

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072823\
 Data File : BG058535.D
 Acq On : 29 Jul 2023 2:36
 Operator : MA/JU
 Sample : 03642-02
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 EFF-WW

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-BG072823.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG058535.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.385	385	391	410	rVB	426123	805613	1.21%	0.229%
2	6.166	518	524	533	rBV	757137	1152197	1.73%	0.328%
3	7.001	642	666	672	rBV2	382825	1396456	2.09%	0.397%
4	7.917	810	822	841	rBV	6717267	18552386	27.81%	5.277%
5	8.981	995	1003	1010	rBV	722494	1262955	1.89%	0.359%
6	9.380	1021	1071	1076	rBV	1751850	10707232	16.05%	3.045%
7	10.620	1178	1282	1285	rBV3	3933154	66711499	100.00%	18.975%
8	13.047	1642	1695	1697	rBV	3677147	32414238	48.59%	9.220%
9	13.088	1697	1702	1711	rVV	1778567	2911574	4.36%	0.828%
10	13.182	1711	1718	1729	rVB	632280	1061982	1.59%	0.302%
11	14.357	1909	1918	1923	rBV	993010	1395861	2.09%	0.397%
12	14.463	1931	1936	1946	rVB	542279	890988	1.34%	0.253%
13	14.803	1988	1994	2003	rVB	3639876	4960291	7.44%	1.411%
14	15.121	2006	2048	2051	rBV	6427518	47659373	71.44%	13.556%
15	15.961	2184	2191	2199	rVV	828814	1326596	1.99%	0.377%
16	16.390	2259	2264	2269	rVV	4803156	9272834	13.90%	2.637%
17	16.443	2269	2273	2278	rVV	7780954	15952140	23.91%	4.537%
18	16.490	2278	2281	2299	rVV	4944613	13161502	19.73%	3.744%
19	16.642	2300	2307	2314	rVV2	1438115	3114690	4.67%	0.886%
20	16.730	2318	2322	2339	rVB3	312557	1196208	1.79%	0.340%
21	16.983	2360	2365	2384	rBV	6397613	13156155	19.72%	3.742%
22	17.212	2399	2404	2411	rVB	574021	828747	1.24%	0.236%
23	18.111	2551	2557	2578	rBV	1646381	3034216	4.55%	0.863%
24	19.022	2707	2712	2720	rBV3	930548	1905101	2.86%	0.542%
25	19.263	2749	2753	2756	rBV	806022	1060812	1.59%	0.302%
26	19.386	2770	2774	2778	rVV	1666345	2211446	3.31%	0.629%
27	19.715	2825	2830	2837	rVB	1238424	1656875	2.48%	0.471%
28	19.827	2844	2849	2855	rBV	2603810	3514664	5.27%	1.000%
29	20.267	2919	2924	2928	rVB	1581016	1807677	2.71%	0.514%
30	20.479	2952	2960	2975	rBV	1191686	2442852	3.66%	0.695%
31	20.779	3006	3011	3016	rVB	1334582	1634199	2.45%	0.465%
32	21.078	3051	3062	3063	rBV2	563972	1494238	2.24%	0.425%
33	21.114	3064	3068	3085	rVB	1229982	2766294	4.15%	0.787%
34	21.302	3095	3100	3108	rVB	1058747	1499982	2.25%	0.427%
35	21.448	3120	3125	3140	rVB	610623	1232937	1.85%	0.351%
36	22.212	3250	3255	3262	rVB	611866	932477	1.40%	0.265%

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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-BG072823.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	22.817	3353	3358	3370	rVB	558522	1017128	1.52%	0.289%
38	23.711	3504	3510	3532	rVV2	279728	1190275	1.78%	0.339%
39	24.515	3639	3647	3661	rVB	359109	1031262	1.55%	0.293%
40	25.802	3853	3866	3882	rVB4	236762	1091080	1.64%	0.310%
41	26.748	4000	4027	4043	rBV2	6661154	33687111	50.50%	9.582%
42	30.033	4553	4586	4630	rVB2	4385759	31081286	46.59%	8.840%
43	31.625	4837	4857	4858	rBV	1303796	5396191	8.09%	1.535%

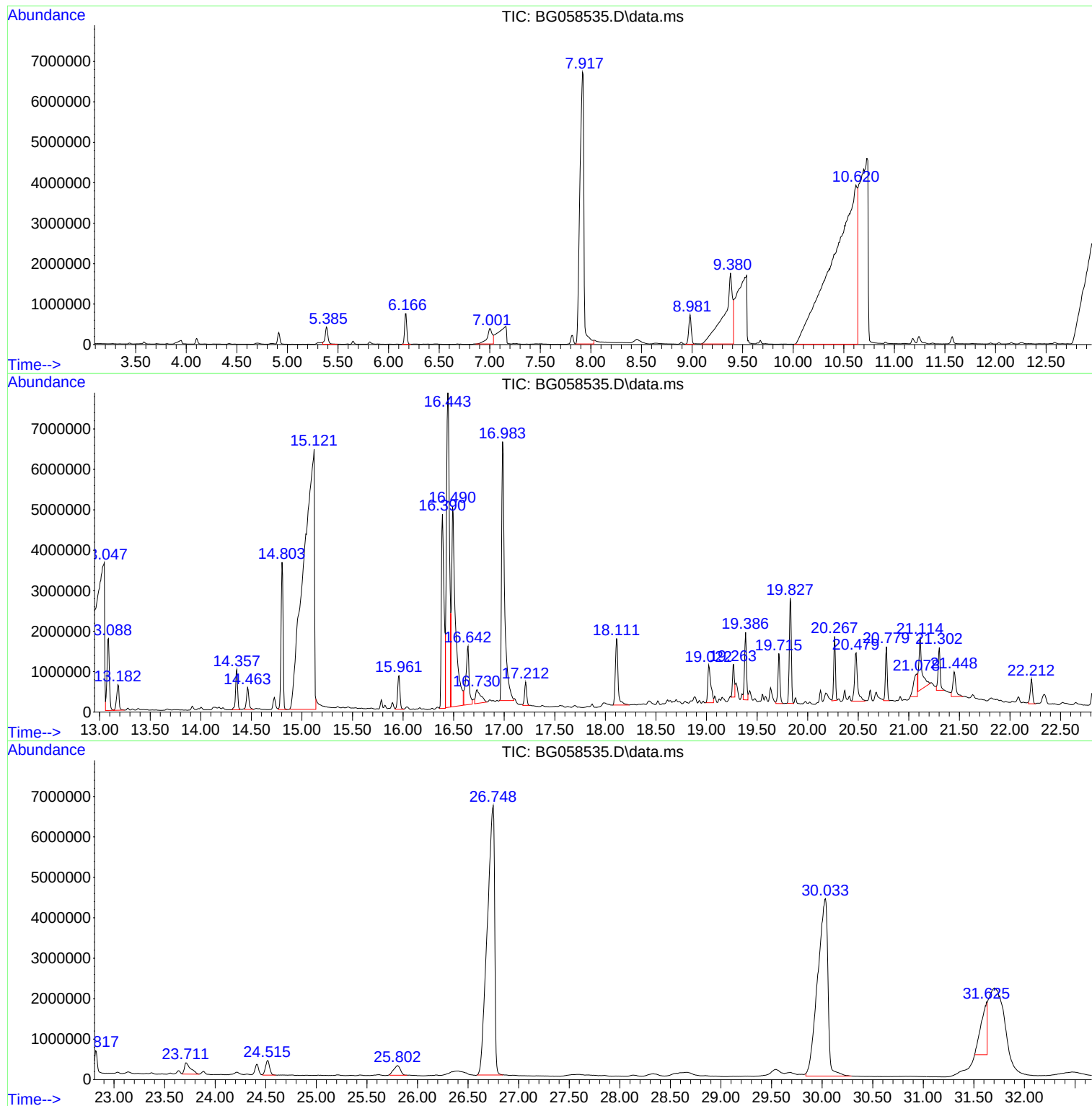
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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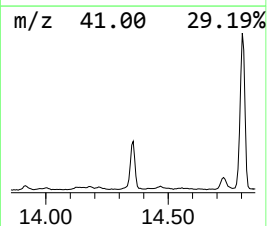
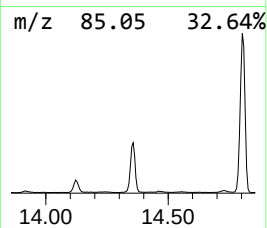
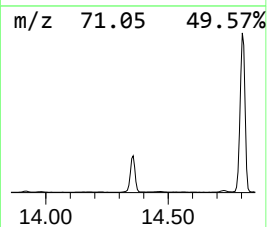
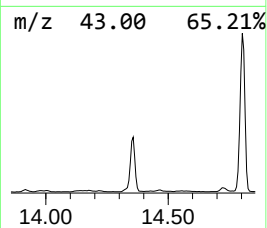
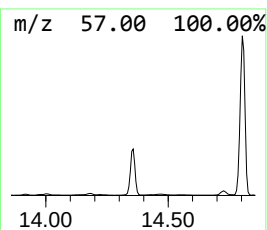
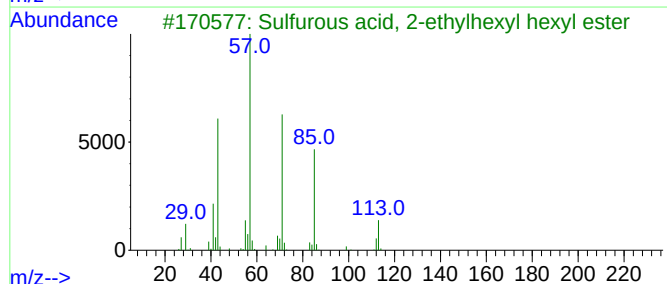
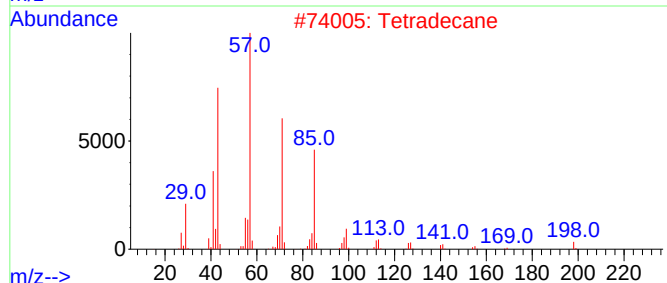
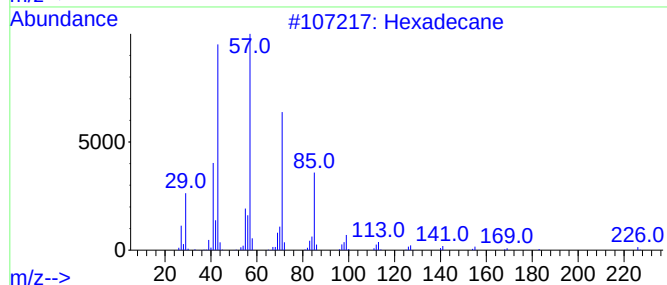
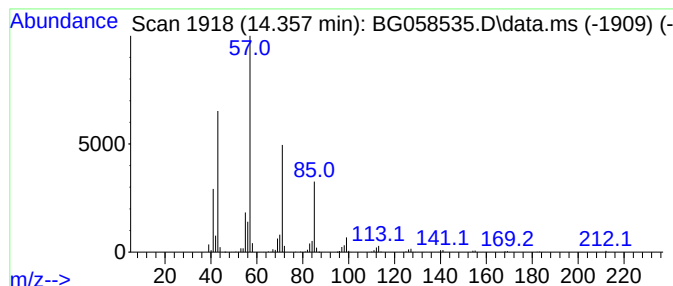
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Hexadecane Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.357	31.33 ng	1395860	Acenaphthene-d10	14.463

