

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG031820\
 Data File : BG044884.D
 Acq On : 19 Mar 2020 4:25
 Operator : CG/JU
 Sample : L1920-02
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 F-2

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-BG031020.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	3.143	4	9	19	rBV2	108717	249132	4.79%	0.835%
2	3.225	19	23	32	rVB	44964	75441	1.45%	0.253%
3	5.610	422	429	442	rBV	1147932	1928954	37.11%	6.465%
4	7.197	690	699	709	rBV	1161841	2082453	40.06%	6.980%
5	8.043	834	843	850	rBV	252689	436543	8.40%	1.463%
6	8.366	889	898	906	rBV	915614	1633021	31.42%	5.474%
7	9.200	1031	1040	1049	rBV	730890	1355787	26.08%	4.544%
8	10.851	1312	1321	1331	rBV	325458	600724	11.56%	2.014%
9	13.301	1730	1738	1746	rBV	1905973	3040953	58.50%	10.193%
10	13.965	1845	1851	1858	rVB4	45963	72408	1.39%	0.243%
11	14.124	1871	1878	1884	rBV	134752	208452	4.01%	0.699%
12	14.676	1965	1972	1982	rBV2	523842	847169	16.30%	2.840%
13	16.157	2218	2224	2237	rBV	1567704	2531191	48.70%	8.484%
14	17.420	2432	2439	2445	rBV	698770	1095634	21.08%	3.672%
15	18.319	2588	2592	2600	rBV3	58408	95506	1.84%	0.320%
16	19.283	2750	2756	2762	rVB2	135768	180818	3.48%	0.606%
17	20.029	2876	2883	2892	rBV	3721096	5197812	100.00%	17.422%
18	20.511	2959	2965	2971	rBV	621913	859707	16.54%	2.882%
19	20.599	2976	2980	2987	rVV7	36479	68058	1.31%	0.228%
20	20.675	2987	2993	2997	rVV	794438	1075845	20.70%	3.606%
21	20.716	2997	3000	3013	rVB3	460175	885412	17.03%	2.968%
22	21.345	3102	3107	3112	rBV2	286625	464869	8.94%	1.558%
23	21.392	3112	3115	3121	rVV3	172999	269819	5.19%	0.904%
24	21.457	3121	3126	3133	rVV2	326890	546943	10.52%	1.833%
25	21.527	3133	3138	3143	rVV	94096	164924	3.17%	0.553%
26	21.604	3147	3151	3156	rVV4	68302	109573	2.11%	0.367%
27	21.686	3158	3165	3176	rVB	788017	1314955	25.30%	4.407%
28	21.903	3199	3202	3208	rVB3	40394	63974	1.23%	0.214%
29	21.974	3210	3214	3222	rVB9	37143	68166	1.31%	0.228%
30	22.144	3238	3243	3248	rVV8	40497	96069	1.85%	0.322%
31	22.414	3283	3289	3296	rBV4	73302	136348	2.62%	0.457%
32	22.532	3304	3309	3317	rVB3	47345	100539	1.93%	0.337%
33	23.219	3422	3426	3432	rVB4	39799	69735	1.34%	0.234%
34	23.413	3452	3459	3465	rBV	142724	274562	5.28%	0.920%

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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-BG031020.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	24.030	3558	3564	3570	rBV6	45092	100484	1.93%	0.337%
36	24.888	3700	3710	3720	rBV	455146	1316553	25.33%	4.413%
37	24.994	3724	3728	3733	rVB7	35826	69361	1.33%	0.232%
38	26.122	3914	3920	3930	rVB7	31143	78743	1.51%	0.264%
39	26.233	3934	3939	3947	rVV9	26418	68076	1.31%	0.228%

