

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG082718\
 Data File : BG036438.D
 Acq On : 27 Aug 2018 19:19
 Operator : JU/SJ
 Sample : J4583-02
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TOD1-SB-01-02-03-0-52

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-BG082318.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	5.168	314	320	327	rBV	46079	70647	1.61%	0.309%
2	5.633	392	399	409	rBV	1111056	1733695	39.60%	7.575%
3	7.219	661	669	683	rBV	1139047	1951181	44.57%	8.526%
4	7.595	725	733	741	rBV	1033589	1778484	40.62%	7.771%
5	8.065	806	813	821	rBV	202681	336269	7.68%	1.469%
6	8.388	860	868	876	rBV	762623	1315273	30.04%	5.747%
7	9.222	1001	1010	1020	rBV	625586	1121731	25.62%	4.901%
8	10.873	1283	1291	1301	rVB	261299	487061	11.12%	2.128%
9	13.318	1699	1707	1716	rBV	1693033	2676068	61.12%	11.693%
10	14.134	1839	1846	1853	rBV	149906	214708	4.90%	0.938%
11	14.687	1931	1940	1952	rVB2	428155	706565	16.14%	3.087%
12	16.173	2186	2193	2206	rBV	1464249	2207608	50.42%	9.646%
13	17.430	2400	2407	2416	rBV	632381	925348	21.14%	4.043%
14	18.318	2553	2558	2566	rBV	71086	109447	2.50%	0.478%
15	20.039	2845	2851	2861	rBV	3361929	4378149	100.00%	19.130%
16	21.349	3069	3074	3094	rBV2	195985	440609	10.06%	1.925%
17	21.696	3126	3133	3140	rBV	673054	1108630	25.32%	4.844%
18	21.913	3164	3170	3175	rBV3	31080	49622	1.13%	0.217%
19	22.525	3269	3274	3279	rBV4	31568	66726	1.52%	0.292%
20	24.035	3526	3531	3537	rVB3	29298	56086	1.28%	0.245%
21	24.910	3669	3680	3690	rBV2	384628	1092842	24.96%	4.775%
22	26.138	3883	3889	3897	rVB4	20806	59167	1.35%	0.259%

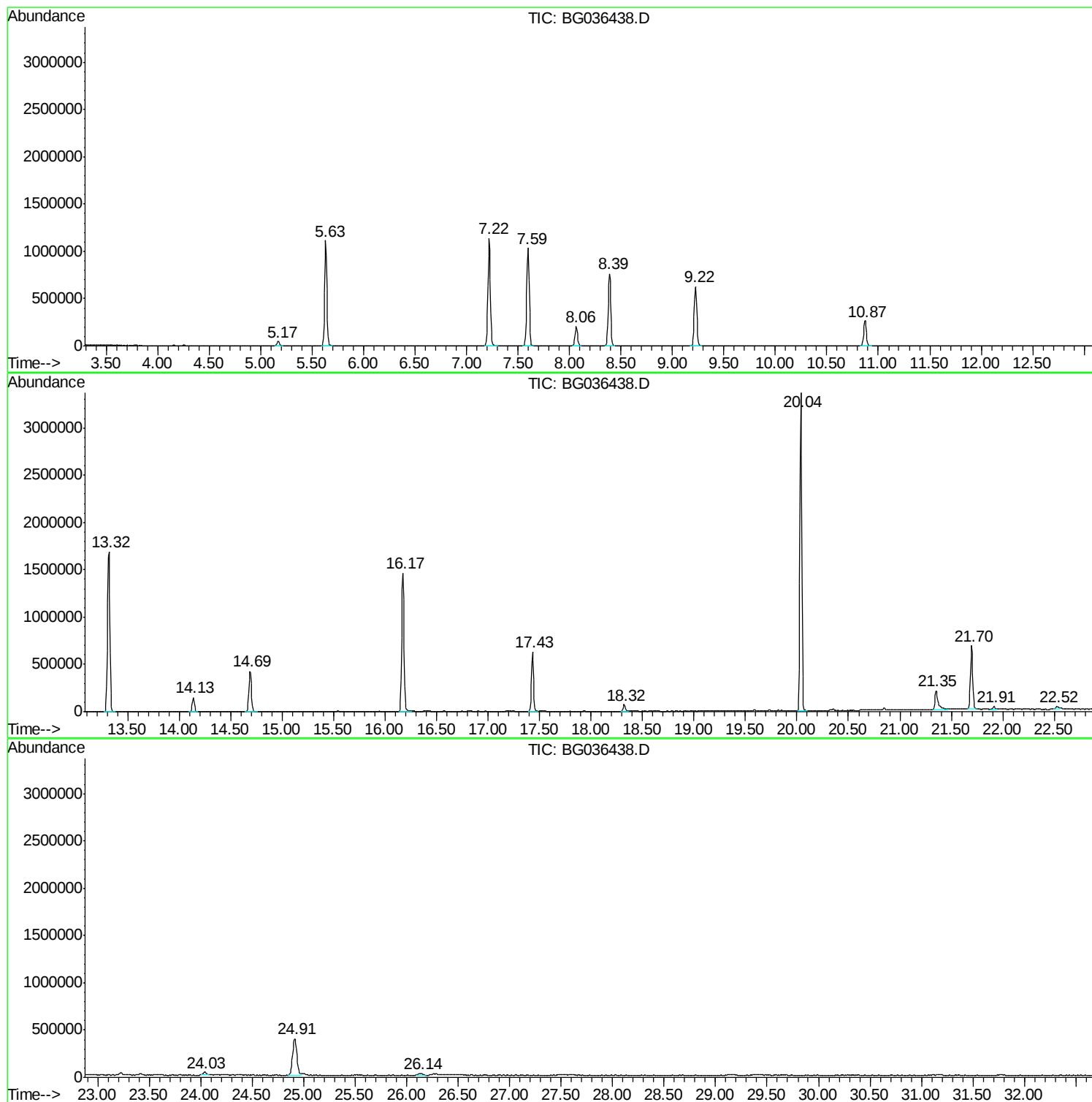
Sum of corrected areas: 22885916

