

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG111618\
 Data File : BG038056.D
 Acq On : 17 Nov 2018 5:48
 Operator : JU/SJ
 Sample : J5968-03
 Misc :
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 MW-3-111418

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-BG111318.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	5.167	314	320	332	rVB2	31475	55195	1.93%	0.366%
2	5.626	392	398	410	rBV	298691	502692	17.61%	3.331%
3	7.230	664	671	685	rBV2	198768	403390	14.13%	2.673%
4	7.612	728	736	744	rBV	576033	1034400	36.23%	6.855%
5	8.082	810	816	826	rBV	172865	306520	10.74%	2.031%
6	8.411	864	872	880	rBV	544242	1002922	35.13%	6.647%
7	9.263	1009	1017	1028	rBV	508349	936986	32.82%	6.210%
8	10.902	1288	1296	1306	rBV	247125	454323	15.91%	3.011%
9	13.340	1702	1711	1721	rBV	1375386	2154787	75.47%	14.280%
10	14.163	1844	1851	1858	rVB	48503	71096	2.49%	0.471%
11	14.721	1939	1946	1954	rBV2	387853	650463	22.78%	4.311%
12	15.097	2001	2010	2020	rBV5	20051	36147	1.27%	0.240%
13	16.207	2192	2199	2207	rBV2	924072	1424391	49.89%	9.440%
14	17.465	2406	2413	2426	rVB2	493038	769601	26.96%	5.100%
15	18.323	2554	2559	2571	rBV2	66328	108511	3.80%	0.719%
16	19.592	2770	2775	2782	rBV4	16979	29557	1.04%	0.196%
17	20.068	2849	2856	2869	rBV	2169125	2855099	100.00%	18.921%
18	21.390	3069	3081	3084	rBV	28796	97266	3.41%	0.645%
19	21.748	3135	3142	3151	rBV2	493866	841099	29.46%	5.574%
20	21.895	3163	3167	3173	rVB	18949	29982	1.05%	0.199%
21	22.512	3267	3272	3279	rBV	26962	43866	1.54%	0.291%
22	23.217	3386	3392	3400	rVB3	31251	65597	2.30%	0.435%
23	23.417	3417	3426	3433	rVB	89295	176117	6.17%	1.167%
24	24.039	3526	3532	3541	rVB2	39914	86375	3.03%	0.572%
25	25.073	3690	3708	3723	rVB	276619	895067	31.35%	5.932%
26	26.172	3888	3895	3903	rVB6	20290	57749	2.02%	0.383%

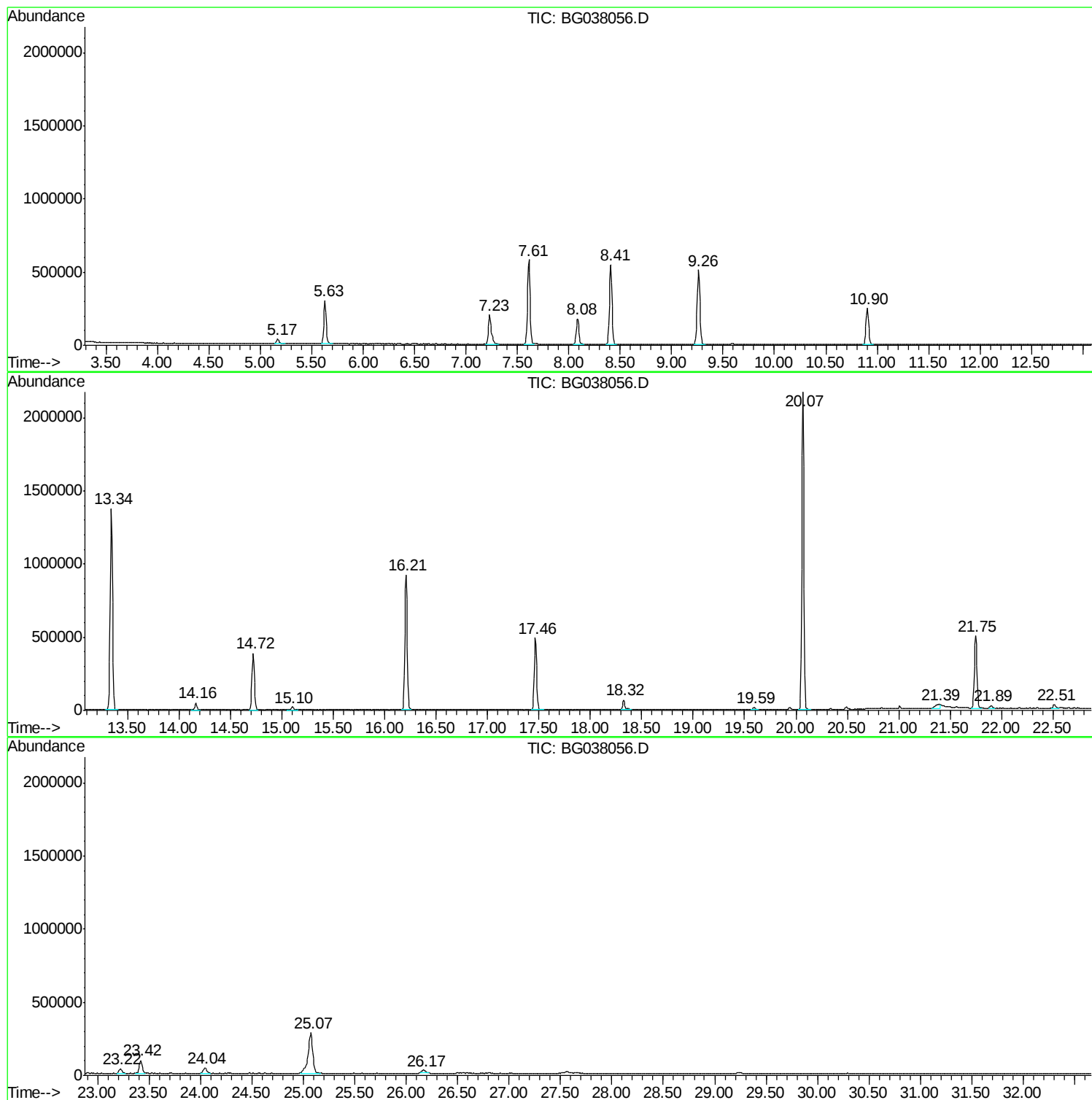
