

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG071618\
 Data File : BG035675.D
 Acq On : 16 Jul 2018 18:35
 Operator : JU/SJ
 Sample : J3991-04
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB-3-A

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-BG071218.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	5.171	314	320	329	rVB	93065	148895	4.08%	0.866%
2	5.641	393	400	410	rBV	740311	1172440	32.09%	6.819%
3	7.227	662	670	684	rBV	781865	1381470	37.81%	8.035%
4	7.597	724	733	740	rBV	709387	1247264	34.14%	7.254%
5	8.055	804	811	819	rBV	123203	216064	5.91%	1.257%
6	8.378	858	866	875	rBV	497607	868223	23.76%	5.050%
7	9.218	1001	1009	1018	rBV	452450	807412	22.10%	4.696%
8	10.857	1282	1288	1298	rVB	159449	301011	8.24%	1.751%
9	13.301	1697	1704	1713	rBV	1252714	1971771	53.97%	11.468%
10	14.123	1834	1844	1852	rBV	205398	291686	7.98%	1.696%
11	14.676	1932	1938	1946	rBV2	305824	509536	13.95%	2.963%
12	16.162	2185	2191	2204	rBV	1099370	1751374	47.93%	10.186%
13	17.419	2398	2405	2413	rBV2	501186	766895	20.99%	4.460%
14	18.300	2550	2555	2564	rBV2	49674	78734	2.15%	0.458%
15	20.021	2842	2848	2855	rBV	2755954	3653678	100.00%	21.250%
16	21.325	3064	3070	3081	rBV2	97084	206593	5.65%	1.202%
17	21.684	3124	3131	3142	rBV2	524702	868225	23.76%	5.050%
18	21.866	3157	3162	3168	rBV	36433	58851	1.61%	0.342%
19	22.477	3262	3266	3270	rBV4	25548	37456	1.03%	0.218%
20	23.170	3380	3384	3391	rVB6	22777	38538	1.05%	0.224%
21	24.903	3668	3679	3690	rBV	291021	817909	22.39%	4.757%

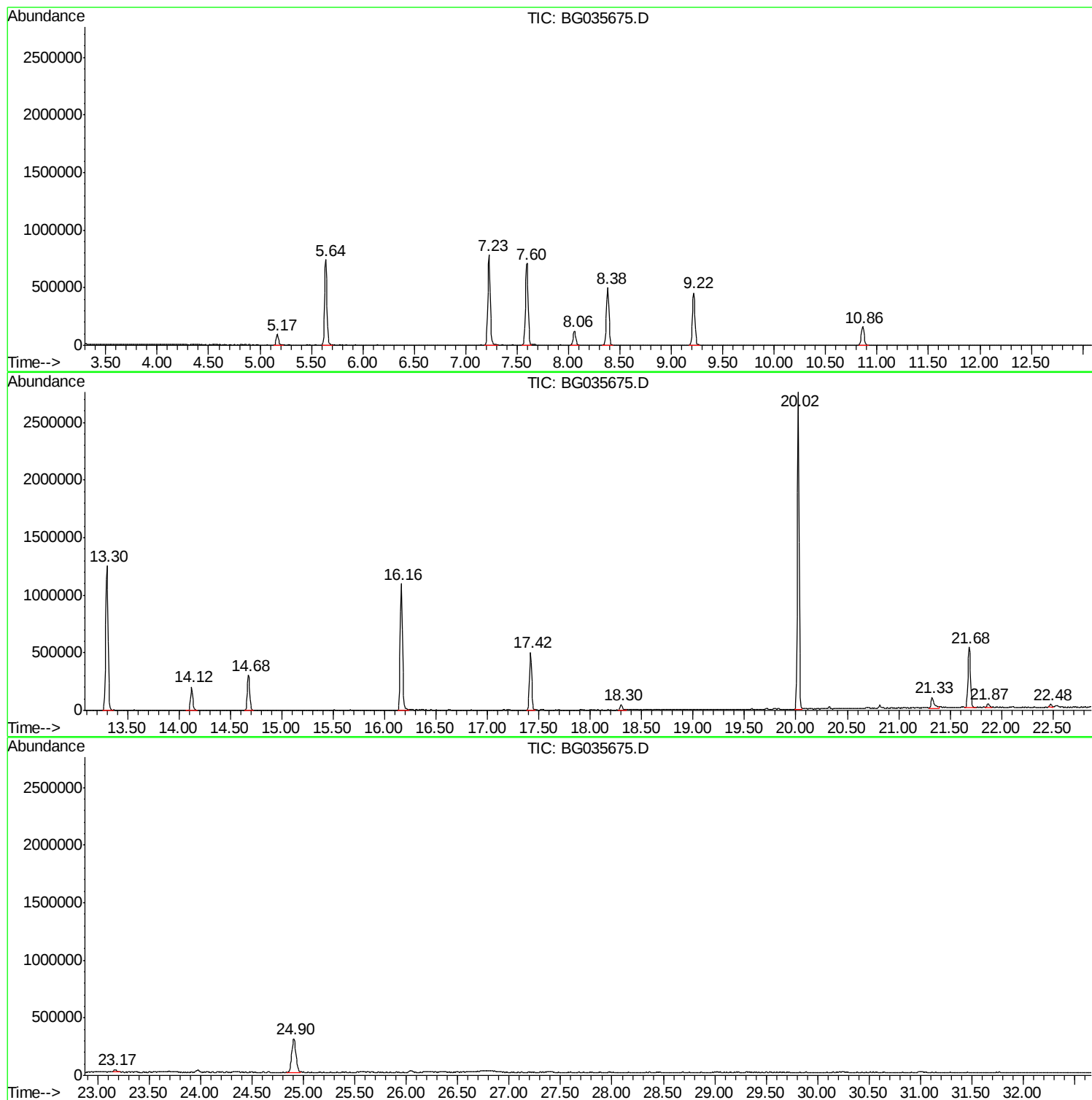
Sum of corrected areas: 17194025

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Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG071218.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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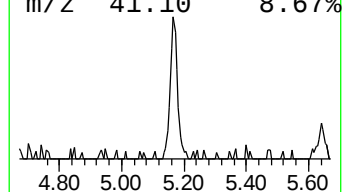
