

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102315\
 Data File : BF082503.D
 Acq On : 24 Oct 2015 10:07
 Operator : UM/IZ
 Sample : G4116-17
 Misc :
 ALS Vial : 32 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 AB-AC-01(0-2)

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-BF101015.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	4.926	240	244	254	rVB	847493	1378510	54.70%	6.212%
2	5.360	279	282	296	rBV	2163808	2223613	88.23%	10.021%
3	5.749	314	316	321	rVB	30725	29163	1.16%	0.131%
4	6.412	371	374	376	rBV	2032919	2208753	87.64%	9.954%
5	6.526	382	384	387	rBV	2416410	2245580	89.10%	10.120%
6	6.755	402	404	406	rBV	628488	554384	22.00%	2.498%
7	6.915	415	418	420	rBV	1506112	1873796	74.35%	8.444%
8	7.326	451	454	457	rBV	1242469	1315847	52.21%	5.930%
9	8.046	514	517	519	rBV	686349	711335	28.22%	3.206%
10	9.120	609	611	614	rBV	2030009	2520258	100.00%	11.357%
11	9.520	644	646	649	rBV	451503	388853	15.43%	1.752%
12	9.795	668	670	673	rBV	664142	805029	31.94%	3.628%
13	10.229	704	708	710	rBV2	80428	103206	4.10%	0.465%
14	10.595	737	740	742	rBV	1336639	1282994	50.91%	5.782%
15	10.698	748	749	756	rVB	47774	70606	2.80%	0.318%
16	11.155	787	789	790	rBV	33634	43457	1.72%	0.196%
17	11.292	798	801	803	rBV	572861	722597	28.67%	3.256%
18	11.578	824	826	832	rVB	29003	31916	1.27%	0.144%
19	11.738	838	840	843	rBV	66182	67143	2.66%	0.303%
20	11.818	845	847	853	rBV	55876	67856	2.69%	0.306%
21	12.698	922	924	926	rBV	104872	92624	3.68%	0.417%
22	12.881	937	940	942	rBV	1816901	1876720	74.47%	8.457%
23	13.407	984	986	988	rBV	75597	65034	2.58%	0.293%
24	13.818	1017	1022	1028	rBV2	54269	148359	5.89%	0.669%
25	13.955	1031	1034	1036	rBV	474627	614789	24.39%	2.770%
26	14.447	1074	1077	1079	rBV2	26174	44798	1.78%	0.202%
27	15.098	1132	1134	1137	rVB	22352	25578	1.01%	0.115%
28	15.430	1160	1163	1170	rBV	469214	610441	24.22%	2.751%
29	15.864	1198	1201	1205	rBV2	18325	34639	1.37%	0.156%
