

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011620\
 Data File : BG044064.D
 Acq On : 16 Jan 2020 11:50
 Operator : JU
 Sample : PB126101BL
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 PB126101BL

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	5.042	326	332	344	rBV	293152	456152	7.11%	0.850%
2	5.518	405	413	425	rBV	1344888	2179955	33.99%	4.060%
3	7.110	675	684	701	rBV	1468170	2543216	39.65%	4.737%
4	7.474	737	746	761	rBV	1398249	2454860	38.27%	4.572%
5	7.938	818	825	833	rBV	288122	492519	7.68%	0.917%
6	8.262	872	880	894	rVB	1045769	1841985	28.72%	3.431%
7	9.096	1012	1022	1043	rBV	805377	1482494	23.11%	2.761%
8	10.741	1294	1302	1317	rBV	377813	712182	11.10%	1.326%
9	13.197	1713	1720	1732	rBV	2308002	3683381	57.43%	6.861%
10	14.025	1855	1861	1866	rBV	42366	69267	1.08%	0.129%
11	14.572	1947	1954	1961	rBV	654213	1038813	16.20%	1.935%
12	16.058	2200	2207	2224	rBV	1888760	3143202	49.01%	5.854%
13	17.316	2415	2421	2432	rBV	852459	1304531	20.34%	2.430%
14	19.930	2859	2866	2876	rBV	4522888	6413863	100.00%	11.946%
15	21.240	3084	3089	3098	rBV	183428	378382	5.90%	0.705%
16	21.470	3123	3128	3133	rBV	123919	171317	2.67%	0.319%
17	21.564	3136	3144	3150	rBV	902644	1596111	24.89%	2.973%
18	21.775	3176	3180	3185	rVB	75730	101830	1.59%	0.190%
19	22.374	3276	3282	3292	rBV2	332806	622750	9.71%	1.160%
20	22.645	3322	3328	3336	rBV	82644	148949	2.32%	0.277%
21	23.009	3383	3390	3394	rBV	272913	589669	9.19%	1.098%
22	23.238	3421	3429	3440	rVB2	535243	1197034	18.66%	2.230%
23	23.749	3512	3516	3522	rVV2	35693	72388	1.13%	0.135%
24	23.826	3523	3529	3534	rVV2	146703	303709	4.74%	0.566%
25	23.890	3534	3540	3552	rVB2	114267	309099	4.82%	0.576%
26	24.266	3594	3604	3616	rBV	846911	2313646	36.07%	4.309%
27	24.519	3643	3647	3657	rVB2	26560	66088	1.03%	0.123%
28	24.678	3664	3674	3681	rBV	548488	1524492	23.77%	2.839%
29	24.742	3681	3685	3696	rVB2	151093	362487	5.65%	0.675%
30	25.541	3808	3821	3840	rBV2	1052686	3743063	58.36%	6.972%
31	25.835	3863	3871	3882	rBV	132267	390259	6.08%	0.727%
32	27.122	4074	4090	4119	rBV2	1099248	5058014	78.86%	9.421%
33	29.102	4408	4427	4450	rBV2	849671	4861667	75.80%	9.055%
34	31.622	4836	4856	4858	rBV3	484672	2062101	32.15%	3.841%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011620\
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Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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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_G\METHODS\8270-BG123019.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

