

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF042420\
 Data File : BF120190.D
 Acq On : 24 Apr 2020 9:45
 Operator : MA/SJ
 Sample : L2330-18
 Misc :
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WB-TWP-1

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-BF040820.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	3.857	294	301	310	rVB	488189	697638	1.74%	0.694%
2	5.269	537	541	552	rBV	2786214	2749600	6.86%	2.734%
3	6.304	713	717	726	rBV	1916941	1855984	4.63%	1.845%
4	6.663	774	778	781	rBV	1015579	870472	2.17%	0.865%
5	6.822	800	805	807	rBV	4113399	3713541	9.27%	3.692%
6	7.234	868	875	878	rVV2	2880803	3553019	8.87%	3.533%
7	7.698	912	954	955	rBV	2725547	16558455	41.32%	16.464%
8	7.716	955	957	962	rVB	1038214	864426	2.16%	0.859%
9	7.945	990	996	999	rBV	1339674	1292349	3.22%	1.285%
10	8.110	1015	1024	1033	rBV	1290831	1713178	4.27%	1.703%
11	8.463	1081	1084	1087	rVB	625739	493630	1.23%	0.491%
12	9.033	1176	1181	1184	rVB	5929449	5887555	14.69%	5.854%
13	9.422	1234	1247	1249	rBV	12860501	40078410	100.00%	39.849%
14	9.439	1249	1250	1253	rVV2	1242408	1216912	3.04%	1.210%
15	9.475	1253	1256	1261	rVB	2877027	2656955	6.63%	2.642%
16	9.716	1293	1297	1300	rVB	1428811	1337282	3.34%	1.330%
17	9.975	1338	1341	1350	rBV	565020	571941	1.43%	0.569%
18	10.216	1380	1382	1395	rVB	443412	515067	1.29%	0.512%
19	10.498	1424	1430	1435	rBV	3638955	3780603	9.43%	3.759%
20	11.186	1543	1547	1550	rVB	1505450	1349914	3.37%	1.342%
21	12.104	1699	1703	1706	rBV	542191	509144	1.27%	0.506%
22	12.780	1812	1818	1821	rBV	5676434	5959330	14.87%	5.925%
23	12.874	1831	1834	1842	rVB	551896	519347	1.30%	0.516%
24	13.815	1991	1994	1998	rBV	1055591	990572	2.47%	0.985%
25	15.221	2228	2233	2236	rBV	668429	840978	2.10%	0.836%

