

Data Path : Z:\SVOASRV\HPCHEM1\BNA_N\DATA\BN110918\
 Data File : BN003493.D
 Acq On : 10 Nov 2018 03:34
 Operator : MJ/SJ
 Sample : J5881-02
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 110718-TIPC-F-D-S

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_N\METHODS\8270-BN102418.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	3.028	3	7	23	rVB	356643	425297	7.59%	1.495%
2	5.411	406	412	420	rBV	509916	714592	12.75%	2.512%
3	6.999	675	682	694	rBV2	303688	597058	10.65%	2.099%
4	7.375	739	746	756	rBV	1065043	1608940	28.71%	5.655%
5	7.846	819	826	832	rBV	346607	531415	9.48%	1.868%
6	8.169	873	881	888	rBV	1510746	2403385	42.88%	8.447%
7	9.016	1017	1025	1034	rBV	1178529	1889009	33.70%	6.639%
8	10.646	1295	1302	1311	rVB	510270	831524	14.84%	2.923%
9	13.104	1713	1720	1726	rBV	3538028	5168495	92.21%	18.166%
10	13.934	1855	1861	1867	rVB	97066	124390	2.22%	0.437%
11	14.481	1948	1954	1962	rBV2	775740	1188948	21.21%	4.179%
12	15.969	2201	2207	2218	rBV	1768528	2504843	44.69%	8.804%
13	17.228	2414	2421	2427	rBV	1014524	1393137	24.86%	4.897%
14	18.098	2563	2569	2580	rBV	137507	199651	3.56%	0.702%
15	19.375	2782	2786	2794	rBV	52668	71989	1.28%	0.253%
16	19.845	2860	2866	2871	rBV	4579320	5604929	100.00%	19.700%
17	21.098	3074	3079	3091	rBV	81931	137977	2.46%	0.485%
18	21.404	3125	3131	3138	rBV	1079163	1285516	22.94%	4.518%
19	22.451	3305	3309	3316	rVB	44968	58645	1.05%	0.206%
20	22.586	3327	3332	3339	rBV	249464	315663	5.63%	1.109%
21	22.974	3394	3398	3404	rVB	49250	73586	1.31%	0.259%
22	23.563	3493	3498	3506	rVB	46272	79853	1.42%	0.281%
23	23.715	3517	3524	3534	rVB2	625902	1183539	21.12%	4.160%
24	24.233	3607	3612	3620	rVB	32165	59175	1.06%	0.208%

