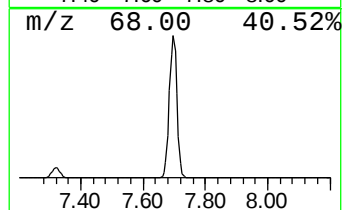
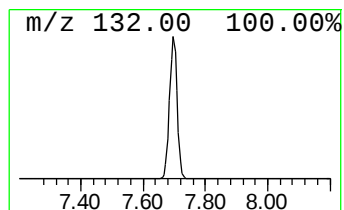
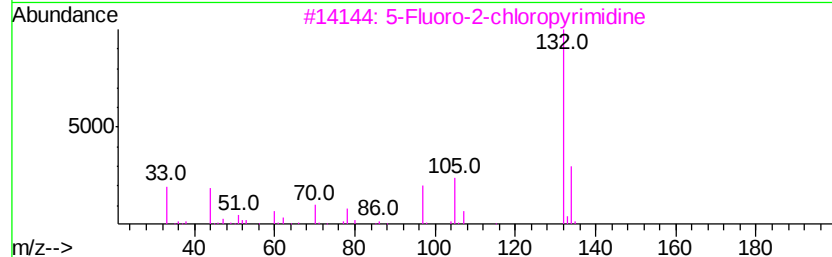
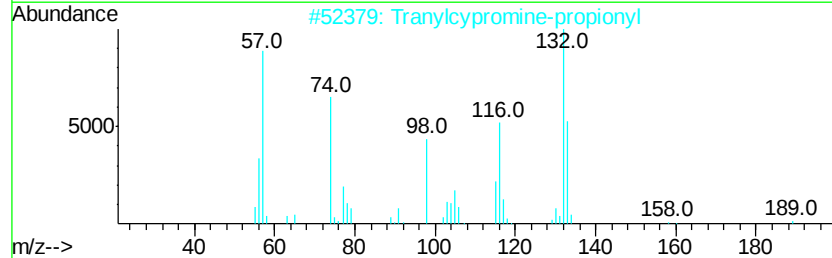
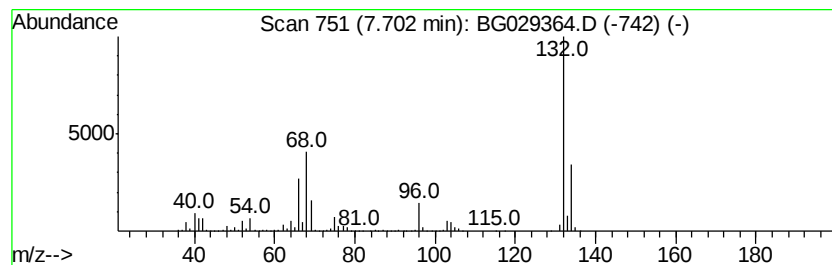
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TIC Library : C:\Database\NIST11.L
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Peak Number 2 unknown7.70 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.70	99.75 ng	1954680	1,4-Dichlorobenzene-d4	8.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
4		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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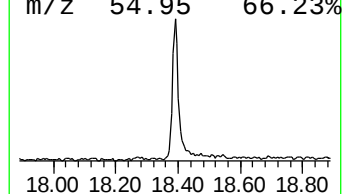
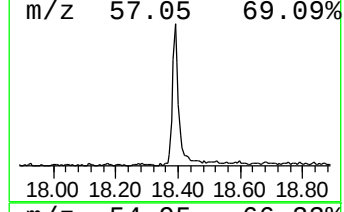
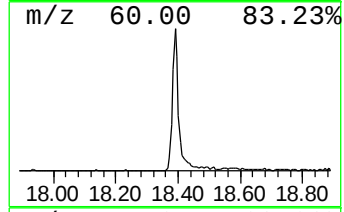
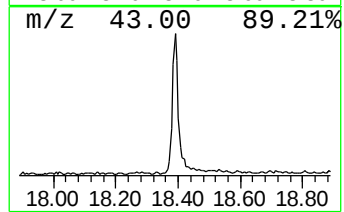
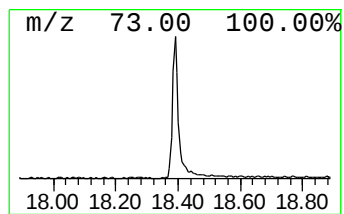
