

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050617\
 Data File : BF094974.D
 Acq On : 8 May 2017 7:50
 Operator : SJ/MA
 Sample : I2947-20
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-07-0-2.0

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	5.037	523	527	547	rBV	128369	249912	10.68%	1.173%
2	5.666	630	634	668	rBV	1328530	2057936	87.97%	9.658%
3	7.260	900	905	921	rBV	1519445	2090027	89.34%	9.808%
4	7.384	921	926	935	rVB	1692287	2339464	100.00%	10.979%
5	7.719	979	983	997	rVB	532646	615556	26.31%	2.889%
6	7.960	1019	1024	1035	rBV	1526149	1816223	77.63%	8.523%
7	8.619	1131	1136	1153	rBV	1103843	1429299	61.10%	6.708%
8	9.736	1322	1326	1340	rBV	620045	834292	35.66%	3.915%
9	11.513	1623	1628	1646	rBV	1781474	2237884	95.66%	10.502%
10	12.201	1741	1745	1759	rBV	296878	397011	16.97%	1.863%
11	12.572	1802	1808	1823	rBV2	580585	858899	36.71%	4.031%
12	13.413	1946	1951	1957	rBV	40674	44872	1.92%	0.211%
13	13.860	2023	2027	2043	rBV	816338	1266346	54.13%	5.943%
14	14.183	2078	2082	2086	rBV	39798	49683	2.12%	0.233%
15	14.918	2203	2207	2211	rBV2	21728	27137	1.16%	0.127%
16	14.971	2211	2216	2221	rBV	586034	767619	32.81%	3.602%
17	15.936	2376	2380	2391	rVB	77131	103200	4.41%	0.484%
18	16.754	2515	2519	2527	rBV	96883	116975	5.00%	0.549%
19	17.012	2559	2563	2567	rBV	112299	148557	6.35%	0.697%
20	17.054	2567	2570	2576	rVB	109859	124644	5.33%	0.585%
21	17.142	2581	2585	2590	rVB	110206	105740	4.52%	0.496%
22	17.189	2590	2593	2596	rBV	47867	50189	2.15%	0.236%
23	17.295	2606	2611	2619	rBV	1485273	1611514	68.88%	7.563%
24	18.065	2737	2742	2746	rBV2	70895	70912	3.03%	0.333%
25	18.636	2826	2839	2843	rBV	585346	773099	33.05%	3.628%
26	18.671	2843	2845	2858	rVB3	61517	102085	4.36%	0.479%
27	18.948	2884	2892	2899	rBV5	12731	25442	1.09%	0.119%
28	19.906	3050	3055	3058	rBV	60533	101181	4.32%	0.475%
29	20.053	3077	3080	3085	rVB4	25025	26805	1.15%	0.126%
