

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082223\
 Data File : BG058804.D
 Acq On : 22 Aug 2023 11:37
 Operator : MA/JU
 Sample : 04090-01
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TP-I

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-BG081823.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG058804.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.379	384	390	400	rBV	283868	445899	21.80%	4.144%
2	6.978	655	662	676	rBV	270223	470292	23.00%	4.371%
3	7.806	796	803	811	rVB	96252	159423	7.80%	1.482%
4	8.969	994	1001	1015	rBV	143673	274281	13.41%	2.549%
5	10.609	1273	1280	1292	rBV	116732	224933	11.00%	2.090%
6	13.070	1692	1699	1713	rBV	358487	585289	28.62%	5.439%
7	13.347	1739	1746	1756	rBV	329634	530379	25.94%	4.929%
8	14.457	1923	1935	1944	rBV	187150	315706	15.44%	2.934%
9	15.944	2182	2188	2200	rBV	317034	560036	27.39%	5.205%
10	16.455	2266	2275	2286	rBV	12090	30731	1.50%	0.286%
11	17.201	2394	2402	2413	rBV	266031	428862	20.97%	3.986%
12	18.094	2547	2554	2569	rBV3	58957	122543	5.99%	1.139%
13	19.034	2710	2714	2720	rVB	37453	55882	2.73%	0.519%
14	19.263	2744	2753	2757	rBV2	21110	32665	1.60%	0.304%
15	19.369	2767	2771	2788	rVB2	25940	53559	2.62%	0.498%
16	19.739	2824	2834	2840	rBV	263812	648878	31.73%	6.030%
17	19.821	2841	2848	2855	rVV	1096763	1780770	87.08%	16.549%
18	19.909	2855	2863	2874	rVV	1143817	2045021	100.00%	19.005%
19	20.021	2877	2882	2889	rVB	82510	132998	6.50%	1.236%
20	20.121	2895	2899	2902	rBV	19821	23332	1.14%	0.217%
21	20.162	2902	2906	2920	rVB	23450	47737	2.33%	0.444%
22	20.567	2969	2975	2979	rBV	25402	38841	1.90%	0.361%
23	20.609	2979	2982	2986	rVB2	39750	43933	2.15%	0.408%
24	21.061	3052	3059	3061	rBV	16657	32429	1.59%	0.301%
25	21.096	3061	3065	3075	rVV2	55954	126142	6.17%	1.172%
26	21.184	3075	3080	3084	rVV	58595	99229	4.85%	0.922%
27	21.226	3084	3087	3096	rVB2	27361	47983	2.35%	0.446%
28	21.443	3118	3124	3135	rBV2	305243	509217	24.90%	4.732%
29	21.613	3148	3153	3158	rVB	34410	49035	2.40%	0.456%
30	21.948	3205	3210	3218	rVB4	20635	41651	2.04%	0.387%
31	22.189	3246	3251	3258	rVB	31514	45244	2.21%	0.420%
32	22.765	3341	3349	3356	rBV3	15168	37106	1.81%	0.345%
33	22.841	3357	3362	3369	rVB2	25292	45068	2.20%	0.419%
34	23.593	3485	3490	3496	rBV3	17714	32370	1.58%	0.301%
35	23.705	3503	3509	3516	rVB6	11261	24381	1.19%	0.227%
36	24.516	3634	3647	3663	rBV	191617	593916	29.04%	5.520%

