

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011320\
 Data File : BG044020.D
 Acq On : 13 Jan 2020 20:19
 Operator : JU
 Sample : PB126031BL
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 PB126031BL

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	3.130	3	7	22	rVB	273576	464861	6.24%	1.111%
2	5.051	328	334	346	rVB	410950	633691	8.50%	1.514%
3	5.527	407	415	427	rBV	1741030	2923321	39.23%	6.986%
4	7.113	677	685	697	rBV	1840607	3280630	44.03%	7.840%
5	7.484	738	748	756	rBV	1817750	3265213	43.82%	7.803%
6	7.948	819	827	836	rBV	357408	614652	8.25%	1.469%
7	8.271	873	882	890	rBV	1457389	2542881	34.13%	6.077%
8	9.099	1013	1023	1035	rBV	1054152	1975639	26.51%	4.721%
9	10.744	1295	1303	1316	rBV	448650	836613	11.23%	1.999%
10	13.200	1714	1721	1736	rBV	2882284	4598158	61.71%	10.989%
11	14.029	1856	1862	1867	rBV	64005	99197	1.33%	0.237%
12	14.575	1947	1955	1964	rBV	725046	1202734	16.14%	2.874%
13	16.068	2201	2209	2223	rBV	2411008	3845792	51.61%	9.191%
14	17.319	2416	2422	2431	rBV	974185	1481258	19.88%	3.540%
15	19.934	2861	2867	2879	rBV	5321268	7451332	100.00%	17.808%
16	21.238	3083	3089	3096	rBV	308977	514359	6.90%	1.229%
17	21.303	3097	3100	3111	rVB	62164	110802	1.49%	0.265%
18	21.567	3138	3145	3156	rBV2	1012463	1704452	22.87%	4.073%
19	21.779	3178	3181	3187	rVB2	61211	86741	1.16%	0.207%
20	22.378	3277	3283	3295	rBV2	99432	206423	2.77%	0.493%
21	23.054	3392	3398	3403	rVB	92787	155689	2.09%	0.372%
22	23.247	3425	3431	3439	rVB4	64054	138706	1.86%	0.331%
23	23.829	3525	3530	3539	rVB2	84089	171682	2.30%	0.410%
24	24.287	3602	3608	3617	rVB2	94483	233028	3.13%	0.557%
25	24.681	3664	3675	3683	rBV2	622233	1736872	23.31%	4.151%
26	25.562	3816	3825	3836	rVB4	107870	360858	4.84%	0.862%
27	25.850	3869	3874	3882	rVB5	54907	146125	1.96%	0.349%
28	27.155	4083	4096	4109	rBV5	135037	572459	7.68%	1.368%
29	29.146	4423	4435	4455	rVB3	96316	489395	6.57%	1.170%

