

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112320\
 Data File : BF122456.D
 Acq On : 23 Nov 2020 19:55
 Operator : JU/CG
 Sample : L4876-03
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TB-2C

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-BF110920.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF122456.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.163	6	13	19	rVB	326153	437524	8.42%	1.081%
2	2.269	27	31	37	rVB	46612	63867	1.23%	0.158%
3	2.987	147	153	160	rVB	150227	245897	4.73%	0.608%
4	4.457	399	403	411	rBV	216285	241555	4.65%	0.597%
5	5.087	503	510	520	rVB	2464051	3577522	68.89%	8.842%
6	5.492	574	579	582	rBV	4646664	4495076	86.56%	11.110%
7	5.881	641	645	648	rBV	361261	308245	5.94%	0.762%
8	6.498	744	750	769	rBV	4391623	4894201	94.24%	12.097%
9	6.863	808	812	815	rBV	1379306	1042354	20.07%	2.576%
10	7.428	902	908	911	rBV	3070130	2920371	56.23%	7.218%
11	8.151	1026	1031	1034	rBV	1464089	1313579	25.29%	3.247%
12	9.228	1209	1214	1217	rBV	5510263	5193222	100.00%	12.836%
13	9.622	1277	1281	1290	rBV	221739	211398	4.07%	0.522%
