

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG103119\
 Data File : BG043446.D
 Acq On : 31 Oct 2019 22:55
 Operator : JU
 Sample : K5599-15
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 Z3-23B

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 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-BG102119.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	3.199	13	19	31	rVB	92588	182237	6.11%	1.176%
2	5.132	340	348	359	rBV	119094	206298	6.92%	1.331%
3	5.614	423	430	447	rBV	603073	1066940	35.80%	6.883%
4	7.207	693	701	720	rBV	641238	1228465	41.22%	7.925%
5	7.565	754	762	776	rBV	673661	1212423	40.68%	7.822%
6	8.023	834	840	848	rBV	151317	260864	8.75%	1.683%
7	8.346	887	895	908	rBV	505467	911951	30.60%	5.883%
8	9.187	1030	1038	1051	rBV	347119	700181	23.49%	4.517%
9	10.832	1310	1318	1328	rBV	151604	322871	10.83%	2.083%
10	13.276	1725	1734	1750	rBV	1066433	1782183	59.80%	11.497%
11	14.104	1869	1875	1888	rBV	59183	113392	3.80%	0.732%
12	14.651	1961	1968	1981	rBV2	302377	504373	16.92%	3.254%
13	16.143	2214	2222	2242	rBV	846627	1541605	51.73%	9.945%
14	17.395	2429	2435	2451	rBV	333865	600951	20.16%	3.877%
15	18.288	2583	2587	2598	rBV6	12310	32033	1.07%	0.207%
16	20.003	2873	2879	2894	rBV	2171173	2980204	100.00%	19.226%
17	21.308	3095	3101	3112	rBV6	25586	76247	2.56%	0.492%
18	21.660	3155	3161	3171	rBV2	392032	742709	24.92%	4.791%
19	22.453	3292	3296	3300	rBV	23215	31423	1.05%	0.203%
20	23.135	3408	3412	3418	rBV5	25038	42997	1.44%	0.277%
21	23.940	3542	3549	3556	rVB5	25483	60020	2.01%	0.387%
22	24.862	3694	3706	3722	rBV	281096	869384	29.17%	5.609%
23	25.996	3892	3899	3905	rBV10	13357	31189	1.05%	0.201%

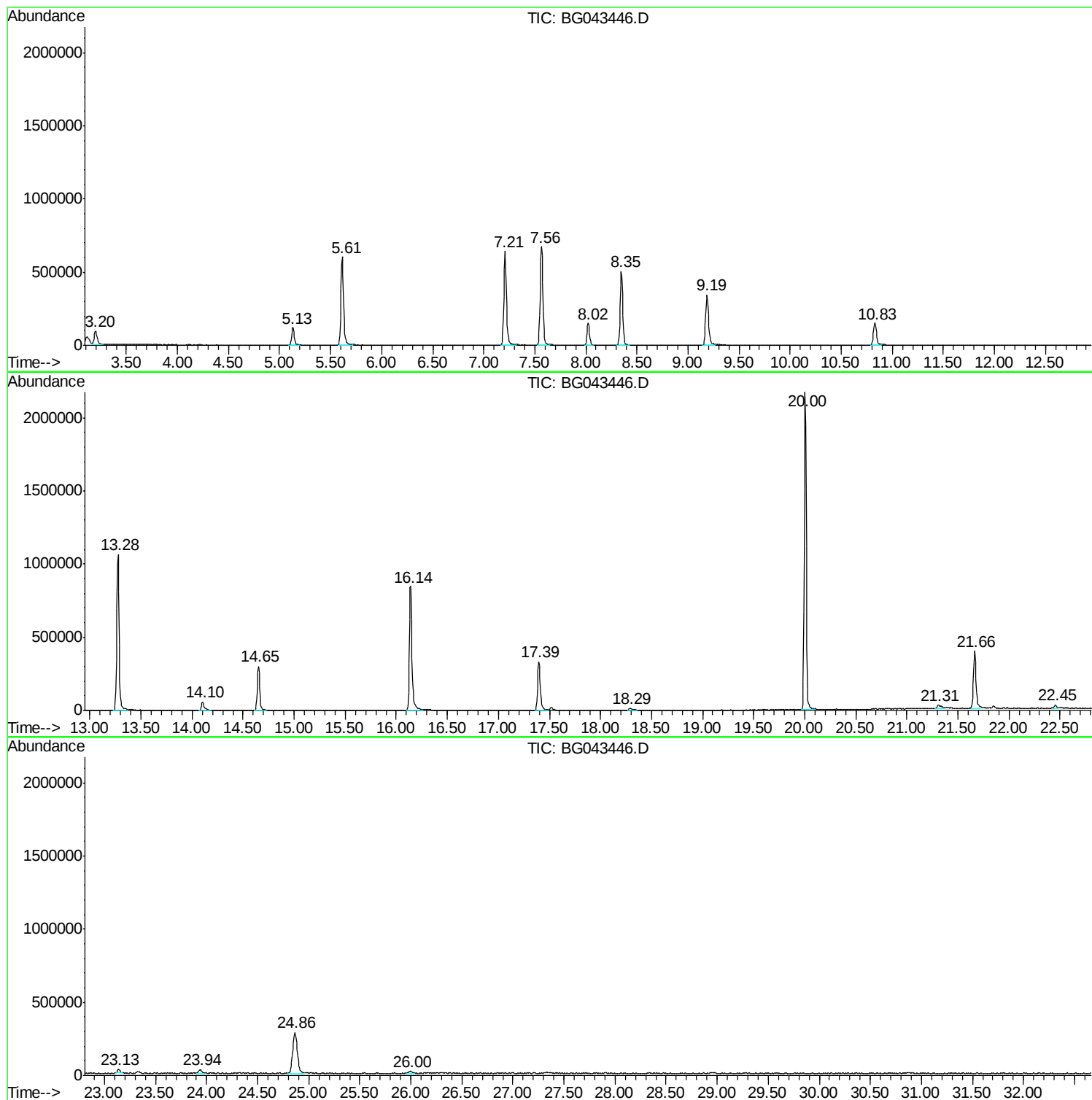
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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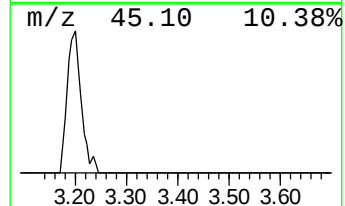
