

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051017\
 Data File : BF095075.D
 Acq On : 11 May 2017 1:26
 Operator : SJ/MA
 Sample : I3046-06
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-12-COMP

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	5.013	519	523	541	rBV	88004	188131	7.92%	0.961%
2	5.648	627	631	664	rBV	1092637	2084711	87.78%	10.651%
3	7.248	899	903	919	rBV	1197288	2009943	84.63%	10.269%
4	7.366	919	923	935	rVV	1573492	2374844	100.00%	12.133%
5	7.460	937	939	944	rVB2	17636	24019	1.01%	0.123%
6	7.707	976	981	994	rVB	436940	525781	22.14%	2.686%
7	7.942	1016	1021	1036	rBV	1471810	1689487	71.14%	8.631%
8	8.607	1129	1134	1152	rBV	846499	1244146	52.39%	6.356%
9	9.724	1320	1324	1337	rBV	487318	707757	29.80%	3.616%
10	11.501	1620	1626	1643	rBV	2004894	2335593	98.35%	11.932%
11	12.195	1739	1744	1755	rBV	299053	402635	16.95%	2.057%
12	12.554	1801	1805	1816	rBV2	485887	685710	28.87%	3.503%
13	13.395	1944	1948	1955	rVB2	22676	27236	1.15%	0.139%
14	13.854	2021	2026	2041	rBV	789001	1200175	50.54%	6.132%
15	14.171	2075	2080	2083	rBV	23357	30621	1.29%	0.156%
16	14.959	2209	2214	2228	rBV	477487	665568	28.03%	3.400%
17	15.924	2372	2378	2386	rBV2	95423	126631	5.33%	0.647%
18	16.747	2513	2518	2524	rBV	27836	36399	1.53%	0.186%
19	17.012	2559	2563	2566	rBV2	28378	38124	1.61%	0.195%
20	17.047	2566	2569	2579	rVV	40218	60530	2.55%	0.309%
21	17.130	2579	2583	2587	rVV	24001	25763	1.08%	0.132%
22	17.283	2604	2609	2619	rBV	1545160	1633604	68.79%	8.346%
23	18.536	2817	2822	2833	rBV5	22732	58025	2.44%	0.296%
24	18.630	2833	2838	2846	rBV	462074	578637	24.37%	2.956%
25	19.500	2982	2986	2992	rVB	57615	63473	2.67%	0.324%
26	19.753	3025	3029	3037	rBV	34473	44288	1.86%	0.226%
27	19.900	3050	3054	3057	rBV	28522	37643	1.59%	0.192%
28	20.247	3109	3113	3117	rBV	28997	38660	1.63%	0.198%
29	20.294	3117	3121	3133	rVV2	434840	574203	24.18%	2.934%
