

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050417\
 Data File : BF094881.D
 Acq On : 4 May 2017 19:02
 Operator : SJ/MA
 Sample : I2956-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 IP-TP(0-5)

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-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	5.037	522	527	544	rBV	202200	382766	14.61%	1.693%
2	5.672	630	635	664	rBV	1653178	2372972	90.55%	10.499%
3	7.266	900	906	921	rBV	1708886	2357830	89.97%	10.432%
4	7.383	921	926	935	rVB	2022077	2537779	96.84%	11.228%
5	7.719	979	983	994	rBV	409121	494380	18.87%	2.187%
6	7.960	1019	1024	1035	rBV	1643370	1914087	73.04%	8.468%
7	8.619	1130	1136	1152	rBV	1148268	1495476	57.07%	6.616%
8	9.742	1322	1327	1337	rBV	456507	597493	22.80%	2.643%
9	11.513	1623	1628	1646	rBV	2021680	2620596	100.00%	11.594%
10	12.201	1741	1745	1753	rBV	208625	262346	10.01%	1.161%
11	12.571	1803	1808	1820	rBV2	519500	722704	27.58%	3.197%
12	13.412	1944	1951	1957	rBV2	23437	29987	1.14%	0.133%
13	13.865	2022	2028	2041	rBV	1163693	1606391	61.30%	7.107%
14	14.189	2079	2083	2086	rBV	31653	40079	1.53%	0.177%
15	14.918	2202	2207	2211	rBV	23825	29535	1.13%	0.131%
16	14.971	2211	2216	2226	rVB	541509	718542	27.42%	3.179%
17	15.936	2374	2380	2390	rBV2	82863	107441	4.10%	0.475%
18	17.295	2606	2611	2615	rBV	2107800	2577673	98.36%	11.404%
19	18.553	2818	2825	2834	rBV5	47553	122138	4.66%	0.540%
20	18.636	2834	2839	2853	rVB	657482	778400	29.70%	3.444%
21	19.771	3024	3032	3036	rBV	48880	53133	2.03%	0.235%
22	20.300	3117	3122	3133	rBV	522690	711916	27.17%	3.150%
23	20.865	3212	3218	3225	rVB8	11871	27132	1.04%	0.120%
24	23.741	3700	3707	3714	rBV9	17379	42031	1.60%	0.186%

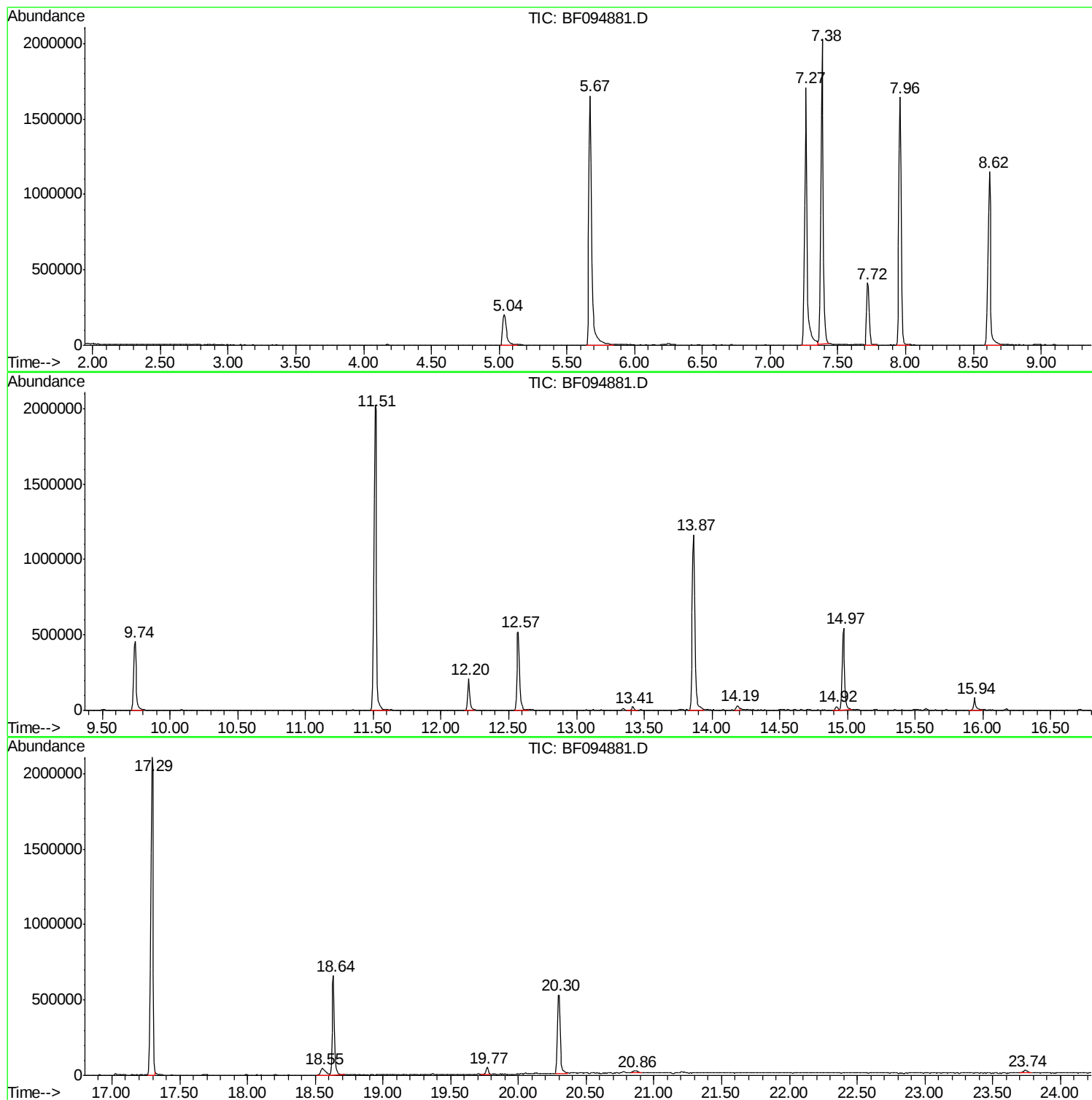
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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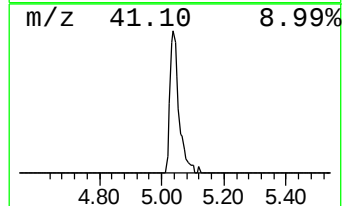
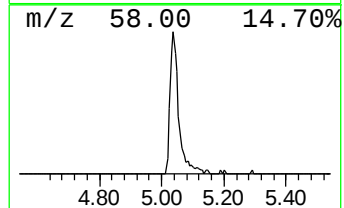