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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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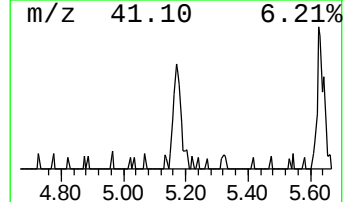
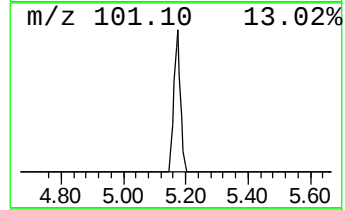
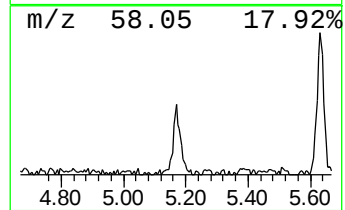
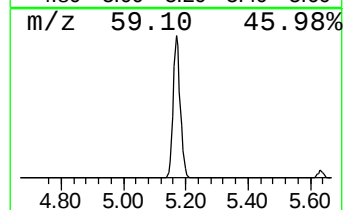
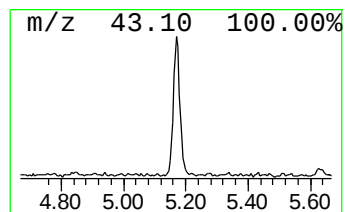
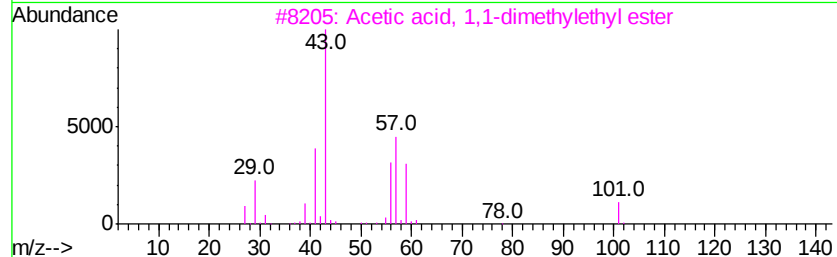
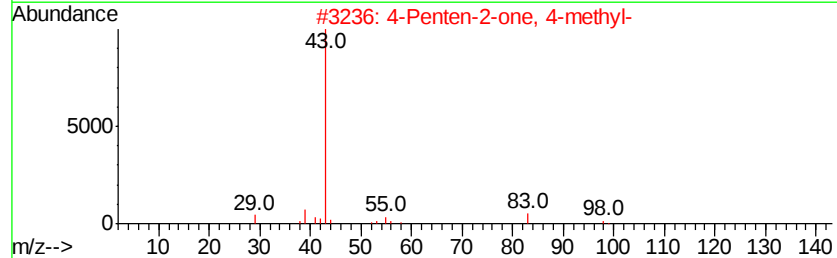
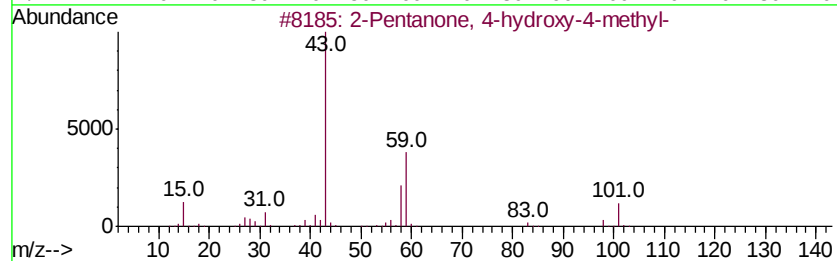
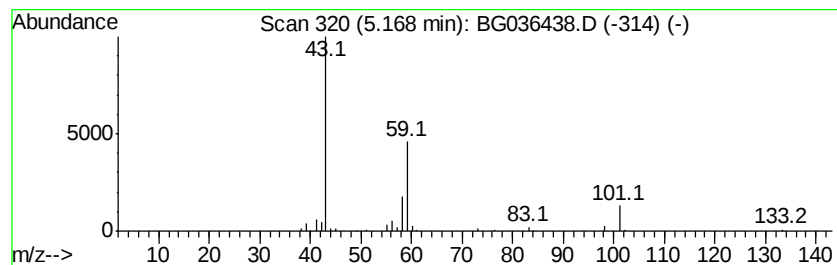
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.17	4.20 ng	70647	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	56
2			4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9
3			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
4			1-Ethylpentyl acetate	158	C9H18O2	005921-83-5	9
5			2-hydroxy-2-methyl-4-heptanone	144	C8H16O2	054862-91-8	9



