

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030321\
 Data File : BF123361.D
 Acq On : 3 Mar 2021 18:07
 Operator : JU/CG
 Sample : M1545-06
 Misc :
 ALS Vial : 10 Sample Multiplier: 4

Instrument :
 BNA_F
 ClientSampleId :
 MH-F

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-BF021921.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123361.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.846	124	129	133	rVB	5441887	6925738	43.47%	5.959%
2	5.569	587	592	595	rBV	6131216	7043269	44.21%	6.060%
3	6.516	747	753	769	rBV	3191896	4958657	31.12%	4.267%
4	6.857	806	811	819	rBV	2928665	2953224	18.54%	2.541%
5	7.428	898	908	911	rBV	5405074	9898541	62.13%	8.517%
6	7.604	931	938	941	rVB	104917	166514	1.05%	0.143%
7	7.663	941	948	953	rBV2	187338	267299	1.68%	0.230%
8	7.939	990	995	1002	rVB2	102067	192640	1.21%	0.166%
9	8.133	1019	1028	1031	rBV	2555993	3949330	24.79%	3.398%
10	8.345	1057	1064	1068	rVB7	96064	177467	1.11%	0.153%
11	8.569	1096	1102	1108	rVB3	126745	239336	1.50%	0.206%
12	8.628	1108	1112	1115	rBV	236202	228598	1.43%	0.197%
13	9.086	1185	1190	1193	rBV	310463	439469	2.76%	0.378%
14	9.127	1193	1197	1202	rVV	638124	673736	4.23%	0.580%
15	9.216	1202	1212	1215	rVV	8385518	15768696	98.97%	13.568%
16	9.280	1218	1223	1226	rBV2	111544	173521	1.09%	0.149%
17	9.327	1226	1231	1234	rVB3	127391	181109	1.14%	0.156%
18	9.604	1274	1278	1281	rVB	229839	226475	1.42%	0.195%
19	9.698	1291	1294	1300	rVB3	142836	196109	1.23%	0.169%
20	9.816	1309	1314	1317	rVB2	123135	178354	1.12%	0.153%
21	9.892	1317	1327	1330	rBV	2975875	4623102	29.02%	3.978%
22	10.698	1451	1464	1467	rBV	6213758	10360507	65.03%	8.914%
23	11.386	1570	1581	1583	rBV	3875799	4418819	27.73%	3.802%
24	11.880	1661	1665	1667	rBV2	233940	318848	2.00%	0.274%
25	11.933	1668	1674	1677	rVV	3746670	5194511	32.60%	4.469%
26	12.198	1716	1719	1723	rVB	268539	296983	1.86%	0.256%
27	12.357	1743	1746	1749	rVV	1379600	1204078	7.56%	1.036%
28	12.410	1753	1755	1760	rVV	320277	338491	2.12%	0.291%
29	12.610	1786	1789	1791	rBV3	271261	294796	1.85%	0.254%
30	12.668	1796	1799	1802	rVV	277196	309026	1.94%	0.266%
31	12.721	1802	1808	1813	rBV	3795373	4331443	27.19%	3.727%
32	12.992	1841	1854	1857	rBV2	9249835	15932332	100.00%	13.709%
33	13.186	1884	1887	1892	rBV3	129036	186512	1.17%	0.160%
34	13.533	1944	1946	1950	rVB2	151923	166878	1.05%	0.144%
35	13.874	2000	2004	2012	rVB	2870239	3231804	20.28%	2.781%
36	14.039	2028	2032	2035	rVB	3702351	4015304	25.20%	3.455%

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030321\
Data File : BF123361.D
Acq On : 3 Mar 2021 18:07
Operator : JU/CG
Sample : M1545-06
Misc :
ALS Vial : 10 Sample Multiplier: 4

Instrument :
BNA_F
ClientSampleId :
MH-F

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-BF021921.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.139	2217	2219	2223	rVB	256576	277160	1.74%	0.238%
38	15.521	2277	2284	2288	rVB	2757063	4328351	27.17%	3.724%
39	15.962	2355	2359	2364	rBV	173865	233868	1.47%	0.201%
40	16.021	2364	2369	2377	rBV	476679	994551	6.24%	0.856%
41	17.174	2560	2565	2575	rBV4	119683	326019	2.05%	0.281%

