

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG121718\
 Data File : BG038659.D
 Acq On : 17 Dec 2018 12:25
 Operator : JU/SJ
 Sample : J6379-09
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 P001-SS004-1824-01

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-BG121218.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	5.144	344	350	359	rVB	29122	51972	2.46%	0.503%
2	5.608	422	429	441	rBV	466789	772432	36.52%	7.475%
3	7.212	695	702	714	rBV	473314	907265	42.90%	8.780%
4	7.588	758	766	776	rBV	455761	800410	37.85%	7.746%
5	8.058	839	846	858	rBV2	74508	133029	6.29%	1.287%
6	8.381	894	901	914	rVB	345007	610222	28.85%	5.906%
7	9.239	1039	1047	1059	rBV	292532	544159	25.73%	5.266%
8	10.878	1318	1326	1333	rBV	94654	175398	8.29%	1.697%
9	13.317	1733	1741	1752	rBV	719091	1127877	53.33%	10.915%
10	14.139	1875	1881	1896	rBV	47329	75478	3.57%	0.730%
11	14.697	1969	1976	1986	rVB3	153130	253901	12.00%	2.457%
12	16.184	2222	2229	2250	rBV	676560	1091220	51.60%	10.561%
13	17.441	2437	2443	2455	rVB2	227839	367963	17.40%	3.561%
14	18.305	2585	2590	2603	rBV2	43030	73886	3.49%	0.715%
15	20.044	2880	2886	2893	rBV	1574201	2114965	100.00%	20.468%
16	21.319	3098	3103	3116	rBV	70098	133722	6.32%	1.294%
17	21.724	3164	3172	3179	rBV2	264053	454106	21.47%	4.395%
18	21.865	3188	3196	3202	rBV2	14915	26778	1.27%	0.259%
19	22.476	3294	3300	3306	rBV3	16691	29044	1.37%	0.281%
20	23.176	3410	3419	3428	rBV3	27419	62011	2.93%	0.600%
21	23.986	3549	3557	3564	rBV3	15396	36339	1.72%	0.352%
22	24.944	3713	3720	3724	rBV4	12952	33047	1.56%	0.320%