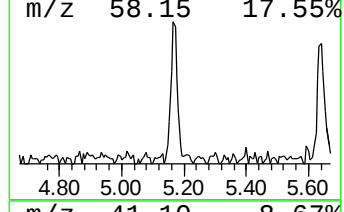
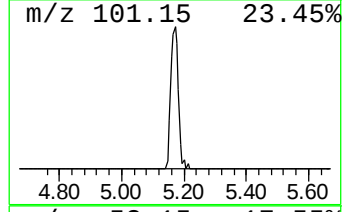
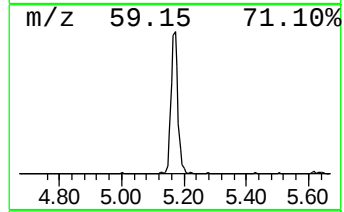
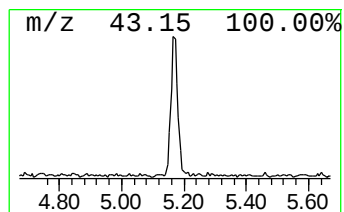
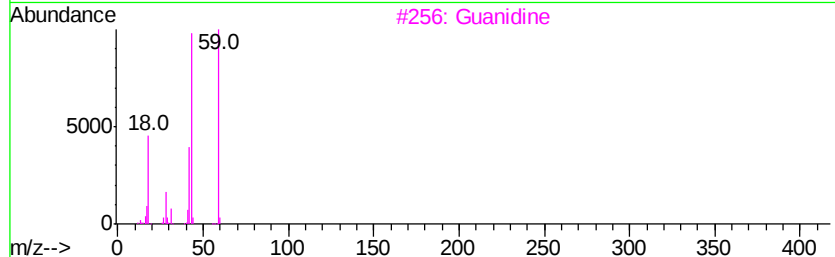
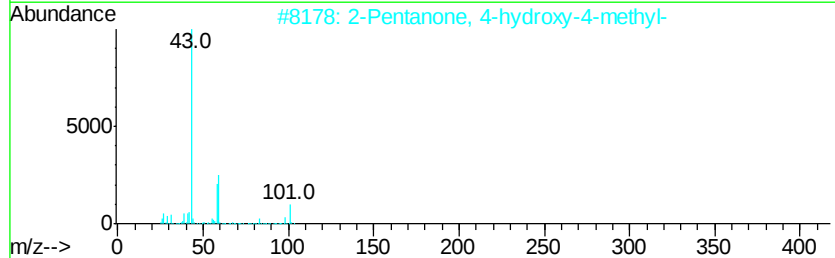
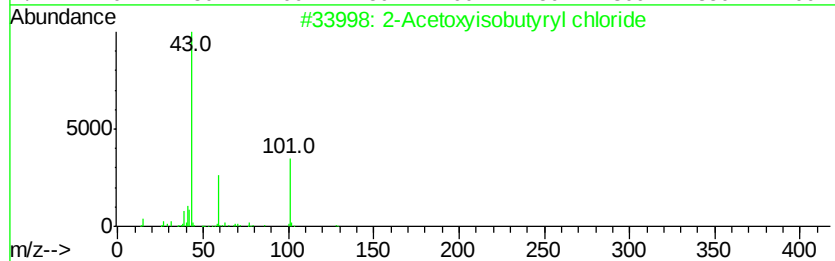
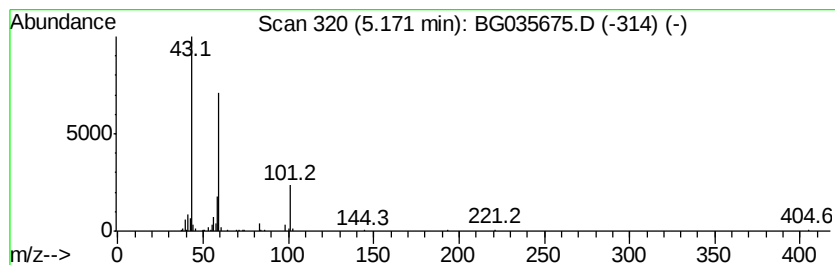
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Acetoxyisobutryl chloride Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.17	13.78 ng	148895	1,4-Dichlorobenzene-d4	8.06

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Acetoxyisobutryl chloride	164	C6H9ClO3	040635-66-3	64
2			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
3			Guanidine	59	CH5N3	000113-00-8	43
4			Dimethadione	129	C5H7NO3	000695-53-4	33
5			n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	28



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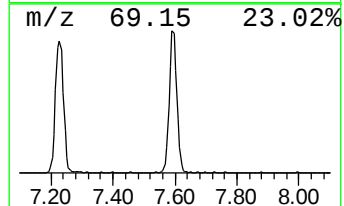
