

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122022\
 Data File : BG056036.D
 Acq On : 20 Dec 2022 19:10
 Operator : CG/JU
 Sample : N6129-04
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 D8

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: BG056036.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.399	14	19	26	rBV	19869	29691	4.24%	0.823%
2	5.415	355	362	369	rBB	46996	72897	10.40%	2.021%
3	5.885	436	442	450	rBB	121429	193399	27.60%	5.363%
4	7.500	709	717	724	rBB	126014	217407	31.03%	6.028%
5	8.370	859	865	871	rBB	37939	63610	9.08%	1.764%
6	9.539	1057	1064	1071	rBB	80702	141277	20.16%	3.917%
7	11.202	1340	1347	1354	rBB	50298	88377	12.61%	2.451%
8	13.605	1749	1756	1763	rBB	273981	416811	59.49%	11.558%
9	14.974	1983	1989	1996	rBV	87129	132762	18.95%	3.681%
10	16.449	2234	2240	2247	rBV	284955	429780	61.34%	11.917%
11	17.712	2448	2455	2459	rBV	116905	178715	25.51%	4.955%
12	17.753	2459	2462	2468	rVB	20504	27189	3.88%	0.754%
13	18.288	2545	2553	2558	rBV	6387	10932	1.56%	0.303%
14	18.429	2571	2577	2582	rBV2	4151	8026	1.15%	0.223%
15	18.558	2595	2599	2607	rBV2	22082	41892	5.98%	1.162%
16	18.628	2607	2611	2616	rVB	10430	16499	2.35%	0.457%
17	18.770	2628	2635	2638	rBV2	12114	23916	3.41%	0.663%
18	18.805	2639	2641	2647	rVB	7525	9632	1.37%	0.267%
19	18.975	2665	2670	2675	rVB3	7493	9756	1.39%	0.271%
20	19.063	2680	2685	2688	rBV2	8893	13378	1.91%	0.371%
21	19.287	2718	2723	2730	rVB8	3682	8818	1.26%	0.245%
22	19.475	2750	2755	2760	rBV	13427	25582	3.65%	0.709%
23	19.533	2760	2765	2769	rVV7	3548	8520	1.22%	0.236%
24	19.616	2775	2779	2783	rBV5	8057	16372	2.34%	0.454%
25	19.739	2794	2800	2805	rBV	58411	86937	12.41%	2.411%
26	19.804	2805	2811	2814	rBV6	7615	15592	2.23%	0.432%
27	20.062	2851	2855	2857	rBV2	11490	15398	2.20%	0.427%
28	20.103	2857	2862	2867	rVV	61257	91441	13.05%	2.536%
29	20.162	2869	2872	2877	rVB7	7044	11184	1.60%	0.310%
30	20.285	2887	2893	2897	rBV	535672	700623	100.00%	19.427%
31	20.332	2897	2901	2906	rVB8	4940	8693	1.24%	0.241%
32	20.573	2934	2942	2947	rBV3	13027	35056	5.00%	0.972%
33	20.891	2993	2996	2999	rBV2	9387	11415	1.63%	0.317%
34	22.019	3180	3188	3193	rBV3	128275	278822	39.80%	7.731%
35	22.066	3193	3196	3203	rVB	30872	51757	7.39%	1.435%
36	25.509	3773	3782	3783	rBV	58132	114249	16.31%	3.168%

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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-BG121322.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

