

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100724\
 Data File : BF139690.D
 Acq On : 07 Oct 2024 17:02
 Operator : RC/JU
 Sample : P4285-03
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WATER-TOTES

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:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF100124.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139690.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.157	3	11	17	rVB	4669645	8095240	98.82%	25.420%
2	2.569	70	81	88	rBV	3865398	8191576	100.00%	25.722%
3	5.487	571	577	588	rVB	969993	1261139	15.40%	3.960%
4	6.492	743	748	759	rBV	608113	814026	9.94%	2.556%
5	6.863	806	811	816	rBV	448345	547108	6.68%	1.718%
6	7.428	900	907	912	rBV	1359748	1823742	22.26%	5.727%
7	8.145	1024	1029	1036	rVV	556494	686424	8.38%	2.155%
8	8.910	1154	1159	1167	rVB	220230	274185	3.35%	0.861%
9	9.222	1206	1212	1217	rBV	2446690	3097437	37.81%	9.726%
10	9.898	1322	1327	1333	rVB	611868	761938	9.30%	2.393%
11	10.163	1367	1372	1389	rBV	127847	200832	2.45%	0.631%
12	10.692	1456	1462	1469	rBV	1399348	1833617	22.38%	5.758%
13	11.386	1575	1580	1587	rBV	607818	750381	9.16%	2.356%
14	11.910	1664	1669	1676	rBV	83223	135078	1.65%	0.424%
15	12.974	1844	1850	1855	rBV	1914585	2457573	30.00%	7.717%
16	14.027	2024	2029	2037	rVB	356545	454573	5.55%	1.427%
17	15.498	2273	2279	2289	rBV	311087	461235	5.63%	1.448%

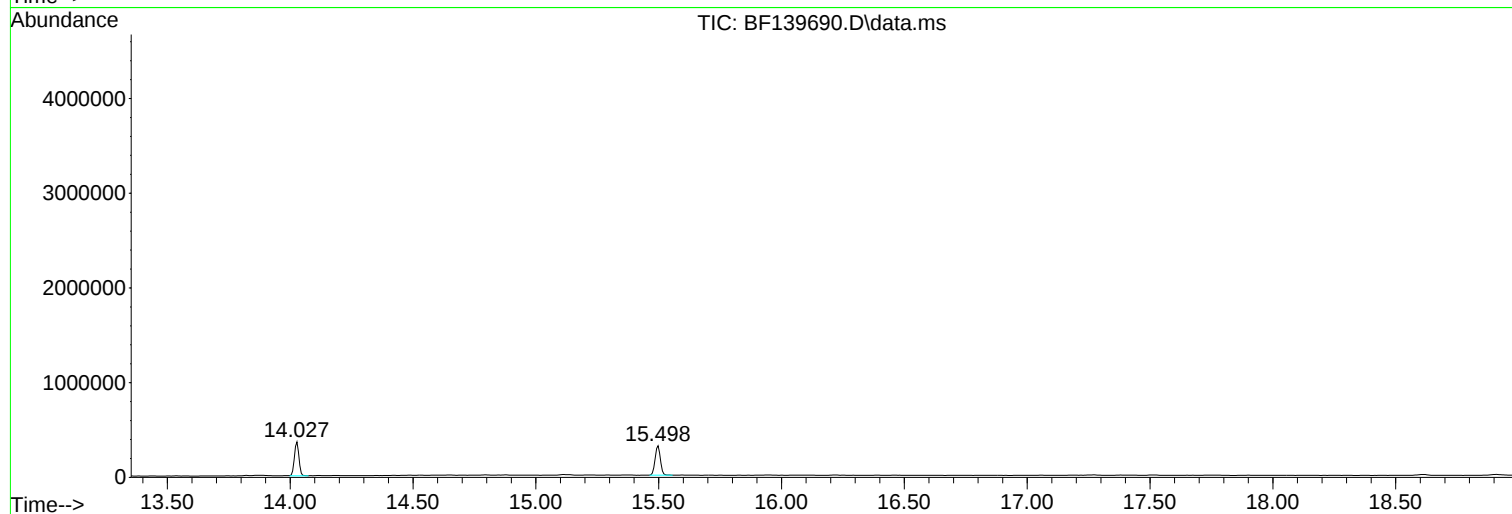
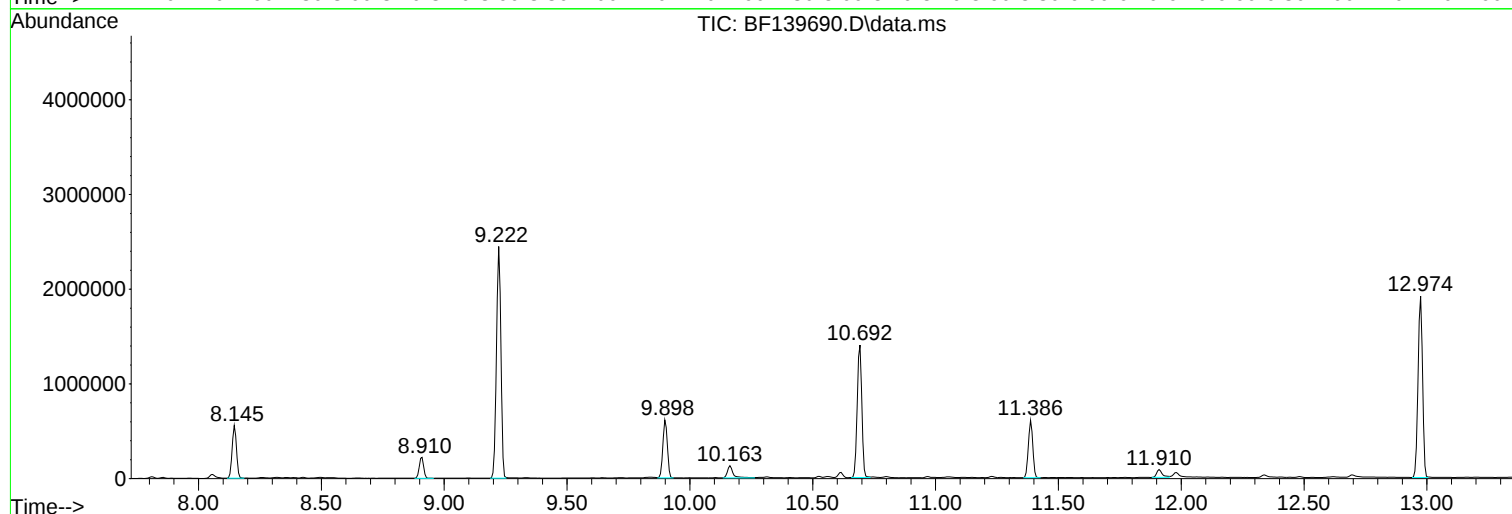
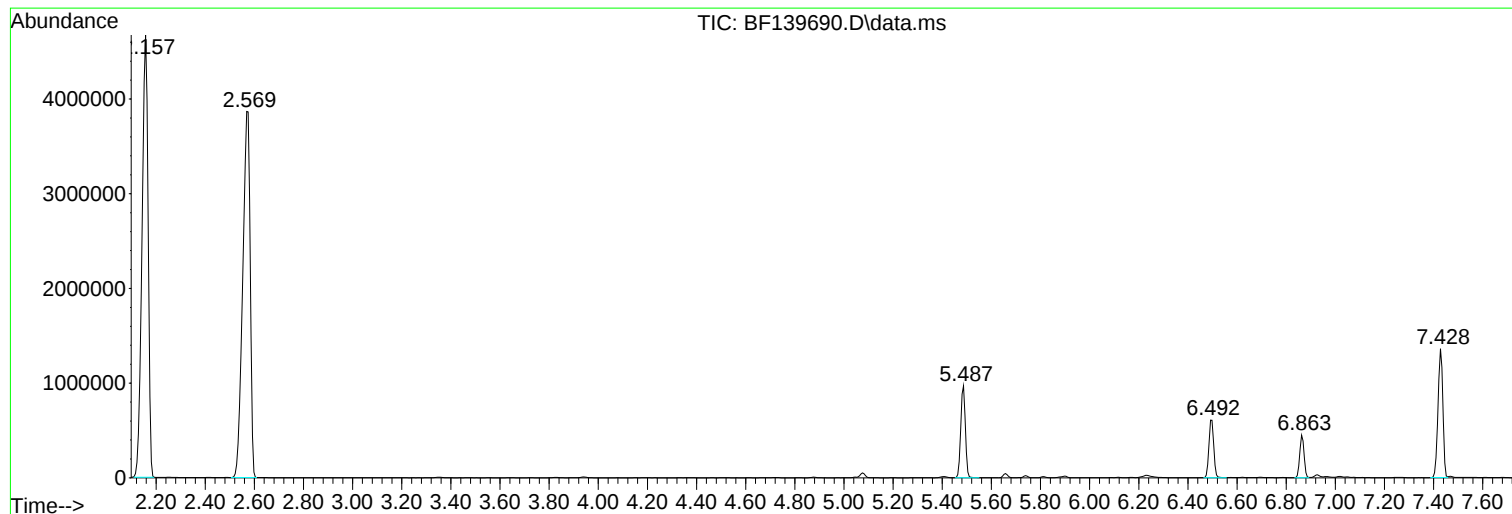
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF100124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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Instrument :
