

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050517\
 Data File : BF094936.D
 Acq On : 6 May 2017 1:33
 Operator : SJ/MA
 Sample : I2950-03
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-10(13-15)20170502

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	5.043	524	528	548	rBV	222185	466814	14.24%	1.780%
2	5.672	630	635	669	rBV	1831859	2714858	82.83%	10.350%
3	7.266	900	906	921	rBV	1904996	2764647	84.35%	10.540%
4	7.384	921	926	936	rVB	2269589	2991084	91.26%	11.403%
5	7.725	980	984	994	rBV	436682	546284	16.67%	2.083%
6	7.960	1019	1024	1039	rBV	1954906	2314835	70.62%	8.825%
7	8.625	1127	1137	1154	rBV	1308601	1780137	54.31%	6.786%
8	9.742	1322	1327	1339	rBV	526278	707636	21.59%	2.698%
9	11.519	1623	1629	1646	rBV	2585889	3277646	100.00%	12.495%
10	12.207	1742	1746	1758	rBV	199038	257092	7.84%	0.980%
11	12.572	1803	1808	1822	rBV2	552954	782600	23.88%	2.983%
12	13.413	1947	1951	1956	rBV	30191	34245	1.04%	0.131%
13	13.866	2022	2028	2043	rBV	1314078	1919131	58.55%	7.316%
14	14.189	2078	2083	2086	rBV	42936	56194	1.71%	0.214%
15	14.918	2201	2207	2211	rBV2	31765	39294	1.20%	0.150%
16	14.971	2211	2216	2228	rVV2	585646	810065	24.71%	3.088%
17	15.936	2376	2380	2389	rBV2	102417	143659	4.38%	0.548%
18	17.024	2562	2565	2576	rBV2	34191	54203	1.65%	0.207%
19	17.301	2606	2612	2623	rBV	2497069	3071975	93.73%	11.711%
20	18.583	2821	2830	2835	rBV8	17048	55219	1.68%	0.211%
21	18.636	2835	2839	2855	rVB	538455	754856	23.03%	2.878%
22	19.771	3027	3032	3035	rBV	54594	56566	1.73%	0.216%
23	20.300	3118	3122	3136	rBV2	357445	561127	17.12%	2.139%
24	21.200	3270	3275	3281	rBV4	18435	35680	1.09%	0.136%
