

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050517\
 Data File : BF094939.D
 Acq On : 6 May 2017 3:10
 Operator : SJ/MA
 Sample : I2950-06
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-11(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	5.048	525	529	549	rBV	242836	503816	14.38%	1.726%
2	5.672	630	635	663	rBV	2036496	3074637	87.76%	10.530%
3	7.266	900	906	921	rBV	1892349	2901424	82.82%	9.937%
4	7.384	921	926	941	rVB	2324165	3255790	92.93%	11.151%
5	7.725	980	984	993	rBV	463415	567983	16.21%	1.945%
6	7.960	1019	1024	1035	rBV	2077731	2506101	71.53%	8.583%
7	8.625	1131	1137	1155	rBV	1392833	1862969	53.18%	6.380%
8	9.742	1322	1327	1341	rBV	542253	747247	21.33%	2.559%
9	11.519	1623	1629	1648	rBV	2766078	3503386	100.00%	11.999%
10	12.207	1741	1746	1757	rBV	250203	320473	9.15%	1.098%
11	12.572	1803	1808	1824	rBV2	630331	859884	24.54%	2.945%
12	13.413	1947	1951	1956	rBV	33748	39102	1.12%	0.134%
13	13.866	2022	2028	2041	rBV	1490266	2151250	61.40%	7.368%
14	14.183	2078	2082	2085	rBV	44614	56756	1.62%	0.194%
15	14.918	2203	2207	2211	rBV2	31214	39452	1.13%	0.135%
16	14.971	2211	2216	2227	rVV	578773	789486	22.53%	2.704%
17	15.942	2376	2381	2390	rBV	278931	337764	9.64%	1.157%
18	17.030	2562	2566	2577	rBV	187600	242049	6.91%	0.829%
19	17.142	2582	2585	2594	rVB2	40247	47696	1.36%	0.163%
20	17.301	2606	2612	2616	rBV2	2615617	3281815	93.68%	11.240%
21	18.583	2821	2830	2835	rBV6	20962	68034	1.94%	0.233%
22	18.636	2835	2839	2844	rVV	627476	787399	22.48%	2.697%
23	18.683	2844	2847	2848	rVV	236249	292339	8.34%	1.001%
24	18.695	2848	2849	2859	rVB	271860	209265	5.97%	0.717%
25	19.771	3028	3032	3037	rBV	59338	65760	1.88%	0.225%
