

Data Path : Z:\HPCHEM1\BNA G\DATA\BG103117\
 Data File : BG030619.D
 Acq On : 31 Oct 2017 19:28
 Operator : SJ/JU
 Sample : I6207-03
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB-04

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-BG101617.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	5.241	326	332	341	rVB	213823	322517	7.96%	1.202%
2	5.717	406	413	422	rBV	1157204	1857700	45.85%	6.922%
3	7.321	677	686	699	rBV	1233973	2268184	55.98%	8.452%
4	7.691	741	749	763	rBV	1185703	2085614	51.48%	7.771%
5	8.161	822	829	836	rBV	277117	459900	11.35%	1.714%
6	8.484	875	884	894	rBV	833862	1475149	36.41%	5.497%
7	9.324	1019	1027	1038	rBV	732004	1323044	32.66%	4.930%
8	10.975	1298	1308	1316	rBV	409053	753013	18.59%	2.806%
9	13.402	1712	1721	1729	rBV	1819794	2826390	69.76%	10.532%
10	14.219	1854	1860	1866	rBV	343727	519763	12.83%	1.937%
11	14.777	1948	1955	1966	rVB2	724682	1172368	28.94%	4.368%
12	16.116	2178	2183	2189	rBV	90830	135187	3.34%	0.504%
13	16.257	2199	2207	2220	rBV	1660722	2578100	63.63%	9.606%
14	17.515	2414	2421	2430	rBV	921057	1381468	34.10%	5.148%
15	18.378	2560	2568	2578	rBV3	44204	87559	2.16%	0.326%
16	20.106	2856	2862	2869	rVB	3036563	4051451	100.00%	15.096%
17	21.404	3077	3083	3091	rBV3	113553	212173	5.24%	0.791%
18	21.786	3141	3148	3156	rVB2	942994	1581516	39.04%	5.893%
19	22.615	3280	3289	3298	rBV4	51286	170676	4.21%	0.636%
20	25.094	3701	3711	3728	rVB2	532456	1575615	38.89%	5.871%

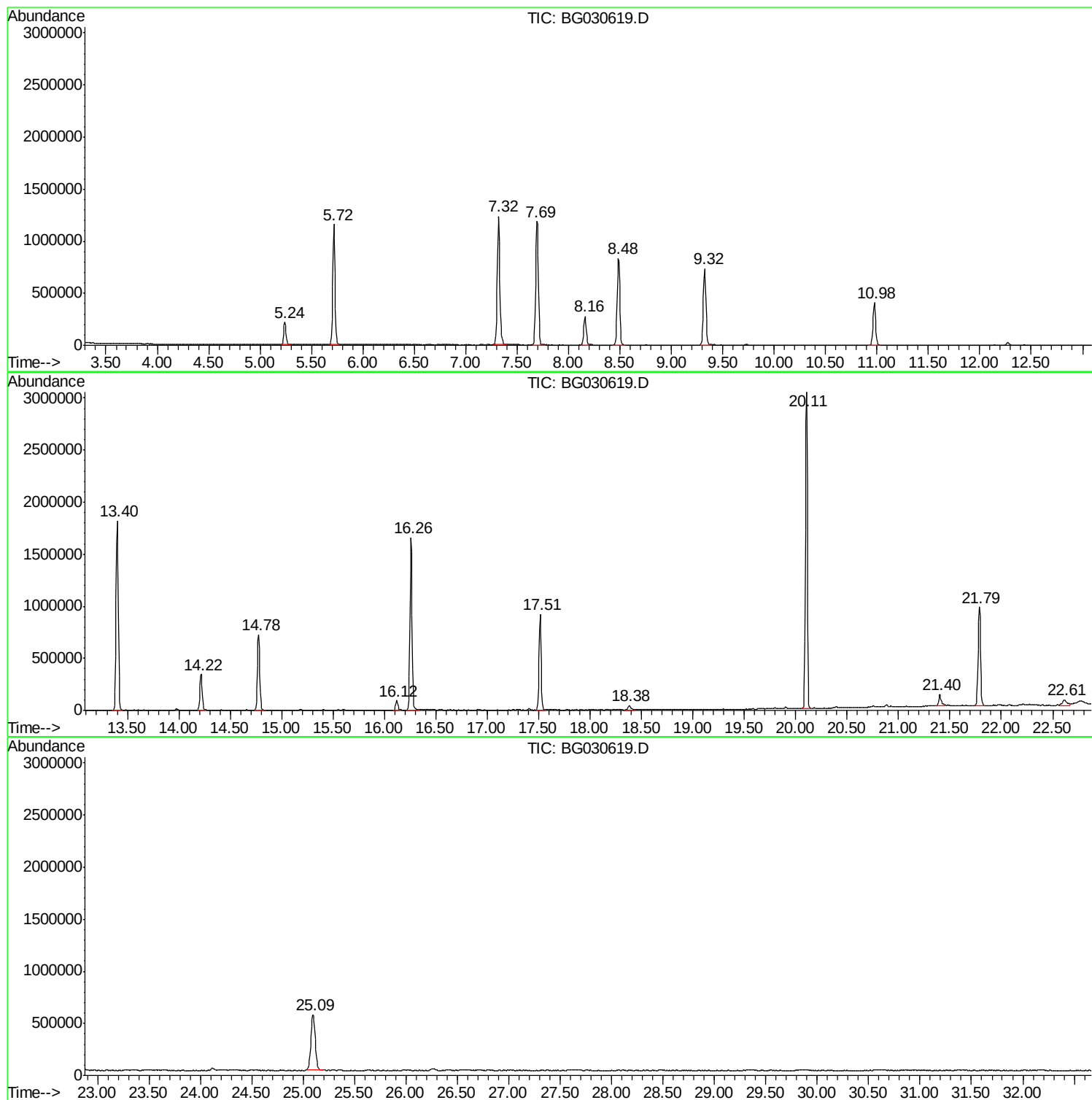
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG101617.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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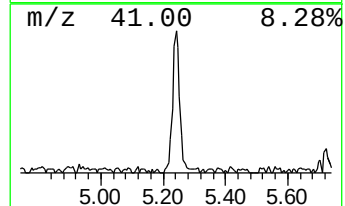