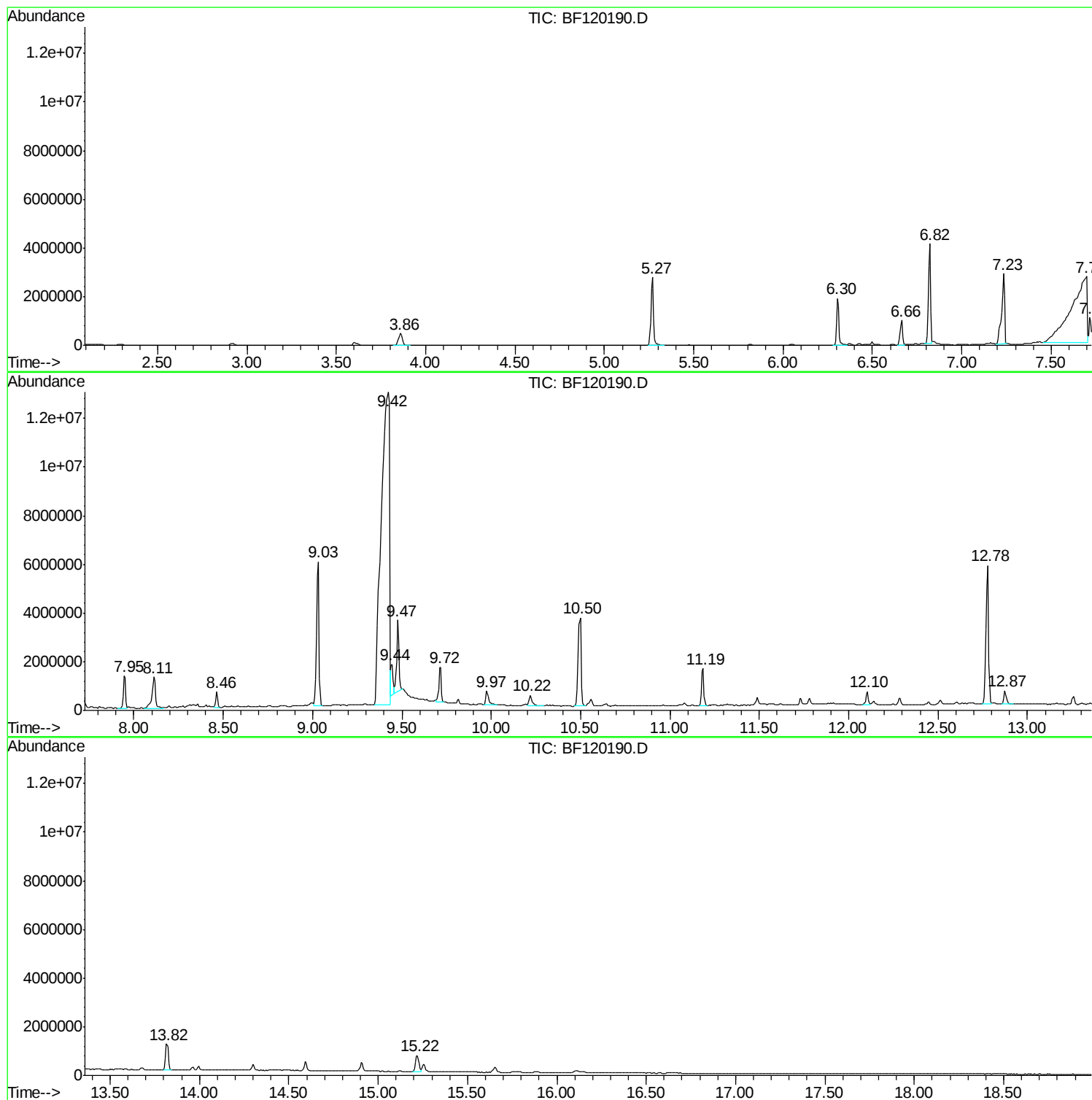
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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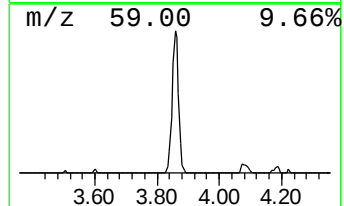
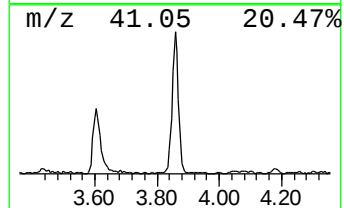
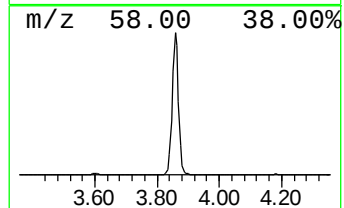
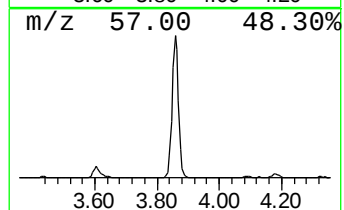
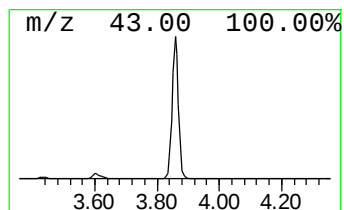
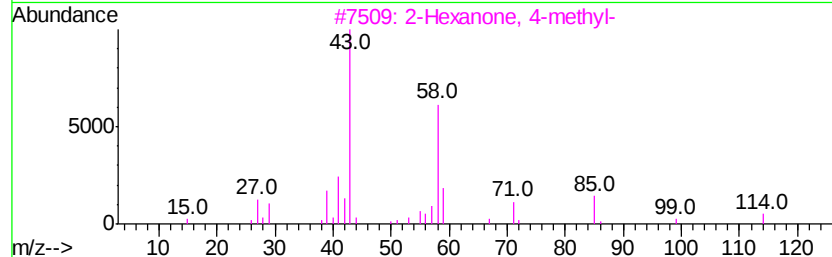
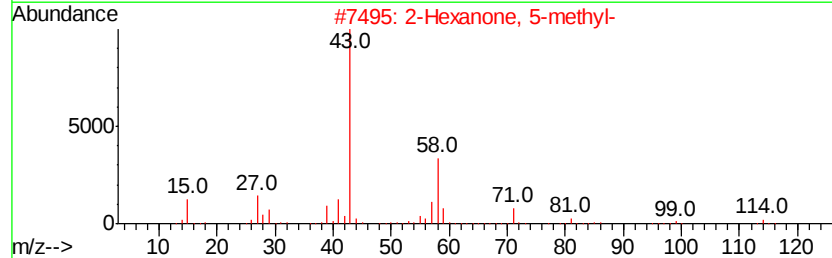
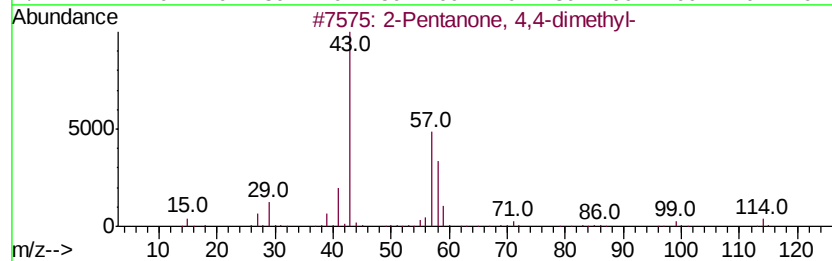
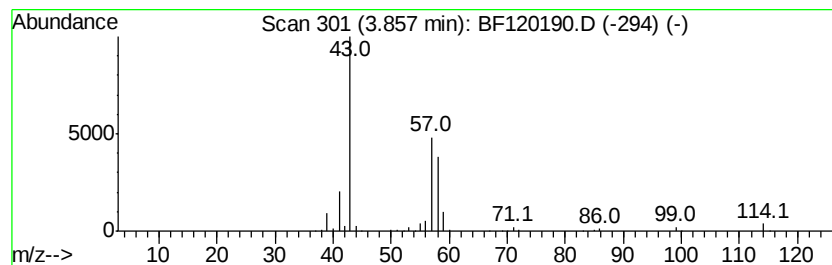
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4,4-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.86	16.03 ng	697638	1,4-Dichlorobenzene-d4	6.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4,4-dimethyl-	114	C7H14O	000590-50-1	90
2		2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	86
3		2-Hexanone, 4-methyl-	114	C7H14O	000105-42-0	59
4		2-Heptanone	114	C7H14O	000110-43-0	45
5		1-Butoxy-2-propanol acetate	174	C9H18O3	085409-76-3	40