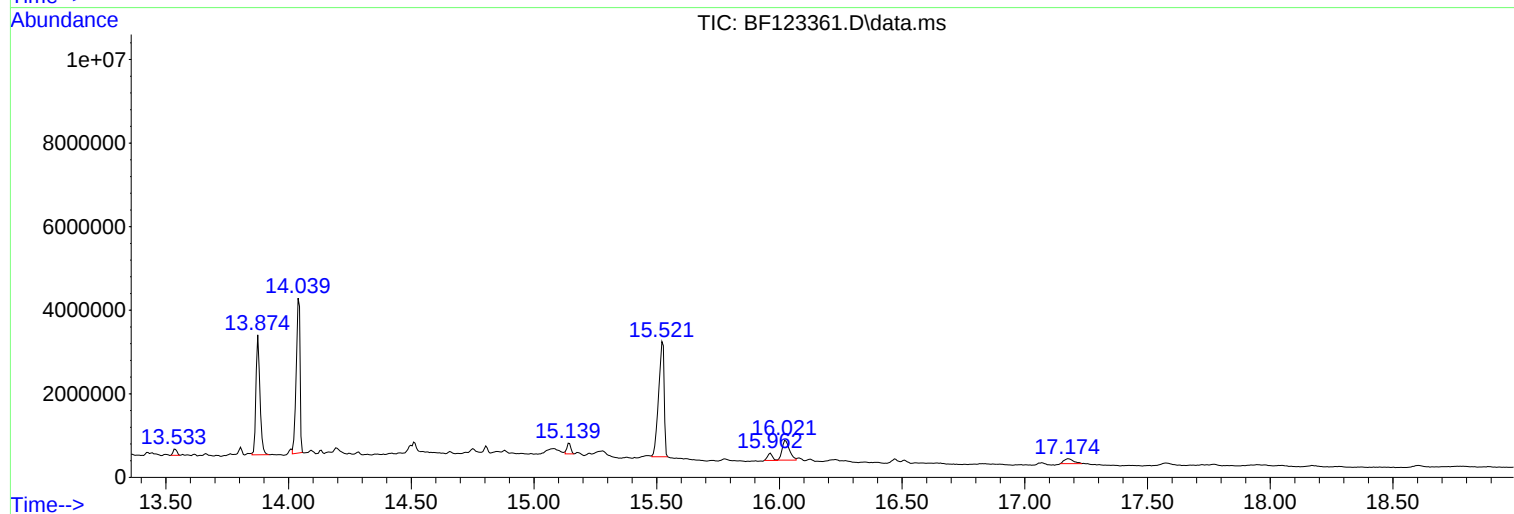
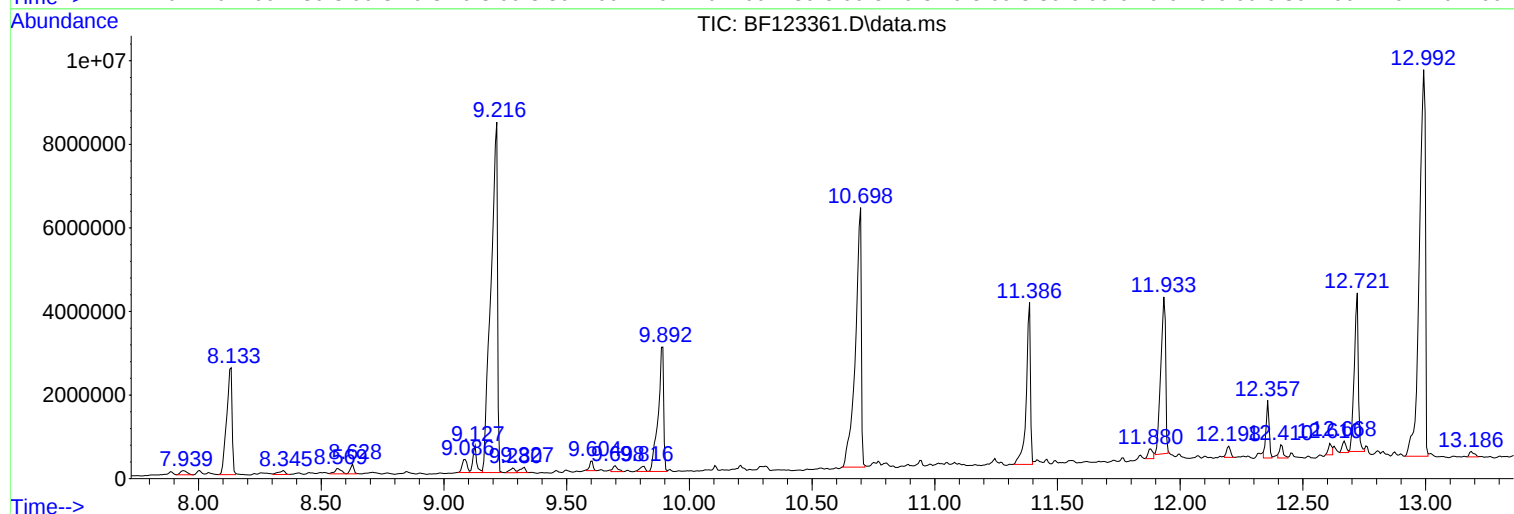
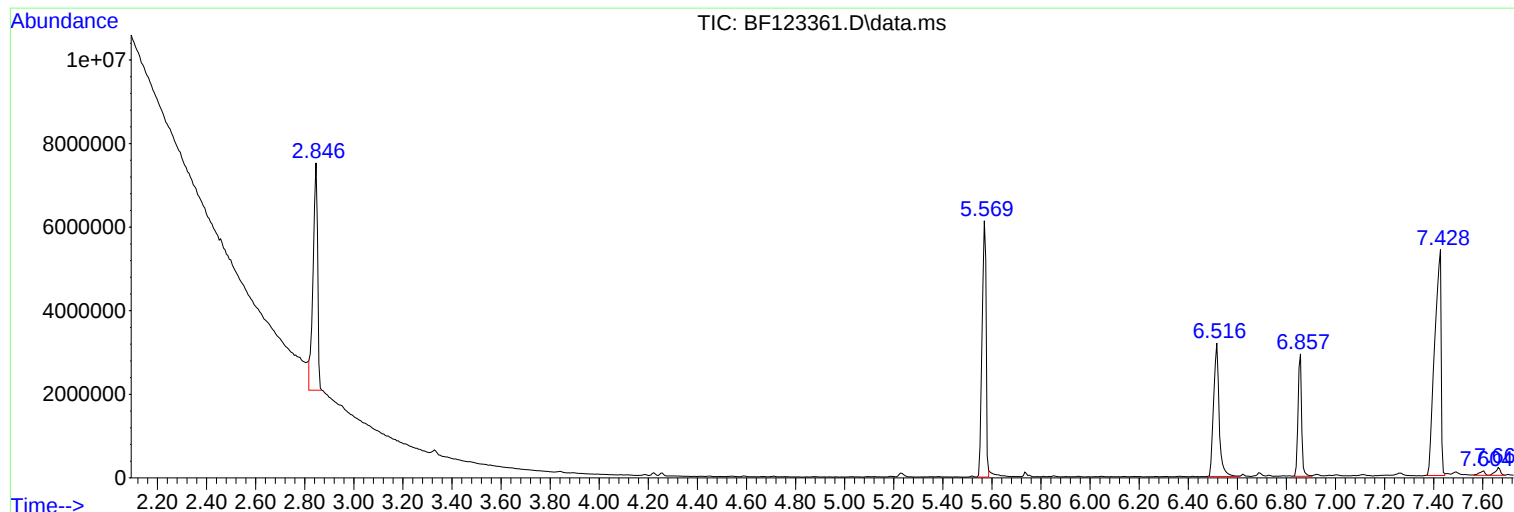
Sum of corrected areas: 116221465