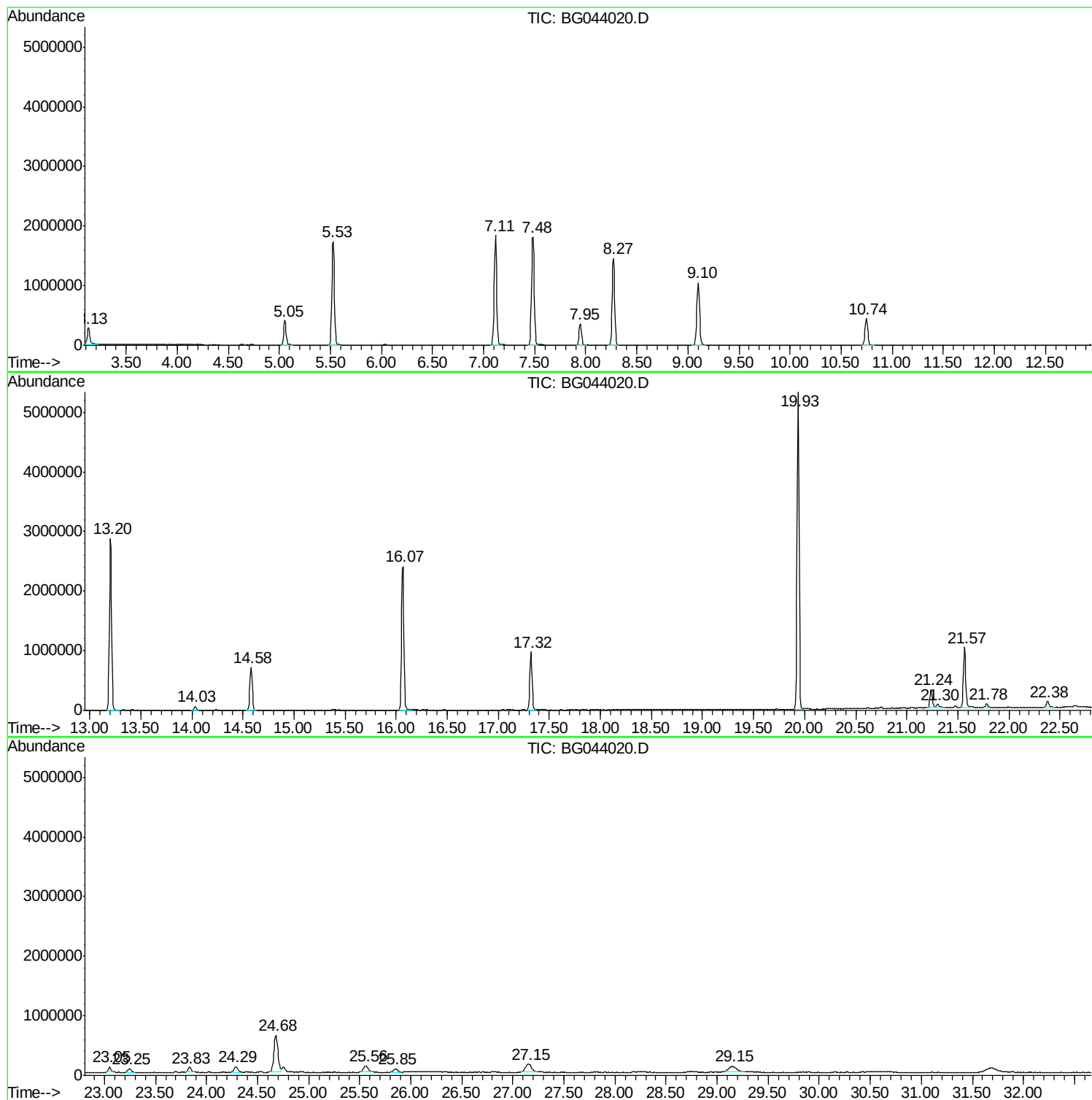
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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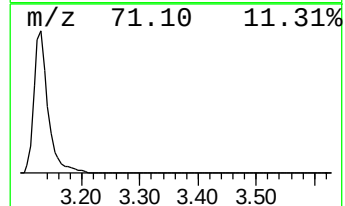
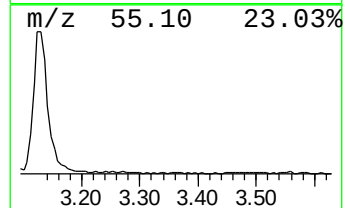
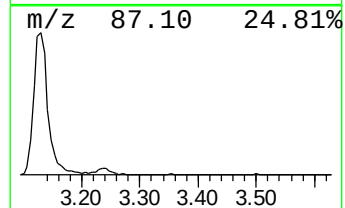
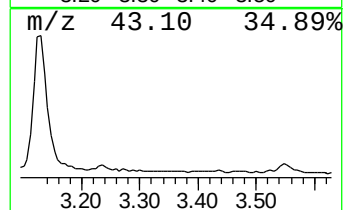
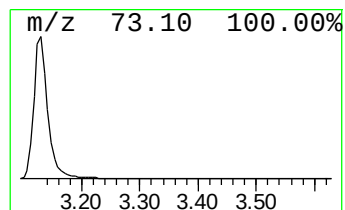
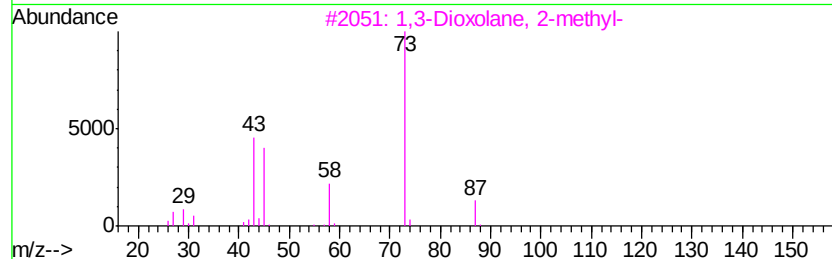
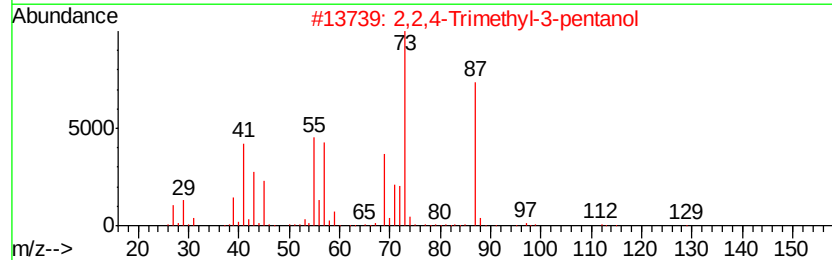
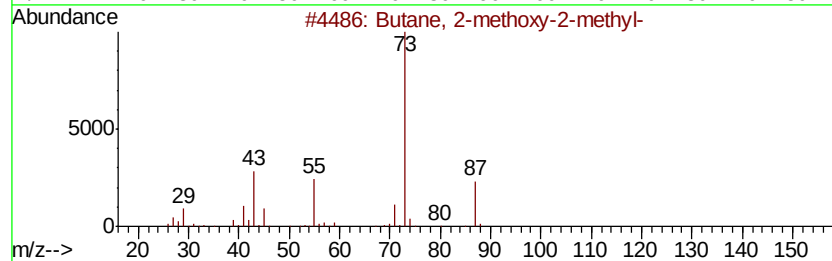
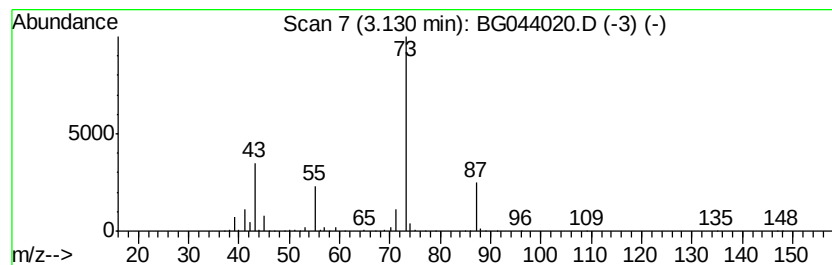
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.13	15.13 ng	464861	1,4-Dichlorobenzene-d4	7.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	86
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5		Silane, tetramethyl-	88	C4H12Si	000075-76-3	9