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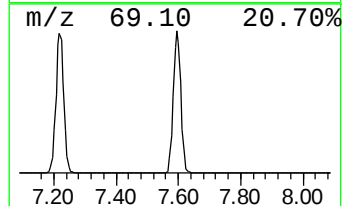
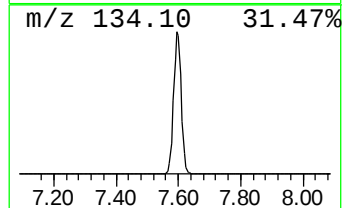
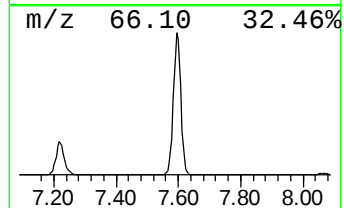
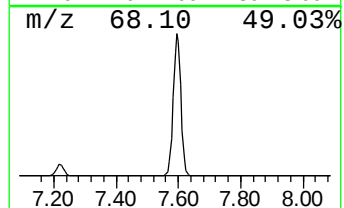
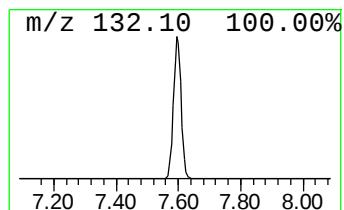
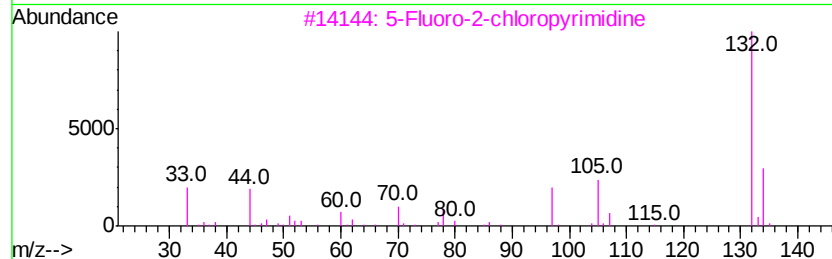
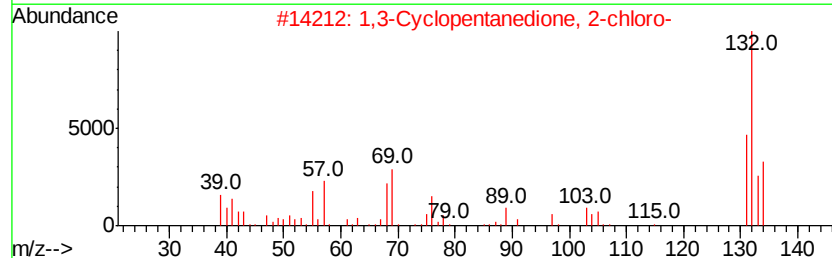
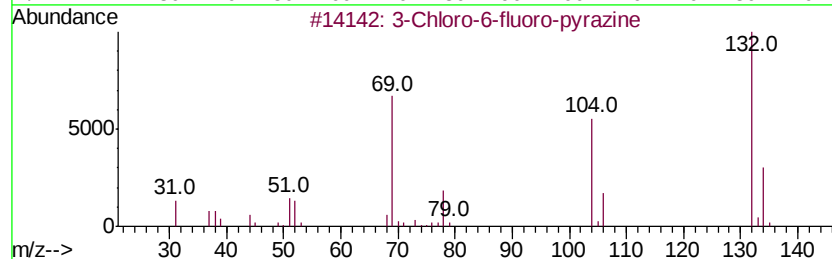
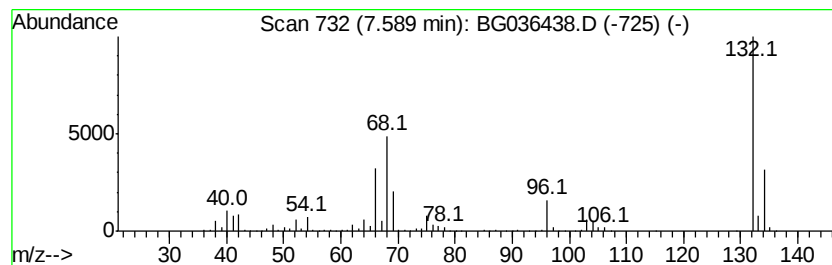
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Peak Number 2 unknown7.59 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.59	105.78 ng	1778480	1,4-Dichlorobenzene-d4	8.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	17
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
5		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10



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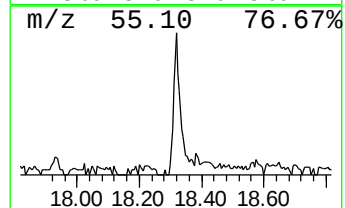
