

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG061518\
 Data File : BG035185.D
 Acq On : 15 Jun 2018 23:36
 Operator : SJ/JU
 Sample : J3518-01
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 EPE-106-7(3-8)

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.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	5.173	315	321	329	rVB	59376	97240	2.50%	0.487%
2	5.632	392	399	413	rBV	849742	1383753	35.52%	6.924%
3	7.218	661	669	681	rBV	964004	1660559	42.63%	8.309%
4	7.594	724	733	741	rBV	866432	1482931	38.07%	7.420%
5	8.064	806	813	820	rVB	154969	264919	6.80%	1.326%
6	8.387	860	868	878	rVB	572608	990271	25.42%	4.955%
7	9.221	1003	1010	1018	rBV	547601	984645	25.28%	4.927%
8	10.866	1284	1290	1299	rVB	211389	369861	9.49%	1.851%
9	13.309	1696	1706	1721	rBV	1425281	2182814	56.04%	10.922%
10	14.132	1840	1846	1851	rBV	175411	256413	6.58%	1.283%
11	14.684	1933	1940	1948	rBV2	377433	618763	15.88%	3.096%
12	16.170	2186	2193	2206	rBV	1505728	2355350	60.46%	11.786%
13	17.427	2401	2407	2415	rBV	563012	855344	21.96%	4.280%
14	18.309	2550	2557	2568	rBV	166103	261342	6.71%	1.308%
15	19.577	2768	2773	2777	rBV2	59492	88940	2.28%	0.445%
16	20.036	2843	2851	2860	rBV	2900780	3895442	100.00%	19.492%
17	21.334	3067	3072	3085	rBV2	170886	366355	9.40%	1.833%
18	21.692	3126	3133	3140	rBV2	591376	985889	25.31%	4.933%
19	24.923	3672	3683	3697	rBV	290937	883770	22.69%	4.422%

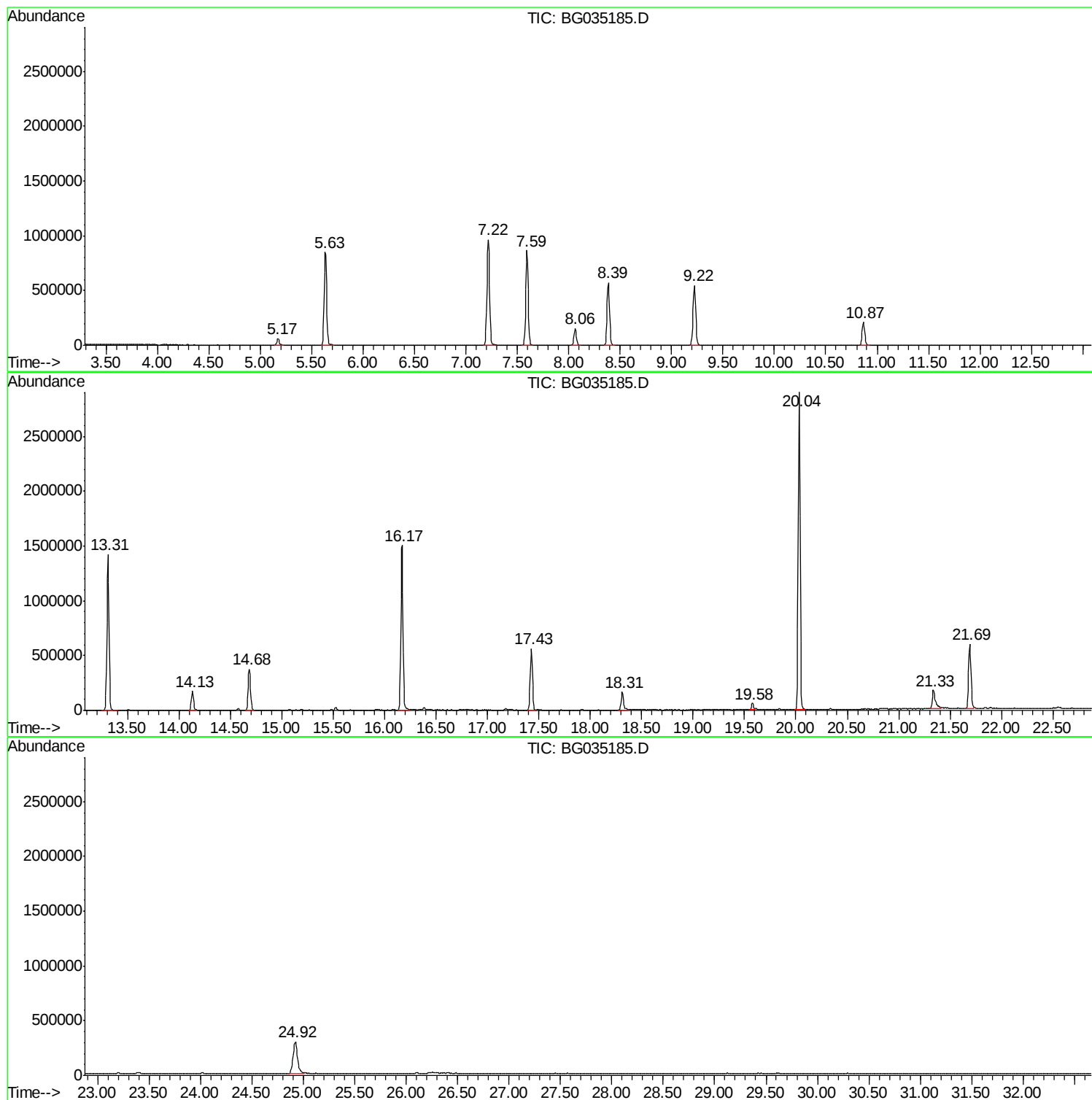
Sum of corrected areas: 19984601

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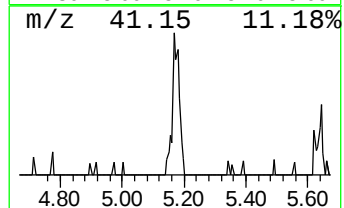
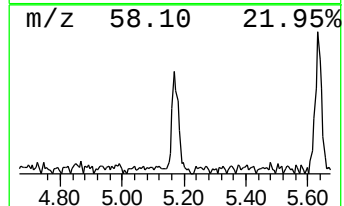
