

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050124\
 Data File : BG061077.D
 Acq On : 1 May 2024 15:22
 Operator : MA/JU
 Sample : P2307-08
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 WC-3

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-BG043024.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG061077.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.152	24	28	35	rVB2	19938	30833	2.07%	0.324%
2	3.675	112	117	126	rVB	14504	24219	1.63%	0.255%
3	5.526	422	432	442	rBV	343998	549996	36.91%	5.781%
4	7.106	692	701	710	rBV	372307	621301	41.69%	6.530%
5	7.935	835	842	849	rBV	115808	186587	12.52%	1.961%
6	9.086	1030	1038	1048	rBV	229814	406740	27.29%	4.275%
7	10.725	1308	1317	1325	rBV	141723	253099	16.98%	2.660%
8	13.187	1729	1736	1742	rBV	624925	963545	64.66%	10.128%
9	14.562	1963	1970	1976	rVB	232717	354987	23.82%	3.731%
10	14.780	1999	2007	2013	rBV5	10740	24930	1.67%	0.262%
11	16.055	2217	2224	2232	rBV	575253	872582	58.55%	9.172%
12	17.312	2430	2438	2442	rBV	290487	453596	30.44%	4.768%
13	17.353	2442	2445	2450	rVB	94753	125549	8.42%	1.320%
14	17.441	2456	2460	2464	rVB	12645	16986	1.14%	0.179%
15	17.823	2520	2525	2528	rBV6	9336	15062	1.01%	0.158%
16	18.211	2583	2591	2600	rVV2	140043	276816	18.58%	2.910%
17	18.375	2614	2619	2624	rBV5	33130	65054	4.37%	0.684%
18	18.411	2624	2625	2631	rVB3	18143	25682	1.72%	0.270%
19	18.587	2649	2655	2659	rBV8	14495	31391	2.11%	0.330%
20	18.687	2668	2672	2674	rBV3	13572	17894	1.20%	0.188%
21	18.722	2675	2678	2683	rVB3	25042	33674	2.26%	0.354%
22	19.104	2739	2743	2748	rVV2	28493	46544	3.12%	0.489%
23	19.239	2764	2766	2771	rVB4	17849	20817	1.40%	0.219%
24	19.362	2782	2787	2794	rVB	277223	382519	25.67%	4.021%
25	19.486	2802	2808	2809	rBV6	33042	52191	3.50%	0.549%
26	19.515	2809	2813	2818	rVB8	38507	58918	3.95%	0.619%
27	19.674	2836	2840	2842	rBV5	47133	65922	4.42%	0.693%
28	19.727	2845	2849	2856	rVB	254229	376732	25.28%	3.960%
29	19.932	2878	2884	2894	rVB	1094656	1490217	100.00%	15.664%
30	21.237	3103	3106	3112	rBV3	58945	91846	6.16%	0.965%
31	21.566	3155	3162	3167	rBV3	329133	707939	47.51%	7.441%
32	21.613	3167	3170	3181	rVB	142701	235348	15.79%	2.474%
33	23.704	3521	3526	3533	rBV3	79786	200771	13.47%	2.110%
34	24.691	3687	3694	3702	rBV	171493	433614	29.10%	4.558%