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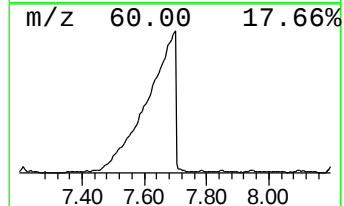
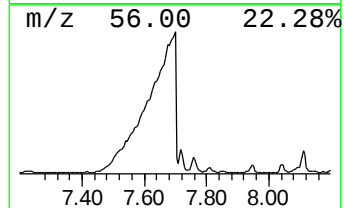
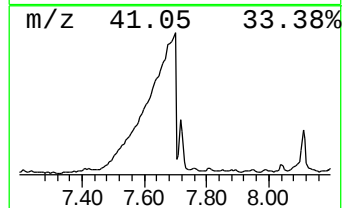
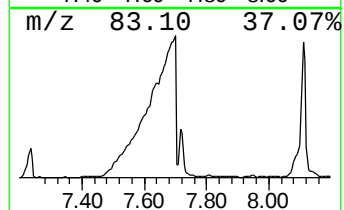
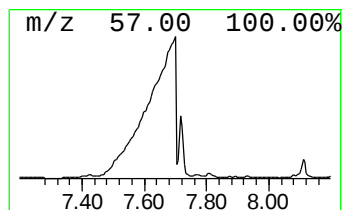
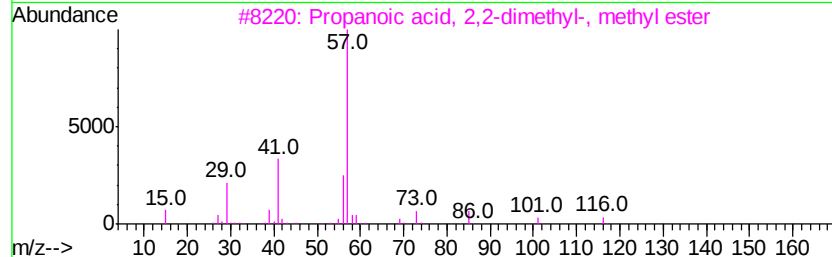
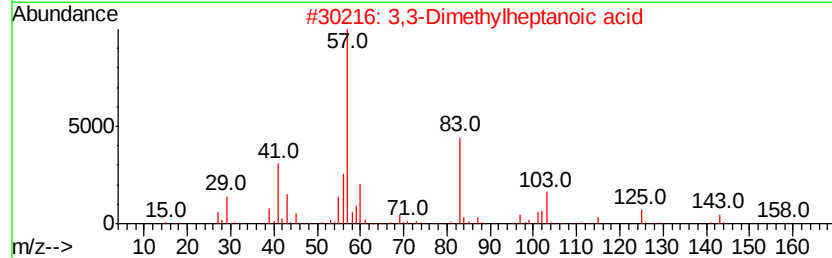
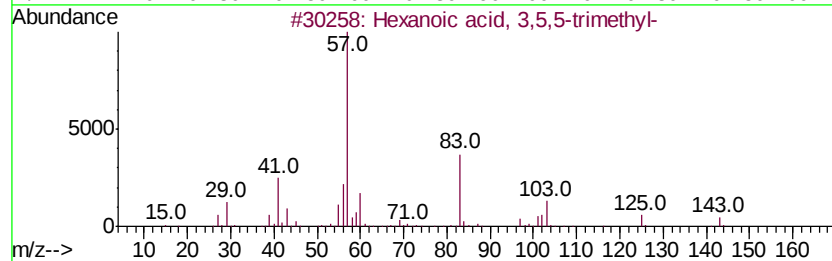
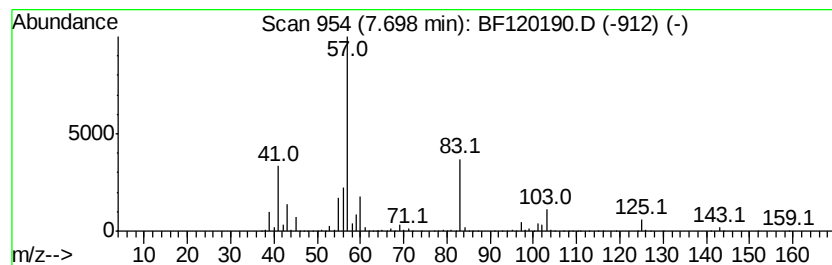
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Peak Number 3 Hexanoic acid, 3,5,5-trimet... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.70	256.25 ng	16558500	Naphthalene-d8	7.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexanoic acid, 3,5,5-trimethyl-	158	C9H18O2	003302-10-1	83
2		3,3-Dimethylheptanoic acid	158	C9H18O2	067061-30-7	83
3		Propanoic acid, 2,2-dimethyl-, m...	116	C6H12O2	000598-98-1	35
4		Hexanoyl chloride, 3,5,5-trimethyl-	176	C9H17ClO	036727-29-4	25
5		Propanoic acid, 2,2-dimethyl-	102	C5H10O2	000075-98-9	22



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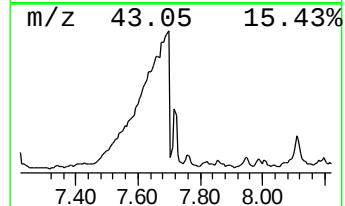
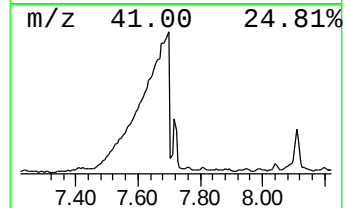
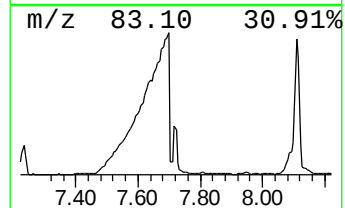
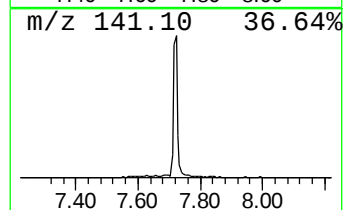
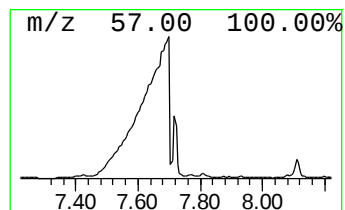
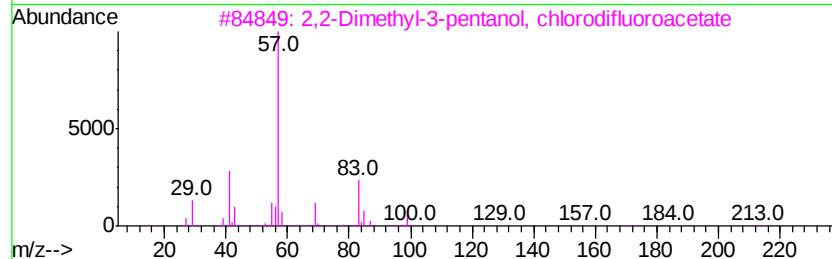
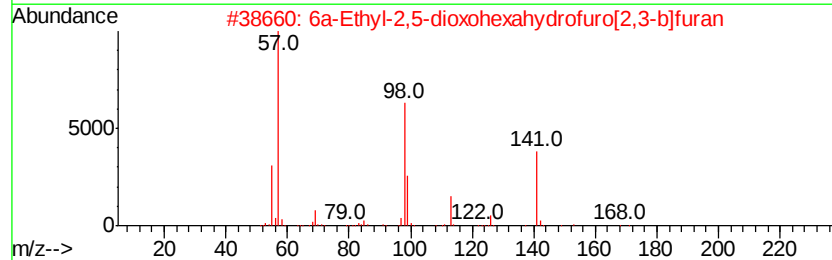
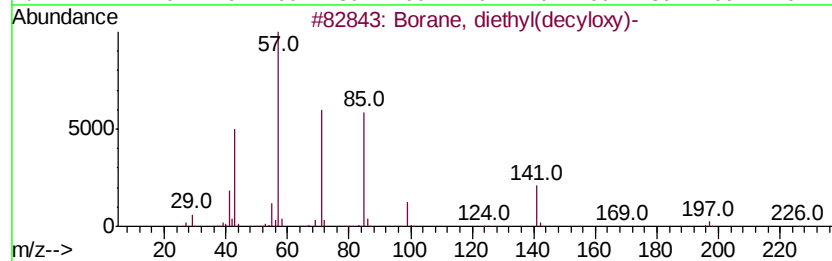
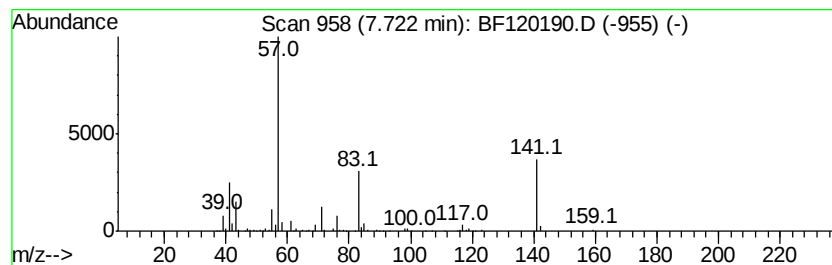
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Peak Number 4 unknown7.72 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.72	13.38 ng	864426	Napthalene-d8	7.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Borane, diethyl(decvloxy)-	226	C14H31BO	1000152-34-3	35
2		6a-Ethyl-2,5-dioxohexahydrofuro[...]	170	C8H10O4	083663-22-3	32
3		2,2-Dimethyl-3-pentanol, chlorod...	228	C9H15ClF2O2	1000376-26-4	25
4		4,4-Dimethyl-2-pentanol, chlorod...	228	C9H15ClF2O2	1000376-27-0	25
5		Heptane, 3,5-dimethyl-	128	C9H20	000926-82-9	14