30	20.759	3195	3200	3205	rBV6	16375	31712	1.34%	0.162%
31	21.612	3341	3345	3351	rBV5	16601	29692	1.25%	0.152%

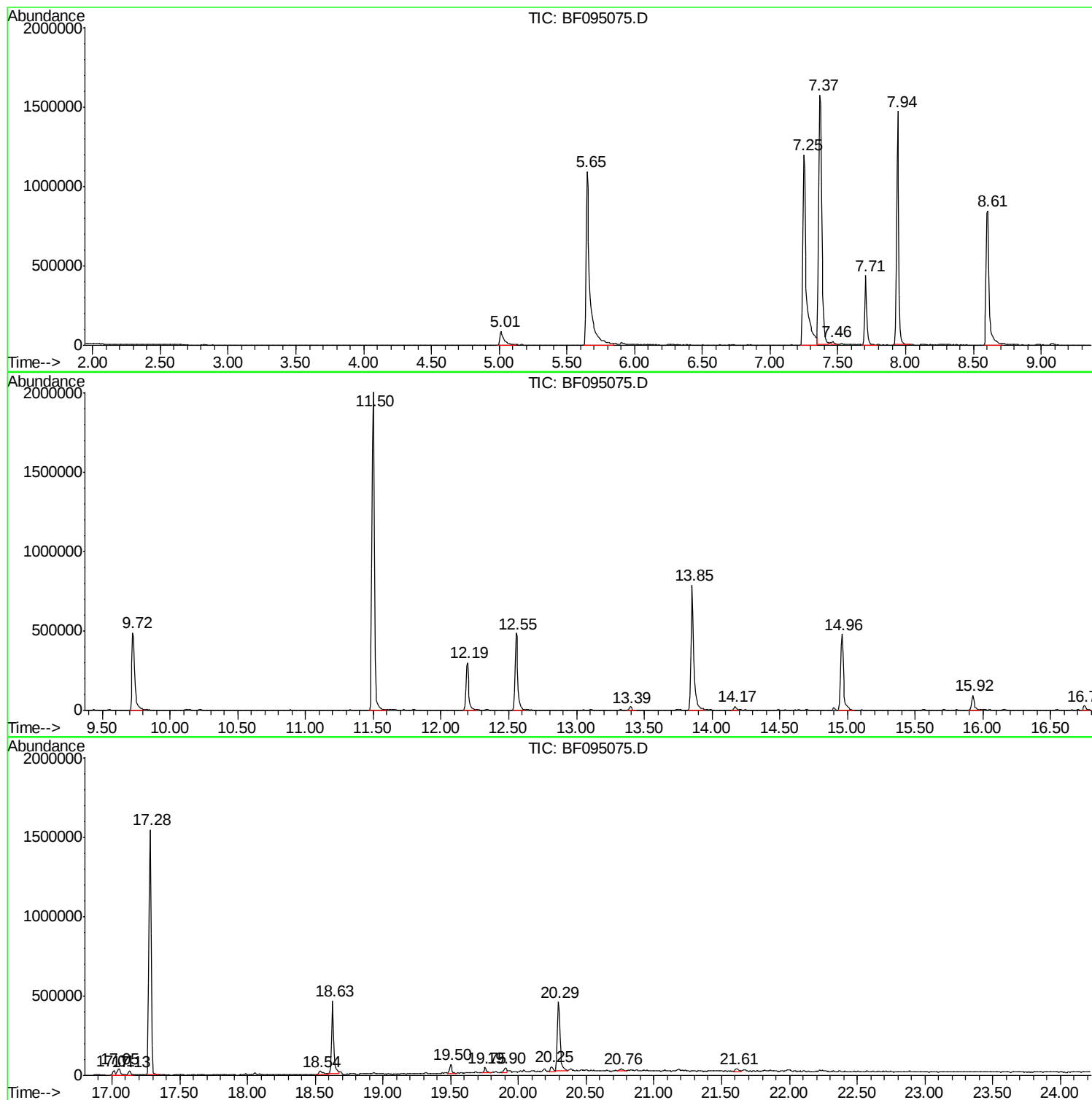
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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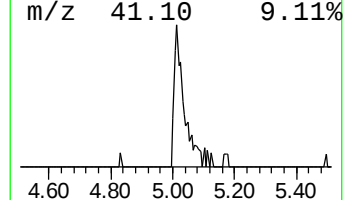
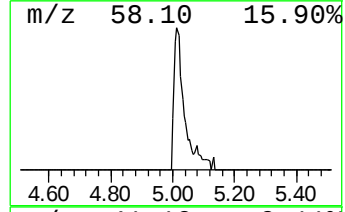
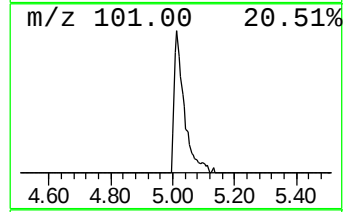
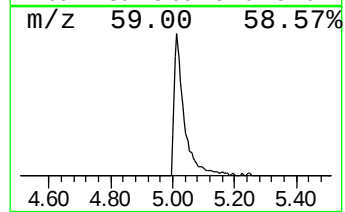
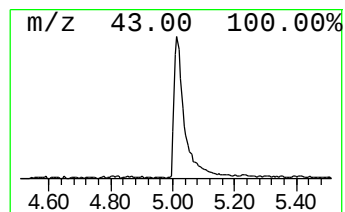
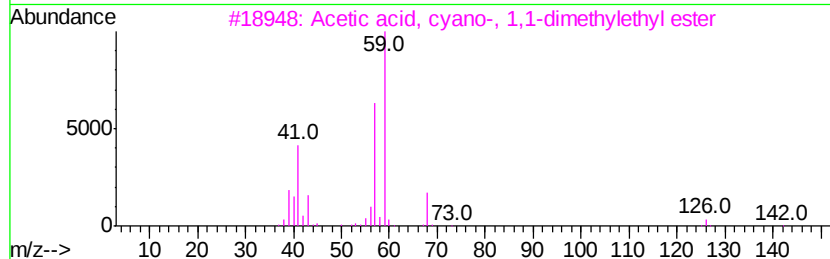
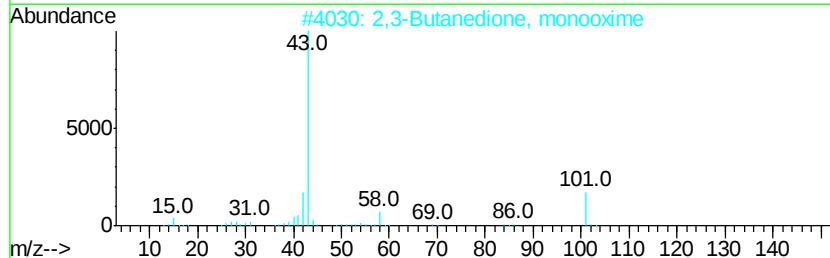
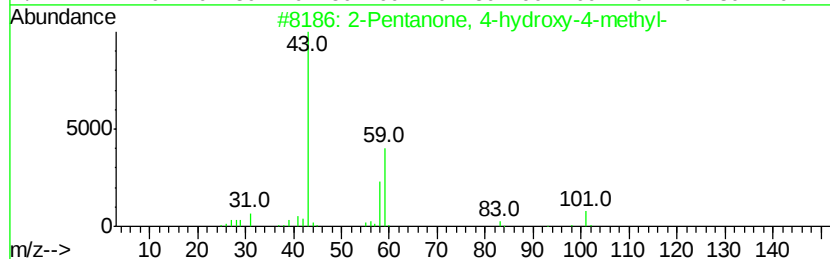
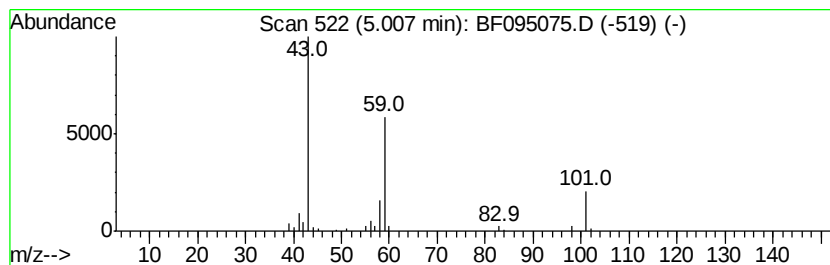
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.01	7.16 ng	188131	1,4-Dichlorobenzene-d4	7.71

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	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17		
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9		
