

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG013120\
 Data File : BG044263.D
 Acq On : 31 Jan 2020 17:07
 Operator : CG/JU
 Sample : L1331-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 C-1_013020

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG013020.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	5.018	323	328	334	rBV	35371	53466	1.21%	0.220%
2	5.494	402	409	421	rBV	986516	1629267	36.77%	6.696%
3	7.086	672	680	699	rBV	1095101	1973735	44.54%	8.112%
4	7.914	814	821	829	rBV	248759	417492	9.42%	1.716%
5	8.237	868	876	890	rBV	800438	1402605	31.65%	5.765%
6	9.072	1010	1018	1036	rBV	645371	1202000	27.12%	4.940%
7	10.717	1289	1298	1311	rBV	345191	651155	14.69%	2.676%
8	13.179	1709	1717	1735	rBV	1916683	3089101	69.71%	12.696%
9	14.007	1849	1858	1867	rBV	215818	342073	7.72%	1.406%
10	14.554	1944	1951	1965	rVB2	677714	1065540	24.05%	4.379%
11	16.040	2197	2204	2222	rBV	1496683	2298218	51.86%	9.446%
12	17.297	2411	2418	2429	rBV	815236	1240470	27.99%	5.098%
13	19.912	2857	2863	2875	rBV	3407121	4431379	100.00%	18.213%
14	21.216	3079	3085	3094	rBV2	131992	262984	5.93%	1.081%
15	21.540	3133	3140	3150	rBV2	757040	1303879	29.42%	5.359%
16	21.751	3172	3176	3184	rVB	56700	79413	1.79%	0.326%
17	22.344	3271	3277	3281	rBV2	66298	108319	2.44%	0.445%
18	23.014	3385	3391	3399	rVB	66722	127145	2.87%	0.523%
19	23.191	3415	3421	3431	rVB	103546	200806	4.53%	0.825%
20	23.784	3515	3522	3531	rBV2	69994	144480	3.26%	0.594%
21	24.219	3590	3596	3603	rVB4	39485	96777	2.18%	0.398%
22	24.642	3657	3668	3688	rBV2	414958	1462017	32.99%	6.009%
23	25.470	3800	3809	3821	rVB2	55774	185765	4.19%	0.764%
24	25.782	3854	3862	3874	rVB2	42705	116038	2.62%	0.477%
25	27.039	4066	4076	4090	rBV7	50571	247129	5.58%	1.016%
26	28.995	4397	4409	4419	rBV6	40571	199386	4.50%	0.819%

