

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG062117\
 Data File : BG027594.D
 Acq On : 22 Jun 2017 13:38
 Operator : SJ/JU
 Sample : I3799-11
 Misc :
 ALS Vial : 35 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB-07-12.5-13.0

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-BG062117.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	5.642	292	298	307	rVB	65207	107384	5.19%	1.118%
2	6.088	365	374	384	rBV	399183	686373	33.20%	7.147%
3	7.640	630	638	648	rBV	406092	740777	35.83%	7.713%
4	8.033	698	705	715	rVB	386022	711099	34.39%	7.404%
5	8.503	778	785	794	rBV2	74282	130377	6.31%	1.358%
6	8.832	833	841	849	rBV	266327	487025	23.56%	5.071%
7	9.667	976	983	992	rBV	226932	429735	20.78%	4.474%
8	11.323	1257	1265	1273	rBV	102611	193437	9.36%	2.014%
9	13.709	1661	1671	1679	rBV	655761	1056798	51.11%	11.004%
10	14.520	1803	1809	1816	rVB	54348	83505	4.04%	0.869%
11	15.090	1899	1906	1913	rVB2	168630	289149	13.99%	3.011%
12	16.570	2151	2158	2172	rVB	677621	1036189	50.12%	10.789%
13	17.833	2366	2373	2382	rBV2	264183	424135	20.51%	4.416%
14	18.674	2511	2516	2525	rBV2	49156	79951	3.87%	0.832%
15	19.931	2725	2730	2739	rBV3	23347	38863	1.88%	0.405%
16	20.413	2806	2812	2819	rBV	1581585	2067547	100.00%	21.528%
17	21.758	3035	3041	3052	rBV2	29902	73009	3.53%	0.760%
18	22.205	3109	3117	3124	rVB	266261	494788	23.93%	5.152%
19	25.842	3720	3736	3748	rBV3	142420	474032	22.93%	4.936%

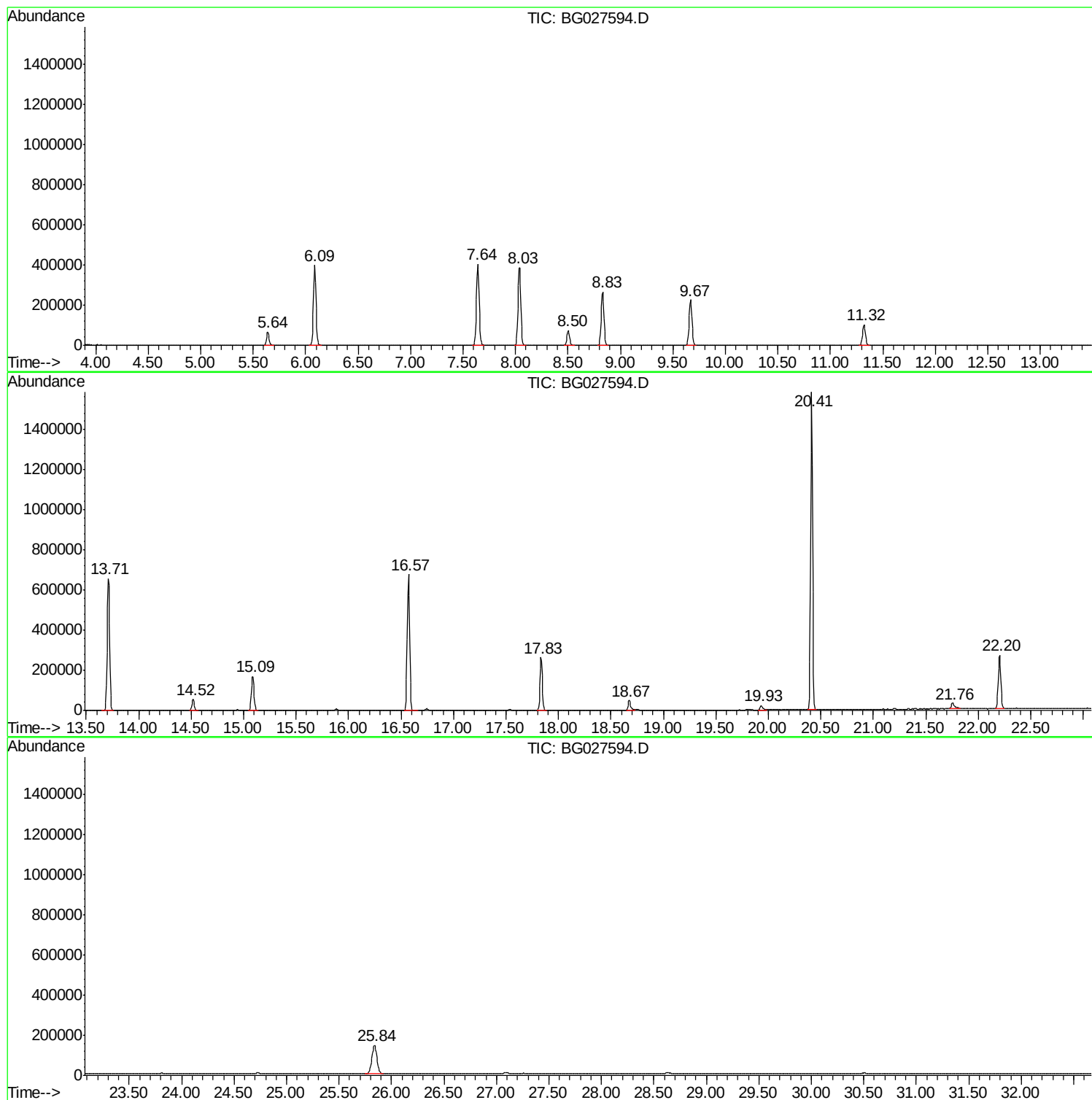
Sum of corrected areas: 9604173

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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG062117.M
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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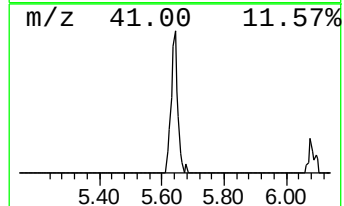
