

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF022317\
Data File : BF093138.D
Acq On : 24 Feb 2017 8:49
Operator : SJ/MA
Sample : I1955-04
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B1-3

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-BF013017.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	2.487	24	35	42	rVV2	20628	96982	2.26%	0.284%
2	2.624	45	47	55	rVB	102414	179799	4.18%	0.526%
3	5.024	254	257	270	rVB	1377543	2022346	47.03%	5.912%
4	5.447	291	294	296	rBV	3814448	3879527	90.22%	11.342%
5	6.487	382	385	387	rBV	3473387	3944940	91.75%	11.533%
6	6.613	393	396	398	rBV	3950718	3994790	92.91%	11.679%
7	6.842	414	416	418	rBV	1007089	863322	20.08%	2.524%
8	7.002	427	430	432	rBV	3109138	3202779	74.49%	9.364%
9	7.413	463	466	468	rBV	2632856	2655910	61.77%	7.765%
10	8.122	526	528	531	rBV	757080	1025358	23.85%	2.998%
11	9.207	620	623	625	rBV	3756509	4299850	100.00%	12.571%
12	9.882	679	682	684	rBV	866916	977070	22.72%	2.857%
13	10.671	748	751	753	rBV	1553847	1832581	42.62%	5.358%
14	11.356	809	811	814	rBV	785812	783697	18.23%	2.291%
15	12.762	932	934	937	rBV	104287	94925	2.21%	0.278%
16	12.945	947	950	952	rBV	3075547	2816700	65.51%	8.235%
17	13.471	994	996	998	rBV	70499	65815	1.53%	0.192%
18	13.997	1039	1042	1044	rBV	814235	767805	17.86%	2.245%
19	15.425	1164	1167	1173	rBV	531209	700674	16.30%	2.048%

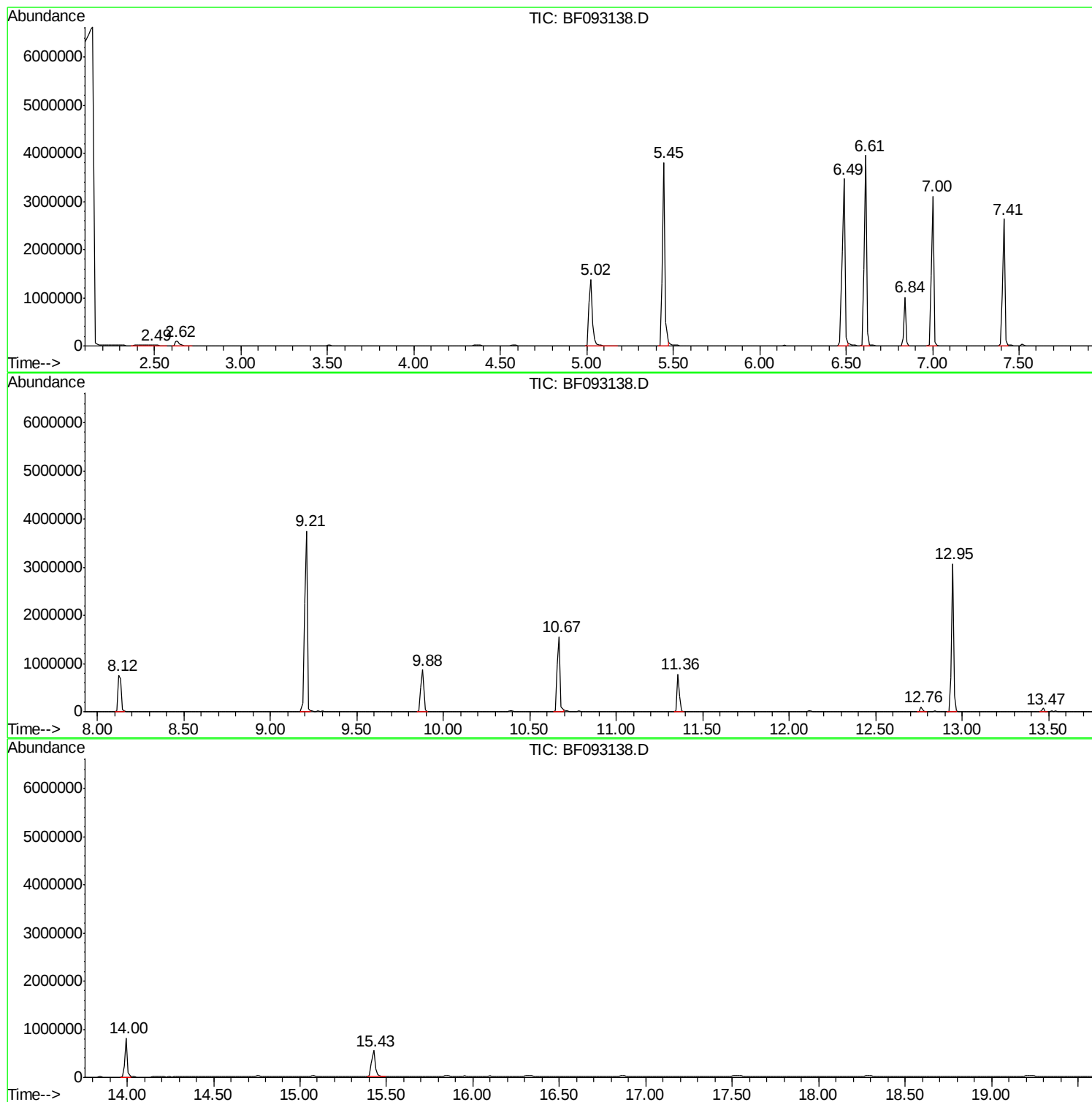
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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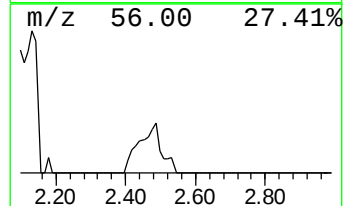
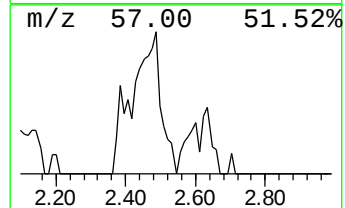
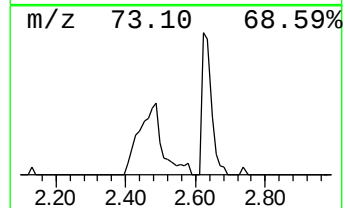
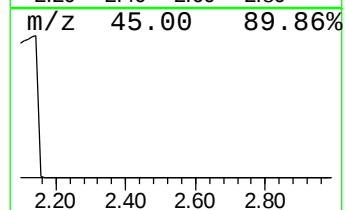
