

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031317\
 Data File : BF093633.D
 Acq On : 14 Mar 2017 3:26
 Operator : SJ/MA
 Sample : I2199-25
 Misc :
 ALS Vial : 33 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 D-101

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON Filtering: 5
 Sampling : 1 Min Area: 3 % of largest Peak
 Start Thrs: 0.2 Max Peaks: 100
 Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.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	2.447	46	49	59	rVB	47699	144262	2.58%	0.308%
2	4.161	197	199	208	rVB	47128	81799	1.46%	0.175%
3	4.413	218	221	230	rVB	35837	84034	1.50%	0.180%
4	4.870	259	261	279	rBV	991994	1889444	33.76%	4.039%
5	5.316	298	300	328	rBV	3695155	5460410	97.57%	11.673%
6	5.716	333	335	346	rVB	56858	111191	1.99%	0.238%
7	6.367	390	392	400	rBV	3318251	5031974	89.91%	10.758%
8	6.481	400	402	405	rVB	4738574	4706216	84.09%	10.061%
9	6.710	420	422	430	rVB	965055	1083962	19.37%	2.317%
10	6.859	433	435	438	rBV	3857636	3868322	69.12%	8.270%
11	7.282	470	472	487	rBV	2996559	3506056	62.65%	7.495%
12	8.002	533	535	544	rBV	1330693	1452845	25.96%	3.106%
13	9.087	627	630	632	rBV	3926742	5596491	100.00%	11.964%
14	9.762	686	689	691	rBV	1268122	1569376	28.04%	3.355%
15	10.550	756	758	761	rBV2	2115942	2927824	52.32%	6.259%
16	11.248	817	819	824	rBV	1696801	1630825	29.14%	3.486%
17	12.654	940	942	945	rBV	161440	138752	2.48%	0.297%
18	12.836	955	958	961	rBV	4458642	5070512	90.60%	10.840%
19	13.362	1002	1004	1006	rBV	82664	87804	1.57%	0.188%
20	13.899	1049	1051	1059	rBV	876044	1356916	24.25%	2.901%
21	15.305	1171	1174	1182	rBV	617387	977264	17.46%	2.089%

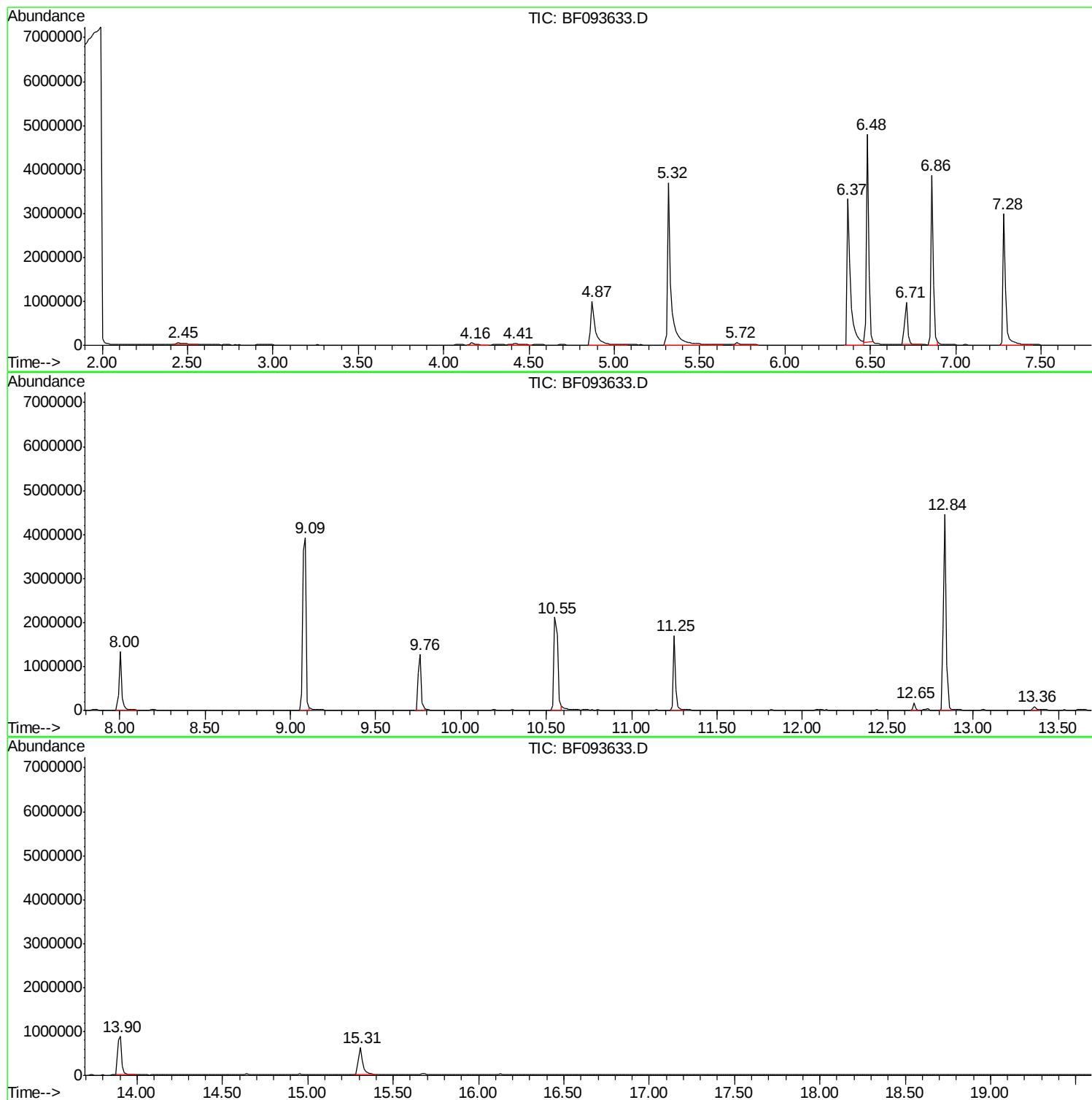
