

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112723\
 Data File : BG059909.D
 Acq On : 27 Nov 2023 20:33
 Operator : MA/JU
 Sample : 05463-01
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 NB-08-11162023

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-BG111623.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG059909.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.344	328	333	339	rVB4	28662	48017	2.18%	0.358%
2	5.802	403	411	419	rBV	655337	1042540	47.24%	7.781%
3	7.436	680	689	698	rBV	676494	1143502	51.82%	8.535%
4	8.311	830	838	844	rBV2	167269	284750	12.90%	2.125%
5	9.510	1034	1042	1051	rVB	476500	813248	36.85%	6.070%
6	11.155	1315	1322	1328	rBV	206426	384254	17.41%	2.868%
7	13.564	1725	1732	1738	rBV	1242026	1898926	86.05%	14.173%
8	13.770	1760	1767	1773	rVB	296181	474078	21.48%	3.538%
9	14.322	1855	1861	1865	rBV8	23232	33416	1.51%	0.249%
10	14.939	1960	1966	1973	rBV	295851	485516	22.00%	3.624%
11	14.998	1974	1976	1982	rVB5	16169	22941	1.04%	0.171%
12	15.985	2138	2144	2147	rBV7	20868	30379	1.38%	0.227%
13	16.425	2211	2219	2226	rBV2	898555	1356366	61.46%	10.124%
14	17.348	2372	2376	2380	rVB6	13804	22172	1.00%	0.165%
15	17.694	2427	2435	2439	rBV	310370	515839	23.38%	3.850%
16	17.736	2439	2442	2447	rVB	124736	177780	8.06%	1.327%
17	17.824	2454	2457	2461	rVB2	27103	38057	1.72%	0.284%
18	18.505	2569	2573	2578	rBV2	96955	126633	5.74%	0.945%
19	18.558	2578	2582	2584	rVV5	22761	34310	1.55%	0.256%
20	18.599	2587	2589	2594	rVB3	30833	40622	1.84%	0.303%
21	18.758	2612	2616	2618	rBV4	19352	24231	1.10%	0.181%
22	18.916	2639	2643	2647	rBV7	24629	33479	1.52%	0.250%
23	19.105	2672	2675	2679	rVB6	29421	38241	1.73%	0.285%
24	19.281	2699	2705	2707	rBV6	19913	33263	1.51%	0.248%
25	19.439	2729	2732	2738	rVB8	45486	61749	2.80%	0.461%
26	19.657	2767	2769	2774	rVB6	23601	28208	1.28%	0.211%
27	19.727	2776	2781	2785	rVV	247888	352405	15.97%	2.630%
28	19.763	2785	2787	2792	rVB6	46516	59094	2.68%	0.441%
29	19.974	2820	2823	2828	rBV7	24003	40357	1.83%	0.301%
30	20.045	2832	2835	2838	rBV5	48860	66927	3.03%	0.500%
31	20.092	2838	2843	2848	rVB	203203	275686	12.49%	2.058%
32	20.268	2867	2873	2879	rBV	1775211	2206756	100.00%	16.471%
33	20.567	2922	2924	2929	rVB4	46143	56622	2.57%	0.423%
34	20.867	2972	2975	2980	rBV7	41568	81711	3.70%	0.610%
35	21.543	3087	3090	3095	rBV7	55888	100121	4.54%	0.747%
36	22.013	3163	3170	3175	rBV3	235407	508417	23.04%	3.795%

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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

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37	22.060	3175	3178	3184	rVB2	89313	137439	6.23%	1.026%
38	25.391	3743	3745	3746	rBV2	41953	32613	1.48%	0.243%
39	25.585	3772	3778	3783	rVB3	115649	287472	13.03%	2.146%