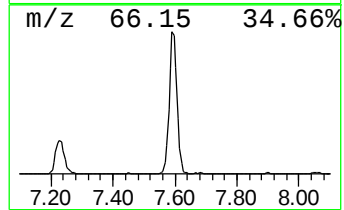
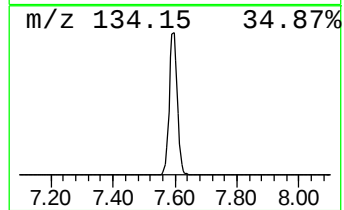
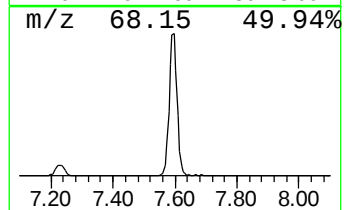
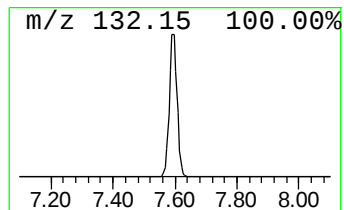
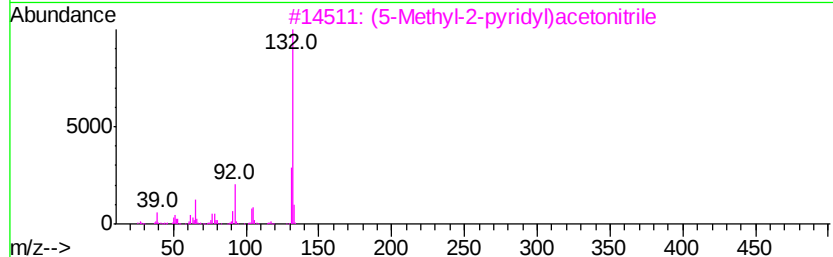
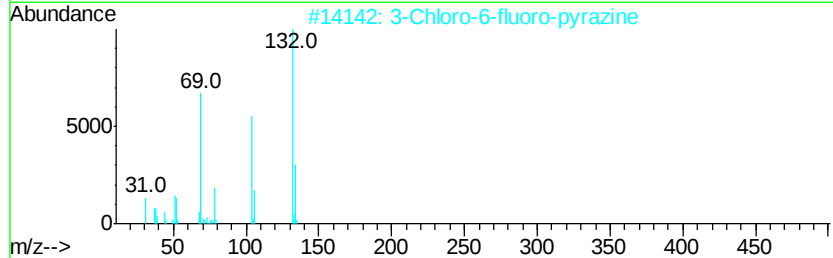
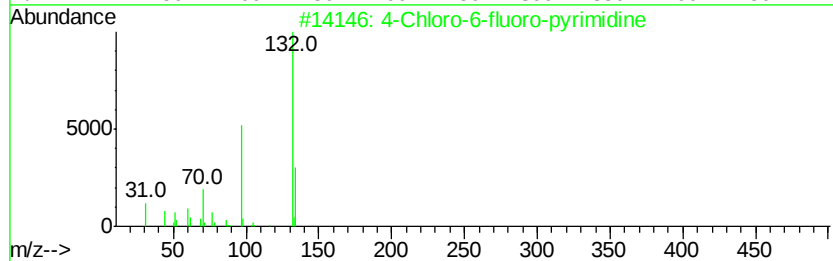
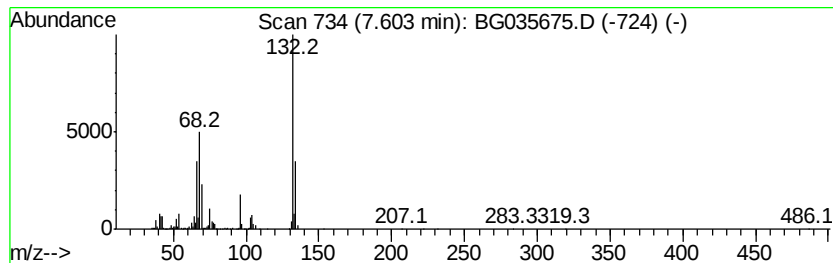
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TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown7.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.60	115.45 ng	1247260	1,4-Dichlorobenzene-d4	8.06

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		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
4		N-(-3,4-Methylenedioxyphenylisop...	267	C17H17NO2	1000378-96-6	10
5		2-Cyclohexen-1-one	96	C6H8O	000930-68-7	10



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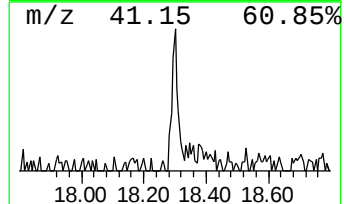
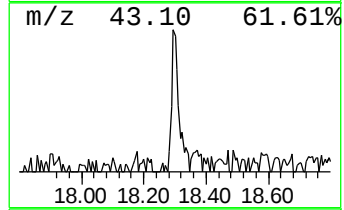
