

Data Path : Z:\HPCHEM1\BNA G\DATA\BG031218\
 Data File : BG033086.D
 Acq On : 12 Mar 2018 13:01
 Operator : SJ/JU
 Sample : J1873-09
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TP-9B-COMP

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_G\METHODS\8270-BG022118.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	3.516	33	39	56	rVB2	32869	75166	3.85%	0.569%
2	5.819	426	431	441	rVB	17874	32809	1.68%	0.248%
3	6.324	509	517	529	rBV	583877	1040309	53.28%	7.875%
4	8.004	795	803	818	rBV	637752	1174879	60.17%	8.893%
5	8.415	865	873	887	rBV	591402	1098646	56.26%	8.316%
6	8.909	947	957	965	rBV	157452	281376	14.41%	2.130%
7	9.244	1006	1014	1024	rBV	414885	766377	39.25%	5.801%
8	10.107	1153	1161	1170	rBV	360770	680052	34.83%	5.148%
9	11.793	1440	1448	1456	rBV	230555	431079	22.08%	3.263%
10	14.149	1841	1849	1863	rBV	893756	1454251	74.47%	11.008%
11	14.942	1976	1984	1989	rBV	69244	102918	5.27%	0.779%
12	15.353	2048	2054	2060	rBV	25078	31661	1.62%	0.240%
13	15.523	2076	2083	2092	rBV2	360377	584531	29.93%	4.425%
14	16.287	2210	2213	2218	rVB	27278	34757	1.78%	0.263%
15	16.992	2327	2333	2349	rBV	701378	1071693	54.88%	8.112%
16	17.145	2354	2359	2371	rVB	25639	43809	2.24%	0.332%
17	18.249	2540	2547	2556	rBV2	452593	694528	35.57%	5.257%
18	19.048	2678	2683	2694	rBV	42969	75643	3.87%	0.573%
19	20.763	2970	2975	2990	rBV	1456635	1952697	100.00%	14.781%
20	22.132	3201	3208	3218	rBV3	38820	125058	6.40%	0.947%
21	22.602	3281	3288	3301	rBV2	364206	735170	37.65%	5.565%
22	24.511	3607	3613	3618	rVB3	16975	33783	1.73%	0.256%
23	26.403	3922	3935	3952	rBV2	183322	689345	35.30%	5.218%

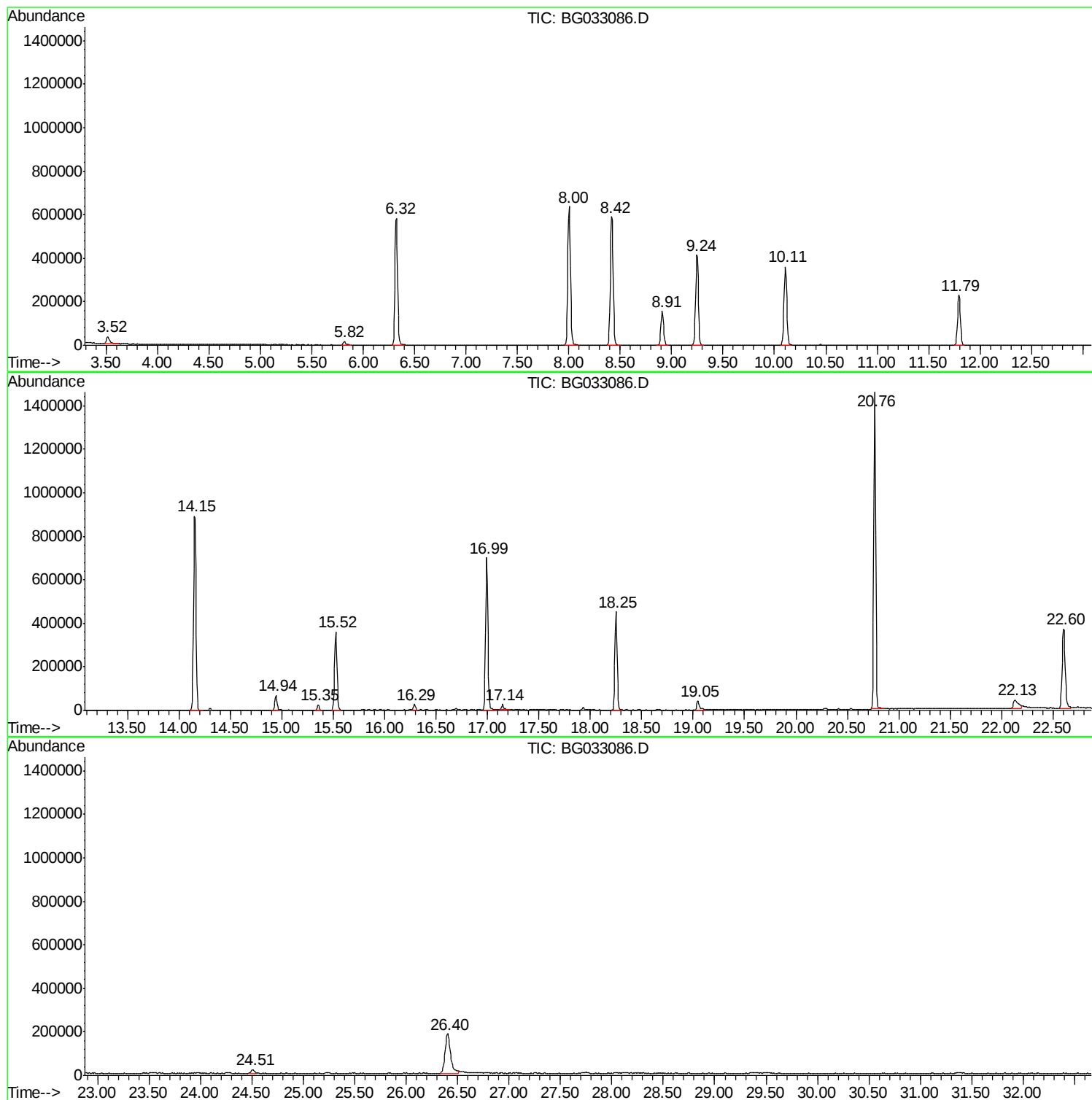