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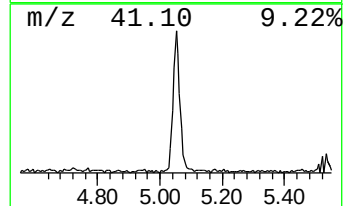
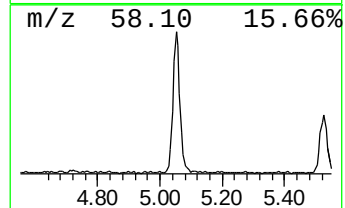
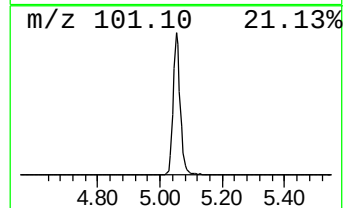
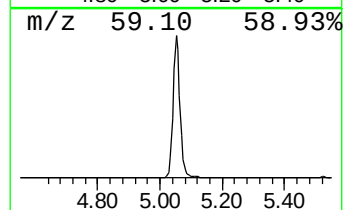
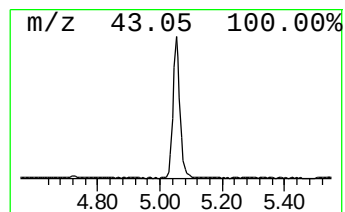
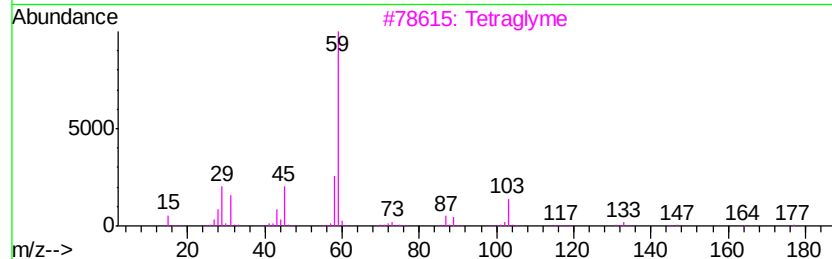
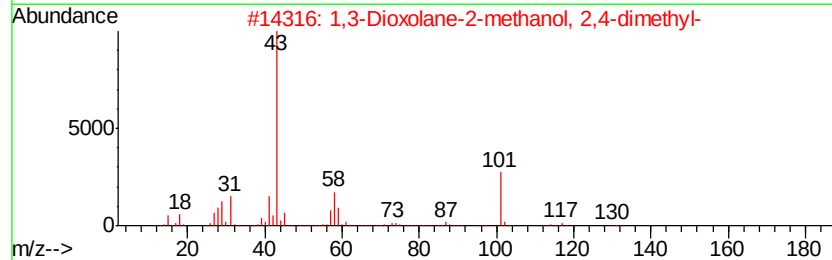
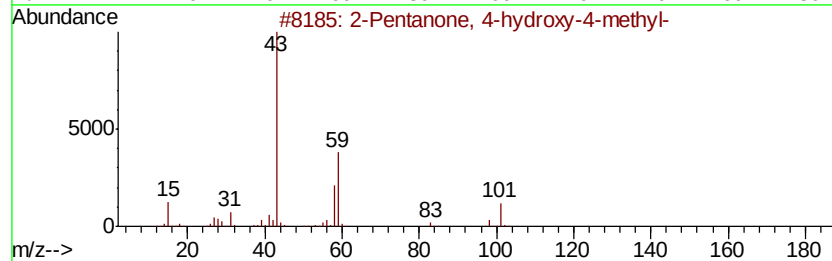
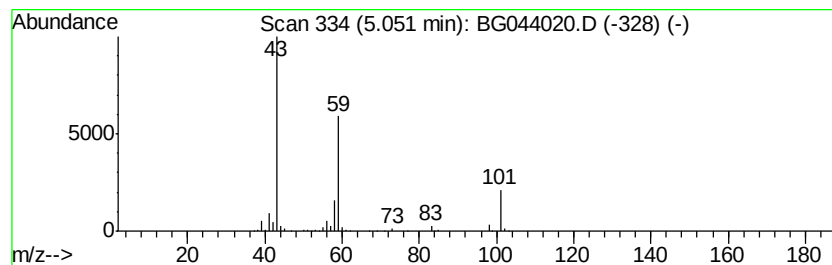
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	20.62 ng	633691	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		1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	28
3		Tetraolyme	222	C10H22O5	000143-24-8	25
4		2,5,8,11-Tetraoxadodecane	178	C8H18O4	000112-49-2	23
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17



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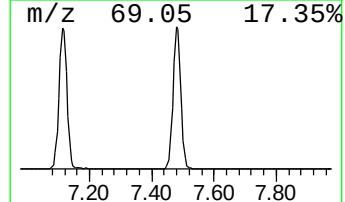
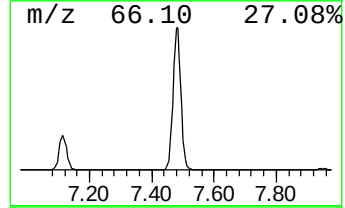
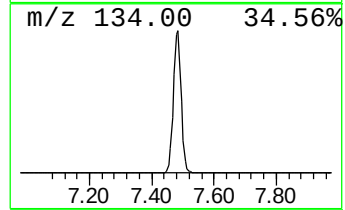
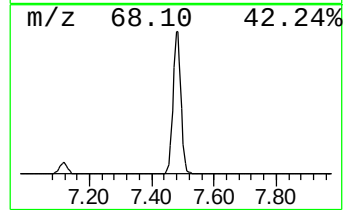
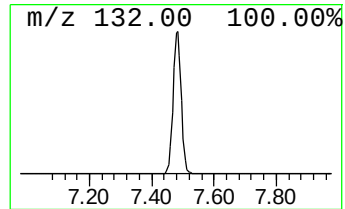
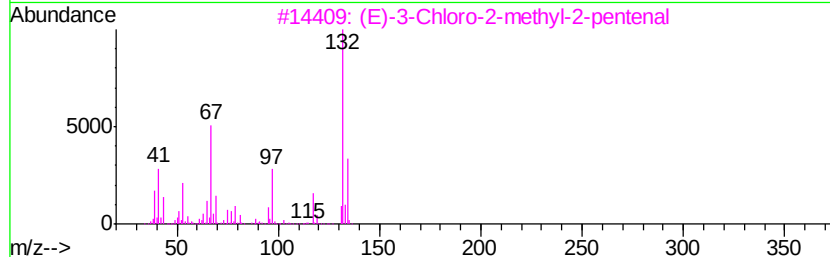
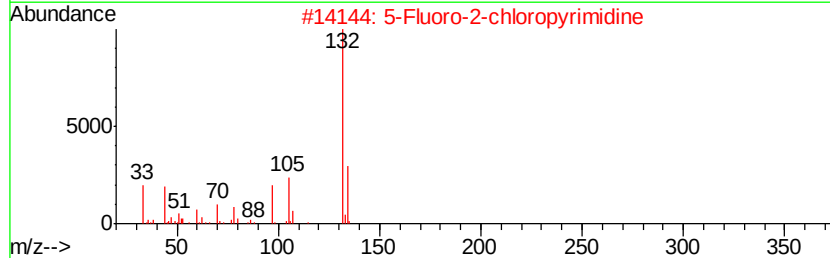
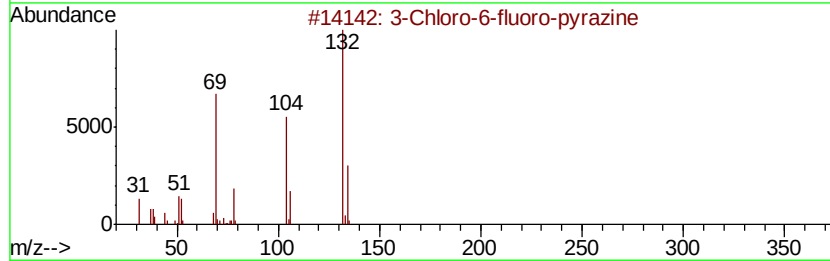
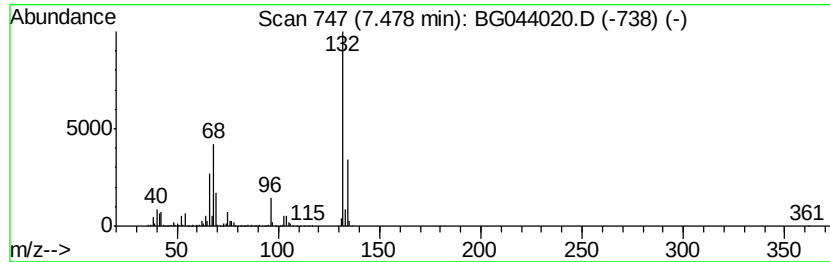
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TIC Library : C:\Database\NIST11.L
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Peak Number 3 unknown7.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.48	106.25 ng	3265210	1,4-Dichlorobenzene-d4	7.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27	
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16	
3	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	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	



