

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052421\
 Data File : BF124041.D
 Acq On : 24 May 2021 17:10
 Operator : JU/CG
 Sample : M2490-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 72-11986

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-BF051421.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124041.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.169	7	14	19	rBV	538402	700730	44.56%	5.204%
2	2.275	27	32	38	rVB	34911	48670	3.09%	0.361%
3	5.104	509	513	524	rVB	271998	332836	21.16%	2.472%
4	5.510	577	582	585	rBV	1418632	1264958	80.44%	9.394%
5	5.904	646	649	653	rBB	30606	24434	1.55%	0.181%
6	6.516	748	753	756	rBV	1387959	1279858	81.38%	9.505%
7	6.716	784	787	793	rBV	45557	47584	3.03%	0.353%
8	6.892	813	817	820	rBV	406141	350343	22.28%	2.602%
9	7.451	907	912	915	rBV	1026599	871334	55.41%	6.471%
10	8.175	1031	1035	1038	rBV	571075	435591	27.70%	3.235%
11	9.251	1214	1218	1221	rBV	2029334	1572609	100.00%	11.679%
12	9.639	1281	1284	1291	rBV	228852	176329	11.21%	1.309%
13	9.927	1330	1333	1337	rBV	613234	509261	32.38%	3.782%
14	10.716	1463	1467	1470	rBV	1211563	1024214	65.13%	7.606%
15	11.416	1582	1586	1589	rBV	615176	510204	32.44%	3.789%
16	11.439	1589	1590	1593	rVB	96138	54654	3.48%	0.406%
17	11.939	1673	1675	1679	rVB2	81739	75310	4.79%	0.559%
18	12.027	1687	1690	1693	rBV2	19294	20023	1.27%	0.149%
19	12.627	1789	1792	1796	rBV	99362	87382	5.56%	0.649%
20	12.857	1826	1831	1834	rBV	95233	99923	6.35%	0.742%
21	13.004	1852	1856	1859	rBV	1595152	1347735	85.70%	10.009%
22	13.086	1863	1870	1872	rBV7	12051	22537	1.43%	0.167%
23	13.233	1890	1895	1897	rBV4	20091	28800	1.83%	0.214%
24	13.904	2006	2009	2018	rBV	241414	347976	22.13%	2.584%
25	14.039	2029	2032	2034	rBV	825080	748035	47.57%	5.555%
26	14.062	2034	2036	2038	rVV	437540	355075	22.58%	2.637%
27	14.086	2038	2040	2042	rVB	44151	32955	2.10%	0.245%
28	14.486	2104	2108	2111	rVB6	15863	23481	1.49%	0.174%
29	14.545	2113	2118	2126	rBV3	100681	179060	11.39%	1.330%
30	14.992	2192	2194	2197	rVB3	36072	29883	1.90%	0.222%
31	15.109	2211	2214	2217	rBV3	35335	50900	3.24%	0.378%
32	15.192	2225	2228	2231	rVB3	49264	52625	3.35%	0.391%
33	15.233	2231	2235	2239	rBV6	47137	74929	4.76%	0.556%
34	15.421	2264	2267	2271	rVB4	35917	42737	2.72%	0.317%
35	15.486	2275	2278	2281	rBV4	26260	31741	2.02%	0.236%
36	15.551	2285	2289	2293	rBV	282669	368721	23.45%	2.738%

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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-BF051421.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.792	2328	2330	2333	rVB4	25423	20389	1.30%	0.151%
38	16.033	2367	2371	2377	rVB3	40006	62382	3.97%	0.463%
39	16.109	2377	2384	2389	rBV8	52643	128073	8.14%	0.951%
40	16.856	2507	2511	2515	rBV6	20377	31118	1.98%	0.231%