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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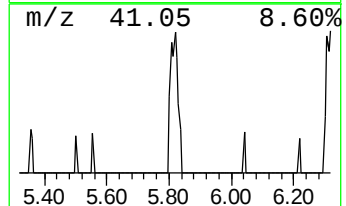
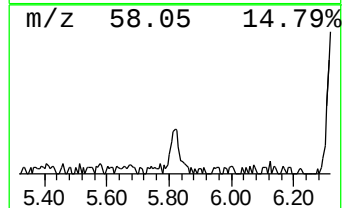
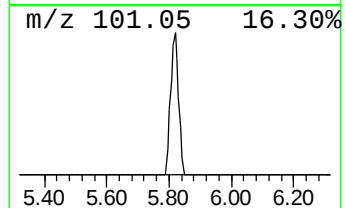
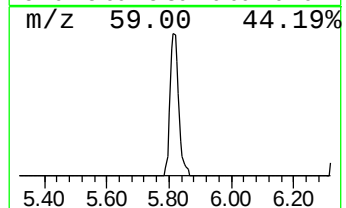
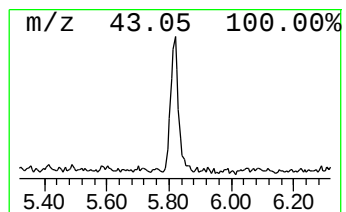
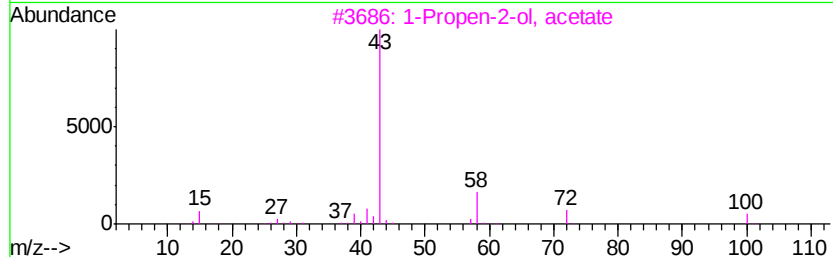
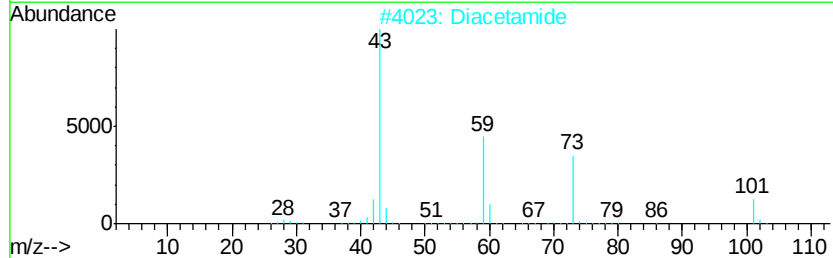
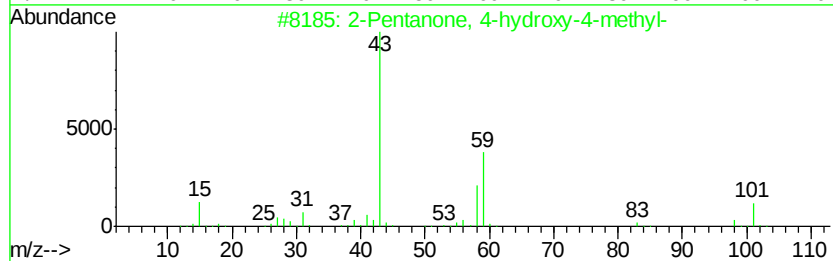
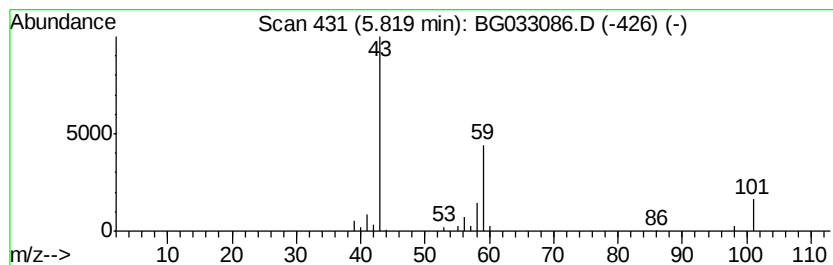
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG022118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.82	2.33 ng	32809	1,4-Dichlorobenzene-d4	8.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	39
2	Diacetamide	101	C4H7NO2	000625-77-4	9
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
4	5-Hexen-2-one	98	C6H10O	000109-49-9	7
5	Propylamine	59	C3H9N	000107-10-8	5



