

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080115\
 Data File : BF080774.D
 Acq On : 1 Aug 2015 11:47
 Operator : TP/UM
 Sample : G3140-03
 Misc :
 ALS Vial : 63 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-3

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-BF073015.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	2.190	6	9	16	rBV	64250	87868	1.73%	0.199%
2	4.407	201	203	208	rVB	158361	182900	3.60%	0.414%
3	5.058	256	260	268	rBV	2376637	3964371	77.96%	8.965%
4	5.458	292	295	298	rBV	3183663	4656254	91.56%	10.529%
5	5.859	328	330	333	rVB	124507	156727	3.08%	0.354%
6	6.487	381	385	387	rBV	3702197	5085394	100.00%	11.500%
7	6.624	394	397	399	rBV	3822273	4780771	94.01%	10.811%
8	6.853	414	417	419	rBV	1090275	975265	19.18%	2.205%
9	7.013	428	431	433	rBV	2296886	3190244	62.73%	7.214%
10	7.413	463	466	468	rBV	2901028	3007665	59.14%	6.801%
11	8.133	526	529	531	rBV	1237311	1212393	23.84%	2.742%
12	9.207	620	623	626	rBV	3938025	4488040	88.25%	10.149%
13	9.607	655	658	660	rBV	1060981	1155159	22.72%	2.612%
14	9.882	679	682	685	rBV	1276674	1291404	25.39%	2.920%
15	10.670	748	751	753	rBV	3014477	3121840	61.39%	7.060%
16	10.796	760	762	765	rVB	50973	62660	1.23%	0.142%
17	11.242	799	801	802	rBV	61692	55037	1.08%	0.124%
18	11.368	809	812	814	rBV	1088801	1250414	24.59%	2.828%
19	11.893	856	858	863	rBV	110469	151297	2.98%	0.342%
20	12.682	925	927	933	rBV	40633	53153	1.05%	0.120%
21	12.774	933	935	937	rVB	64707	58514	1.15%	0.132%
22	12.945	948	950	953	rBV	2889441	3788865	74.50%	8.568%
23	13.985	1039	1041	1044	rBV	643746	781776	15.37%	1.768%
24	15.402	1162	1165	1168	rBV	495096	663094	13.04%	1.499%

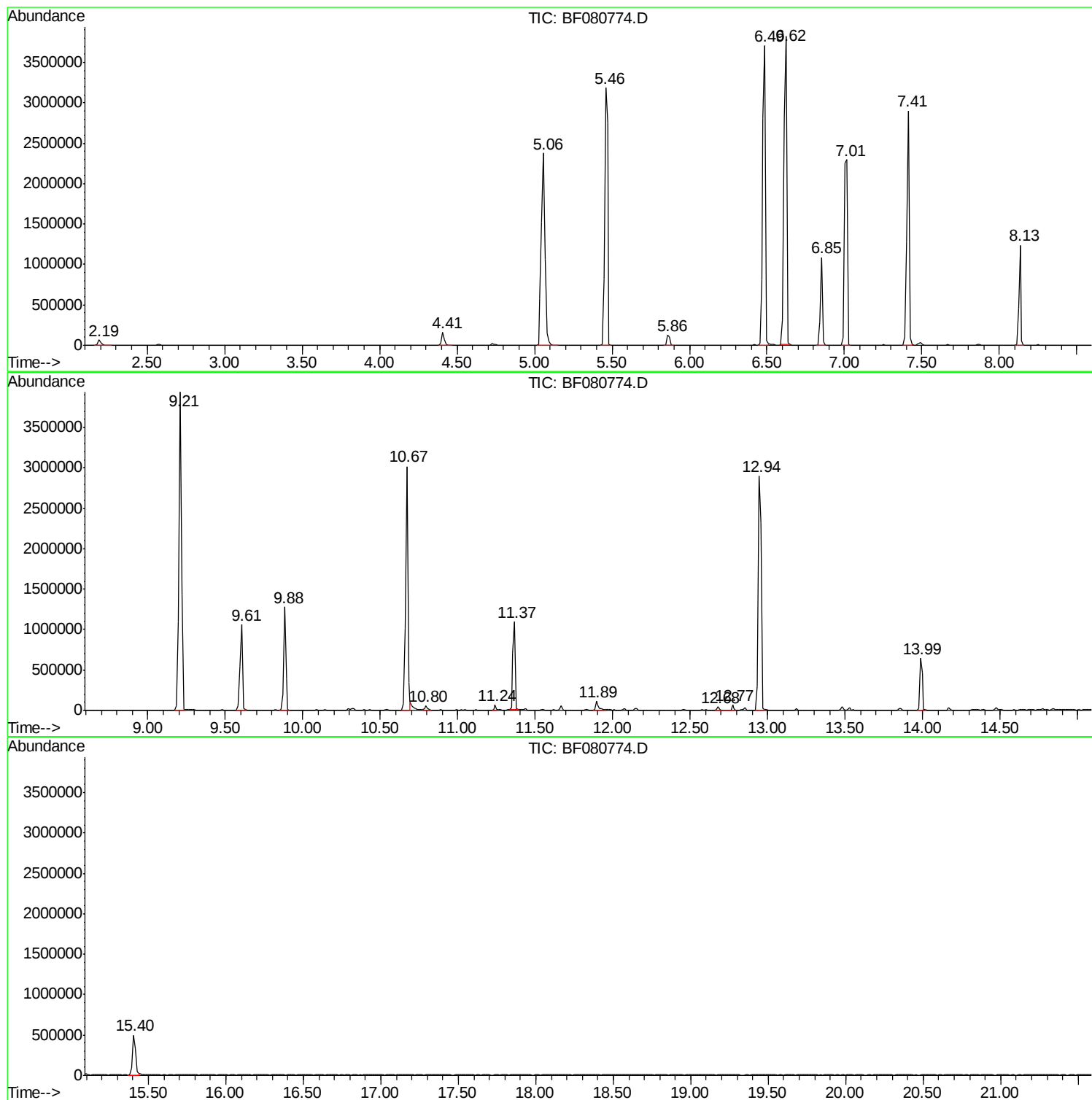
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF073015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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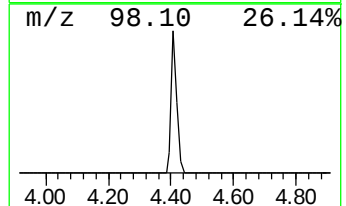
