

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122122\
 Data File : BG056047.D
 Acq On : 21 Dec 2022 13:58
 Operator : CG/JU
 Sample : N6038-24
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 RB-41-(0-2)

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-BG121322.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG056047.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.385	12	16	23	rBV	17247	24816	3.29%	0.528%
2	5.400	354	359	365	rBB	14094	19928	2.64%	0.424%
3	5.876	434	440	447	rBB	110217	172632	22.90%	3.676%
4	7.492	708	715	722	rBB	115424	198651	26.35%	4.230%
5	8.361	857	863	869	rBB	27220	43124	5.72%	0.918%
6	9.531	1055	1062	1069	rBB	70826	123813	16.42%	2.636%
7	11.193	1337	1345	1351	rBV	39038	64602	8.57%	1.376%
8	13.596	1747	1754	1761	rVB	262528	401770	53.29%	8.555%
9	14.701	1935	1942	1946	rBV2	4402	8293	1.10%	0.177%
10	14.965	1981	1987	1994	rVB	74190	116259	15.42%	2.475%
11	16.305	2209	2215	2221	rVB	44439	64287	8.53%	1.369%
12	16.446	2232	2239	2248	rVB	312170	481257	63.83%	10.247%
13	17.703	2445	2453	2457	rBV	112906	165823	21.99%	3.531%
14	17.744	2457	2460	2467	rVB	21715	29396	3.90%	0.626%
15	18.549	2591	2597	2605	rBV3	36665	53100	7.04%	1.131%
16	18.620	2605	2609	2614	rVB2	6110	9383	1.24%	0.200%
17	18.761	2627	2633	2638	rBV5	6307	14267	1.89%	0.304%
18	19.061	2677	2684	2687	rBV	5087	7884	1.05%	0.168%
19	19.096	2687	2690	2695	rVV4	7403	10358	1.37%	0.221%
20	19.472	2746	2754	2758	rBV4	7290	13435	1.78%	0.286%
21	19.613	2773	2778	2781	rBV3	5793	11082	1.47%	0.236%
22	19.730	2793	2798	2804	rVB	75509	113214	15.02%	2.411%
23	19.801	2804	2810	2820	rVB7	9051	21516	2.85%	0.458%
24	19.883	2820	2824	2828	rBV	6537	9994	1.33%	0.213%
25	19.995	2835	2843	2847	rVB2	7069	13554	1.80%	0.289%
26	20.054	2849	2853	2854	rVV3	8630	9897	1.31%	0.211%
27	20.095	2855	2860	2866	rVB	87149	126181	16.74%	2.687%
28	20.159	2866	2871	2876	rBV5	6192	9919	1.32%	0.211%
29	20.277	2885	2891	2896	rBV	599275	753977	100.00%	16.054%
30	20.400	2905	2912	2913	rBV6	9517	13016	1.73%	0.277%
31	20.418	2913	2915	2922	rVB6	10811	16058	2.13%	0.342%
32	20.571	2930	2941	2948	rVB	15289	44327	5.88%	0.944%
33	20.676	2955	2959	2963	rBV	9804	17288	2.29%	0.368%
34	20.735	2964	2969	2973	rVV2	14337	23068	3.06%	0.491%
35	20.876	2989	2993	2998	rBV2	12805	17298	2.29%	0.368%
36	20.923	2998	3001	3007	rVB	10225	14504	1.92%	0.309%

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Stop Thrs : 0

Peak Location: TOP

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37	21.364	3073	3076	3082	rVB2	10513	18977	2.52%	0.404%
38	21.558	3107	3109	3112	rBV2	6508	8095	1.07%	0.172%
39	21.593	3112	3115	3121	rVB3	31432	52454	6.96%	1.117%
40	21.652	3121	3125	3131	rBV2	8938	16671	2.21%	0.355%
41	21.710	3131	3135	3143	rVB2	9420	21838	2.90%	0.465%
42	21.945	3171	3175	3178	rBV3	20546	33813	4.48%	0.720%
43	22.004	3178	3185	3190	rVV2	136507	320249	42.47%	6.819%
44	22.057	3190	3194	3200	rVB	51511	88992	11.80%	1.895%
45	22.169	3208	3213	3217	rBV7	4559	9976	1.32%	0.212%
46	22.280	3230	3232	3240	rVB3	9220	14639	1.94%	0.312%
47	22.791	3310	3319	3324	rBV2	11577	29163	3.87%	0.621%
48	22.838	3324	3327	3328	rVV2	7951	9263	1.23%	0.197%
49	22.868	3328	3332	3340	rVB5	13959	28863	3.83%	0.615%
50	23.079	3364	3368	3370	rBV5	5428	7597	1.01%	0.162%
51	23.244	3392	3396	3402	rVB6	7180	12703	1.68%	0.270%
52	23.802	3486	3491	3501	rVB3	19857	41930	5.56%	0.893%
53	24.125	3544	3546	3554	rVB8	5360	7769	1.03%	0.165%
54	24.372	3581	3588	3598	rBV4	38264	141133	18.72%	3.005%
55	24.654	3633	3636	3646	rVB2	12627	32601	4.32%	0.694%
56	25.165	3714	3723	3732	rBV	30199	84297	11.18%	1.795%
57	25.324	3742	3750	3762	rVB3	44170	135474	17.97%	2.885%
58	25.494	3767	3779	3787	rBV2	75539	229363	30.42%	4.884%
59	26.082	3873	3879	3883	rVB8	5057	11742	1.56%	0.250%
60	29.495	4450	4460	4462	rBV2	17311	46297	6.14%	0.986%
61	30.759	4663	4675	4681	rBV2	13255	54559	7.24%	1.162%