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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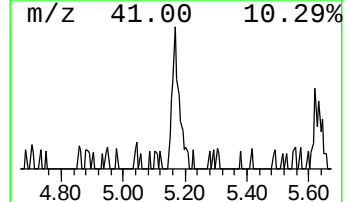
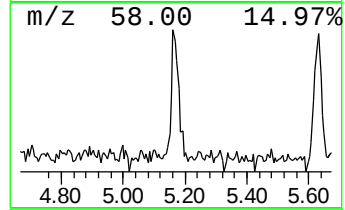
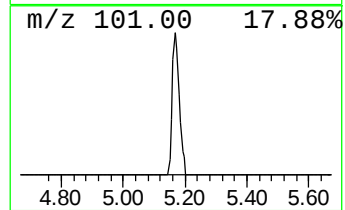
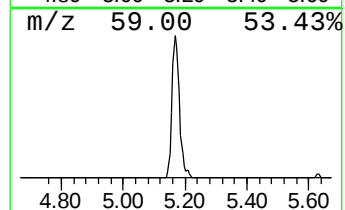
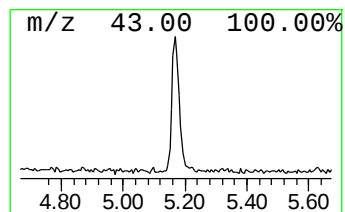
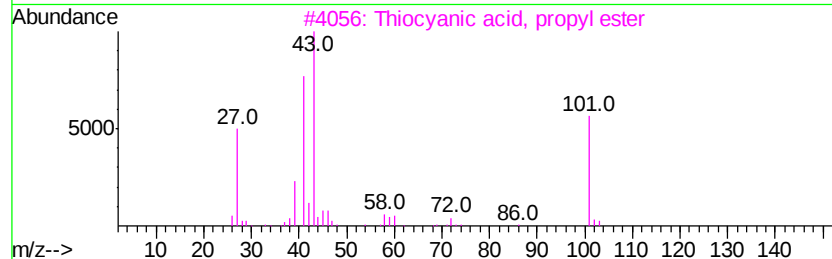
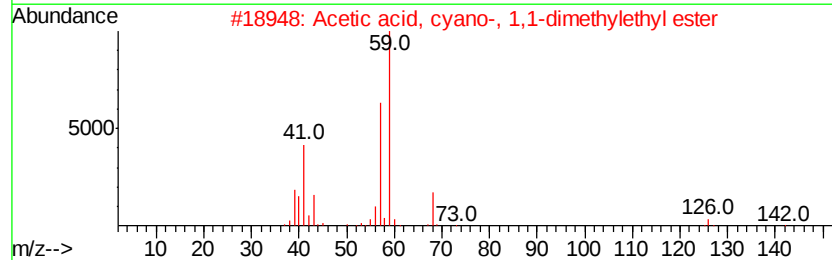
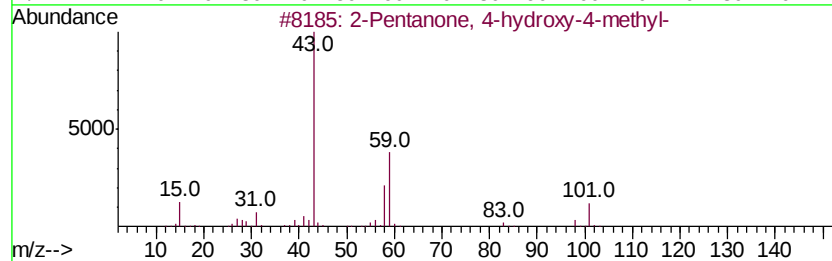
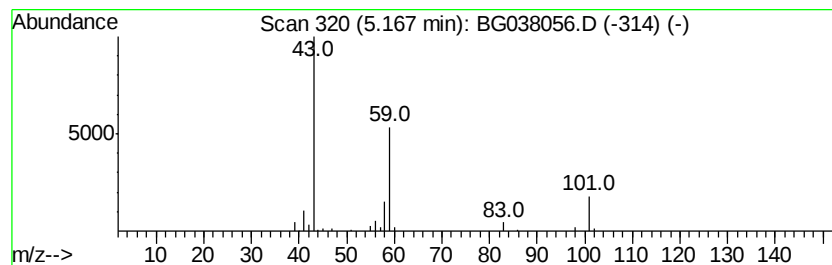
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG111318.M
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown5.17 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.17	3.60 ng	55195	1,4-Dichlorobenzene-d4	8.08

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	39
2			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3			Thiocyanic acid, propyl ester	101	C4H7NS	004251-16-5	9
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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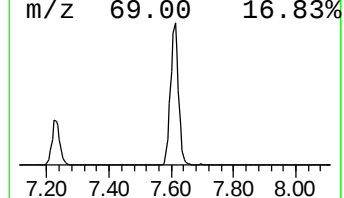