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9		



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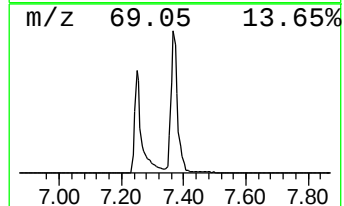
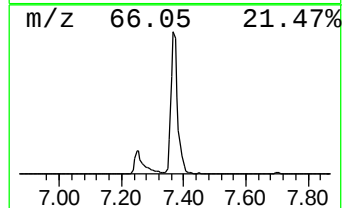
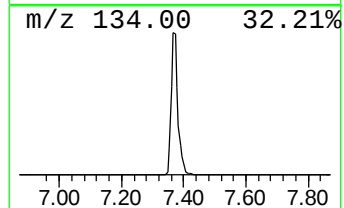
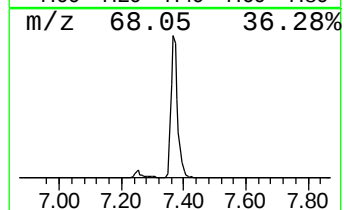
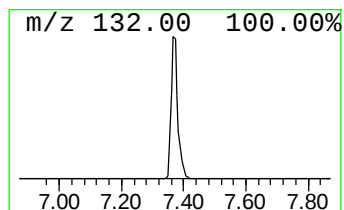
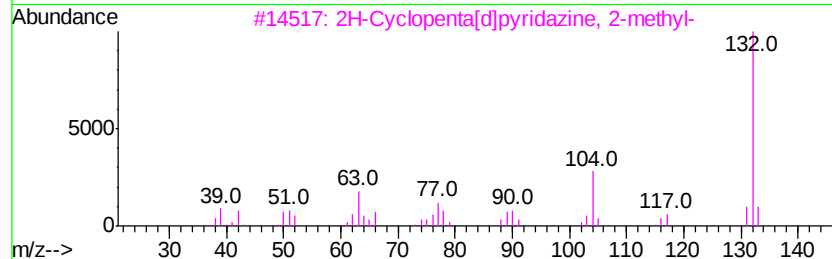
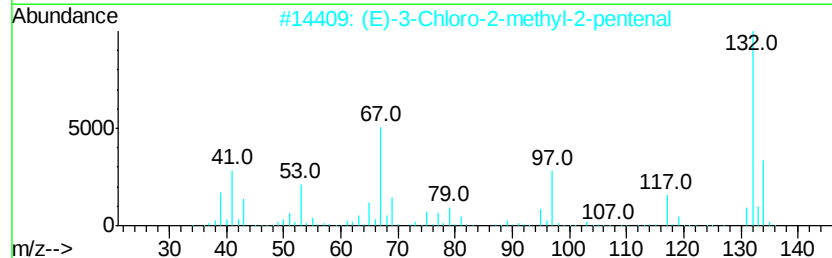
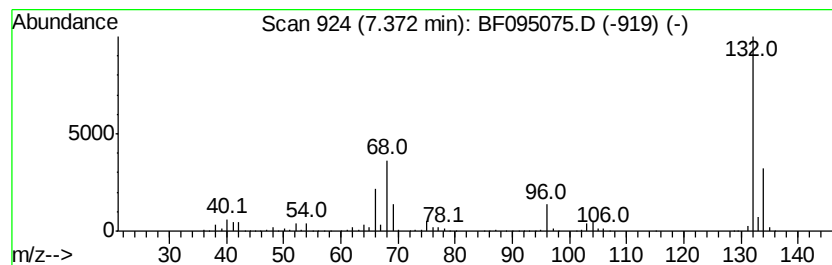
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Peak Number 2 unknown7.37 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.37	90.34 ng	2374840	1,4-Dichlorobenzene-d4	7.71

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		2H-Cyclopentaf[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9



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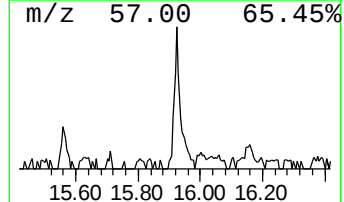
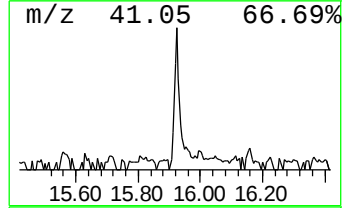
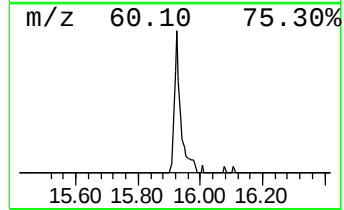