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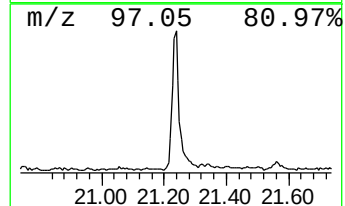
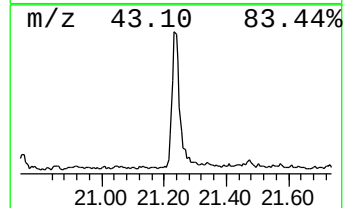
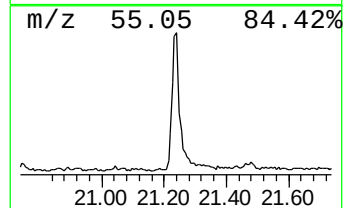
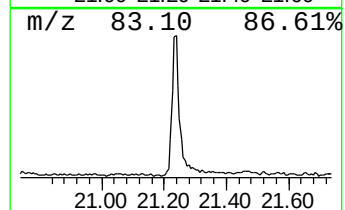
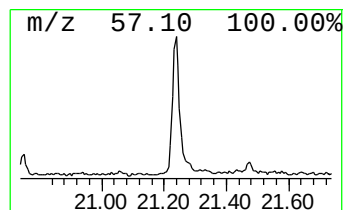
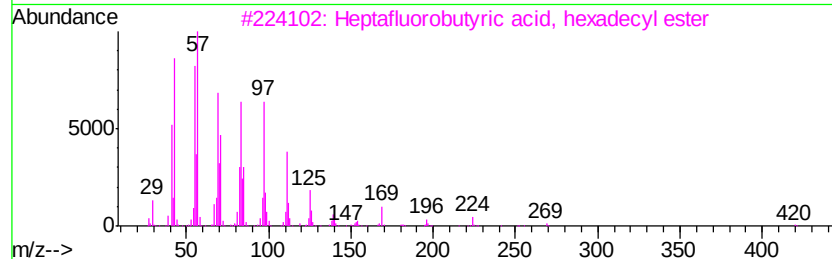
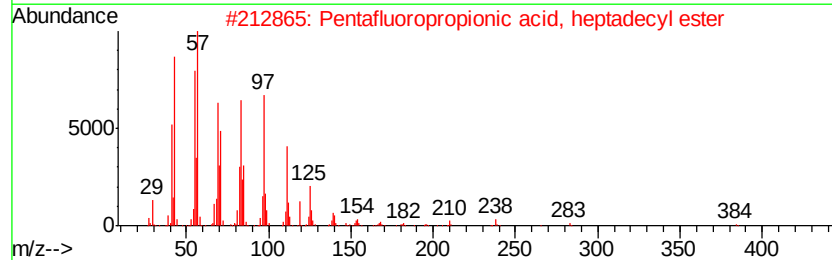
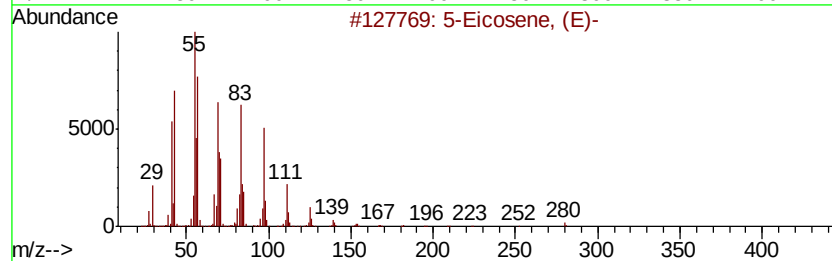
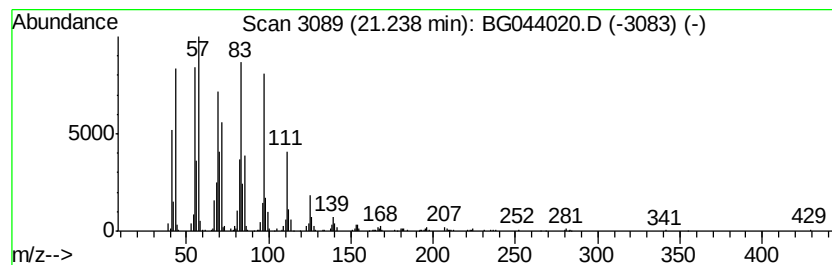
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Peak Number 5 5-Eicosene, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
21.24	6.04 ng	514359	Chrysene-d12		21.57	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-		280	C20H40	074685-30-6	97
2	Pentafluoropropionic acid, hepta...		402	C20H35F5O2	959218-78-1	94
3	Heptafluorobutyric acid, hexadec...		438	C20H33F7O2	006385-15-5	94
4	Nonadecyl pentafluoropropionate		430	C22H39F5O2	1000351-88-8	94
5	Heptadecyl heptafluorobutyrate		452	C21H35F7O2	959085-66-6	94



