

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP111519\
 Data File : BP001048.D
 Acq On : 15 Nov 2019 19:25
 Operator : JU
 Sample : K5832-04
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 9-(2-4)

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:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110619.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	2.340	37	43	53	rVB	522095	801135	9.54%	1.293%
2	5.740	614	621	635	rBV	515548	852517	10.15%	1.376%
3	6.310	711	718	722	rBV	3802358	4843529	57.66%	7.819%
4	7.816	966	974	981	rBV	3573857	5482043	65.26%	8.850%
5	8.010	1000	1007	1011	rBV	4424252	5566067	66.26%	8.985%
6	8.369	1062	1068	1073	rVB	1230051	1428741	17.01%	2.306%
7	8.610	1102	1109	1113	rBV	3858433	4584526	54.58%	7.401%
8	9.245	1209	1217	1221	rBV	2713367	3382089	40.26%	5.460%
9	10.392	1406	1412	1417	rBV	1576808	1836345	21.86%	2.964%
10	12.175	1706	1715	1719	rBV	5860053	7377704	87.83%	11.910%
11	12.833	1822	1827	1834	rBV	524856	611019	7.27%	0.986%
12	13.251	1892	1898	1905	rBV	1938162	2403434	28.61%	3.880%
13	14.545	2110	2118	2140	rBV	4337166	5713049	68.01%	9.223%
14	15.645	2300	2305	2310	rBV	2287562	2598867	30.94%	4.195%
15	16.527	2450	2455	2468	rBV2	241867	343597	4.09%	0.555%
16	17.927	2687	2693	2697	rBV	7645341	8399775	100.00%	13.560%
17	19.162	2898	2903	2918	rBV	360353	696017	8.29%	1.124%
18	19.280	2918	2923	2928	rBV	2153977	2317597	27.59%	3.741%
19	19.568	2969	2972	2980	rBV	94628	107279	1.28%	0.173%
20	19.962	3035	3039	3042	rBV	98788	109754	1.31%	0.177%
21	20.339	3099	3103	3107	rBV	95173	104746	1.25%	0.169%
22	20.733	3167	3170	3180	rBV	83694	133545	1.59%	0.216%
23	21.062	3220	3226	3235	rVB	1578856	2152416	25.62%	3.475%
