

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011320\
 Data File : BG044022.D
 Acq On : 13 Jan 2020 21:38
 Operator : JU
 Sample : PB126048BL
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 PB126048BL

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-BG123019.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	5.050	328	334	346	rBV	377930	581568	8.32%	1.551%
2	5.526	408	415	429	rBV	1745452	2803589	40.13%	7.477%
3	7.112	676	685	695	rBV	1758977	3115886	44.60%	8.309%
4	7.482	738	748	758	rBV	1763822	3095110	44.30%	8.254%
5	7.947	819	827	836	rBV	384892	638890	9.15%	1.704%
6	8.270	873	882	890	rBV	1365893	2389323	34.20%	6.372%
7	9.098	1014	1023	1037	rBV	1001345	1841440	26.36%	4.911%
8	10.743	1296	1303	1314	rBV	462176	869303	12.44%	2.318%
9	13.205	1714	1722	1735	rBV	2639720	4318414	61.82%	11.516%
10	14.574	1949	1955	1968	rBV	763027	1248686	17.87%	3.330%
11	16.061	2201	2208	2227	rBV	2223101	3577479	51.21%	9.540%
12	17.318	2415	2422	2435	rBV	1014331	1549603	22.18%	4.132%
13	19.938	2861	2868	2883	rBV	4495488	6985973	100.00%	18.630%
14	21.572	3139	3146	3157	rBV2	977237	1714336	24.54%	4.572%
15	23.270	3430	3435	3442	rVB2	40941	91762	1.31%	0.245%
16	24.316	3607	3613	3625	rVB3	69416	193339	2.77%	0.516%
17	24.692	3666	3677	3698	rBV2	475453	1771536	25.36%	4.724%
18	25.614	3824	3834	3847	rBV5	81797	296844	4.25%	0.792%
19	27.236	4099	4110	4128	rVB9	85816	415556	5.95%	1.108%