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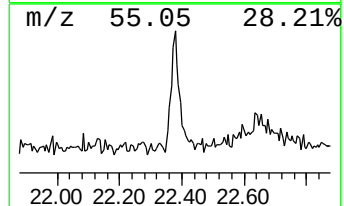
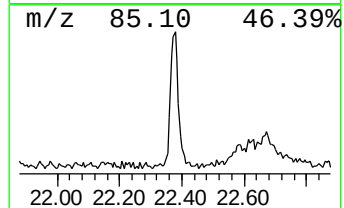
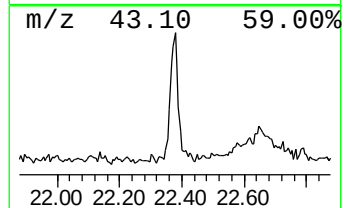
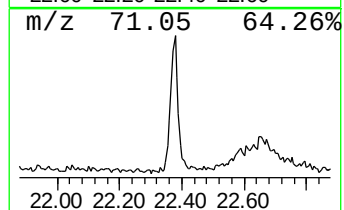
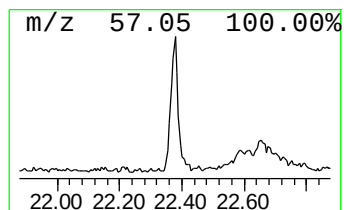
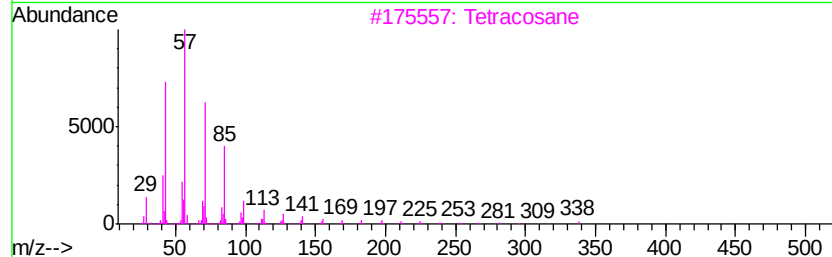
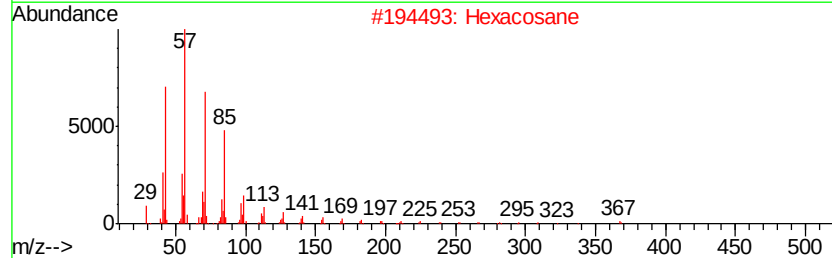
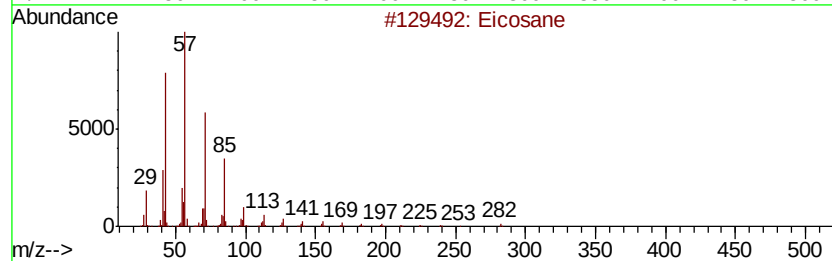
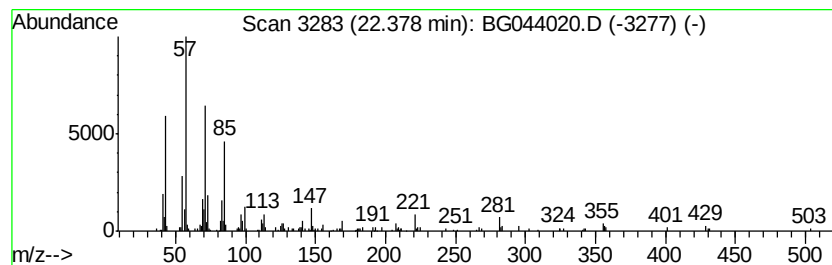
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TIC Library : C:\Database\NIST11.L
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Peak Number 6 Eicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.38	2.42 ng	206423	Chrysene-d12	21.57

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	86
2		Hexacosane	366	C26H54	000630-01-3	70
3		Tetracosane	338	C24H50	000646-31-1	70
4		Tricosane	324	C23H48	000638-67-5	70
5		Docosane	310	C22H46	000629-97-0	62