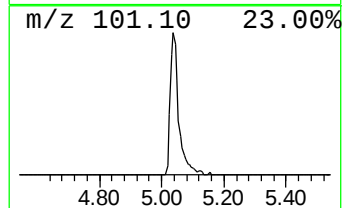
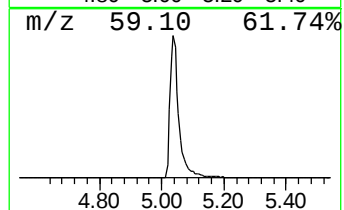
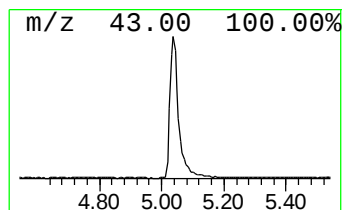
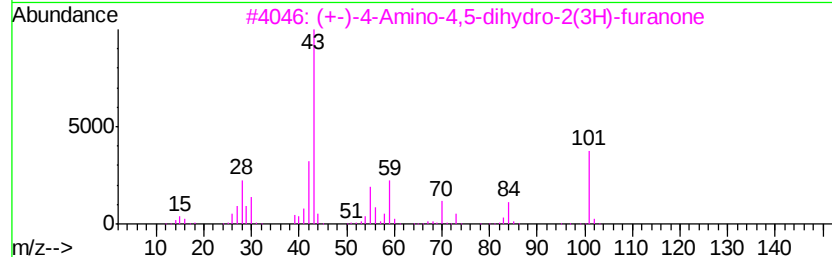
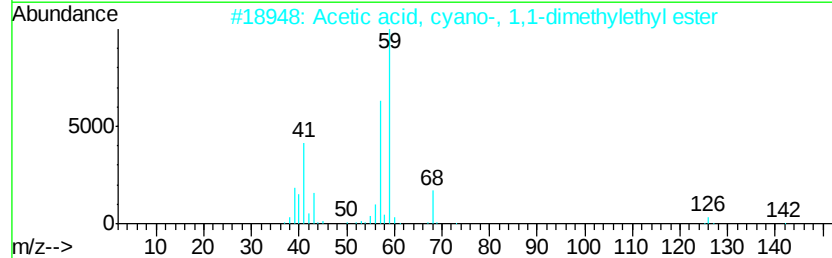
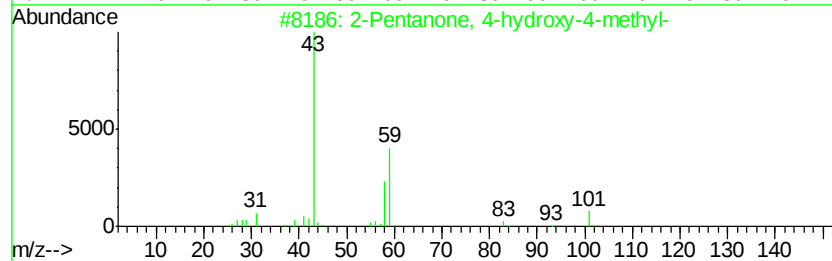
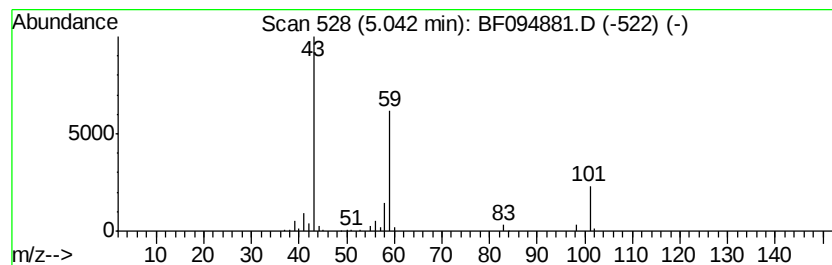
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.04	15.48 ng	382766	1,4-Dichlorobenzene-d4	7.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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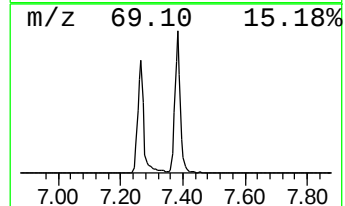
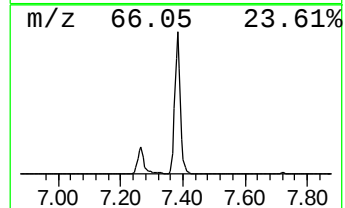
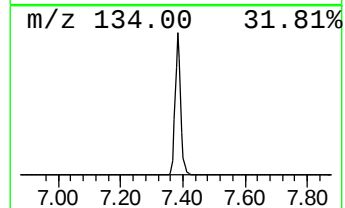
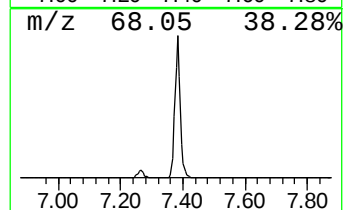
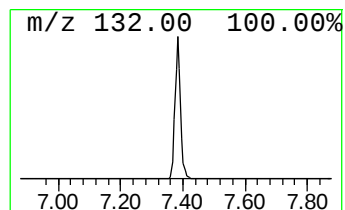
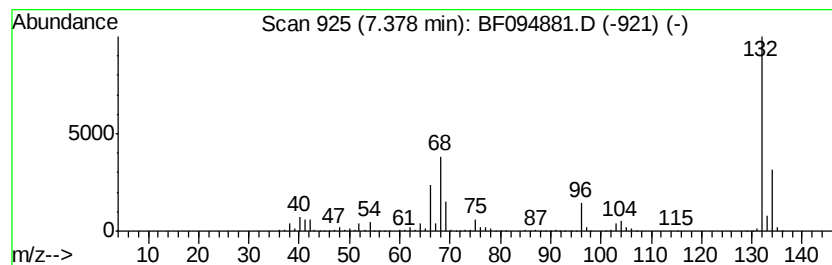
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown7.38 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.38	102.67 ng	2537780	1,4-Dichlorobenzene-d4	7.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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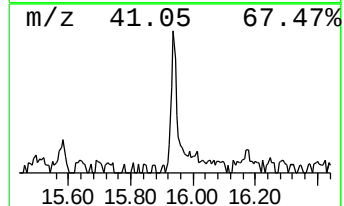
