

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040623\
 Data File : BG057012.D
 Acq On : 6 Apr 2023 14:47
 Operator : CG/JU
 Sample : 02208-01
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 RO-124035

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-BG033023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057012.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.447	315	325	333	rBV	421695	681787	79.72%	11.183%
2	5.922	400	406	414	rBB	193471	311379	36.41%	5.108%
3	7.544	674	682	691	rBV	300925	513351	60.02%	8.420%
4	8.413	824	830	836	rBV	55082	91813	10.74%	1.506%
5	9.588	1022	1030	1040	rBB	209626	372880	43.60%	6.116%
6	11.250	1304	1313	1321	rBV	66319	120850	14.13%	1.982%
7	11.415	1336	1341	1347	rBV	10656	16319	1.91%	0.268%
8	13.647	1713	1721	1729	rBV	434919	653472	76.41%	10.719%
9	15.022	1949	1955	1962	rBV2	111480	176641	20.65%	2.897%
10	15.175	1975	1981	1992	rVB9	22917	76701	8.97%	1.258%
11	16.355	2177	2182	2186	rVB	18741	23992	2.81%	0.394%
12	16.502	2200	2207	2212	rVB	258924	393053	45.96%	6.447%
13	17.113	2306	2311	2315	rVB5	7114	12130	1.42%	0.199%
14	17.618	2392	2397	2402	rVB	21670	28860	3.37%	0.473%
15	17.718	2410	2414	2416	rBV3	14595	18687	2.18%	0.307%
16	17.759	2416	2421	2432	rVB	142777	234720	27.44%	3.850%
17	17.883	2435	2442	2447	rBV	15223	26412	3.09%	0.433%
18	18.082	2471	2476	2480	rBV	21739	26295	3.07%	0.431%
19	18.382	2521	2527	2531	rBV	59884	79339	9.28%	1.301%
20	18.435	2531	2536	2542	rVV4	16700	40504	4.74%	0.664%
21	18.499	2544	2547	2552	rVB	15422	20446	2.39%	0.335%
22	18.599	2555	2564	2571	rBV3	73342	132493	15.49%	2.173%
23	18.799	2594	2598	2602	rBV	23290	28802	3.37%	0.472%
24	19.069	2640	2644	2649	rBV	61974	79063	9.24%	1.297%
25	19.163	2656	2660	2663	rBV5	7039	10028	1.17%	0.164%
26	19.363	2690	2694	2699	rBV6	7740	16023	1.87%	0.263%
27	19.733	2755	2757	2762	rBV5	10421	13873	1.62%	0.228%
28	19.845	2773	2776	2781	rVB5	24645	29659	3.47%	0.486%
29	20.044	2806	2810	2811	rBV4	9016	13350	1.56%	0.219%
30	20.121	2818	2823	2828	rBV8	11820	22230	2.60%	0.365%
31	20.197	2834	2836	2843	rBV6	13209	33361	3.90%	0.547%
32	20.326	2852	2858	2863	rBV	677673	855255	100.00%	14.029%
33	20.526	2888	2892	2897	rBV6	18894	40099	4.69%	0.658%
34	20.597	2902	2904	2909	rVB5	11248	13395	1.57%	0.220%
35	20.732	2925	2927	2931	rBV5	9171	12265	1.43%	0.201%
36	20.973	2965	2968	2970	rBV4	15053	17737	2.07%	0.291%

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37	21.096	2987	2989	2992	rBV3	9058	10368	1.21%	0.170%
38	21.278	3016	3020	3028	rBV8	20485	39088	4.57%	0.641%
39	21.366	3033	3035	3041	rVB6	12908	22215	2.60%	0.364%
40	21.454	3046	3050	3051	rBV4	12682	17476	2.04%	0.287%
41	21.642	3078	3082	3086	rBV2	34066	45786	5.35%	0.751%
42	22.077	3150	3156	3166	rBV	134221	278223	32.53%	4.564%
43	22.611	3244	3247	3248	rBV3	11419	11295	1.32%	0.185%
44	22.888	3290	3294	3300	rBV7	10806	22878	2.67%	0.375%
45	23.029	3314	3318	3325	rVB4	23008	41648	4.87%	0.683%
46	23.475	3388	3394	3396	rBV7	7901	14364	1.68%	0.236%
47	23.640	3421	3422	3432	rVB9	13124	20293	2.37%	0.333%
48	24.527	3571	3573	3581	rVB7	11812	16350	1.91%	0.268%
49	25.431	3719	3727	3732	rBV9	9472	28035	3.28%	0.460%
50	25.613	3748	3758	3769	rVB2	82175	263313	30.79%	4.319%
51	30.090	4512	4520	4522	rBV8	13398	27908	3.26%	0.458%

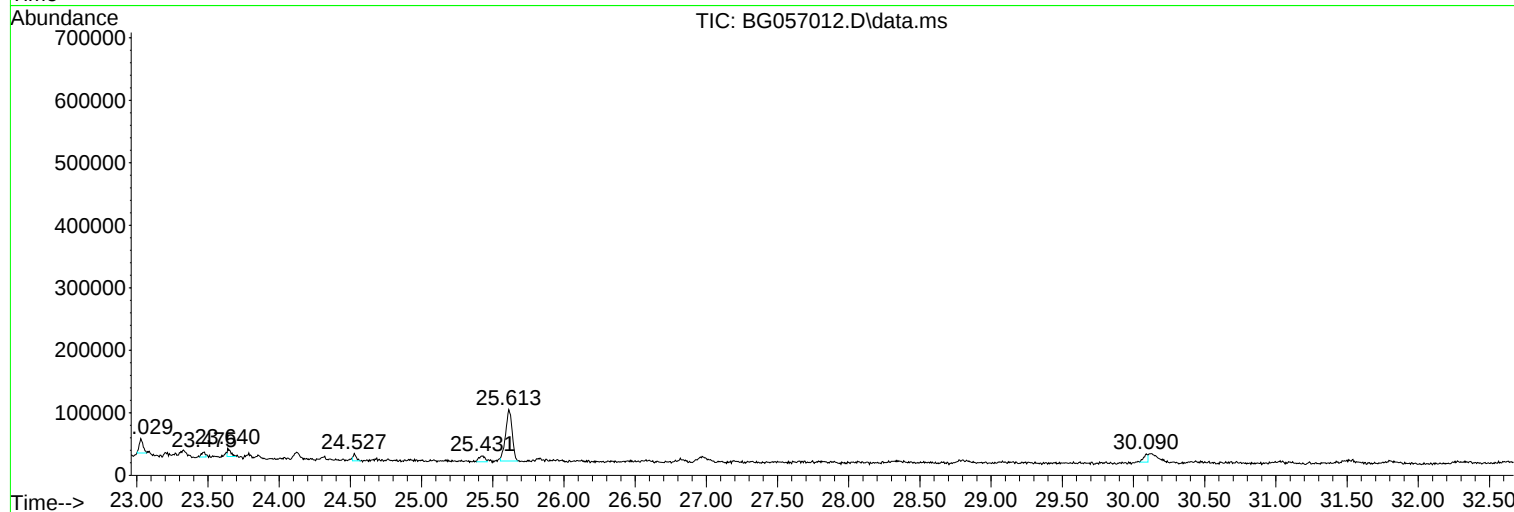
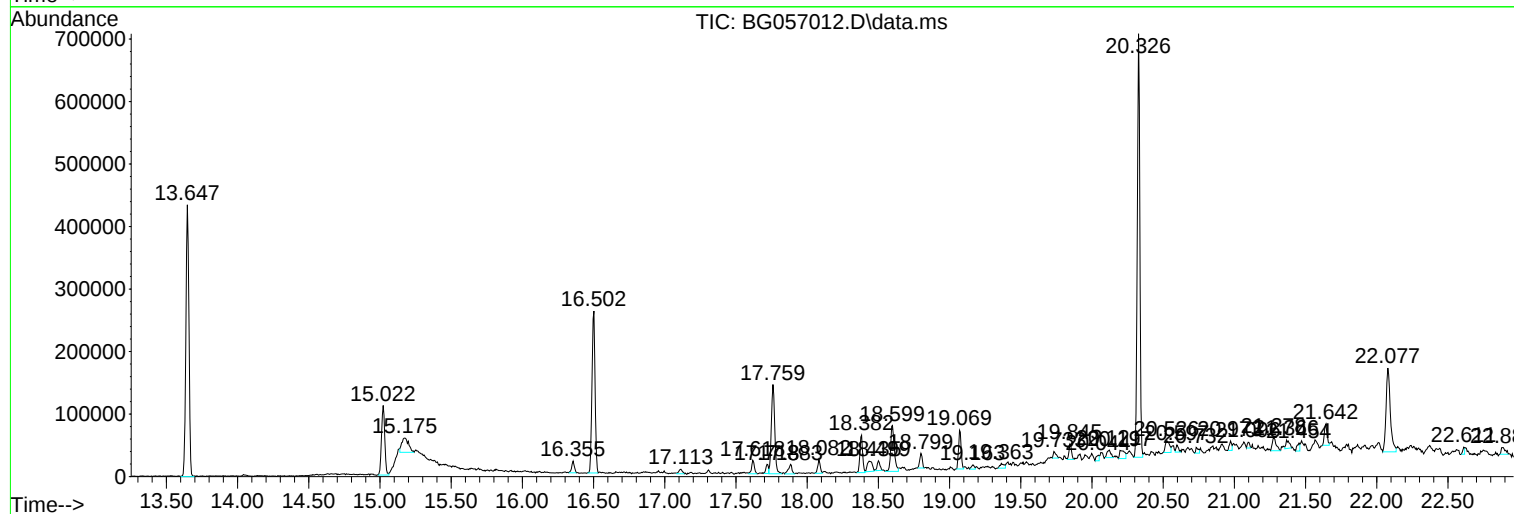
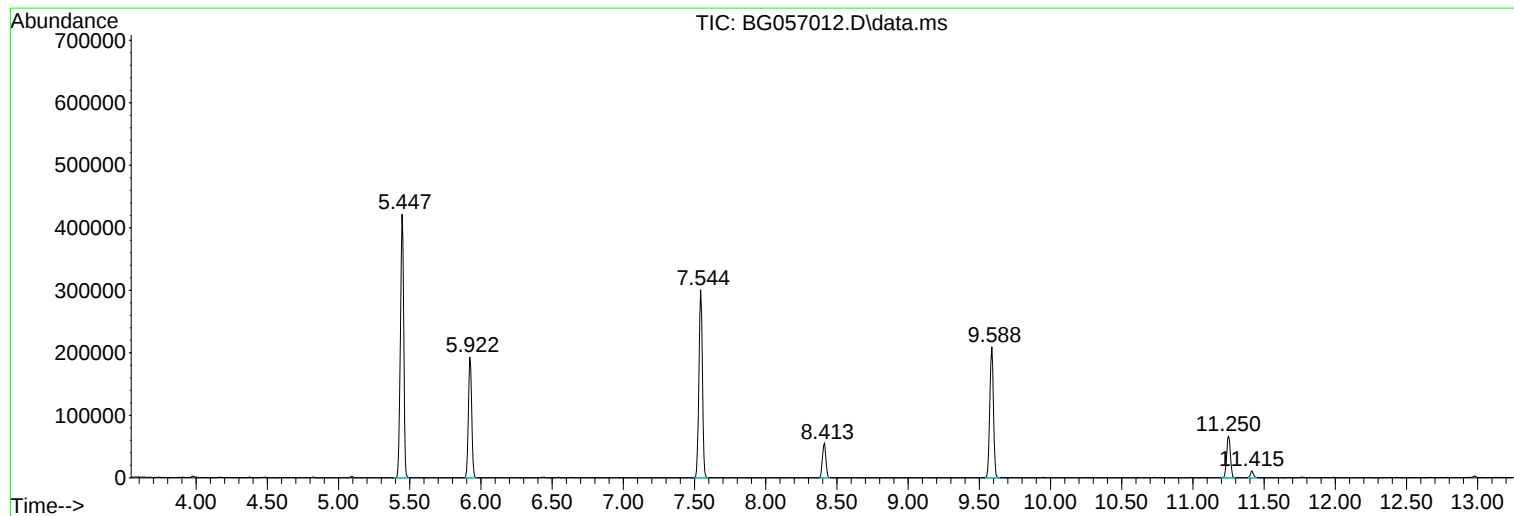
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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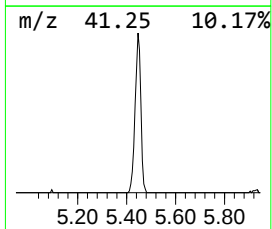
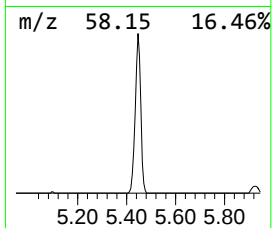
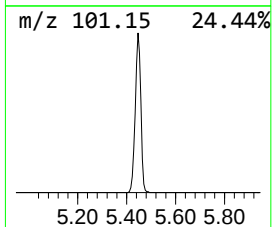
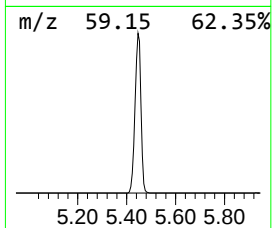
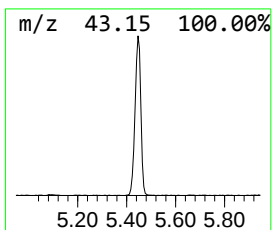
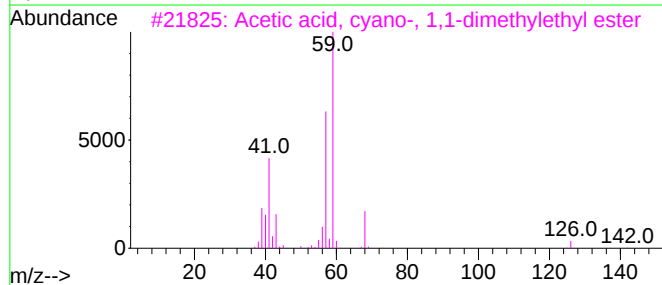
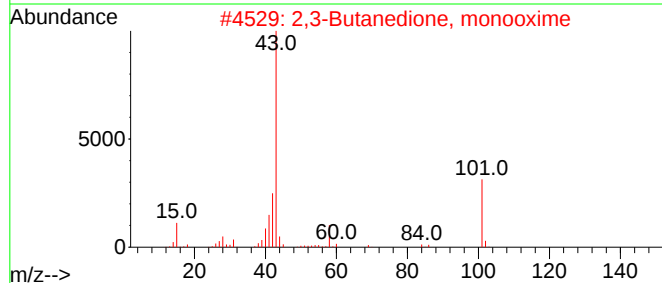
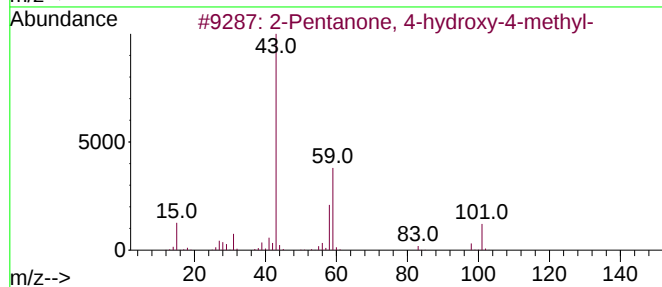
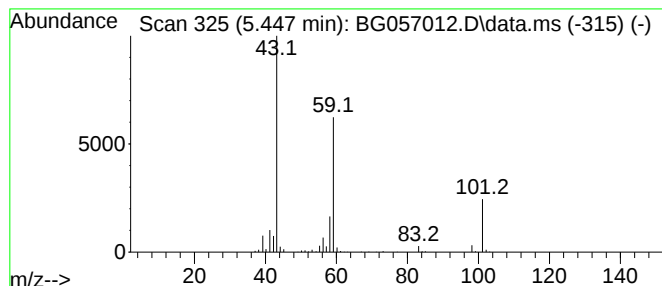
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.447	148.52 ng	681787	1,4-Dichlorobenzene-d4	8.413