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane	226	C16H34	000544-76-3	90
2			Tetradecane	198	C14H30	000629-59-4	86
3			Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	80
4			Tridecane	184	C13H28	000629-50-5	78
5			Nonane, 3,7-dimethyl-	156	C11H24	017302-32-8	68



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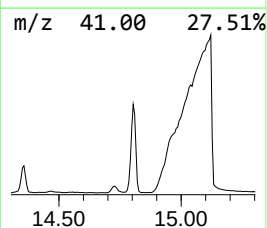
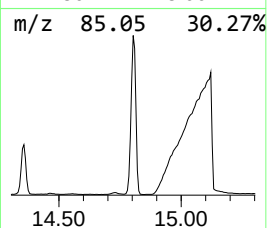
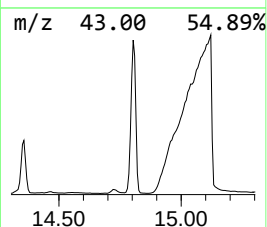
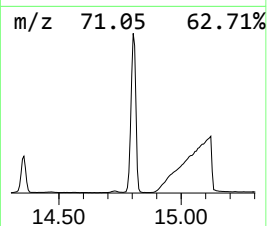
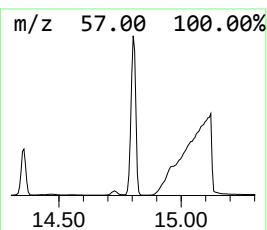
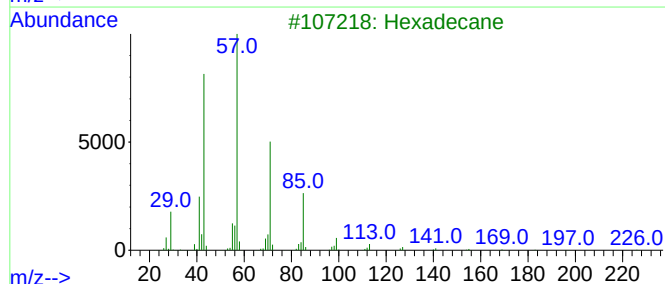
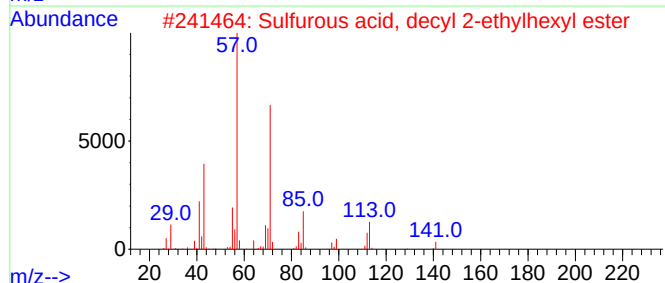
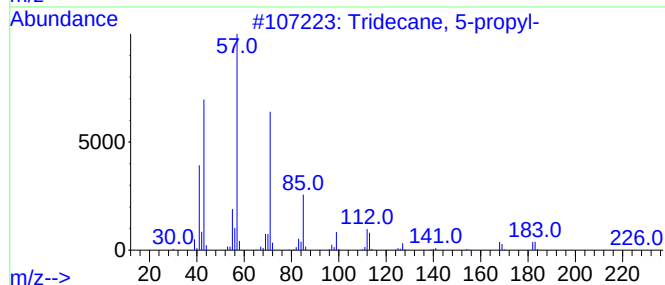
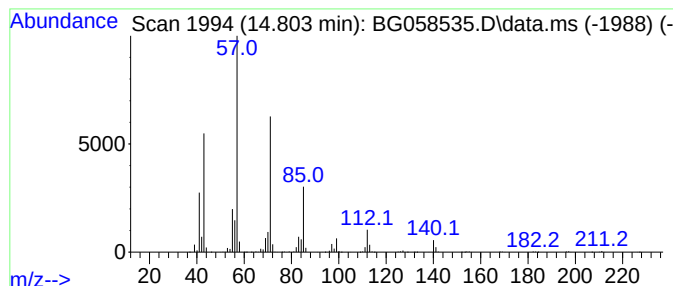
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Tridecane, 5-propyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.803	111.34 ng	4960290	Acenaphthene-d10	14.463

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane, 5-propyl-	226	C16H34	055045-11-9	87
2			Sulfurous acid, decyl 2-ethylhex...	334	C18H38O3S	1000309-19-3	80
3			Hexadecane	226	C16H34	000544-76-3	80
4			Nonane, 2-methyl-5-propyl-	184	C13H28	031081-17-1	80
5			Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	78



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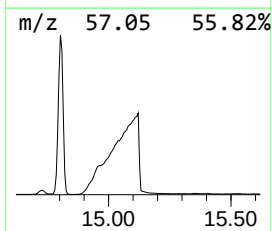
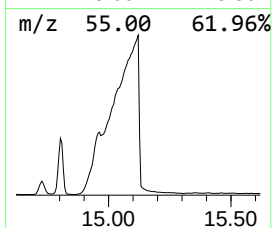
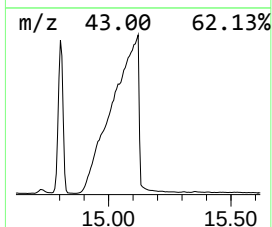
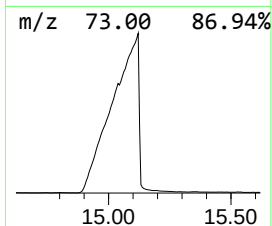
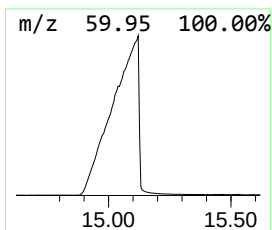
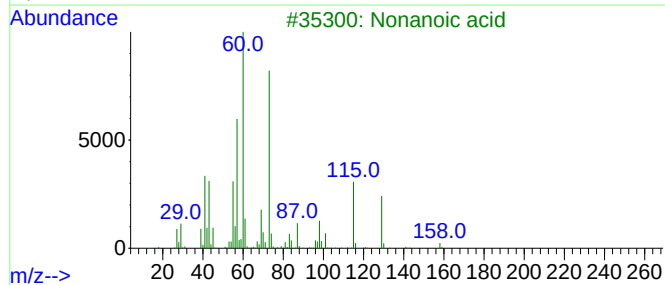
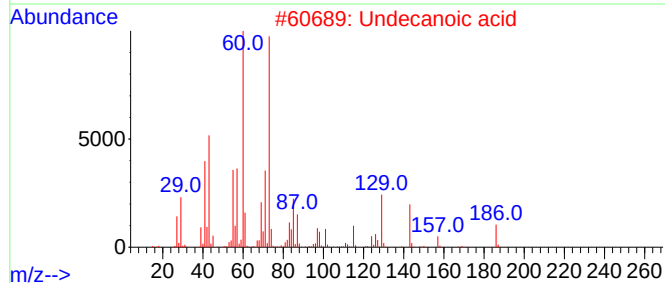
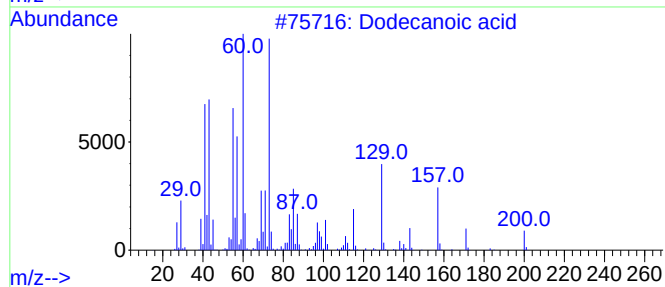
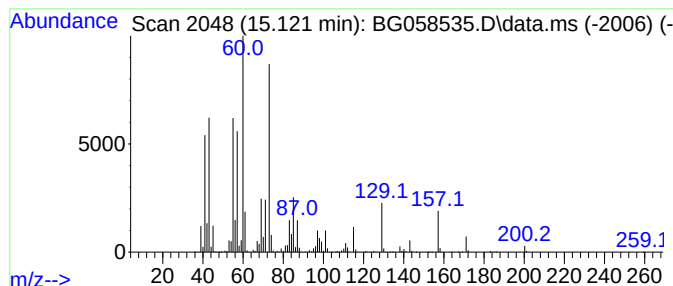
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Dodecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.121	1069.81 ng	47659400	Acenaphthene-d10	14.463