26	20.300	3118	3122	3135	rBV	398338	602326	17.19%	2.063%
27	20.777	3198	3203	3209	rBV3	28134	45075	1.29%	0.154%
28	20.859	3212	3217	3223	rBV8	15456	38913	1.11%	0.133%

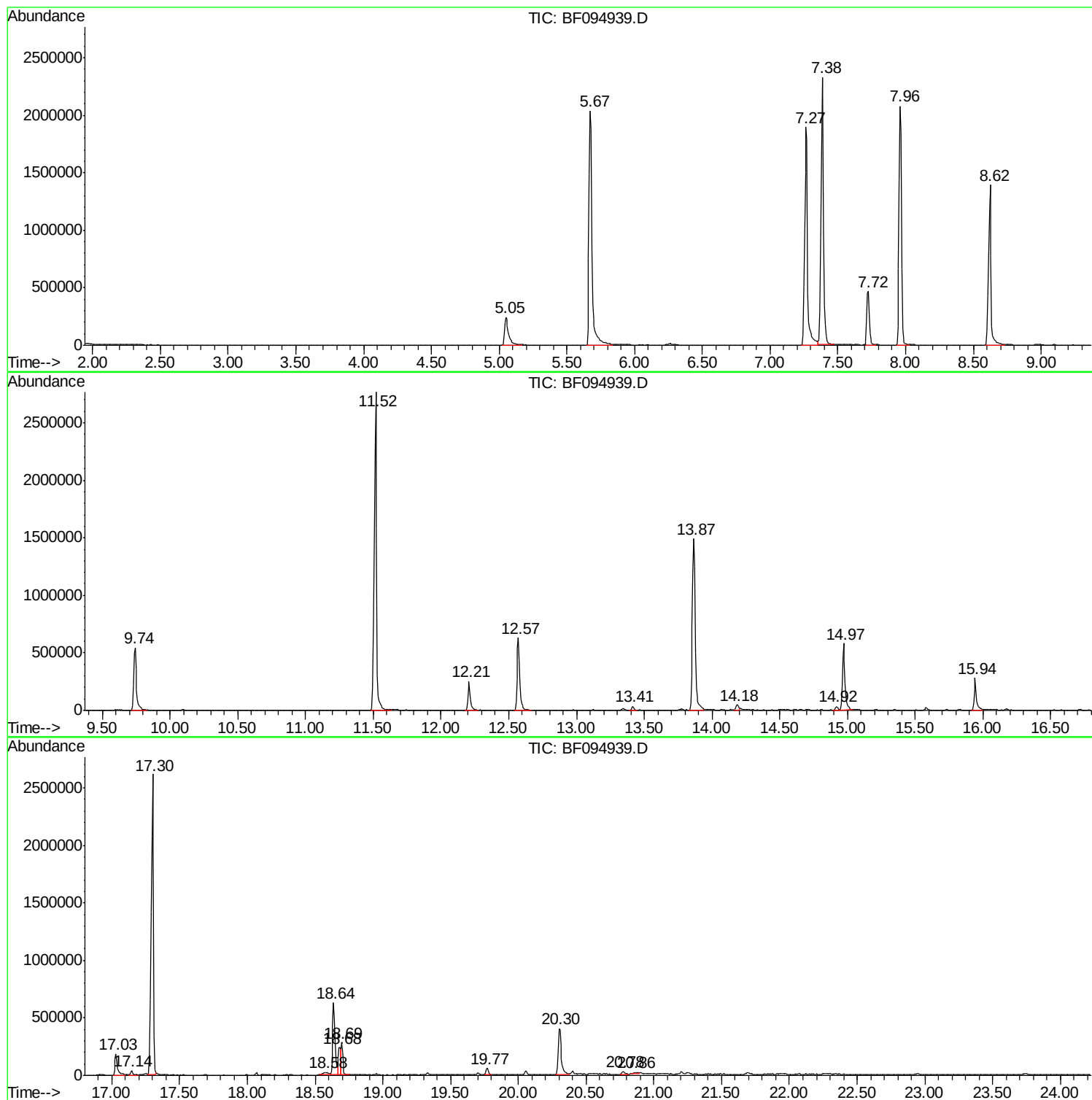
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ClientSampleId :
SB-11(13-15)20170502

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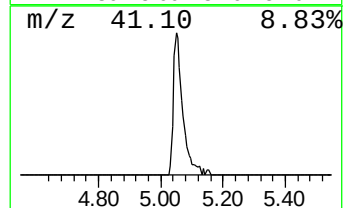
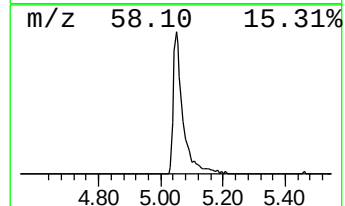
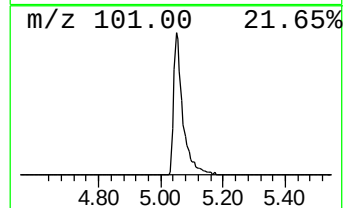
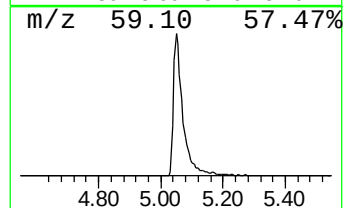
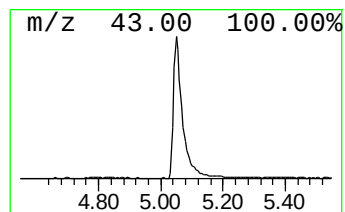
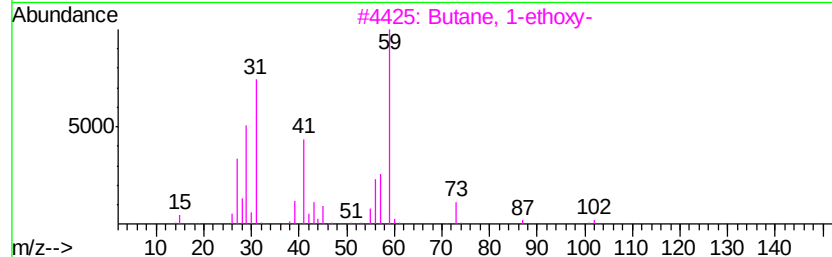
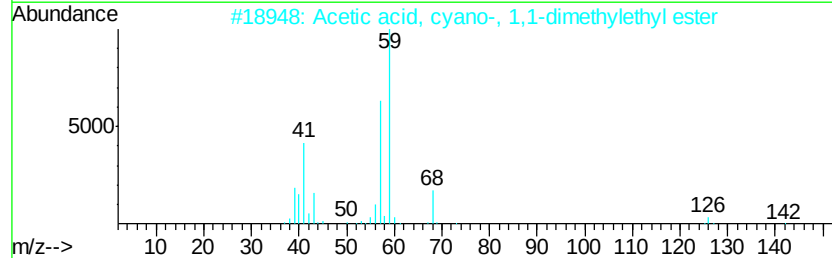
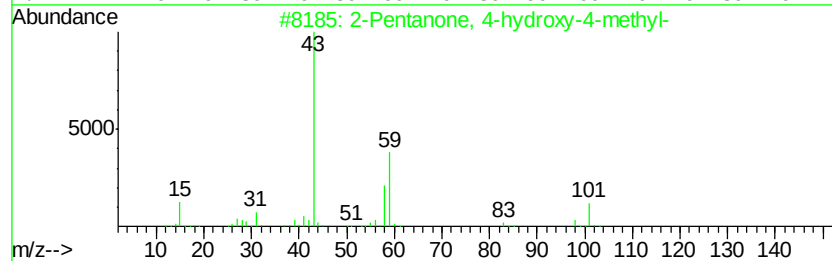
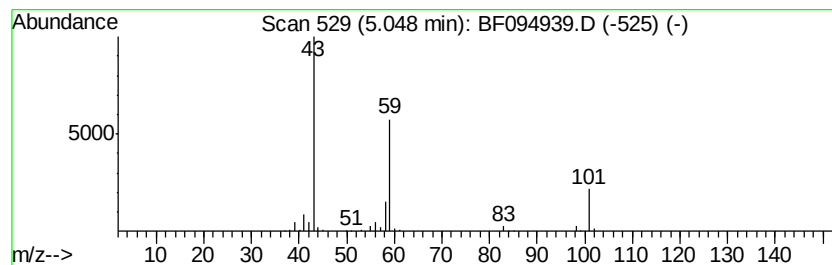