Sum of corrected areas: 9513901

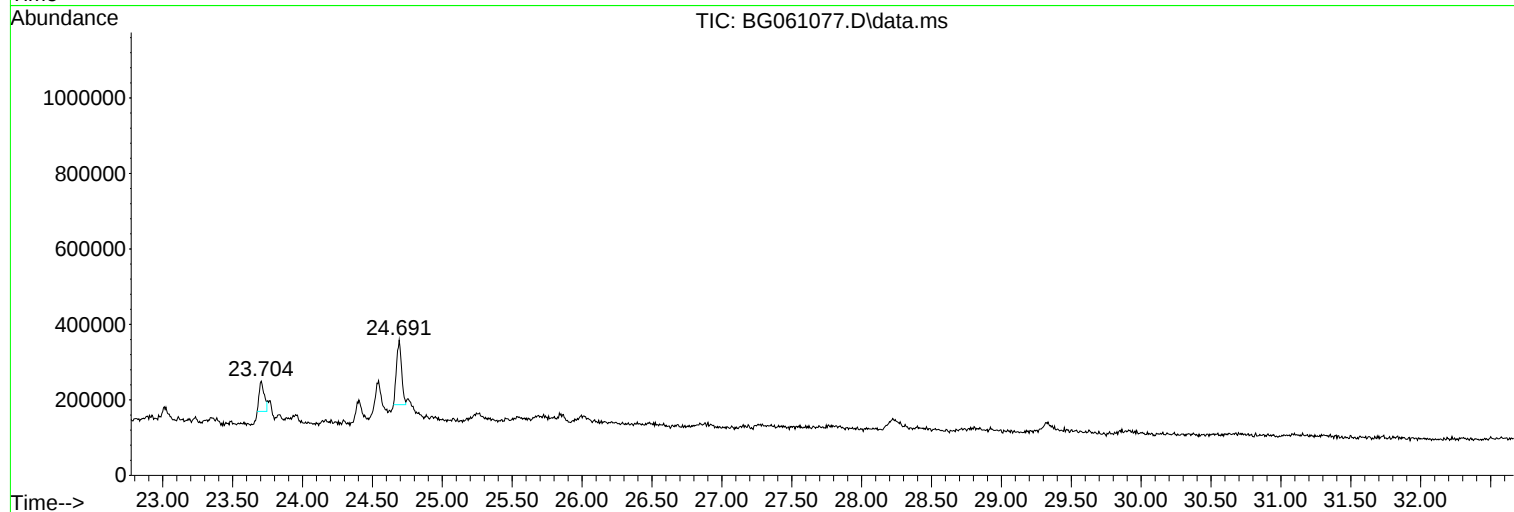
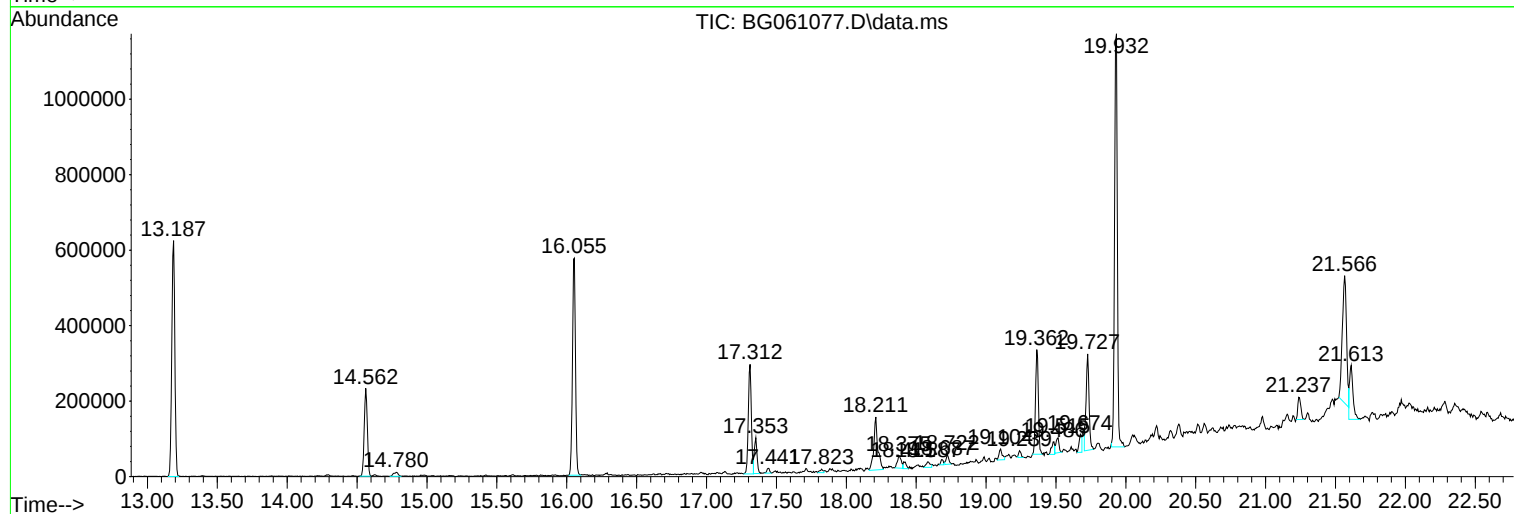
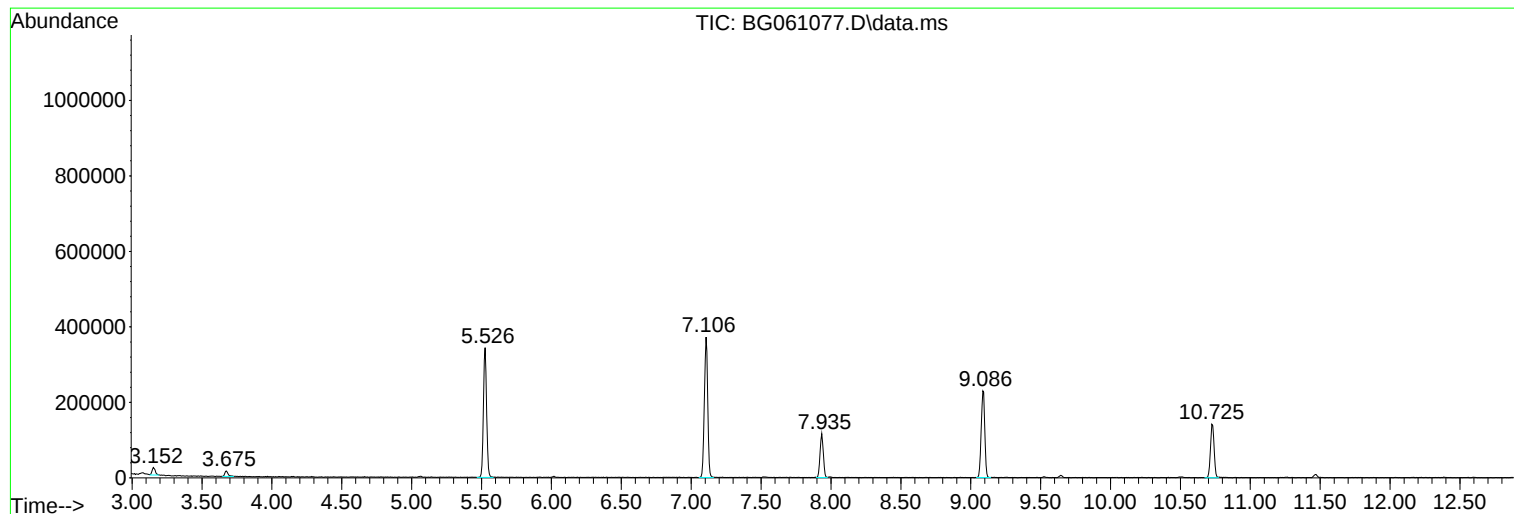
Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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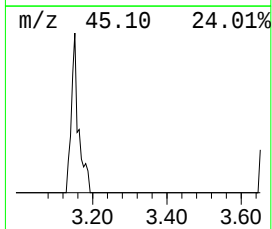
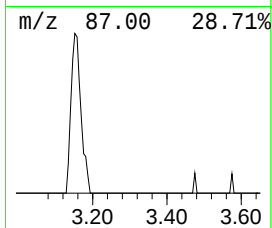
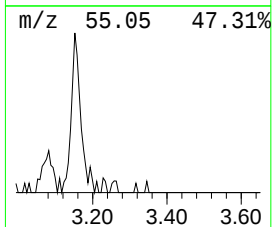
