

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052421\
 Data File : BF124042.D
 Acq On : 24 May 2021 17:42
 Operator : JU/CG
 Sample : M2486-01
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 OR-03-052121

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: BF124042.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	7	13	22	rBB	545786	672634	47.11%	5.527%
2	2.269	27	31	37	rVB	35981	46172	3.23%	0.379%
3	5.104	509	513	522	rVB	258405	279055	19.54%	2.293%
4	5.510	577	582	585	rBV	1197999	1096673	76.81%	9.011%
5	5.904	646	649	652	rBV	25187	20115	1.41%	0.165%
6	6.516	748	753	756	rBV	1203484	1115484	78.12%	9.166%
7	6.716	784	787	792	rBV2	37039	40909	2.87%	0.336%
8	6.892	813	817	820	rBV	443367	370767	25.97%	3.046%
9	7.451	907	912	915	rBV	915818	762206	53.38%	6.263%
10	8.175	1031	1035	1038	rBV	613926	478698	33.53%	3.933%
11	9.251	1214	1218	1221	rBV	1808154	1427836	100.00%	11.732%
12	9.639	1281	1284	1288	rBV	235732	170692	11.95%	1.403%
13	9.927	1329	1333	1337	rBV	688848	567555	39.75%	4.663%
14	10.716	1463	1467	1471	rBV	1116932	939614	65.81%	7.721%
15	11.416	1582	1586	1589	rBV	666324	554450	38.83%	4.556%
16	11.439	1589	1590	1593	rVB	70700	37332	2.61%	0.307%
17	11.939	1673	1675	1680	rBV2	74700	70373	4.93%	0.578%
18	12.210	1716	1721	1724	rBV5	9791	17257	1.21%	0.142%
19	12.468	1762	1765	1769	rVB2	15068	18048	1.26%	0.148%
20	12.627	1790	1792	1795	rBV	88160	75778	5.31%	0.623%
21	12.857	1827	1831	1834	rBV	78981	84347	5.91%	0.693%
22	13.004	1852	1856	1859	rBV	1654905	1310312	91.77%	10.766%
23	13.233	1890	1895	1897	rBV4	17217	24695	1.73%	0.203%
24	13.692	1971	1973	1977	rBV4	19445	19684	1.38%	0.162%
25	13.910	2006	2010	2020	rBV	219650	305898	21.42%	2.513%
26	14.062	2029	2036	2038	rBV	481211	517982	36.28%	4.256%
27	14.086	2038	2040	2047	rVB	43860	51710	3.62%	0.425%
28	14.233	2062	2065	2068	rBV5	12095	20340	1.42%	0.167%
29	14.445	2099	2101	2105	rVB5	22836	21826	1.53%	0.179%
30	14.480	2105	2107	2110	rBV4	15433	20848	1.46%	0.171%
31	14.551	2116	2119	2125	rVB8	47027	65949	4.62%	0.542%
32	14.921	2180	2182	2185	rBV4	22891	25341	1.77%	0.208%
33	14.992	2192	2194	2199	rVB6	33950	35117	2.46%	0.289%
34	15.109	2211	2214	2216	rBV2	33485	32016	2.24%	0.263%
35	15.192	2225	2228	2231	rVB	65392	63452	4.44%	0.521%
36	15.239	2232	2236	2240	rVB7	31708	50273	3.52%	0.413%

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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	15.421	2265	2267	2270	rVB3	29589	31297	2.19%	0.257%
38	15.486	2275	2278	2281	rBV5	34942	32496	2.28%	0.267%
39	15.551	2284	2289	2293	rBV	298338	379853	26.60%	3.121%
40	15.792	2327	2330	2333	rBV5	33739	36882	2.58%	0.303%
41	16.033	2367	2371	2376	rVB2	88605	133438	9.35%	1.096%
42	16.104	2380	2383	2390	rVB7	45106	85484	5.99%	0.702%
43	16.280	2410	2413	2422	rVB9	29238	59381	4.16%	0.488%