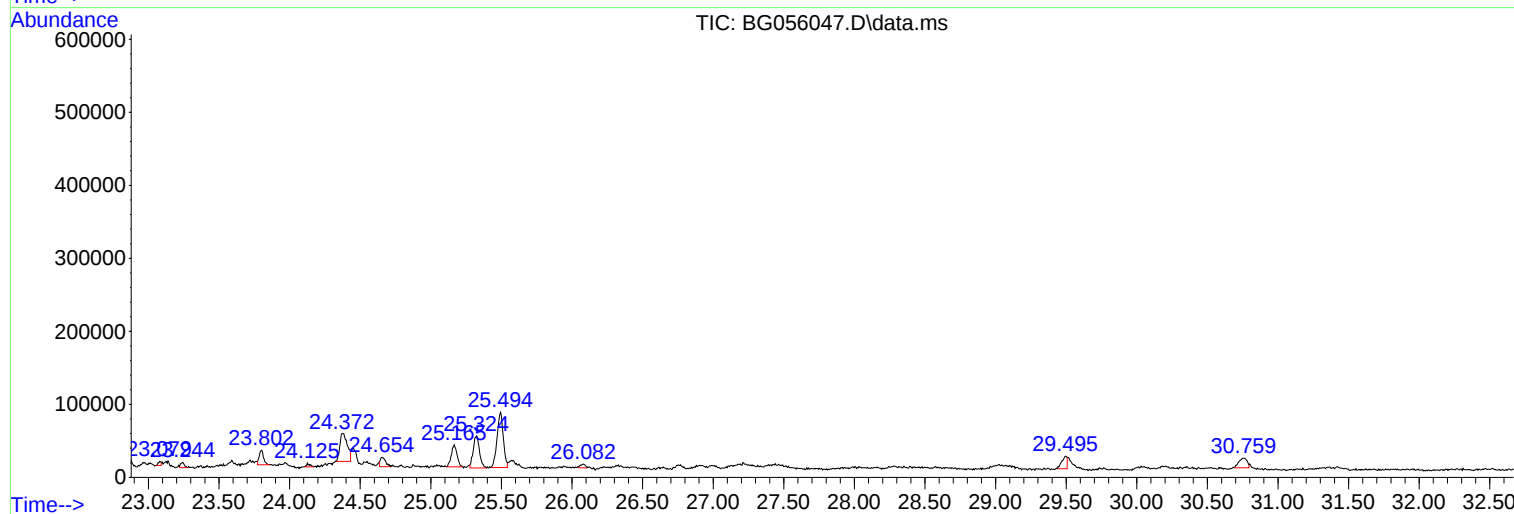
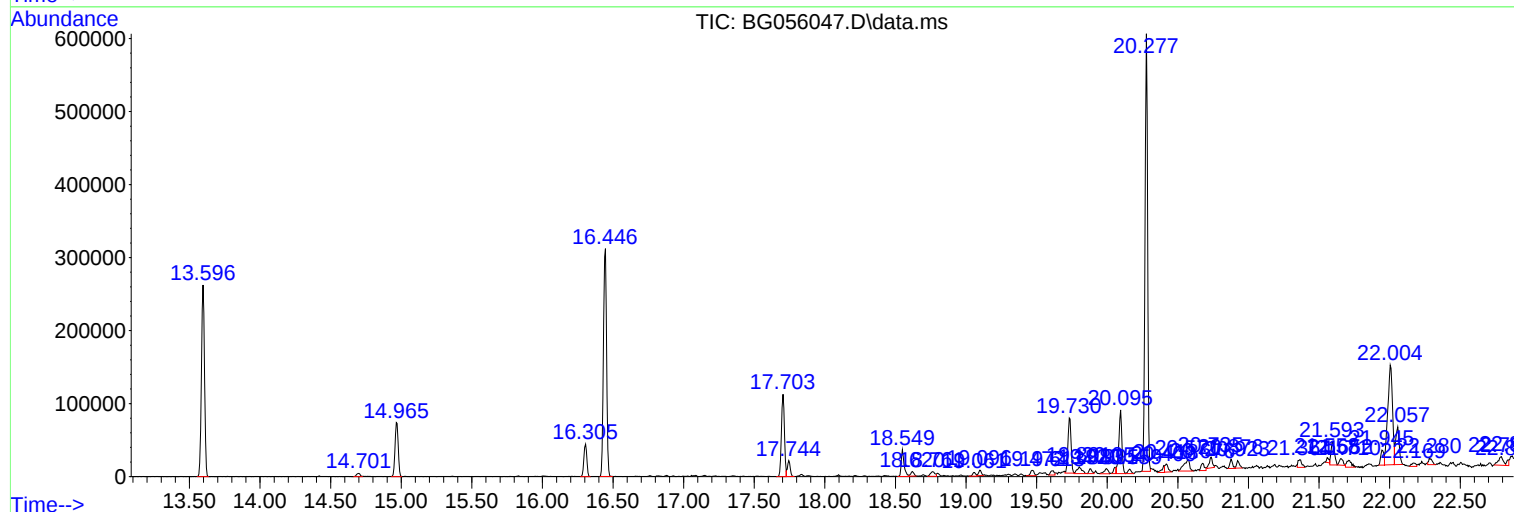
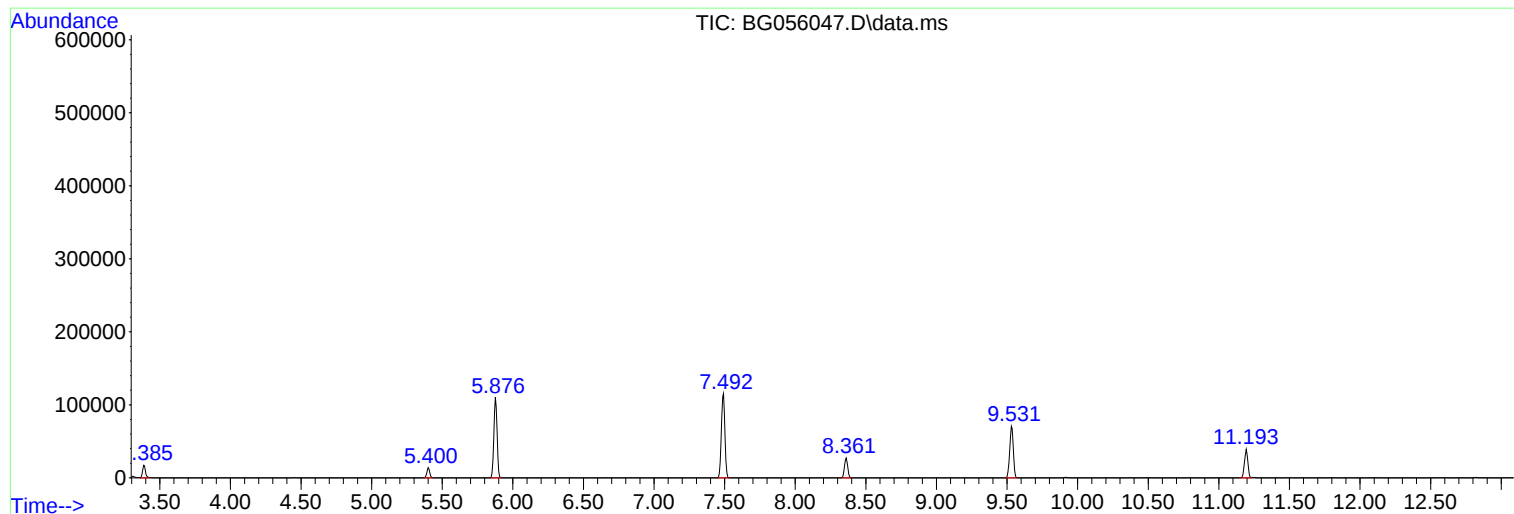
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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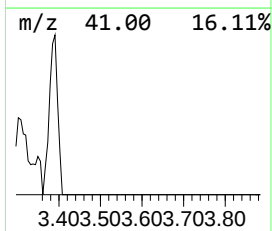
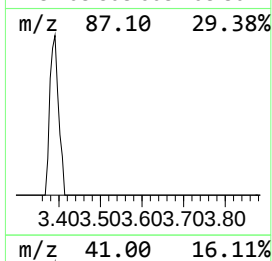
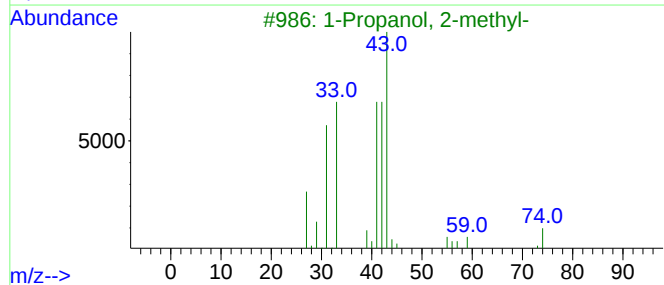
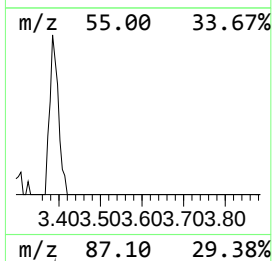
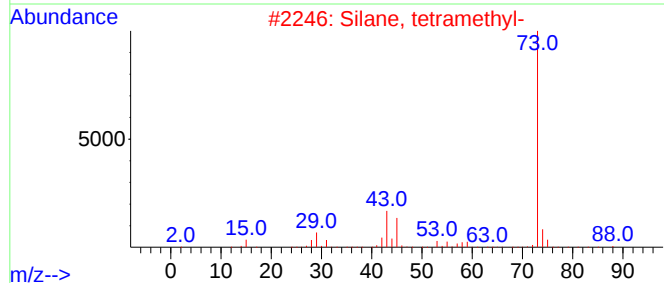
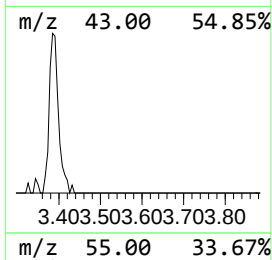
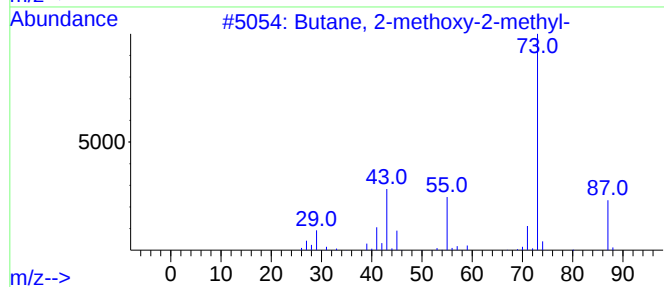
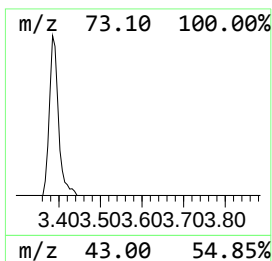
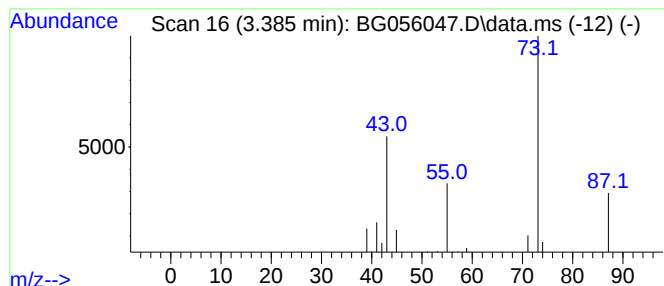
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.385	11.51 ng	24816	1,4-Dichlorobenzene-d4	8.361

