

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062123\
 Data File : BG057790.D
 Acq On : 21 Jun 2023 18:44
 Operator : CG/JU
 Sample : 03289-16
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB-06-12.0-14.0

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-BG061923.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057790.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.026	324	330	339	rBV	117866	170057	8.09%	1.401%
2	5.491	402	409	421	rBV	467337	738017	35.11%	6.080%
3	7.083	671	680	687	rBV	511491	837052	39.82%	6.896%
4	7.923	817	823	829	rBV	101931	160219	7.62%	1.320%
5	9.081	1011	1020	1030	rVB	285922	499139	23.74%	4.112%
6	10.726	1293	1300	1310	rVB	149220	259699	12.35%	2.139%
7	13.182	1711	1718	1727	rVB	788883	1171219	55.72%	9.649%
8	14.556	1945	1952	1958	rBV	259593	397555	18.91%	3.275%
9	15.914	2176	2183	2189	rVB	97478	143466	6.82%	1.182%
10	16.043	2198	2205	2218	rBV	751350	1112923	52.94%	9.169%
11	16.695	2311	2316	2322	rBV3	22828	37436	1.78%	0.308%
12	17.300	2413	2419	2424	rBV	376125	548390	26.09%	4.518%
13	17.465	2442	2447	2455	rVB3	17491	24158	1.15%	0.199%
14	18.064	2545	2549	2558	rBV	43167	70970	3.38%	0.585%
15	18.193	2565	2571	2581	rBV	273214	433436	20.62%	3.571%
16	19.345	2759	2767	2775	rBV4	55691	129936	6.18%	1.070%
17	19.462	2783	2787	2799	rBV	68709	107143	5.10%	0.883%
18	19.709	2823	2829	2839	rVB3	23237	55355	2.63%	0.456%
19	19.915	2858	2864	2870	rVB	1603382	2102116	100.00%	17.318%
20	20.191	2904	2911	2914	rBV8	11897	25483	1.21%	0.210%
21	20.285	2924	2927	2933	rVV3	16704	23257	1.11%	0.192%
22	20.720	2996	3001	3004	rBV2	28801	35299	1.68%	0.291%
23	21.166	3071	3077	3080	rBV2	66201	131037	6.23%	1.080%
24	21.207	3080	3084	3092	rVV3	165197	384573	18.29%	3.168%
25	21.284	3093	3097	3104	rVV	312468	442363	21.04%	3.644%
26	21.554	3136	3143	3149	rBV2	370146	609152	28.98%	5.018%
27	21.748	3173	3176	3181	rVB	42846	64393	3.06%	0.530%
28	22.353	3274	3279	3285	rBV	36351	64371	3.06%	0.530%
29	23.035	3391	3395	3403	rVB2	25970	44493	2.12%	0.367%
30	23.217	3419	3426	3434	rVB	279843	549284	26.13%	4.525%
31	24.703	3670	3679	3695	rVB2	234757	696024	33.11%	5.734%
32	25.972	3891	3895	3907	rVB9	25359	70420	3.35%	0.580%