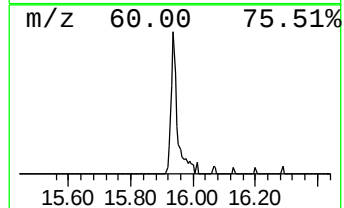
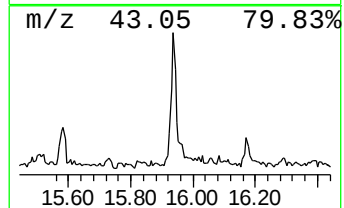
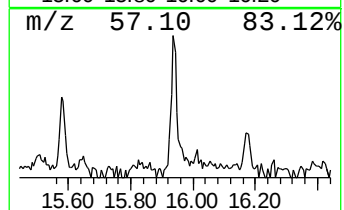
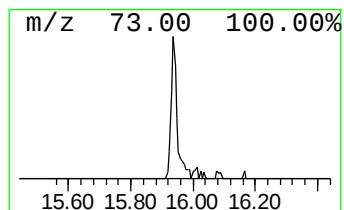
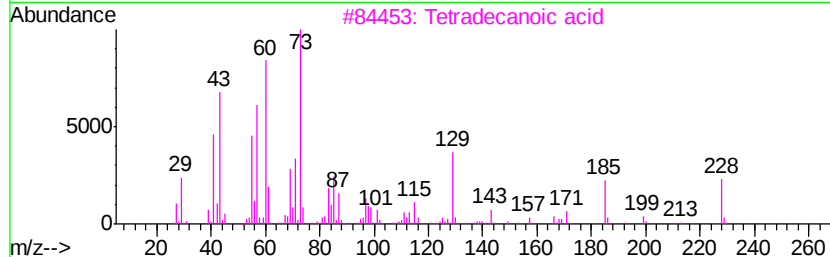
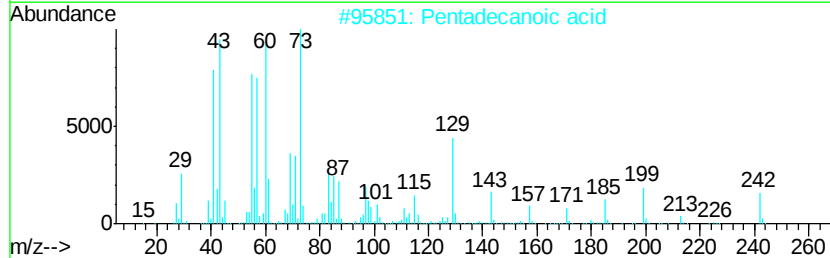
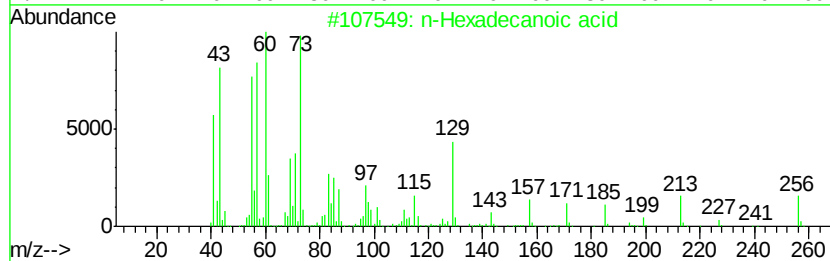
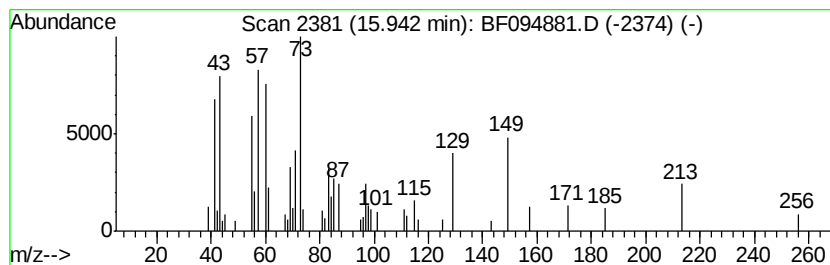
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.94	2.99 ng	107441	Phenanthrene-d10	14.97

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	91
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	86
4		Tridecanoic acid	214	C13H26O2	000638-53-9	80
5		Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	18



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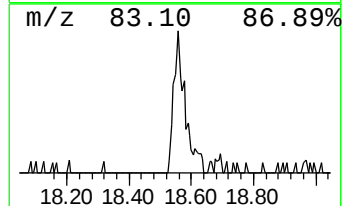
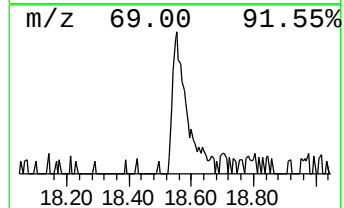
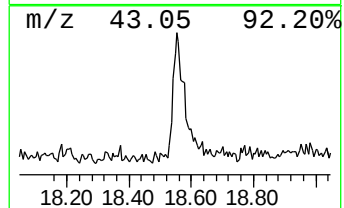