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecanoic acid	200	C12H24O2	000143-07-7	91
2			Undecanoic acid	186	C11H22O2	000112-37-8	80
3			Nonanoic acid	158	C9H18O2	000112-05-0	64
4			Octanoic acid	144	C8H16O2	000124-07-2	60
5			Hexanoic acid	116	C6H12O2	000142-62-1	43



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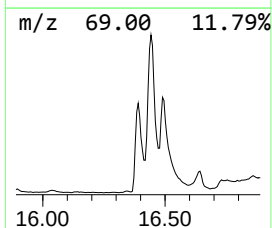
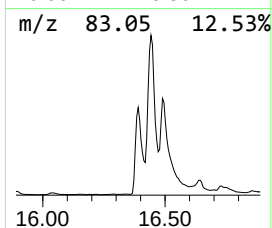
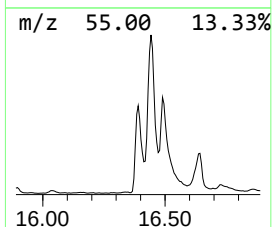
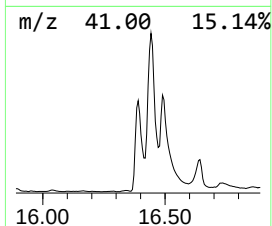
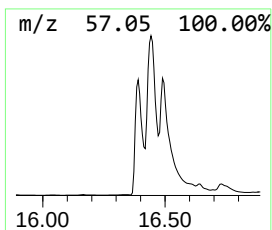
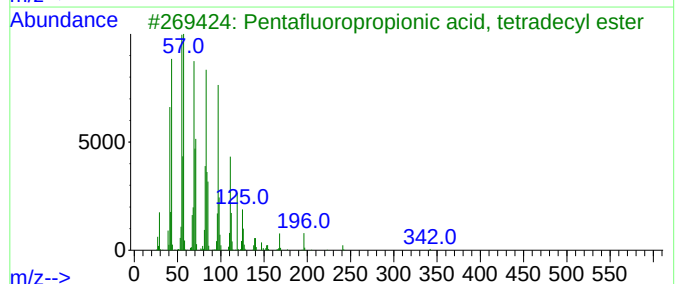
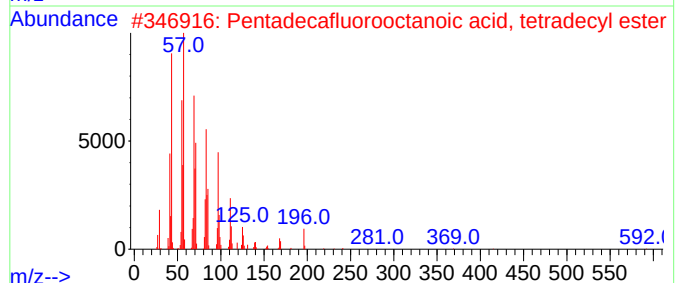
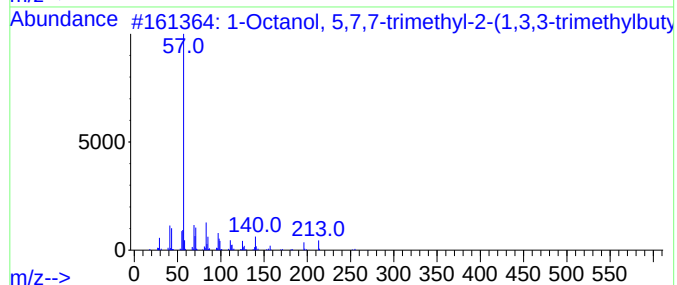
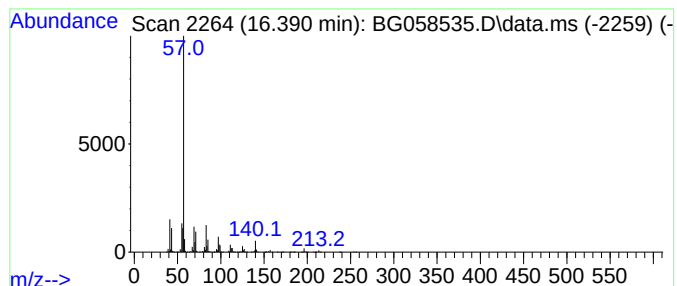
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 1-Octanol, 5,7,7-trimethyl-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.390	223.78 ng	9272830	Phenanthrene-d10	17.212

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octanol, 5,7,7-trimethyl-2-(1,...	270	C18H38O	036400-98-3	90		
2	Pentadecafluorooctanoic acid, te...	610	C22H29F15O2	1000406-04-4	64		
3	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	59		
4	3-Propionyloxytridecane	256	C16H32O2	1000245-62-5	59		
5	1-Dodecanol, 3,7,11-trimethyl-	228	C15H32O	006750-34-1	59		



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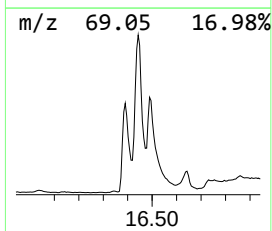
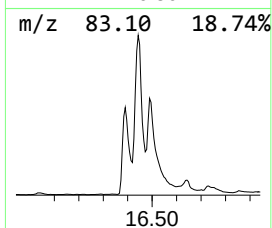
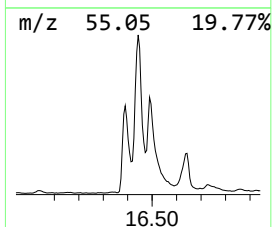
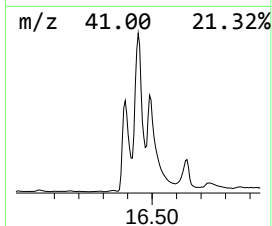
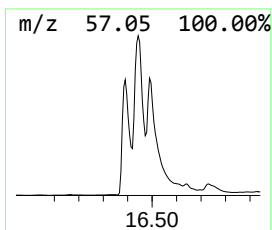
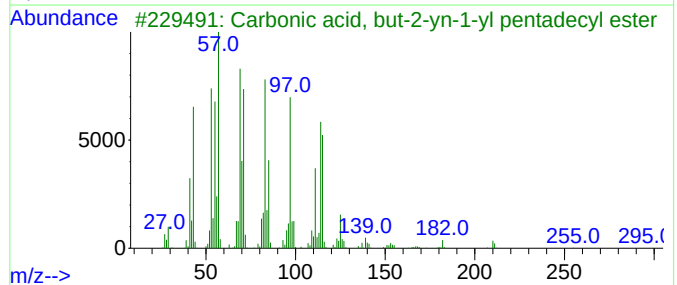
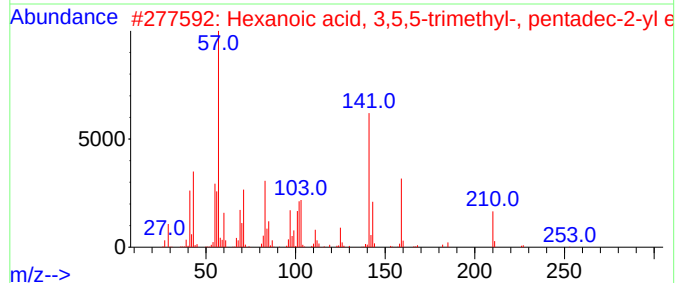
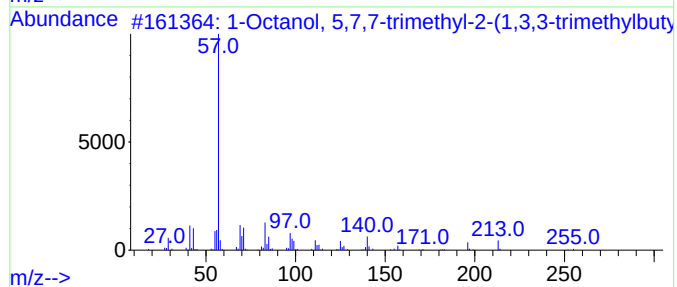
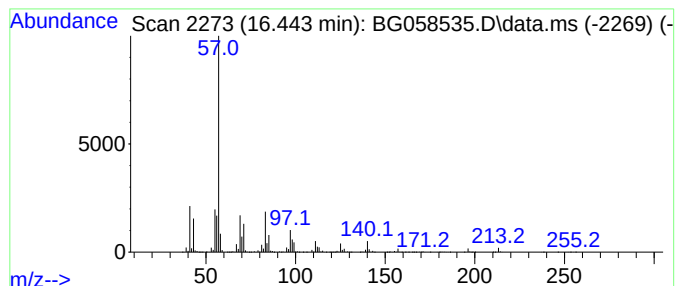
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Hexanoic acid, 3,5,5-trimet... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.443	384.97 ng	15952100	Phenanthrene-d10	17.212