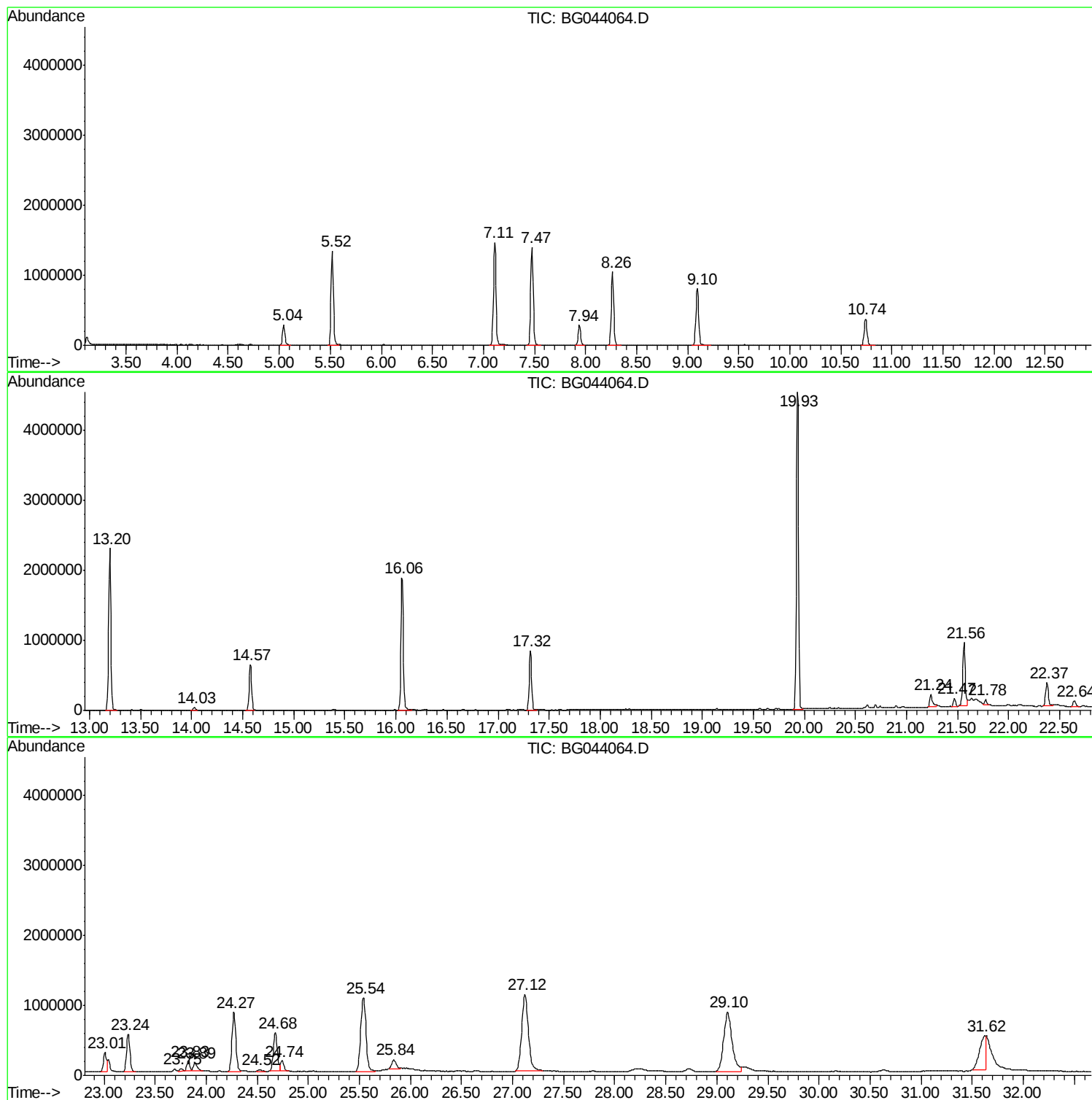
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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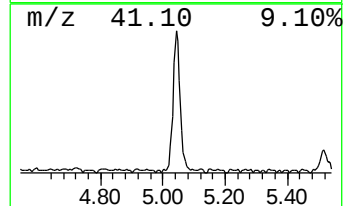
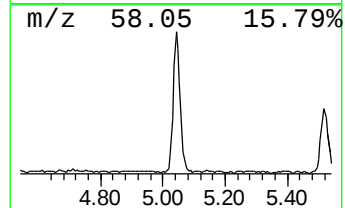
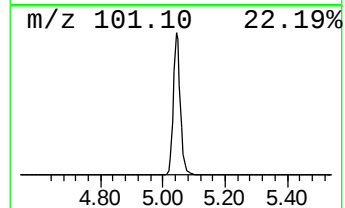
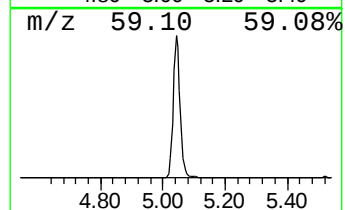
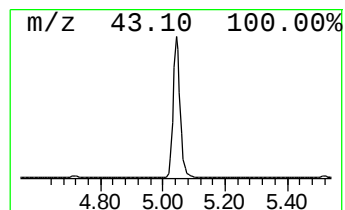
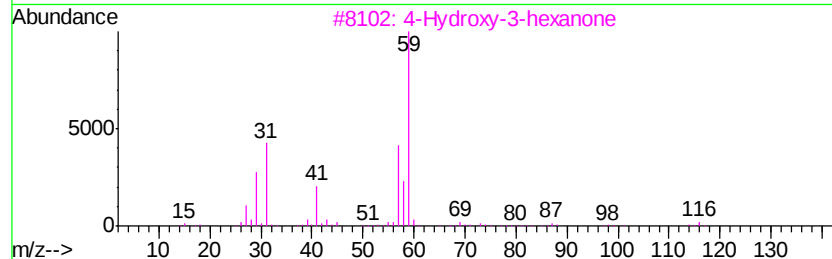
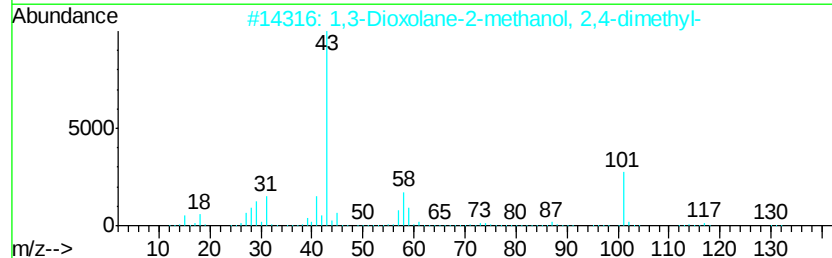
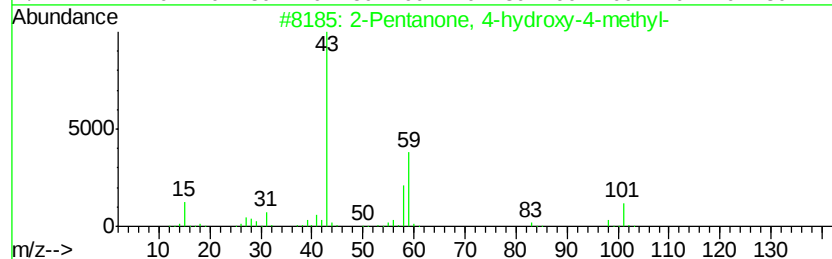
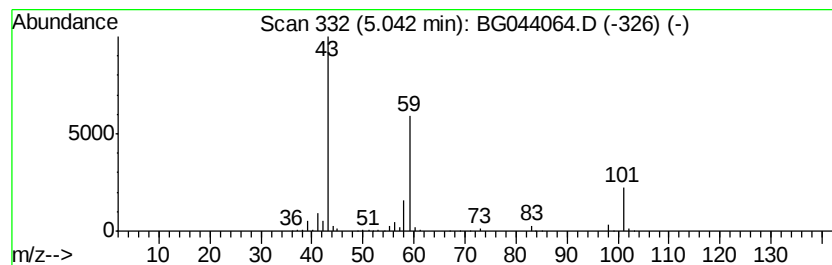
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.04	18.52 ng	456152	1,4-Dichlorobenzene-d4	7.94

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	25
3		4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	17
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5		Acetone	58	C3H6O	000067-64-1	10



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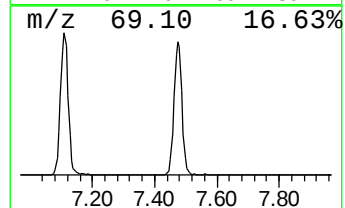
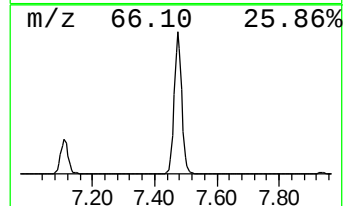
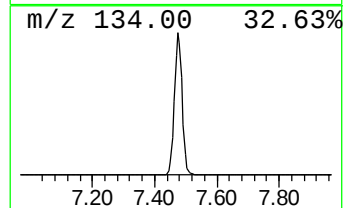
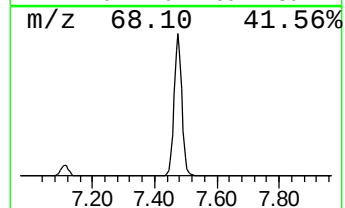
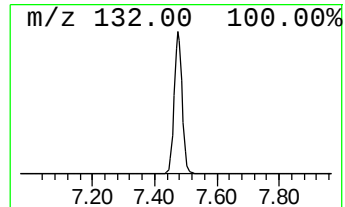
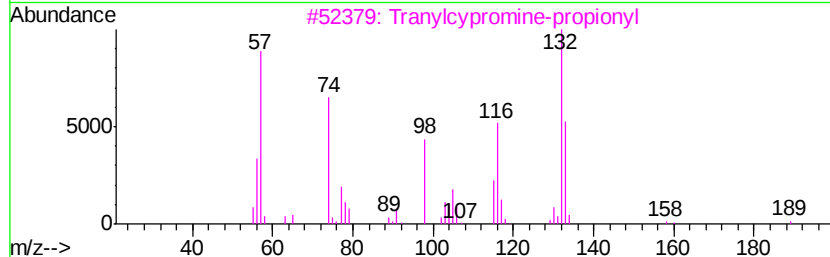
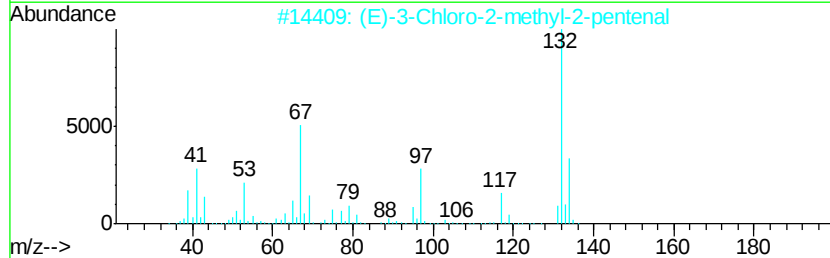
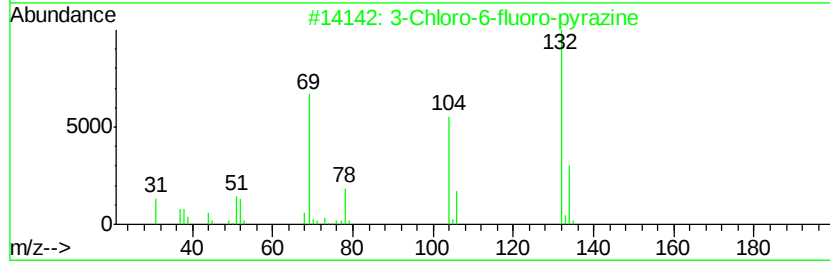
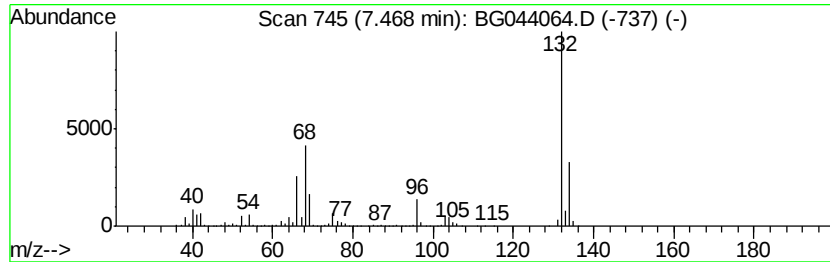
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown7.47 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.47	99.69 ng	2454860	1,4-Dichlorobenzene-d4	7.94