30	20.189	3099	3103	3108	rBV	38393	50537	2.16%	0.237%
31	20.247	3110	3113	3118	rBV	51379	61000	2.61%	0.286%
32	20.300	3118	3122	3136	rVB	508604	624650	26.70%	2.931%
33	20.777	3199	3203	3209	rVB6	22563	34569	1.48%	0.162%
34	21.612	3341	3345	3352	rVV3	17400	33051	1.41%	0.155%

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35	21.989	3406	3409	3420	rVB2	14688	35062	1.50%	0.165%
36	23.741	3705	3707	3716	rVB8	15663	27270	1.17%	0.128%

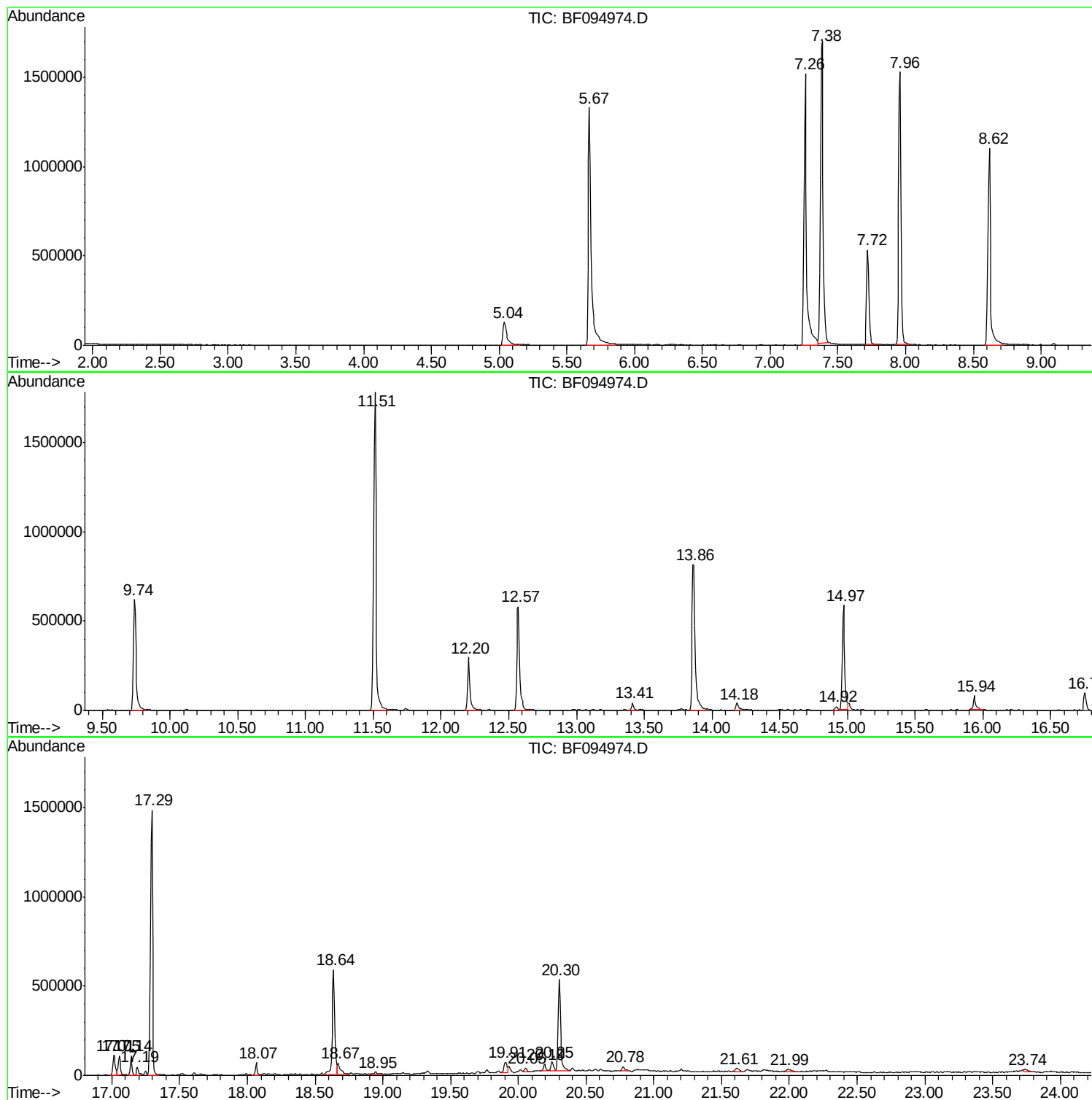
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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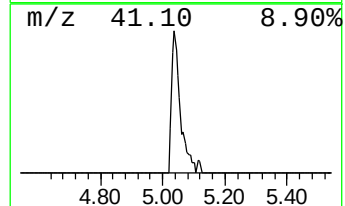
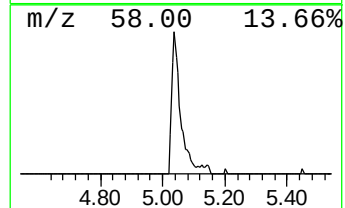
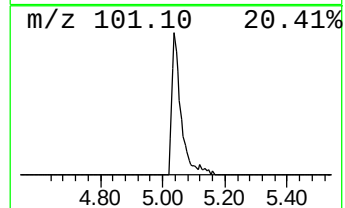
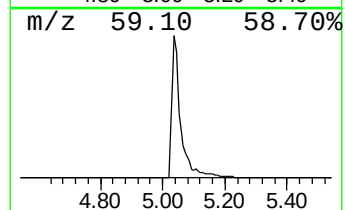
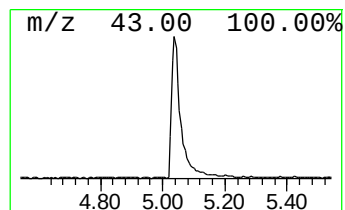
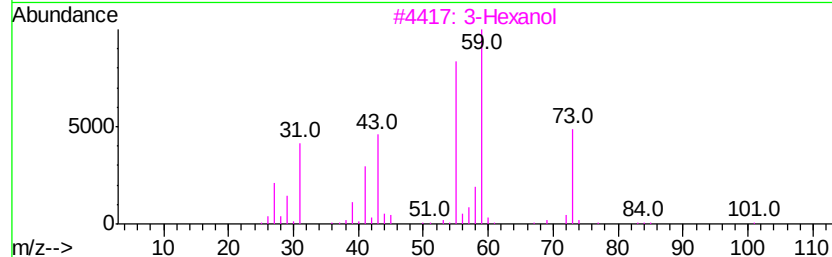
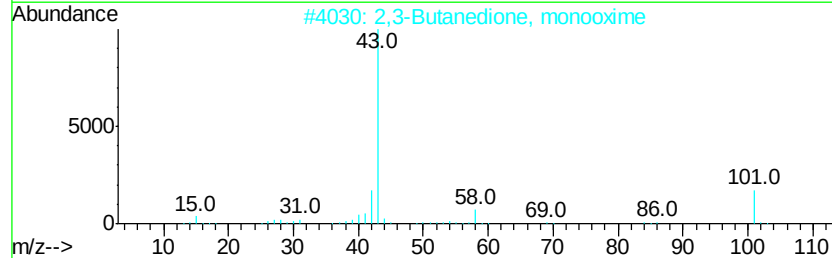
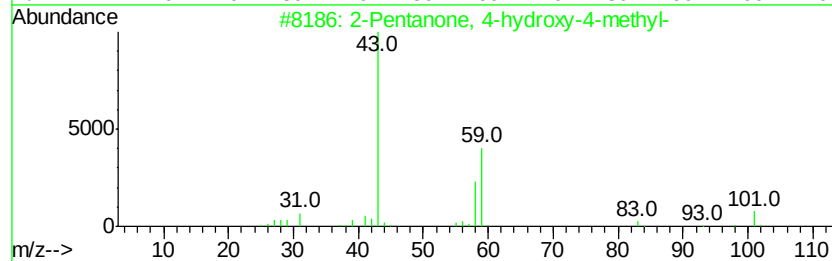
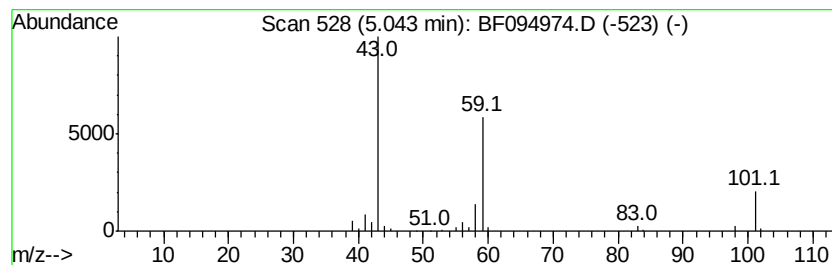