24	21.180	3243	3246	3252	rVB	74712	100625	1.20%	0.162%

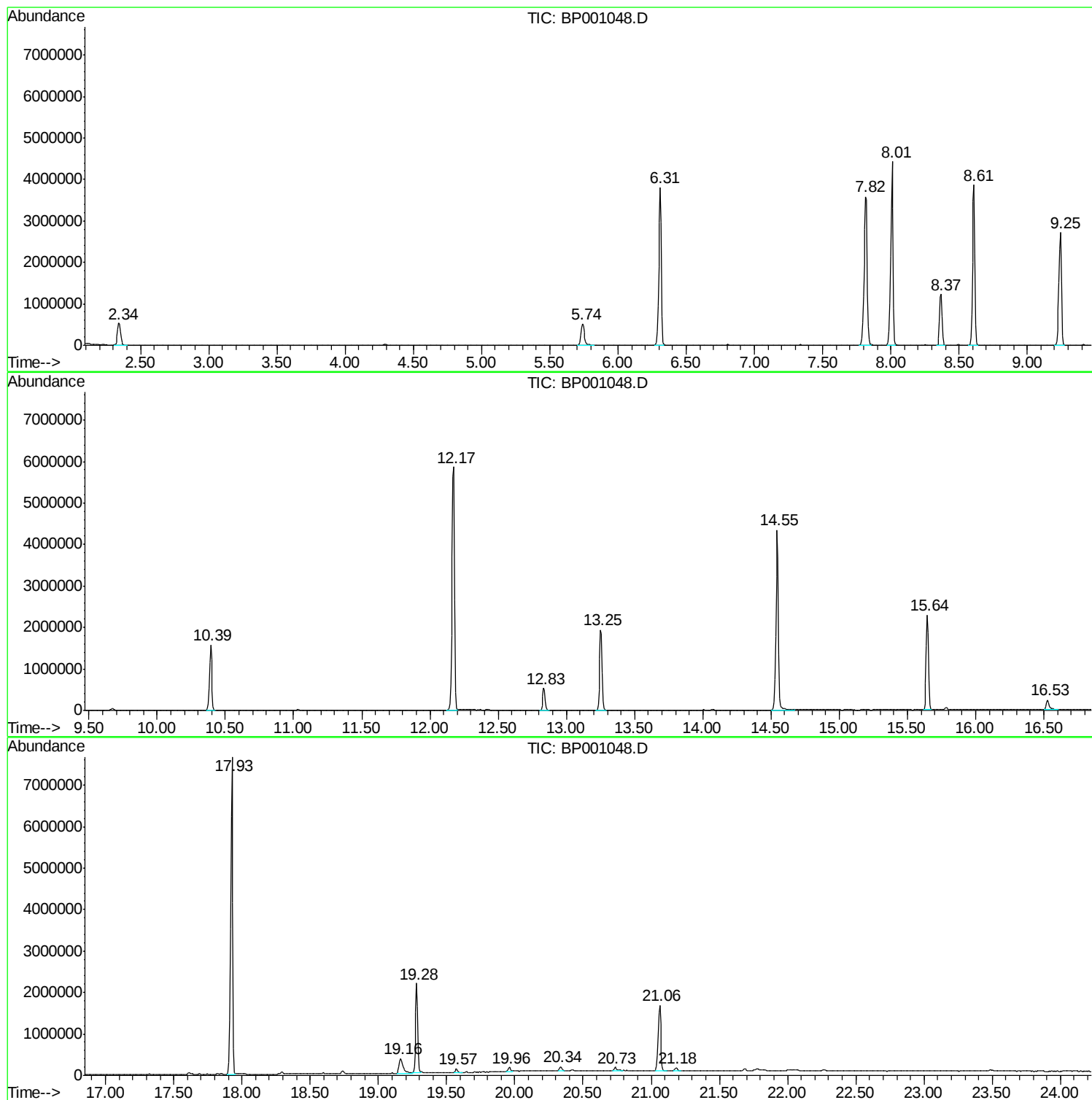
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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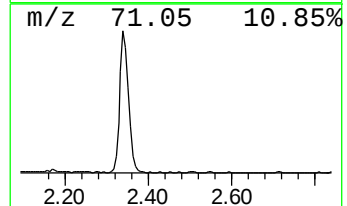
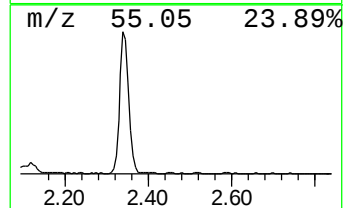
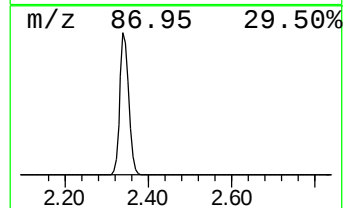
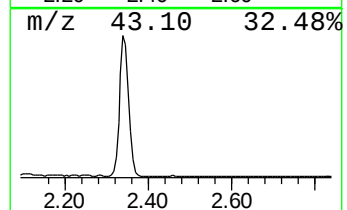
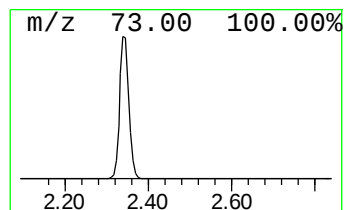
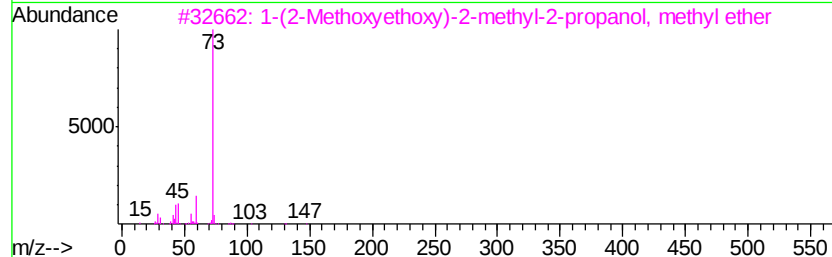
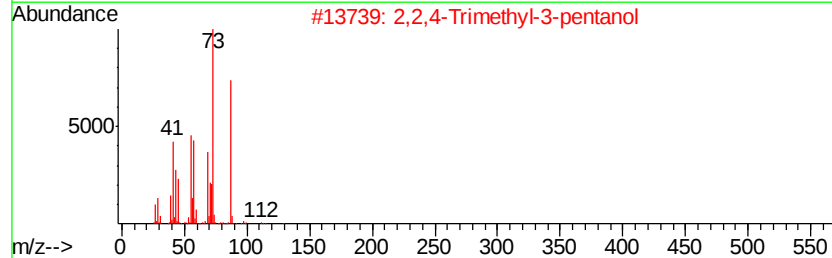
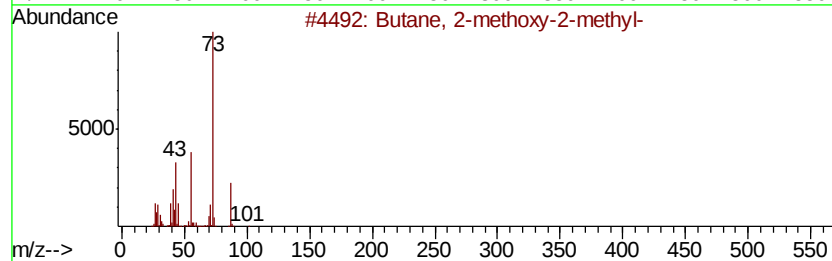
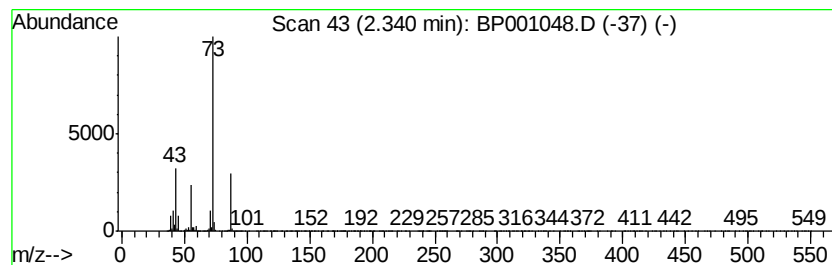
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.34	11.21 ng	801135	1,4-Dichlorobenzene-d4	8.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3		1-(2-Methoxyethoxy)-2-methyl-2-propanol	162	C8H18O3	1000364-24-4	25
4		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5		N-Ethylformamide	73	C3H7NO	000627-45-2	9