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030321\
Data File : BF123361.D
Acq On : 3 Mar 2021 18:07
Operator : JU/CG
Sample : M1545-06
Misc :
ALS Vial : 10 Sample Multiplier: 4

Instrument :
BNA_F
ClientSampleId :
MH-F

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030321\
Data File : BF123361.D
Acq On : 3 Mar 2021 18:07
Operator : JU/CG
Sample : M1545-06
Misc :
ALS Vial : 10 Sample Multiplier: 4

Instrument :
BNA_F
ClientSampleId :
MH-F

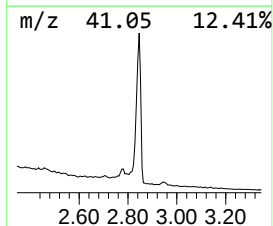
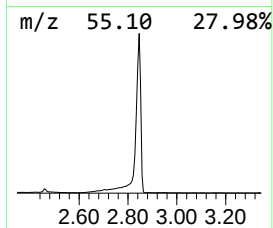
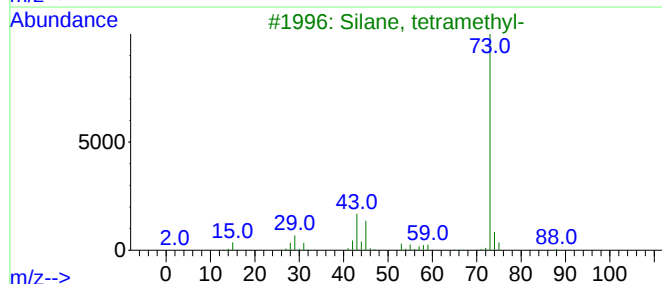
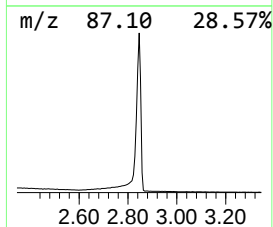
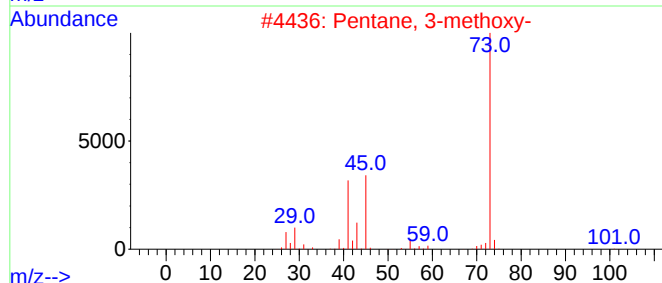
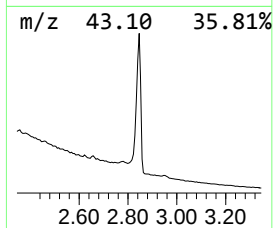
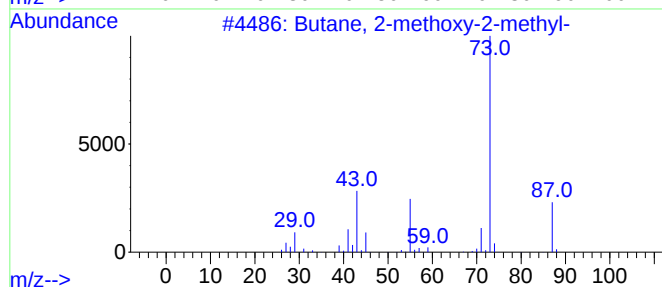
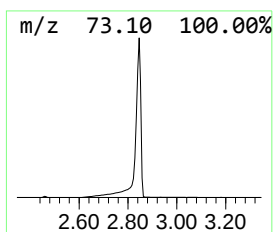
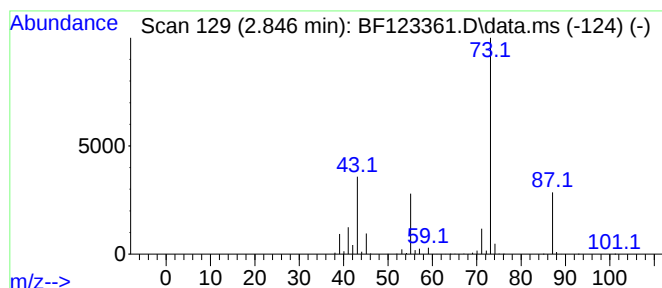
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.846	46.90 ng	6925740	1,4-Dichlorobenzene-d4	6.857