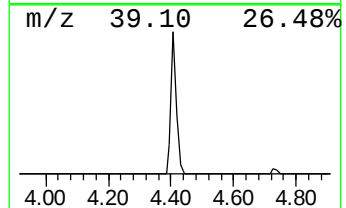
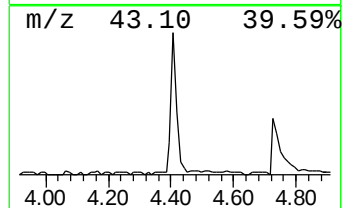
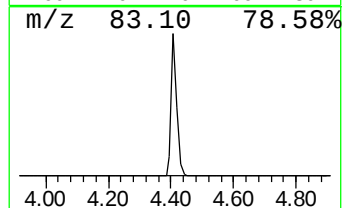
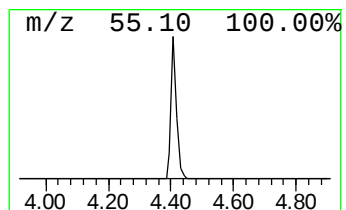
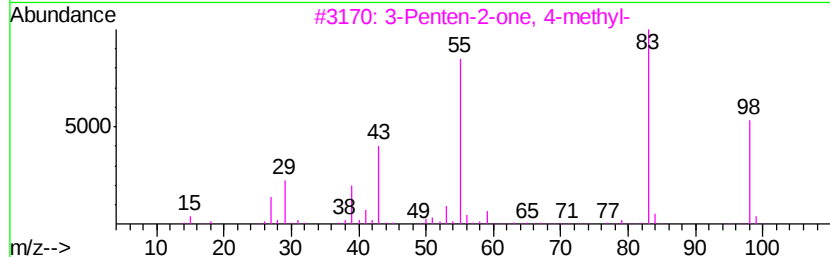
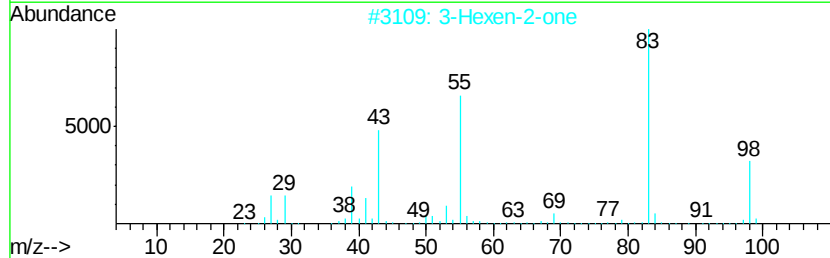
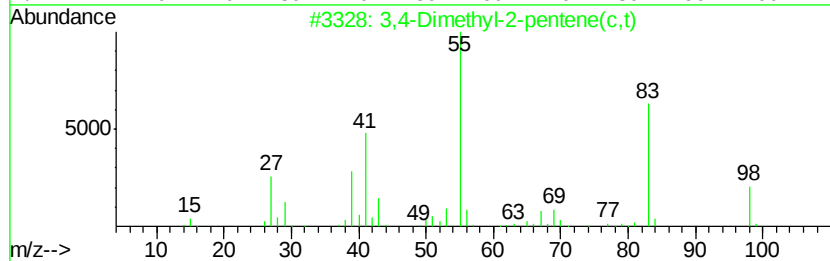
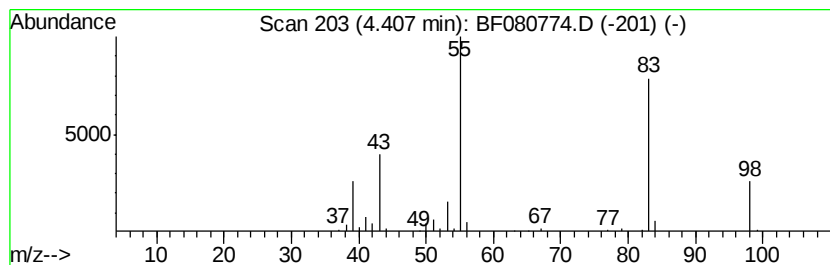
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF073015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3,4-Dimethyl-2-pentene(c,t) Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.41	3.75 ng	182900	1,4-Dichlorobenzene-d4	6.85

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3,4-Dimethyl-2-pentene(c,t)	98	C7H14	1000118-16-5	86
2			3-Hexen-2-one	98	C6H10O	000763-93-9	80
3			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	78