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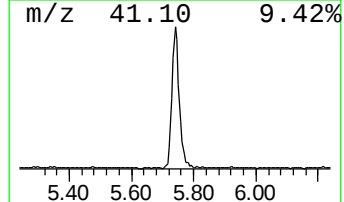
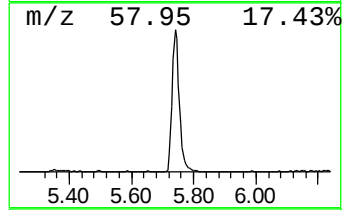
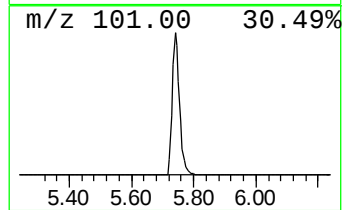
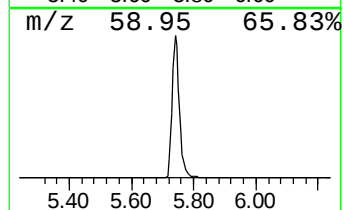
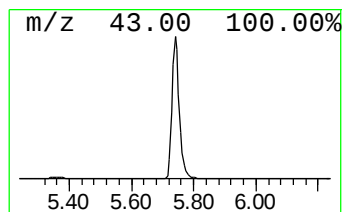
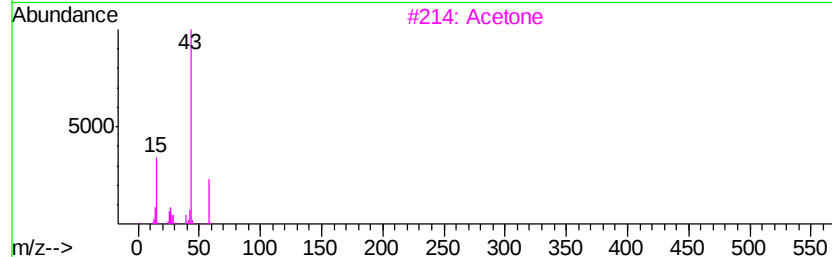
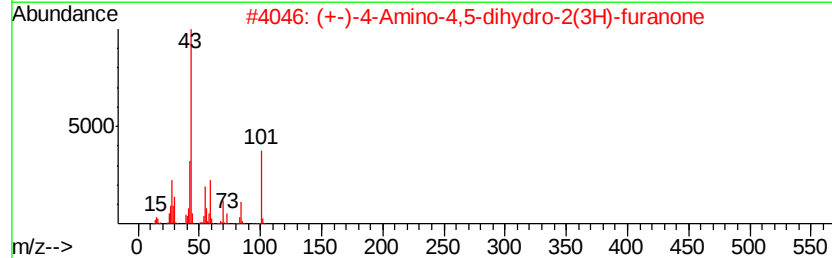
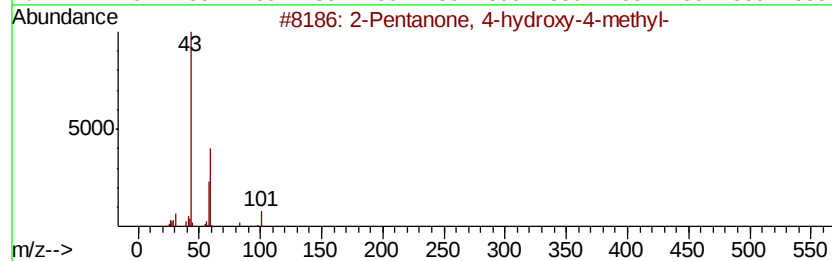
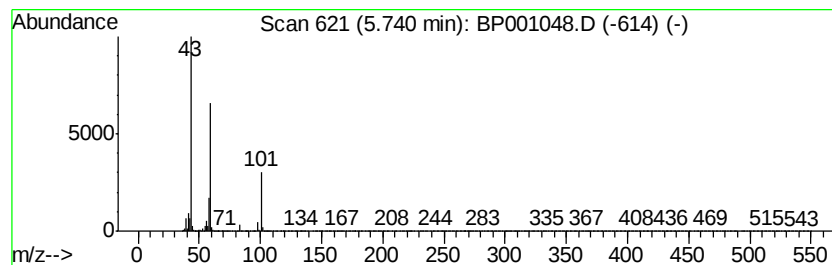
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.74	11.93 ng	852517	1,4-Dichlorobenzene-d4	8.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
2		(+)-4-Amino-4,5-dihydro-2(3H)-furanone	101	C4H7NO2	016504-58-8	37
3		Acetone	58	C3H6O	000067-64-1	10
4		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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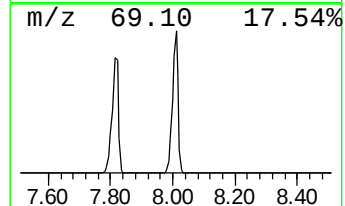