14	9.910	1321	1330	1341	rBV	1618423	1506294	29.00%	3.723%
15	10.698	1459	1464	1475	rBV	3527211	3288681	63.33%	8.128%
16	11.398	1579	1583	1586	rBV	1443442	1380403	26.58%	3.412%
17	11.921	1669	1672	1680	rBV	182395	211212	4.07%	0.522%
18	12.610	1786	1789	1792	rBV	155059	139734	2.69%	0.345%
19	12.710	1802	1806	1812	rBV5	47837	63989	1.23%	0.158%
20	12.839	1821	1828	1831	rBV	132809	134360	2.59%	0.332%
21	12.986	1849	1853	1857	rBV	5100790	4748310	91.43%	11.736%
22	13.898	2004	2008	2018	rBV	223326	412125	7.94%	1.019%
23	14.039	2027	2032	2035	rBV	1388658	1485562	28.61%	3.672%
24	14.062	2035	2036	2042	rVB	106379	97219	1.87%	0.240%
25	15.086	2207	2210	2219	rVB	144663	283321	5.46%	0.700%
26	15.392	2259	2262	2268	rVB	70135	95450	1.84%	0.236%
27	15.457	2269	2273	2278	rVB	114294	136903	2.64%	0.338%
28	15.521	2279	2284	2288	rBV	1191197	1467396	28.26%	3.627%
29	16.086	2376	2380	2383	rBV6	34329	63470	1.22%	0.157%

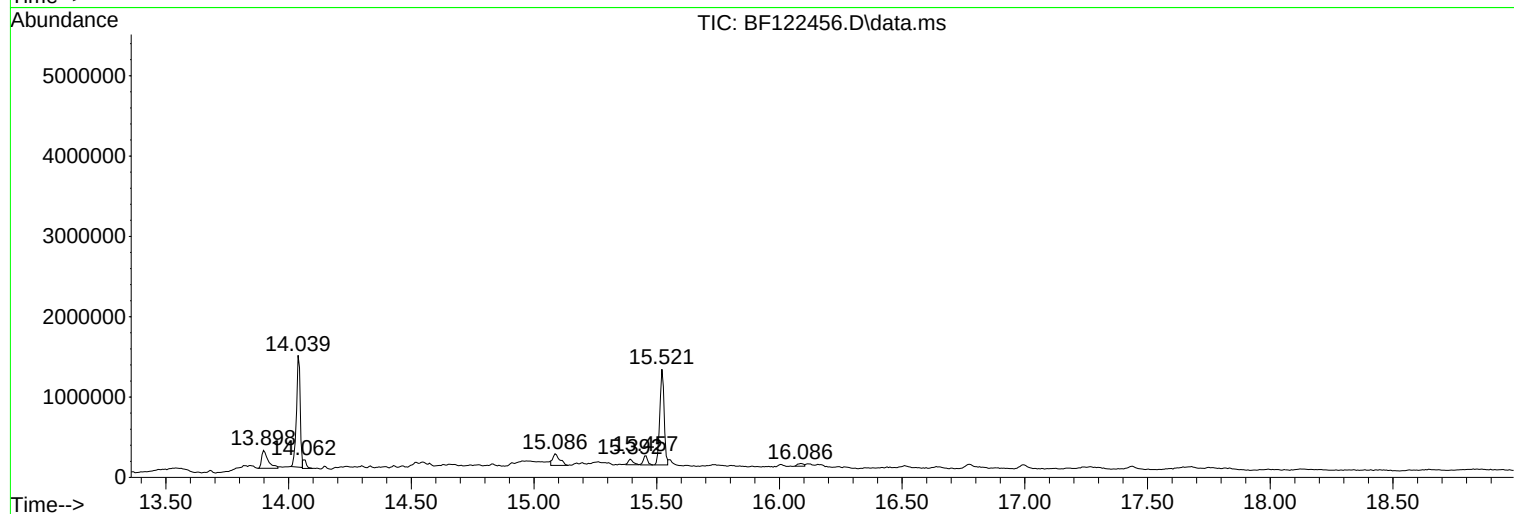
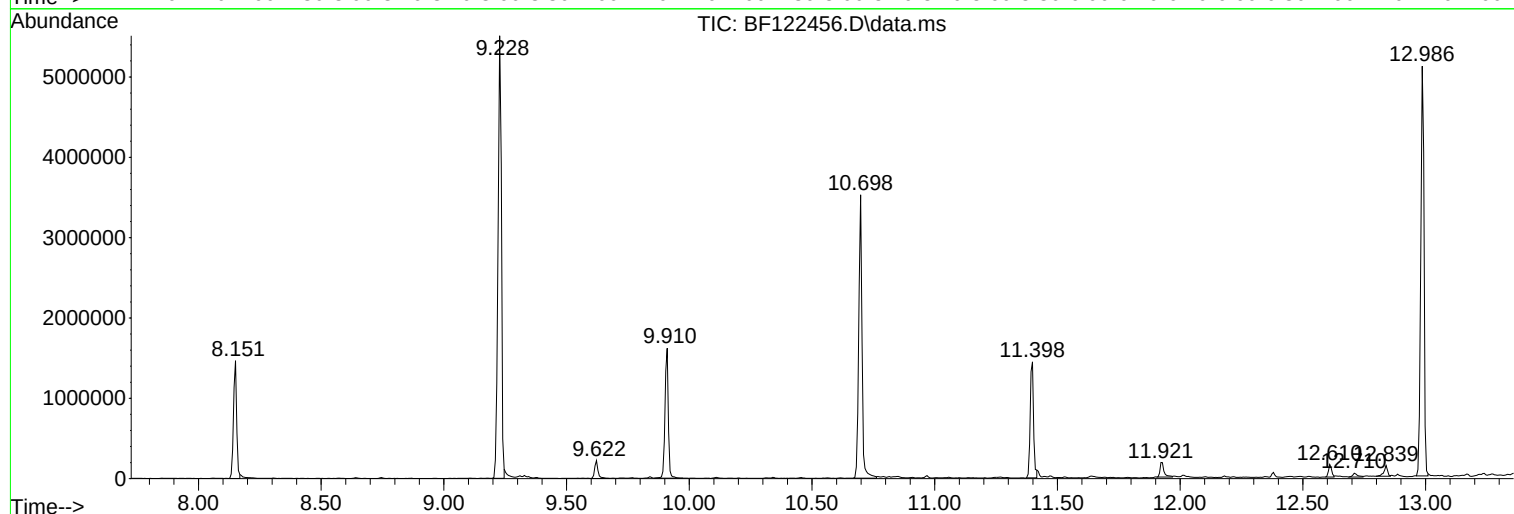
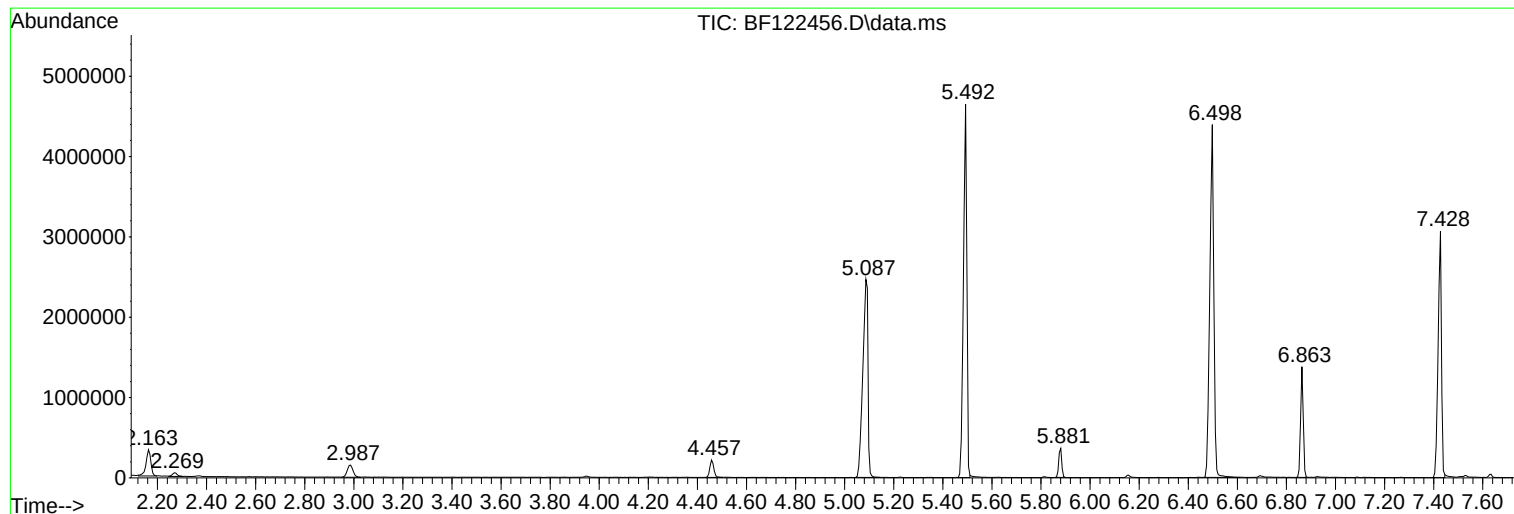