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9		



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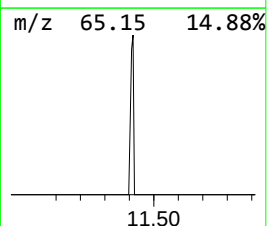
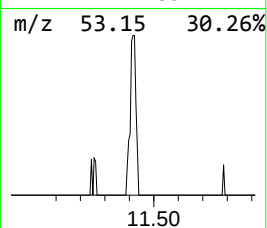
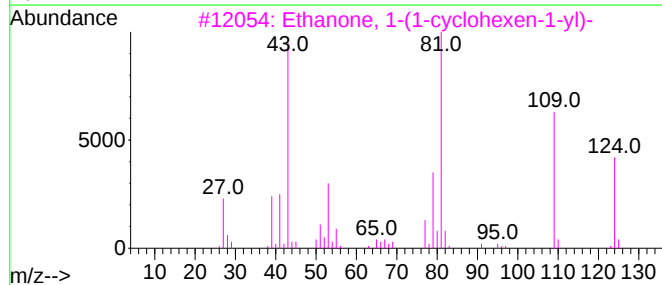
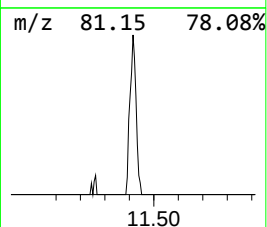
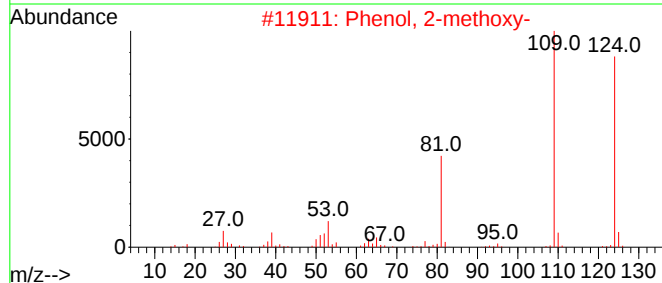
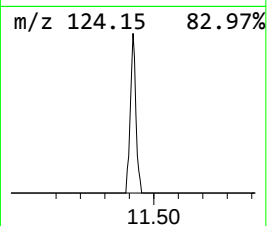
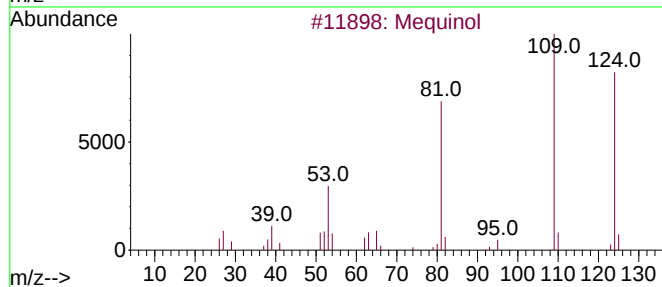
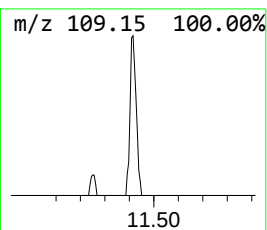
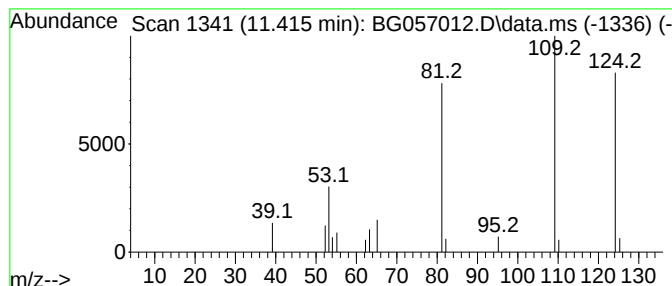
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Mequinol Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.415	2.70 ng	16319	Naphthalene-d8	11.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Mequinol	124	C7H8O2	000150-76-5	91
2			Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	91
3			Ethanone, 1-(1-cyclohexen-1-yl)-	124	C8H12O	000932-66-1	72
4			5-Ethyl-2-furaldehyde	124	C7H8O2	023074-10-4	53
5			Ethanone, 1-(2-methyl-1-cyclopent-1-en-1-yl)-	124	C8H12O	003168-90-9	50



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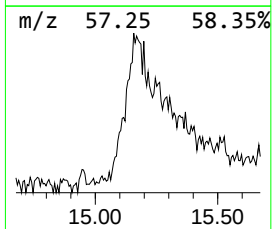
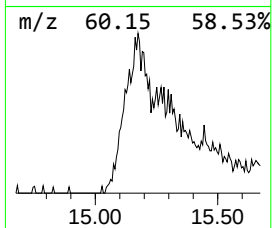
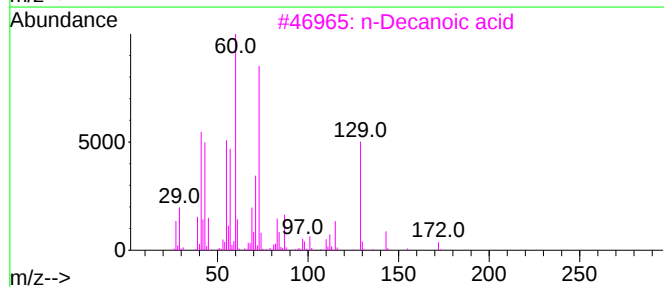
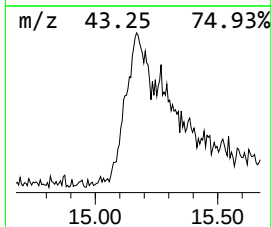
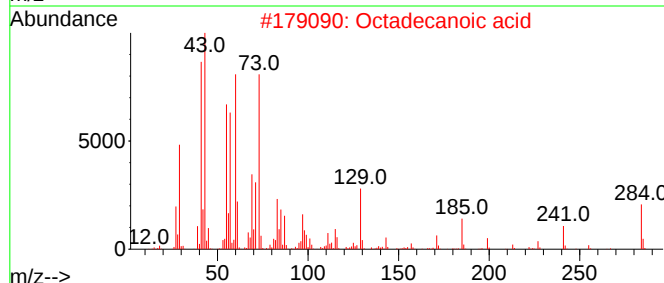
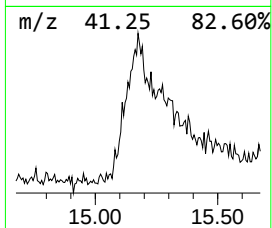
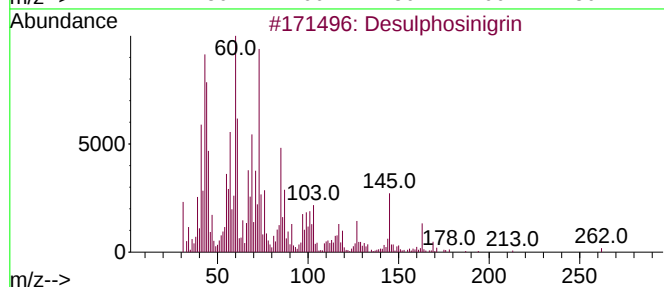
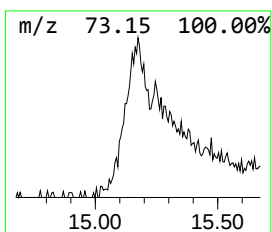
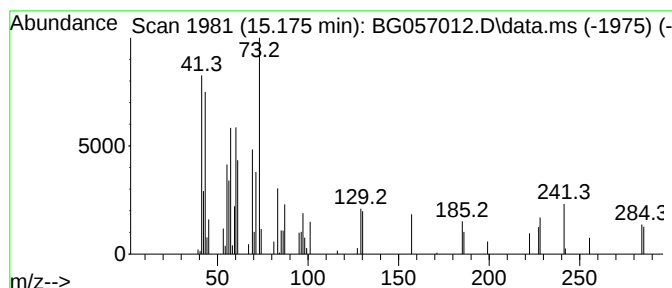
Instrument :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown15.175 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.175	8.68 ng	76701	Acenaphthene-d10	15.022	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Desulphosinigrin	279	C10H17NO6S	005115-81-1	43
2	Octadecanoic acid	284	C18H36O2	000057-11-4	43
3	n-Decanoic acid	172	C10H20O2	000334-48-5	38
4	11-Bromoundecanoic acid	264	C11H21BrO2	002834-05-1	35
5	d-Gulopyranose	180	C6H12O6	000530-27-8	35