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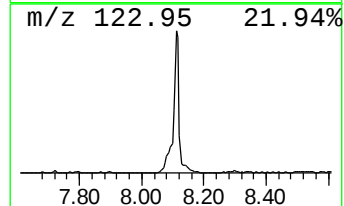
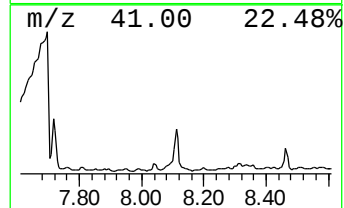
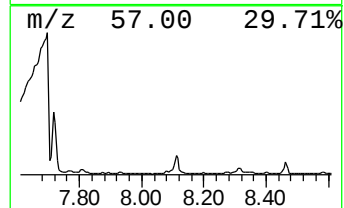
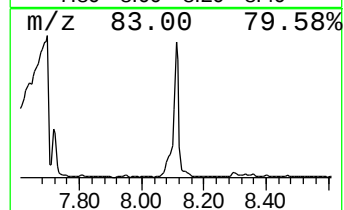
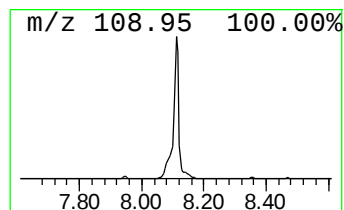
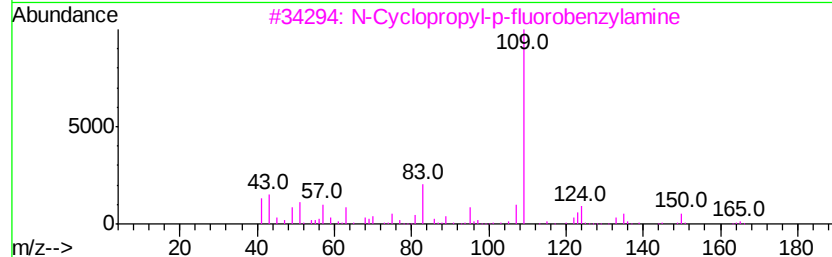
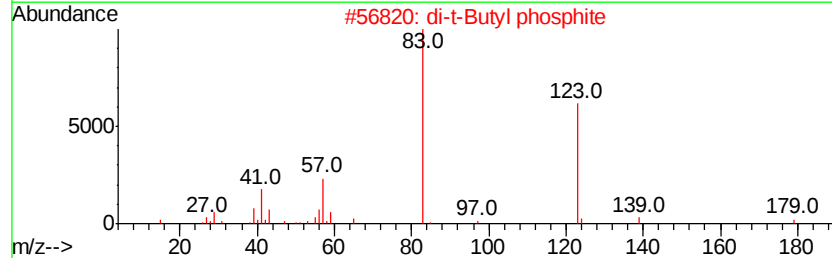
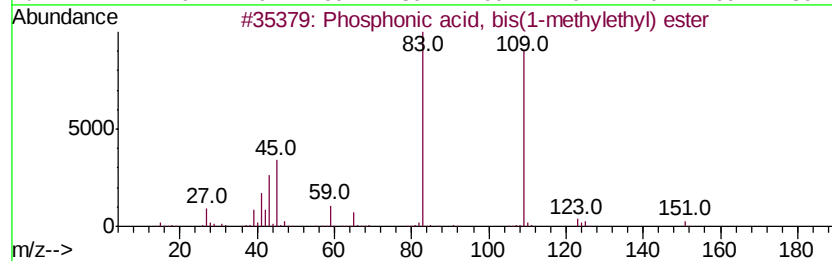
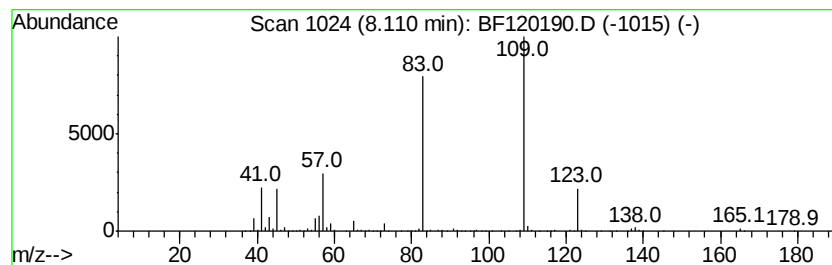
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Peak Number 5 unknown8.11 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.11	26.51 ng	1713180	Napthalene-d8	7.95

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Phosphonic acid, bis(1-methylethyl)	166	C6H15O3P	001809-20-7	33
2		di-t-Butyl phosphite	194	C8H19O3P	013086-84-5	17
3		N-Cyclopropyl-p-fluorobenzylamine	165	C10H12FN	1000250-88-9	9
4		3,4-Pyridinediamine	109	C5H7N3	000054-96-6	9
5		1H-Imidazol-2-amine	83	C3H5N3	007720-39-0	9