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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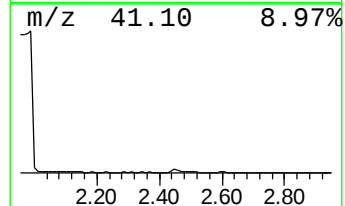
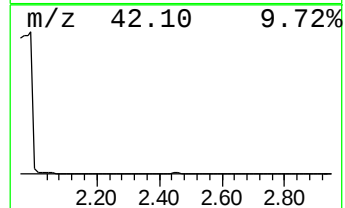
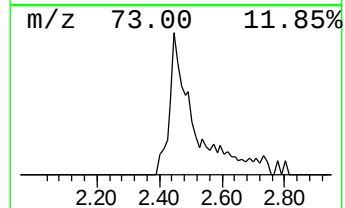
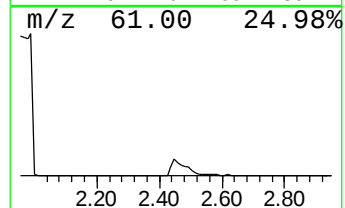
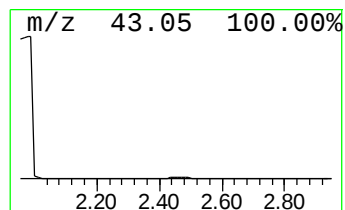
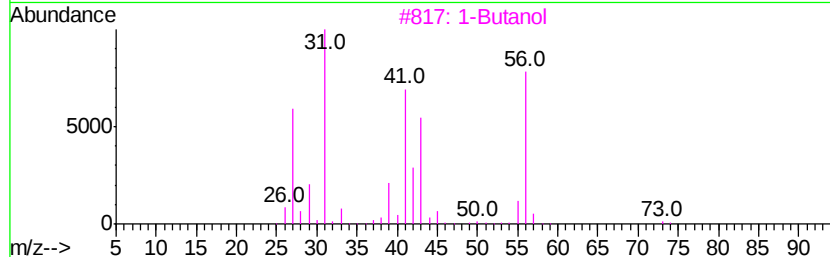
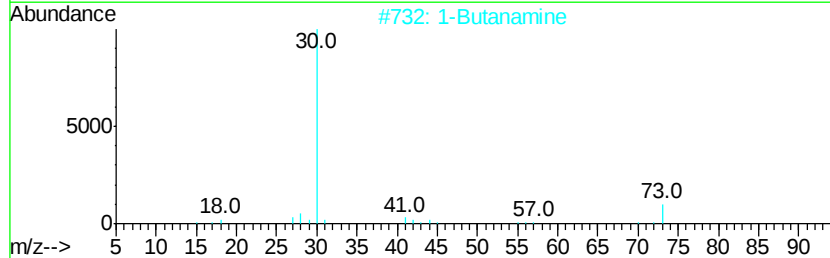
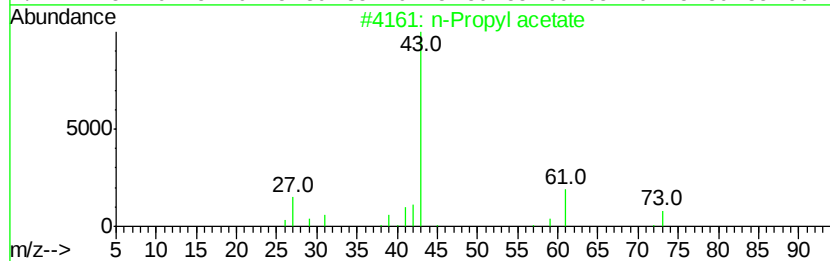
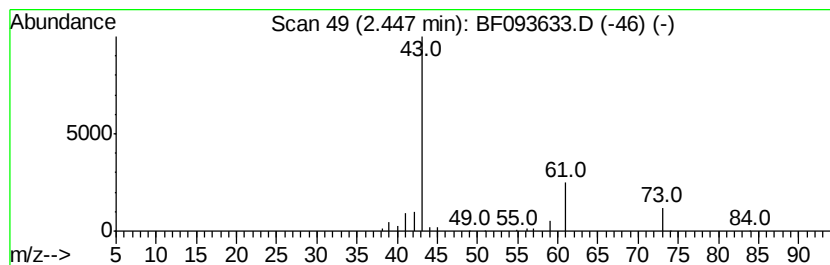
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Propyl acetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.45	2.66 ng	144262	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Propyl acetate	102	C5H10O2	000109-60-4	64
2		1-Butanamine	73	C4H11N	000109-73-9	5
3		1-Butanol	74	C4H10O	000071-36-3	5
4		Isobutylamine	73	C4H11N	000078-81-9	4
5		Hydrogen azide	43	HN3	007782-79-8	4