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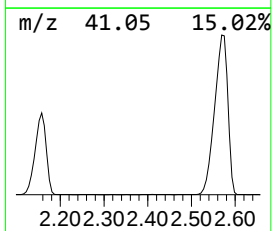
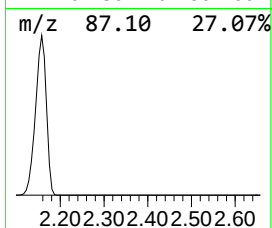
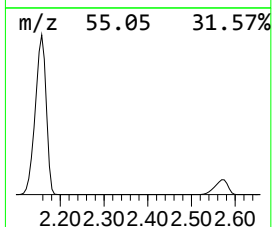
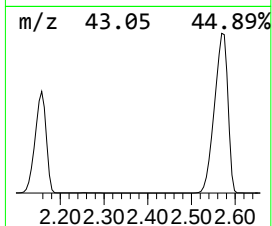
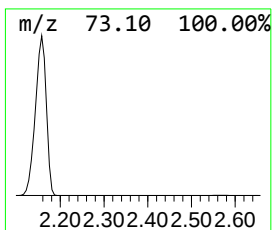
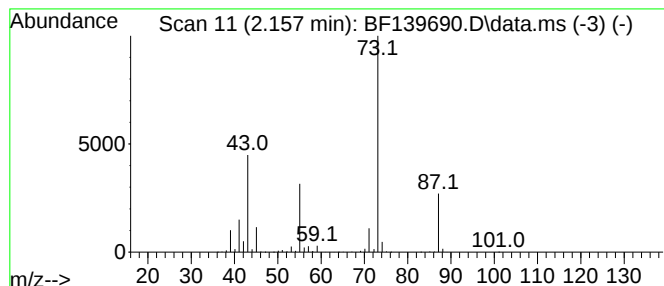
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.157	295.93 ng	8095240	1,4-Dichlorobenzene-d4	6.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



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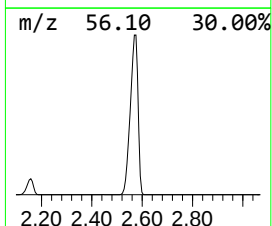
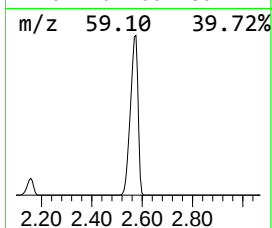
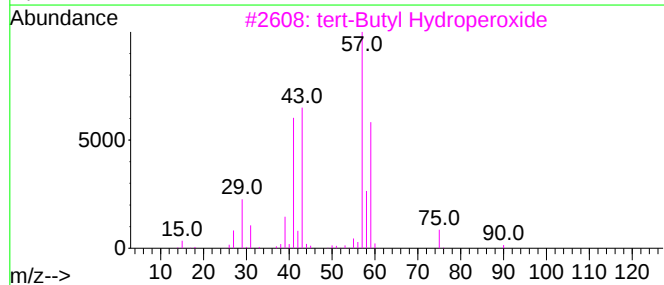
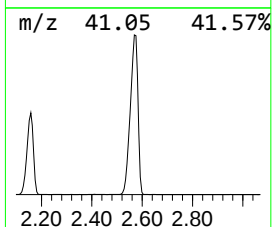
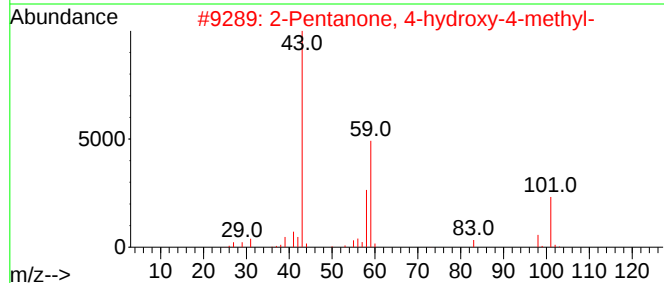
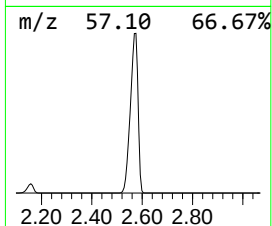
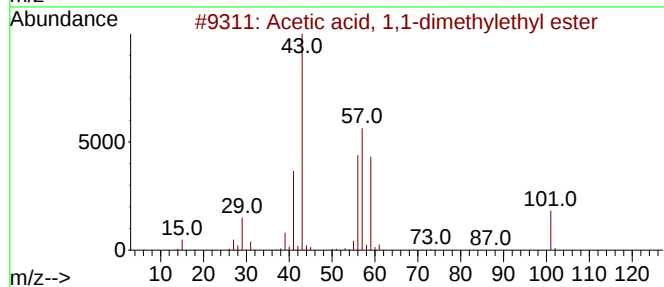
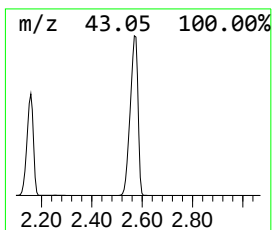
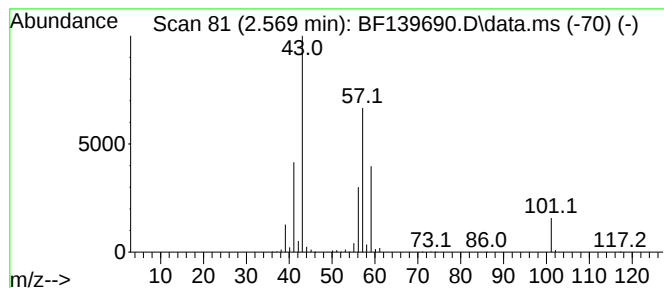