30	16.870	1286	1289	1293	rVB2	13888	32728	1.30%	0.147%

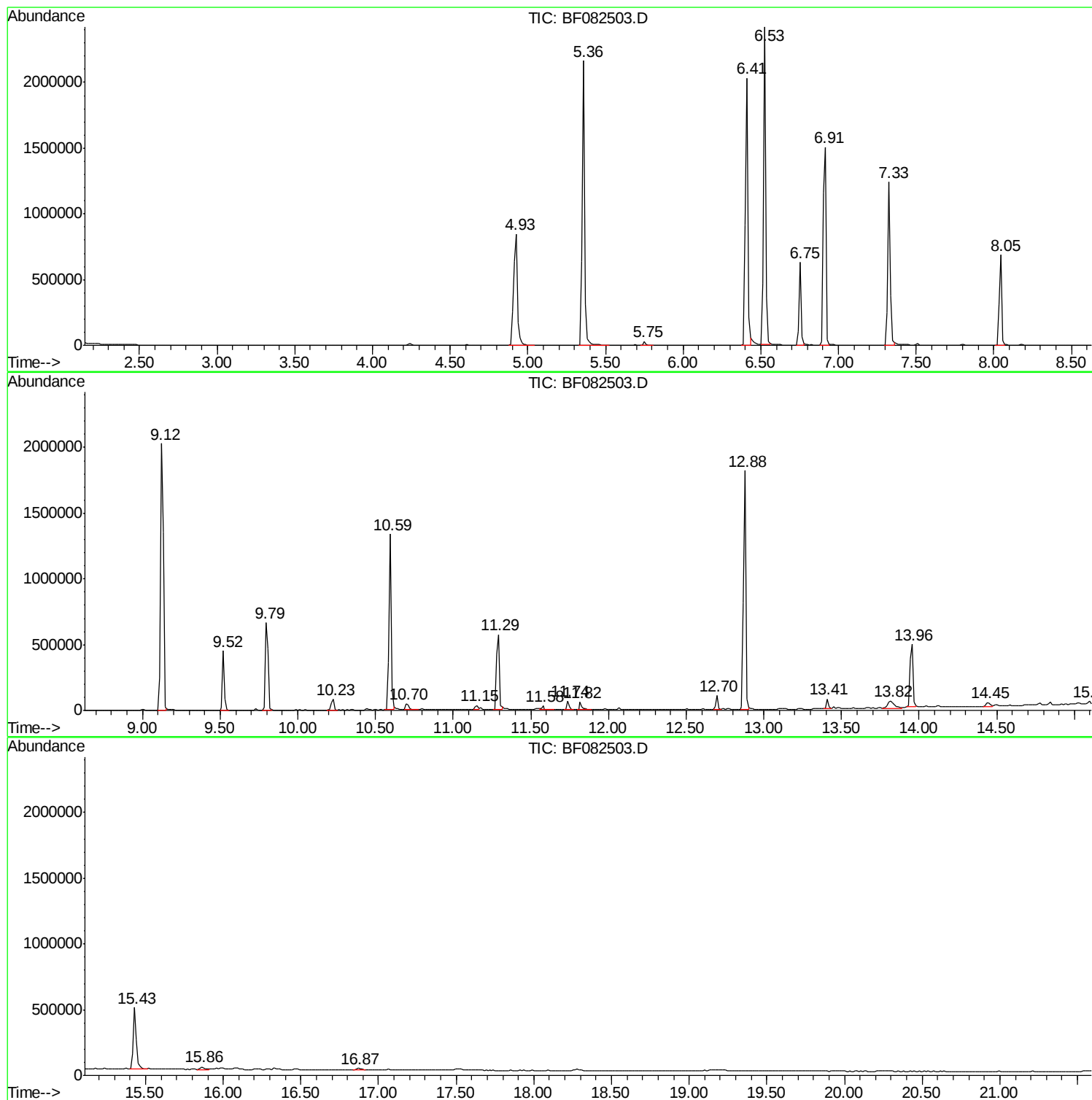
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AB-AC-01(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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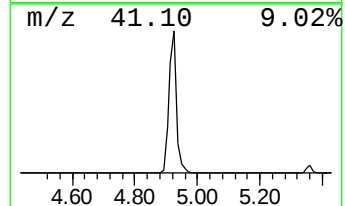
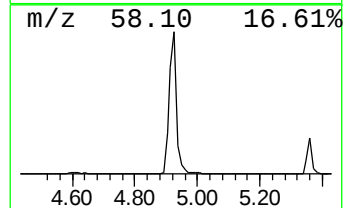
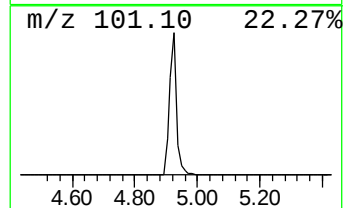
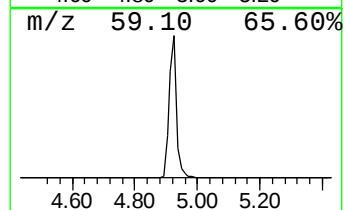
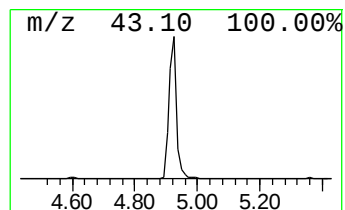
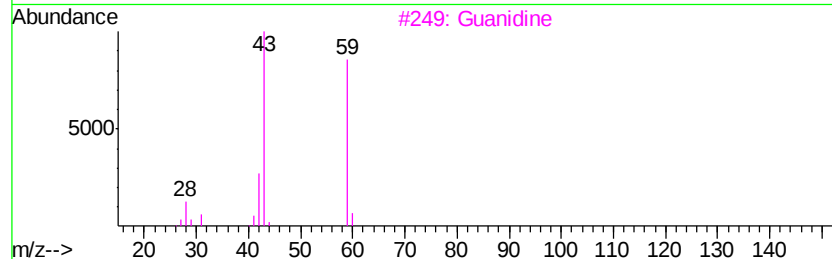
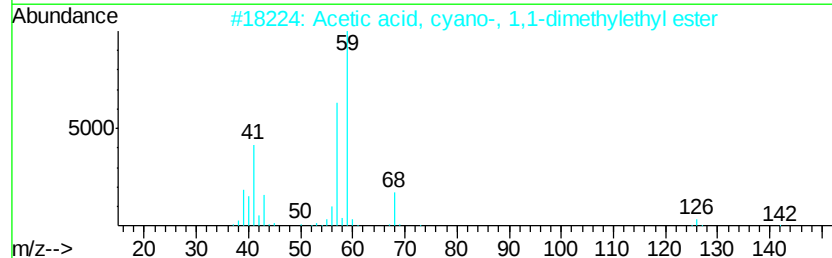
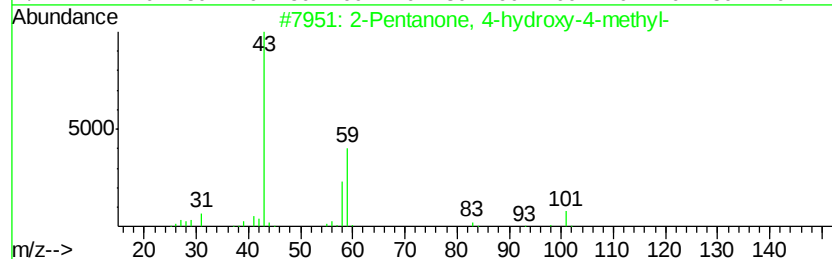
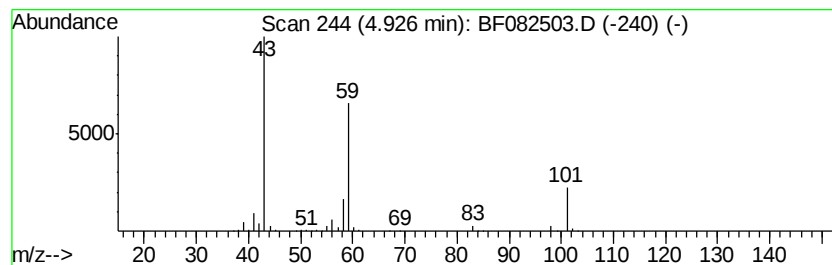
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.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.
4.93	49.73 ng	1378510	1,4-Dichlorobenzene-d4	6.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3		Guanidine	59	CH5N3	000113-00-8	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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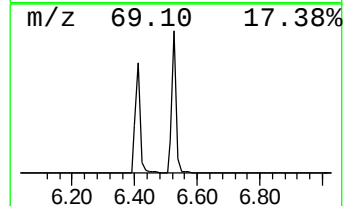