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Octanol, 5,7,7-trimethyl-2-(1,...	270	C18H38O	036400-98-3	72
2			Hexanoic acid, 3,5,5-trimethyl-,...	368	C24H48O2	1000406-27-2	53
3			Carbonic acid, but-2-yn-1-yl pen...	324	C20H36O3	1010383-21-0	50
4			Butyl tetradecyl ether	270	C18H38O	1000406-40-4	50
5			Isobutyl tetradecyl ether	270	C18H38O	1000406-32-7	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072823\
Data File : BG058535.D
Acq On : 29 Jul 2023 2:36
Operator : MA/JU
Sample : 03642-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
EFF-WW

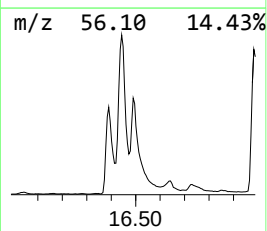
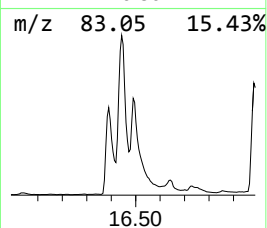
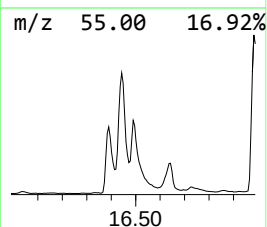
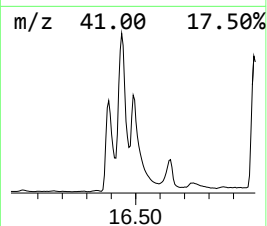
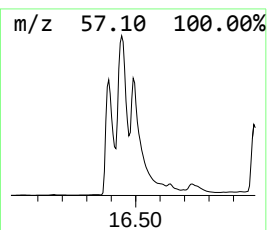
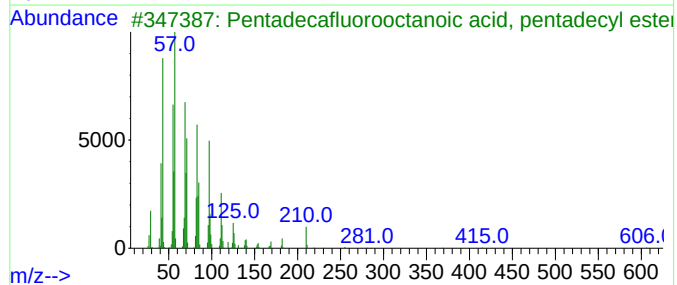
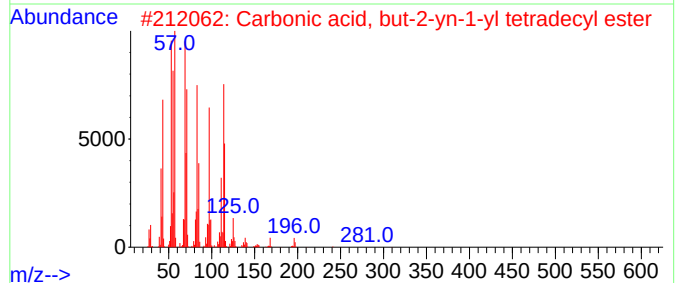
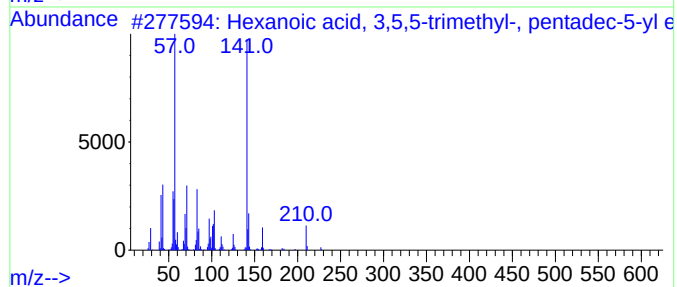
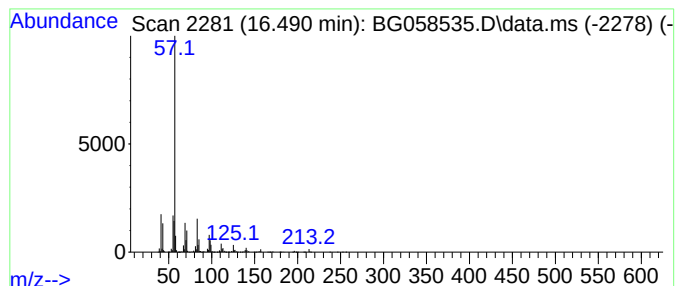
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Carbonic acid, but-2-yn-1-y... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.490	317.62 ng	13161500	Phenanthrene-d10	17.212

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid, 3,5,5-trimethyl-,...	368	C24H48O2	1000406-27-5	53
2			Carbonic acid, but-2-yn-1-yl tet...	310	C19H34O3	1010383-20-9	53
3			Pentadecafluorooctanoic acid, pe...	624	C23H31F15O2	1000406-04-5	53
4			Hexanoic acid, 3,5,5-trimethyl-,...	354	C23H46O2	1000406-26-9	53
5			Hexanoic acid, 3,5,5-trimethyl-,...	368	C24H48O2	1000406-27-4	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072823\
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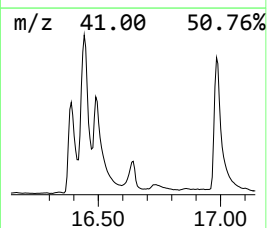
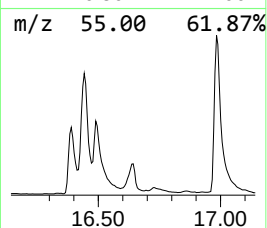
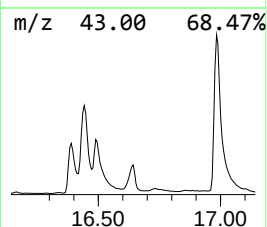
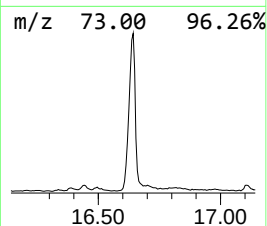
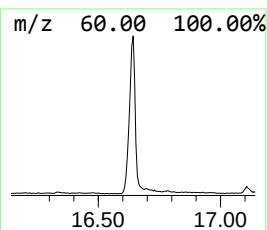
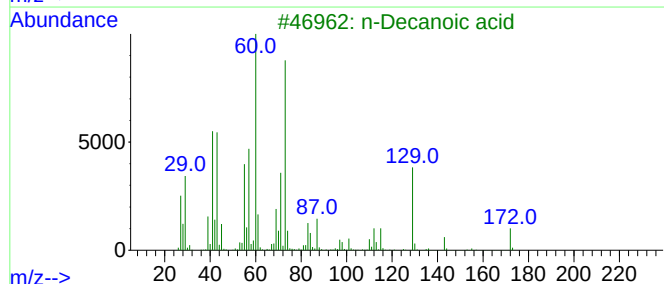
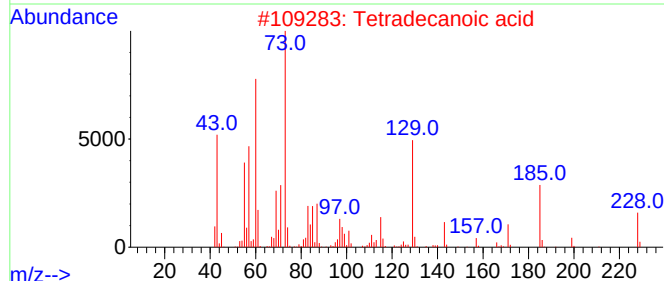
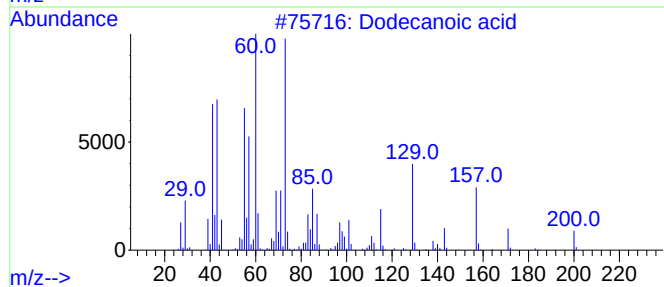
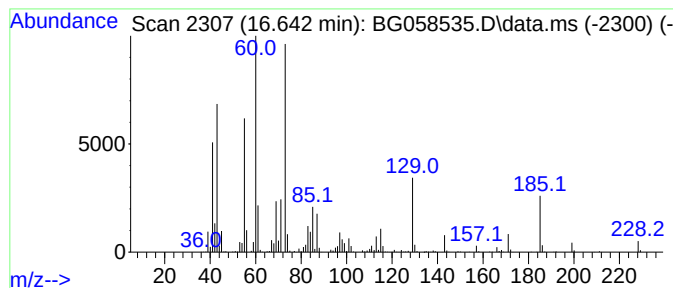
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tetradecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.642	75.17 ng	3114690	Phenanthrene-d10	17.212

