

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032421\
 Data File : BF123440.D
 Acq On : 24 Mar 2021 15:41
 Operator : JU/CG
 Sample : M1770-06
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-105D

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-BF032321.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123440.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.252	20	28	33	rBV	4123114	5330549	66.63%	10.825%
2	2.357	41	46	52	rVB	161170	189983	2.37%	0.386%
3	5.140	512	519	525	rVB	136454	166483	2.08%	0.338%
4	5.534	581	586	589	rBV	3973488	3888037	48.60%	7.895%
5	6.528	750	755	760	rBV	2849917	2683572	33.54%	5.450%
6	6.910	817	820	824	rBV	1622361	1418924	17.74%	2.881%
7	7.475	910	916	919	rBV	4639921	4925341	61.57%	10.002%
8	8.198	1034	1039	1042	rBV	2245241	1858995	23.24%	3.775%
9	8.586	1098	1105	1109	rBV	474853	541357	6.77%	1.099%
10	9.280	1217	1223	1226	rBV	8384878	8000104	100.00%	16.246%
11	9.357	1232	1236	1240	rBV	118928	94227	1.18%	0.191%
12	9.669	1285	1289	1293	rBV	151066	161382	2.02%	0.328%
13	9.710	1293	1296	1299	rVB	123066	103129	1.29%	0.209%
14	9.957	1334	1338	1342	rVB	2534031	2056300	25.70%	4.176%
15	10.157	1368	1372	1378	rVB	118502	121359	1.52%	0.246%
16	10.751	1467	1473	1476	rBV	5450030	5161991	64.52%	10.482%
17	11.022	1516	1519	1522	rVB	124005	98291	1.23%	0.200%
18	11.445	1588	1591	1595	rBV	1971021	1841532	23.02%	3.740%
19	11.974	1677	1681	1688	rBV	732358	715942	8.95%	1.454%
20	12.433	1756	1759	1762	rVB	135710	112520	1.41%	0.228%
21	12.763	1811	1815	1823	rBV	291759	283390	3.54%	0.575%
22	13.045	1858	1863	1866	rBV	6809660	6132761	76.66%	12.454%
23	13.939	2012	2015	2024	rBV	711145	808758	10.11%	1.642%
24	14.092	2037	2041	2045	rBV	1127560	1104105	13.80%	2.242%
25	14.280	2068	2073	2079	rBV5	53631	91293	1.14%	0.185%
26	15.598	2292	2297	2302	rBV	902103	1186335	14.83%	2.409%
27	16.162	2389	2393	2401	rBV3	82606	167402	2.09%	0.340%

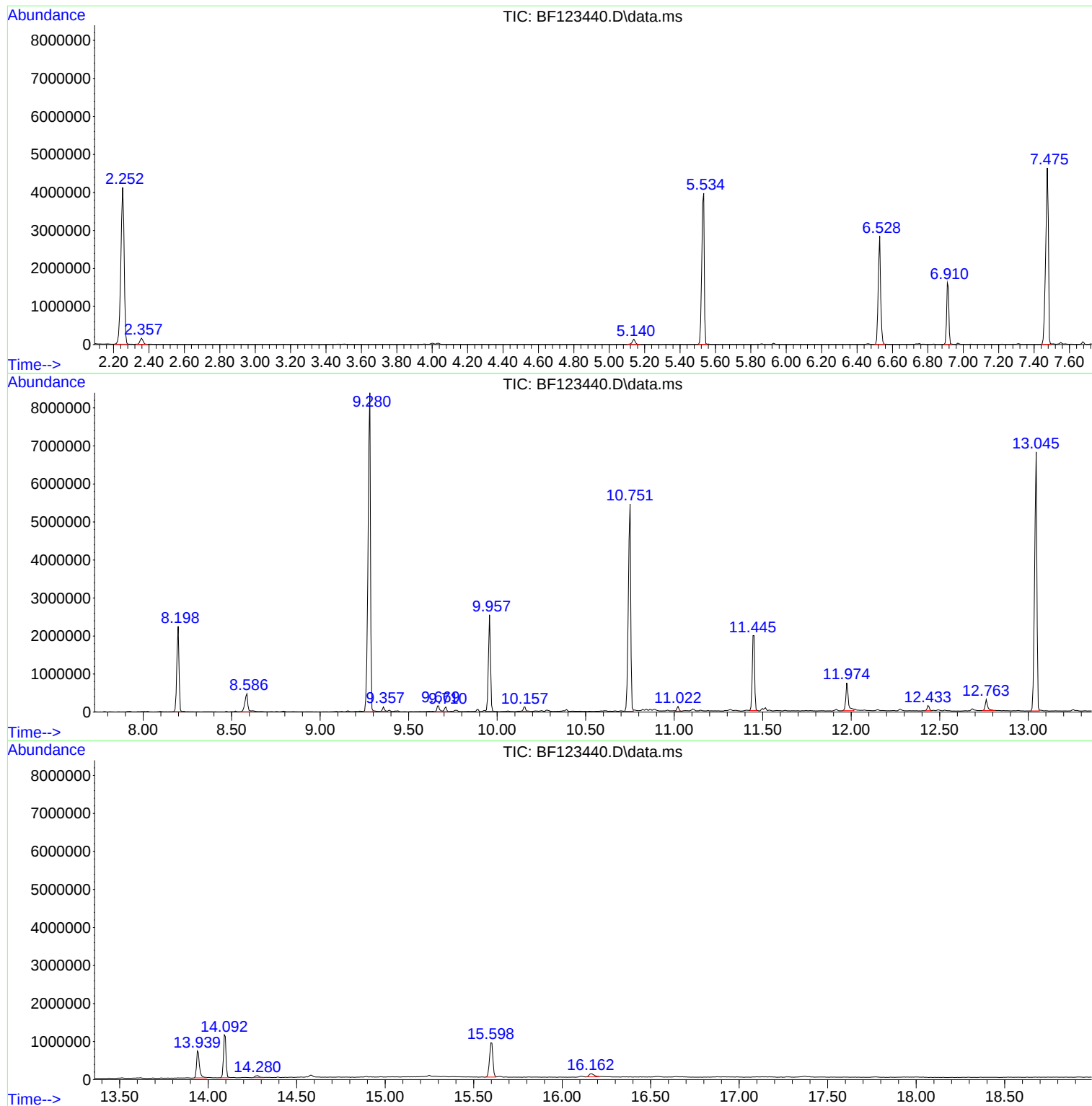
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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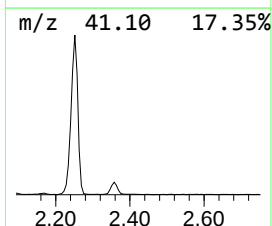