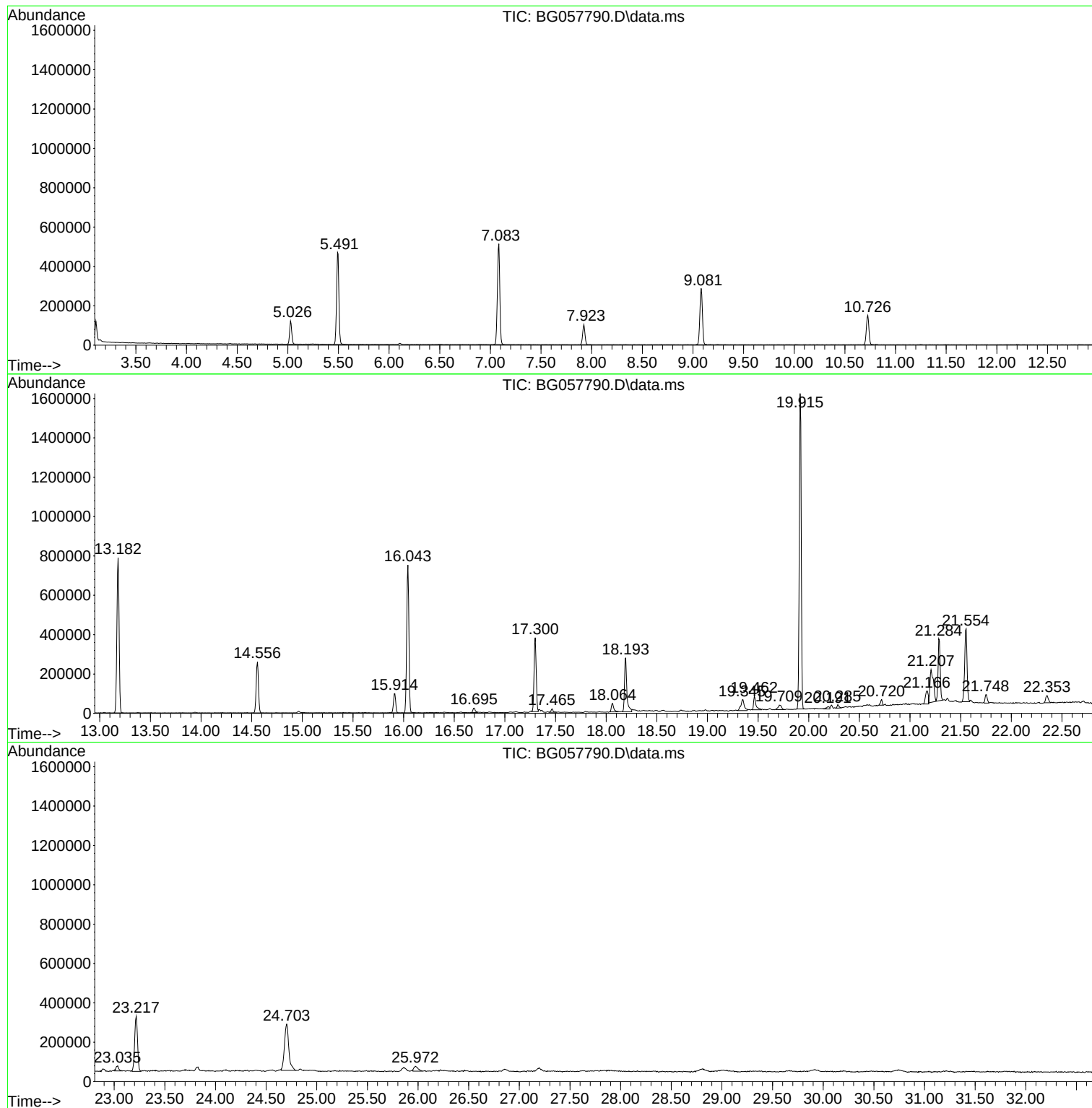
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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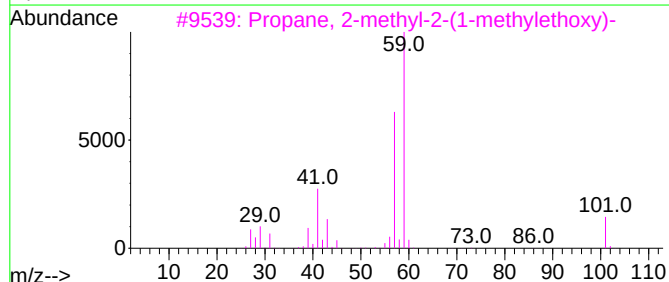
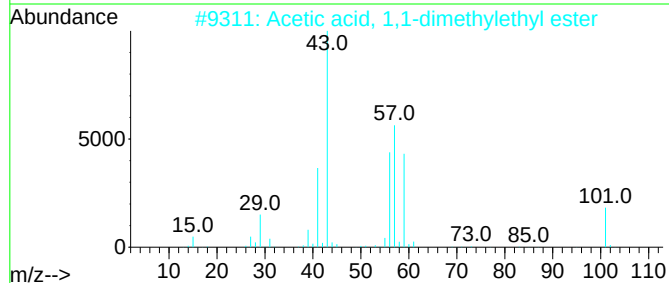
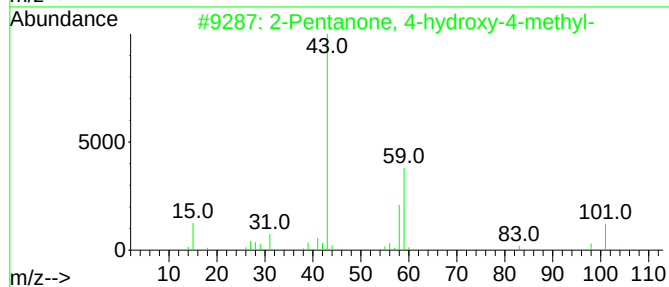
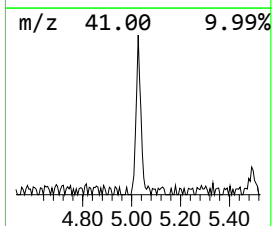
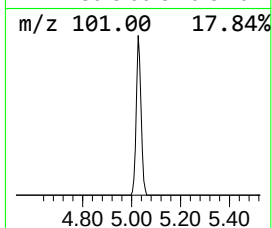
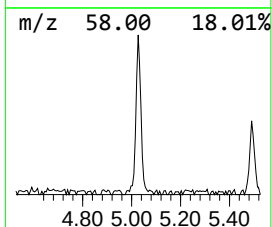
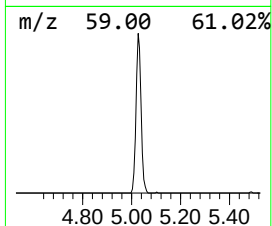
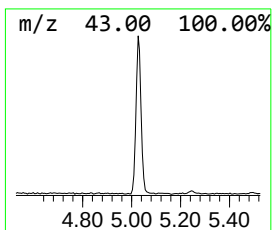
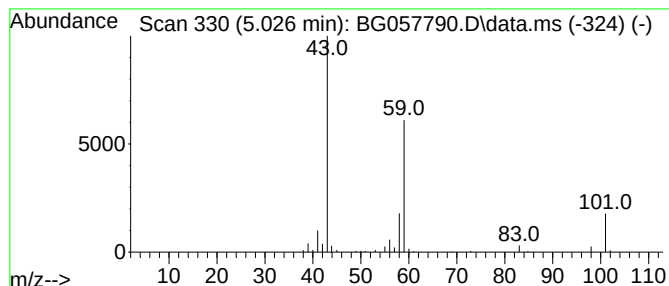
Instrument :
BNA_G
ClientSampleId :
SB-06-12.0-14.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.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.	
5.026	21.23 ng	170057	1,4-Dichlorobenzene-d4	7.923	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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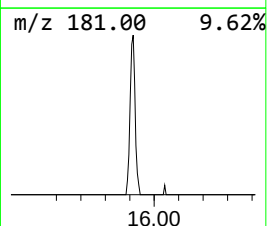
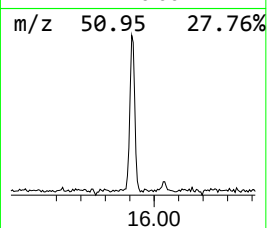
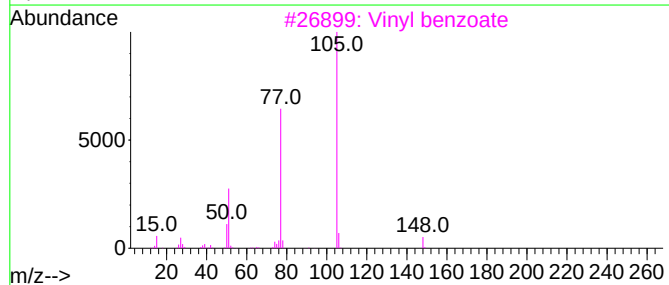
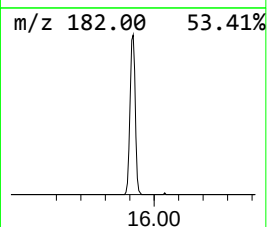
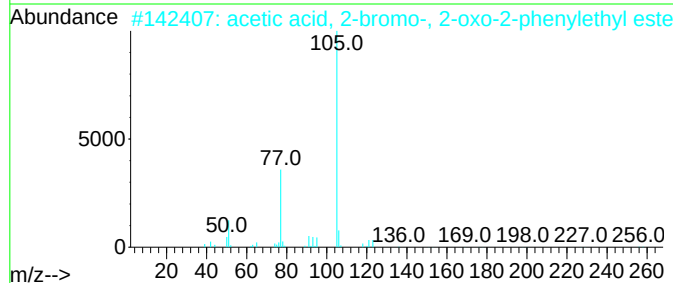
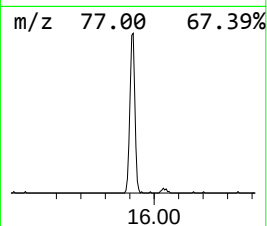
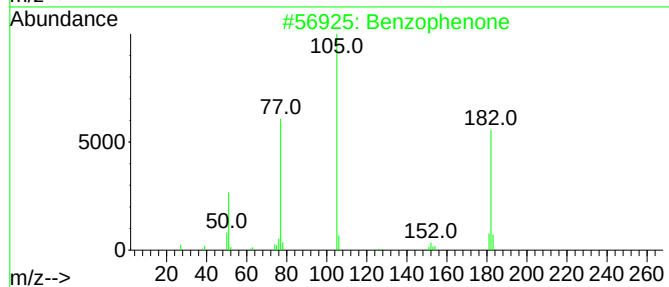
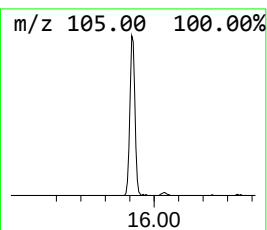
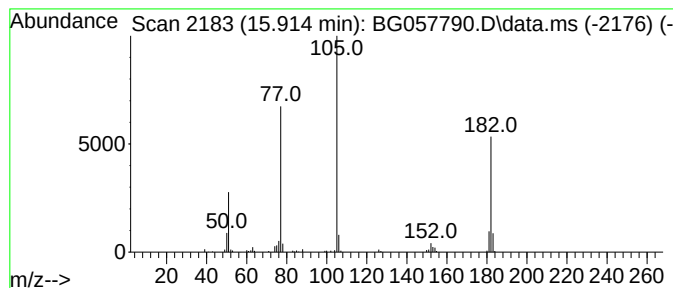
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Benzophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.914	7.22 ng	143466	Acenaphthene-d10	14.557

