

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061317\
 Data File : BF095905.D
 Acq On : 13 Jun 2017 21:18
 Operator : SJ/MA
 Sample : I3624-01
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 NB-RO6151-060917

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_F\METHODS\8270-BF060517.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	4.551	501	504	527	rBV	48210	155203	8.46%	1.134%
2	5.239	617	621	657	rBV	724130	1549844	84.45%	11.326%
3	6.916	902	906	917	rBV	898343	1394635	75.99%	10.192%
4	7.004	917	921	943	rVB	1071719	1835189	100.00%	13.412%
5	7.351	976	980	997	rBB	281433	388548	21.17%	2.840%
6	7.586	1015	1020	1036	rBV	916876	1215809	66.25%	8.885%
7	8.269	1132	1136	1170	rBV	603834	951765	51.86%	6.956%
8	9.380	1321	1325	1344	rBV	320047	504968	27.52%	3.690%
9	11.157	1622	1627	1645	rBV	1217849	1542542	84.05%	11.273%
10	11.863	1743	1747	1757	rBV	84743	129655	7.06%	0.948%
11	12.204	1800	1805	1810	rBV2	368042	500943	27.30%	3.661%
12	13.057	1945	1950	1956	rBV	21824	27023	1.47%	0.197%
13	13.498	2020	2025	2041	rBV	490164	772969	42.12%	5.649%
14	13.827	2076	2081	2088	rBV2	20227	31611	1.72%	0.231%
15	14.598	2208	2212	2224	rVB	298460	443586	24.17%	3.242%
16	15.615	2381	2385	2394	rBV2	64131	83377	4.54%	0.609%
17	16.433	2521	2524	2527	rBV	23291	27676	1.51%	0.202%
18	16.733	2569	2575	2584	rBV	43458	78463	4.28%	0.573%
19	16.968	2610	2615	2623	rVB	917692	1060249	57.77%	7.748%
20	17.345	2674	2679	2682	rBV5	20439	37696	2.05%	0.275%
21	17.380	2682	2685	2687	rVB4	15658	19934	1.09%	0.146%
22	18.233	2826	2830	2836	rBV2	96066	166715	9.08%	1.218%
23	18.315	2840	2844	2853	rBV	328533	458055	24.96%	3.348%
24	19.991	3126	3129	3137	rVB2	216344	306936	16.73%	2.243%

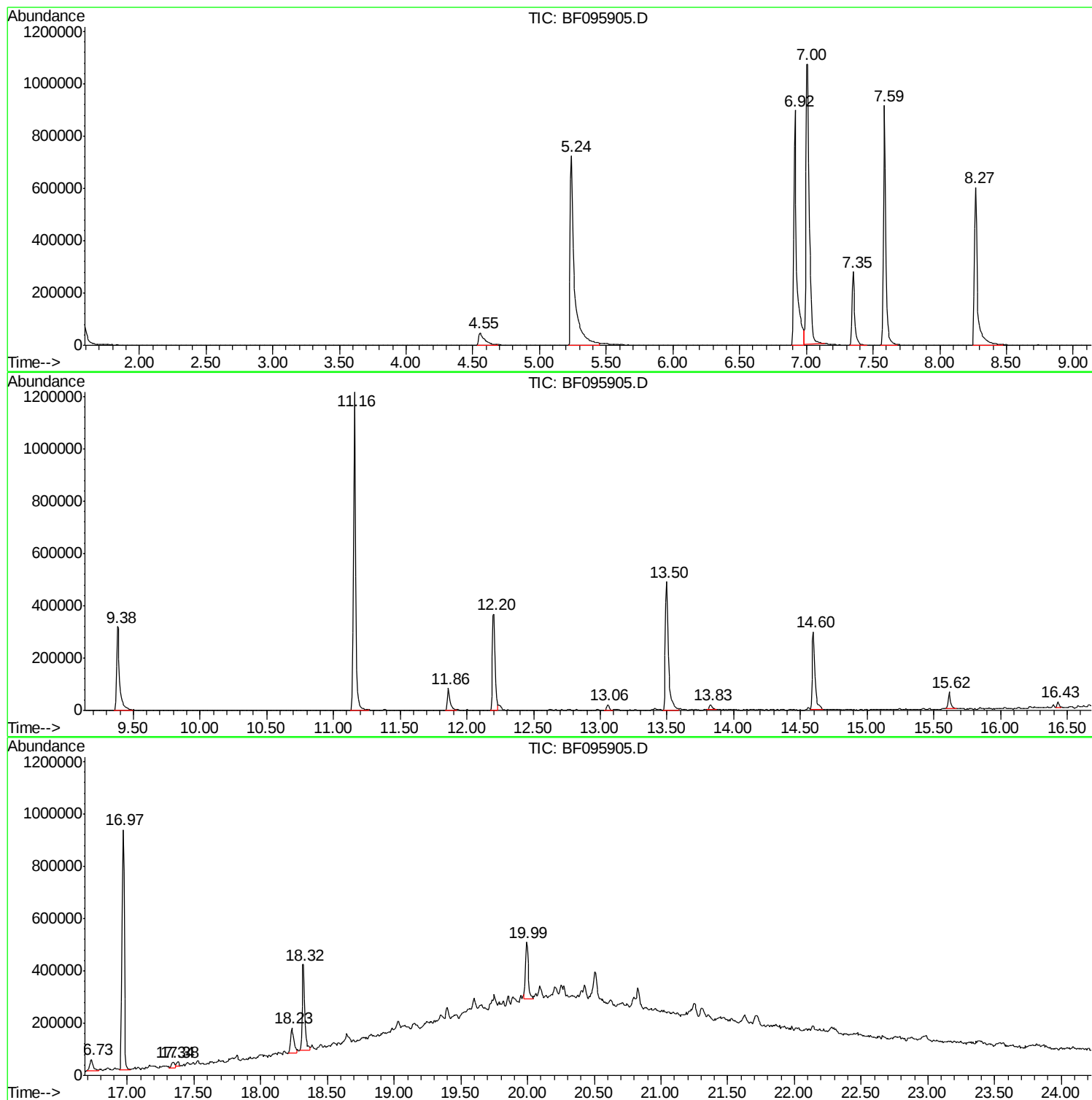
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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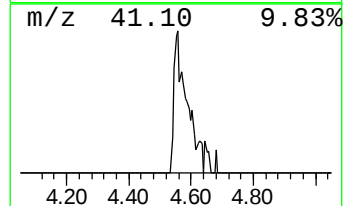
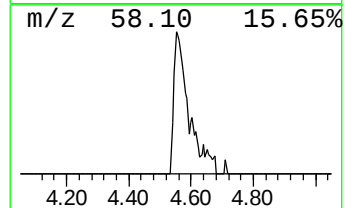
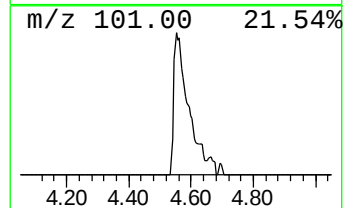
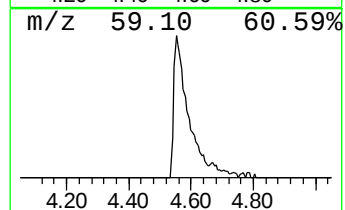