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.04	8.12 ng	249912	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	56
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
3			3-Hexanol	102	C6H14O	000623-37-0	28
4			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
5			Propanamide, N-ethyl-	101	C5H11NO	005129-72-6	9



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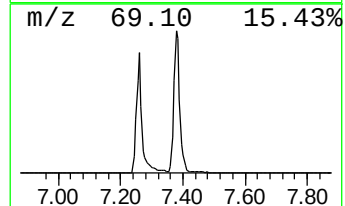
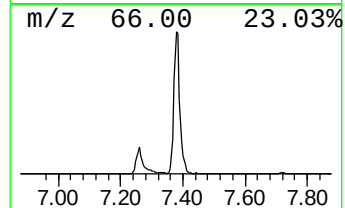
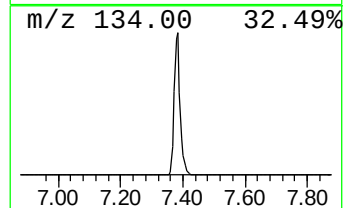
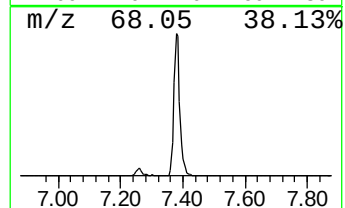
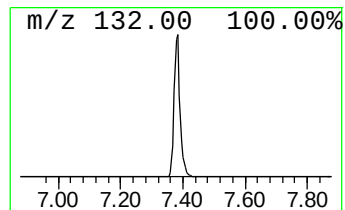
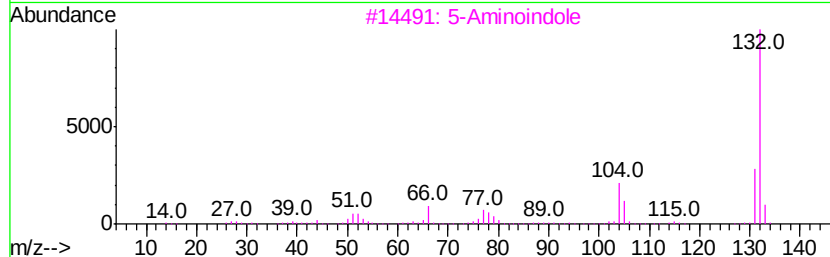
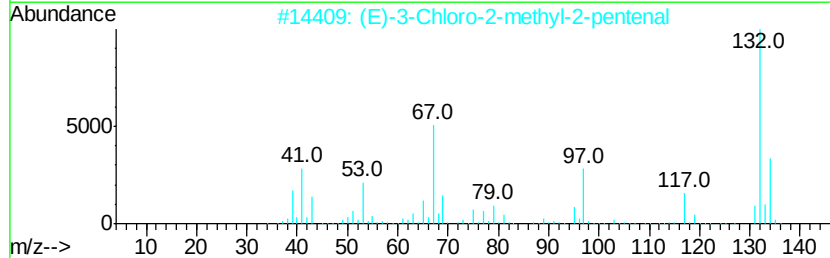
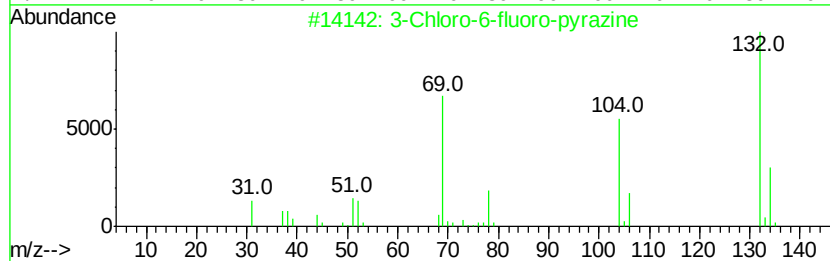
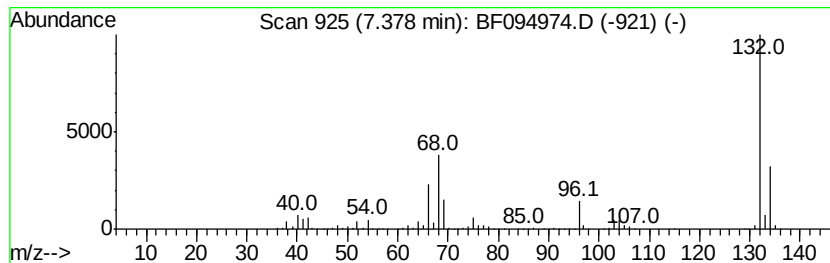
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Peak Number 2 unknown7.38 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.38	76.01 ng	2339460	