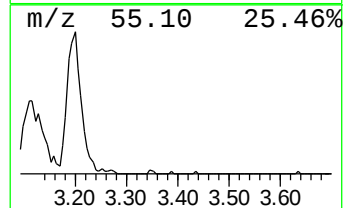
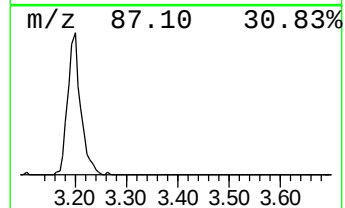
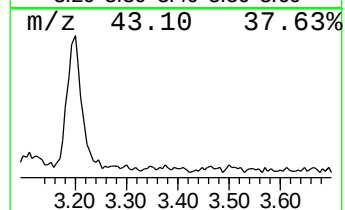
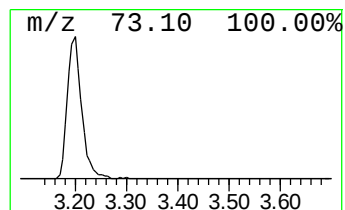
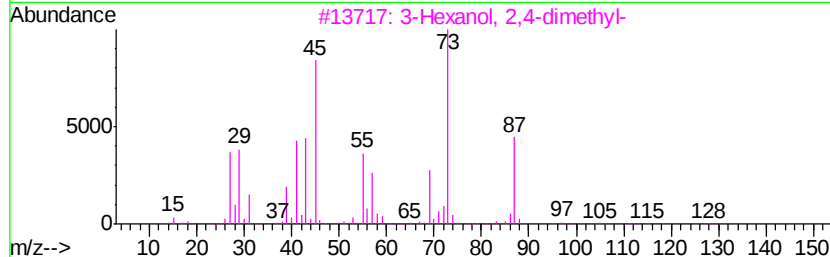
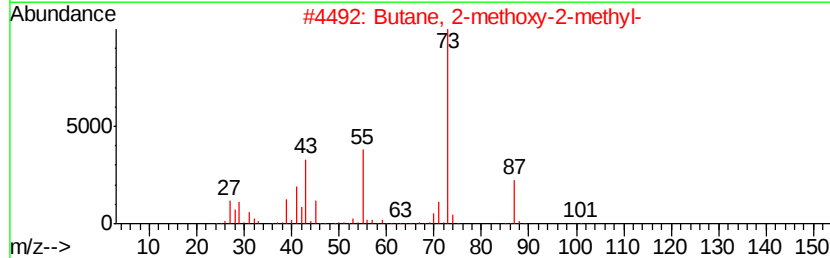
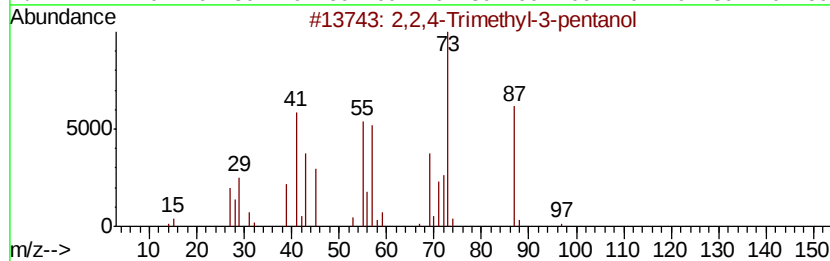
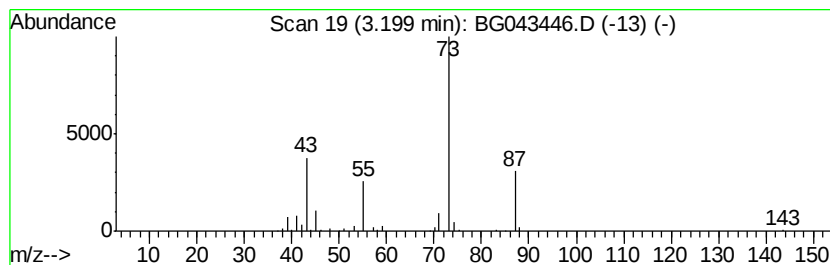
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2,2,4-Trimethyl-3-pentanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.20	13.97 ng	182237	1,4-Dichlorobenzene-d4	8.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	64
2		Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	56
3		3-Hexanol, 2,4-dimethyl-	130	C8H18O	013432-25-2	38
4		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	12
5		N-Ethylformamide	73	C3H7NO	000627-45-2	9



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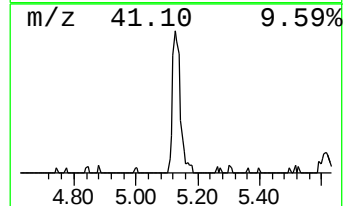
