

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111622\
 Data File : BG055654.D
 Acq On : 16 Nov 2022 19:42
 Operator : CG/JU
 Sample : N5607-11
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB-40A

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-BG111622.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055654.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.303	337	343	351	rBV	84154	129573	6.38%	1.009%
2	5.779	417	424	436	rBV	503750	809196	39.85%	6.304%
3	7.389	690	698	710	rBV	568157	968987	47.72%	7.549%
4	8.253	836	845	853	rBV	149103	253229	12.47%	1.973%
5	9.422	1034	1044	1052	rBV	346089	606930	29.89%	4.728%
6	10.826	1276	1283	1296	rBV	34298	66848	3.29%	0.521%
7	11.079	1318	1326	1333	rBV	215281	393318	19.37%	3.064%
8	13.500	1729	1738	1746	rBV	940807	1456525	71.72%	11.347%
9	13.664	1760	1766	1774	rBV3	15764	24600	1.21%	0.192%
10	14.152	1843	1849	1854	rBV2	101549	154418	7.60%	1.203%
11	14.716	1941	1945	1948	rVB	20377	25859	1.27%	0.201%
12	14.763	1948	1953	1957	rVB2	26437	38379	1.89%	0.299%
13	14.875	1964	1972	1978	rBV	370878	581629	28.64%	4.531%
14	16.150	2183	2189	2195	rBV3	19191	27718	1.36%	0.216%
15	16.349	2216	2223	2235	rBV	738857	1147884	56.53%	8.943%
16	17.613	2432	2438	2444	rBV	458999	698773	34.41%	5.444%
17	18.253	2543	2547	2552	rBV	19067	22001	1.08%	0.171%
18	18.353	2558	2564	2571	rBV6	9919	23960	1.18%	0.187%
19	18.418	2571	2575	2580	rBV	27765	42204	2.08%	0.329%
20	18.470	2580	2584	2596	rVV	145159	229018	11.28%	1.784%
21	18.764	2630	2634	2640	rBV3	14348	22766	1.12%	0.177%
22	19.587	2771	2774	2777	rBV4	13885	21975	1.08%	0.171%
23	19.646	2777	2784	2791	rVV	56753	120040	5.91%	0.935%
24	19.734	2795	2799	2810	rVB	65799	108218	5.33%	0.843%
25	20.010	2841	2846	2851	rVB	39245	65043	3.20%	0.507%
26	20.198	2872	2878	2885	rBV	1513032	2030751	100.00%	15.821%
27	20.486	2925	2927	2933	rVB5	17180	23221	1.14%	0.181%
28	20.668	2955	2958	2966	rVB3	27395	42918	2.11%	0.334%
29	20.844	2983	2988	2992	rBV	236915	329720	16.24%	2.569%
30	20.879	2992	2994	3003	rVB2	71065	109893	5.41%	0.856%
31	20.991	3010	3013	3016	rVB2	18966	21697	1.07%	0.169%
32	21.520	3098	3103	3118	rBV3	66618	170698	8.41%	1.330%
33	21.772	3141	3146	3153	rVB	95896	137224	6.76%	1.069%
34	21.908	3162	3169	3176	rBV	456115	812108	39.99%	6.327%
35	22.736	3305	3310	3319	rBV4	56042	123092	6.06%	0.959%
36	25.321	3740	3750	3761	rBV2	268835	830109	40.88%	6.467%