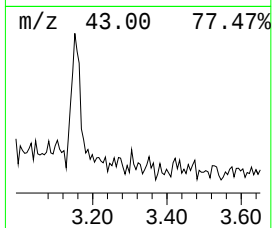
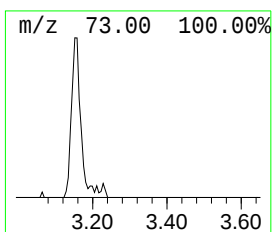
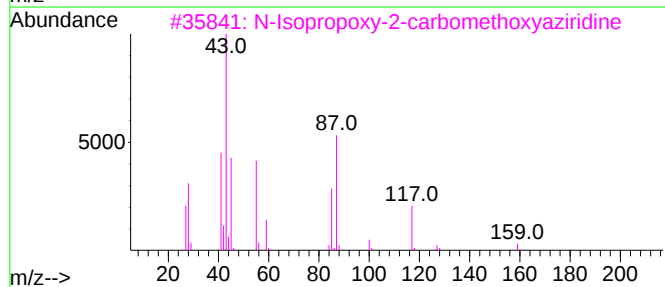
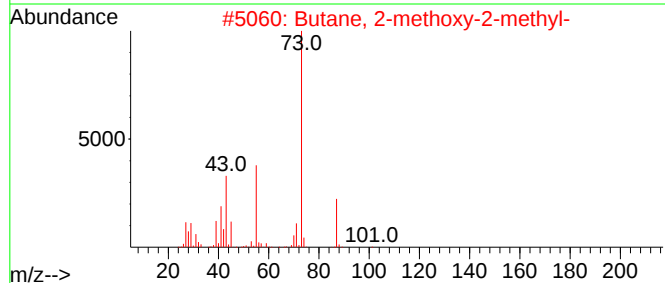
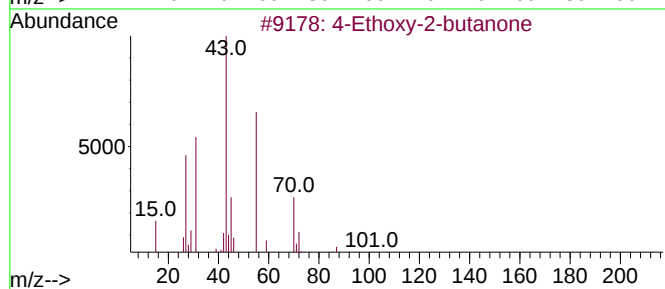
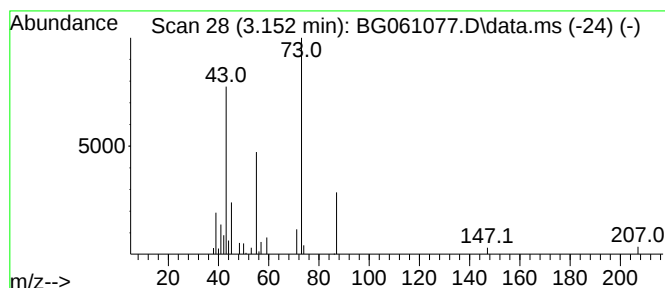
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown3.152 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.152	3.30 ng	30833	1,4-Dichlorobenzene-d4	7.935