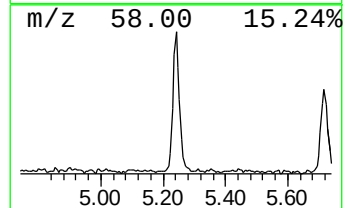
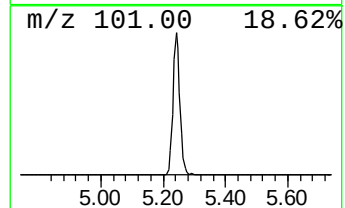
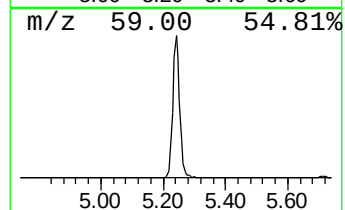
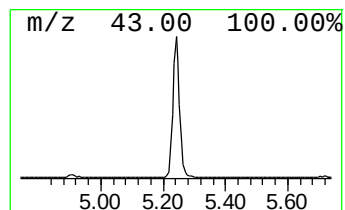
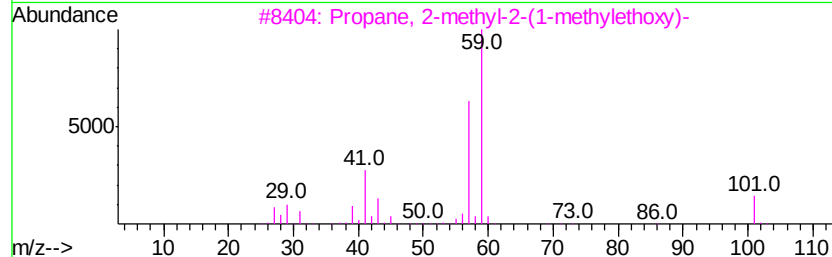
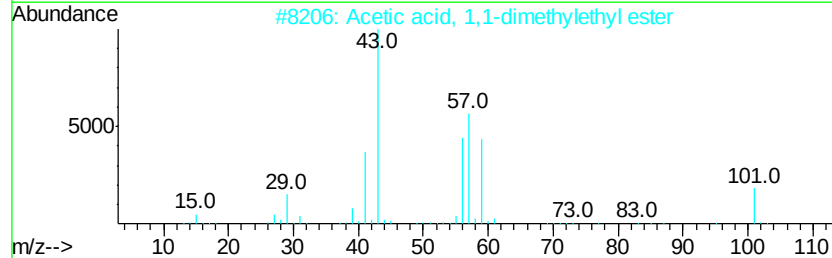
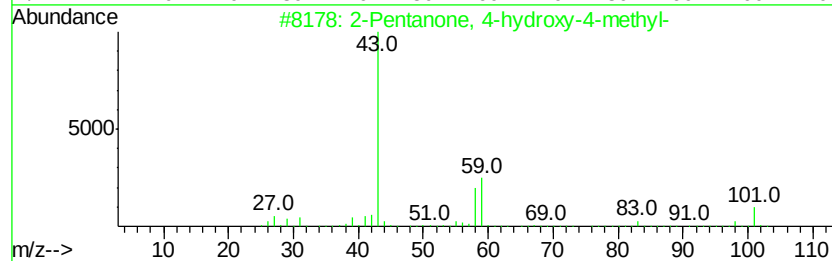
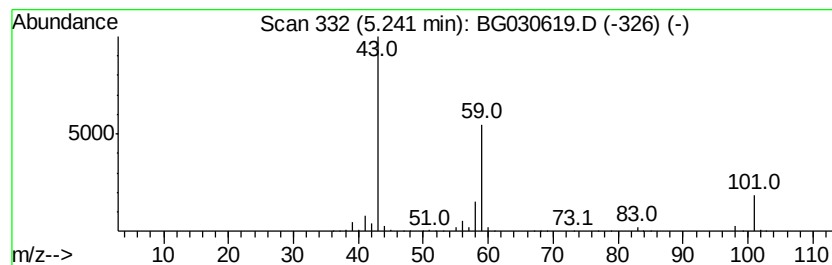
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.24	14.03 ng	322517	1,4-Dichlorobenzene-d4	8.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16



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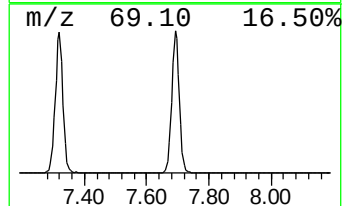
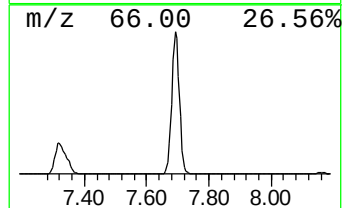
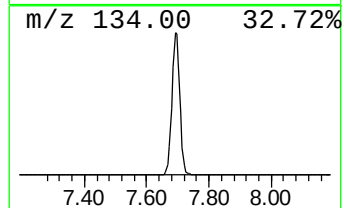
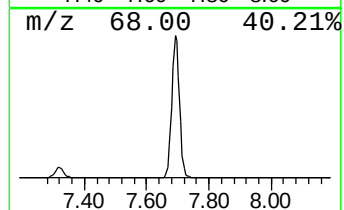
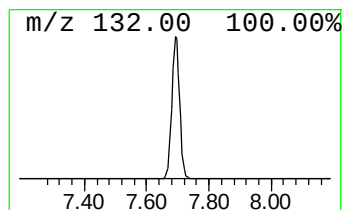
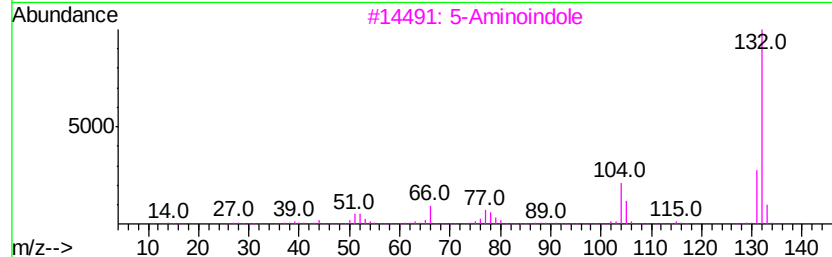
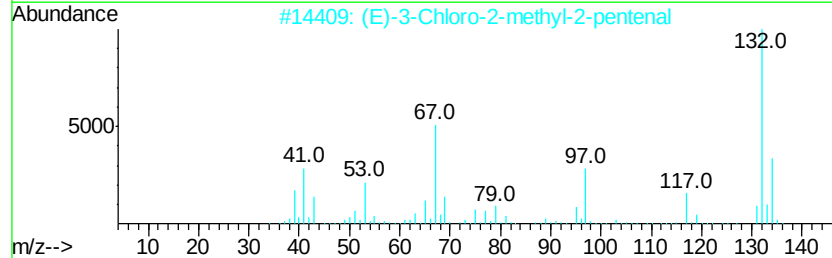
