

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG062618\
 Data File : BG035420.D
 Acq On : 26 Jun 2018 21:30
 Operator : JU/SJ
 Sample : J3688-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 EPE-109-6(60-62)

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:\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	5.162	314	319	326	rBV	87602	139218	3.47%	0.636%
2	5.632	391	399	412	rBV	996823	1641989	40.91%	7.506%
3	7.212	660	668	680	rBV	1075943	1890838	47.11%	8.644%
4	7.588	723	732	743	rBV	1001608	1736236	43.26%	7.937%
5	8.052	804	811	819	rBV	197650	326766	8.14%	1.494%
6	8.375	857	866	875	rBV	737592	1281974	31.94%	5.860%
7	9.209	1000	1008	1016	rBV	606861	1117834	27.85%	5.110%
8	10.854	1280	1288	1297	rBV	246262	425076	10.59%	1.943%
9	13.298	1697	1704	1714	rBV	1712161	2625978	65.43%	12.004%
10	14.120	1838	1844	1850	rBV	257763	381036	9.49%	1.742%
11	14.673	1931	1938	1948	rBV2	411425	663885	16.54%	3.035%
12	16.159	2183	2191	2204	rBV	1553056	2304985	57.43%	10.537%
13	17.416	2398	2405	2412	rBV2	566218	865505	21.56%	3.957%
14	18.297	2549	2555	2563	rBV	124806	187843	4.68%	0.859%
15	19.560	2765	2770	2779	rBV3	46671	72734	1.81%	0.332%
16	20.018	2842	2848	2854	rBV	2958653	4013665	100.00%	18.348%
17	21.322	3064	3070	3080	rBV3	79994	195375	4.87%	0.893%
18	21.681	3123	3131	3140	rBV2	600021	1010684	25.18%	4.620%
19	22.527	3270	3275	3280	rBV8	28608	55591	1.39%	0.254%
20	24.894	3666	3678	3690	rBV2	332746	938053	23.37%	4.288%

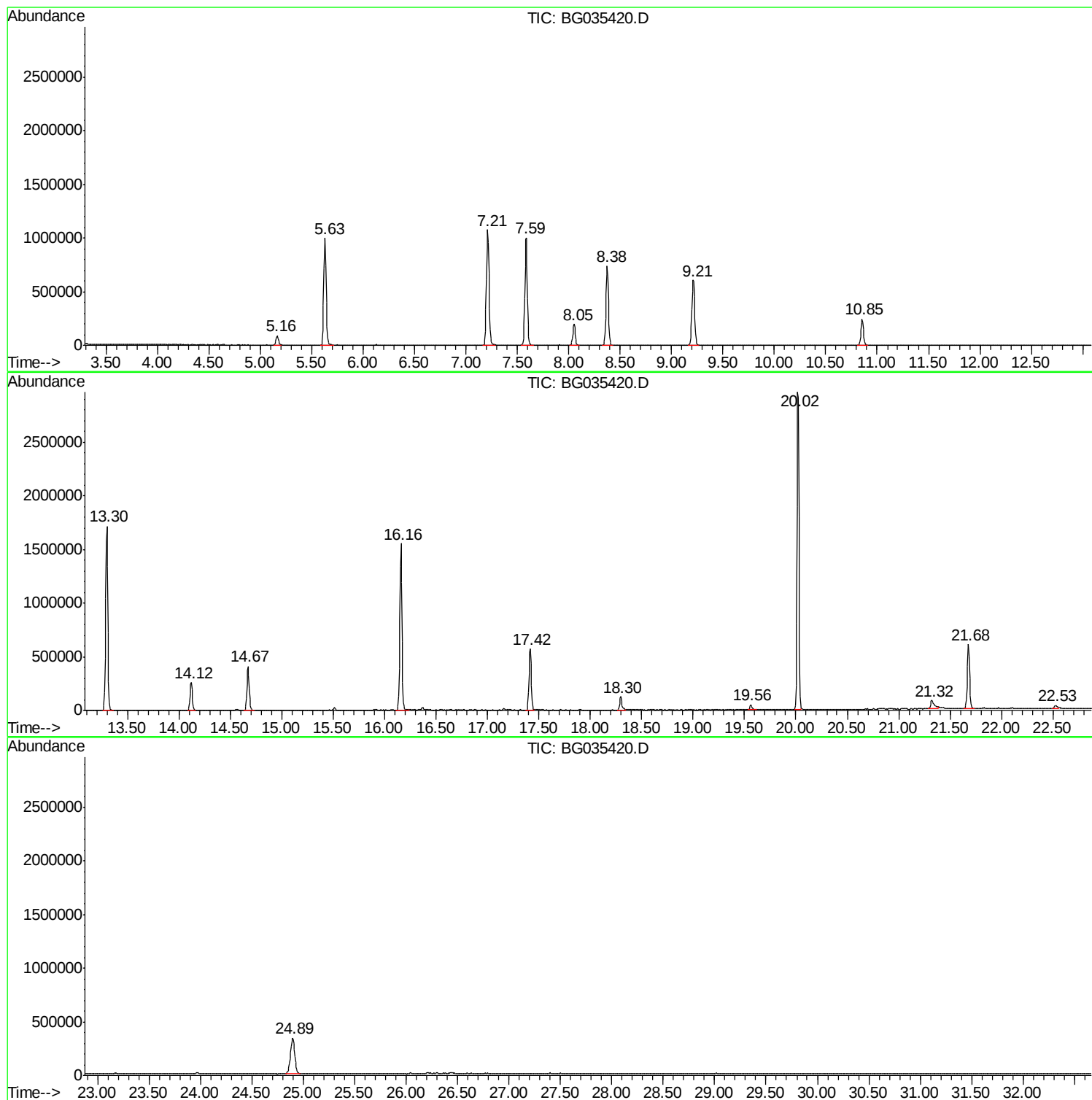
Sum of corrected areas: 21875265