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030321\
Data File : BF123361.D
Acq On : 3 Mar 2021 18:07
Operator : JU/CG
Sample : M1545-06
Misc :
ALS Vial : 10 Sample Multiplier: 4

Instrument :
BNA_F
ClientSampleId :
MH-F

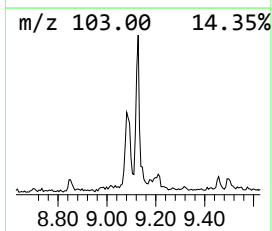
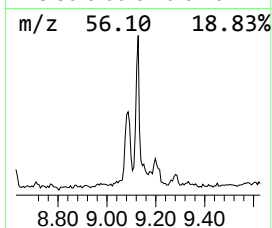
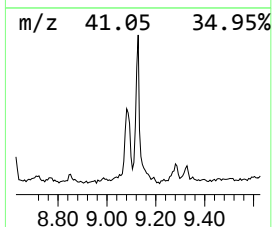
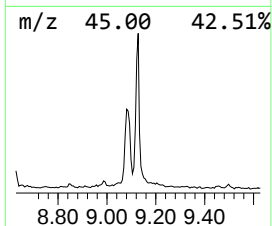
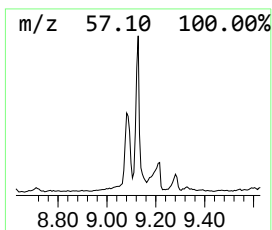
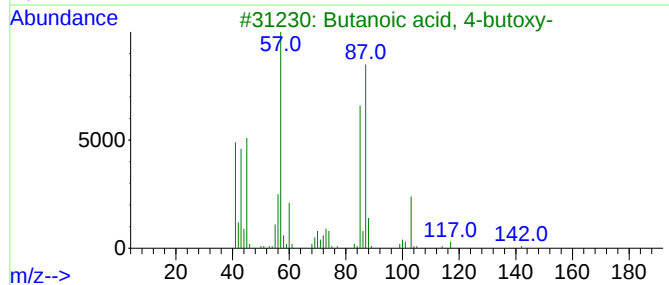
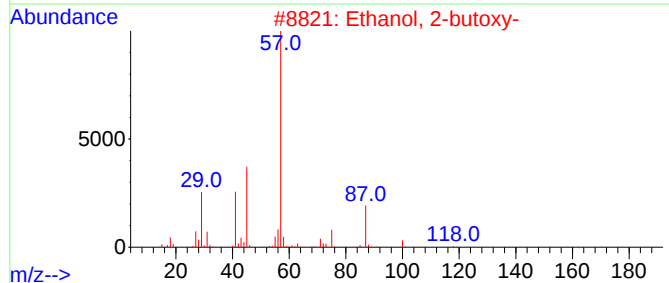
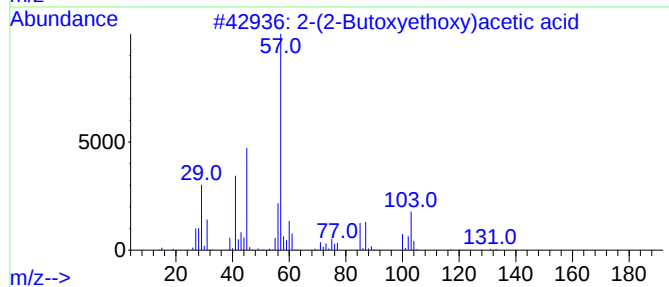
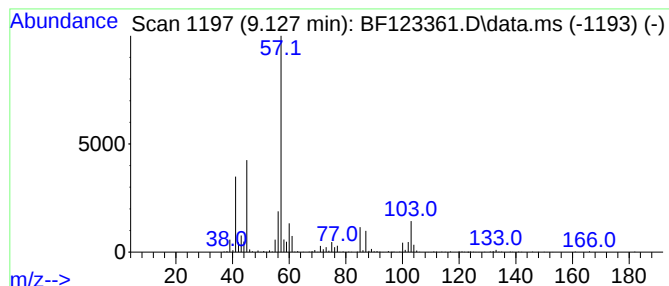
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-(2-Butoxyethoxy)acetic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.127	2.91 ng	673736	Acenaphthene-d10	9.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-(2-Butoxyethoxy)acetic acid	176	C8H16O4	082941-26-2	64
2			Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	43
3			Butanoic acid, 4-butoxy-	160	C8H16O3	055724-73-7	38
4			2-Pentanol, 4,4-dimethyl-	116	C7H16O	006144-93-0	38
5			2-(2-Butoxyethoxy)ethyl isobutyl...	262	C13H26O5	1000378-28-1	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030321\
Data File : BF123361.D
Acq On : 3 Mar 2021 18:07
Operator : JU/CG
Sample : M1545-06
Misc :
ALS Vial : 10 Sample Multiplier: 4