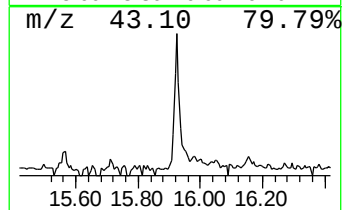
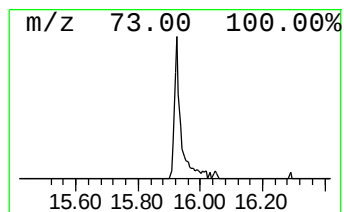
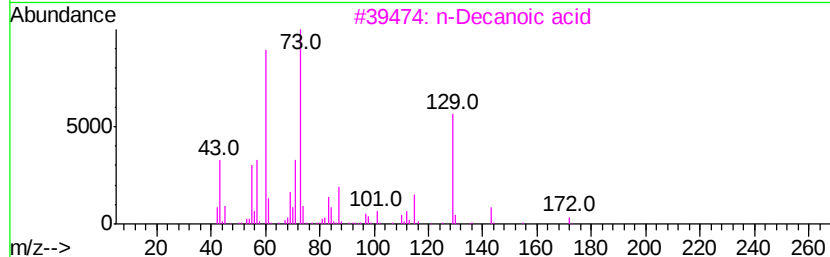
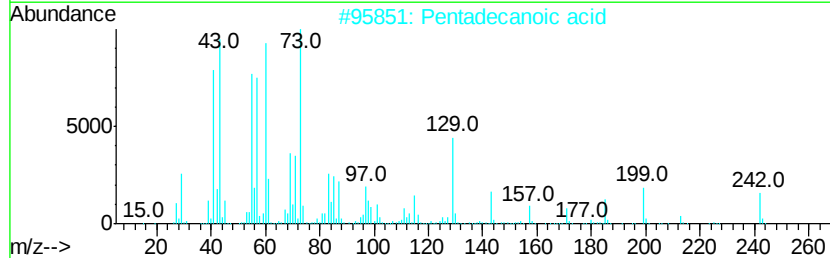
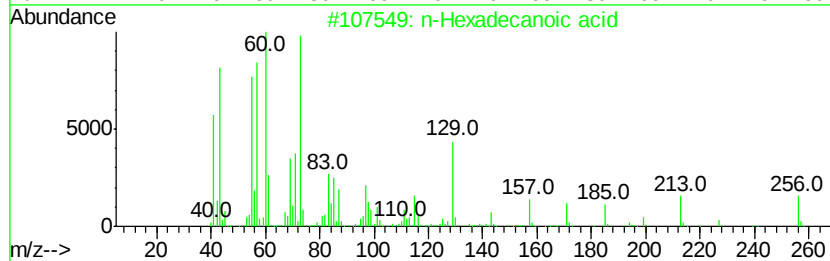
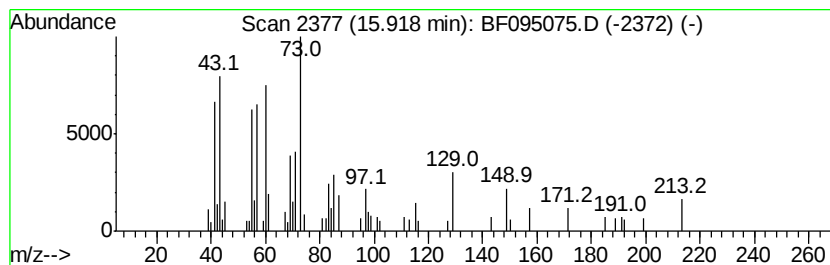
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.92	3.81 ng	126631	Phenanthrene-d10	14.96

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	81
3		n-Decanoic acid	172	C10H20O2	000334-48-5	43
4		Oxalic acid, dodecyl propyl ester	300	C17H32O4	1000309-26-5	20
5		N-Cyclooct-4-enylacetamide	167	C10H17NO	170952-69-9	18



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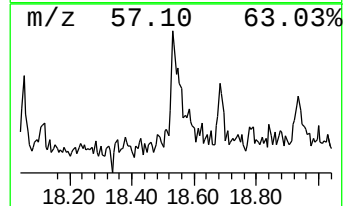
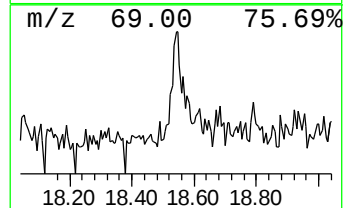
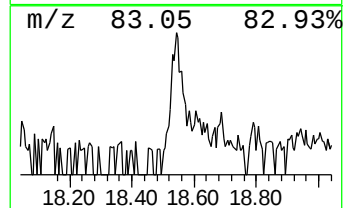
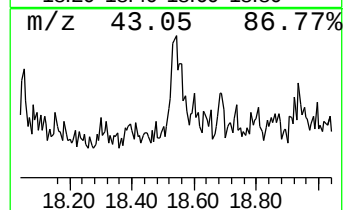
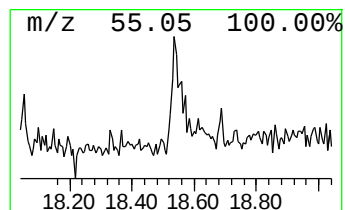
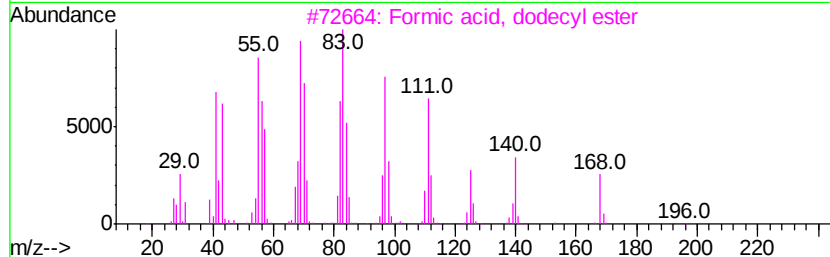
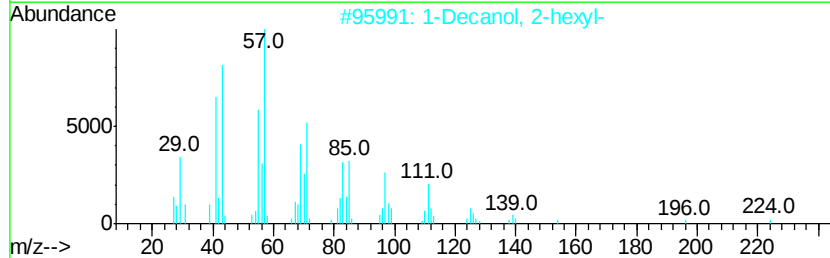