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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-BG111622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	26.555	3954	3960	3971	rVB2	57129	165550	8.15%	1.290%
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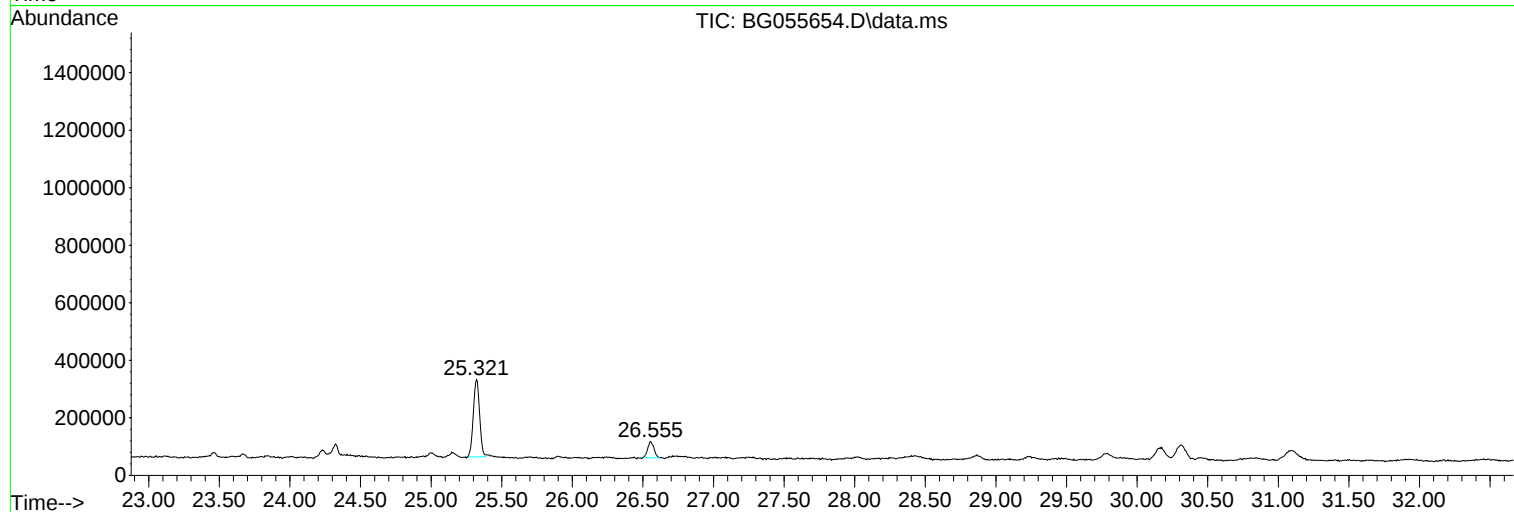
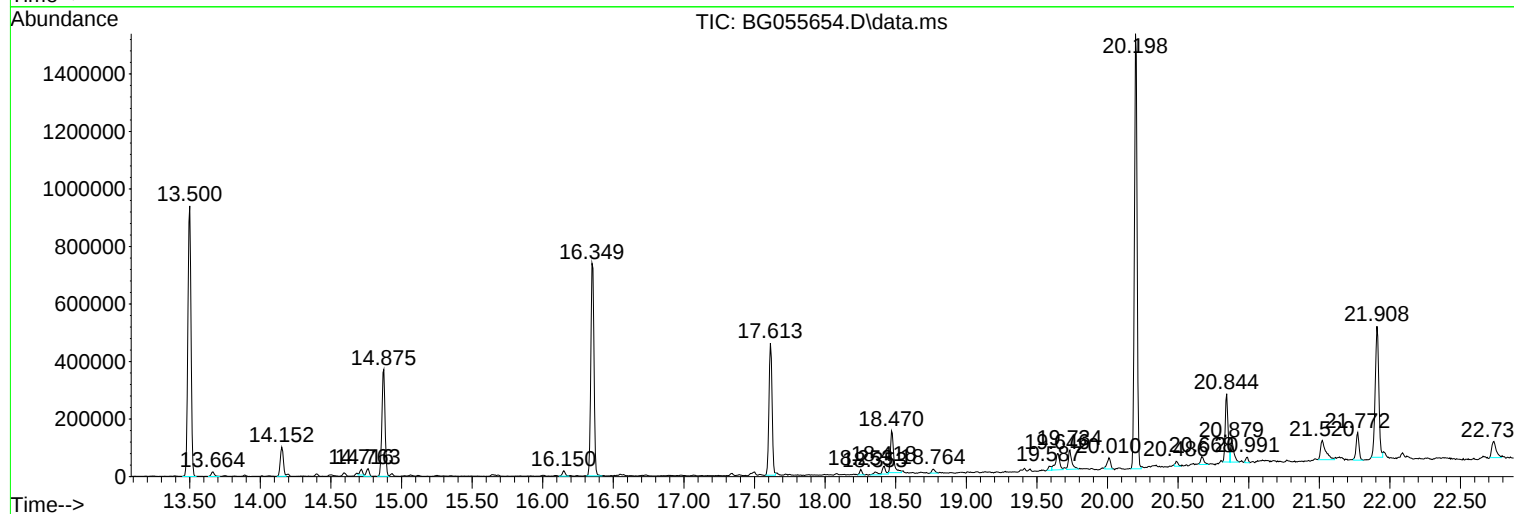
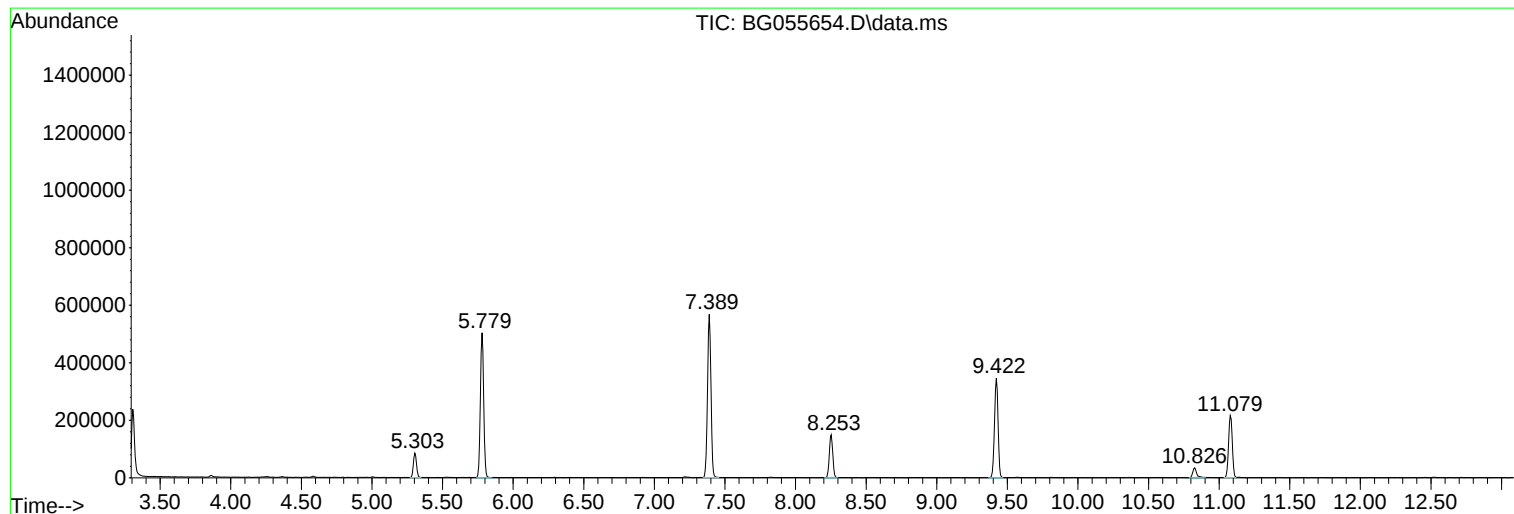
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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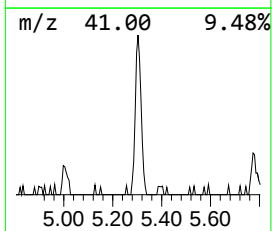
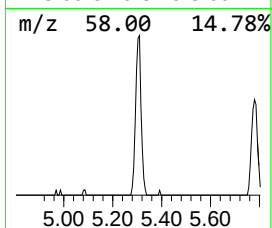
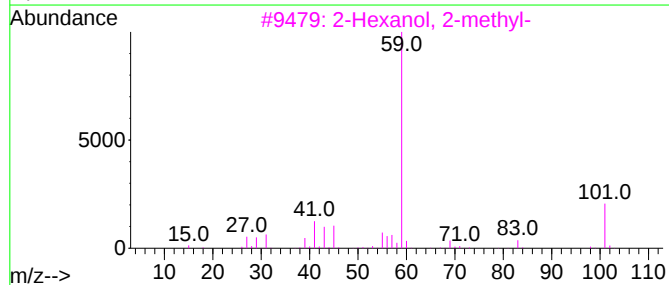
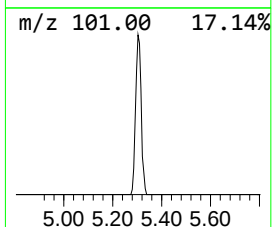
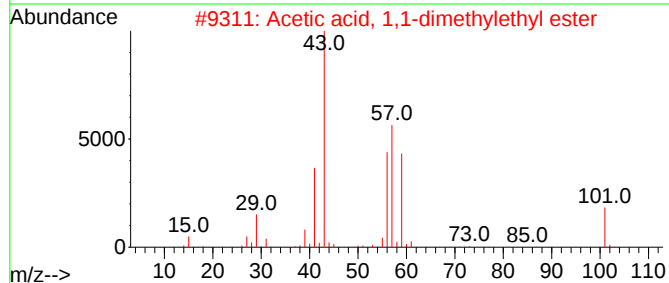
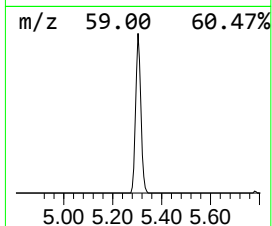
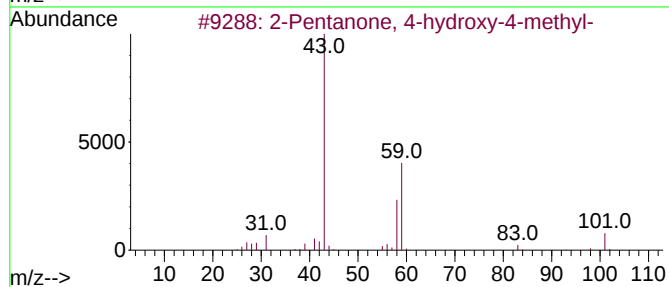
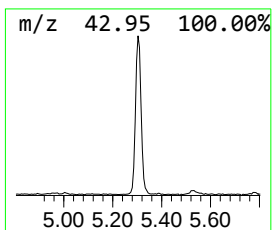
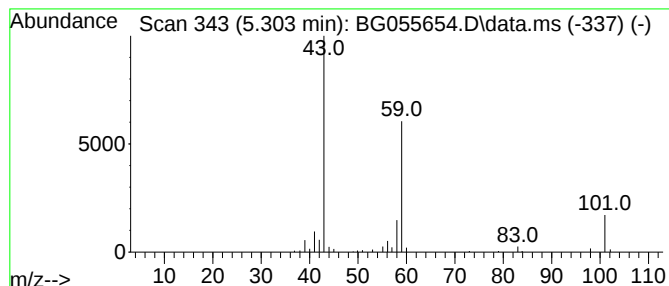
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.303	10.23 ng	129573	1,4-Dichlorobenzene-d4	8.253