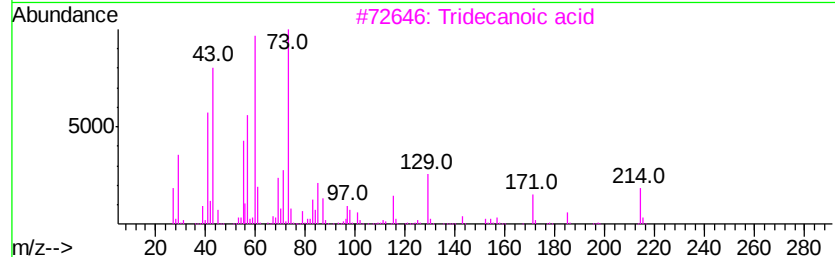
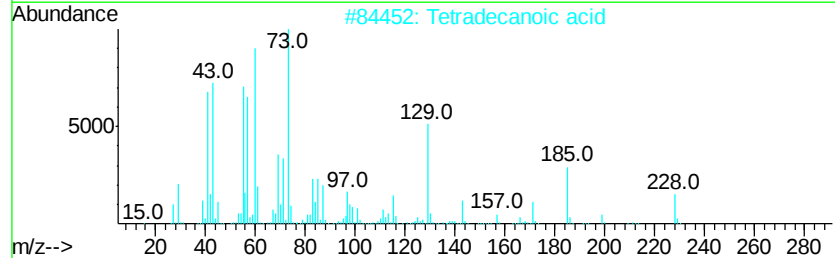
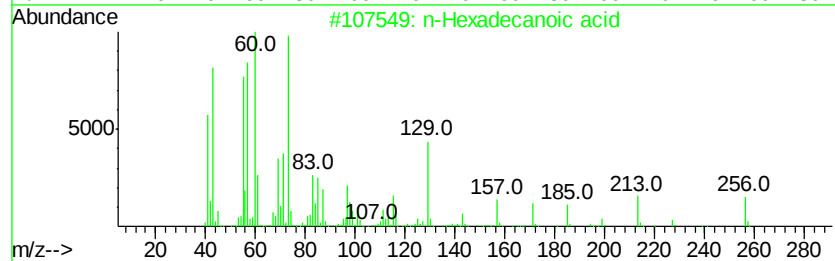
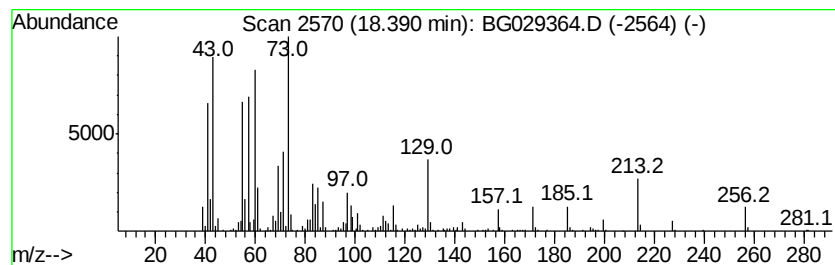
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.39	6.35 ng	424768	Phenanthrene-d10	17.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	89
3	Tridecanoic acid	214	C13H26O2	000638-53-9	76
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
5	Nonanoic acid	158	C9H18O2	000112-05-0	45



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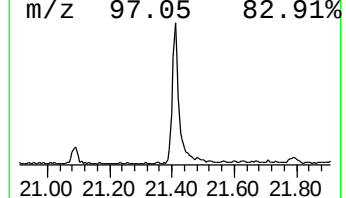
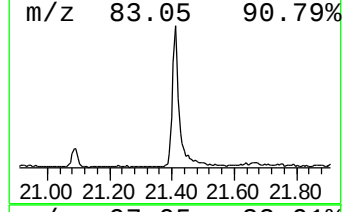
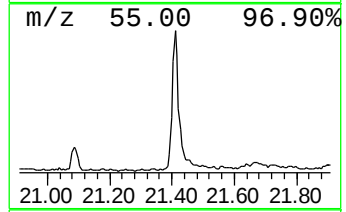
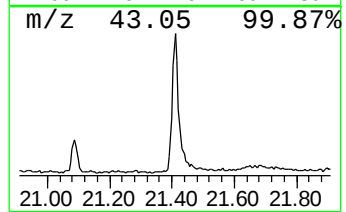
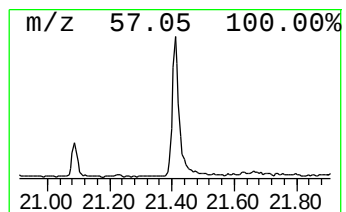
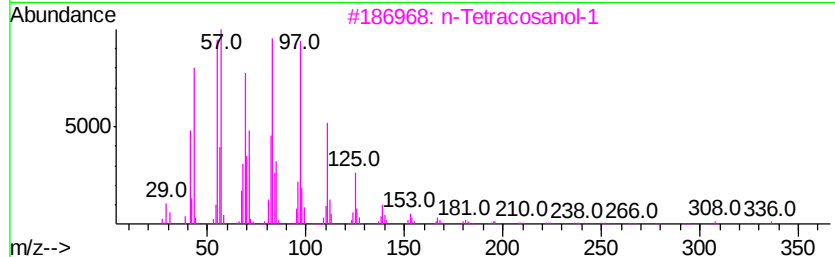
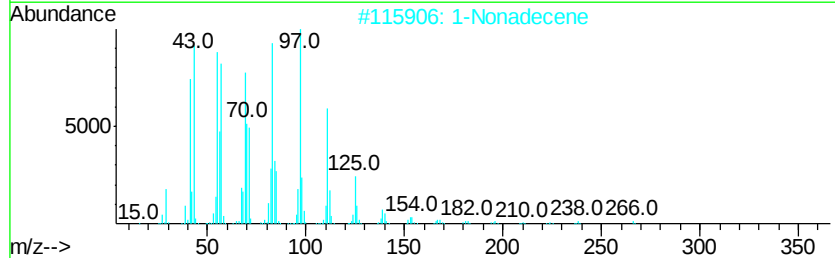
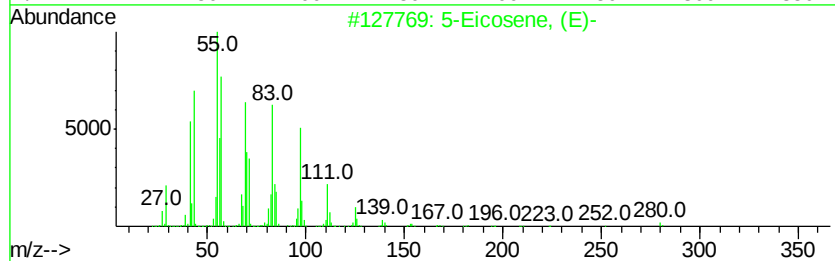
