

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050517\
 Data File : BF094931.D
 Acq On : 5 May 2017 22:51
 Operator : SJ/MA
 Sample : I2949-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-07-7.5-8.0

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	5.042	524	528	543	rBV	190042	364774	12.65%	1.636%
2	5.672	630	635	663	rBV	1536875	2284313	79.23%	10.246%
3	7.266	900	906	921	rBV	1580326	2240978	77.72%	10.051%
4	7.383	921	926	935	rVB	1950008	2519751	87.39%	11.302%
5	7.725	979	984	996	rVB	403593	490942	17.03%	2.202%
6	7.960	1019	1024	1034	rBV	1749300	2027696	70.33%	9.095%
7	8.619	1131	1136	1152	rBV	1151810	1537923	53.34%	6.898%
8	9.742	1323	1327	1347	rVB	485607	674758	23.40%	3.026%
9	11.519	1623	1629	1647	rBV	2163022	2883316	100.00%	12.932%
10	12.207	1743	1746	1755	rBV	112181	156370	5.42%	0.701%
11	12.571	1803	1808	1821	rBV2	526930	746587	25.89%	3.349%
12	13.865	2022	2028	2042	rBV	1132284	1686830	58.50%	7.566%
13	14.189	2079	2083	2085	rBV	29407	34731	1.20%	0.156%
14	14.971	2211	2216	2228	rVV	513903	730757	25.34%	3.278%
15	15.936	2375	2380	2387	rBV2	78276	108573	3.77%	0.487%
16	17.300	2606	2612	2615	rBV	2077325	2519806	87.39%	11.302%
17	18.577	2818	2829	2835	rBV6	11677	36756	1.27%	0.165%
18	18.636	2835	2839	2857	rVB	467430	644274	22.34%	2.890%
19	18.824	2864	2871	2876	rVB	44071	46902	1.63%	0.210%
20	19.771	3028	3032	3036	rBV	75822	73930	2.56%	0.332%
21	20.306	3118	3123	3135	rBV	323382	485636	16.84%	2.178%

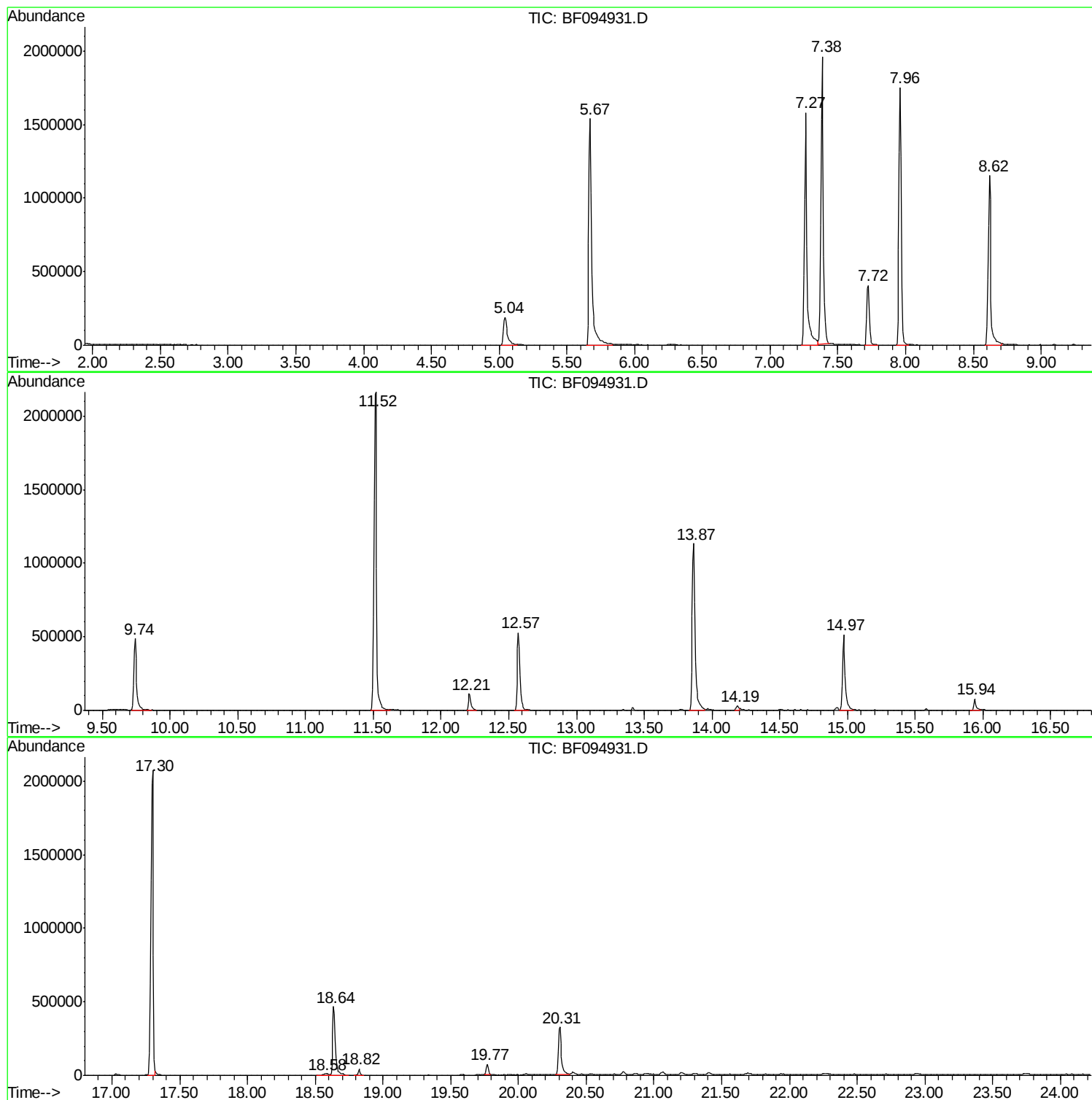
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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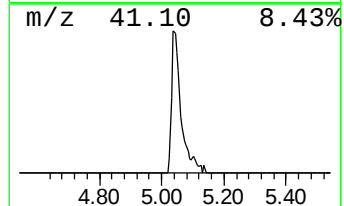