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38		
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28		
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		



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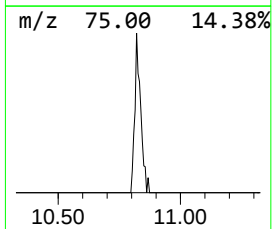
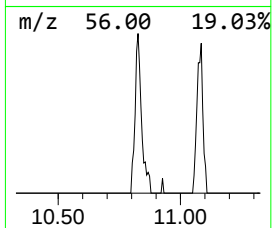
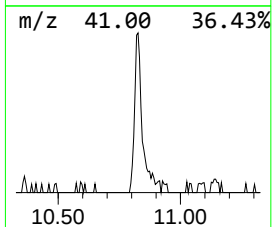
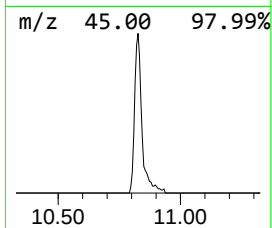
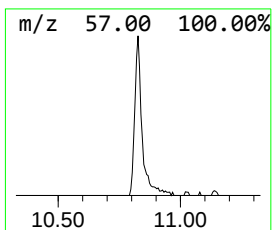
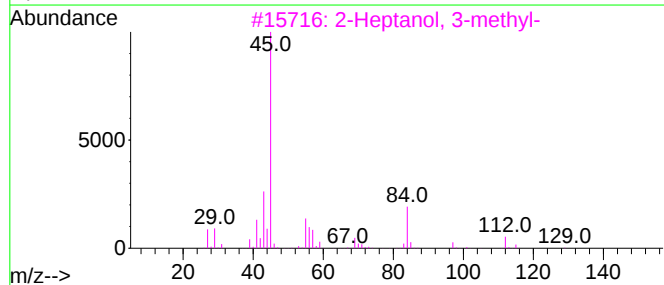
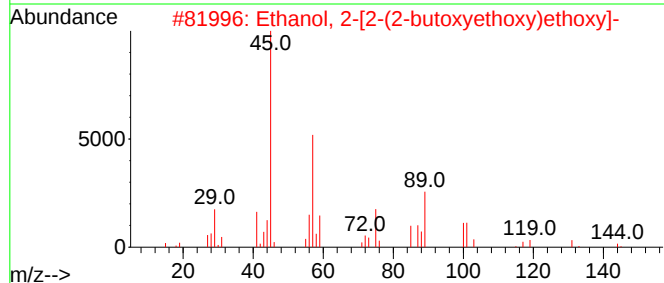
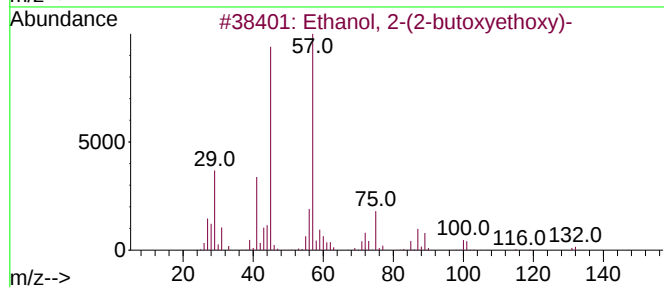
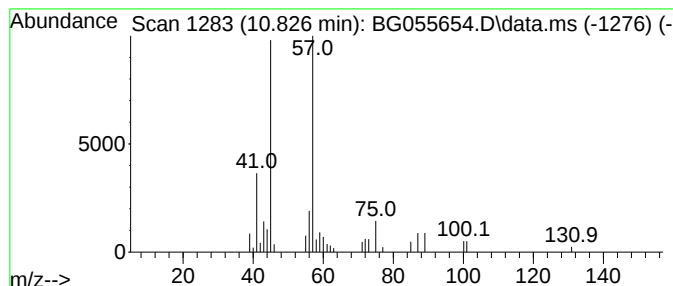
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.826	3.40 ng	66848	Naphthalene-d8	11.079

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	80
2			Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	64
3			2-Heptanol, 3-methyl-	130	C8H18O	031367-46-1	64
4			Propanoic acid, 2-hydroxy-, 2-me...	146	C7H14O3	000585-24-0	56
5			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56



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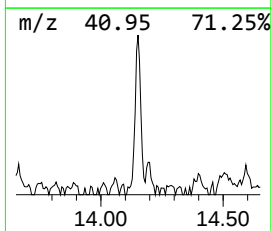
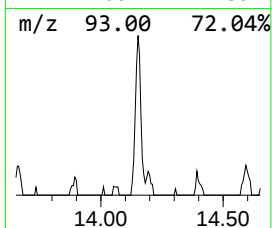
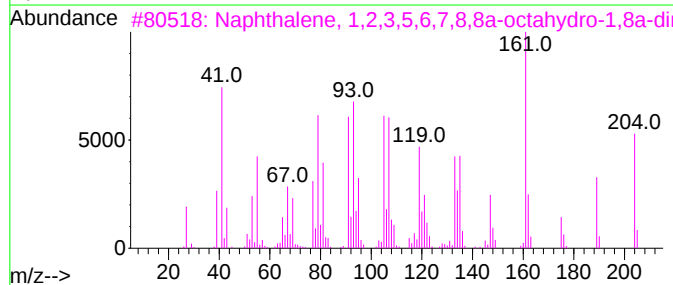
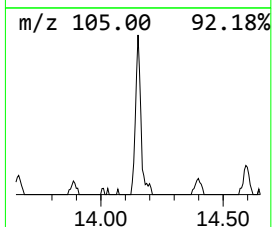
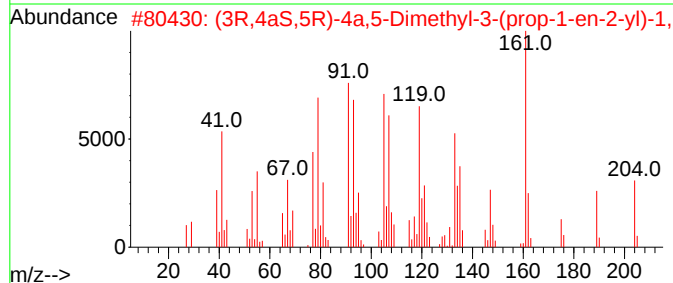
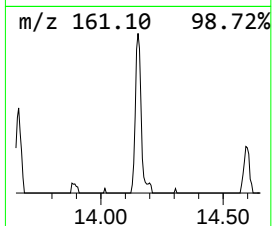
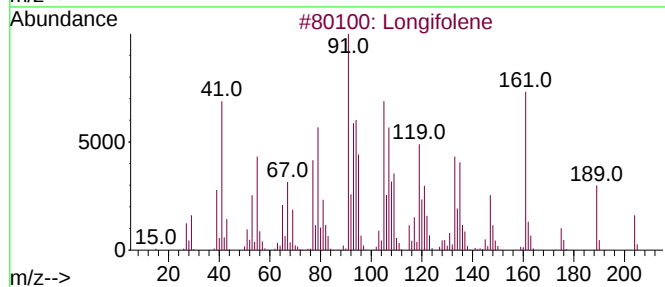
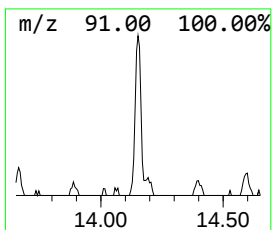
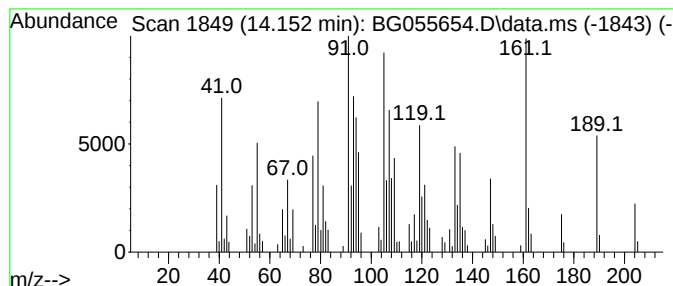
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Longifolene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.152	5.31 ng	154418	Acenaphthene-d10	14.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Longifolene	204	C15H24	000475-20-7	99
2			(3R,4aS,5R)-4a,5-Dimethyl-3-(pro...	204	C15H24	024741-64-8	95
3			Naphthalene, 1,2,3,5,6,7,8,8a-oc...	204	C15H24	010219-75-7	95
4			Naphthalene, 1,2,3,5,6,7,8,8a-oc...	204	C15H24	004630-07-3	95
5			Spiro[5.5]undec-2-ene, 3,7,7-tri...	204	C15H24	018431-82-8	89