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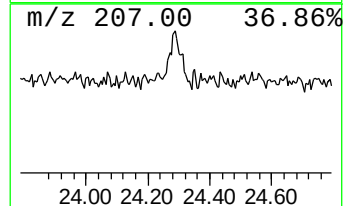
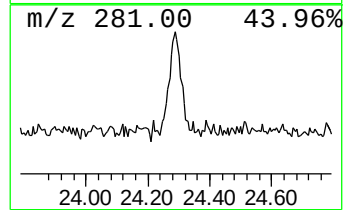
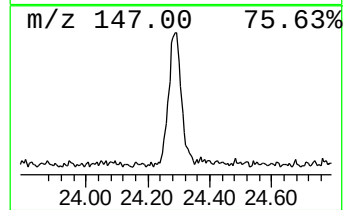
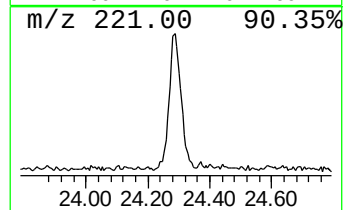
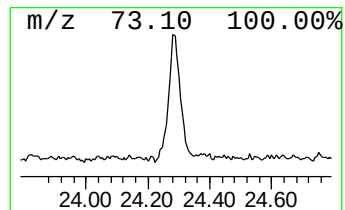
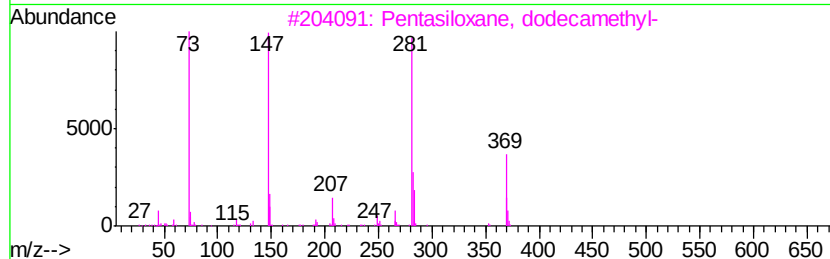
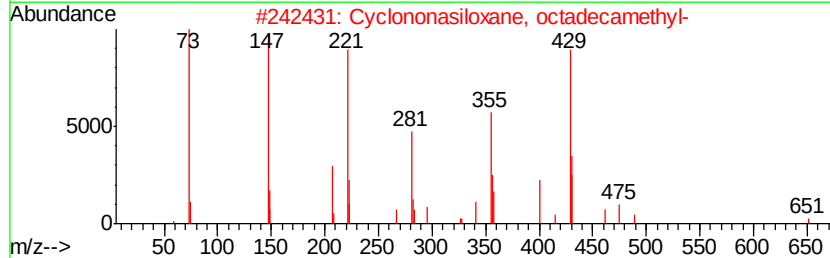
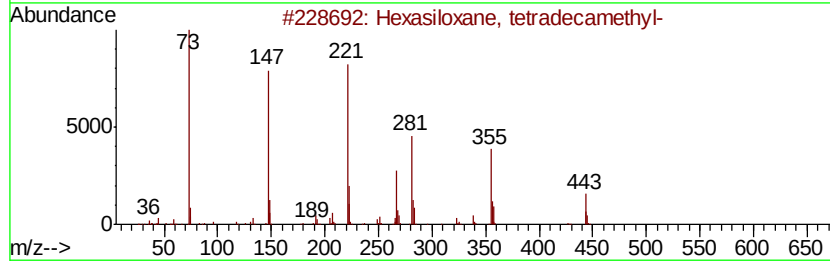
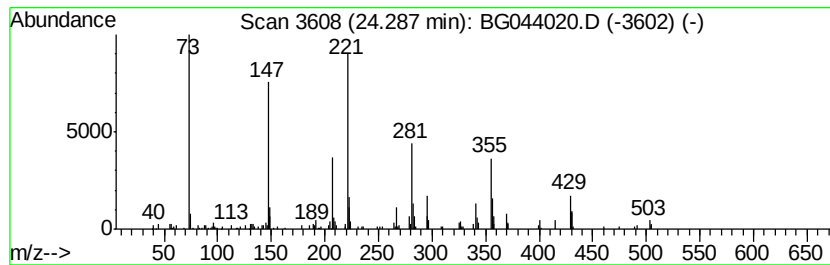
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ClientSampleId :
PB126031BL

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 7 Hexasiloxane, tetradecamethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.
24.29	2.68 ng	233028	Perylene-d12		24.68
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	56
2	Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	53
3	Pentasiloxane, dodecamethyl-	384	C12H36O4Si5	000141-63-9	41
4	Mercaptoacetic acid, bis(trimeth...	236	C8H20O2SSi2	006398-62-5	38
5	3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	35



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011320\
Data File : BG044020.D
Acq On : 13 Jan 2020 20:19
Operator : JU
Sample : PB126031BL
Misc :
ALS Vial : 7 Sample Multiplier: 1

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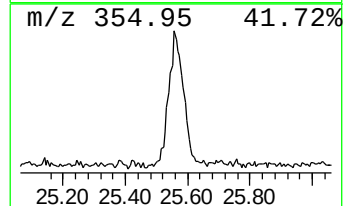
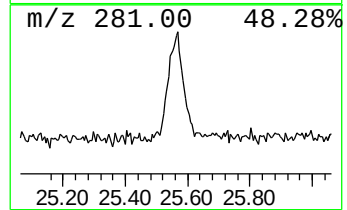
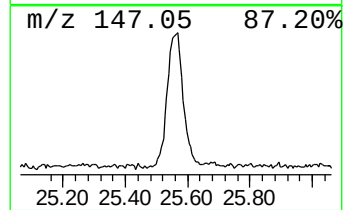
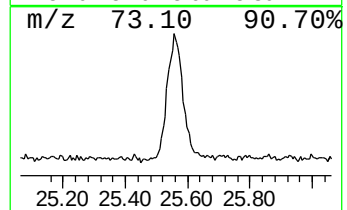
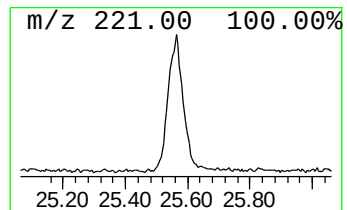
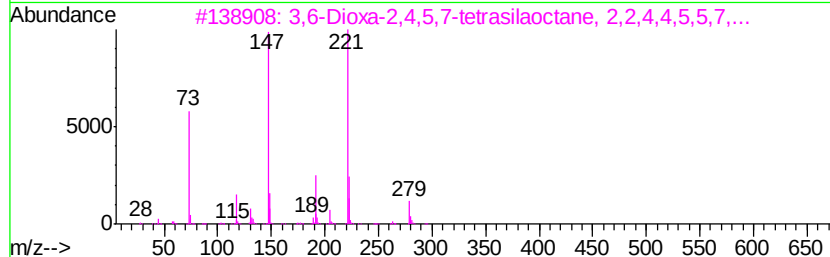
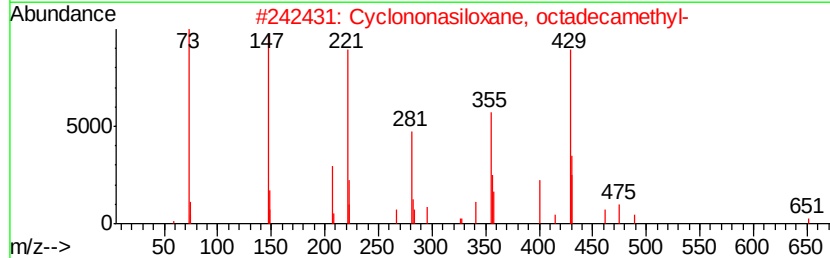
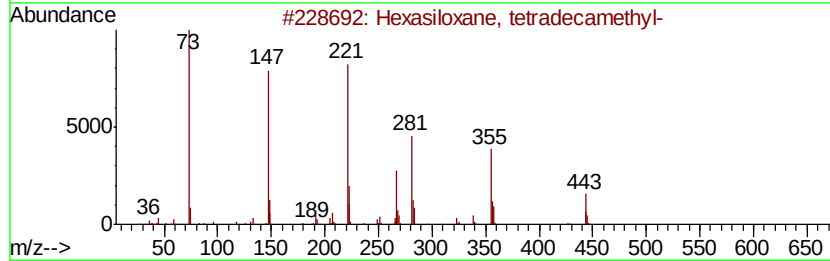
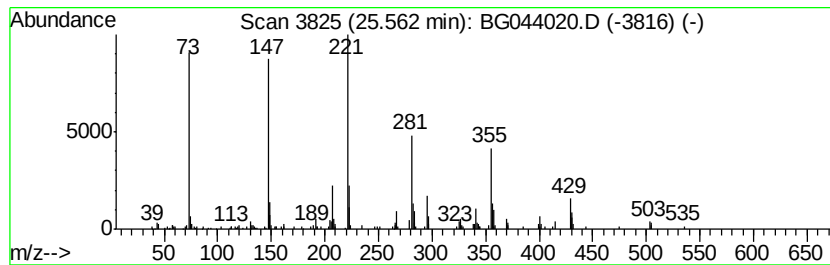
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Cyclononasiloxane, octadeca... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.56	4.16 ng	360858	Perylene-d12	24.68