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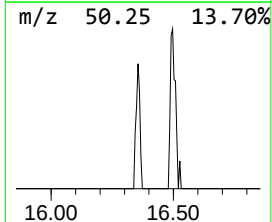
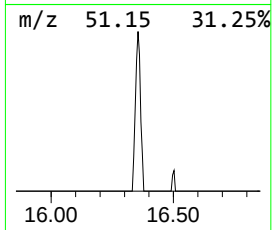
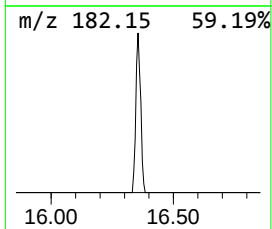
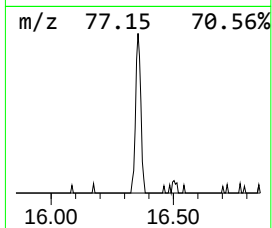
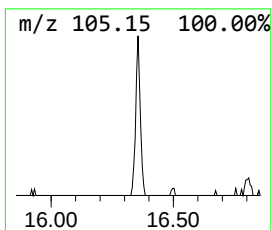
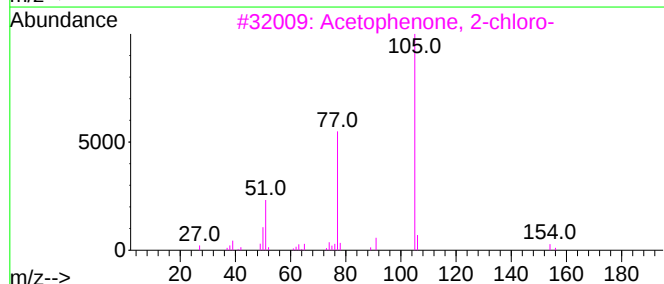
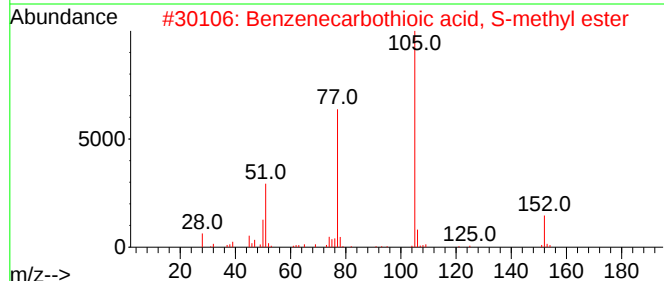
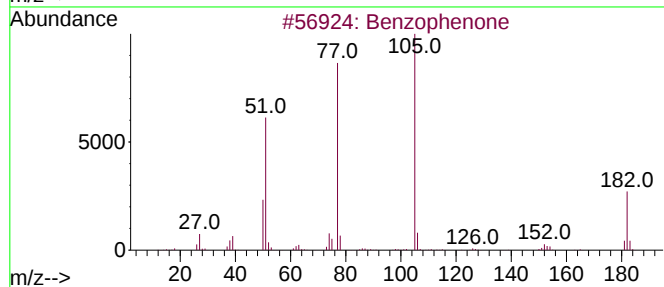
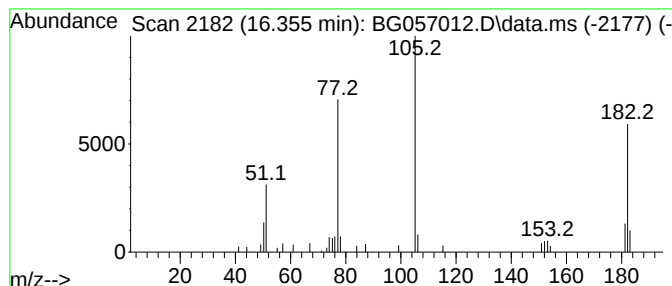
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzophenone Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.355	2.72 ng	23992	Acenaphthene-d10	15.022

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	93
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	46
3			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	43
4			1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	38
5			Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	38



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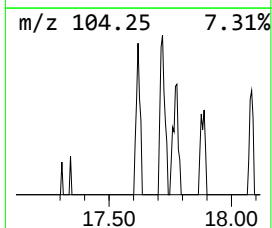
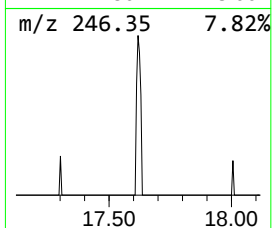
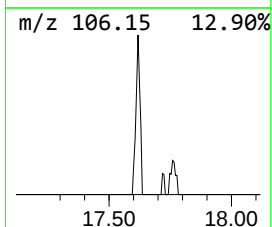
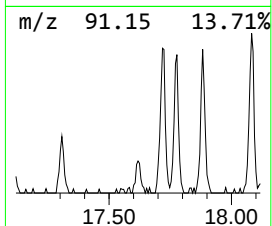
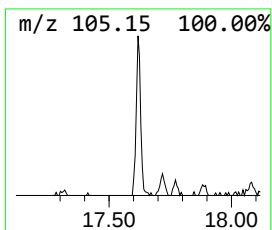
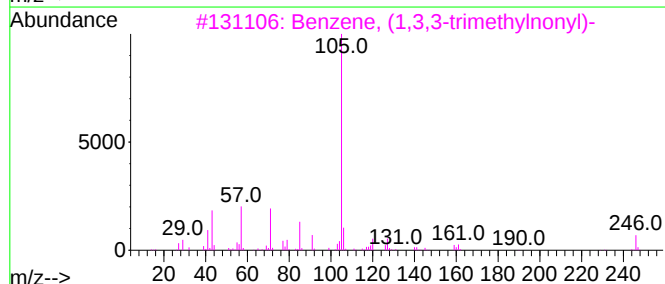
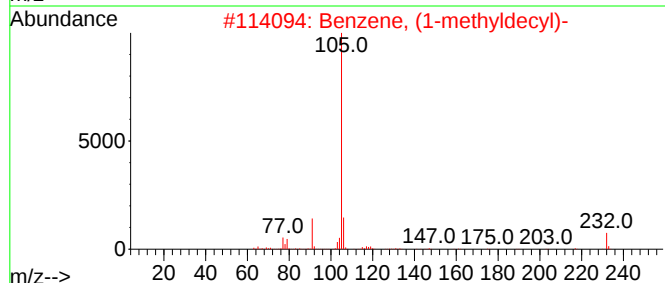
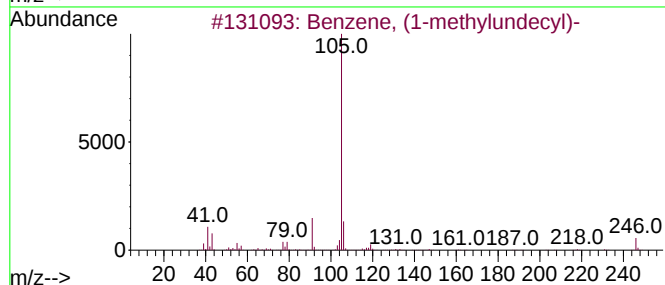
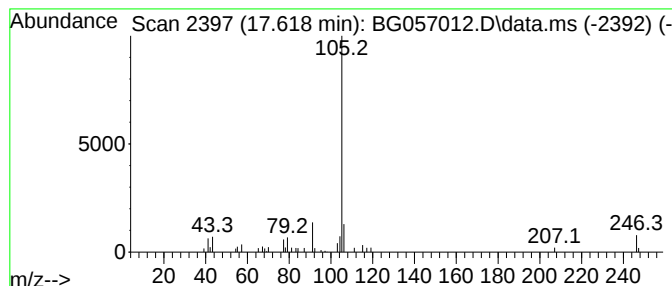
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Benzene, (1-methylundecyl)- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.618	2.46 ng	28860	Phenanthrene-d10	17.759

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (1-methylundecyl)-	246	C18H30	002719-61-1	93
2			Benzene, (1-methyldecyl)-	232	C17H28	004536-88-3	72
3			Benzene, (1,3,3-trimethylnonyl)-	246	C18H30	054986-44-6	72
4			Benzene, (1-methylnonyl)-	218	C16H26	004537-13-7	64
5			1-Hexene, 6-phenyl-4-(1-phenylet...	280	C20H24O	1010190-48-6	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040623\
Data File : BG057012.D
Acq On : 6 Apr 2023 14:47
Operator : CG/JU
Sample : 02208-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RO-124035

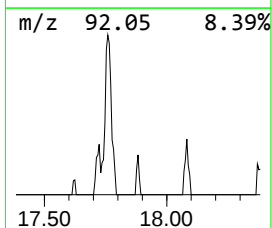
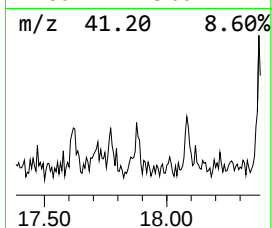
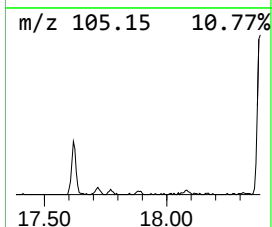
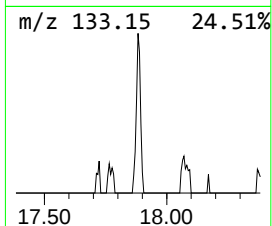
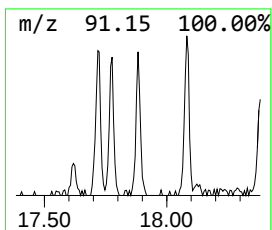
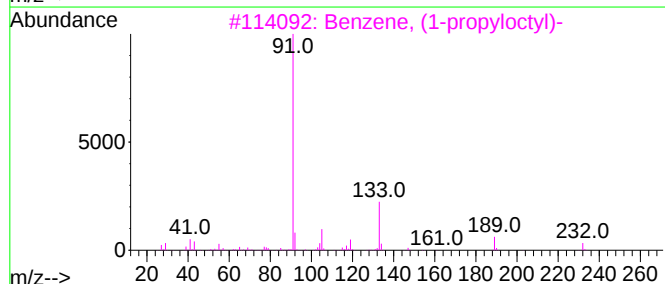
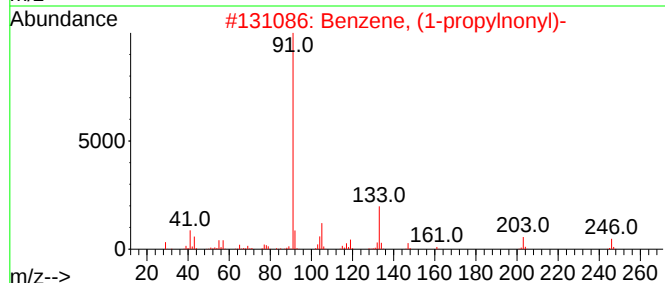
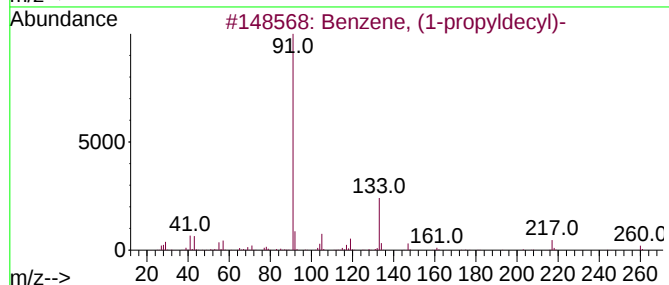
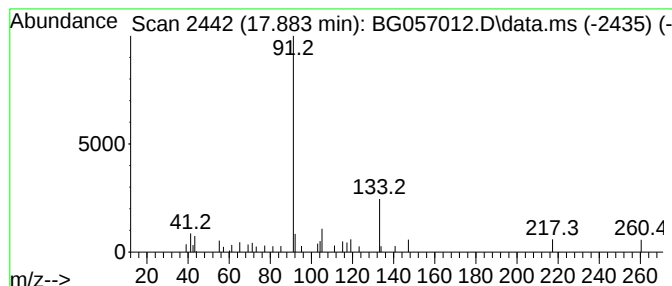
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Benzene, (1-propyldecyl)- Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.883	2.25 ng	26412	Phenanthrene-d10	17.759

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (1-propyldecyl)-	260	C19H32	004534-51-4	91
2			Benzene, (1-propylnonyl)-	246	C18H30	002719-64-4	72
3			Benzene, (1-propyloctyl)-	232	C17H28	004536-86-1	59
4			Benzene, (1-ethyldecyl)-	246	C18H30	002400-00-2	50
5			Benzene, (1-ethylundecyl)-	260	C19H32	004534-52-5	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040623\
Data File : BG057012.D
Acq On : 6 Apr 2023 14:47
Operator : CG/JU
Sample : 02208-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RO-124035