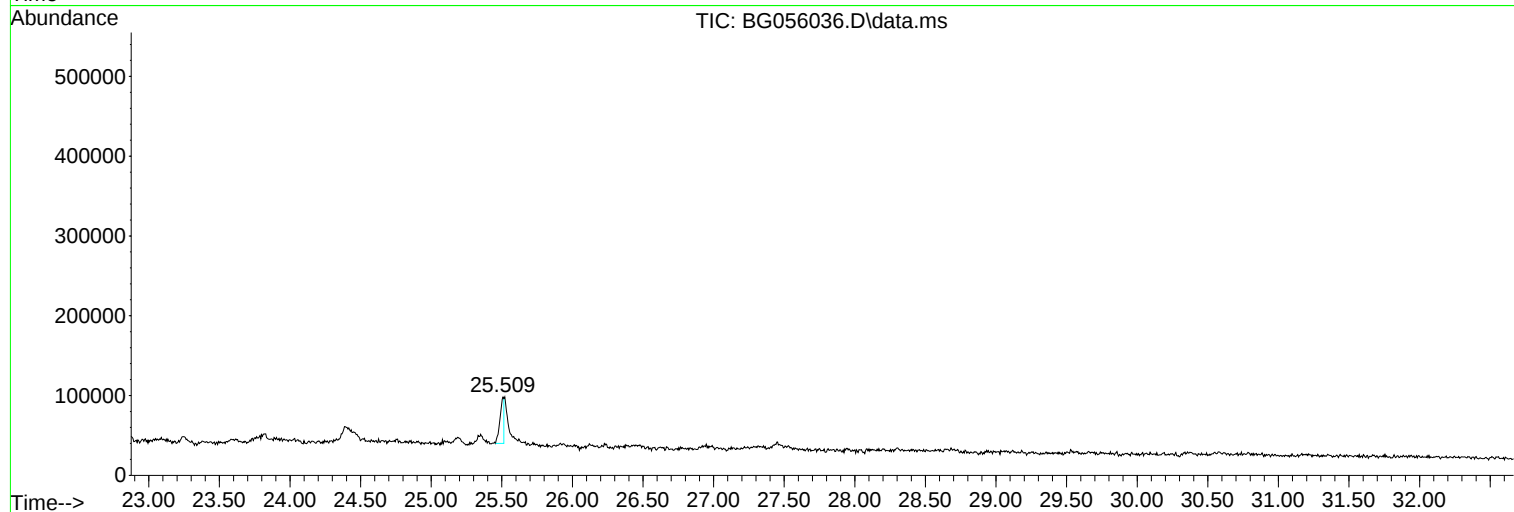
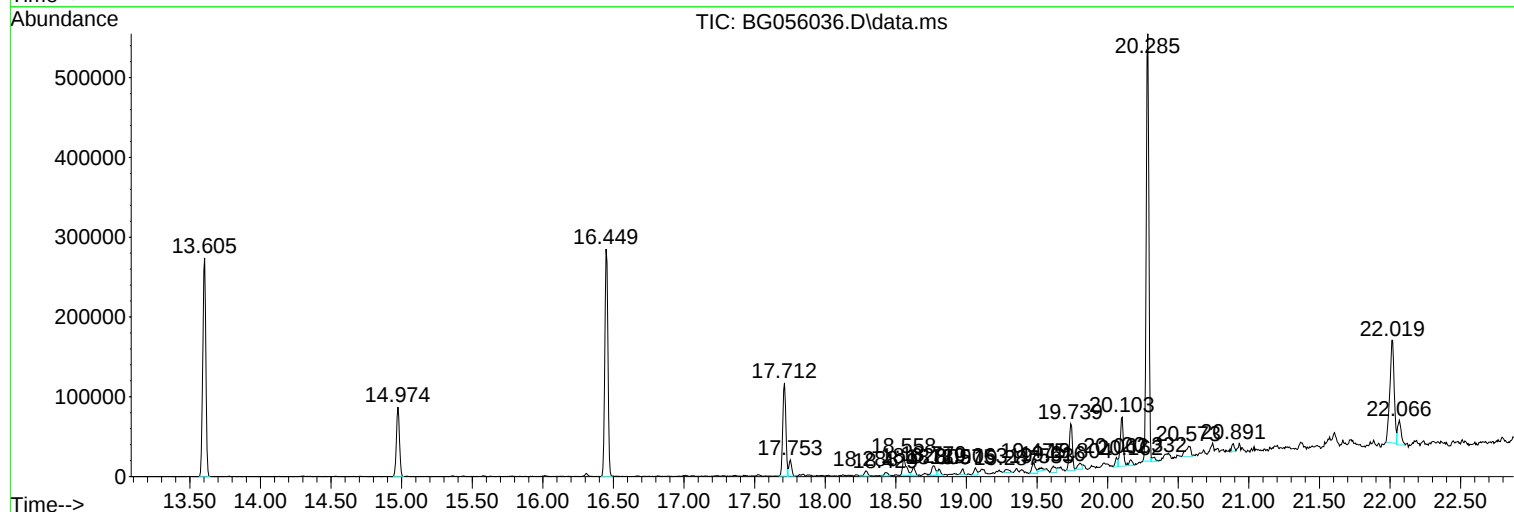
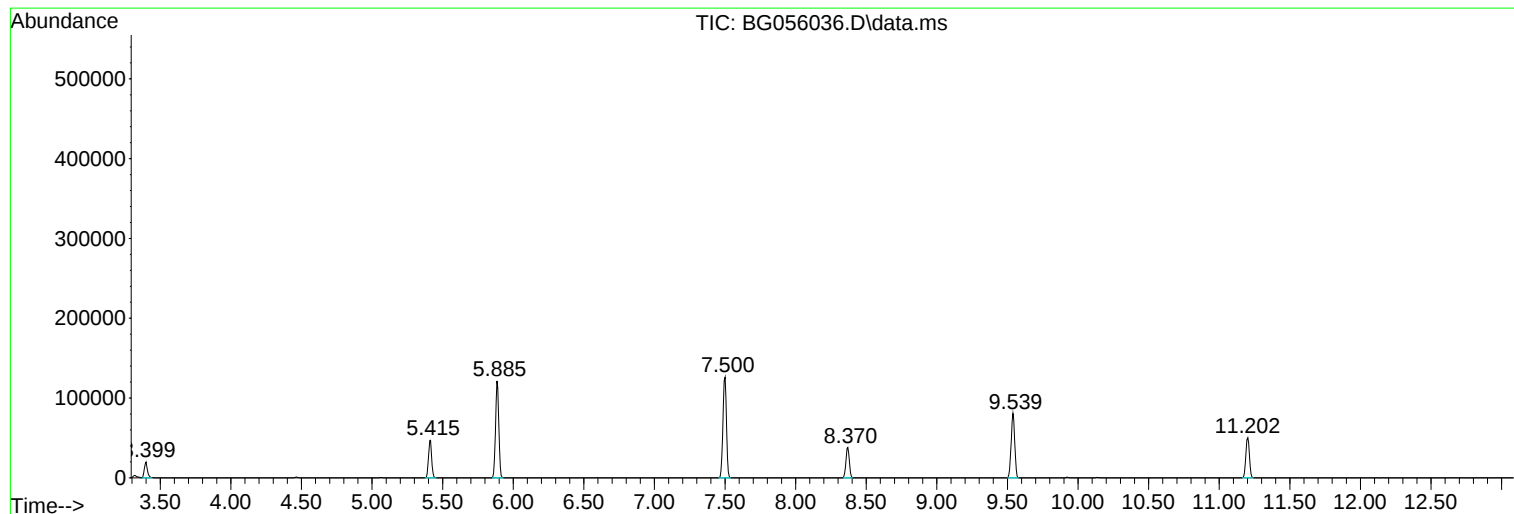
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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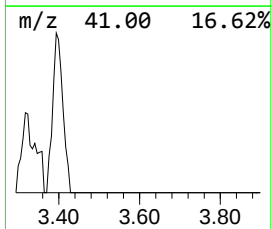
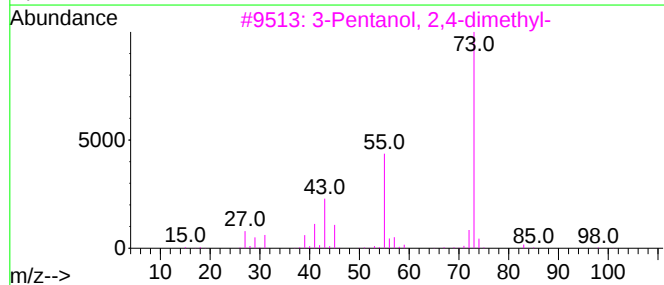
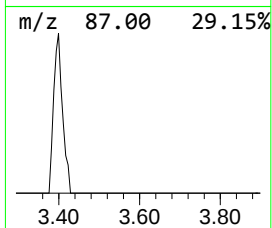