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Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG060718.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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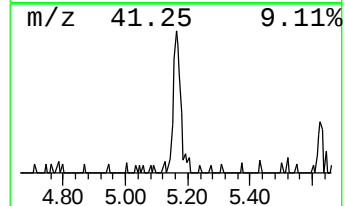
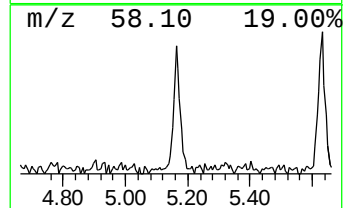
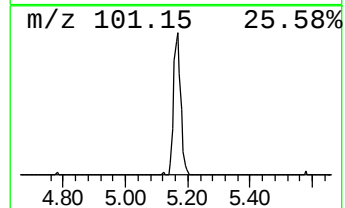
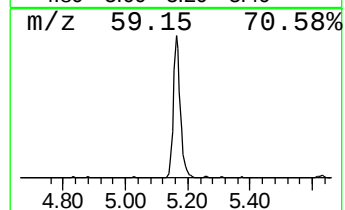
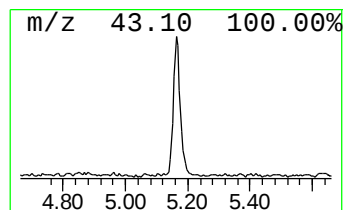
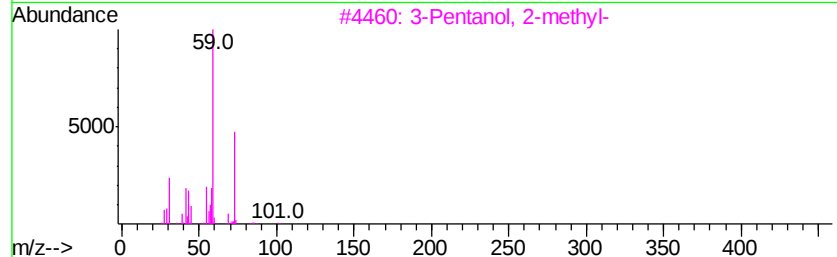
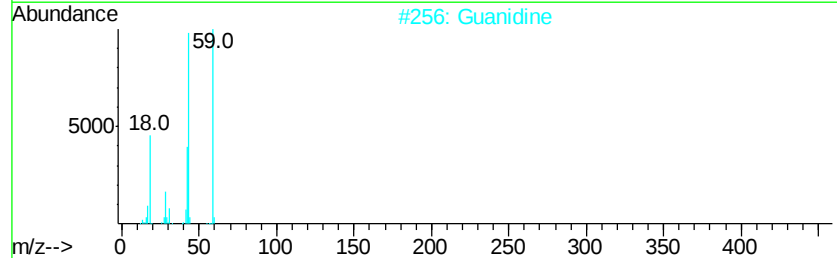
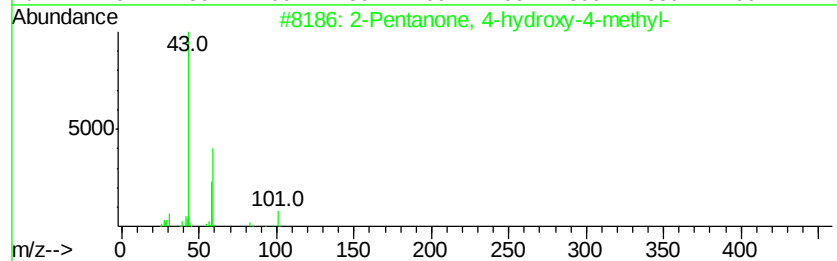
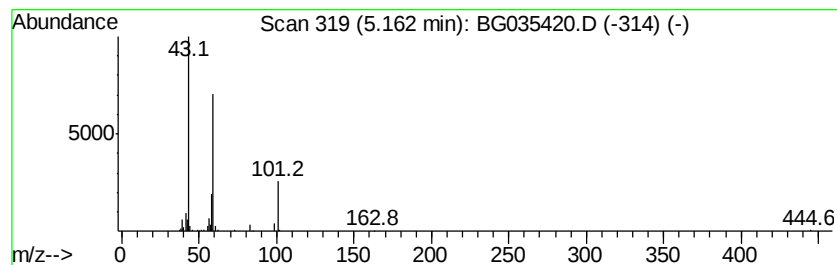
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.16	8.52 ng	139218	1,4-Dichlorobenzene-d4	8.05

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Guanidine	59	CH5N3	000113-00-8	43