23	25.026	3724	3734	3747	rVB3	142694	434644	20.55%	4.206%
24	26.090	3909	3915	3923	rBV5	8043	23163	1.10%	0.224%

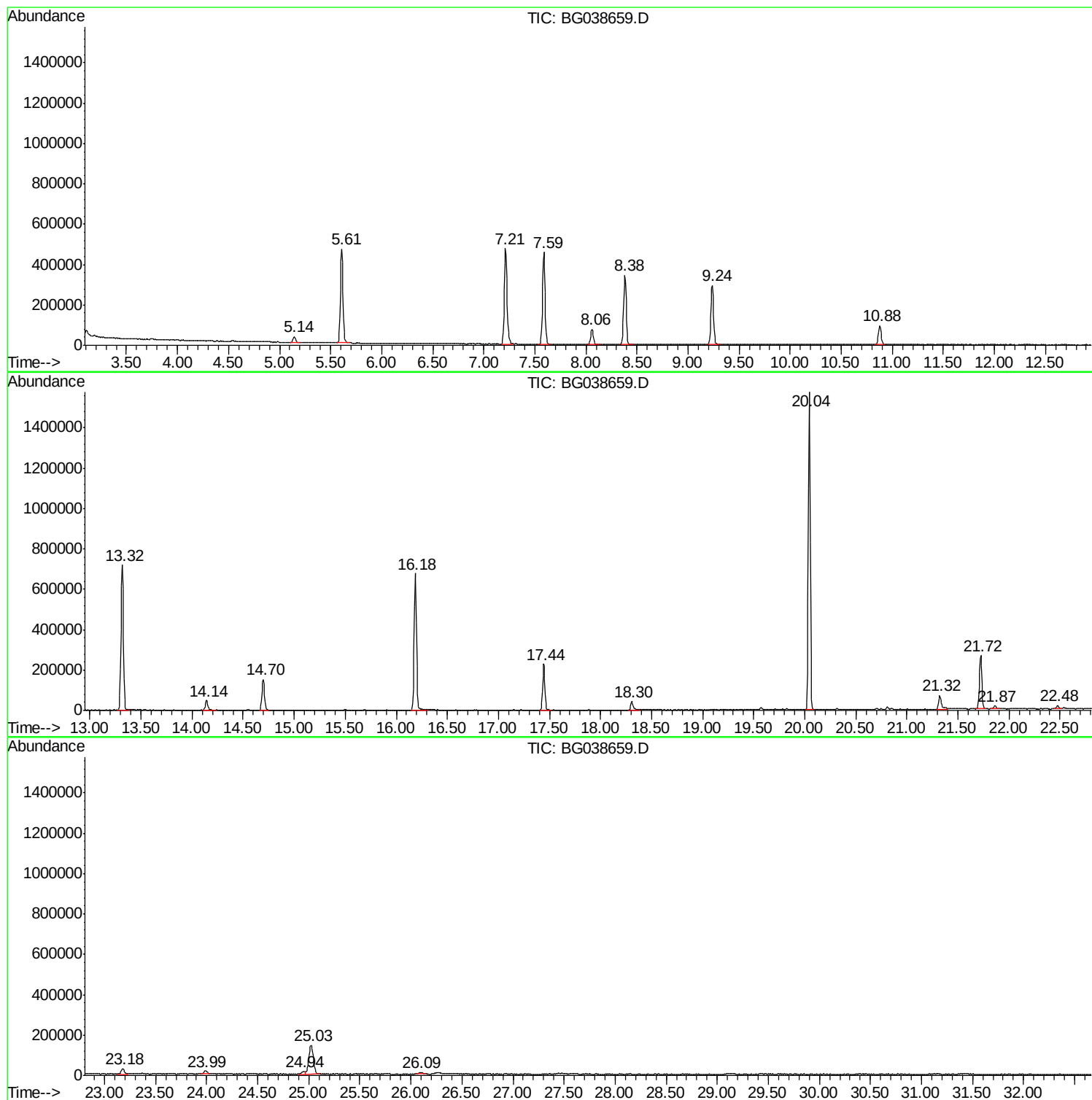
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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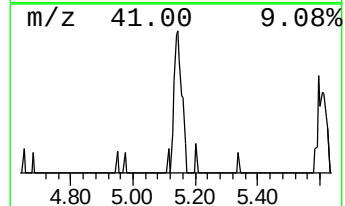
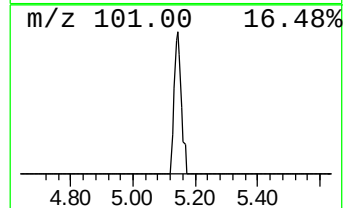
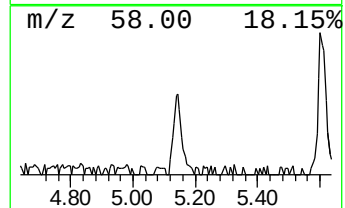
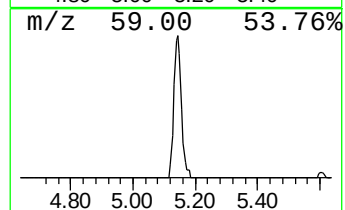
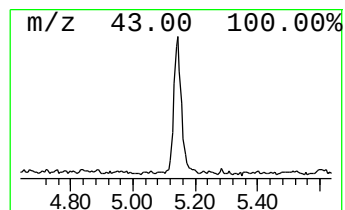
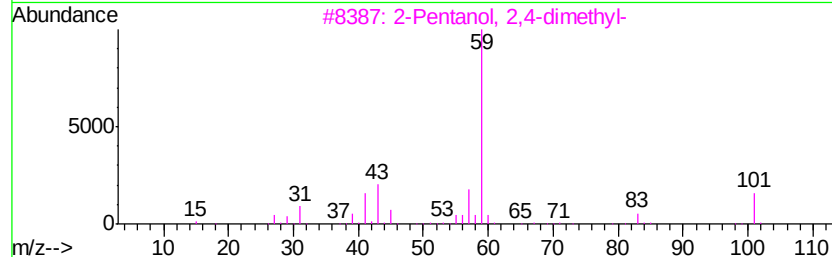
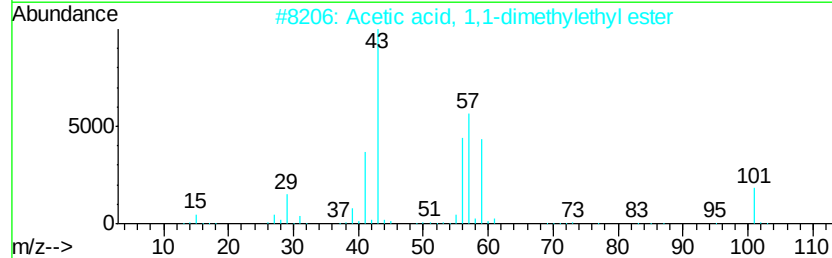
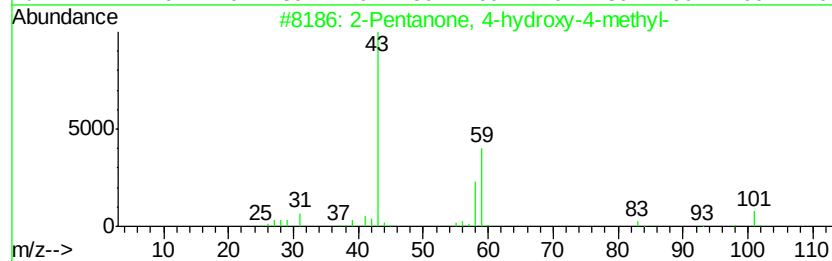
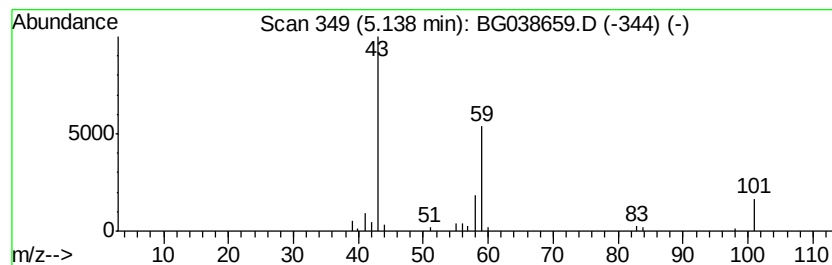
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.14	7.81 ng	51972	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	50