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		Tranvlcvpromine-propionyl	189	C12H15NO	1000123-86-3	12
4		Xenon	132	Xe	007440-63-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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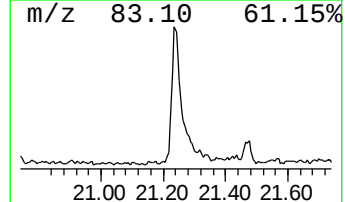
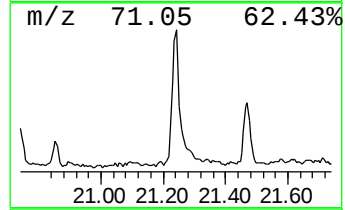
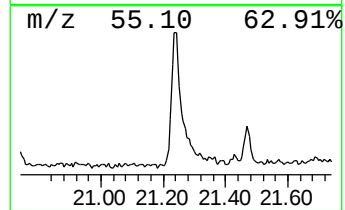
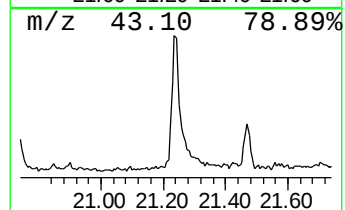
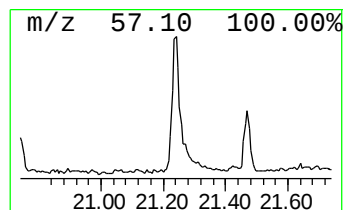
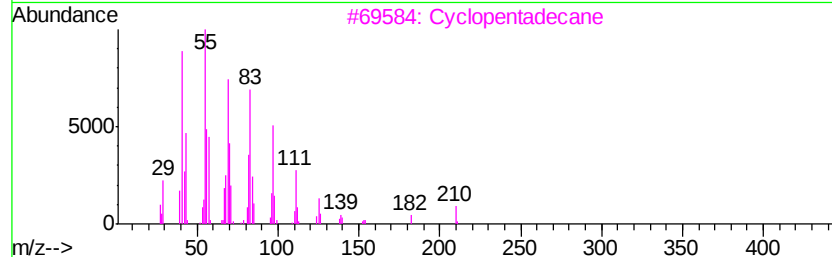
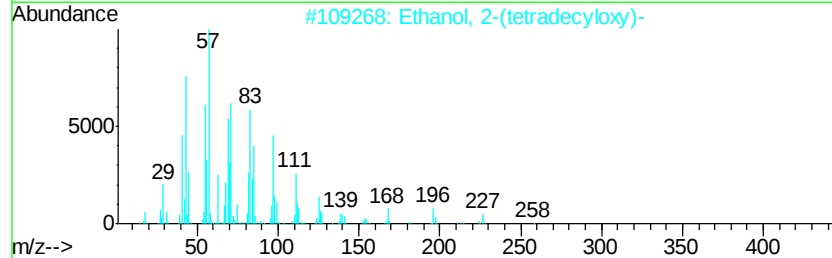
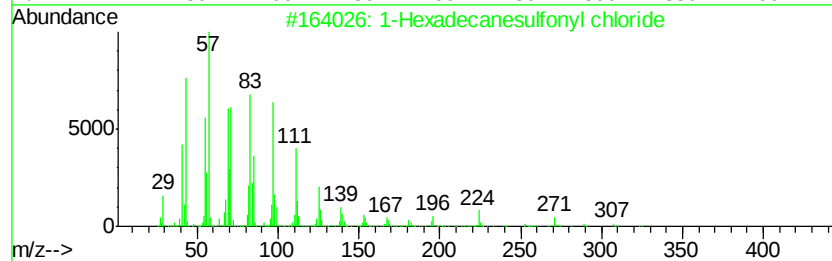
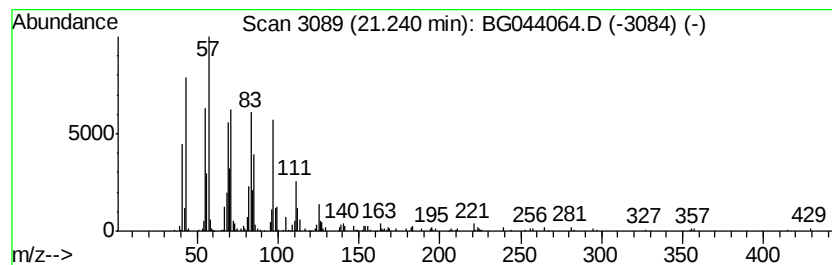
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Hexadecanesulfonyl chloride Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.24	4.74 ng	378382	Chrysene-d12	21.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	91
2		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
3		Cyclopentadecane	210	C15H30	000295-48-7	90
4		Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	87
5		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	87