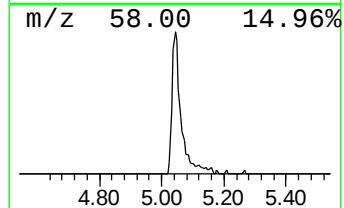
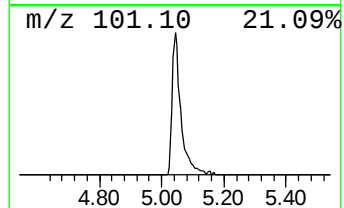
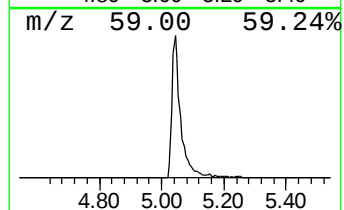
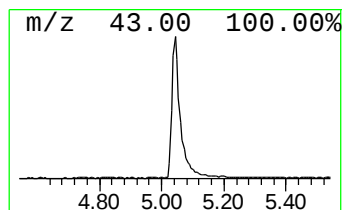
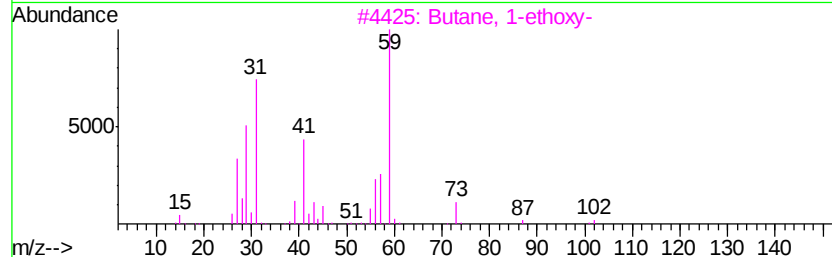
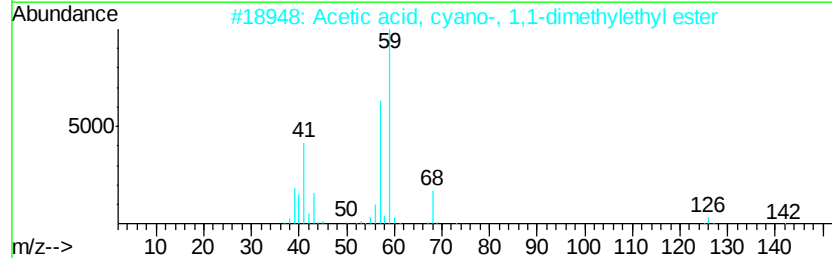
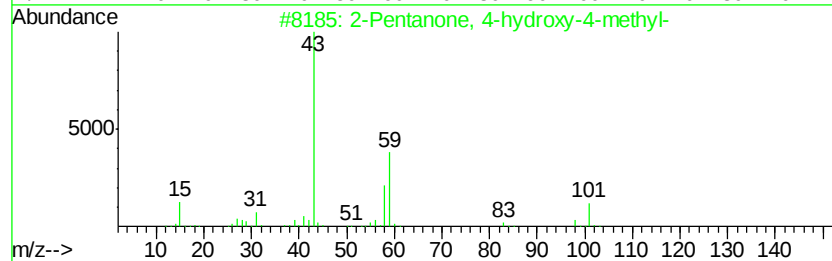
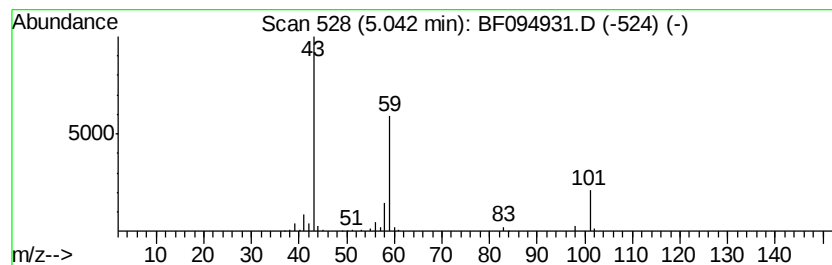
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	14.86 ng	364774	1,4-Dichlorobenzene-d4	7.72

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	47
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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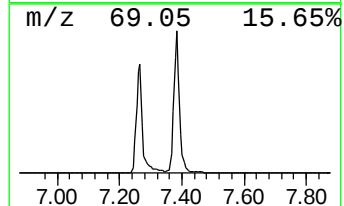
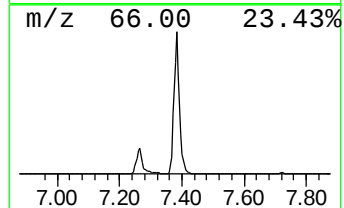
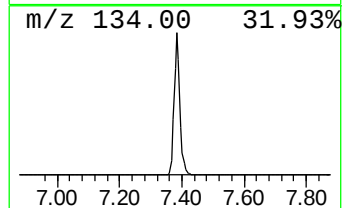