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	25
4			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	23
5			Acetamide	59	C2H5NO	000060-35-5	9



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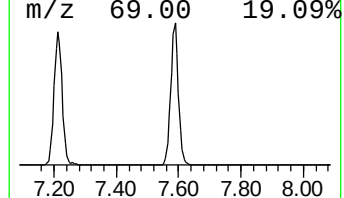
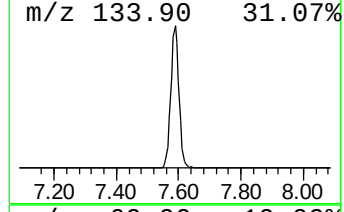
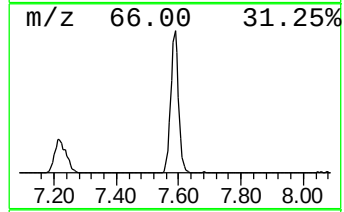
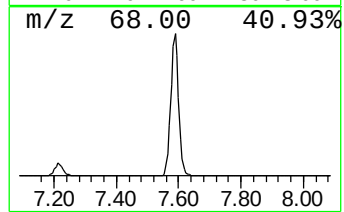
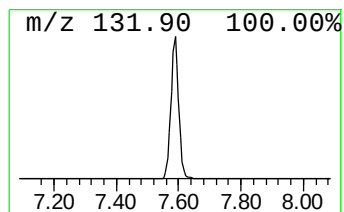
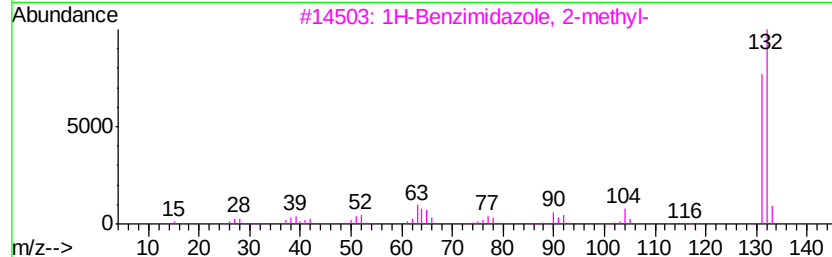
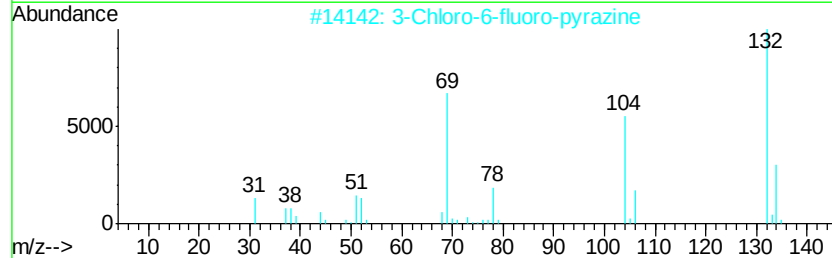
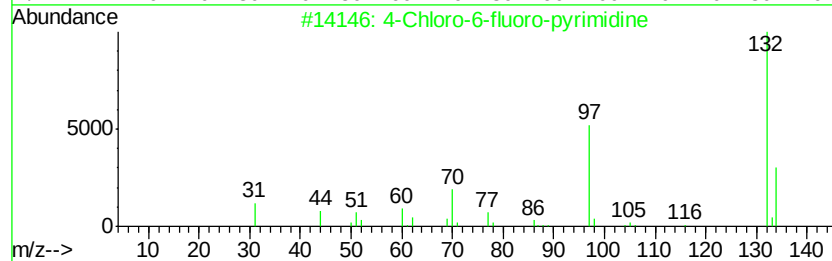
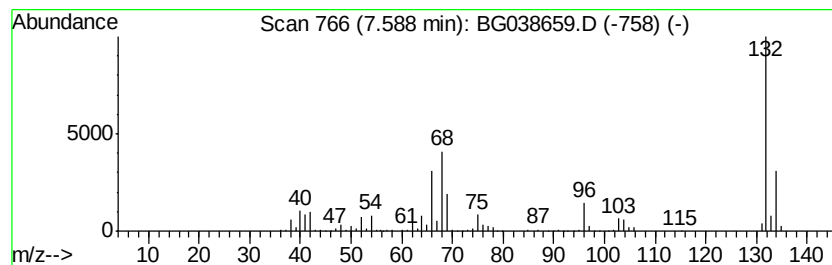
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TIC Library : C:\Database\NIST11.L