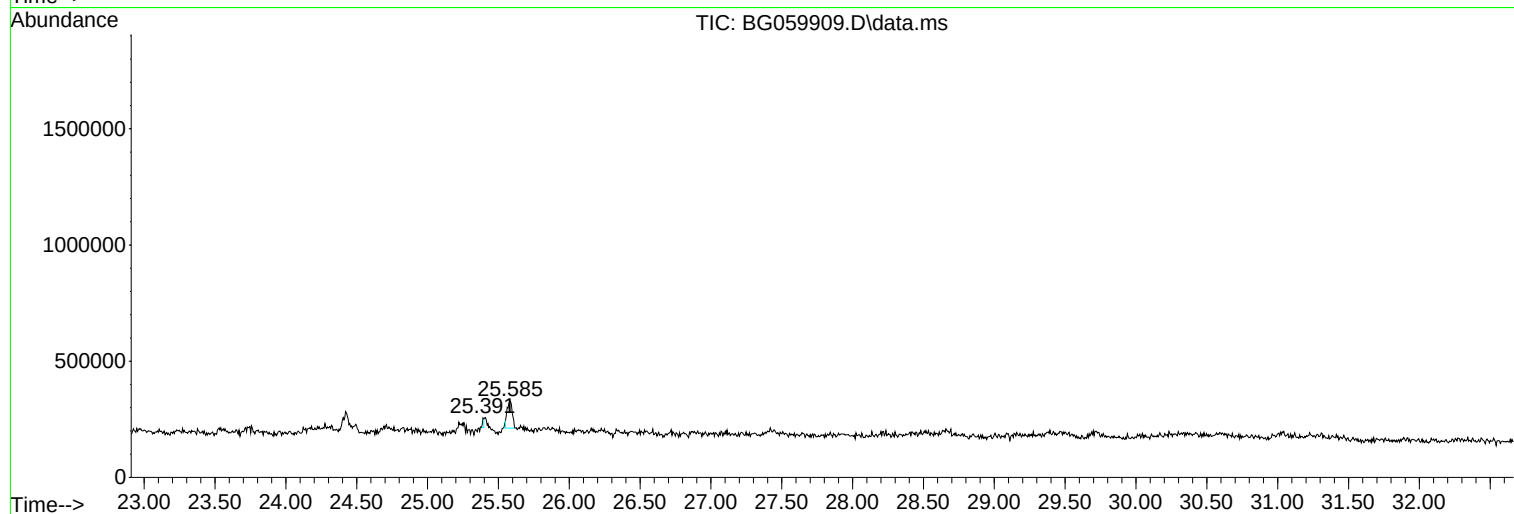
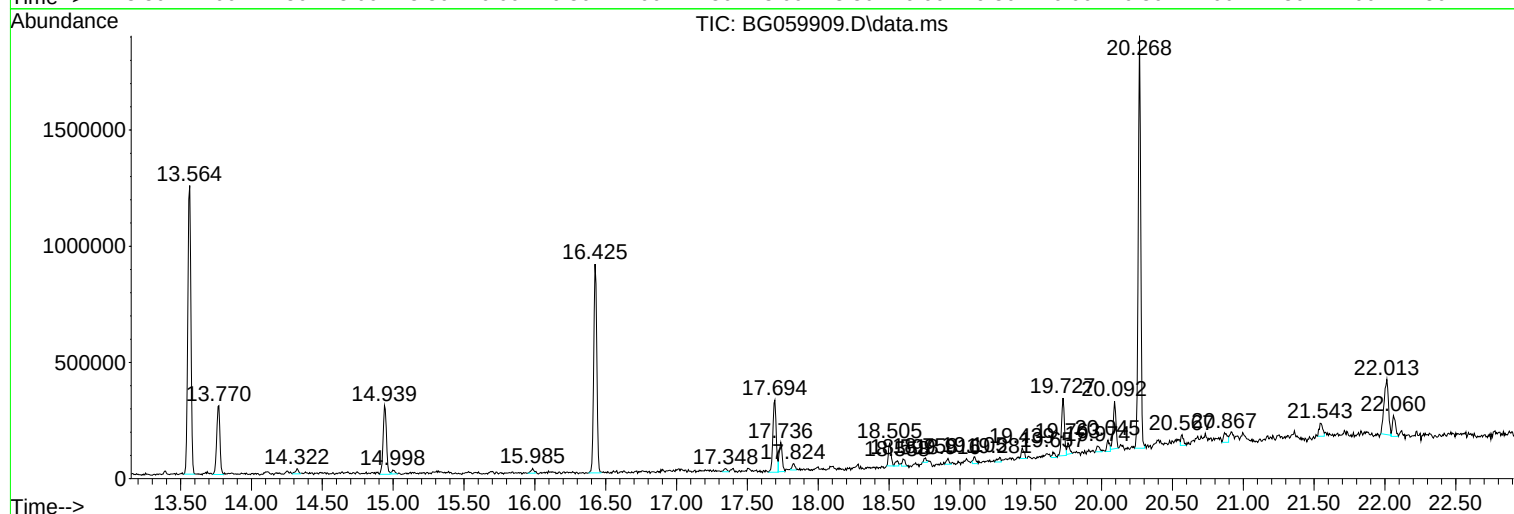
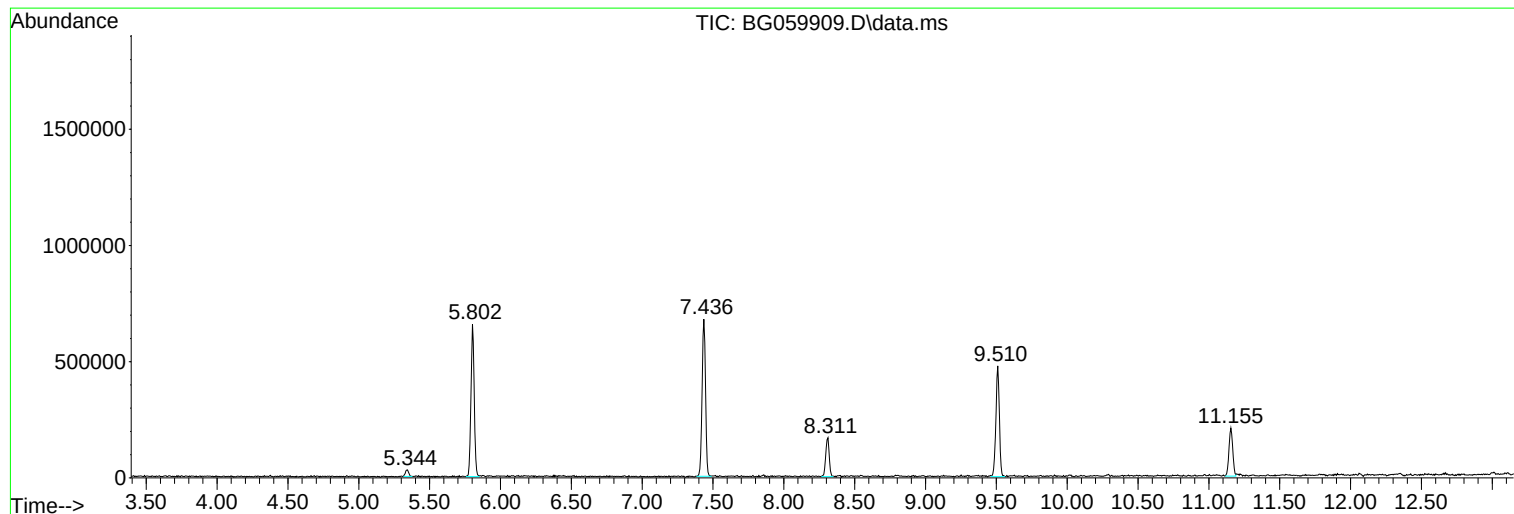
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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NB-08-11162023