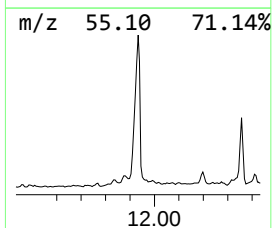
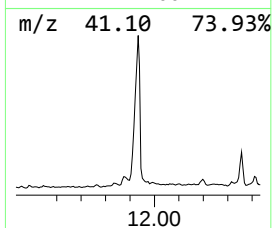
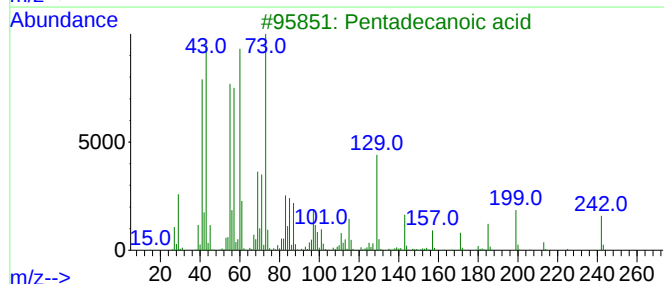
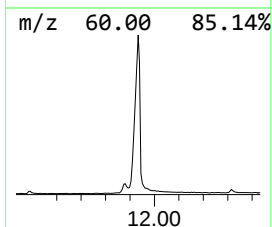
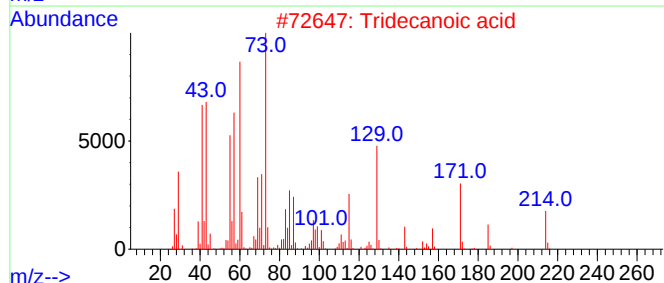
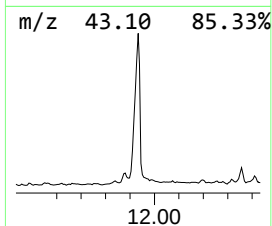
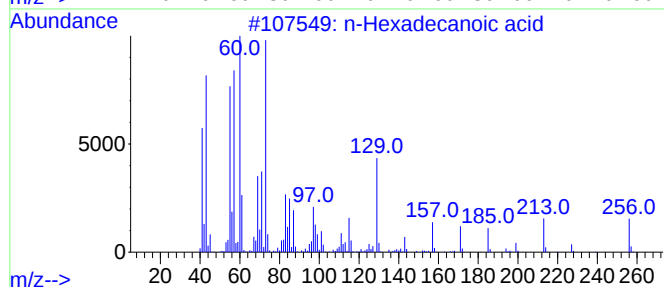
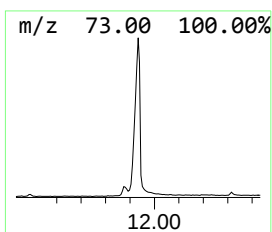
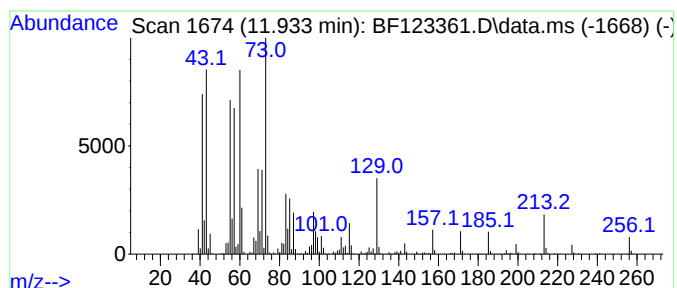
Instrument :
BNA_F
ClientSampleId :
MH-F

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.933	23.51 ng	5194510	Phenanthrene-d10	11.386	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5	Estra-1,3,5(10)-trien-17.β.-ol	256	C18H24O	002529-64-8	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030321\
Data File : BF123361.D
Acq On : 3 Mar 2021 18:07
Operator : JU/CG
Sample : M1545-06
Misc :
ALS Vial : 10 Sample Multiplier: 4

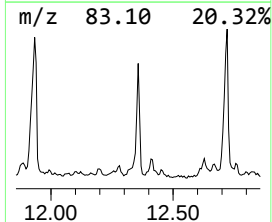
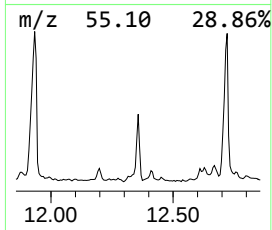
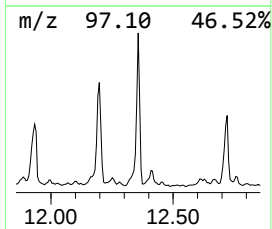
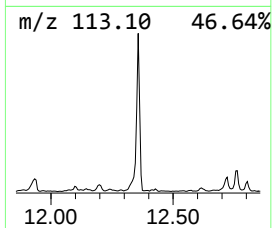
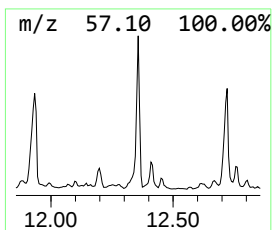
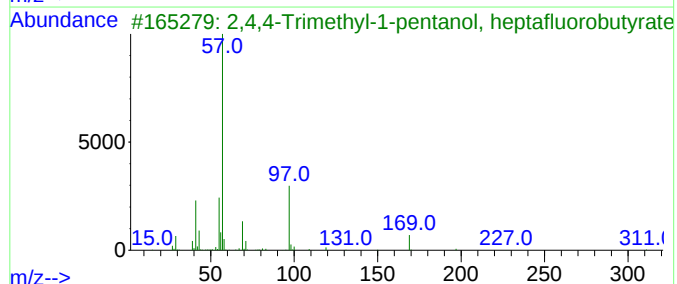
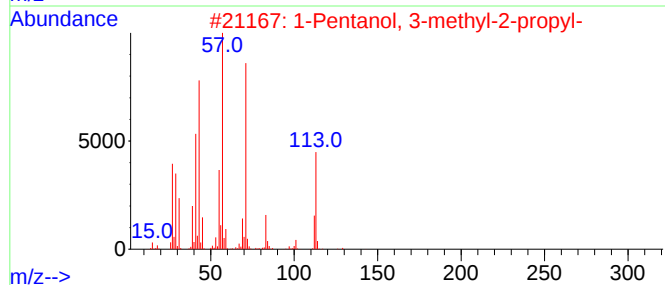
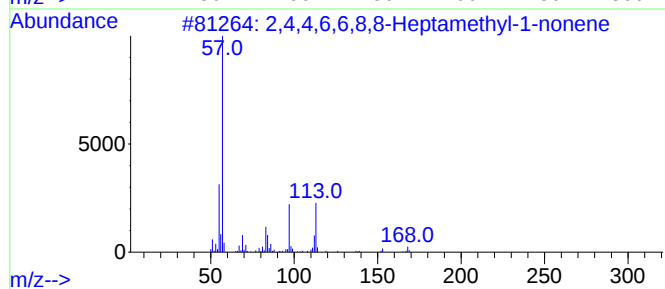
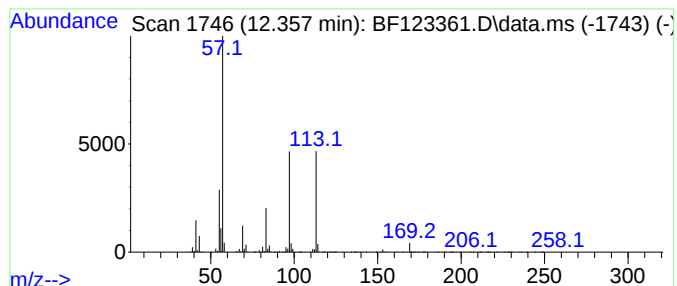
Instrument :
BNA_F
ClientSampleId :
MH-F