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	90
2			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	58
3			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	40
4			2-Amino-2-oxo-acetic acid, N-[3,...	221	C12H15NO3	024451-17-0	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\BG011320\
Data File : BG044020.D
Acq On : 13 Jan 2020 20:19
Operator : JU
Sample : PB126031BL
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB126031BL

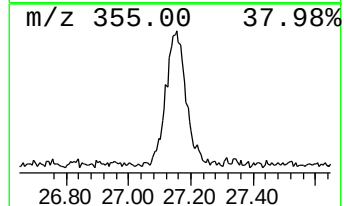
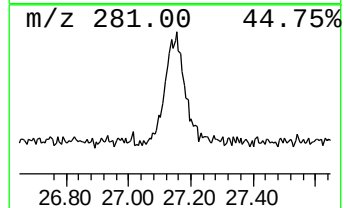
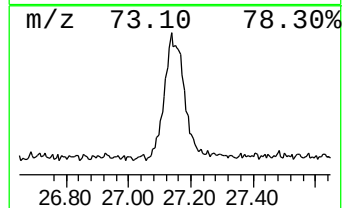
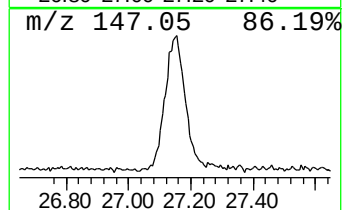
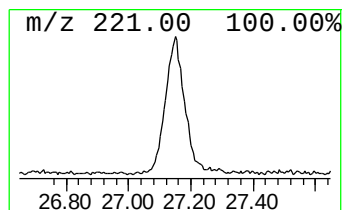
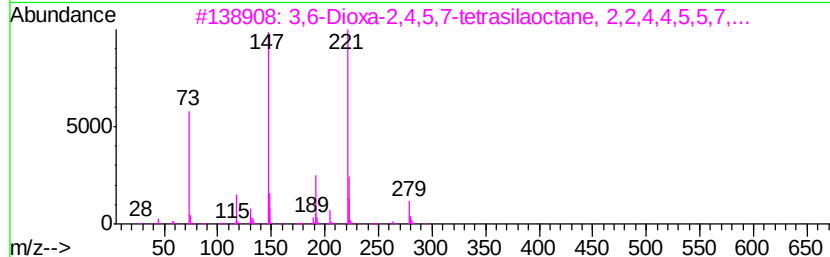
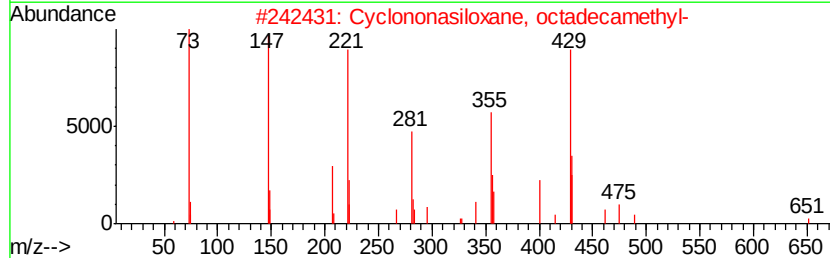
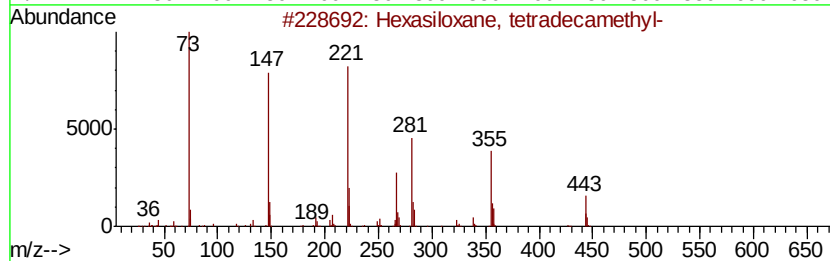
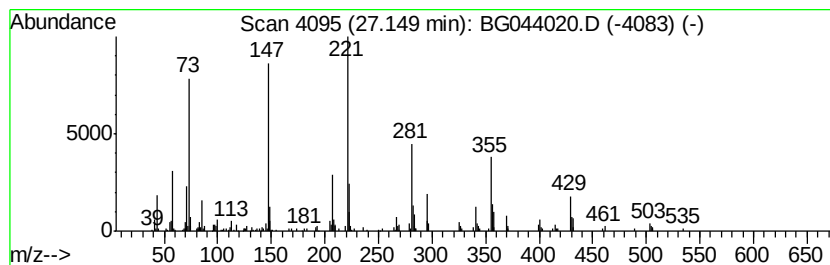
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown27.15 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.15	6.59 ng	572459	Perylene-d12	24.68