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	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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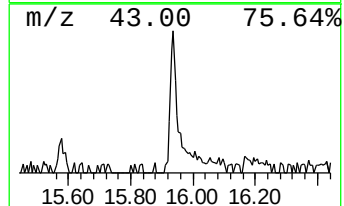
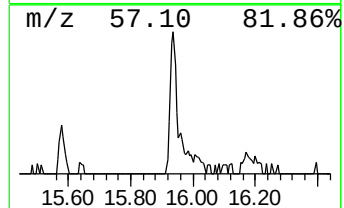
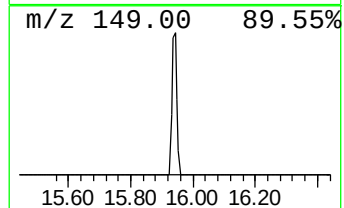
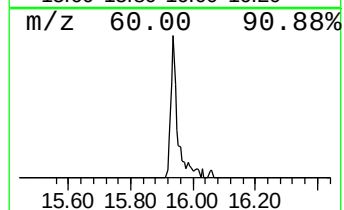
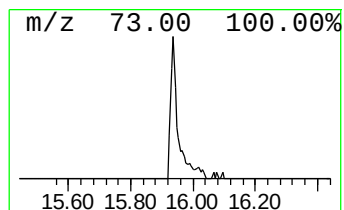
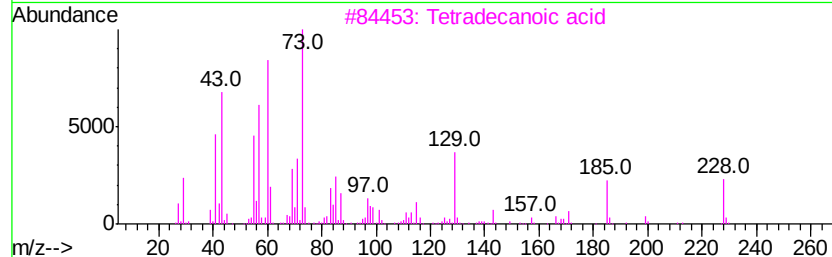
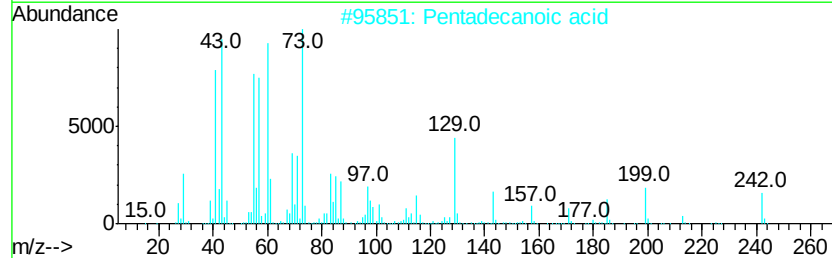
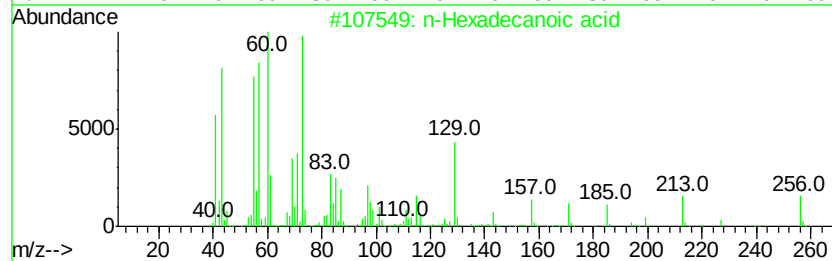
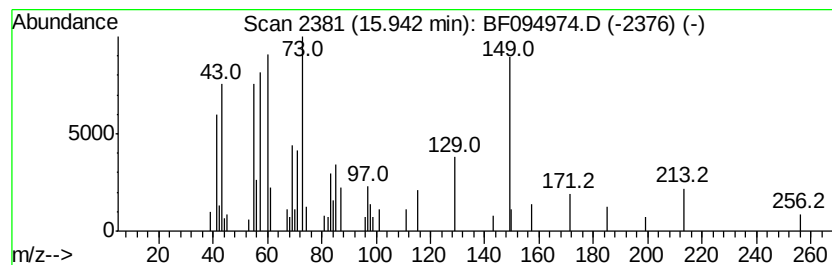
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.94	2.69 ng	103200	Phenanthrene-d10	14.97	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	58
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
4	Tridecanoic acid	214	C13H26O2	000638-53-9	53
5	Dodecanoic acid	200	C12H24O2	000143-07-7	53



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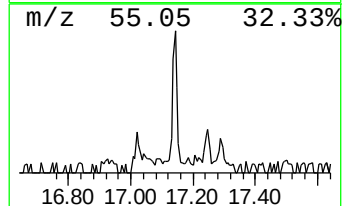
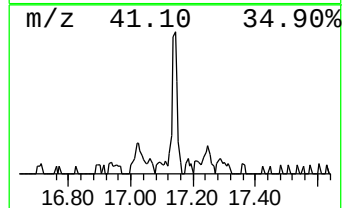