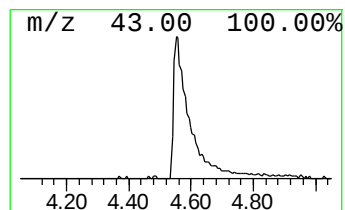
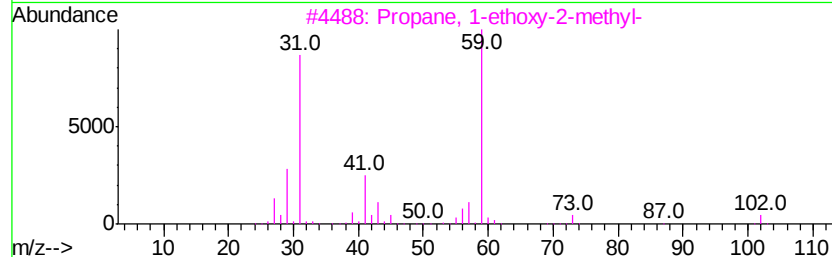
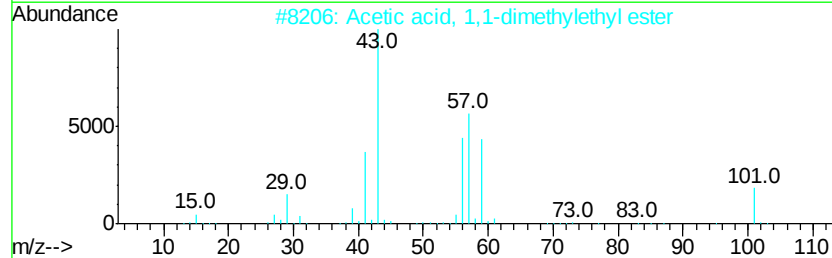
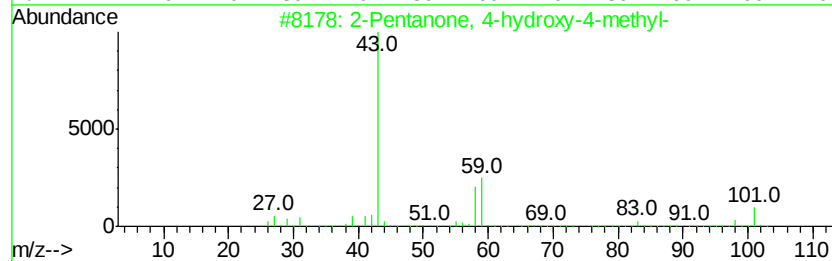
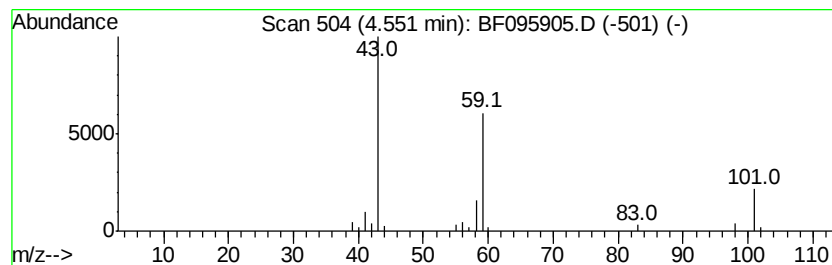
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.55	7.99 ng	155203	1,4-Dichlorobenzene-d4	7.35

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			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, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	25
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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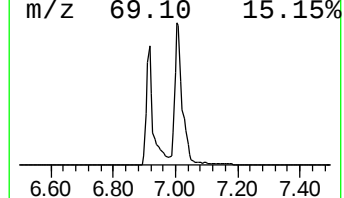
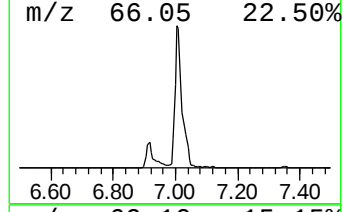
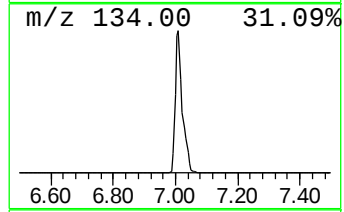
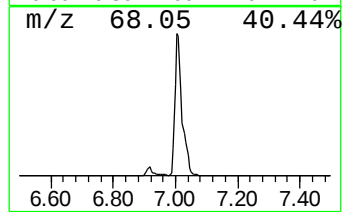
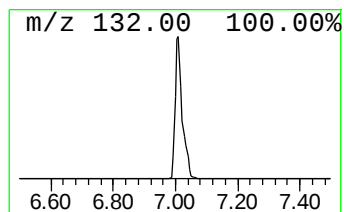
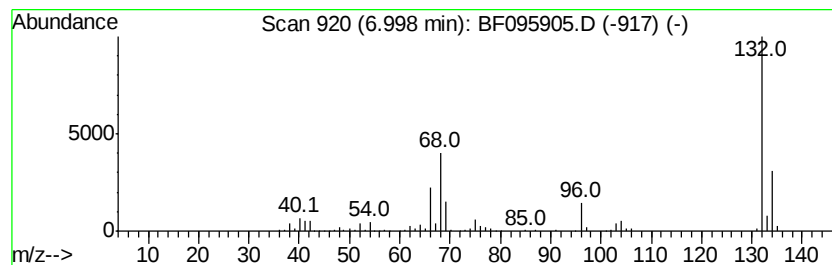
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown7.00 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.00	94.46 ng	1835190	1,4-Dichlorobenzene-d4	7.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9