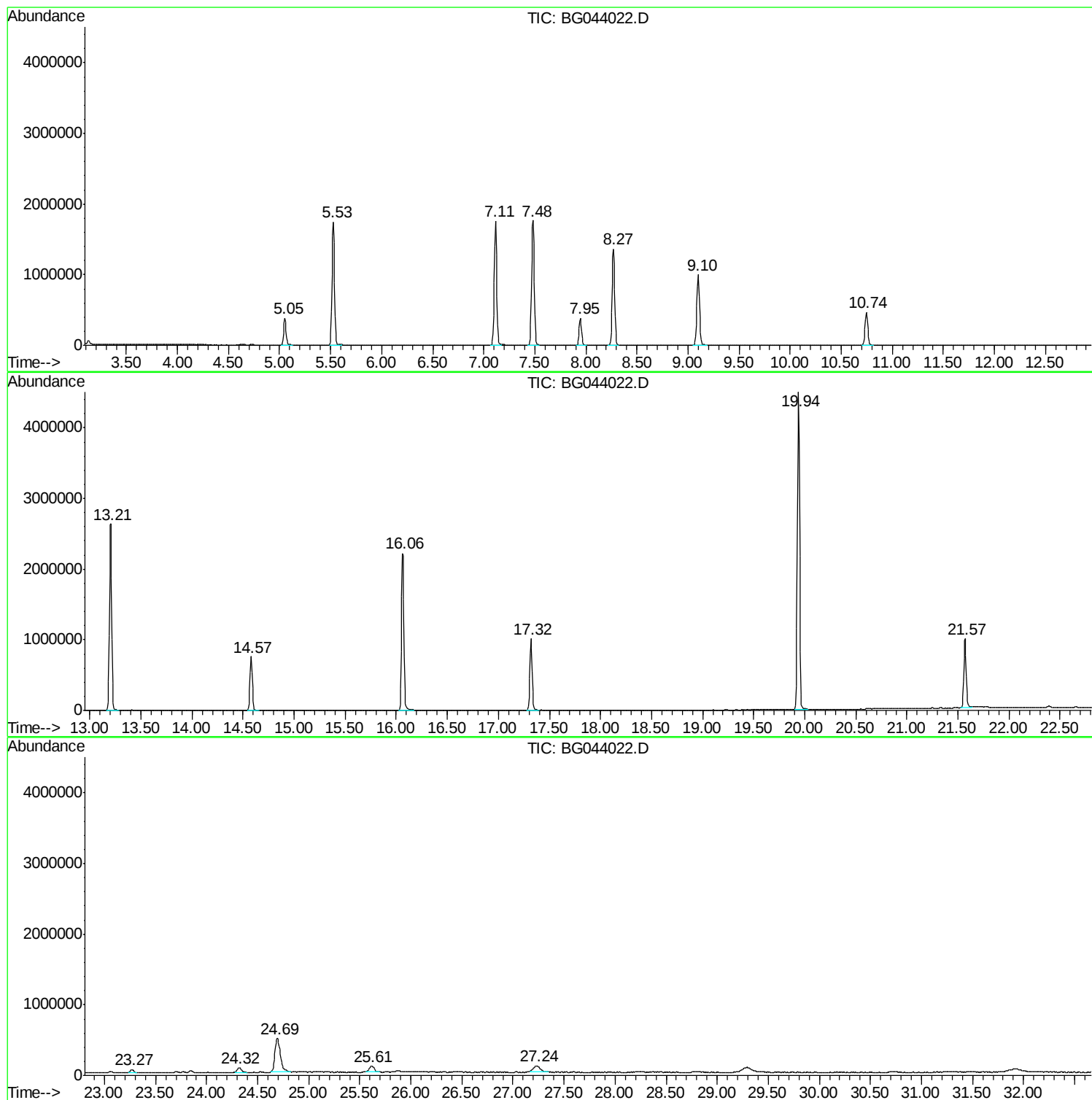
Sum of corrected areas: 37498637

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011320\
Data File : BG044022.D
Acq On : 13 Jan 2020 21:38
Operator : JU
Sample : PB126048BL
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB126048BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG123019.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\BG011320\
Data File : BG044022.D
Acq On : 13 Jan 2020 21:38
Operator : JU
Sample : PB126048BL
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB126048BL

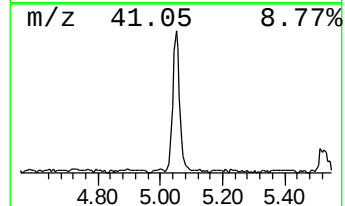
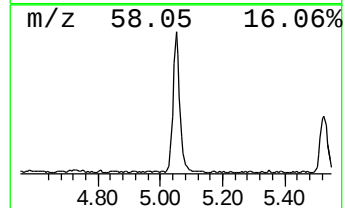