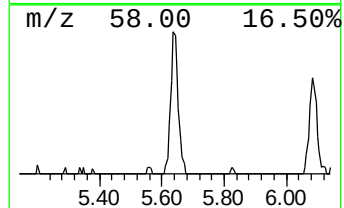
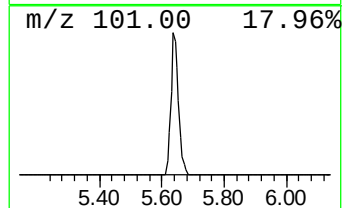
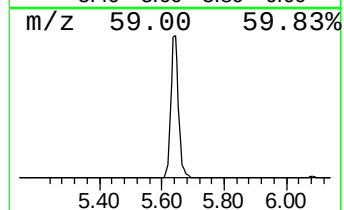
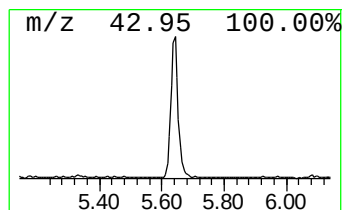
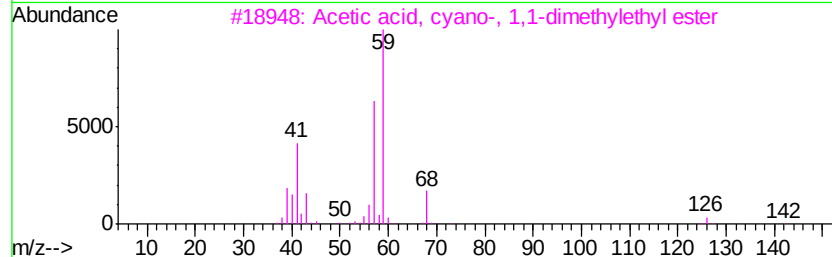
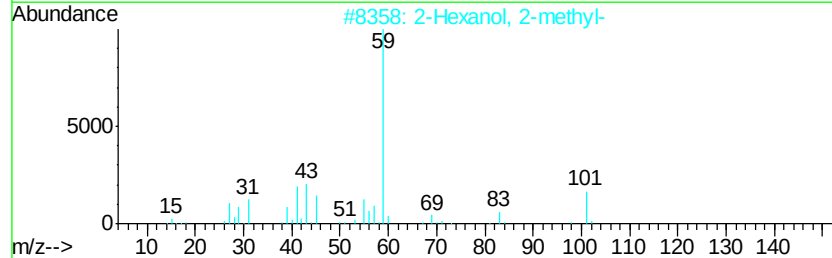
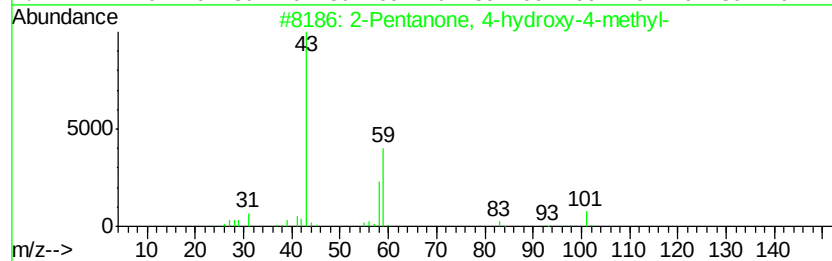
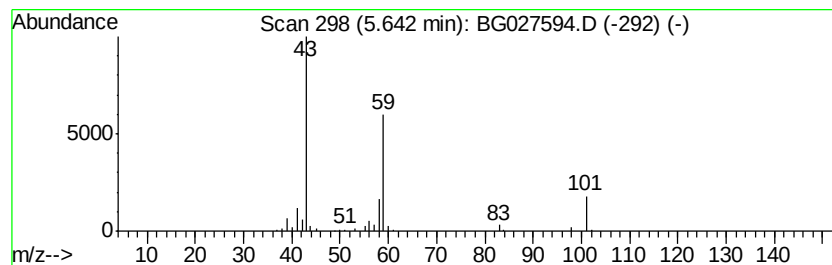
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.64	16.47 ng	107384	1,4-Dichlorobenzene-d4	8.50

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	38
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	37
4			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
5			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	32



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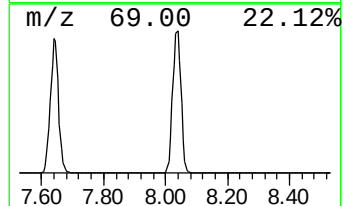