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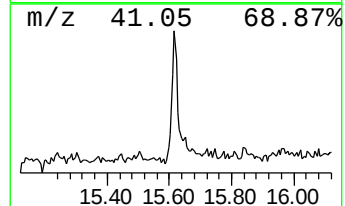
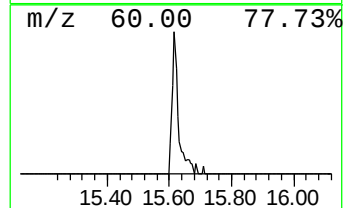
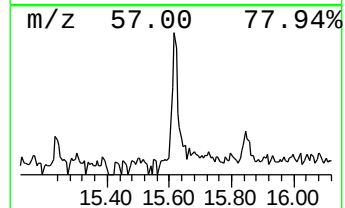
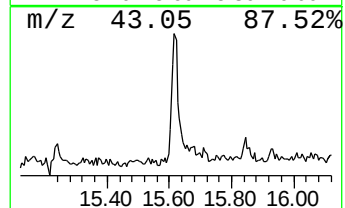
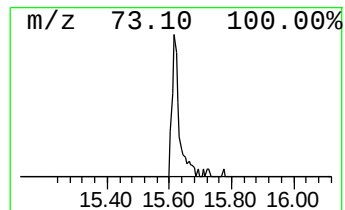
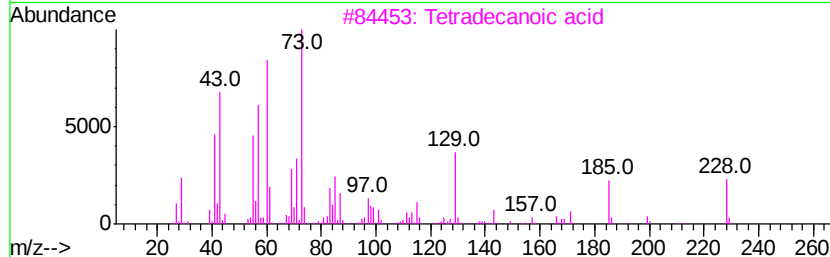
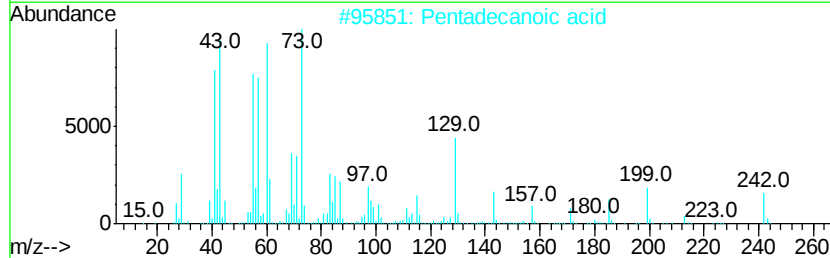
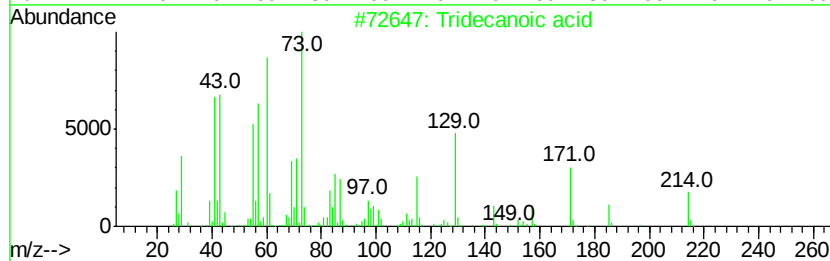
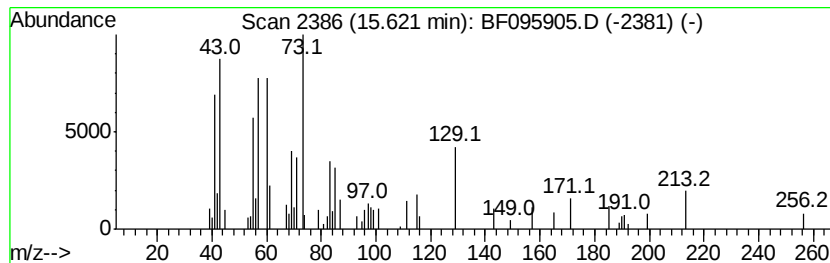
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Peak Number 4 Tridecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.62	3.76 ng	83377	Phenanthrene-d10	14.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	86
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	Undecanoic acid	186	C11H22O2	000112-37-8	72
5	Dodecanoic acid	200	C12H24O2	000143-07-7	53



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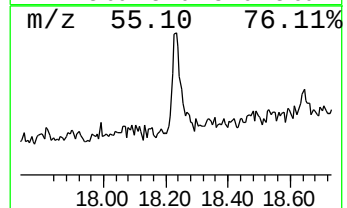
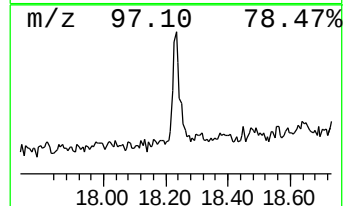
