

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060516\
 Data File : BF087733.D
 Acq On : 6 Jun 2016 3:51
 Operator : UM/SJ
 Sample : H3378-16
 Misc :
 ALS Vial : 69 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-10

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-BF060416.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	1.781	12	17	19	rBV	4295841	8670232	100.00%	21.135%
2	1.907	26	28	49	rVB	1596543	3768861	43.47%	9.187%
3	2.170	49	51	62	rVB	107934	183620	2.12%	0.448%
4	5.062	301	304	311	rVB	216773	340559	3.93%	0.830%
5	5.462	336	339	342	rBV	2553052	2868055	33.08%	6.991%
6	6.490	425	429	431	rBV	2473769	2895669	33.40%	7.059%
7	6.628	438	441	443	rBV	2882825	3074679	35.46%	7.495%
8	6.856	459	461	464	rBV	870384	715638	8.25%	1.744%
9	7.016	472	475	477	rBV	2670627	2504082	28.88%	6.104%
10	7.428	507	511	513	rBV	1567010	2195801	25.33%	5.353%
11	8.148	571	574	576	rBV	706677	936507	10.80%	2.283%
12	9.222	665	668	671	rBV	3115787	3498626	40.35%	8.529%
13	9.611	700	702	705	rBV	195967	218307	2.52%	0.532%
14	9.896	724	727	730	rBV	1162659	1072951	12.38%	2.616%
15	10.685	793	796	799	rBV	1983519	2082393	24.02%	5.076%
16	11.382	854	857	859	rBV	1065300	1094083	12.62%	2.667%
17	12.800	978	981	983	rBV	93221	116279	1.34%	0.283%
18	12.971	993	996	998	rBV	3135761	3257283	37.57%	7.940%
19	14.011	1084	1087	1089	rBV	946113	864625	9.97%	2.108%
20	15.440	1209	1212	1215	rBV	547629	664303	7.66%	1.619%

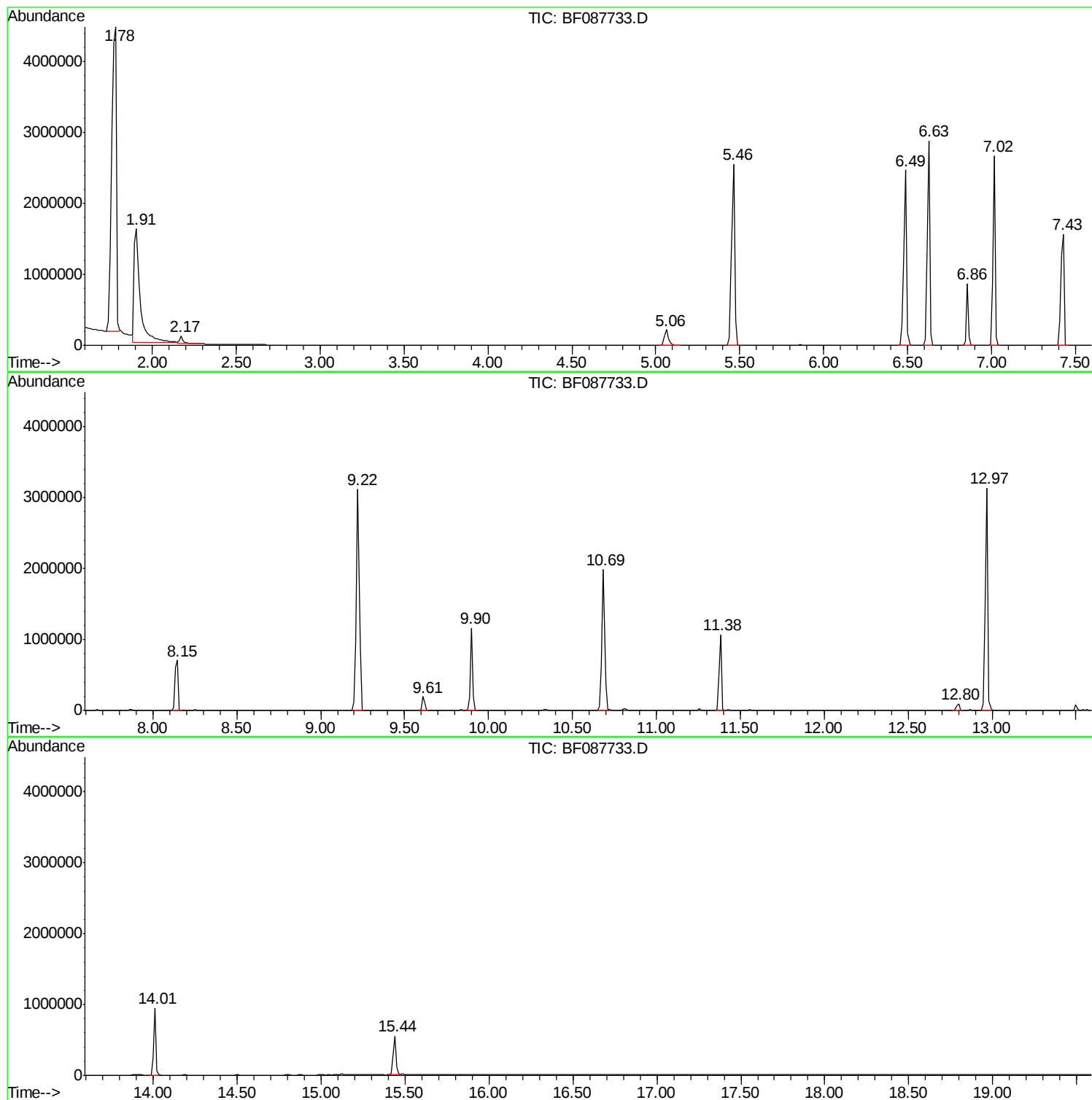
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ClientSampled :
SB-10

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF060416.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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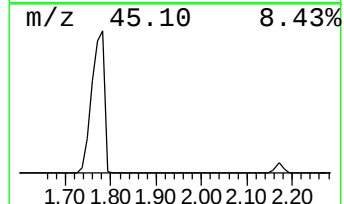
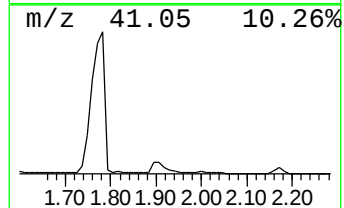
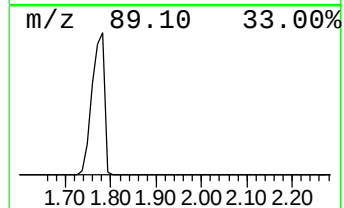