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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-BG081823.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	24.815	3690	3698	3705	rVB5	8910	24538	1.20%	0.228%
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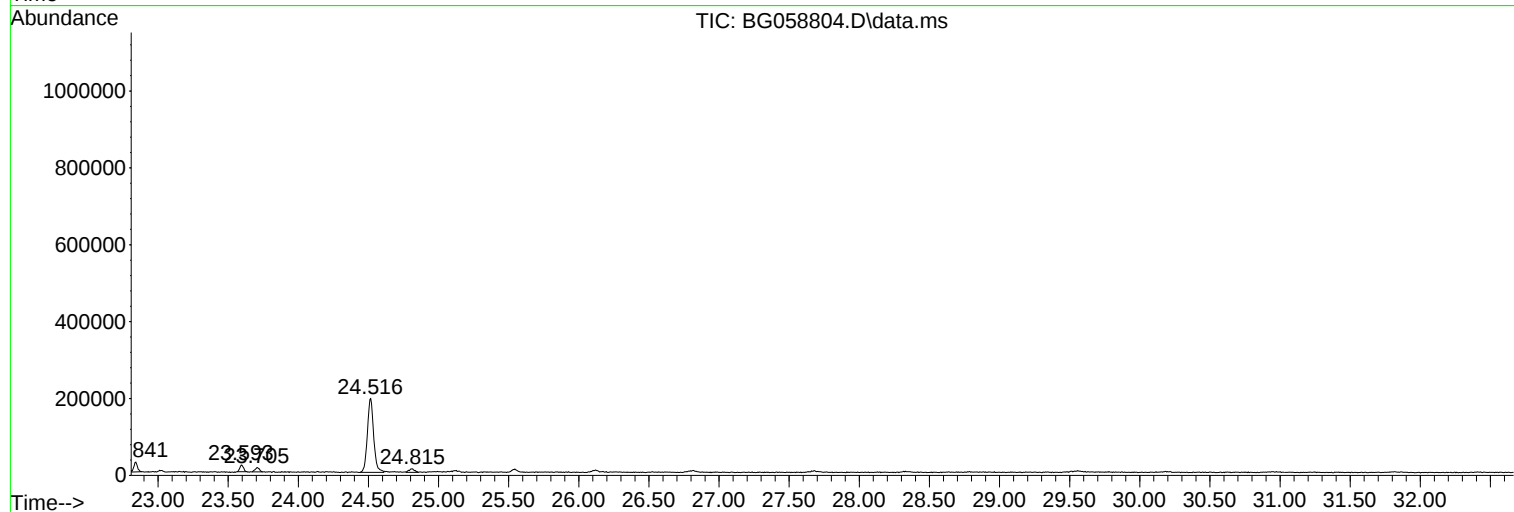
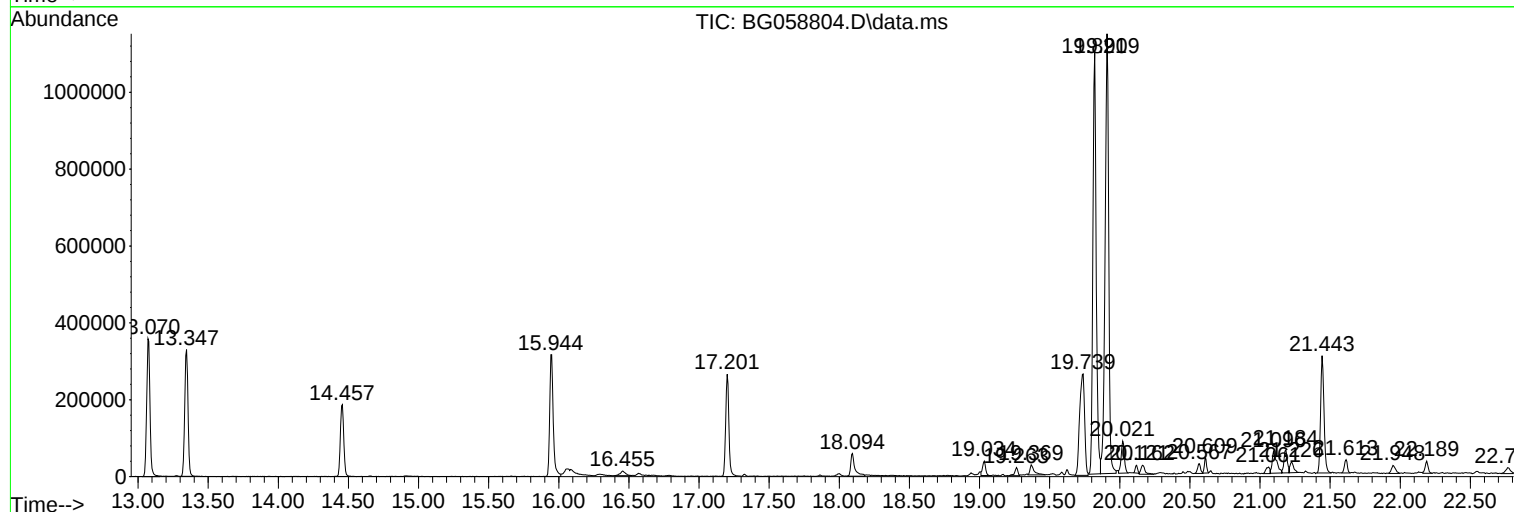
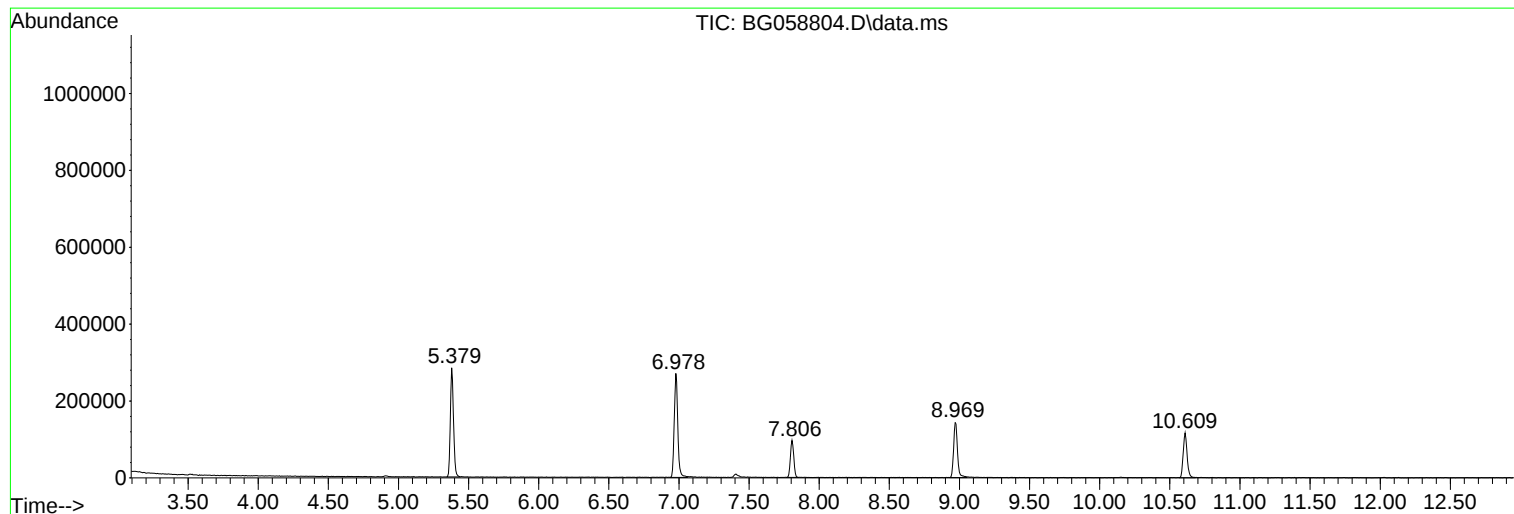
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG081823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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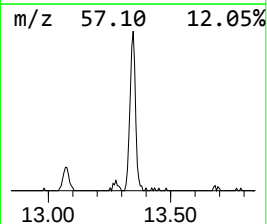
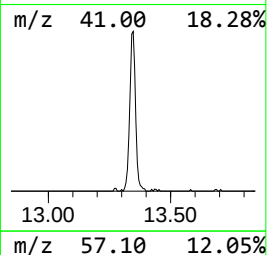
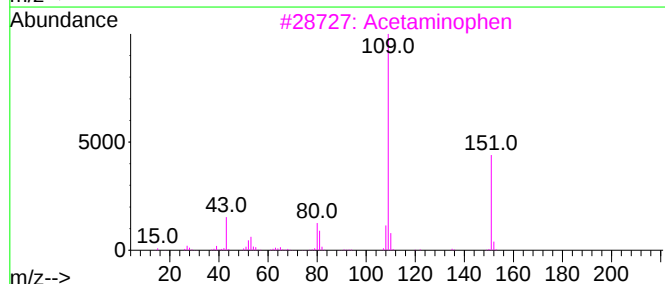
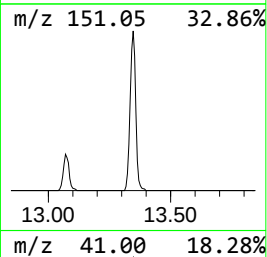
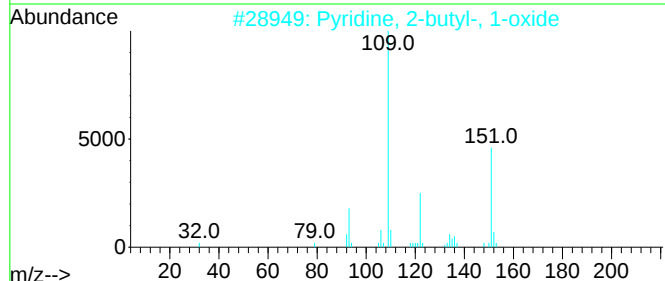
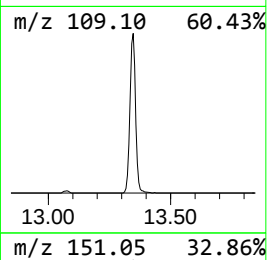
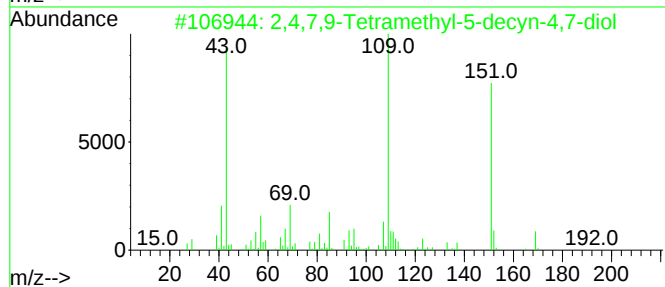
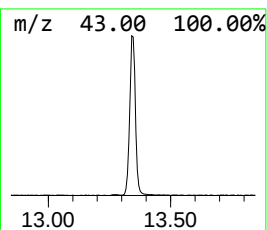
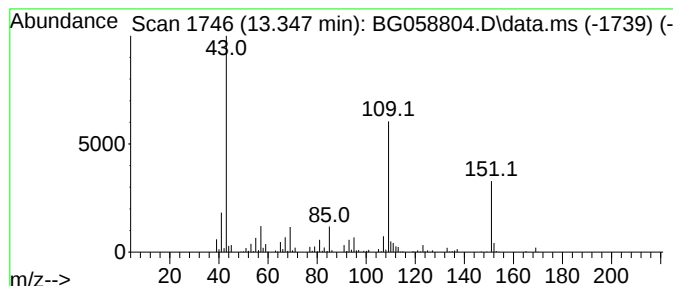
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.347	33.60 ng	530379	Acenaphthene-d10	14.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	87		
2	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	53		
3	Acetaminophen	151	C8H9NO2	000103-90-2	49		
4	Metacetamol	151	C8H9NO2	000621-42-1	47		
5	2-Thiophenecarbonitrile	109	C5H3NS	001003-31-2	43		