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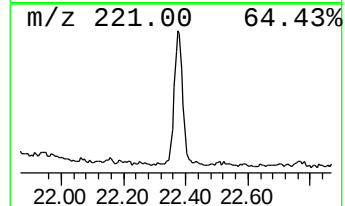
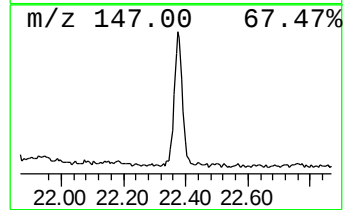
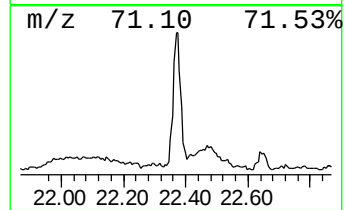
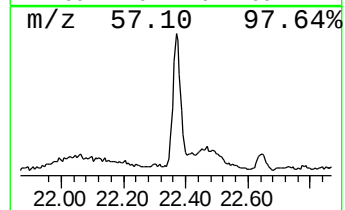
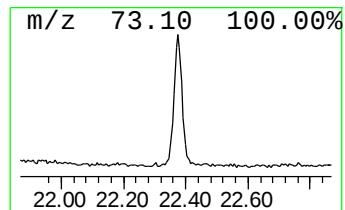
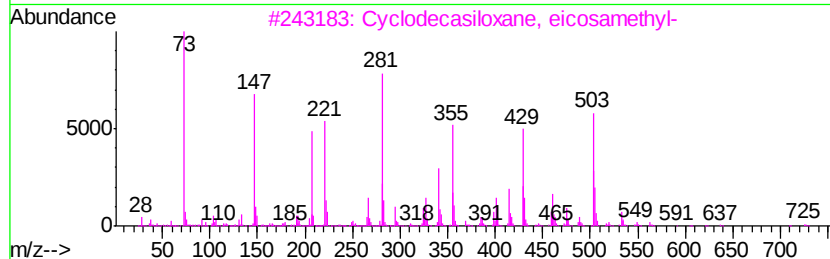
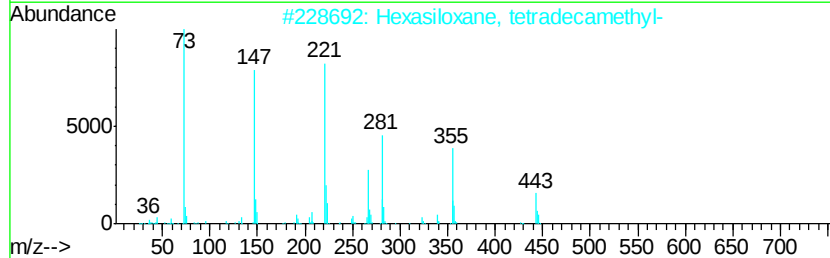
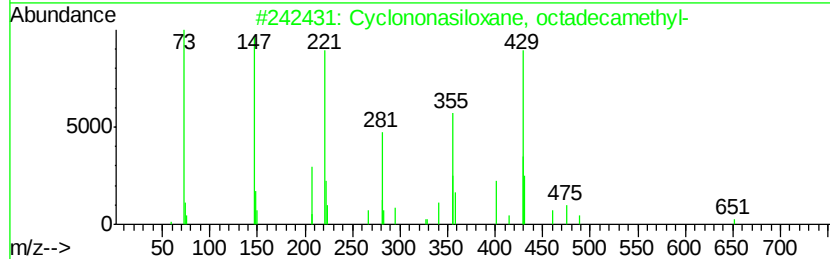
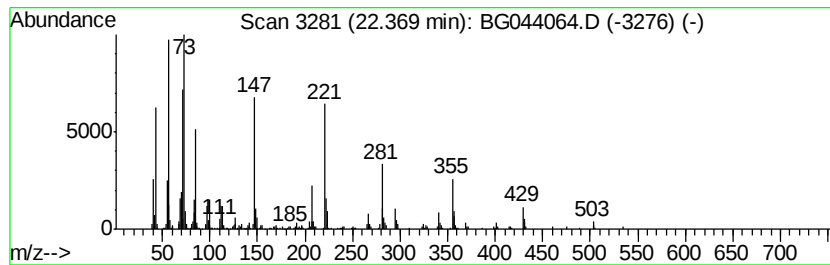
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Cyclononasiloxane, octadeca... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.37	7.80 ng	622750	Chrysene-d12	21.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclononasiloxane, octadecamethyl-	666	C18H5409Si9	000556-71-8	52
2		Hexasiloxane, tetradecamethyl-	458	C14H4205Si6	000107-52-8	50
3		Cyclodecasiloxane, eicosamethyl-	740	C20H60010Si10	018772-36-6	43
4		Heptasiloxane, hexadecamethyl-	532	C16H4806Si7	000541-01-5	27
5		Silane, [[(3.beta.,11.beta.,20S)...]	638	C33H6604Si4	032221-72-0	11