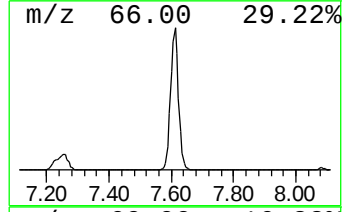
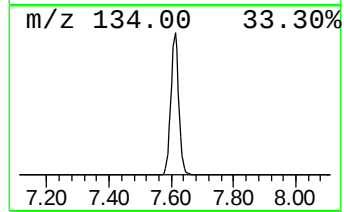
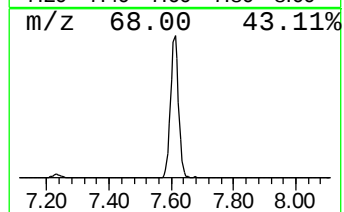
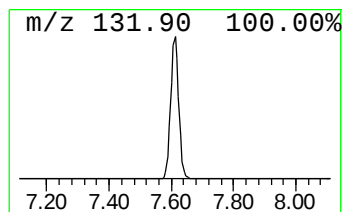
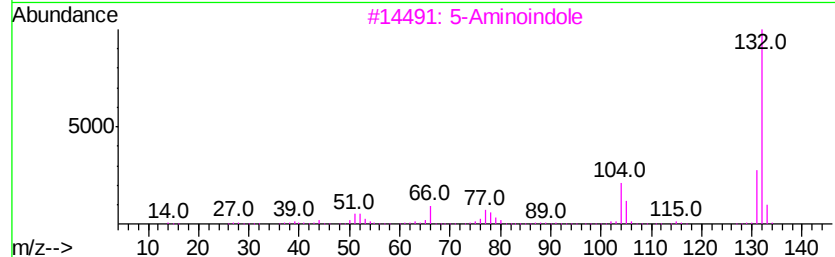
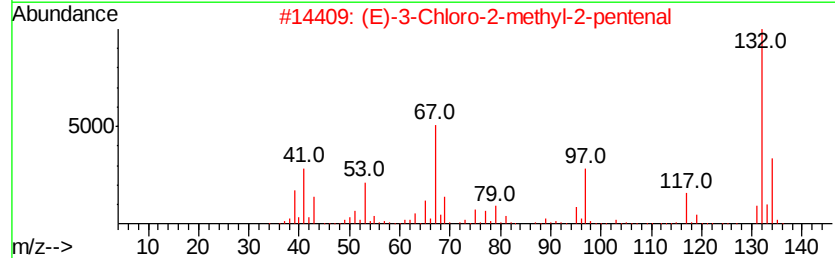
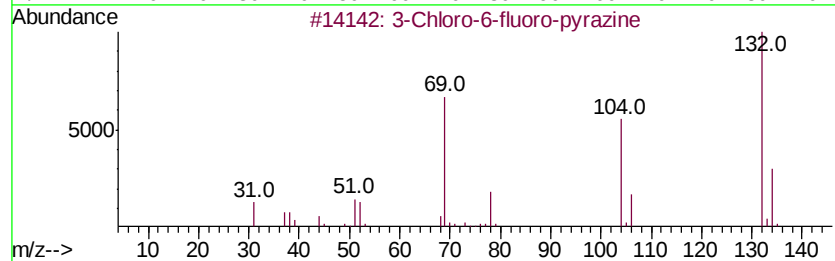
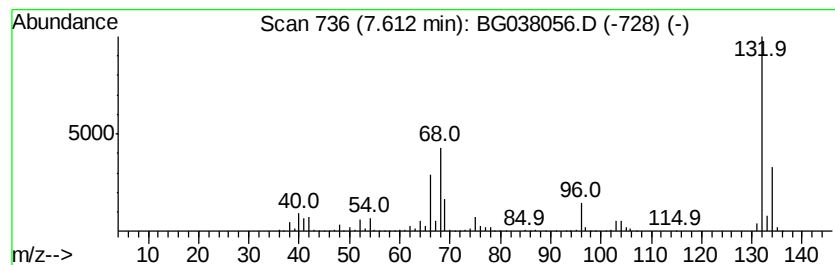
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Peak Number 2 unknown7.61 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.61	67.49 ng	1034400	1,4-Dichlorobenzene-d4	8.08

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		1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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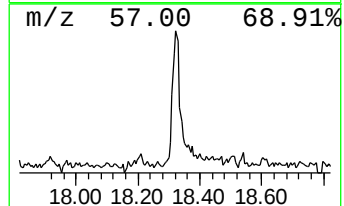
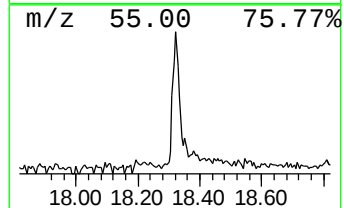
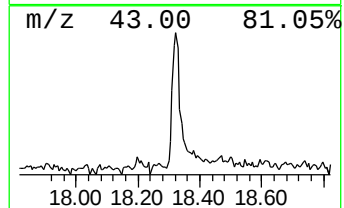
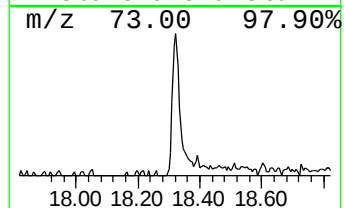