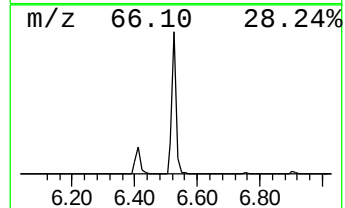
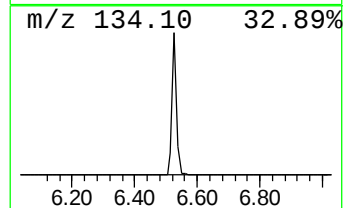
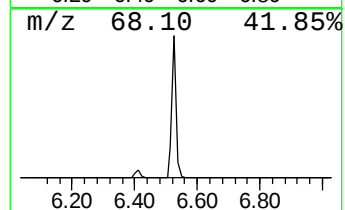
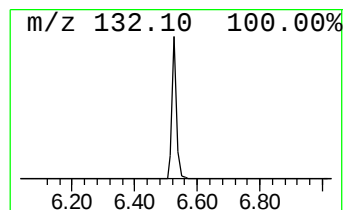
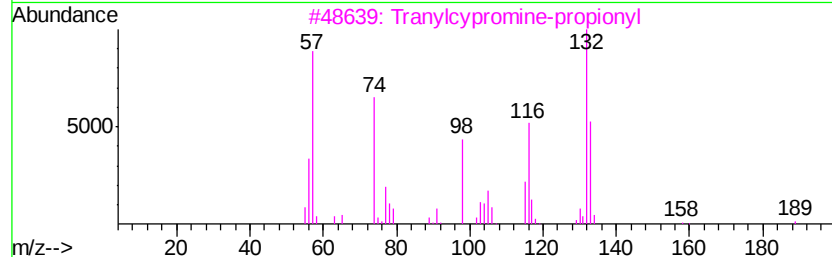
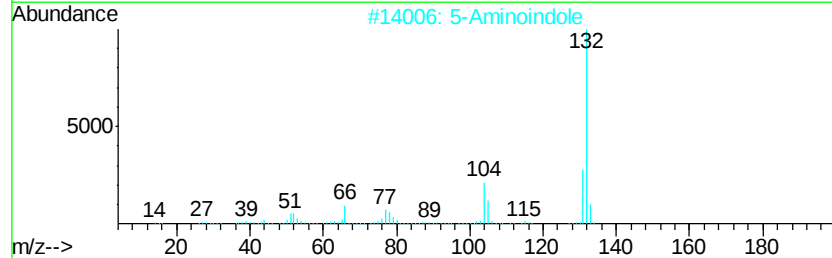
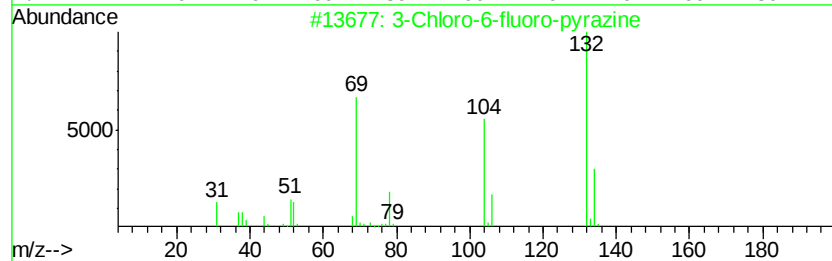
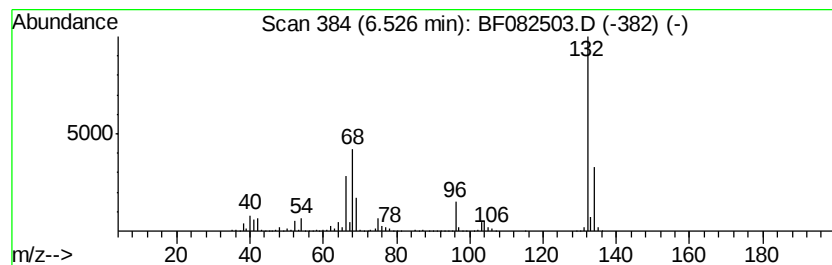
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Peak Number 2 unknown6.53 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.53	81.01 ng	2245580	1,4-Dichlorobenzene-d4	6.75

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			5-Aminoindole	132	C8H8N2	005192-03-0	12
3			Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4			Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9
5			(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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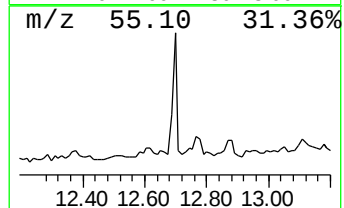