25	21.689	3352	3358	3365	rBV4	15490	35183	1.07%	0.134%

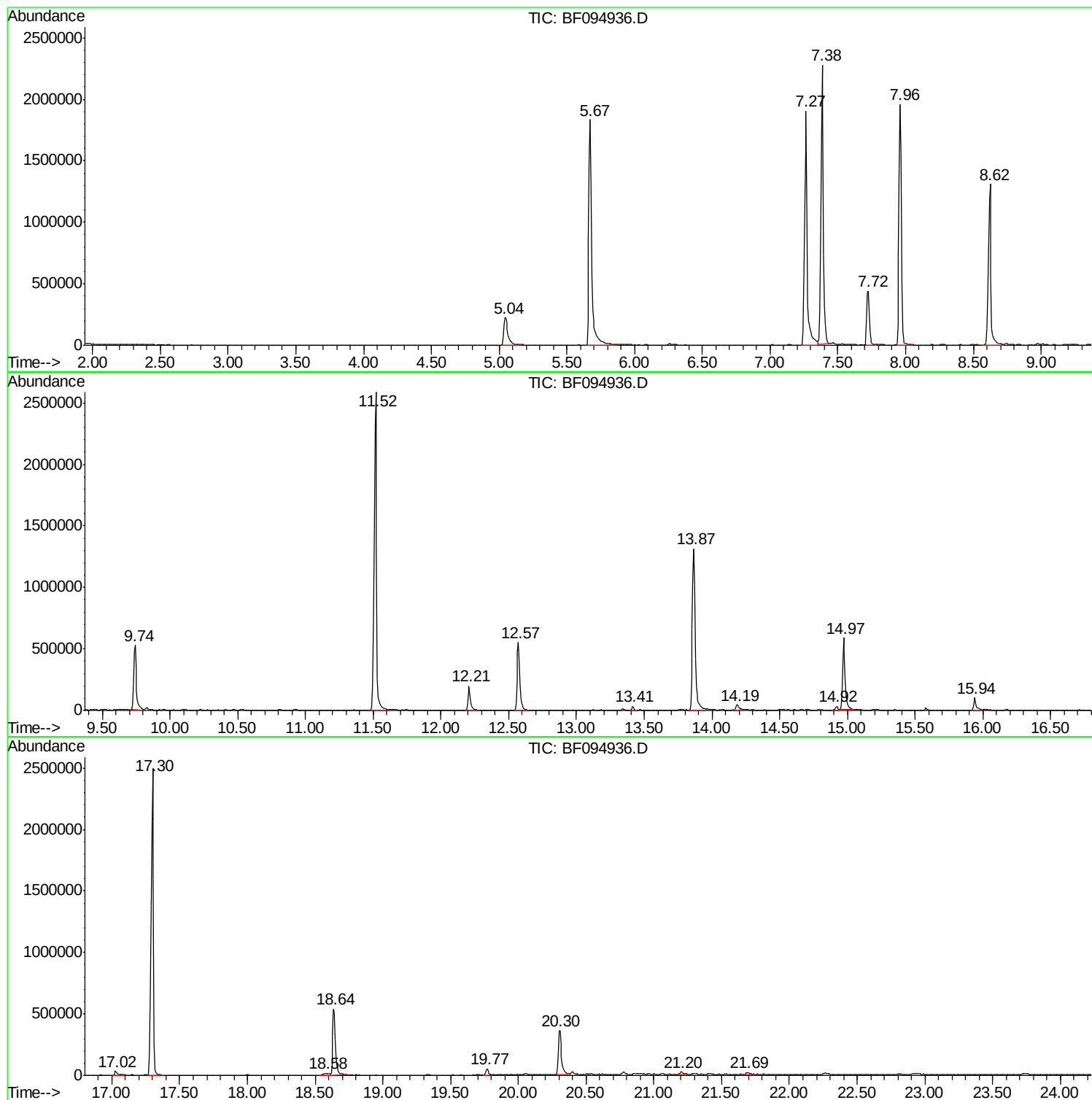
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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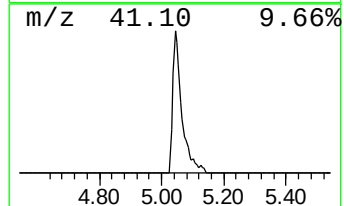
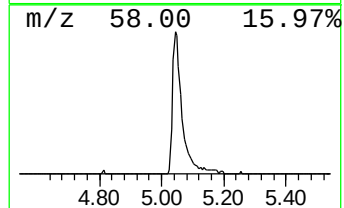
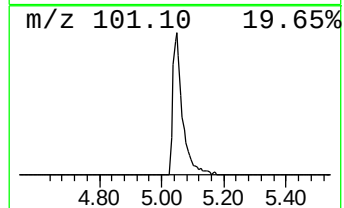
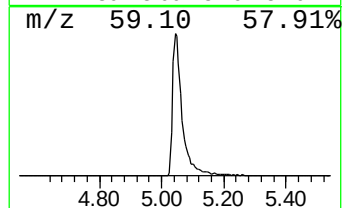
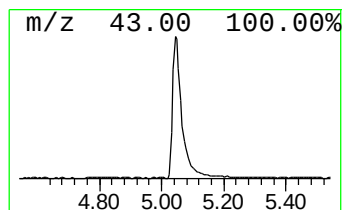
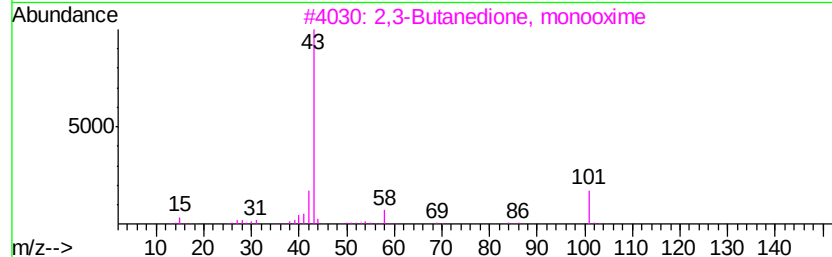
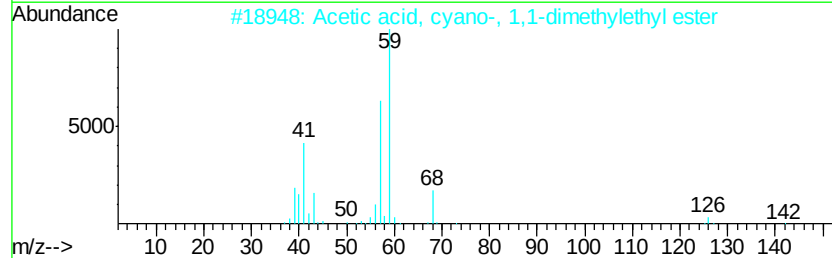
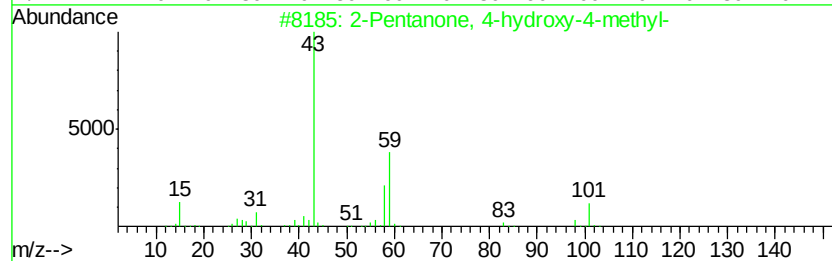
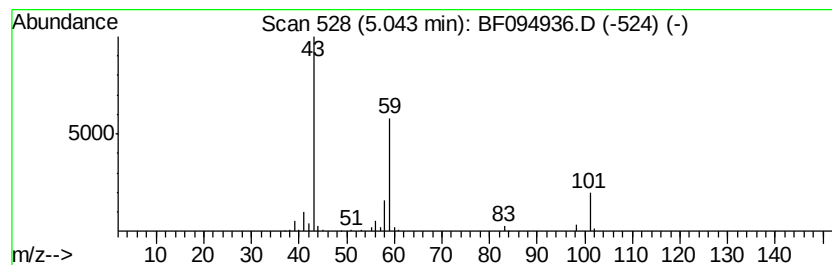
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	17.09 ng	466814	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	72
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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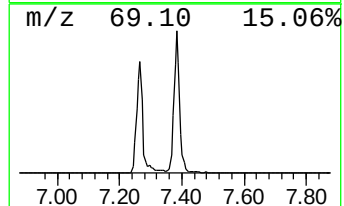