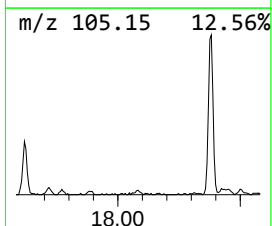
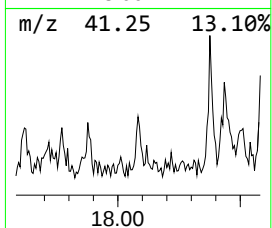
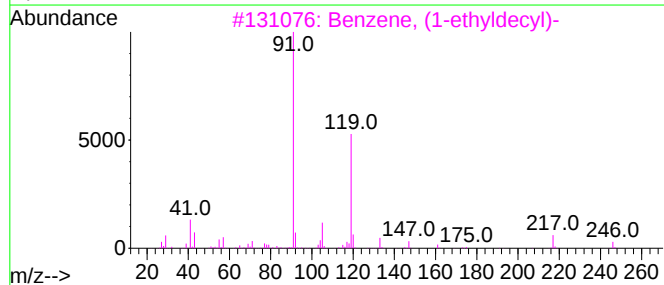
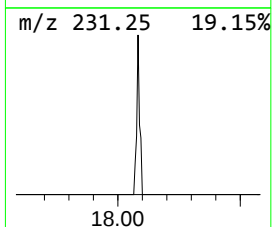
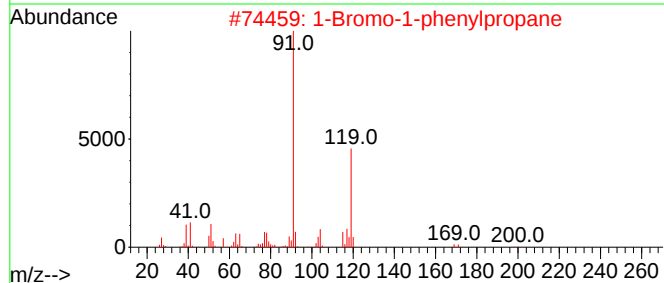
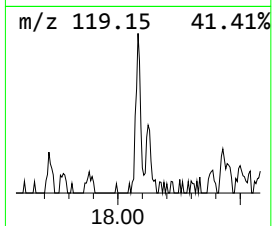
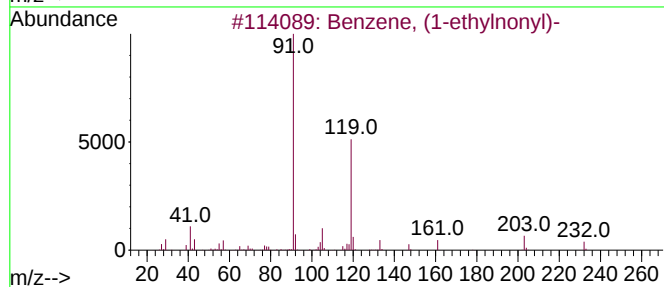
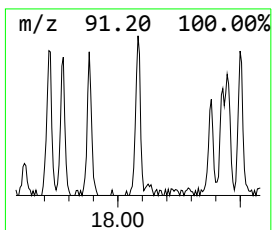
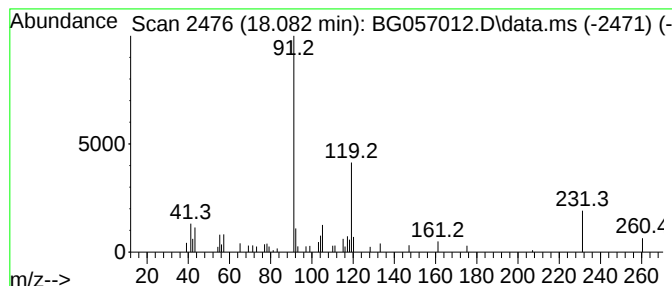
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Benzene, (1-ethylnonyl)- Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.082	2.24 ng	26295	Phenanthrene-d10	17.759

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (1-ethylnonyl)-	232	C17H28	004536-87-2	59
2			1-Bromo-1-phenylpropane	198	C9H11Br	002114-36-5	53
3			Benzene, (1-ethyldecyl)-	246	C18H30	002400-00-2	53
4			Benzene, (1-nitropropyl)-	165	C9H11NO2	005279-14-1	50
5			Hexane, 3,4-diphenyl-	238	C18H22	005789-31-1	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040623\
Data File : BG057012.D
Acq On : 6 Apr 2023 14:47
Operator : CG/JU
Sample : 02208-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RO-124035

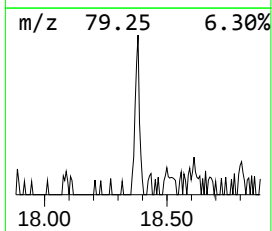
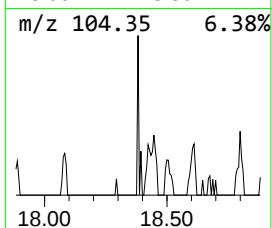
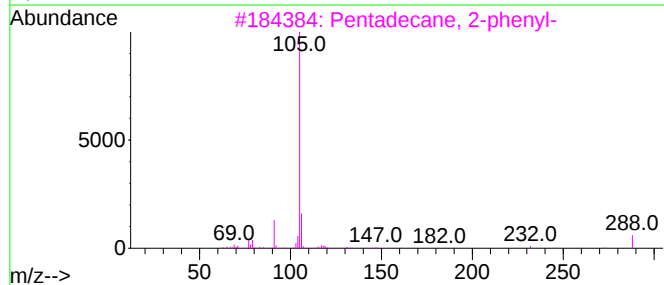
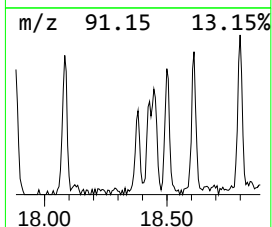
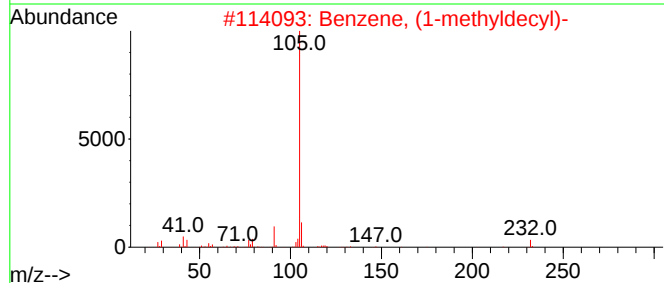
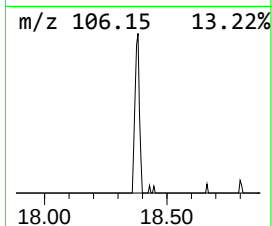
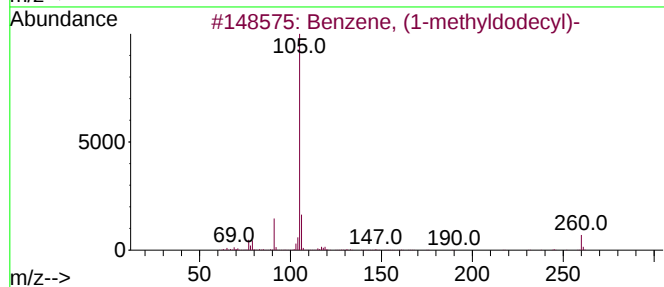
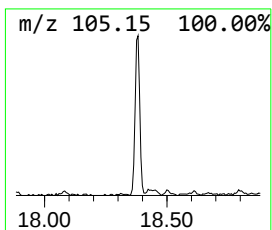
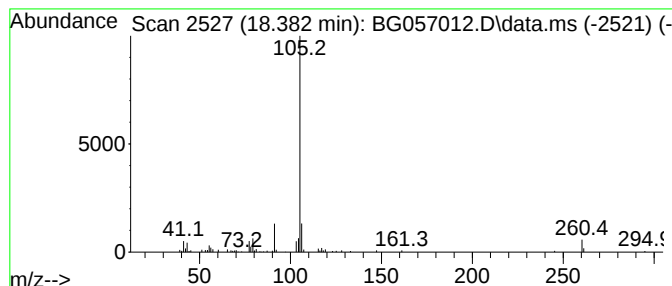
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Benzene, (1-methyldodecyl)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.382	6.76 ng	79339	Phenanthrene-d10	17.759

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (1-methyldodecyl)-	260	C19H32	004534-53-6	91
2			Benzene, (1-methyldecyl)-	232	C17H28	004536-88-3	64
3			Pentadecane, 2-phenyl-	288	C21H36	004534-66-1	59
4			Benzene, (1-methylundecyl)-	246	C18H30	002719-61-1	59
5			Benzene, (1-methylnonyl)-	218	C16H26	004537-13-7	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040623\
Data File : BG057012.D
Acq On : 6 Apr 2023 14:47
Operator : CG/JU
Sample : 02208-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RO-124035

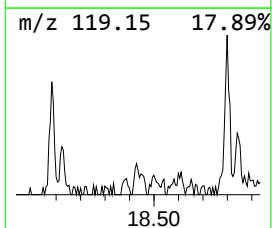
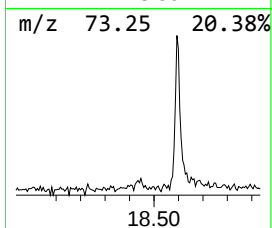
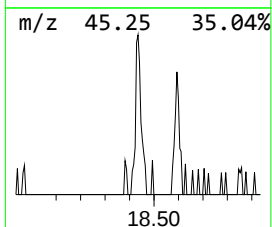
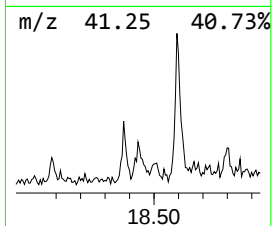
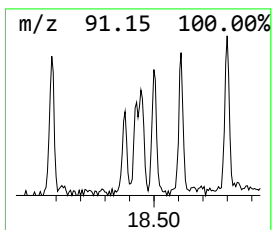
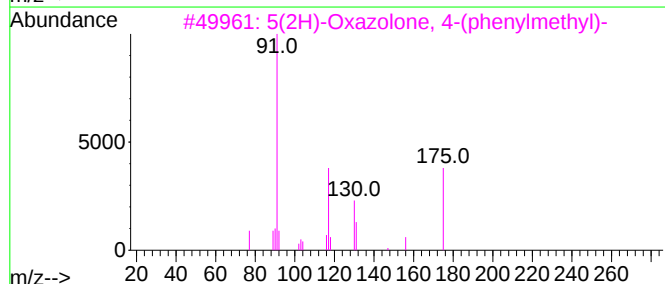
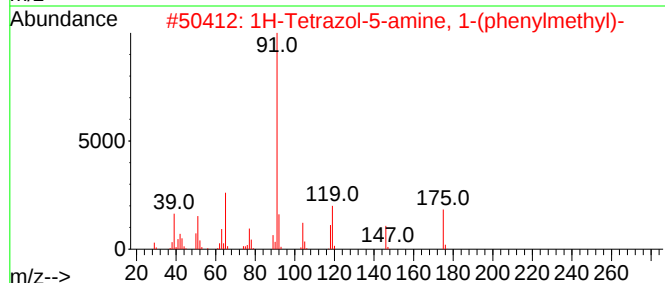
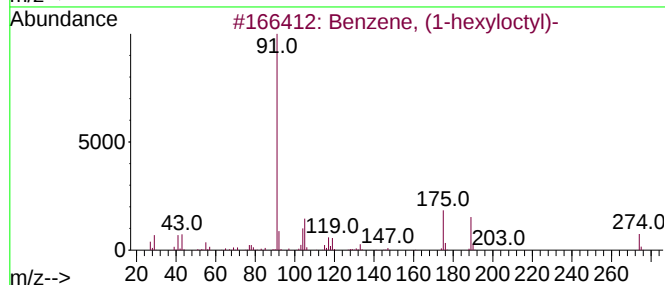
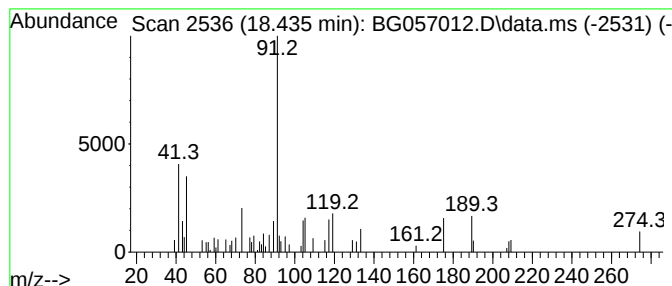
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Benzene, (1-hexyloctyl)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.435	3.45 ng	40504	Phenanthrene-d10	17.759