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			acetic acid, 2-bromo-, 2-oxo-2-p...	256	C10H9BrO3	1000401-50-0	47
3			Vinyl benzoate	148	C9H8O2	000769-78-8	47
4			Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	47
5			2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	47



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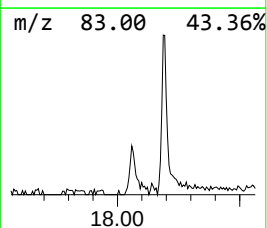
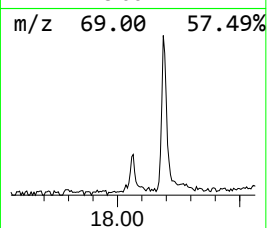
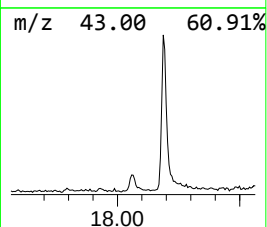
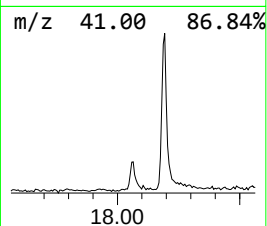
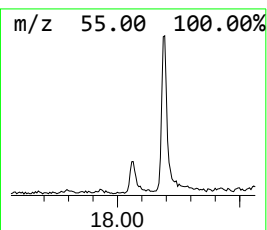
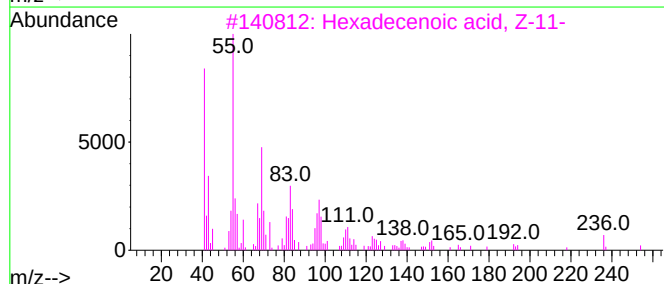
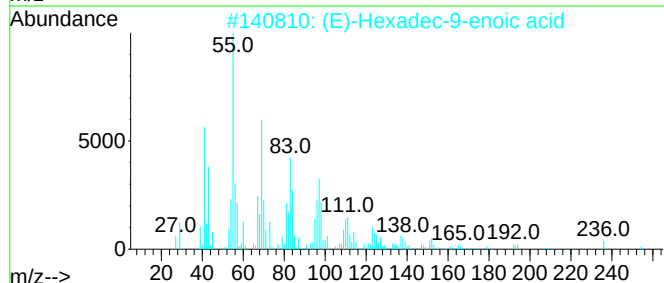
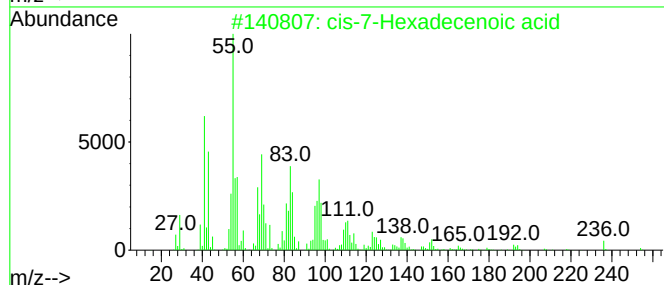
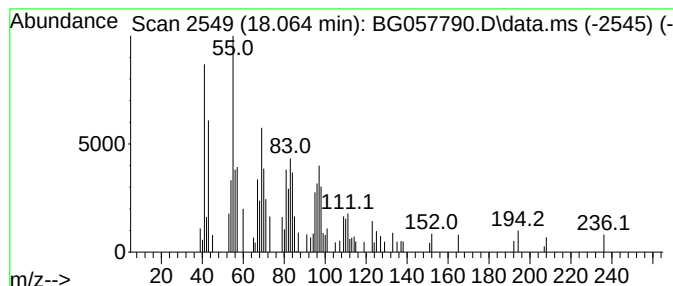
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 cis-7-Hexadecenoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.064	2.59 ng	70970	Phenanthrene-d10	17.300

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			cis-7-Hexadecenoic acid	254	C16H30O2	002416-19-5	83
2			(E)-Hexadec-9-enoic acid	254	C16H30O2	010030-73-6	72
3			Hexadecenoic acid, Z-11-	254	C16H30O2	002416-20-8	64
4			Myristoleic acid	226	C14H26O2	000544-64-9	64
5			E-9-Tetradecenoic acid	226	C14H26O2	050286-30-1	62



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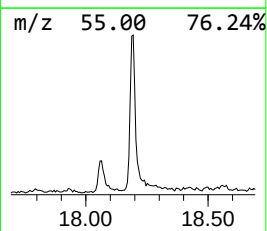
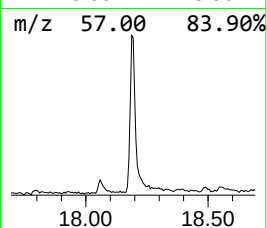
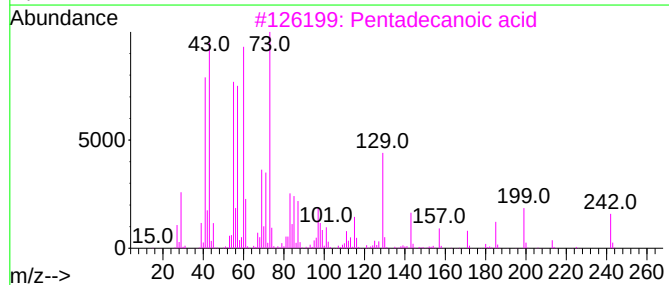
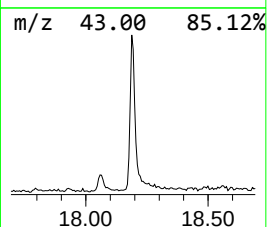
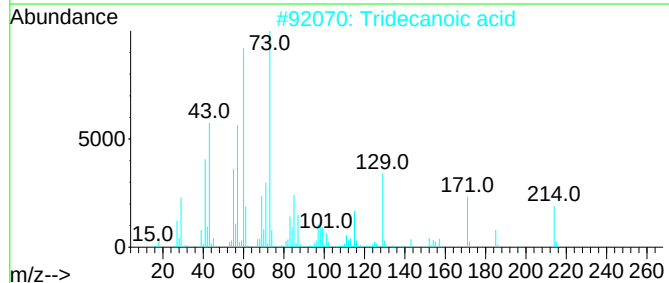
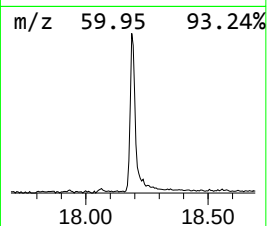
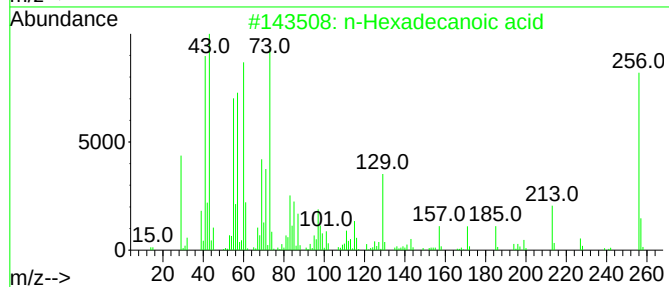
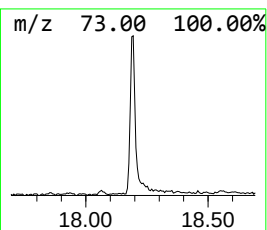
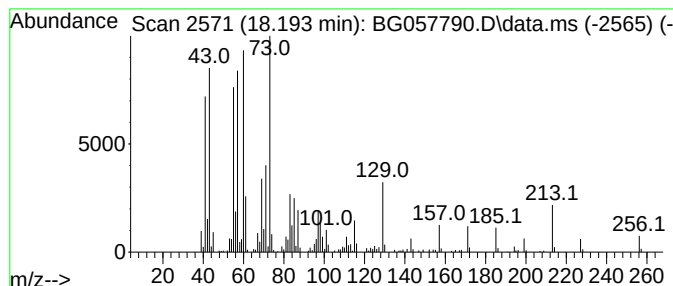
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.193	15.81 ng	433436	Phenanthrene-d10		17.300	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	99
2	Tridecanoic acid		214	C13H26O2	000638-53-9	87
3	Pentadecanoic acid		242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid		228	C14H28O2	000544-63-8	76
5	8-Methylnonanoic acid		172	C10H20O2	005963-14-4	53