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Peak Number 2 unknown7.59 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.59	120.34 ng	800410	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		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4		5-Aminoindole	132	C8H8N2	005192-03-0	22
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	12



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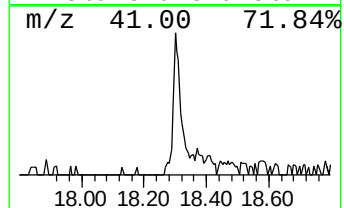
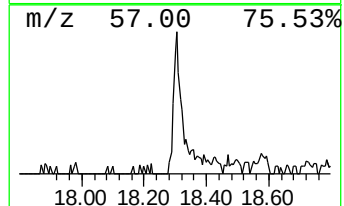
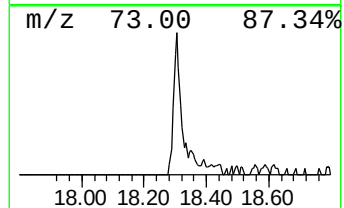
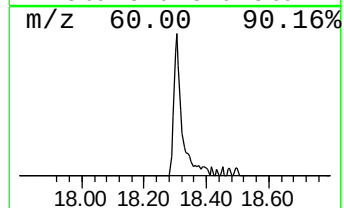
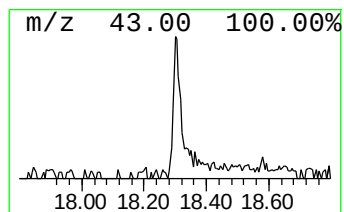
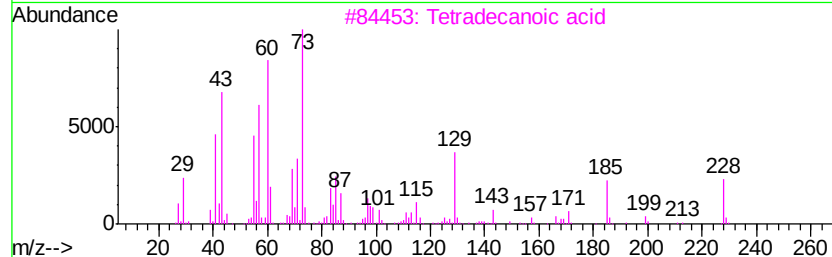
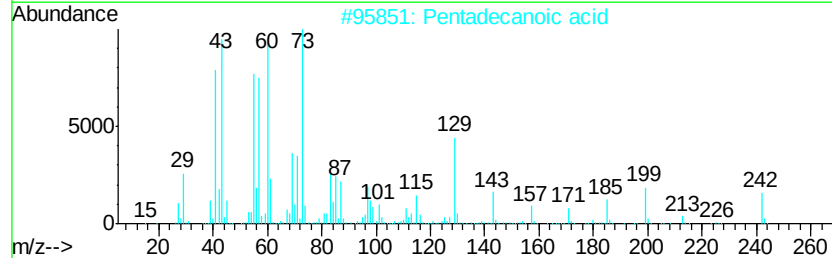
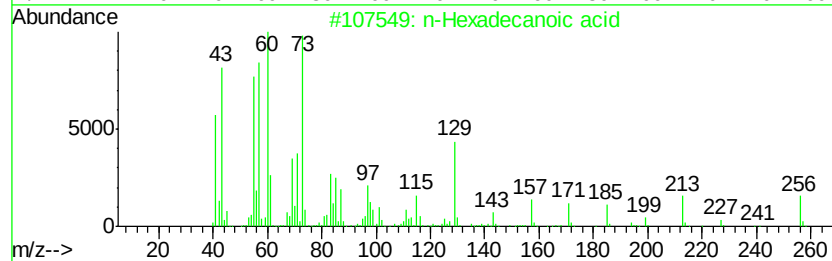
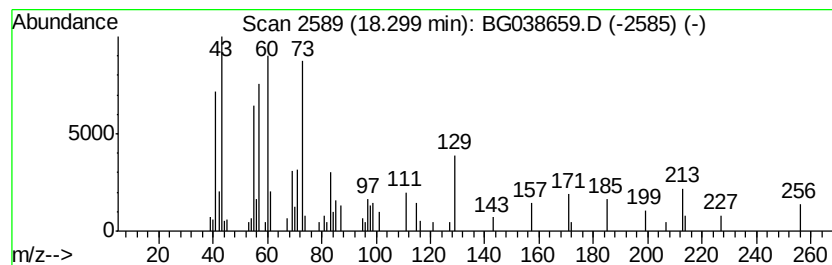
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