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Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TB-2C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.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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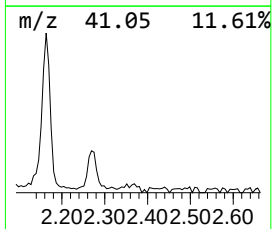
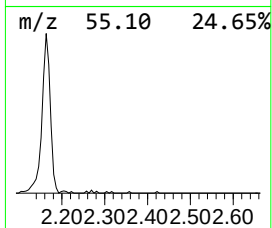
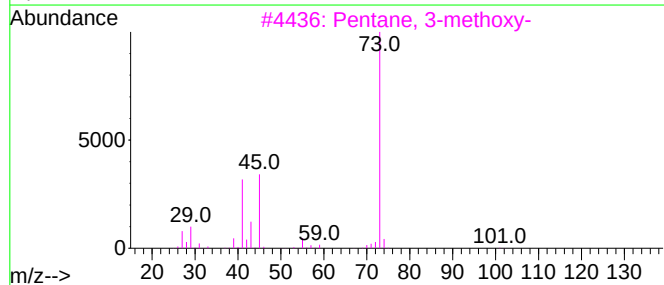
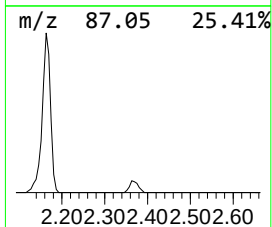
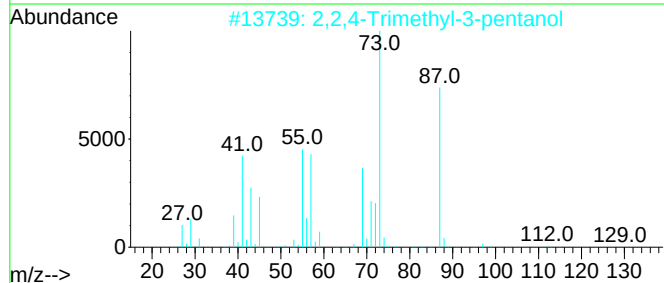
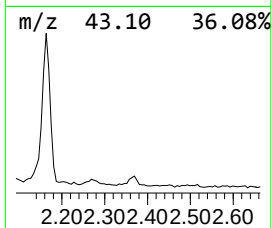
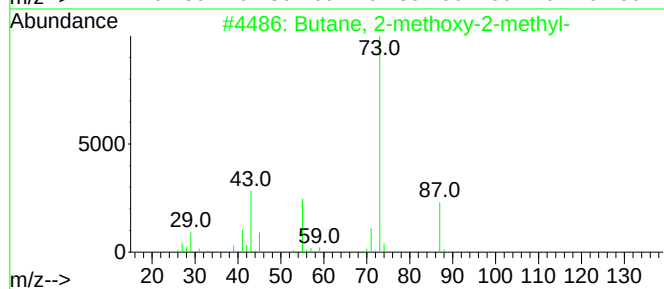
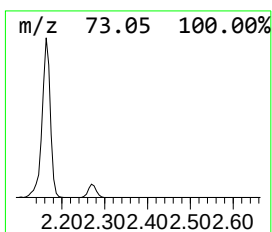
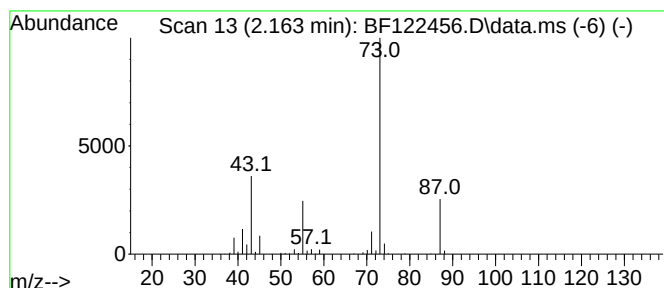
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.163	8.39 ng	437524	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	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	10
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9



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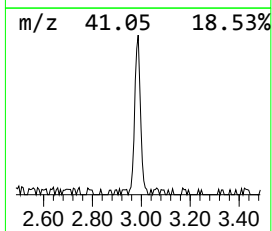
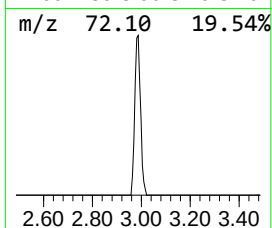
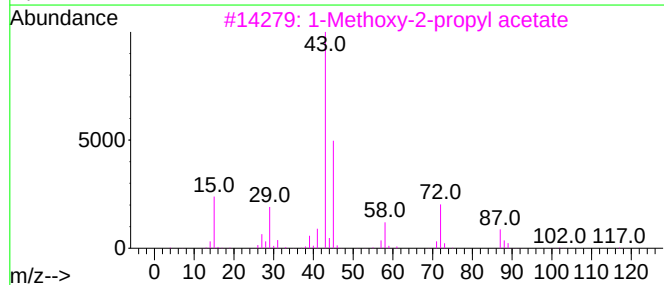
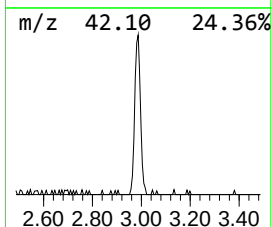