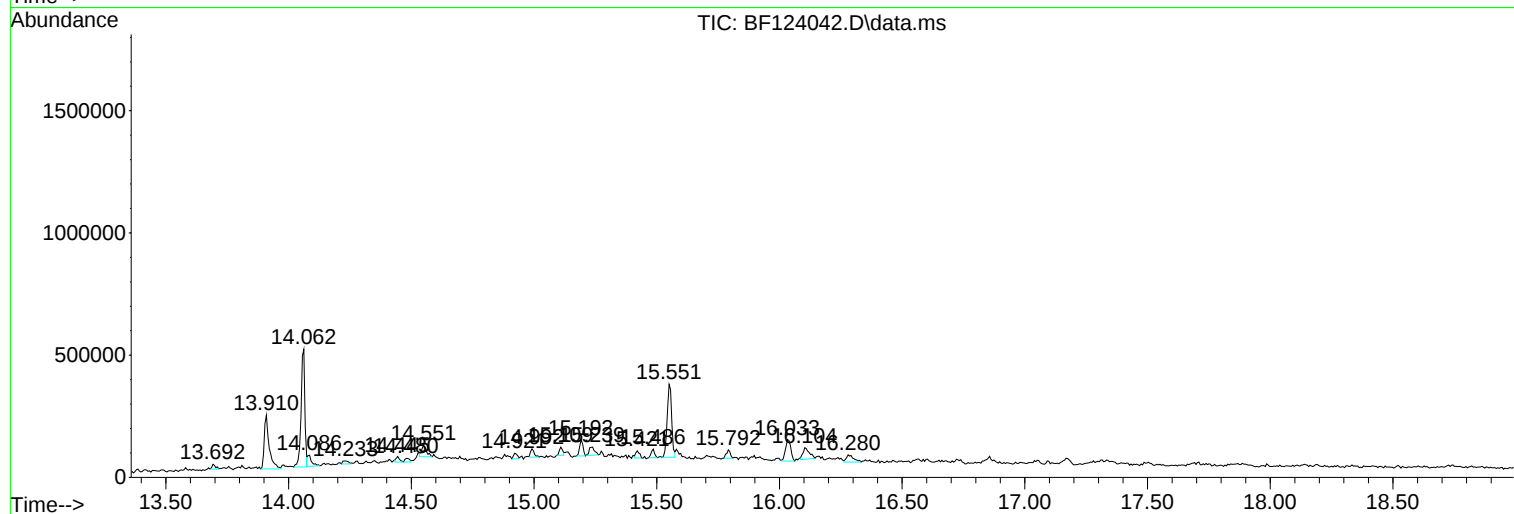
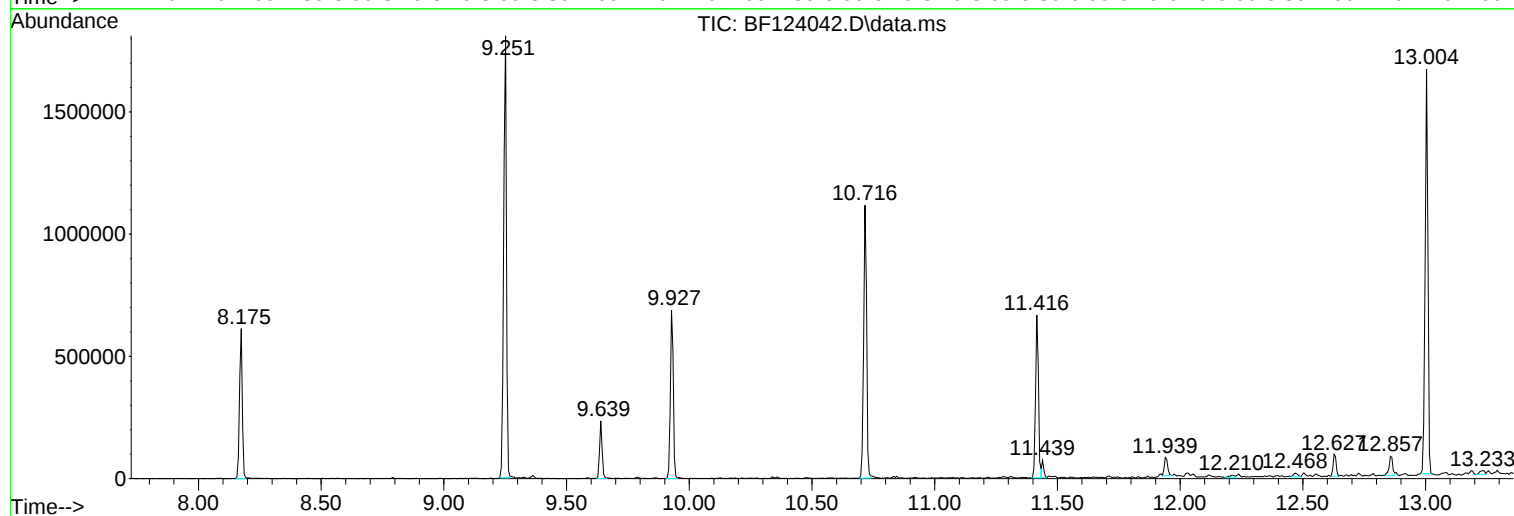
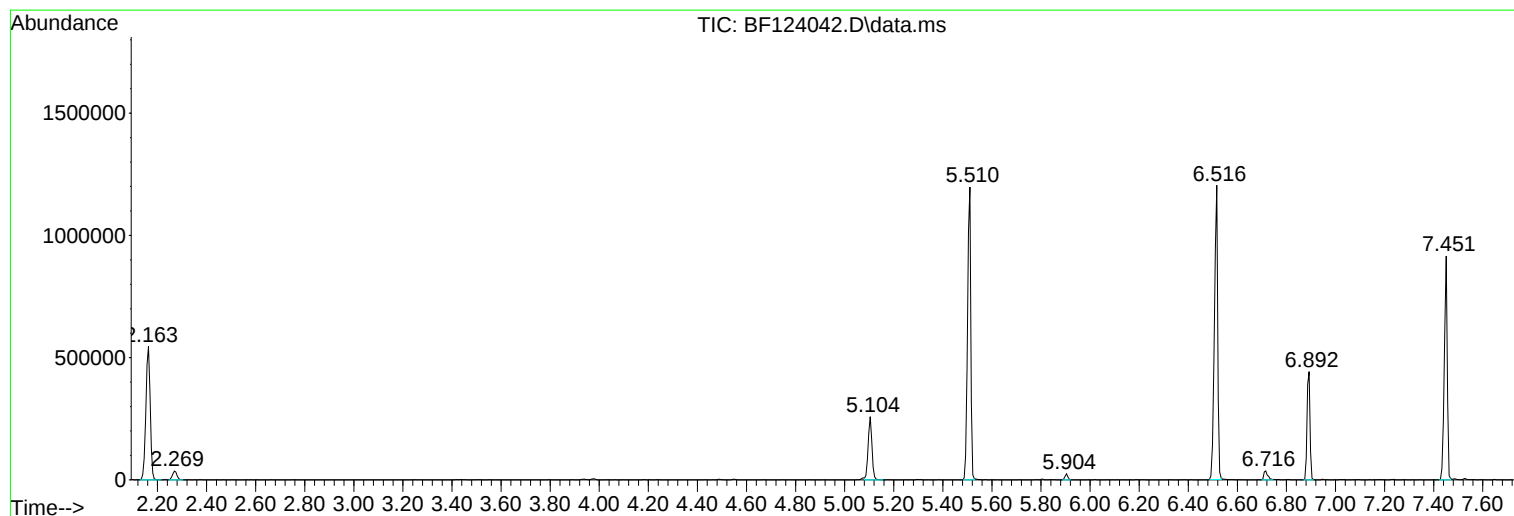
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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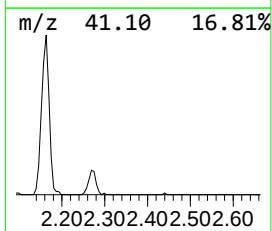
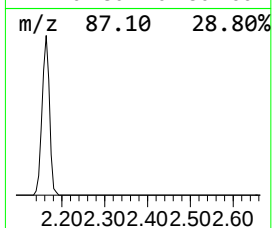
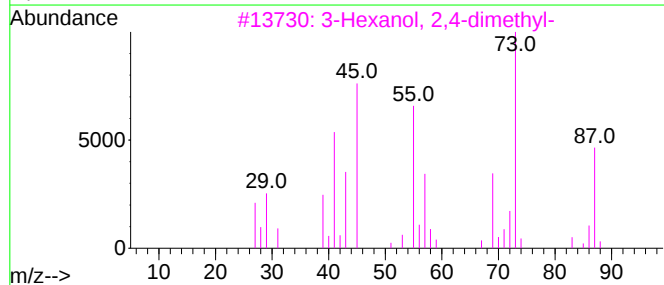
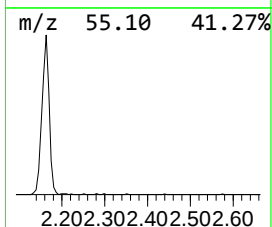
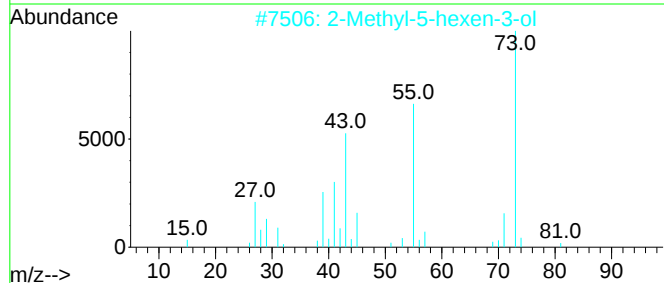
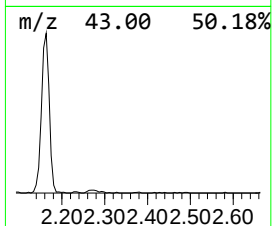
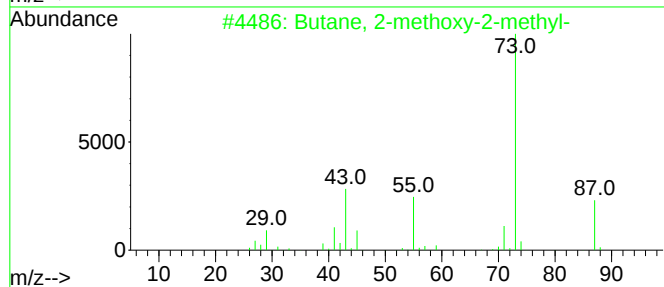
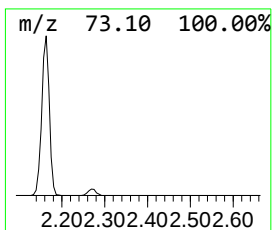
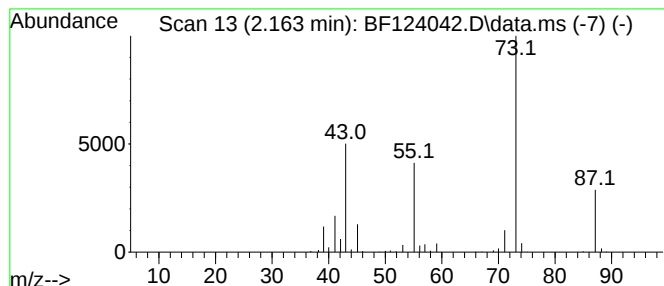
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.163	36.28 ng	672634	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	37
3			3-Hexanol, 2,4-dimethyl-	130	C8H18O	013432-25-2	36
4			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	36
5			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	25