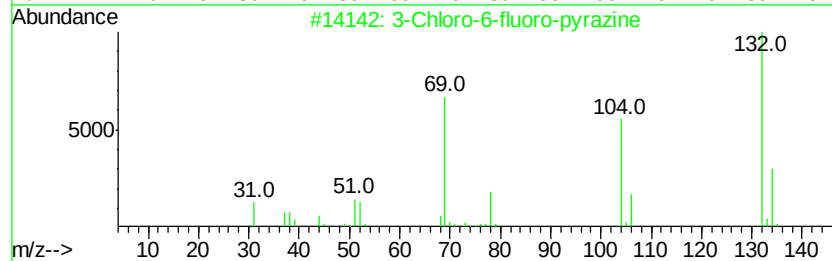
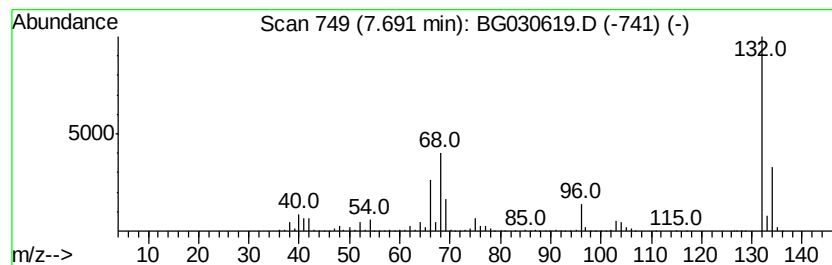
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Peak Number 2 unknown7.69 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.69	90.70 ng	2085610	1,4-Dichlorobenzene-d4	8.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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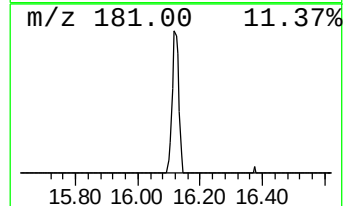
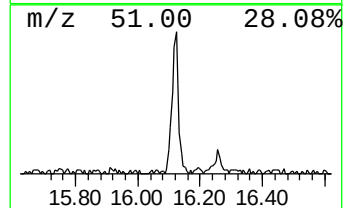
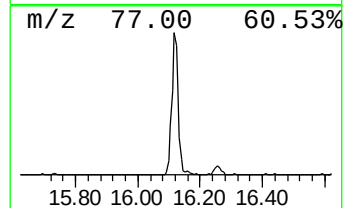
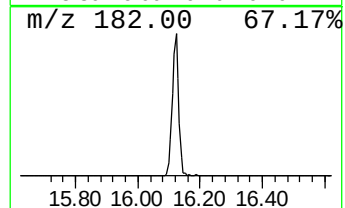
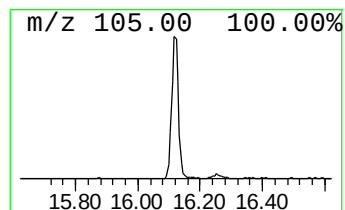
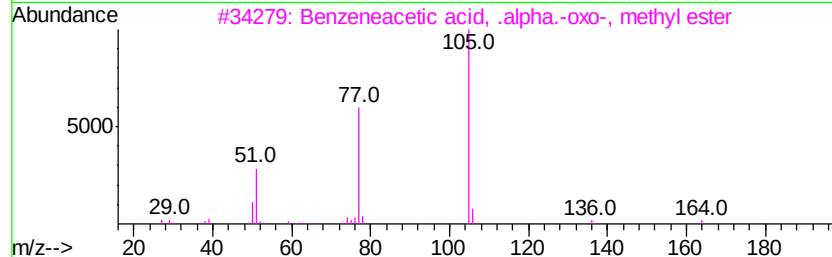
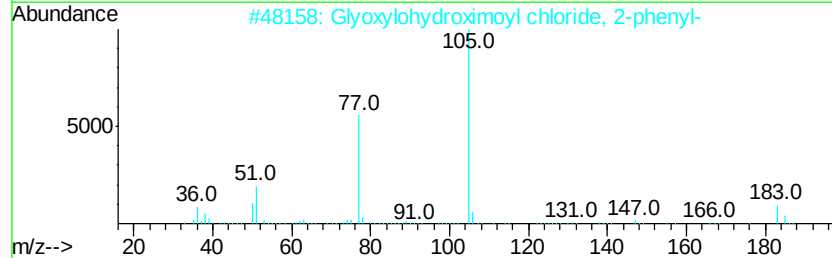
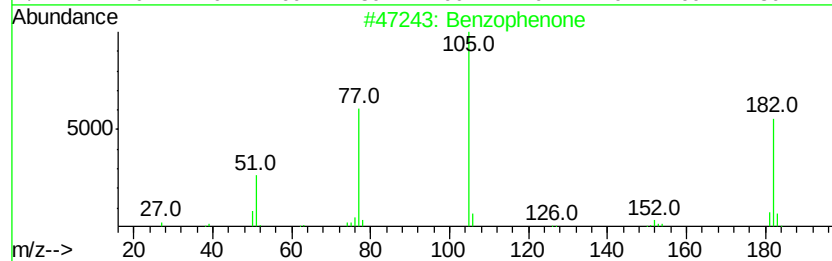
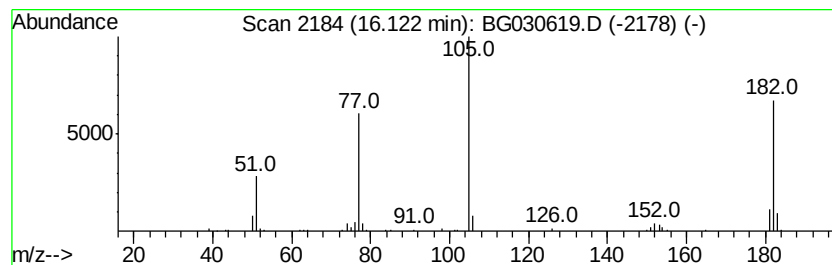
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Peak Number 4 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.12	2.31 ng	135187	Acenaphthene-d10	14.78