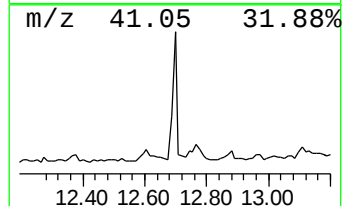
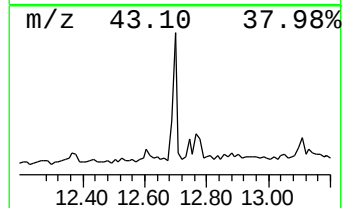
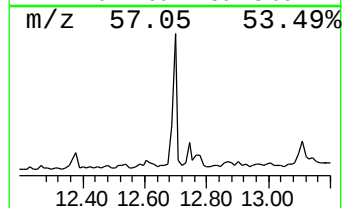
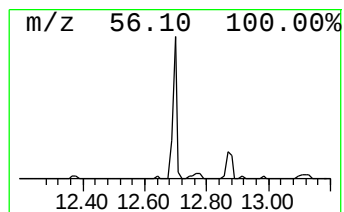
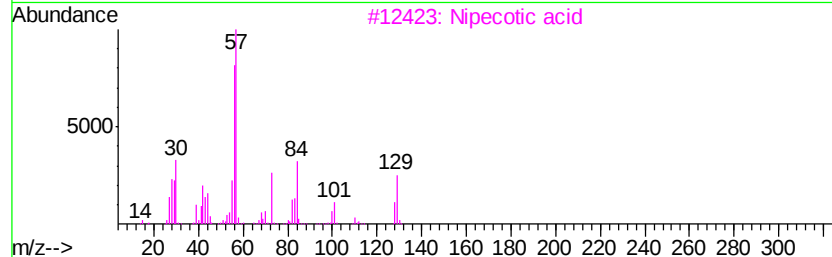
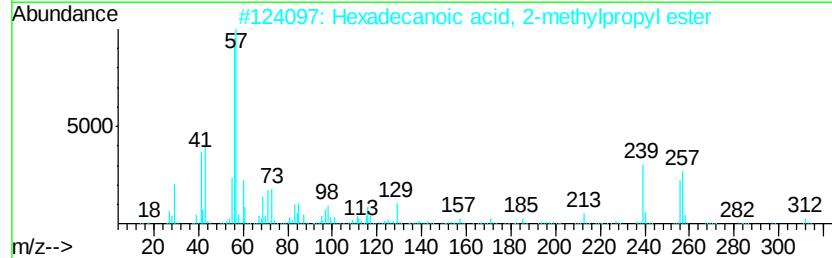
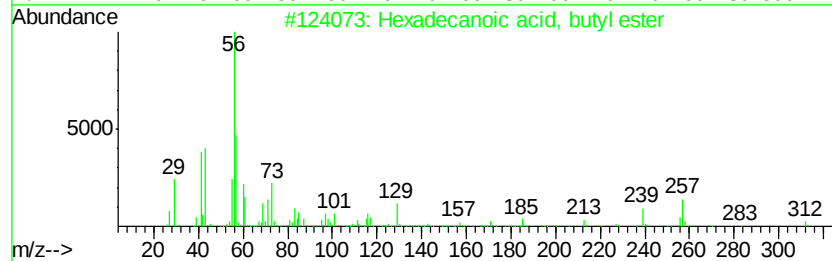
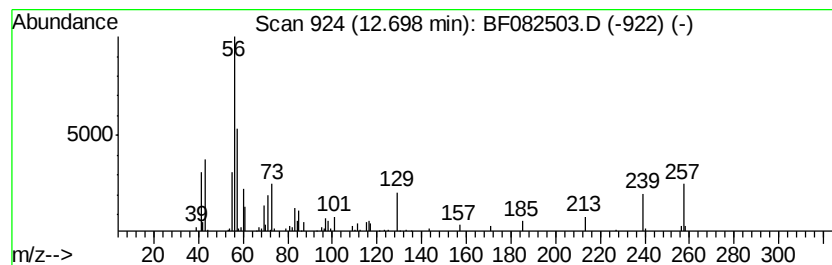
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TIC Integration Parameters: LSCINT.P

Peak Number 4 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.70	3.01 ng	92624	Chrysene-d12	13.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	74
2		Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	50
3		Nipecotic acid	129	C6H11NO2	000498-95-3	43
4		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	35
5		Cyclopentanone, 2,2-dimethyl-	112	C7H12O	004541-32-6	25



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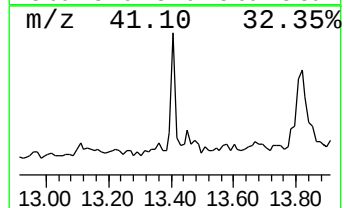
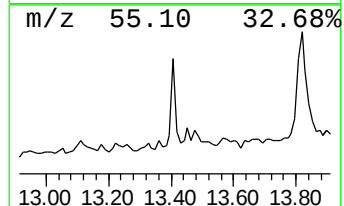
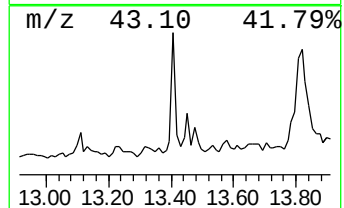