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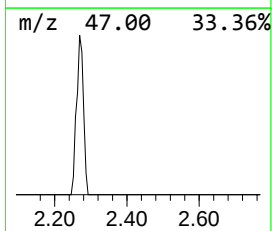
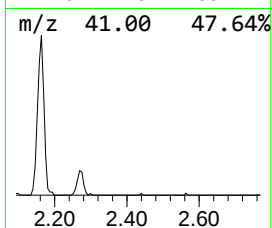
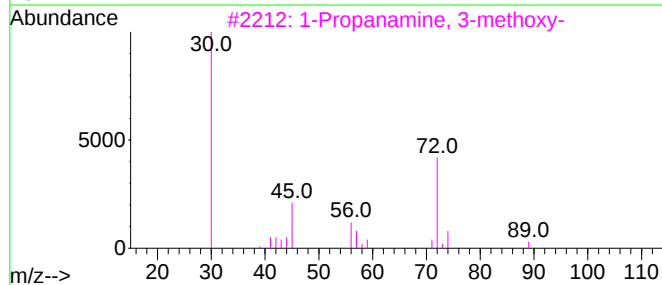
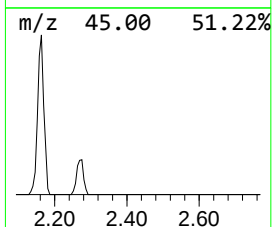
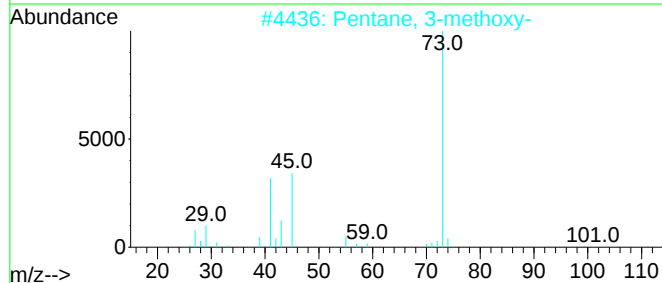
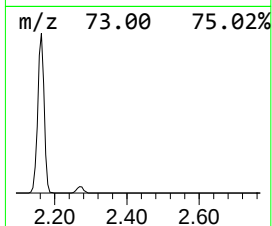
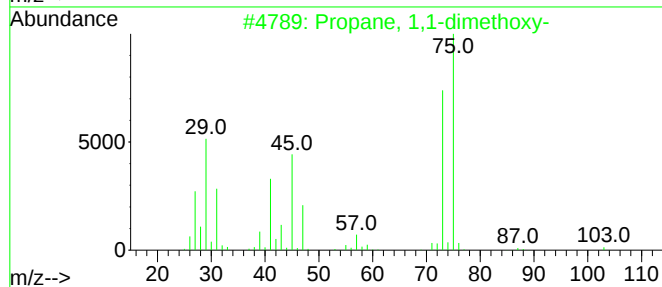
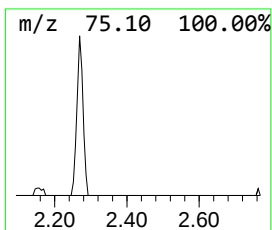
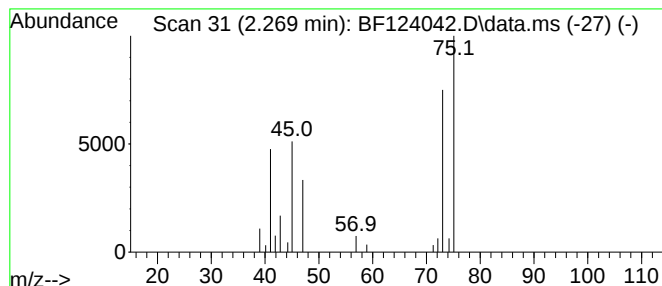
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.269	2.49 ng	46172	1,4-Dichlorobenzene-d4	6.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	27
3			1-Propanamine, 3-methoxy-	89	C4H11NO	005332-73-0	9
4			1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	9
5			1-Propene-1-thiol	74	C3H6S	000925-89-3	9



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ALS Vial : 10 Sample Multiplier: 1

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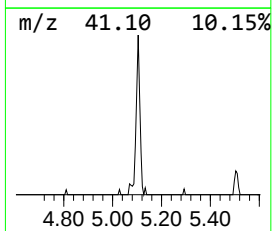
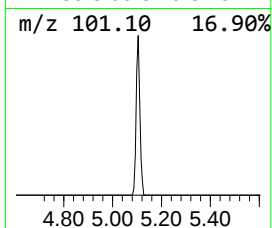
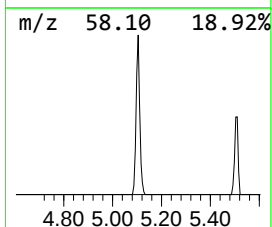
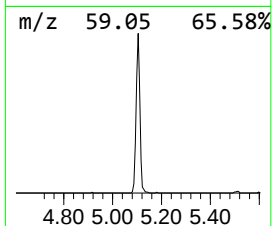
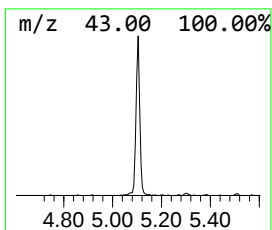
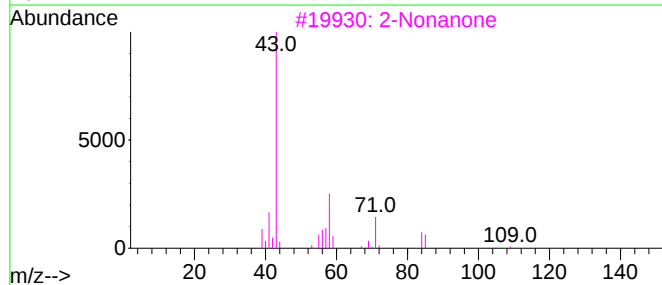
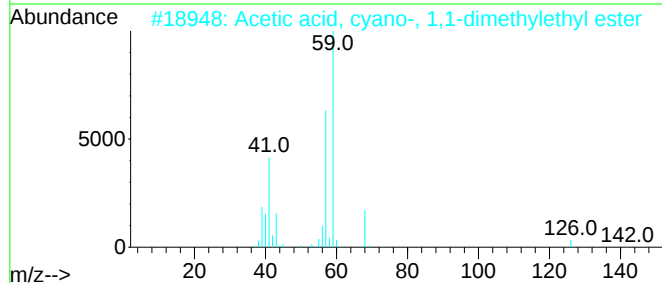
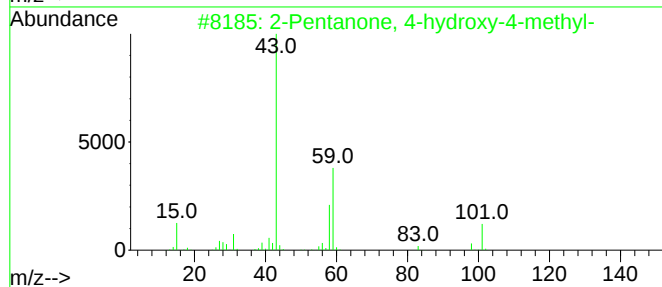
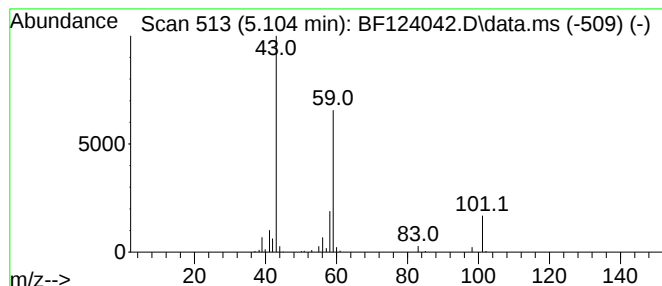
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.104	15.05 ng	279055	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			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3			2-Nonanone	142	C9H18O	000821-55-6	17
4			Acetone	58	C3H6O	000067-64-1	12
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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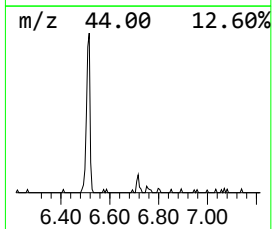
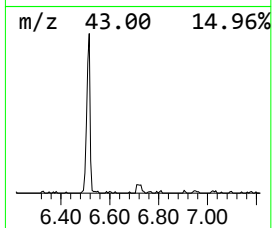
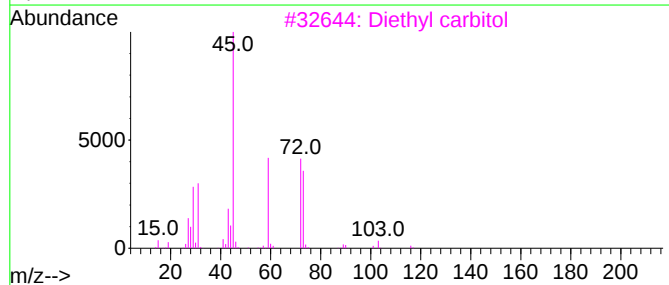
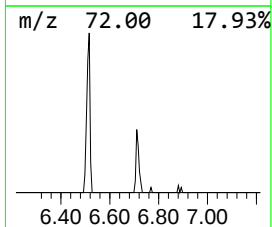
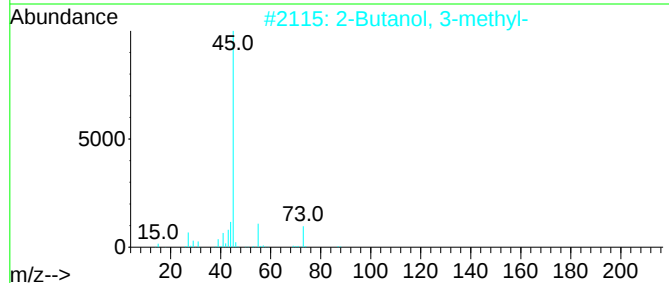
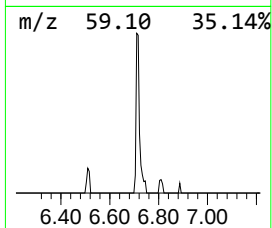
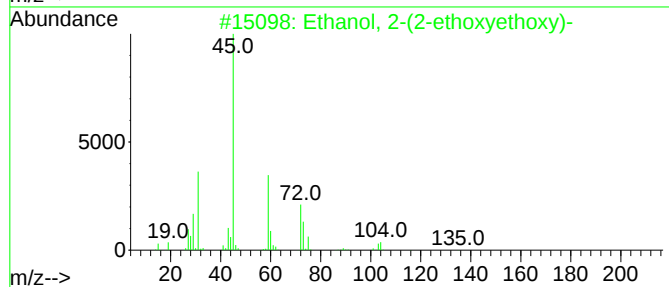
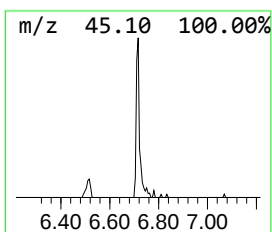
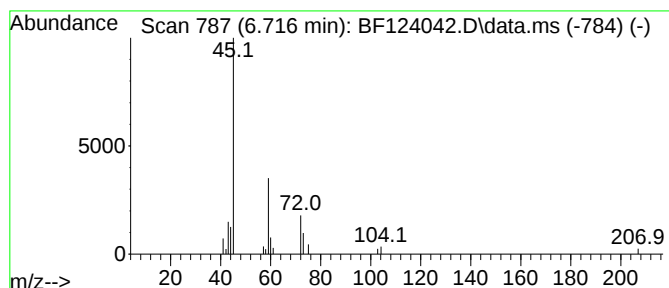
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.716	2.21 ng	40909	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	78
2			2-Butanol, 3-methyl-	88	C5H12O	000598-75-4	33
3			Diethyl carbitol	162	C8H18O3	000112-36-7	9
4			Ethyl ether	74	C4H10O	000060-29-7	9
5			2-Propanol, 1-propoxy-	118	C6H14O2	001569-01-3	9