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF100124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Acetic acid, 1,1-dimethylet... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.569	299.45 ng	8191580	1,4-Dichlorobenzene-d4	6.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	83
2			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
3			tert-Butyl Hydroperoxide	90	C4H10O2	000075-91-2	28
4			Butyl isocyanatoacetate	157	C7H11NO3	017046-22-9	10
5			1-Butanol, 3,3-dimethyl-	102	C6H14O	000624-95-3	10



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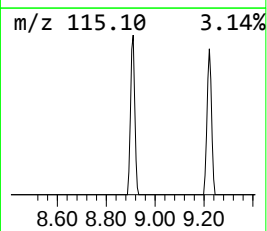
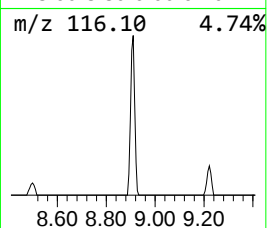
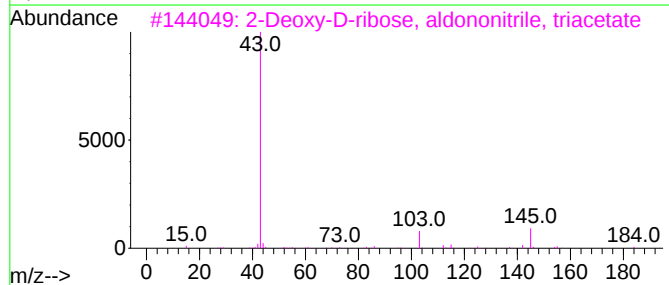
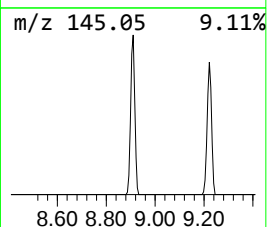
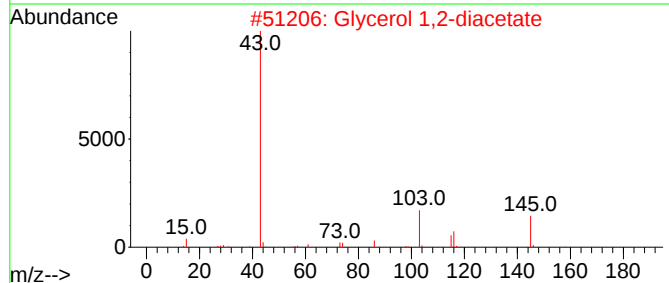
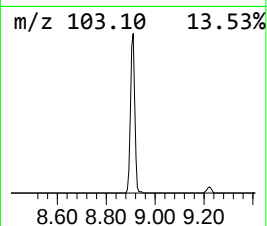
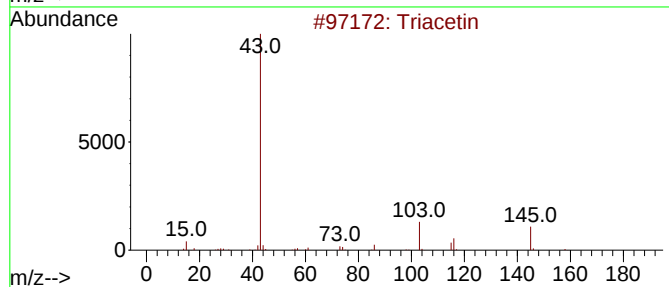