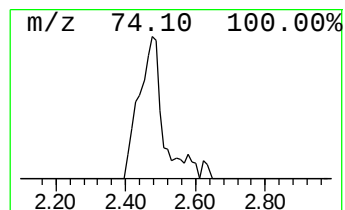
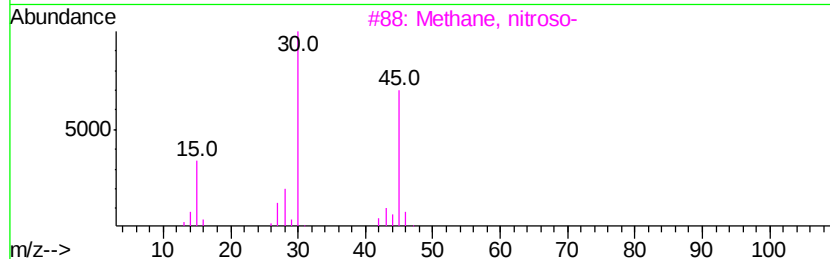
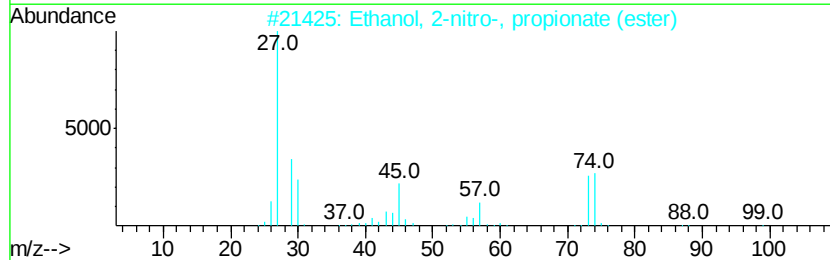
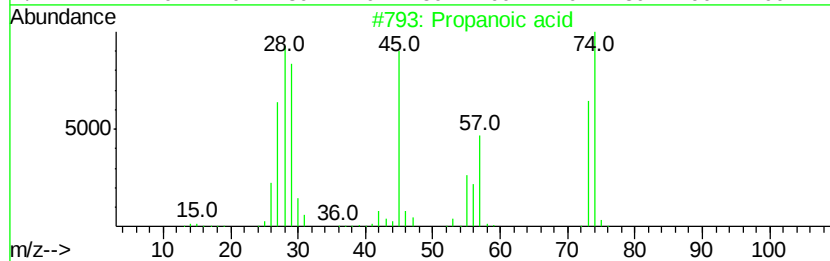
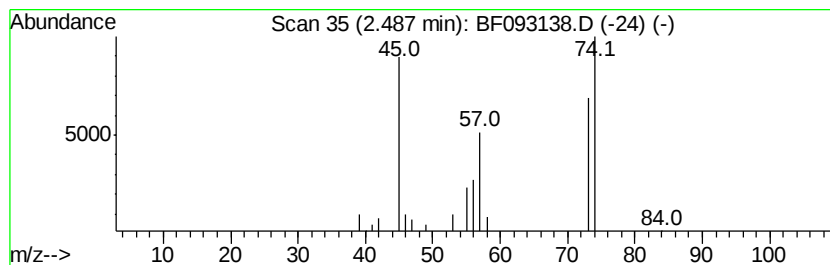
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Propanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.49	2.25 ng	96982	1,4-Dichlorobenzene-d4	6.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propanoic acid	74	C3H6O2	000079-09-4	90
2		Ethanol, 2-nitro-, propionate (e...	147	C5H9NO4	005390-28-3	9
3		Methane, nitroso-	45	CH3NO	000865-40-7	5
4		Thiirane, methyl-	74	C3H6S	001072-43-1	4
5		Allyl mercaptan	74	C3H6S	000870-23-5	4



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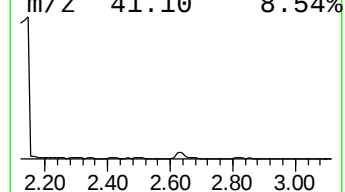
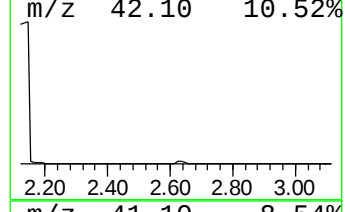