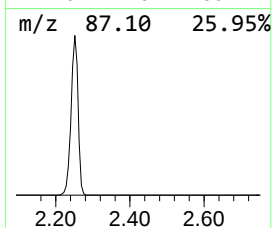
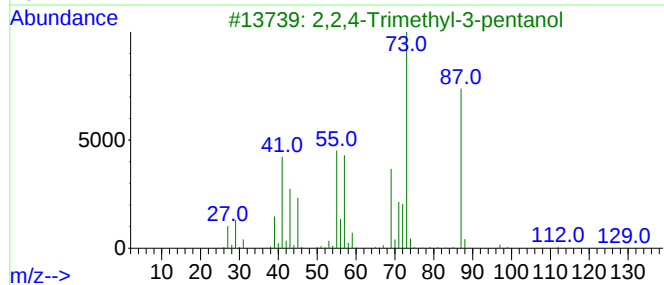
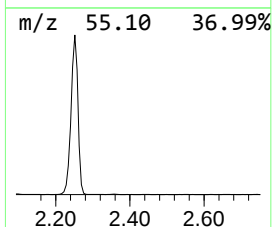
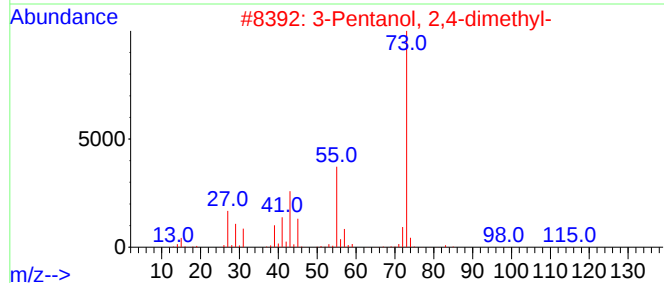
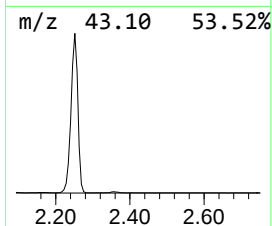
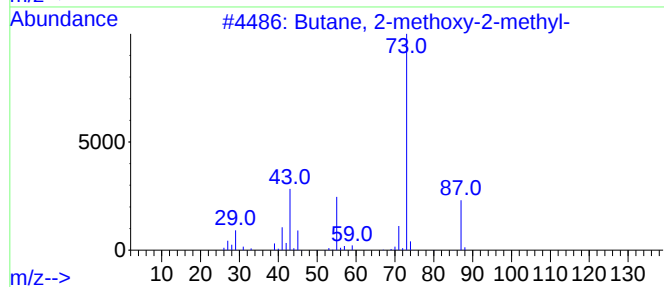
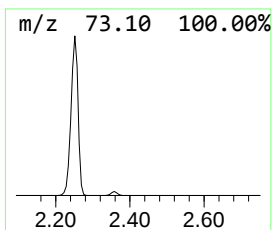
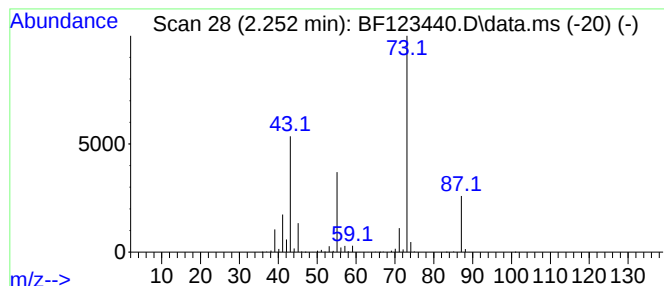
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.252	75.14 ng	5330550	1,4-Dichlorobenzene-d4	6.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	32



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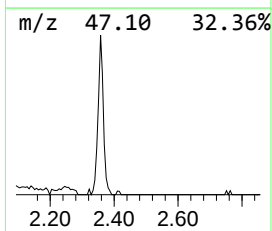
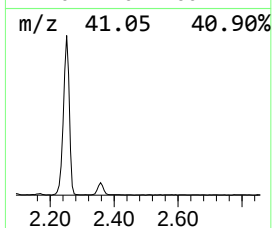
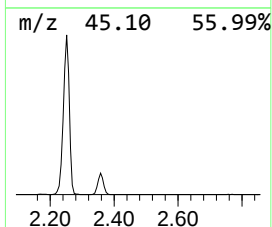
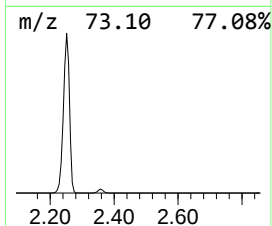
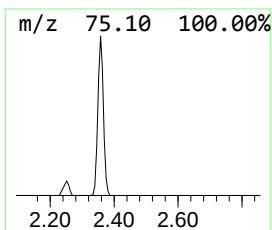
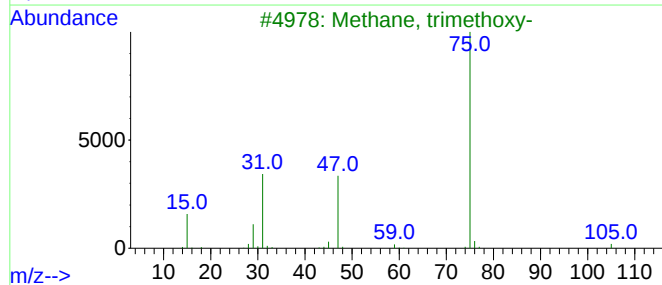
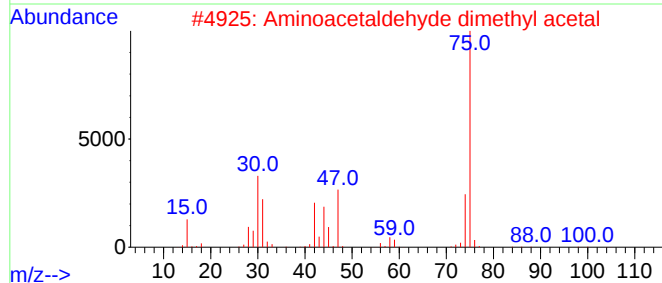
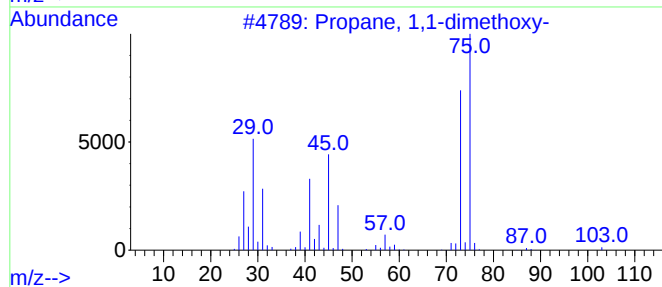
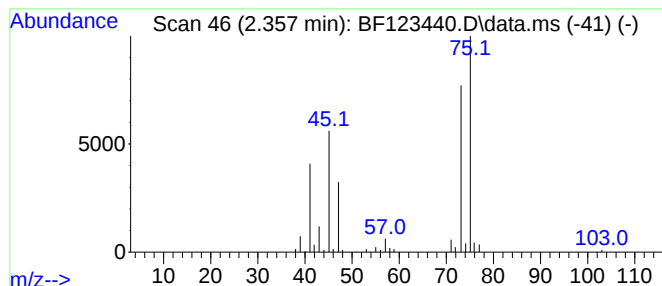