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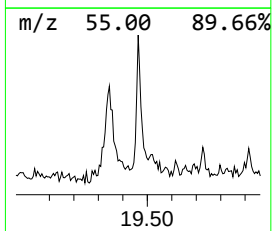
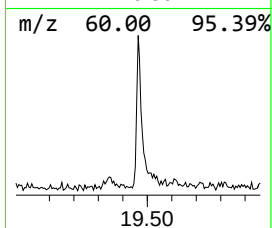
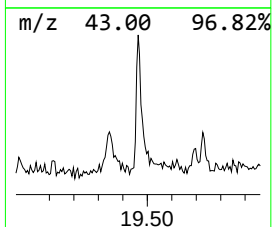
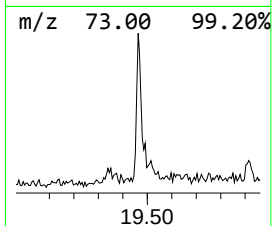
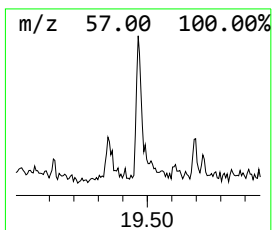
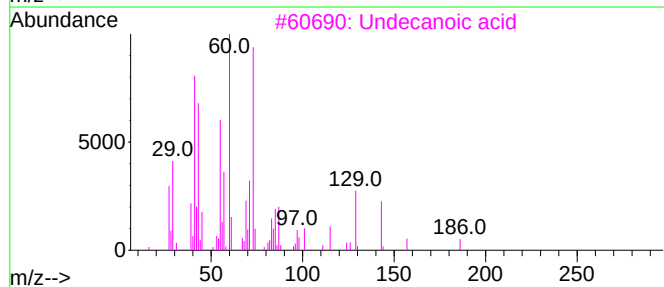
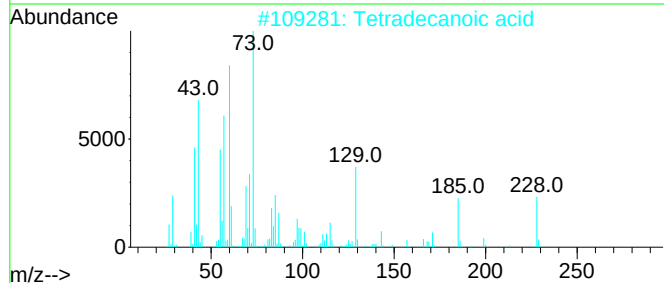
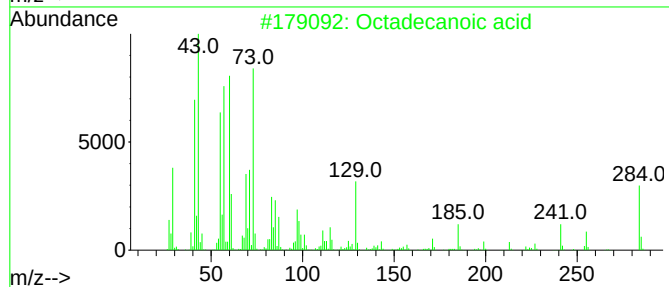
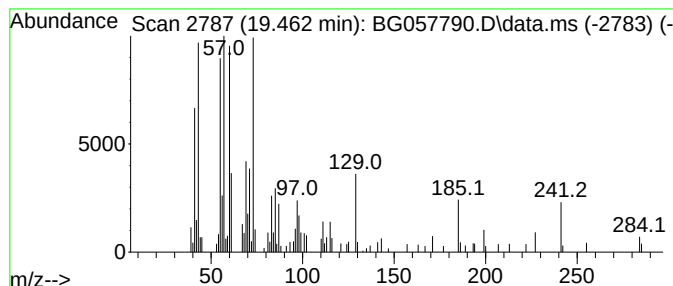
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.462	3.52 ng	107143	Chrysene-d12	21.554

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	95
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
3			Undecanoic acid	186	C11H22O2	000112-37-8	62
4			Tridecanoic acid	214	C13H26O2	000638-53-9	59
5			n-Decanoic acid	172	C10H20O2	000334-48-5	53



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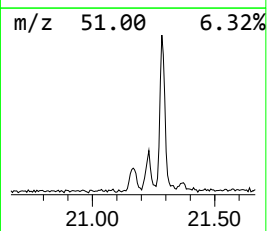
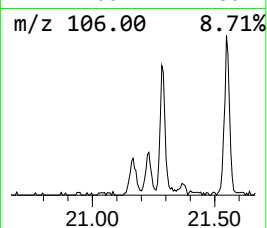
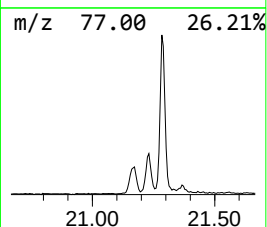
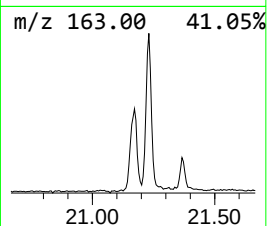
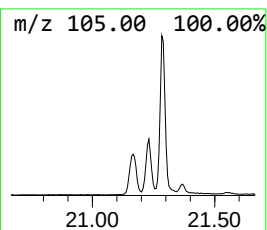
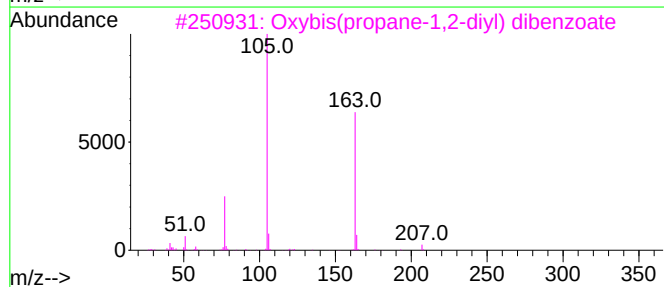
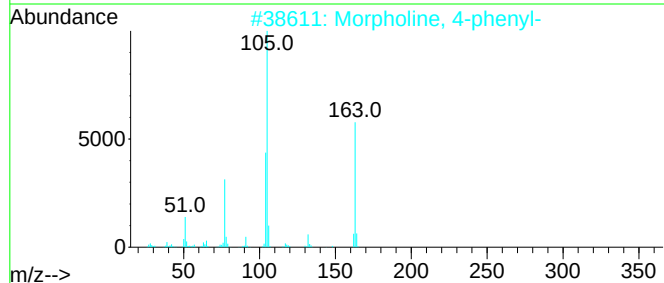
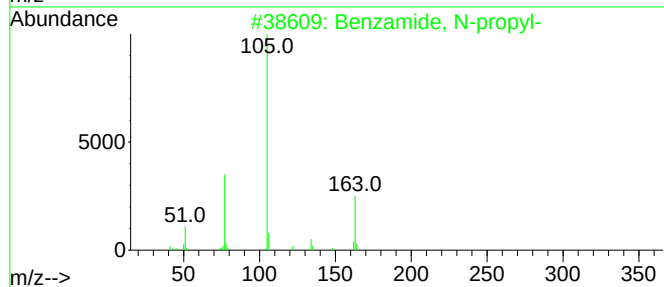
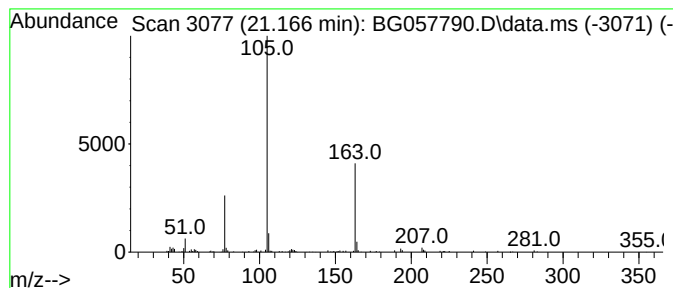
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzamide, N-propyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.166	4.30 ng	131037	Chrysene-d12	21.554