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.05	17.74 ng	503816	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	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		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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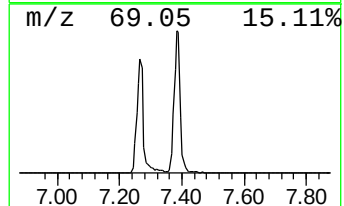
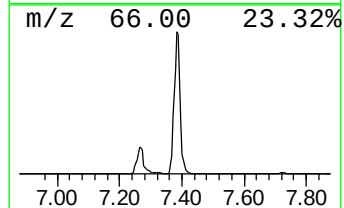
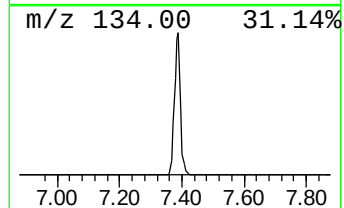
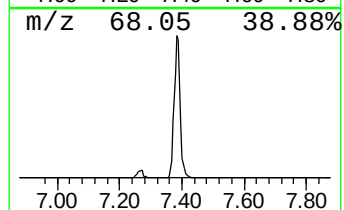
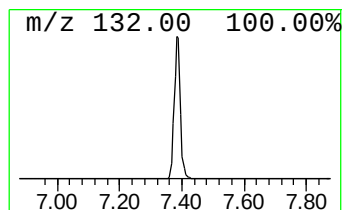
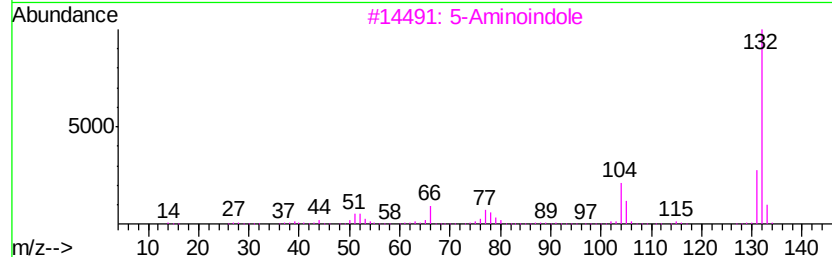
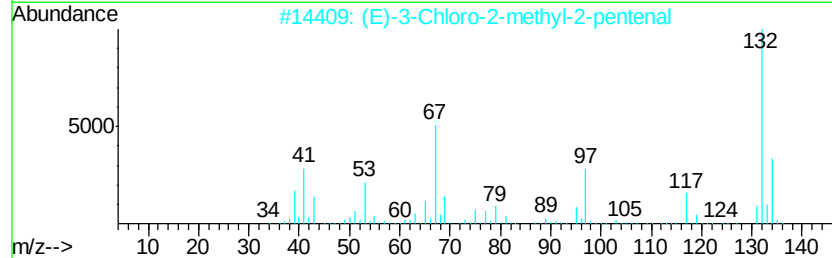
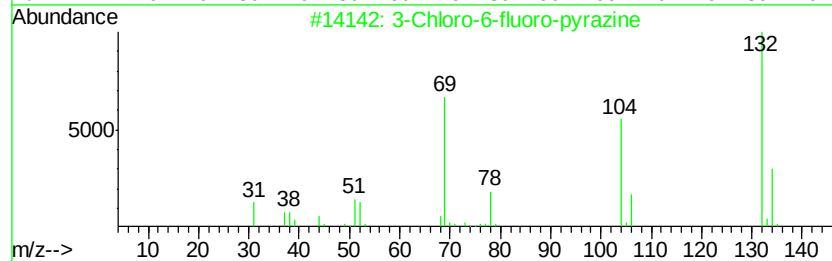
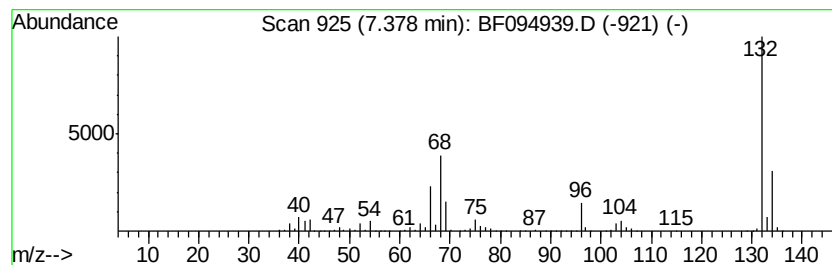
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Peak Number 2 unknown7.38 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.38	114.64 ng	3255790	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	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