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.357	2.68 ng	189983	1,4-Dichlorobenzene-d4	6.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	64
2			Aminoacetaldehyde dimethyl acetal	105	C4H11NO2	022483-09-6	33
3			Methane, trimethoxy-	106	C4H10O3	000149-73-5	28
4			Acetic acid, dimethoxy-, methyl ...	134	C5H10O4	000089-91-8	28
5			1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	12



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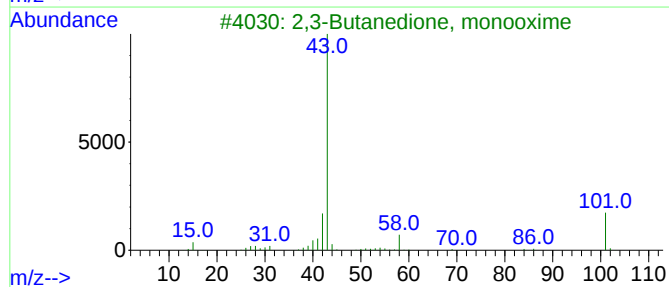
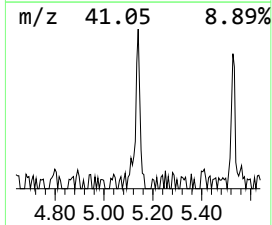
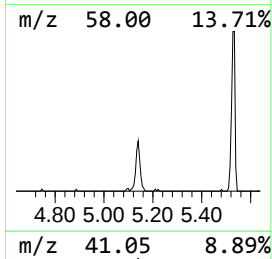
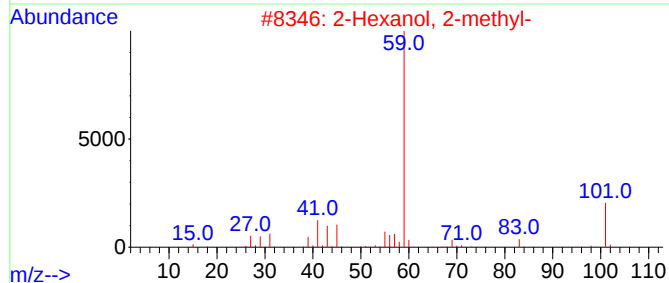
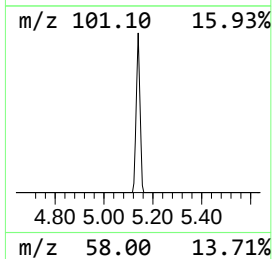
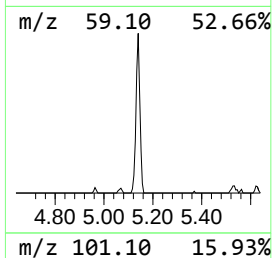
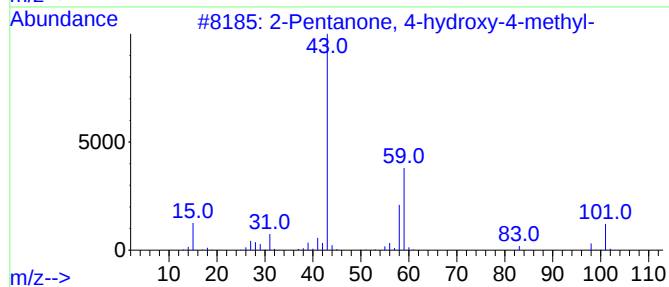
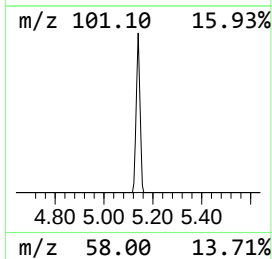
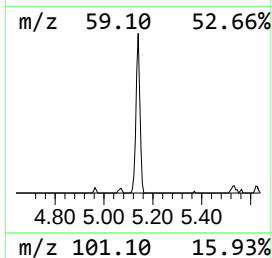
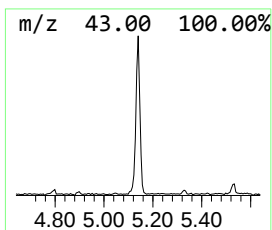
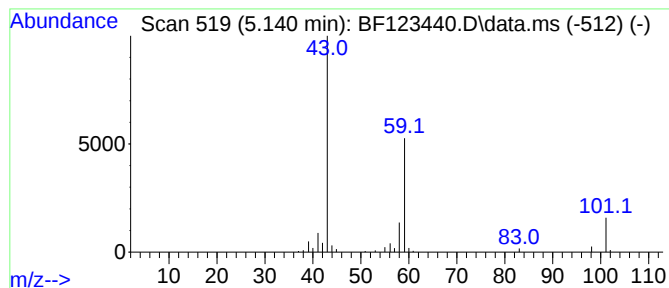
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.140	2.35 ng	166483	1,4-Dichlorobenzene-d4	6.916

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