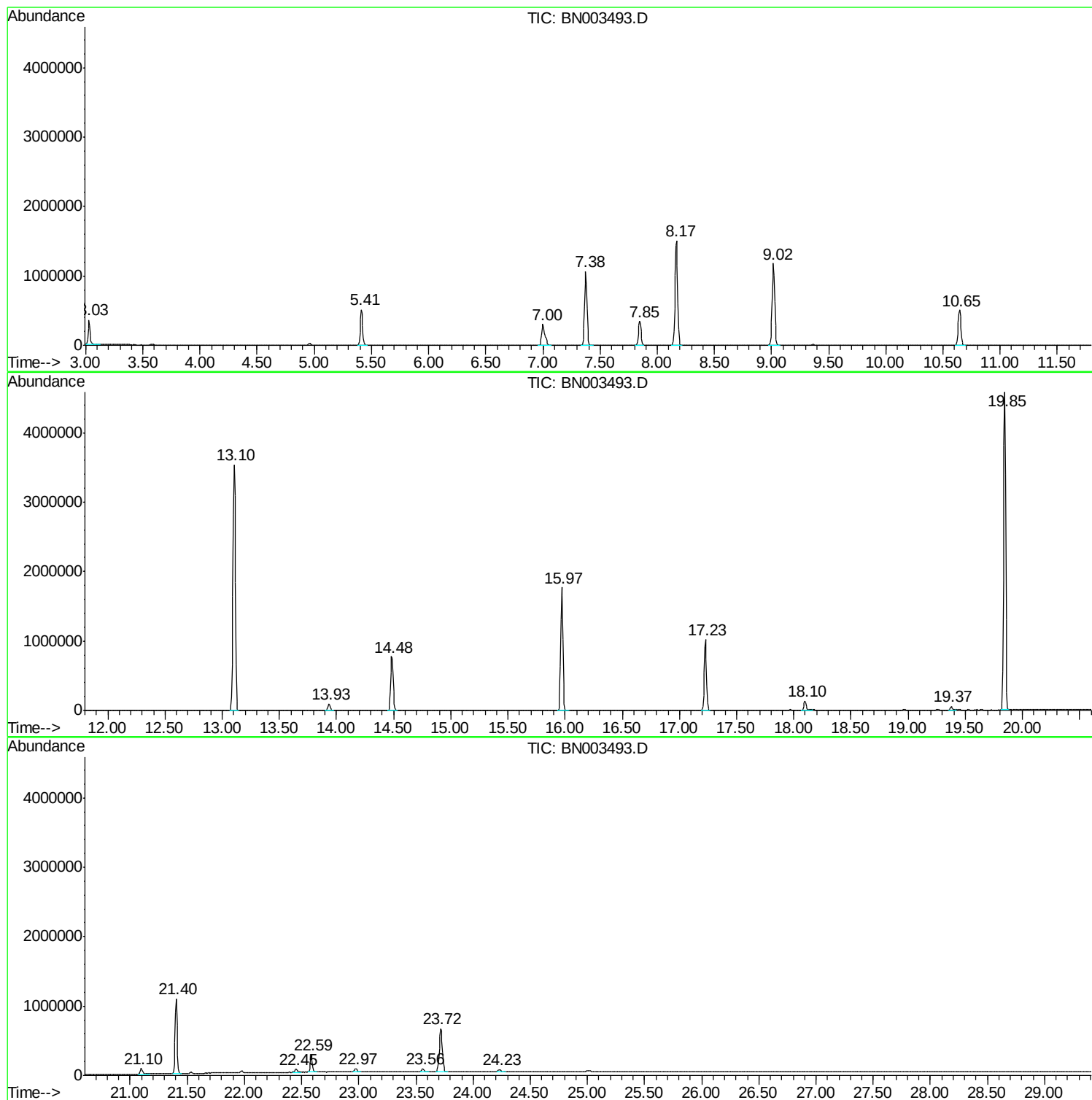
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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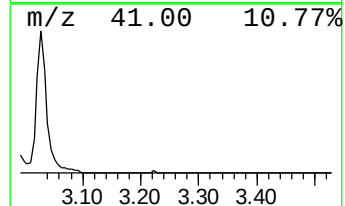
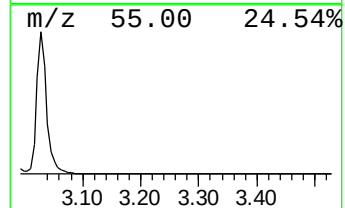
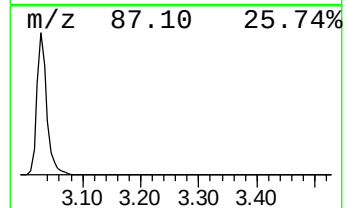
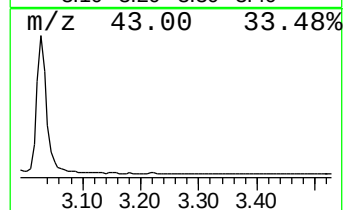
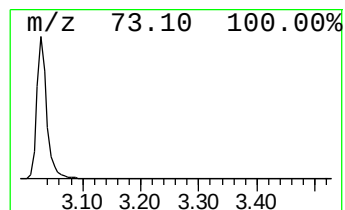
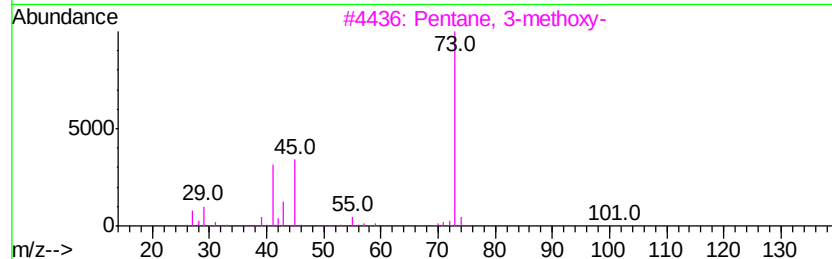
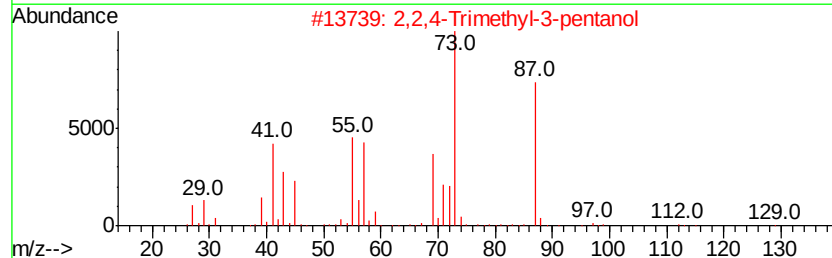
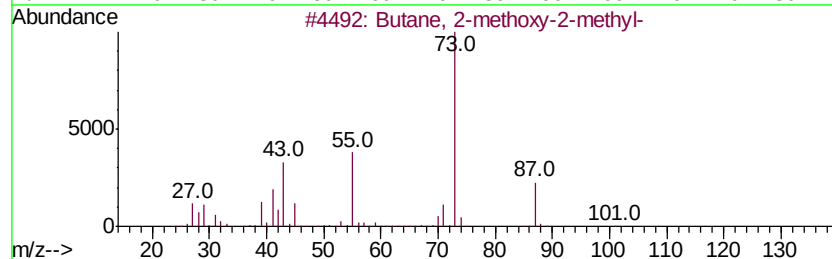
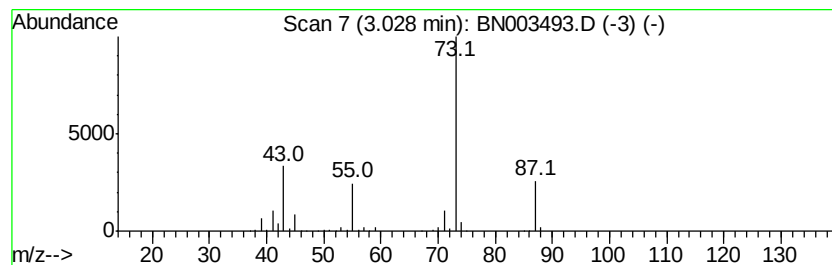
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
3.03	16.01 ng	425297	1,4-Dichlorobenzene-d4	7.85	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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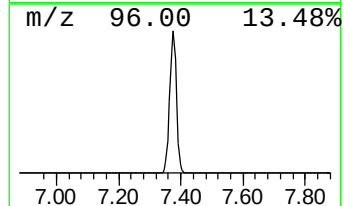
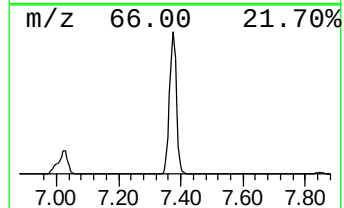
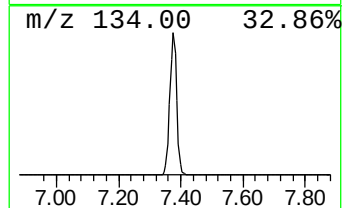
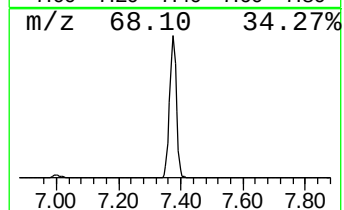