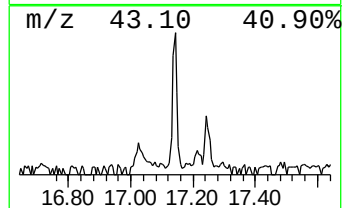
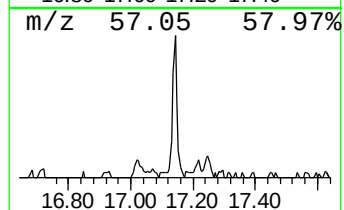
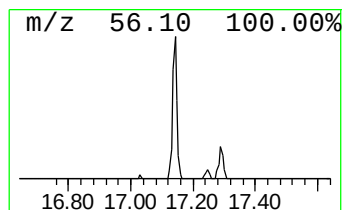
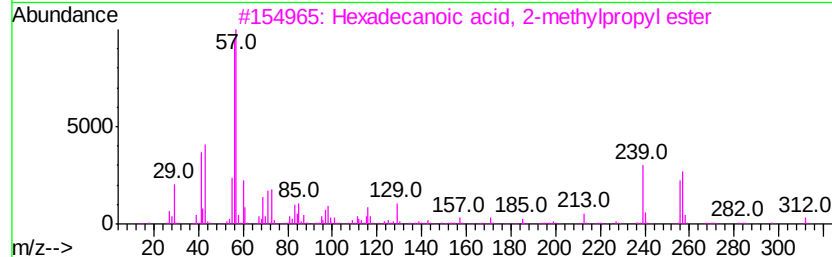
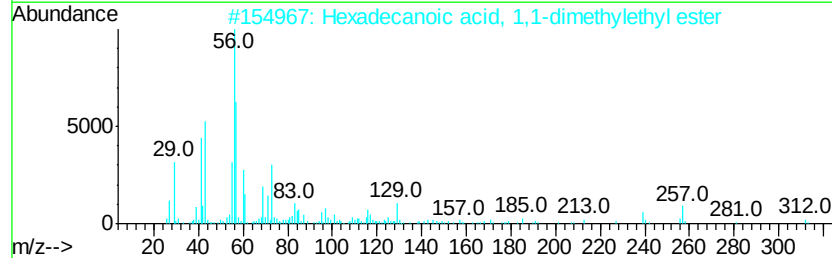
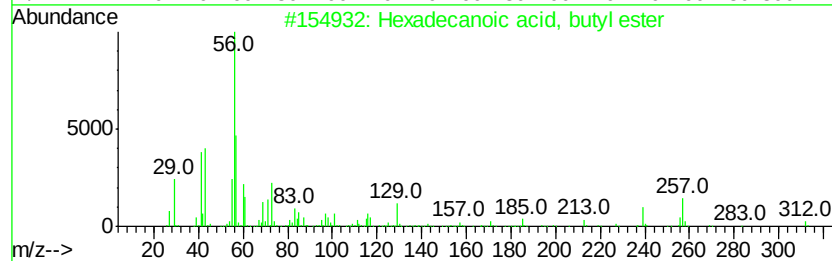
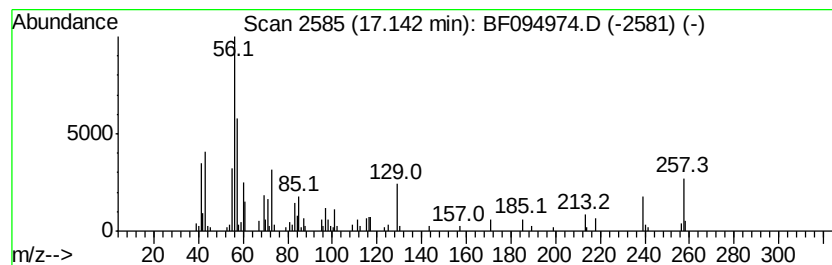
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Hexadecanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.14	2.74 ng	105740	Chrysene-d12	18.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	74
3		Hexadecanoic acid, 2-methylpropyl...	312	C20H40O2	000110-34-9	72
4		Nipecotic acid	129	C6H11NO2	000498-95-3	47
5		Cyclopropane, 1-(1-methylethyl)-...	210	C15H30	041977-39-3	35



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.04	8.1	ng	249912	1	7.72	615556	20.0
unknown7.38	7.38	76.0	ng	2339460	1	7.72	615556	20.0
n-Hexadecanoic acid	15.94	2.7	ng	103200	4	14.97	767619	20.0
Hexadecanoic acid...	17.14	2.7	ng	105740	5	18.64	773099	20.0