4		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5		Butane	58	C4H10	000106-97-8	9



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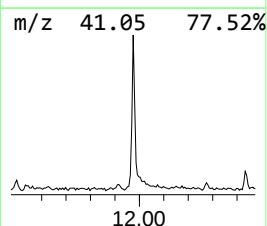
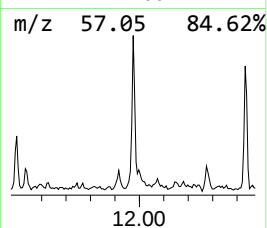
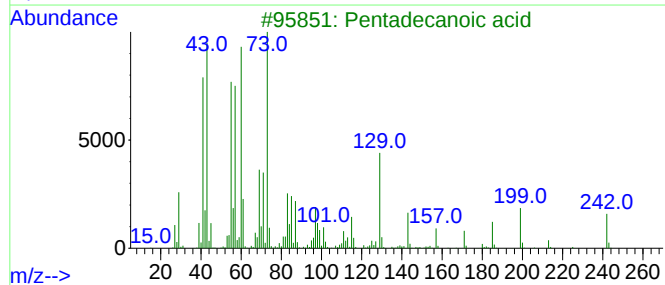
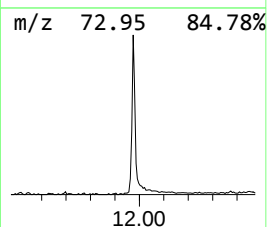
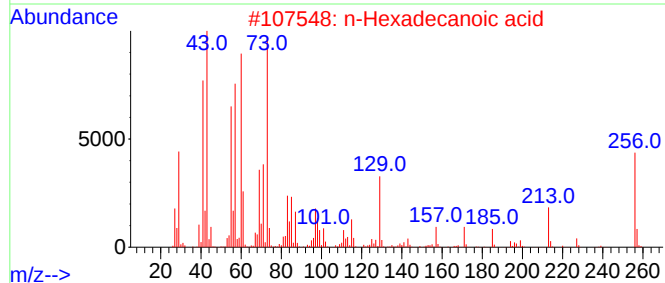
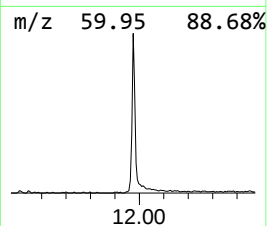
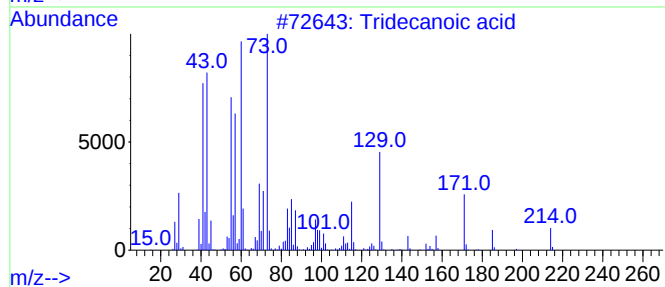
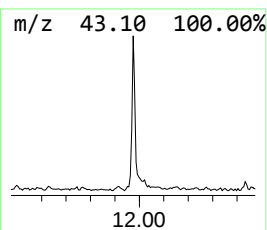
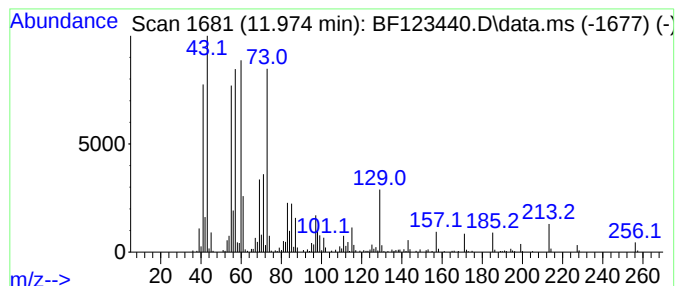
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Peak Number 4 Tridecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.974	7.78 ng	715942	Phenanthrene-d10	11.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid	214	C13H26O2	000638-53-9	93
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5			n-Decanoic acid	172	C10H20O2	000334-48-5	58



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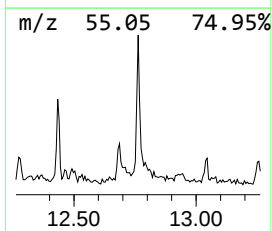
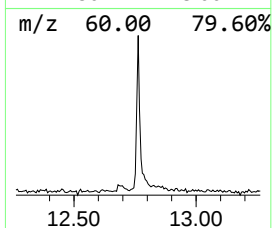
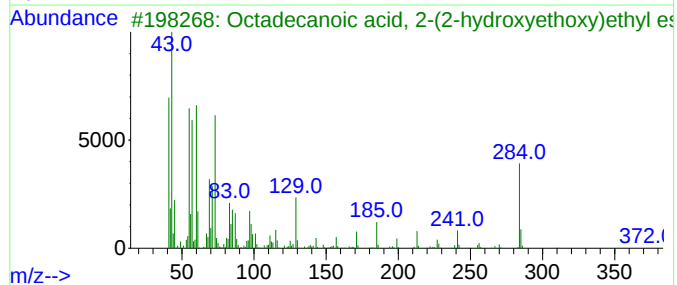