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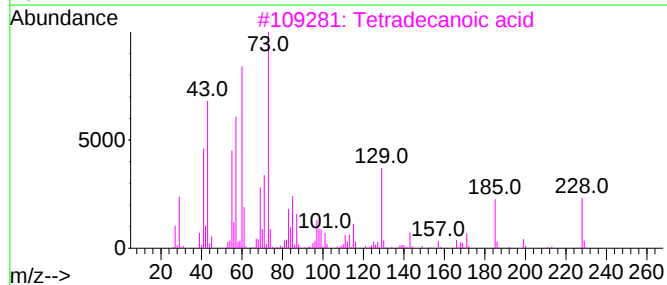
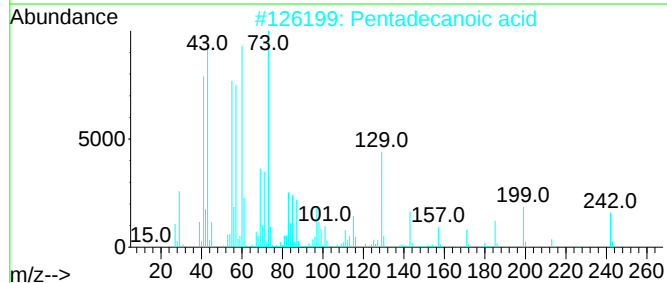
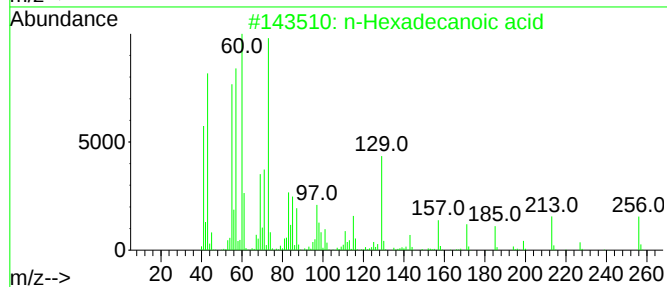
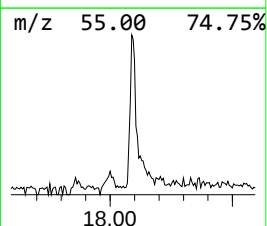
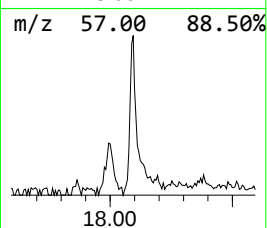
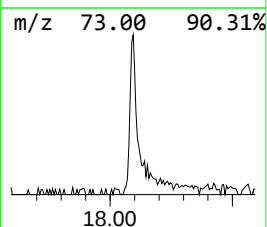
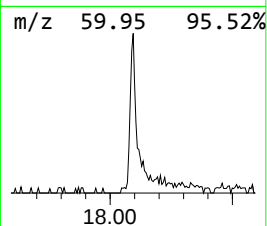
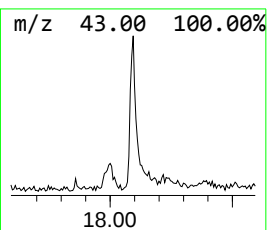
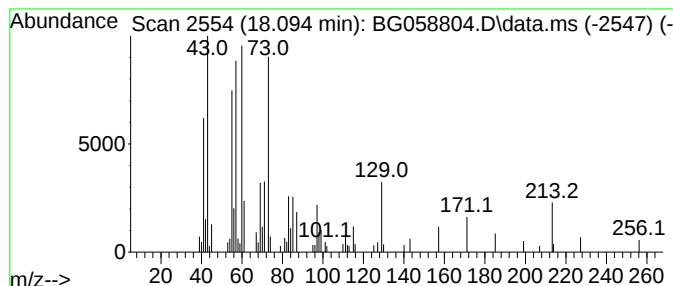
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG081823.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.094	5.71 ng	122543	Phenanthrene-d10	17.201