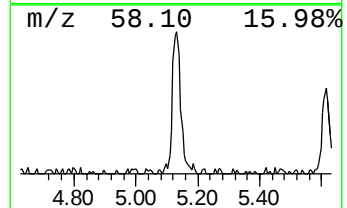
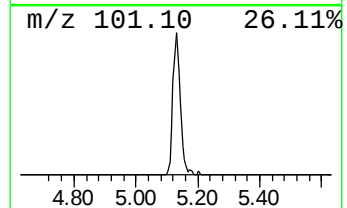
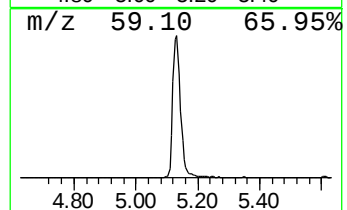
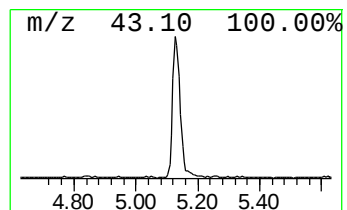
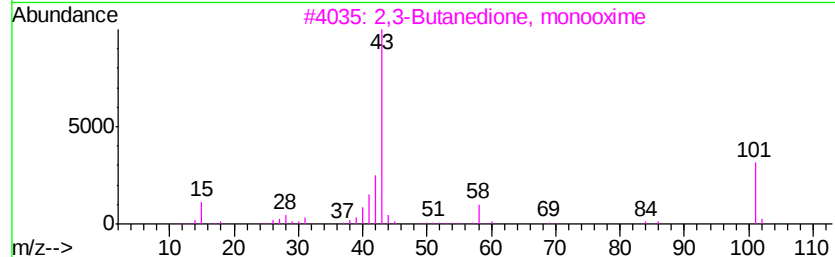
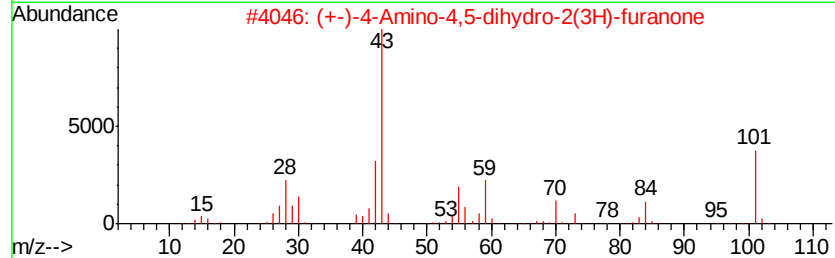
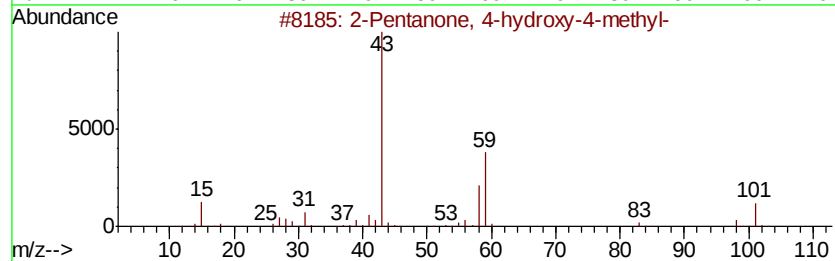
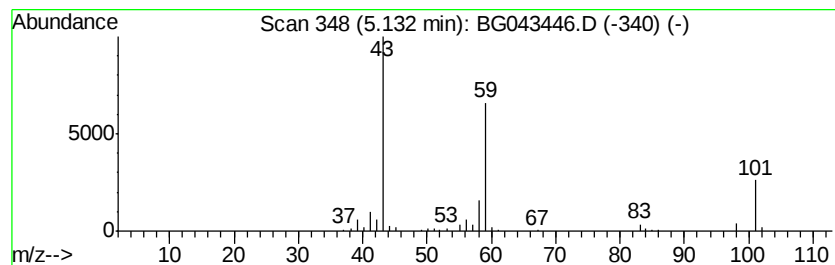
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	15.82 ng	206298	1,4-Dichlorobenzene-d4	8.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		(+)-4-Amino-4,5-dihydro-2(3H)-furanone	101	C4H7NO2	016504-58-8	47
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4		Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	25
5		Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	17



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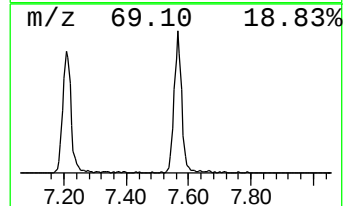
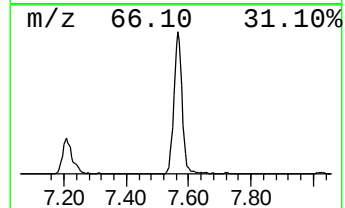
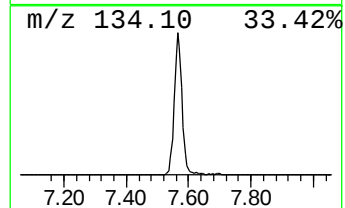