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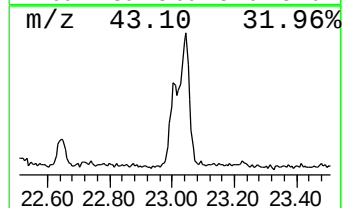
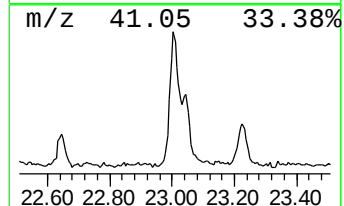
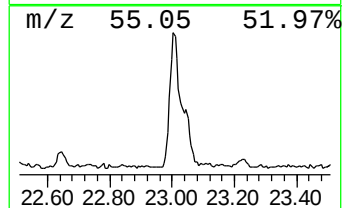
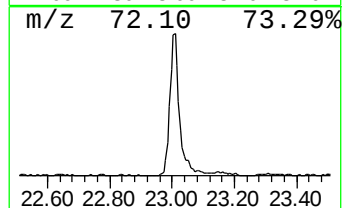
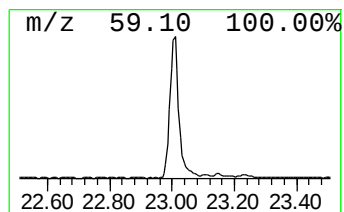
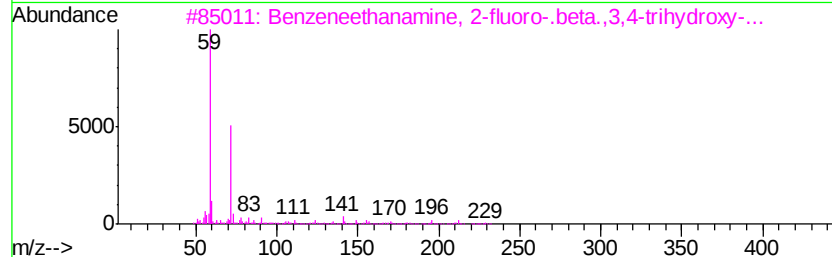
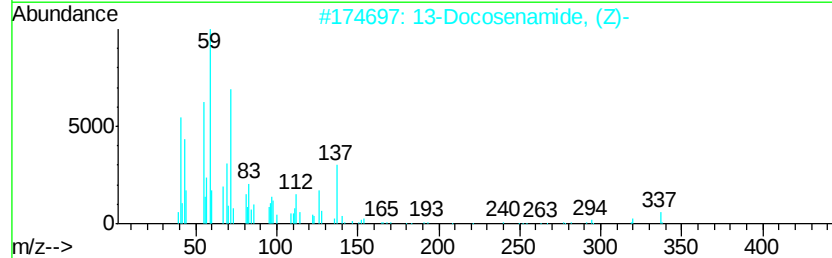
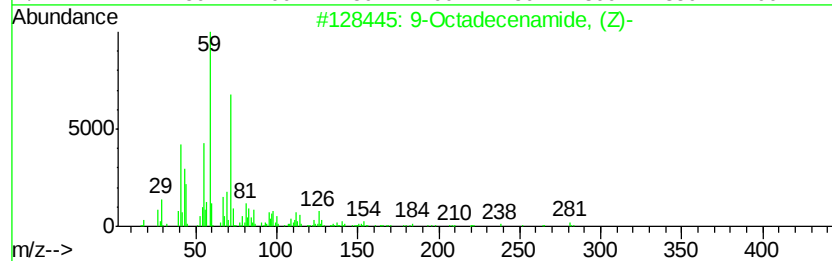
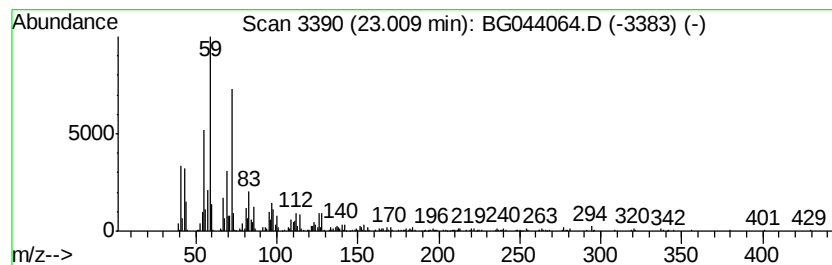
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Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.01	7.39 ng	589669	Chrysene-d12	21.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	93
2		13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	87
3		Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	50
4		Tetradecanamide	227	C14H29NO	000638-58-4	50
5		Octadecanamide	283	C18H37NO	000124-26-5	47



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011620\
Data File : BG044064.D
Acq On : 16 Jan 2020 11:50
Operator : JU
Sample : PB126101BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB126101BL

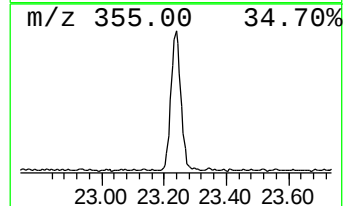
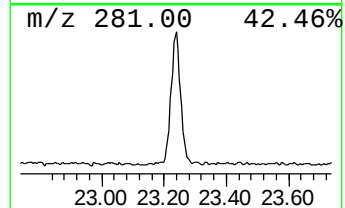
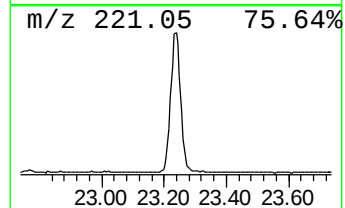
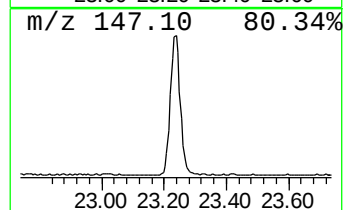
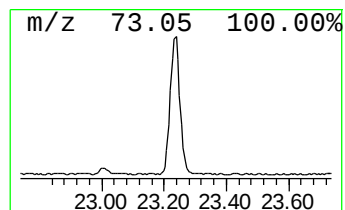
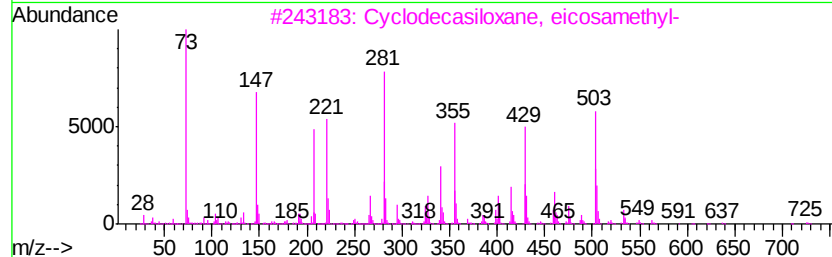
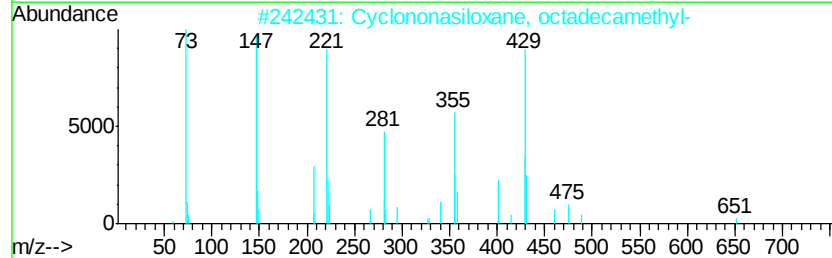
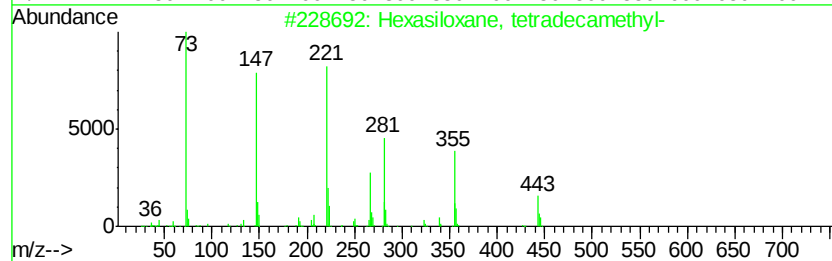
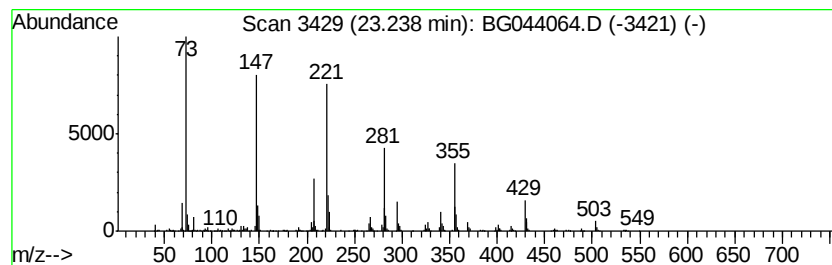
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexasiloxane, tetradecamethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.24	15.70 ng	1197030	Perylene-d12	24.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	83
2		Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	80
3		Cyclodecasiloxane, eicosamethyl-	740	C20H60O10Si10	018772-36-6	43
4		N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	38
5		Pentasiloxane, dodecamethyl-	384	C12H36O4Si5	000141-63-9	35