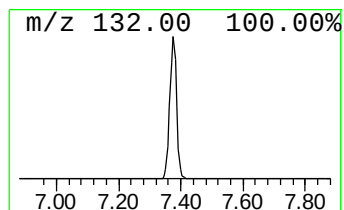
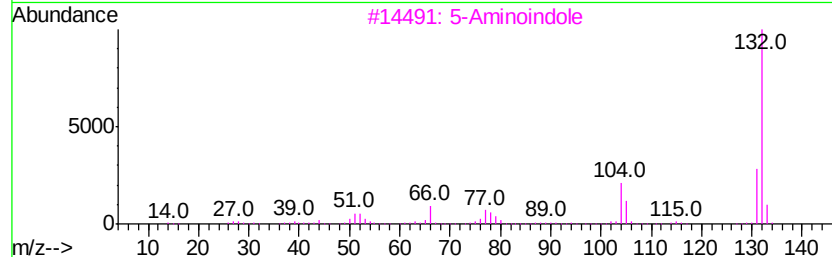
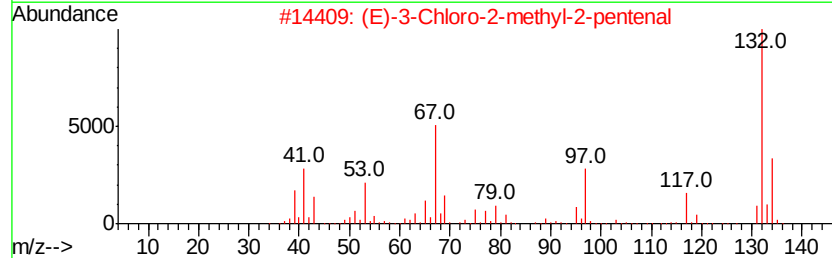
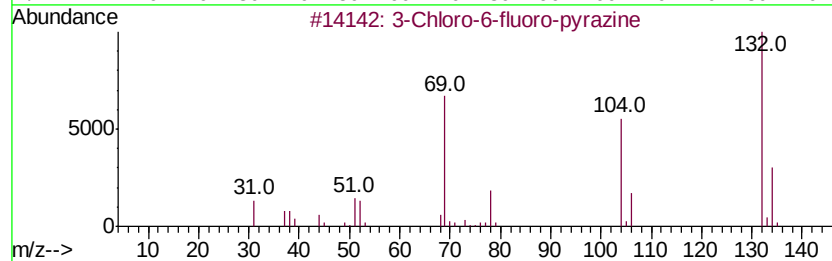
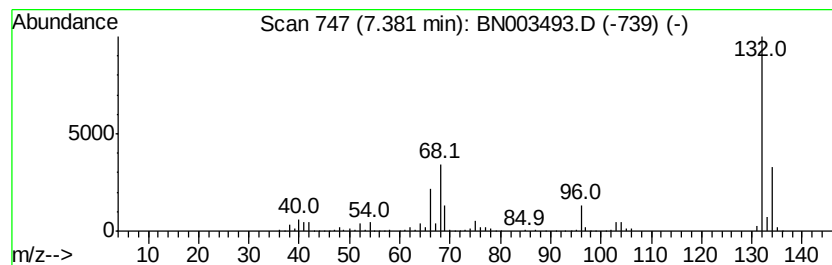
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Peak Number 2 unknown7.38 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.38	60.55 ng	1608940	1,4-Dichlorobenzene-d4	7.85

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			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			4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5			4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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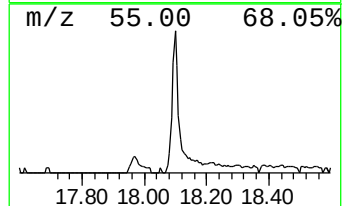
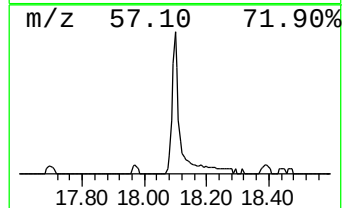
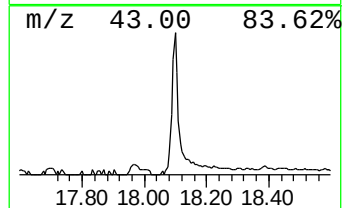
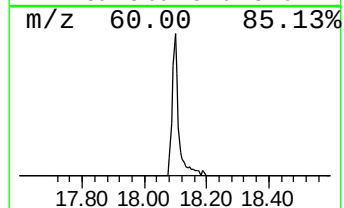