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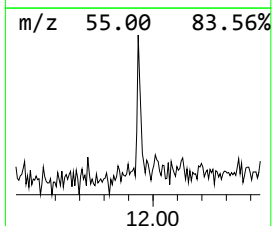
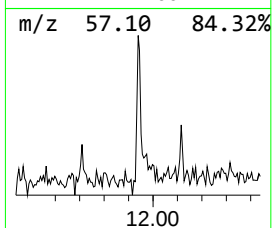
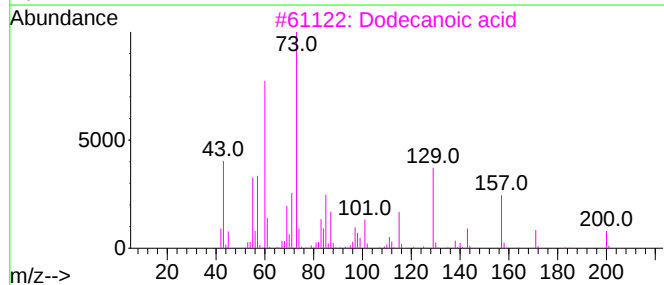
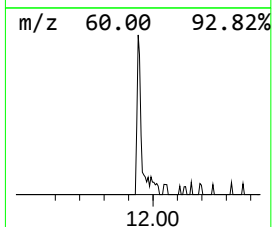
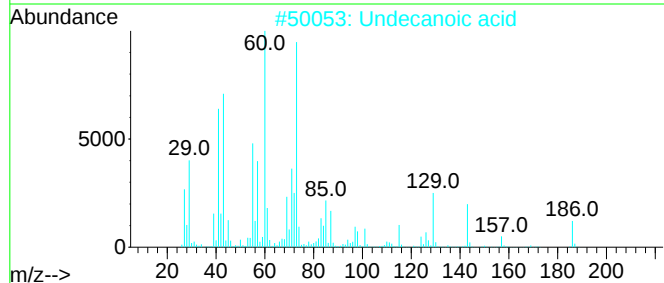
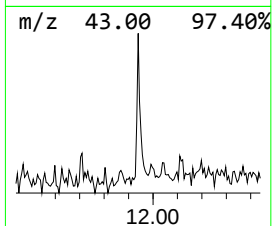
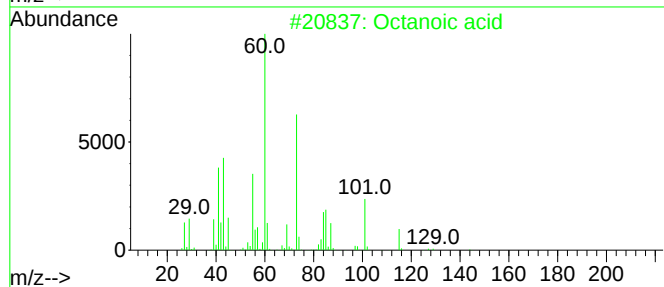
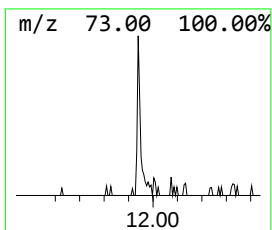
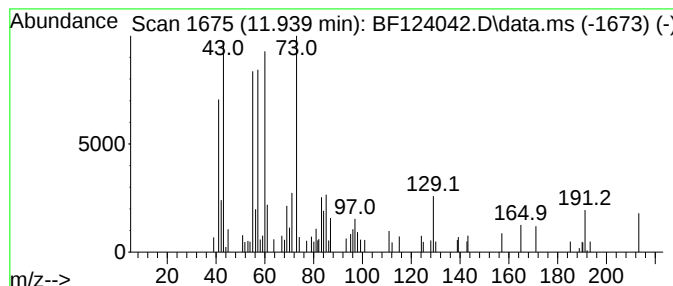
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Octanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.939	2.54 ng	70373	Phenanthrene-d10	11.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octanoic acid	144	C8H16O2	000124-07-2	50
2			Undecanoic acid	186	C11H22O2	000112-37-8	50
3			Dodecanoic acid	200	C12H24O2	000143-07-7	47
4			Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	47
5			n-Decanoic acid	172	C10H20O2	000334-48-5	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052421\
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Acq On : 24 May 2021 17:42
Operator : JU/CG
Sample : M2486-01
Misc :
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ClientSampleId :
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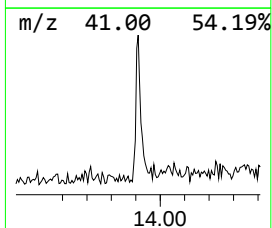
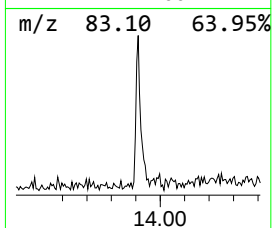
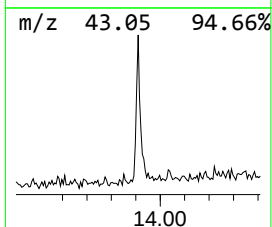
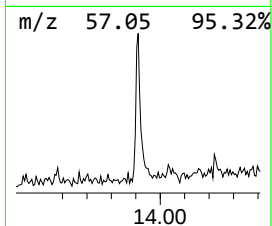
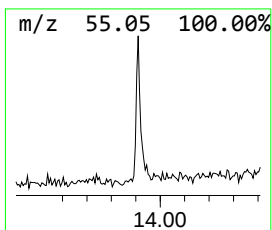
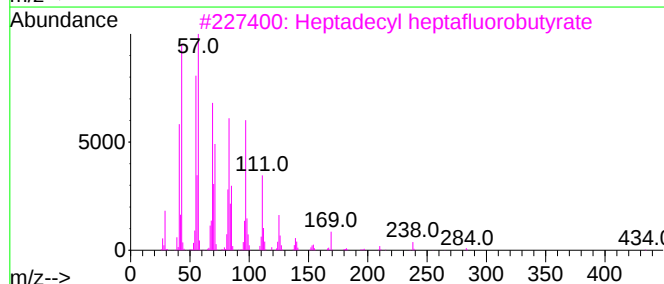
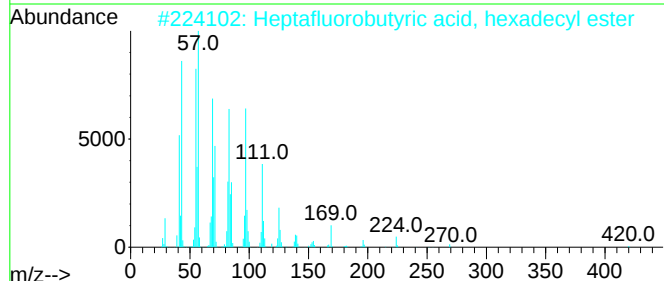
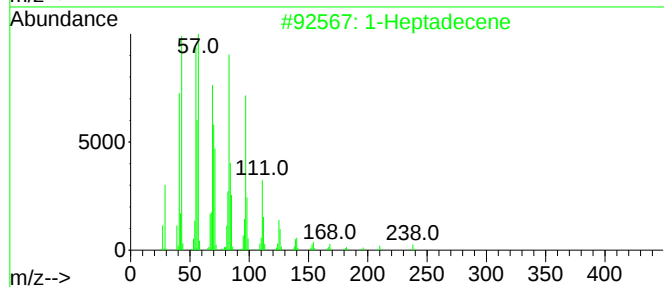
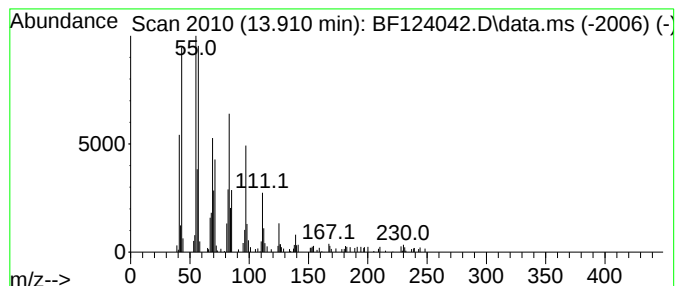
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Heptadecene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.910	11.81 ng	305898	Chrysene-d12	14.063