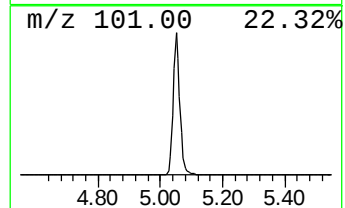
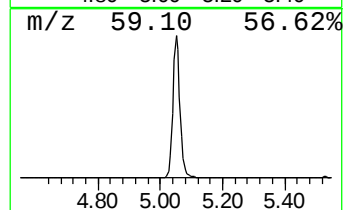
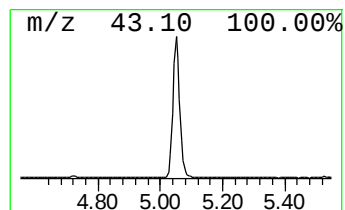
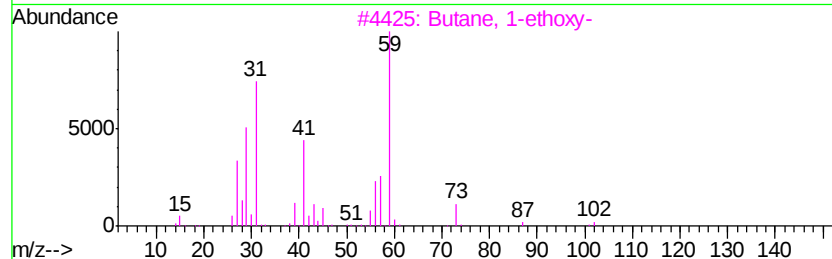
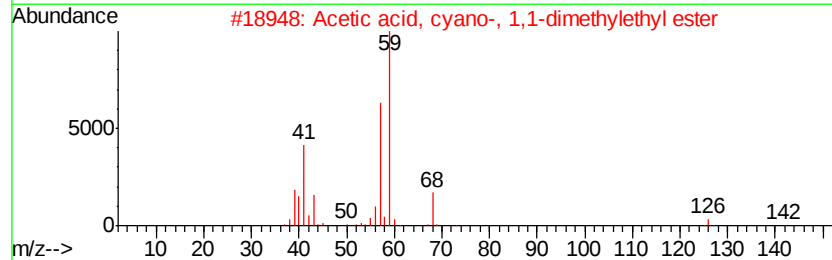
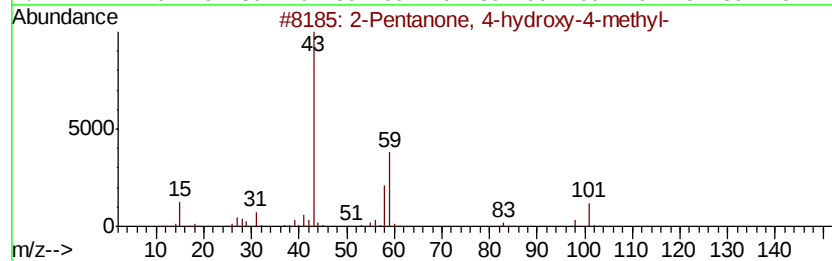
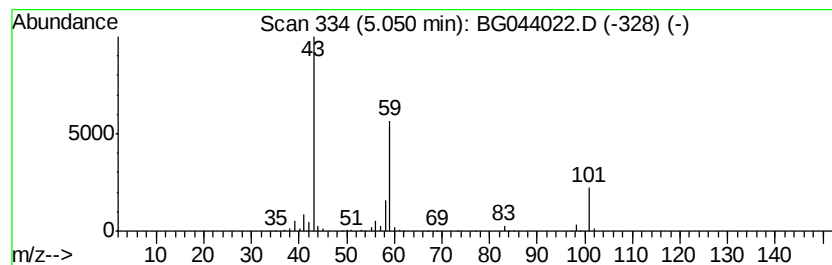
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	18.21 ng	581568	1,4-Dichlorobenzene-d4	7.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	32
3		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011320\
Data File : BG044022.D
Acq On : 13 Jan 2020 21:38
Operator : JU
Sample : PB126048BL
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB126048BL