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			Silane, tetramethyl-	88	C4H12Si	000075-76-3	25
3			1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	10
4			1-Propene-1-thiol	74	C3H6S	000925-89-3	9
5			Acetic acid, methyl ester	74	C3H6O2	000079-20-9	9



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ALS Vial : 7 Sample Multiplier: 1

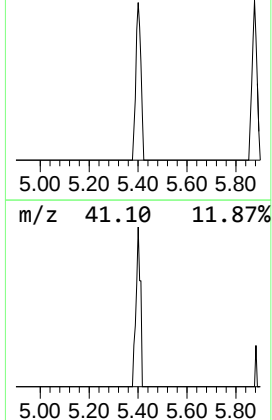
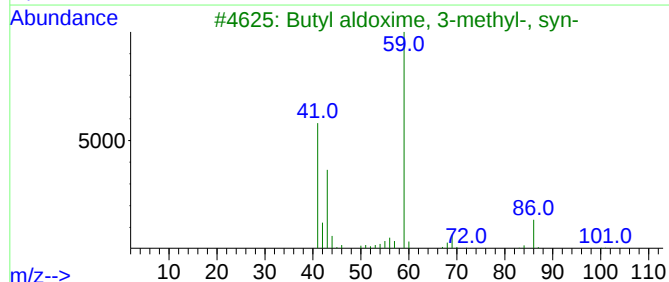
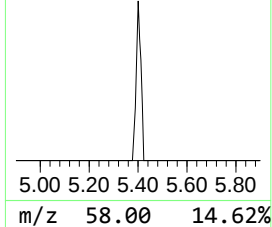
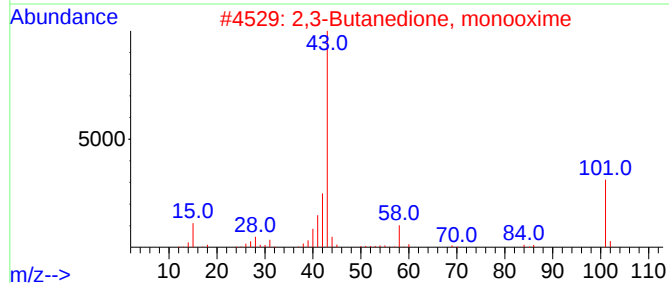
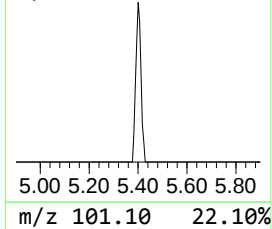
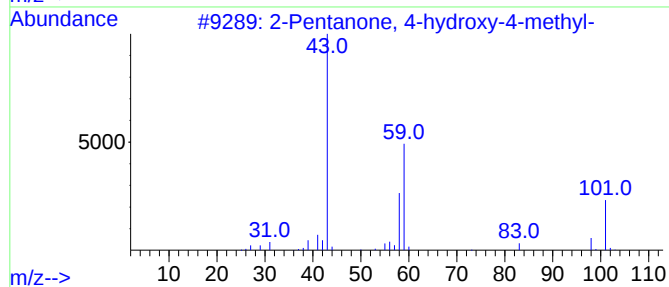
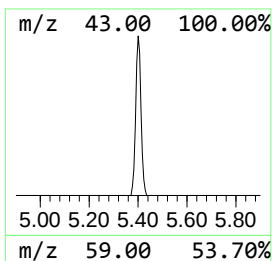
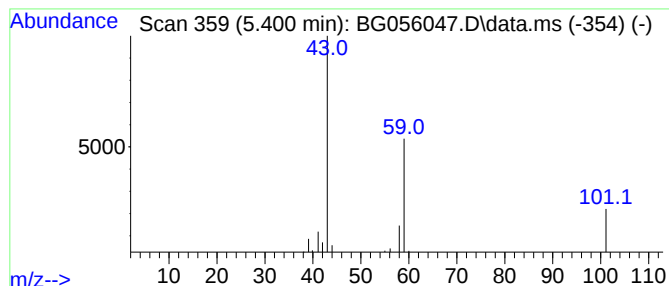
Instrument :
BNA_G
ClientSampleId :
RB-41-(0-2)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD		R.T.	
5.400	9.24 ng	19928	1,4-Dichlorobenzene-d4		8.361	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	56
2	2,3-Butanedione, monooxime		101	C4H7NO2	000057-71-6	32
3	Butyl aldoxime, 3-methyl-, syn-		101	C5H11NO	005780-40-5	23
4	Propylamine		59	C3H9N	000107-10-8	9
5	Morpholine, 4-methyl-		101	C5H11NO	000109-02-4	9