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (1-hexyloctyl)-	274	C20H34	004534-54-7	60
2			1H-Tetrazol-5-amine, 1-(phenylme...	175	C8H9N5	031694-90-3	27
3			5(2H)-Oxazolone, 4-(phenylmethyl)-	175	C10H9N02	049656-77-1	25
4			Diglycolic acid, 2-acetylphenyl ...	280	C14H16O6	1000382-71-6	22
5			Benzene, (1-hexylheptyl)-	260	C19H32	002400-01-3	17



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040623\
Data File : BG057012.D
Acq On : 6 Apr 2023 14:47
Operator : CG/JU
Sample : 02208-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

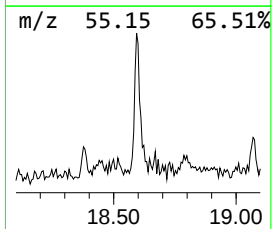
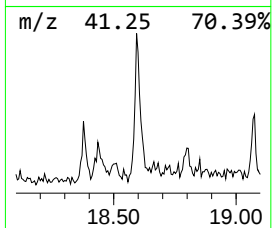
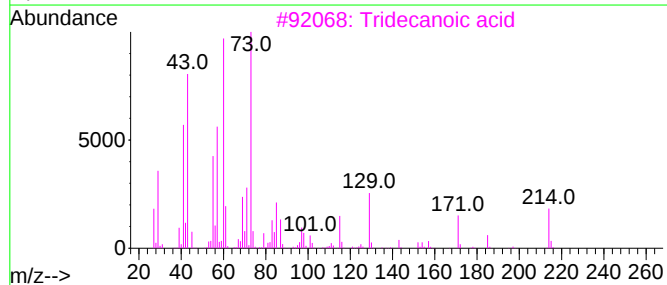
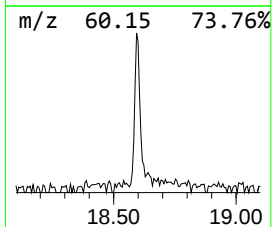
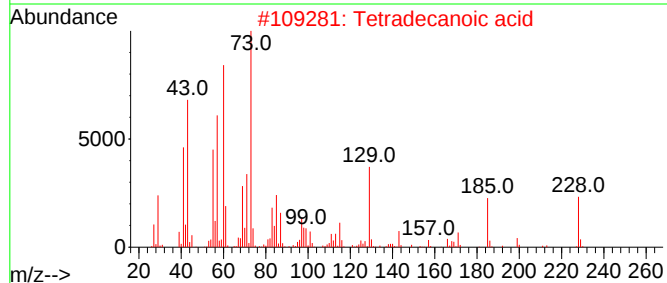
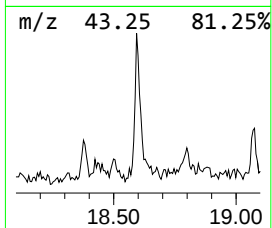
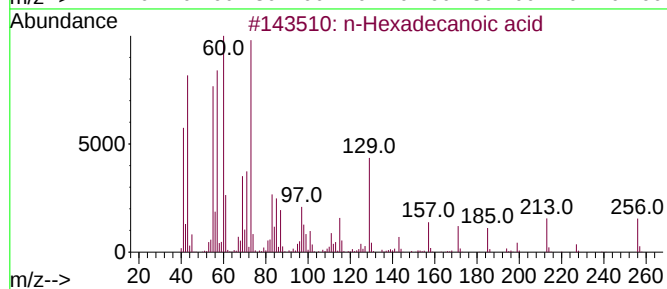
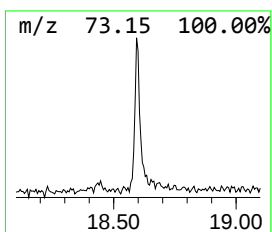
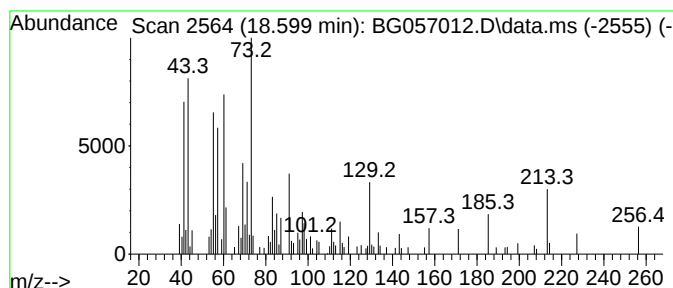
Instrument :
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ClientSampleId :
RO-124035

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.599	11.29 ng	132493	Phenanthrene-d10	17.759	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	68
3	Tridecanoic acid	214	C13H26O2	000638-53-9	64
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	47
5	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040623\
Data File : BG057012.D
Acq On : 6 Apr 2023 14:47
Operator : CG/JU
Sample : 02208-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RO-124035

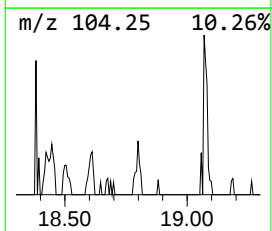
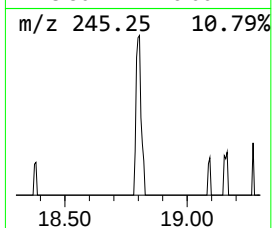
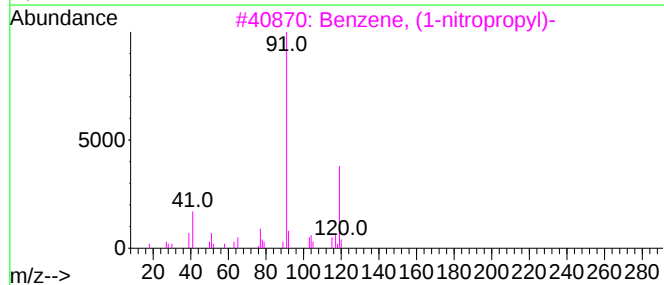
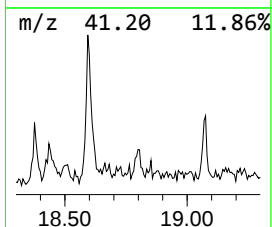
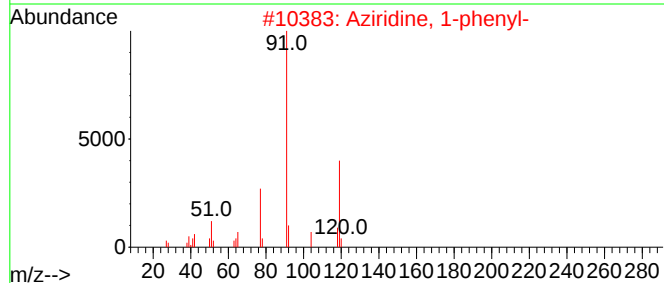
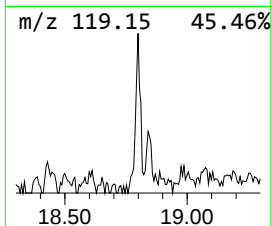
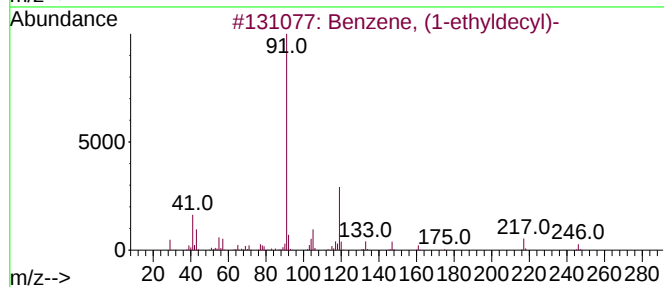
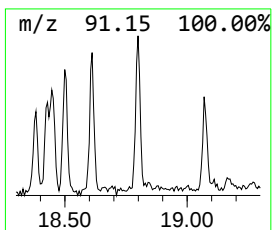
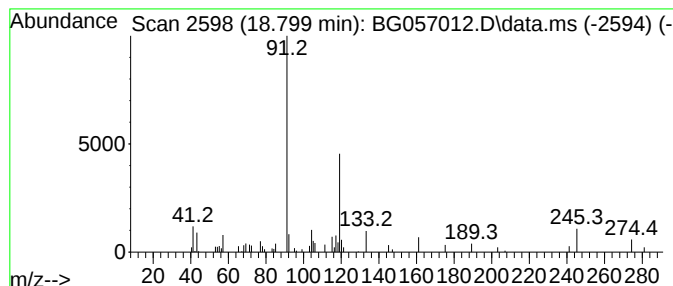
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Benzene, (1-ethyldecyl)- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.799	2.45 ng	28802	Phenanthrene-d10	17.759

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (1-ethyldecyl)-	246	C18H30	002400-00-2	50
2			Aziridine, 1-phenyl-	119	C8H9N	000696-18-4	50
3			Benzene, (1-nitropropyl)-	165	C9H11NO2	005279-14-1	50
4			Diglycolic acid, di(2-acetylphen...	370	C20H18O7	1000382-73-0	47
5			2-Phenylbutyryl chloride	182	C10H11ClO	036854-57-6	40



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040623\
Data File : BG057012.D
Acq On : 6 Apr 2023 14:47
Operator : CG/JU
Sample : 02208-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

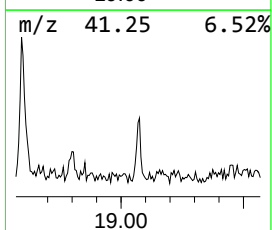
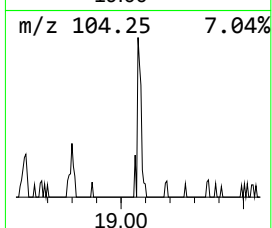
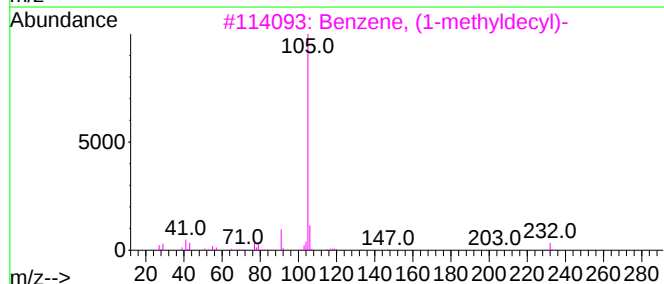
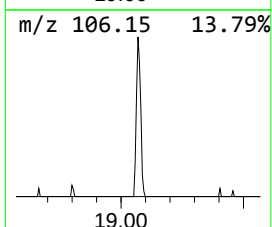
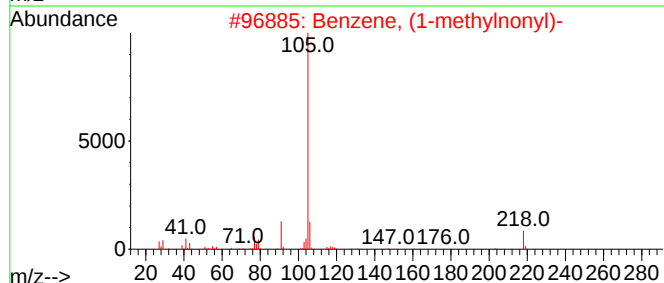
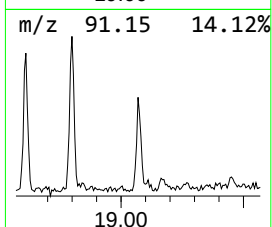
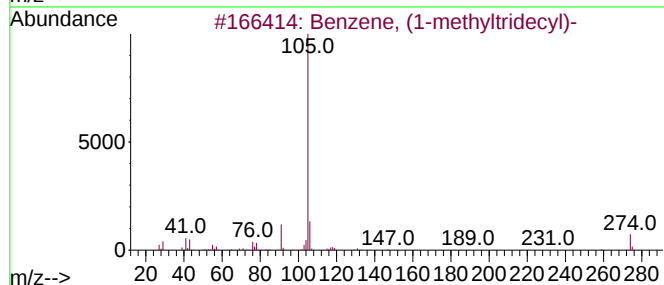
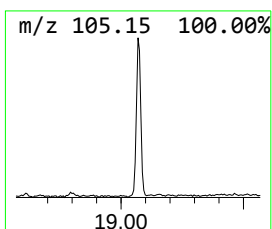
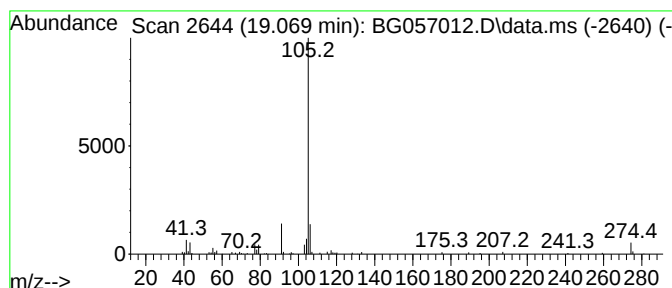
Instrument :
BNA_G
ClientSampleId :
RO-124035