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzophenone	182 C13H10O	000119-61-9 96
2		Glyoxylohydroximoyl chloride, 2-...	183 C8H6ClNO2	004937-87-5 47
3		Benzeneacetic acid, .alpha.-oxo-...	164 C9H8O3	015206-55-0 43
4		Benzenecarbothioic acid, S-methy...	152 C8H8OS	005925-68-8 43
5		N-[2,2-Dichloro-1-(toluene-4-sul...	371 C16H15Cl2NO3S	136800-77-6 43



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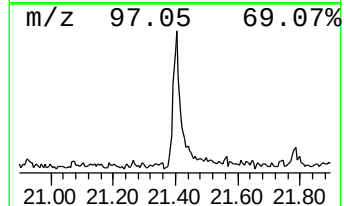
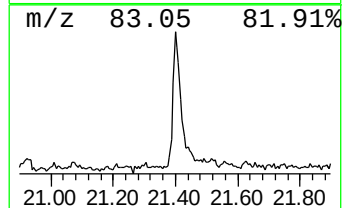
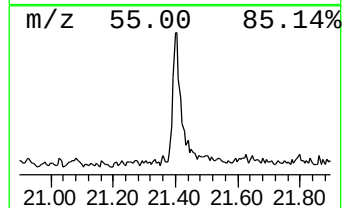
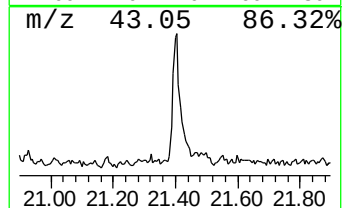
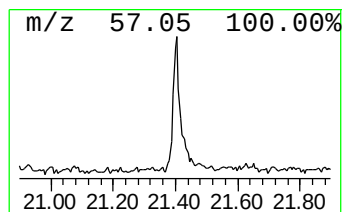
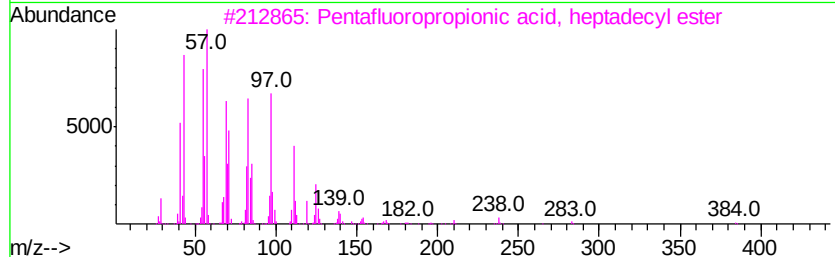
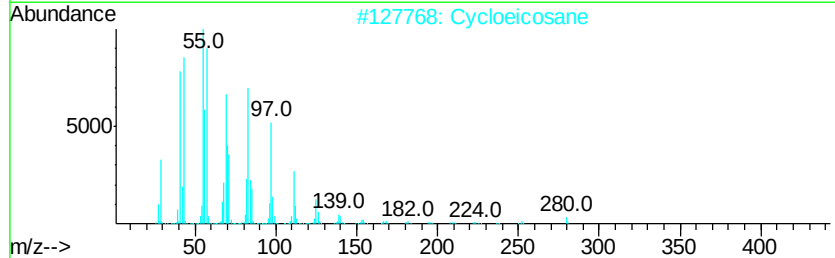
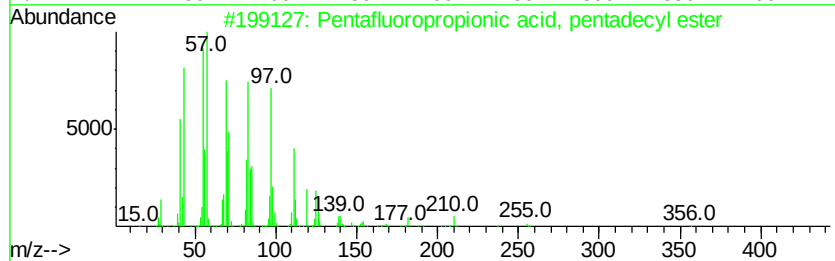
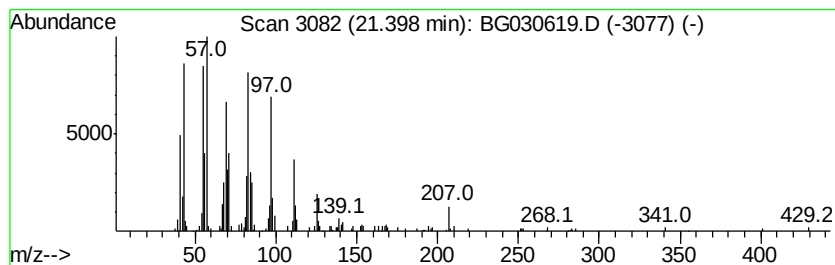