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	78
2		Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	52
3		3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	40
4		N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	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 : BG044020.D
Acq On : 13 Jan 2020 20:19
Operator : JU
Sample : PB126031BL
Misc :
ALS Vial : 7 Sample Multiplier: 1

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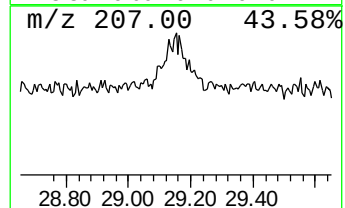
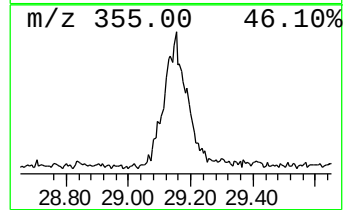
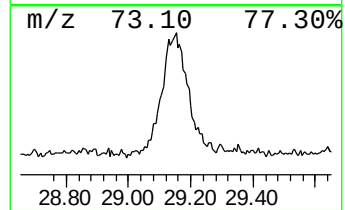
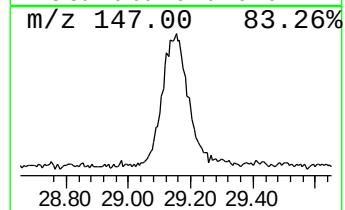
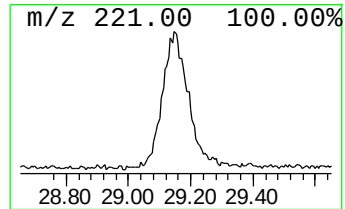
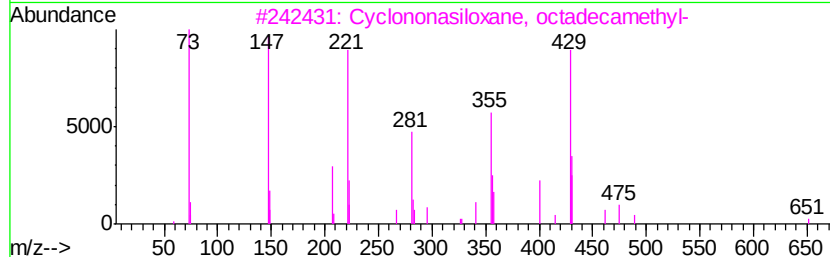
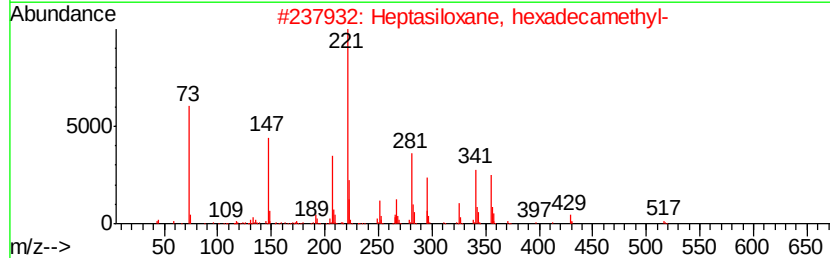
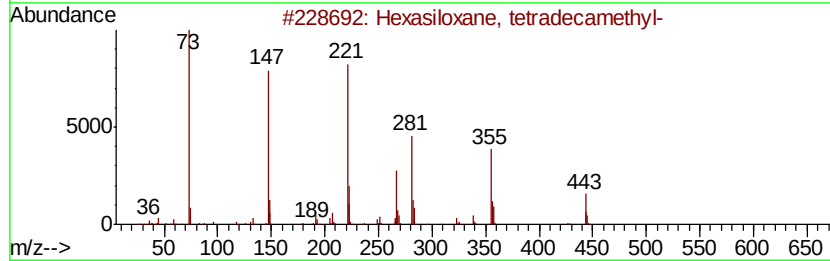
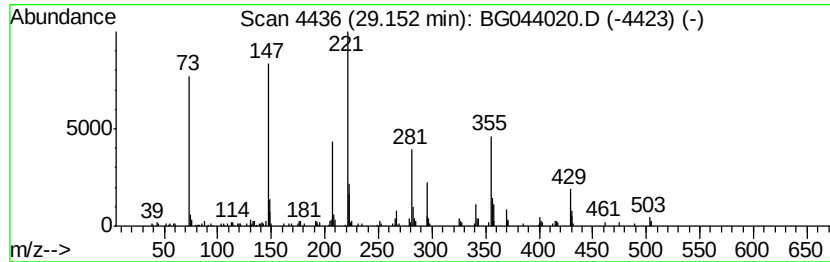
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heptasiloxane, hexadecamethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
29.15	5.64 ng	489395	Perylene-d12	24.68

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	59
2			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	50
3			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	47
4			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	32
5			Pentasiloxane, dodecamethyl-	384	C12H36O4Si5	000141-63-9	30



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG011320\
Data File : BG044020.D
Acq On : 13 Jan 2020 20:19
Operator : JU
Sample : PB126031BL
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB126031BL

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
Butane, 2-methoxy...	3.13	15.1	ng	464861	1	7.95	614652	20.0
2-Pentanone, 4-hy...	5.05	20.6	ng	633691	1	7.95	614652	20.0
unknown7.48	7.48	106.3	ng	3265210	1	7.95	614652	20.0
5-Eicosene, (E)-	21.24	6.0	ng	514359	5	21.57	1704450	20.0
Eicosane	22.38	2.4	ng	206423	5	21.57	1704450	20.0
Hexasiloxane, tet...	24.29	2.7	ng	233028	6	24.68	1736870	20.0
Cyclononasiloxane...	25.56	4.2	ng	360858	6	24.68	1736870	20.0
unknown27.15	27.15	6.6	ng	572459	6	24.68	1736870	20.0
Heptasiloxane, he...	29.15	5.6	ng	489395	6	24.68	1736870	20.0