

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080115\
 Data File : BF080773.D
 Acq On : 1 Aug 2015 11:16
 Operator : TP/UM
 Sample : PB84692TB
 Misc :
 ALS Vial : 62 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB84692TB

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	4.430	201	205	208	rBV	3133628	5276372	76.51%	10.694%
2	5.081	257	262	264	rBV	3791826	6896694	100.00%	13.978%
3	5.470	293	296	298	rBV	4069650	4351681	63.10%	8.820%
4	5.870	328	331	333	rBV	362426	369292	5.35%	0.748%
5	6.476	381	384	387	rBV	2922105	4003396	58.05%	8.114%
6	6.613	394	396	399	rBV	2918117	4136004	59.97%	8.383%
7	6.853	415	417	419	rVB	942355	916042	13.28%	1.857%
8	7.002	428	430	433	rBV	2384571	3001379	43.52%	6.083%
9	7.413	463	466	468	rBV	2660920	2847575	41.29%	5.771%
10	8.133	526	529	531	rBV	1212450	1188889	17.24%	2.410%
11	9.208	620	623	626	rBV	3693090	4276618	62.01%	8.668%
12	9.882	679	682	685	rBV	1255134	1249638	18.12%	2.533%
13	10.671	748	751	753	rBV	3000186	3027915	43.90%	6.137%
14	11.368	809	812	814	rBV	1154016	1317673	19.11%	2.671%
15	12.774	933	935	938	rBV	334567	321917	4.67%	0.652%
16	12.957	948	951	953	rBV	3227219	4444724	64.45%	9.008%
17	13.482	995	997	999	rBV	263338	220513	3.20%	0.447%
18	13.985	1039	1041	1044	rBV	632030	845344	12.26%	1.713%
19	15.403	1162	1165	1168	rBV	489330	647846	9.39%	1.313%

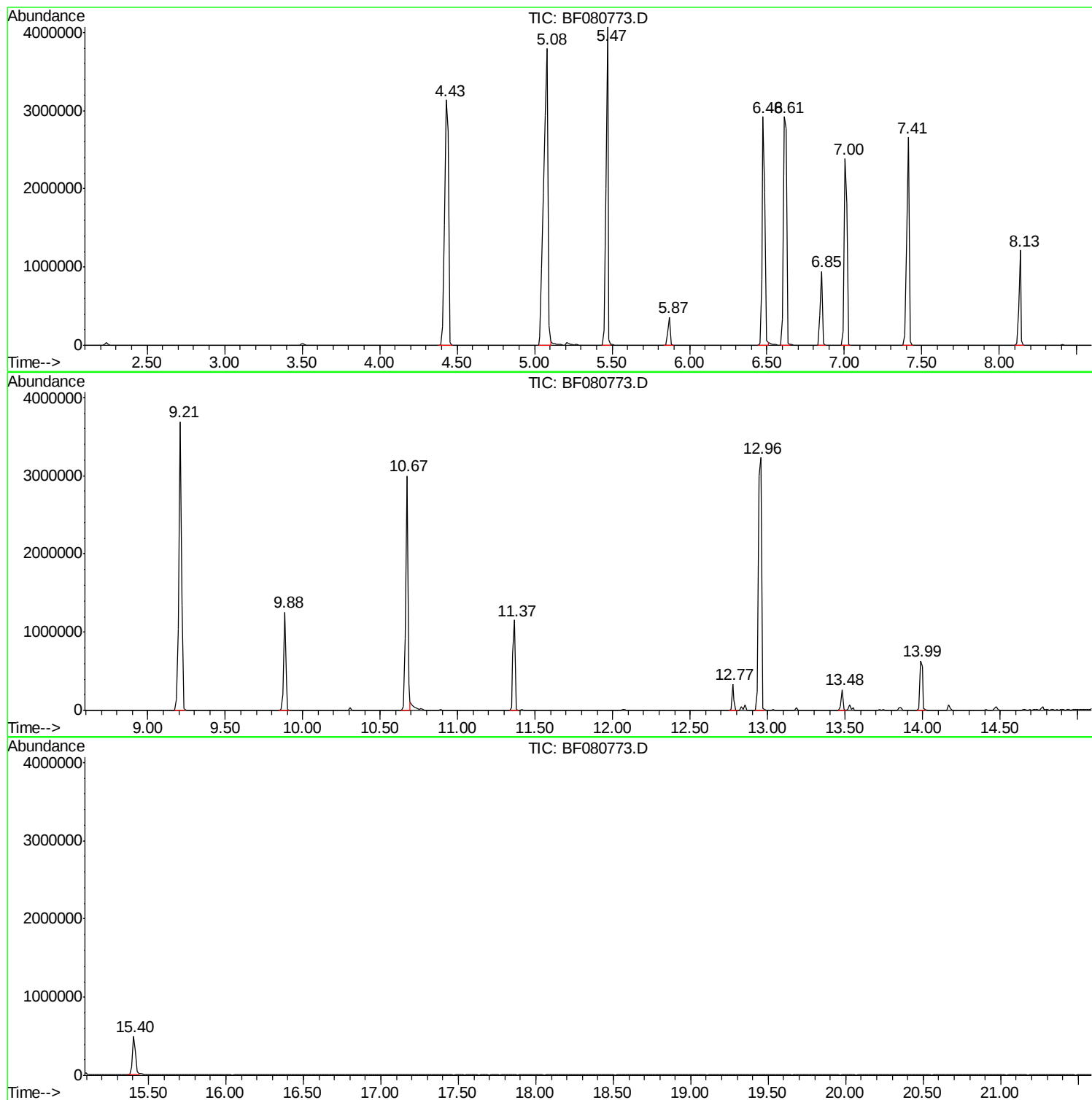
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF073015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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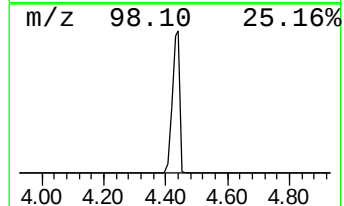
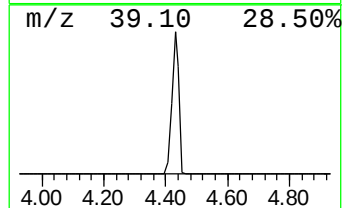
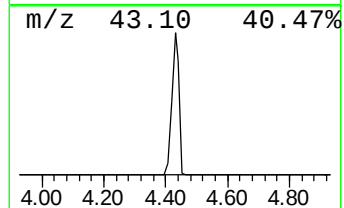