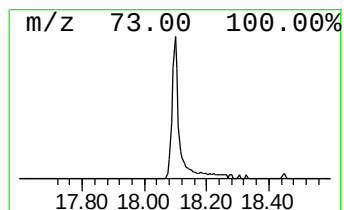
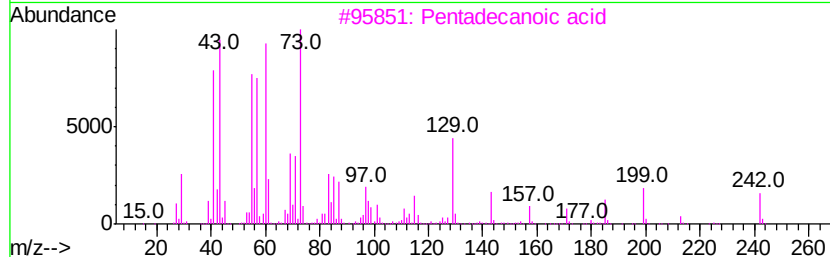
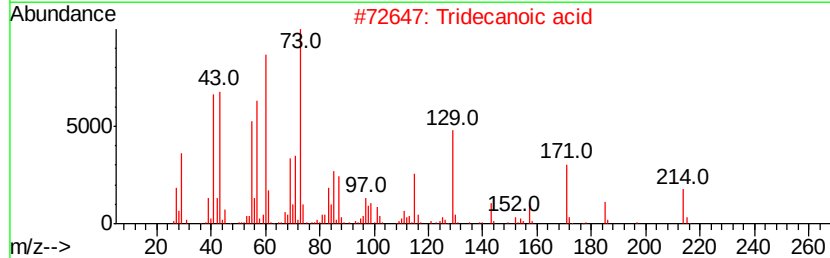
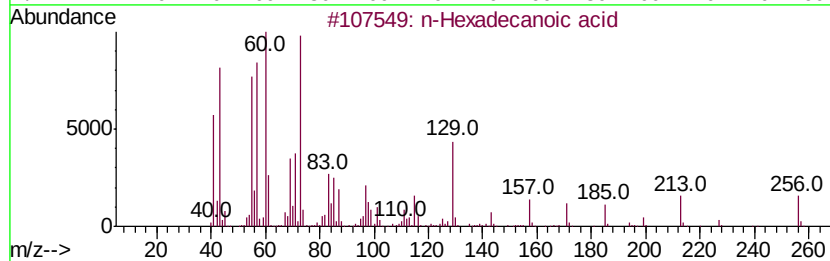
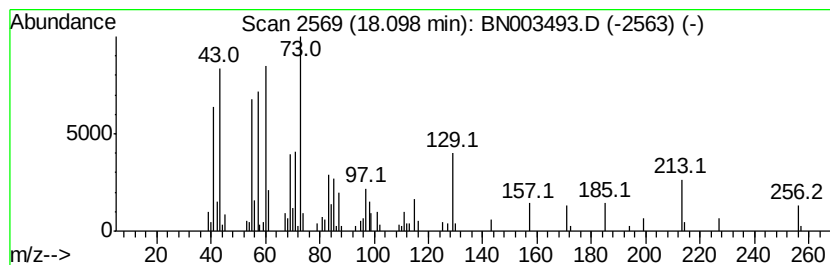
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.10	2.87 ng	199651	Phenanthrene-d10	17.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	93
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5		n-Decanoic acid	172	C10H20O2	000334-48-5	76



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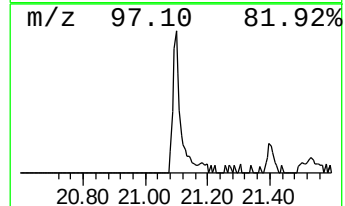
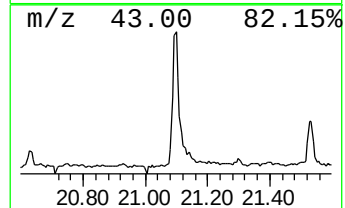
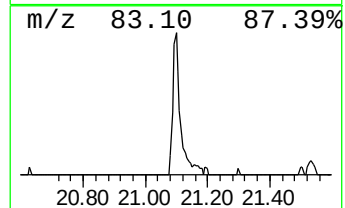
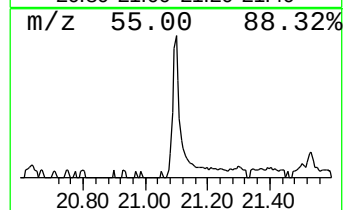
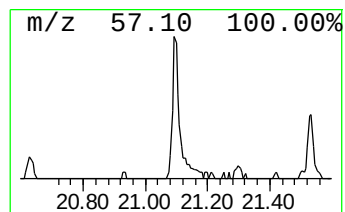
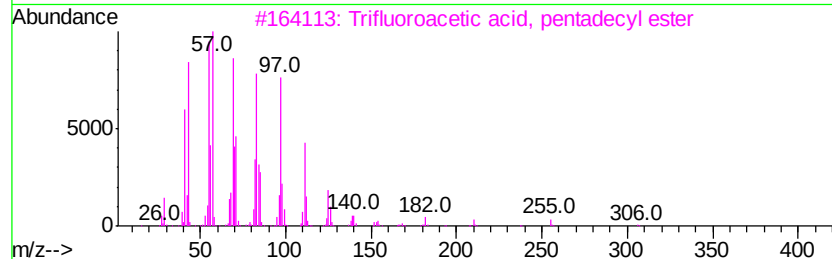
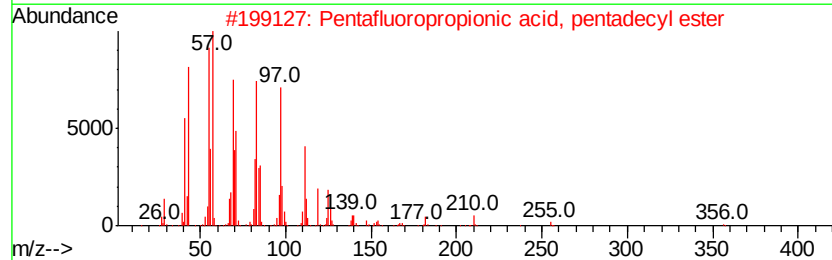
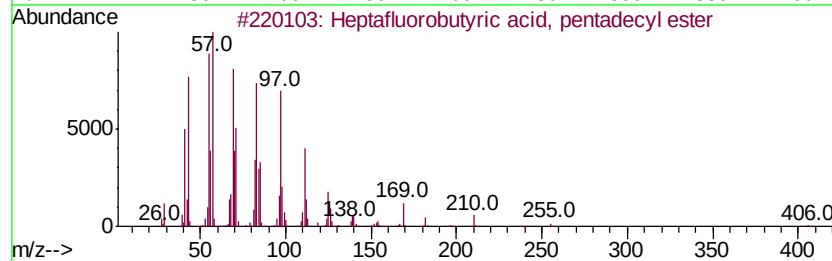