4			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	78
5			2-Pentene, 3,4-dimethyl-	98	C7H14	024910-63-2	64



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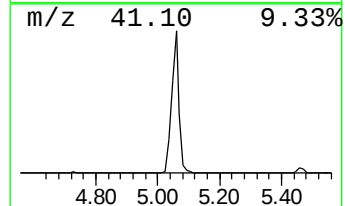
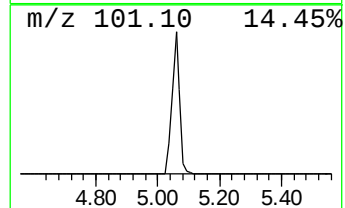
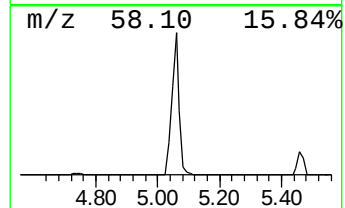
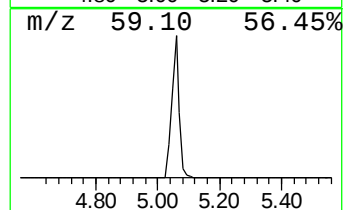
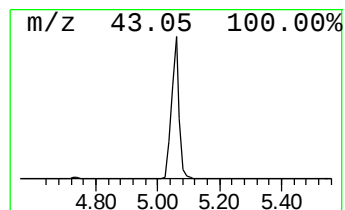
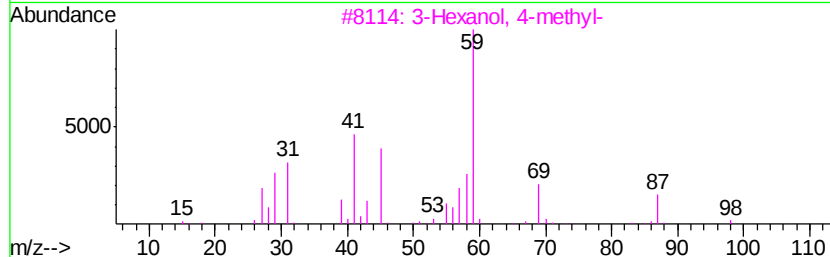
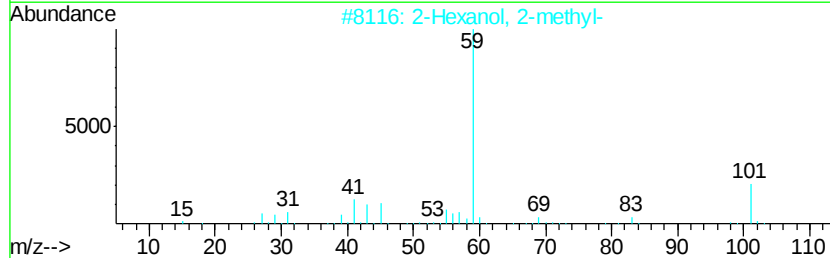
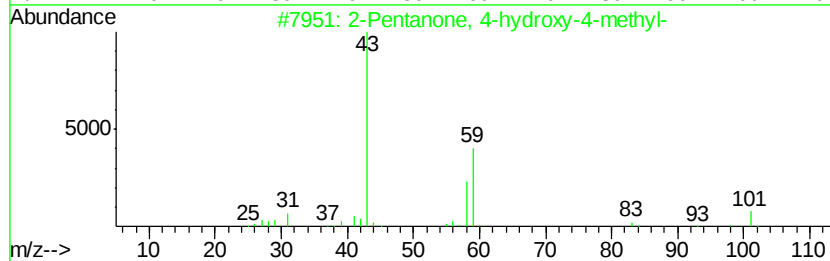
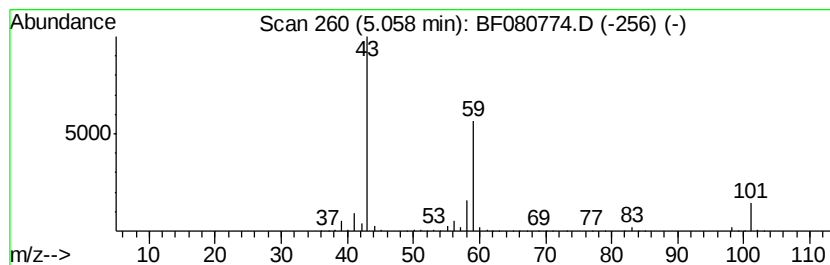
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.		
5.06	81.30 ng	3964370	1,4-Dichlorobenzene-d4	6.85		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64	
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33	
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33	
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28	
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25	