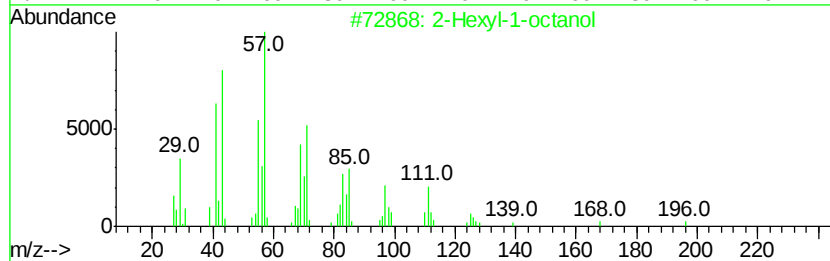
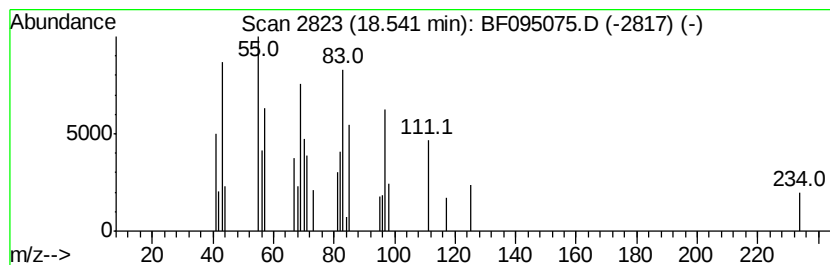
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 2-Hexyl-1-octanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.54	2.01 ng	58025	Chrysene-d12	18.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Hexyl-1-octanol	214	C14H30O	019780-79-1	53
2		1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	50
3		Formic acid, dodecyl ester	214	C13H26O2	028303-42-6	49
4		Acetic acid, trifluoro-, dodecyl...	282	C14H25F3O2	006222-00-0	47
5		Trichloroacetic acid, dodecyl ester	330	C14H25Cl3O2	074339-50-7	43



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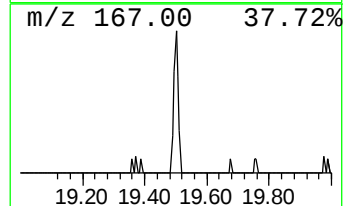
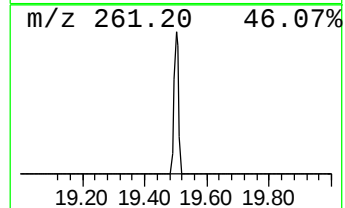
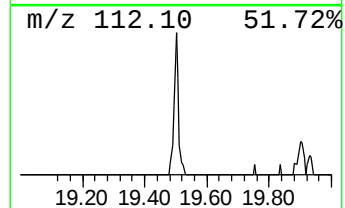
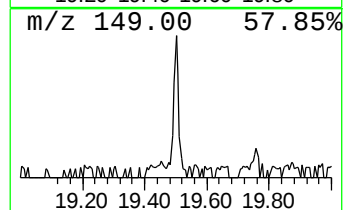
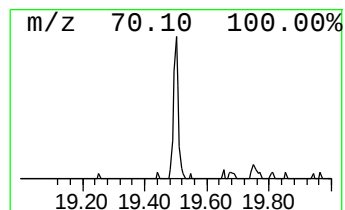
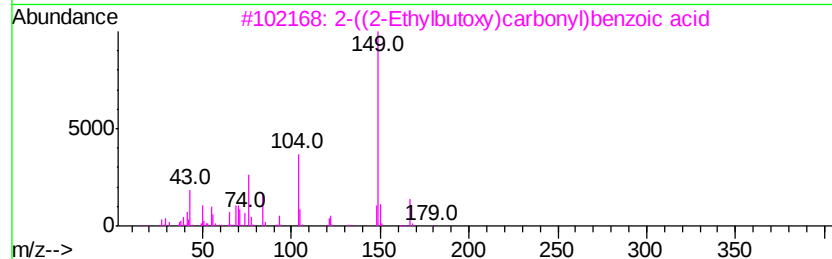
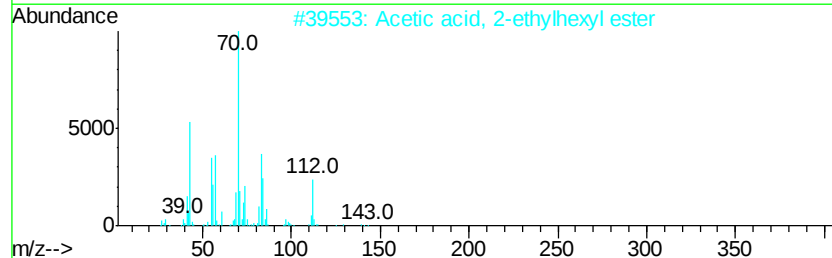