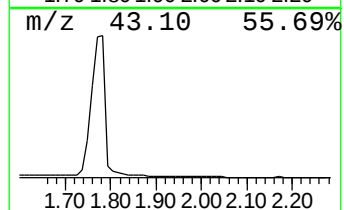
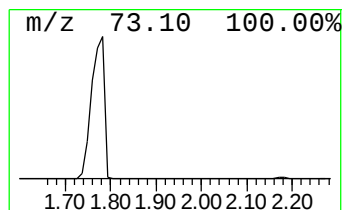
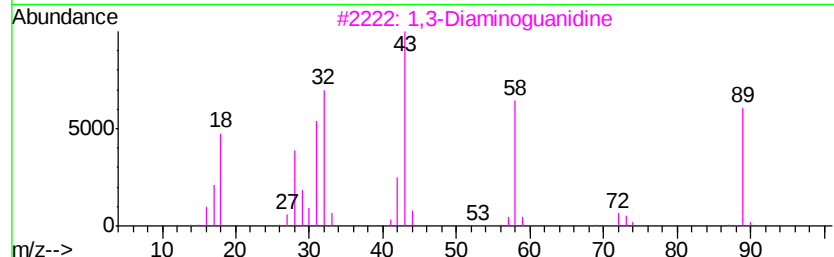
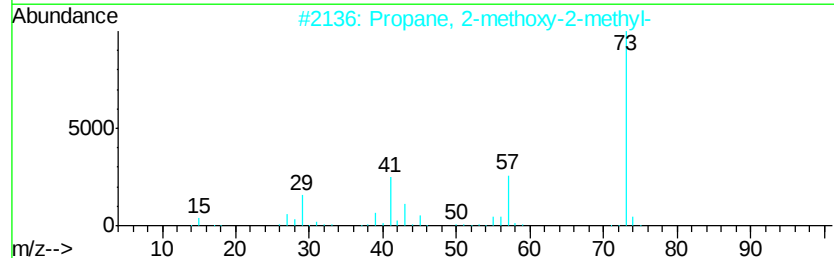
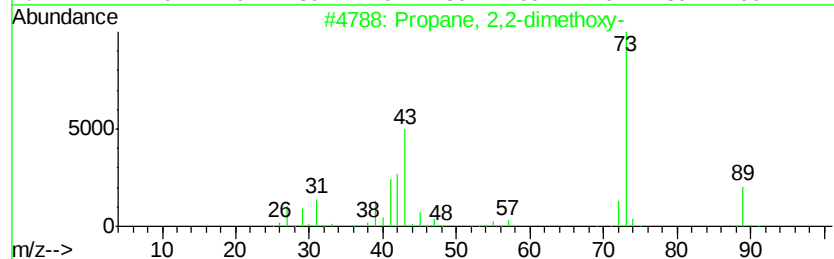
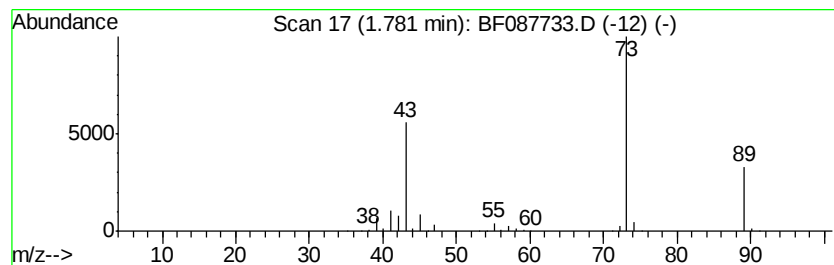
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.78	242.31 ng	8670230	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	56
2		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	17
3		1,3-Diaminoquanidine	89	CH7N5	004364-78-7	9
4		N-Ethylformamide	73	C3H7NO	000627-45-2	9
5		2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9



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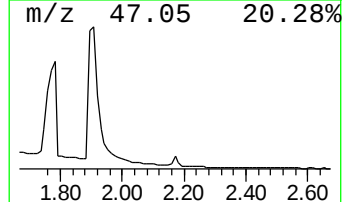
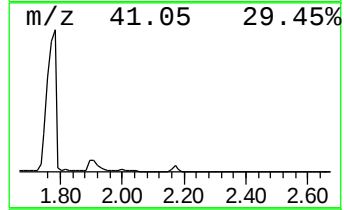
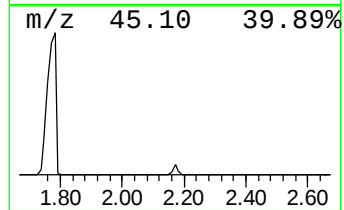
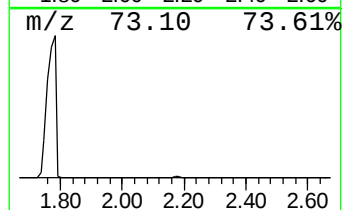
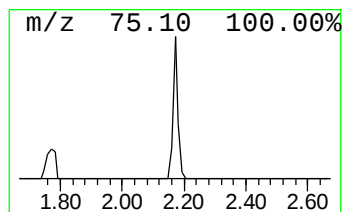
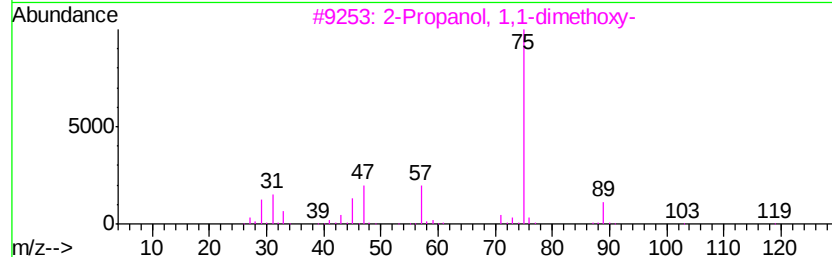
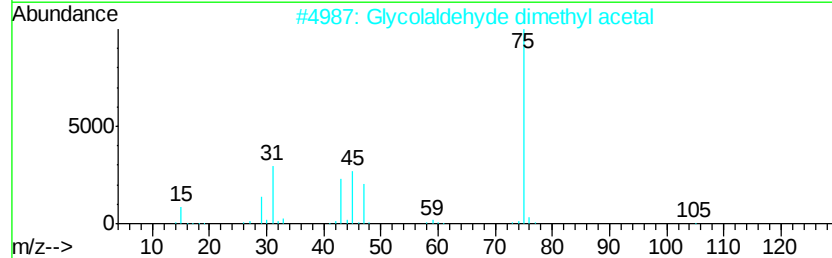