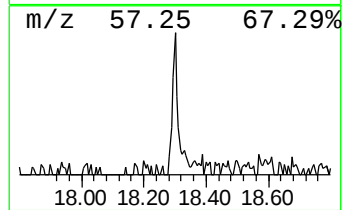
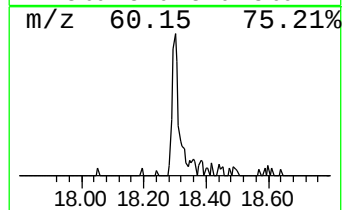
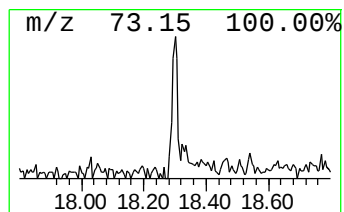
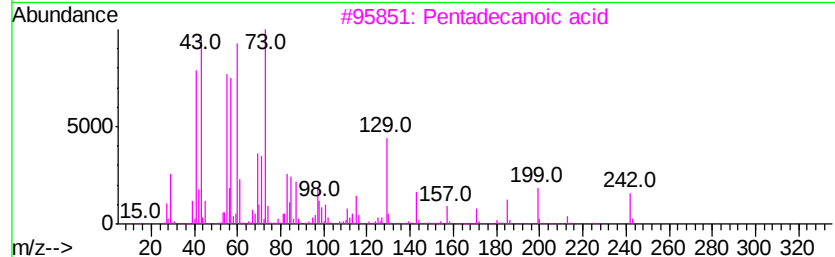
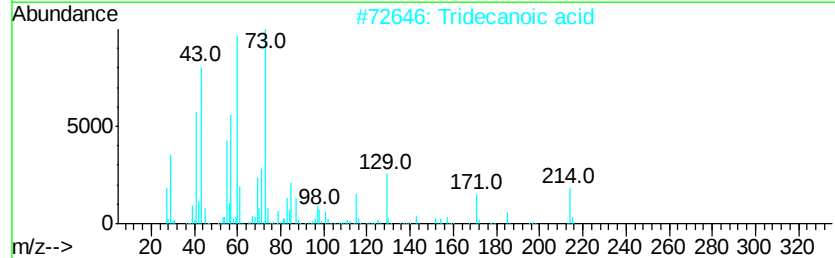
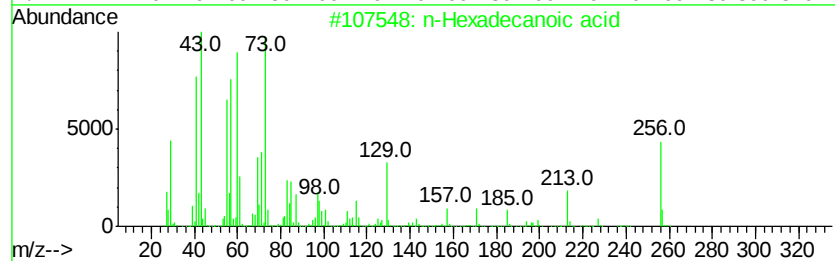
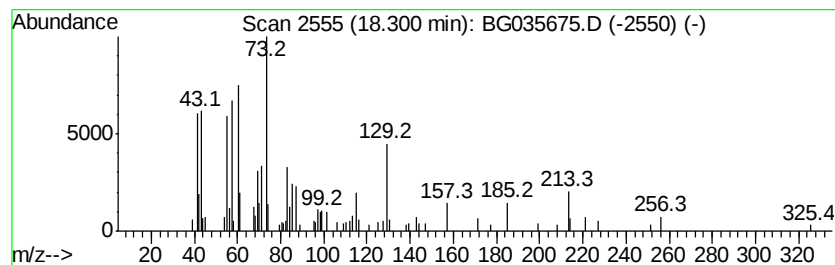
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.30	2.05 ng	78734	Phenanthrene-d10	17.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2		Tridecanoic acid	214	C13H26O2	000638-53-9	90
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5		n-Decanoic acid	172	C10H20O2	000334-48-5	58



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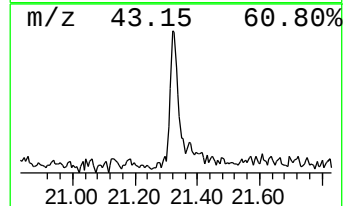
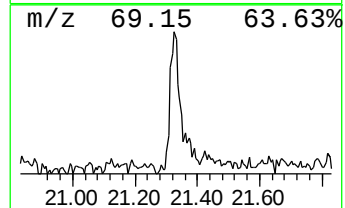
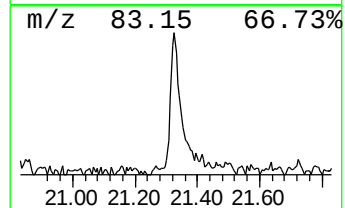
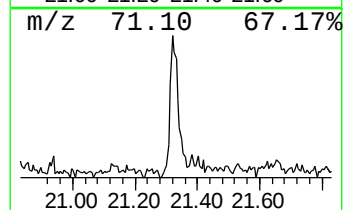
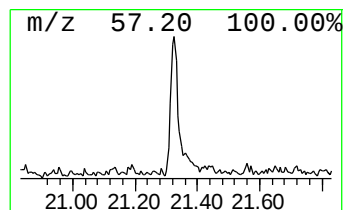
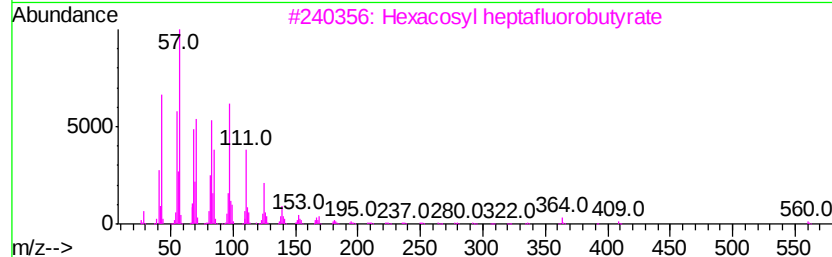
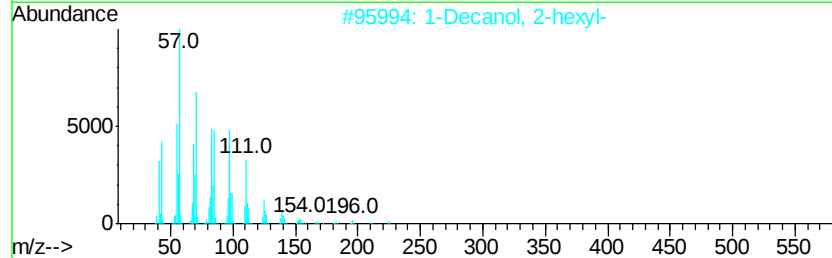