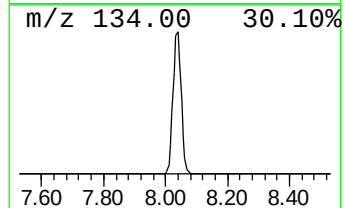
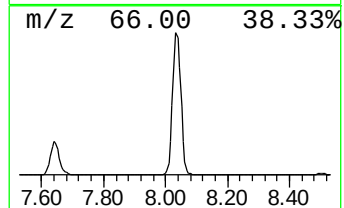
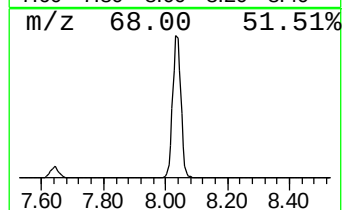
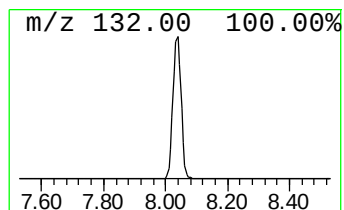
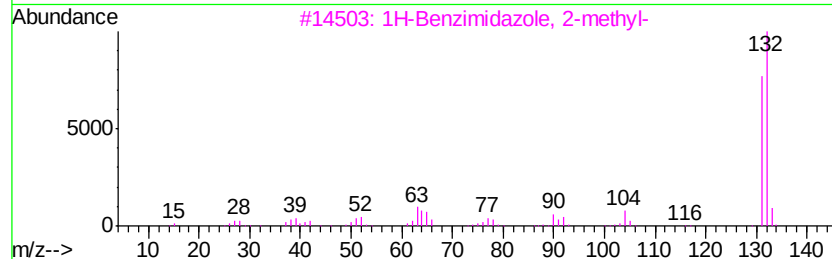
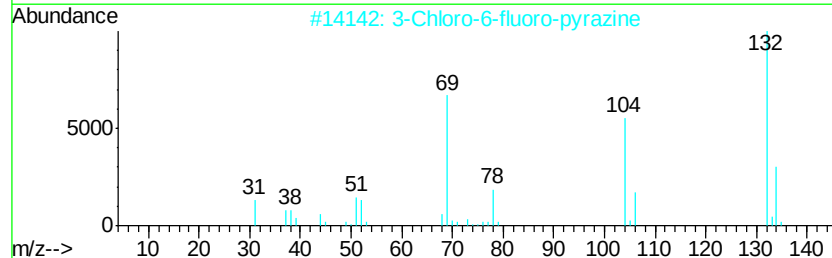
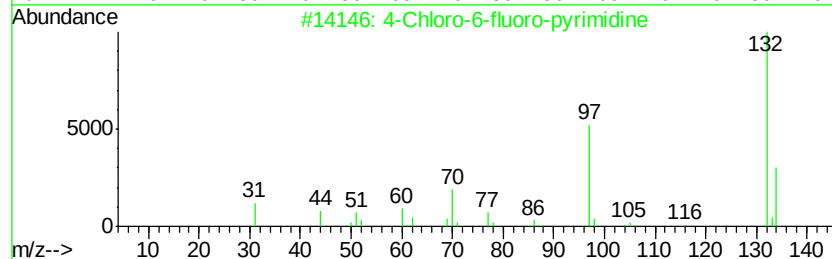
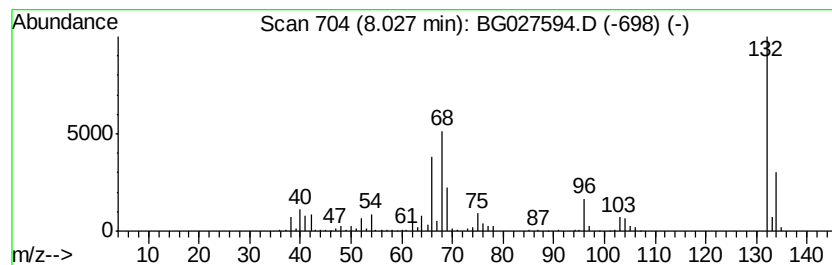
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Peak Number 2 unknown8.03 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.03	109.08 ng	711099	1,4-Dichlorobenzene-d4	8.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4		5-Aminoindole	132	C8H8N2	005192-03-0	22
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12



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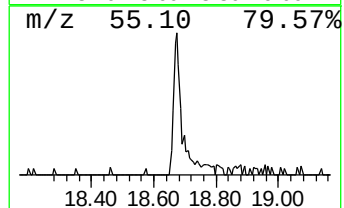
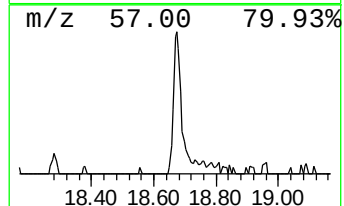
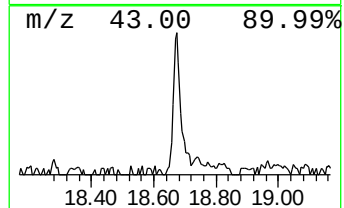