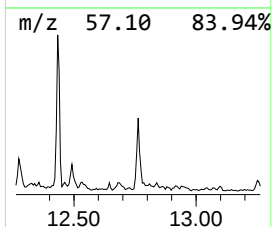
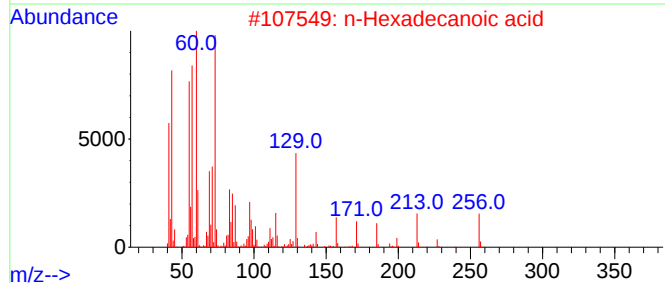
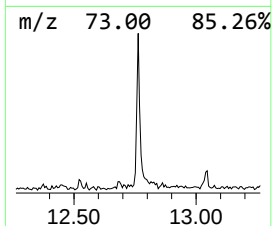
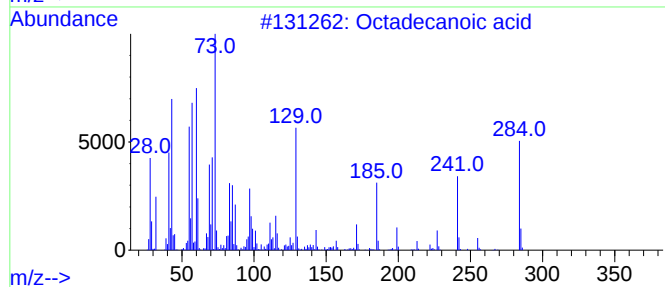
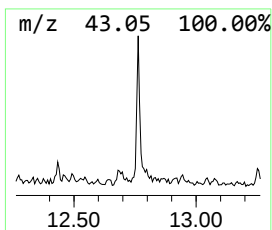
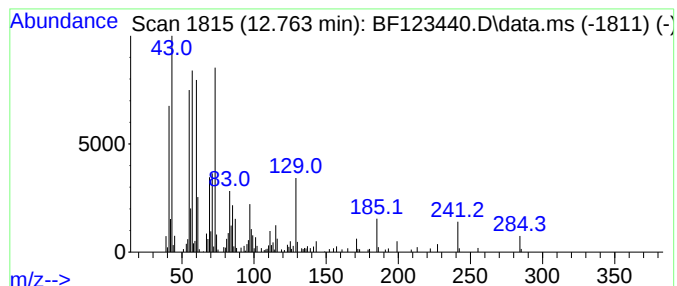
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Peak Number 5 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.763	3.08 ng	283390	Phenanthrene-d10	11.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
3			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	68
5			n-Decanoic acid	172	C10H20O2	000334-48-5	60



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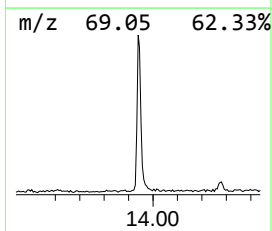
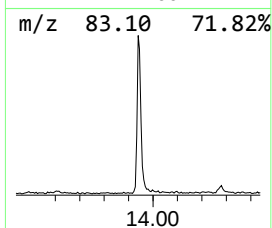
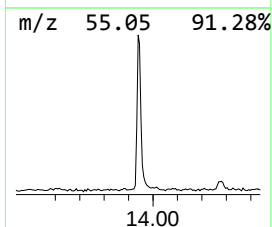
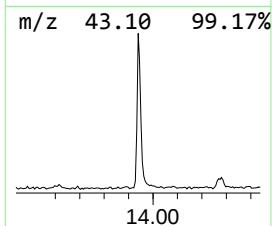
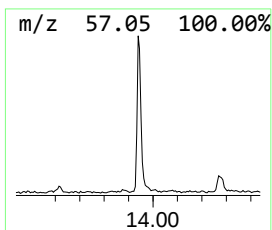
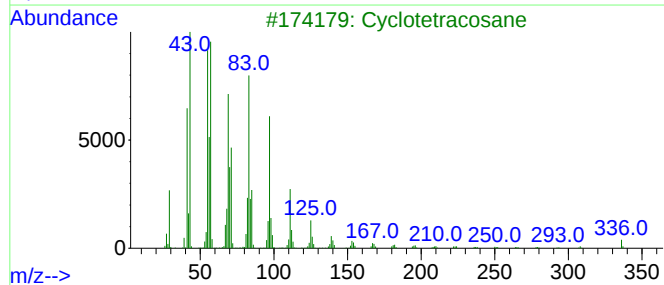
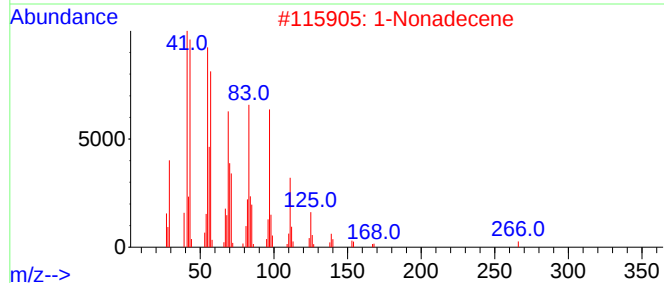
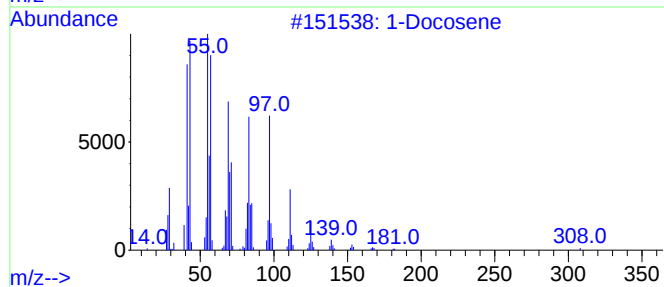
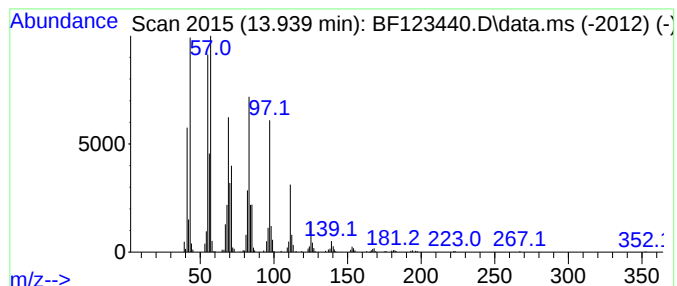