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heptadecene	238	C17H34	006765-39-5	94
2			Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
3			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93
4			Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91
5			n-Tetracosanol-1	354	C24H50O	000506-51-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052421\
Data File : BF124042.D
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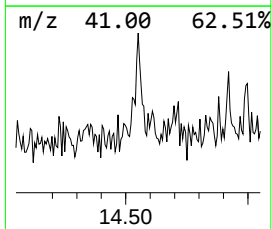
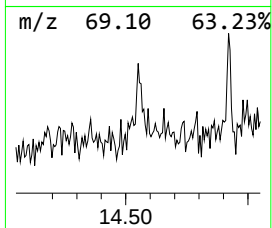
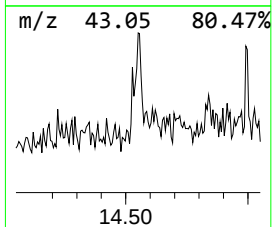
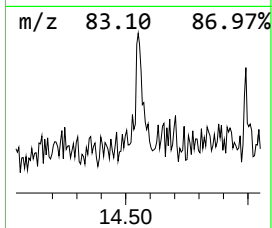
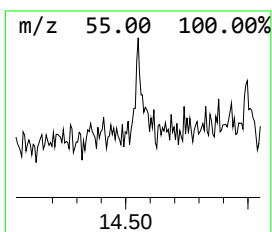
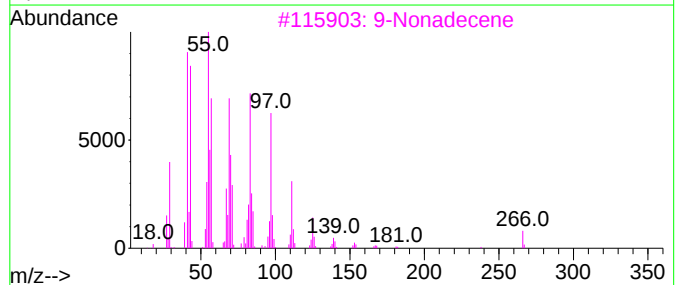
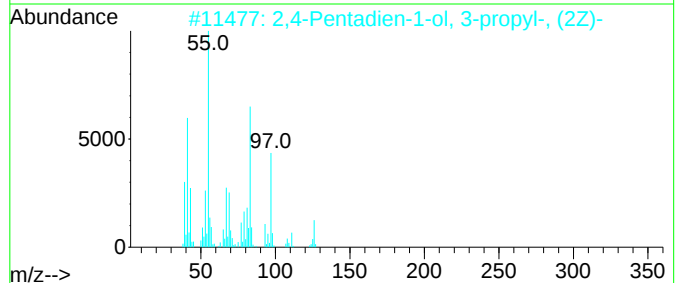
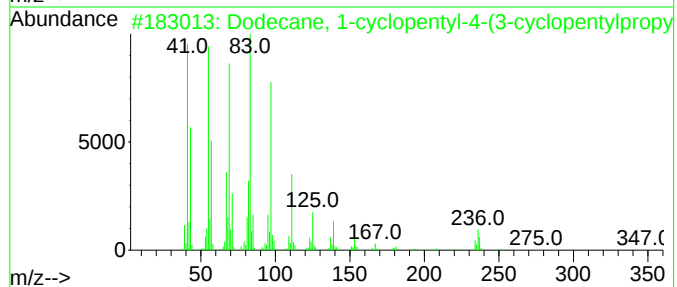
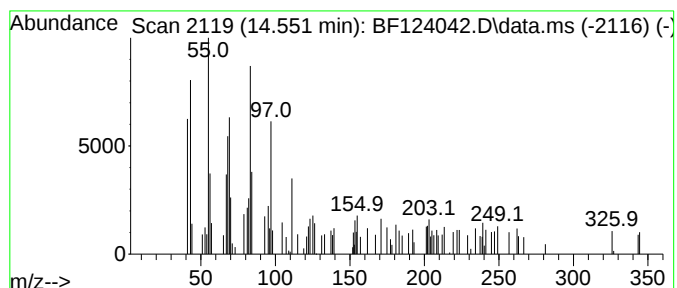
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown14.55 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.551	2.55 ng	65949	Chrysene-d12	14.063