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzamide, N-propyl-	163	C10H13NO	010546-70-0	72
2			Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	72
3			Oxybis(propane-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	53
4			(3-Phenyloxiran-2-yl)methyl benz...	254	C16H14O3	1000366-96-1	50
5			Hydrazinecarboxylic acid, 2-benz...	208	C10H12N2O3	010465-97-1	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062123\
Data File : BG057790.D
Acq On : 21 Jun 2023 18:44
Operator : CG/JU
Sample : 03289-16
Misc :
ALS Vial : 7 Sample Multiplier: 1

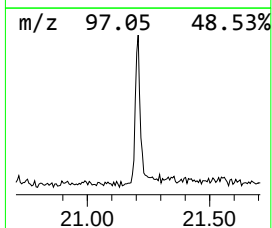
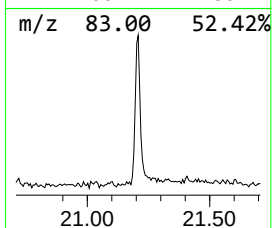
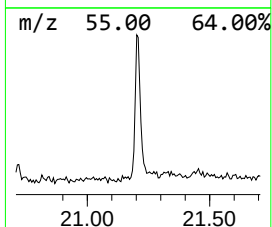
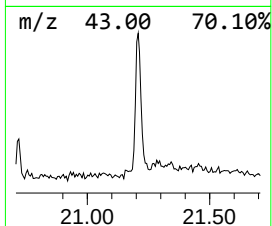
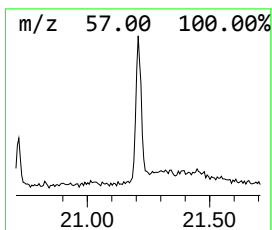
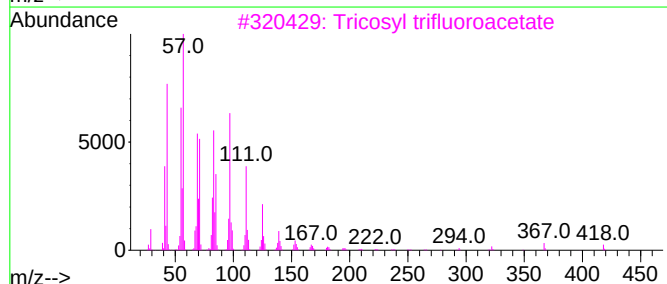
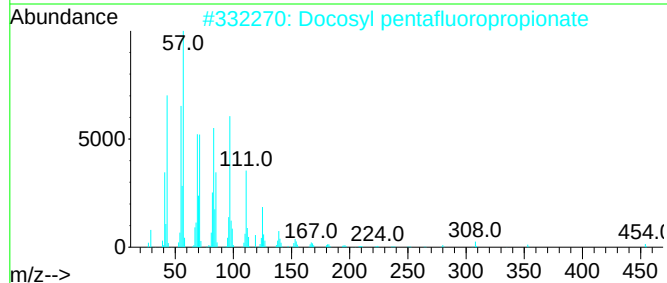
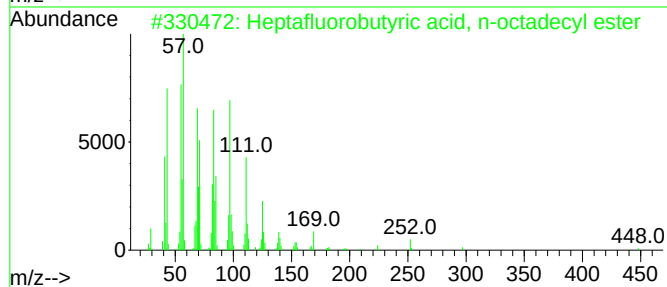
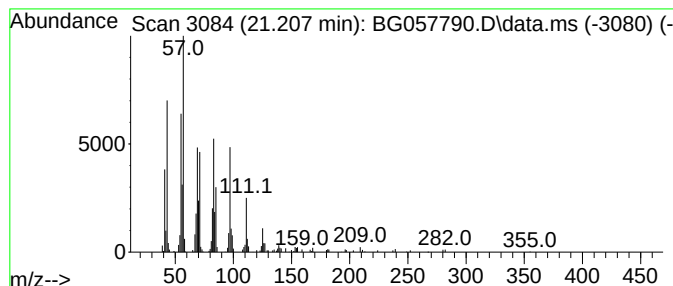
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptafluorobutyric acid, n-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
21.208	12.63 ng	384573	Chrysene-d12		21.554	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, n-octad...		466	C22H37F7O2	000400-57-7	91
2	Docosyl pentafluoropropionate		472	C25H45F5O2	1000351-80-9	91
3	Tricosyl trifluoroacetate		436	C25H47F3O2	1000351-75-1	91
4	Octadecyl trifluoroacetate		366	C20H37F3O2	079392-43-1	91
5	Heneicosyl heptafluorobutyrate		508	C25H43F7O2	1000351-83-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062123\
Data File : BG057790.D
Acq On : 21 Jun 2023 18:44
Operator : CG/JU
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Instrument :
BNA_G
ClientSampleId :
SB-06-12.0-14.0