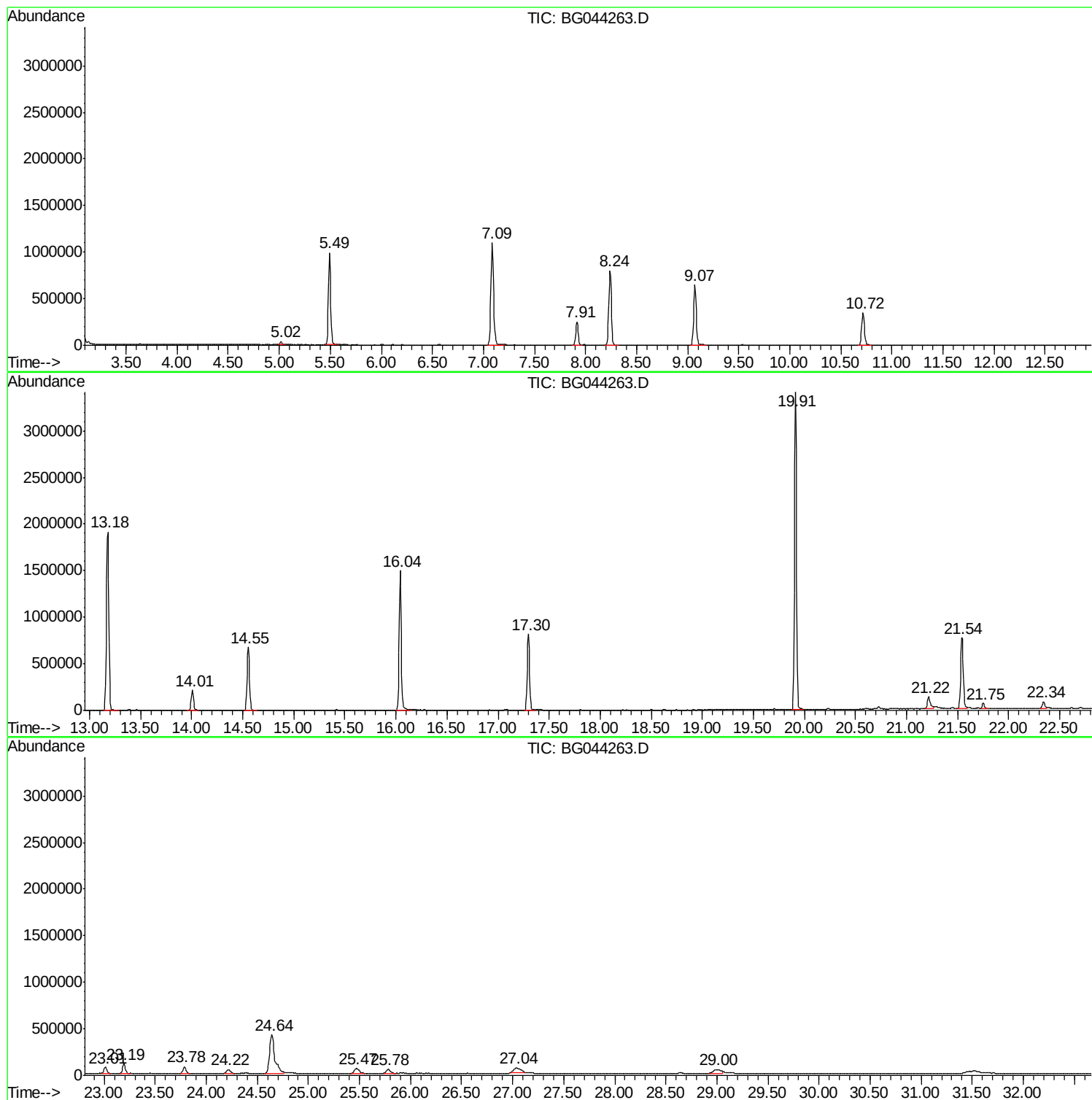
Sum of corrected areas: 24330639

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG013120\
Data File : BG044263.D
Acq On : 31 Jan 2020 17:07
Operator : CG/JU
Sample : L1331-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C-1_013020

Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG013020.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 G\DATA\BG013120\
Data File : BG044263.D
Acq On : 31 Jan 2020 17:07
Operator : CG/JU
Sample : L1331-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C-1_013020