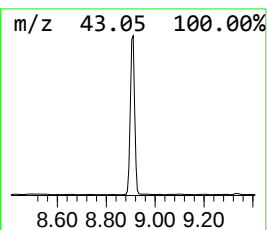
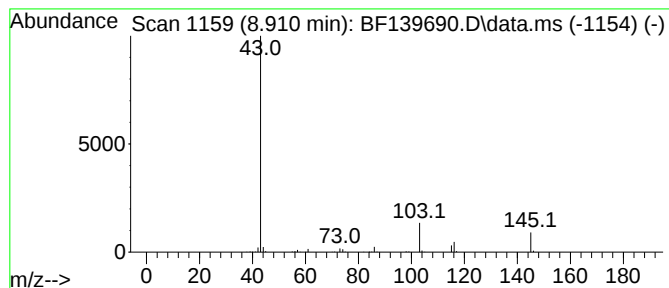
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Triacetin Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.910	7.99 ng	274185	Naphthalene-d8	8.145

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triacetin	218	C9H14O6	000102-76-1	90
2			Glycerol 1,2-diacetate	176	C7H12O5	000102-62-5	83
3			2-Deoxy-D-ribose, aldonitrile,...	257	C11H15N06	1000380-43-1	64
4			1,1,2-Triacetoxymethane	204	C8H12O6	002983-35-9	50
5			1,2,3,4-butanetetrol, tetraacetate	290	C12H18O8	073977-54-5	50



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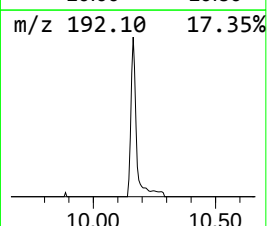
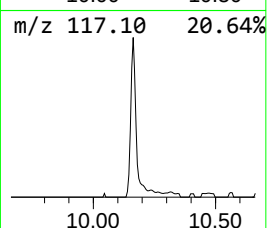
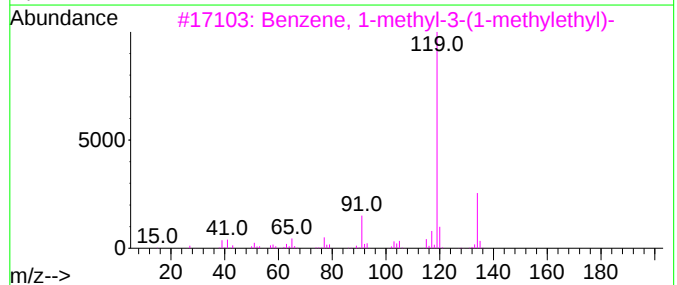
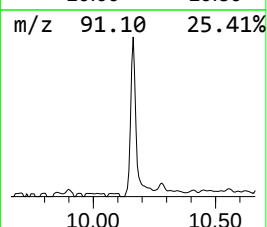
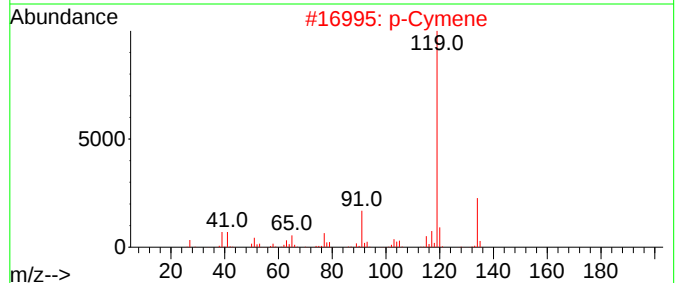