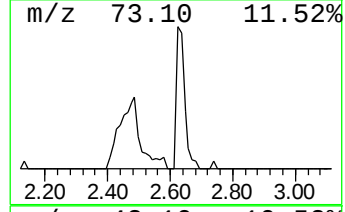
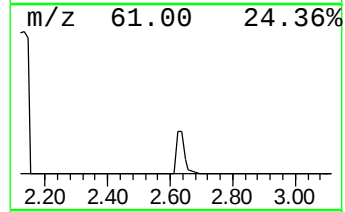
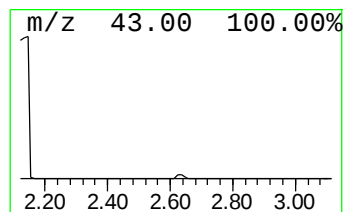
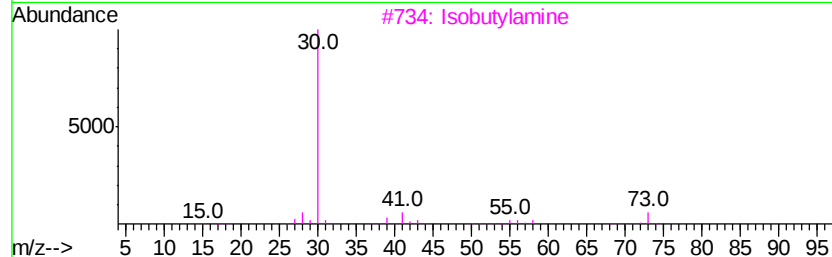
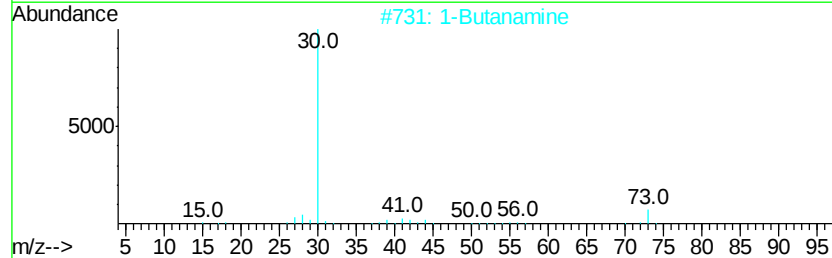
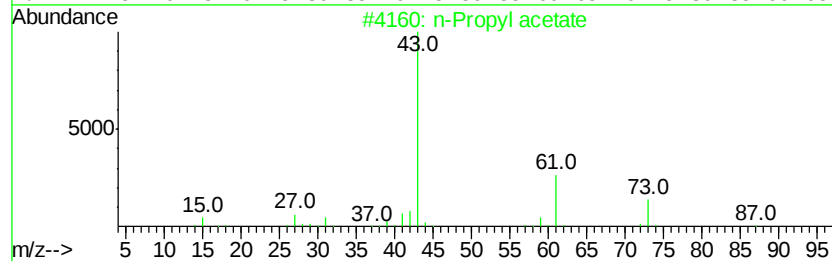
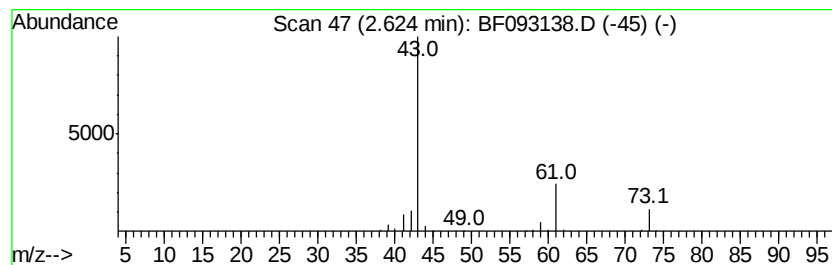
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Propyl acetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.62	4.17 ng	179799	1,4-Dichlorobenzene-d4	6.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Propyl acetate	102	C5H10O2	000109-60-4	83
2		1-Butanamine	73	C4H11N	000109-73-9	5
3		Isobutylamine	73	C4H11N	000078-81-9	4
4		Hydrogen azide	43	HN3	007782-79-8	4
5		1,4-Diacetoxybutane	174	C8H14O4	033934-62-2	4



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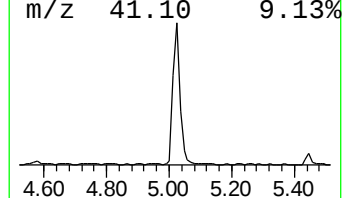
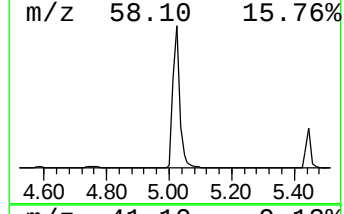