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011620\
Data File : BG044064.D
Acq On : 16 Jan 2020 11:50
Operator : JU
Sample : PB126101BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

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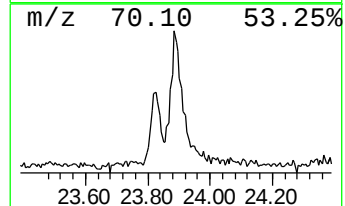
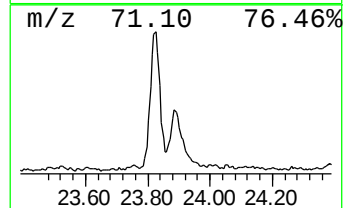
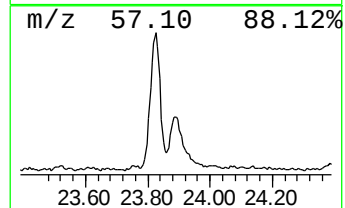
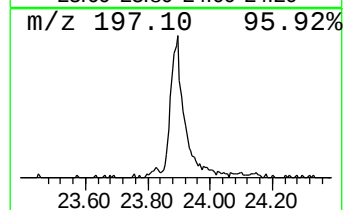
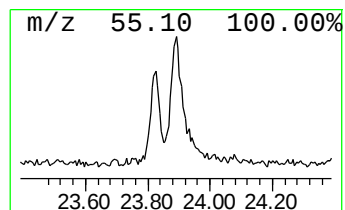
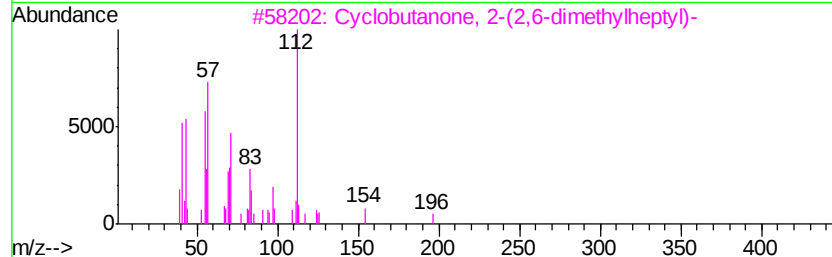
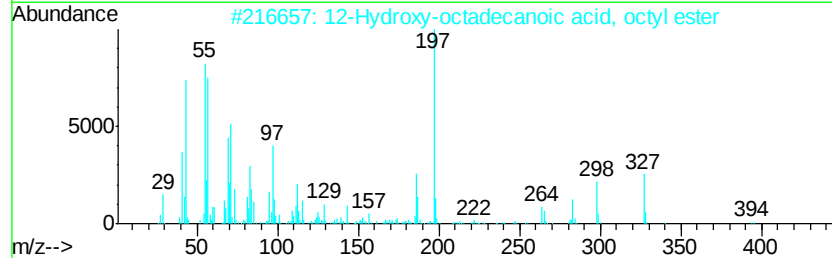
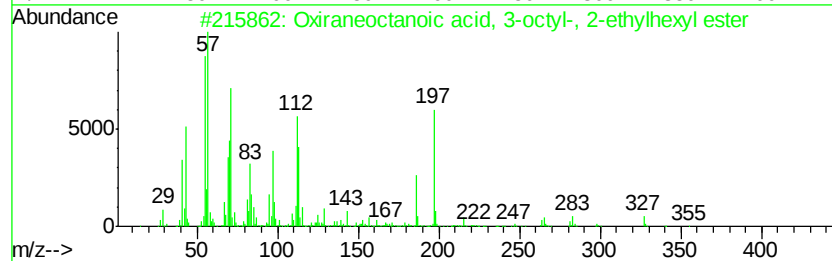
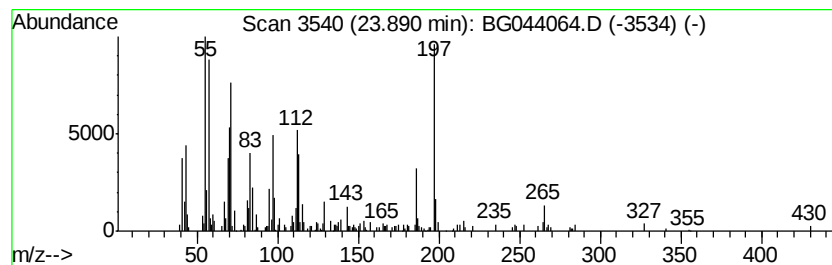
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 12-Hydroxy-octadecanoic aci... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.89	4.06 ng	309099	Perylene-d12	24.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Oxiraneoctanoic acid, 3-octyl-, ...	410	C26H50O3	000141-38-8	81
2		12-Hydroxy-octadecanoic acid, oc...	412	C26H52O3	074819-90-2	53
3		Cyclobutanone, 2-(2,6-dimethylhe...	196	C13H24O	065147-64-0	35
4		2-Ethyl-1-dodecanol	214	C14H30O	019780-33-7	27
5		3-Cyclopentylpropionamide, N-met...	195	C12H21NO	1000340-38-1	22



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011620\
Data File : BG044064.D
Acq On : 16 Jan 2020 11:50
Operator : JU
Sample : PB126101BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

