

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052317\
 Data File : BF095360.D
 Acq On : 23 May 2017 19:57
 Operator : SJ/MA
 Sample : I3243-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-7-TP-8

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:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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	5.125	537	542	563	rBV	230784	608366	16.61%	2.216%
2	5.719	639	643	675	rBV	1310472	2775251	75.77%	10.108%
3	7.301	907	912	927	rBV	1861510	2906801	79.36%	10.587%
4	7.419	927	932	949	rVB	2147027	3330206	90.92%	12.129%
5	7.754	985	989	1001	rVB	455160	553371	15.11%	2.015%
6	7.989	1025	1029	1044	rBV	1860602	2442765	66.69%	8.897%
7	8.660	1138	1143	1174	rBV	1078898	1867342	50.98%	6.801%
8	9.778	1328	1333	1357	rBV	387010	796560	21.75%	2.901%
9	10.960	1529	1534	1544	rBV2	19266	38199	1.04%	0.139%
10	11.542	1628	1633	1655	rBV	2558381	3662700	100.00%	13.340%
11	12.242	1748	1752	1769	rBV	288175	482529	13.17%	1.757%
12	12.607	1809	1814	1834	rBV2	551605	897132	24.49%	3.267%
13	13.436	1952	1955	1960	rBV	45087	49905	1.36%	0.182%
14	13.518	1965	1969	1977	rVB2	30923	48583	1.33%	0.177%
15	13.901	2029	2034	2053	rBV	1125593	1896112	51.77%	6.906%
16	14.213	2082	2087	2090	rBV	41198	54421	1.49%	0.198%
17	15.012	2218	2223	2227	rBV	447597	650517	17.76%	2.369%
18	15.048	2227	2229	2244	rVV	123334	222319	6.07%	0.810%
19	15.965	2379	2385	2400	rVB5	55760	147385	4.02%	0.537%
20	16.801	2523	2527	2540	rBV	77586	121996	3.33%	0.444%
21	17.106	2573	2579	2587	rBV	93830	133382	3.64%	0.486%
22	17.330	2611	2617	2630	rBV	1963330	2370364	64.72%	8.633%
23	18.583	2824	2830	2841	rBV5	29737	95994	2.62%	0.350%
24	18.683	2843	2847	2867	rVV	325378	572692	15.64%	2.086%
25	19.689	3014	3018	3029	rBV	176132	241149	6.58%	0.878%
26	20.359	3128	3132	3142	rVV	312964	490588	13.39%	1.787%

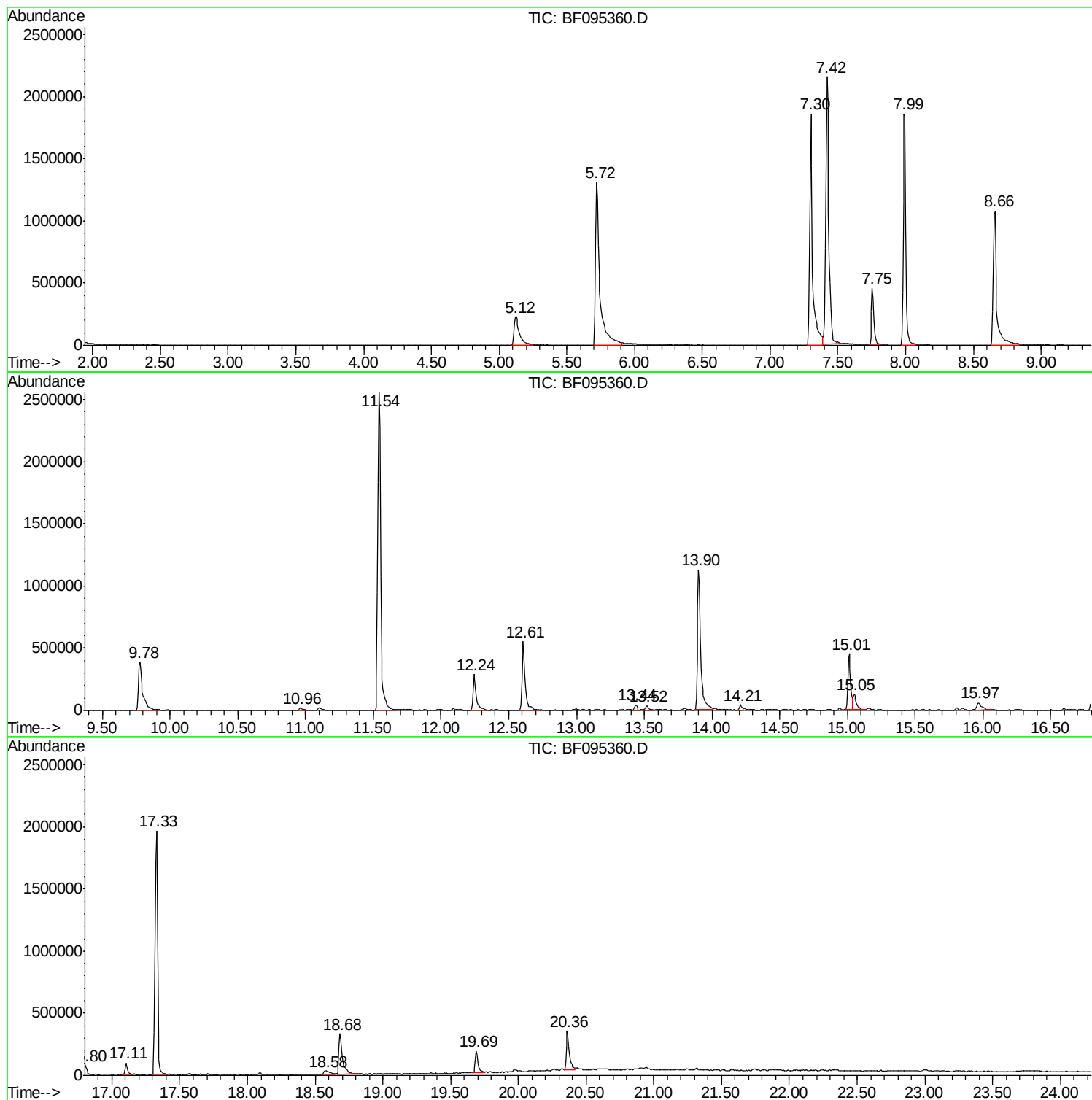