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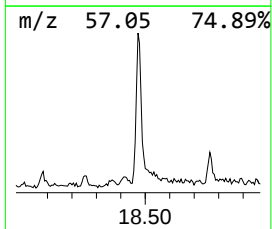
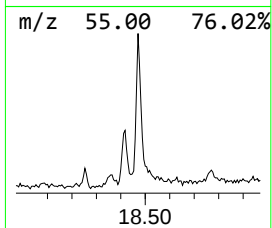
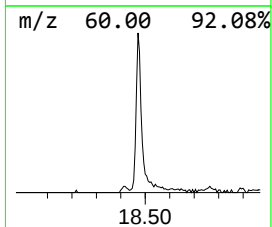
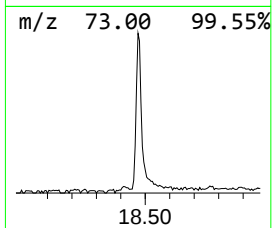
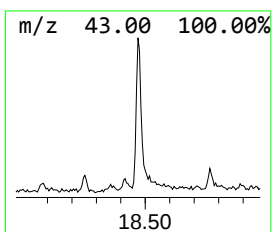
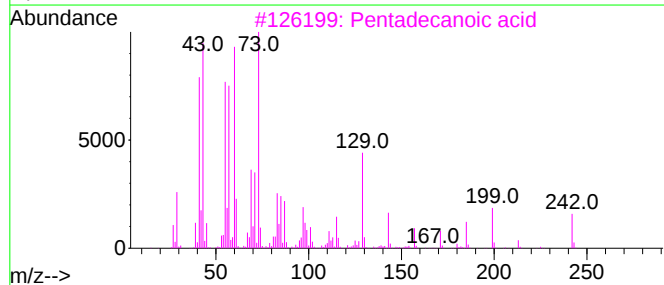
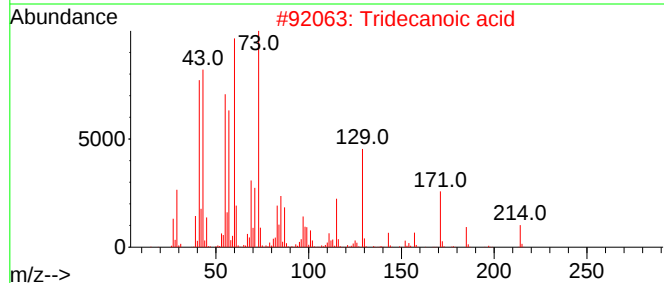
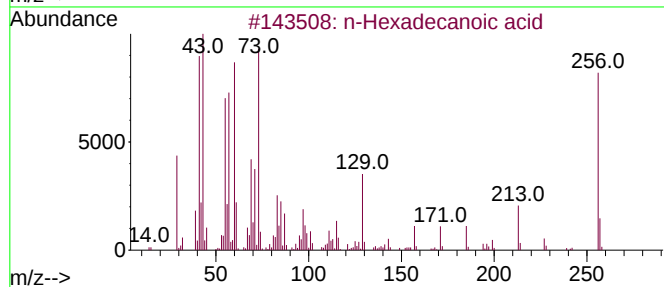
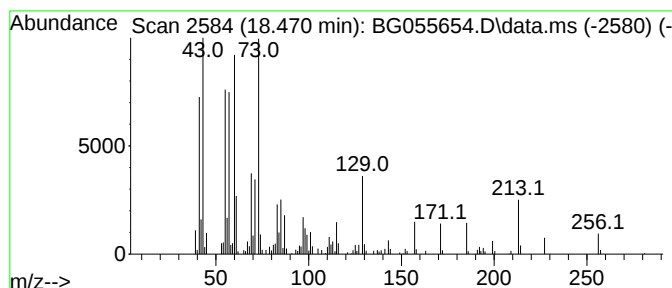
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.470	6.55 ng	229018	Phenanthrene-d10	17.613

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4			Undecanoic acid	186	C11H22O2	000112-37-8	70
5			n-Decanoic acid	172	C10H20O2	000334-48-5	53



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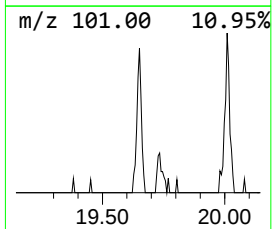
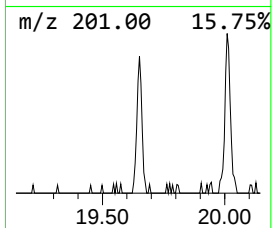
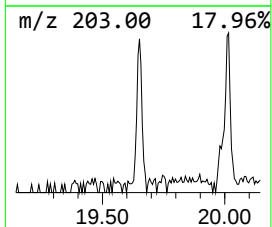
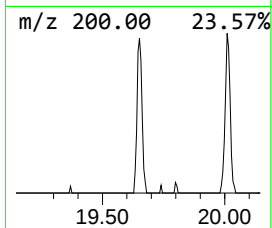
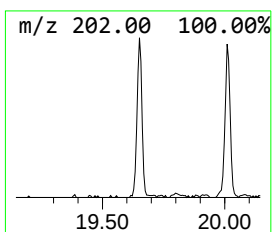
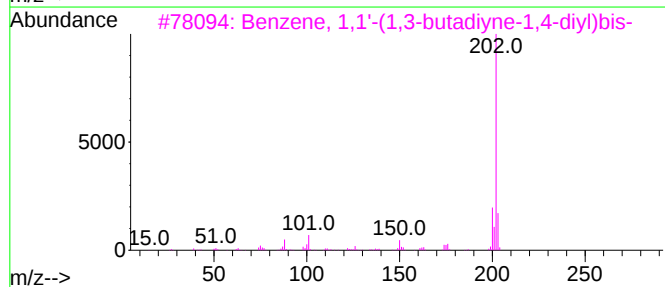
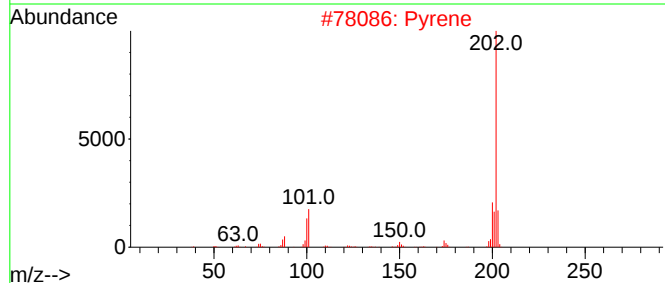
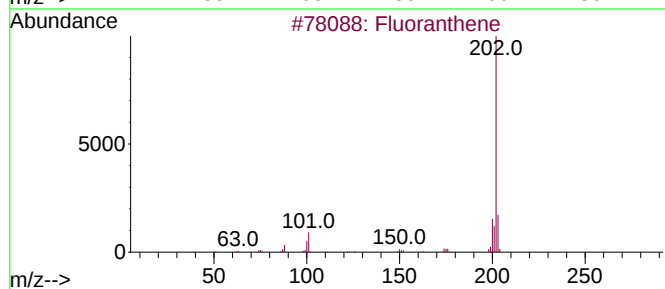
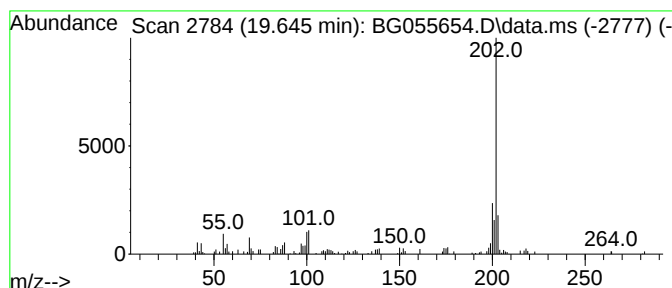
Instrument :
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SB-40A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Benzene, 1,1'-(1,3-butadiyn... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.645	3.44 ng	120040	Phenanthrene-d10	17.613	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fluoranthene	202	C16H10	000206-44-0	93
2	Pyrene	202	C16H10	000129-00-0	90
3	Benzene, 1,1'-(1,3-butadiyne-1,4...	202	C16H10	000886-66-8	76
4	7H-Furo[3,2-g][1]benzopyran-7-on...	202	C11H6O4	002009-24-7	47
5	2-Butenamide, 3-methyl-N-1H-puri...	217	C10H11N5O	021589-34-4	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111622\
Data File : BG055654.D
Acq On : 16 Nov 2022 19:42
Operator : CG/JU
Sample : N5607-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-40A