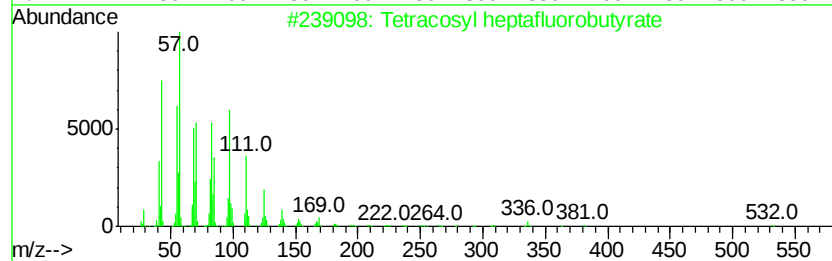
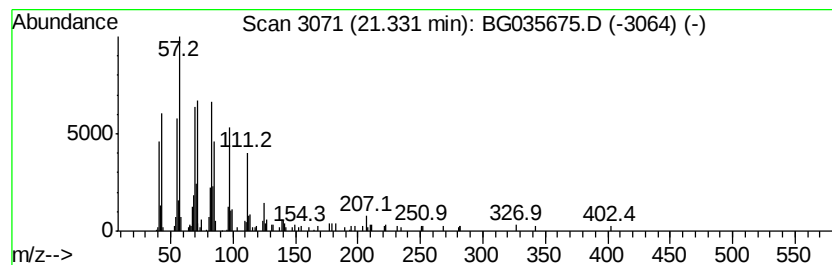
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Peak Number 5 Tetracosyl heptafluorobutyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.33	4.76 ng	206593	Chrysene-d12	21.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetracosyl heptafluorobutvrate	550	C28H49F7O2	1000351-83-7	87
2		1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	83
3		Hexacosyl heptafluorobutvrate	578	C30H53F7O2	1000351-83-3	81
4		Hexatriacontyl pentafluoropropio...	669	C39H73F5O2	1000351-89-0	81
5		Octacosyl heptafluorobutyrate	606	C32H57F7O2	1000351-83-6	81



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Acetoxyisobutyr...	5.17	13.8	ng	148895	1	8.06	216064	20.0
unknown7.60	7.60	115.5	ng	1247260	1	8.06	216064	20.0
n-Hexadecanoic acid	18.30	2.0	ng	78734	4	17.42	766895	20.0
Tetracosyl heptaf...	21.33	4.8	ng	206593	5	21.68	868225	20.0