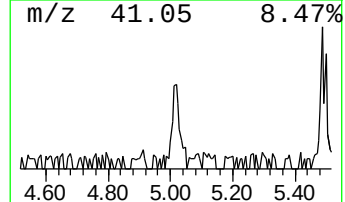
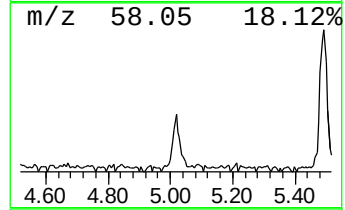
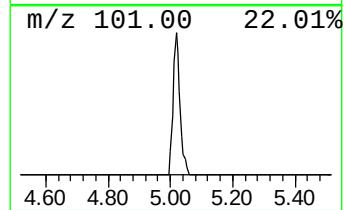
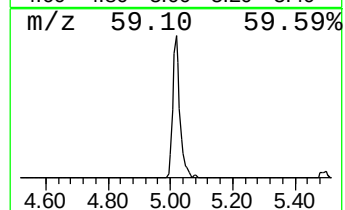
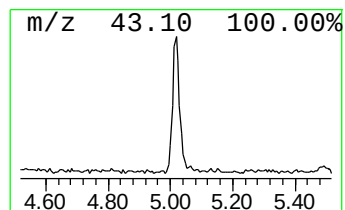
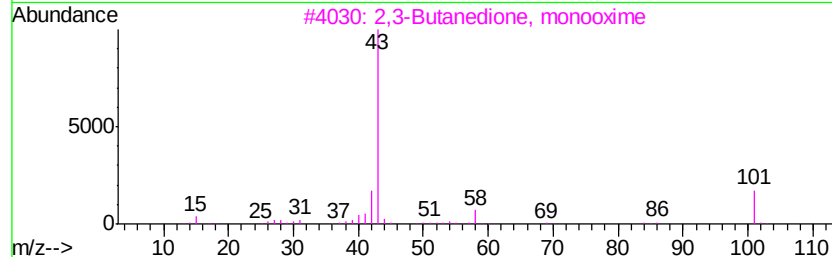
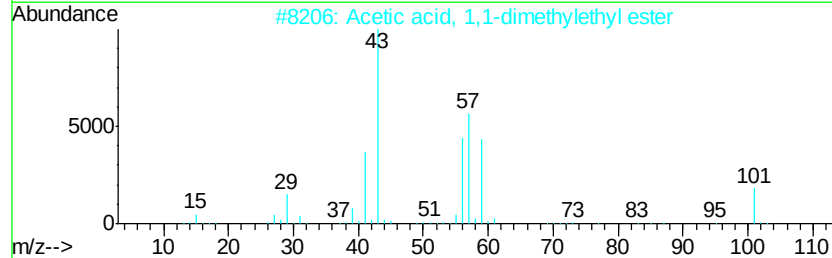
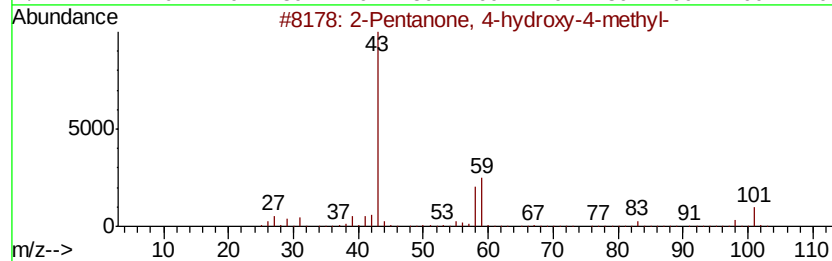
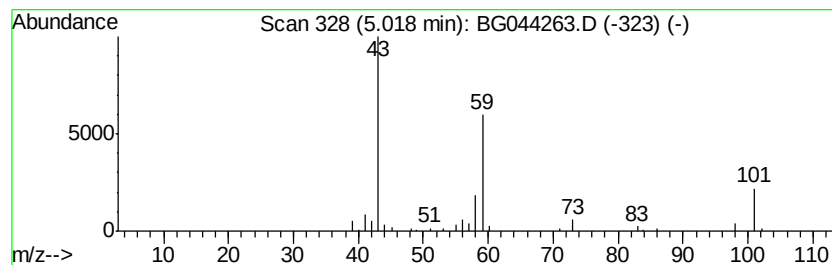
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG013020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	2.56 ng	53466	1,4-Dichlorobenzene-d4	7.91