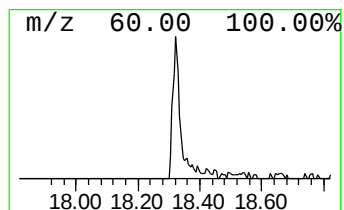
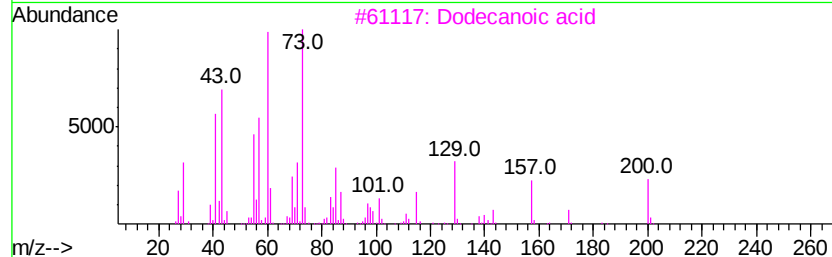
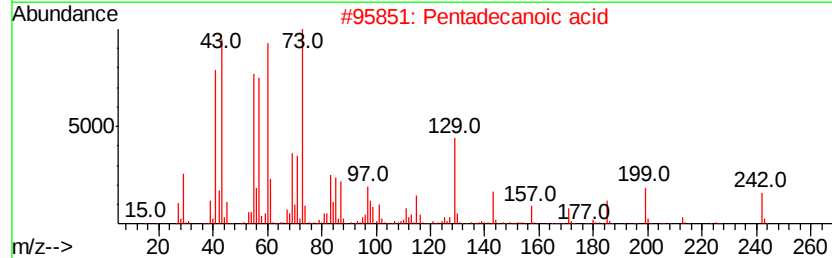
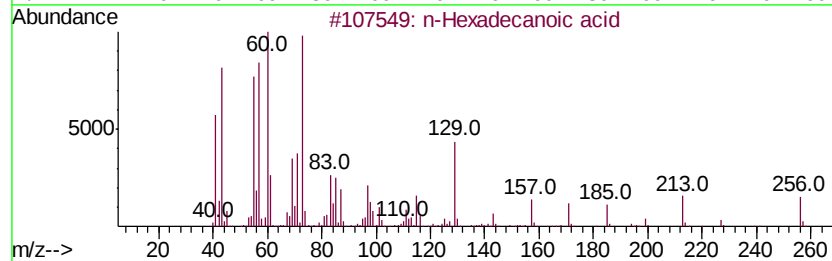
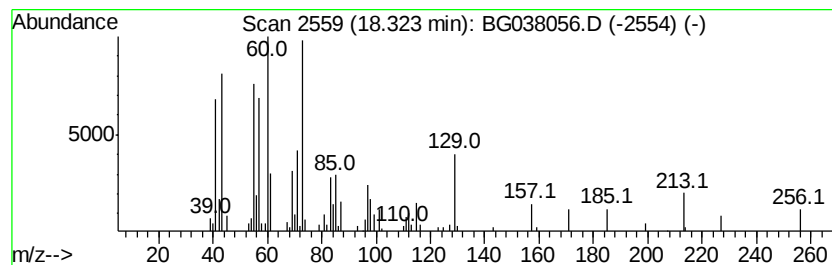
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.32	2.82 ng	108511	Phenanthrene-d10		17.46	
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	90
3		Dodecanoic acid	200	C12H24O2	000143-07-7	64
4		Tridecanoic acid	214	C13H26O2	000638-53-9	62
5		1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	11



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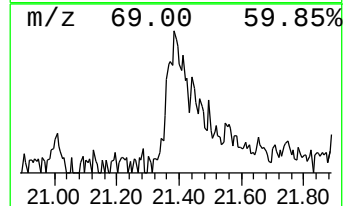
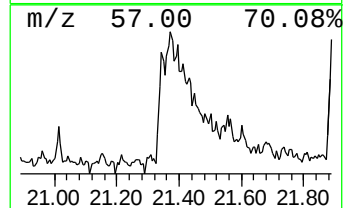
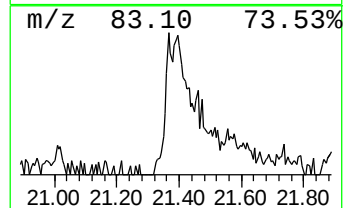
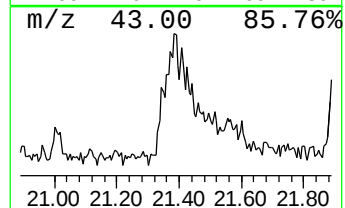
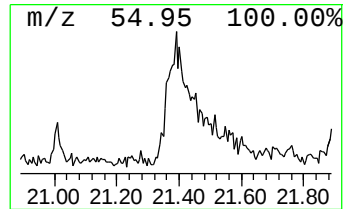
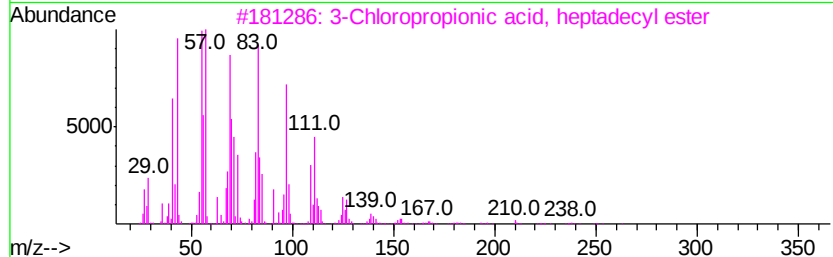
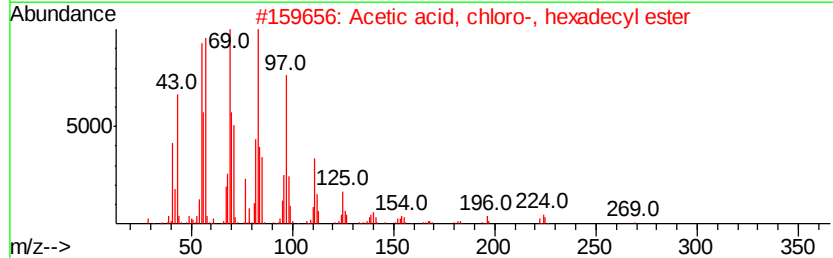
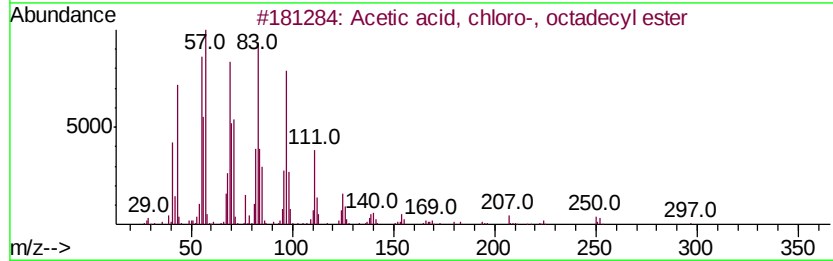
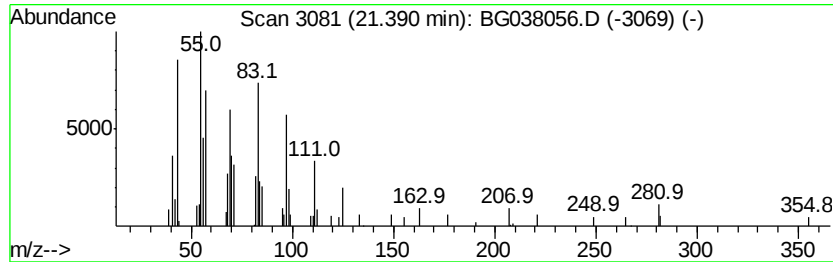