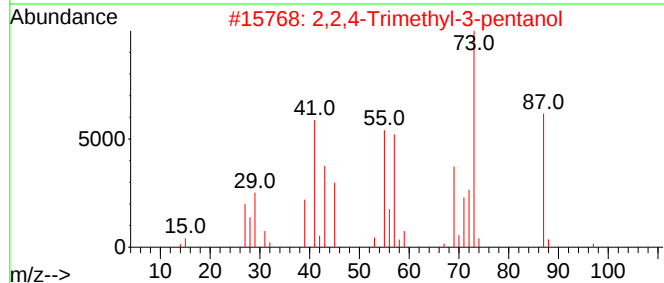
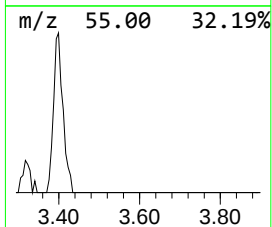
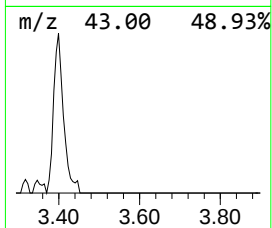
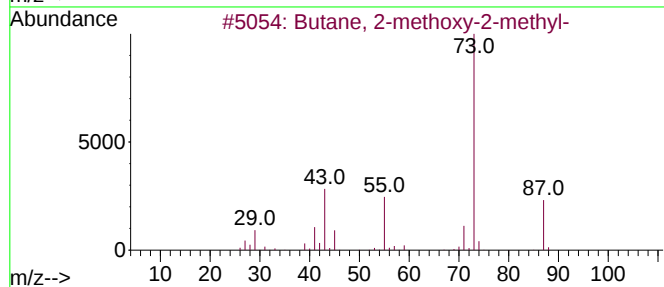
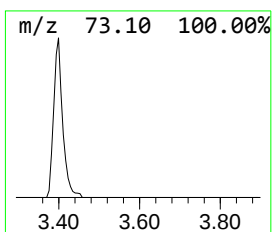
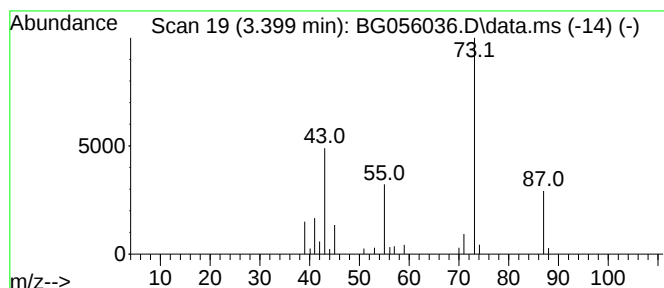
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.399	9.34 ng	29691	1,4-Dichlorobenzene-d4	8.370