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	74
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4			Dodecanoic acid	200	C12H24O2	000143-07-7	59
5			Undecanoic acid	186	C11H22O2	000112-37-8	53



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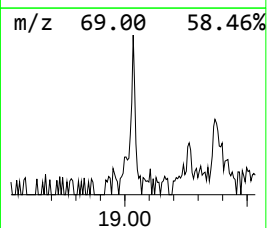
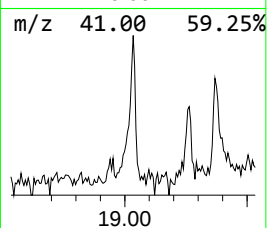
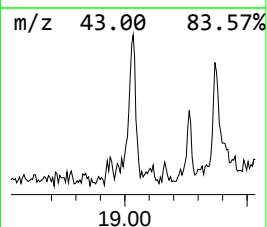
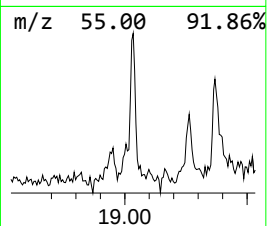
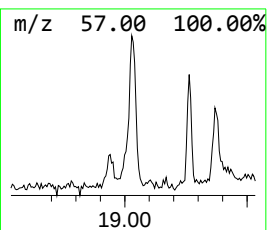
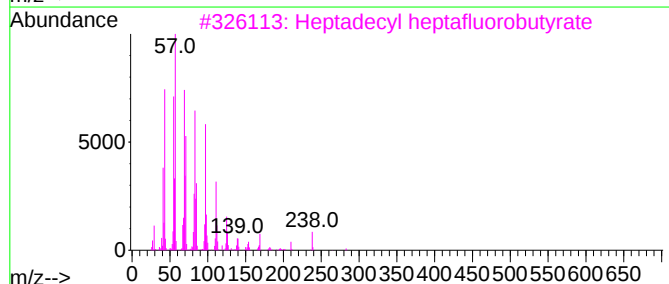
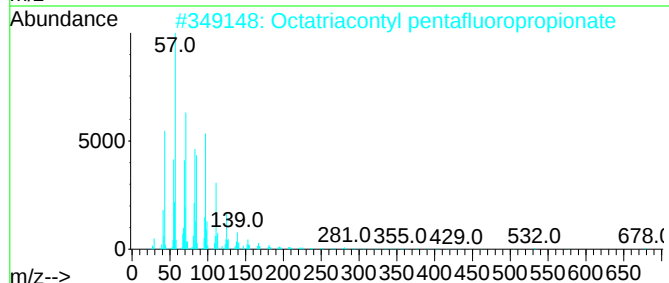
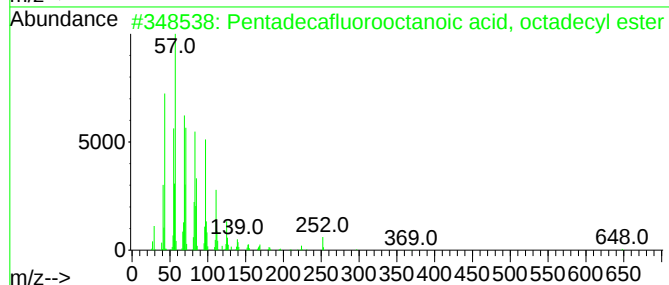
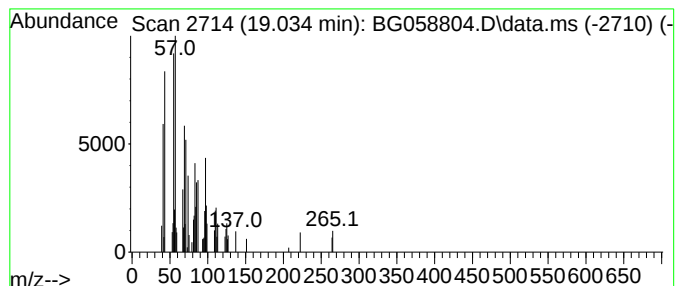
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG081823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Pentadecafluorooctanoic aci... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.034	2.61 ng	55882	Phenanthrene-d10	17.201

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	62
2			Octatriacontyl pentafluoropropio...	697	C41H77F5O2	1000351-89-1	53
3			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	52
4			Triacontyl heptafluorobutyrate	634	C34H61F7O2	1000351-83-2	49
5			Trifluoroacetic acid,n-tridecyl ...	296	C15H27F3O2	053800-02-5	49