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		4-Ethoxy-2-butanone	116	C6H12O2	060044-74-8	35
2		Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	28
3		N-Isopropoxy-2-carbomethoxyaziri...	159	C7H13NO3	053084-32-5	28
4		3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	25
5		Butanoic acid, 2-hydroxy-2-methy...	132	C6H12O3	032793-34-3	25



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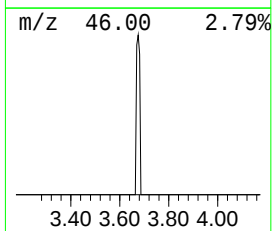
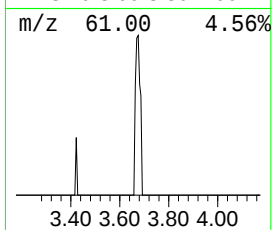
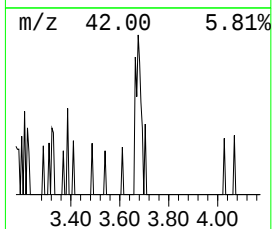
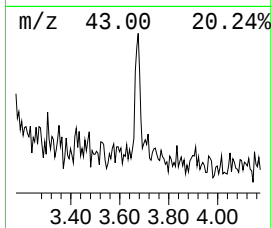
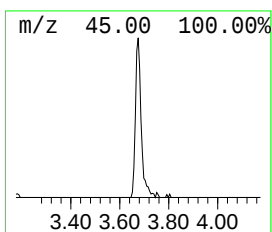
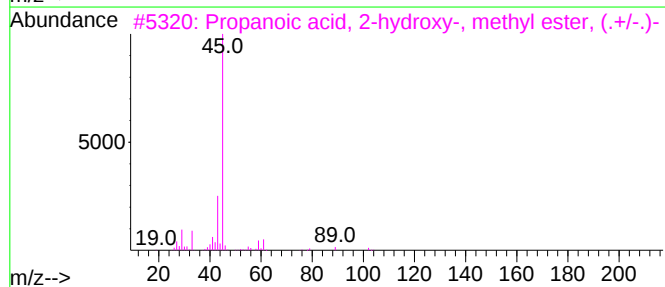
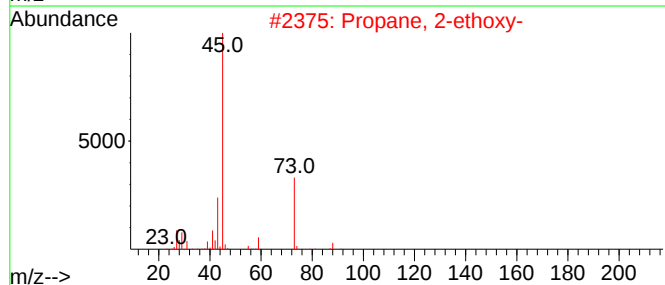
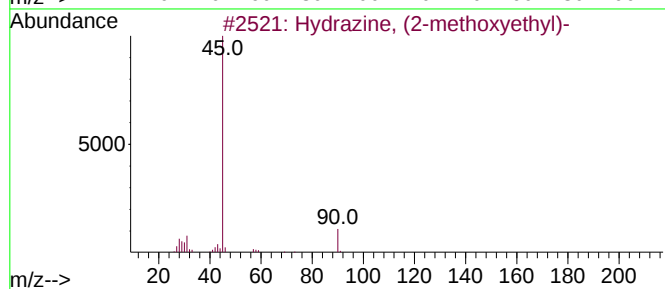
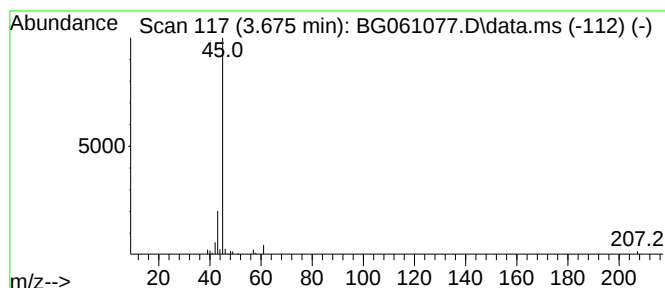
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown3.675 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.675	2.60 ng	24219	1,4-Dichlorobenzene-d4	7.935