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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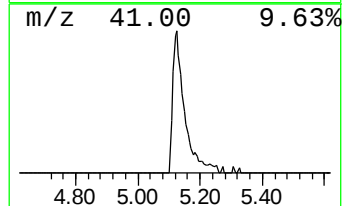
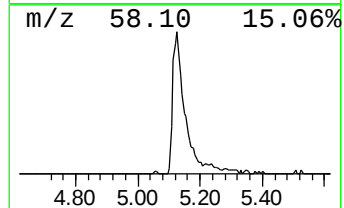
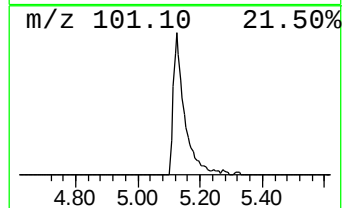
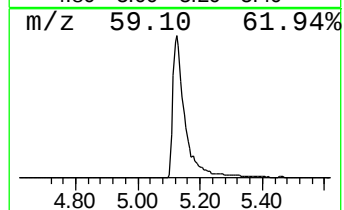
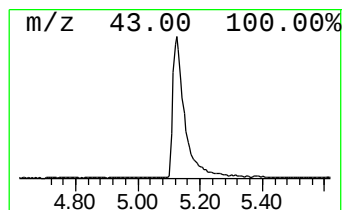
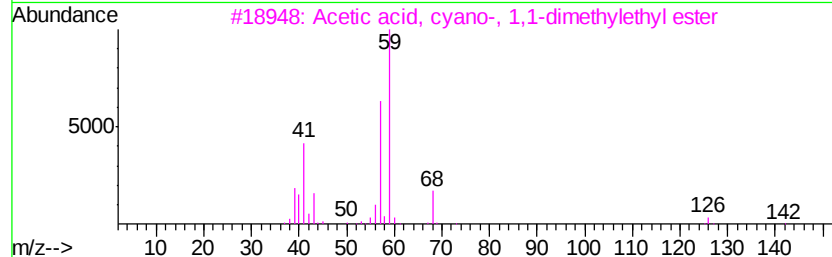
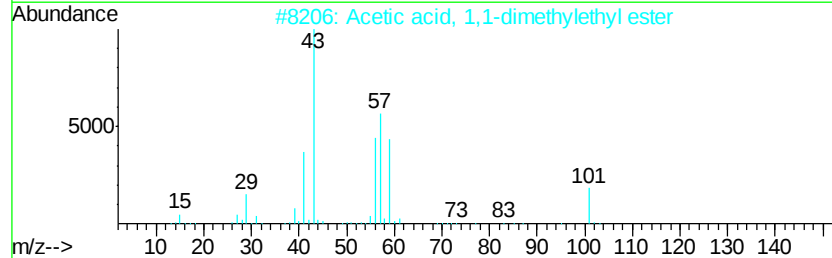
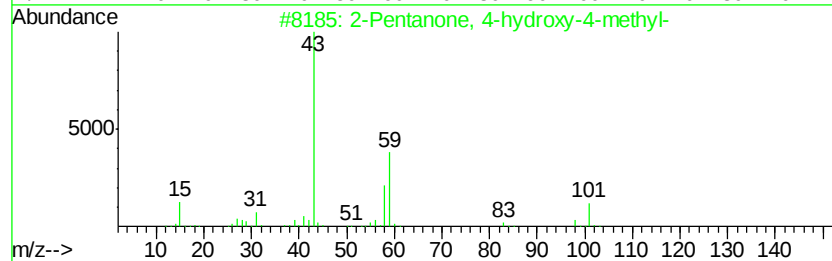
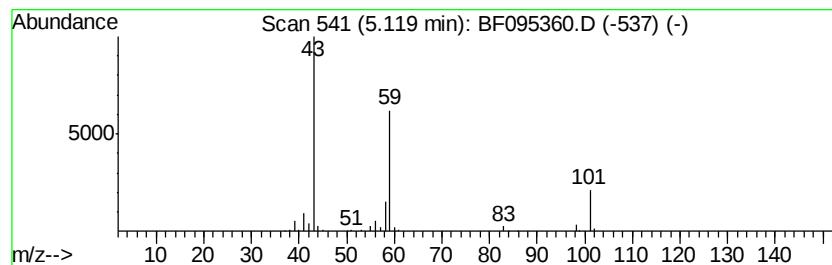
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.12	21.99 ng	608366	1,4-Dichlorobenzene-d4	7.75

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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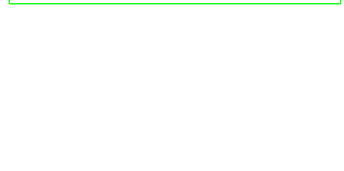
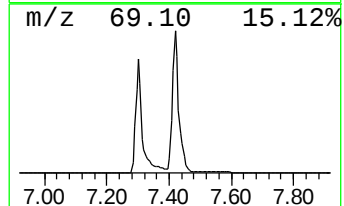
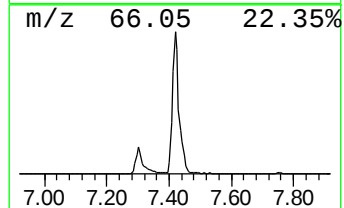
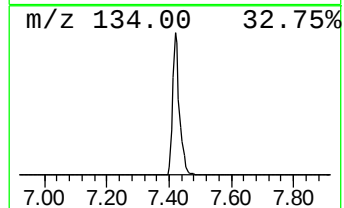
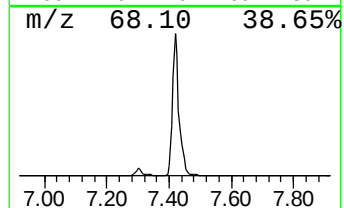
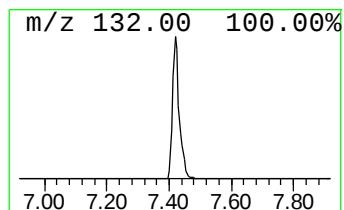