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ALS Vial : 7 Sample Multiplier: 1

Instrument :
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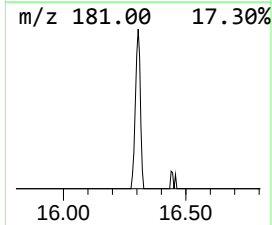
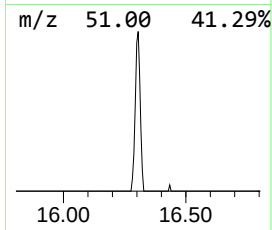
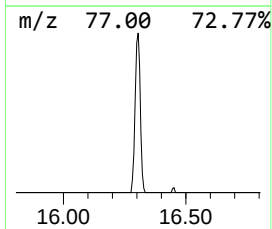
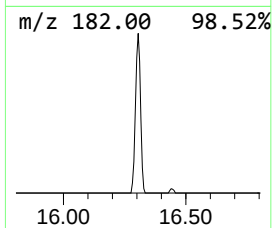
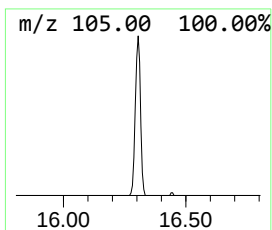
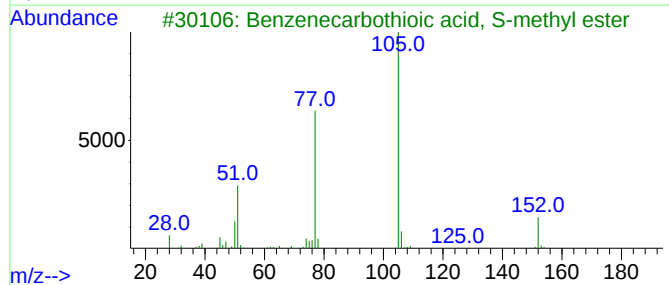
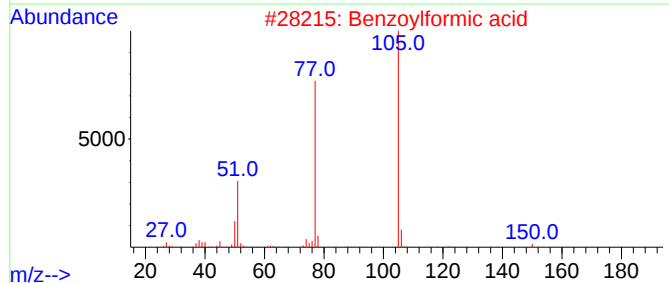
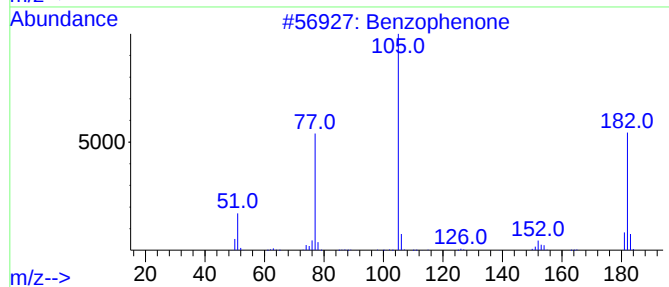
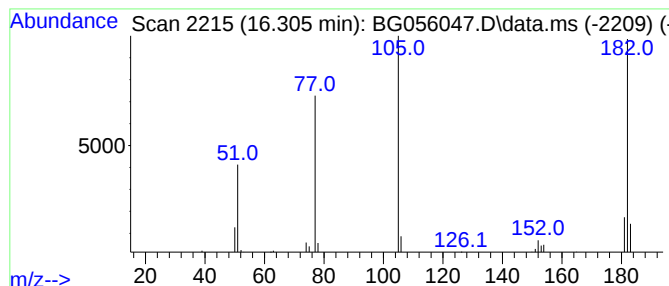
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.305	11.06 ng	64287	Acenaphthene-d10	14.965

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	95
2			Benzoylformic acid	150	C8H6O3	000611-73-4	46
3			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	45
4			2,4,6-Trimethoxytoluene	182	C10H14O3	014107-97-2	38
5			7-Phosphabicyclo[2.2.1]hept-2-en...	182	C11H19P	1000151-83-5	38



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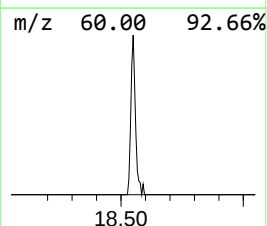
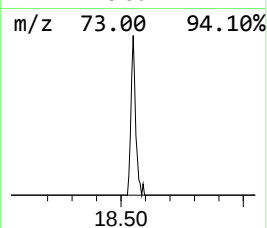
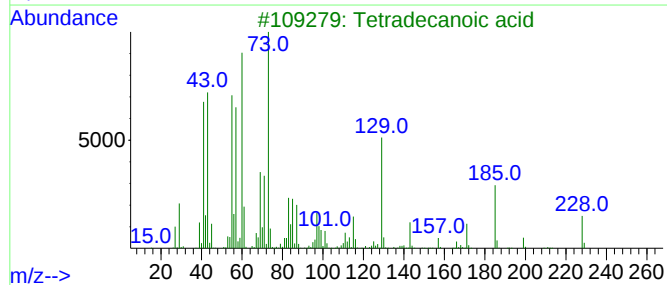
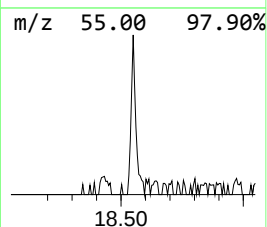
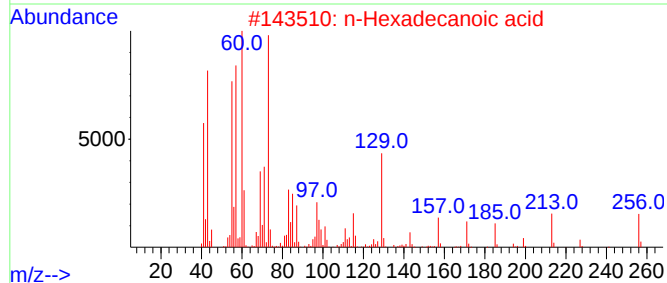
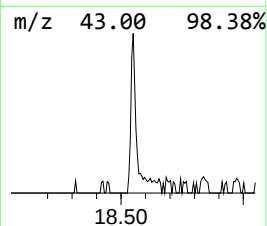
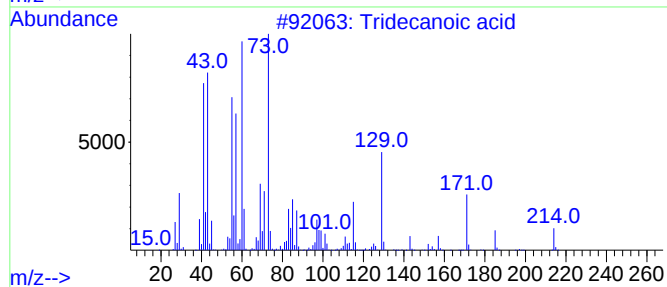
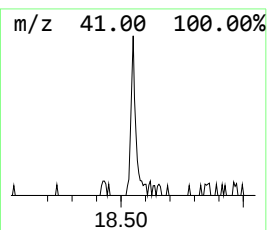
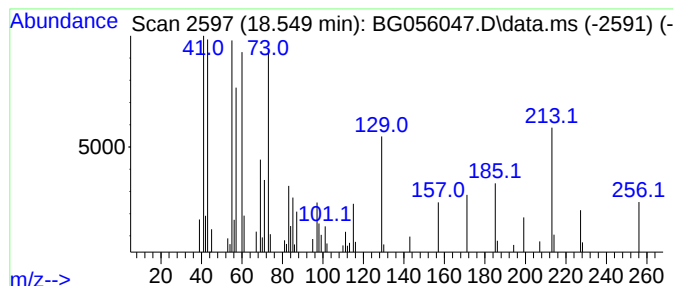
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Tridecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.549	6.40 ng	53100	Phenanthrene-d10	17.703