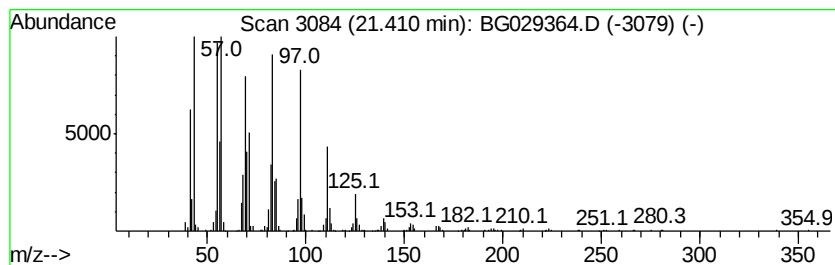
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Peak Number 5 5-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.41	7.71 ng	648293	Chrysene-d12	21.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Eicosene, (E)-	280	C20H40	074685-30-6	99
2		1-Nonadecene	266	C19H38	018435-45-5	99
3		n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
5		n-Nonadecanol-1	284	C19H40O	001454-84-8	94



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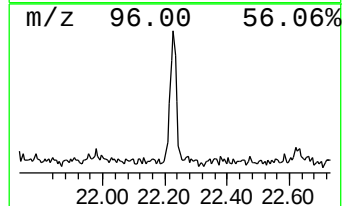
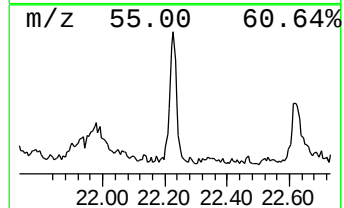
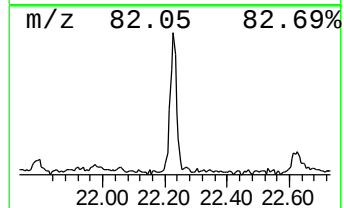
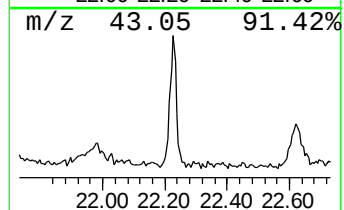
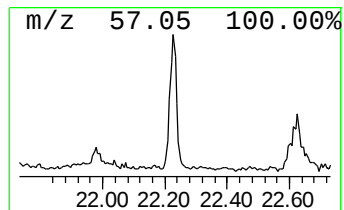
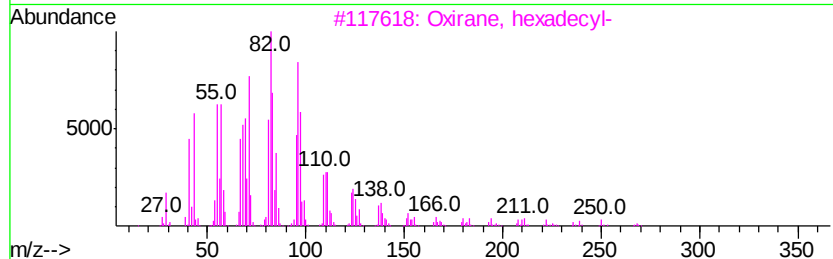
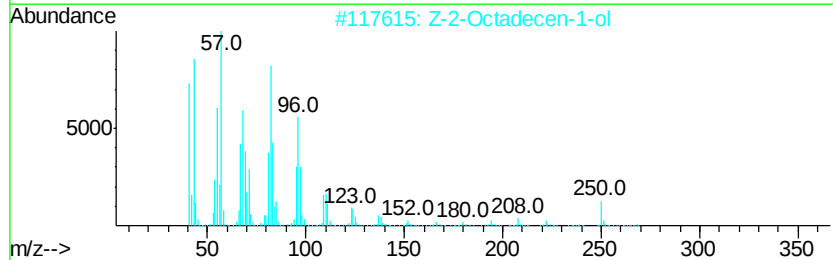
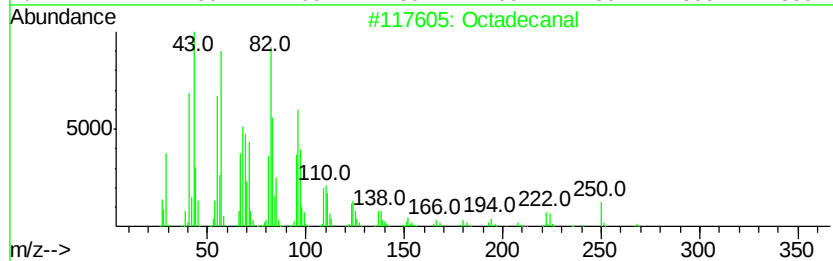