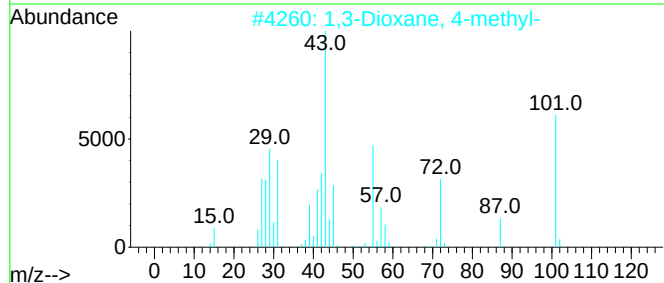
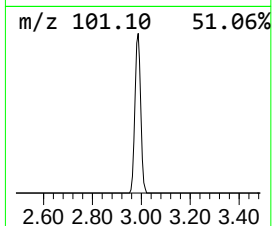
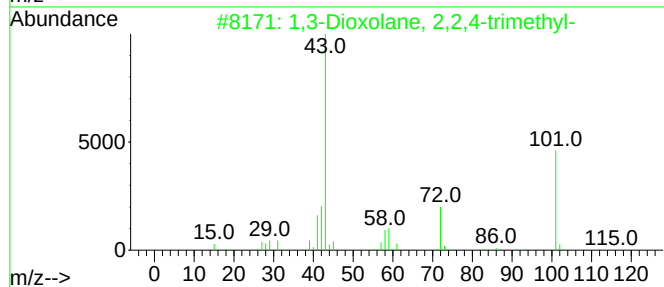
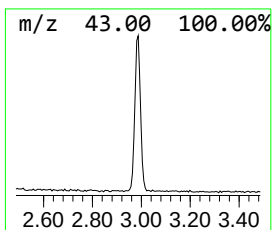
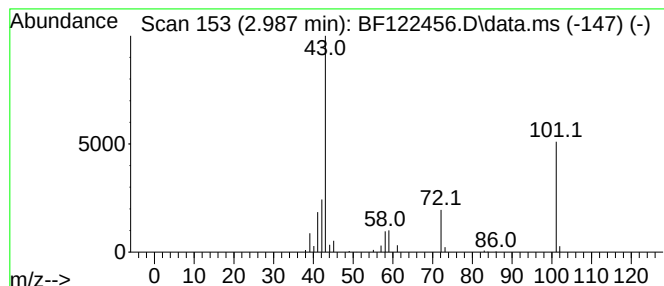
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 1,3-Dioxolane, 2,2,4-trimet... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.987	4.72 ng	245897	1,4-Dichlorobenzene-d4	6.863

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,3-Dioxolane, 2,2,4-trimethyl-	116	C6H12O2	001193-11-9	90
2		1,3-Dioxane, 4-methyl-	102	C5H10O2	001120-97-4	50
3		1-Methoxy-2-propyl acetate	132	C6H12O3	000108-65-6	12
4		Ethanedithioic acid, S-(dihydro-2,...	174	C6H6O4S	006953-60-2	10
5		2-Oxazolidinone, 3-methyl-	101	C4H7NO2	019836-78-3	9



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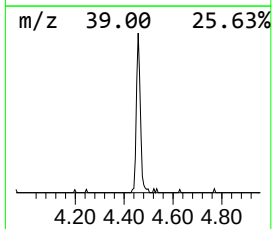
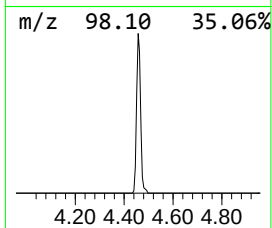
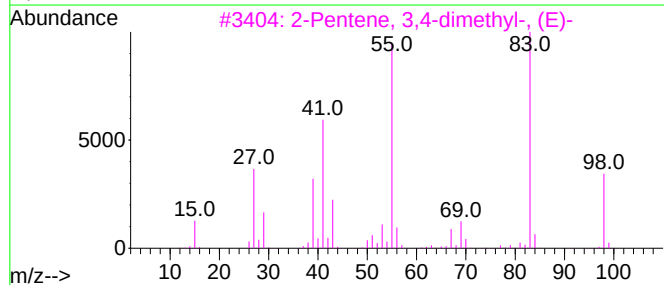
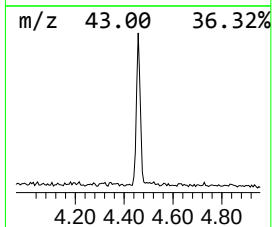
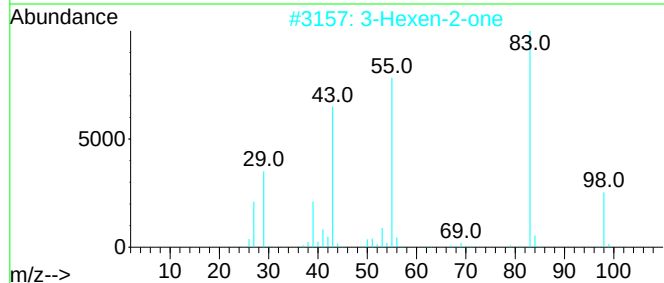
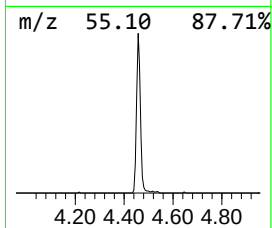
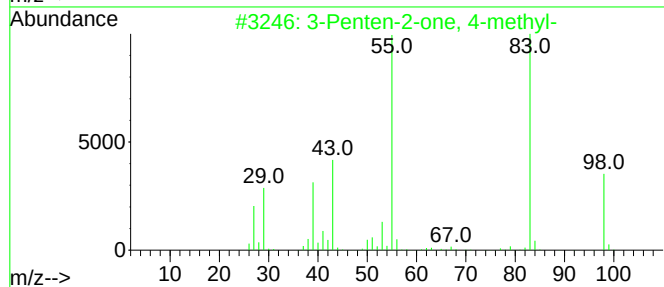