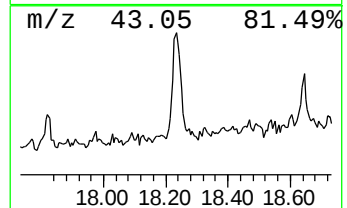
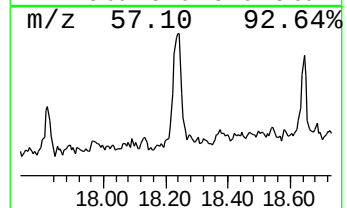
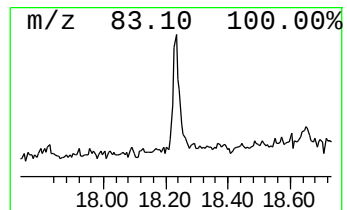
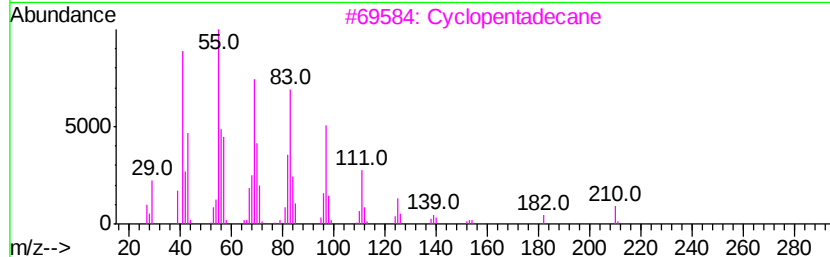
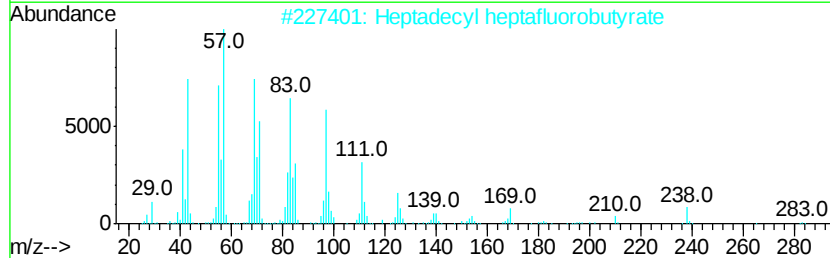
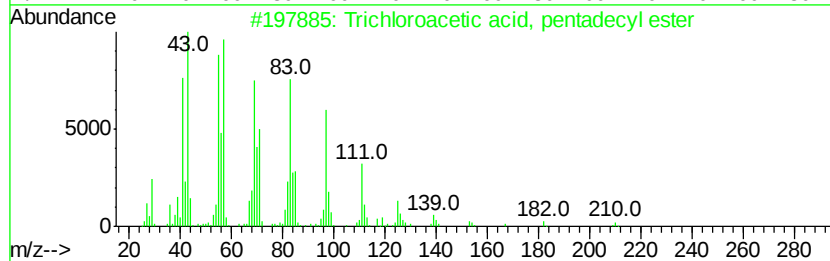
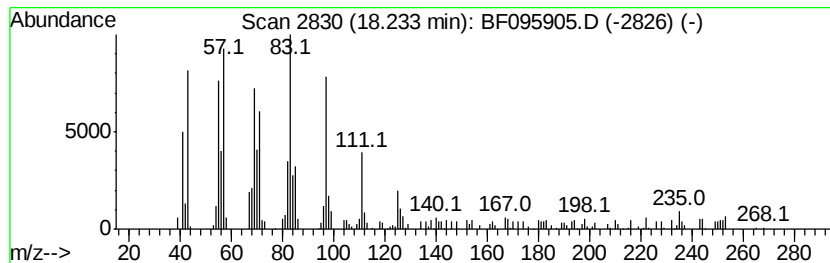
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Peak Number 6 Trichloroacetic acid, penta... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.23	7.28 ng	166715	Chrysene-d12	18.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
2		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
3		Cyclopentadecane	210	C15H30	000295-48-7	91
4		1-Docosene	308	C22H44	001599-67-3	91
5		E-7-Octadecene	252	C18H36	1000130-92-0	90



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.55	8.0	ng	155203	1	7.35	388548	20.0
unknown7.00	7.00	94.5	ng	1835190	1	7.35	388548	20.0
Tridecanoic acid	15.62	3.8	ng	83377	4	14.60	443586	20.0
Trichloroacetic a...	18.23	7.3	ng	166715	5	18.32	458055	20.0