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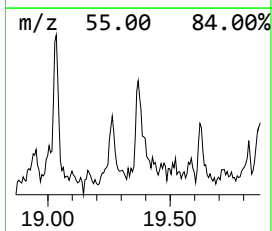
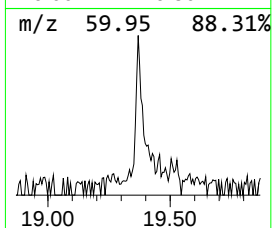
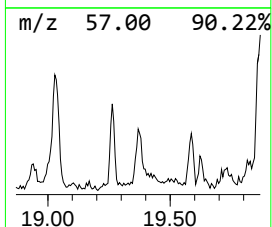
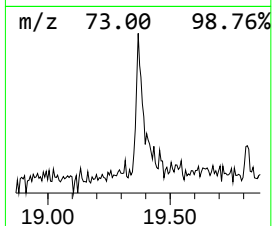
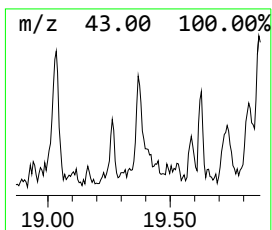
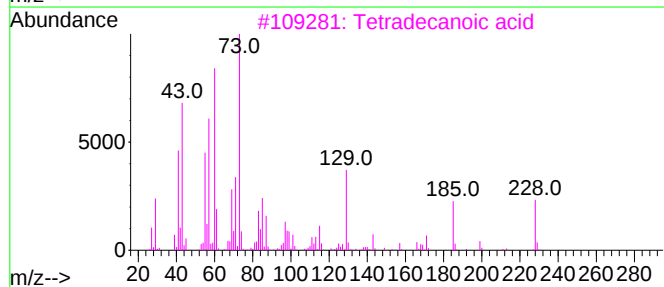
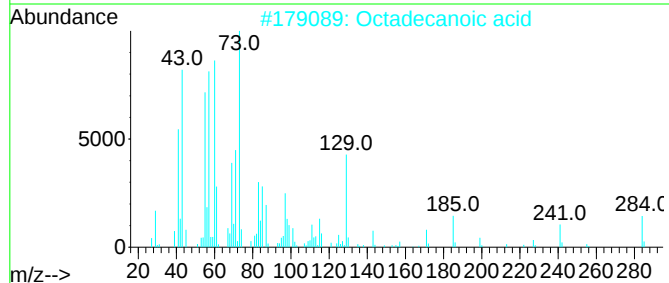
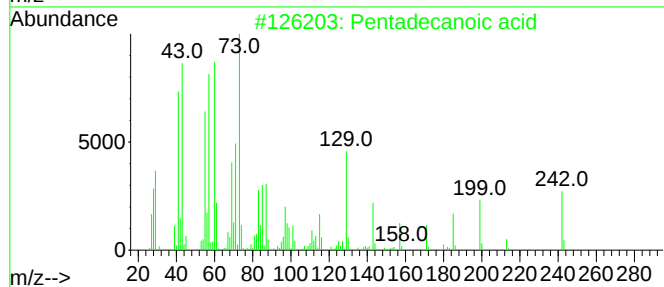
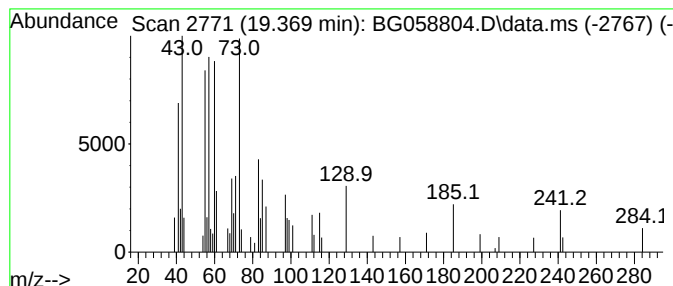
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Pentadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.369	2.10 ng	53559	Chrysene-d12	21.443

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
2			Octadecanoic acid	284	C18H36O2	000057-11-4	81
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	50
4			Dodecanoic acid	200	C12H24O2	000143-07-7	49
5			Tridecanoic acid	214	C13H26O2	000638-53-9	49



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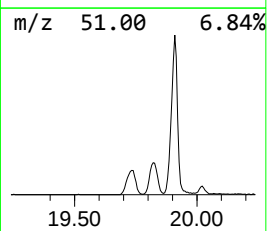
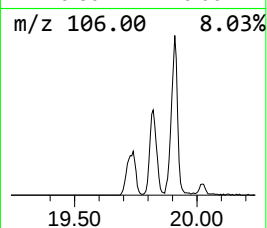
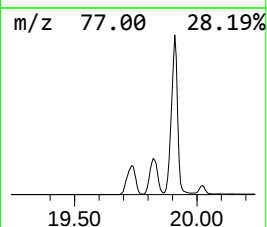
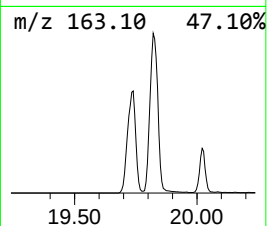
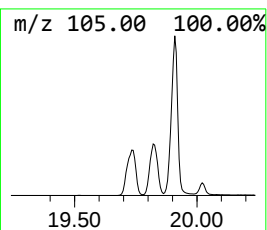
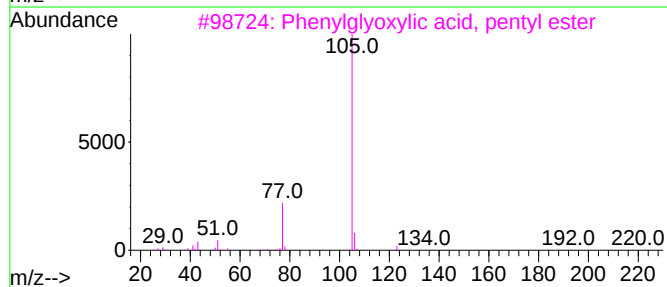
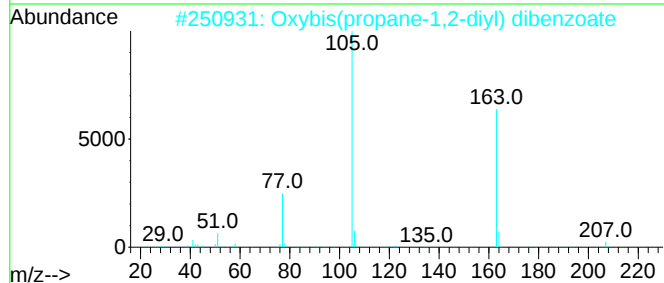
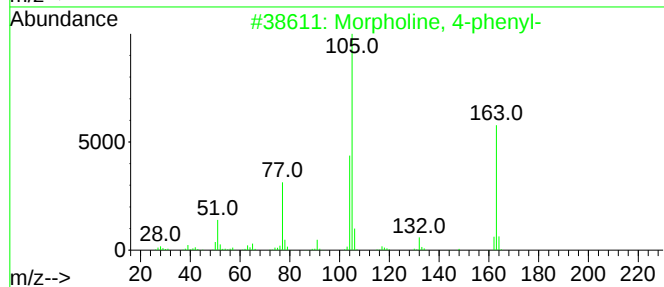
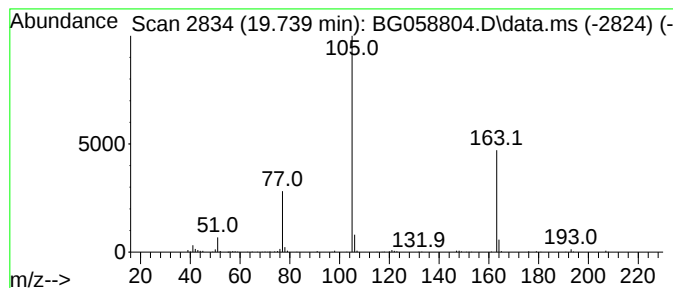
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Morpholine, 4-phenyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.739	25.49 ng	648878	Chrysene-d12	21.443