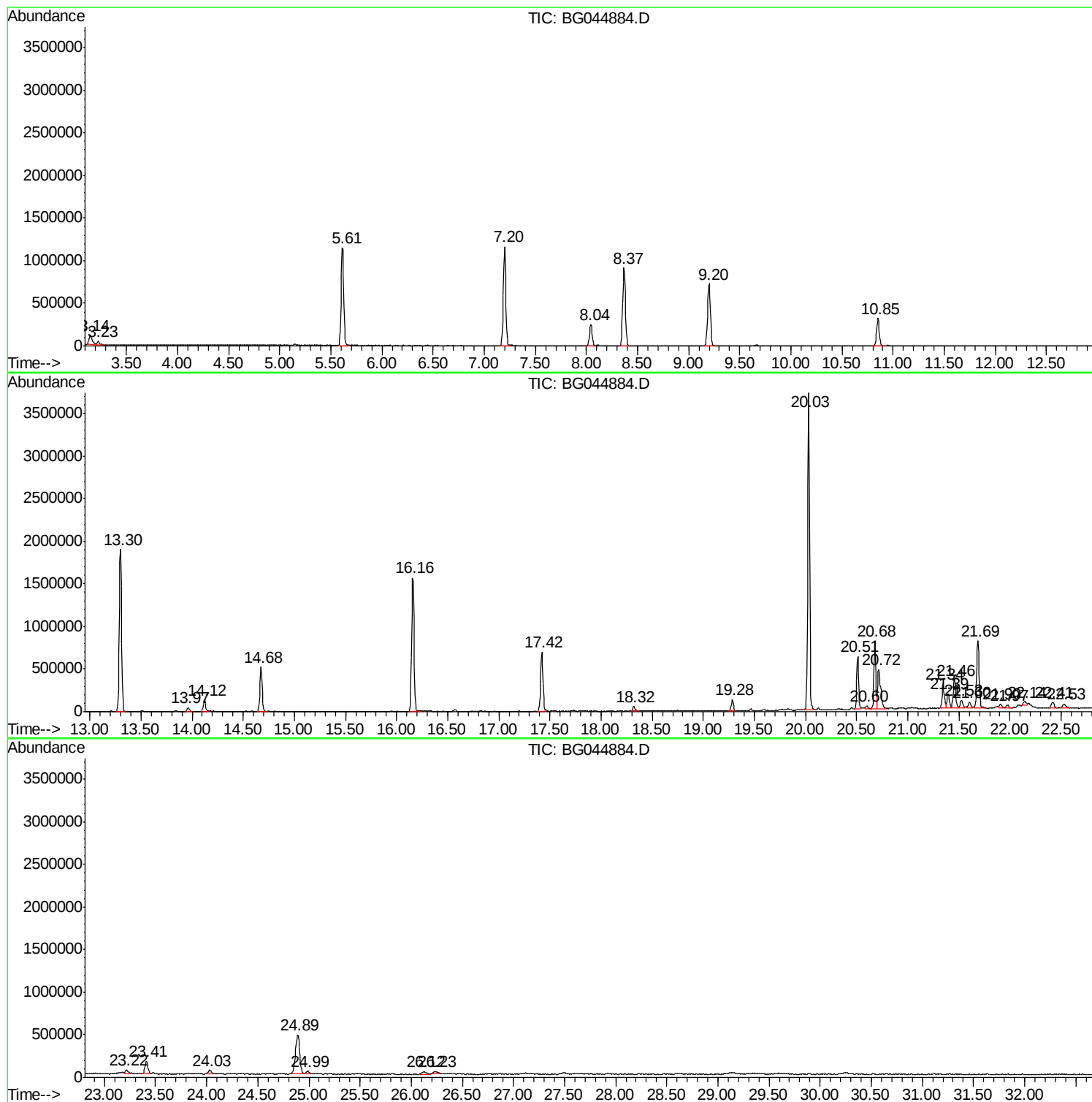
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG031020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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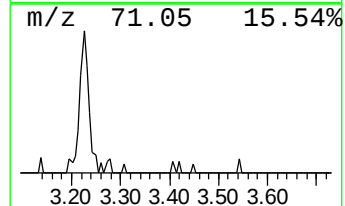
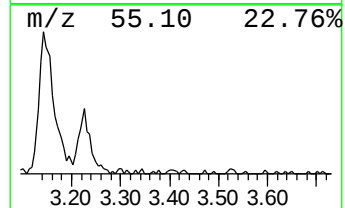
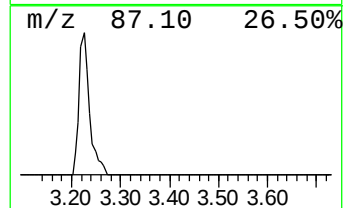
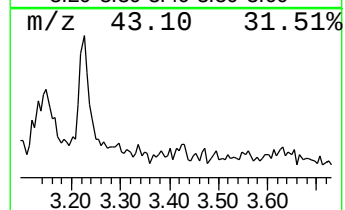
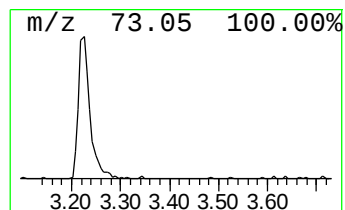
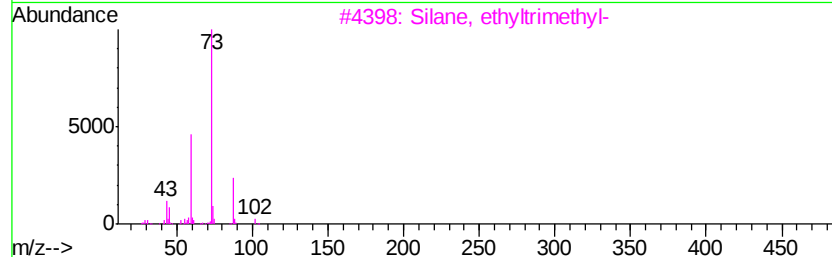
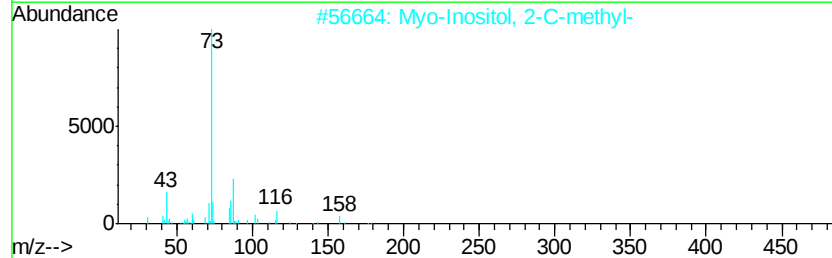
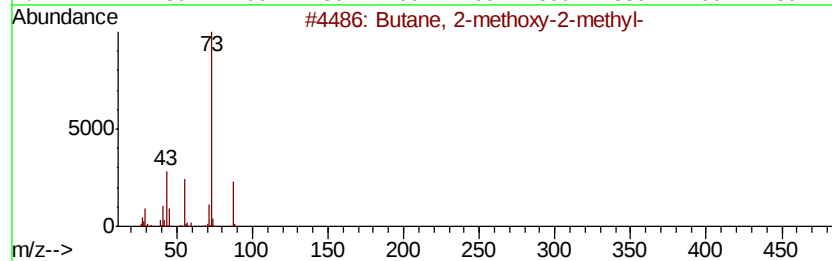
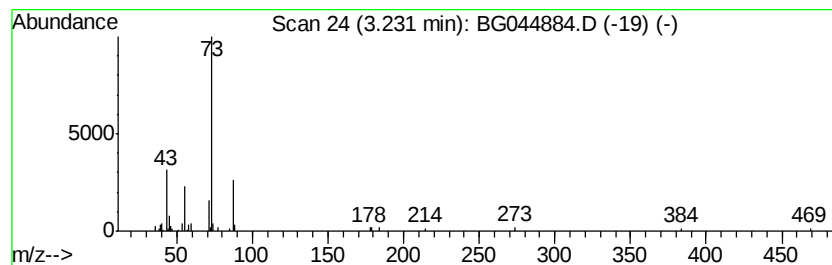
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG031020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown3.23 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.23	3.46 ng	75441	1,4-Dichlorobenzene-d4	8.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	45
2		Myo-Inositol, 2-C-methyl-	194	C7H14O6	000472-96-8	39
3		Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	28
4		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5		Acetaldehyde, O-ethyloxime-	87	C4H9NO	1000288-34-6	9



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Misc :
ALS Vial : 18 Sample Multiplier: 1

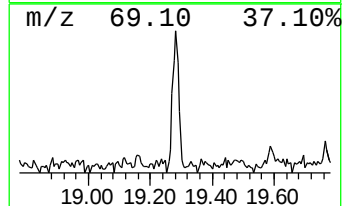
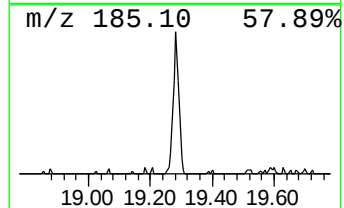
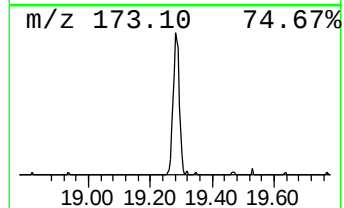
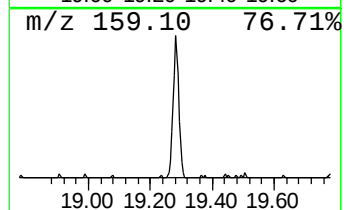
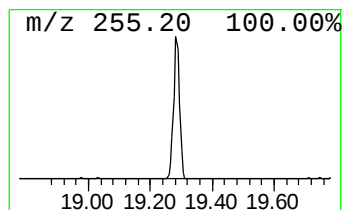
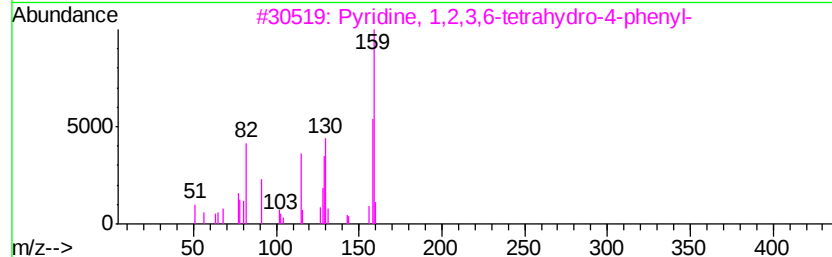
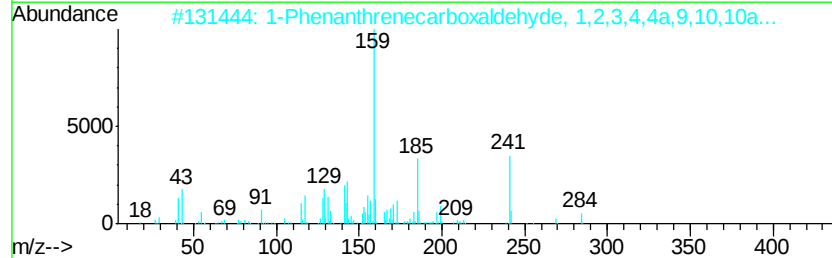
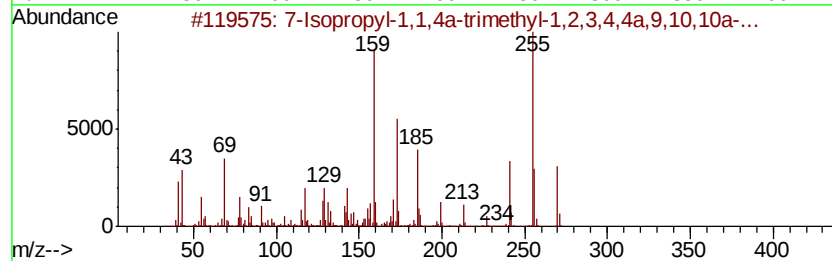
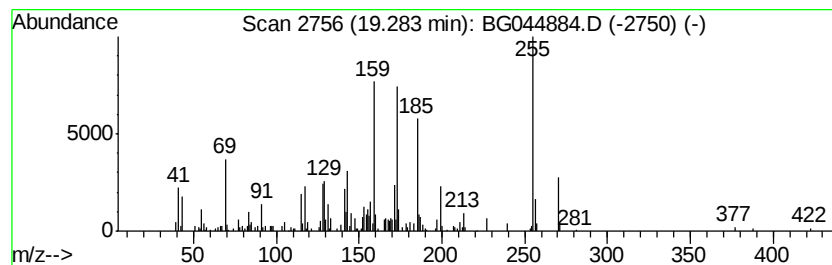
Instrument :
BNA_G
ClientSampled :
F-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG031020.M
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 7-Isopropyl-1,1,4a-trimethy... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.28	3.30 ng	180818	Phenanthrene-d10	17.42	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Isopropyl-1,1,4a-trimethyl-1,2...	270	C20H30	1000210-28-9	58
2	1-Phenanthrenecarboxaldehyde, 1,...	284	C20H28O	024035-50-5	22
3	Pyridine, 1,2,3,6-tetrahydro-4-p...	159	C11H13N	010338-69-9	15
4	S-Indacene-1,7-dione, 2,3,5,6-te...	270	C18H22O2	055591-16-7	14
5	1H-Indene, 2,3-dihydro-1,1,5,6-t...	174	C13H18	000942-43-8	11