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	96
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	49
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	43
5	Dodecanoic acid	200	C12H24O2	000143-07-7	41



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RB-41-(0-2)

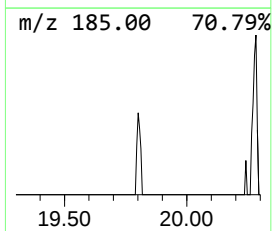
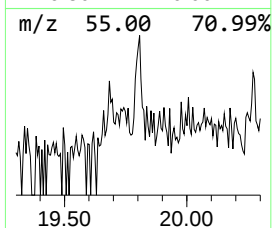
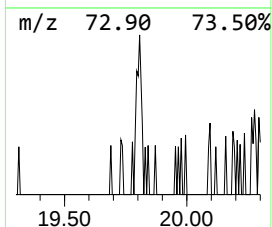
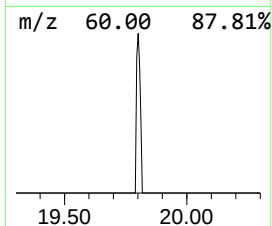
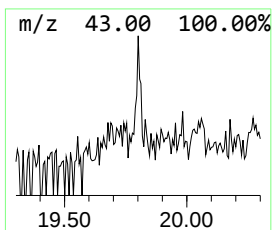
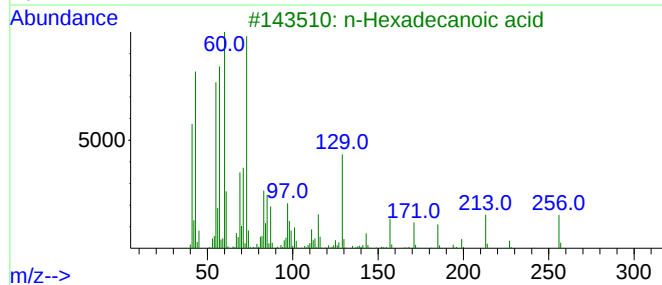
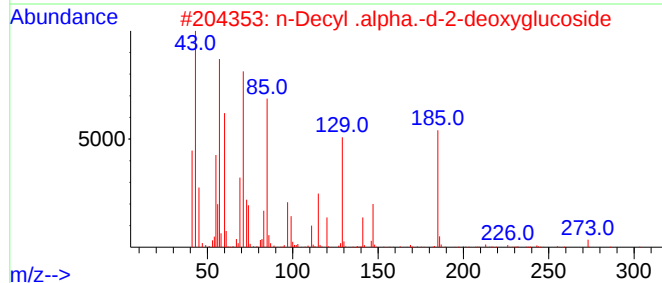
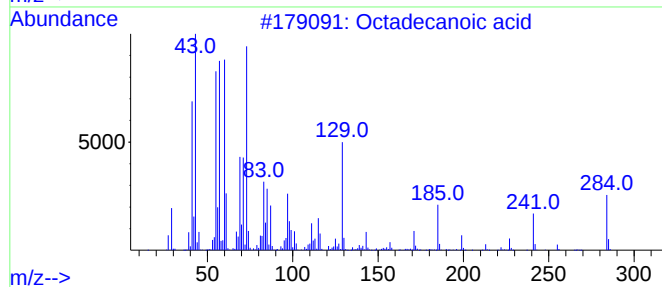
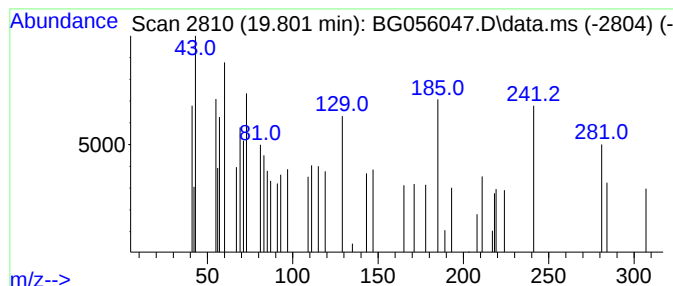
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown19.801 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.801	2.60 ng	21516	Phenanthrene-d10	17.703

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	38
2			n-Decyl .alpha.-d-2-deoxyglucoside	304	C16H32O5	1000211-42-8	32
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	12
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	12
5			Tridecanoic acid	214	C13H26O2	000638-53-9	12



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122122\
Data File : BG056047.D
Acq On : 21 Dec 2022 13:58
Operator : CG/JU
Sample : N6038-24
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RB-41-(0-2)