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	32
4			(2,3,3-Trimethyloxiran-yl)methanol	116	C6H12O2	1000306-64-7	28
5			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	23



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG013120\
Data File : BG044263.D
Acq On : 31 Jan 2020 17:07
Operator : CG/JU
Sample : L1331-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

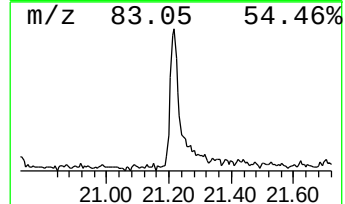
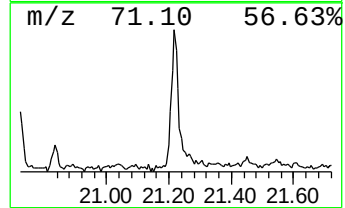
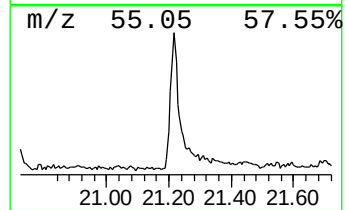
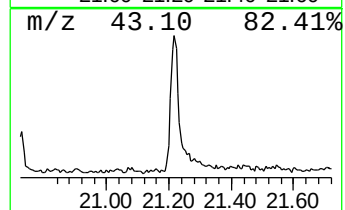
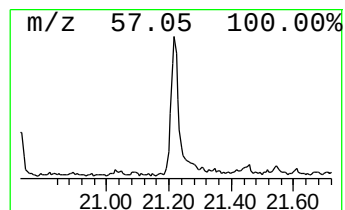
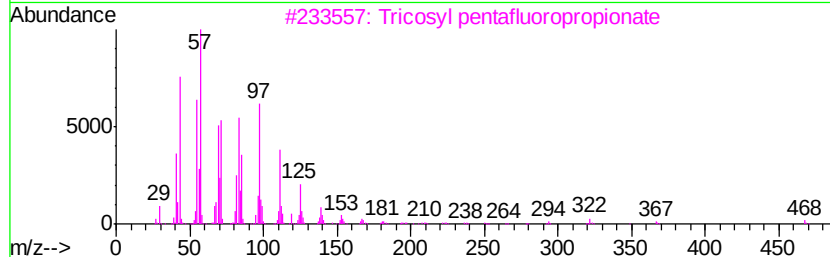
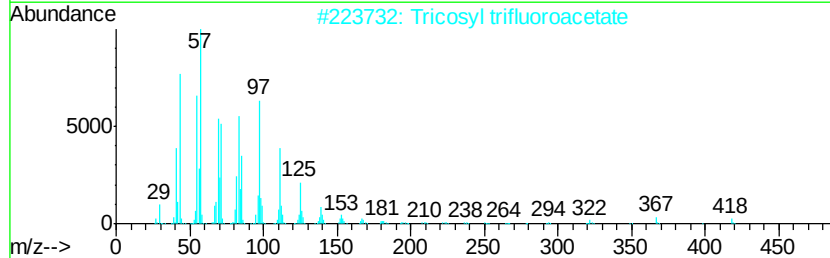
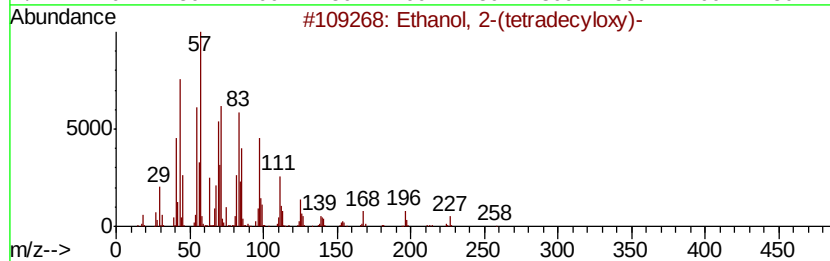
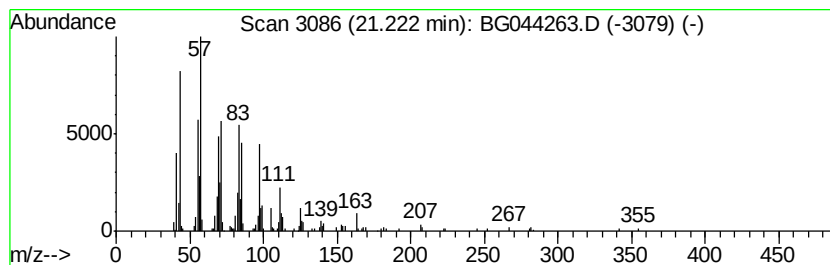
Instrument :
BNA_G
ClientSampleId :
C-1_013020

Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG013020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Ethanol, 2-(tetradecyloxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.		
21.22	4.03 ng	262984	Chrysene-d12	21.54		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
2		Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	90
3		Tricosyl pentafluoropropionate	486	C26H47F5O2	1000351-81-0	87
4		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	87
5		Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	81



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG013120\
Data File : BG044263.D
Acq On : 31 Jan 2020 17:07
Operator : CG/JU
Sample : L1331-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C-1_013020