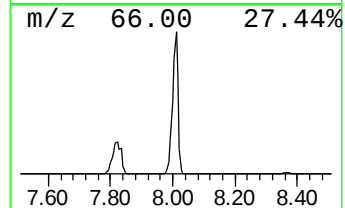
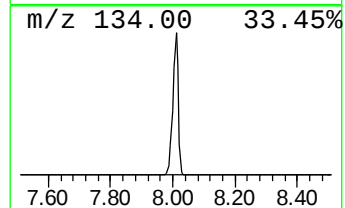
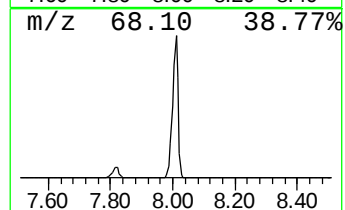
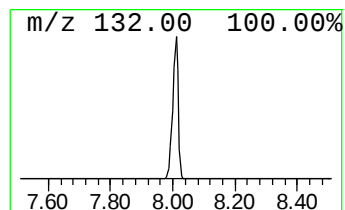
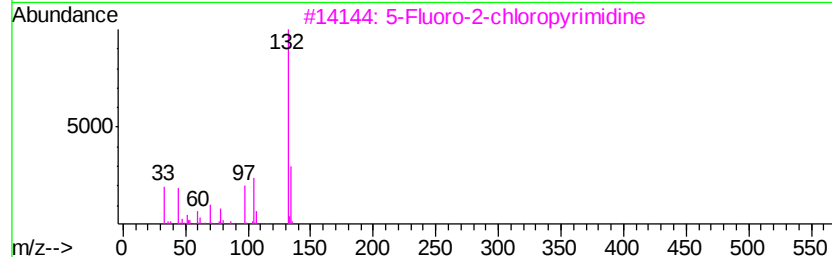
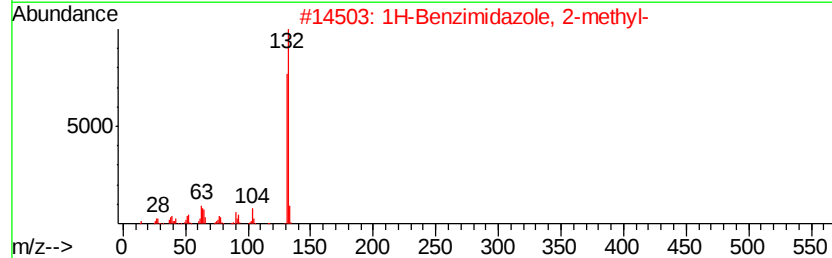
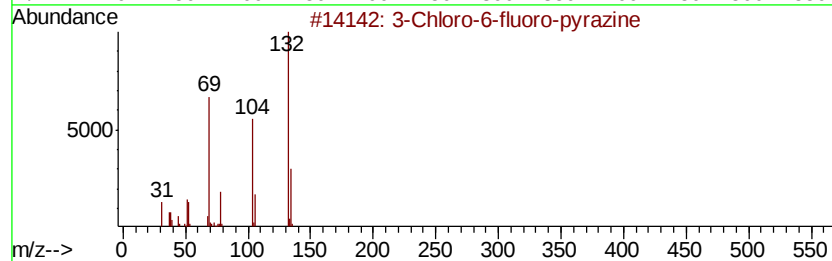
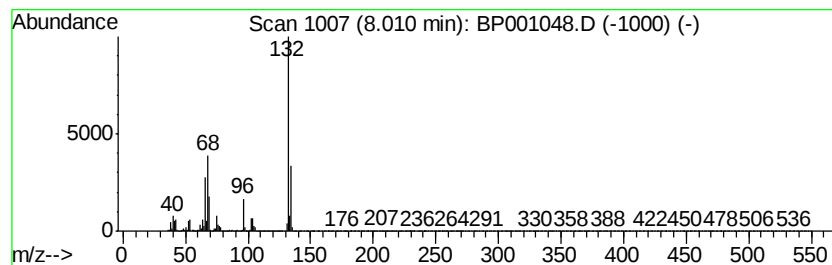
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown8.01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.01	77.92 ng	5566070	1,4-Dichlorobenzene-d4	8.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
5		5-Aminoindole	132	C8H8N2	005192-03-0	12



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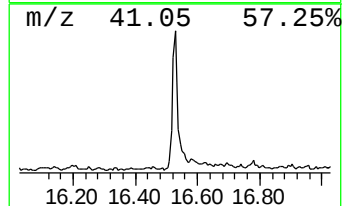
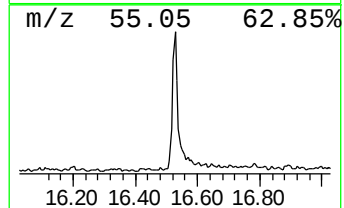
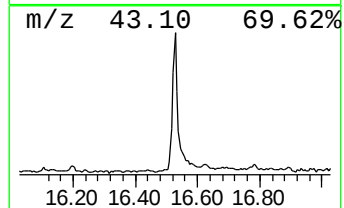
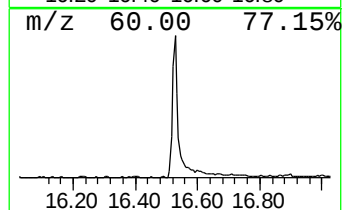
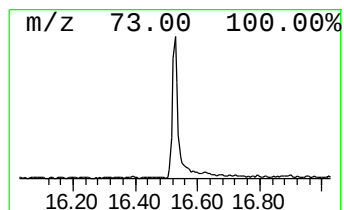