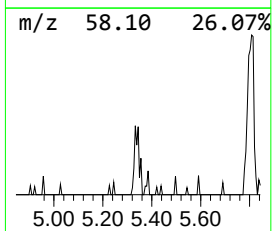
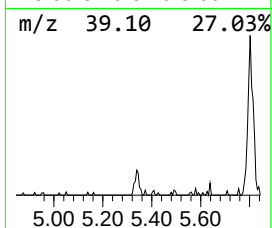
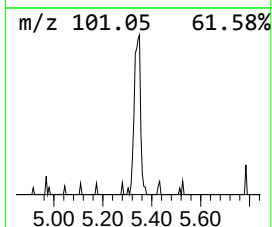
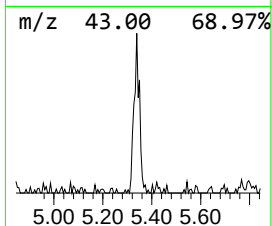
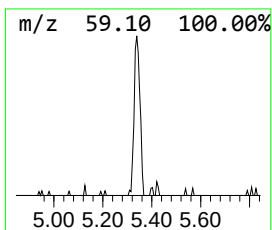
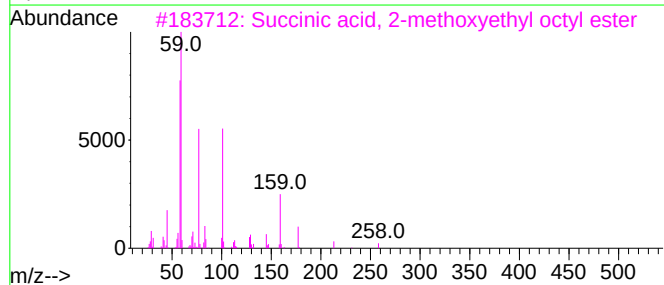
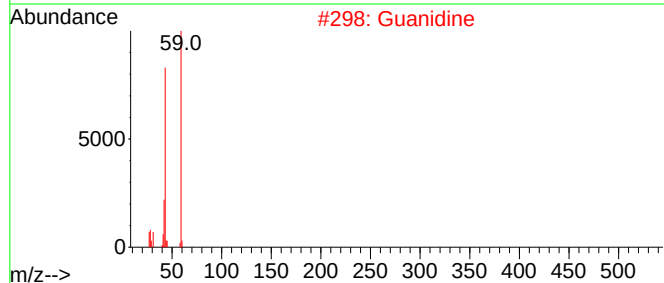
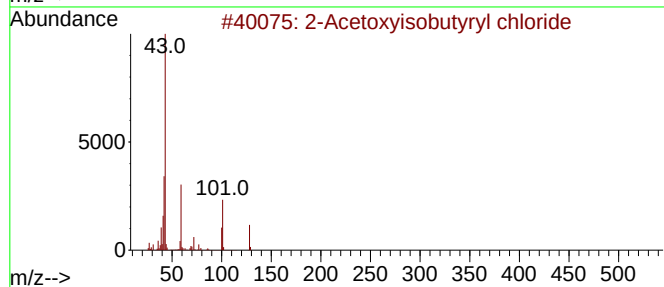
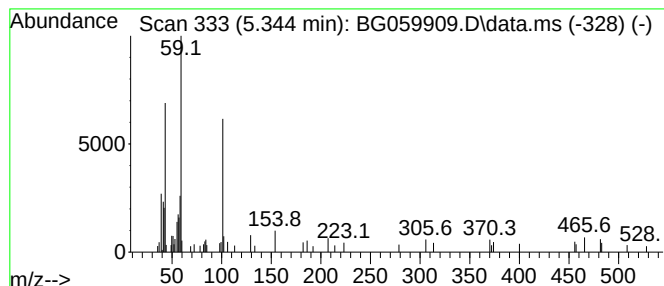
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown5.344 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.344	3.37 ng	48017	1,4-Dichlorobenzene-d4	8.311

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Acetoxyisobutyryl chloride	164	C6H9ClO3	040635-66-3	45		
2	Guanidine	59	CH5N3	000113-00-8	43		
3	Succinic acid, 2-methoxyethyl oc...	288	C15H28O5	1000325-80-8	38		
4	Oxirane, tetramethyl-	100	C6H12O	005076-20-0	37		
5	2-Propanol, 1,1,1-trichloro-2-me...	176	C4H7Cl3O	000057-15-8	32		