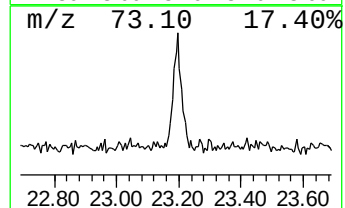
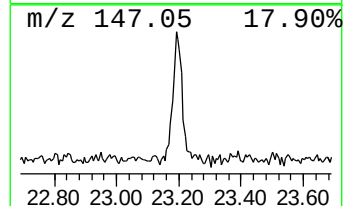
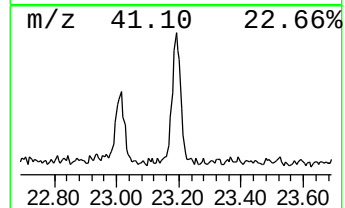
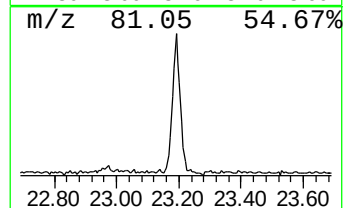
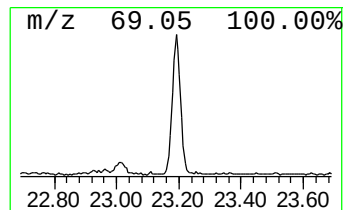
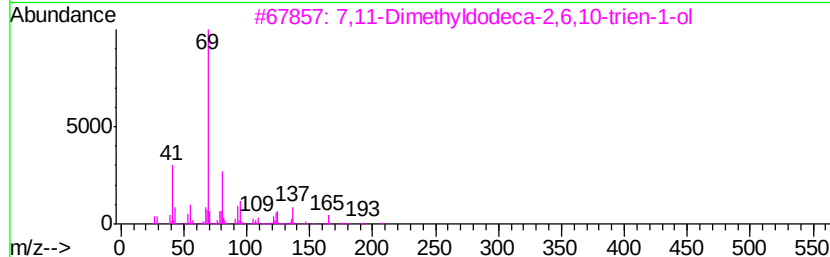
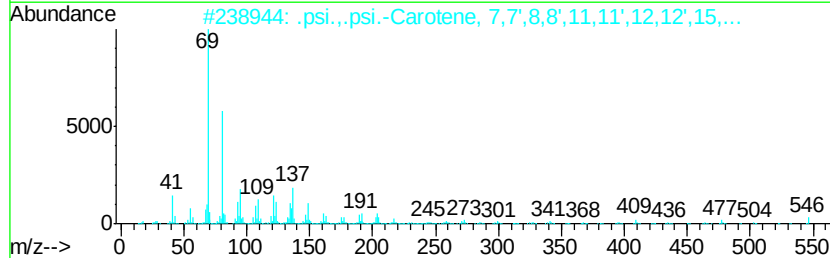
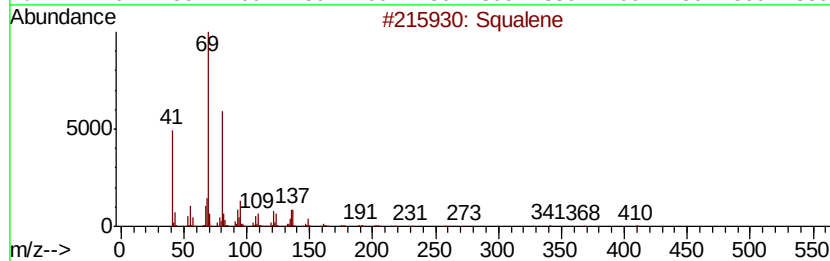
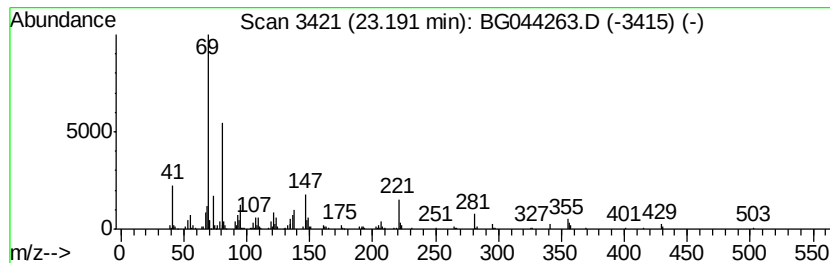
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG013020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.19	2.75 ng	200806	Perylene-d12	24.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	68
2		.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	59
3		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	59
4		Supraene	410	C30H50	007683-64-9	58
5		4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	53



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG013120\
Data File : BG044263.D
Acq On : 31 Jan 2020 17:07
Operator : CG/JU
Sample : L1331-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