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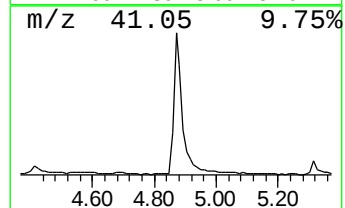
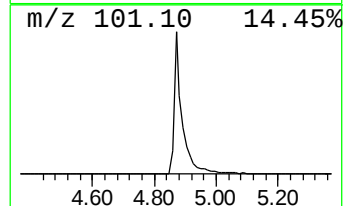
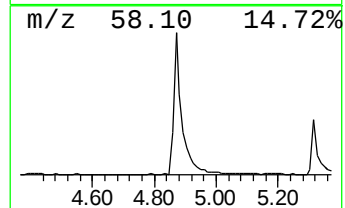
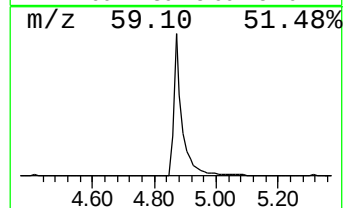
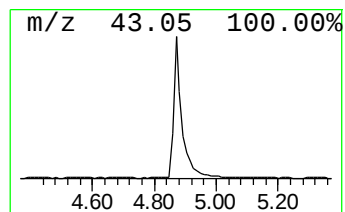
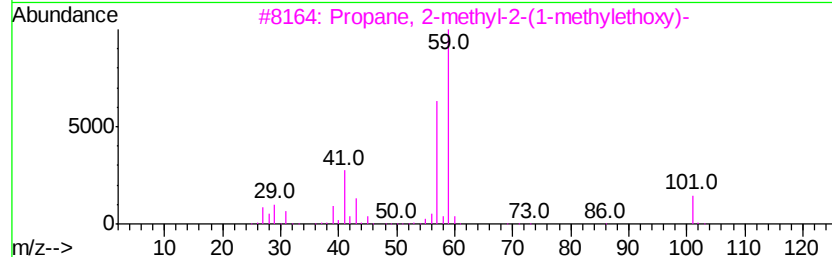
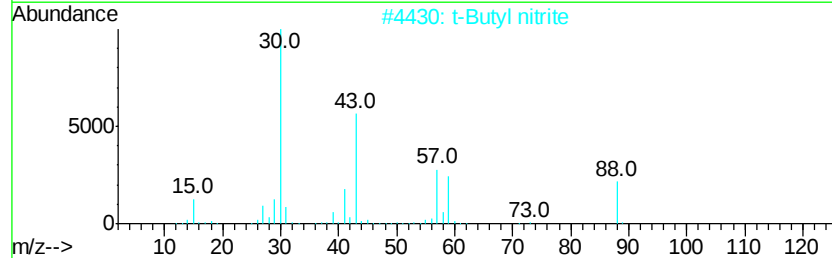
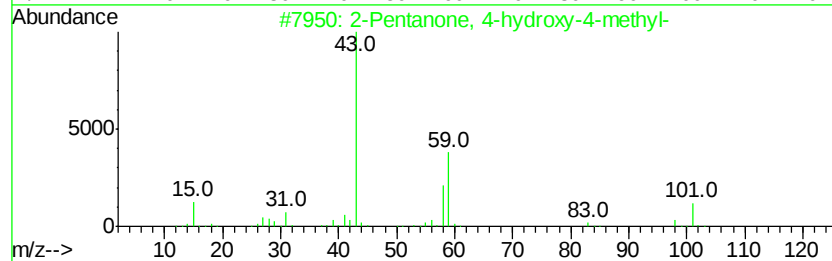
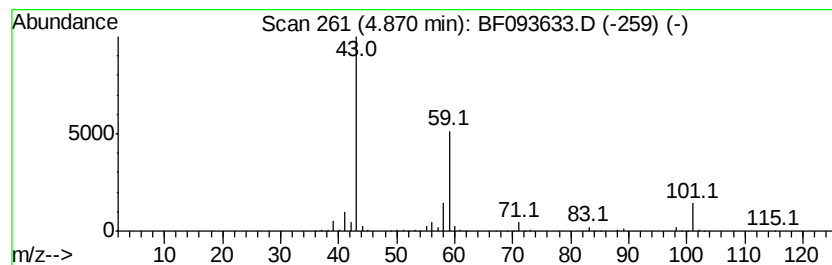
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.87	34.86 ng	1889440	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2		t-Butyl nitrite	103	C4H9NO2	000540-80-7	39
3		Propane, 2-methyl-2-(1-methylethoxy)-	116	C7H16O	017348-59-3	33
4		4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	25
5		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25



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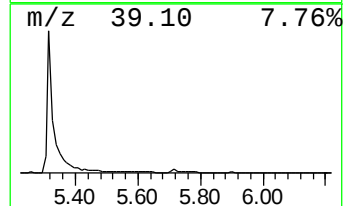