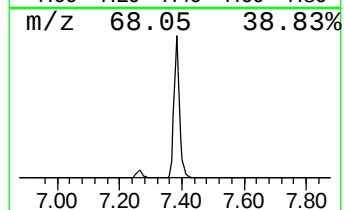
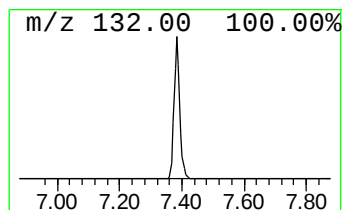
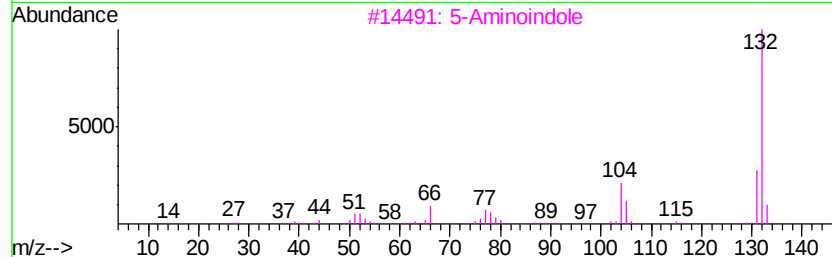
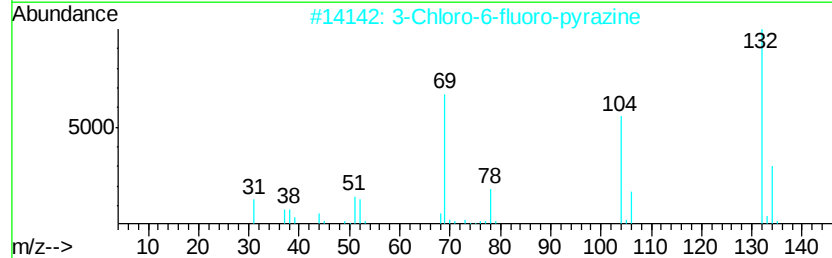
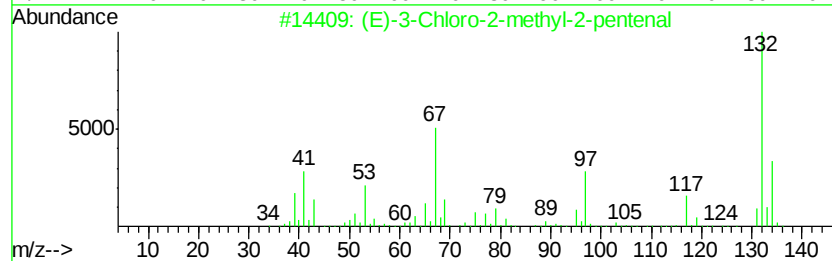
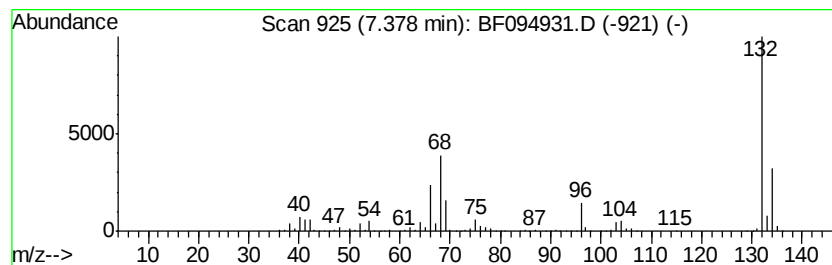
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Peak Number 2 unknown7.38 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.38	102.65 ng	2519750	1,4-Dichlorobenzene-d4	7.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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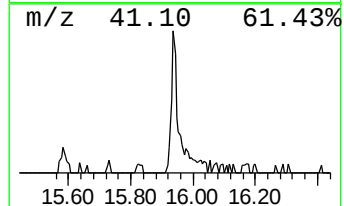
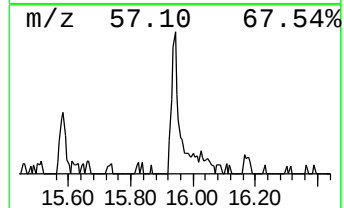
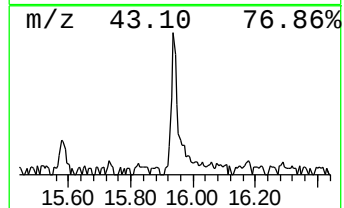
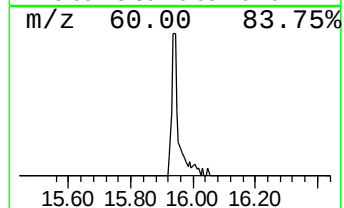
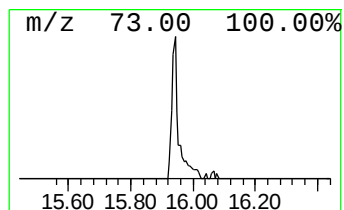
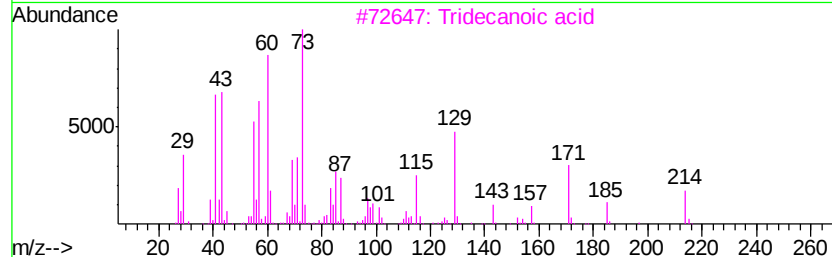