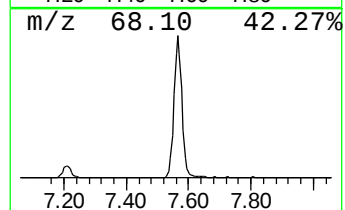
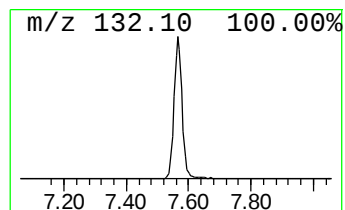
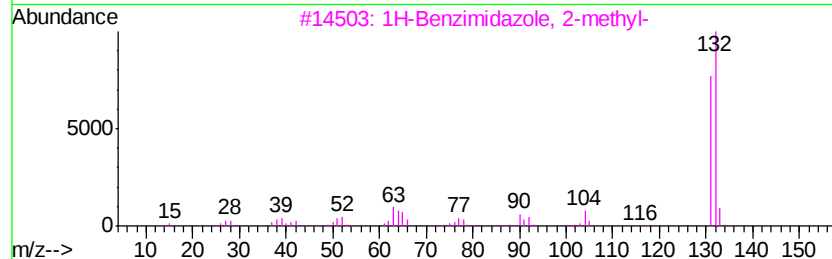
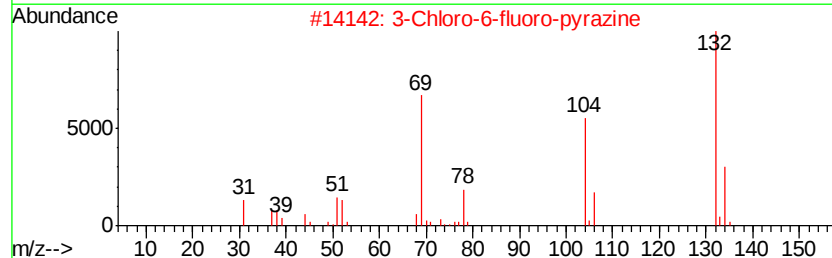
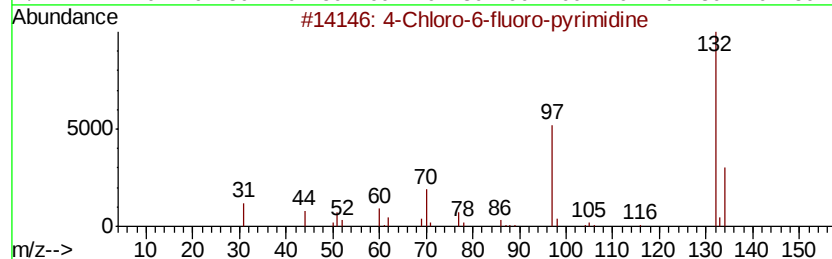
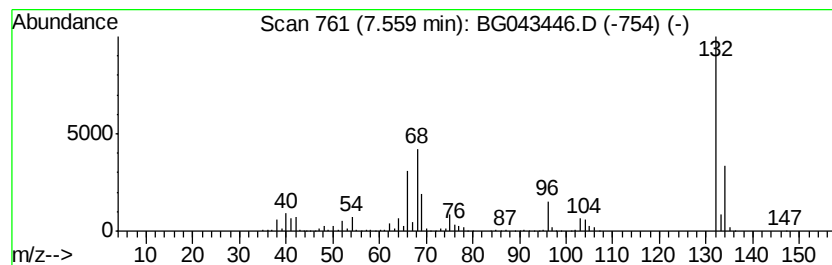
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Peak Number 3 unknown7.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.56	92.95 ng	1212420	1,4-Dichlorobenzene-d4	8.02

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-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5		5-Aminoindole	132	C8H8N2	005192-03-0	12



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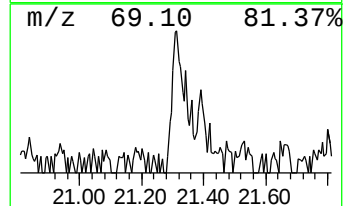
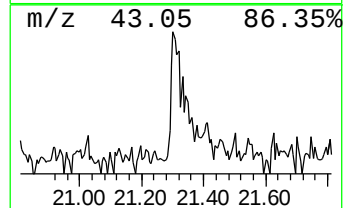
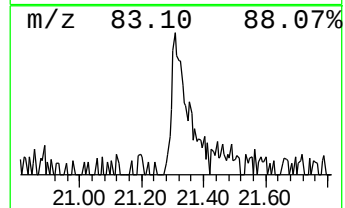
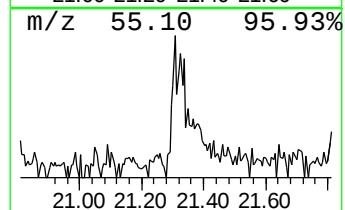
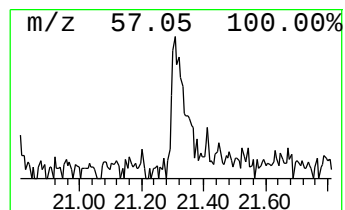
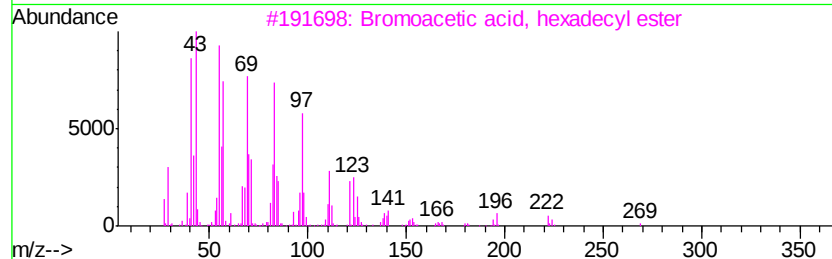
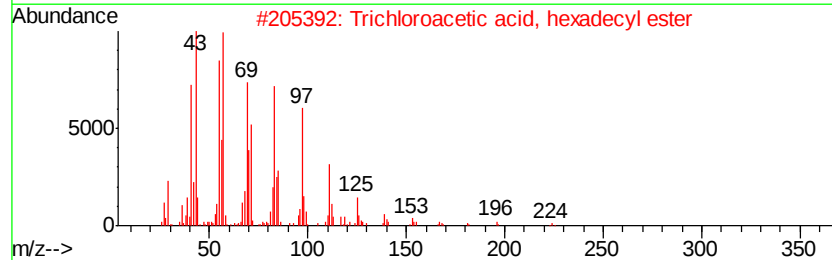