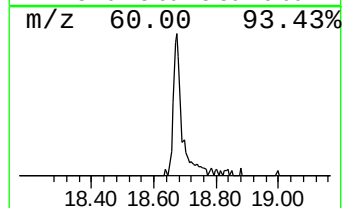
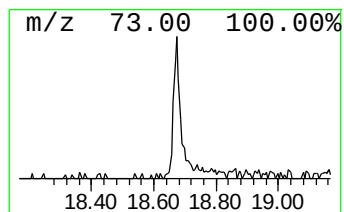
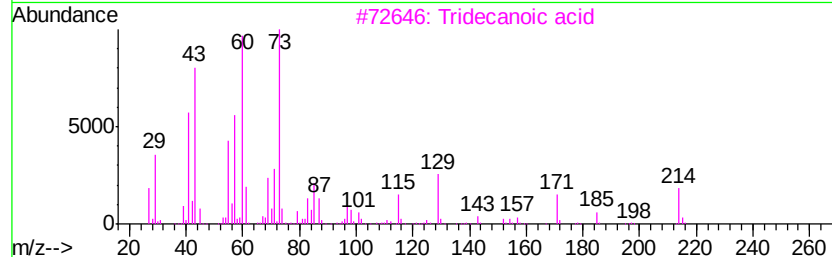
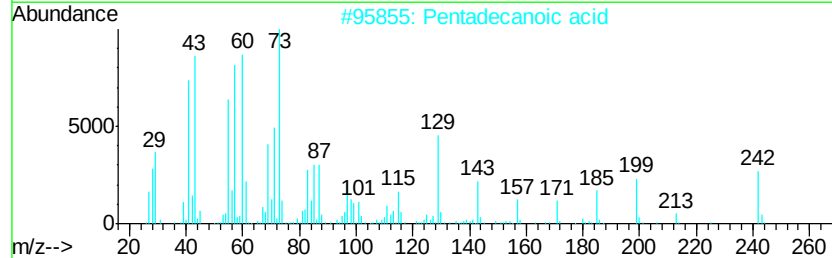
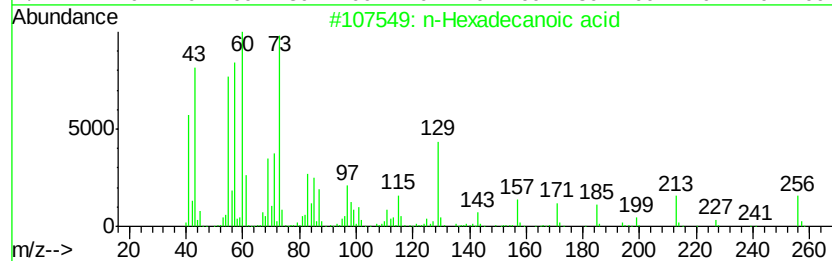
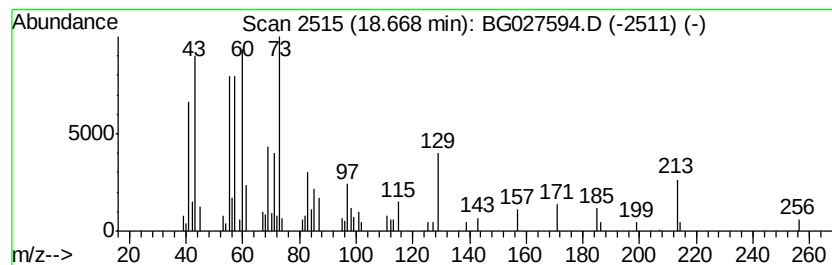
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.67	3.77 ng	79951	Phenanthrene-d10	17.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3		Tridecanoic acid	214	C13H26O2	000638-53-9	81
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5		n-Decanoic acid	172	C10H20O2	000334-48-5	52



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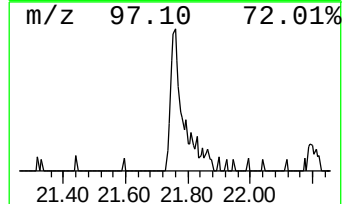
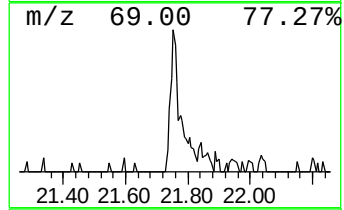
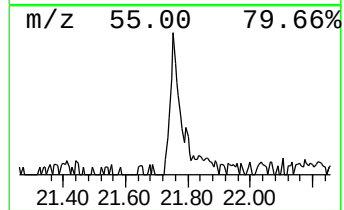
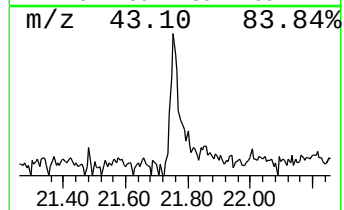
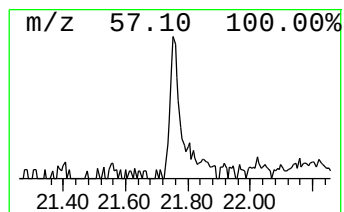
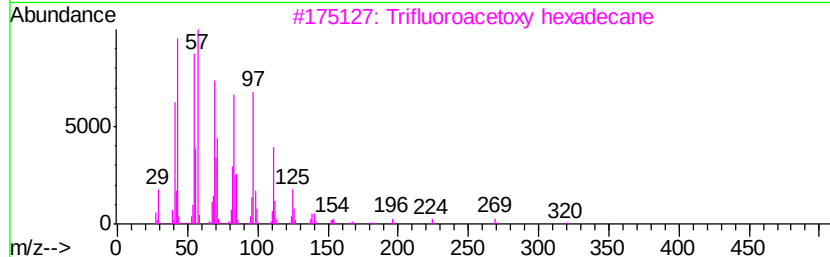