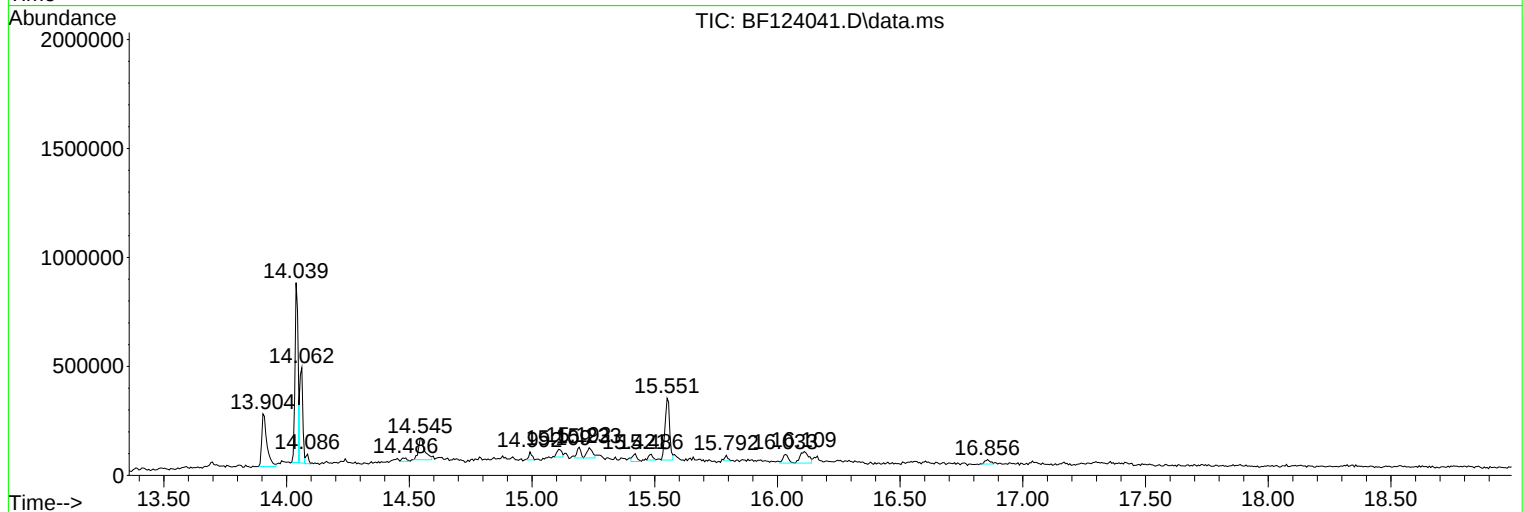
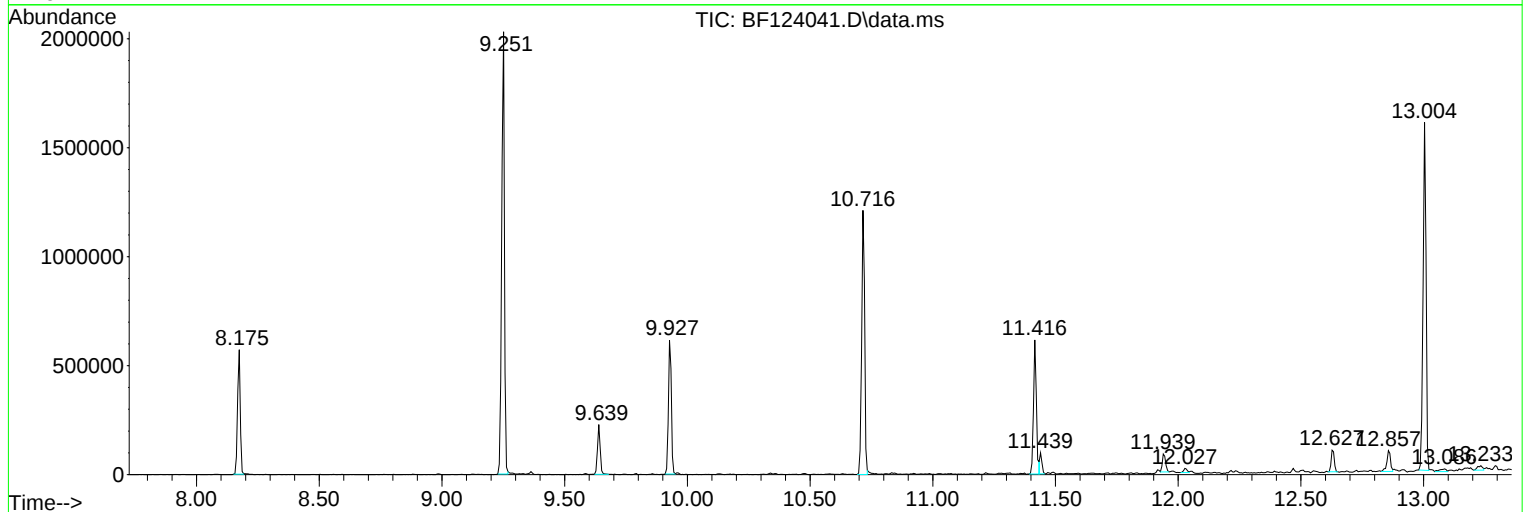
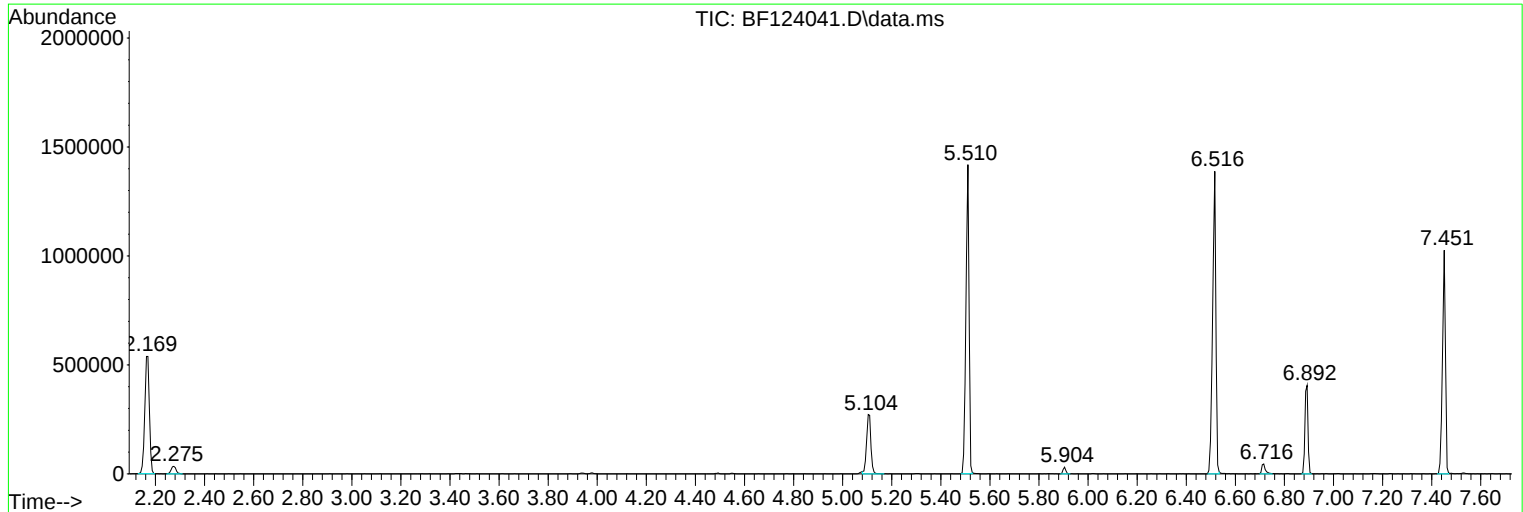
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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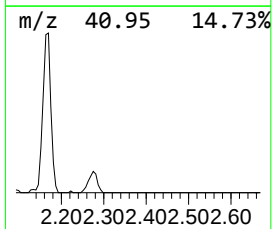
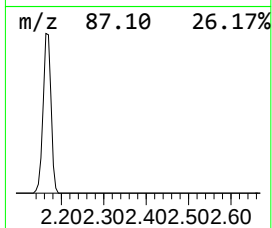
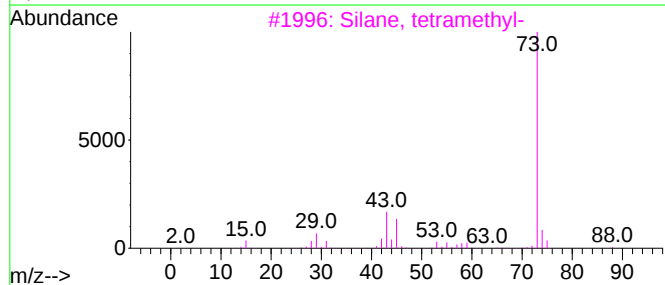
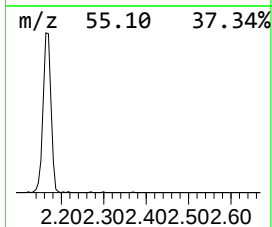
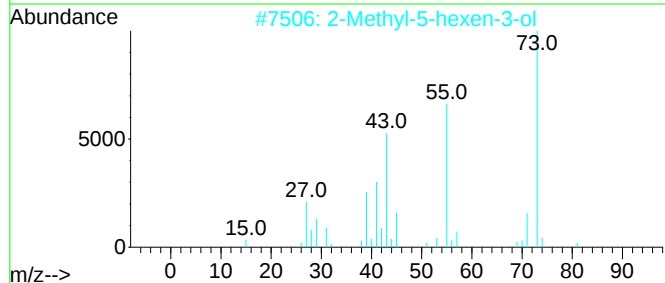
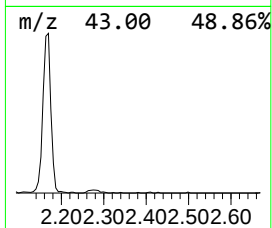
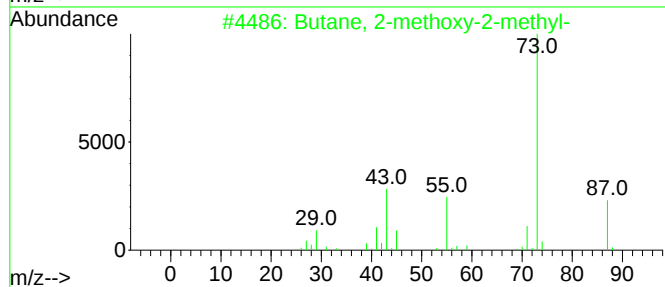
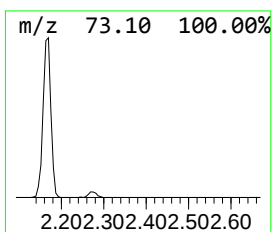
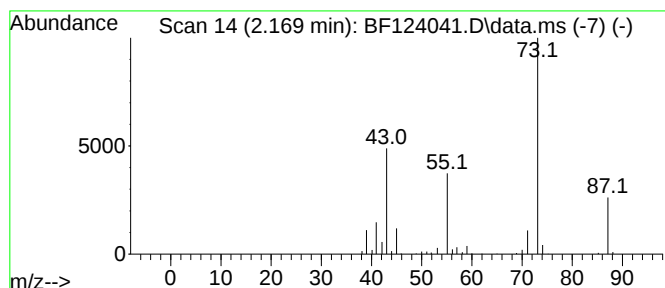
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.169	40.00 ng	700730	1,4-Dichlorobenzene-d4	6.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	25
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	16
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	9



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ALS Vial : 9 Sample Multiplier: 1