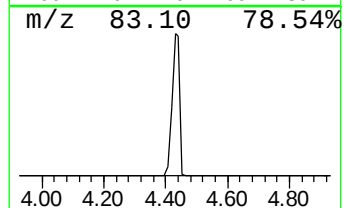
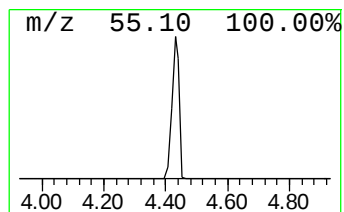
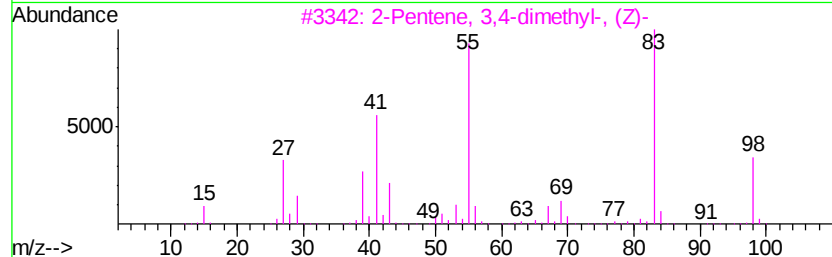
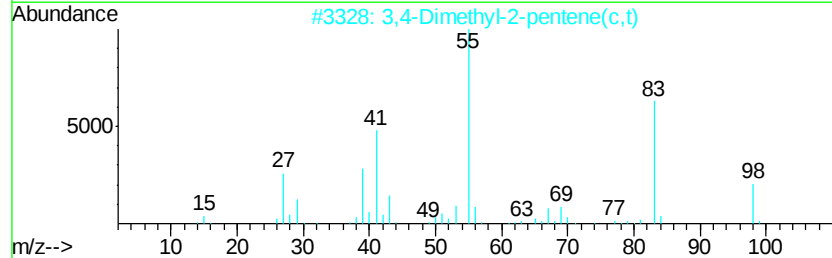
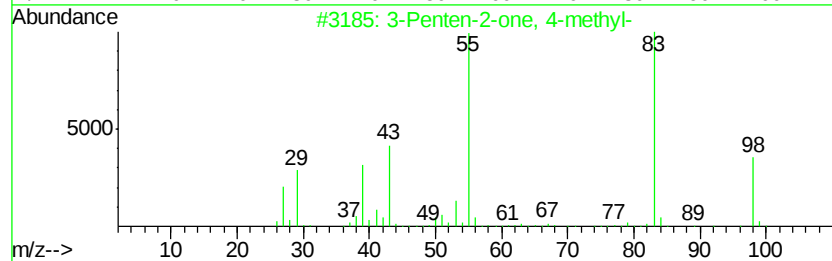
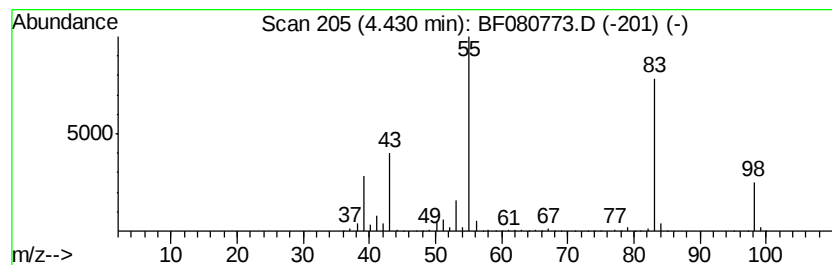
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.43	115.20 ng	5276370	1,4-Dichlorobenzene-d4	6.85

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	90
2			3,4-Dimethyl-2-pentene(c,t)	98	C7H14	1000118-16-5	86
3			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	80
4			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80
5			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	80



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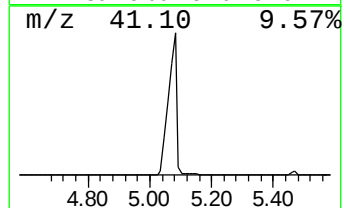
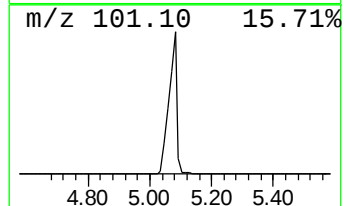
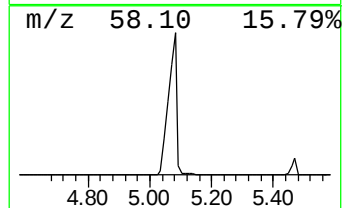