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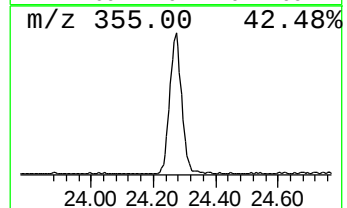
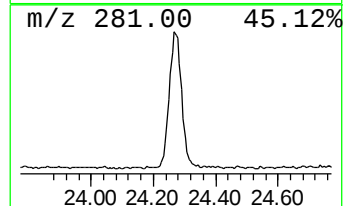
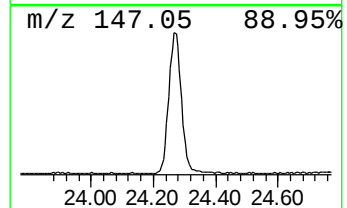
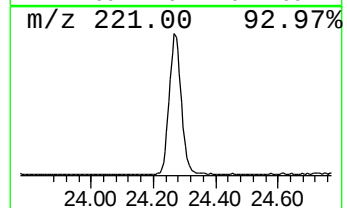
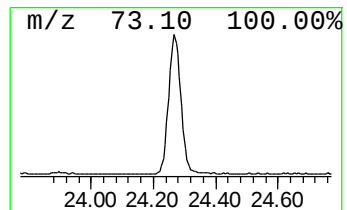
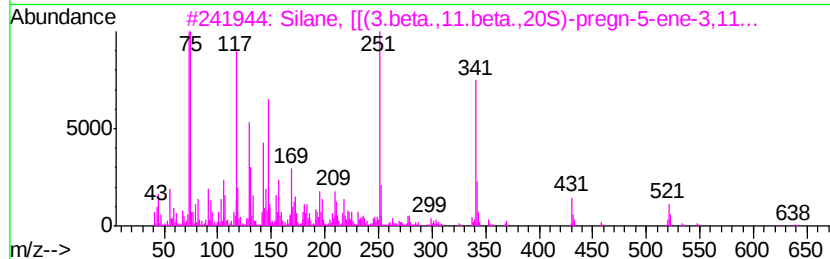
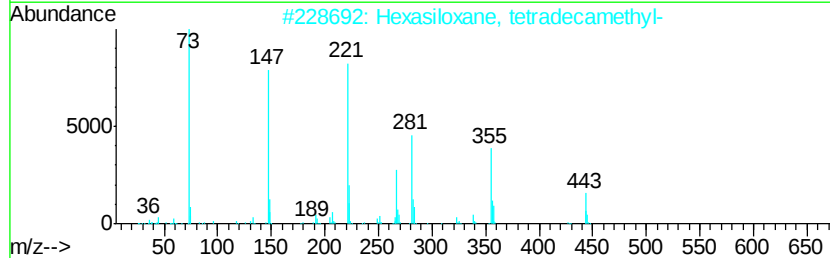
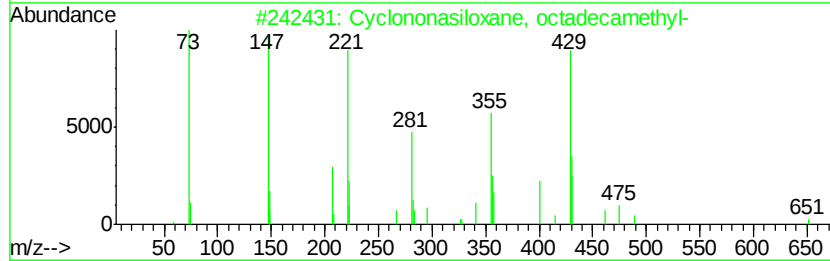
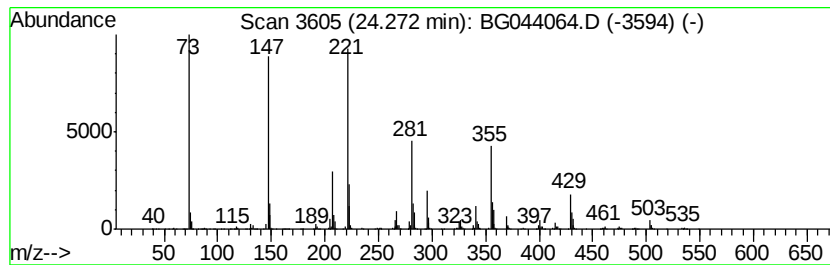
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Silane, [(3.beta.,11.beta.... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.27	30.35 ng	2313650	Perylene-d12	24.68

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	91
2			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	87
3			Silane, [(3.beta.,11.beta.,20S)...]	638	C33H66O4Si4	032221-72-0	62
4			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	40
5			Mercaptoacetic acid, bis(trimeth...	236	C8H20O2SSi2	006398-62-5	40



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011620\
Data File : BG044064.D
Acq On : 16 Jan 2020 11:50
Operator : JU
Sample : PB126101BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