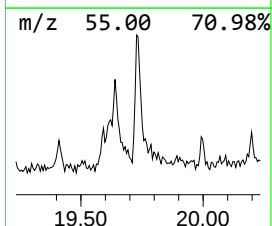
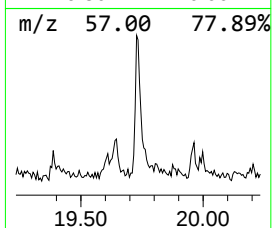
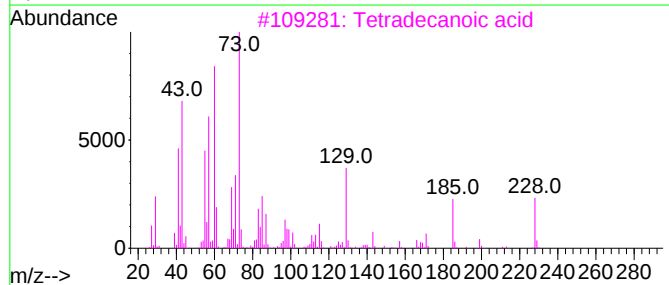
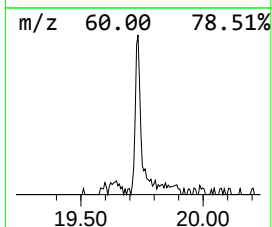
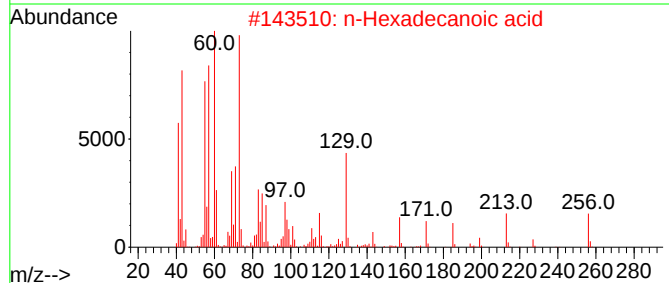
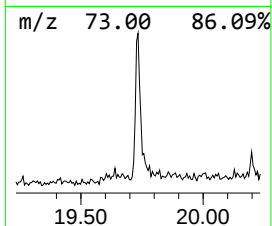
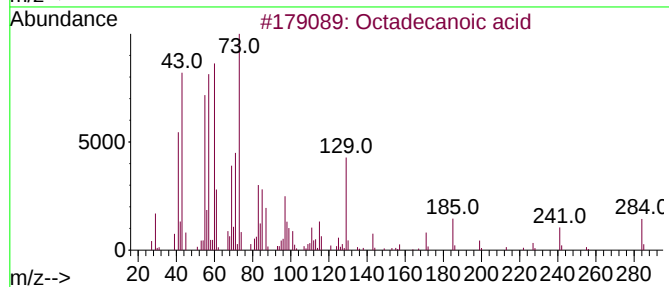
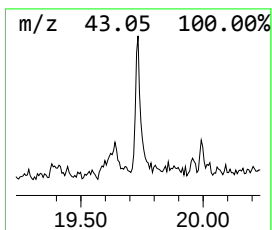
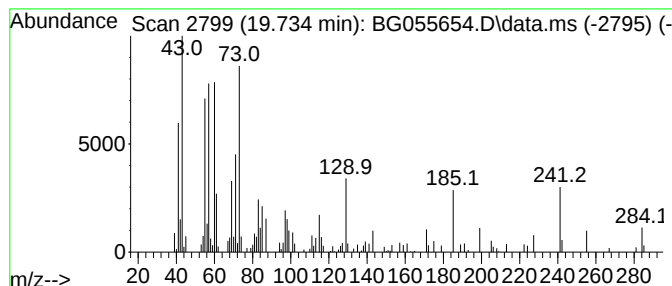
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.734	3.10 ng	108218	Phenanthrene-d10	17.613

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	98
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	68
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4			Tridecanoic acid	214	C13H26O2	000638-53-9	52
5			n-Decanoic acid	172	C10H20O2	000334-48-5	52



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111622\
Data File : BG055654.D
Acq On : 16 Nov 2022 19:42
Operator : CG/JU
Sample : N5607-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-40A