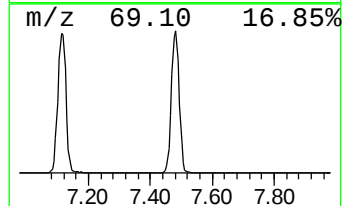
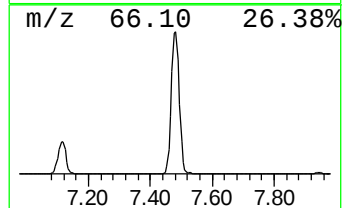
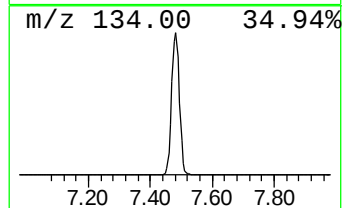
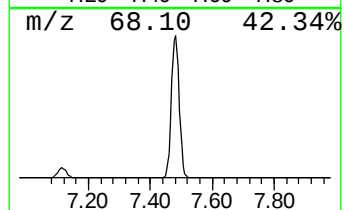
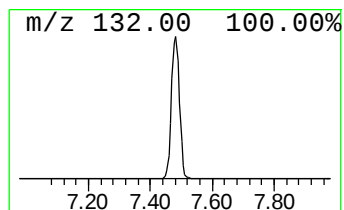
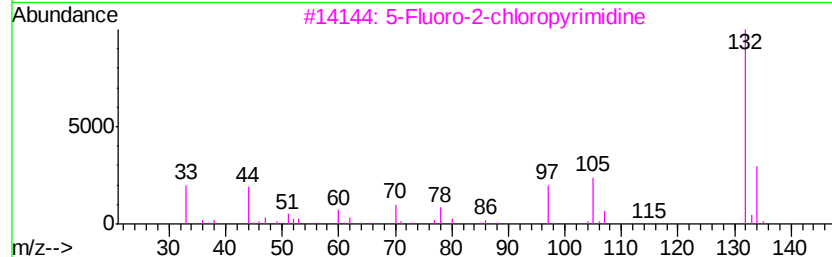
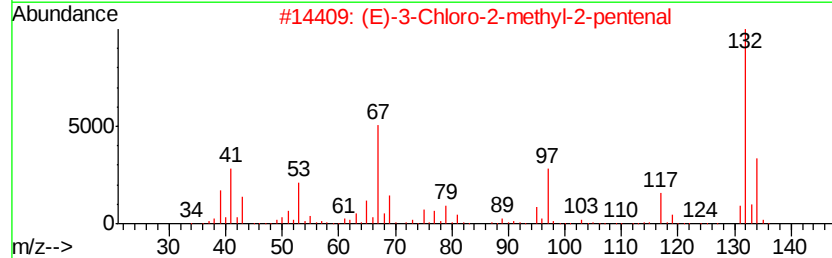
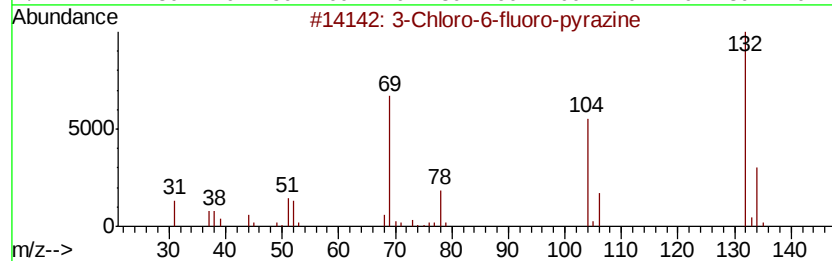
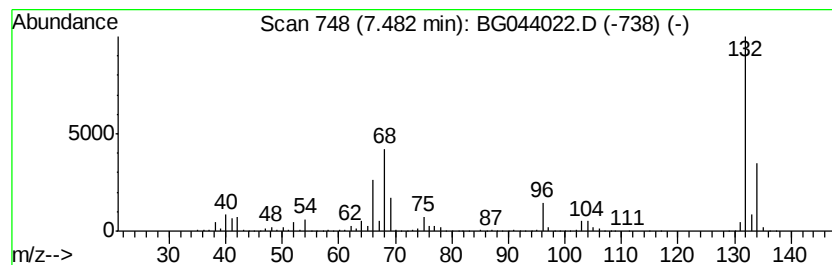
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown7.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.48	96.89 ng	3095110	1,4-Dichlorobenzene-d4	7.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4		Tranvlcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011320\
Data File : BG044022.D
Acq On : 13 Jan 2020 21:38
Operator : JU
Sample : PB126048BL
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB126048BL