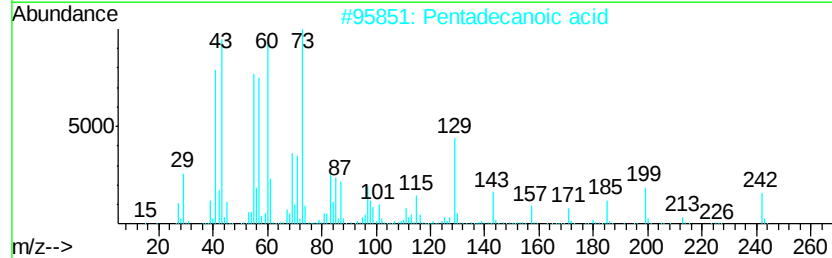
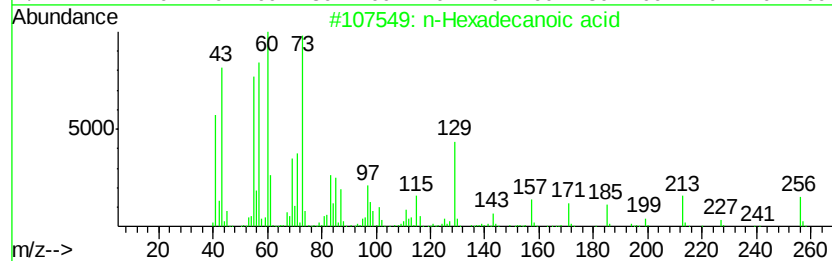
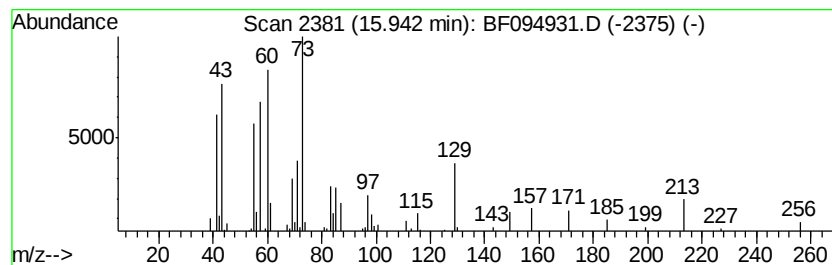
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.94	2.97 ng	108573	Phenanthrene-d10	14.97

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3		Tridecanoic acid	214	C13H26O2	000638-53-9	86
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5		Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	64



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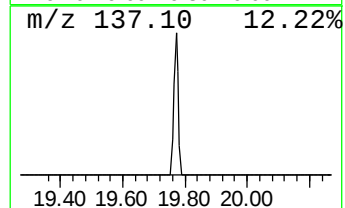
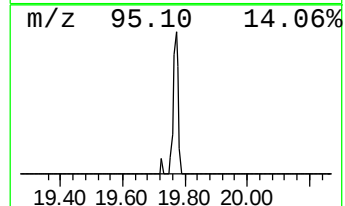
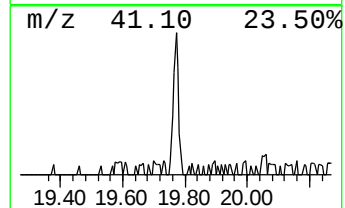
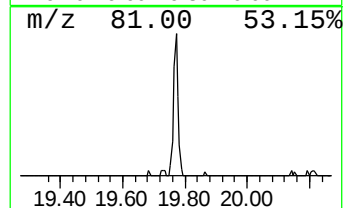
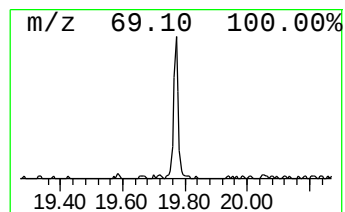
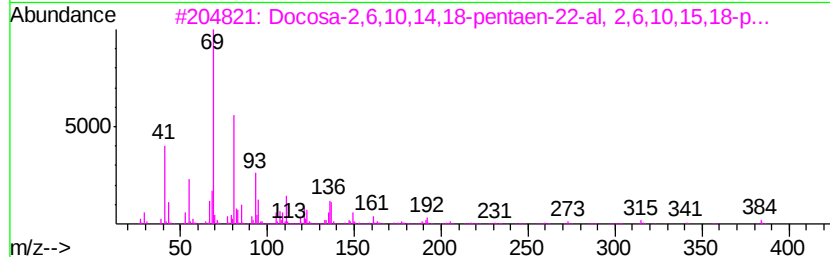
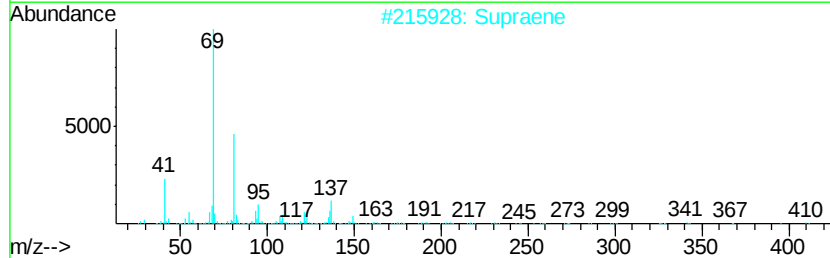