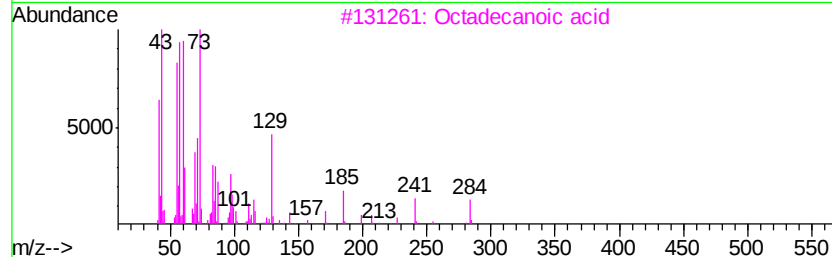
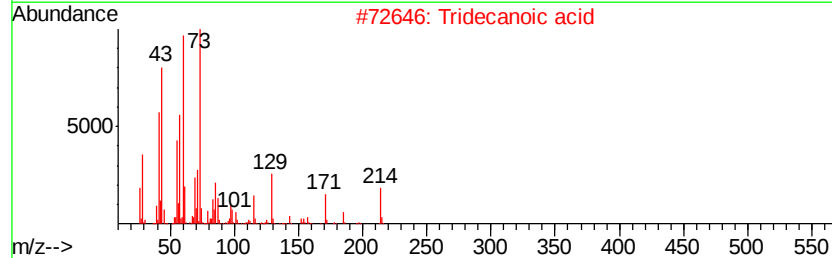
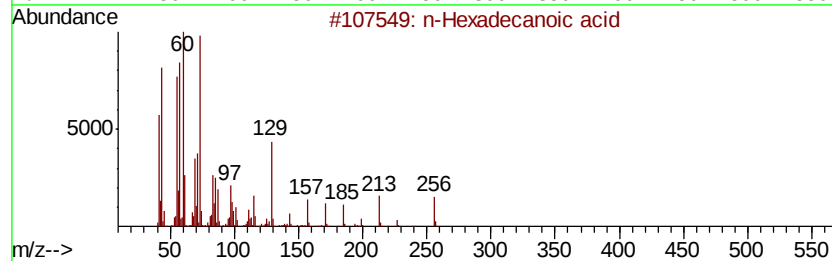
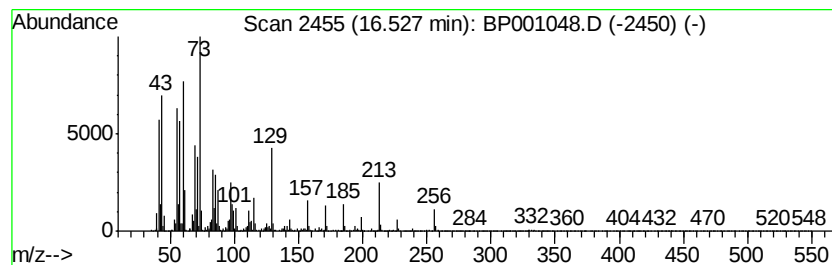
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.53	2.64 ng	343597	Phenanthrene-d10	15.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	91
3		Octadecanoic acid	284	C18H36O2	000057-11-4	87
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	83
5		Undecanoic acid	186	C11H22O2	000112-37-8	72



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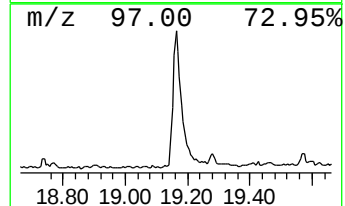
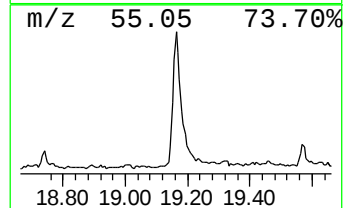
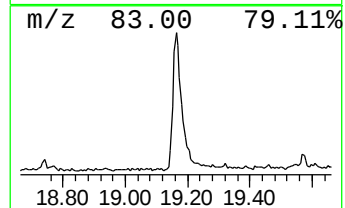
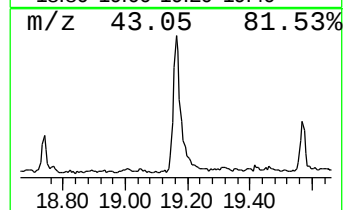
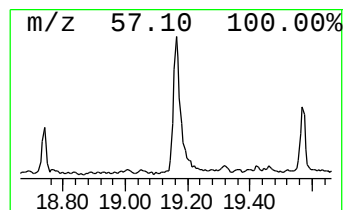
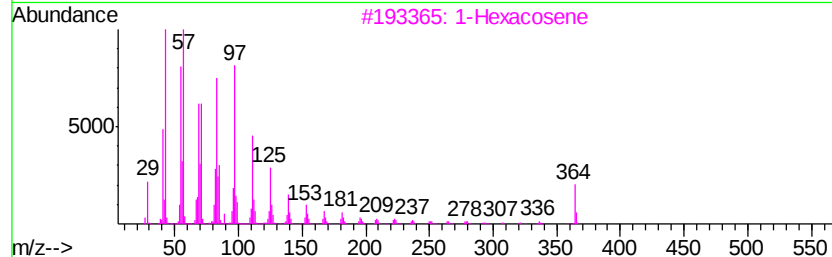
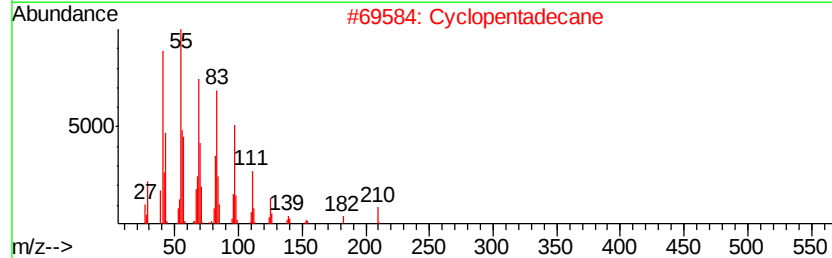
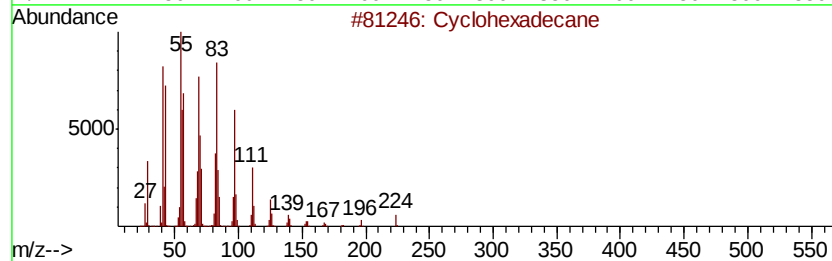