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 2,4,4,6,6,8,8-Heptamethyl-1... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.357	5.45 ng	1204080	Phenanthrene-d10	11.386	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	56
2	1-Pentanol, 3-methyl-2-propyl-	144	C9H20O	054004-40-9	40
3	2,4,4-Trimethyl-1-pentanol, hept...	326	C12H17F7O2	1000365-01-4	32
4	2,4,4-Trimethyl-1-pentanol, pent...	276	C11H17F5O2	1000365-51-0	27
5	Octane, 2-bromo-	192	C8H17Br	000557-35-7	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030321\
Data File : BF123361.D
Acq On : 3 Mar 2021 18:07
Operator : JU/CG
Sample : M1545-06
Misc :
ALS Vial : 10 Sample Multiplier: 4

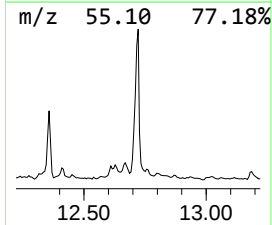
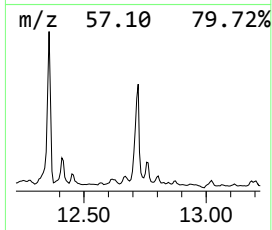
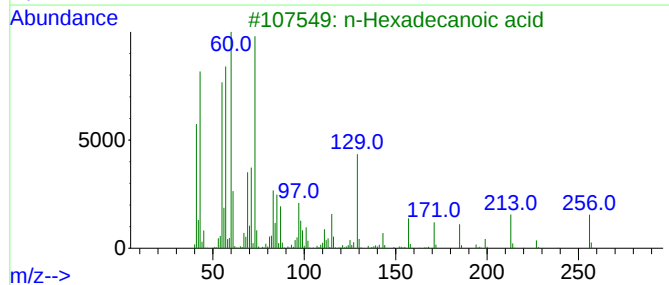
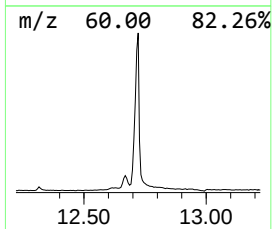
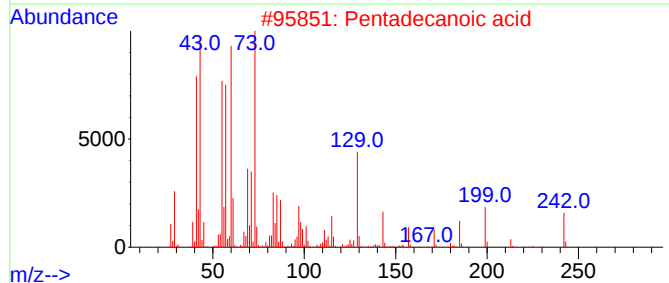
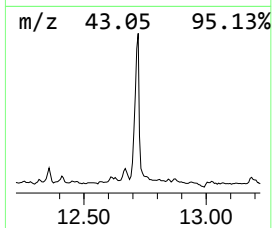
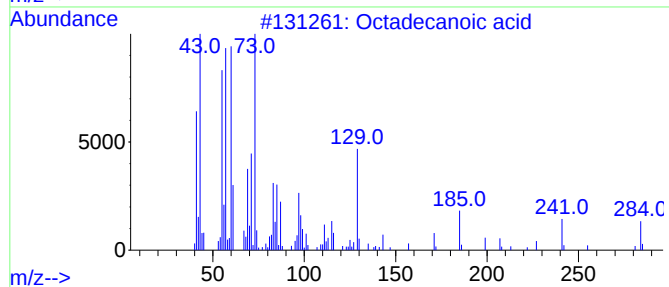
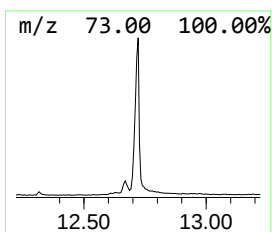
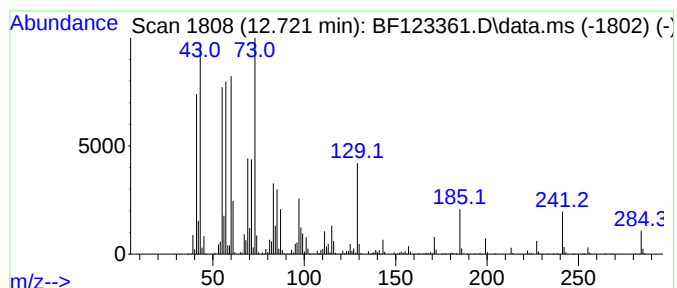
Instrument :
BNA_F
ClientSampleId :
MH-F