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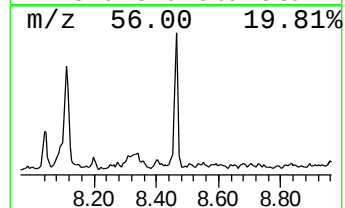
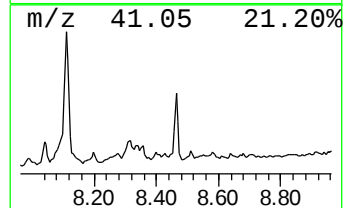
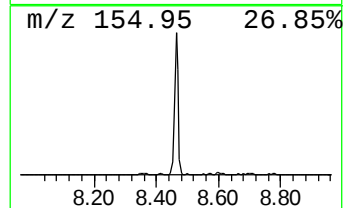
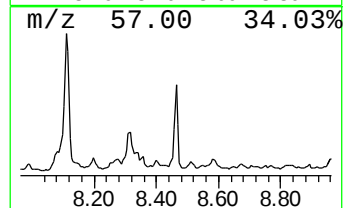
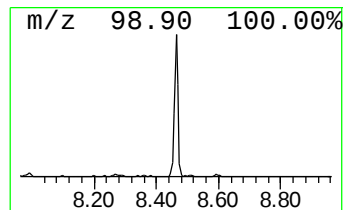
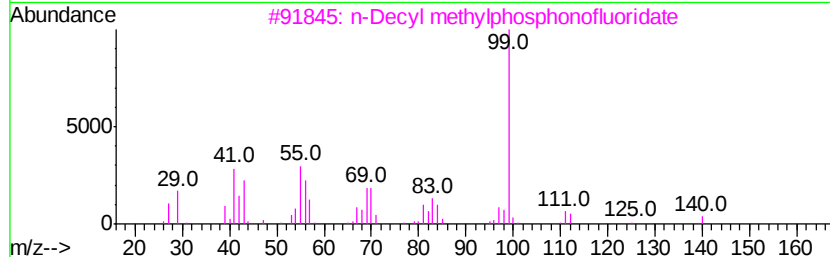
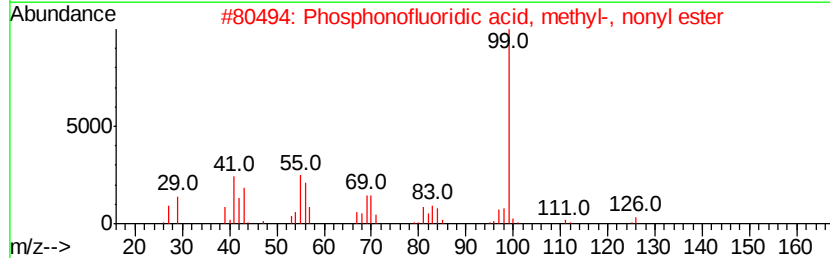
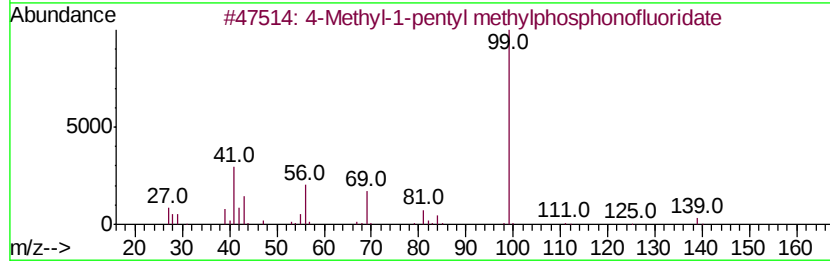
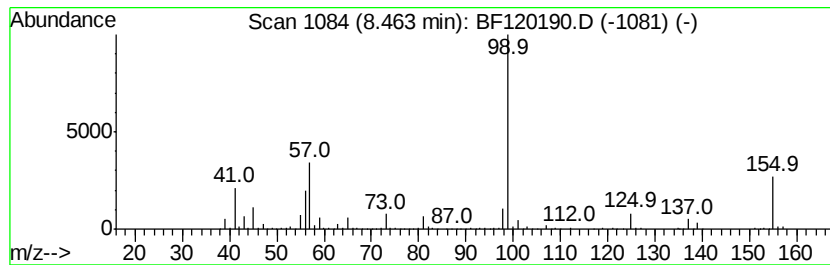
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TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown8.46 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.46	7.64 ng	493630	Naphthalene-d8	7.95

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Methyl-1-pentyl		methylphosphon...	182	C7H16F02P	1000216-68-2	40
2	Phosphonofluoridic acid, methyl-		...	224	C10H22F02P	211192-74-4	36
3	n-Decyl		methylphosphonofluoridate	238	C11H24F02P	193090-25-4	36
4	n-Butyl		methylphosphonofluoridate	154	C5H12F02P	000352-63-6	33
5	Phosphonofluoridic acid, methyl-		...	182	C7H16F02P	000660-21-9	25