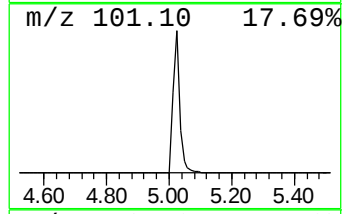
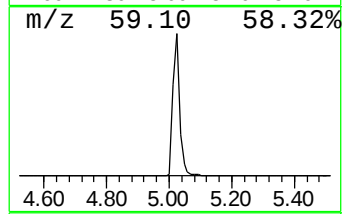
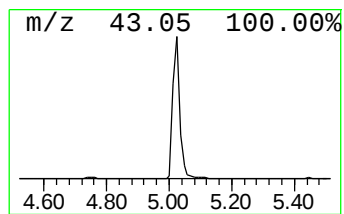
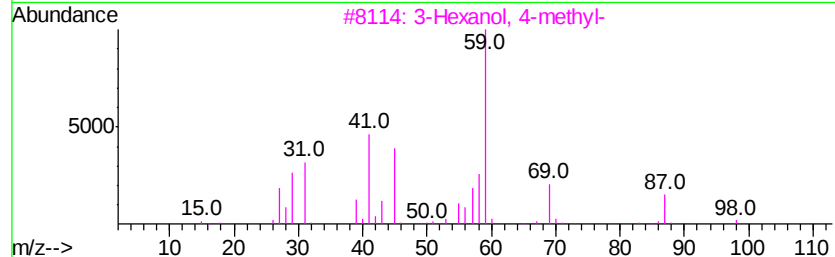
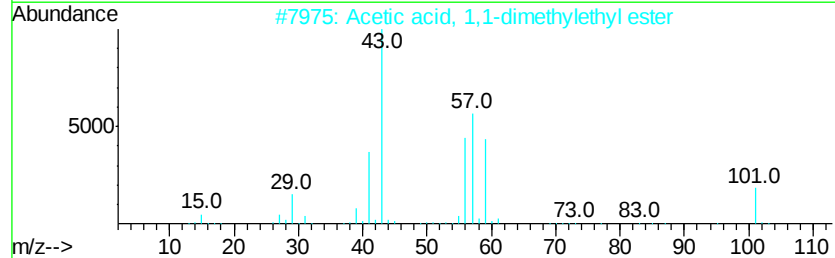
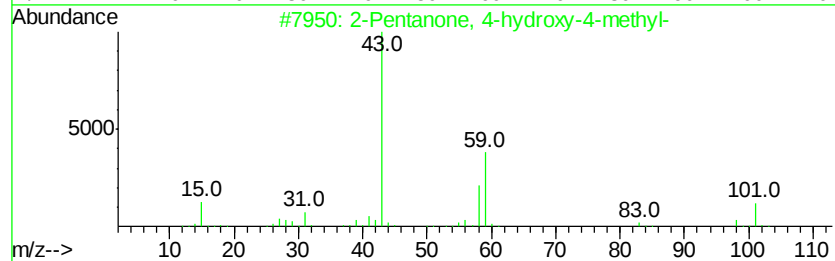
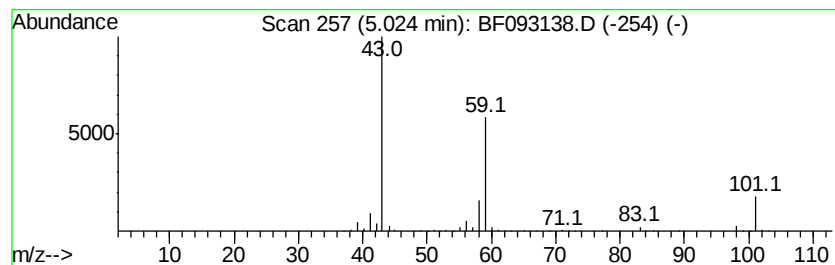
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	46.85 ng	2022350	1,4-Dichlorobenzene-d4	6.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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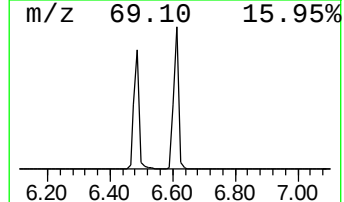
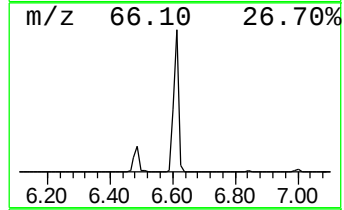
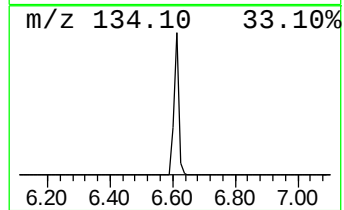
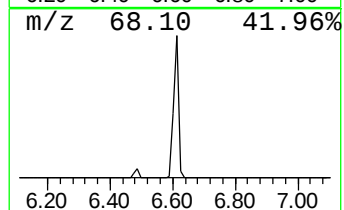
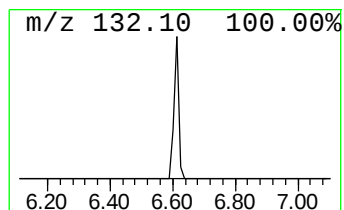
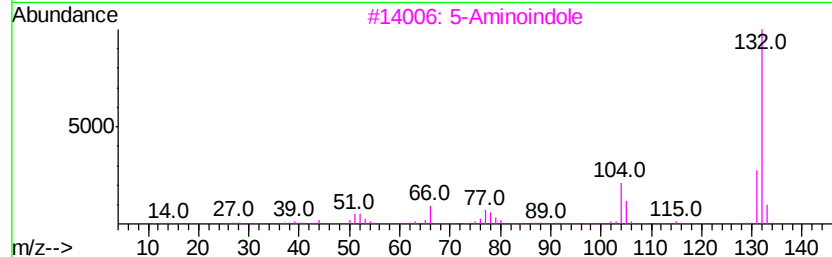
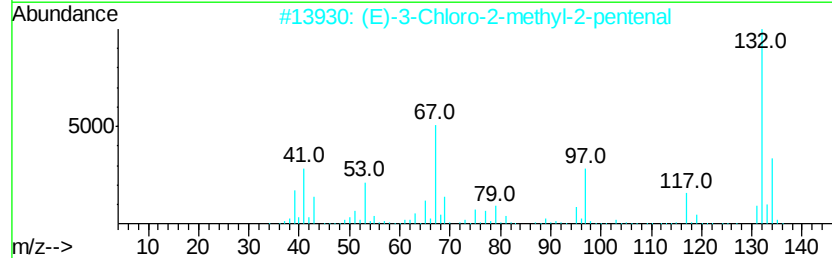
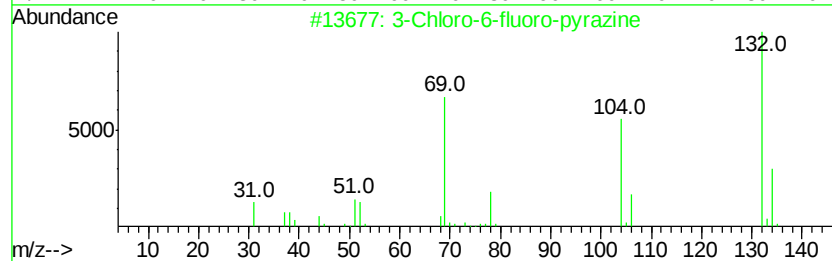