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecanoic acid	200	C12H24O2	000143-07-7	80
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	62
3			n-Decanoic acid	172	C10H20O2	000334-48-5	58
4			Tridecanoic acid	214	C13H26O2	000638-53-9	50
5			Methyl-.alpha.-d-ribofuranoside	164	C6H12O5	1000129-83-1	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072823\
Data File : BG058535.D
Acq On : 29 Jul 2023 2:36
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Sample : 03642-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

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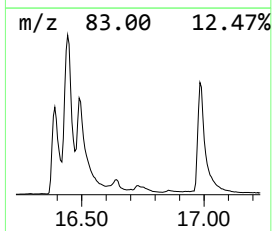
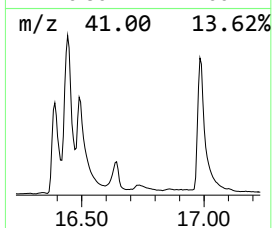
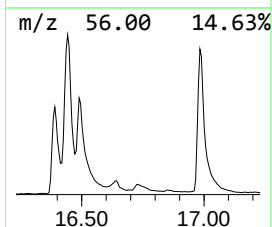
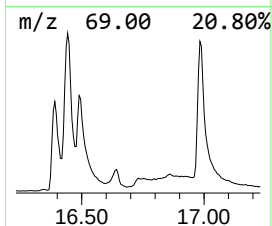
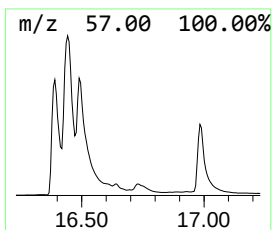
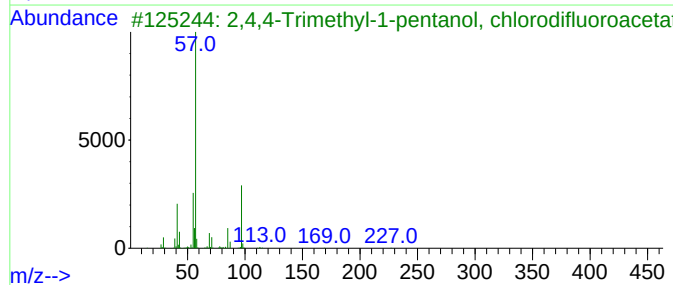
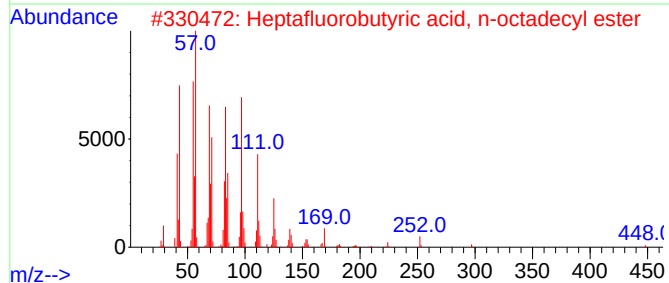
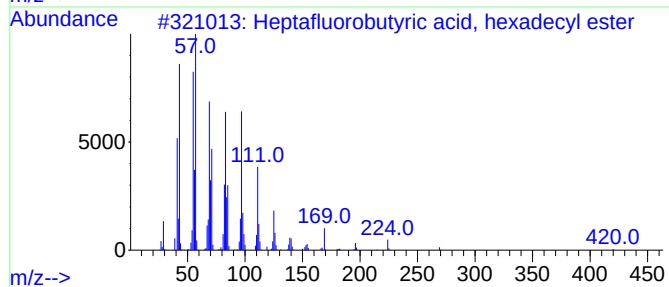
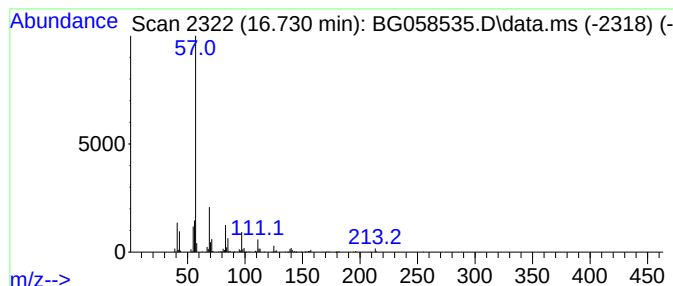
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptafluorobutyric acid, he... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.730	28.87 ng	1196210	Phenanthrene-d10	17.212

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	50
2			Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	50
3			2,4,4-Trimethyl-1-pentanol, chlo...	242	C10H17ClF2O2	1000447-27-2	50
4			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	50
5			2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072823\
Data File : BG058535.D
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Misc :
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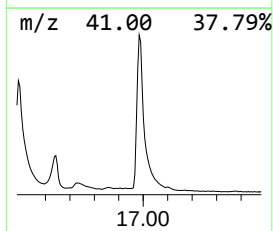
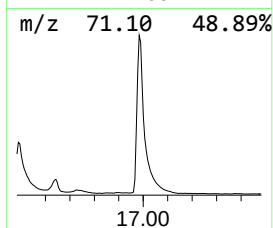
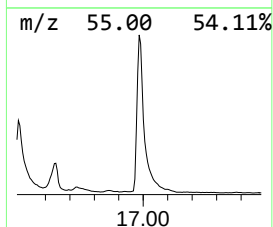
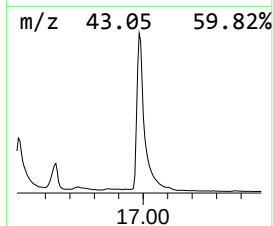
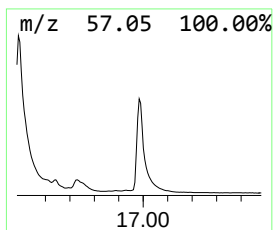
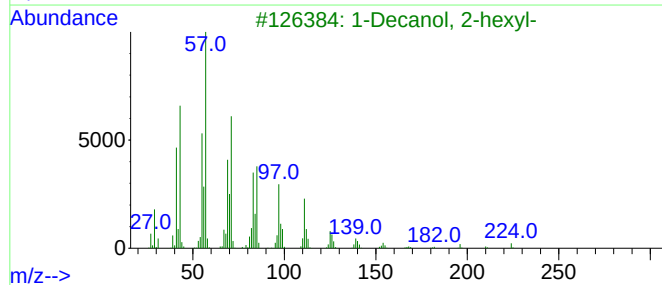
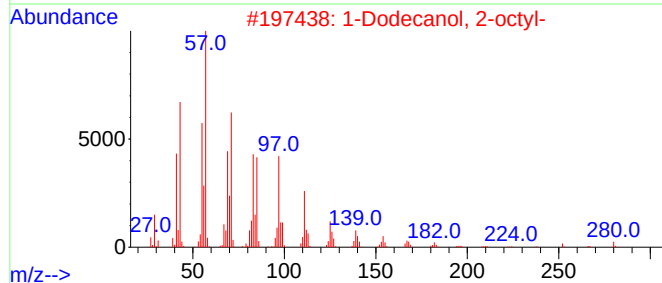
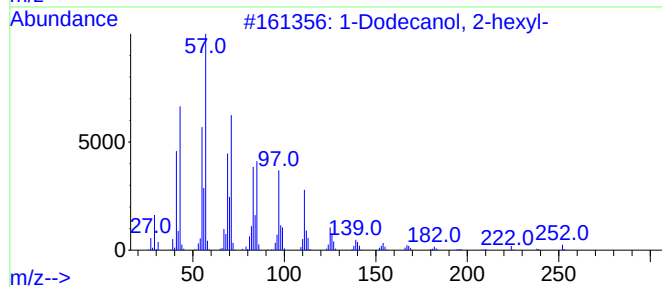
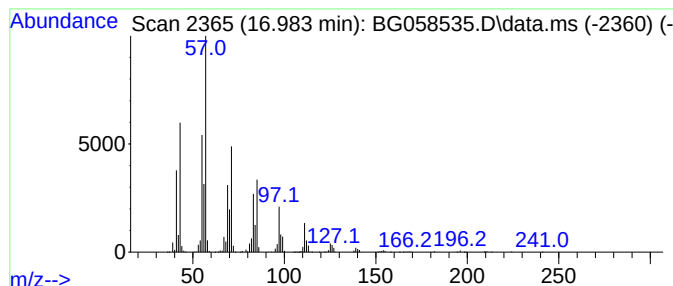
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1-Dodecanol, 2-hexyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.983	317.50 ng	13156200	Phenanthrene-d10	17.212