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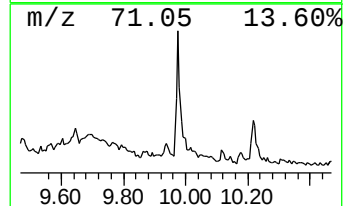
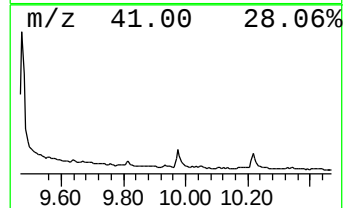
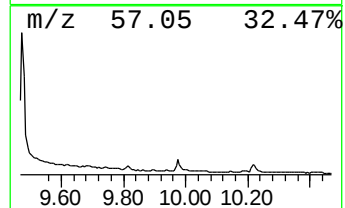
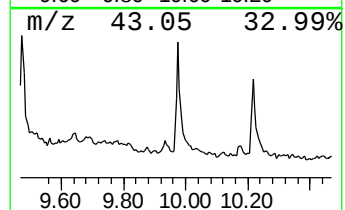
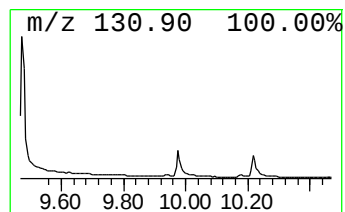
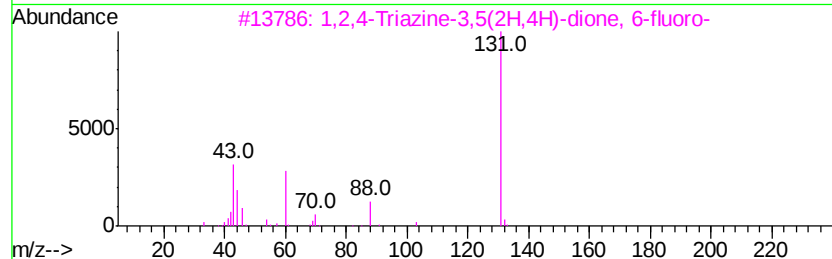
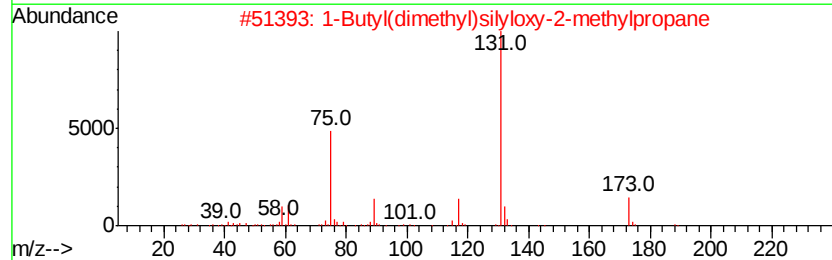
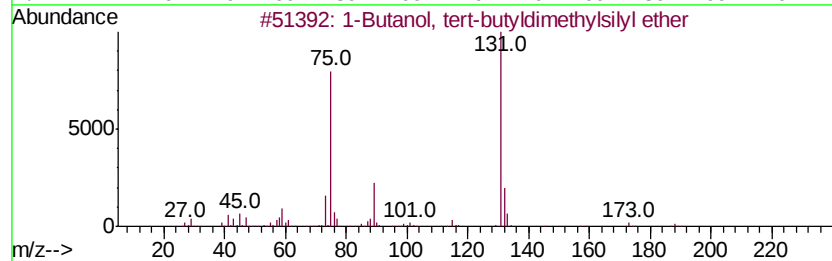
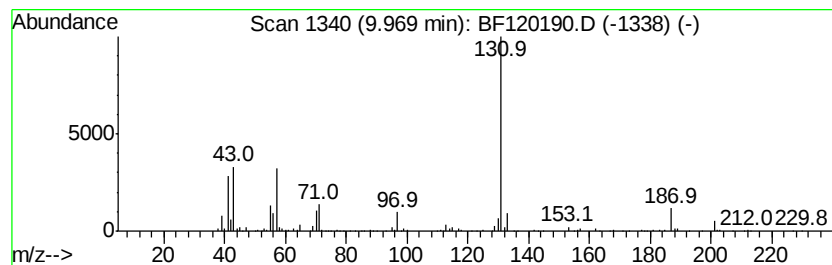
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown9.97 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.97	8.55 ng	571941	Acenaphthene-d10	9.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Butanol, tert-butyl(dimethyl)silyl ether	188	C10H24OSi	1000333-04-7	7
2		1-Butyl(dimethyl)silyloxy-2-methylpropane	188	C10H24OSi	1000282-45-2	5
3		1,2,4-Triazine-3,5(2H,4H)-dione, 6-fluoro-	131	C3H2FN3O2	082736-95-6	5
4		Pyrrolo[2,3-d]pyrimidine	131	C7H5N3	000254-61-5	4
5		2-Oxazolidinethione, 4,4-dimethyl-	131	C5H9NOS	054013-55-7	4



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF042420\
Data File : BF120190.D
Acq On : 24 Apr 2020 9:45
Operator : MA/SJ
Sample : L2330-18
Misc :
ALS Vial : 27 Sample Multiplier: 1

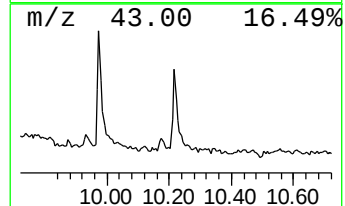
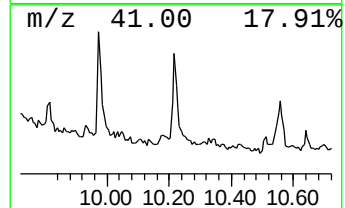
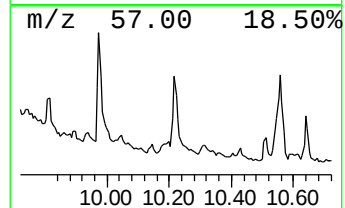
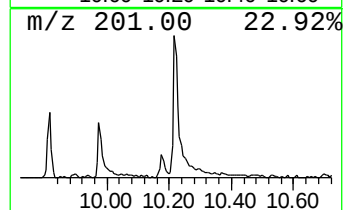
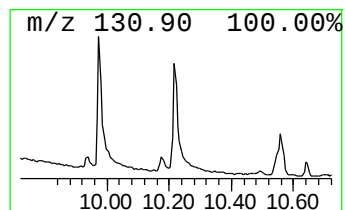
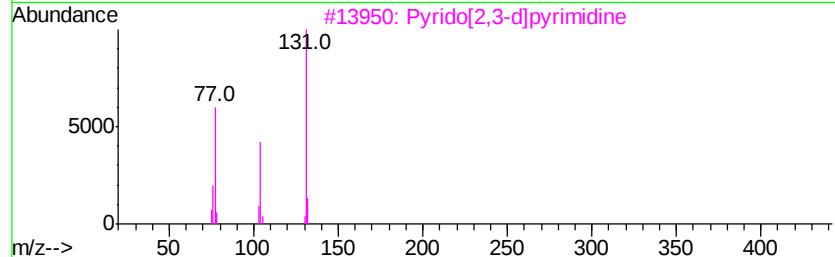
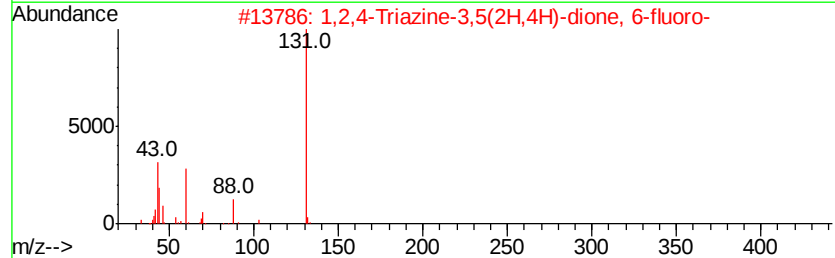
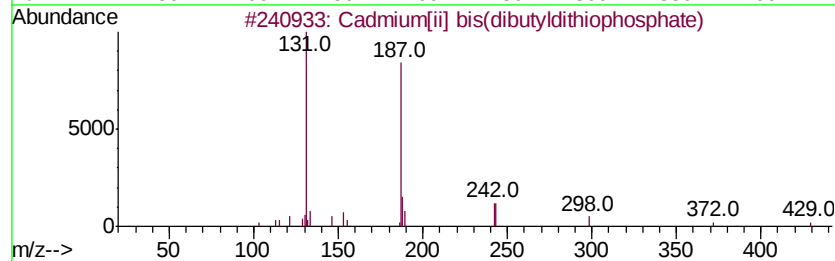
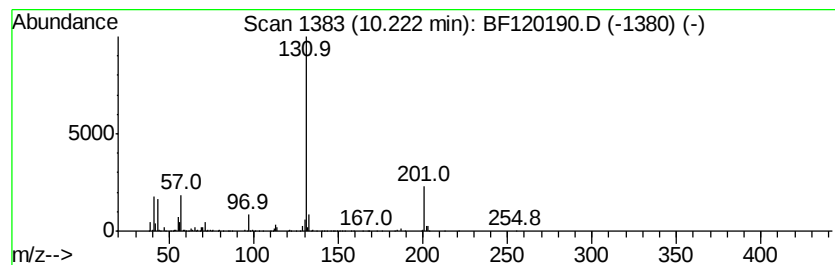
Instrument :
BNA_F
ClientSampleId :
WB-TWP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF040820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown10.22 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.		
10.22	7.70 ng	515067	Acenaphthene-d10		9.72		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cadmium[II] bis(dibutylthiophospho...	596	C16H36CdO4P2S4	043159-11-1	39
2			1,2,4-Triazine-3,5(2H,4H)-dione,...	131	C3H2FN3O2	082736-95-6	7
3			Pyrido[2,3-d]pyrimidine	131	C7H5N3	000254-61-5	4
4			1,2,4-Triazolidin-3-one, 4-methy...	131	C3H5N3OS	022244-61-7	4
5			2-Oxazolidinethione, 4,4-dimethyl-	131	C5H9NOS	054013-55-7	4