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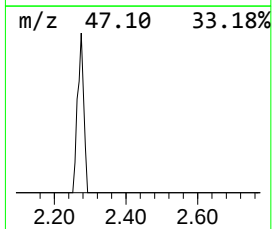
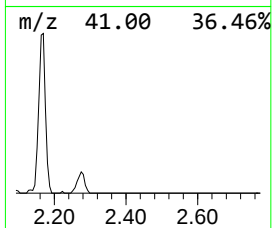
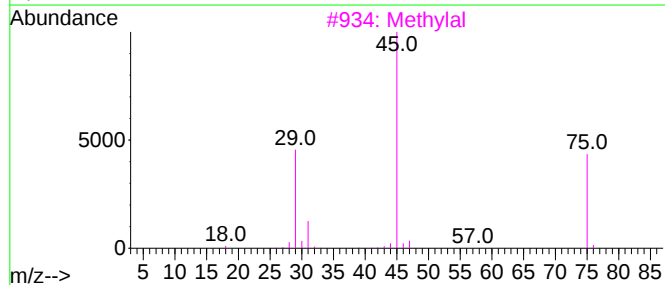
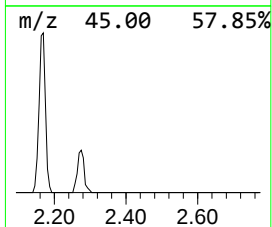
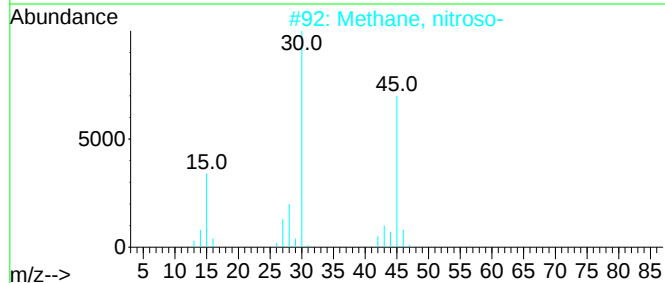
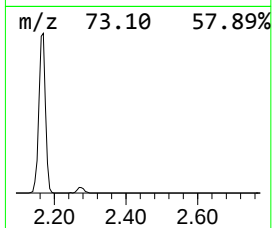
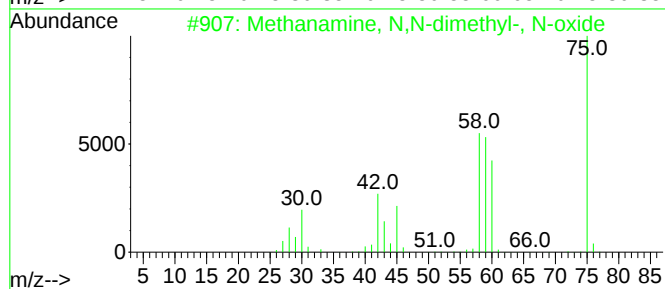
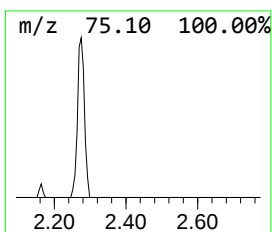
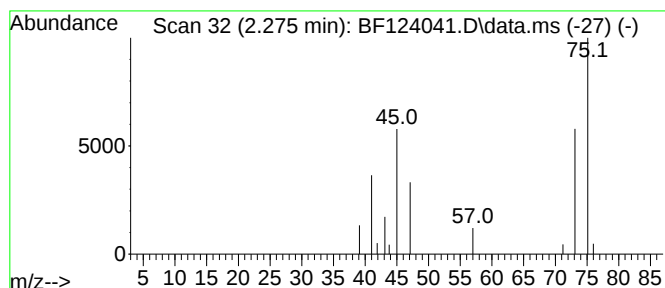
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown2,27 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.275	2.78 ng	48670	1,4-Dichlorobenzene-d4	6.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methanamine, N,N-dimethyl-, N-oxide	75	C3H9NO	001184-78-7	5
2			Methane, nitroso-	45	CH3NO	000865-40-7	4
3			Methylal	76	C3H8O2	000109-87-5	4
4			Glycine	75	C2H5NO2	000056-40-6	4
5			2-Hydrazinoethanol	76	C2H8N2O	000109-84-2	4



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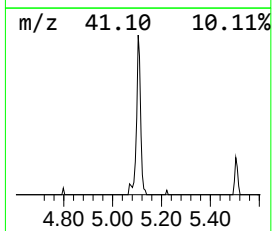
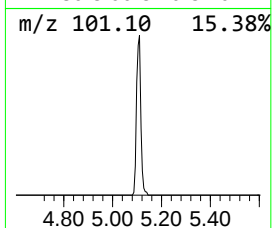
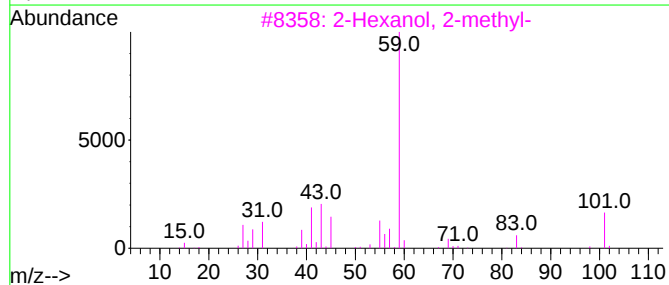
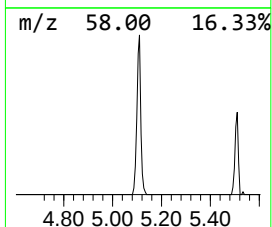
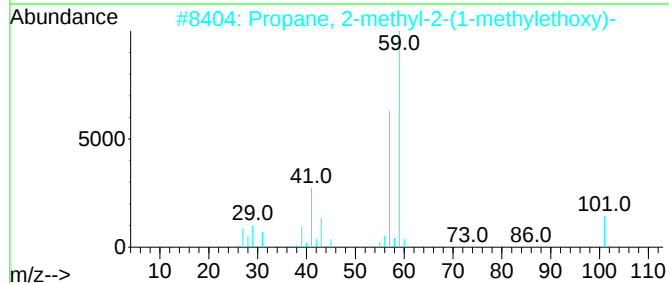
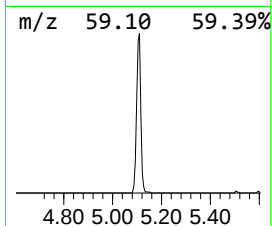
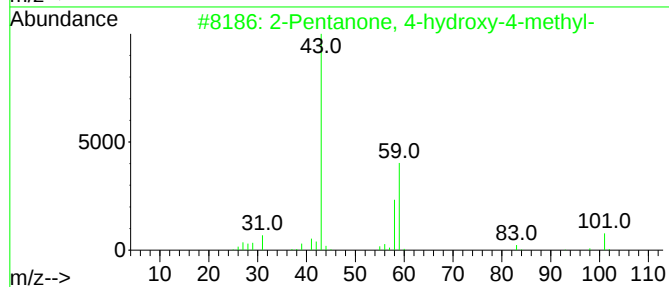
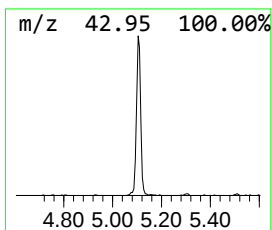
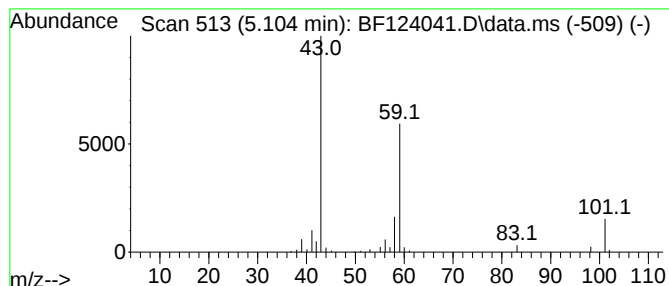
Instrument :
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD		R.T.	
5.104	19.00 ng	332836	1,4-Dichlorobenzene-d4		6.892	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	50
2	Propane, 2-methyl-2-(1-methyleth...		116	C7H16O	017348-59-3	42
3	2-Hexanol, 2-methyl-		116	C7H16O	000625-23-0	40
4	3-Hexanol, 4-methyl-		116	C7H16O	000615-29-2	33
5	3-Octanol		130	C8H18O	000589-98-0	33