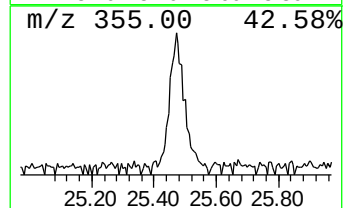
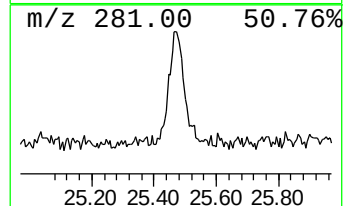
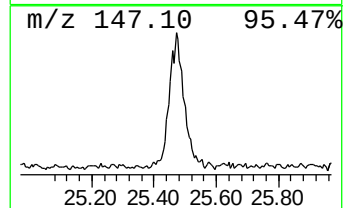
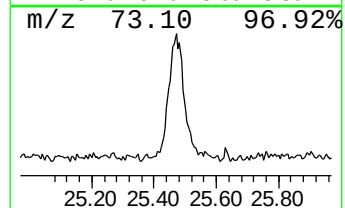
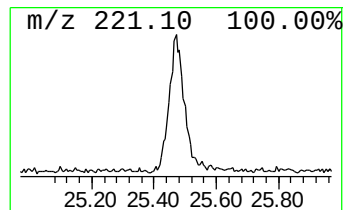
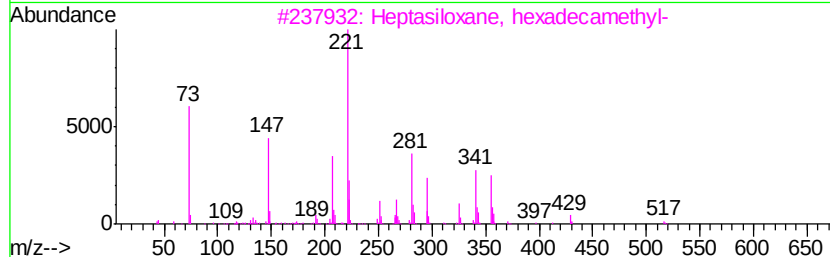
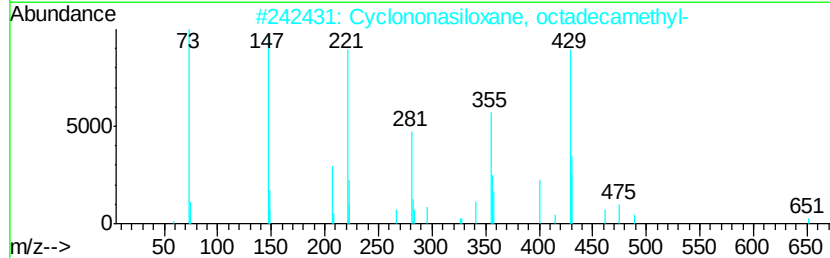
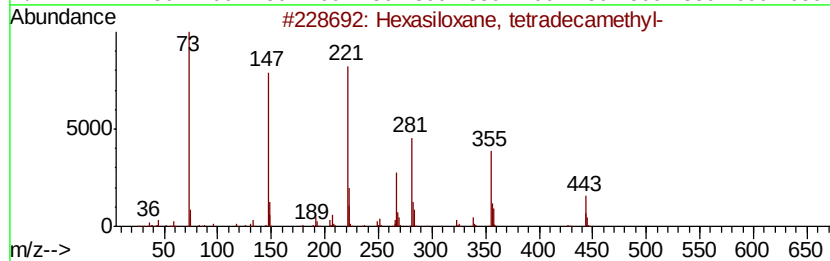
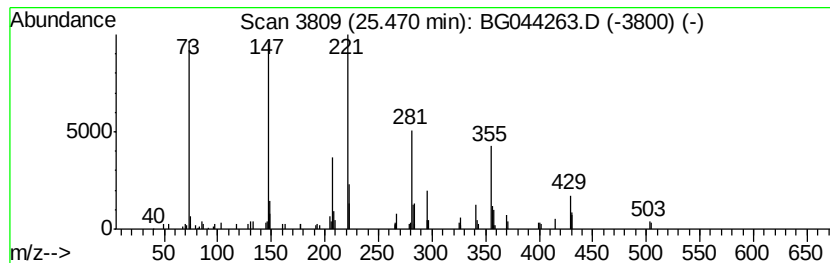
Instrument :
BNA_G
ClientSampleId :
C-1_013020

Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG013020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Hexasiloxane, tetradecamethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
25.47	2.54 ng	185765	Perylene-d12		24.64
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	87
2	Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	83
3	Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	50
4	3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	38
5	1,1,1,5,7,7,7-Heptamethyl-3,3-bi...	444	C13H40O5Si6	038147-00-1	38



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG013120\
Data File : BG044263.D
Acq On : 31 Jan 2020 17:07
Operator : CG/JU
Sample : L1331-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C-1_013020