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hydrazine, (2-methoxyethyl)-	90	C3H10N2O	003044-15-3	9
2			Propane, 2-ethoxy-	88	C5H12O	000625-54-7	9
3			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	9
4			L-Lactic acid	90	C3H6O3	000079-33-4	9
5			2-Propanone, 1-methoxy-	88	C4H8O2	005878-19-3	9



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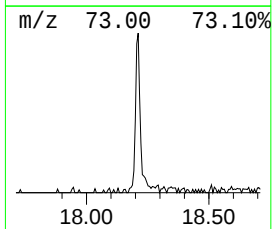
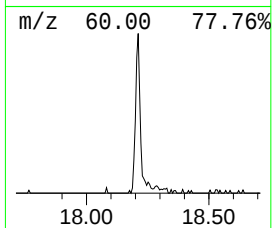
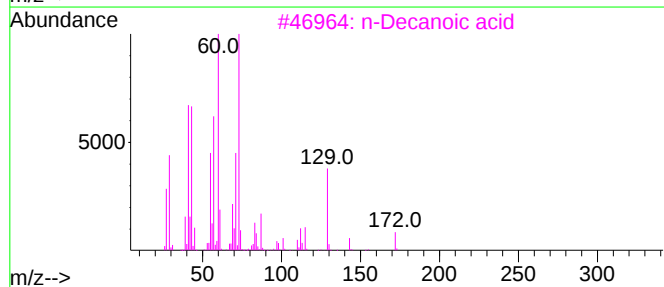
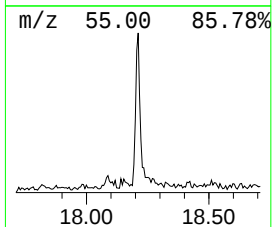
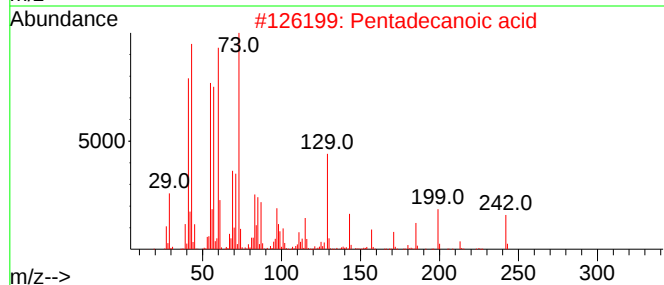
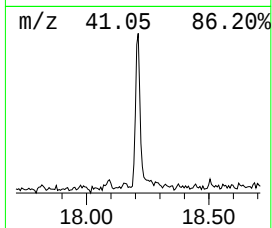
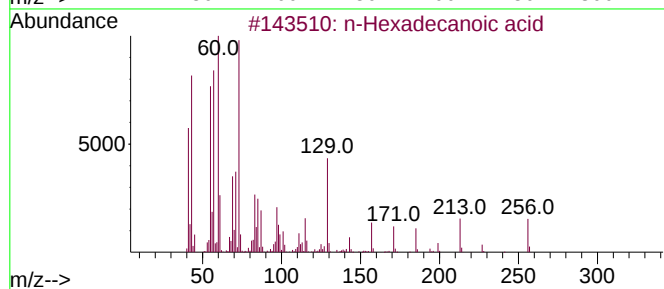
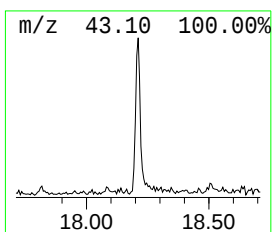
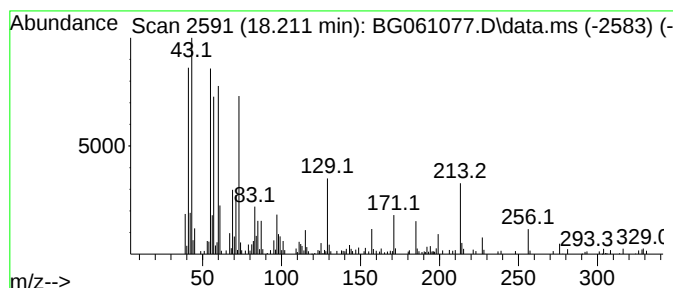
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.211	12.21 ng	276816	Phenanthrene-d10	17.312