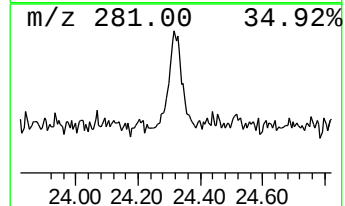
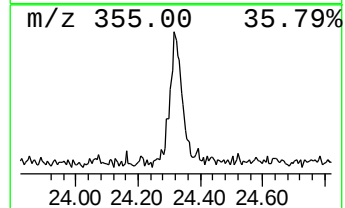
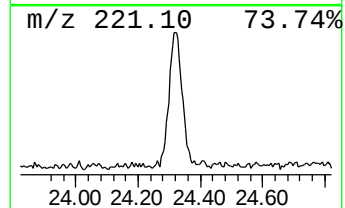
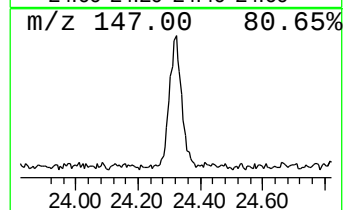
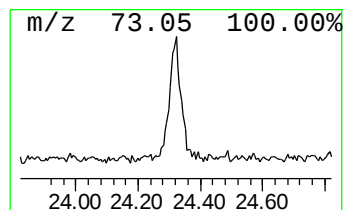
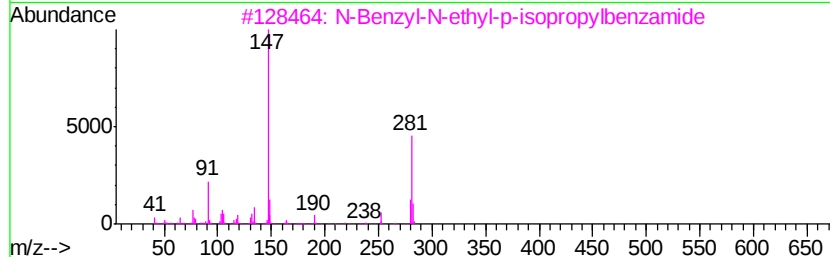
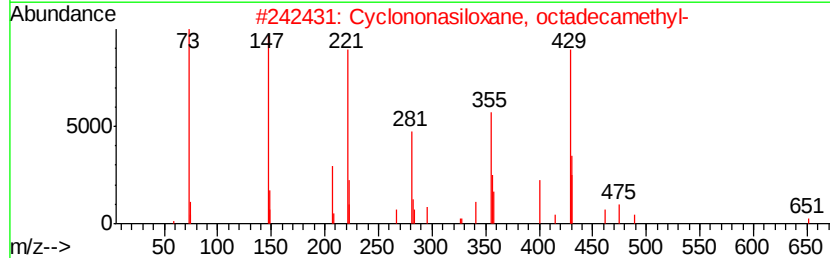
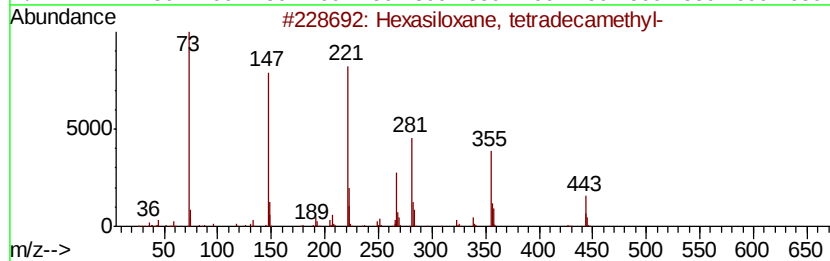
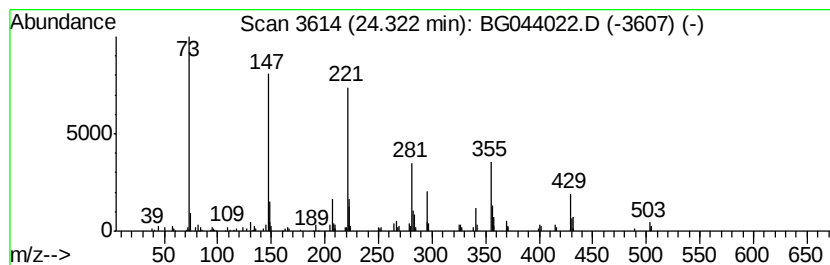
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Hexasiloxane, tetradecamethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.32	2.18 ng	193339	Perylene-d12	24.70