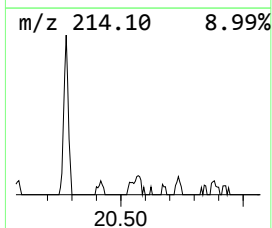
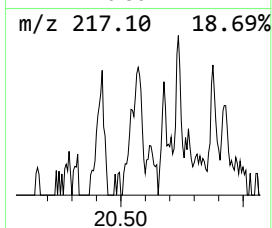
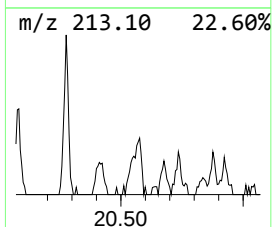
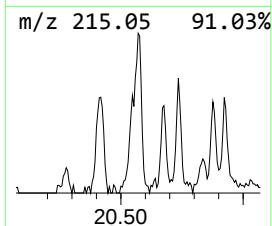
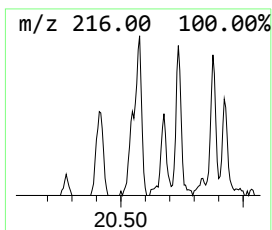
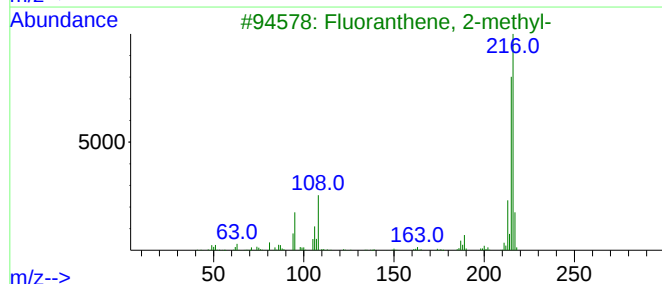
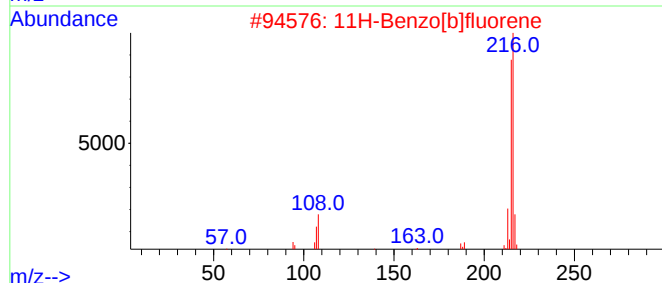
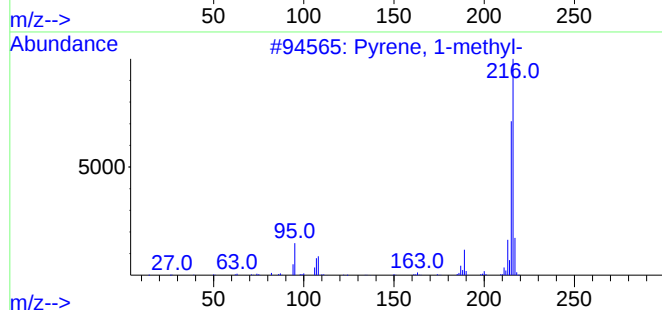
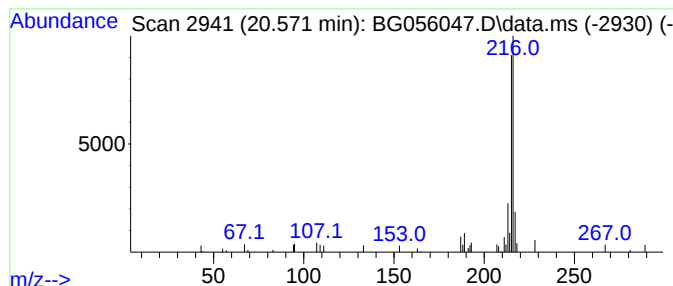
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Pyrene, 1-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.570	2.77 ng	44327	Chrysene-d12	22.004

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pyrene, 1-methyl-	216	C17H12	002381-21-7	91
2		11H-Benzo[b]fluorene	216	C17H12	000243-17-4	87
3		Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	87
4		11H-Benzo[a]fluorene	216	C17H12	000238-84-6	87
5		7H-Benzo[c]fluorene	216	C17H12	000205-12-9	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122122\
Data File : BG056047.D
Acq On : 21 Dec 2022 13:58
Operator : CG/JU
Sample : N6038-24
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
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ClientSampleId :
RB-41-(0-2)

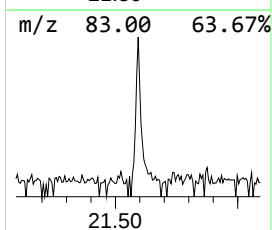
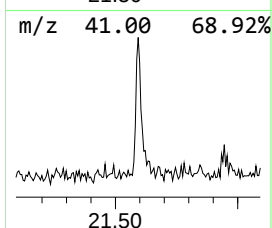
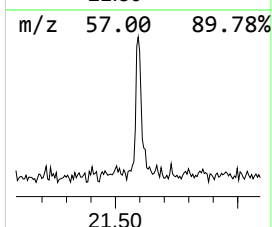
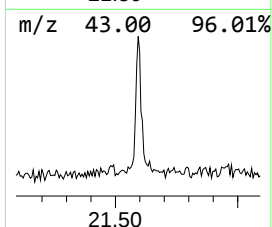
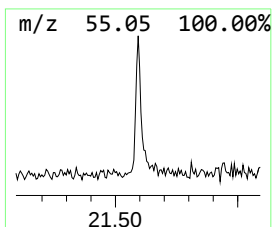
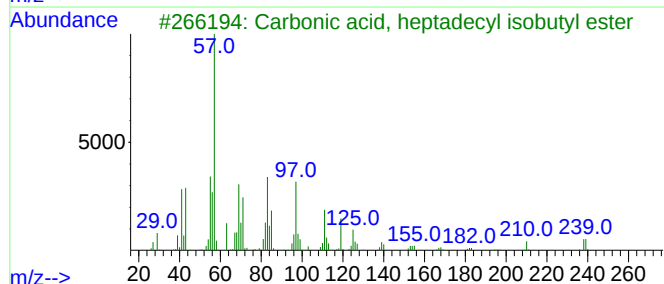
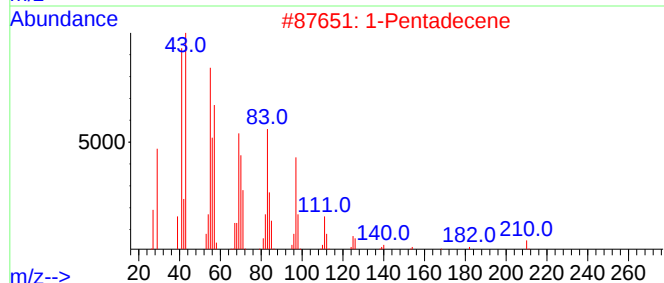
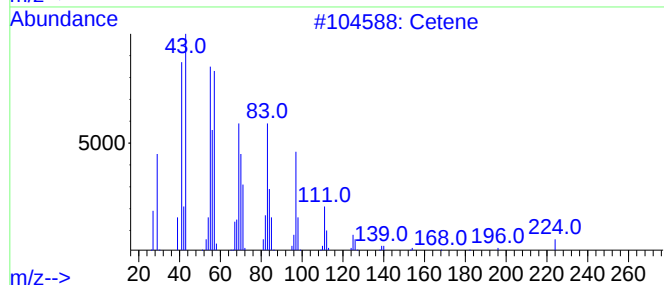
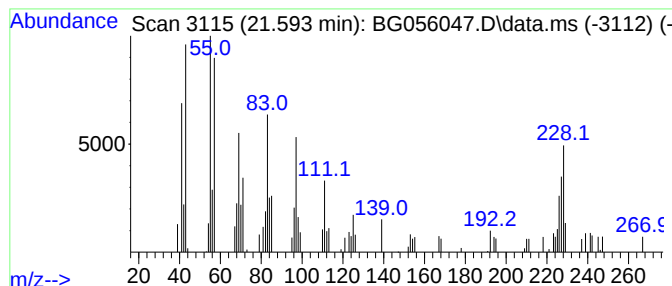
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Cetene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.593	3.28 ng	52454	Chrysene-d12	22.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cetene	224	C16H32	000629-73-2	64
2			1-Pentadecene	210	C15H30	013360-61-7	64
3			Carbonic acid, heptadecyl isobut...	356	C22H44O3	1000314-61-4	49
4			Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	49
5			1-Octadecanol	270	C18H38O	000112-92-5	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122122\
Data File : BG056047.D
Acq On : 21 Dec 2022 13:58
Operator : CG/JU
Sample : N6038-24
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RB-41-(0-2)