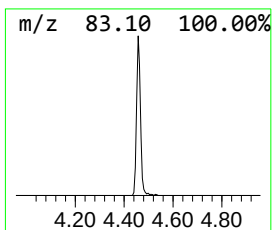
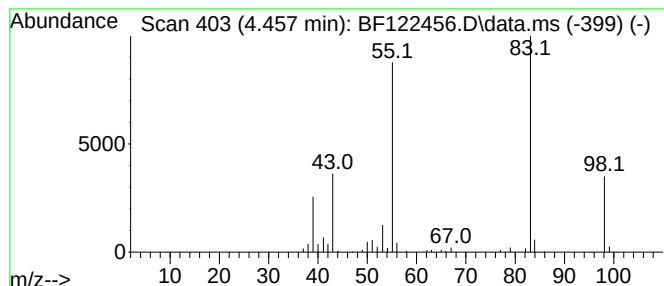
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 3-Penten-2-one, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.457	4.63 ng	241555	1,4-Dichlorobenzene-d4	6.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
2			3-Hexen-2-one	98	C6H10O	000763-93-9	91
3			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	87
5			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86



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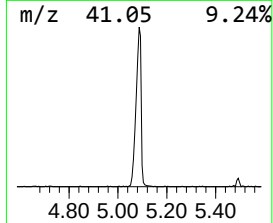
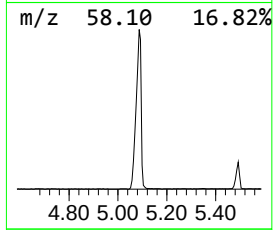
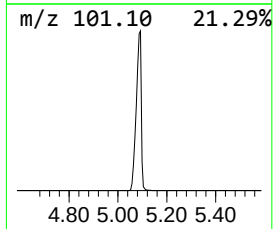
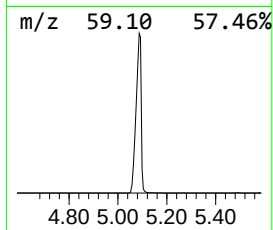
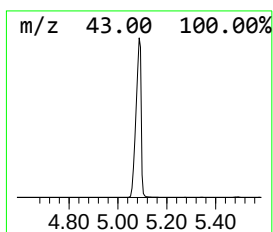
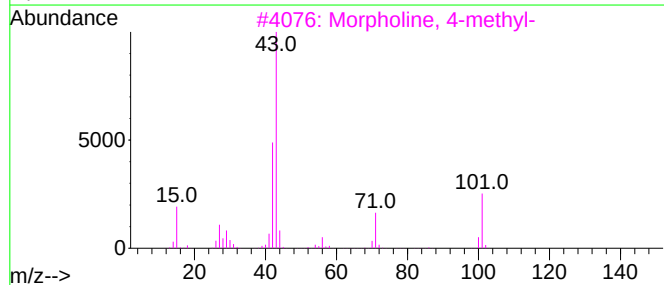
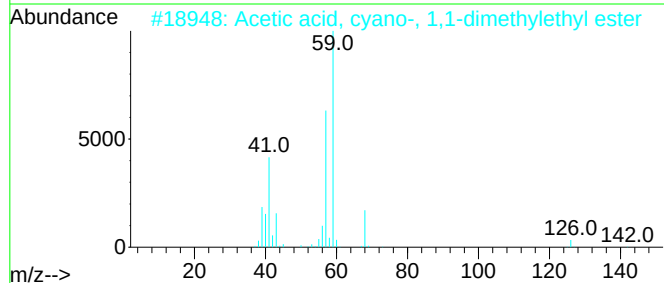
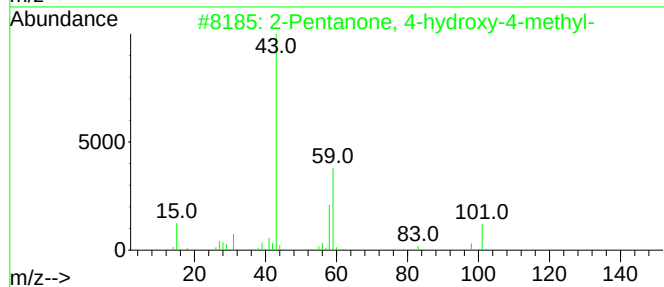
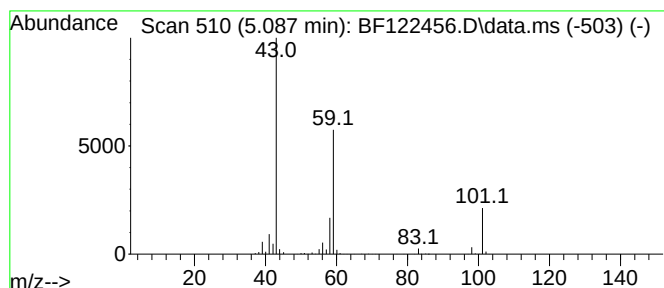
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.087	68.64 ng	3577520	1,4-Dichlorobenzene-d4	6.863	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9