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 1-cyclopentyl-4-(3-cyclopentylpropyl)-	348	C25H48	007225-68-5	46
2			2,4-Pentadien-1-ol, 3-propyl-, (2Z)-	126	C8H14O	1000142-17-9	46
3			9-Nonadecene	266	C19H38	031035-07-1	46
4			1-Hexadecene, 16-bromo-	302	C16H31Br	118625-56-2	43
5			Cycloheptanol, 2-methylene	126	C8H14O	016240-38-3	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052421\
Data File : BF124042.D
Acq On : 24 May 2021 17:42
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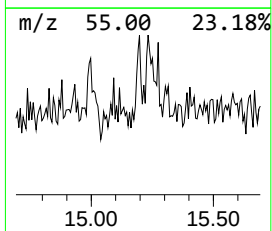
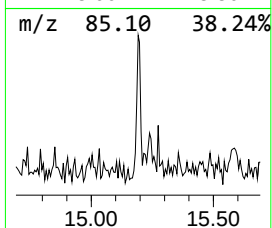
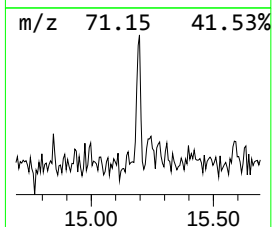
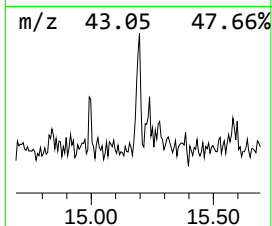
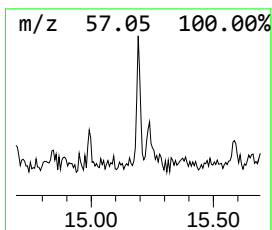
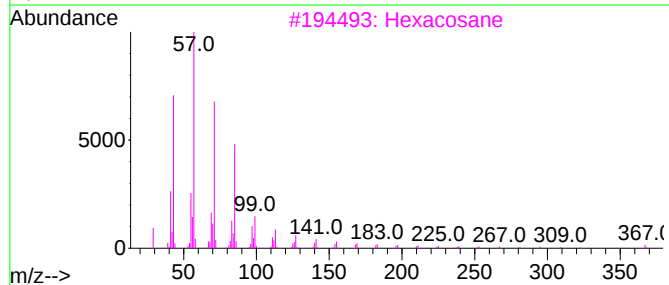
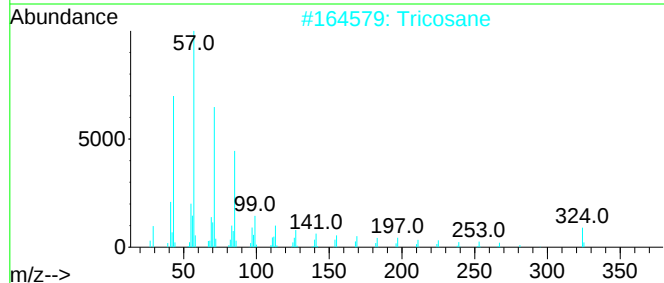
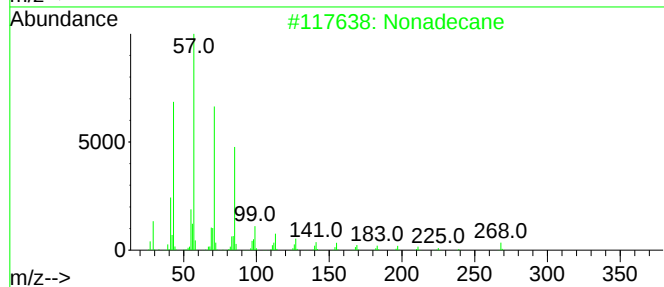
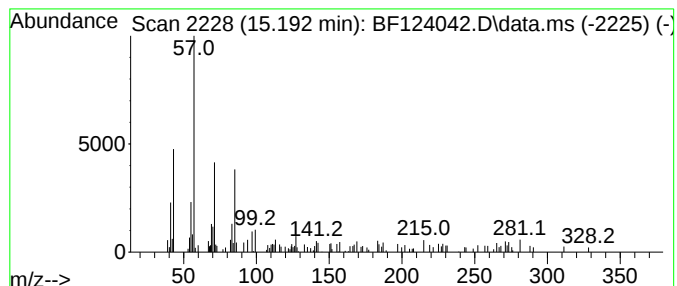
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Nonadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.192	3.34 ng	63452	Perylene-d12	15.551

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	70
2			Tricosane	324	C23H48	000638-67-5	64
3			Hexacosane	366	C26H54	000630-01-3	64
4			Heptadecane	240	C17H36	000629-78-7	64
5			Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052421\
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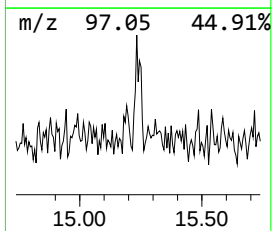
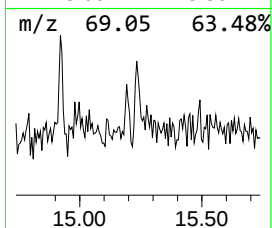
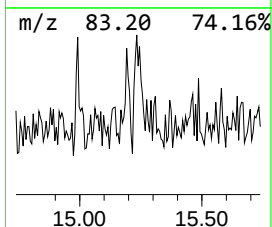
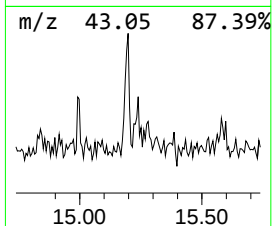
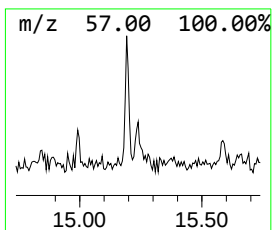
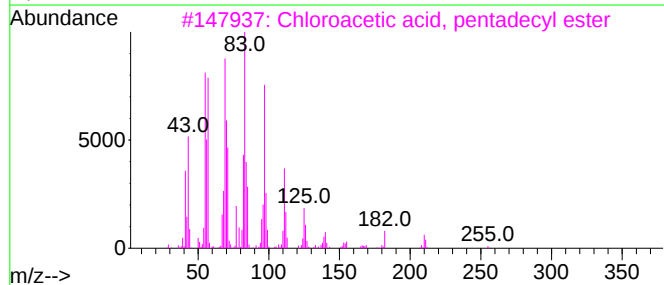
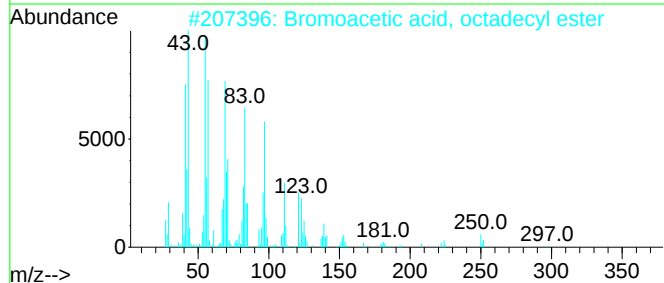
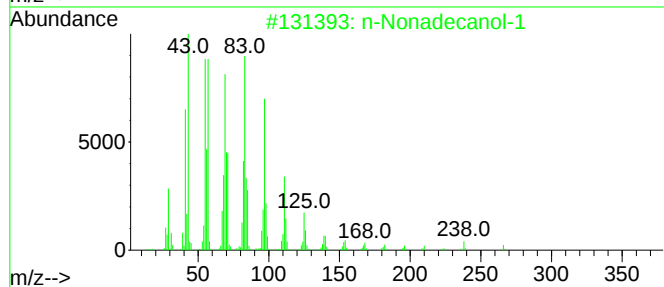
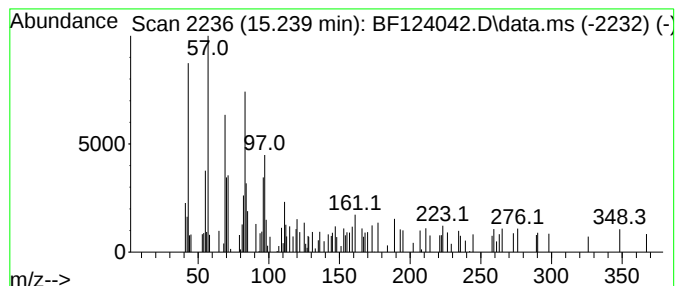
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 n-Nonadecanol-1 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.239	2.65 ng	50273	Perylene-d12	15.551