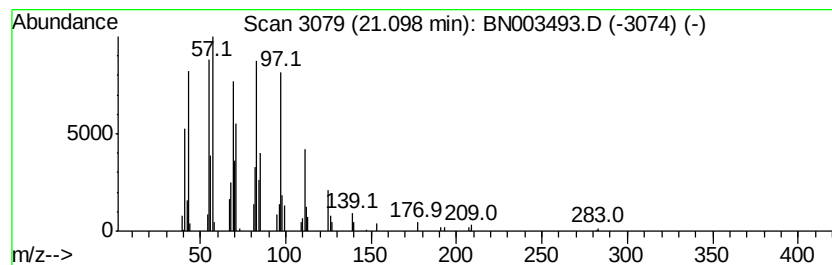
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Peak Number 5 Heptafluorobutyric acid, pe... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.10	2.15 ng	137977	Chrysene-d12	21.40

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	95
2		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	95
3		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	95
4		Trifluoroacetoxv hexadecane	338	C18H33F3O2	006222-03-3	95
5		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94



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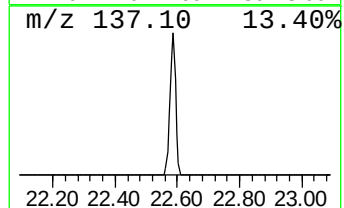
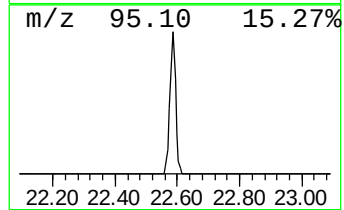
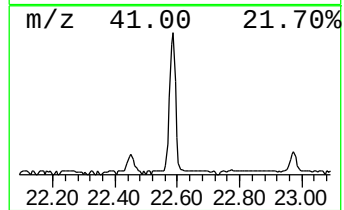
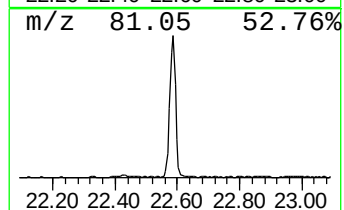
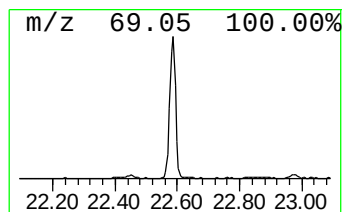
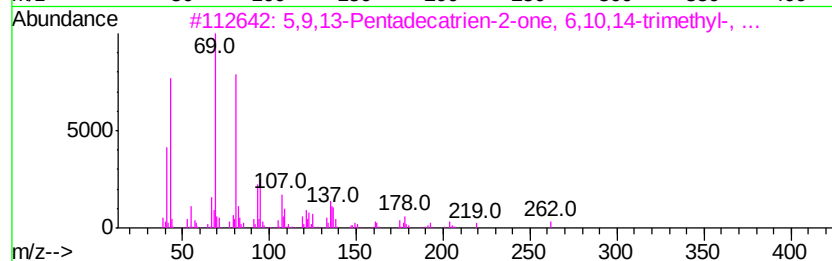
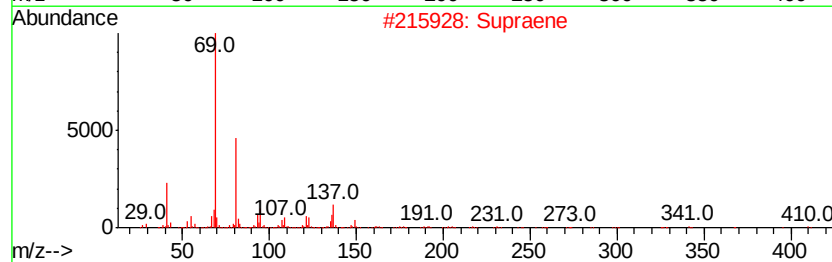