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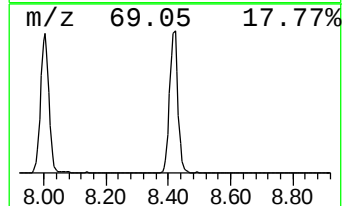
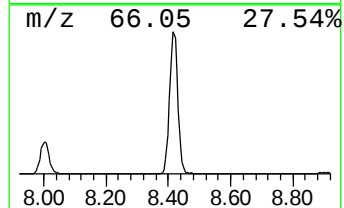
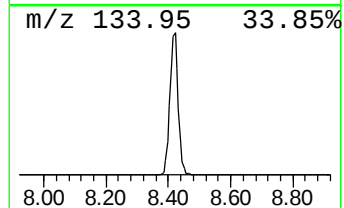
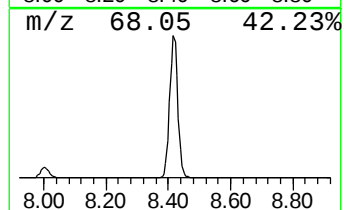
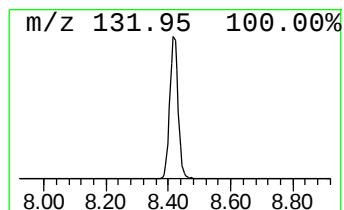
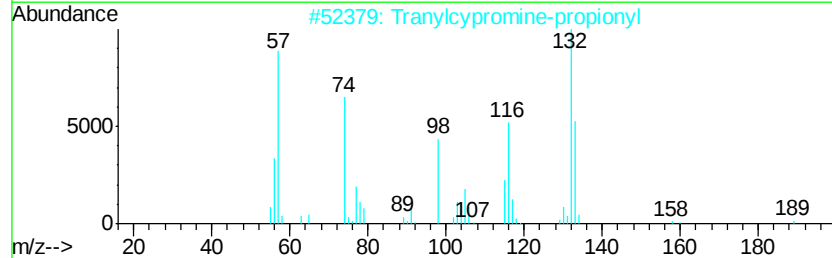
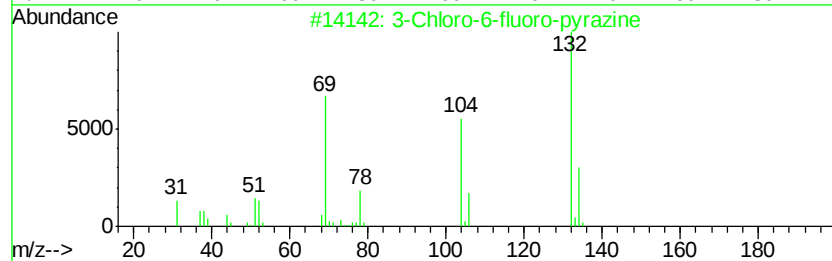
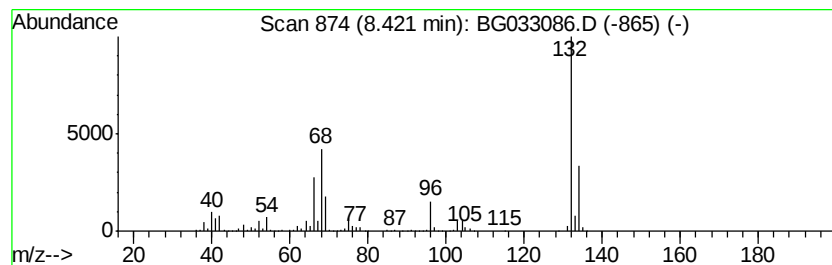
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TIC Library : C:\Database\NIST11.L
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Peak Number 3 unknown8.42 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.42	78.09 ng	1098650	1,4-Dichlorobenzene-d4	8.91

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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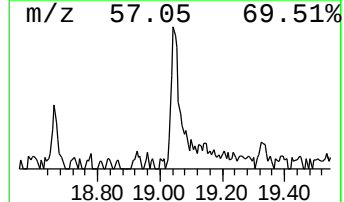
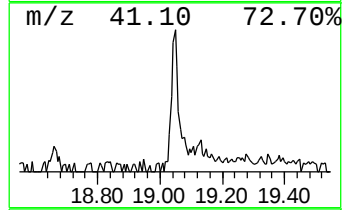