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Nonadecanol-1	284	C19H40O	001454-84-8	62
2			Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	62
3			Chloroacetic acid, pentadecyl ester	304	C17H33ClO2	070301-47-2	62
4			Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	58
5			Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052421\
Data File : BF124042.D
Acq On : 24 May 2021 17:42
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Misc :
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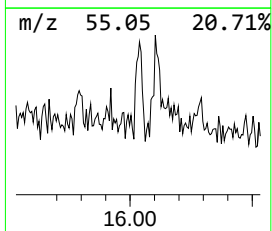
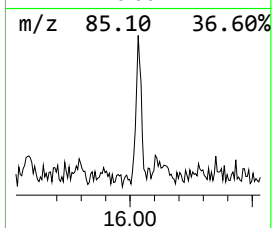
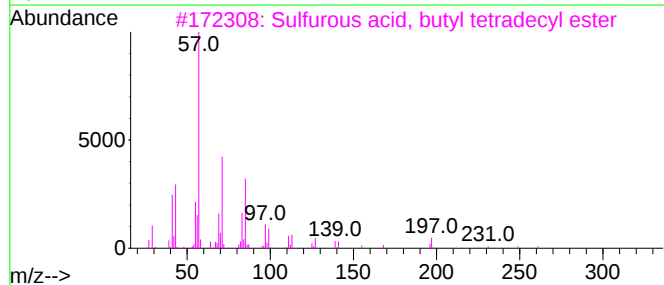
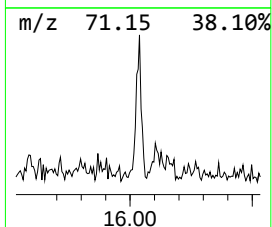
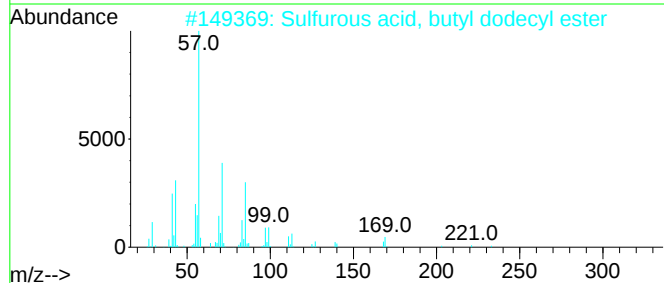
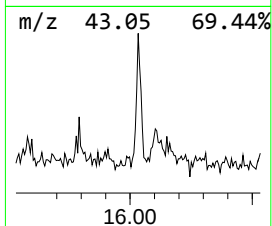
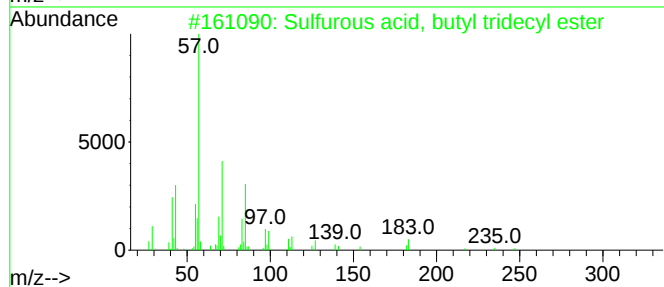
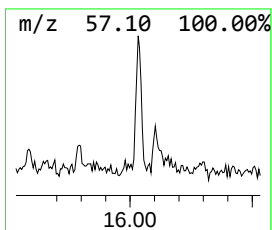
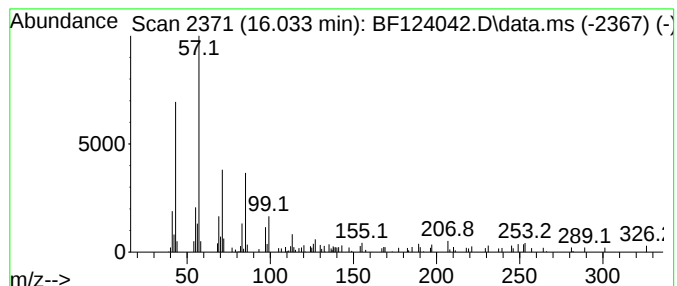
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Sulfurous acid, butyl tridec... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.033	7.03 ng	133438	Perylene-d12	15.551

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, butyl tridecyl e...	320	C17H36O3S	1000309-18-0	83
2			Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	80
3			Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1000309-18-1	72
4			Sulfurous acid, butyl undecyl ester	292	C15H32O3S	1000309-17-8	72
5			1-Iodoundecane	282	C11H23I	004282-44-4	68



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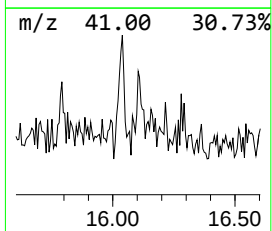
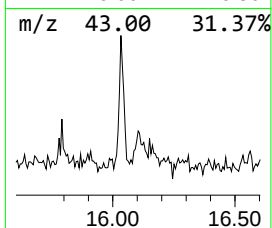
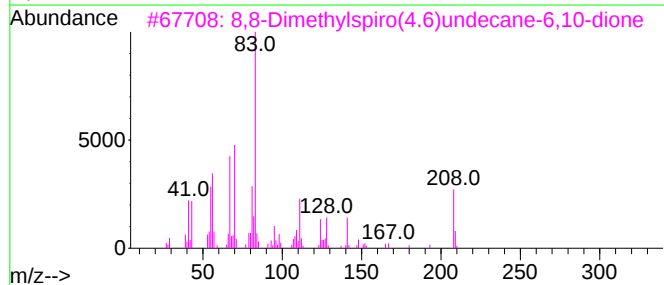
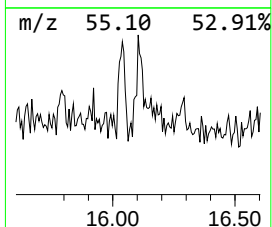
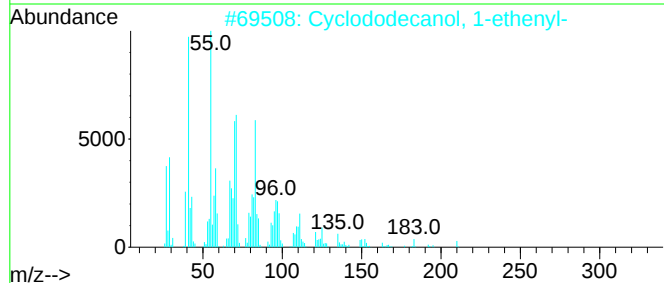
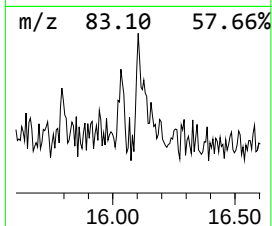
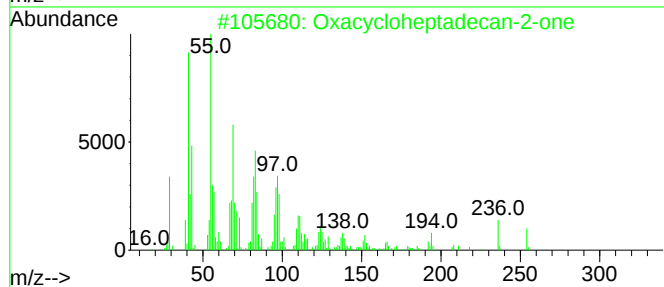
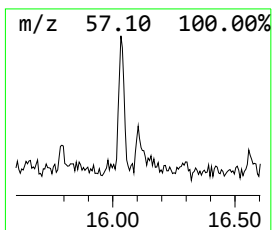
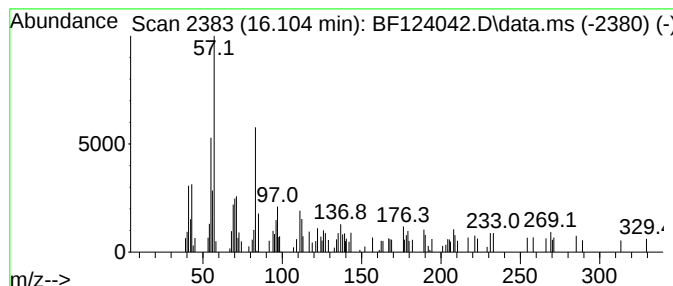
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Oxacycloheptadecan-2-one Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.104	4.50 ng	85484	Perylene-d12	15.551