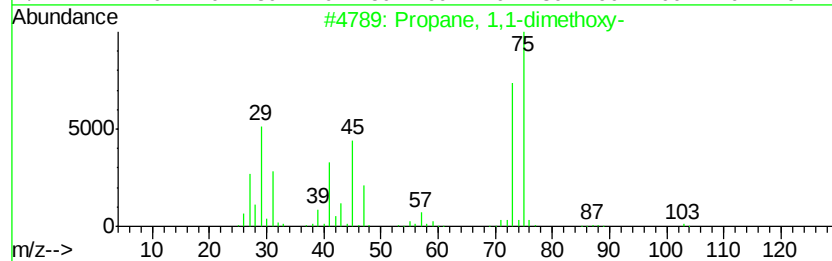
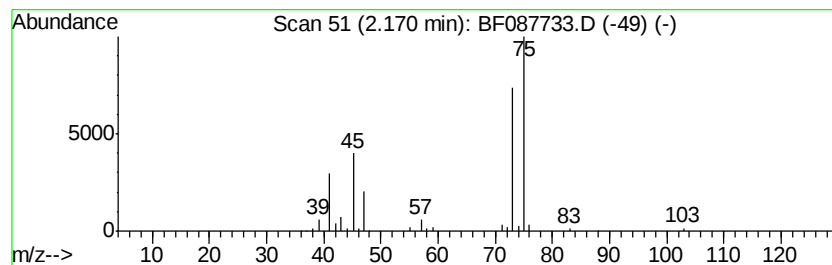
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TIC Integration Parameters: LSCINT.P

Peak Number 3 Propane, 1,1-dimethoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.17	5.13 ng	183620	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	64
2		Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	50
3		2-Propanol, 1,1-dimethoxy-	120	C5H12O3	042919-42-6	42
4		Ethane, 1,1,2-trimethoxy-	120	C5H12O3	024332-20-5	28
5		1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	27



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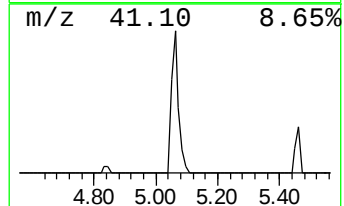
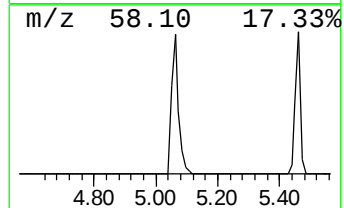
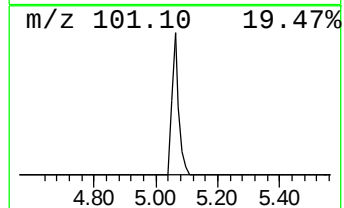
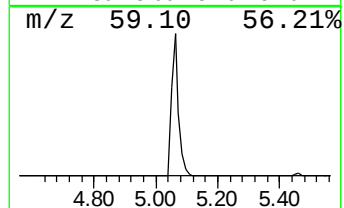
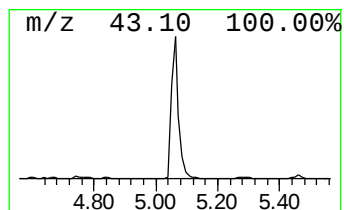
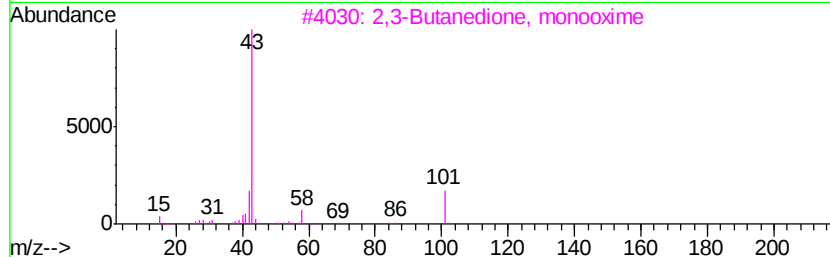
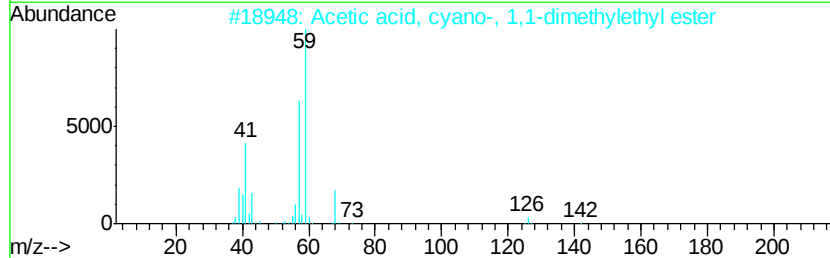