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.721	21.57 ng	4331440	Chrysene-d12	14.039	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	80
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030321\
Data File : BF123361.D
Acq On : 3 Mar 2021 18:07
Operator : JU/CG
Sample : M1545-06
Misc :
ALS Vial : 10 Sample Multiplier: 4

Instrument :
BNA_F
ClientSampleId :
MH-F

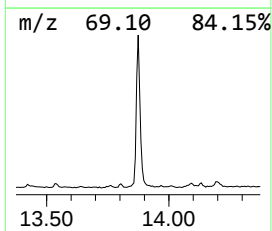
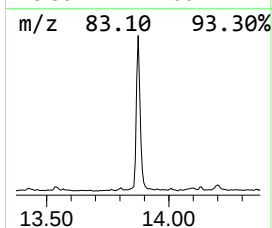
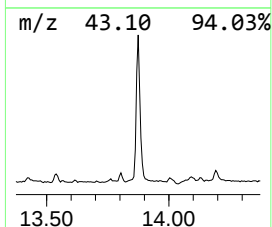
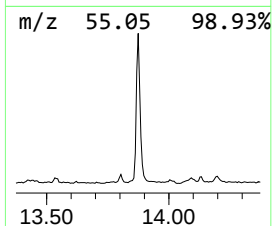
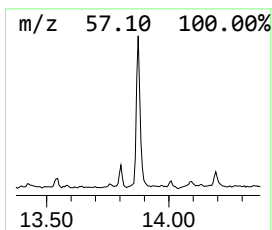
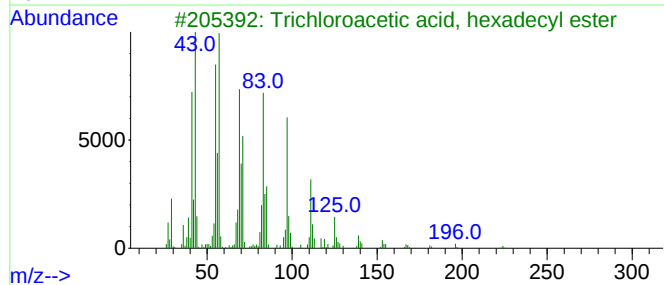
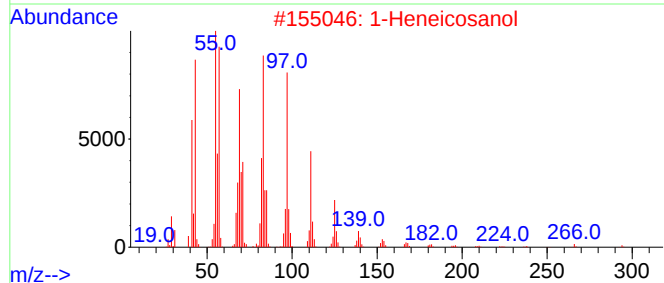
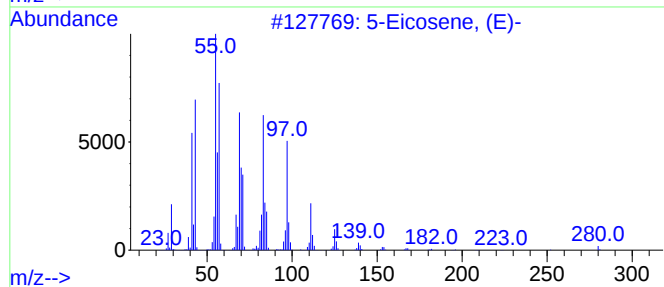
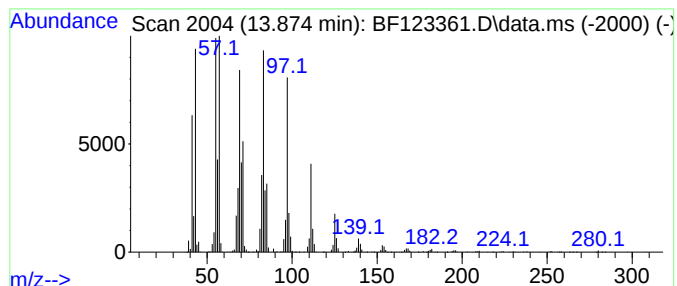
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 5-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	16.10 ng	3231800	Chrysene-d12	14.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Eicosene, (E)-	280	C20H40	074685-30-6	99
2			1-Heneicosanol	312	C21H44O	015594-90-8	95
3			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
4			Behenic alcohol	326	C22H46O	000661-19-8	94
5			n-Tetracosanol-1	354	C24H50O	000506-51-4	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030321\
Data File : BF123361.D
Acq On : 3 Mar 2021 18:07
Operator : JU/CG
Sample : M1545-06
Misc :
ALS Vial : 10 Sample Multiplier: 4