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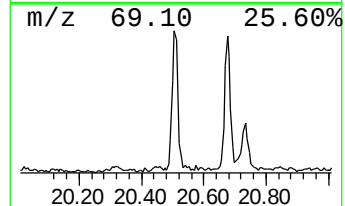
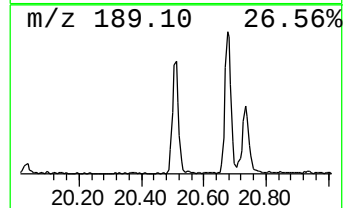
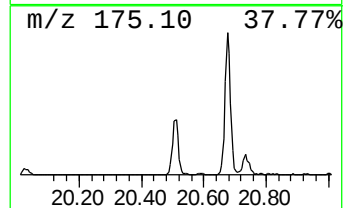
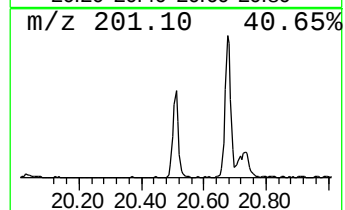
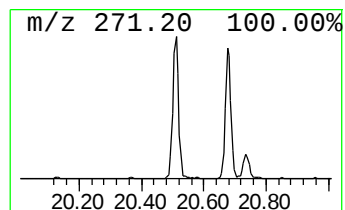
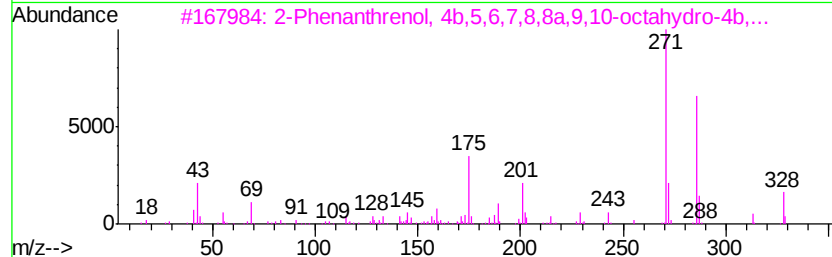
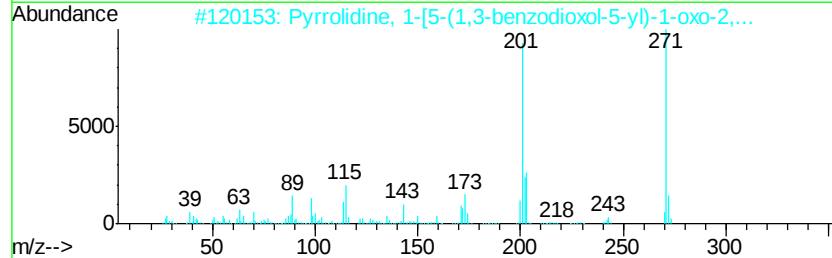
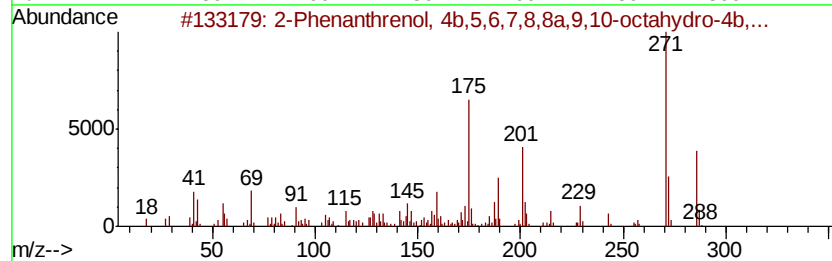
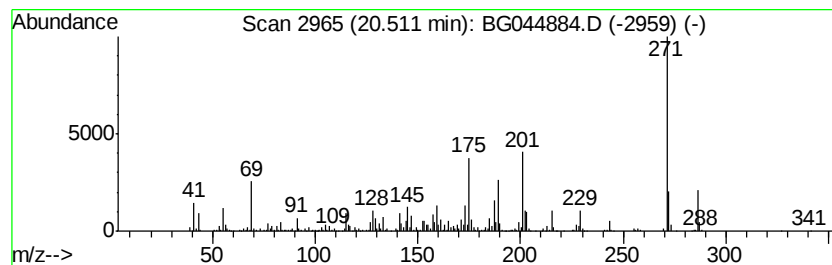
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 2-Phenanthrenol, 4b,5,6,7,8... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.51	13.08 ng	859707	Chrysene-d12	21.69

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Phenanthrenol, 4b,5,6,7,8,8a,9...	286	C20H30O	000511-15-9	70
2		Pyrrolidine, 1-[5-(1,3-benzodiox...	271	C16H17NO3	025924-78-1	49
3		2-Phenanthrenol, 4b,5,6,7,8,8a,9...	328	C22H32O2	015340-82-6	43
4		(+)-4-Methoxy-6-ketomorphinan	271	C17H21NO2	1000129-08-5	38
5		Crinan-1-one	271	C16H17NO3	098301-98-5	38