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Peak Number 5 Acetic acid, chloro-, octadec... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
21.39	2.31 ng	97266	Chrysene-d12		21.75	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, chloro-, octadecyl ...	346	C20H39ClO2	005348-82-3	90	
2	Acetic acid, chloro-, hexadecyl ...	318	C18H35ClO2	052132-58-8	87	
3	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	87	
4	E-15-Heptadecenal	252	C17H32O	1000130-97-9	87	
5	Carbonic acid, tetradecyl 2,2,2-...	388	C17H31Cl3O3	1000314-56-0	83	



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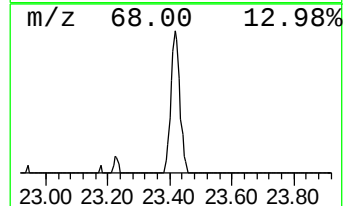
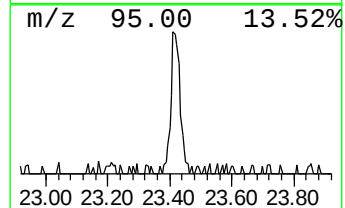
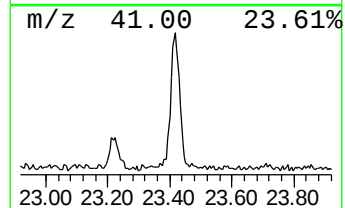
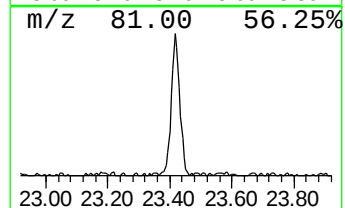
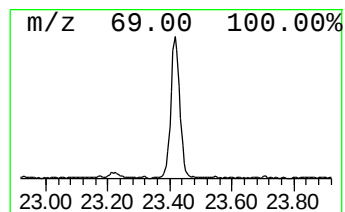
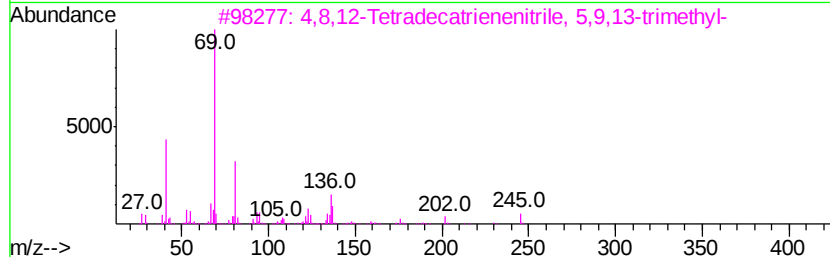
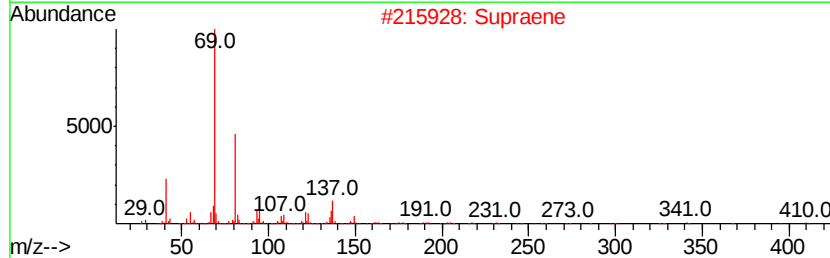
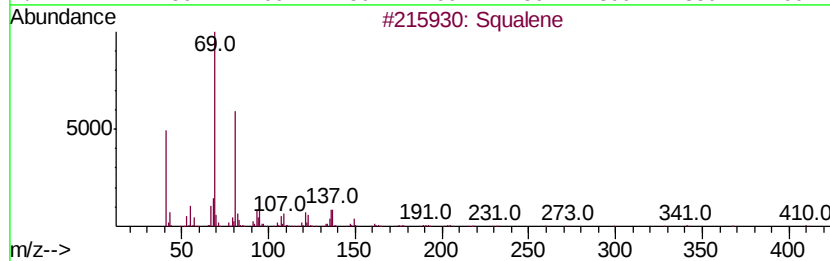