18.30	4.02 ng	73886	Phenanthrene-d10		17.44
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	Dodecanoic acid	200	C12H24O2	000143-07-7	64
5	Tridecanoic acid	214	C13H26O2	000638-53-9	52



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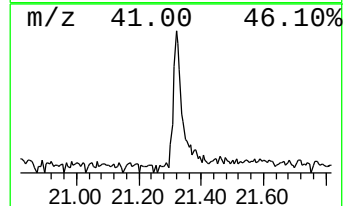
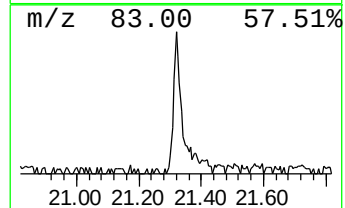
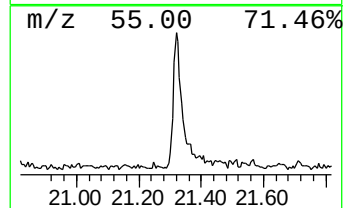
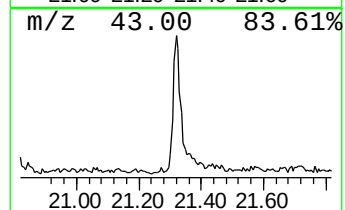
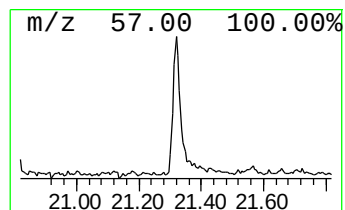
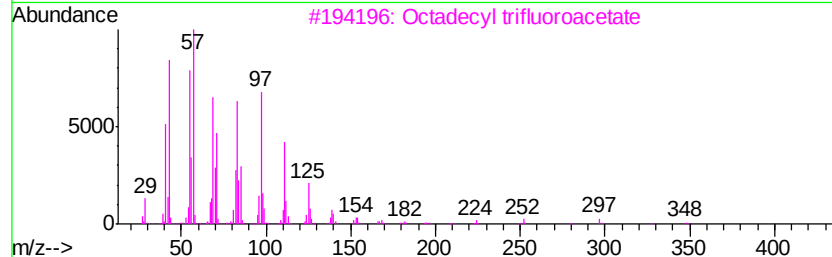
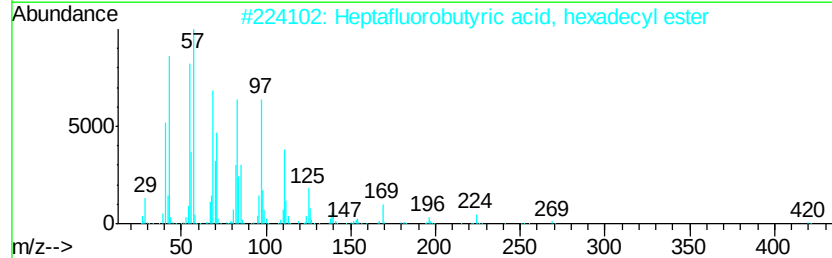
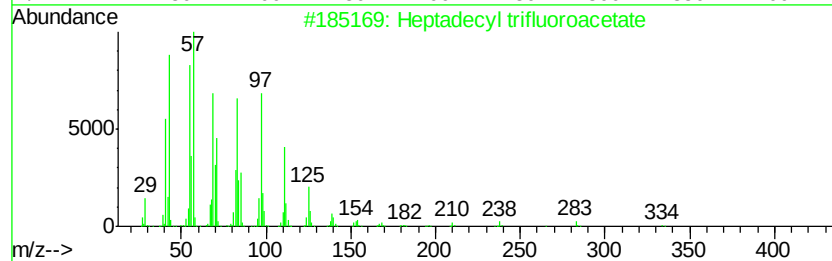
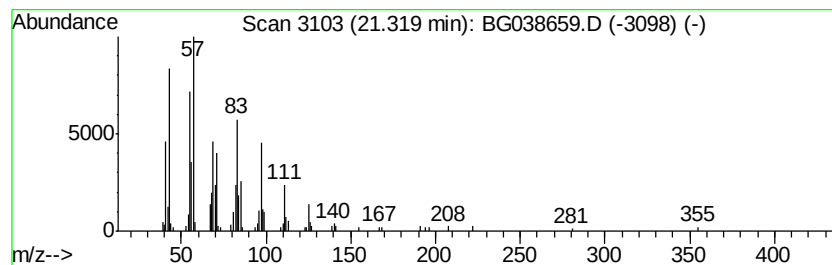
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Peak Number 5 Heptadecyl trifluoroacetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.		