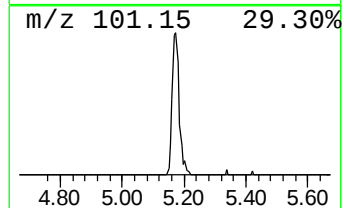
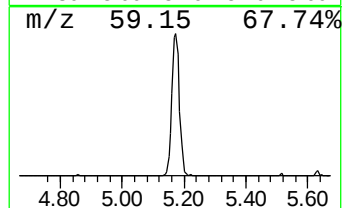
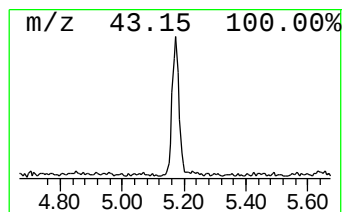
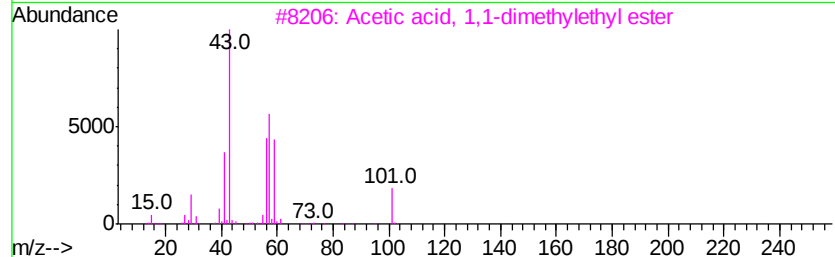
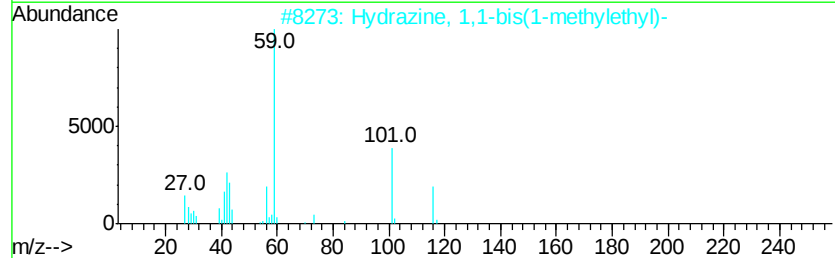
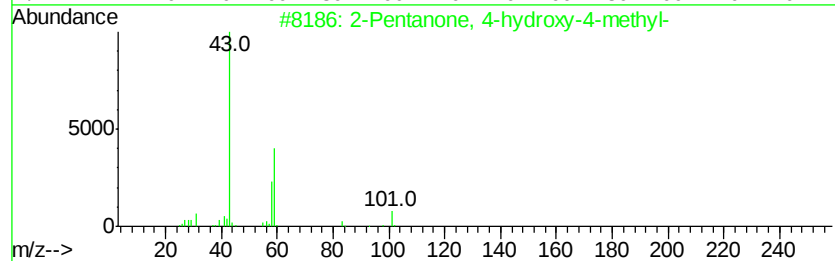
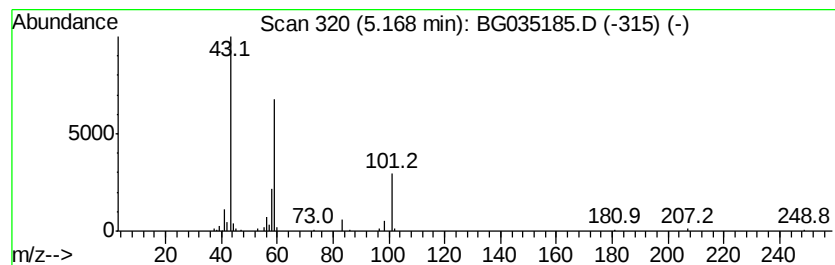
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.17	7.34 ng	97240	1,4-Dichlorobenzene-d4	8.06

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	50
3			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
4			3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	25
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25



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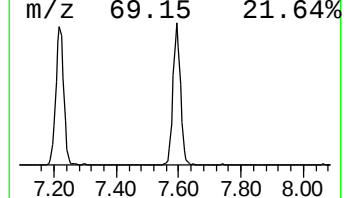
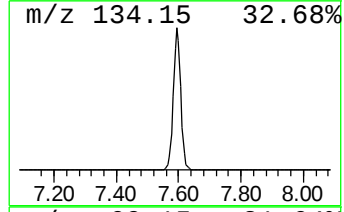
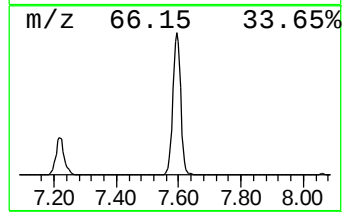