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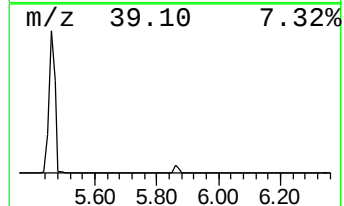
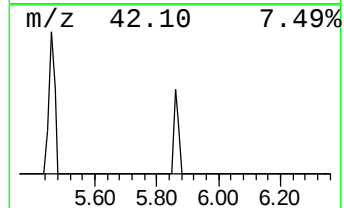
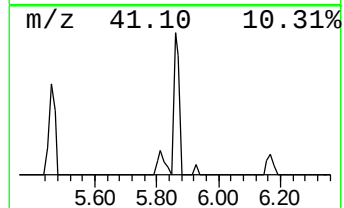
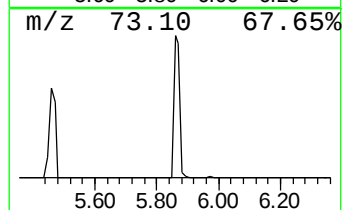
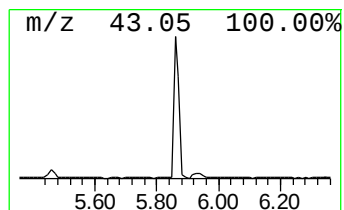
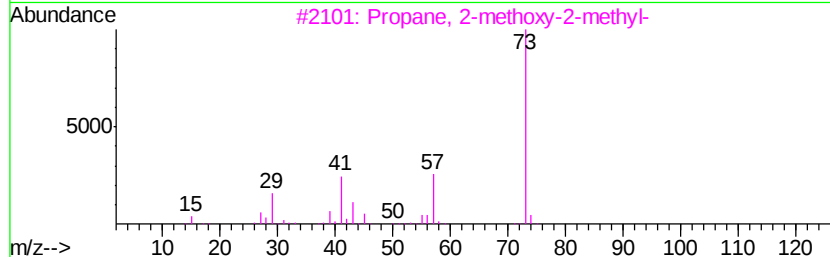
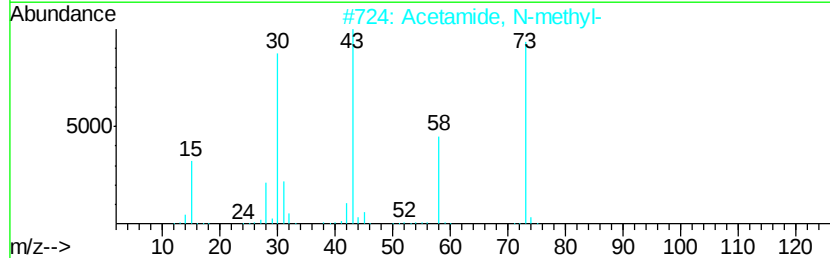
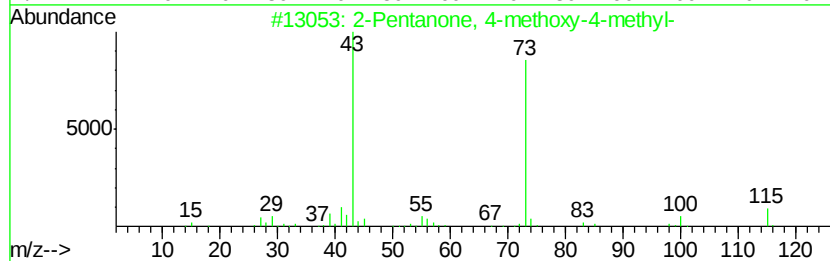
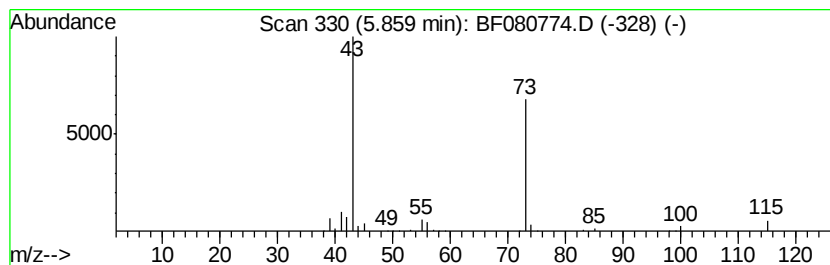
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Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.86	3.21 ng	156727	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	78
2		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	47
3		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	17
4		N,N'-Bis(2-methyl-2-nitrosopenta...	258	C12H22N2O4	094514-30-4	12
5		1,3-Dioxolane, 2-ethenyl-	100	C5H8O2	003984-22-3	9