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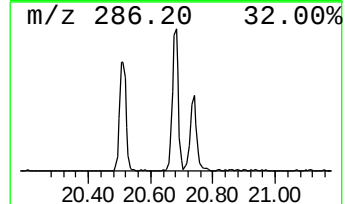
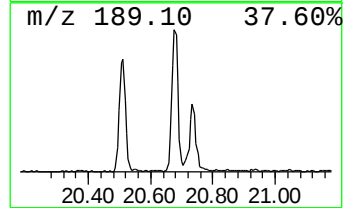
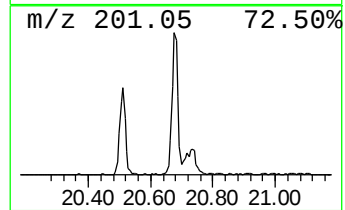
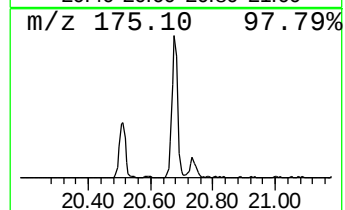
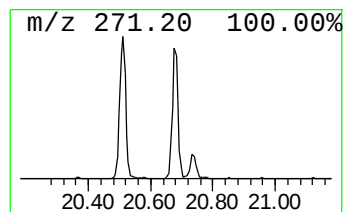
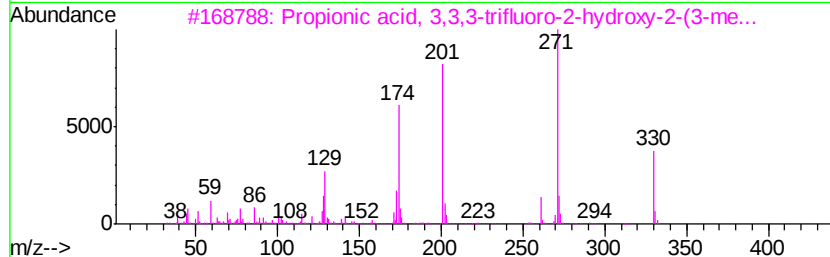
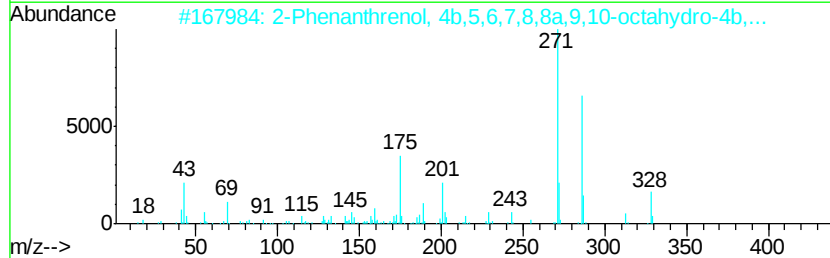
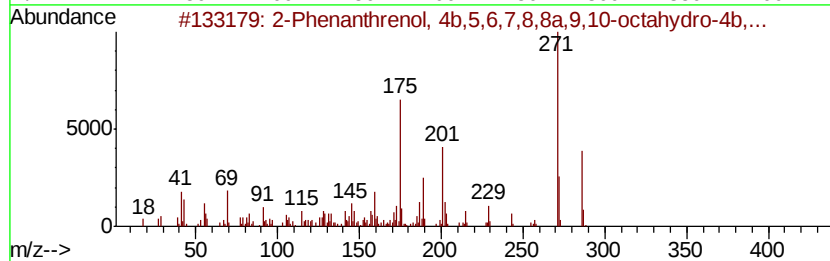
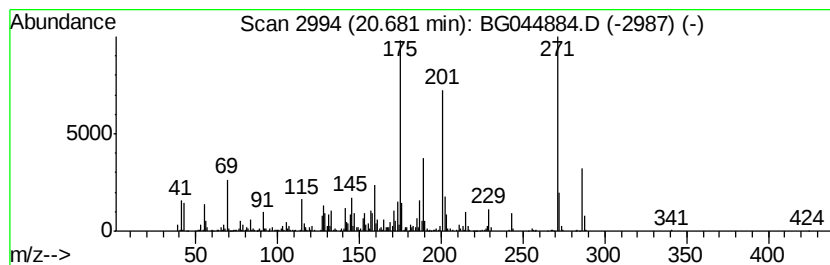
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TIC Library : C:\Database\NIST11.L
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Peak Number 6 unknown20.68 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.68	16.36 ng	1075850	Chrysene-d12	21.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Phenanthrenol, 4b,5,6,7,8,8a,9...	286	C20H30O	000511-15-9	93
2		2-Phenanthrenol, 4b,5,6,7,8,8a,9...	328	C22H32O2	015340-82-6	90
3		Propionic acid, 3,3,3-trifluoro-...	330	C15H13F3O3S	1000276-91-1	35
4		Pyrrolidine, 1-[5-(1,3-benzodiox...	271	C16H17NO3	025924-78-1	35
5		Silane, diethyl(3-chlorophenoxy)...	300	C15H25ClO2Si	1000363-83-3	25



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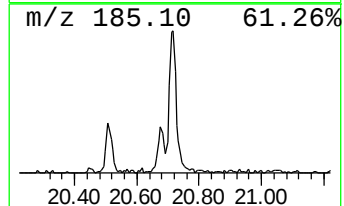
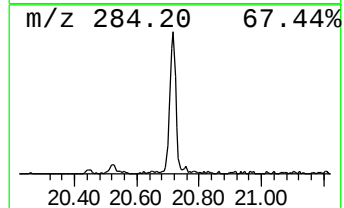
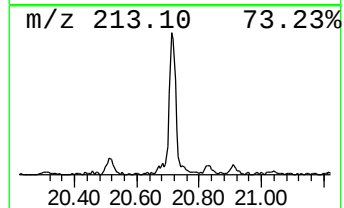
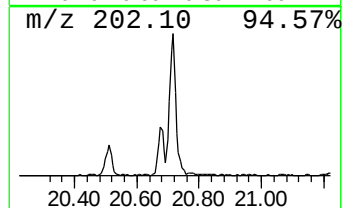
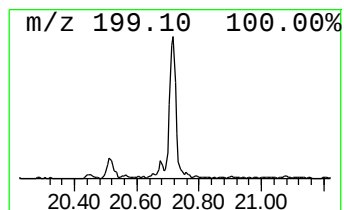
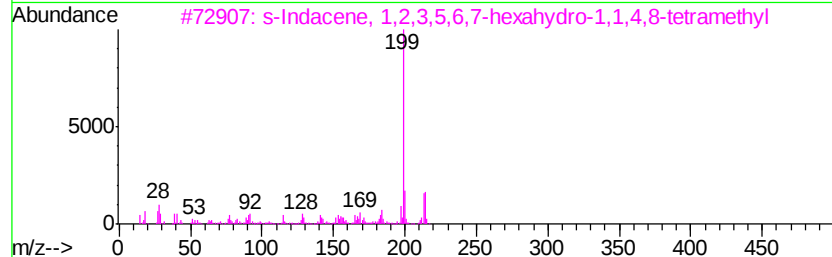
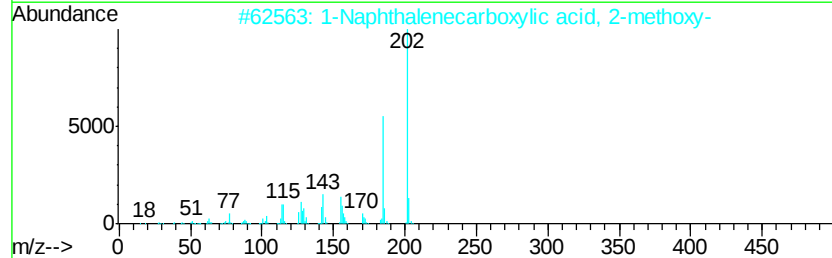
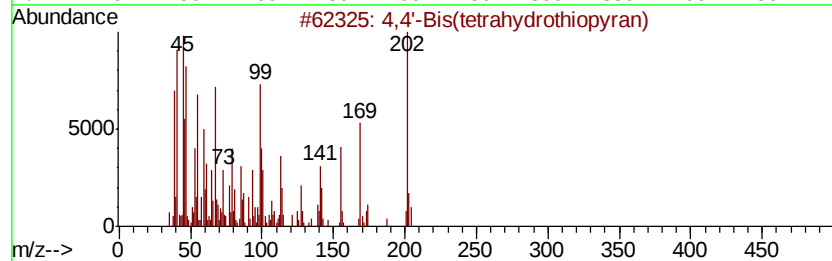
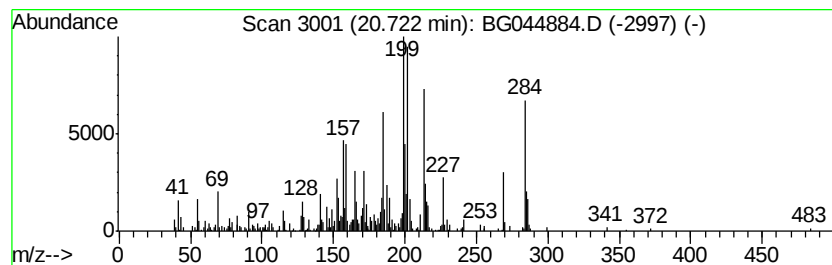
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TIC Integration Parameters: LSCINT.P