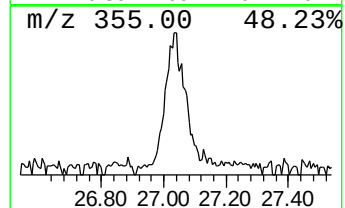
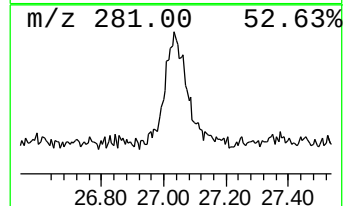
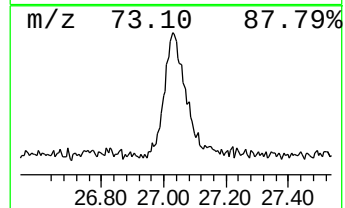
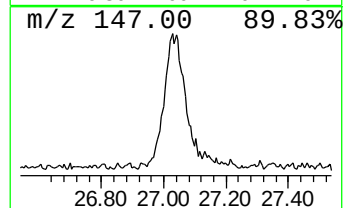
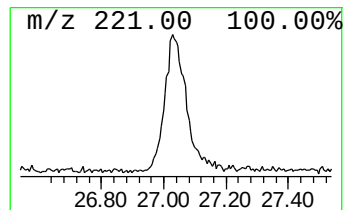
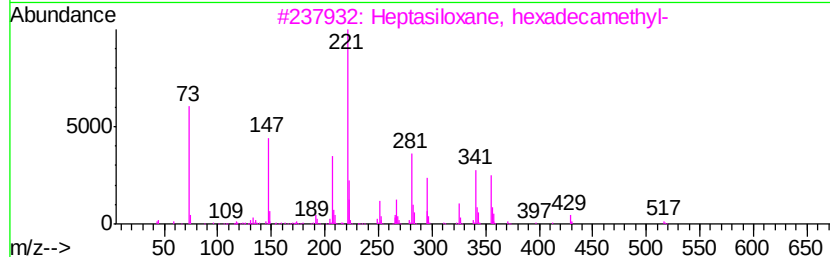
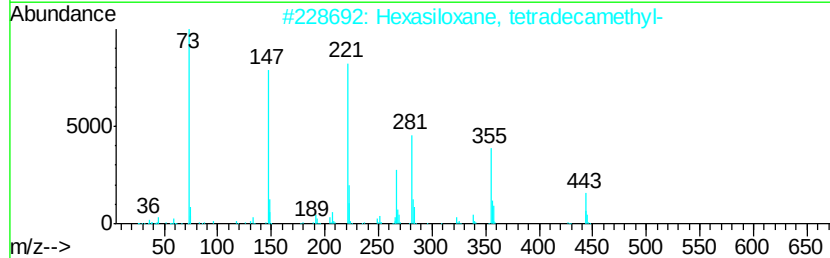
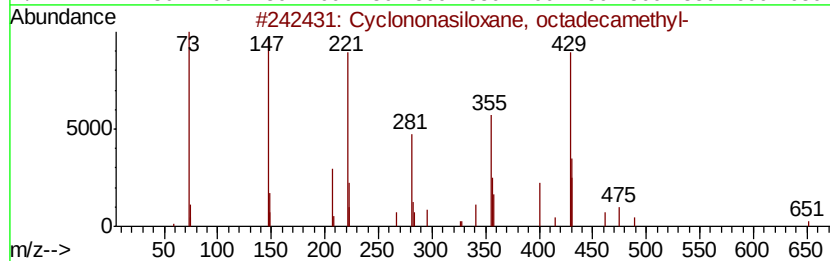
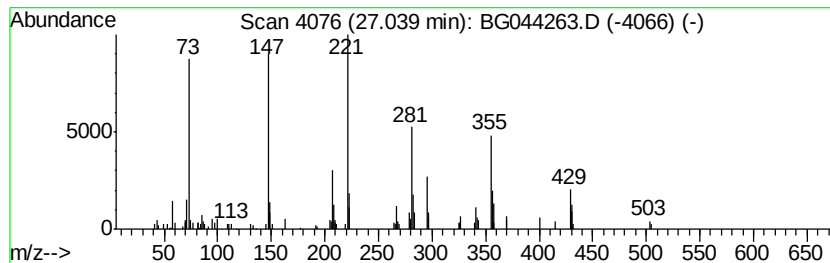
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG013020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Cyclononasiloxane, octadeca... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.04	3.38 ng	247129	Perylene-d12	24.64

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclononasiloxane, octadecamethyl-	666	C18H5409Si9	000556-71-8	72
2		Hexasiloxane, tetradecamethyl-	458	C14H4205Si6	000107-52-8	45
3		Heptasiloxane, hexadecamethyl-	532	C16H4806Si7	000541-01-5	35
4		3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H3002Si4	004342-25-0	32
5		3-Isopropoxy-1,1,1,7,7,7-hexamet...	576	C18H5207Si7	071579-69-6	32



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG013120\
Data File : BG044263.D
Acq On : 31 Jan 2020 17:07
Operator : CG/JU
Sample : L1331-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