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Docosene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.939	14.65 ng	808758	Chrysene-d12	14.098

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene			308	C22H44	001599-67-3	94
2	1-Nonadecene			266	C19H38	018435-45-5	91
3	Cyclotetracosane			336	C24H48	000297-03-0	91
4	5-Eicosene, (E)-			280	C20H40	074685-30-6	91
5	Heptafluorobutyric acid, hexadec...			438	C20H33F7O2	006385-15-5	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032421\
Data File : BF123440.D
Acq On : 24 Mar 2021 15:41
Operator : JU/CG
Sample : M1770-06
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-105D

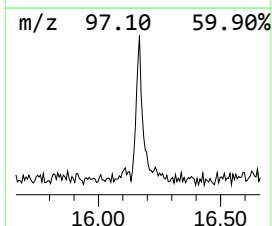
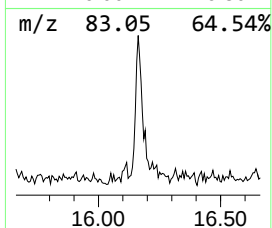
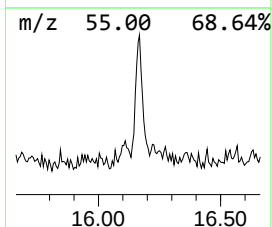
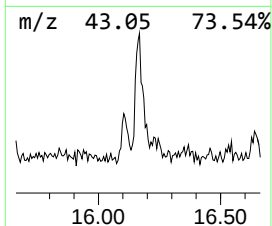
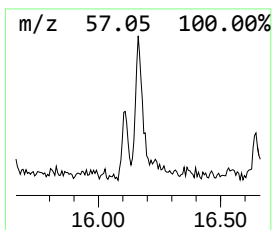
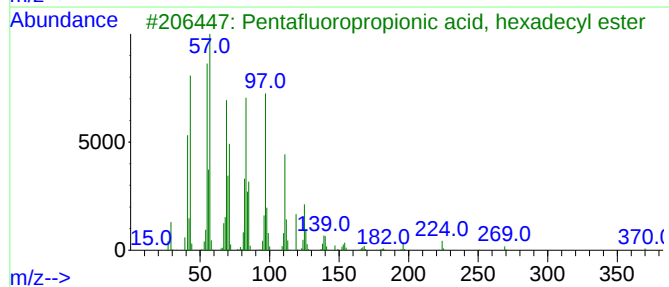
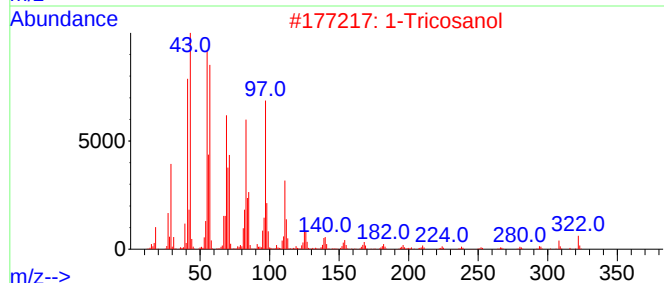
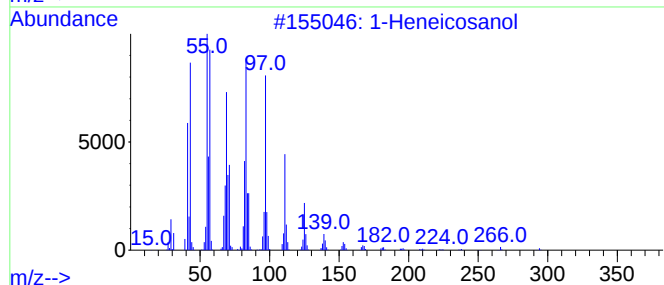
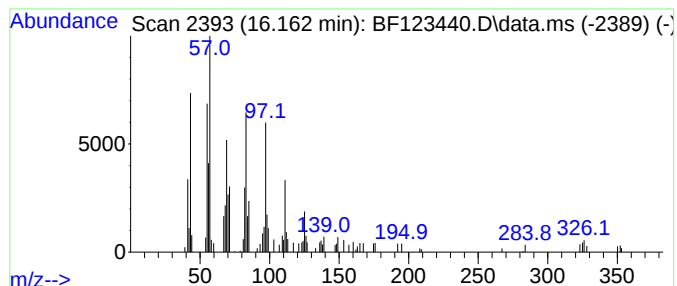
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.162	2.82 ng	167402	Perylene-d12	15.604

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol			312	C21H44O	015594-90-8	87
2	1-Tricosanol			340	C23H48O	003133-01-5	83
3	Pentafluoropropionic acid, hexadecyl ester			388	C19H33F5O2	006222-07-7	76
4	Behenic alcohol			326	C22H46O	000661-19-8	76
5	Heptadecyl trifluoroacetate			352	C19H35F3O2	1000351-87-0	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032421\
Data File : BF123440.D
Acq On : 24 Mar 2021 15:41
Operator : JU/CG
Sample : M1770-06
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-105D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.252	75.1	ng	5330550	1	6.916	1418920	20.0
Propane, 1,1-di...	2.357	2.7	ng	189983	1	6.916	1418920	20.0
2-Pentanone, 4-...	5.140	2.4	ng	166483	1	6.916	1418920	20.0
Tridecanoic acid	11.974	7.8	ng	715942	4	11.451	1841530	20.0
Octadecanoic acid	12.763	3.1	ng	283390	4	11.451	1841530	20.0
1-Docosene	13.939	14.7	ng	808758	5	14.098	1104110	20.0
1-Heneicosanol	16.162	2.8	ng	167402	6	15.604	1186340	20.0