Peak Number 7 4,4'-Bis(tetrahydrothiopyran) Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.72	13.47 ng	885412	Chrysene-d12	21.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4,4'-Bis(tetrahydrothiopyran)	202	C10H18S2	116196-83-9	56
2		1-Naphthalenecarboxylic acid, 2-...	202	C12H10O3	000947-62-6	38
3		s-Indacene, 1,2,3,5,6,7-hexahydr...	214	C16H22	055030-60-9	30
4		[1,2,5]-Oxadiazolo[3,4-a]cinnoli...	202	C10H10N4O	1000260-59-4	30
5		Methallenestril	286	C18H22O3	000517-18-0	22



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG031820\
Data File : BG044884.D
Acq On : 19 Mar 2020 4:25
Operator : CG/JU
Sample : L1920-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

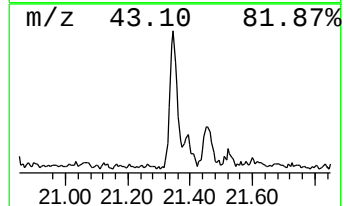
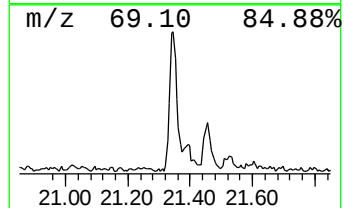
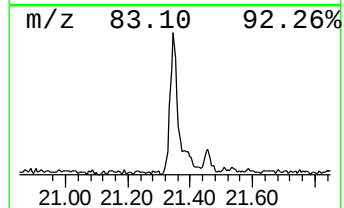
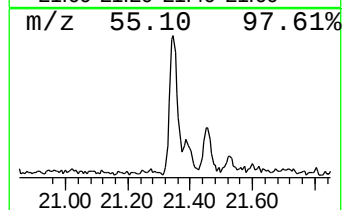
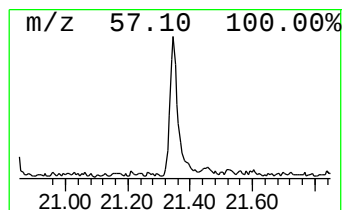
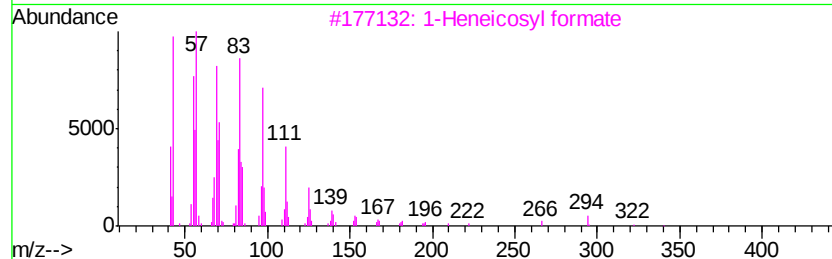
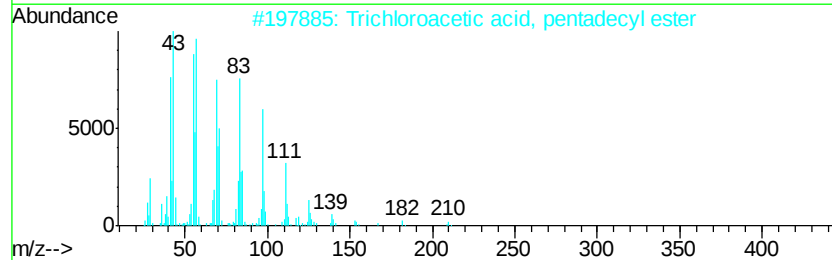
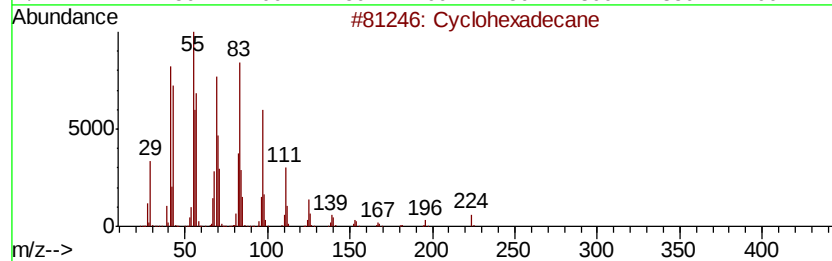
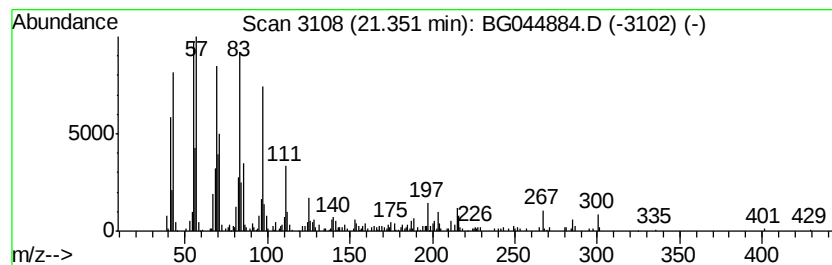
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG031020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Cyclohexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.		
21.35	7.07 ng	464869	Chrysene-d12	21.69		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cvclohexadecane	224	C16H32	000295-65-8	98
2		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
3		1-Heneicosvl formate	340	C22H44O2	077899-03-7	94
4		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
5		Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91