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	62
3			n-Decanoic acid	172	C10H20O2	000334-48-5	60
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	47
5			Nonanoic acid	158	C9H18O2	000112-05-0	43



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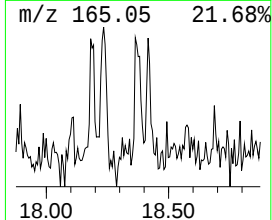
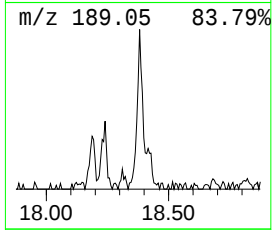
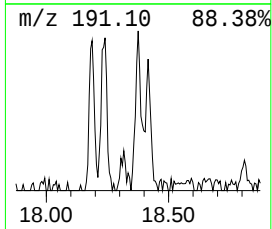
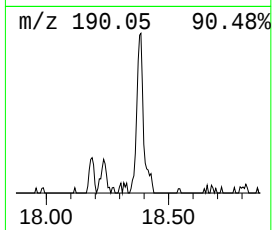
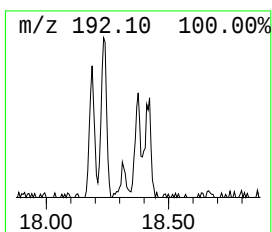
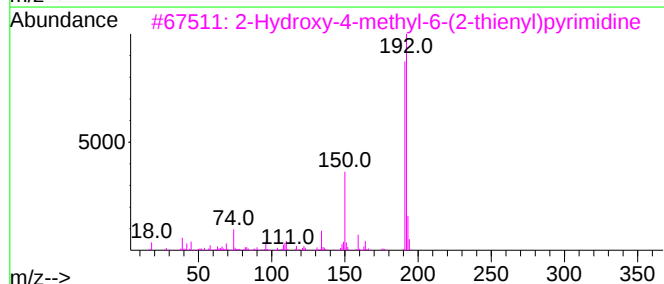
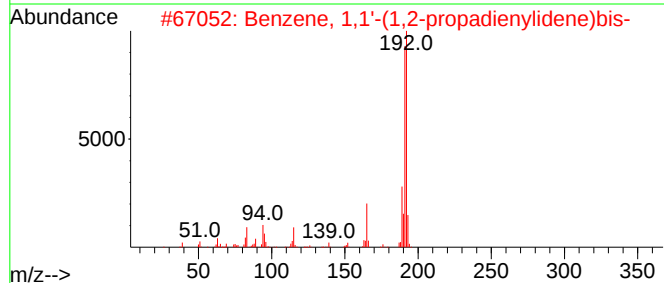
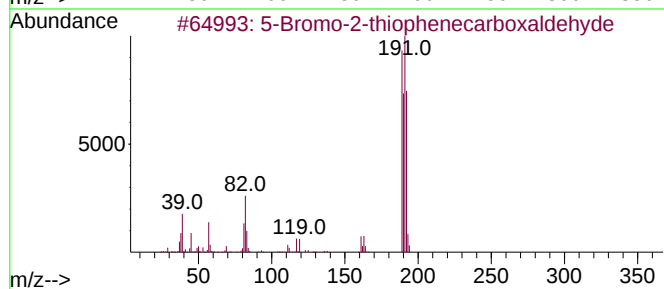
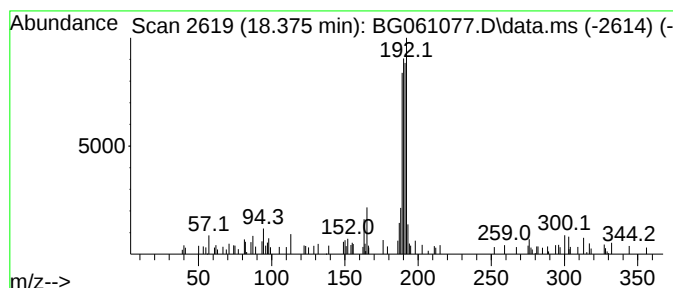
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TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 4 5-Bromo-2-thiophenecarboxal... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.375	2.87 ng	65054	Phenanthrene-d10	17.312	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Bromo-2-thiophenecarboxaldehyde	190	C5H3BrOS	004701-17-1	72
2	Benzene, 1,1'-(1,2-propadienyli...	192	C15H12	014251-57-1	43
3	2-Hydroxy-4-methyl-6-(2-thienyl)...	192	C9H8N2OS	026963-45-1	42
4	8,9-Dihydrocyclopenta[def]phenan...	192	C15H12	027410-55-5	41
5	5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	41