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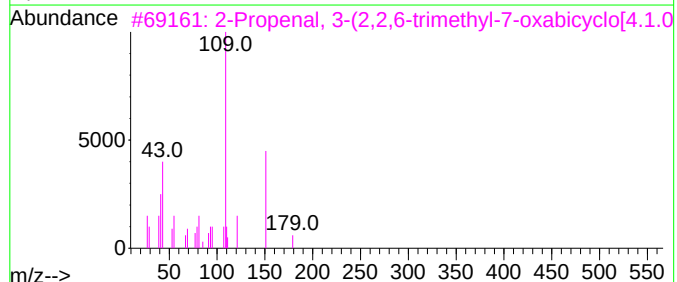
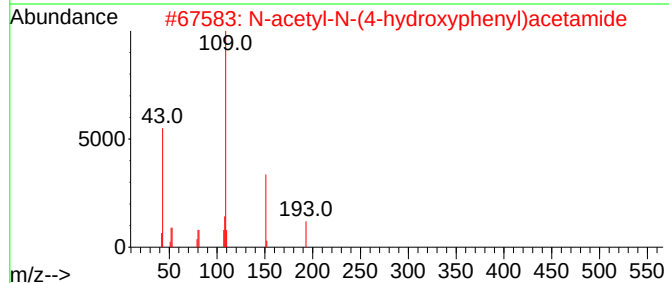
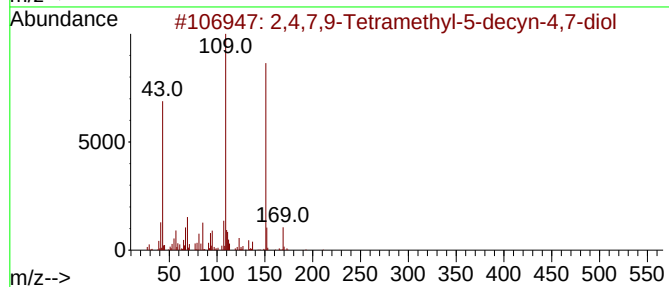
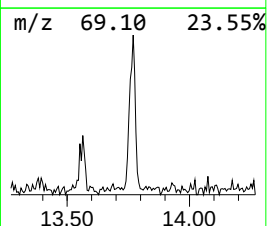
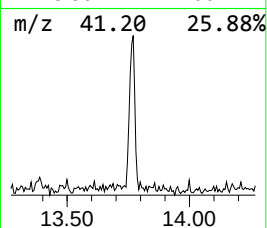
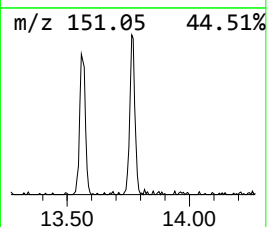
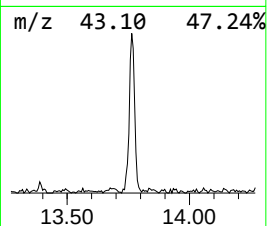
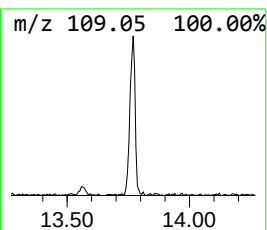
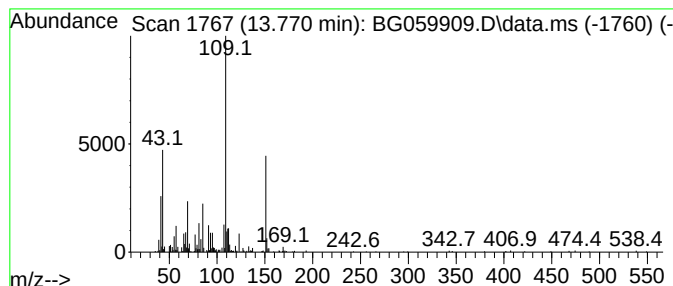
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Peak Number 2 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.770	19.53 ng	474078	Acenaphthene-d10	14.939	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	80
2	N-acetyl-N-(4-hydroxyphenyl)acet...	193	C10H11NO3	1000389-51-9	59
3	2-Propenal, 3-(2,2,6-trimethyl-7...	194	C12H18O2	055759-91-6	59
4	Acetaminophen	151	C8H9NO2	000103-90-2	58
5	Metacetamol	151	C8H9NO2	000621-42-1	53