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF042420\
 Data File : BF120190.D
 Acq On : 24 Apr 2020 9:45
 Operator : MA/SJ
 Sample : L2330-18
 Misc :
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WB-TWP-1

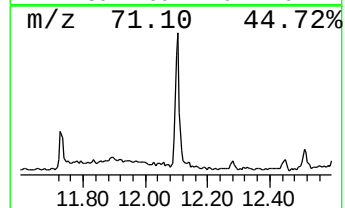
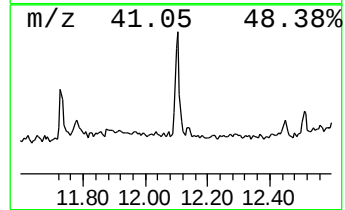
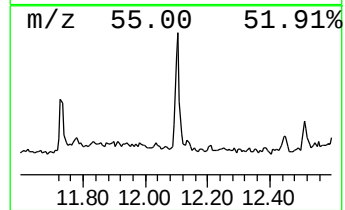
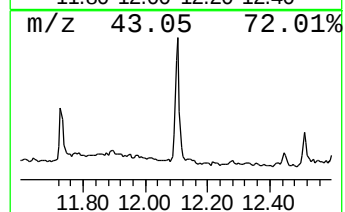
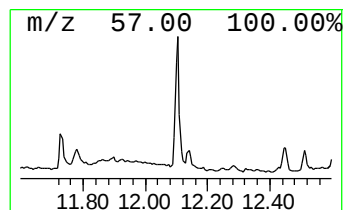
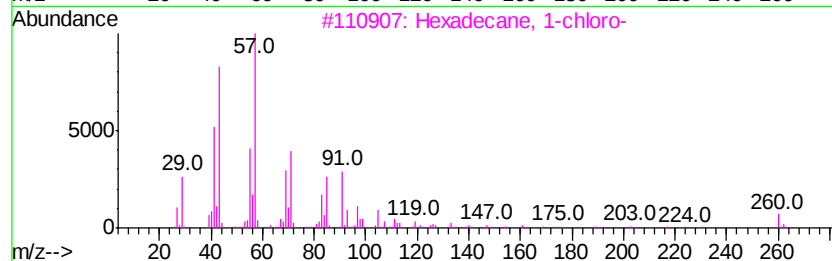
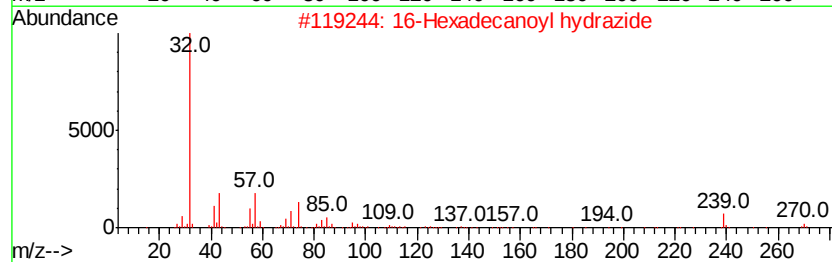
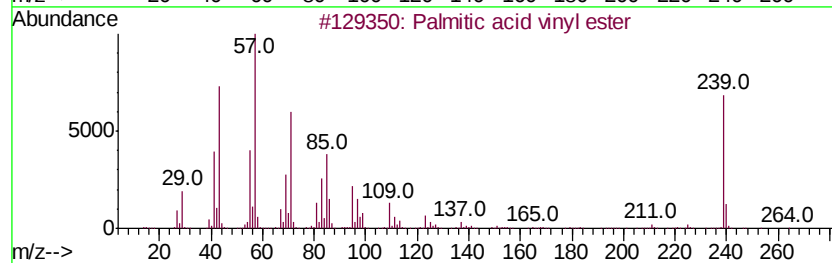
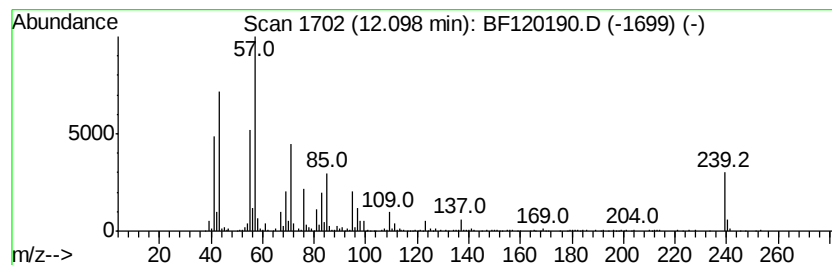
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 9 Palmitic acid vinyl ester Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.10	7.54 ng	509144	Phenanthrene-d10	11.19