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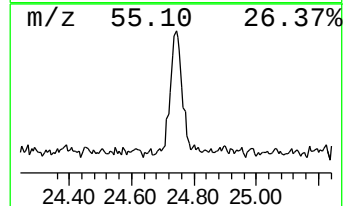
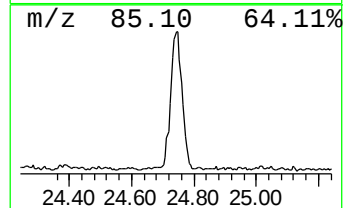
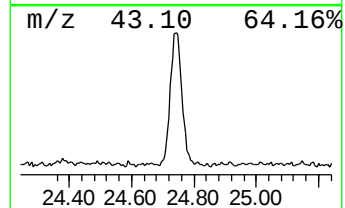
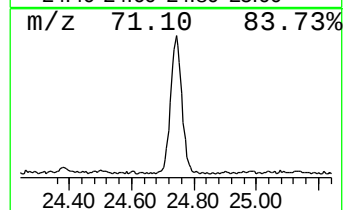
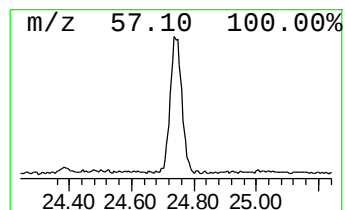
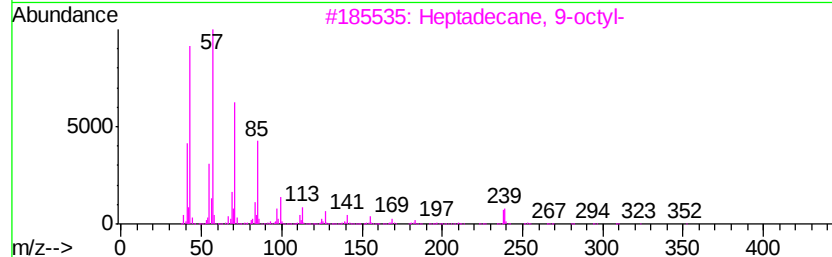
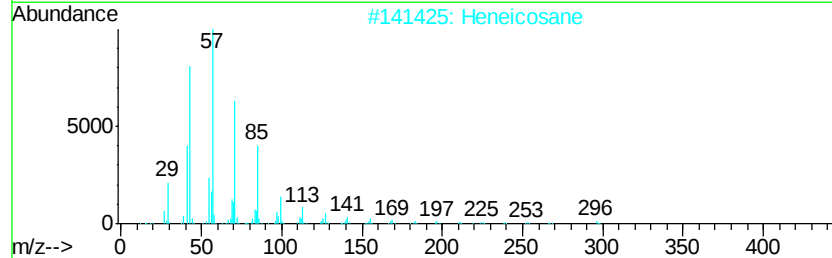
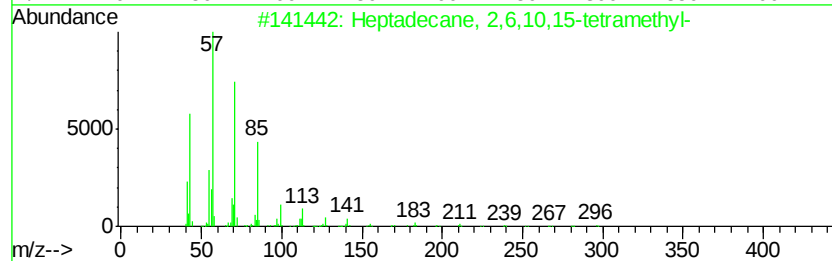
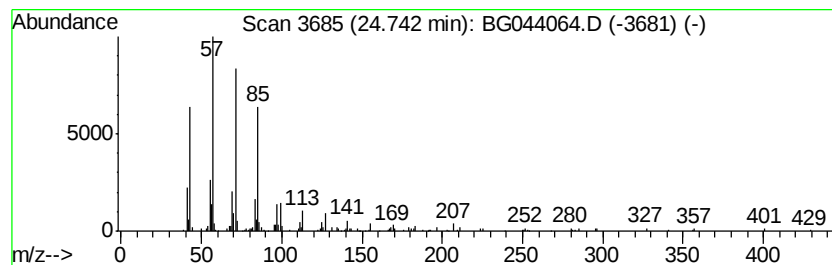
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Heptadecane, 2,6,10,15-tetr... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.74	4.76 ng	362487	Perylene-d12	24.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	93
2		Heneicosane	296	C21H44	000629-94-7	92
3		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4		Heptadecane, 9-hexyl-	324	C23H48	055124-79-3	90
5		2-Bromotetradecane	276	C14H29Br	074036-95-6	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011620\
Data File : BG044064.D
Acq On : 16 Jan 2020 11:50
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Sample : PB126101BL
Misc :
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Instrument :
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ClientSampleId :
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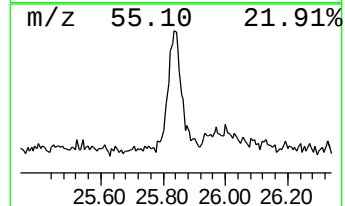
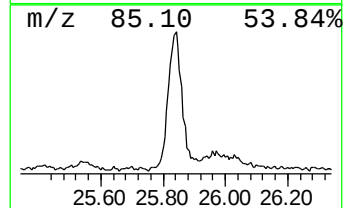
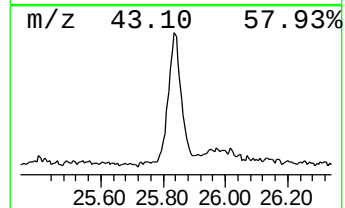
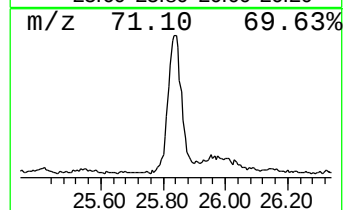
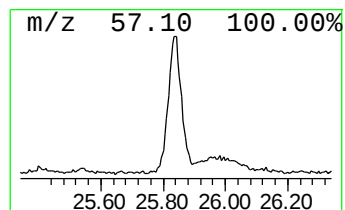
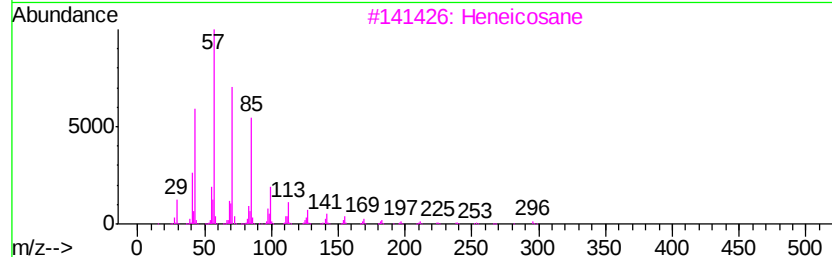
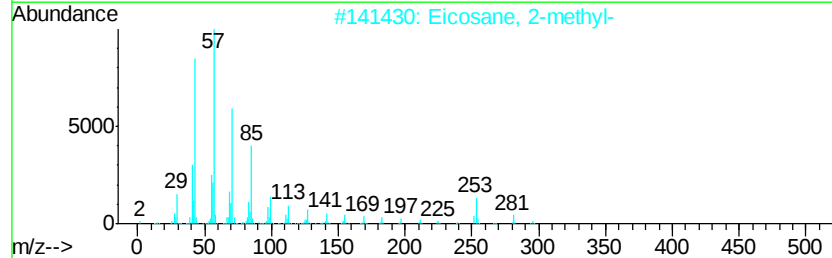
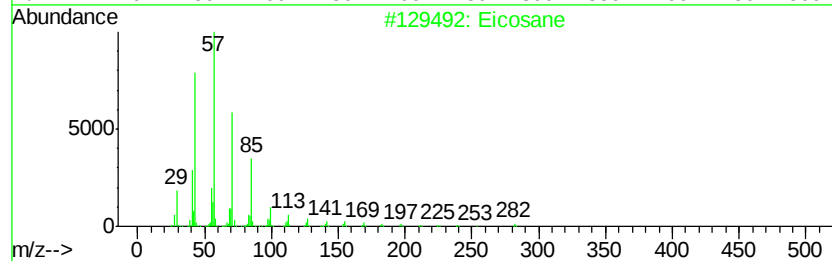
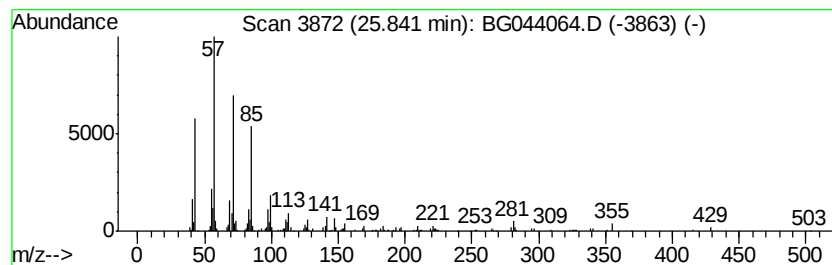
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Eicosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.84	5.12 ng	390259	Perylene-d12	24.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	86
2		Eicosane, 2-methyl-	296	C21H44	001560-84-5	83
3		Heneicosane	296	C21H44	000629-94-7	81
4		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	81
5		Tetracosane	338	C24H50	000646-31-1	76



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG011620\
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 Acq On : 16 Jan 2020 11:50
 Operator : JU
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 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
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 ClientSampleId :
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 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
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unknown7.47	7.47	99.7	ng	2454860	1	7.94	492519	20.0
1-Hexadecanesulfo...	21.24	4.7	ng	378382	5	21.56	1596110	20.0
Cyclononasiloxane...	22.37	7.8	ng	622750	5	21.56	1596110	20.0
9-Octadecenamide,...	23.01	7.4	ng	589669	5	21.56	1596110	20.0
Hexasiloxane, tet...	23.24	15.7	ng	1197030	6	24.68	1524490	20.0
12-Hydroxy-octade...	23.89	4.1	ng	309099	6	24.68	1524490	20.0
Silane, [(3.beta...	24.27	30.4	ng	2313650	6	24.68	1524490	20.0
Heptadecane, 2,6,...	24.74	4.8	ng	362487	6	24.68	1524490	20.0
Eicosane	25.84	5.1	ng	390259	6	24.68	1524490	20.0