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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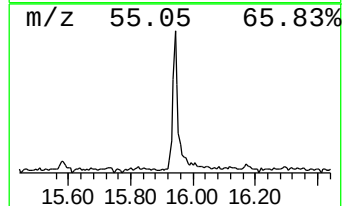
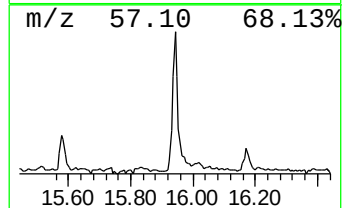
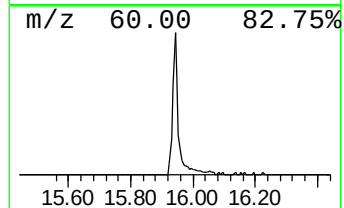
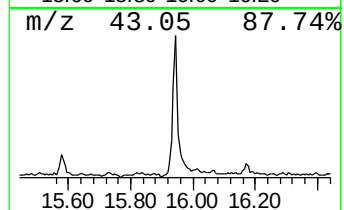
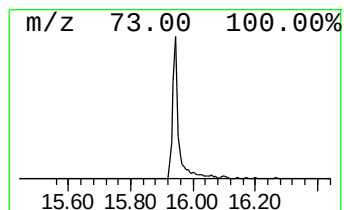
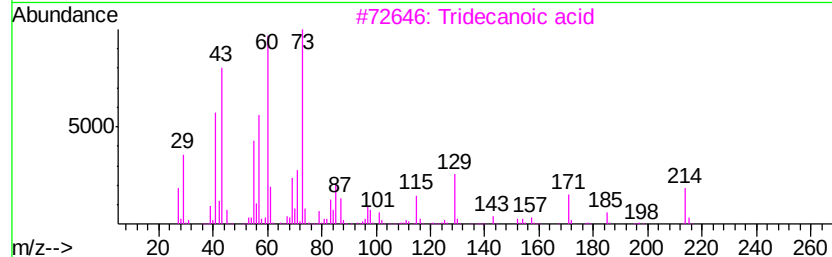
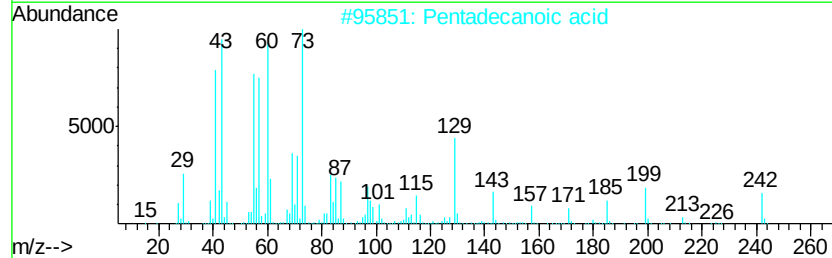
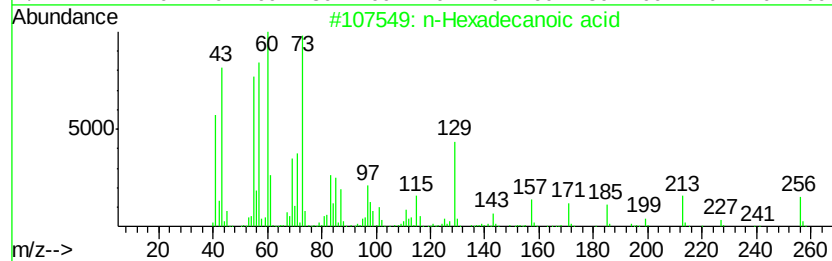
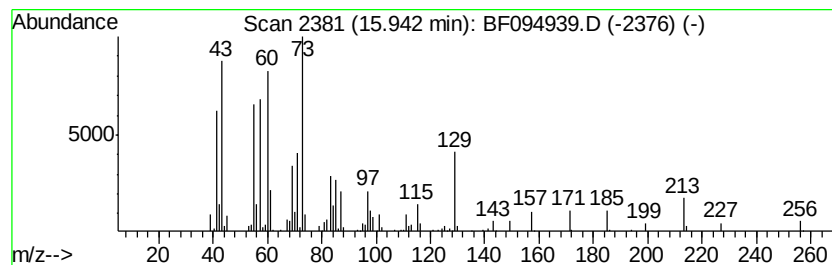
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.		
15.94	8.56 ng	337764	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	94
3		Tridecanoic acid	214	C13H26O2	000638-53-9	93
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	86
5		n-Decanoic acid	172	C10H20O2	000334-48-5	68



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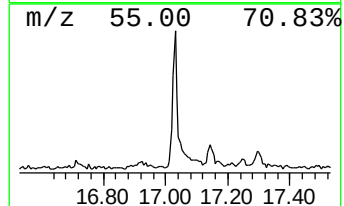