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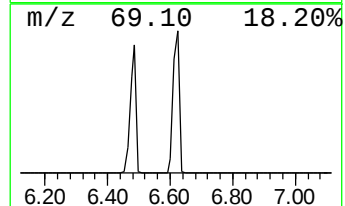
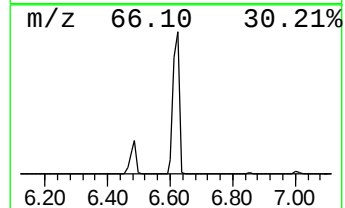
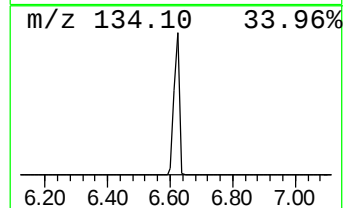
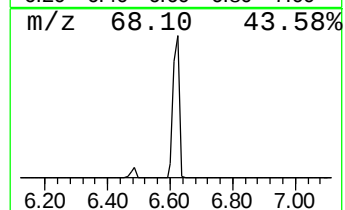
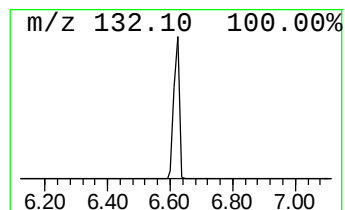
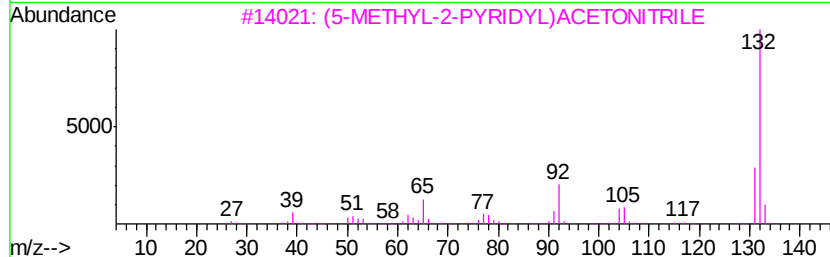
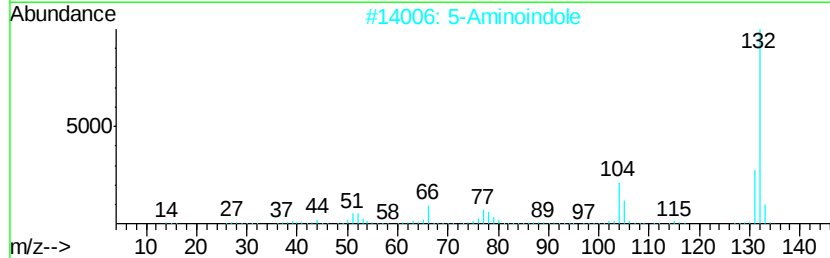
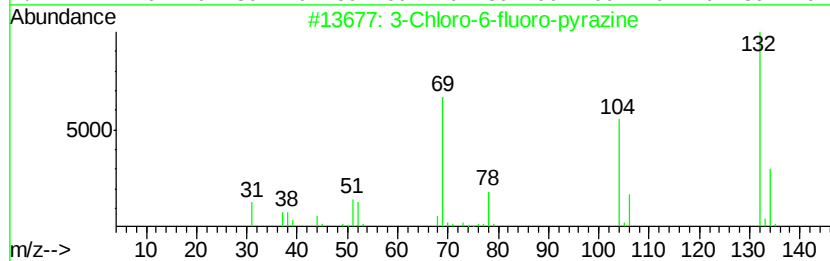
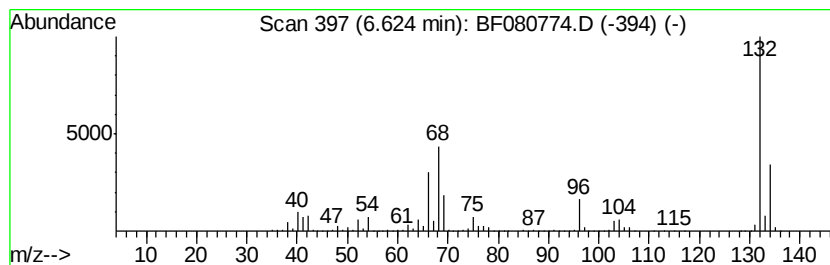
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Peak Number 4 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	98.04 ng	4780770	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9



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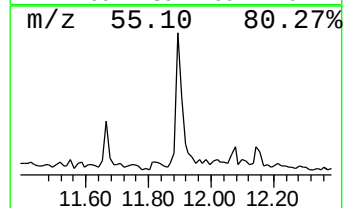
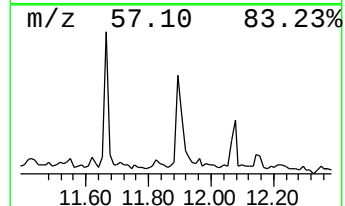
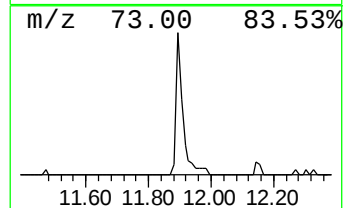
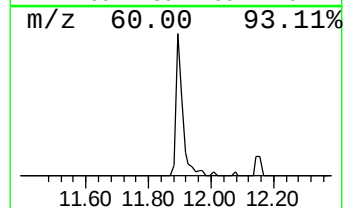
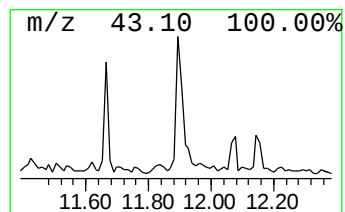
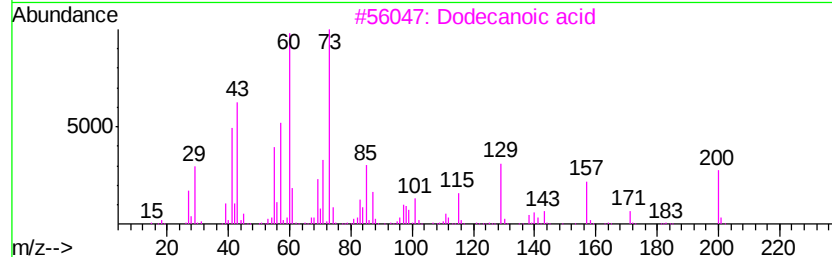