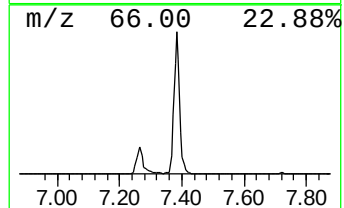
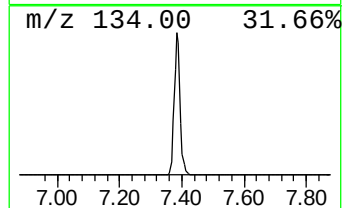
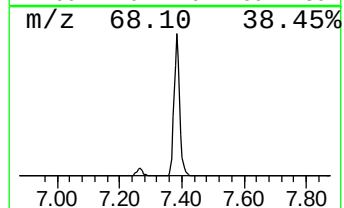
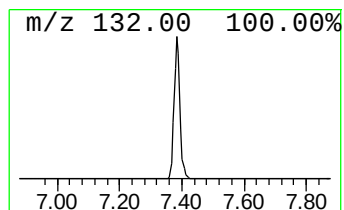
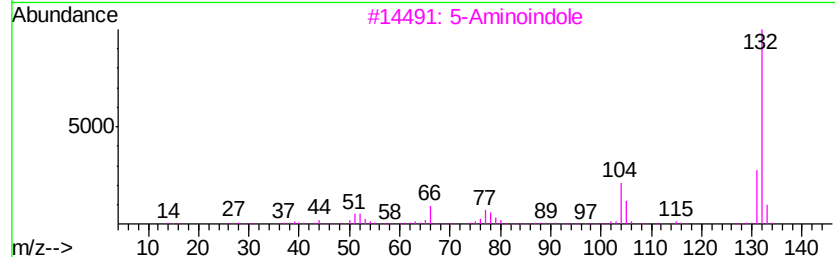
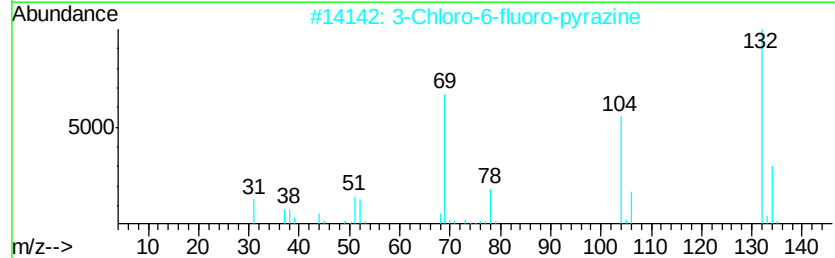
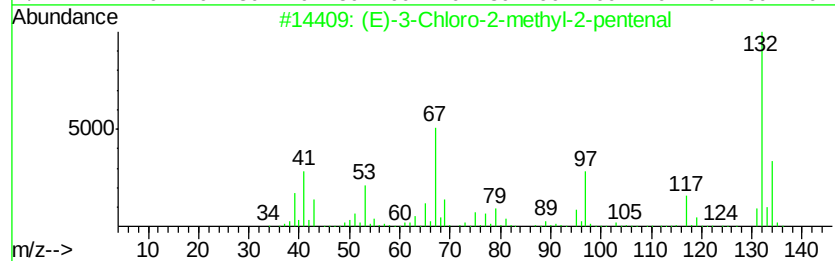
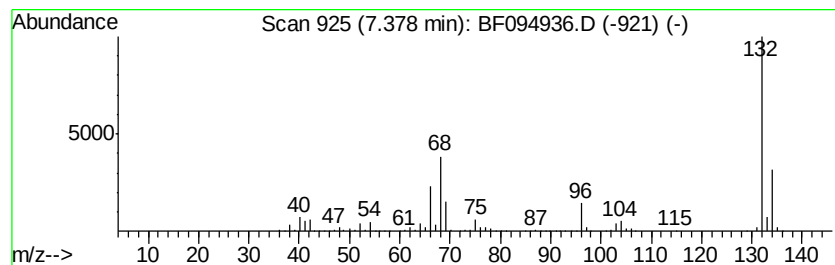
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Peak Number 2 unknown7.38 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.38	109.51 ng	2991080	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	17
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10



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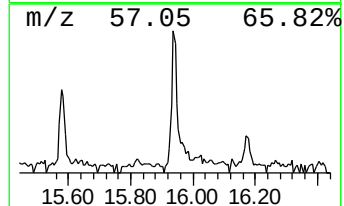
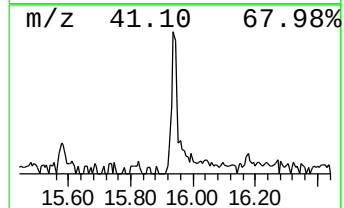
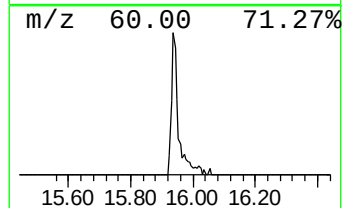
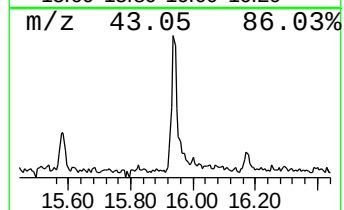