3			3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	38
4			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	37
5			Succinic acid, heptyl 2-methoxye...	274	C14H26O5	1000325-80-7	33



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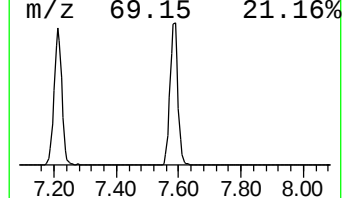
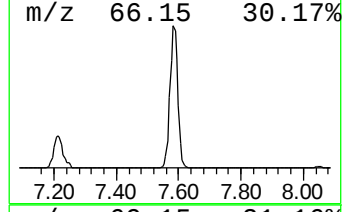
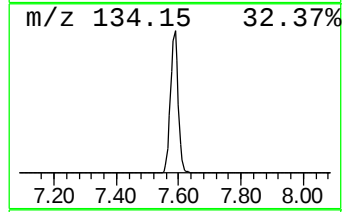
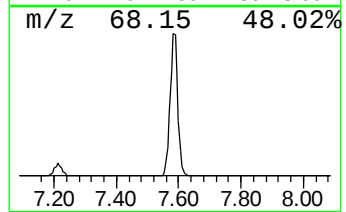
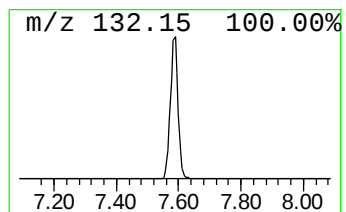
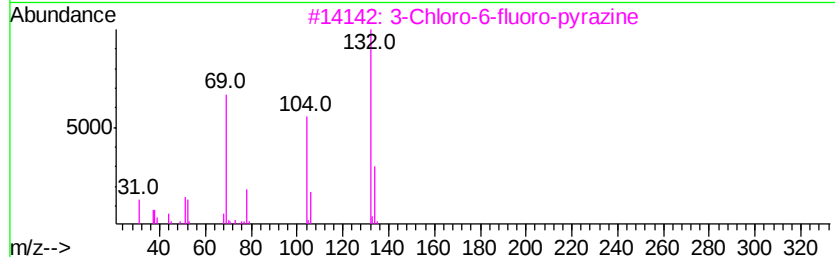
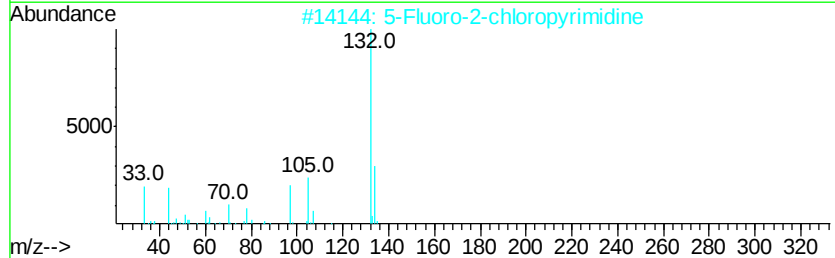
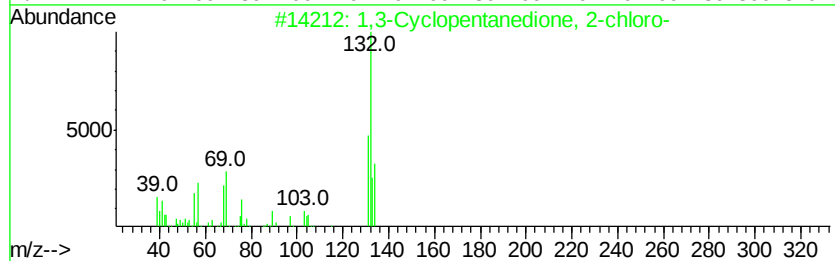
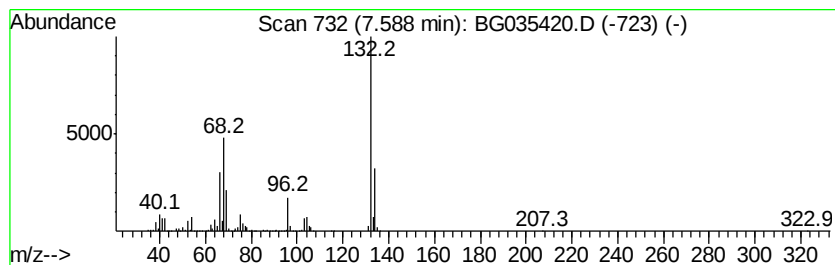
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Peak Number 2 unknown7.59 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.59	106.27 ng	1736240	1,4-Dichlorobenzene-d4	8.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	25