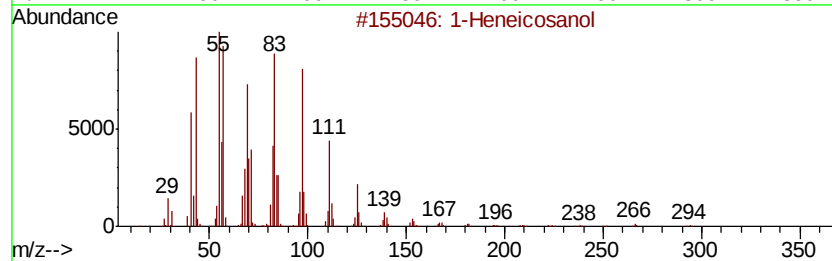
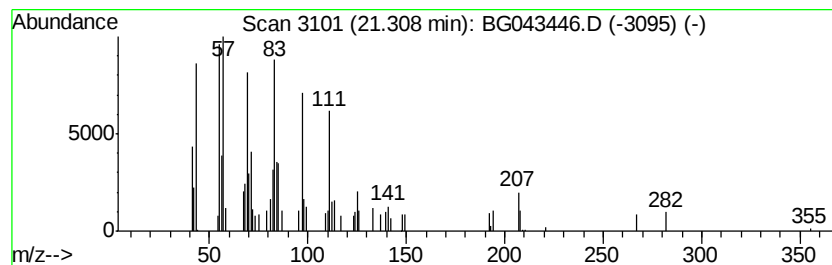
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Peak Number 5 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.31	2.05 ng	76247	Chrysene-d12	21.66
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Heneicosanol	312 C21H44O	015594-90-8	76
2	Trichloroacetic acid, hexadecyl ...	386 C18H33Cl3O2	074339-54-1	68
3	Bromoacetic acid, hexadecyl ester	362 C18H35BrO2	005454-48-8	62
4	Pentafluoropropionic acid, penta...	374 C18H31F5O2	959092-08-1	60
5	Trifluoroacetic acid, pentadecyl...	324 C17H31F3O2	959010-23-2	53



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2,2,4-Trimethyl-3...	3.20	14.0	ng	182237	1	8.02	260864	20.0
2-Pentanone, 4-hy...	5.13	15.8	ng	206298	1	8.02	260864	20.0
unknown7.56	7.56	93.0	ng	1212420	1	8.02	260864	20.0
1-Heneicosanol	21.31	2.0	ng	76247	5	21.66	742709	20.0