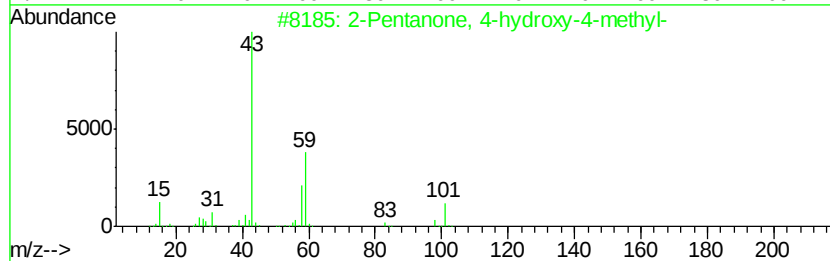
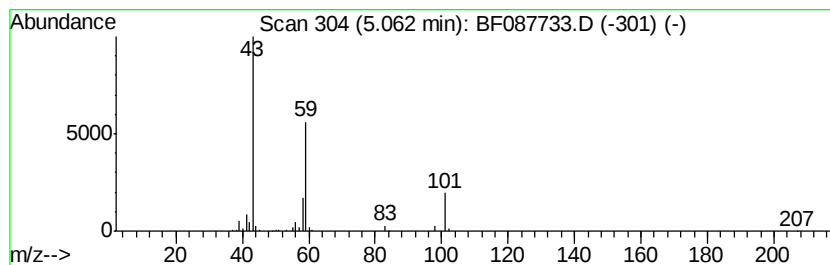
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Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.06	9.52 ng	340559	1,4-Dichlorobenzene-d4	6.86

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53	
2	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17	
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9	
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9	
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9	



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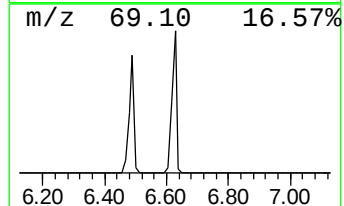
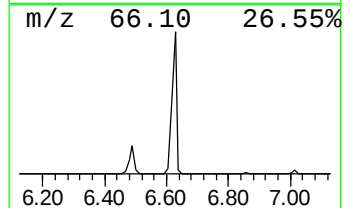
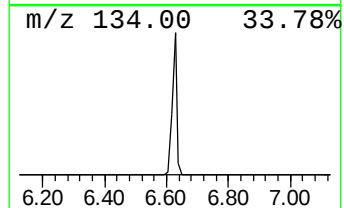
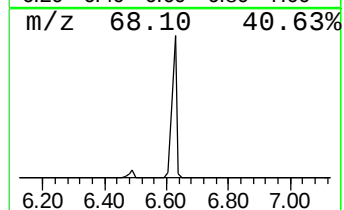
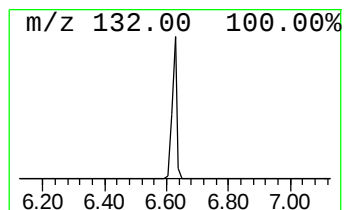
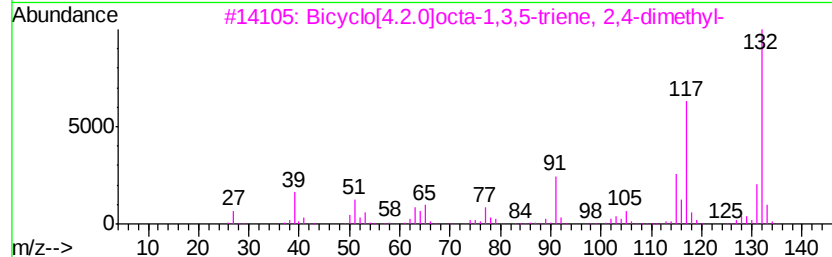
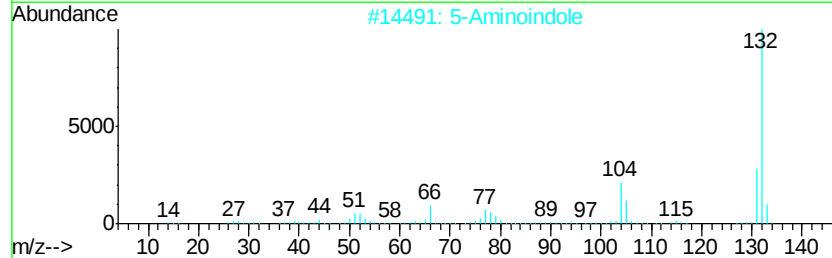
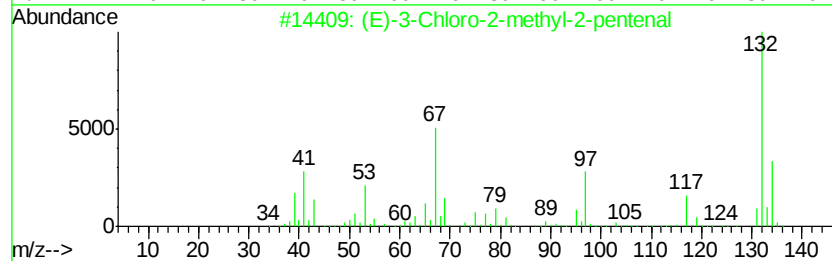