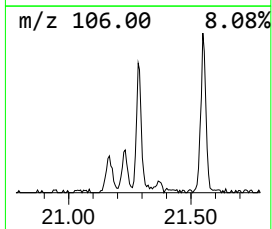
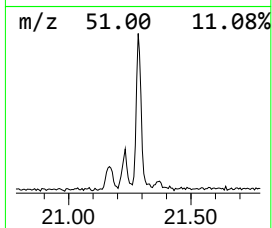
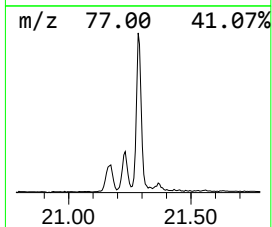
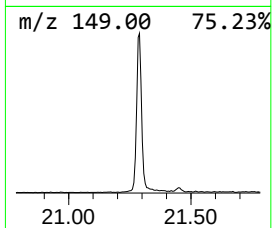
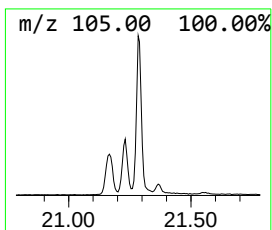
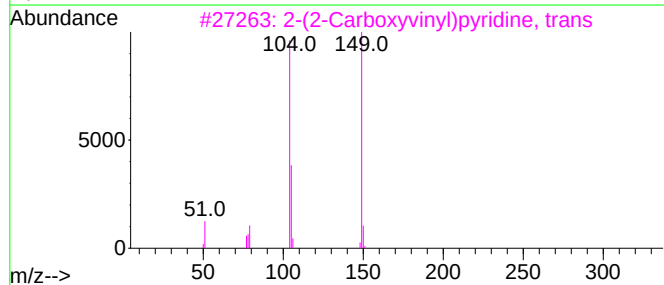
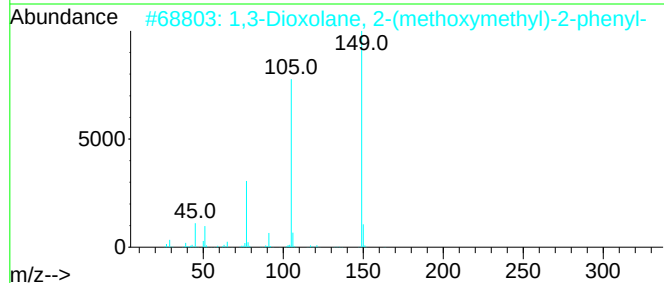
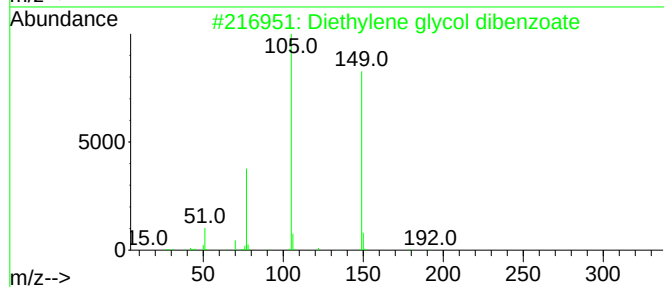
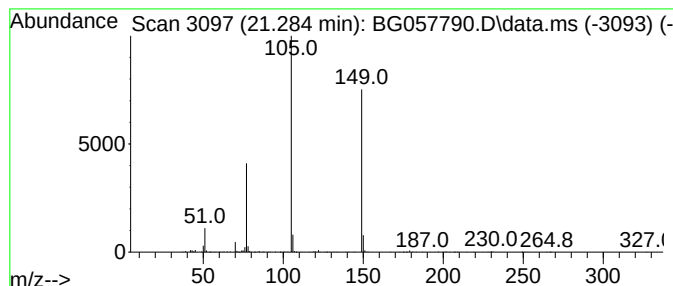
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Diethylene glycol dibenzoate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.284	14.52 ng	442363	Chrysene-d12	21.554

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	90
2			1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	59
3			2-(2-Carboxyvinyl)pyridine, trans	149	C8H7NO2	007340-22-9	49
4			2-Methyl-4-hydroxybenzoxazole	149	C8H7NO2	051110-60-2	43
5			N-(4-Methylthiazol-2-yl)benzamide	218	C11H10N2OS	037529-67-2	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062123\
Data File : BG057790.D
Acq On : 21 Jun 2023 18:44
Operator : CG/JU
Sample : 03289-16
Misc :
ALS Vial : 7 Sample Multiplier: 1

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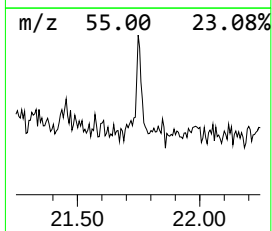
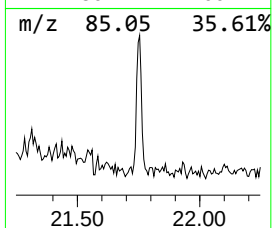
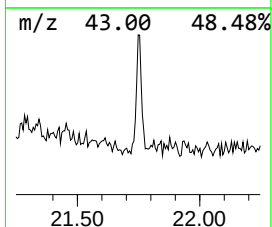
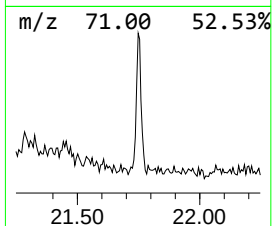
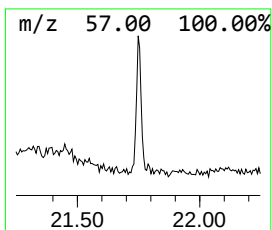
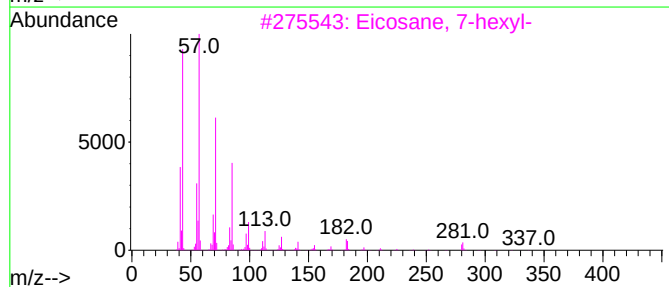
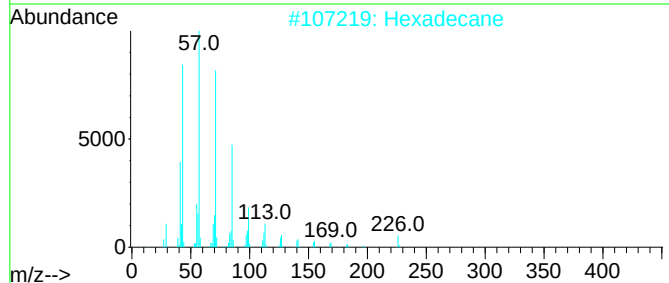
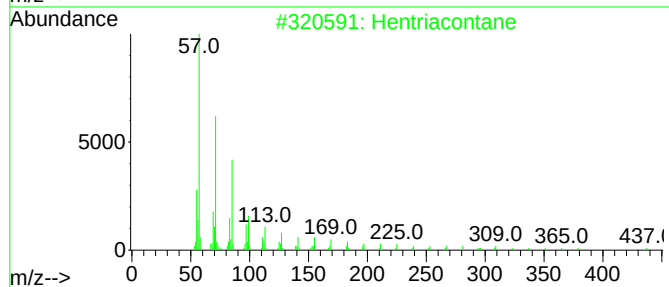
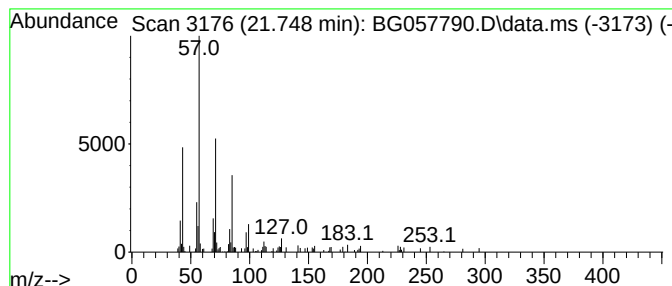
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hentriacontane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.748	2.11 ng	64393	Chrysene-d12	21.554