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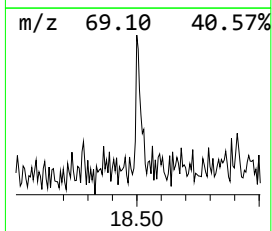
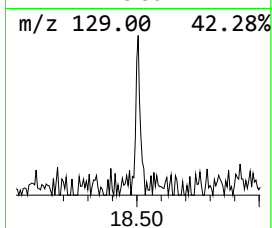
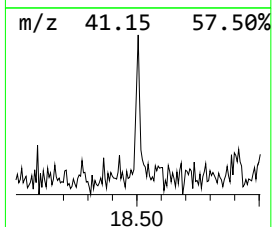
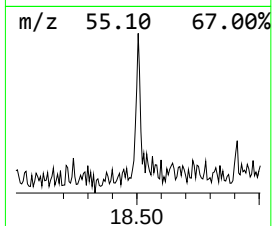
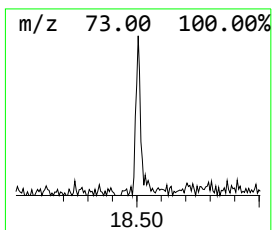
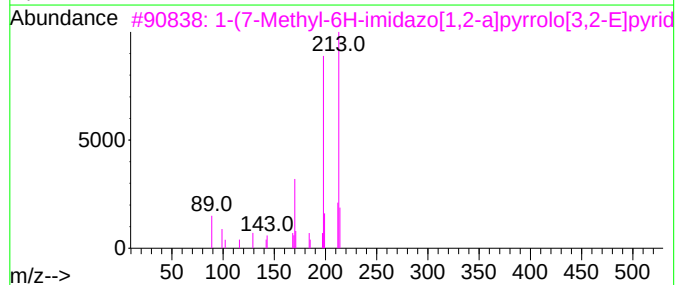
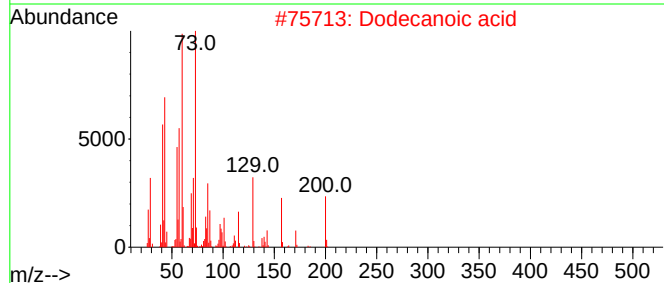
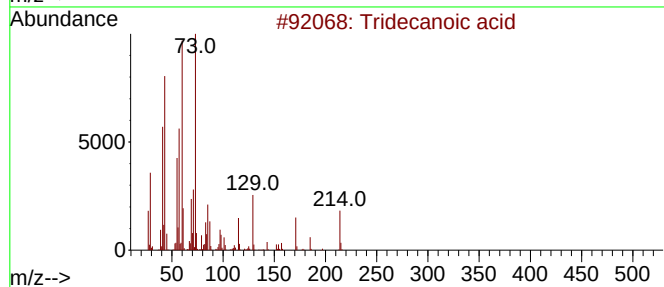
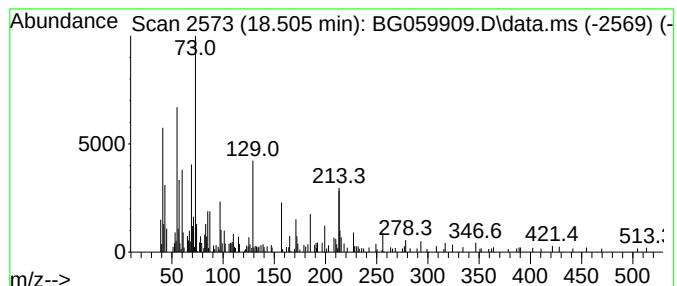
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Tridecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.505	4.91 ng	126633	Phenanthrene-d10	17.694

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid	214	C13H26O2	000638-53-9	55
2			Dodecanoic acid	200	C12H24O2	000143-07-7	27
3			1-(7-Methyl-6H-imidazo[1,2-a]pyr...	213	C12H11N3O	959007-34-2	22
4			.alpha.-D-Glucopyranoside, methy...	334	C17H34O6	1000157-24-7	22
5			As-Indacen-1(2H)-one, 3,6,7,8-te...	228	C16H20O	055591-18-9	14



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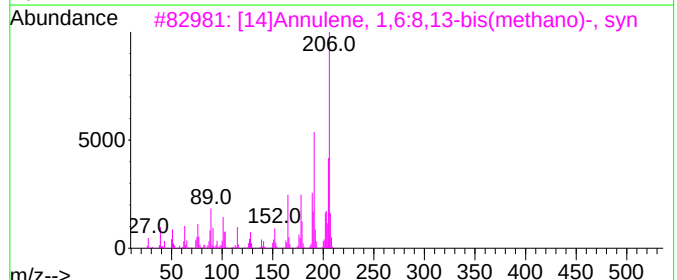
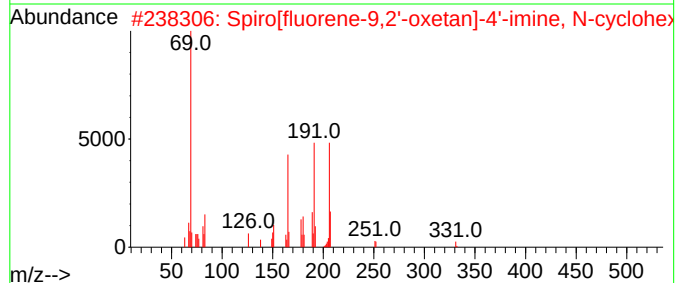
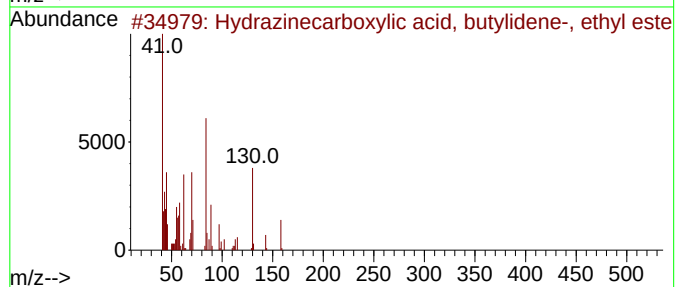
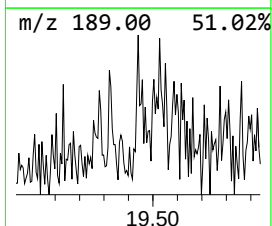
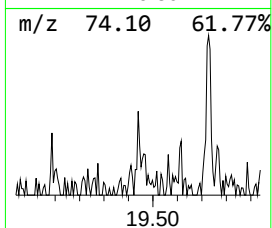
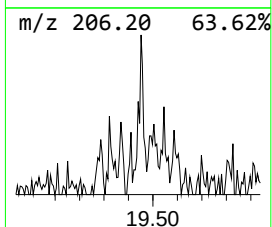
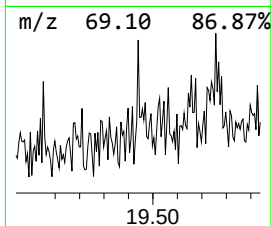
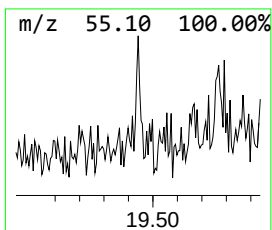
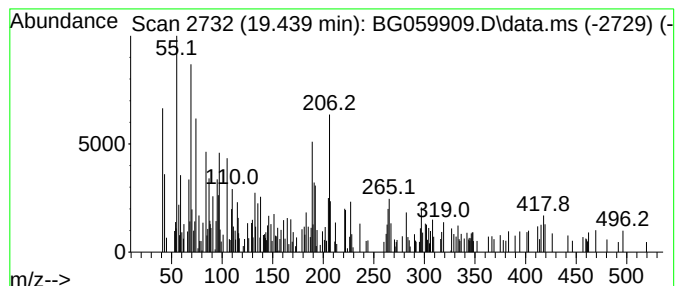
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 unknown19.439 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.439	2.39 ng	61749	Phenanthrene-d10	17.694