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	83
2			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	72
3			N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	30
4			Trisiloxane, 1,1,1,5,5,5-hexamet...	384	C12H36O4Si5	003555-47-3	27
5			Acetamide, 2-(5,7-dimethyl-[1,2,...	389	C21H19N5OS	1000304-63-9	25



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011320\
Data File : BG044022.D
Acq On : 13 Jan 2020 21:38
Operator : JU
Sample : PB126048BL
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB126048BL

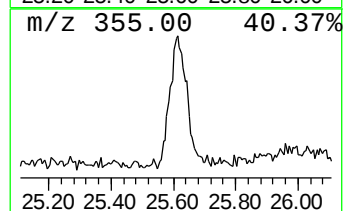
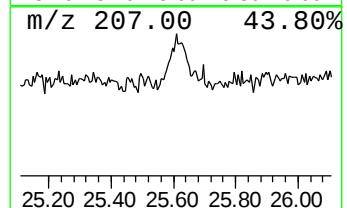
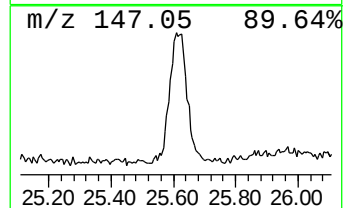
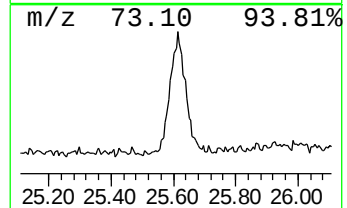
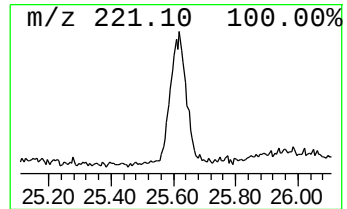
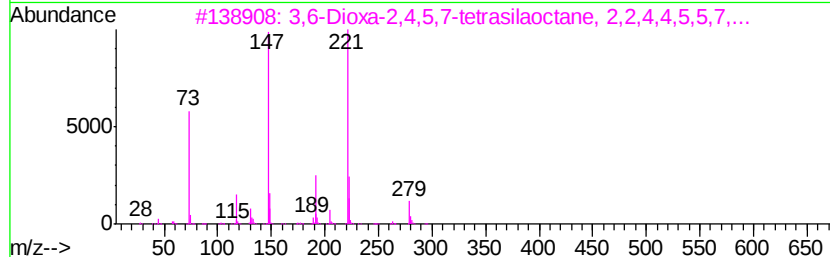
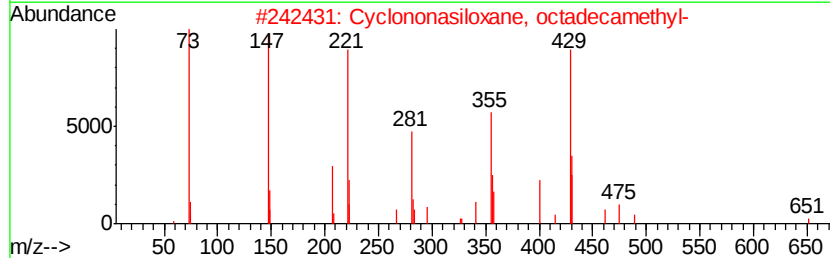
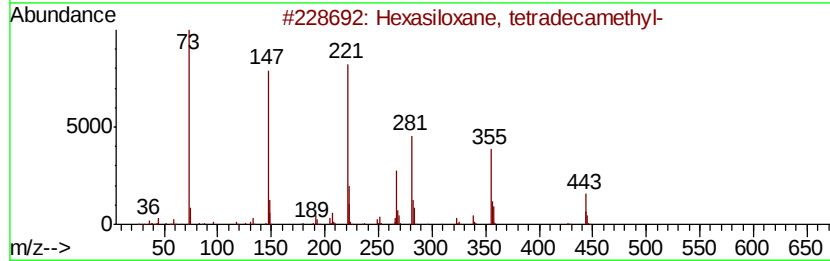
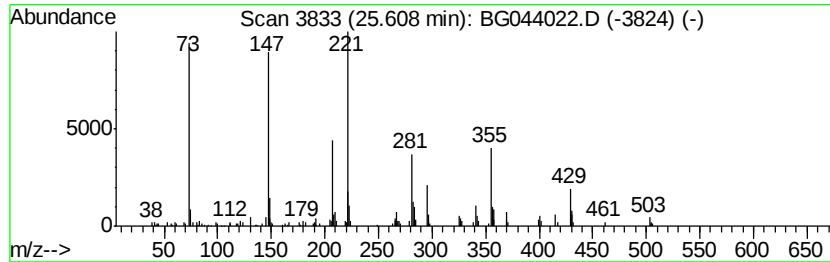
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Cyclononasiloxane, octadeca... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.61	3.35 ng	296844	Perylene-d12	24.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	80
2		Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	72
3		3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	33
4		N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	30
5		Pentasiloxane, dodecamethyl-	384	C12H36O4Si5	000141-63-9	27



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011320\
Data File : BG044022.D
Acq On : 13 Jan 2020 21:38
Operator : JU
Sample : PB126048BL
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB126048BL