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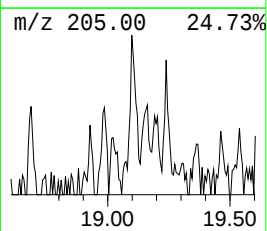
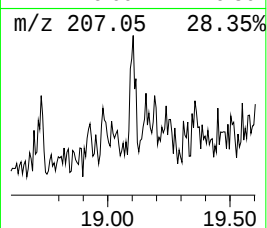
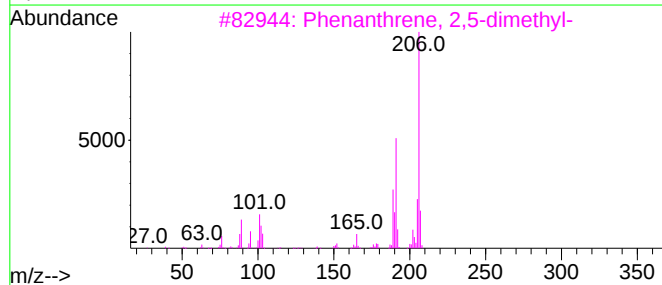
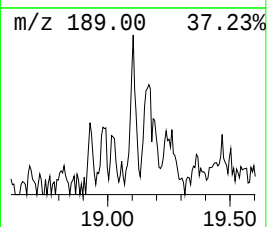
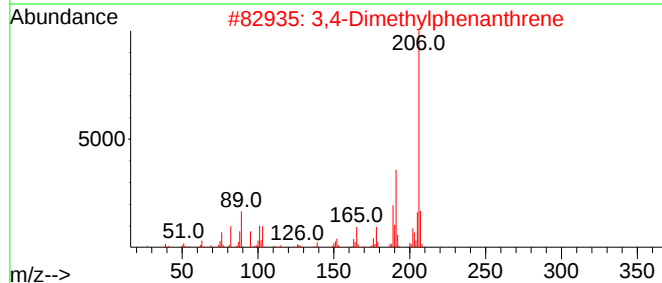
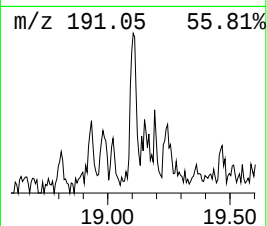
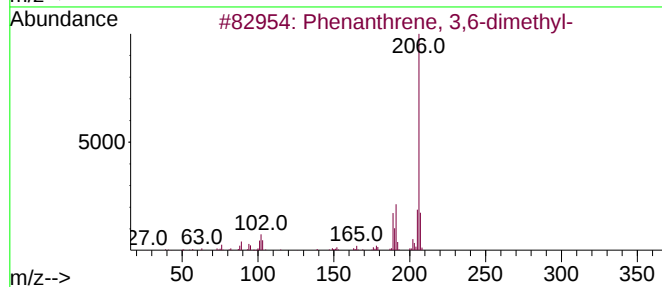
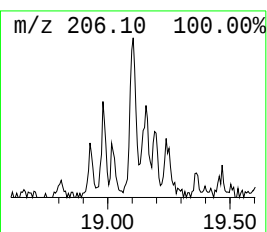
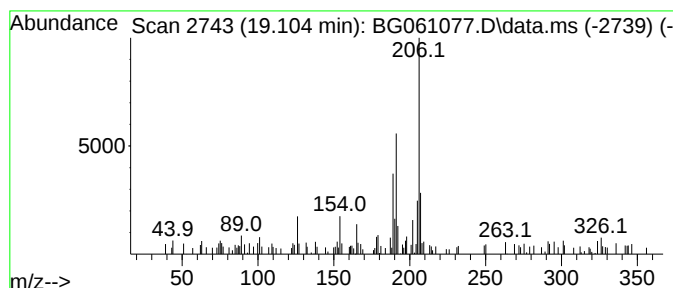
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Peak Number 5 Phenanthrene, 3,6-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.104	2.05 ng	46544	Phenanthrene-d10	17.312

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	87
2			3,4-Dimethylphenanthrene	206	C16H14	1000452-24-5	83
3			Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	83
4			9,10-Dimethylantracene	206	C16H14	000781-43-1	81
5			di-p-Tolylacetylene	206	C16H14	002789-88-0	80