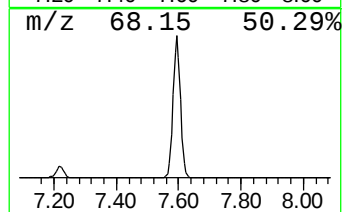
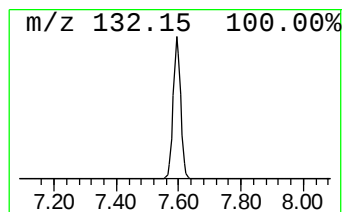
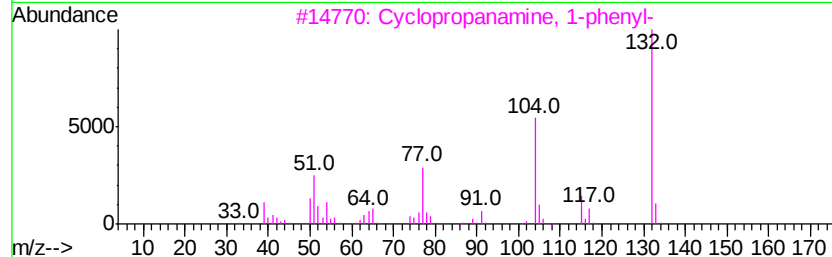
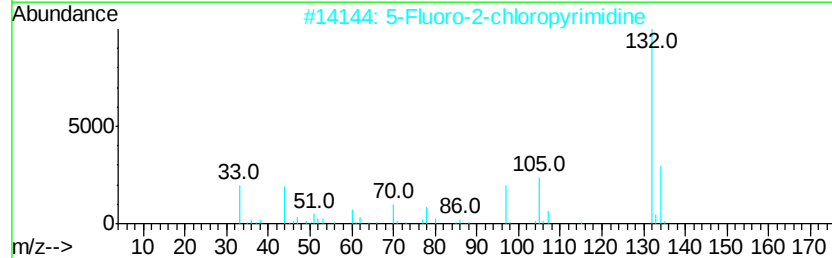
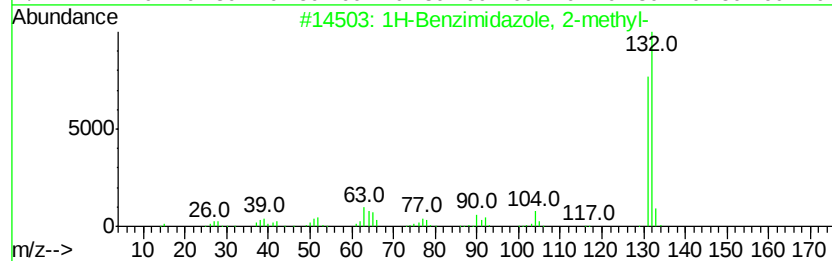
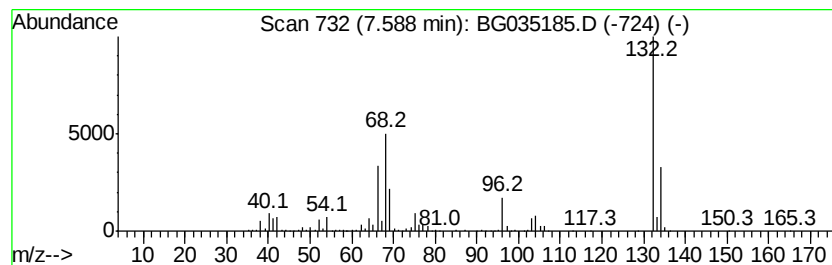
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Peak Number 2 unknown7.59 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.59	111.95 ng	1482930	1,4-Dichlorobenzene-d4	8.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
4		5-Aminoindole	132	C8H8N2	005192-03-0	10
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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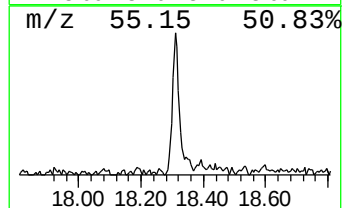
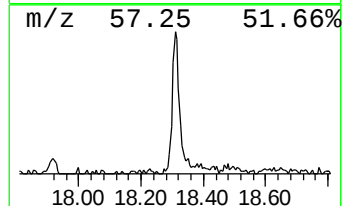
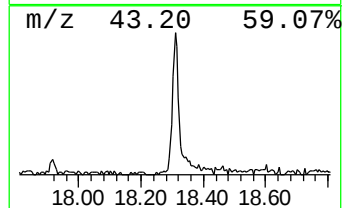
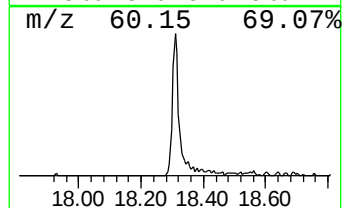