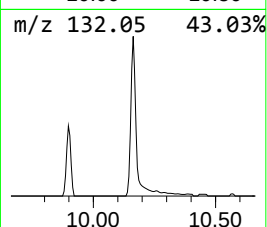
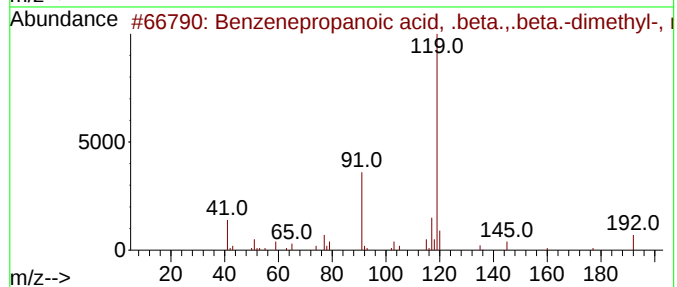
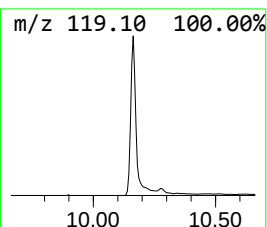
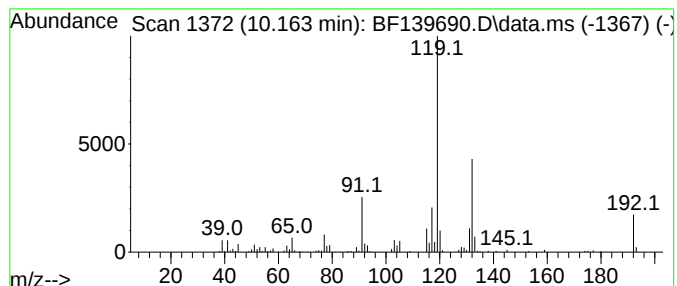
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 4 Benzenepropanoic acid, .bet... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.163	5.27 ng	200832	Acenaphthene-d10	9.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzenepropanoic acid, .beta.,.b...	192	C12H16O2	025080-84-6	50
2			p-Cymene	134	C10H14	000099-87-6	43
3			Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	43
4			o-Cymene	134	C10H14	000527-84-4	43
5			4-Methylbenzoic acid, propargyl ...	174	C11H10O2	1000325-59-9	43



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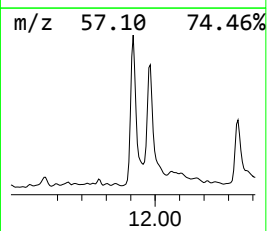
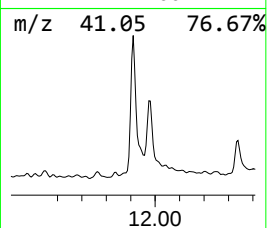
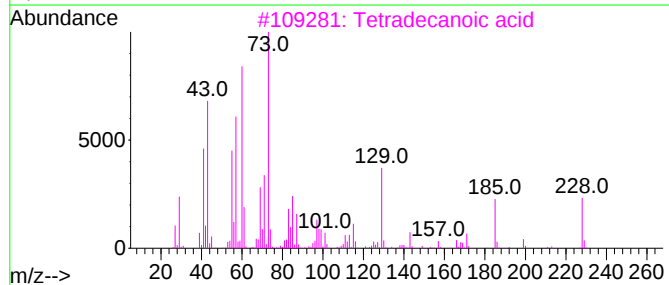
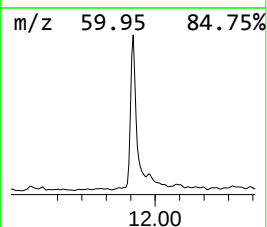