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	72
2			Oxybis(propane-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	43
3			Phenylglyoxylic acid, pentyl ester	220	C13H16O3	1000453-46-0	38
4			Phenylglyoxylic acid, butyl ester	206	C12H14O3	1000453-46-6	38
5			Ethanone, 2-(acetyloxy)-1-phenyl-	178	C10H10O3	002243-35-8	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082223\
Data File : BG058804.D
Acq On : 22 Aug 2023 11:37
Operator : MA/JU
Sample : 04090-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
TP-I

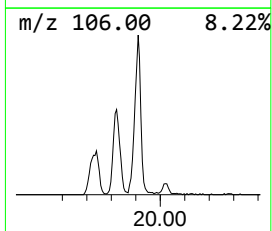
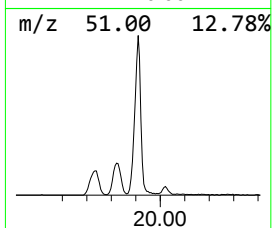
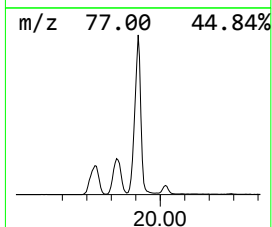
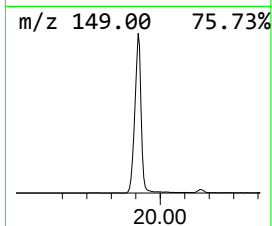
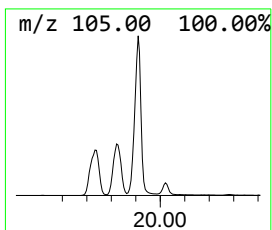
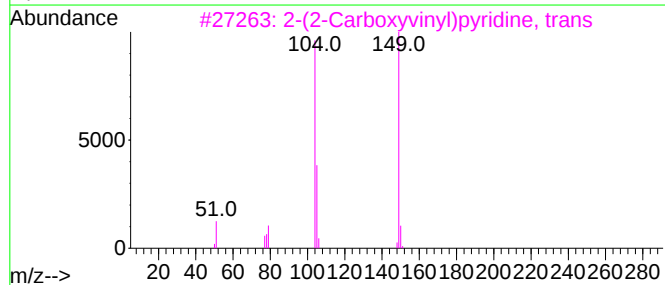
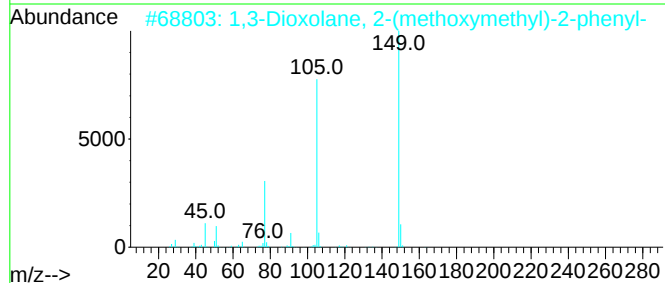
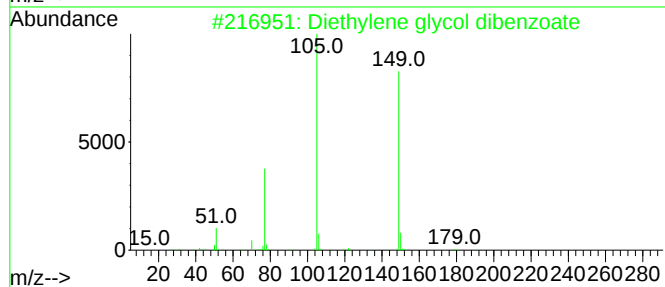
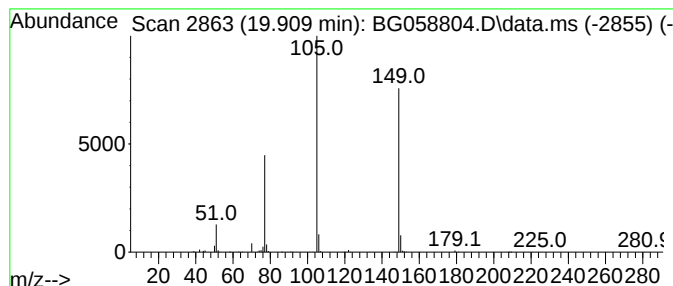
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Diethylene glycol dibenzoate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.909	80.32 ng	2045020	Chrysene-d12	21.443