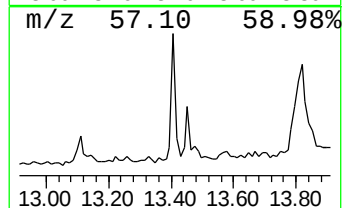
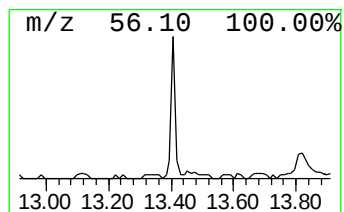
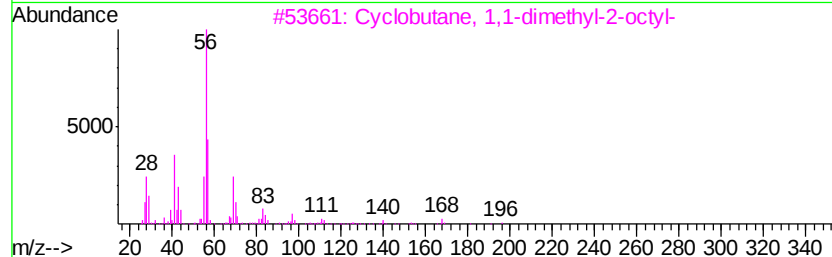
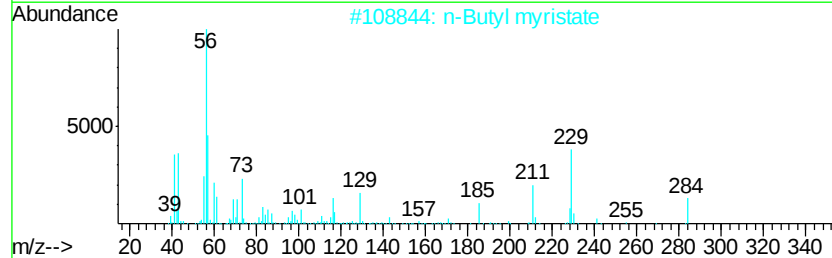
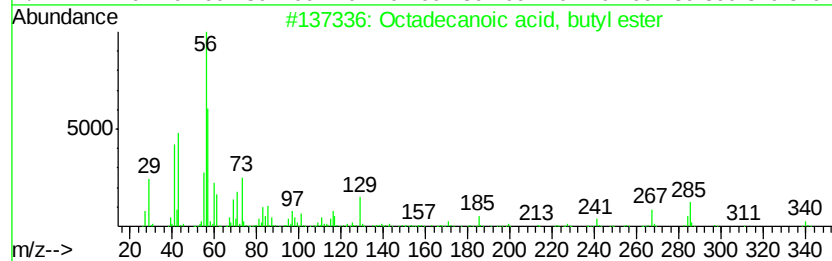
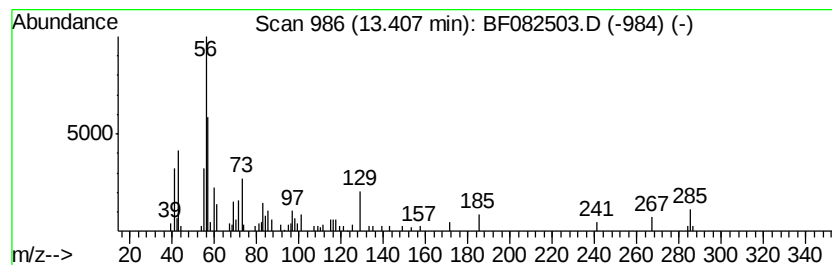
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Peak Number 5 Octadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.41	2.12 ng	65034	Chrysene-d12	13.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	86
2		n-Butyl myristate	284	C18H36O2	000110-36-1	80
3		Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	38
4		Decane, 2,2,3-trimethyl-	184	C13H28	062338-09-4	38
5		Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	35



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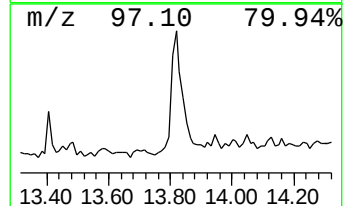
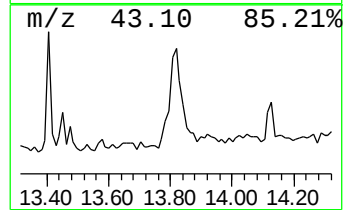
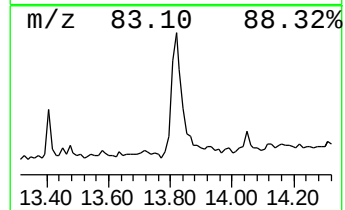
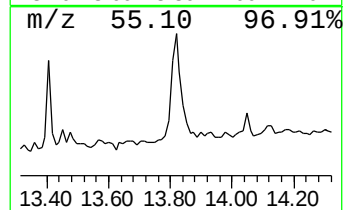
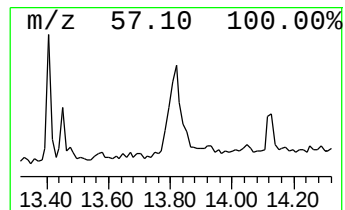