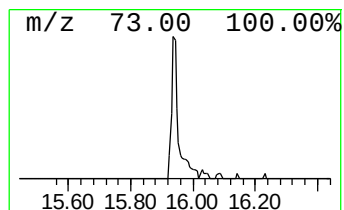
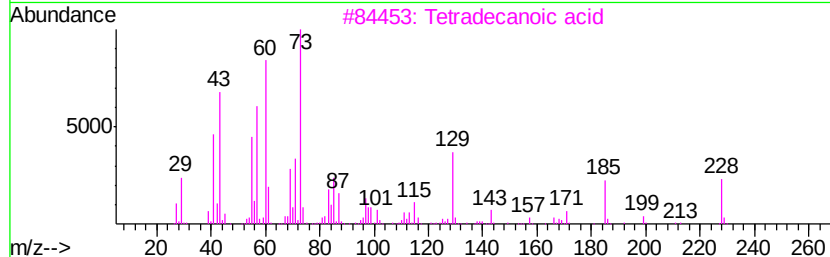
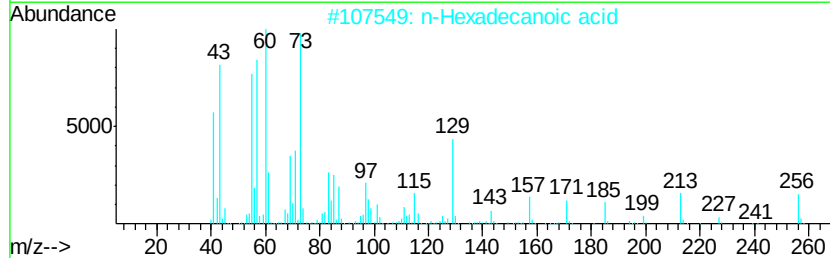
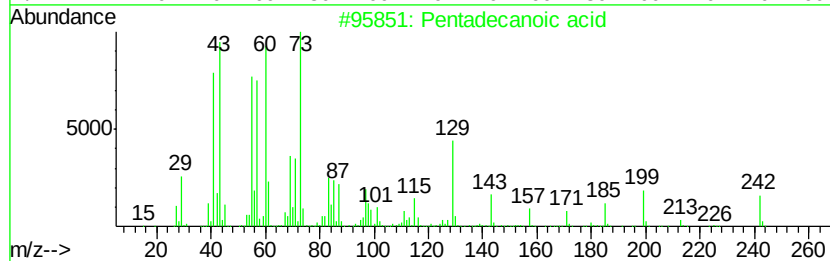
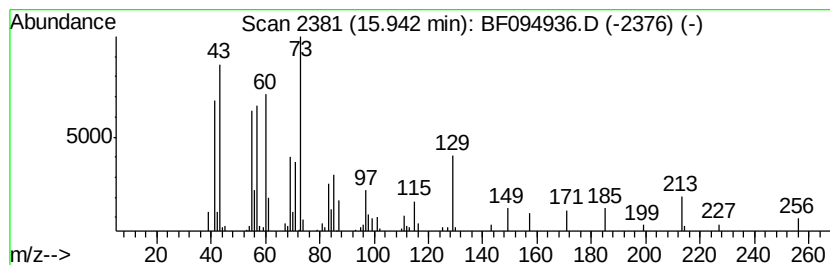
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Peak Number 4 Pentadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.94	3.55 ng	143659	Phenanthrene-d10	14.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4	Tridecanoic acid	214	C13H26O2	000638-53-9	72
5	Trehalose	342	C12H22O11	000099-20-7	35



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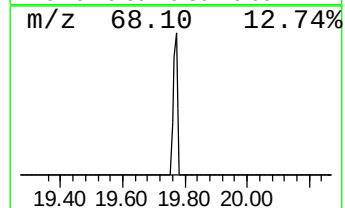
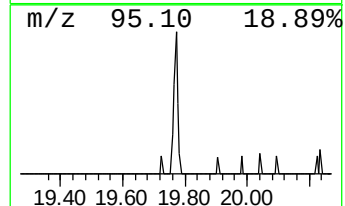
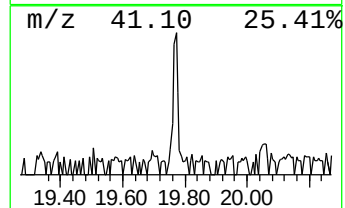
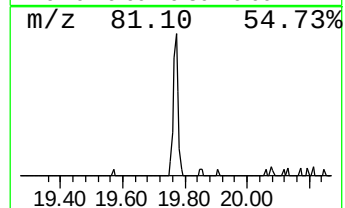
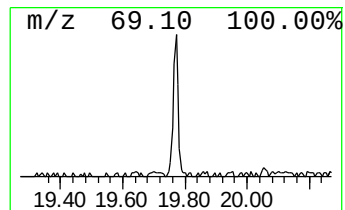
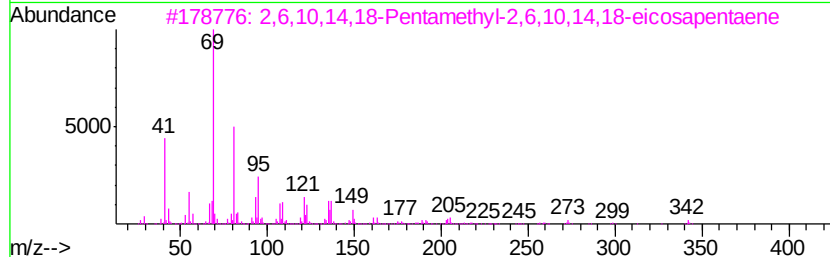