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Benzene, (1-methyltridecyl)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.069	6.74 ng	79063	Phenanthrene-d10	17.759	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1-methyltridecyl)-	274	C20H34	004534-59-2	87
2	Benzene, (1-methylnonyl)-	218	C16H26	004537-13-7	78
3	Benzene, (1-methyldecyl)-	232	C17H28	004536-88-3	72
4	Benzene, (1-methylundecyl)-	246	C18H30	002719-61-1	64
5	Benzene, (1-methyldodecyl)-	260	C19H32	004534-53-6	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040623\
Data File : BG057012.D
Acq On : 6 Apr 2023 14:47
Operator : CG/JU
Sample : 02208-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

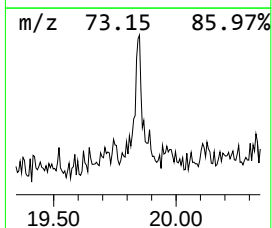
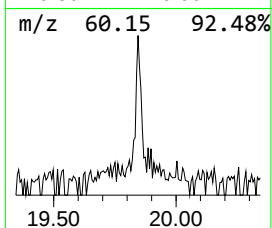
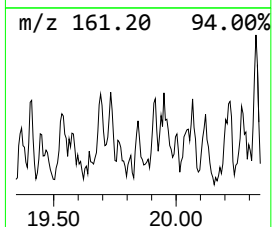
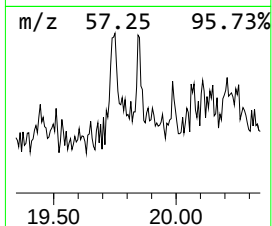
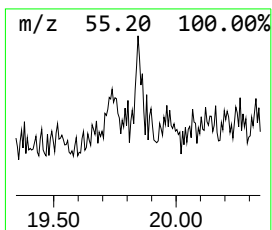
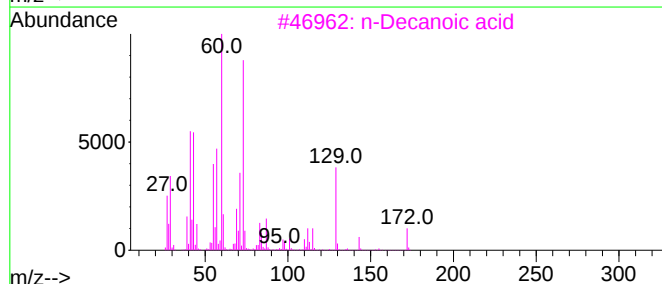
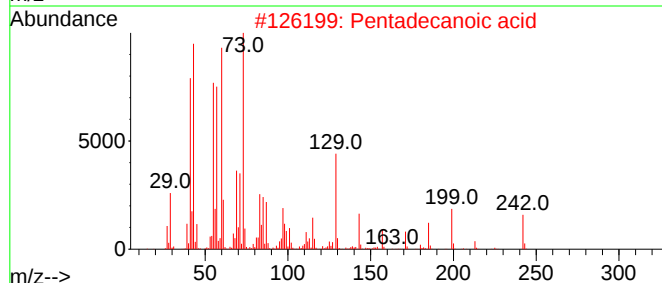
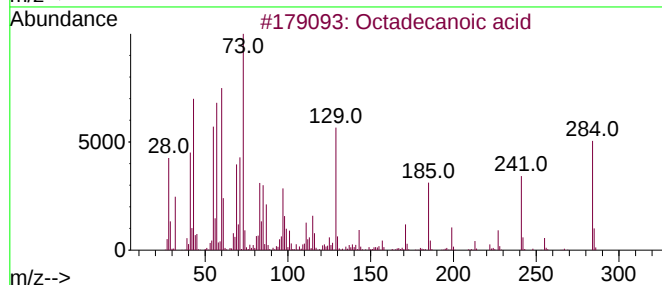
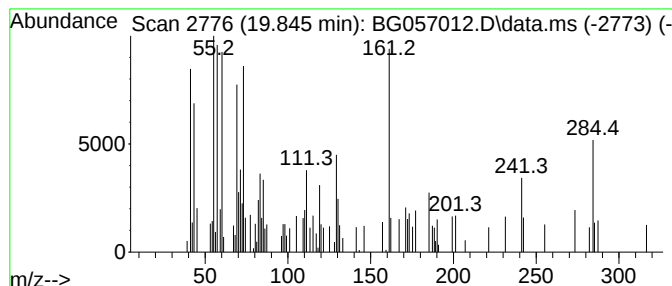
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Octadecanoic acid Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD		R.T.	
19.845	2.53 ng	29659	Phenanthrene-d10		17.759	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Octadecanoic acid		284	C18H36O2	000057-11-4	50
2	Pentadecanoic acid		242	C15H30O2	001002-84-2	35
3	n-Decanoic acid		172	C10H20O2	000334-48-5	18
4	Ethanone, 1-(4,5-dihydro-2-thiaz...		129	C5H7NOS	029926-41-8	18
5	Tetradecanoic acid		228	C14H28O2	000544-63-8	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040623\
Data File : BG057012.D
Acq On : 6 Apr 2023 14:47
Operator : CG/JU
Sample : 02208-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RO-124035

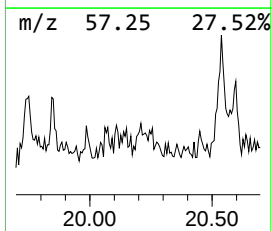
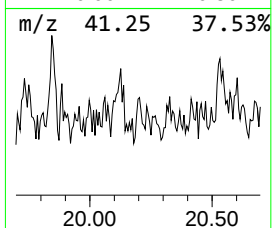
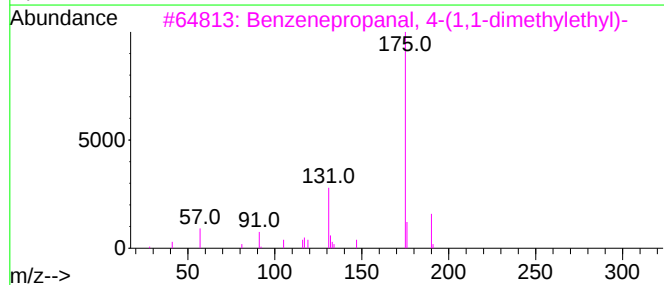
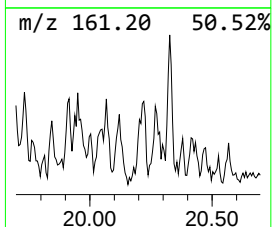
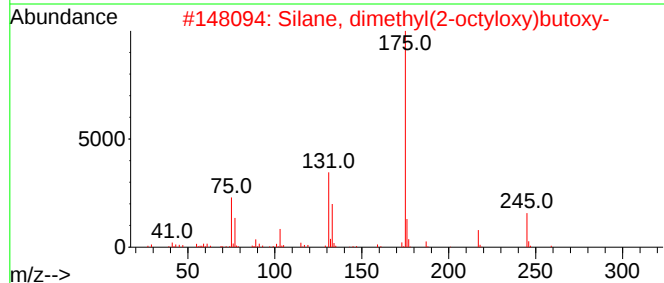
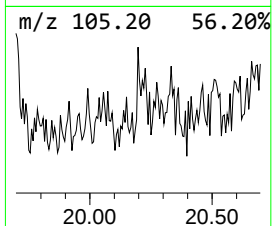
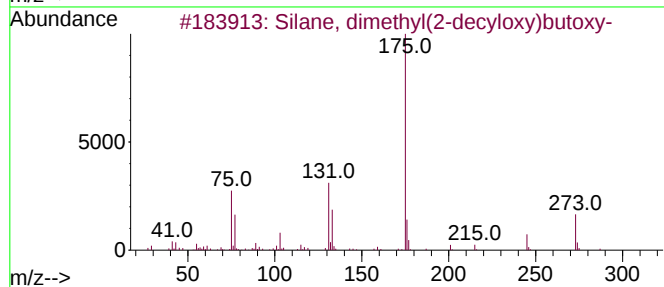
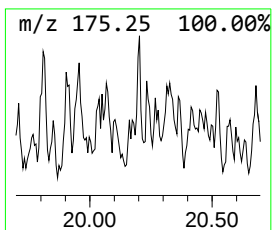
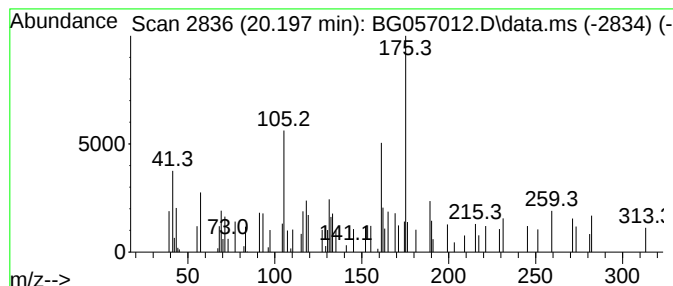
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 14 unknown20.197 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.197	2.40 ng	33361	Chrysene-d12	22.077

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Silane, dimethyl(2-decyloxy)butoxy-	288	C16H36O2Si	1000347-61-7	38
2			Silane, dimethyl(2-octyloxy)butoxy-	260	C14H32O2Si	1000346-84-1	35
3			Benzenepropanal, 4-(1,1-dimethyl...)	190	C13H18O	018127-01-0	27
4			p-Pentylacetophenone	190	C13H18O	037593-02-5	25
5			Benzene, 1,4-bis(1,1-dimethyleth...)	190	C14H22	001012-72-2	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040623\
Data File : BG057012.D
Acq On : 6 Apr 2023 14:47
Operator : CG/JU
Sample : 02208-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RO-124035

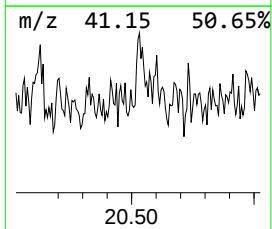
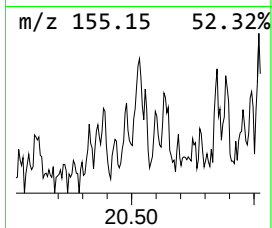
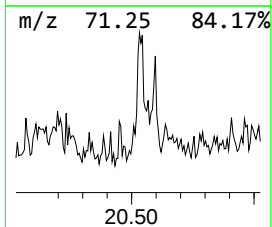
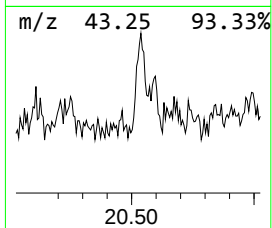
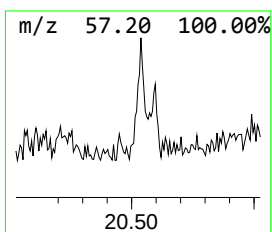
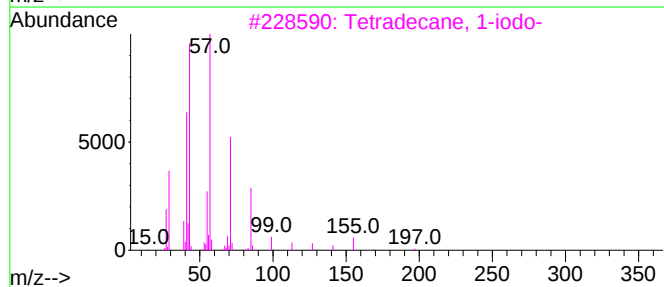
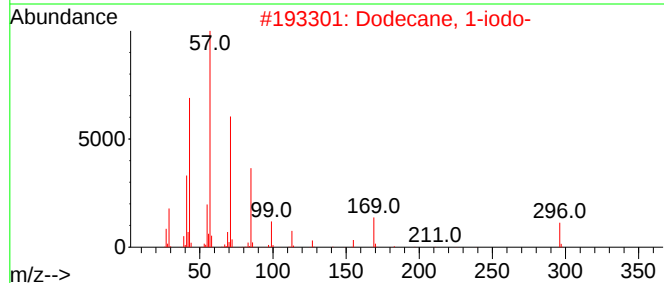
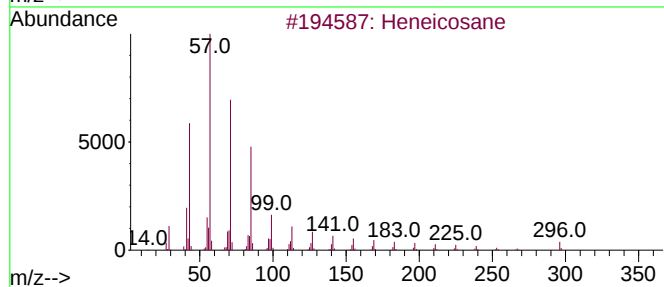
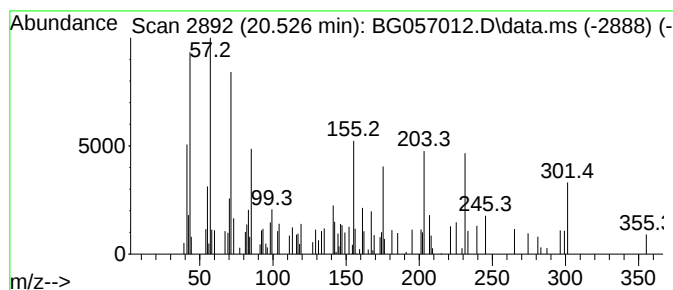
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 15 unknown20.526 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.526	2.88 ng	40099	Chrysene-d12	22.077