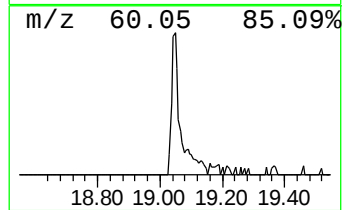
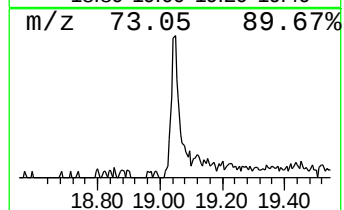
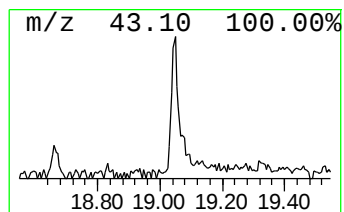
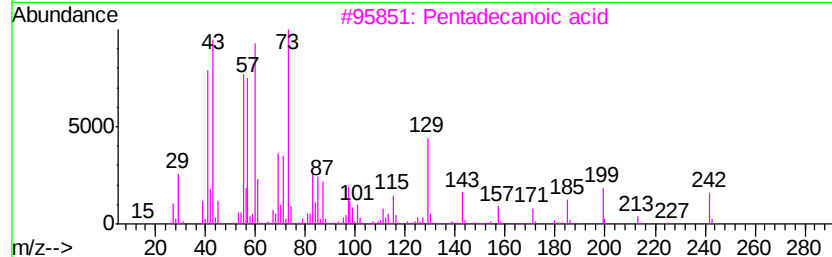
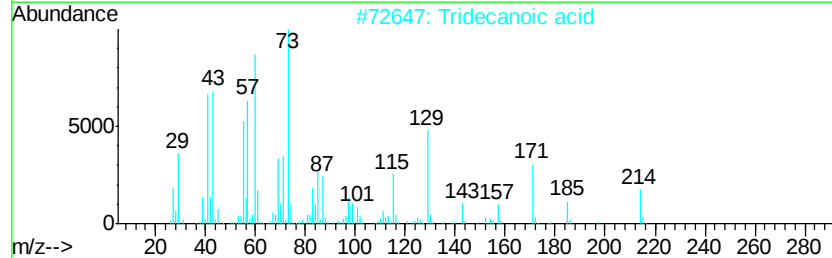
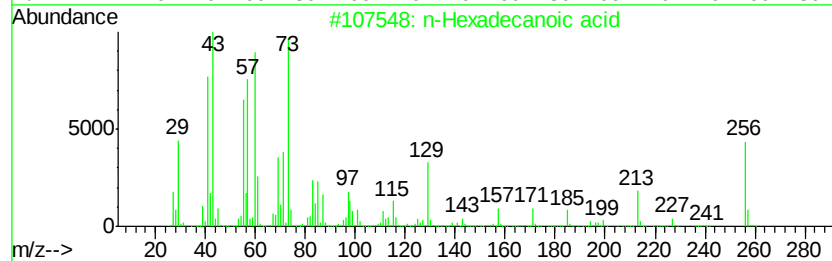
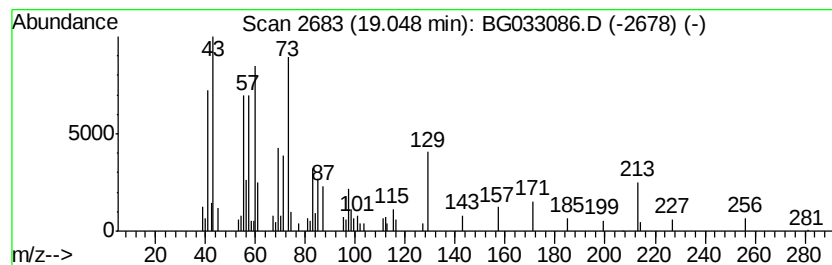
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.05	2.18 ng	75643	Phenanthrene-d10	18.25

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2		Tridecanoic acid	214	C13H26O2	000638-53-9	91
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5		n-Decanoic acid	172	C10H20O2	000334-48-5	53



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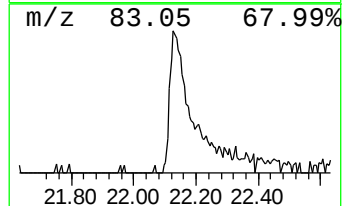
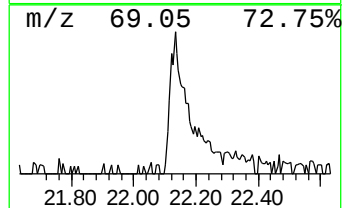
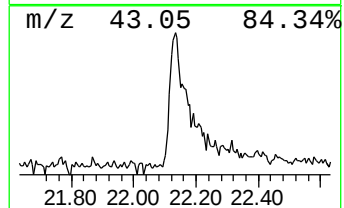
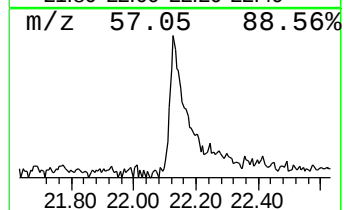
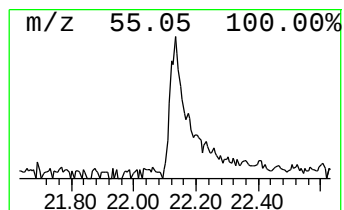