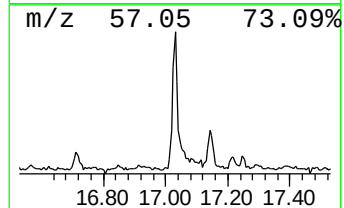
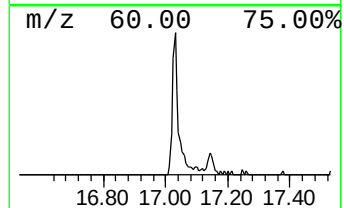
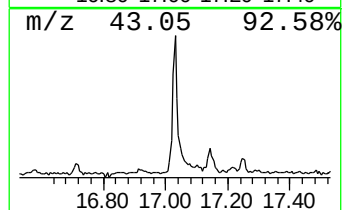
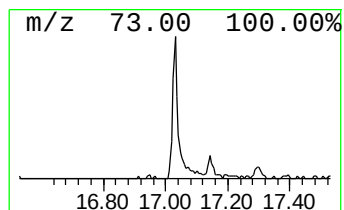
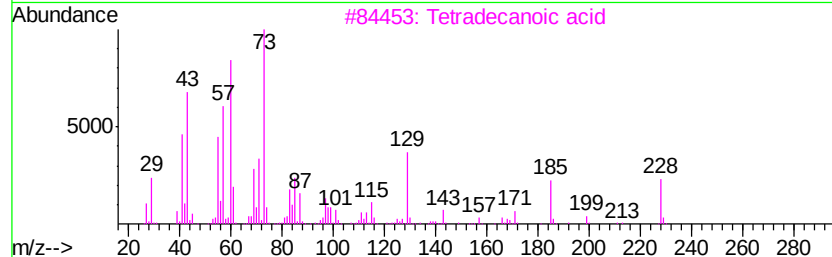
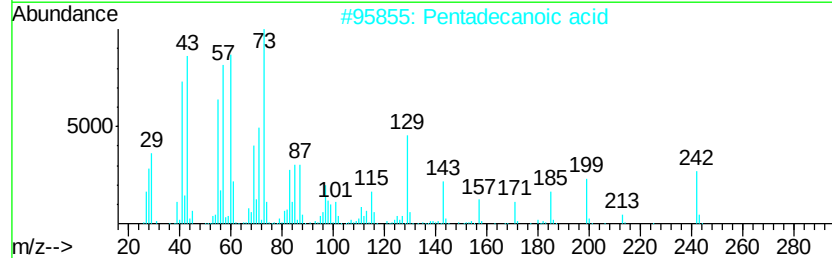
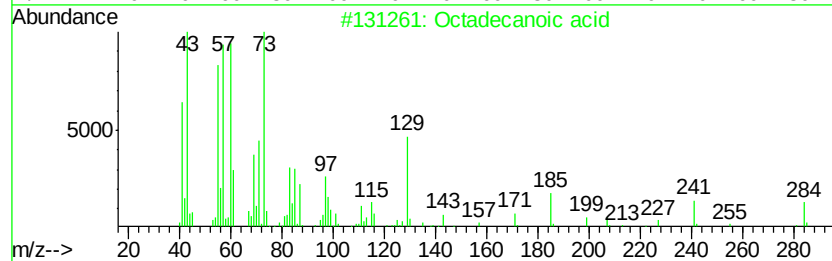
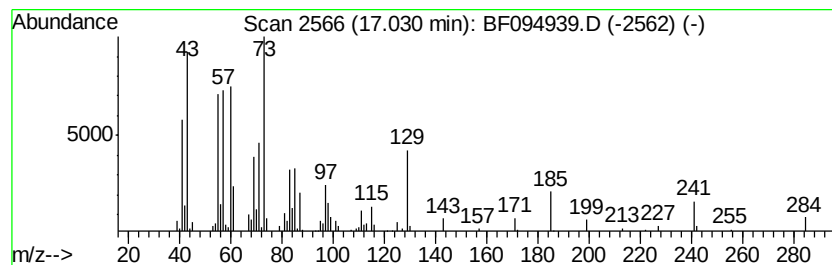
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
17.03	6.15 ng	242049	Chrysene-d12		18.64
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	n-Decanoic acid	172	C10H20O2	000334-48-5	49
5	n-PROPYL NONYL ETHER	186	C12H26O	1000130-69-3	25



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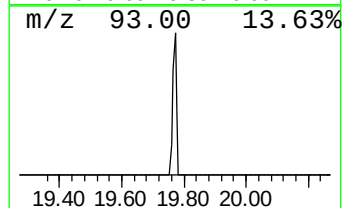
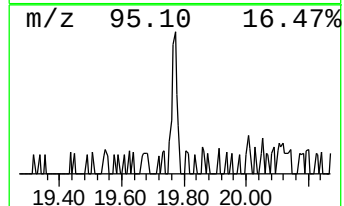
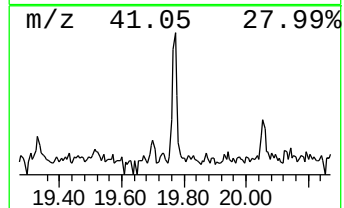
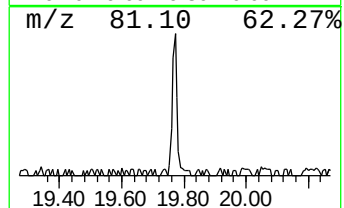