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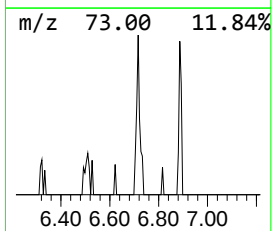
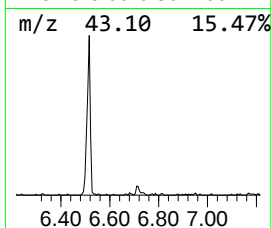
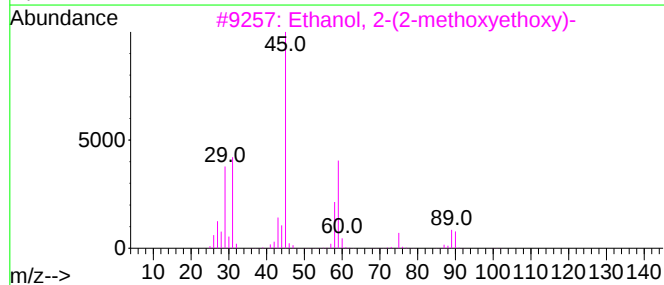
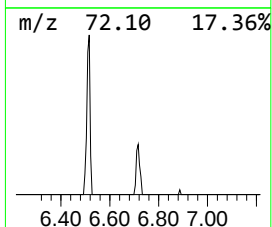
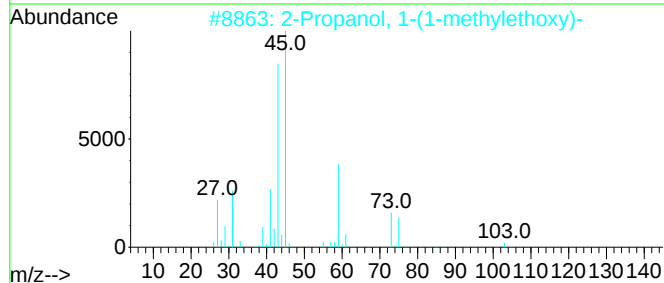
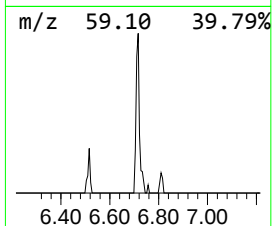
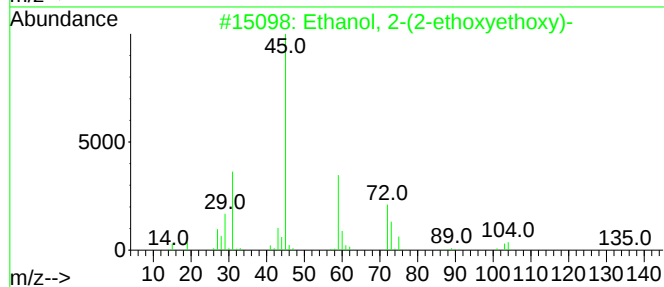
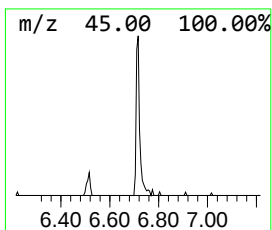
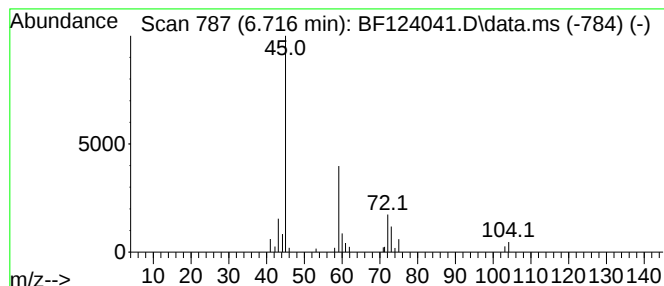
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.716	2.72 ng	47584	1,4-Dichlorobenzene-d4	6.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	83
2			2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	56
3			Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	50
4			Carbonic acid, dimethyl ester	90	C3H6O3	000616-38-6	39
5			Diethyl carbitol	162	C8H18O3	000112-36-7	28



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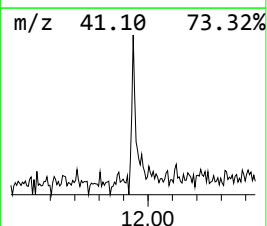
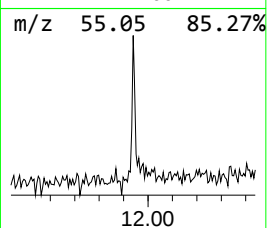
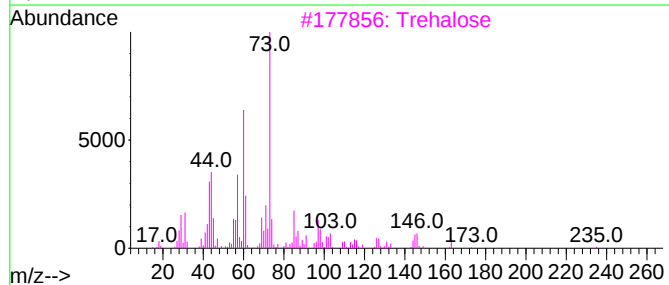
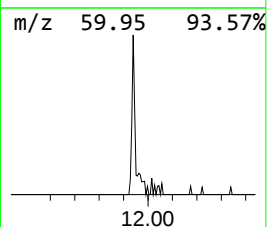
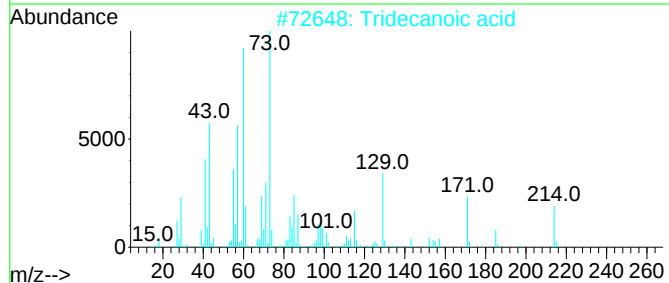
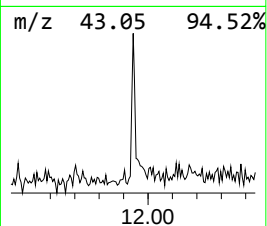
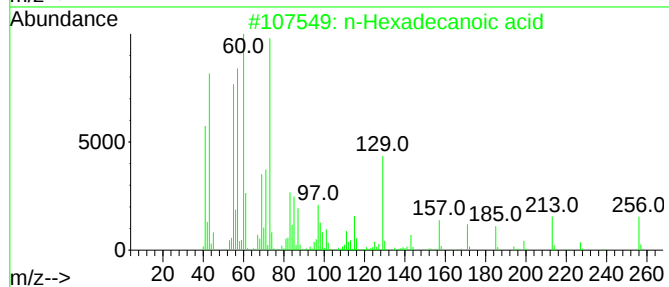
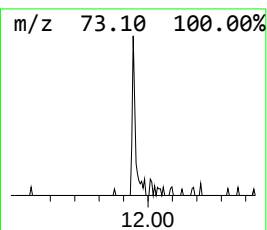
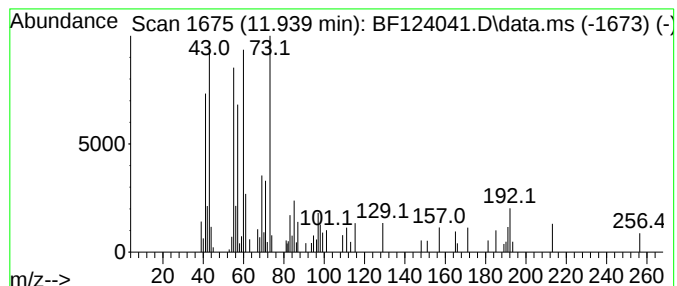
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.939	2.95 ng	75310	Phenanthrene-d10	11.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2			Tridecanoic acid	214	C13H26O2	000638-53-9	53
3			Trehalose	342	C12H22O11	000099-20-7	43
4			Dodecanoic acid	200	C12H24O2	000143-07-7	43
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	42