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ClientSampleId :
WC-3

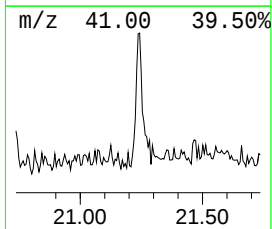
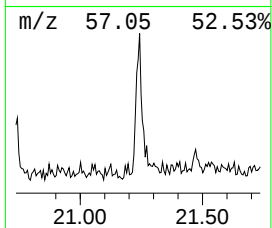
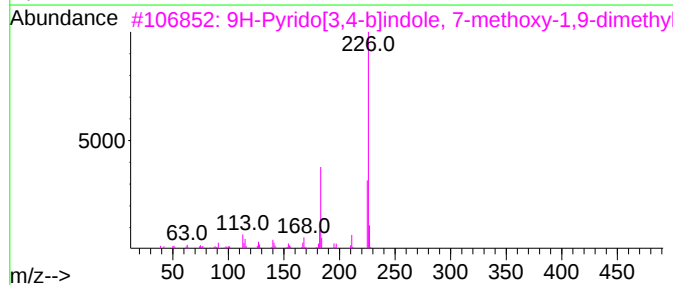
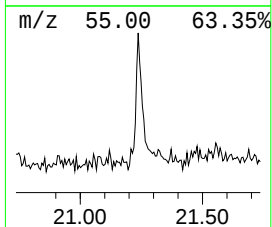
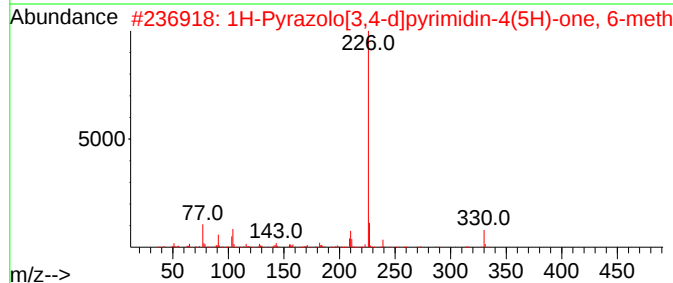
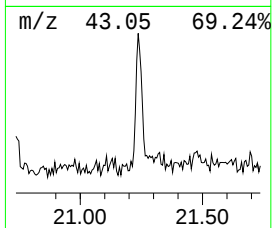
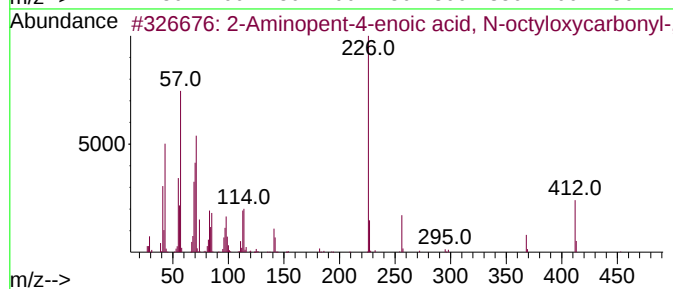
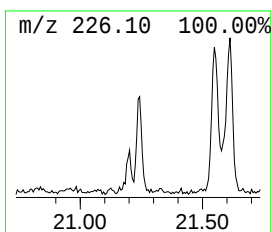
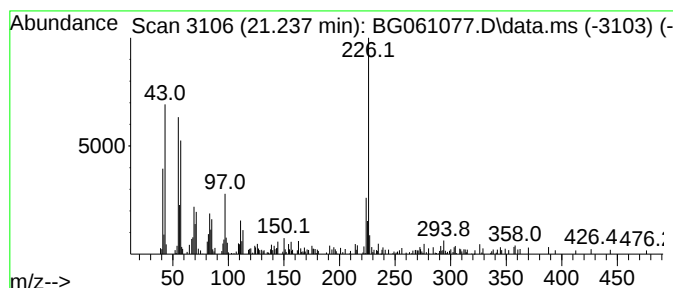
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown21.237 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.237	2.59 ng	91846	Chrysene-d12	21.566

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Aminopent-4-enoic acid, N-octy...	453	C27H51N04	1000393-15-9	40
2		1H-Pyrazolo[3,4-d]pyrimidin-4(5H...	330	C20H18N4O	301322-28-1	37
3		9H-Pyrido[3,4-b]indole, 7-methox...	226	C14H14N2O	143502-37-8	37
4		2-Phenyl-4,5-methylenedioxybenza...	226	C14H10O3	004432-95-5	37
5		Acridin-9-amine, 1,2,3,4-tetrahy...	226	C15H18N2	1000300-57-6	37



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050124\
Data File : BG061077.D
Acq On : 1 May 2024 15:22
Operator : MA/JU
Sample : P2307-08
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown3.152	3.152	3.3	ng	30833	1	7.935	186587	20.0
unknown3.675	3.675	2.6	ng	24219	1	7.935	186587	20.0
n-Hexadecanoic ...	18.211	12.2	ng	276816	4	17.312	453596	20.0
5-Bromo-2-thiop...	18.375	2.9	ng	65054	4	17.312	453596	20.0
Phenanthrene, 3...	19.104	2.0	ng	46544	4	17.312	453596	20.0
unknown21.237	21.237	2.6	ng	91846	5	21.566	707939	20.0