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heneicosane	296	C21H44	000629-94-7	38
2		Dodecane, 1-iodo-	296	C12H25I	004292-19-7	38
3		Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	35
4		Undecane	156	C11H24	001120-21-4	25
5		1-Nonene, 4,6,8-trimethyl-	168	C12H24	054410-98-9	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040623\
Data File : BG057012.D
Acq On : 6 Apr 2023 14:47
Operator : CG/JU
Sample : 02208-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

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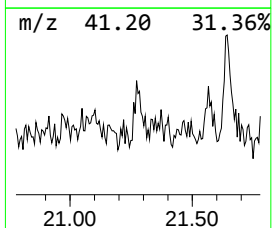
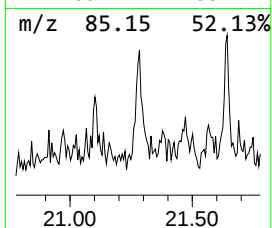
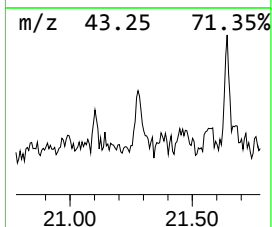
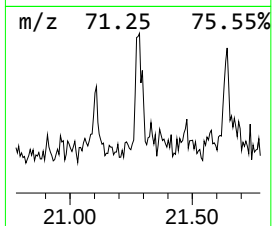
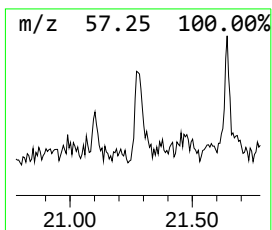
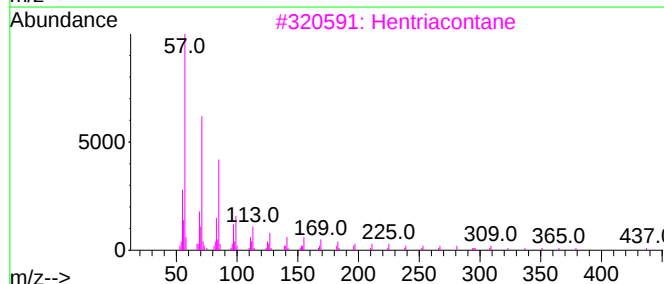
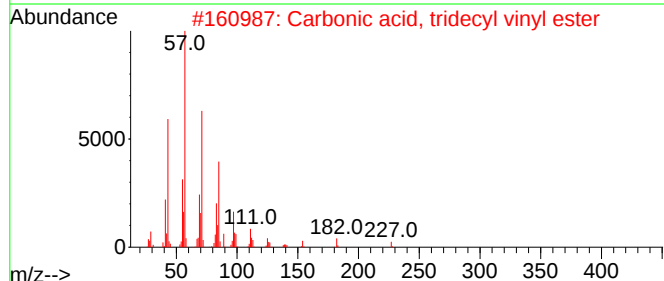
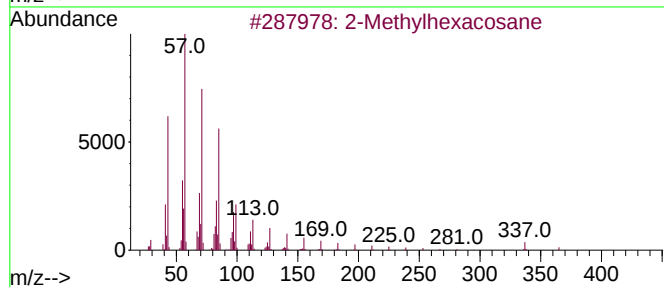
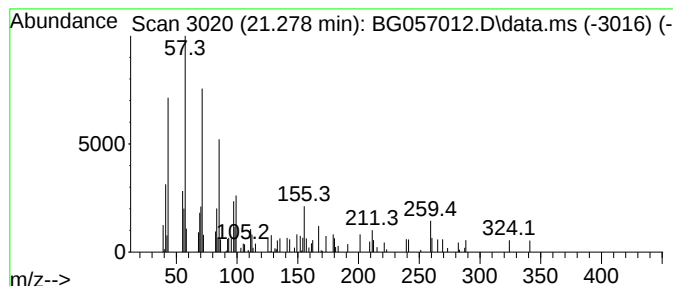
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 16 2-Methylhexacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.278	2.81 ng	39088	Chrysene-d12	22.077

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Methylhexacosane	380	C27H56	001561-02-0	64
2		Carbonic acid, tridecyl vinyl ester	270	C16H30O3	1000382-54-7	58
3		Hentriacontane	437	C31H64	000630-04-6	58
4		Carbonic acid, tetradecyl vinyl ...	284	C17H32O3	1000382-54-5	58
5		Eicosane	282	C20H42	000112-95-8	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040623\
Data File : BG057012.D
Acq On : 6 Apr 2023 14:47
Operator : CG/JU
Sample : 02208-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
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ClientSampleId :
RO-124035

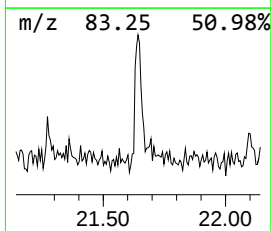
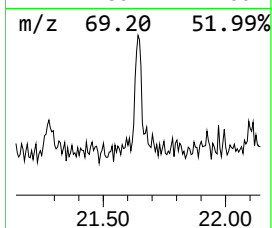
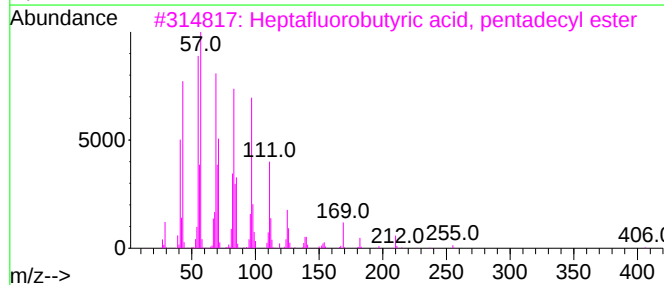
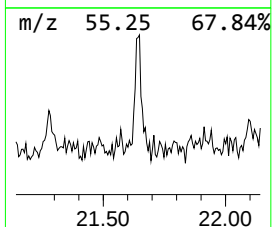
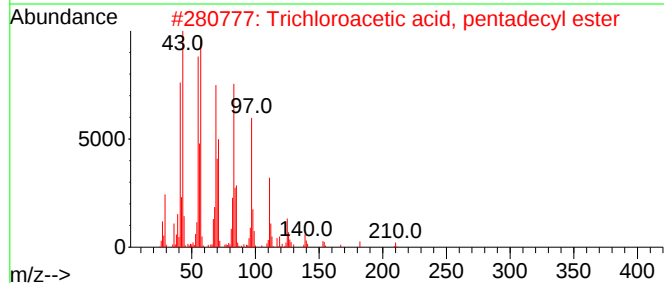
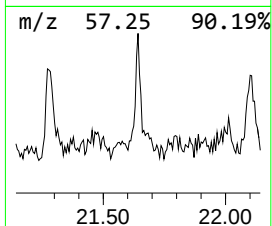
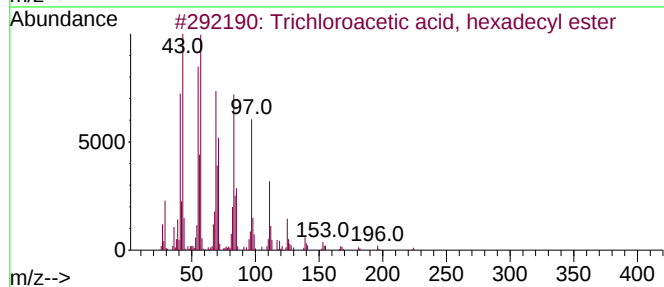
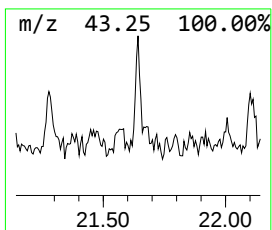
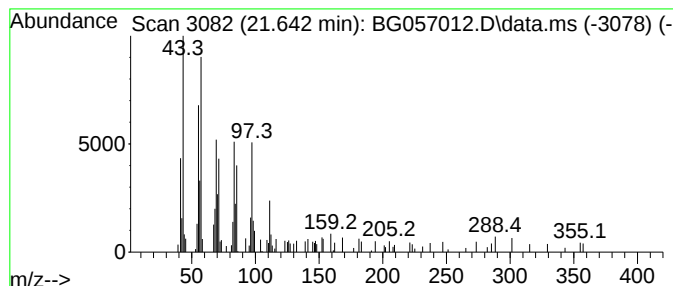
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 17 Trichloroacetic acid, hexad... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.642	3.29 ng	45786	Chrysene-d12	22.077

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	81
2			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	76
3			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	74
4			1-Tricosene	322	C23H46	018835-32-0	74
5			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040623\
Data File : BG057012.D
Acq On : 6 Apr 2023 14:47
Operator : CG/JU
Sample : 02208-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

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ClientSampleId :
RO-124035

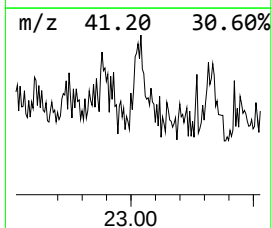
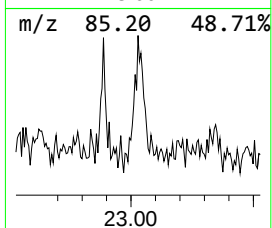
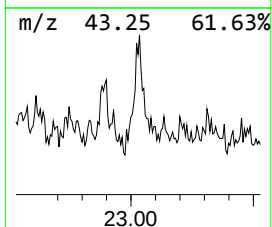
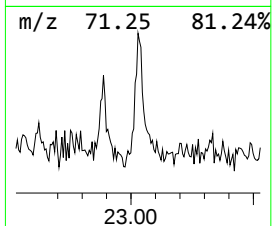
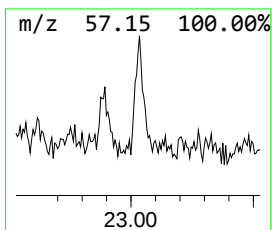
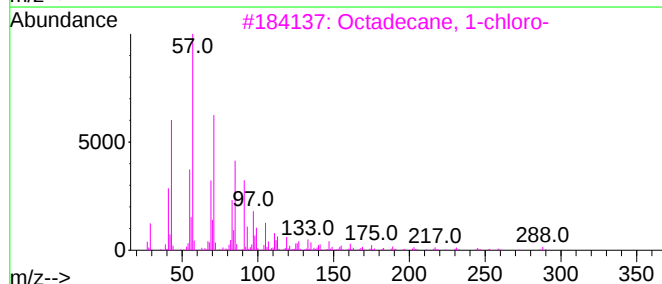
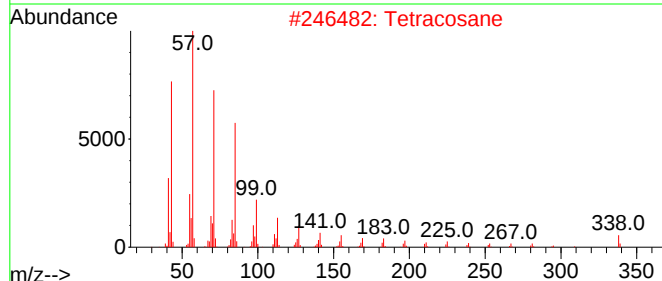
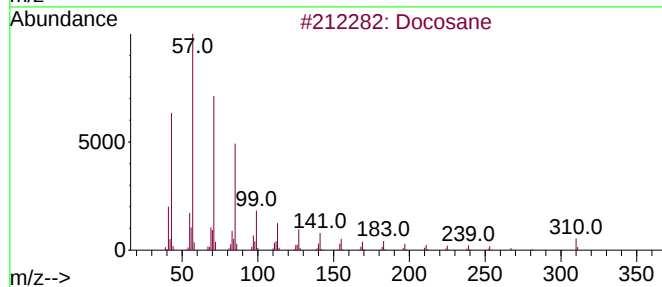
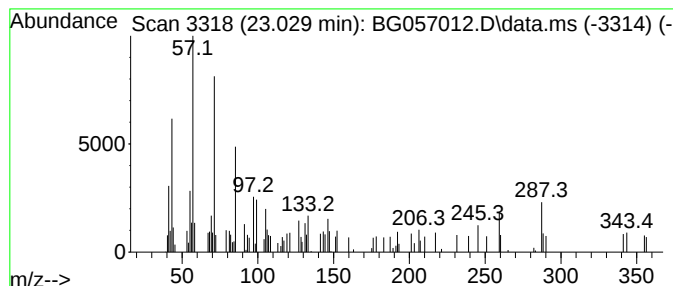
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 18 Docosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.029	2.99 ng	41648	Chrysene-d12	22.077