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052421\
Data File : BF124041.D
Acq On : 24 May 2021 17:10
Operator : JU/CG
Sample : M2490-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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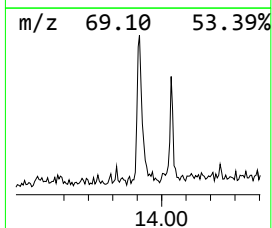
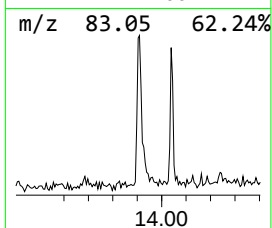
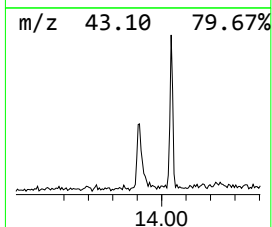
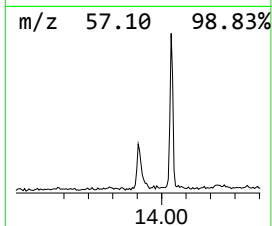
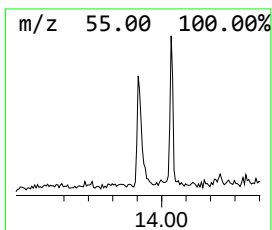
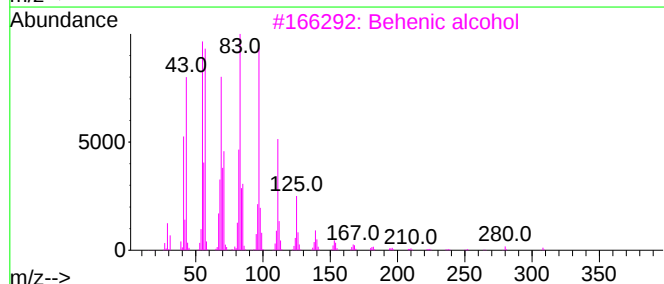
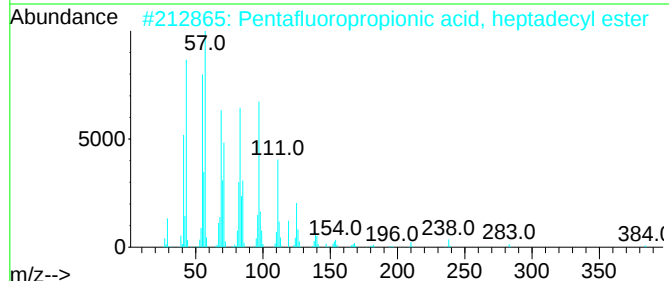
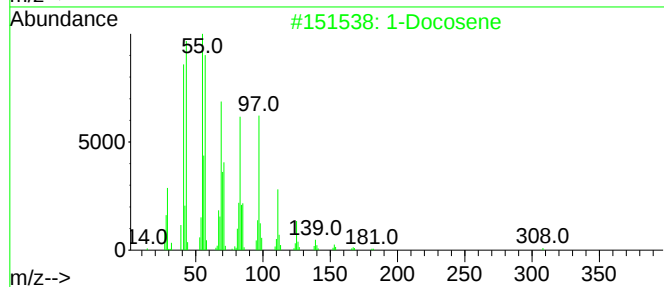
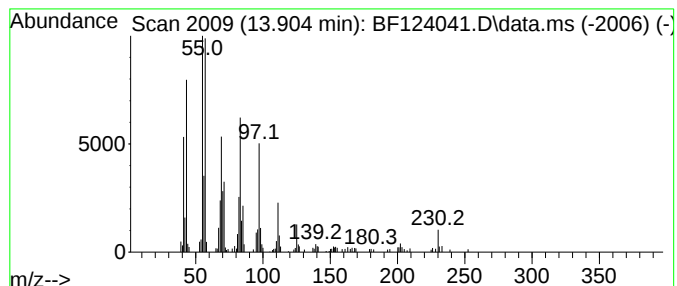
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
13.904	19.60 ng	347976	Chrysene-d12	14.062