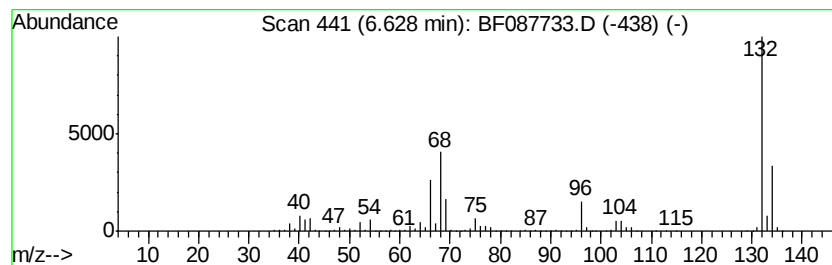
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Peak Number 5 unknown6.63 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	85.93 ng	3074680	1,4-Dichlorobenzene-d4	6.86

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
2			5-Aminoindole	132	C8H8N2	005192-03-0	12
3			Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4			4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5			4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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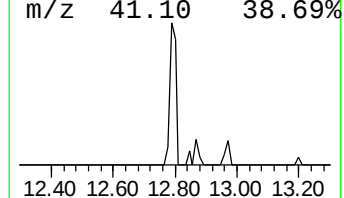
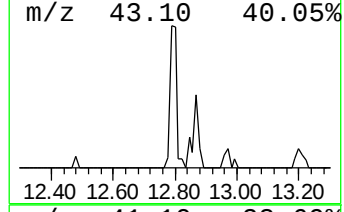
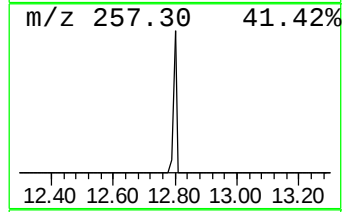
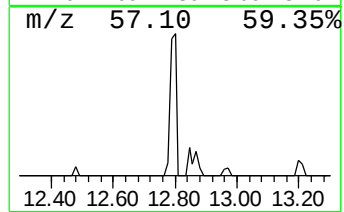
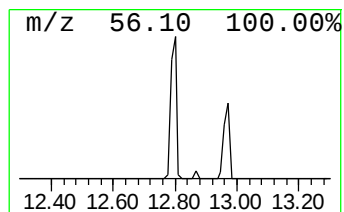
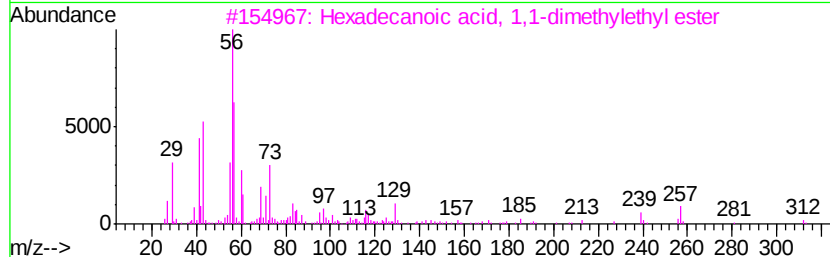
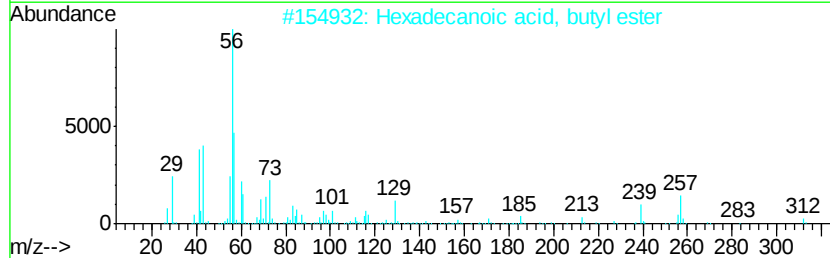
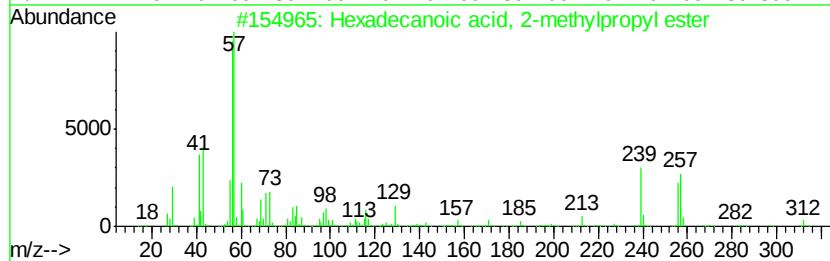
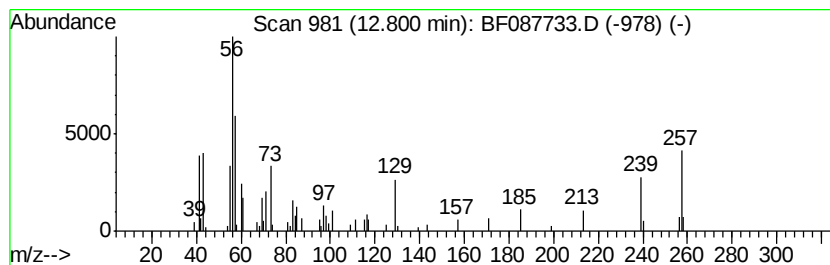
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TIC Library : C:\Database\NIST11.L
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Peak Number 7 Hexadecanoic acid, 2-methyl... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.80	2.69 ng	116279	Chrysene-d12	14.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, 2-methylpropyl...	312	C20H40O2	000110-34-9	64
2		Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	58
3		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	49
4		Nipecotic acid	129	C6H11NO2	000498-95-3	38
5		1-Hexene, 2-methyl-	98	C7H14	006094-02-6	22



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 2,2-dime...	1.78	242.3	ng	8670230	1	6.86	715638	20.0
Propane, 1,1-dime...	2.17	5.1	ng	183620	1	6.86	715638	20.0
2-Pentanone, 4-hy...	5.06	9.5	ng	340559	1	6.86	715638	20.0
unknown6.63	6.63	85.9	ng	3074680	1	6.86	715638	20.0
Hexadecanoic acid...	12.80	2.7	ng	116279	5	14.01	864625	20.0