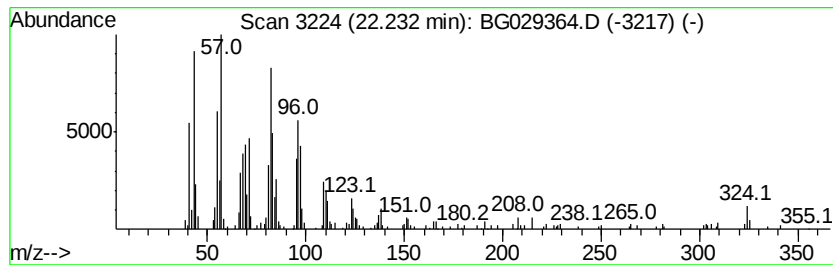
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Peak Number 6 Octadecanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
22.23	2.62 ng	220681	Chrysene-d12	21.79	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal	268	C18H36O	000638-66-4	96
2	Z-2-Octadecen-1-ol	268	C18H36O	1000131-11-0	93
3	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	93
4	Tetracosanal	352	C24H48O	057866-08-7	90
5	E-11(13-Methyl)tetradecen-1-ol a...	268	C17H32O2	1000130-80-4	86



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.24	16.1	ng	315145	1	8.17	391923	20.0
unknown7.70	7.70	99.8	ng	1954680	1	8.17	391923	20.0
n-Hexadecanoic acid	18.39	6.3	ng	424768	4	17.52	1338860	20.0
5-Eicosene, (E)-	21.41	7.7	ng	648293	5	21.79	1681590	20.0
Octadecanal	22.23	2.6	ng	220681	5	21.79	1681590	20.0