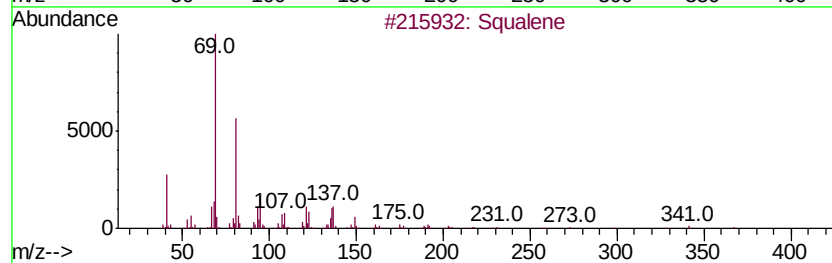
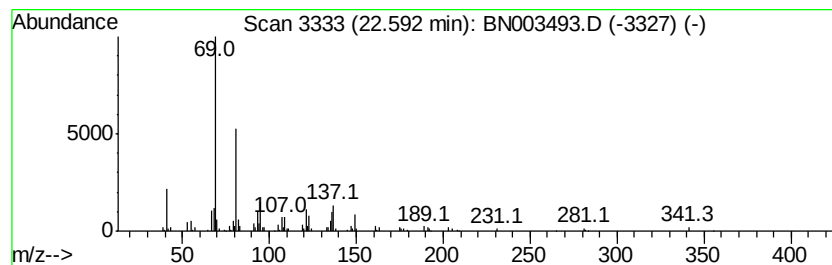
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Peak Number 6 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.59	5.33 ng	315663	Perylene-d12	23.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	94
2		Supraene	410	C30H50	007683-64-9	91
3		5,9,13-Pentadecatrien-2-one, 6,1...	262	C18H30O	001117-52-8	59
4		4-Methyl-1,5-Heptadiene	110	C8H14	000998-94-7	52
5		Cyclopropanecarboxylic acid, 3-m...	176	C11H12O2	1000307-52-1	43



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	3.03	16.0	ng	425297	1	7.85	531415	20.0
unknown7.38	7.38	60.5	ng	1608940	1	7.85	531415	20.0
n-Hexadecanoic acid	18.10	2.9	ng	199651	4	17.23	1393140	20.0
Heptafluorobutyri...	21.10	2.1	ng	137977	5	21.40	1285520	20.0
Squalene	22.59	5.3	ng	315663	6	23.72	1183540	20.0