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene			308	C22H44	001599-67-3	90
2	Pentafluoropropionic acid, hepta...			402	C20H35F5O2	959218-78-1	87
3	Behenic alcohol			326	C22H46O	000661-19-8	87
4	Heptadecyl trifluoroacetate			352	C19H35F3O2	1000351-87-0	87
5	Pentafluoropropionic acid, octad...			416	C21H37F5O2	959261-25-7	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052421\
Data File : BF124041.D
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Operator : JU/CG
Sample : M2490-01
Misc :
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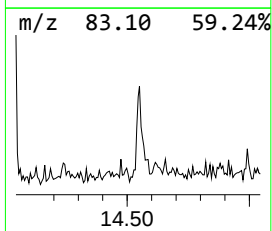
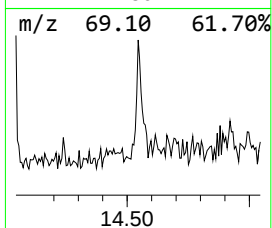
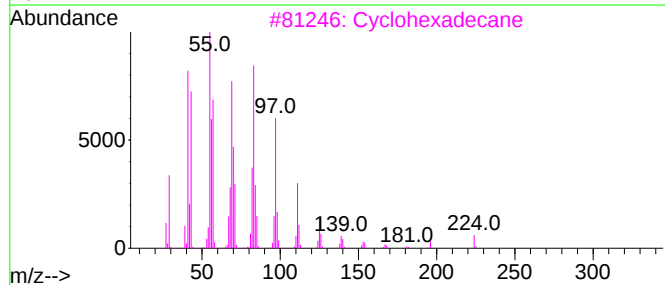
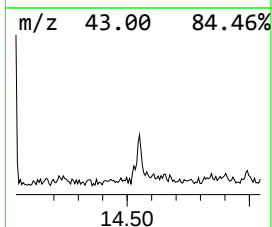
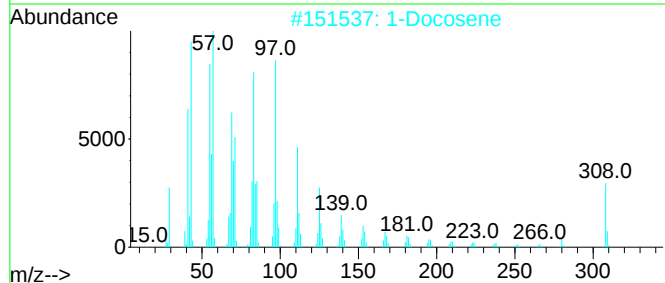
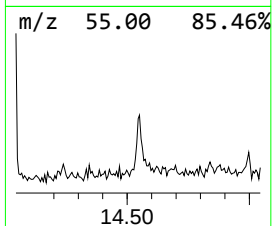
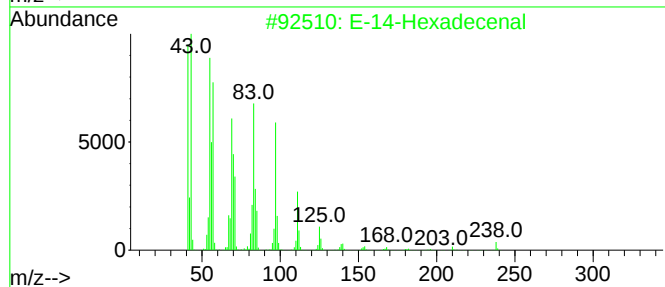
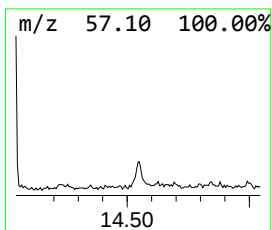
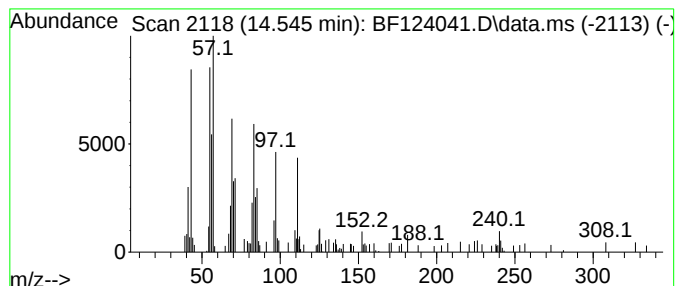
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 E-14-Hexadecenal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
14.545	10.09 ng	179060	Chrysene-d12		14.062	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	E-14-Hexadecenal		238	C16H30O	330207-53-9	86
2	1-Docosene		308	C22H44	001599-67-3	83
3	Cyclohexadecane		224	C16H32	000295-65-8	83
4	Cycloeicosane		280	C20H40	000296-56-0	68
5	Heptafluorobutyric acid, hexadec...		438	C20H33F7O2	006385-15-5	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052421\
Data File : BF124041.D
Acq On : 24 May 2021 17:10
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Sample : M2490-01
Misc :
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Instrument :
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ClientSampleId :
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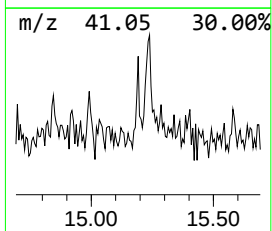
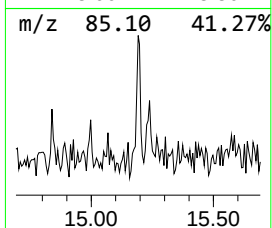
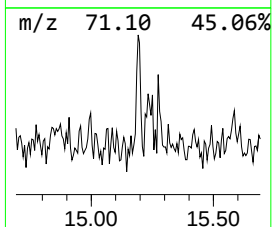
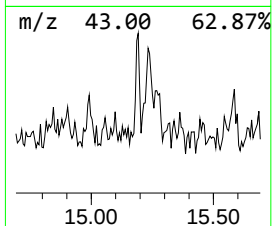
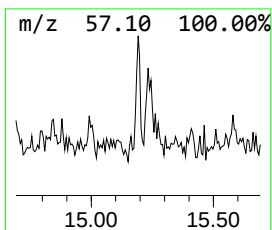
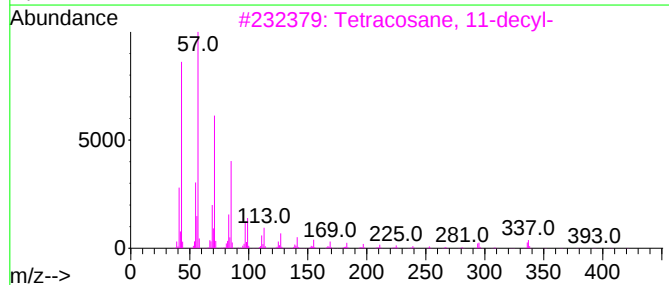
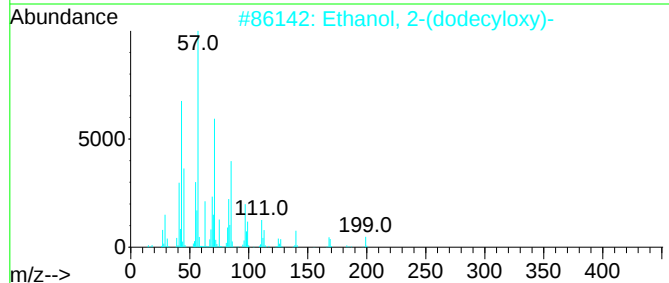
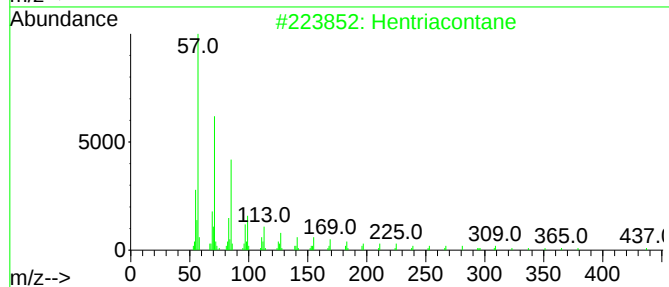
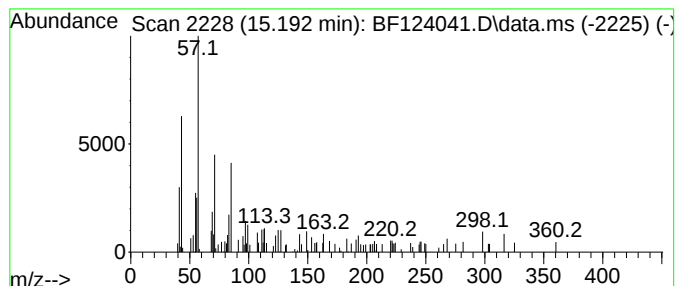
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown15.19 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.192	2.85 ng	52625	Perylene-d12	15.551

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hentriacontane	437	C31H64	000630-04-6	47
2			Ethanol, 2-(dodecyloxy)-	230	C14H30O2	004536-30-5	47
3			Tetracosane, 11-decyl-	479	C34H70	055429-84-0	47
4			Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	47
5			Octadecane	254	C18H38	000593-45-3	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052421\
Data File : BF124041.D
Acq On : 24 May 2021 17:10
Operator : JU/CG
Sample : M2490-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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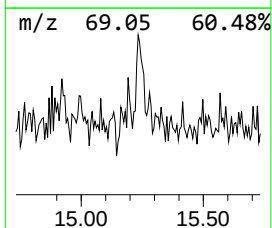
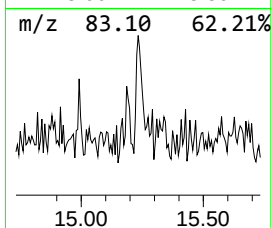
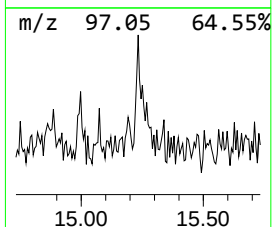
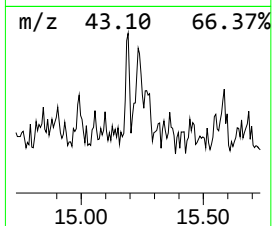
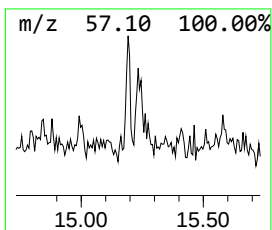
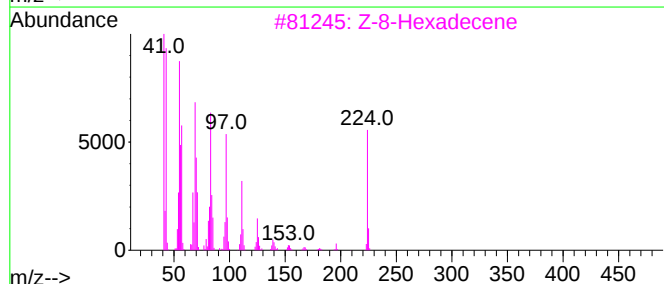
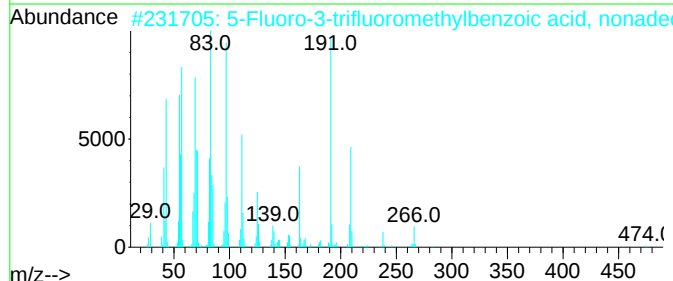
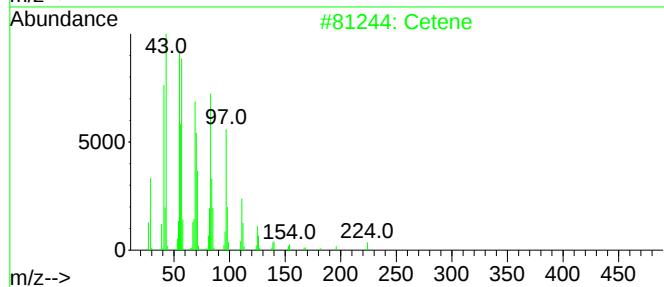
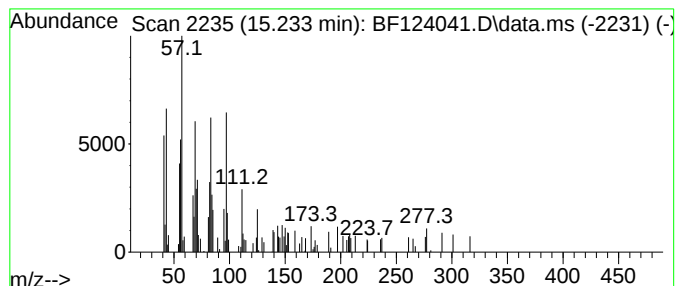
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Cetene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.233	4.06 ng	74929	Perylene-d12	15.551