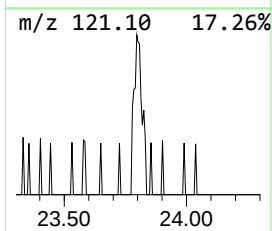
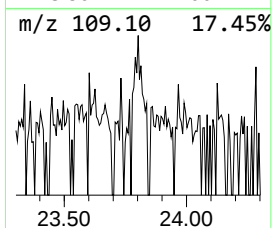
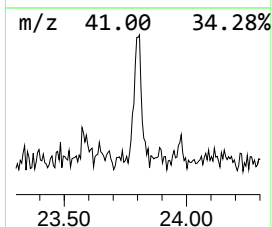
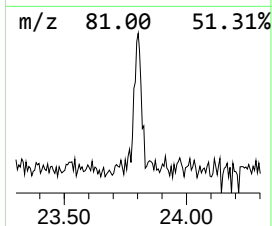
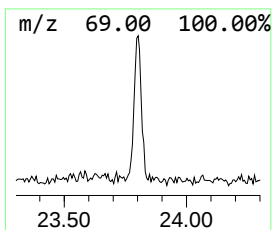
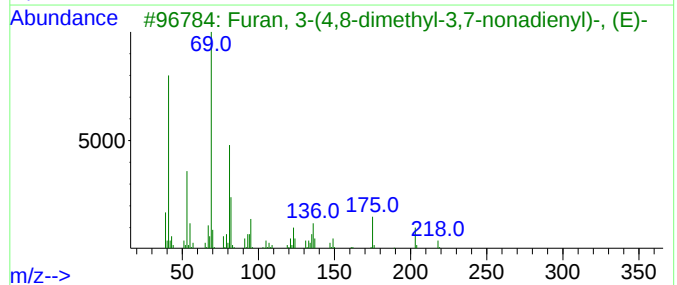
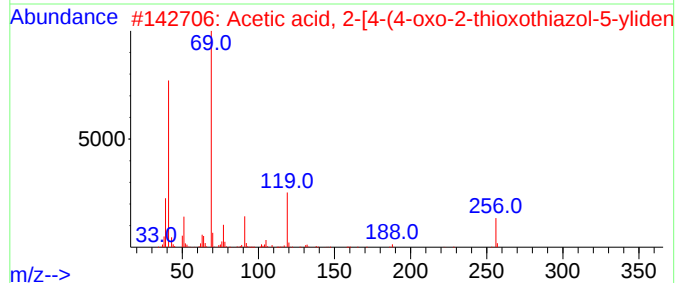
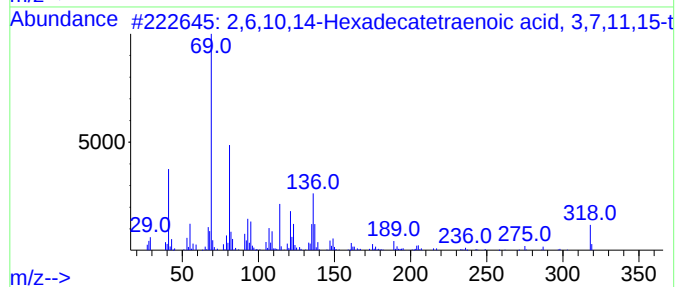
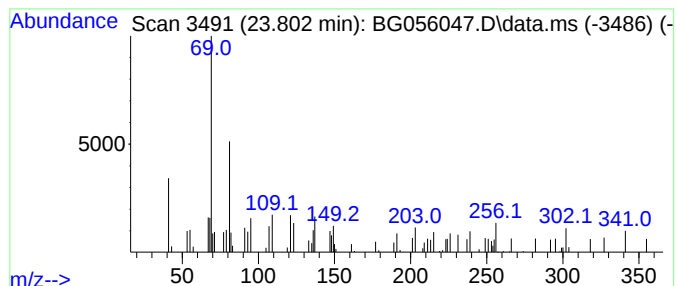
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown23.802 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.802	3.66 ng	41930	Perylene-d12	25.494

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6,10,14-Hexadecatetraenoic aci...	318	C21H34O2	042207-88-5	47		
2	Acetic acid, 2-[4-(4-oxo-2-thiox...	256	C13H12N4O2	1000265-00-3	47		
3	Furan, 3-(4,8-dimethyl-3,7-nonad...	218	C15H22O	023262-34-2	38		
4	Diethylmalonic acid, monochlorid...	302	C14H16Cl2O3	1000370-12-3	33		
5	Succinic acid, 2,2,3,3-tetraflu...	368	C17H24F4O4	1000391-23-5	28		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122122\
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Operator : CG/JU
Sample : N6038-24
Misc :
ALS Vial : 7 Sample Multiplier: 1

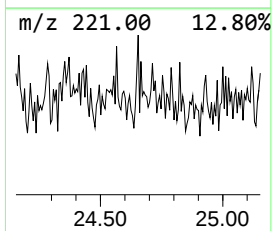
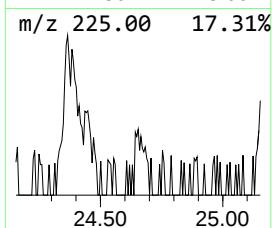
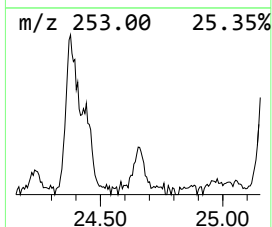
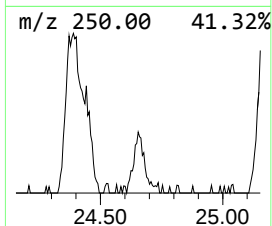
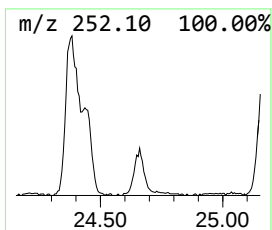
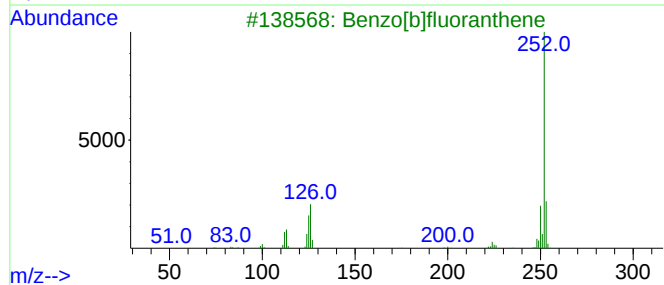
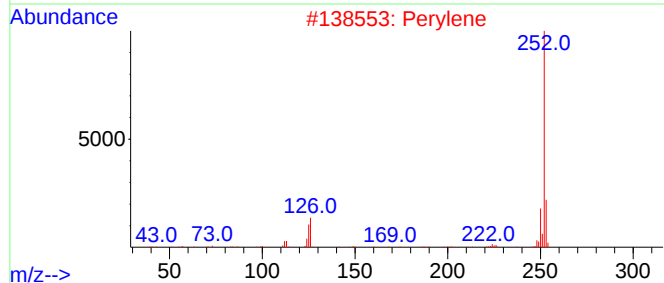
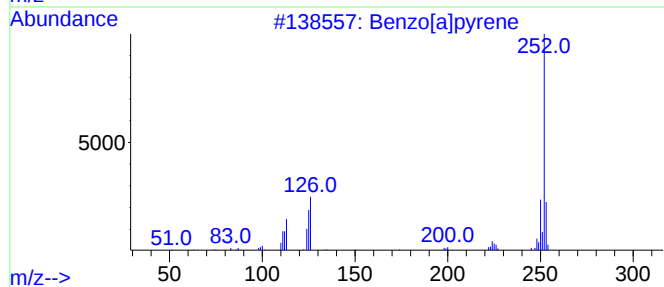
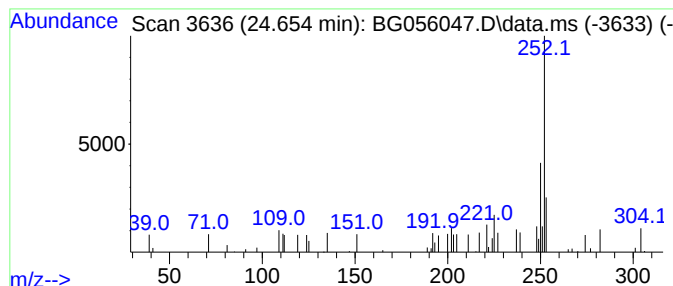
Instrument :
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ClientSampleId :
RB-41-(0-2)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown24.654 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.	
24.654	2.84 ng	32601	Perylene-d12		25.494	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Benzo[a]pyrene		252	C20H12	000050-32-8	55
2	Perylene		252	C20H12	000198-55-0	49
3	Benzo[b]fluoranthene		252	C20H12	000205-99-2	49
4	Benzo[k]fluoranthene		252	C20H12	000207-08-9	47
5	Benzo[e]pyrene		252	C20H12	000192-97-2	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122122\
Data File : BG056047.D
Acq On : 21 Dec 2022 13:58
Operator : CG/JU
Sample : N6038-24
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RB-41-(0-2)