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	36
3			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	25
4			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	25
5			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	17



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Misc :
ALS Vial : 13 Sample Multiplier: 1

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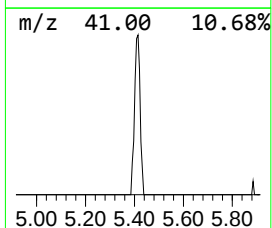
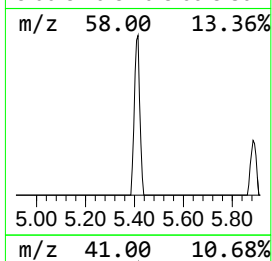
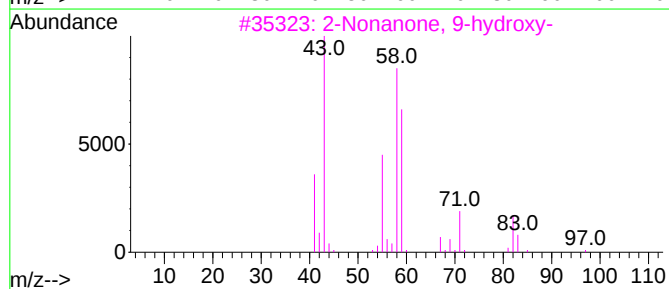
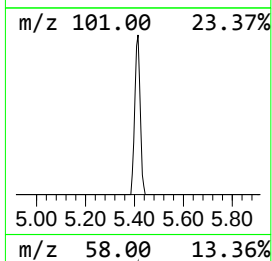
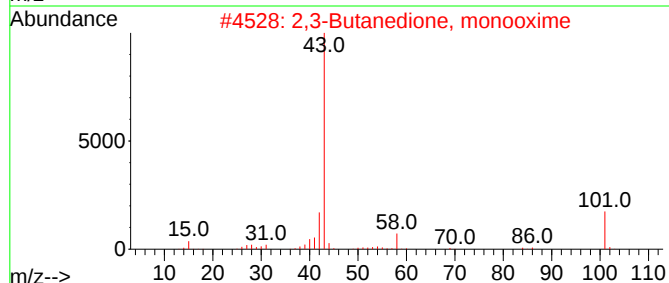
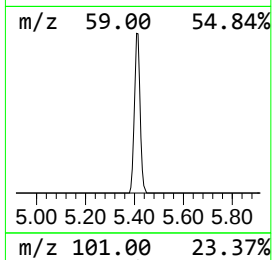
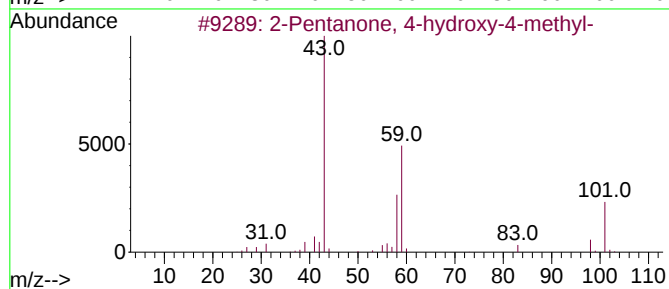
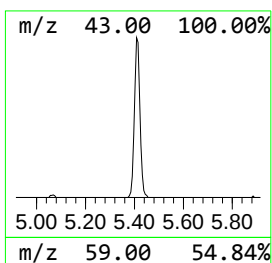
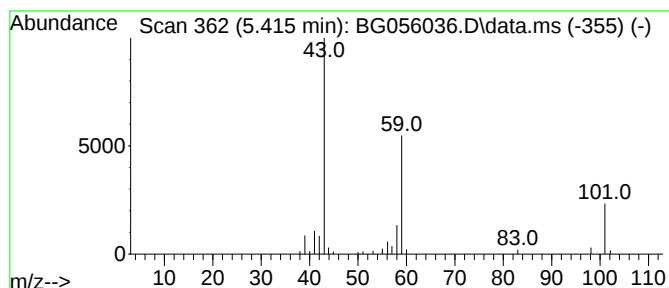
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.415	22.92 ng	72897	1,4-Dichlorobenzene-d4	8.370