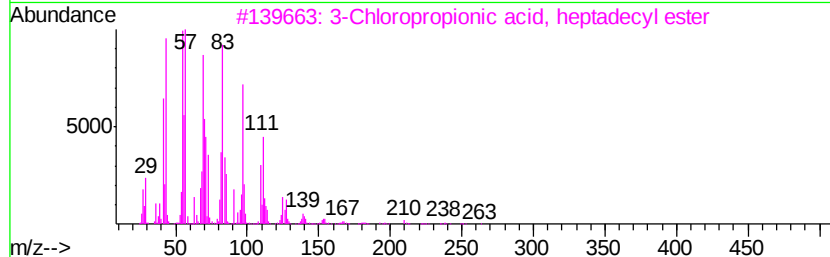
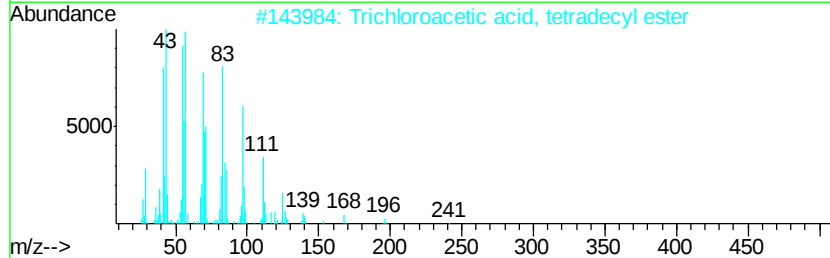
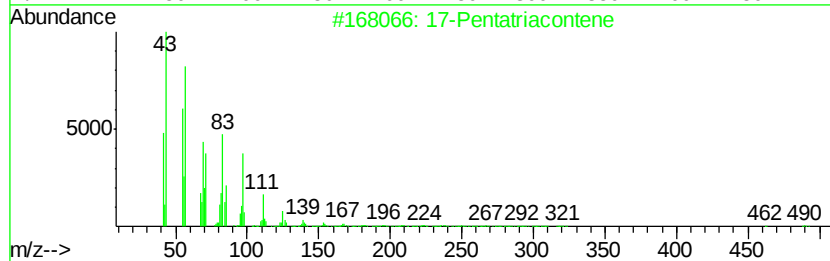
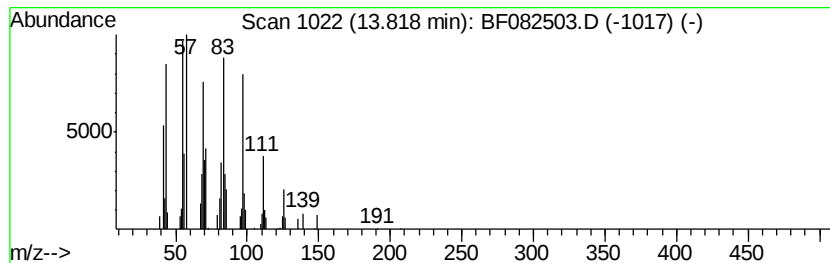
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 6 17-Pentatriacontene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	4.83 ng	148359	Chrysene-d12	13.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	17-Pentatriacontene	491	C35H70	006971-40-0	80
2		Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	80
3		3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	76
4		1-Pentadecanol	228	C15H32O	000629-76-5	74
5		5-Eicosene, (E)-	280	C20H40	074685-30-6	68



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.93	49.7	ng	1378510	1	6.75	554384	20.0
unknown6.53	6.53	81.0	ng	2245580	1	6.75	554384	20.0
Hexadecanoic acid...	12.70	3.0	ng	92624	5	13.96	614789	20.0
Octadecanoic acid...	13.41	2.1	ng	65034	5	13.96	614789	20.0
17-Pentatriacontene	13.82	4.8	ng	148359	5	13.96	614789	20.0