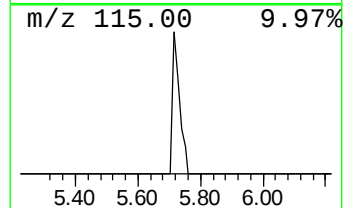
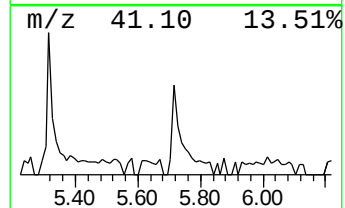
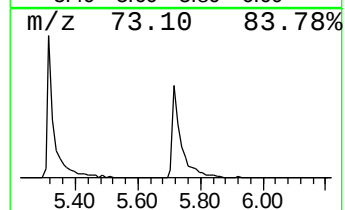
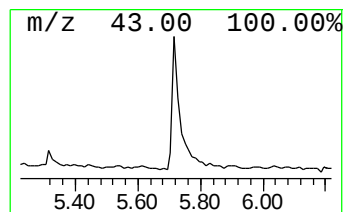
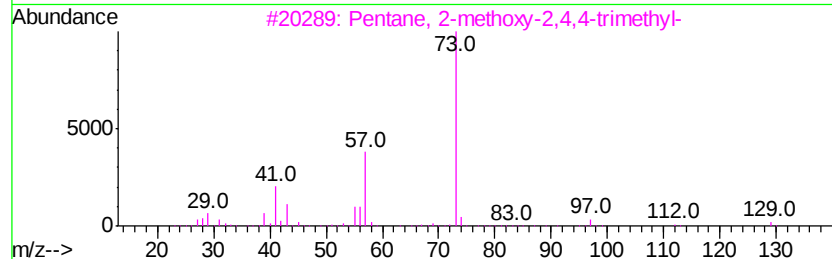
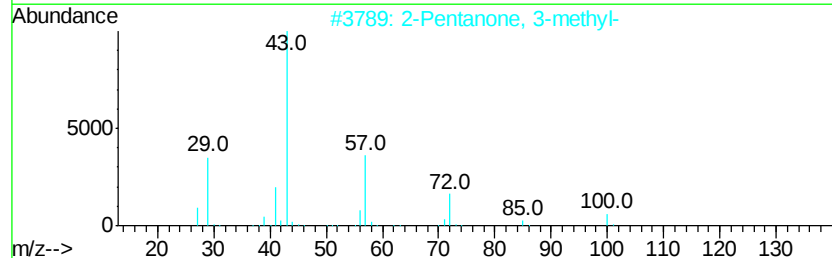
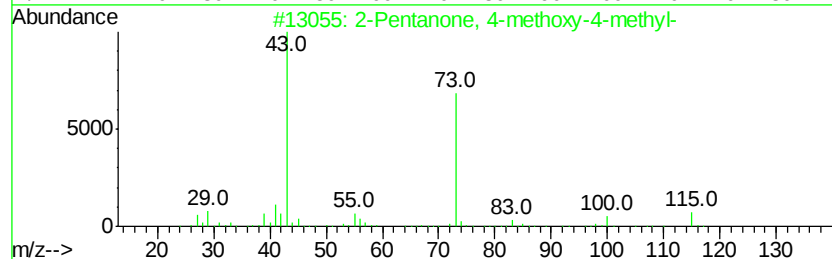
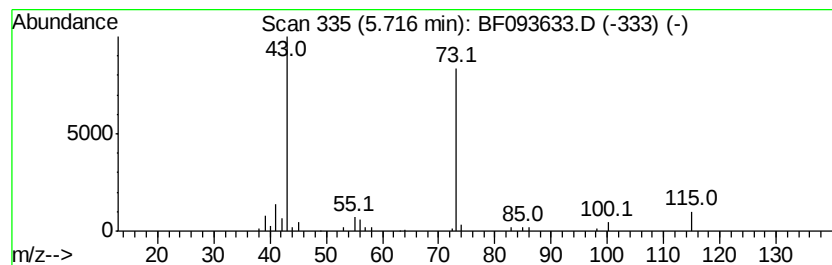
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Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.72	2.05 ng	111191	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2		2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	27
3		Pentane, 2-methoxy-2,4,4-trimethyl-	144	C9H20O	062108-41-2	12
4		2-Nonanone	142	C9H18O	000821-55-6	10
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9



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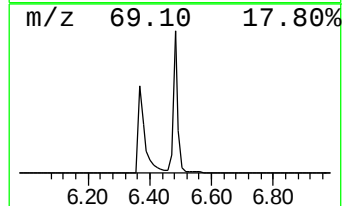
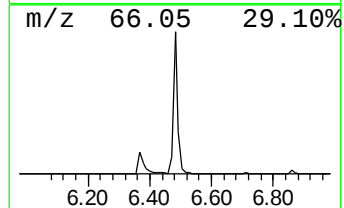