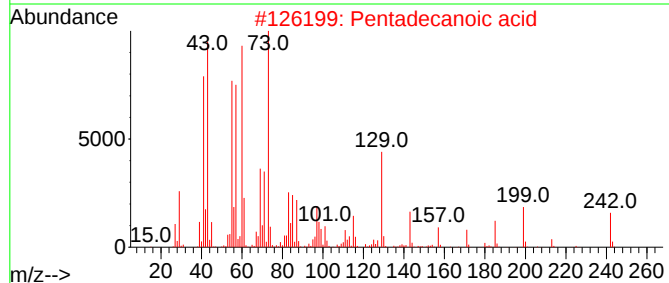
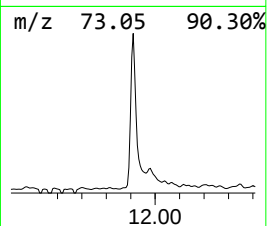
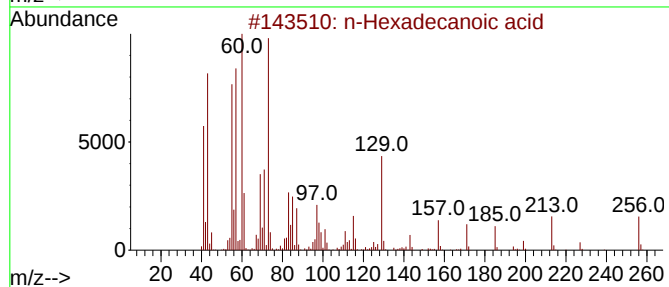
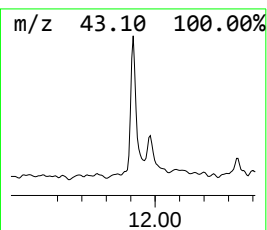
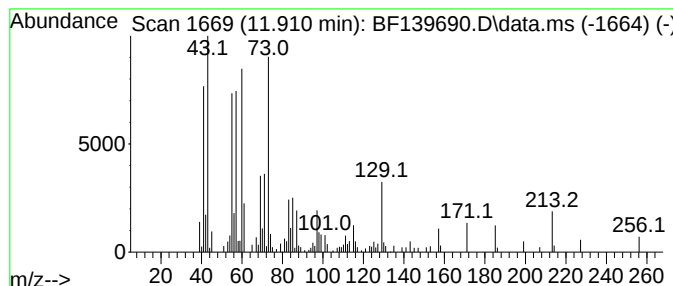
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.910	3.60 ng	135078	Phenanthrene-d10	11.386

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4			Tridecanoic acid	214	C13H26O2	000638-53-9	68
5			n-Decanoic acid	172	C10H20O2	000334-48-5	50



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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.157	295.9	ng	8095240	1	6.863	547108	20.0
Acetic acid, 1,...	2.569	299.4	ng	8191580	1	6.863	547108	20.0
Triacetin	8.910	8.0	ng	274185	2	8.145	686424	20.0
Benzenepropanoi...	10.163	5.3	ng	200832	3	9.898	761938	20.0
n-Hexadecanoic ...	11.910	3.6	ng	135078	4	11.386	750381	20.0