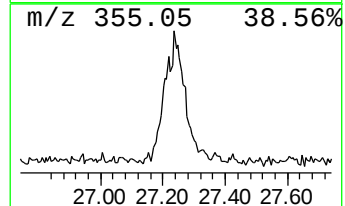
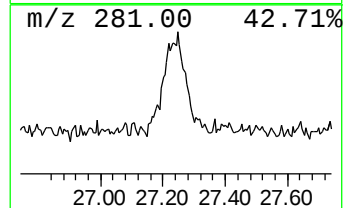
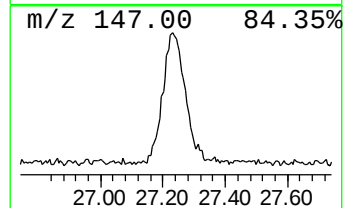
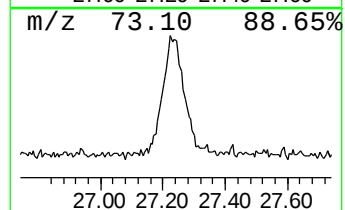
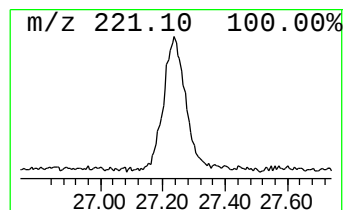
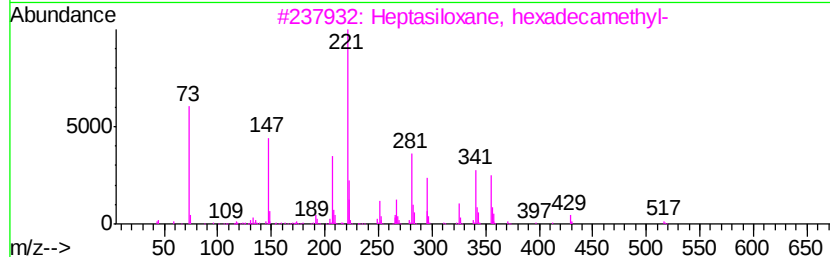
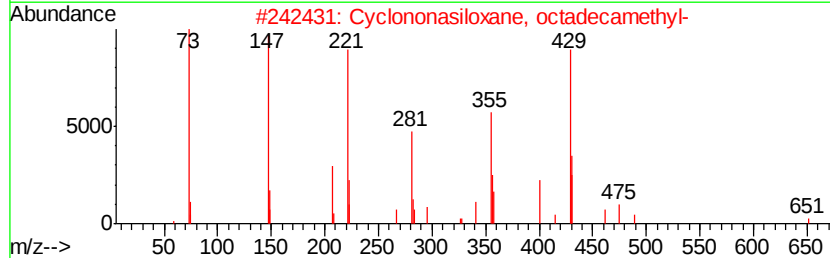
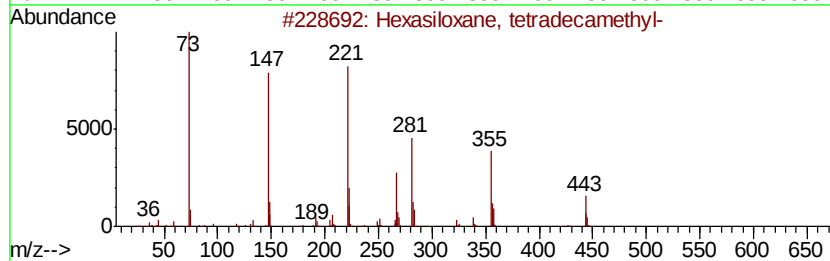
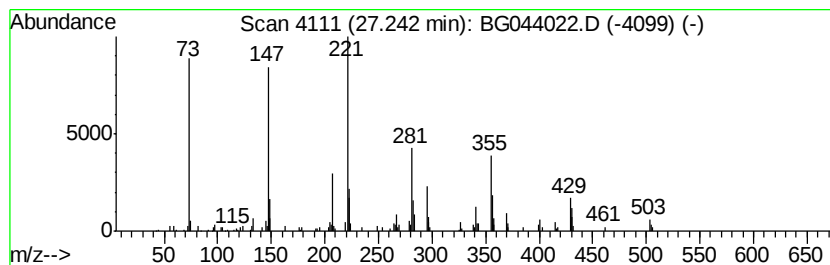
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown27.24 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.24	4.69 ng	415556	Perylene-d12	24.70

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	80
2			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	58
3			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	49
4			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	38
5			Pentasiloxane, dodecamethyl-	384	C12H36O4Si5	000141-63-9	30



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG011320\
Data File : BG044022.D
Acq On : 13 Jan 2020 21:38
Operator : JU
Sample : PB126048BL
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB126048BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.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...	5.05	18.2	ng	581568	1	7.95	638890	20.0
unknown7.48	7.48	96.9	ng	3095110	1	7.95	638890	20.0
Hexasiloxane, tet...	24.32	2.2	ng	193339	6	24.70	1771540	20.0
Cyclononasiloxane...	25.61	3.4	ng	296844	6	24.70	1771540	20.0
unknown27.24	27.24	4.7	ng	415556	6	24.70	1771540	20.0