Instrument :
BNA_F
ClientSampleId :
MH-F

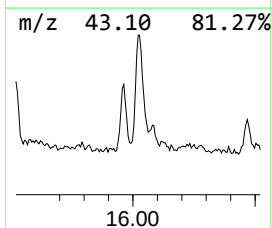
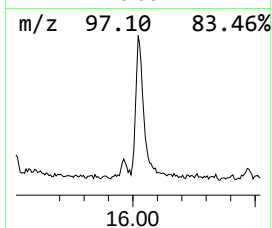
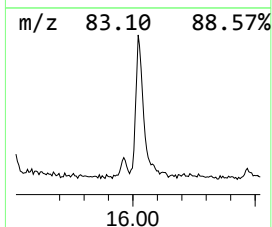
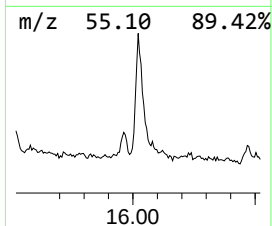
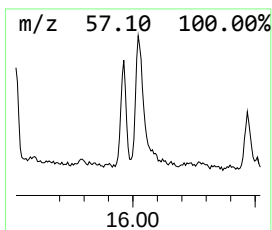
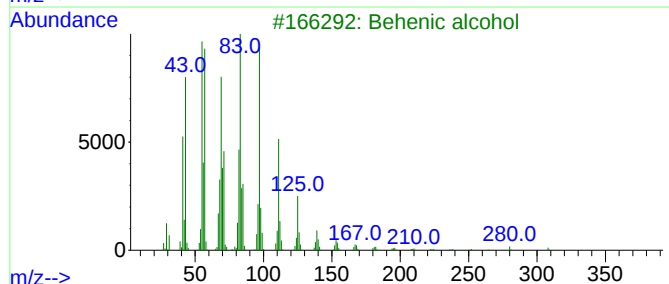
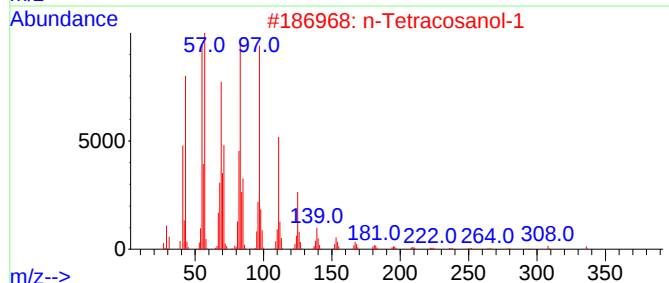
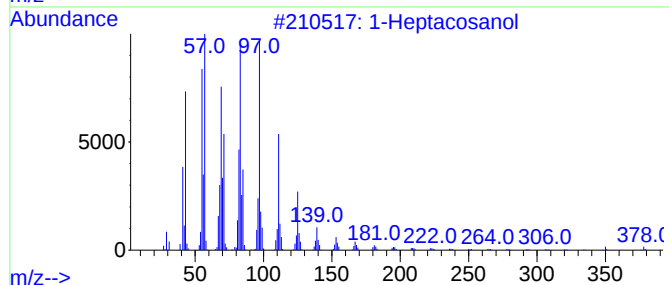
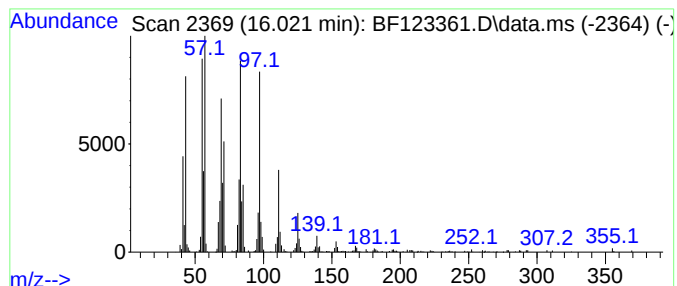
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Heptacosanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.021	4.60 ng	994551	Perylene-d12	15.521

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heptacosanol	396	C27H56O	002004-39-9	95
2			n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3			Behenic alcohol	326	C22H46O	000661-19-8	93
4			1-Heneicosanol	312	C21H44O	015594-90-8	93
5			Octacosanol	410	C28H58O	000557-61-9	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030321\
Data File : BF123361.D
Acq On : 3 Mar 2021 18:07
Operator : JU/CG
Sample : M1545-06
Misc :
ALS Vial : 10 Sample Multiplier: 4

Instrument :
BNA_F
ClientSampleId :
MH-F

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021921.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...	2.846	46.9	ng	6925740	1	6.857	2953220	20.0
2-(2-Butoxyetho...	9.127	2.9	ng	673736	3	9.892	4623100	20.0
n-Hexadecanoic ...	11.933	23.5	ng	5194510	4	11.386	4418820	20.0
2,4,4,6,6,8,8-H...	12.357	5.5	ng	1204080	4	11.386	4418820	20.0
Octadecanoic acid	12.721	21.6	ng	4331440	5	14.039	4015300	20.0
5-Eicosene, (E)-	13.874	16.1	ng	3231800	5	14.039	4015300	20.0
1-Heptacosanol	16.021	4.6	ng	994551	6	15.521	4328350	20.0