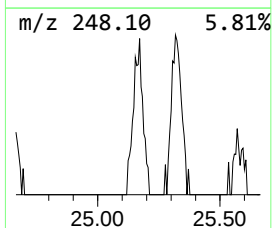
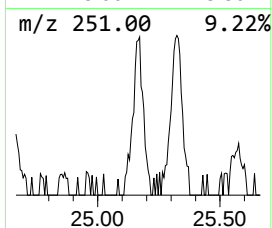
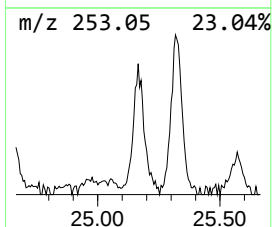
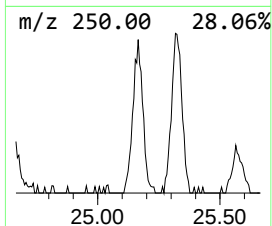
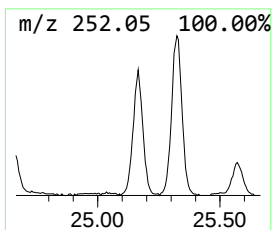
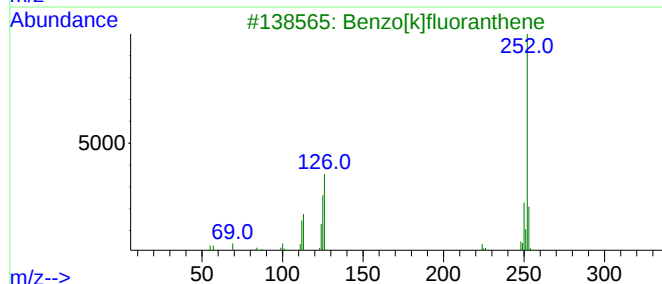
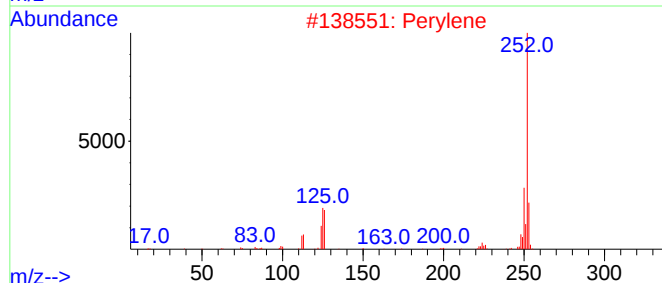
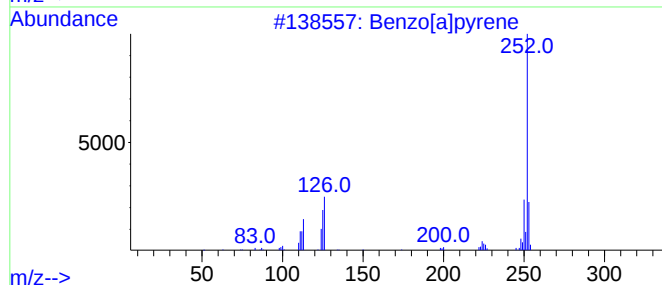
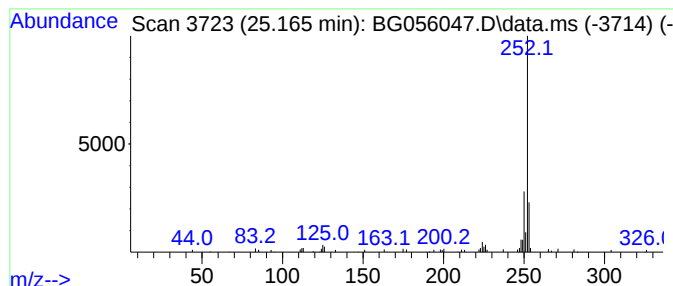
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Perylene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.165	7.35 ng	84297	Perylene-d12	25.494

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzo[a]pyrene	252	C20H12	000050-32-8	89
2		Perylene	252	C20H12	000198-55-0	89
3		Benzo[k]fluoranthene	252	C20H12	000207-08-9	81
4		Benzo[e]pyrene	252	C20H12	000192-97-2	81
5		Benzo[j]fluoranthene	252	C20H12	000205-82-3	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122122\
Data File : BG056047.D
Acq On : 21 Dec 2022 13:58
Operator : CG/JU
Sample : N6038-24
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RB-41-(0-2)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.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
Butane, 2-metho...	3.385	11.5	ng	24816	1	8.361	43124	20.0
2-Pentanone, 4-...	5.400	9.2	ng	19928	1	8.361	43124	20.0
Benzophenone	16.305	11.1	ng	64287	3	14.965	116259	20.0
Tridecanoic acid	18.549	6.4	ng	53100	4	17.703	165823	20.0
unknown19.801	19.801	2.6	ng	21516	4	17.703	165823	20.0
Pyrene, 1-methyl-	20.570	2.8	ng	44327	5	22.004	320249	20.0
Cetene	21.593	3.3	ng	52454	5	22.004	320249	20.0
unknown23.802	23.802	3.7	ng	41930	6	25.494	229363	20.0
unknown24.654	24.654	2.8	ng	32601	6	25.494	229363	20.0
Perylene	25.165	7.3	ng	84297	6	25.494	229363	20.0