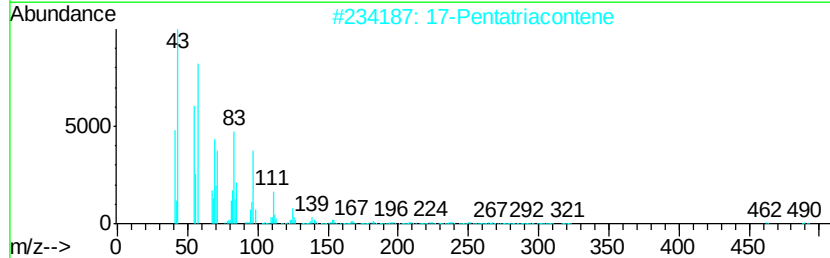
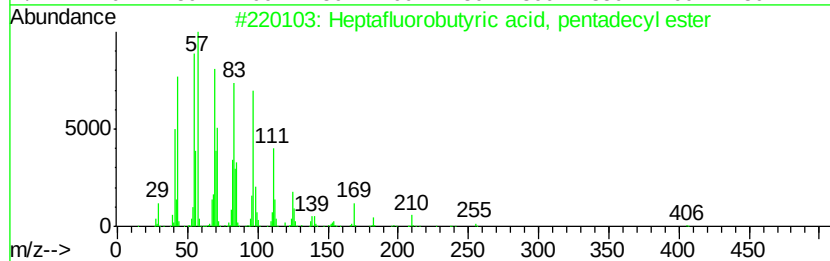
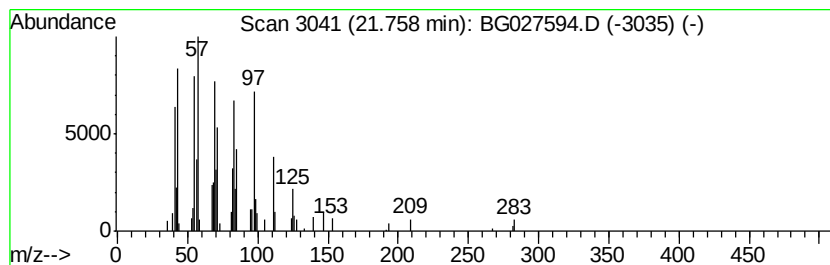
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Peak Number 5 Heptafluorobutyric acid, pe... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.76	2.95 ng	73009	Chrysene-d12	22.20

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93
2		17-Pentatriacontene	491	C35H70	006971-40-0	91
3		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	87
4		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	87
5		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	87



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.64	16.5	ng	107384	1	8.50	130377	20.0
unknown8.03	8.03	109.1	ng	711099	1	8.50	130377	20.0
n-Hexadecanoic acid	18.67	3.8	ng	79951	4	17.83	424135	20.0
Heptafluorobutyri...	21.76	3.0	ng	73009	5	22.20	494788	20.0