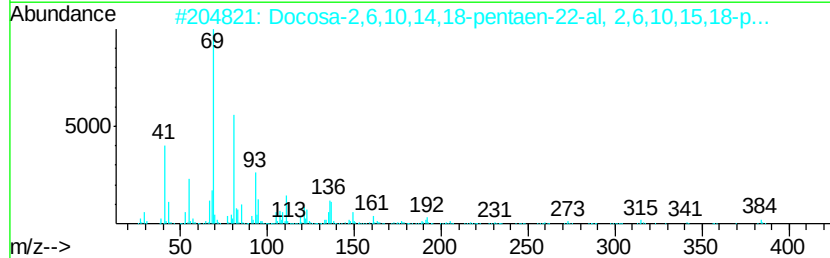
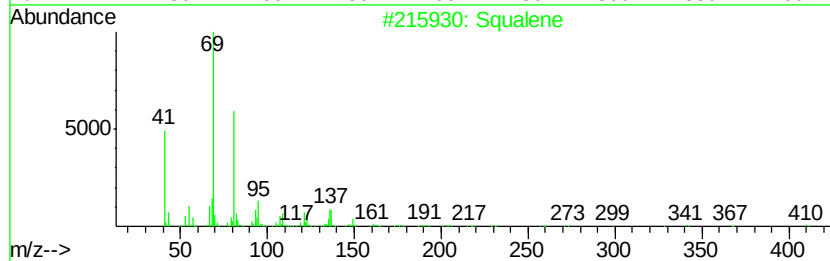
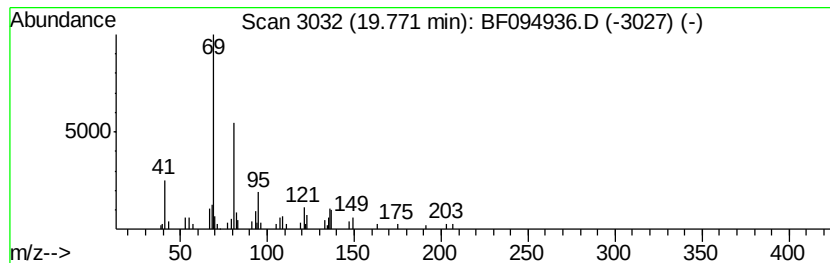
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Peak Number 5 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.77	2.02 ng	56566	Perylene-d12	20.31

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	91
2		Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	86
3		2,6,10,14,18-Pentamethyl-2,6,10,...	342	C25H42	075581-03-2	86
4		Supraene	410	C30H50	007683-64-9	80
5		Hexadeca-2,6,10,14-tetraen-1-ol,...	290	C20H34O	007614-21-3	78



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.04	17.1	ng	466814	1	7.72	546284	20.0
unknown7.38	7.38	109.5	ng	2991080	1	7.72	546284	20.0
Pentadecanoic acid	15.94	3.5	ng	143659	4	14.97	810065	20.0
Squalene	19.77	2.0	ng	56566	6	20.31	561127	20.0