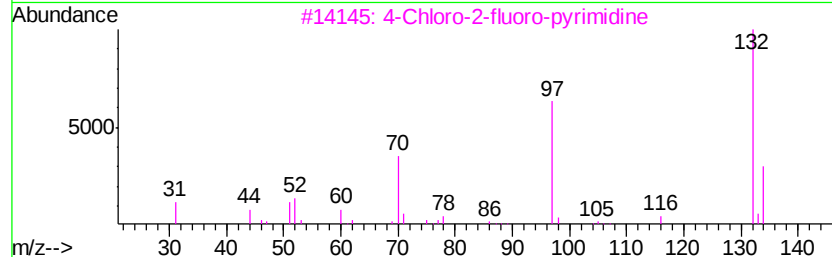
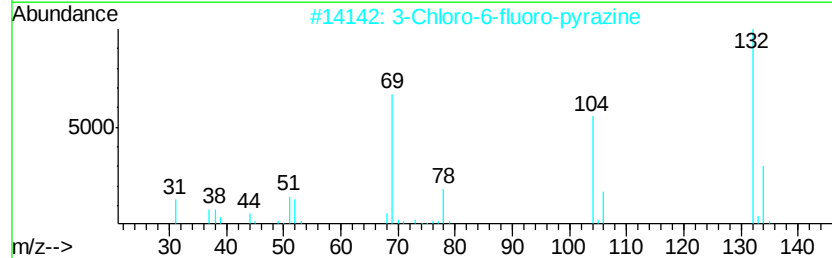
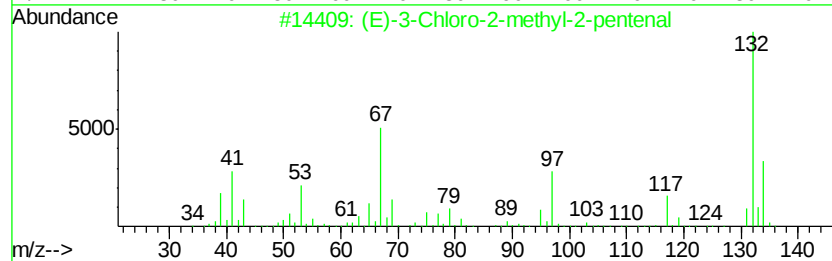
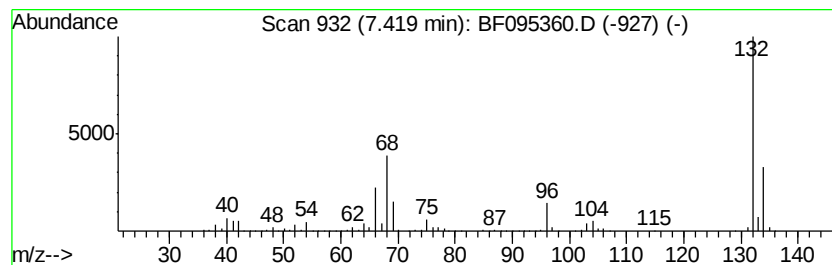
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Peak Number 2 unknown7.42 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.42	120.36 ng	3330210	1,4-Dichlorobenzene-d4	7.75

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27	
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16	
3	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9	
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9	
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9	



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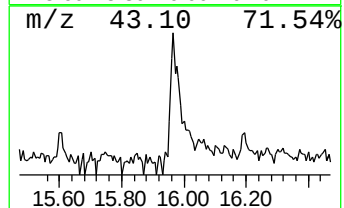
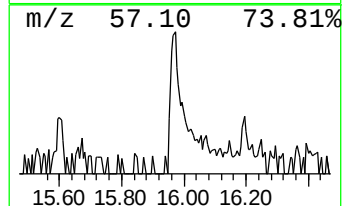
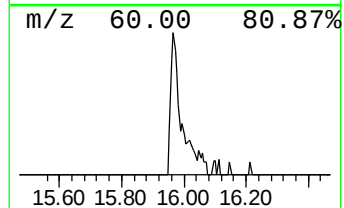
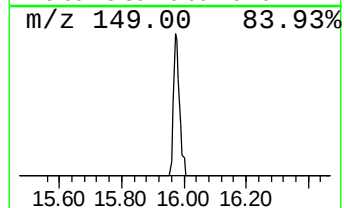
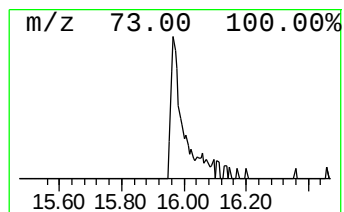