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Dodecanol, 2-hexyl-			270	C18H38O	110225-00-8	91
2	1-Dodecanol, 2-octyl-			298	C20H42O	005333-42-6	91
3	1-Decanol, 2-hexyl-			242	C16H34O	002425-77-6	91
4	Carbonic acid, octadecyl prop-1-...			354	C22H42O3	1000383-11-5	81
5	Decyl isobutyl carbonate			258	C15H30O3	959226-07-4	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072823\
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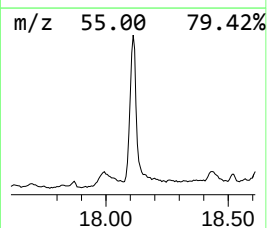
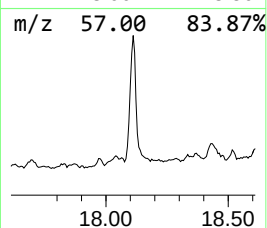
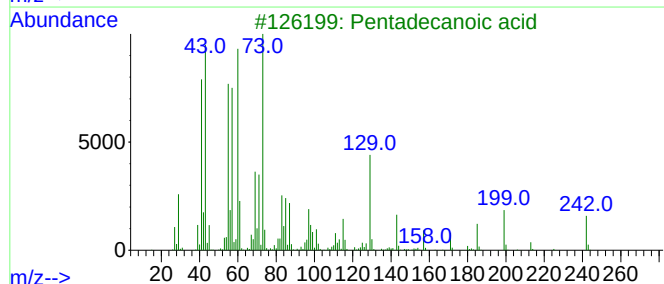
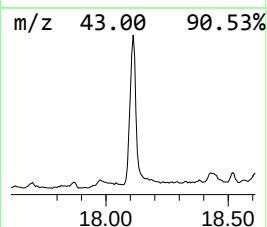
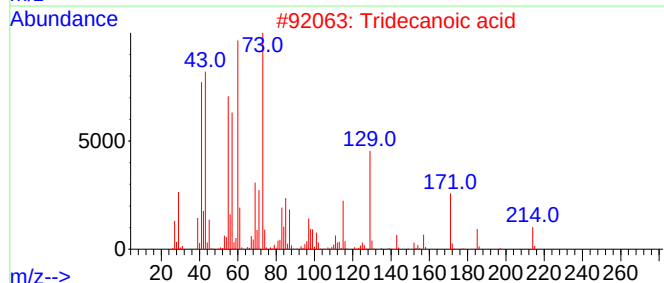
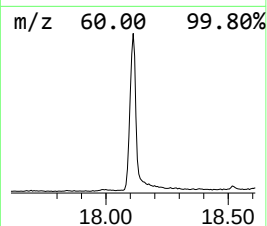
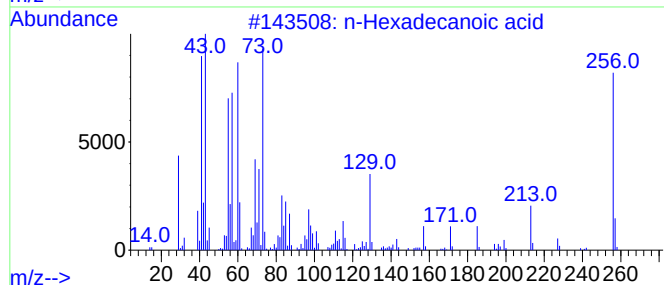
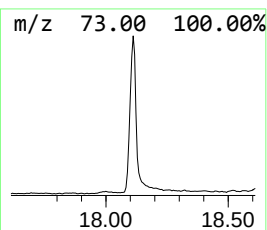
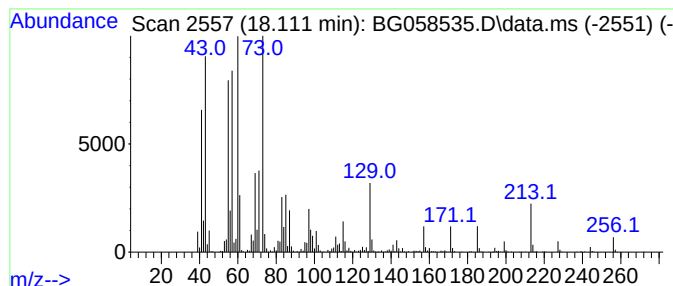
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 n-Hexadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.111	73.22 ng	3034220	Phenanthrene-d10	17.212

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	90
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			Undecanoic acid	186	C11H22O2	000112-37-8	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072823\
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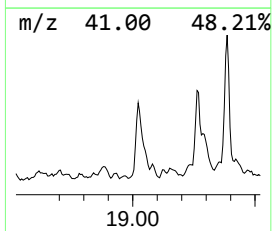
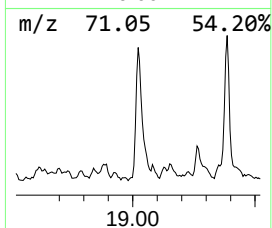
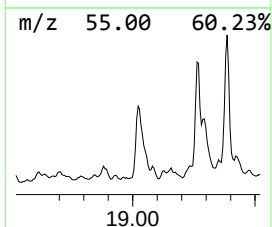
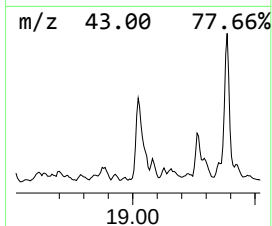
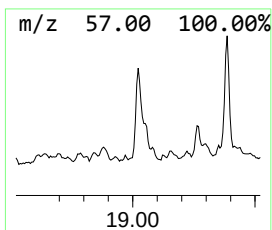
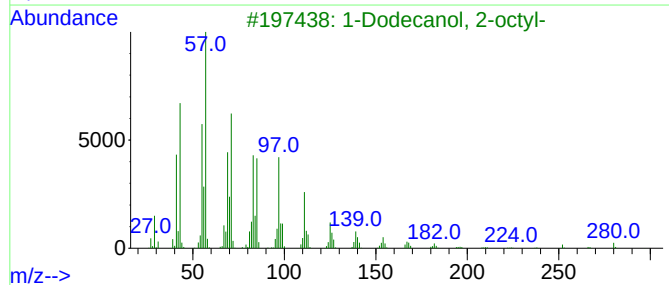
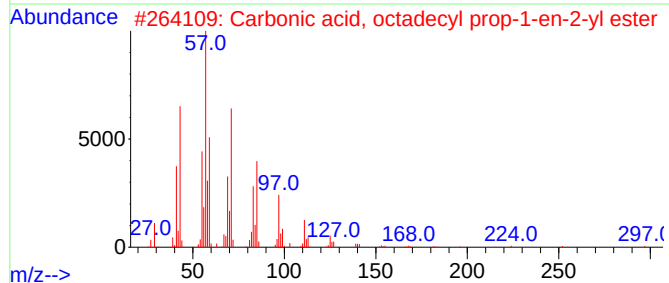
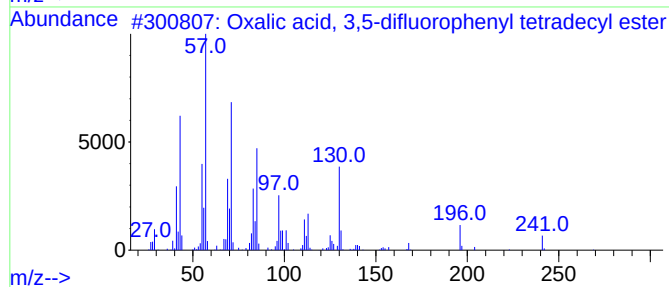
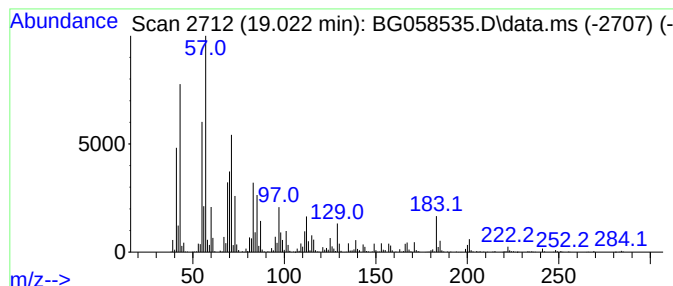
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 unknown19.022 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.022	45.98 ng	1905100	Phenanthrene-d10	17.212

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxalic acid, 3,5-difluorophenyl ...	398	C22H32F2O4	1000309-67-8	49
2			Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	46
3			1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	46
4			Silane, trichlorodocosyl-	442	C22H45Cl3Si	007325-84-0	46
5			Eicosyl octyl ether	410	C28H58O	1000406-38-8	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072823\
Data File : BG058535.D
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ALS Vial : 16 Sample Multiplier: 1