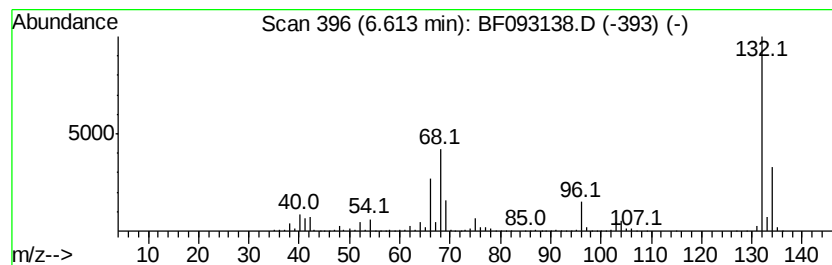
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 4 unknown6.61 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.61	92.54 ng	3994790	1,4-Dichlorobenzene-d4	6.84

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3			5-Aminoindole	132	C8H8N2	005192-03-0	12
4			Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5			Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9



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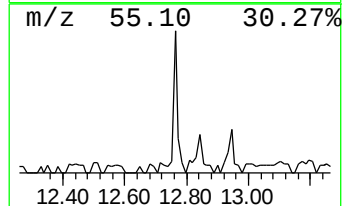
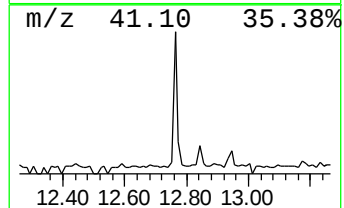
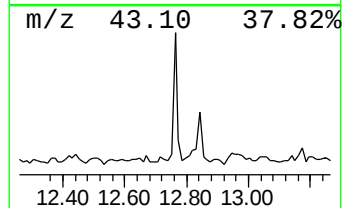
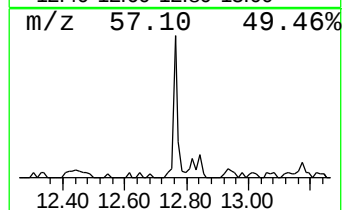
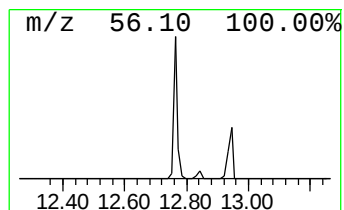
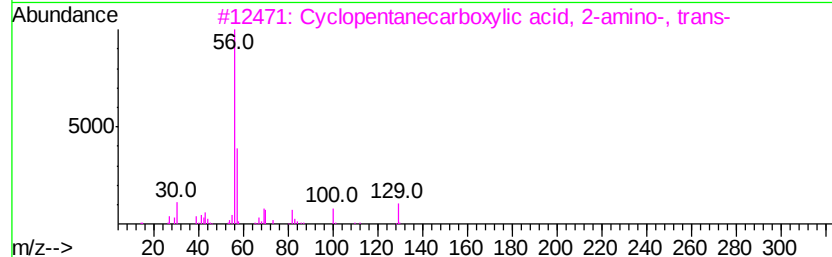
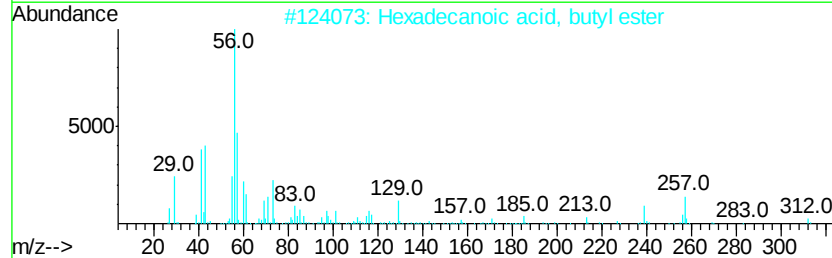
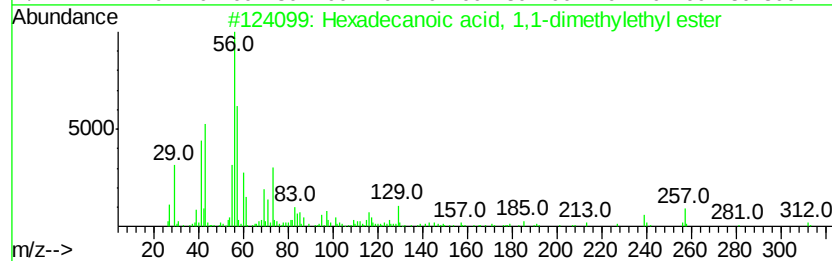