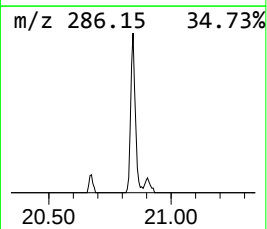
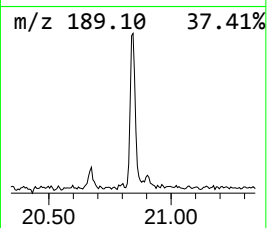
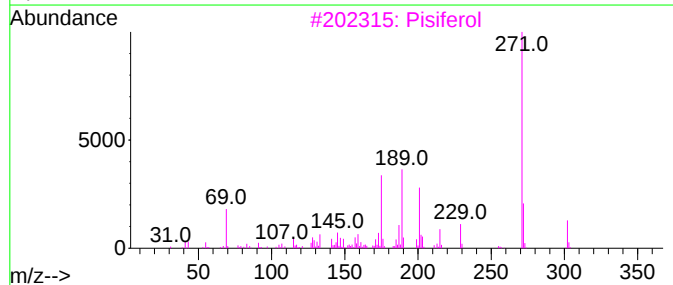
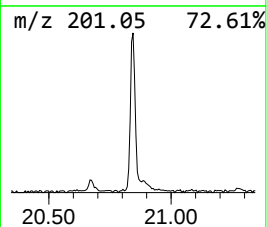
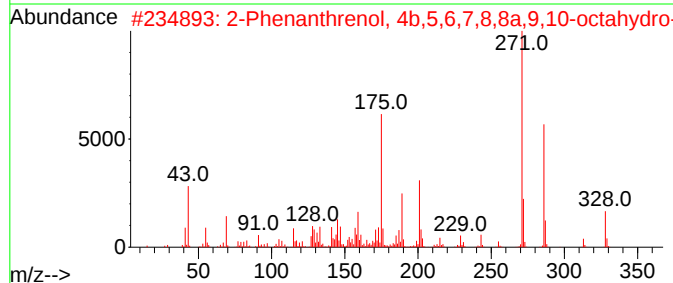
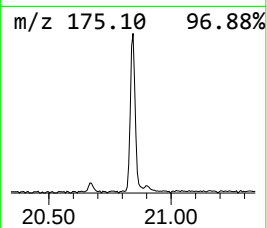
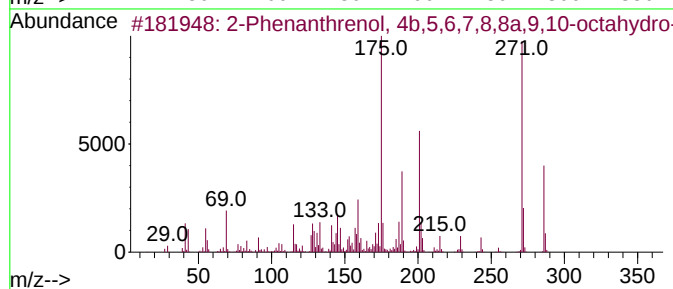
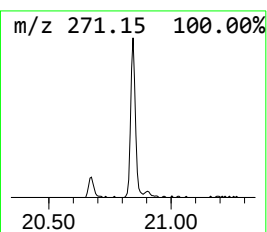
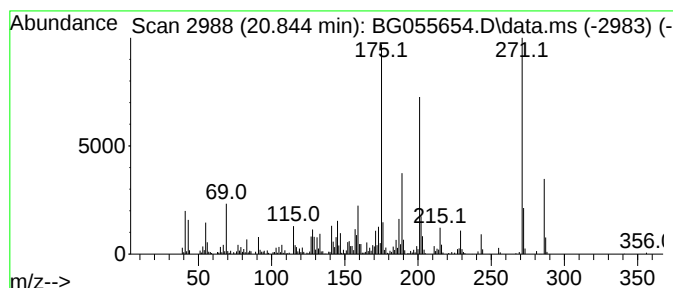
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 2-Phenanthrenol, 4b,5,6,7,8... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.844	8.12 ng	329720	Chrysene-d12	21.908

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Phenanthrenol, 4b,5,6,7,8,8a,9...	286	C20H30O	000511-15-9	99		
2	2-Phenanthrenol, 4b,5,6,7,8,8a,9...	328	C22H32O2	015340-82-6	91		
3	Pisiferol	302	C20H30O2	024035-36-7	46		
4	13-Isopropylpodocarpene-12-ol-20-al	300	C20H28O2	024035-37-8	43		
5	Silane, dimethyl(2-chloro-5-meth...	286	C14H23ClO2Si	1000347-54-6	41		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111622\
Data File : BG055654.D
Acq On : 16 Nov 2022 19:42
Operator : CG/JU
Sample : N5607-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

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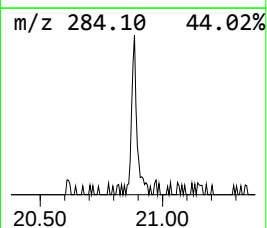
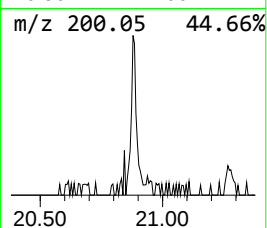
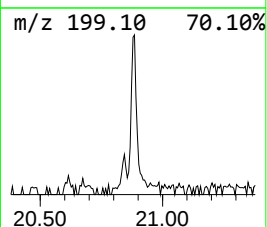
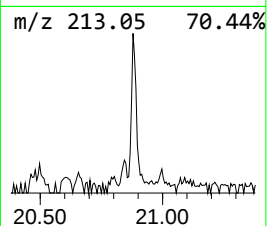
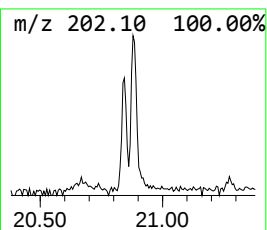
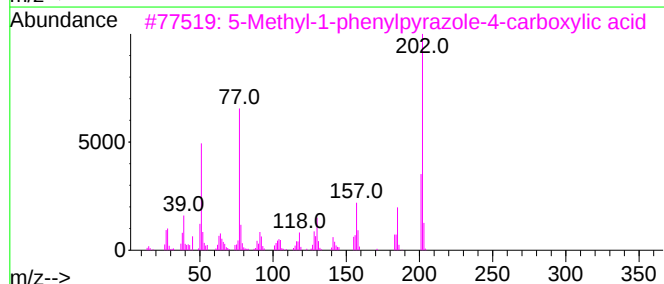
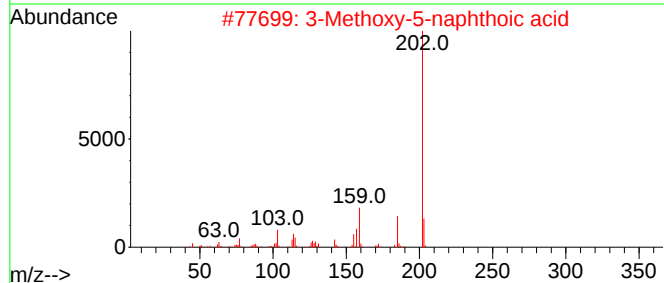
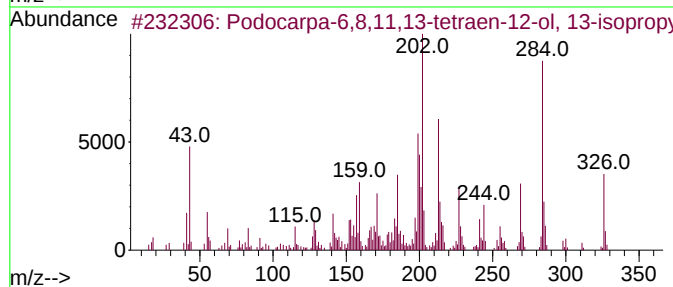
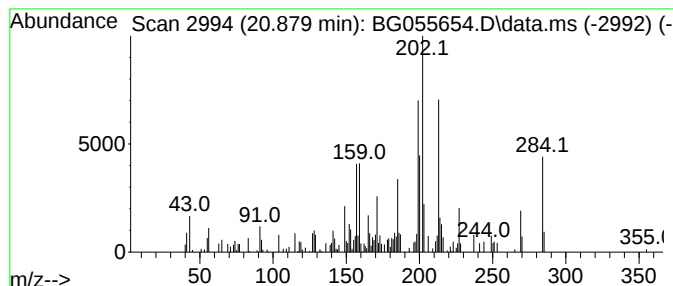
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown20.879 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.879	2.71 ng	109893	Chrysene-d12	21.908