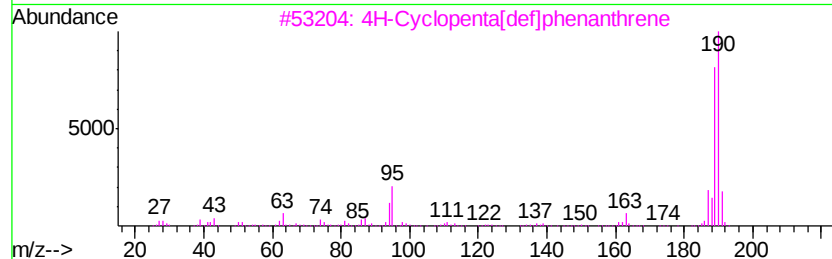
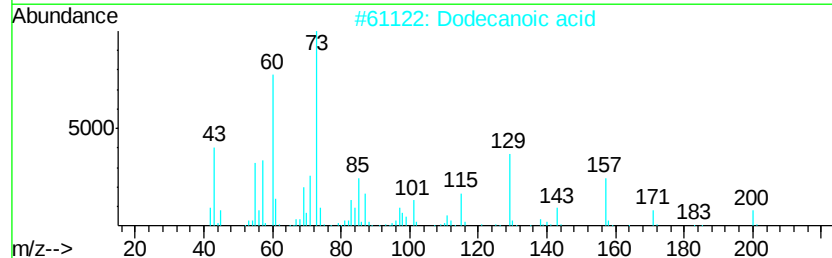
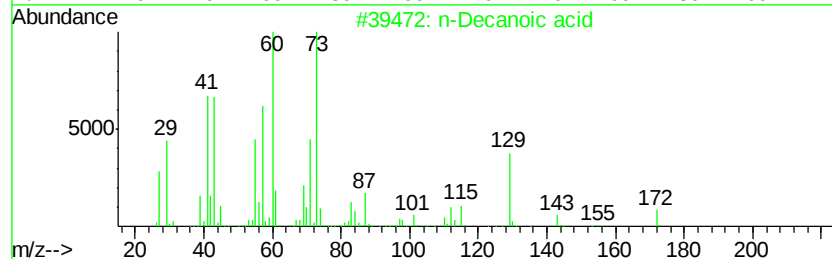
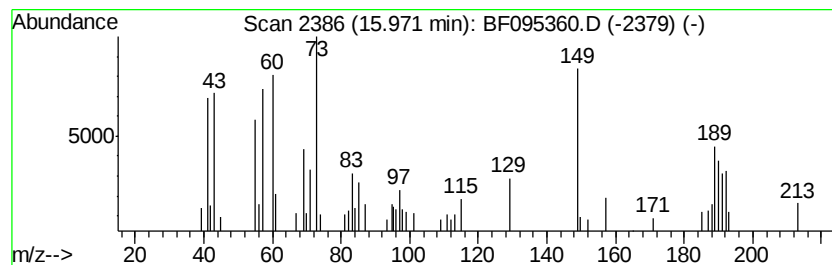
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Peak Number 4 unknown15.97 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
15.97	4.53 ng	147385	Phenanthrene-d10		15.01
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Decanoic acid	172	C10H20O2	000334-48-5	22
2	Dodecanoic acid	200	C12H24O2	000143-07-7	22
3	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	22
4	Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	22
5	Cyclohepta[cd][2]benzothiophene, ...	190	C12H14S	199807-57-3	14



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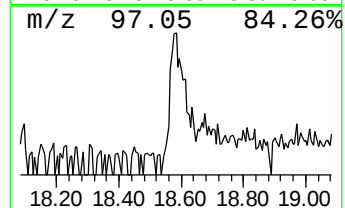
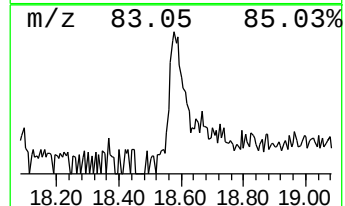
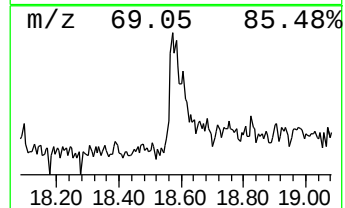
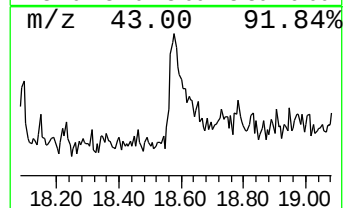
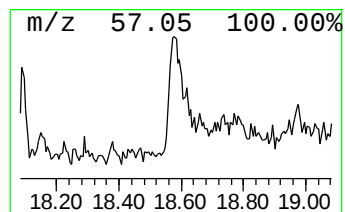