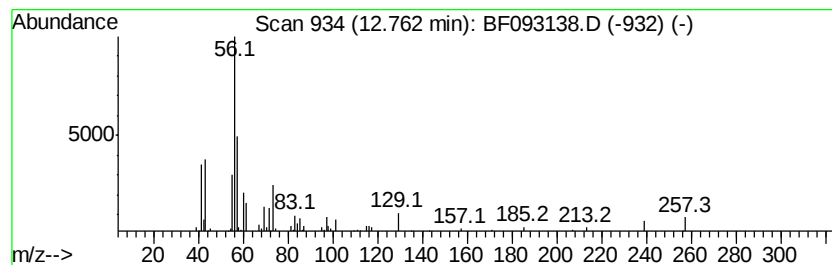
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Peak Number 6 Hexadecanoic acid, 1,1-dime... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.76	2.47 ng	94925	Chrysene-d12	14.00

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	58
2		Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	49
3		Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	43
4		Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	037910-65-9	43
5		Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propanoic acid	2.49	2.3	ng	96982	1	6.84	863322	20.0
n-Propyl acetate	2.62	4.2	ng	179799	1	6.84	863322	20.0
2-Pentanone, 4-hy...	5.02	46.9	ng	2022350	1	6.84	863322	20.0
unknown6.61	6.61	92.5	ng	3994790	1	6.84	863322	20.0
Hexadecanoic acid...	12.76	2.5	ng	94925	5	14.00	767805	20.0