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Podocarpa-6,8,11,13-tetraen-12-o...	326	C22H30O2	022160-86-7	32
2			3-Methoxy-5-naphthoic acid	202	C12H10O3	007498-58-0	22
3			5-Methyl-1-phenylpyrazole-4-carb...	202	C11H10N2O2	091138-00-0	15
4			5-Ethyl-4,7-dihydro-2-methyl-7-o...	202	C10H10N4O	903195-75-5	14
5			4-Chloro-1-tripropylsilyloxybenzene	284	C15H25ClOSi	1000307-84-1	11



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111622\
Data File : BG055654.D
Acq On : 16 Nov 2022 19:42
Operator : CG/JU
Sample : N5607-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

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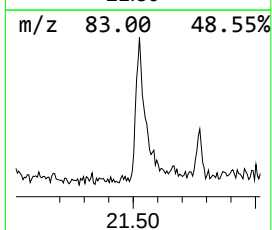
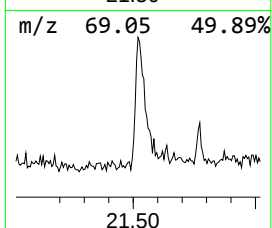
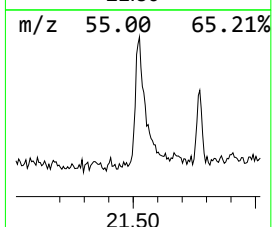
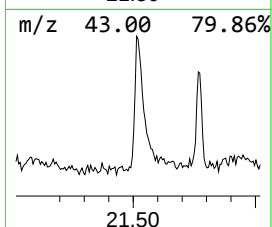
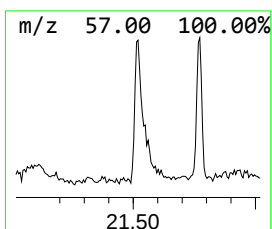
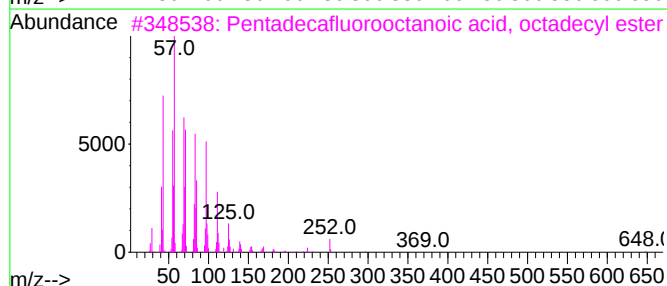
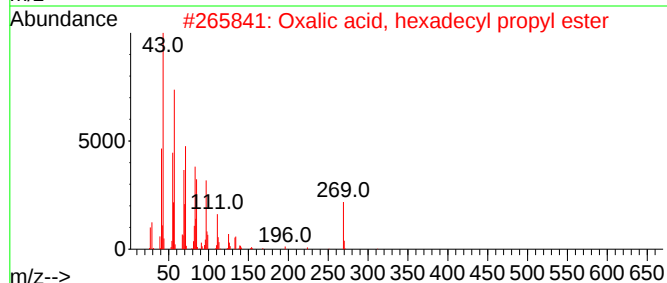
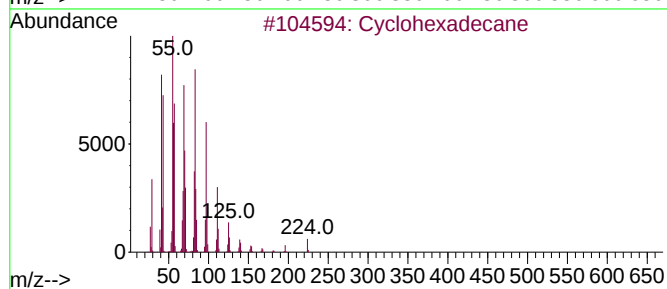
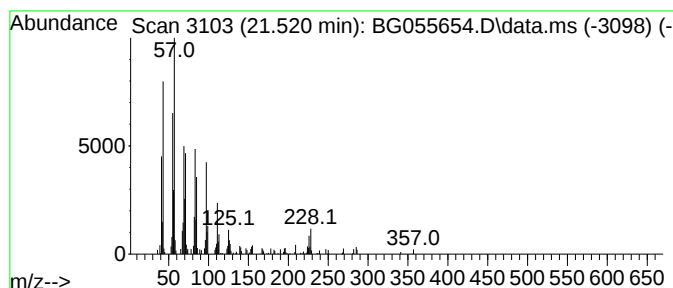
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Cyclohexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.520	4.20 ng	170698	Chrysene-d12	21.908

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexadecane	224	C16H32	000295-65-8	94
2			Oxalic acid, hexadecyl propyl ester	356	C21H40O4	1000309-26-9	87
3			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	87
4			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	74
5			Hexadecanoic acid, 2-hydroxy-, m...	286	C17H34O3	016742-51-1	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111622\
Data File : BG055654.D
Acq On : 16 Nov 2022 19:42
Operator : CG/JU
Sample : N5607-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

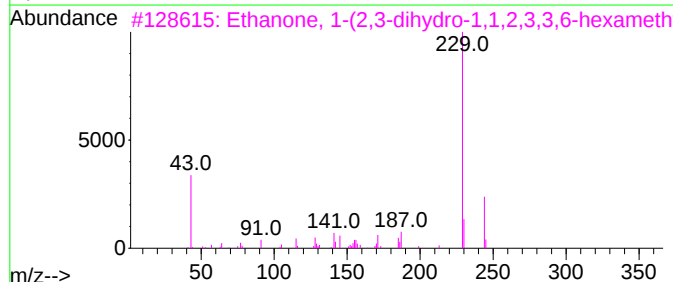
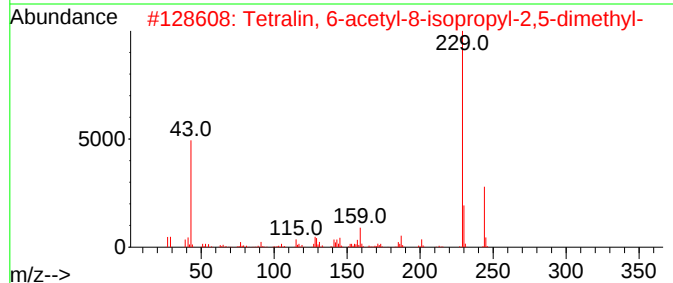
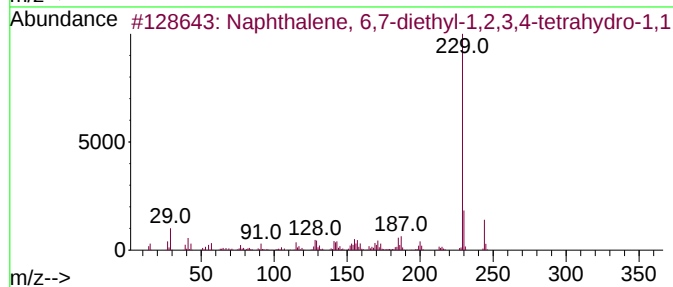
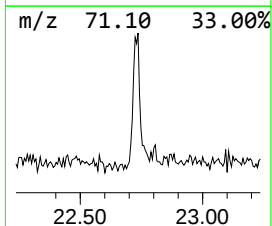
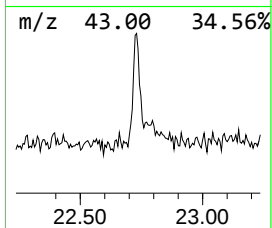
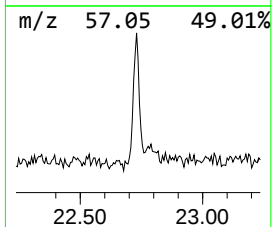
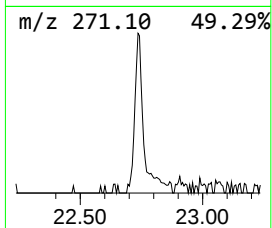
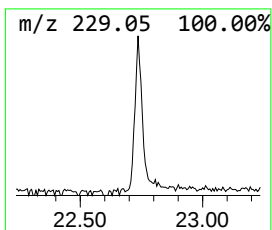
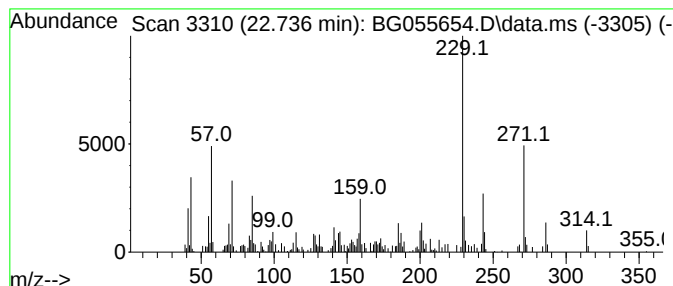
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Naphthalene, 6,7-diethyl-1,... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD		R.T.	
22.736	3.03 ng	123092	Chrysene-d12		21.908	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Naphthalene, 6,7-diethyl-1,2,3,4...		244	C18H28	055741-10-1	56
2	Tetralin, 6-acetyl-8-isopropyl-2...		244	C17H24O	1000155-43-5	46
3	Ethanone, 1-(2,3-dihydro-1,1,2,3...		244	C17H24O	015323-35-0	46
4	N-(7-Chloro-2-phenazinyl)acetamide		271	C14H10ClN3O	023677-13-6	43
5	10H-Phenothiazine, 3-methoxy-		229	C13H11NOS	001771-19-3	42