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hydrazinecarboxylic acid, butyli...	158	C7H14N2O2	007400-28-4	38
2			Spiro[fluorene-9,2'-oxetan]-4'-i...	331	C23H25NO	015183-47-8	25
3			[14]Annulene, 1,6:8,13-bis(metha...	206	C16H14	085385-68-8	15
4			Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	11
5			1,4-Diphenyl-1,3-butadiene	206	C16H14	000886-65-7	11



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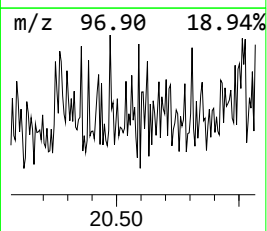
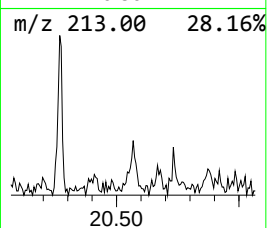
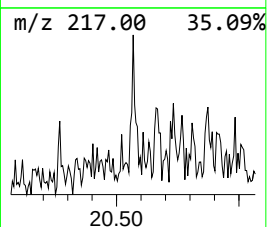
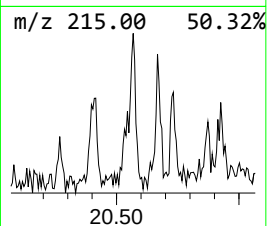
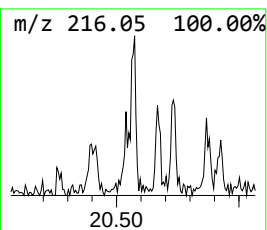
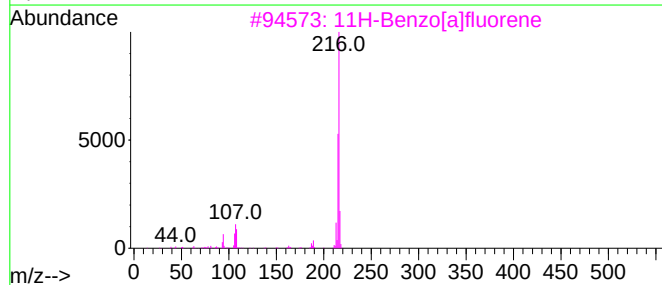
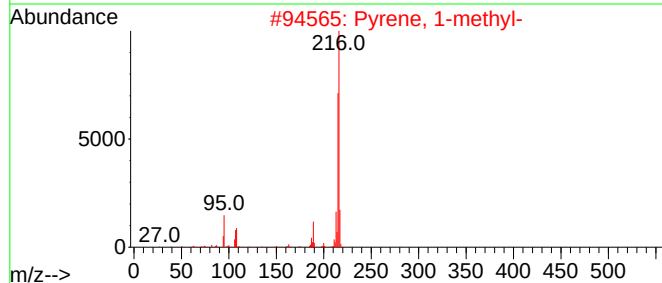
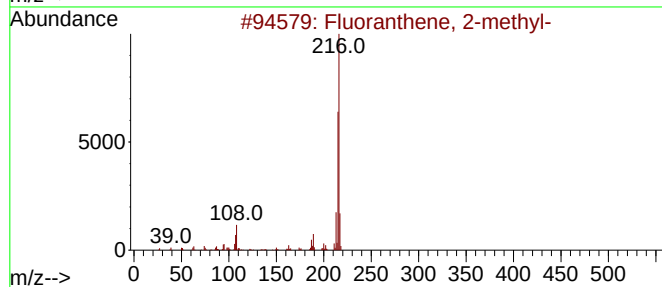
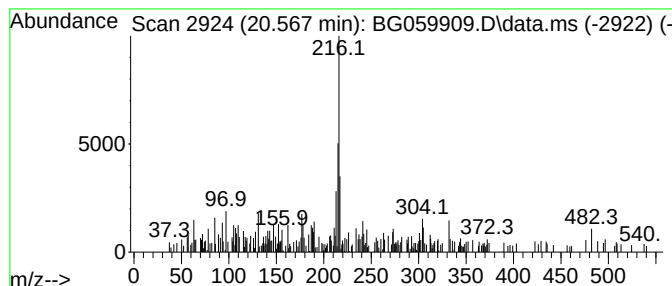
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Fluoranthene, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.567	2.23 ng	56622	Chrysene-d12	22.013