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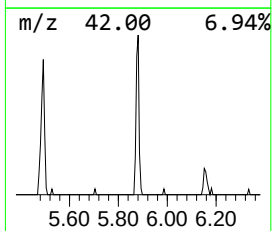
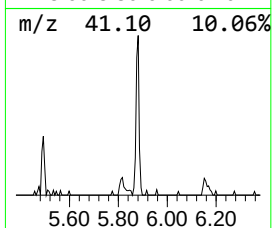
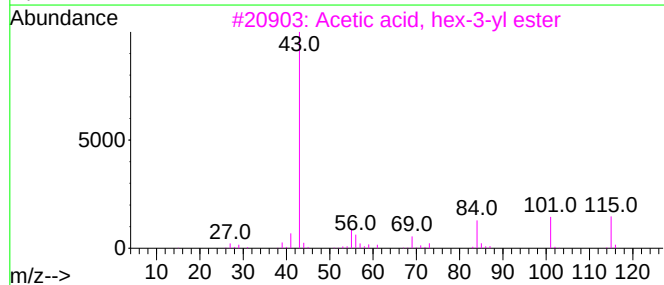
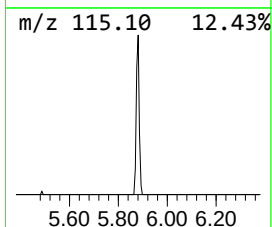
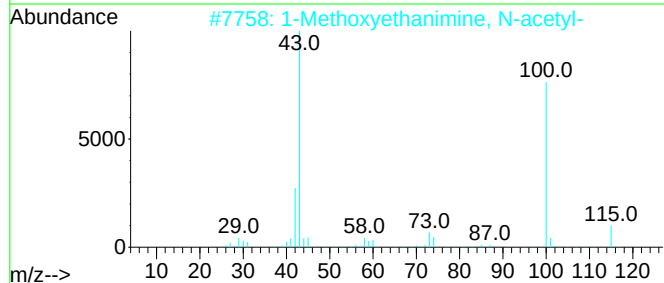
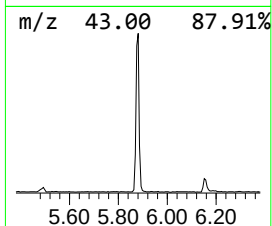
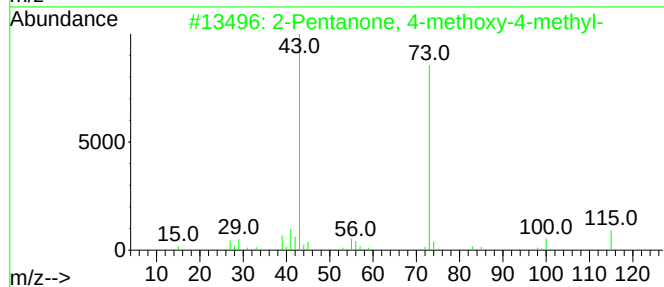
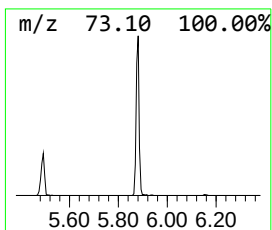
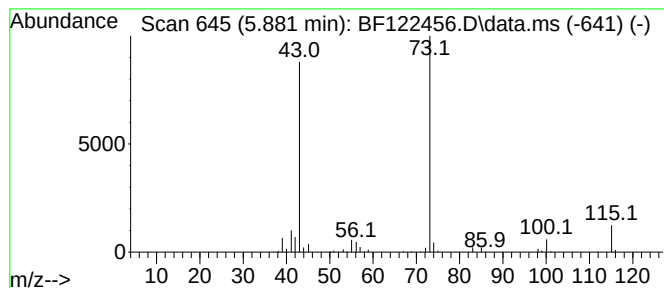
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.881	5.91 ng	308245	1,4-Dichlorobenzene-d4	6.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2			1-Methoxyethanimine, N-acetyl-	115	C5H9NO2	099028-43-0	38
3			Acetic acid, hex-3-yl ester	144	C8H16O2	1000367-94-5	37
4			N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	33
5			1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	10



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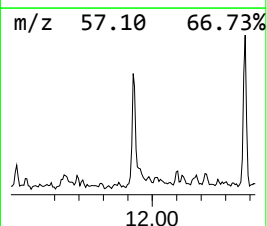
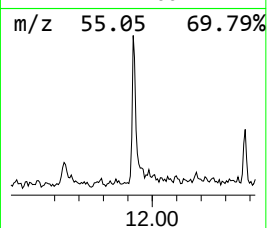
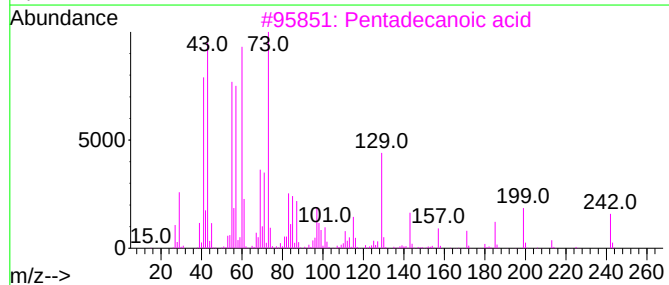
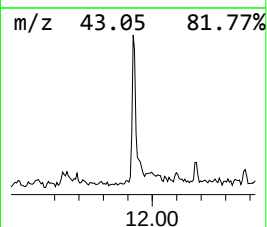
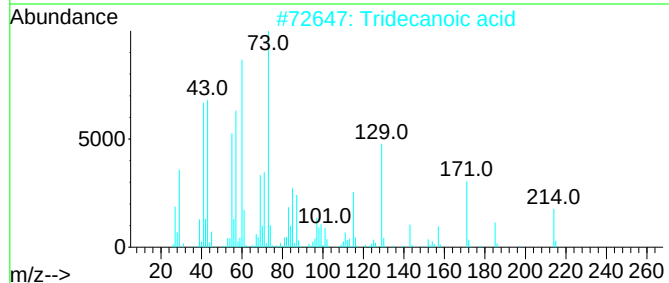