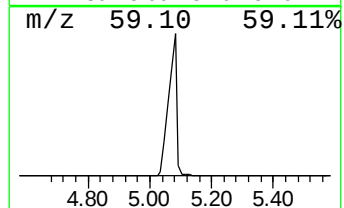
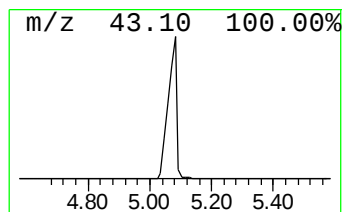
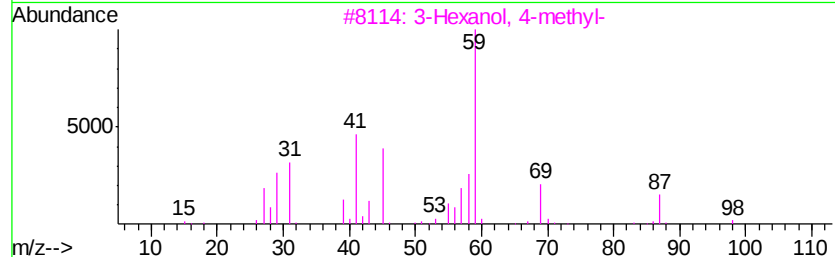
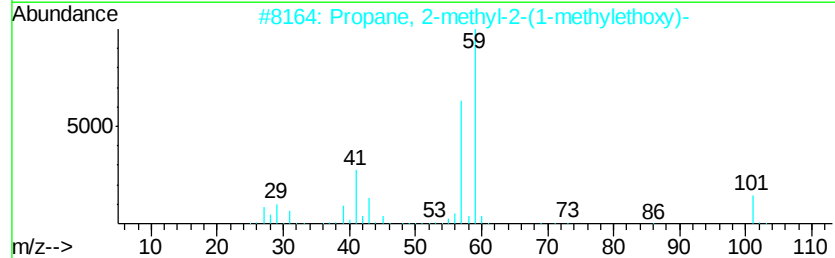
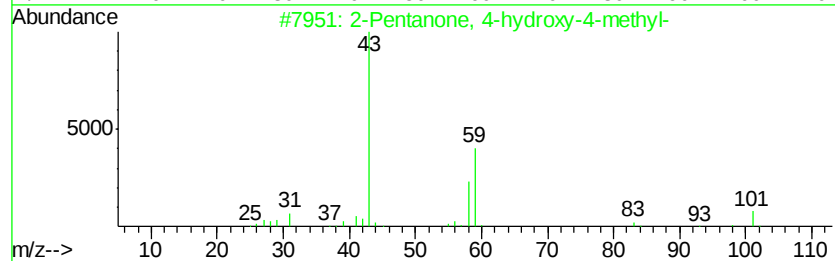
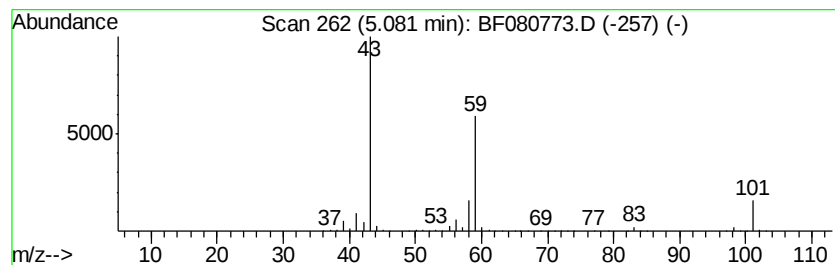
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.08	150.58 ng	6896690	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	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32



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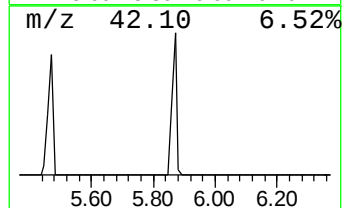
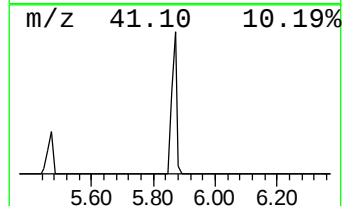
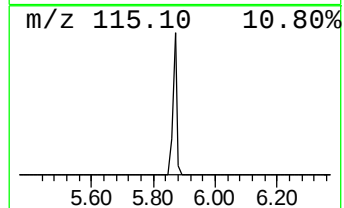
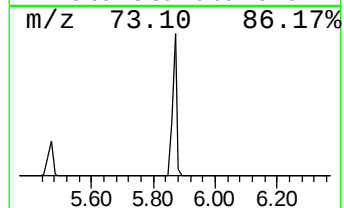
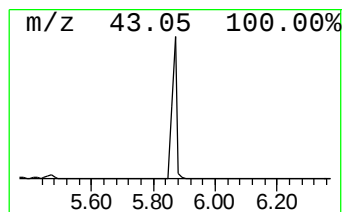
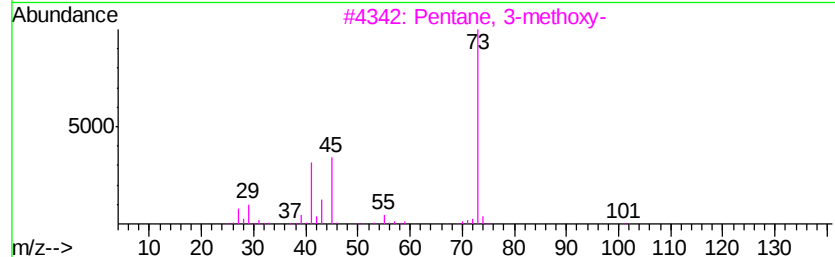
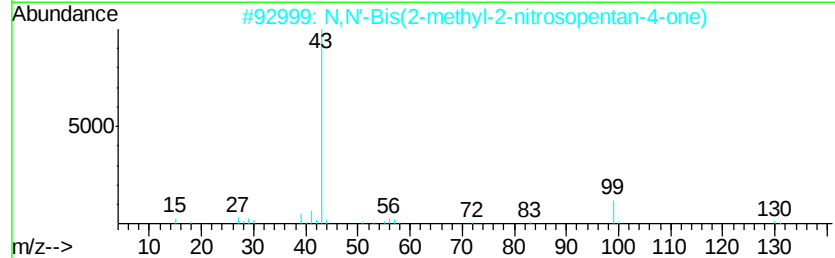
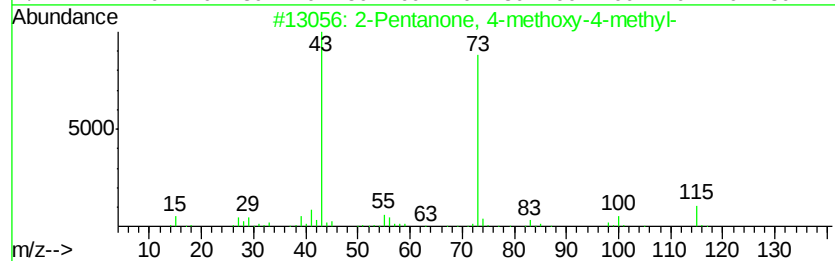