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	76
2			Pyrene, 1-methyl-	216	C17H12	002381-21-7	64
3			11H-Benzo[a]fluorene	216	C17H12	000238-84-6	64
4			1,3-Dihydro-5,6-dimethyl-1-(2-pr...	216	C12H12N2S	080276-22-8	59
5			8-Phosphadispiro[2.1.2.2]nonane,...	216	C14H17P	1010162-94-6	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112723\
Data File : BG059909.D
Acq On : 27 Nov 2023 20:33
Operator : MA/JU
Sample : 05463-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
NB-08-11162023

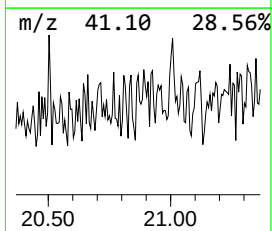
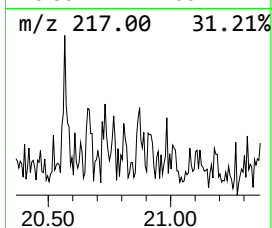
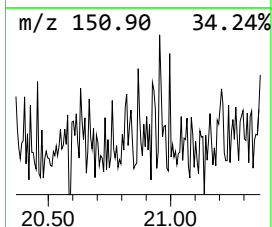
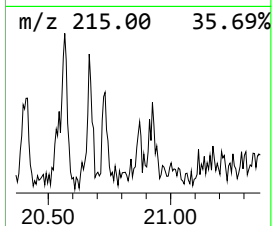
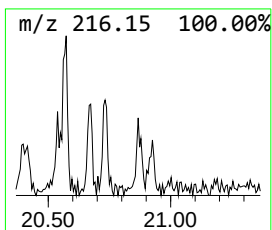
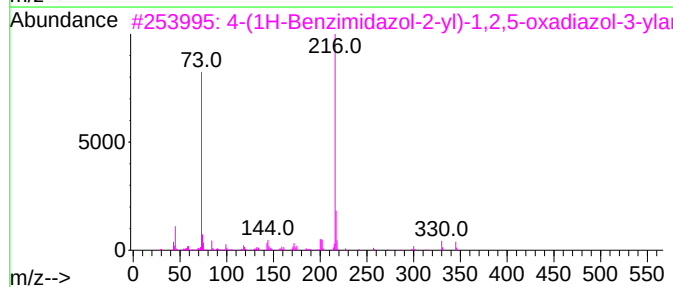
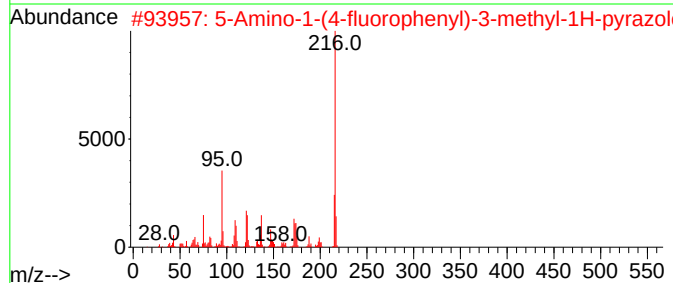
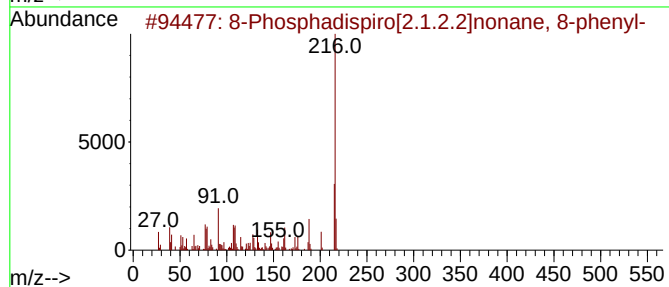
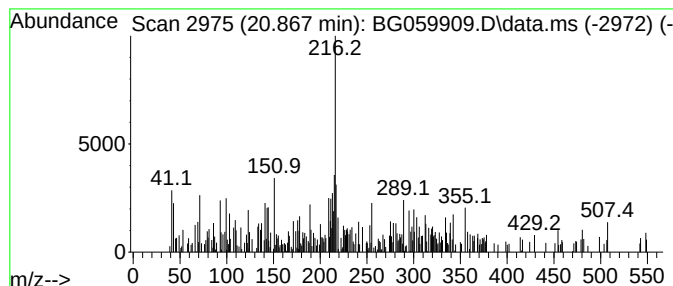
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 8-Phosphadispiro[2.1.2.2]no... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.867	3.21 ng	81711	Chrysene-d12	22.013

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			8-Phosphadispiro[2.1.2.2]nonane,...	216	C14H17P	1010162-94-6	50
2			5-Amino-1-(4-fluorophenyl)-3-met...	216	C11H9FN4	051516-82-6	43
3			4-(1H-Benzimidazol-2-yl)-1,2,5-o...	345	C15H23N5OSi2	1000470-95-5	43
4			Cyclohexanecarboxamide, N,N-dibe...	307	C21H25NO	1000450-96-8	43
5			4-((2-Methylphenyl)diazonyl)-1...	216	C10H12N6	057770-59-9	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112723\
Data File : BG059909.D
Acq On : 27 Nov 2023 20:33
Operator : MA/JU
Sample : 05463-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
NB-08-11162023