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
3			2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	33
4			3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	23
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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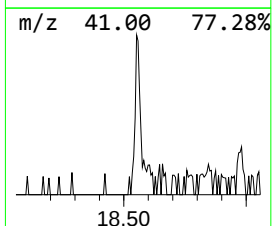
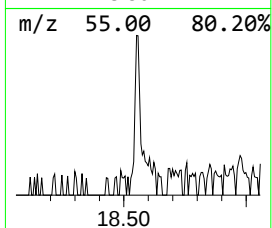
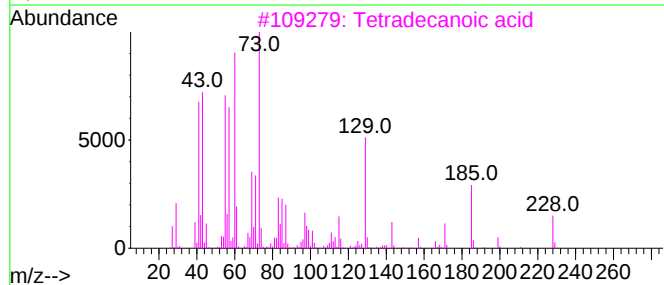
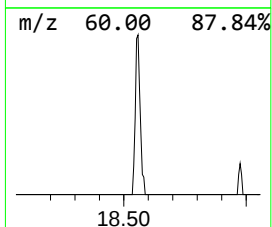
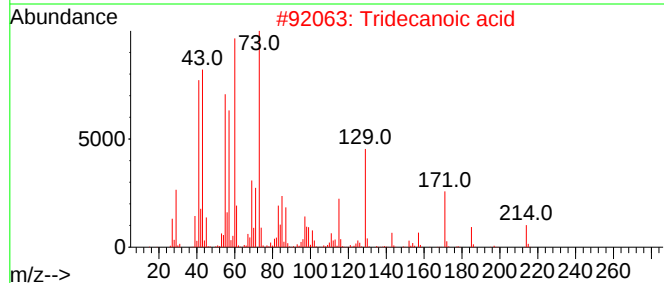
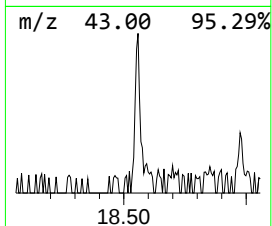
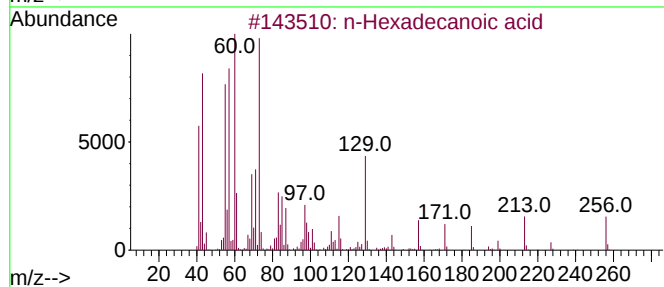
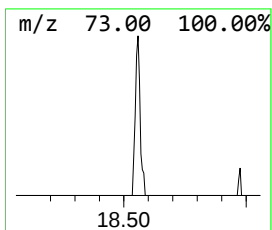
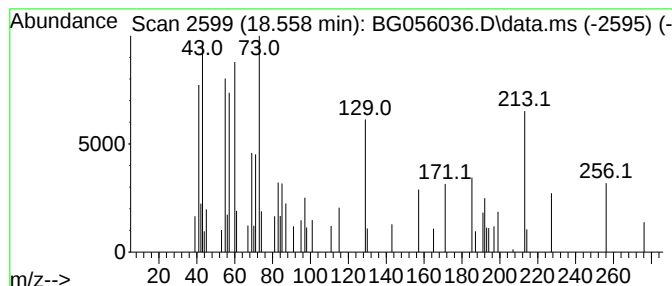
Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.558	4.69 ng	41892	Phenanthrene-d10		17.712	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	91
2	Tridecanoic acid		214	C13H26O2	000638-53-9	89
3	Tetradecanoic acid		228	C14H28O2	000544-63-8	45
4	8-Methylnonanoic acid		172	C10H20O2	005963-14-4	38
5	n-Decanoic acid		172	C10H20O2	000334-48-5	35