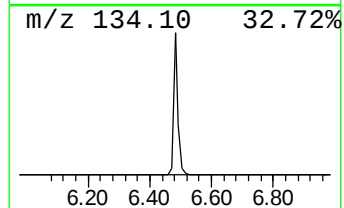
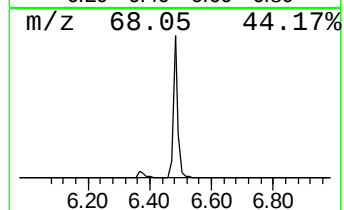
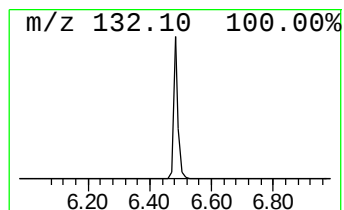
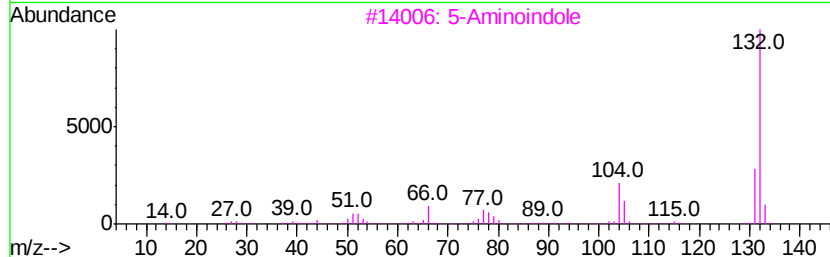
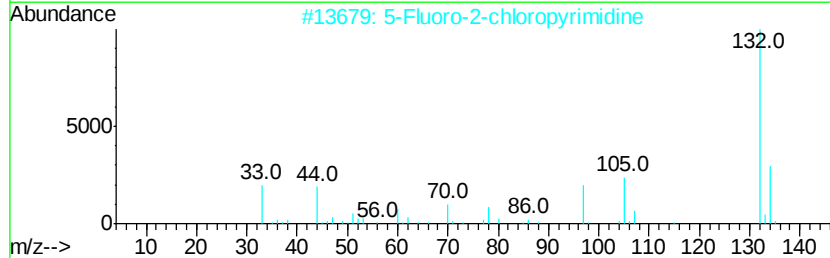
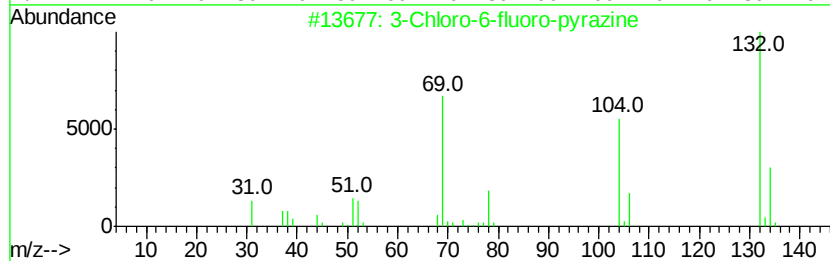
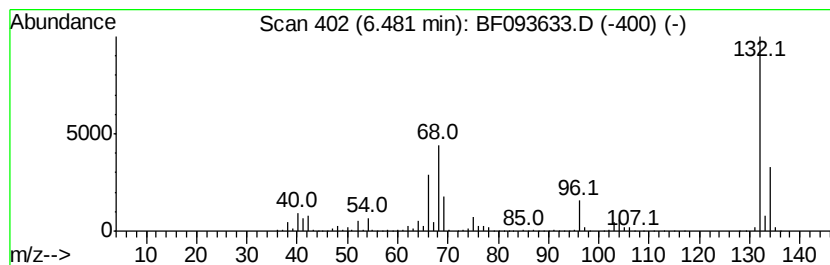
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 4 unknown6.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	86.83 ng	4706220	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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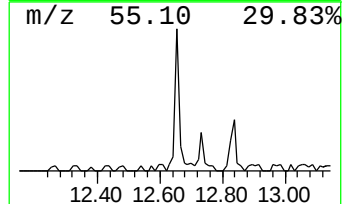
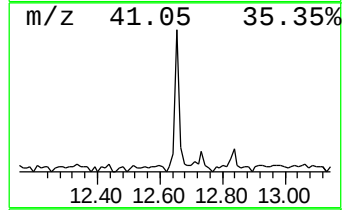
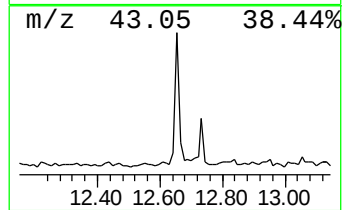
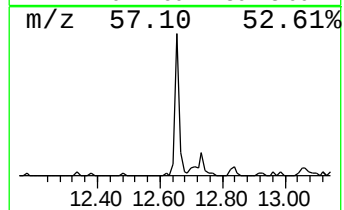
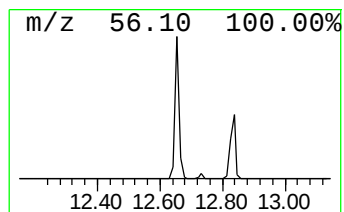
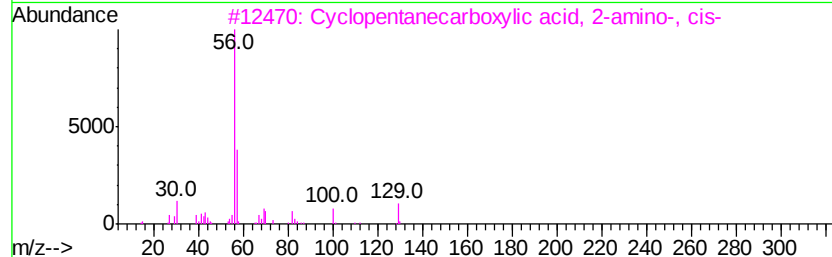
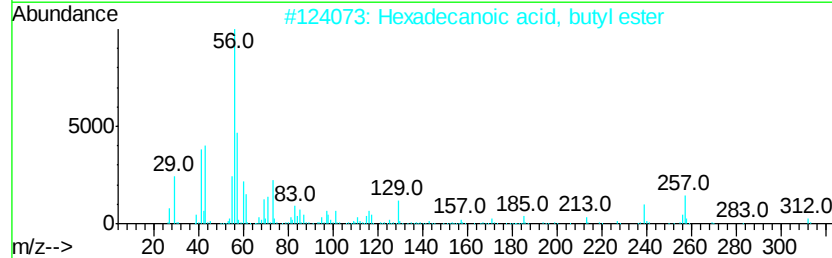