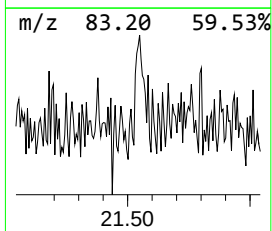
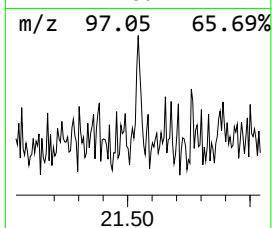
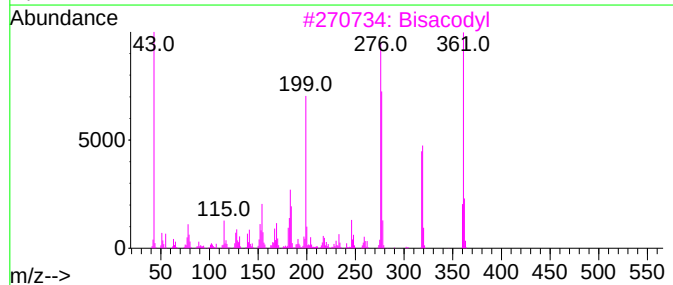
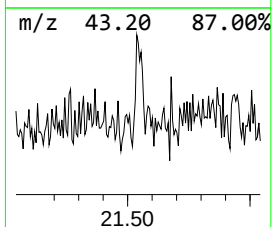
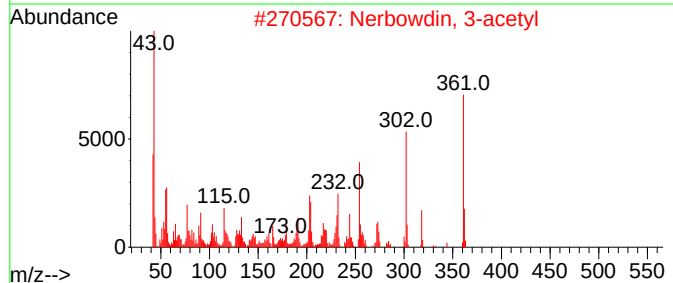
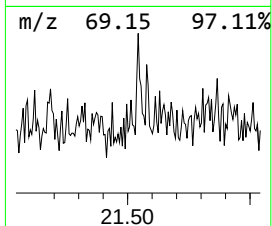
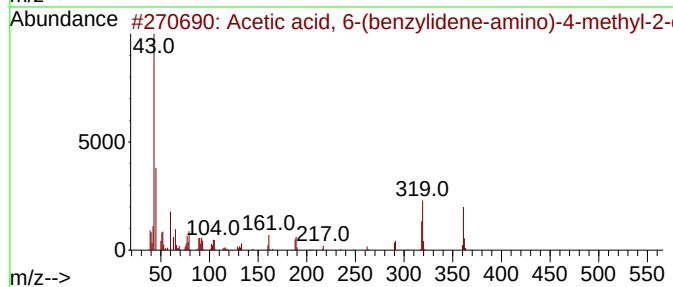
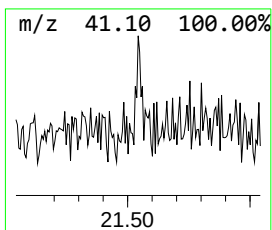
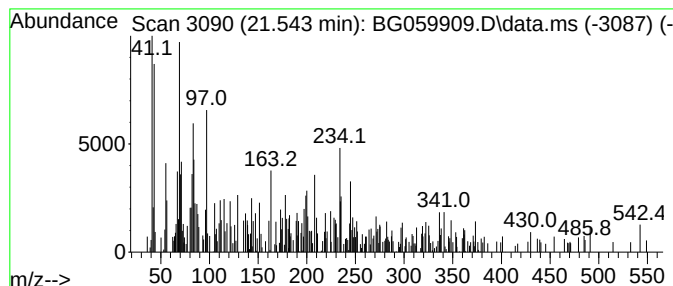
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown21.543 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.543	3.94 ng	100121	Chrysene-d12	22.013

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, 6-(benzylidene-amin...	361	C21H15NO5	1000294-68-2	14
2			Nerbowdin, 3-acetyl	361	C19H23NO6	100196-22-3	11
3			Bisacodyl	361	C22H19NO4	000603-50-9	10
4			N-[9-(Hydroxyimino)-2-methyl-5,1...	251	C7H5N7O4	1000436-04-1	10
5			5-Phthalimido-6-methoxy-8-acetam...	361	C20H15N3O4	1000227-45-3	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112723\
Data File : BG059909.D
Acq On : 27 Nov 2023 20:33
Operator : MA/JU
Sample : 05463-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
NB-08-11162023

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.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
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2,4,7,9-Tetrame...	13.770	19.5	ng	474078	3	14.939	485516	20.0
Tridecanoic acid	18.505	4.9	ng	126633	4	17.694	515839	20.0
unknown19.439	19.439	2.4	ng	61749	4	17.694	515839	20.0
Fluoranthene, 2...	20.567	2.2	ng	56622	5	22.013	508417	20.0
8-Phosphadispir...	20.867	3.2	ng	81711	5	22.013	508417	20.0
unknown21.543	21.543	3.9	ng	100121	5	22.013	508417	20.0