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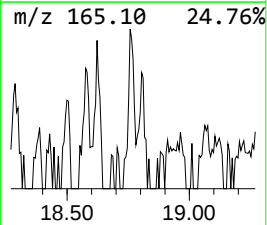
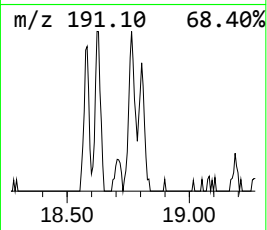
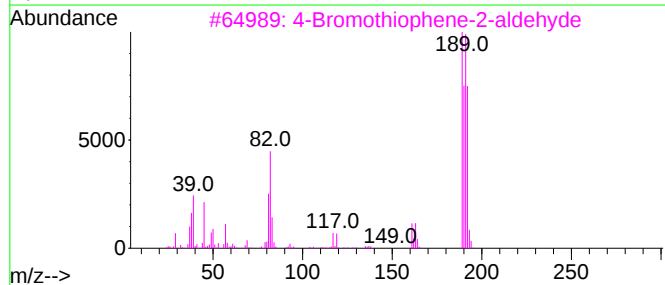
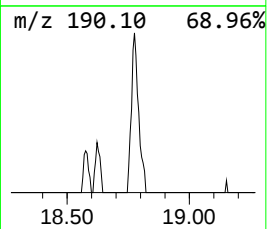
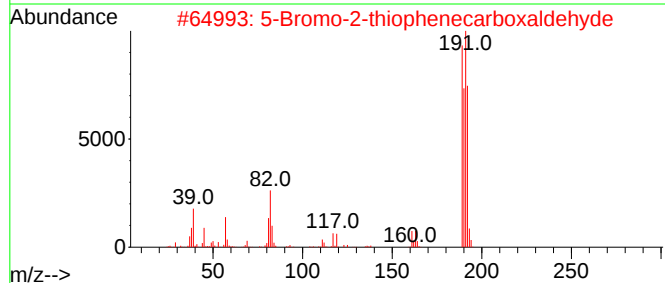
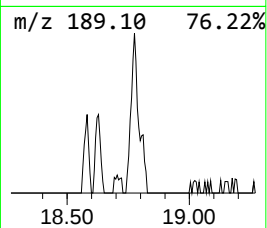
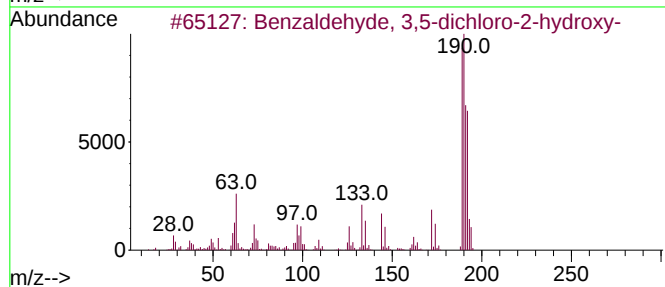
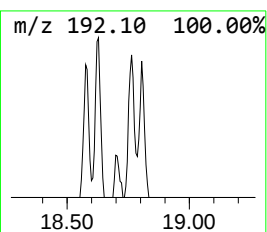
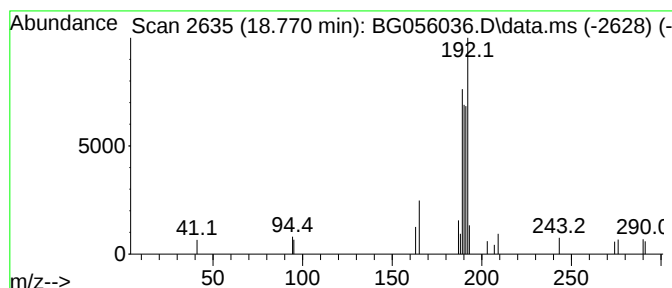
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzaldehyde, 3,5-dichloro-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.770	2.68 ng	23916	Phenanthrene-d10	17.712

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	52
2			5-Bromo-2-thiophenecarboxaldehyde	190	C5H3BrOS	004701-17-1	52
3			4-Bromothiophene-2-aldehyde	190	C5H3BrOS	018791-75-8	52
4			Benzene, 1,1'-(2-cyclopropen-1-y...	192	C15H12	022825-21-4	43
5			Anthracene, 9-methyl-	192	C15H12	000779-02-2	43