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Peak Number 5 Pentafluoropropionic acid, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.40	2.68 ng	212173	Chrysene-d12	21.79

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
2		Cycloeicosane	280	C20H40	000296-56-0	93
3		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	93
4		Behenic alcohol	326	C22H46O	000661-19-8	93
5		1-Docosene	308	C22H44	001599-67-3	91



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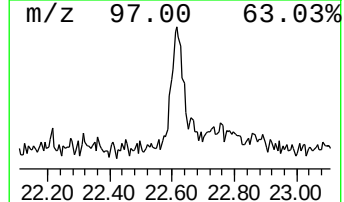
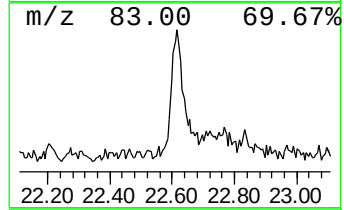
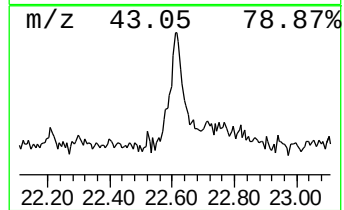
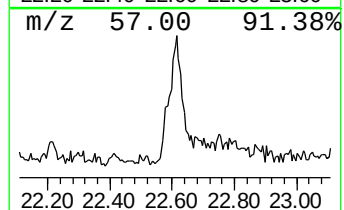
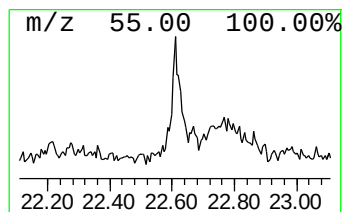
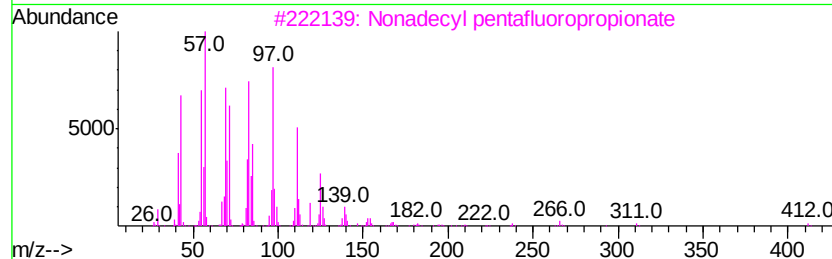
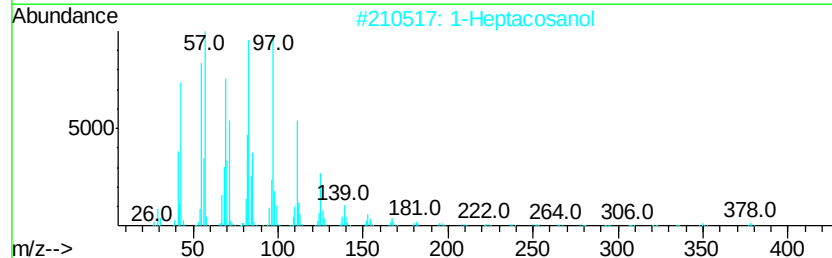
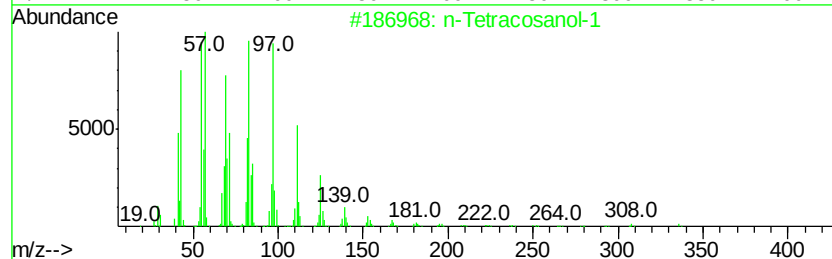
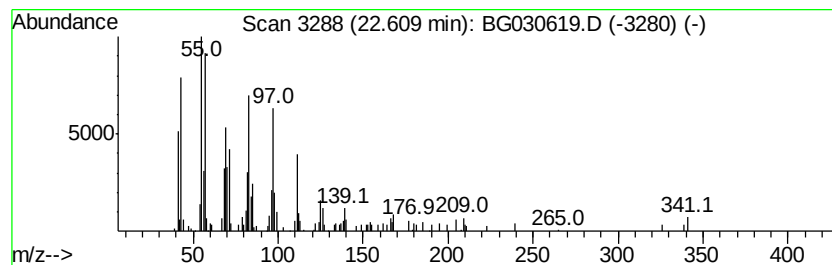
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Peak Number 6 n-Tetracosanol-1 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.61	2.16 ng	170676	Chrysene-d12	21.79
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		n-Tetracosanol-1	354 C24H50O	000506-51-4 93
2		1-Heptacosanol	396 C27H56O	002004-39-9 91
3		Nonadecyl pentafluoropropionate	430 C22H39F5O2	1000351-88-8 91
4		Nonadecyl trifluoroacetate	380 C21H39F3O2	1000351-76-3 91
5		Eicosyl pentafluoropropionate	444 C23H41F5O2	1000351-80-8 87



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.24	14.0	ng	322517	1	8.16	459900	20.0
unknown7.69	7.69	90.7	ng	2085610	1	8.16	459900	20.0
Benzophenone	16.12	2.3	ng	135187	3	14.78	1172370	20.0
Pentafluoropropio...	21.40	2.7	ng	212173	5	21.79	1581520	20.0
n-Tetracosanol-1	22.61	2.2	ng	170676	5	21.79	1581520	20.0