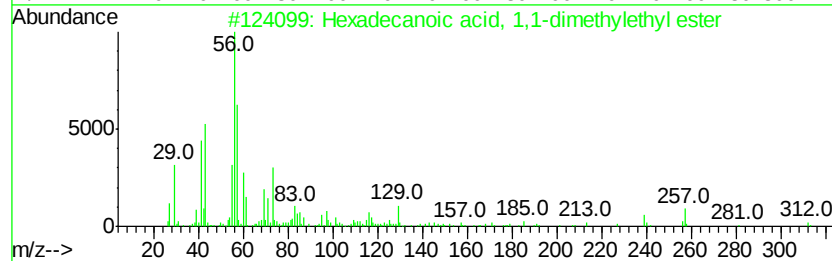
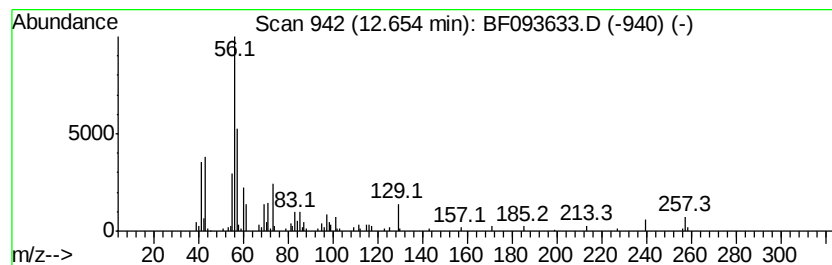
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Peak Number 6 Hexadecanoic acid, 1,1-dime... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.65	2.05 ng	138752	Chrysene-d12	13.90

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	90
2		Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	83
3		Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	037910-65-9	43
4		Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	43
5		Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Propyl acetate	2.45	2.7	ng	144262	1	6.71	1083960	20.0
2-Pentanone, 4-hy...	4.87	34.9	ng	1889440	1	6.71	1083960	20.0
2-Pentanone, 4-me...	5.72	2.0	ng	111191	1	6.71	1083960	20.0
unknown6.48	6.48	86.8	ng	4706220	1	6.71	1083960	20.0
Hexadecanoic acid...	12.65	2.0	ng	138752	5	13.90	1356920	20.0