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
4		Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10
5		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10



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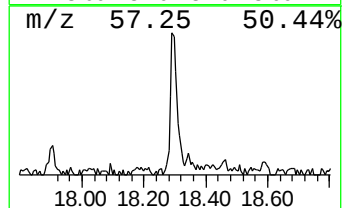
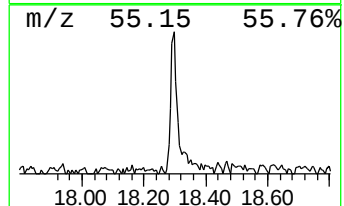
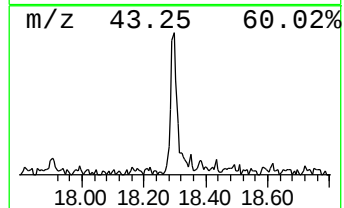
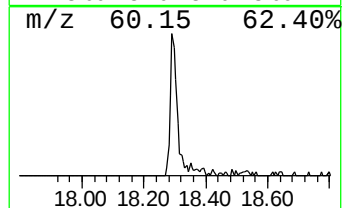
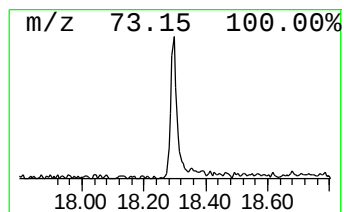
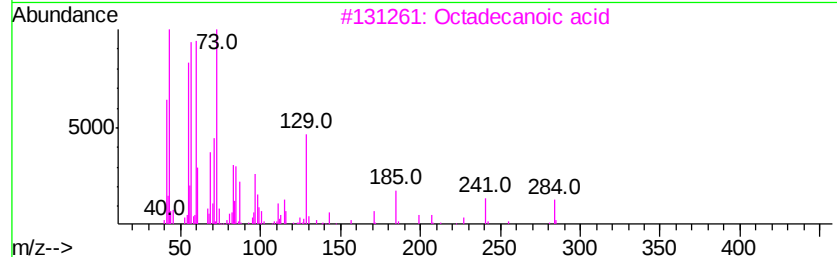
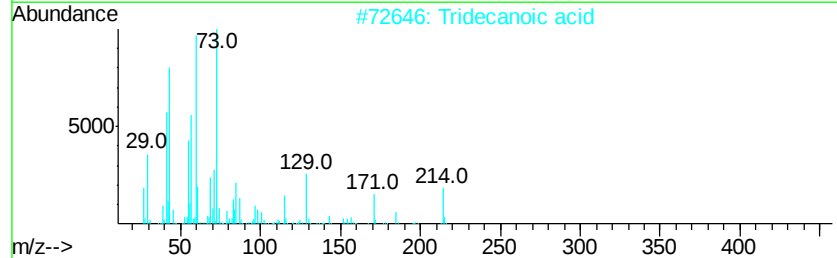
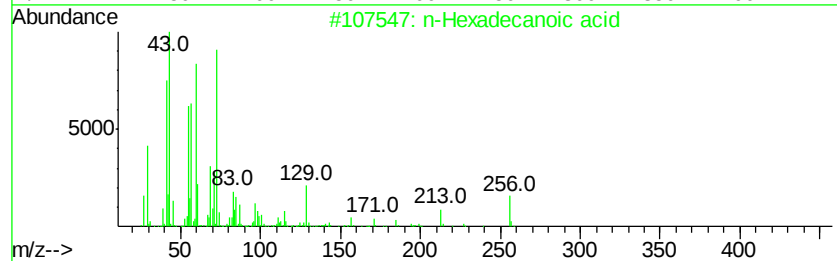
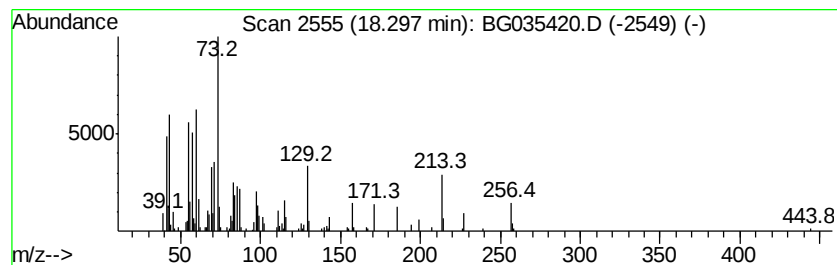
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.		