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Docosane	310	C22H46	000629-97-0	50
2		Tetracosane	338	C24H50	000646-31-1	50
3		Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	50
4		2-Bromononane	206	C9H19Br	002216-35-5	43
5		Undecane, 2-methyl-	170	C12H26	007045-71-8	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040623\
Data File : BG057012.D
Acq On : 6 Apr 2023 14:47
Operator : CG/JU
Sample : 02208-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RO-124035

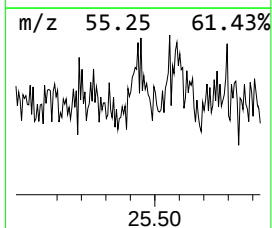
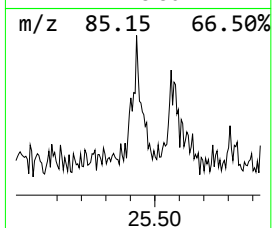
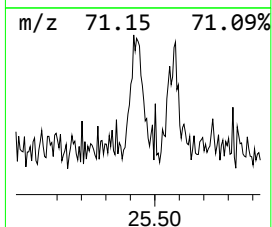
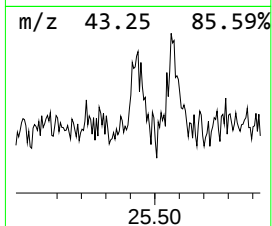
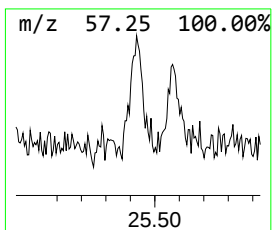
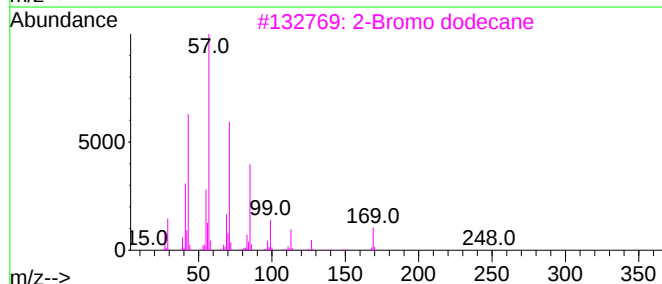
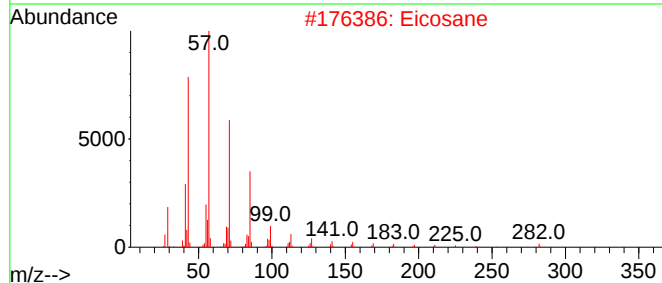
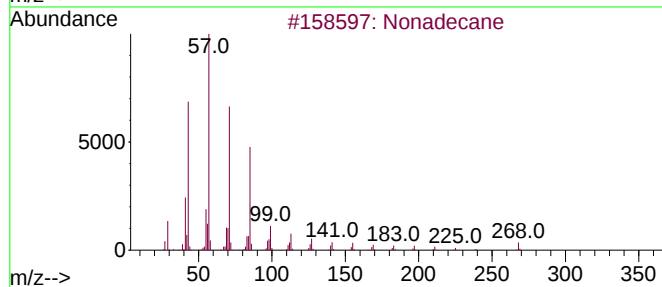
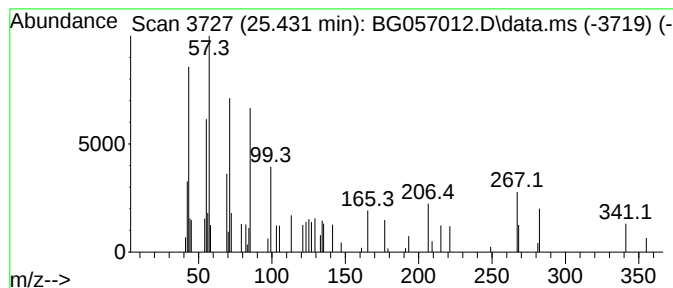
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 19 unknown25.431 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.431	2.13 ng	28035	Perylene-d12	25.613

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Nonadecane	268	C19H40	000629-92-5	46
2		Eicosane	282	C20H42	000112-95-8	46
3		2-Bromo dodecane	248	C12H25Br	013187-99-0	35
4		Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	27
5		Heptadecane	240	C17H36	000629-78-7	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040623\
Data File : BG057012.D
Acq On : 6 Apr 2023 14:47
Operator : CG/JU
Sample : 02208-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

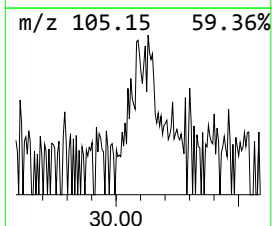
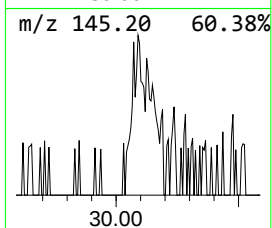
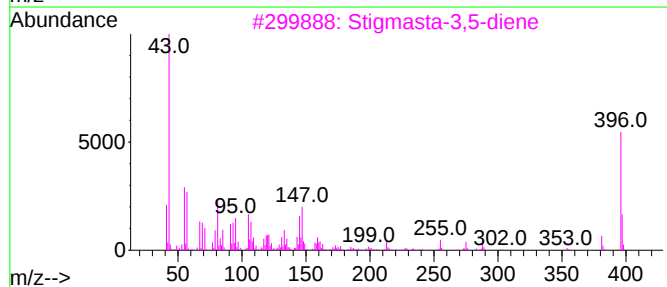
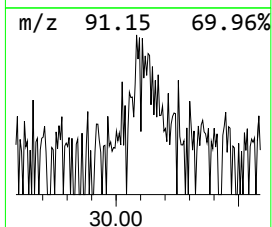
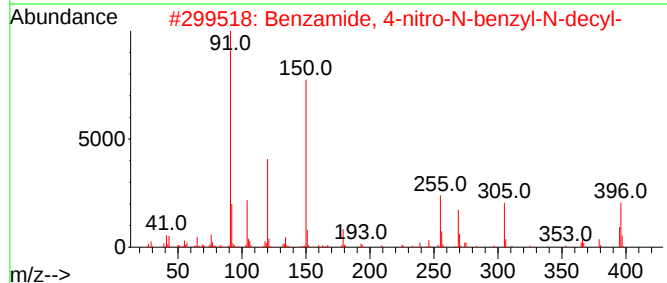
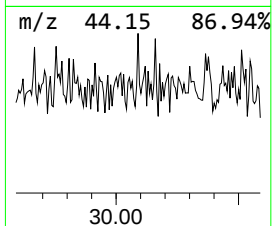
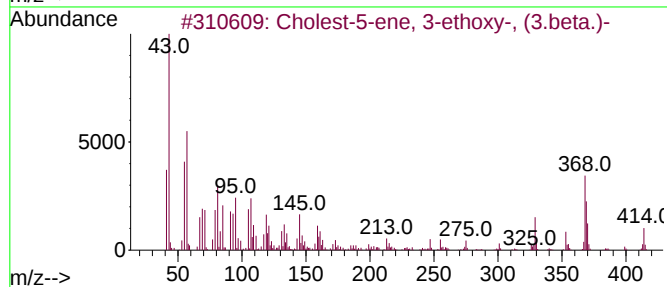
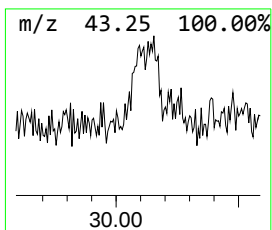
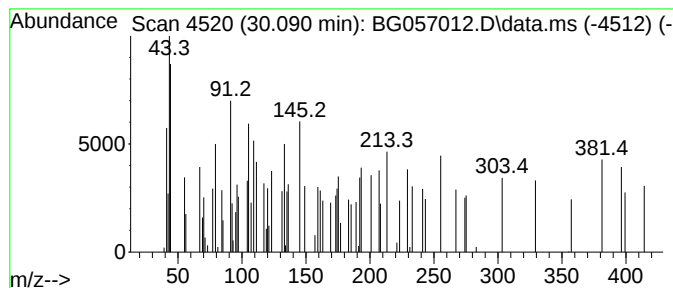
Instrument :
BNA_G
ClientSampleId :
RO-124035

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 20 unknown30.090 Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.	
30.090	2.12 ng	27908	Perylene-d12	25.613	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cholest-5-ene, 3-ethoxy-, (3.bet...	414	C29H50O	000986-19-6	9
2	Benzamide, 4-nitro-N-benzyl-N-de...	396	C24H32N2O3	1000446-50-8	9
3	Stigmasta-3,5-diene	396	C29H48	004970-37-0	7
4	Ethyl 3-[(5-amino-1-benzyl-1,2,4...	329	C17H23N5O2	1000435-35-2	4
5	.beta.-Sitosterol acetate	456	C31H52O2	000915-05-9	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040623\
Data File : BG057012.D
Acq On : 6 Apr 2023 14:47
Operator : CG/JU
Sample : 02208-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RO-124035

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.447	148.5	ng	681787	1	8.413	91813	20.0
Mequinol	11.415	2.7	ng	16319	2	11.250	120850	20.0
unknown15.175	15.175	8.7	ng	76701	3	15.022	176641	20.0
Benzophenone	16.355	2.7	ng	23992	3	15.022	176641	20.0
Benzene, (1-met...	17.618	2.5	ng	28860	4	17.759	234720	20.0
Benzene, (1-pro...	17.883	2.3	ng	26412	4	17.759	234720	20.0
Benzene, (1-eth...	18.082	2.2	ng	26295	4	17.759	234720	20.0
Benzene, (1-met...	18.382	6.8	ng	79339	4	17.759	234720	20.0
Benzene, (1-hex...	18.435	3.5	ng	40504	4	17.759	234720	20.0
n-Hexadecanoic ...	18.599	11.3	ng	132493	4	17.759	234720	20.0
Benzene, (1-eth...	18.799	2.5	ng	28802	4	17.759	234720	20.0
Benzene, (1-met...	19.069	6.7	ng	79063	4	17.759	234720	20.0
Octadecanoic acid	19.845	2.5	ng	29659	4	17.759	234720	20.0
unknown20.197	20.197	2.4	ng	33361	5	22.077	278223	20.0
unknown20.526	20.526	2.9	ng	40099	5	22.077	278223	20.0
2-Methylhexacosane	21.278	2.8	ng	39088	5	22.077	278223	20.0
Trichloroacetic...	21.642	3.3	ng	45786	5	22.077	278223	20.0
Docosane	23.029	3.0	ng	41648	5	22.077	278223	20.0
unknown25.431	25.431	2.1	ng	28035	6	25.613	263313	20.0
unknown30.090	30.090	2.1	ng	27908	6	25.613	263313	20.0