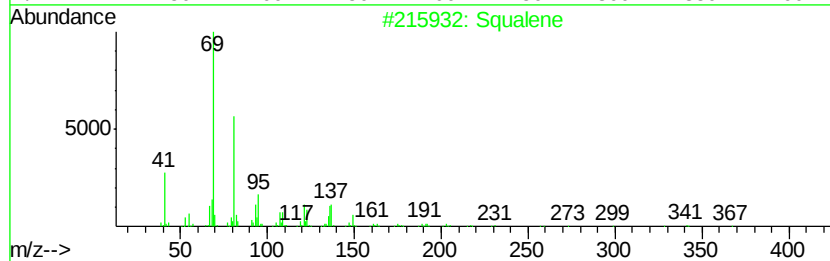
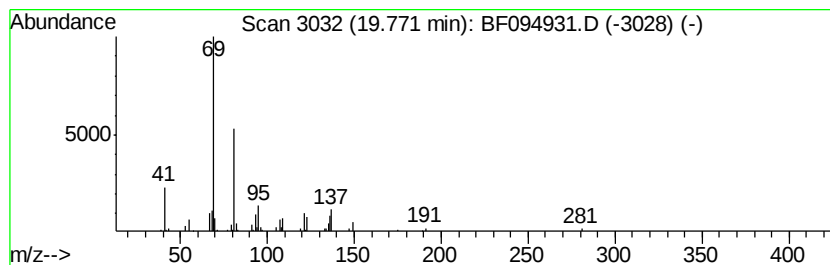
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Peak Number 5 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.77	3.04 ng	73930	Perylene-d12	20.31

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	91
2		Supraene	410	C30H50	007683-64-9	91
3		Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	90
4		.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	83
5		Propanoic acid, 2,2-dimethyl-, [...	306	C20H34O2	1000164-38-8	72



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.04	14.9	ng	364774	1	7.72	490942	20.0
unknown7.38	7.38	102.7	ng	2519750	1	7.72	490942	20.0
n-Hexadecanoic acid	15.94	3.0	ng	108573	4	14.97	730757	20.0
Squalene	19.77	3.0	ng	73930	6	20.31	485636	20.0