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Palmitic acid vinyl ester	282	C18H34O2	000693-38-9	83
2			16-Hexadecanoyl hydrazide	270	C16H34N2O	002619-88-7	59
3			Hexadecane, 1-chloro-	260	C16H33Cl	004860-03-1	43
4			Heptadecane	240	C17H36	000629-78-7	38
5			Hexadecane	226	C16H34	000544-76-3	27



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF042420\
Data File : BF120190.D
Acq On : 24 Apr 2020 9:45
Operator : MA/SJ
Sample : L2330-18
Misc :
ALS Vial : 27 Sample Multiplier: 1

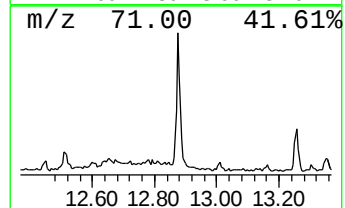
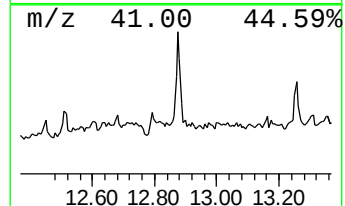
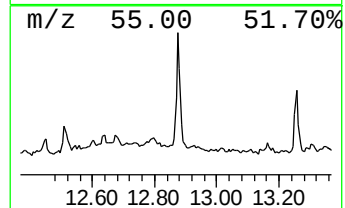
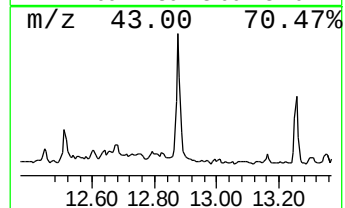
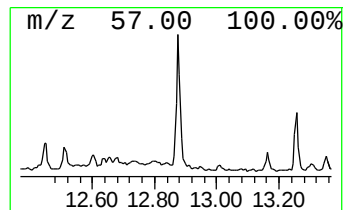
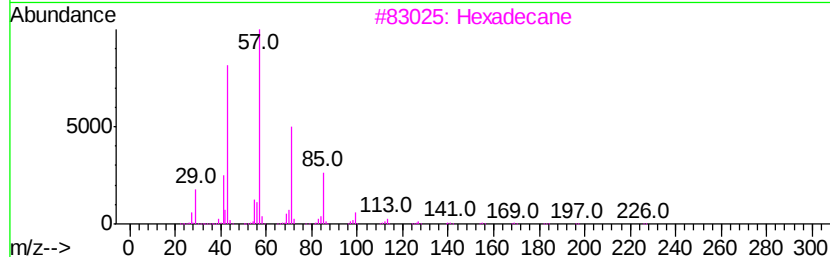
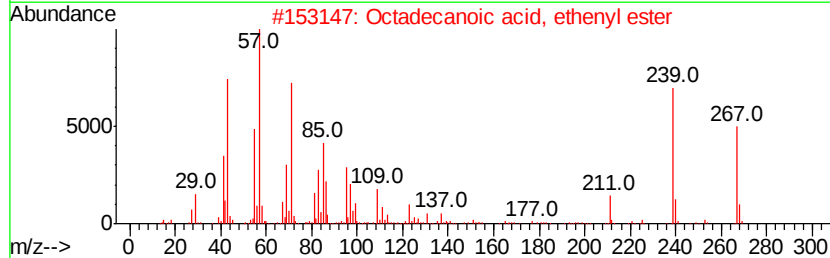
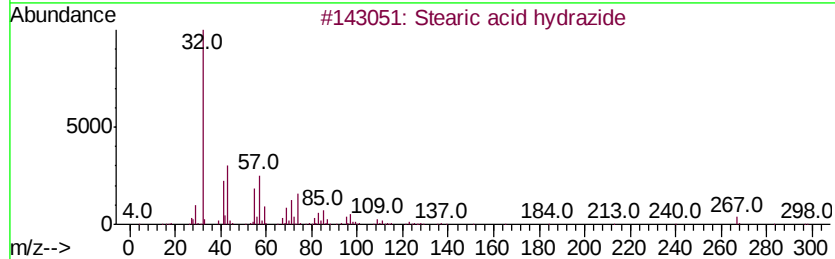
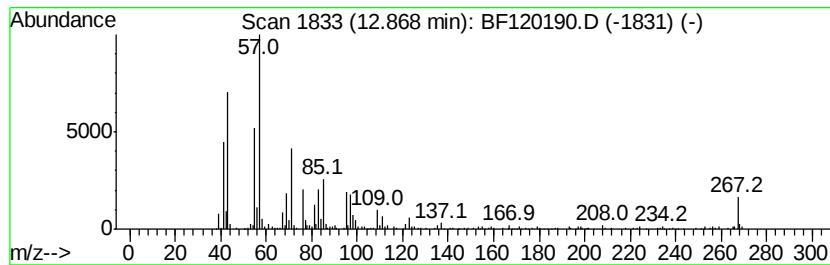
Instrument :
BNA_F
ClientSampleId :
WB-TWP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF040820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Stearic acid hydrazide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.87	10.49 ng	519347	Chrysene-d12	13.82	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Stearic acid hydrazide	298	C18H38N2O	004130-54-5	64
2	Octadecanoic acid, ethenyl ester	310	C20H38O2	000111-63-7	53
3	Hexadecane	226	C16H34	000544-76-3	35
4	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	35
5	Sulfurous acid, decyl 2-propyl e...	264	C13H28O3S	1000309-12-1	27



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF042420\
Data File : BF120190.D
Acq On : 24 Apr 2020 9:45
Operator : MA/SJ
Sample : L2330-18
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WB-TWP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040820.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
2-Pentanone, 4,4-...	3.86	16.0	ng	697638	1	6.66	870472	20.0
Hexanoic acid, 3,...	7.70	256.3	ng	16558500	2	7.95	1292350	20.0
unknown7.72	7.72	13.4	ng	864426	2	7.95	1292350	20.0
unknown8.11	8.11	26.5	ng	1713180	2	7.95	1292350	20.0
unknown8.46	8.46	7.6	ng	493630	2	7.95	1292350	20.0
unknown9.97	9.97	8.6	ng	571941	3	9.72	1337280	20.0
unknown10.22	10.22	7.7	ng	515067	3	9.72	1337280	20.0
Palmitic acid vin...	12.10	7.5	ng	509144	4	11.19	1349910	20.0
Stearic acid hydr...	12.87	10.5	ng	519347	5	13.82	990572	20.0