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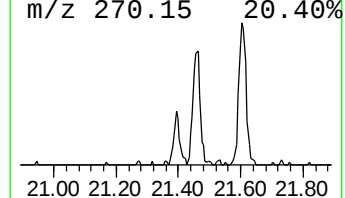
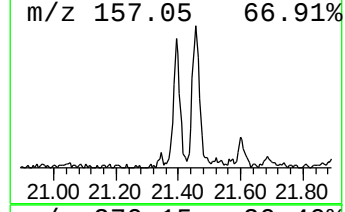
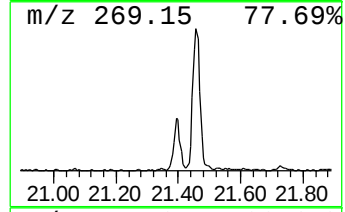
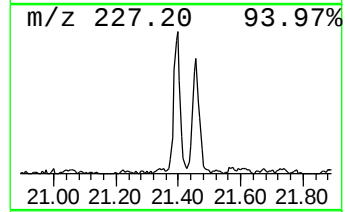
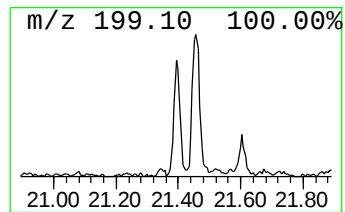
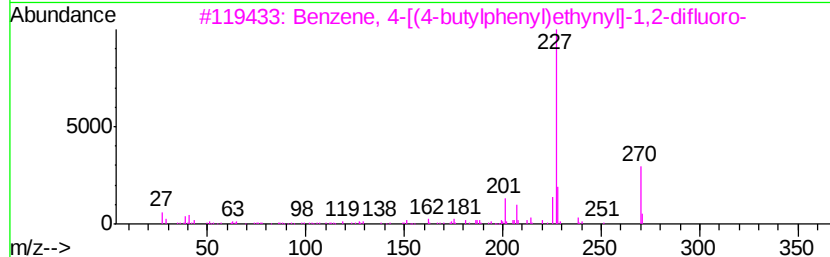
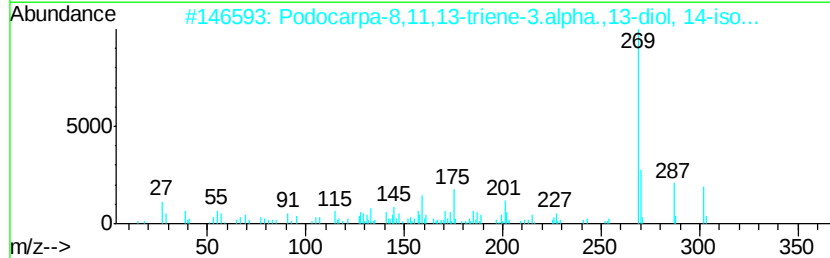
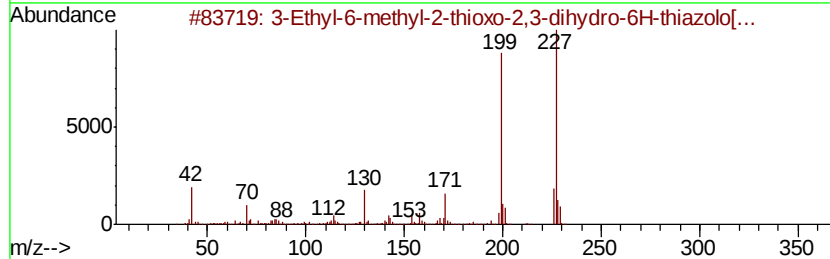
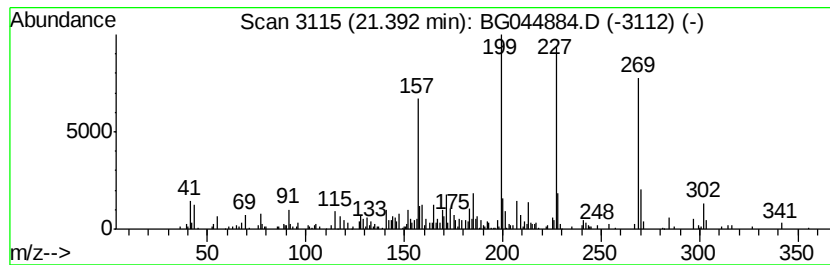
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown21.39 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.39	4.10 ng	269819	Chrysene-d12	21.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Ethyl-6-methyl-2-thioxo-2,3-di...	227	C8H9N3OS2	1000275-34-5	45
2		Podocarpa-8,11,13-triene-3.alpha...	302	C20H30O2	018325-87-6	38
3		Benzene, 4-[(4-butylphenyl)ethyn...	270	C18H16F2	109970-65-2	35
4		Phenylethylene, 2-nitro-2',3',4'...	269	C12H15NO6	082261-07-2	35
5		3-Ethenyl-6-dimethylaminomethyle...	199	C12H13N3	193695-67-9	30



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG031820\
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ClientSampleId :
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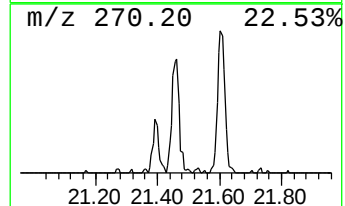
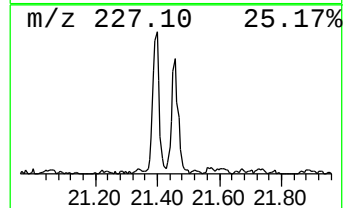
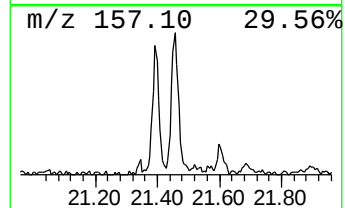
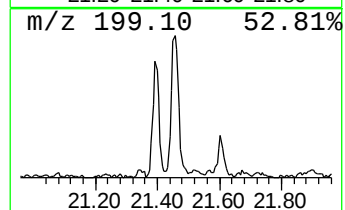
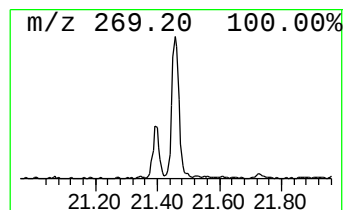
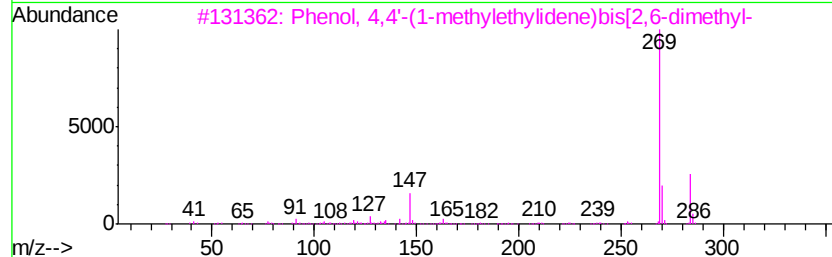
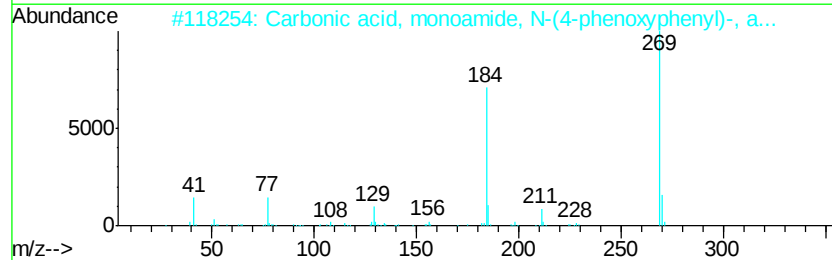
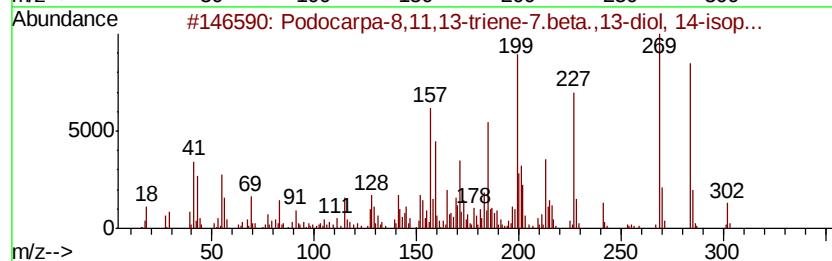
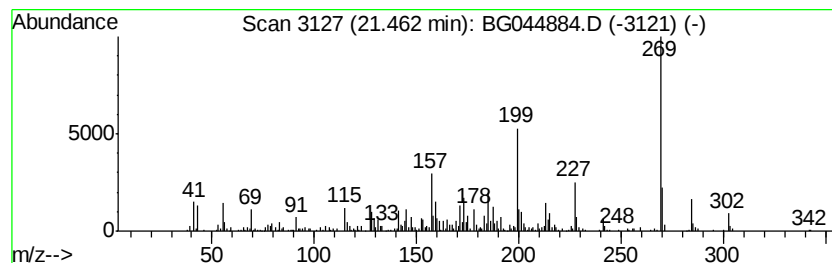
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Podocarpa-8,11,13-triene-7... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.46	8.32 ng	546943	Chrysene-d12	21.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Podocarpa-8,11,13-triene-7.beta....	302	C20H30O2	024338-19-0	60
2		Carbonic acid, monoamide, N-(4-p...	269	C16H15NO3	1000340-18-7	30
3		Phenol, 4,4'-(1-methylethylidene)...	284	C19H24O2	005613-46-7	27
4		Pivalamide, N-(4-phenoxyphenyl)-	269	C17H19NO2	1000340-13-6	27
5		4-Acetylphenyl 5-acetyl-2-methox...	284	C17H16O4	007251-24-3	22