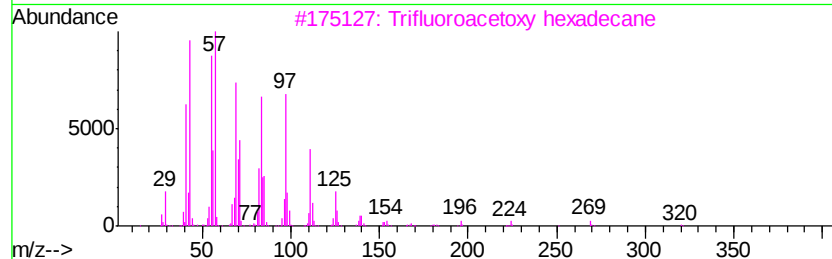
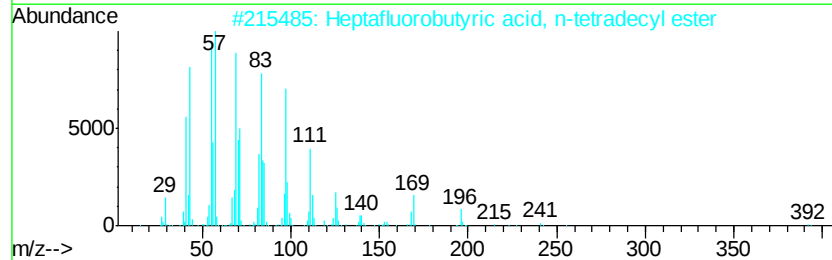
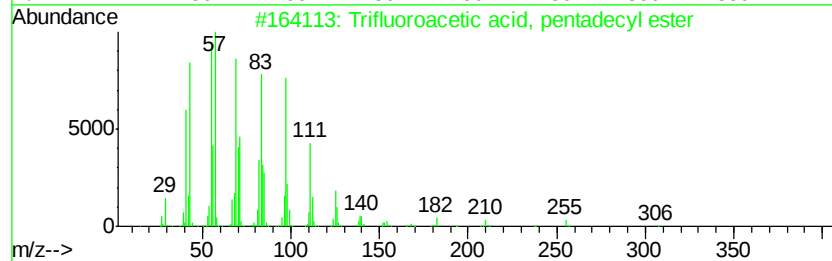
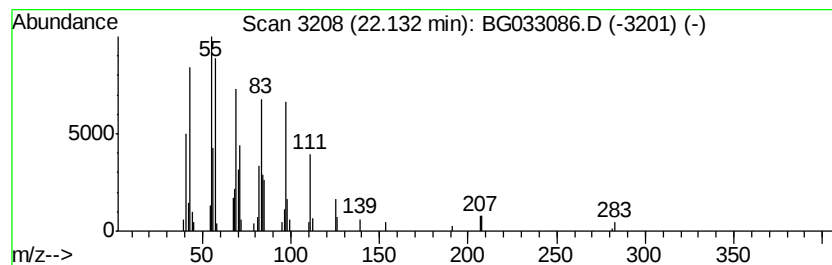
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Peak Number 6 Trifluoroacetic acid, penta... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.13	3.40 ng	125058	Chrysene-d12	22.60

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
2		Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	91
3		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
4		Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91
5		Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.82	2.3	ng	32809	1	8.91	281376	20.0
unknown8.42	8.42	78.1	ng	1098650	1	8.91	281376	20.0
n-Hexadecanoic acid	19.05	2.2	ng	75643	4	18.25	694528	20.0
Trifluoroacetic a...	22.13	3.4	ng	125058	5	22.60	735170	20.0