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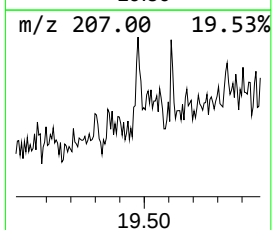
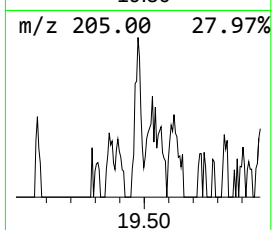
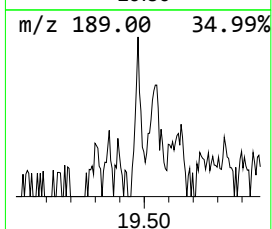
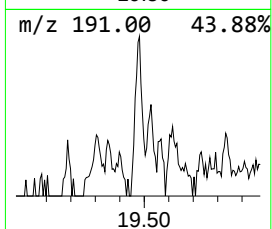
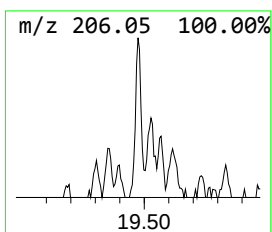
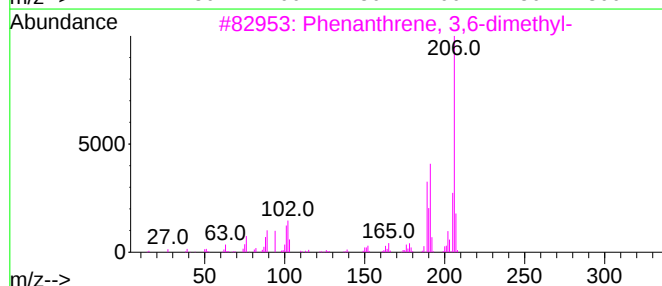
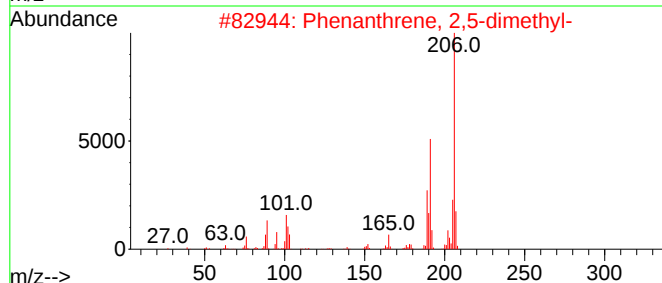
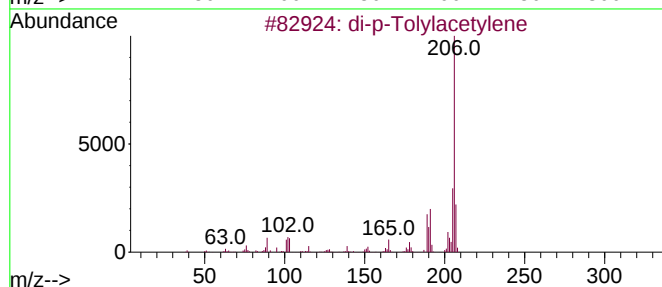
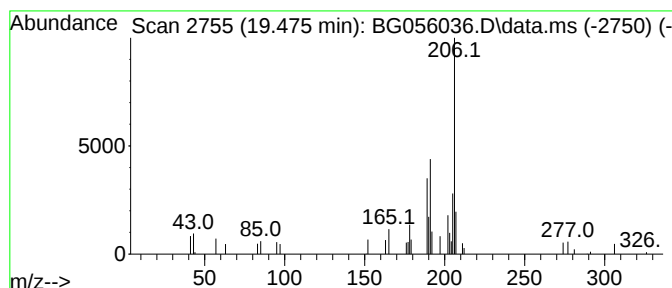
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 di-p-Tolylacetylene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.475	2.86 ng	25582	Phenanthrene-d10	17.712

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			di-p-Tolylacetylene	206	C16H14	002789-88-0	93
2			Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	90
3			Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	90
4			Phenanthrene, 2,7-dimethyl-	206	C16H14	001576-69-8	90
5			9,10-Dimethylanthracene	206	C16H14	000781-43-1	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122022\
Data File : BG056036.D
Acq On : 20 Dec 2022 19:10
Operator : CG/JU
Sample : N6129-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
D8