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG031820\
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Acq On : 19 Mar 2020 4:25
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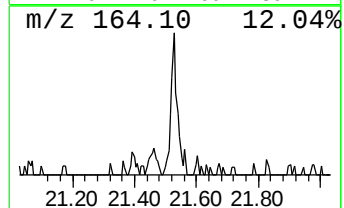
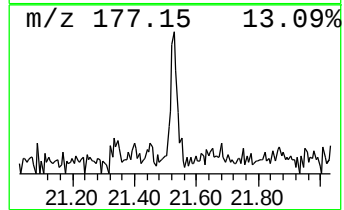
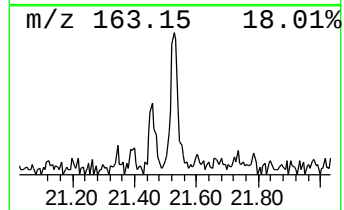
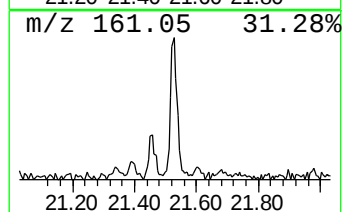
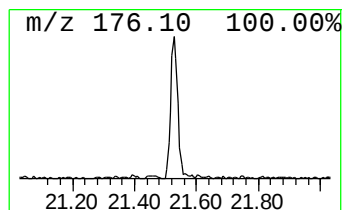
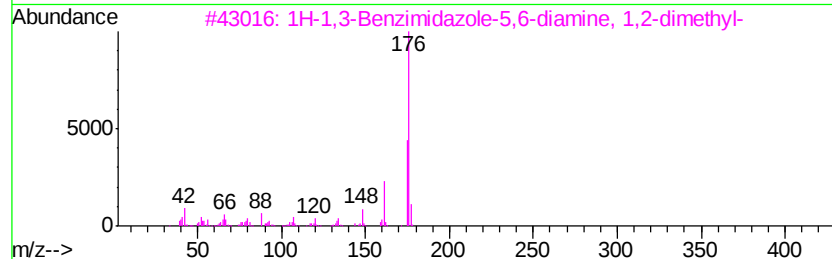
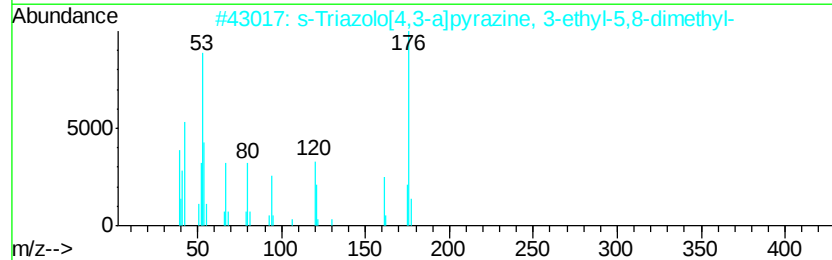
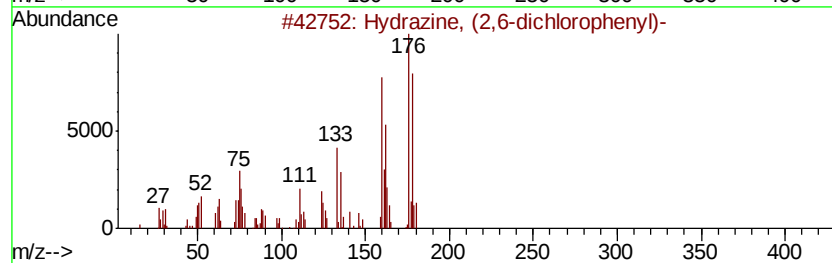
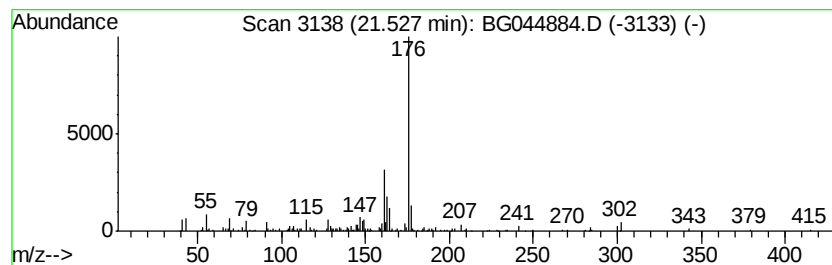
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Hydrazine, (2,6-dichlorophe... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.53	2.51 ng	164924	Chrysene-d12	21.69	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hvdrazine, (2,6-dichlorophenvl)-	176	C6H6Cl2N2	014763-24-7	86
2	s-Triazolo[4,3-a]pyrazine, 3-eth...	176	C9H12N4	019848-81-8	64
3	1H-1,3-Benzimidazole-5,6-diamine...	176	C9H12N4	1000319-10-3	64
4	Furan, 2,2'-methylenebis[5-methyl-	176	C11H12O2	013679-43-1	59
5	Benzo[b]thiophene, 2,5,7-trimethyl-	176	C11H12S	016587-65-8	59



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG031820\
Data File : BG044884.D
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Operator : CG/JU
Sample : L1920-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

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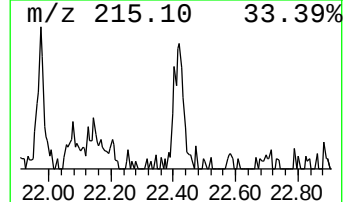
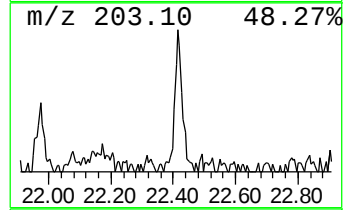
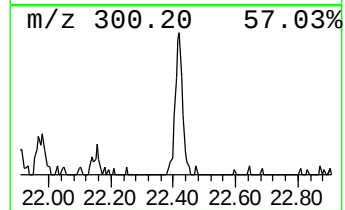
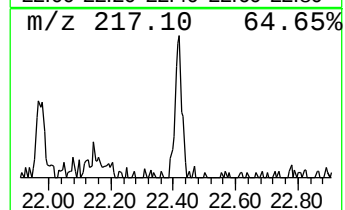
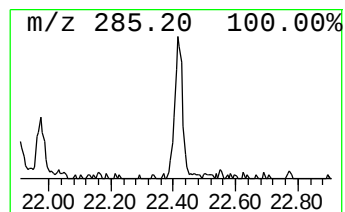
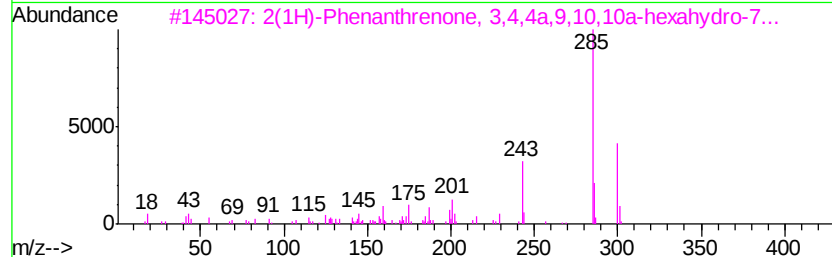
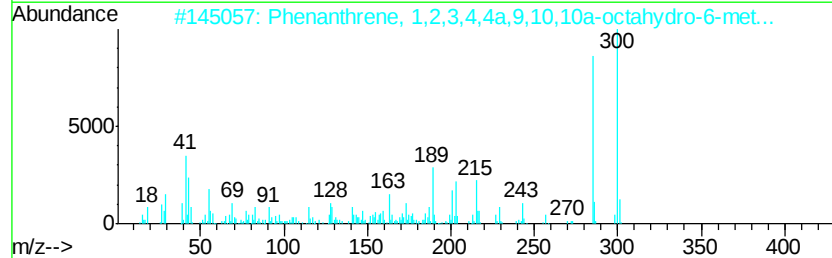
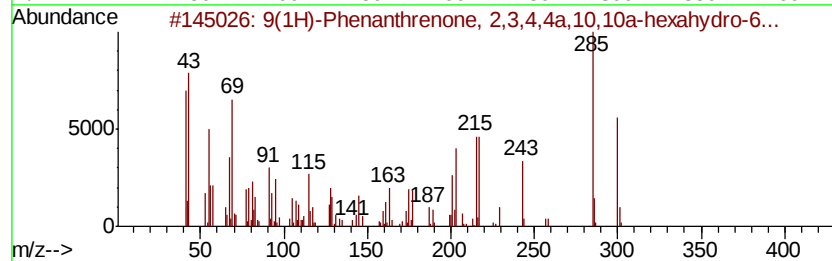
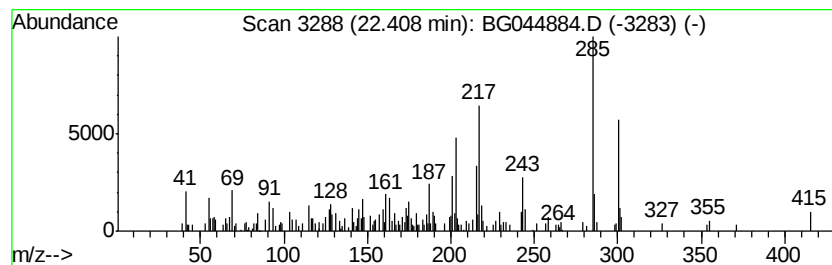
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 9(1H)-Phenanthrenone, 2,3,4... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.41	2.07 ng	136348	Chrysene-d12	21.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9(1H)-Phenanthrenone, 2,3,4,4a,1...	300	C20H28O2	000511-05-7	93
2		Phenanthrene, 1,2,3,4,4a,9,10,10...	300	C21H32O	010064-26-3	89
3		2(1H)-Phenanthrenone, 3,4,4a,9,1...	300	C20H28O2	006755-93-7	47
4		Podocarpa-8,11,13-trien-3-one, 1...	342	C22H30O3	018468-20-7	43
5		Epibuphanisine	285	C17H19NO3	006835-79-6	30