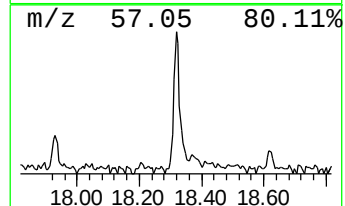
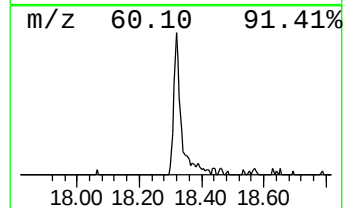
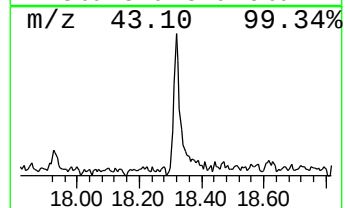
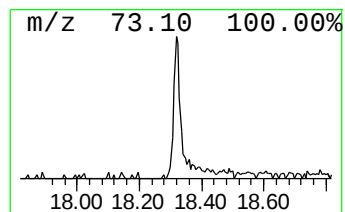
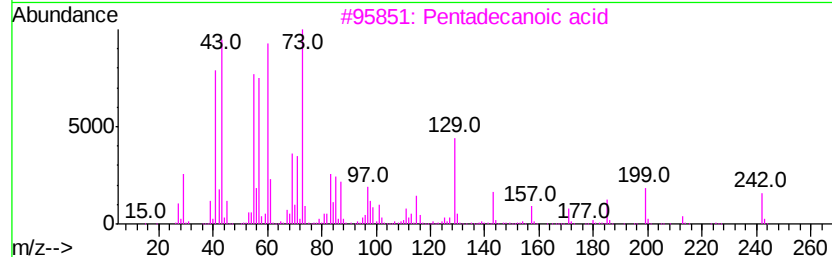
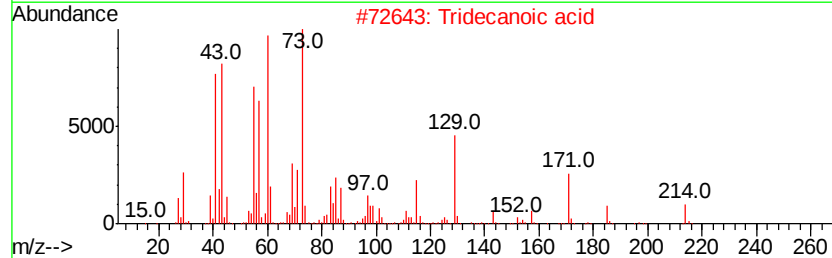
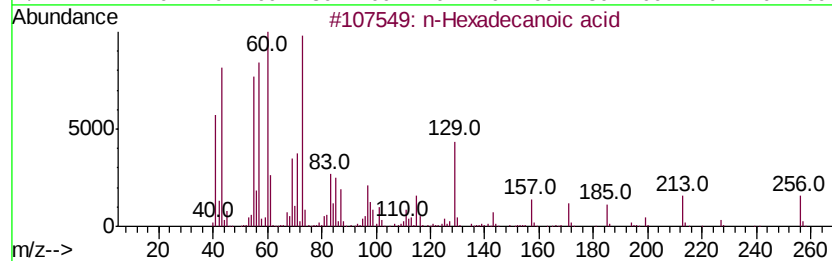
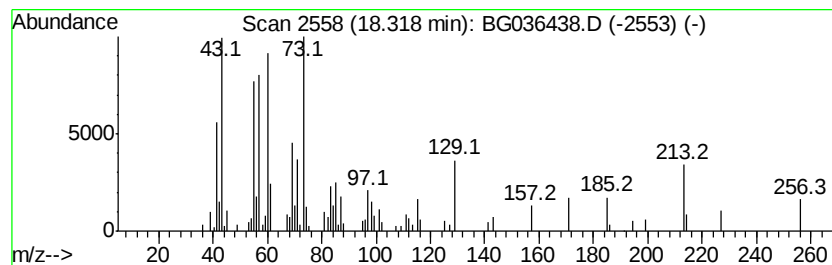
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.32	2.37 ng	109447	Phenanthrene-d10	17.43

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	93
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4		Undecanoic acid	186	C11H22O2	000112-37-8	70
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	64



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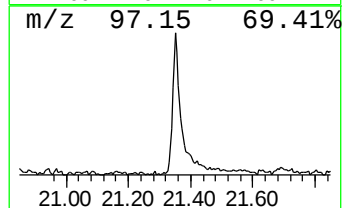
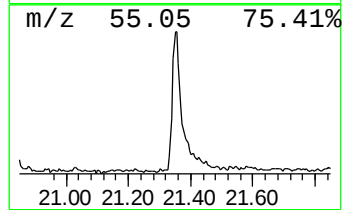
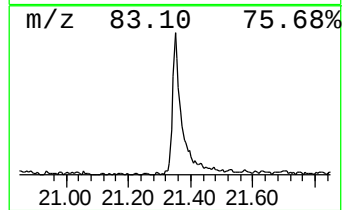
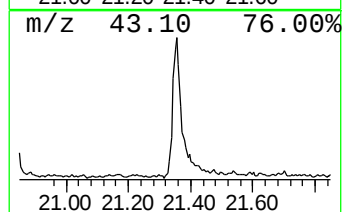