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxacycloheptadecan-2-one	254	C16H30O2	000109-29-5	55
2			Cyclododecanol, 1-ethenyl-	210	C14H26O	006244-49-1	49
3			8,8-Dimethylspiro(4.6)undecane-6...	208	C13H20O2	068181-81-7	46
4			1-Hexadecanethiol	258	C16H34S	002917-26-2	45
5			Spiro[2.3]hexan-4-one, 5,5-dieth...	180	C12H20O	1000152-13-6	41



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052421\
Data File : BF124042.D
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Misc :
ALS Vial : 10 Sample Multiplier: 1

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ClientSampleId :
OR-03-052121

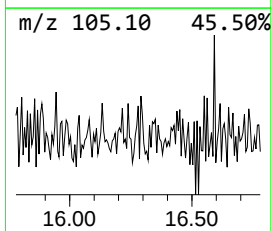
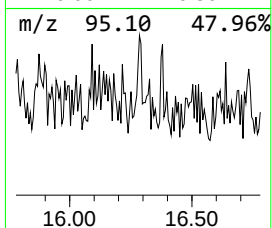
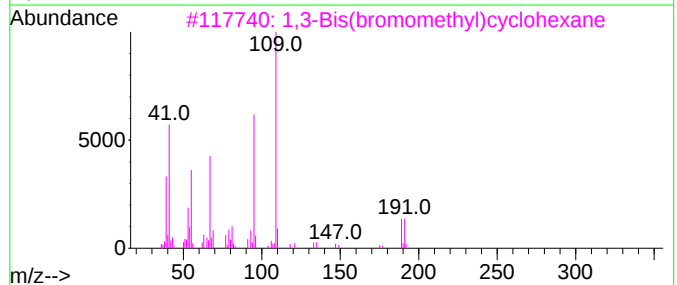
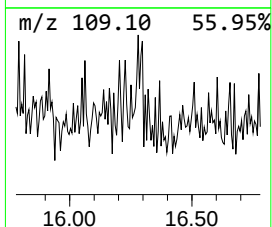
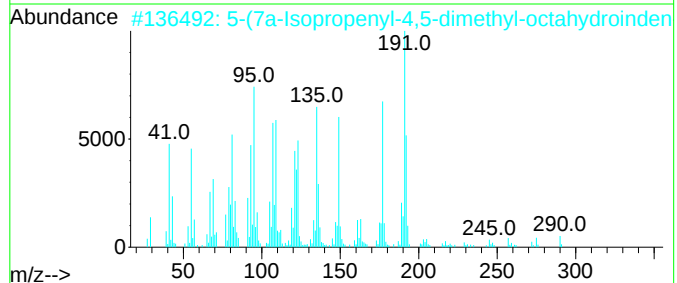
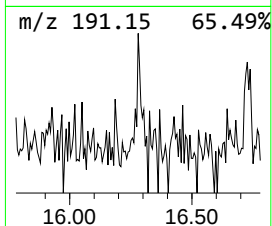
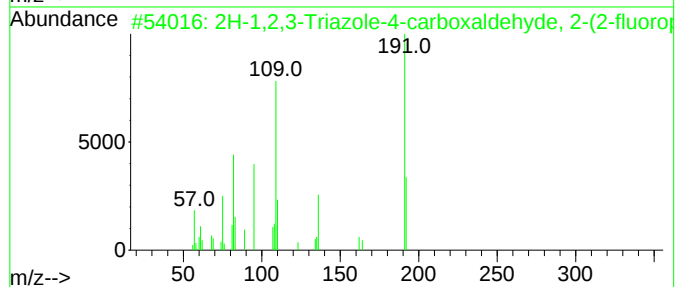
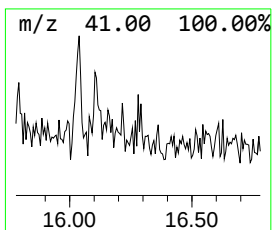
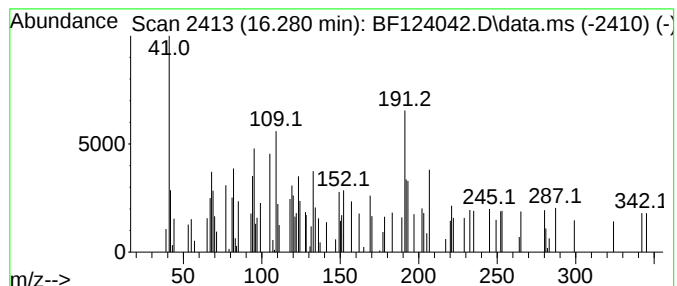
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown16.28 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.280	3.13 ng	59381	Perylene-d12	15.551

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2H-1,2,3-Triazole-4-carboxaldehy...	191	C9H6FN3O	051306-43-5	27		
2	5-(7a-Isopropenyl-4,5-dimethyl-o...	290	C20H34O	1000193-54-0	25		
3	1,3-Bis(bromomethyl)cyclohexane	268	C8H14Br2	1000216-89-9	14		
4	2H-1,2,3-Triazole-4-carboxylic a...	207	C9H6FN3O2	051306-44-6	14		
5	4,7,7-Trimethylbicyclo[2.2.1]hep...	207	C13H21NO	1000210-89-8	12		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052421\
Data File : BF124042.D
Acq On : 24 May 2021 17:42
Operator : JU/CG
Sample : M2486-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OR-03-052121

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...	2.163	36.3	ng	672634	1	6.892	370767	20.0
Propane, 1,1-di...	2.269	2.5	ng	46172	1	6.892	370767	20.0
2-Pentanone, 4-...	5.104	15.1	ng	279055	1	6.892	370767	20.0
Ethanol, 2-(2-e...	6.716	2.2	ng	40909	1	6.892	370767	20.0
Octanoic acid	11.939	2.5	ng	70373	4	11.416	554450	20.0
1-Heptadecene	13.910	11.8	ng	305898	5	14.063	517982	20.0
unknown14.55	14.551	2.5	ng	65949	5	14.063	517982	20.0
Nonadecane	15.192	3.3	ng	63452	6	15.551	379853	20.0
n-Nonadecanol-1	15.239	2.6	ng	50273	6	15.551	379853	20.0
Sulfurous acid,...	16.033	7.0	ng	133438	6	15.551	379853	20.0
Oxacycloheptade...	16.104	4.5	ng	85484	6	15.551	379853	20.0
unknown16.28	16.280	3.1	ng	59381	6	15.551	379853	20.0