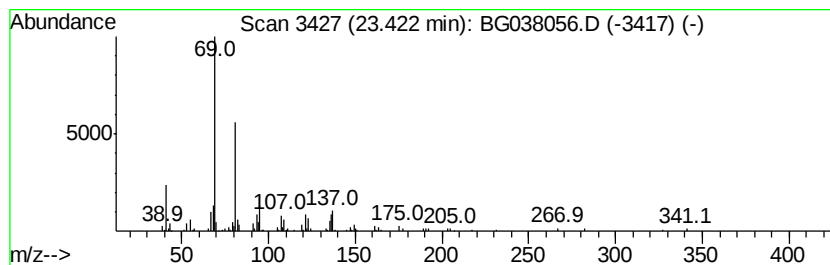
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Peak Number 6 Squalene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.42	3.94 ng	176117	Perylene-d12	25.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	91
2		Supraene	410	C30H50	007683-64-9	90
3		4,8,12-Tetradecatrienenitrile, 5...	245	C17H27N	005981-31-7	72
4		Propanoic acid, 2,2-dimethyl-, [...	306	C20H34O2	1000164-38-8	72
5		1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	52



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TIC Top Hit name	RT	EstConc	Units	Response	---Internal Standard---			
					#	RT	Resp	Conc
unknown5.17	5.17	3.6	ng	55195	1	8.08	306520	20.0
unknown7.61	7.61	67.5	ng	1034400	1	8.08	306520	20.0
n-Hexadecanoic acid	18.32	2.8	ng	108511	4	17.46	769601	20.0
Acetic acid, chlo...	21.39	2.3	ng	97266	5	21.75	841099	20.0
Squalene	23.42	3.9	ng	176117	6	25.07	895067	20.0