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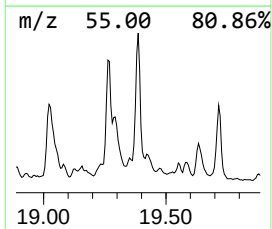
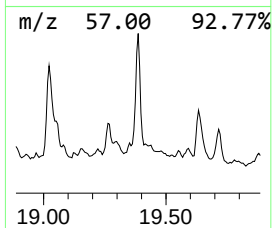
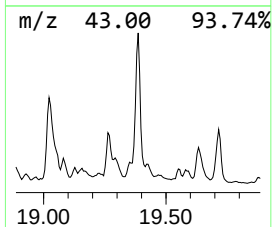
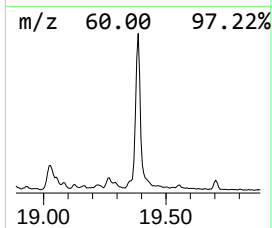
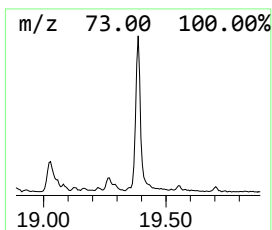
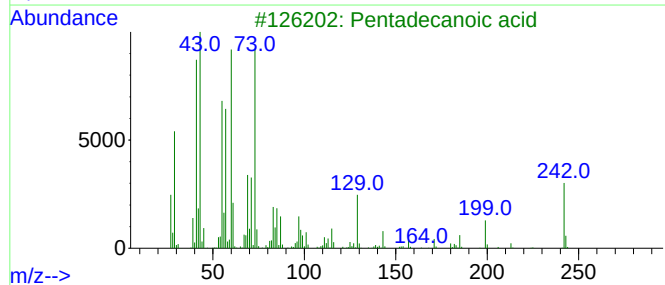
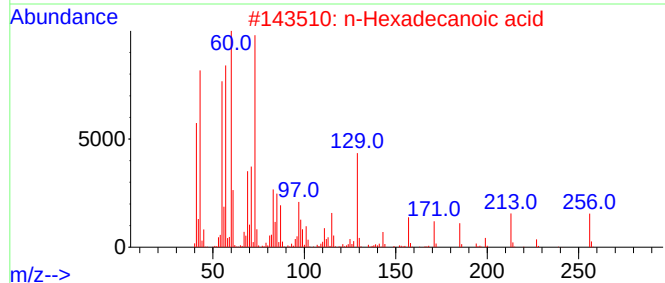
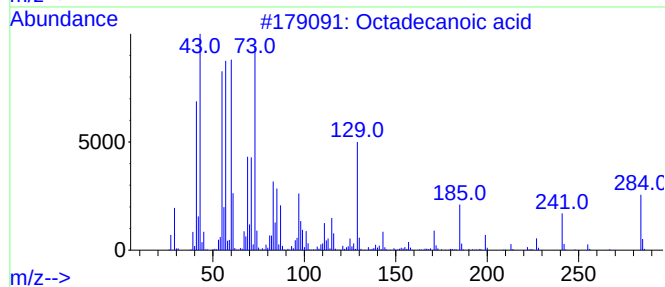
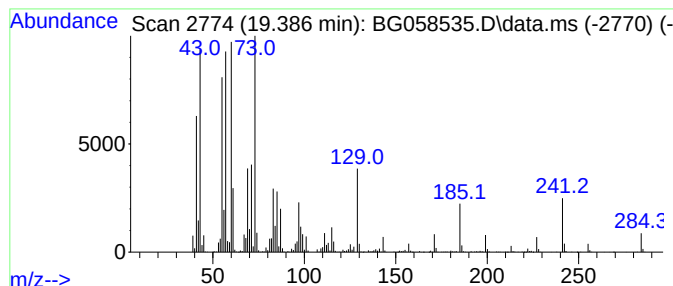
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Octadecanoic acid Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.386	35.87 ng	2211450	Chrysene-d12	21.448

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	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5			n-Decanoic acid	172	C10H20O2	000334-48-5	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072823\
Data File : BG058535.D
Acq On : 29 Jul 2023 2:36
Operator : MA/JU
Sample : 03642-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
EFF-WW

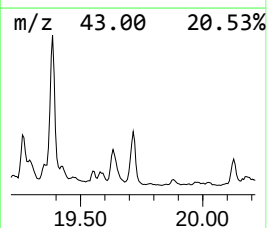
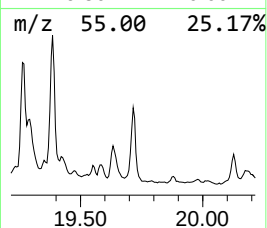
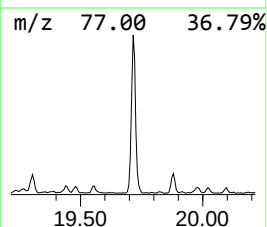
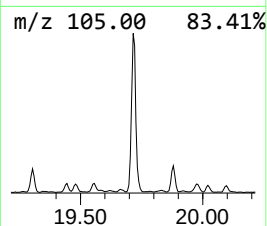
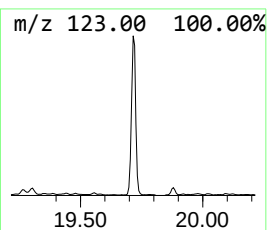
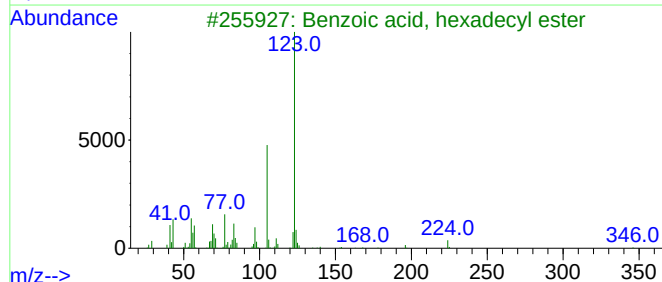
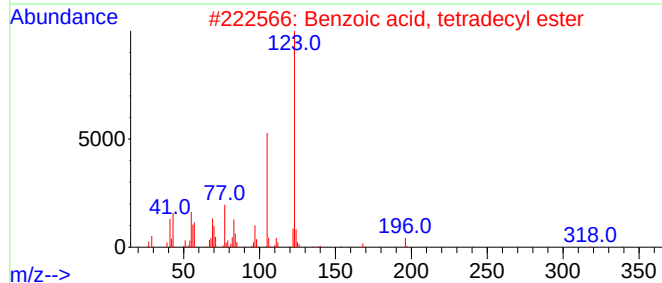
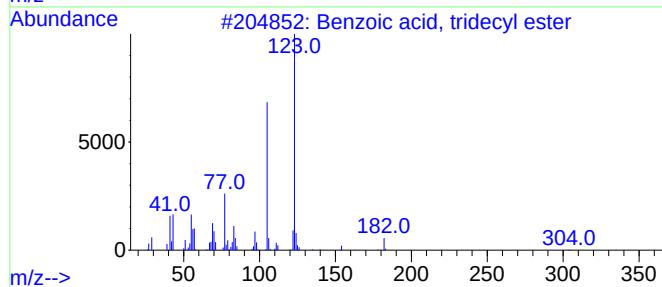
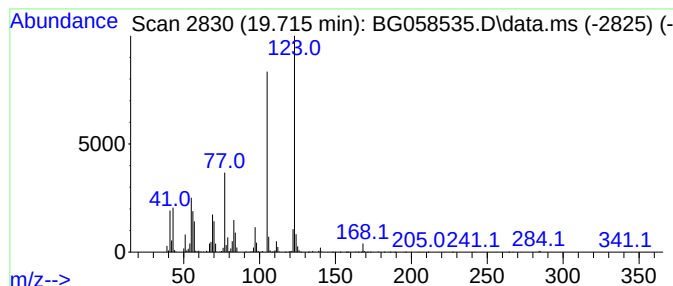
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Benzoic acid, tridecyl ester Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.715	26.88 ng	1656880	Chrysene-d12	21.448

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, tridecyl ester	304	C20H32O2	1010340-22-6	91
2			Benzoic acid, tetradecyl ester	318	C21H34O2	1000340-22-7	86
3			Benzoic acid, hexadecyl ester	346	C23H38O2	1000340-22-9	80
4			Benzoic acid, pentadecyl ester	332	C22H36O2	1000340-22-8	80
5			Benzoic acid, heptyl ester	220	C14H20O2	007155-12-6	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072823\
Data File : BG058535.D
Acq On : 29 Jul 2023 2:36
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Sample : 03642-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