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cetene	224	C16H32	000629-73-2	81
2			5-Fluoro-3-trifluoromethylbenzoi...	474	C27H42F4O2	1000338-91-1	76
3			Z-8-Hexadecene	224	C16H32	1000130-87-5	72
4			1-Octadecene	252	C18H36	000112-88-9	72
5			E-15-Heptadecenal	252	C17H32O	1000130-97-9	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052421\
Data File : BF124041.D
Acq On : 24 May 2021 17:10
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Sample : M2490-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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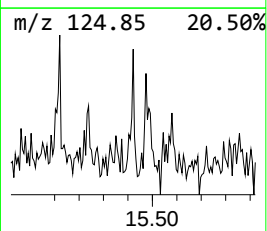
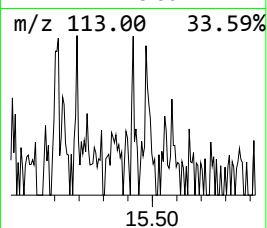
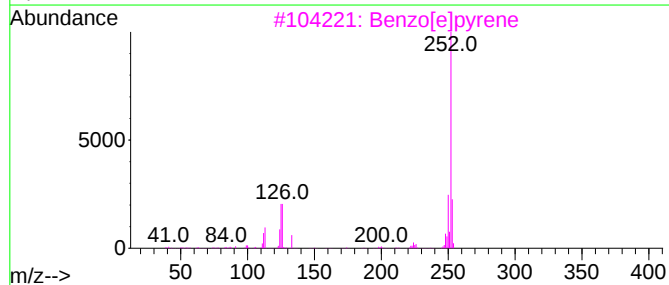
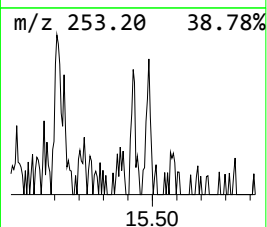
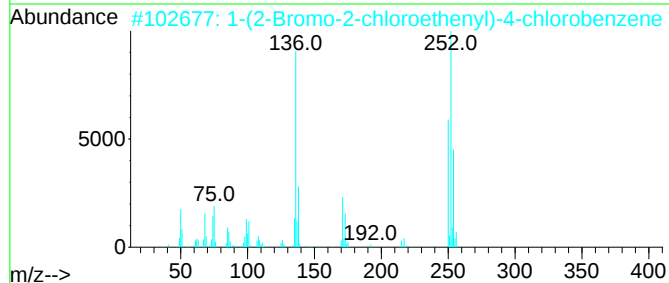
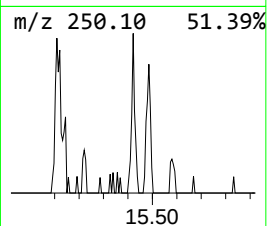
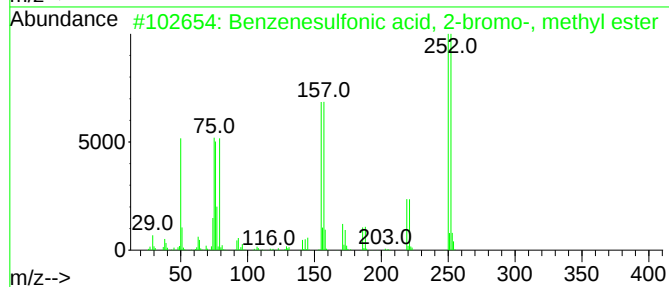
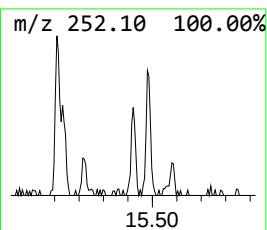
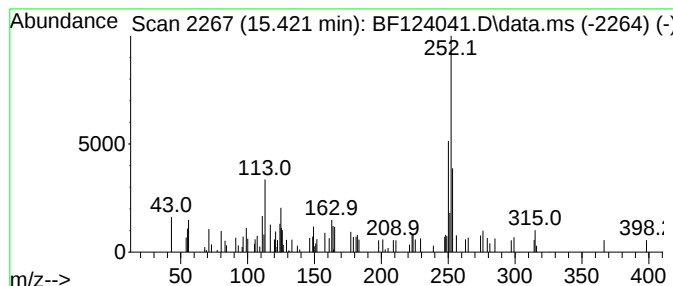
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown15.42 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.421	2.32 ng	42737	Perylene-d12	15.551

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzenesulfonic acid, 2-bromo-, ...	250	C7H7BrO3S	1000163-27-7	38
2			1-(2-Bromo-2-chloroethenyl)-4-ch...	250	C8H5BrCl2	1000305-36-0	38
3			Benzo[e]pyrene	252	C20H12	000192-97-2	38
4			Benzo[k]fluoranthene	252	C20H12	000207-08-9	35
5			4'-Methoxyflavone	252	C16H12O3	004143-74-2	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052421\
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Sample : M2490-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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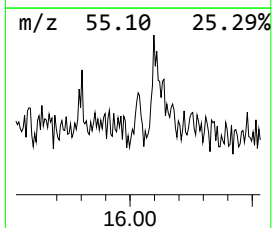
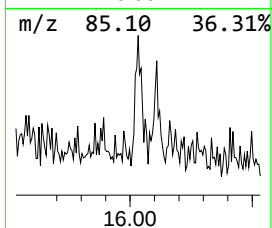
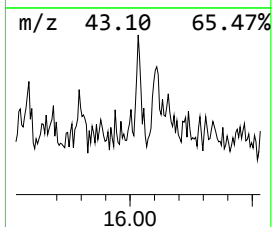
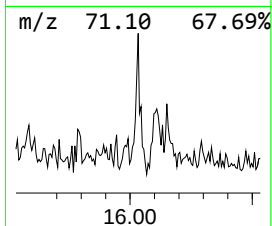
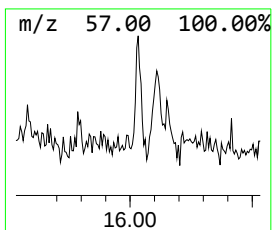
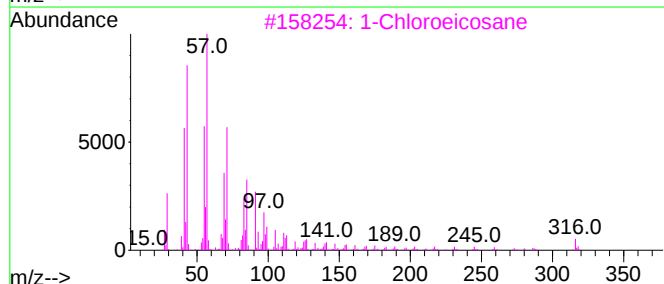
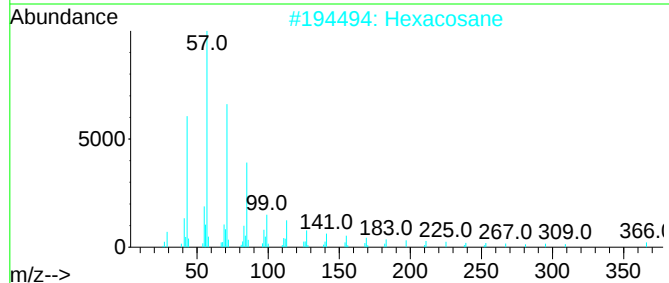
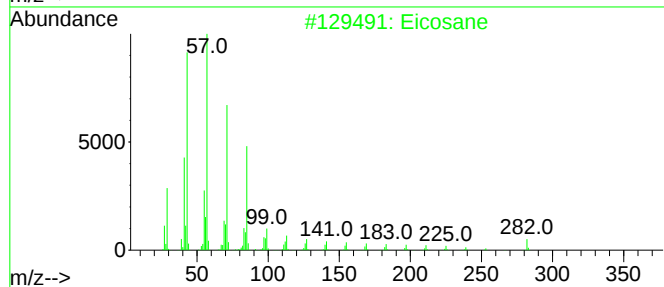
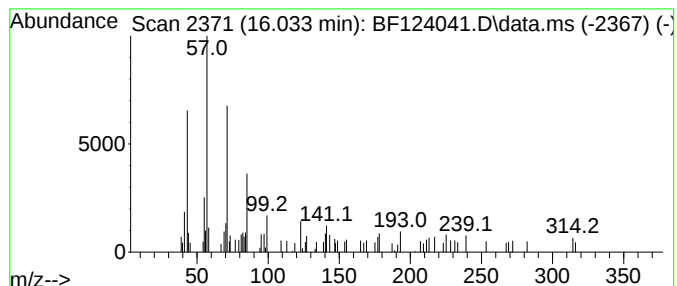
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.033	3.38 ng	62382	Perylene-d12	15.551