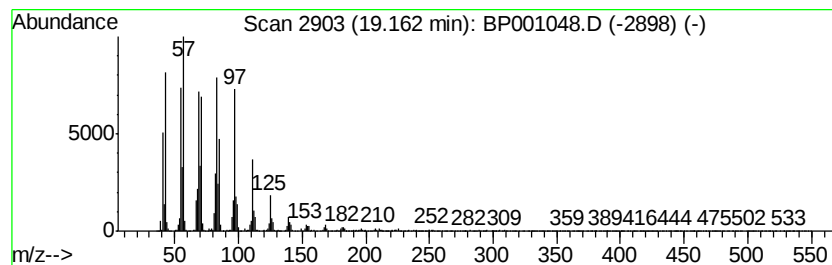
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Cyclohexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.16	6.01 ng	696017	Chrysene-d12	19.28
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Cyclohexadecane	224 C16H32	000295-65-8 99
2		Cyclopentadecane	210 C15H30	000295-48-7 96
3		1-Hexacosene	364 C26H52	018835-33-1 94
4		Nonadecyl pentafluoropropionate	430 C22H39F5O2	1000351-88-8 94
5		Heptafluorobutyric acid, pentade...	424 C19H31F7O2	959261-23-5 93



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.34	11.2	ng	801135	1	8.37	1428740	20.0
2-Pentanone, 4-hy...	5.74	11.9	ng	852517	1	8.37	1428740	20.0
unknown8.01	8.01	77.9	ng	5566070	1	8.37	1428740	20.0
n-Hexadecanoic acid	16.53	2.6	ng	343597	4	15.65	2598870	20.0
Cyclohexadecane	19.16	6.0	ng	696017	5	19.28	2317600	20.0