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hentriacontane	437	C31H64	000630-04-6	86
2		Hexadecane	226	C16H34	000544-76-3	86
3		Eicosane, 7-hexyl-	366	C26H54	055333-99-8	80
4		2-Bromo dodecane	248	C12H25Br	013187-99-0	80
5		Octacosane	394	C28H58	000630-02-4	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062123\
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Sample : 03289-16
Misc :
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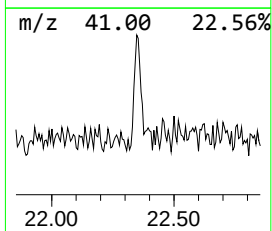
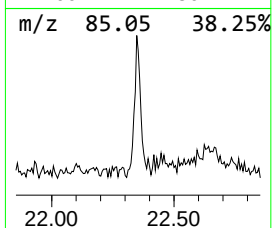
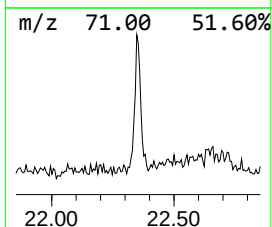
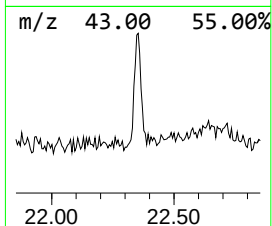
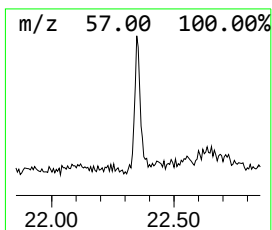
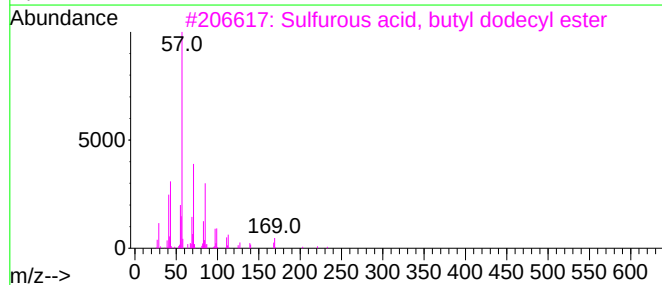
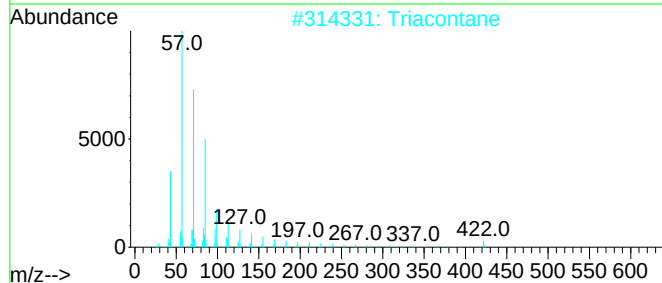
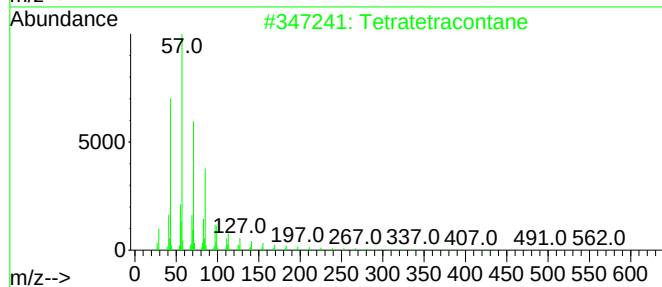
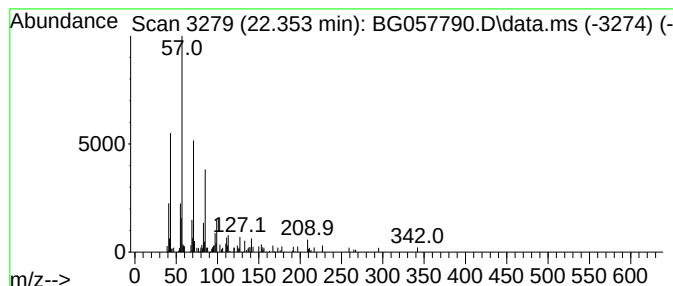
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Tetratetracontane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
22.353	2.11 ng	64371	Chrysene-d12	21.554	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratetracontane	619	C44H90	007098-22-8	83
2	Triacontane	422	C30H62	000638-68-6	83
3	Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	83
4	Heneicosane, 11-decyl-	437	C31H64	055320-06-4	83
5	4-Methylheneicosane	310	C22H46	025117-29-7	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062123\
Data File : BG057790.D
Acq On : 21 Jun 2023 18:44
Operator : CG/JU
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Misc :
ALS Vial : 7 Sample Multiplier: 1

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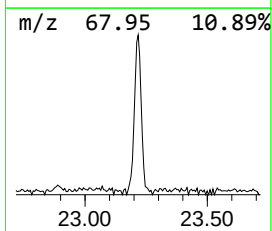
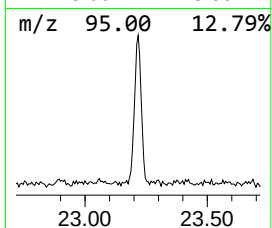
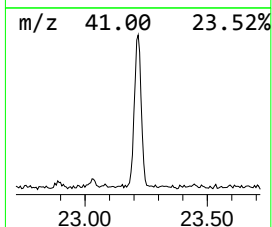
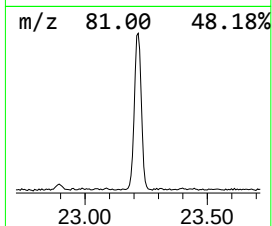
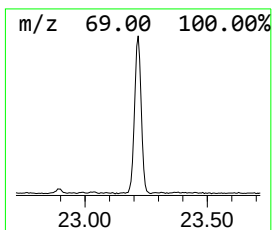
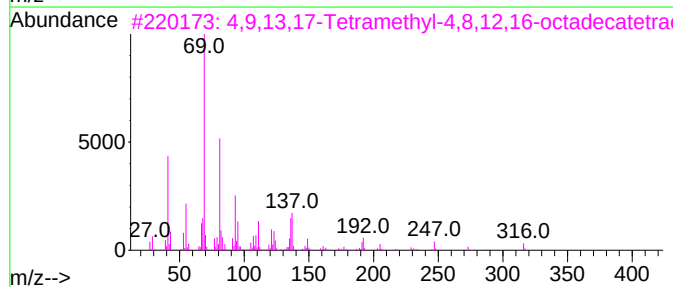
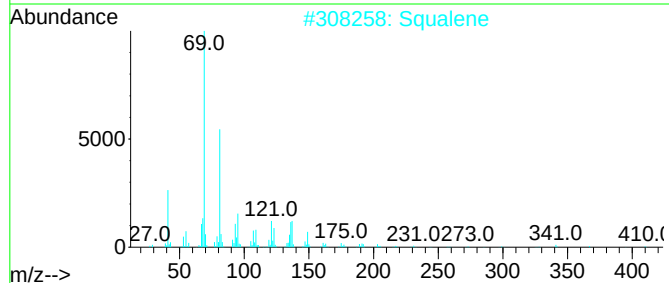
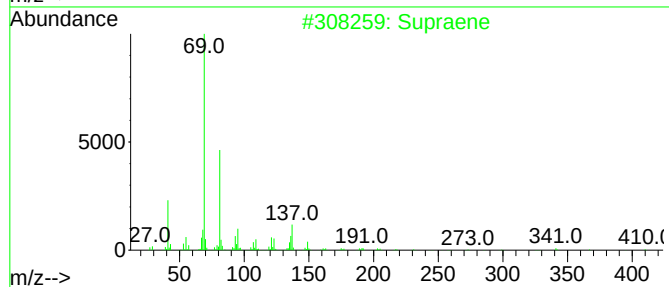
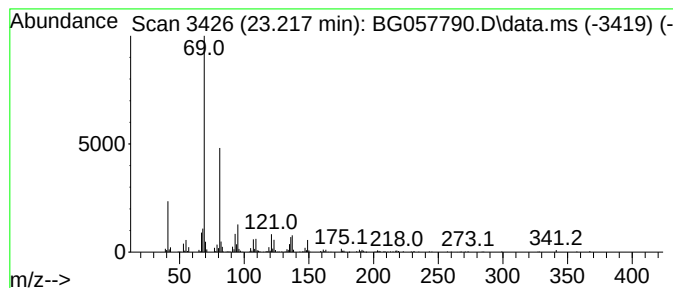
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Supraene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.217	15.78 ng	549284	Perylene-d12	24.703