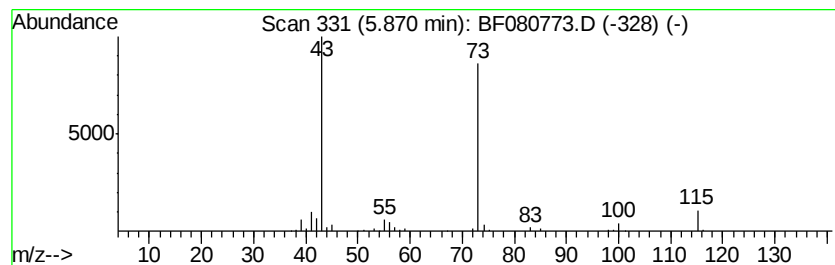
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Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.87	8.06 ng	369292	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	83
2		N,N'-Bis(2-methyl-2-nitrosopenta...	258	C12H22N2O4	094514-30-4	10
3		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	10
4		1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	9
5		4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9



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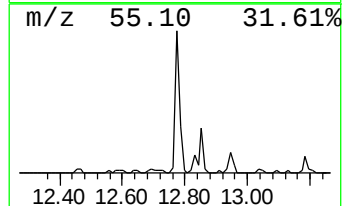
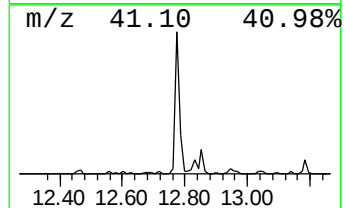
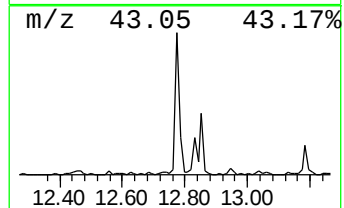
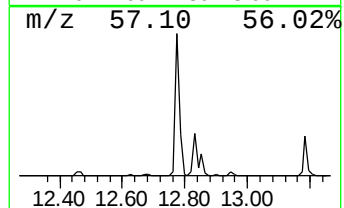
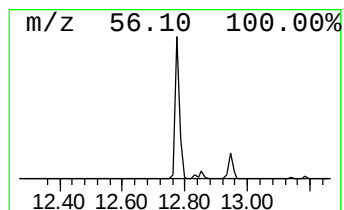
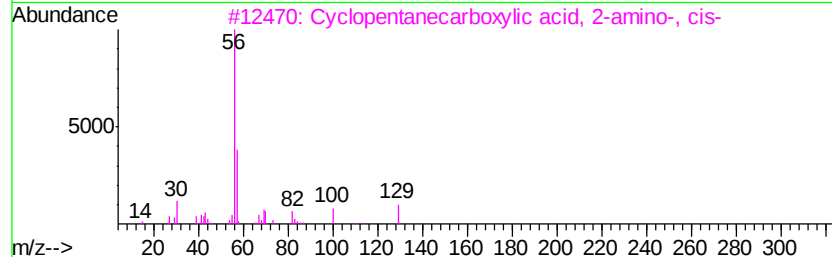
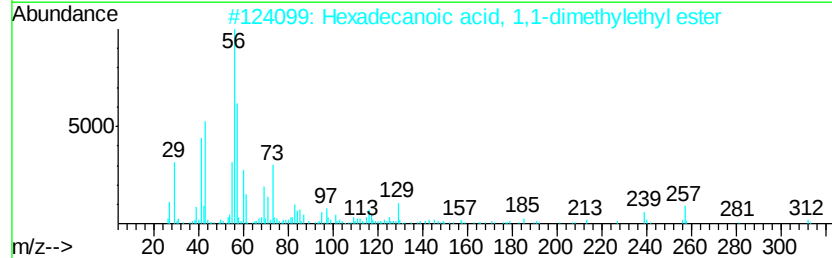
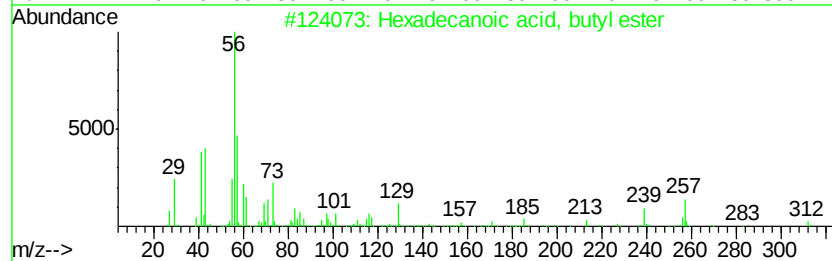