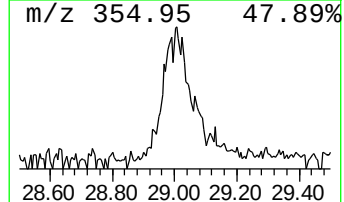
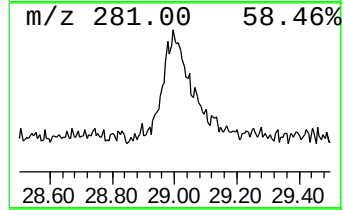
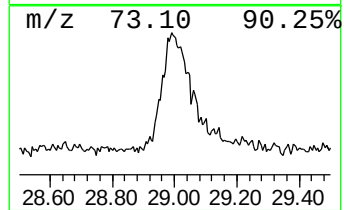
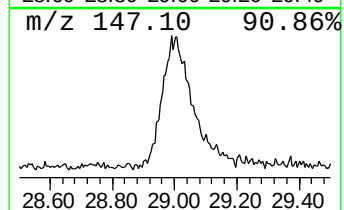
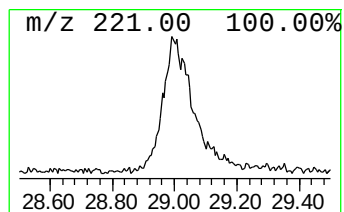
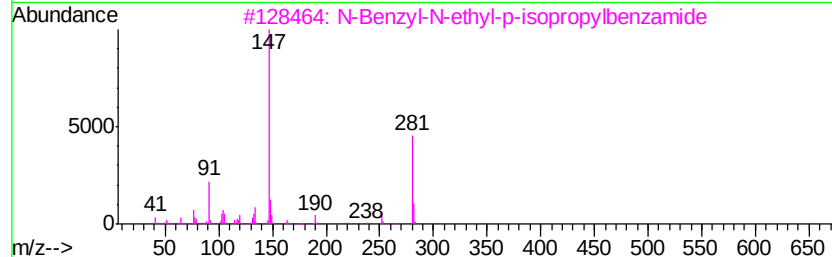
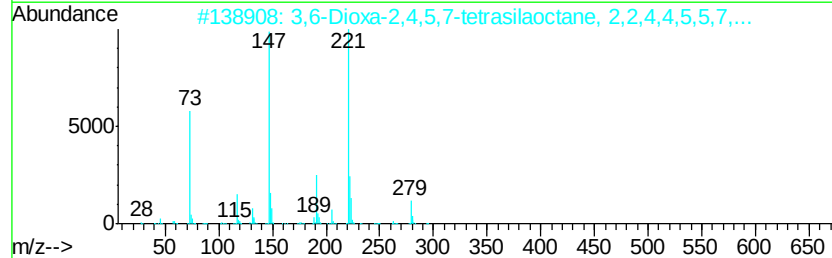
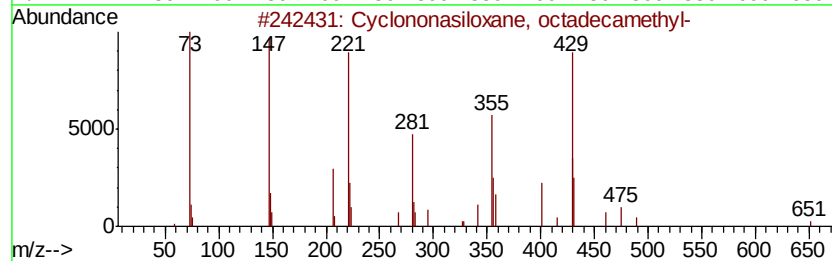
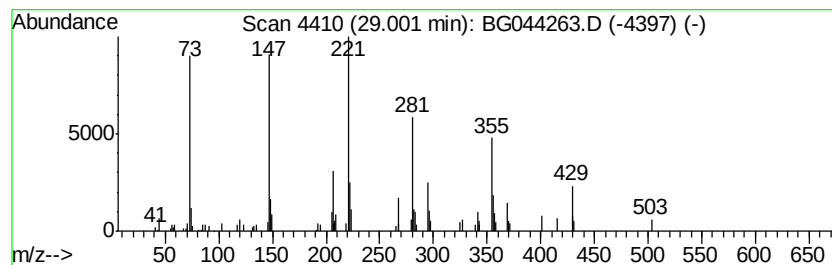
Instrument :
BNA_G
ClientSampleId :
C-1_013020

Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG013020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown29.00 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
29.00	2.73 ng	199386	Perylene-d12	24.64	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	38
2	3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	28
3	N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	22
4	Tetrahydropyran-4-carboxamide, 4...	369	C22H27NO4	1000310-01-9	18
5	2-Amino-2-oxo-acetic acid, N-[3,...	221	C12H15NO3	024451-17-0	16



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG013120\
Data File : BG044263.D
Acq On : 31 Jan 2020 17:07
Operator : CG/JU
Sample : L1331-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C-1_013020

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG013020.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-hy...	5.02	2.6	ng	53466	1	7.91	417492	20.0
Ethanol, 2-(tetra...	21.22	4.0	ng	262984	5	21.54	1303880	20.0
Squalene	23.19	2.8	ng	200806	6	24.64	1462020	20.0
Hexasiloxane, tet...	25.47	2.5	ng	185765	6	24.64	1462020	20.0
Cyclononasiloxane...	27.04	3.4	ng	247129	6	24.64	1462020	20.0
unknown29.00	29.00	2.7	ng	199386	6	24.64	1462020	20.0