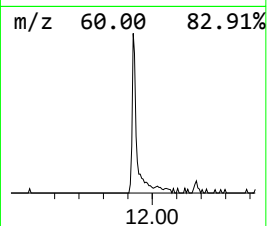
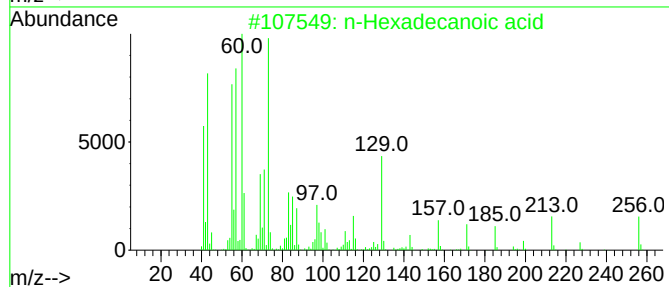
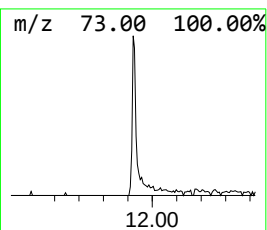
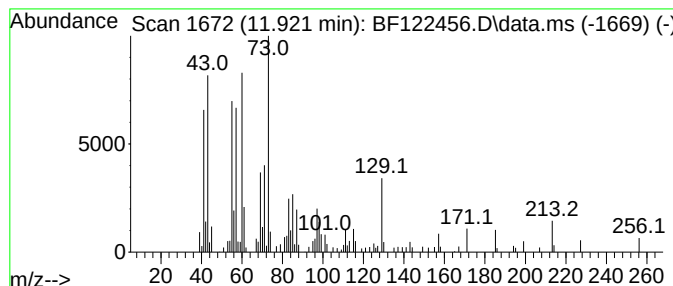
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.922	3.06 ng	211212	Phenanthrene-d10	11.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2			Tridecanoic acid	214	C13H26O2	000638-53-9	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4			Undecanoic acid	186	C11H22O2	000112-37-8	87
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112320\
Data File : BF122456.D
Acq On : 23 Nov 2020 19:55
Operator : JU/CG
Sample : L4876-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

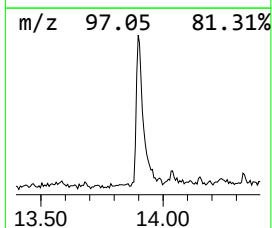
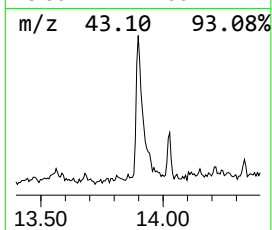
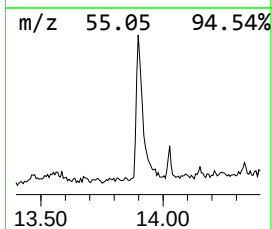
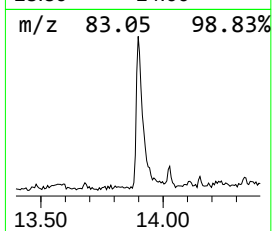
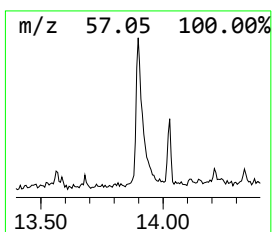
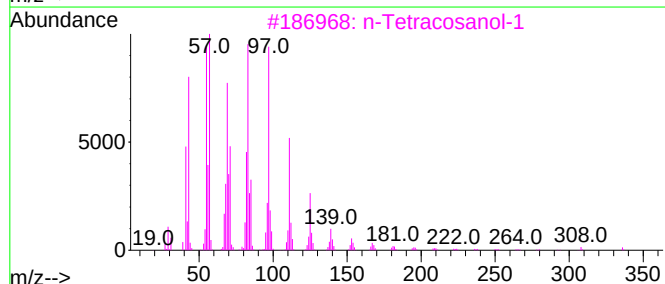
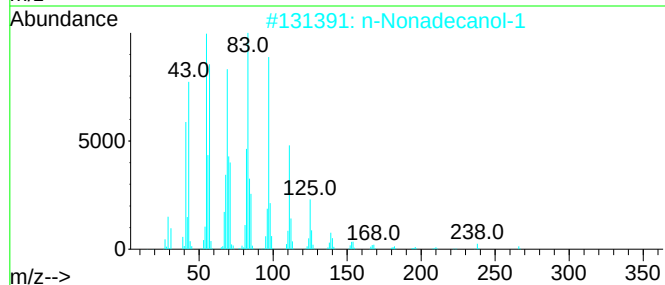
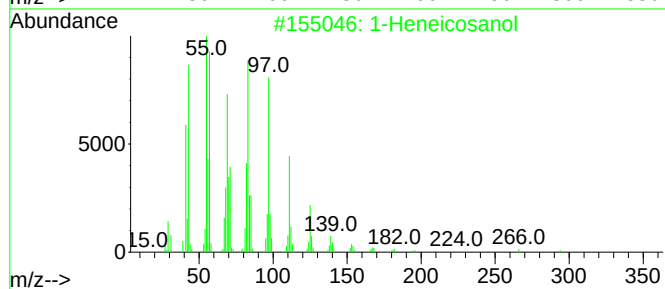
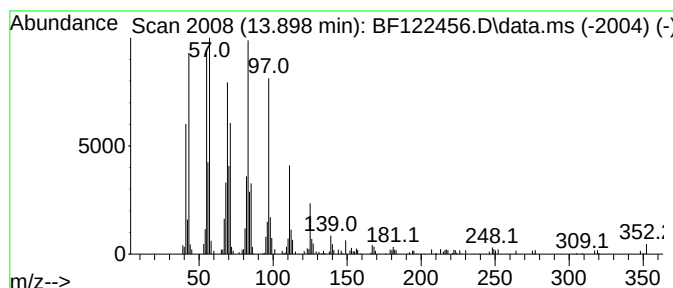
Instrument :
BNA_F
ClientSampled :
TB-2C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.898	5.55 ng	412125	Chrysene-d12	14.039	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	93
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	91
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
4	Trichloroacetic acid, pentadecyl...	372	C17H31Cl13O2	074339-53-0	90
5	n-Heptadecanol-1	256	C17H36O	001454-85-9	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112320\
Data File : BF122456.D
Acq On : 23 Nov 2020 19:55
Operator : JU/CG
Sample : L4876-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TB-2C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.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...	2.163	8.4	ng	437524	1	6.863	1042350	20.0
1,3-Dioxolane, ...	2.987	4.7	ng	245897	1	6.863	1042350	20.0
3-Penten-2-one,...	4.457	4.6	ng	241555	1	6.863	1042350	20.0
2-Pentanone, 4-...	5.087	68.6	ng	3577520	1	6.863	1042350	20.0
2-Pentanone, 4-...	5.881	5.9	ng	308245	1	6.863	1042350	20.0
n-Hexadecanoic ...	11.922	3.1	ng	211212	4	11.398	1380400	20.0
1-Heneicosanol	13.898	5.5	ng	412125	5	14.039	1485560	20.0