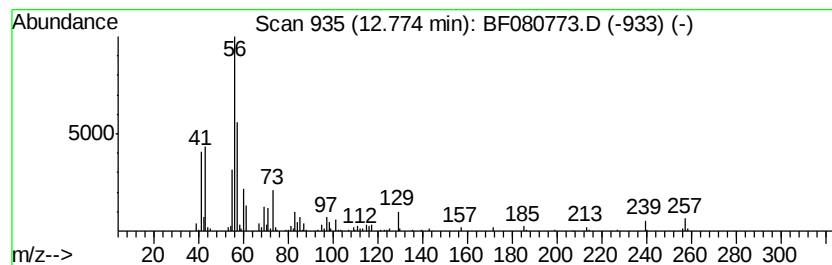
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Peak Number 6 Hexadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.77	7.62 ng	321917	Chrysene-d12	14.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	58
3		Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	037910-65-9	43
4		Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	43
5		Cyclopentanone, 2,2-dimethyl-	112	C7H12O	004541-32-6	38



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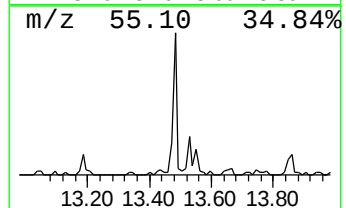
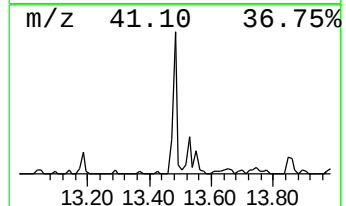
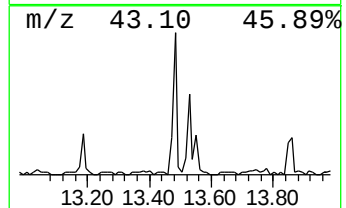
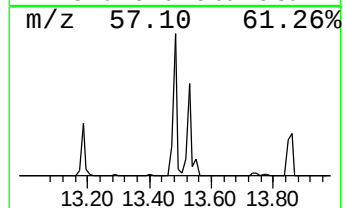
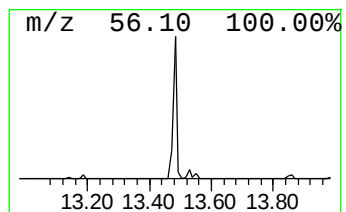
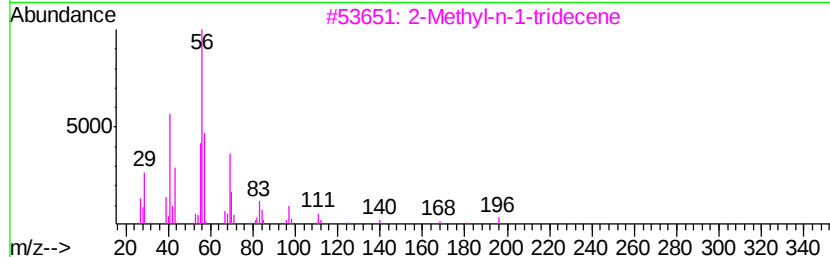
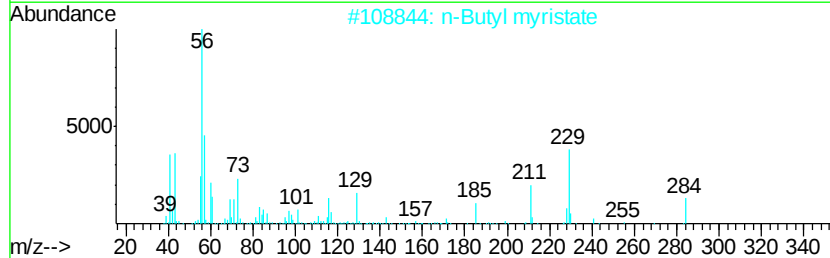
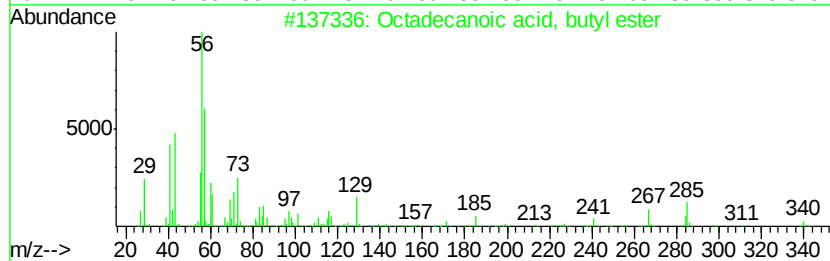