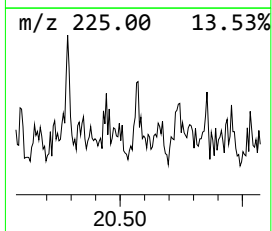
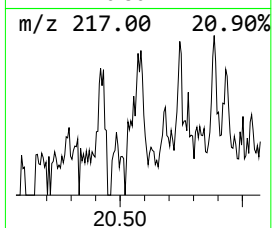
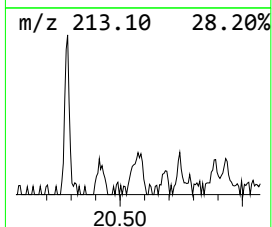
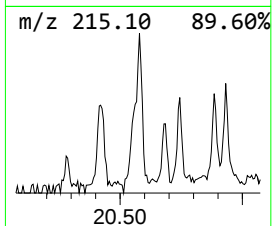
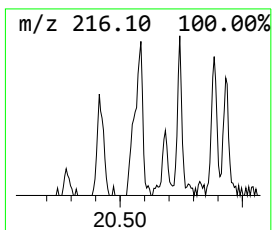
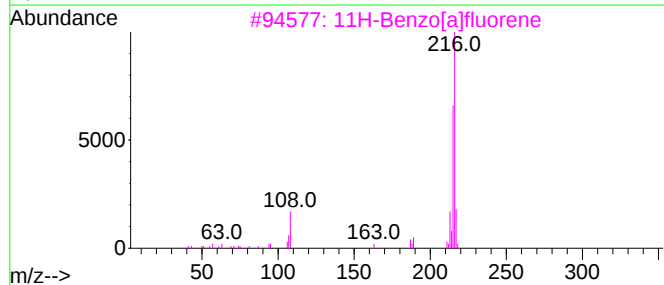
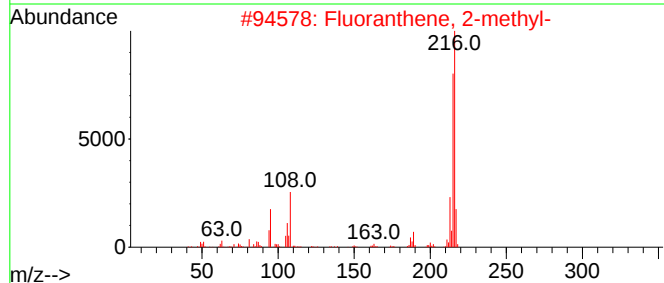
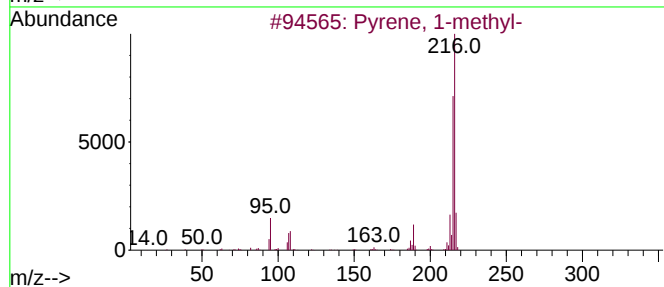
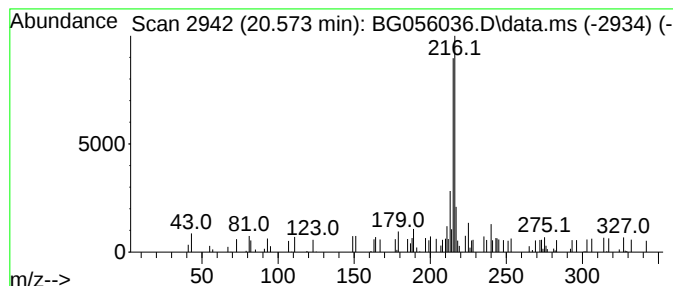
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.573	2.51 ng	35056	Chrysene-d12	22.019

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pyrene, 1-methyl-	216	C17H12	002381-21-7	72
2			Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	72
3			11H-Benzo[a]fluorene	216	C17H12	000238-84-6	72
4			6H-Thiazolo[5,4-e]indole, 2,7,8-...	216	C12H12N2S	1000338-32-0	64
5			11H-Benzo[b]fluorene	216	C17H12	000243-17-4	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122022\
Data File : BG056036.D
Acq On : 20 Dec 2022 19:10
Operator : CG/JU
Sample : N6129-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
D8

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...	3.399	9.3	ng	29691	1	8.370	63610	20.0
2-Pentanone, 4-...	5.415	22.9	ng	72897	1	8.370	63610	20.0
n-Hexadecanoic ...	18.558	4.7	ng	41892	4	17.712	178715	20.0
Benzaldehyde, 3...	18.770	2.7	ng	23916	4	17.712	178715	20.0
di-p-Tolylacety...	19.475	2.9	ng	25582	4	17.712	178715	20.0
Pyrene, 1-methyl-	20.573	2.5	ng	35056	5	22.019	278822	20.0