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Supraene	410	C30H50	007683-64-9	91
2		Squalene	410	C30H50	000111-02-4	91
3		4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	83
4		.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	83
5		1-(Phenylthio)-3,7,11-trimethyl-...	314	C21H30S	028413-57-2	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062123\
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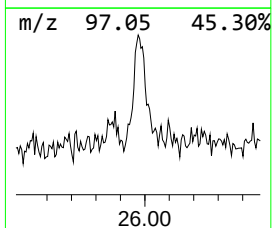
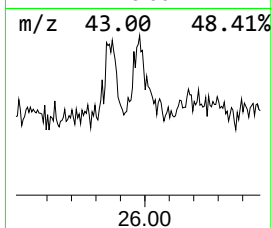
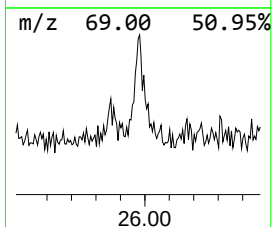
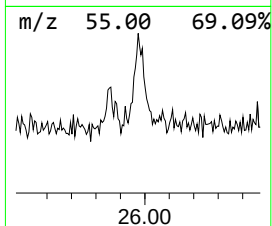
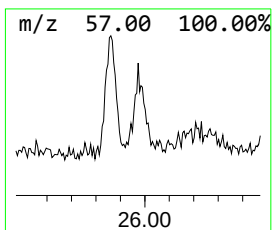
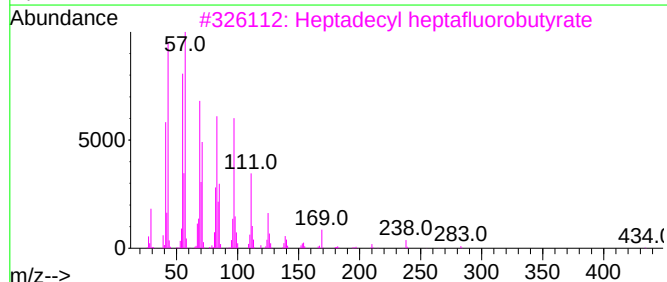
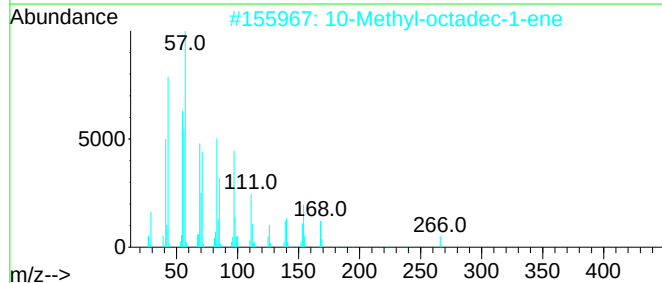
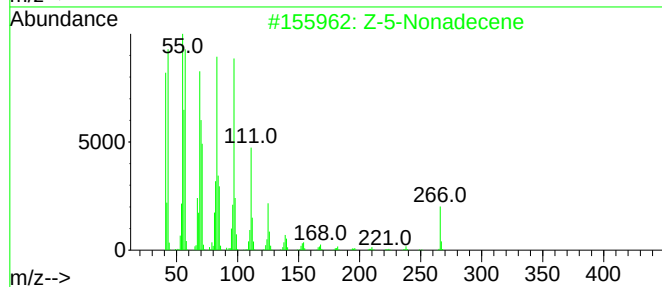
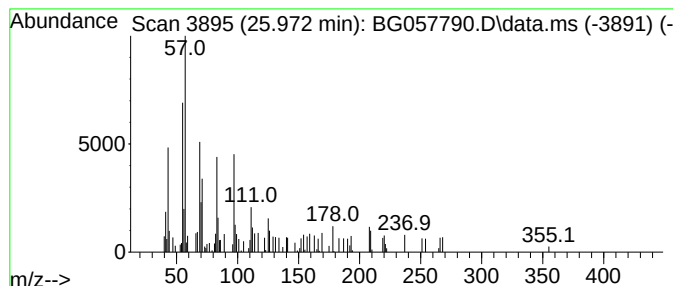
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Z-5-Nonadecene Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD		R.T.	
25.973	2.02 ng	70420	Perylene-d12		24.703	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Z-5-Nonadecene		266	C19H38	1000131-11-8	76
2	10-Methyl-octadec-1-ene		266	C19H38	1000192-60-5	76
3	Heptadecyl heptafluorobutyrate		452	C21H35F7O2	959085-66-6	62
4	Pentadecafluorooctanoic acid, oc...		666	C26H37F15O2	1000406-04-8	62
5	2- Chloropropionic acid, octadec...		360	C21H41ClO2	088104-31-8	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062123\
Data File : BG057790.D
Acq On : 21 Jun 2023 18:44
Operator : CG/JU
Sample : 03289-16
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-06-12.0-14.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.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-...	5.026	21.2	ng	170057	1	7.923	160219	20.0
Benzophenone	15.914	7.2	ng	143466	3	14.557	397555	20.0
cis-7-Hexadecen...	18.064	2.6	ng	70970	4	17.300	548390	20.0
n-Hexadecanoic ...	18.193	15.8	ng	433436	4	17.300	548390	20.0
Octadecanoic acid	19.462	3.5	ng	107143	5	21.554	609152	20.0
Benzamide, N-pr...	21.166	4.3	ng	131037	5	21.554	609152	20.0
Heptafluorobuty...	21.208	12.6	ng	384573	5	21.554	609152	20.0
Diethylene glyc...	21.284	14.5	ng	442363	5	21.554	609152	20.0
Hentriacontane	21.748	2.1	ng	64393	5	21.554	609152	20.0
Tetratetracontane	22.353	2.1	ng	64371	5	21.554	609152	20.0
Supraene	23.217	15.8	ng	549284	6	24.703	696024	20.0
Z-5-Nonadecene	25.973	2.0	ng	70420	6	24.703	696024	20.0