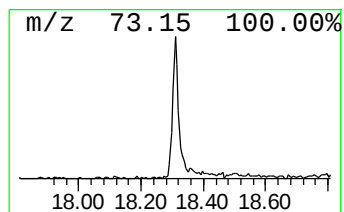
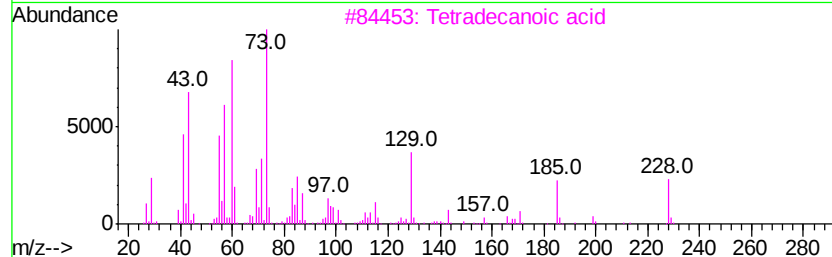
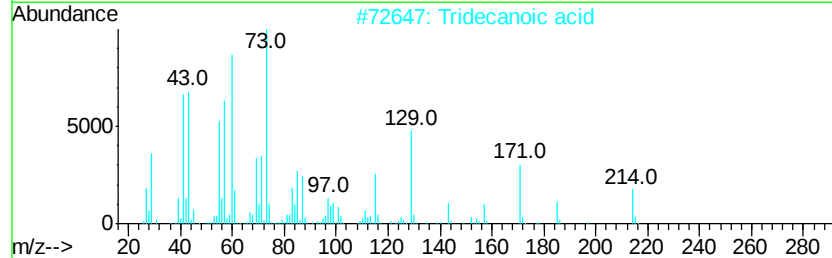
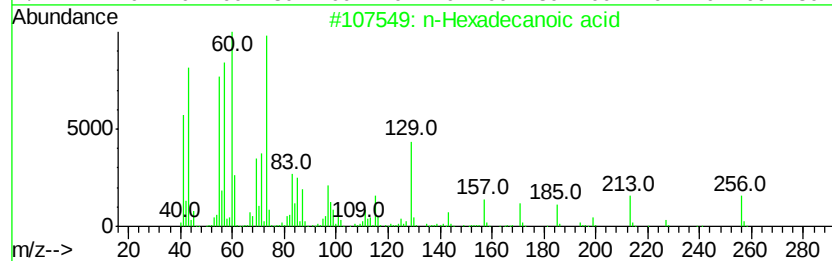
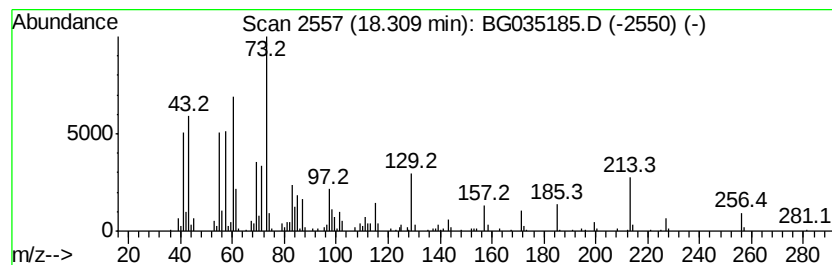
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.31	6.11 ng	261342	Phenanthrene-d10	17.43	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	60
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	46
5	Trehalose	342	C12H22O11	000099-20-7	38



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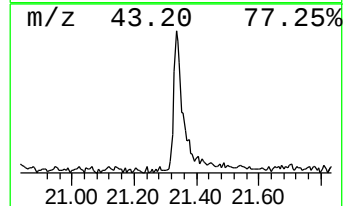
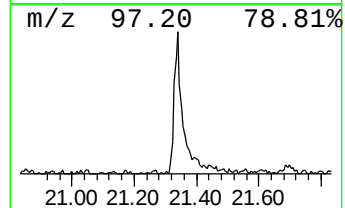
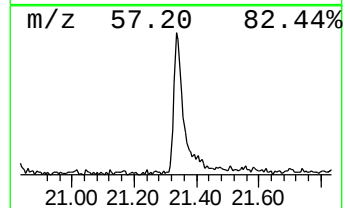
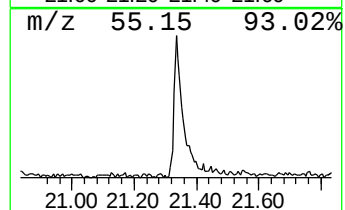
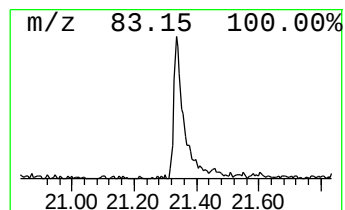
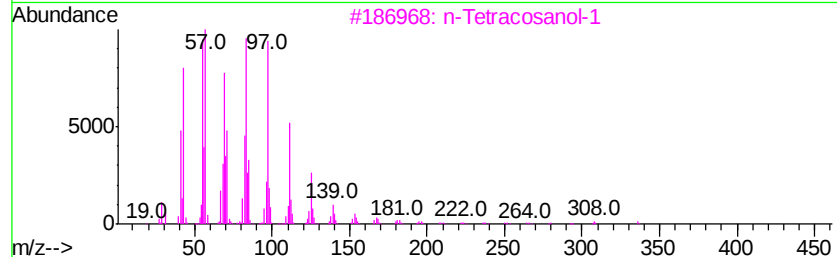
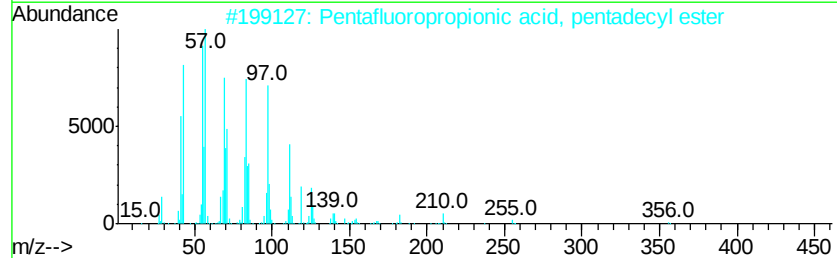