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111622\
Data File : BG055654.D
Acq On : 16 Nov 2022 19:42
Operator : CG/JU
Sample : N5607-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-40A

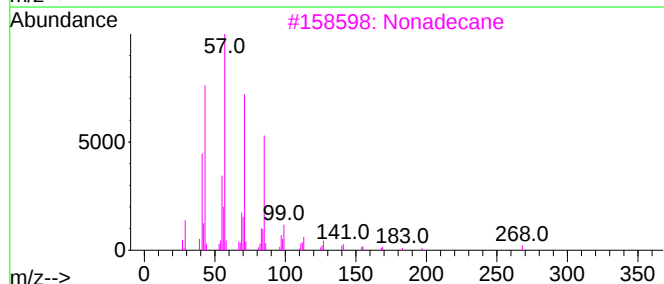
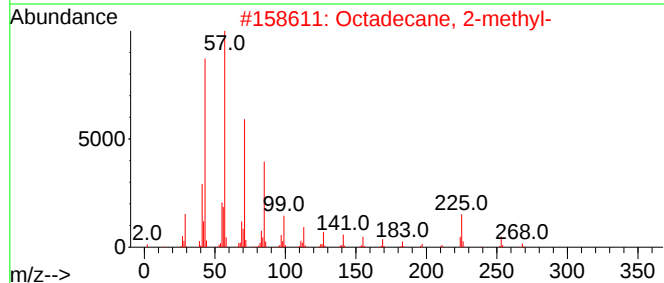
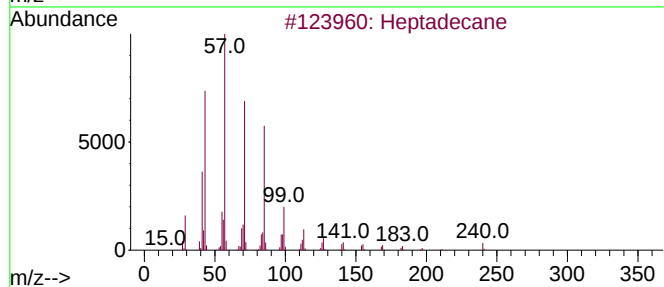
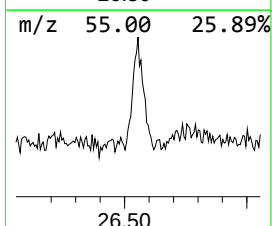
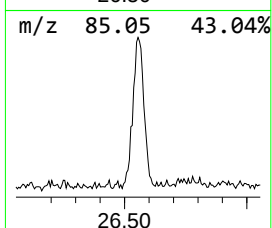
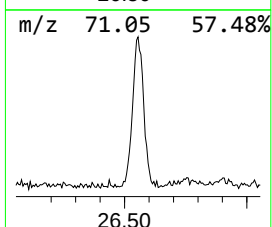
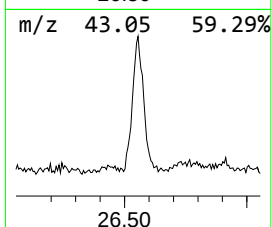
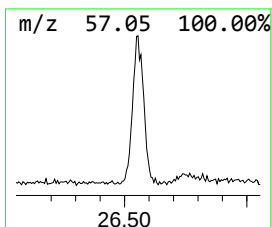
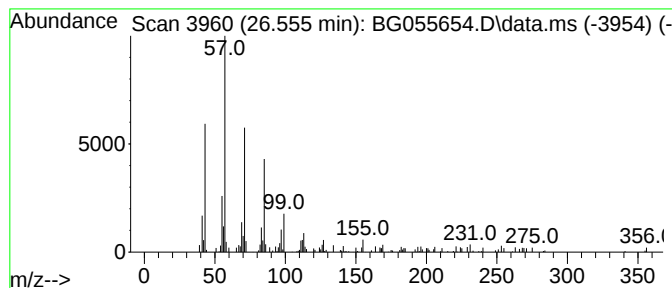
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Heptadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.555	3.99 ng	165550	Perylene-d12	25.321

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecane	240	C17H36	000629-78-7	90
2		Octadecane, 2-methyl-	268	C19H40	001560-88-9	90
3		Nonadecane	268	C19H40	000629-92-5	90
4		Hexadecane, 2-methyl-	240	C17H36	001560-92-5	87
5		Hentriacontane	437	C31H64	000630-04-6	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111622\
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Operator : CG/JU
Sample : N5607-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-40A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.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-...	5.303	10.2	ng	129573	1	8.253	253229	20.0
Ethanol, 2-(2-b...	10.826	3.4	ng	66848	2	11.079	393318	20.0
Longifolene	14.152	5.3	ng	154418	3	14.875	581629	20.0
n-Hexadecanoic ...	18.470	6.5	ng	229018	4	17.613	698773	20.0
Benzene, 1,1'-(...	19.645	3.4	ng	120040	4	17.613	698773	20.0
Octadecanoic acid	19.734	3.1	ng	108218	4	17.613	698773	20.0
2-Phenanthrenol...	20.844	8.1	ng	329720	5	21.908	812108	20.0
unknown20.879	20.879	2.7	ng	109893	5	21.908	812108	20.0
Cyclohexadecane	21.520	4.2	ng	170698	5	21.908	812108	20.0
Naphthalene, 6,...	22.736	3.0	ng	123092	5	21.908	812108	20.0
Heptadecane	26.555	4.0	ng	165550	6	25.321	830109	20.0