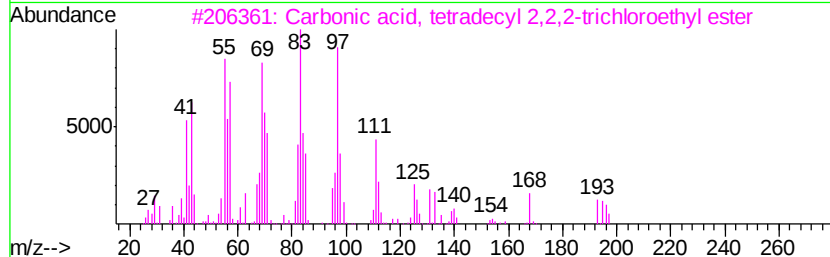
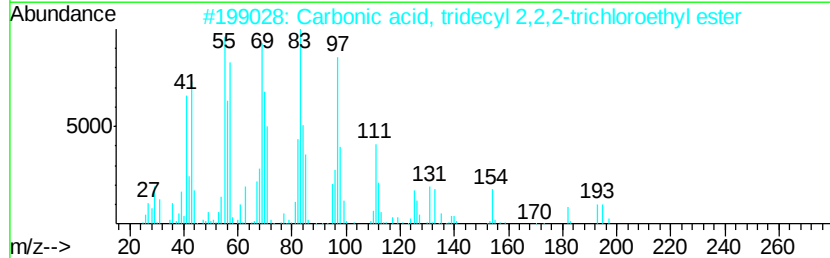
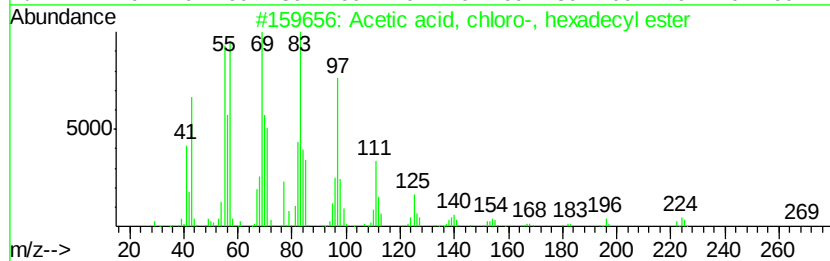
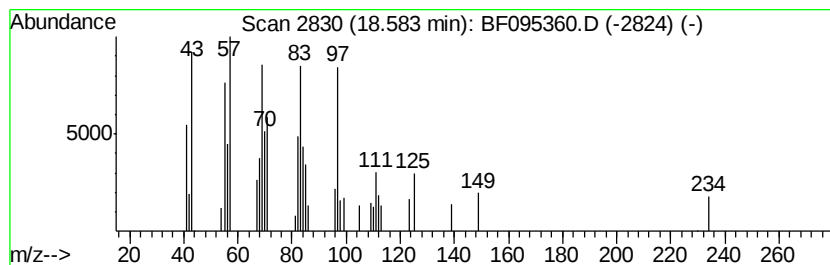
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Peak Number 5 Acetic acid, chloro-, hexad... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.58	3.35 ng	95994	Chrysene-d12	18.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Acetic acid, chloro-, hexadecyl ...	318	C18H35ClO2	052132-58-8	87
2		Carbonic acid, tridecyl 2,2,2-tr...	374	C16H29Cl3O3	1000314-55-9	87
3		Carbonic acid, tetradecyl 2,2,2-...	388	C17H31Cl3O3	1000314-56-0	87
4		n-Tetracosanol-1	354	C24H50O	000506-51-4	83
5		Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	83



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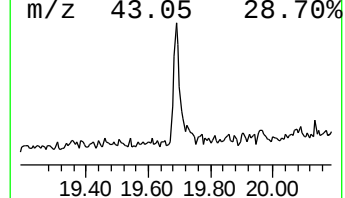
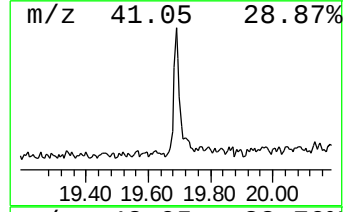
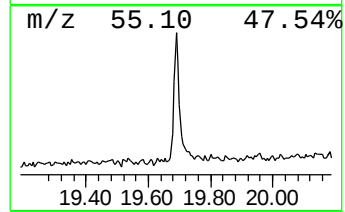
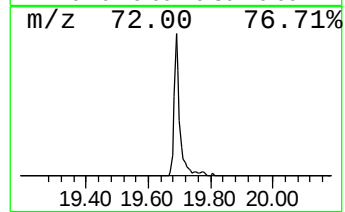