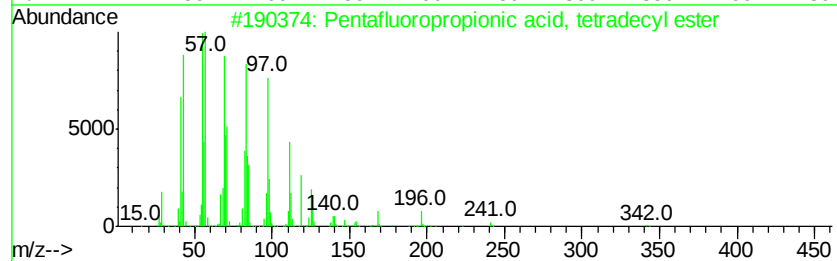
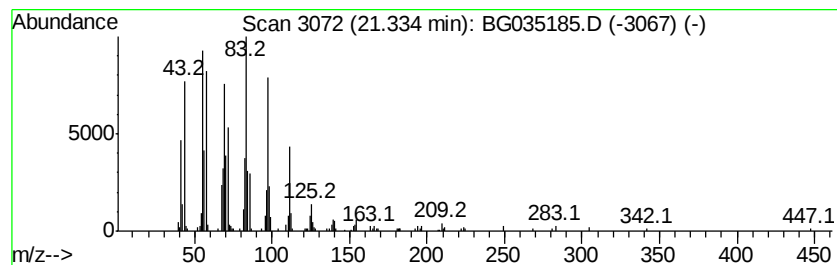
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Peak Number 5 Pentafluoropropionic acid, ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.33	7.43 ng	366355	Chrysene-d12	21.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	91
2		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91
3		n-Tetracosanol-1	354	C24H50O	000506-51-4	91
4		n-Nonadecanol-1	284	C19H40O	001454-84-8	90
5		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	90



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.17	7.3	ng	97240	1	8.06	264919	20.0
unknown7.59	7.59	112.0	ng	1482930	1	8.06	264919	20.0
n-Hexadecanoic acid	18.31	6.1	ng	261342	4	17.43	855344	20.0
Pentafluoropropio...	21.33	7.4	ng	366355	5	21.69	985889	20.0