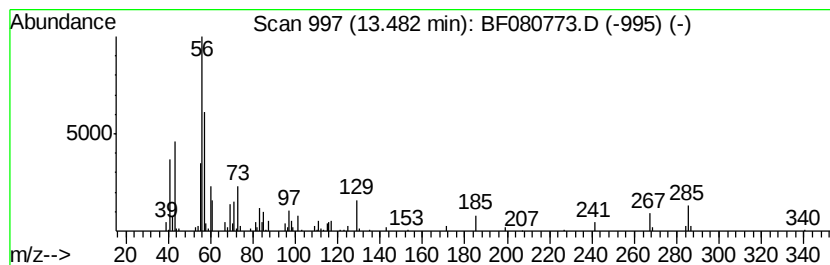
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Octadecanoic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.48	5.22 ng	220513	Chrysene-d12	14.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	91
2		n-Butyl myristate	284	C18H36O2	000110-36-1	83
3		2-Methyl-n-1-tridecene	196	C14H28	018094-01-4	38
4		Cyclopropane, 1-(1-methylethyl)-...	210	C15H30	041977-39-3	32
5		Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	32



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	4.43	115.2	ng	5276370	1	6.85	916042	20.0
2-Pentanone, 4-hy...	5.08	150.6	ng	6896690	1	6.85	916042	20.0
2-Pentanone, 4-me...	5.87	8.1	ng	369292	1	6.85	916042	20.0
Hexadecanoic acid...	12.77	7.6	ng	321917	5	14.00	845344	20.0
Octadecanoic acid...	13.48	5.2	ng	220513	5	14.00	845344	20.0