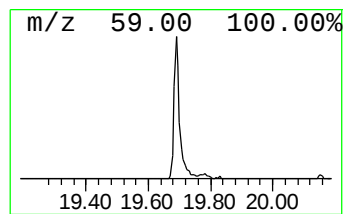
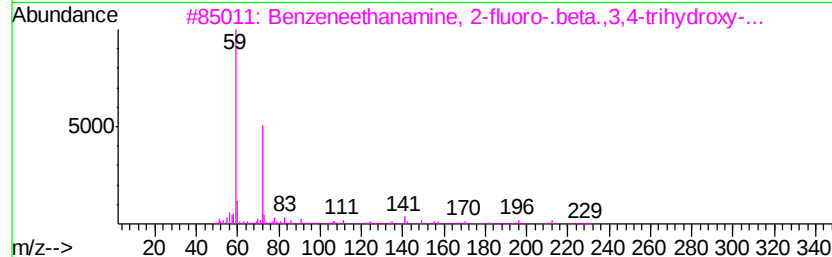
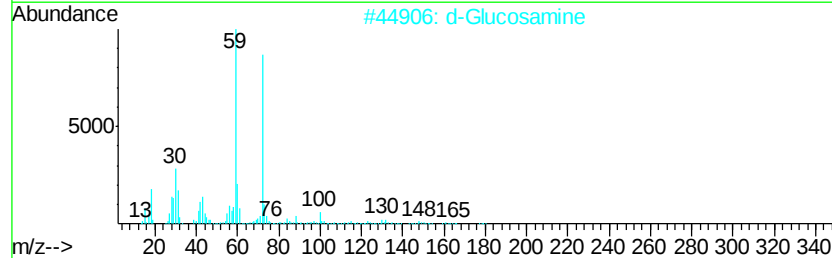
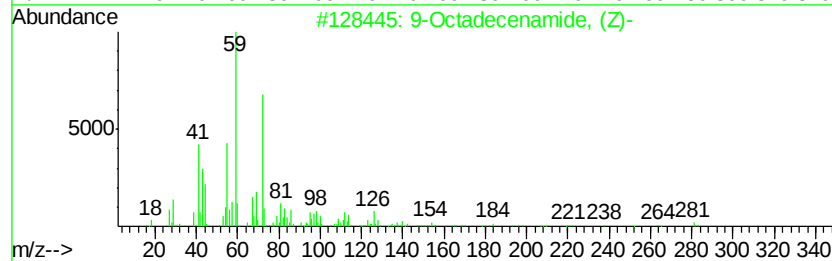
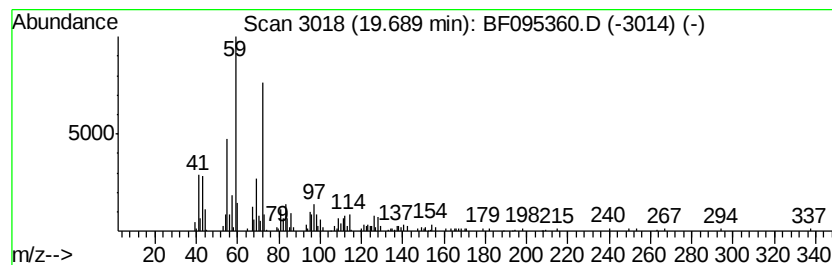
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Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.69	9.83 ng	241149	Perylene-d12	20.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2		d-Glucosamine	179	C6H13NO5	000090-77-7	59
3		Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	47
4		Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	47
5		Tetradecanamide	227	C14H29NO	000638-58-4	47



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.12	22.0	ng	608366	1	7.75	553371	20.0
unknown7.42	7.42	120.4	ng	3330210	1	7.75	553371	20.0
unknown15.97	15.97	4.5	ng	147385	4	15.01	650517	20.0
Acetic acid, chlo...	18.58	3.4	ng	95994	5	18.68	572692	20.0
9-Octadecenamide,...	19.69	9.8	ng	241149	6	20.36	490588	20.0