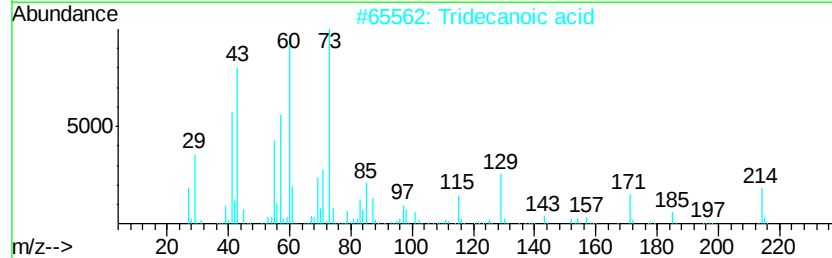
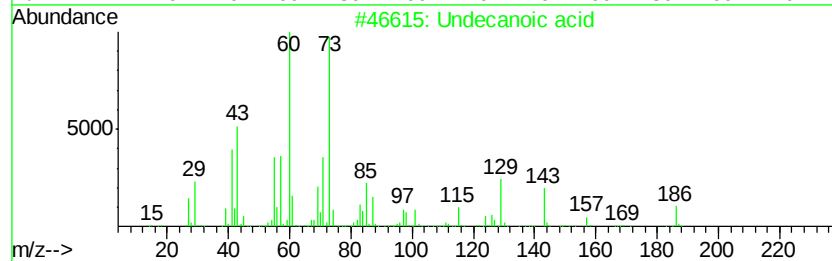
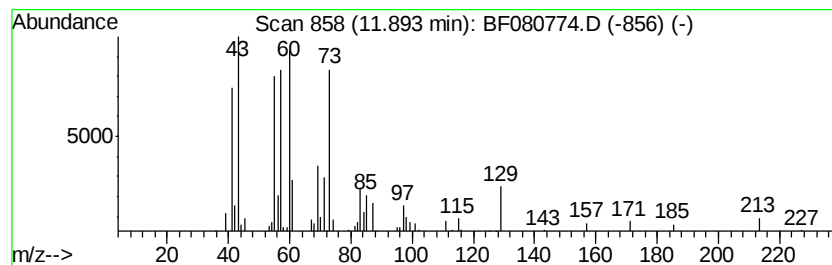
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Undecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.89	2.42 ng	151297	Phenanthrene-d10		11.37
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid	186	C11H22O2	000112-37-8	86
2	Tridecanoic acid	214	C13H26O2	000638-53-9	86
3	Dodecanoic acid	200	C12H24O2	000143-07-7	47
4	n-Decanoic acid	172	C10H20O2	000334-48-5	38
5	Methyl 2,6-anhydro-.alpha.-d-alt...	176	C7H12O5	1000130-02-0	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3,4-Dimethyl-2-pe...	4.41	3.8	ng	182900	1	6.85	975265	20.0
2-Pentanone, 4-hy...	5.06	81.3	ng	3964370	1	6.85	975265	20.0
2-Pentanone, 4-me...	5.86	3.2	ng	156727	1	6.85	975265	20.0
unknown6.62	6.62	98.0	ng	4780770	1	6.85	975265	20.0
Undecanoic acid	11.89	2.4	ng	151297	4	11.37	1250410	20.0