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	50
4			Phenylglyoxylic acid, neopentyl ...	220	C13H16O3	1000453-45-9	38
5			N-(Methoxymethyl)benzamide	165	C9H11NO2	013156-28-0	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082223\
Data File : BG058804.D
Acq On : 22 Aug 2023 11:37
Operator : MA/JU
Sample : 04090-01
Misc :
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Instrument :
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ClientSampleId :
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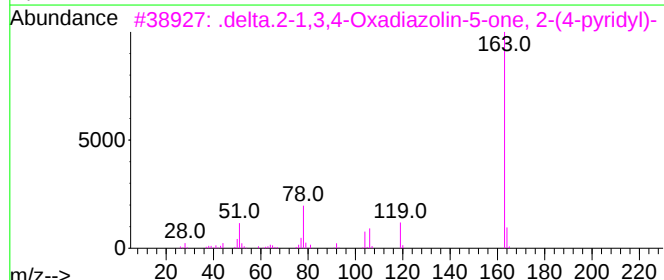
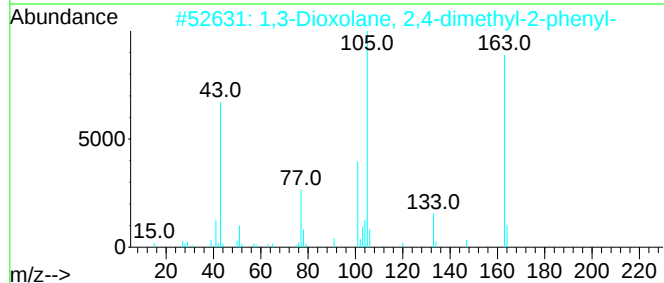
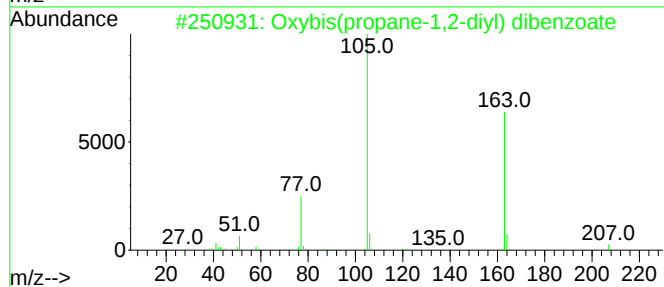
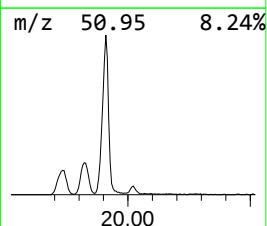
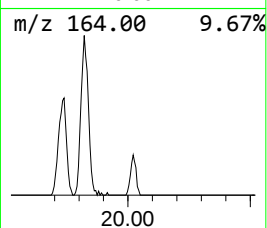
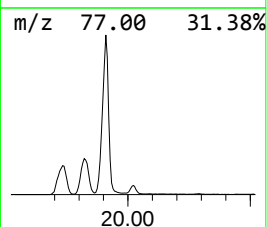
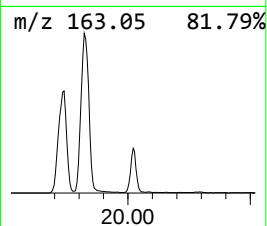
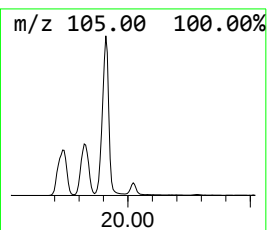
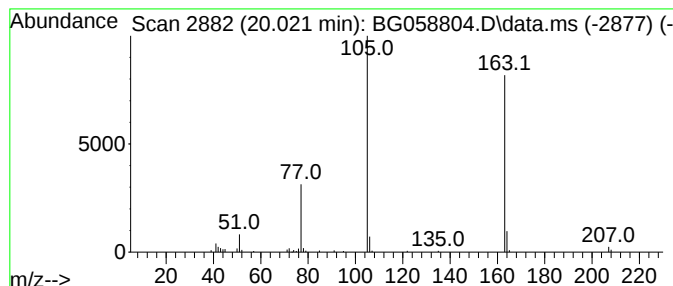
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Oxybis(propene-1,2-diyl) di... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.021	5.22 ng	132998	Chrysene-d12	21.443

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxybis(propene-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	90
2			1,3-Dioxolane, 2,4-dimethyl-2-ph...	178	C11H14O2	004359-30-2	64
3			.delta.2-1,3,4-Oxadiazolin-5-one...	163	C7H5N3O2	002845-82-1	53
4			phenol, 2-chloro-6-nitro-, benzo...	277	C13H8ClNO4	1010397-11-4	22
5			Phenylglyoxylic acid, neopentyl ...	220	C13H16O3	1000453-45-9	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082223\
Data File : BG058804.D
Acq On : 22 Aug 2023 11:37
Operator : MA/JU
Sample : 04090-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-I

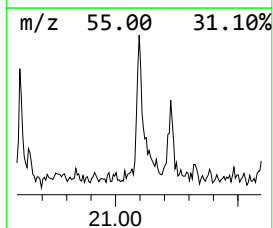
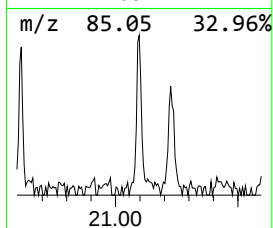
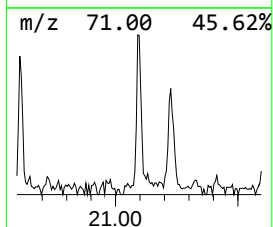
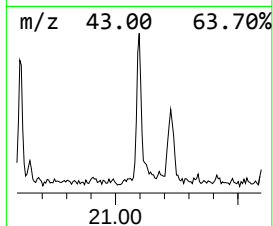
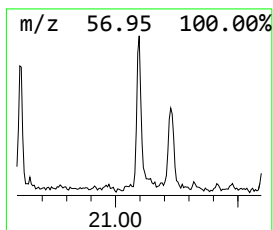
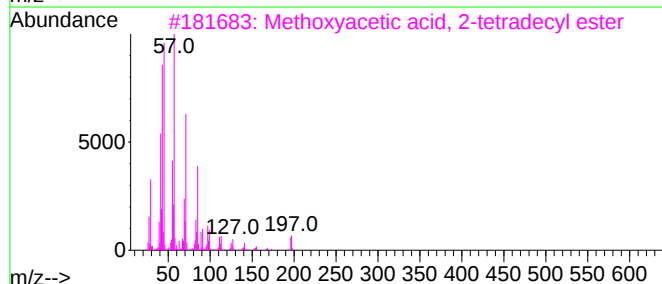
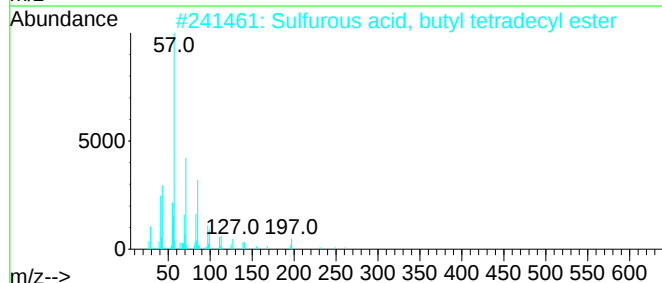
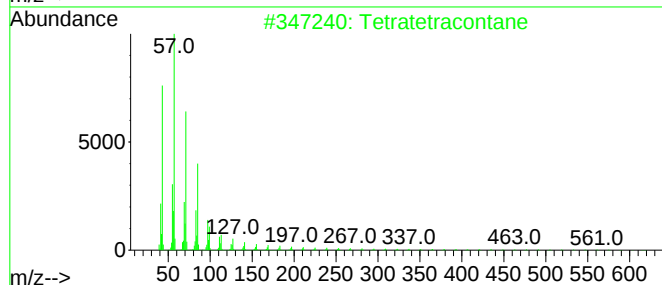
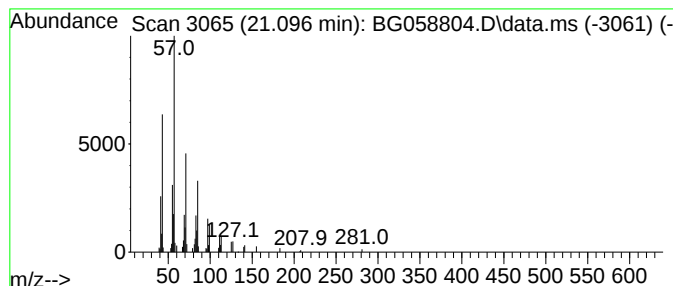
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tetratetracontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.096	4.95 ng	126142	Chrysene-d12	21.443