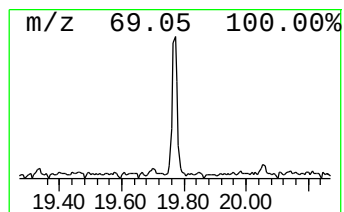
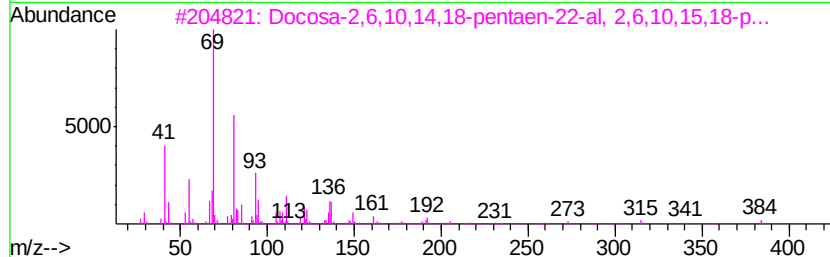
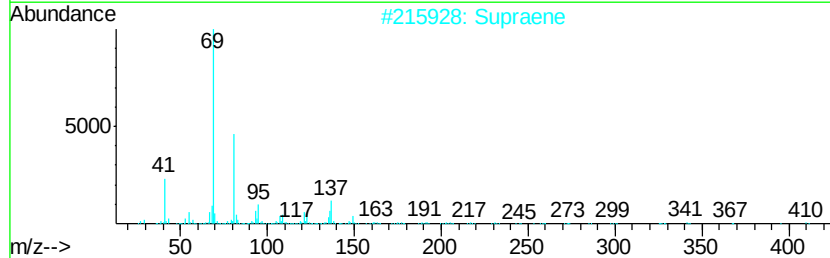
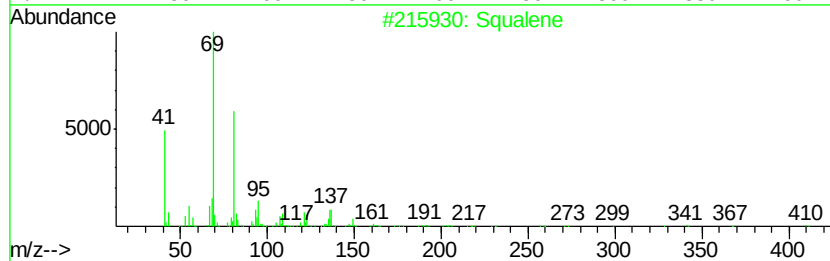
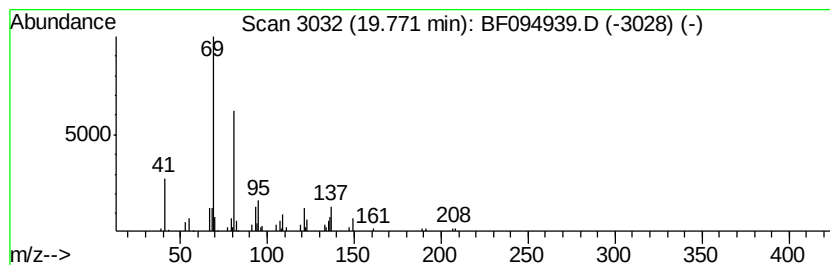
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.77	2.18 ng	65760	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	86
3		Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	78
4		trans-Farnesol	222	C15H26O	000106-28-5	64
5		2-Octene, 2-methyl-6-methylene-	138	C10H18	010054-09-8	53



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.05	17.7	ng	503816	1	7.72	567983	20.0
unknown7.38	7.38	114.6	ng	3255790	1	7.72	567983	20.0
n-Hexadecanoic acid	15.94	8.6	ng	337764	4	14.97	789486	20.0
Octadecanoic acid	17.03	6.2	ng	242049	5	18.64	787399	20.0
Squalene	19.77	2.2	ng	65760	6	20.31	602326	20.0