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG031820\
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Sample : L1920-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

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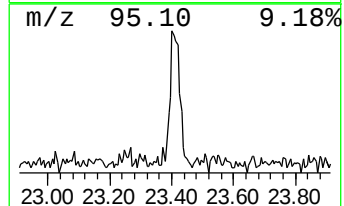
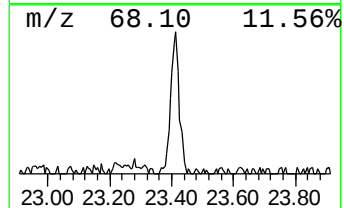
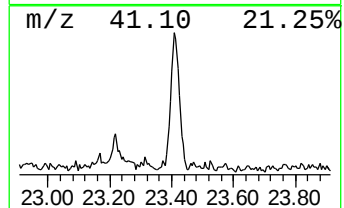
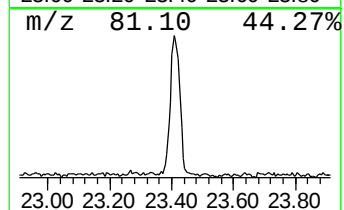
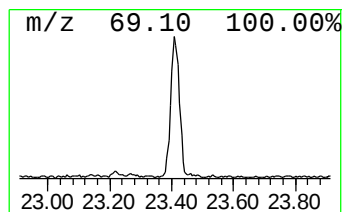
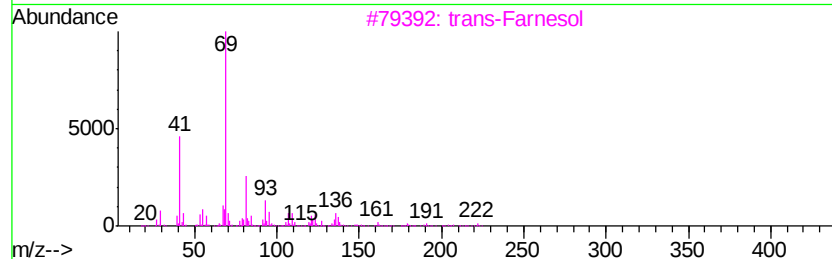
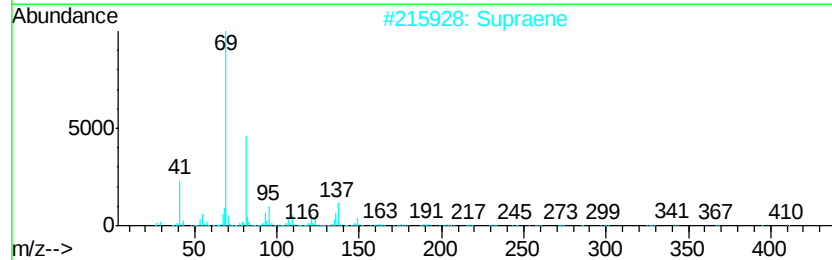
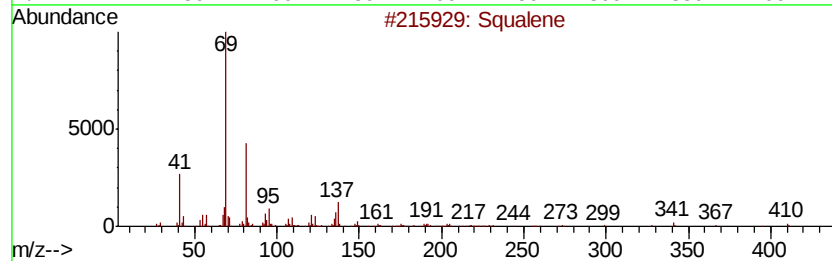
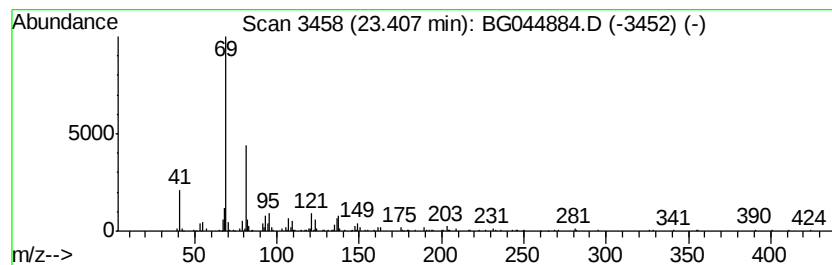
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Squalene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.41	4.17 ng	274562	Perylene-d12	24.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	91
2		Supraene	410	C30H50	007683-64-9	91
3		trans-Farnesol	222	C15H26O	000106-28-5	80
4		2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	78
5		Trifluoroacetyl-lavandulol	250	C12H17F3O2	028673-24-7	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG031820\
 Data File : BG044884.D
 Acq On : 19 Mar 2020 4:25
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 Sample : L1920-02
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
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 ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG031020.M
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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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7-Isopropyl-1,1,4...	19.28	3.3	ng	180818	4	17.42	1095630	20.0
2-Phenanthrenol, ...	20.51	13.1	ng	859707	5	21.69	1314960	20.0
unknown20.68	20.68	16.4	ng	1075850	5	21.69	1314960	20.0
4,4'-Bis(tetrahyd...	20.72	13.5	ng	885412	5	21.69	1314960	20.0
Cyclohexadecane	21.35	7.1	ng	464869	5	21.69	1314960	20.0
unknown21.39	21.39	4.1	ng	269819	5	21.69	1314960	20.0
Podocarpa-8,11,13...	21.46	8.3	ng	546943	5	21.69	1314960	20.0
Hydrazine, (2,6-d...	21.53	2.5	ng	164924	5	21.69	1314960	20.0
9(1H)-Phenanthren...	22.41	2.1	ng	136348	5	21.69	1314960	20.0
Squalene	23.41	4.2	ng	274562	6	24.89	1316550	20.0