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetratetracontane	619	C44H90	007098-22-8	91
2			Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1010309-18-1	91
3			Methoxyacetic acid, 2-tetradecyl...	286	C17H34O3	1000282-04-8	91
4			Heneicosane	296	C21H44	000629-94-7	87
5			Hexacosane	366	C26H54	000630-01-3	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082223\
Data File : BG058804.D
Acq On : 22 Aug 2023 11:37
Operator : MA/JU
Sample : 04090-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

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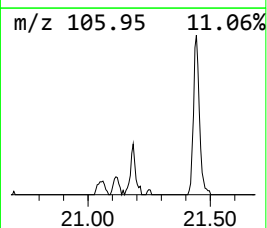
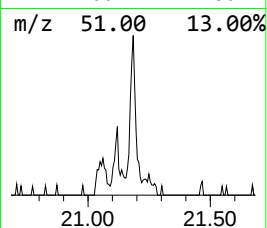
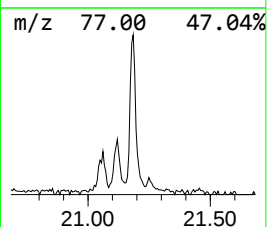
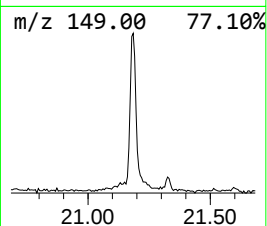
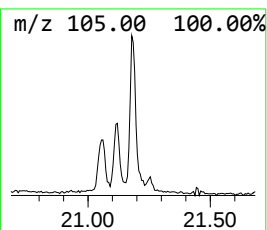
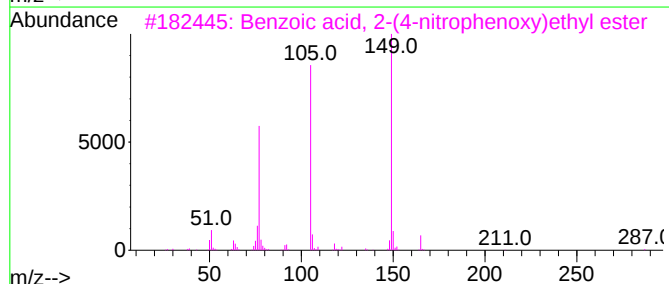
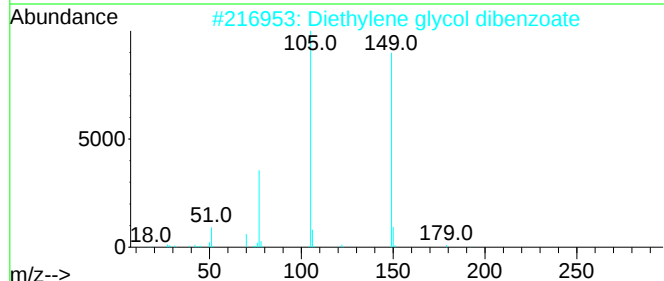
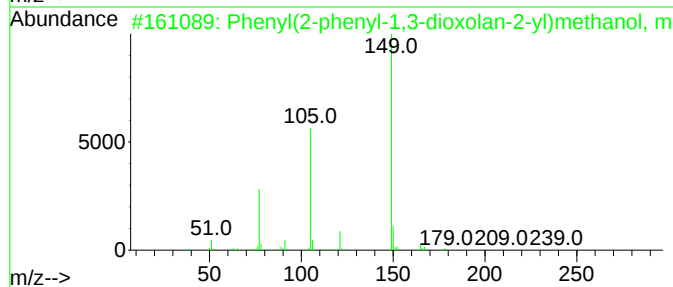
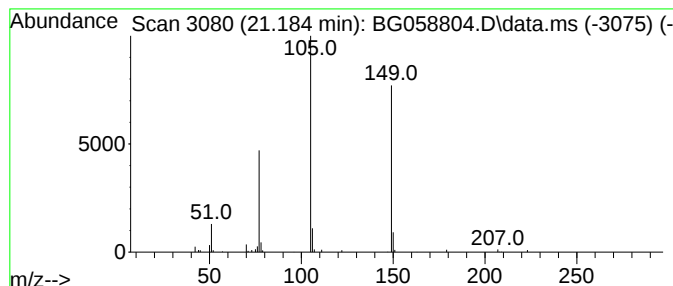
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Phenyl(2-phenyl-1,3-dioxola... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.184	3.90 ng	99229	Chrysene-d12	21.443

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenyl(2-phenyl-1,3-dioxolan-2-y...	270	C17H18O3	1000507-07-6	83
2			Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	83
3			Benzoic acid, 2-(4-nitrophenoxy)...	287	C15H13NO5	1000368-92-7	78
4			Benzoic acid, 2-(3-nitrophenyl)e...	271	C15H13NO4	1000368-22-4	78
5			2-Methyl-4-hydroxybenzoxazole	149	C8H7NO2	051110-60-2	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082223\
Data File : BG058804.D
Acq On : 22 Aug 2023 11:37
Operator : MA/JU
Sample : 04090-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-I

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG081823.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
2,4,7,9-Tetrame...	13.347	33.6	ng	530379	3	14.451	315706	20.0
n-Hexadecanoic ...	18.094	5.7	ng	122543	4	17.201	428862	20.0
Pentadecafluoro...	19.034	2.6	ng	55882	4	17.201	428862	20.0
Pentadecanoic acid	19.369	2.1	ng	53559	5	21.443	509217	20.0
Morpholine, 4-p...	19.739	25.5	ng	648878	5	21.443	509217	20.0
Diethylene glyc...	19.909	80.3	ng	2045020	5	21.443	509217	20.0
Oxybis(propane-...	20.021	5.2	ng	132998	5	21.443	509217	20.0
Tetratetracontane	21.096	5.0	ng	126142	5	21.443	509217	20.0
Phenyl(2-phenyl...	21.184	3.9	ng	99229	5	21.443	509217	20.0