18.30	4.34 ng	187843	Phenanthrene-d10	17.42		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2		Tridecanoic acid	214	C13H26O2	000638-53-9	64
3		Octadecanoic acid	284	C18H36O2	000057-11-4	64
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	62
5		l-(+)-Ascorbic acid 2,6-dihexade...	652	C38H68O8	028474-90-0	50



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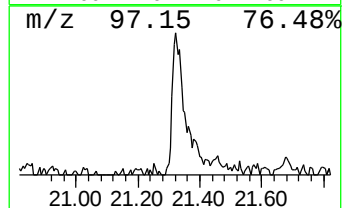
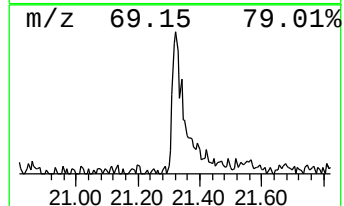
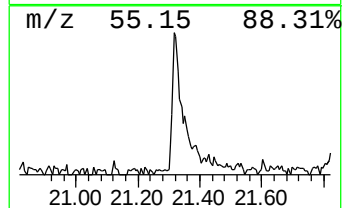
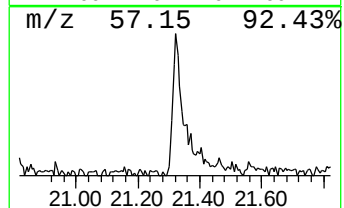
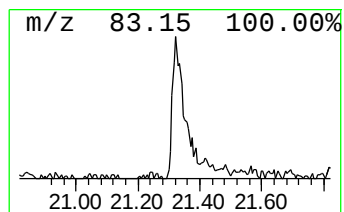
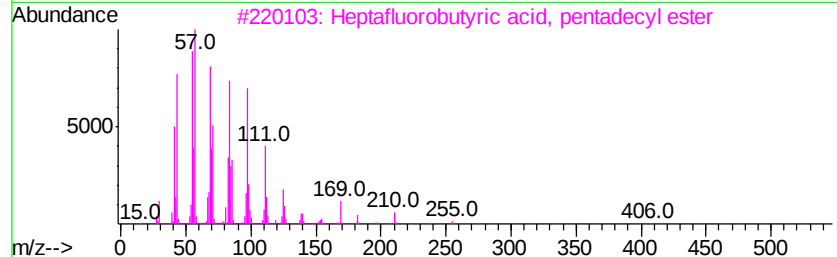
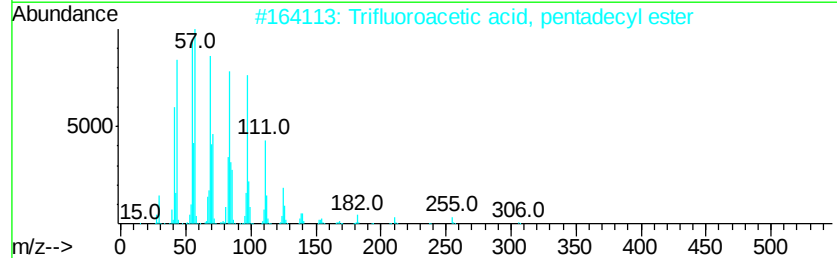
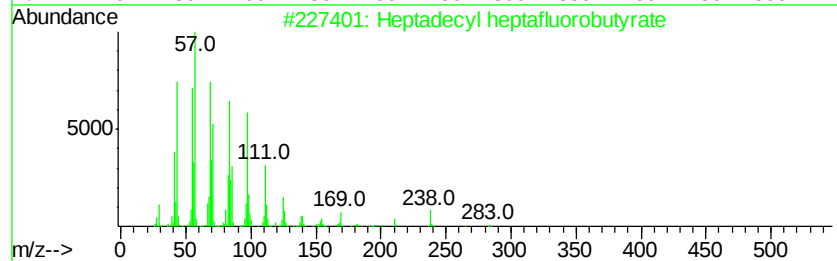
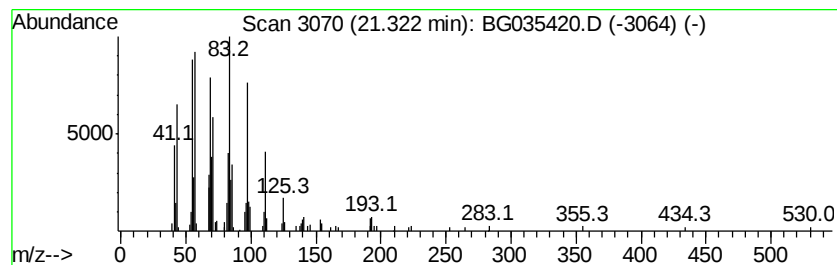
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Peak Number 5 Heptadecyl heptafluorobutyrate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.32	3.87 ng	195375	Chrysene-d12	21.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
2		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	91
3		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	87
4		Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	87
5		1-Pentadecene	210	C15H30	013360-61-7	76



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.16	8.5	ng	139218	1	8.05	326766	20.0
unknown7.59	7.59	106.3	ng	1736240	1	8.05	326766	20.0
n-Hexadecanoic acid	18.30	4.3	ng	187843	4	17.42	865505	20.0
Heptadecyl heptaf...	21.32	3.9	ng	195375	5	21.67	1010680	20.0