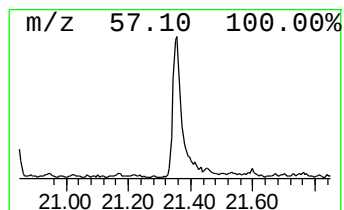
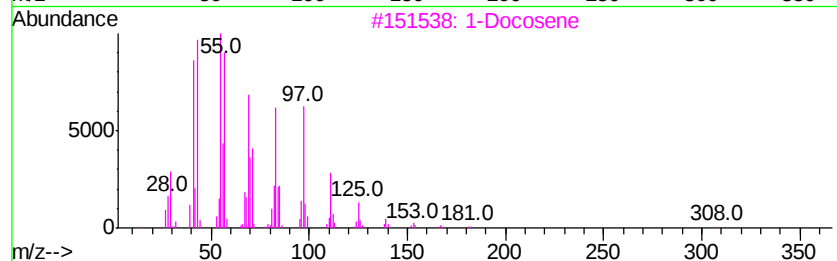
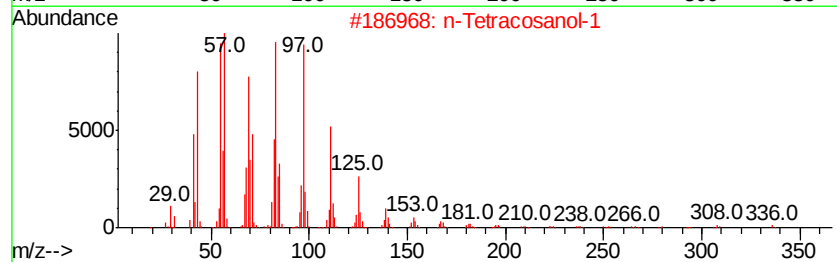
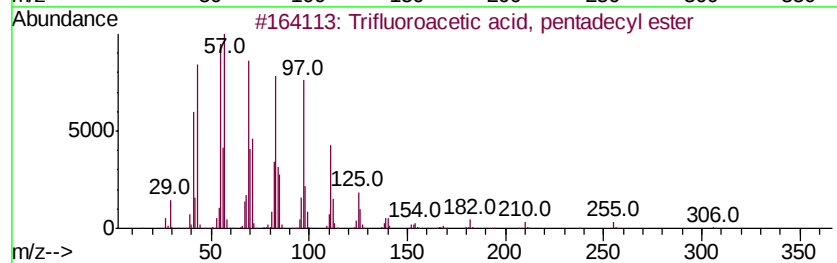
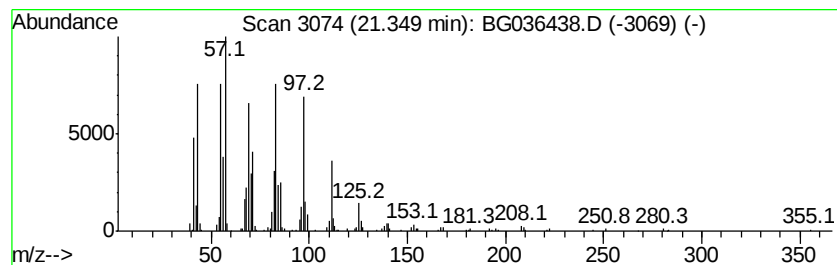
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Peak Number 5 Trifluoroacetic acid, penta... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.35	7.95 ng	440609	Chrysene-d12	21.70

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
2		n-Tetracosanol-1	354	C24H50O	000506-51-4	91
3		1-Docosene	308	C22H44	001599-67-3	91
4		1-Heptacosanol	396	C27H56O	002004-39-9	91
5		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.17	4.2	ng	70647	1	8.06	336269	20.0
unknown7.59	7.59	105.8	ng	1778480	1	8.06	336269	20.0
n-Hexadecanoic acid	18.32	2.4	ng	109447	4	17.43	925348	20.0
Trifluoroacetic a...	21.35	8.0	ng	440609	5	21.70	1108630	20.0