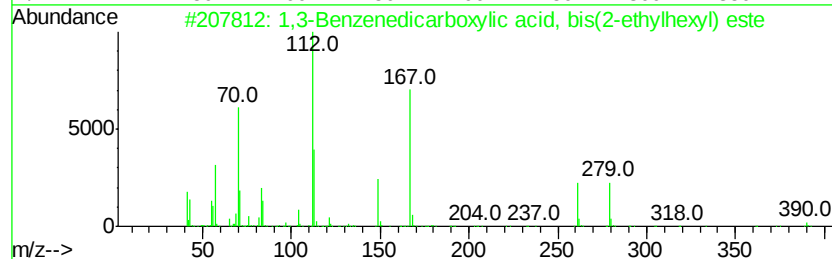
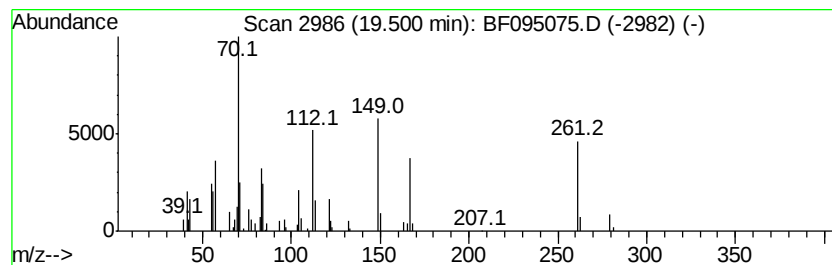
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Peak Number 7 1,3-Benzenedicarboxylic aci... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.50	2.21 ng	63473	Perylene-d12	20.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	59
2		Acetic acid, 2-ethylhexyl ester	172	C10H20O2	000103-09-3	38
3		2-((2-Ethylbutoxy)carbonyl)benzo...	250	C14H18O4	1000373-62-8	22
4		Bromoacetic acid, 2-ethylhexyl e...	250	C10H19BrO2	068144-73-0	22
5		4-Nitrobenzoic acid, cyclobutyl ...	221	C11H11NO4	070335-00-1	16



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.01	7.2	ng	188131	1	7.71	525781	20.0
unknown7.37	7.37	90.3	ng	2374840	1	7.71	525781	20.0
n-Hexadecanoic acid	15.92	3.8	ng	126631	4	14.96	665568	20.0
2-Hexyl-1-octanol	18.54	2.0	ng	58025	5	18.63	578637	20.0
1,3-Benzenedicarb...	19.50	2.2	ng	63473	6	20.29	574203	20.0