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	55
2			Hexacosane	366	C26H54	000630-01-3	49
3			1-Chloroeicosane	316	C20H41Cl	042217-02-7	49
4			Sulfurous acid, decyl pentyl ester	292	C15H32O3S	1000309-14-3	47
5			Docosane	310	C22H46	000629-97-0	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052421\
Data File : BF124041.D
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Sample : M2490-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

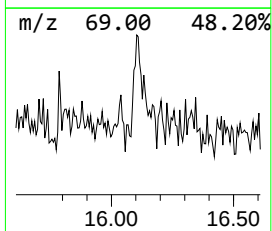
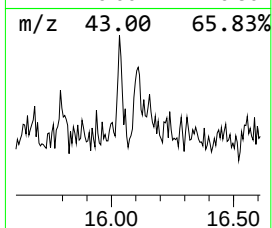
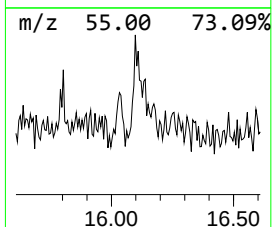
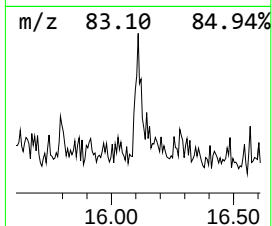
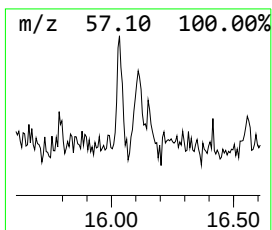
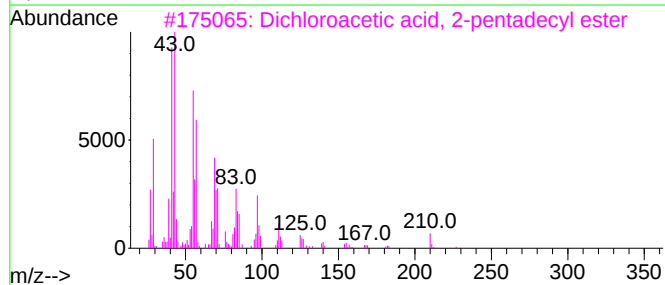
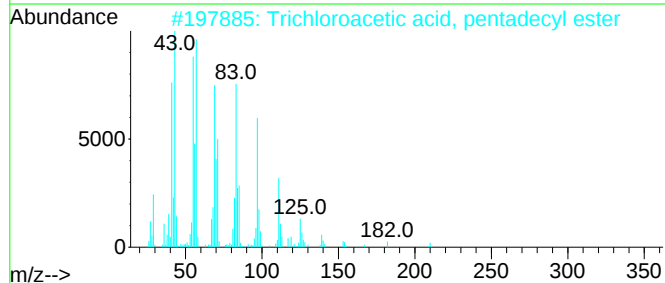
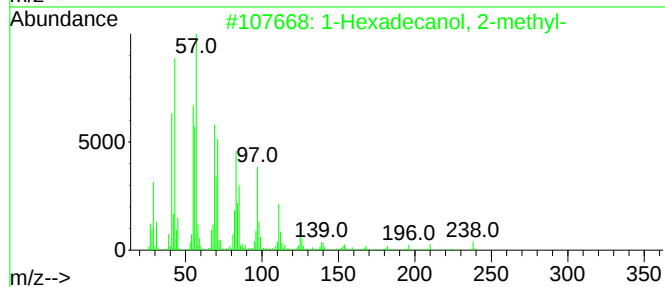
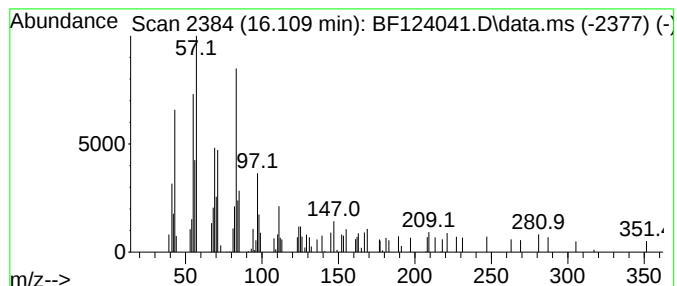
Instrument :
BNA_F
ClientSampleId :
72-11986

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 1-Hexadecanol, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.109	6.95 ng	128073	Perylene-d12	15.551	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexadecanol, 2-methyl-	256	C17H36O	002490-48-4	62
2	Trichloroacetic acid, pentadecyl...	372	C17H31Cl13O2	074339-53-0	58
3	Dichloroacetic acid, 2-pentadecyl...	338	C17H32Cl12O2	1000280-64-7	58
4	Trichloroacetic acid, tetradecyl...	358	C16H29Cl13O2	074339-52-9	58
5	2- Bromopropionic acid, pentadec...	362	C18H35BrO2	1000292-44-2	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052421\
Data File : BF124041.D
Acq On : 24 May 2021 17:10
Operator : JU/CG
Sample : M2490-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11986

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.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...	2.169	40.0	ng	700730	1	6.892	350343	20.0
unknown2,27	2.275	2.8	ng	48670	1	6.892	350343	20.0
2-Pentanone, 4-...	5.104	19.0	ng	332836	1	6.892	350343	20.0
Ethanol, 2-(2-e...	6.716	2.7	ng	47584	1	6.892	350343	20.0
n-Hexadecanoic ...	11.939	3.0	ng	75310	4	11.416	510204	20.0
1-Docosene	13.904	19.6	ng	347976	5	14.062	355075	20.0
E-14-Hexadecenal	14.545	10.1	ng	179060	5	14.062	355075	20.0
unknown15.19	15.192	2.9	ng	52625	6	15.551	368721	20.0
Cetene	15.233	4.1	ng	74929	6	15.551	368721	20.0
unknown15.42	15.421	2.3	ng	42737	6	15.551	368721	20.0
Eicosane	16.033	3.4	ng	62382	6	15.551	368721	20.0
1-Hexadecanol, ...	16.109	7.0	ng	128073	6	15.551	368721	20.0