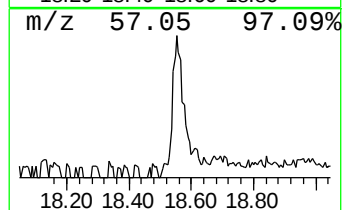
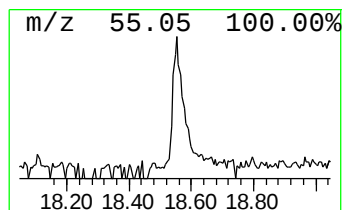
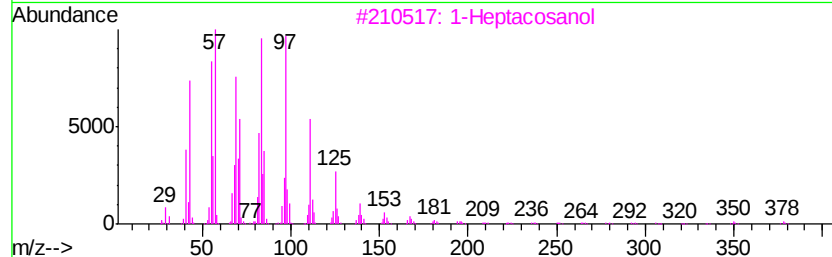
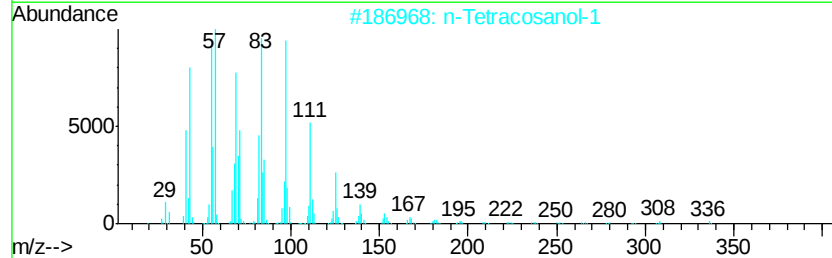
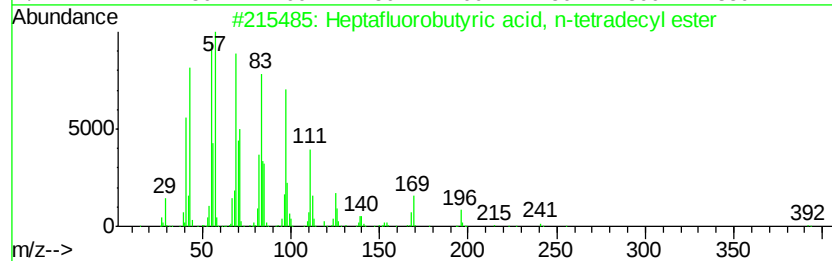
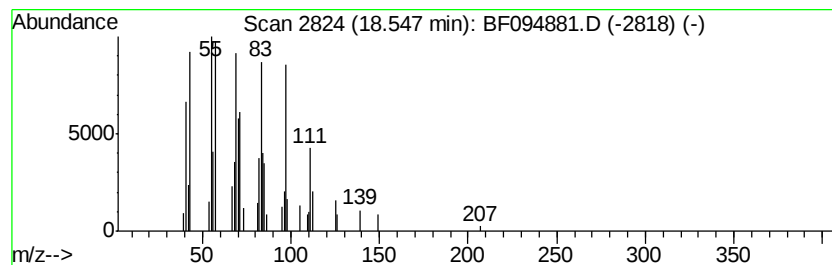
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Peak Number 5 Heptafluorobutyric acid, n-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.55	3.14 ng	122138	Chrysene-d12	18.64

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	95
2		n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3		1-Heptacosanol	396	C27H56O	002004-39-9	91
4		Behenic alcohol	326	C22H46O	000661-19-8	91
5		n-Pentadecanol	228	C15H32O	000629-76-5	90



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.04	15.5	ng	382766	1	7.72	494380	20.0
unknown7.38	7.38	102.7	ng	2537780	1	7.72	494380	20.0
n-Hexadecanoic acid	15.94	3.0	ng	107441	4	14.97	718542	20.0
Heptafluorobutyri...	18.55	3.1	ng	122138	5	18.64	778400	20.0