21.32	5.89 ng	133722	Chrysene-d12	21.72		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94
2		Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
3		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
4		Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	91
5		Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91



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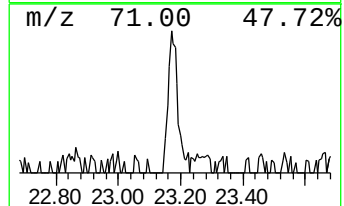
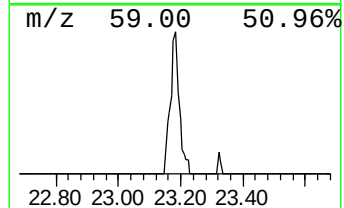
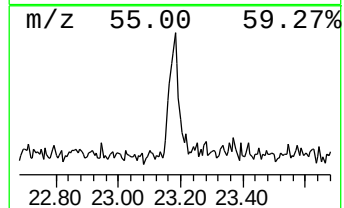
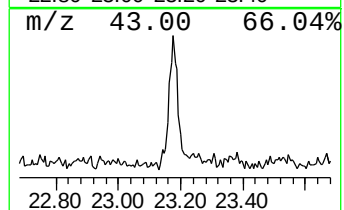
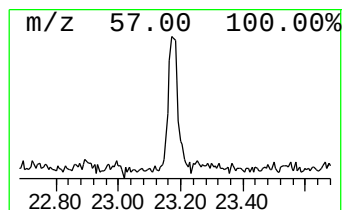
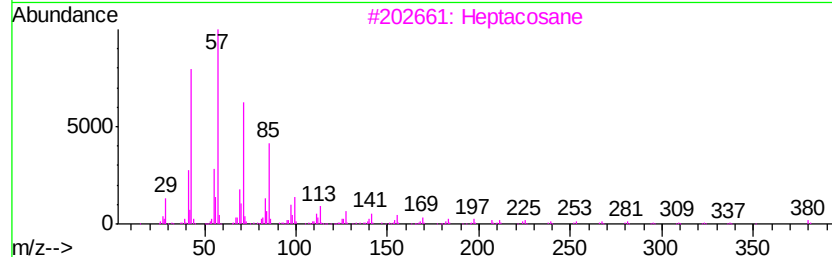
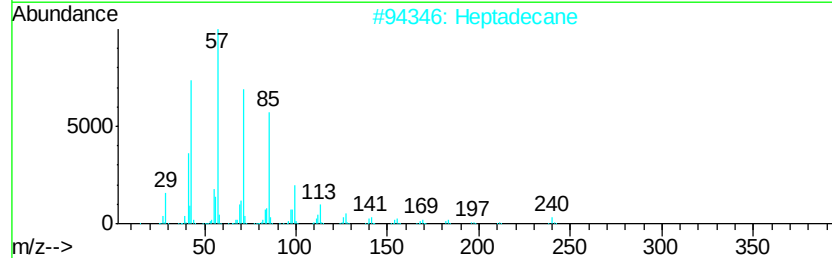
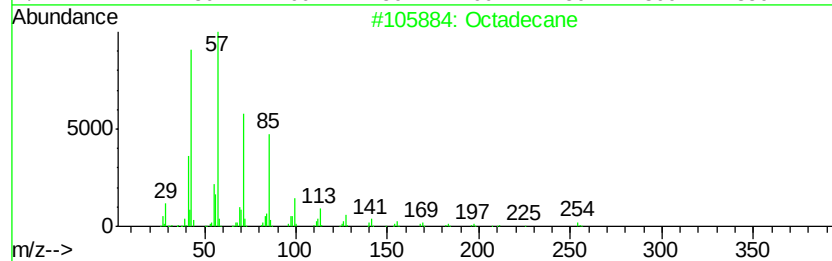
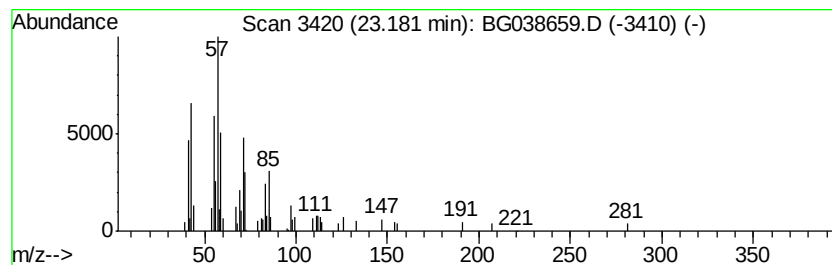
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Peak Number 6 unknown23.18 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.18	2.73 ng	62011	Chrysene-d12	21.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecane	254	C18H38	000593-45-3	49
2		Heptadecane	240	C17H36	000629-78-7	47
3		Heptacosane	380	C27H56	000593-49-7	47
4		Heneicosane	296	C21H44	000629-94-7	47
5		Nonadecane	268	C19H40	000629-92-5	47



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.14	7.8	ng	51972	1	8.06	133029	20.0
unknown7.59	7.59	120.3	ng	800410	1	8.06	133029	20.0
n-Hexadecanoic acid	18.30	4.0	ng	73886	4	17.44	367963	20.0
Heptadecyl triflu...	21.32	5.9	ng	133722	5	21.72	454106	20.0
unknown23.18	23.18	2.7	ng	62011	5	21.72	454106	20.0