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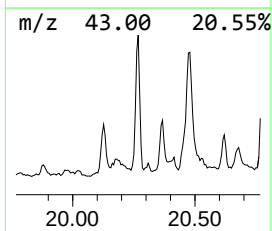
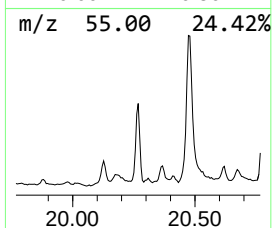
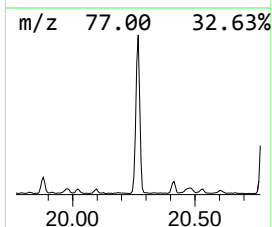
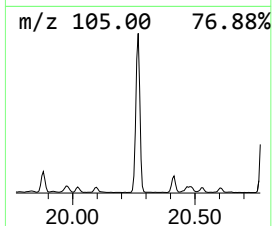
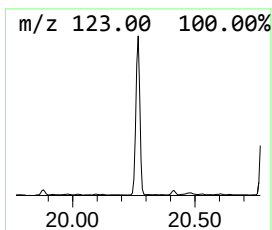
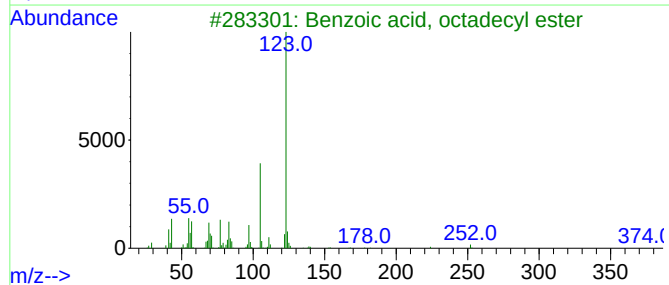
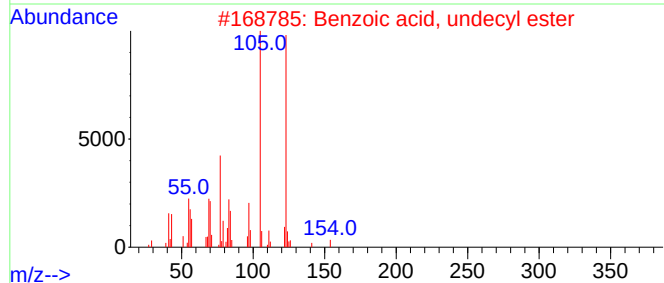
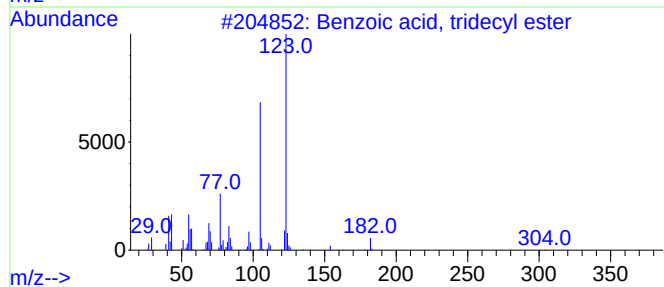
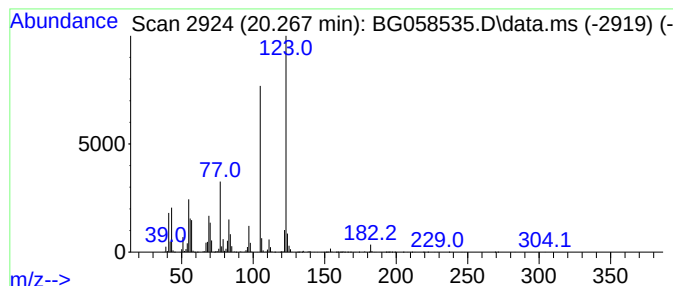
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Benzoic acid, undecyl ester Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.267	29.32 ng	1807680	Chrysene-d12	21.448

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, tridecyl ester	304	C20H32O2	1010340-22-6	91
2			Benzoic acid, undecyl ester	276	C18H28O2	006316-30-9	90
3			Benzoic acid, octadecyl ester	374	C25H42O2	010578-34-4	87
4			Benzoic acid, heptadecyl ester	360	C24H40O2	1000340-23-0	86
5			Benzoic acid, nonadecyl ester	388	C26H44O2	1000340-23-2	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072823\
Data File : BG058535.D
Acq On : 29 Jul 2023 2:36
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Sample : 03642-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

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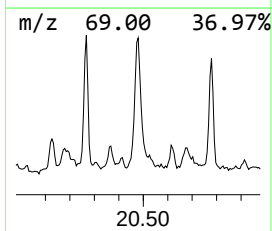
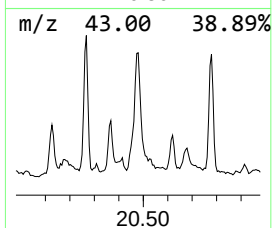
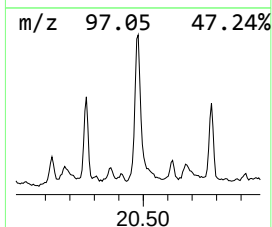
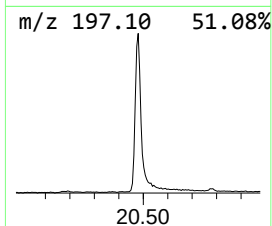
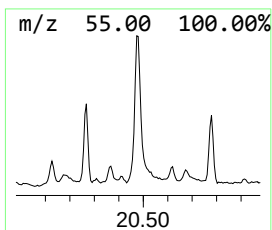
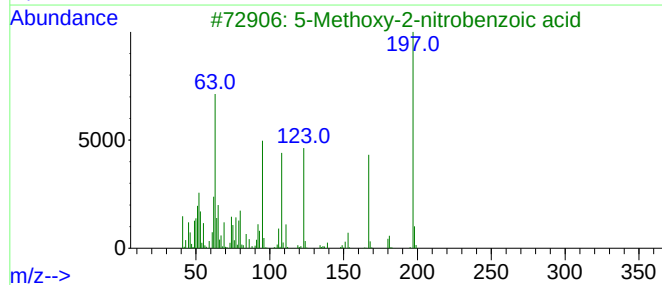
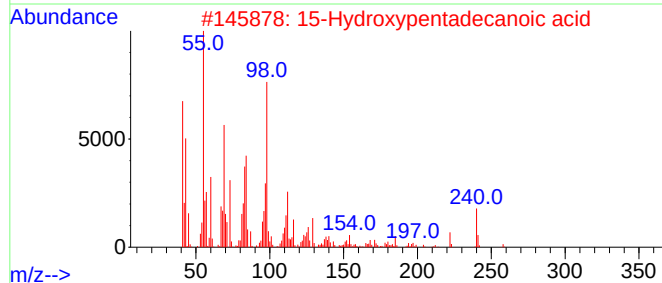
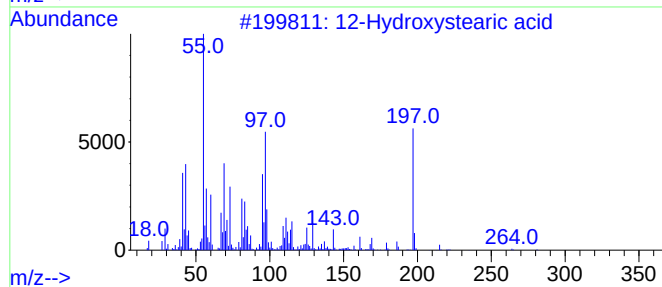
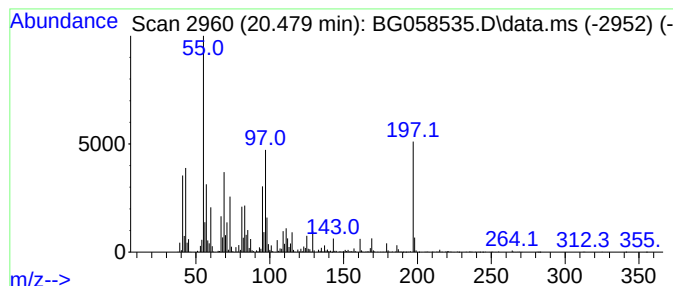
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 12-Hydroxystearic acid Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.479	39.63 ng	2442850	Chrysene-d12	21.448

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			12-Hydroxystearic acid	300	C18H36O3	000106-14-9	91
2			15-Hydroxypentadecanoic acid	258	C15H30O3	004617-33-8	35
3			5-Methoxy-2-nitrobenzoic acid	197	C8H7NO5	001882-69-5	27
4			Succinic acid, 2,2-dichloroethyl...	310	C9H11Cl2F3O4	1000390-84-2	22
5			Tetradecanoic acid, 2-oxo-, ethy...	270	C16H30O3	160941-13-9	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072823\
Data File : BG058535.D
Acq On : 29 Jul 2023 2:36
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Sample : 03642-02
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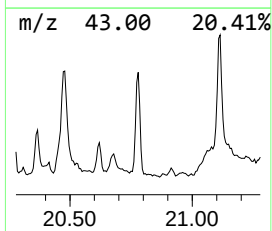
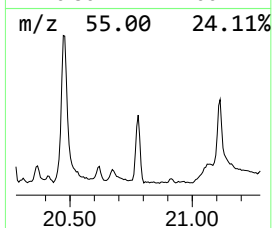
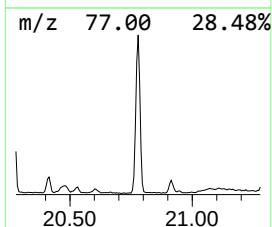
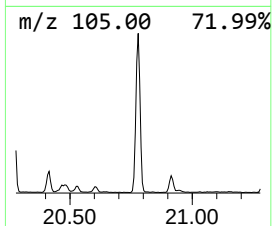
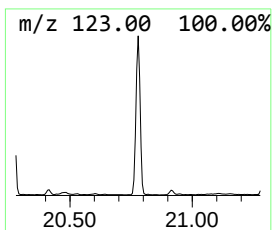
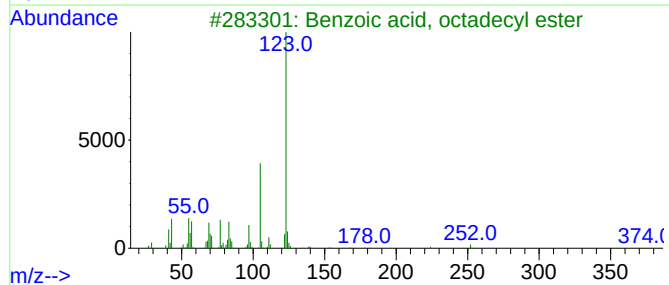
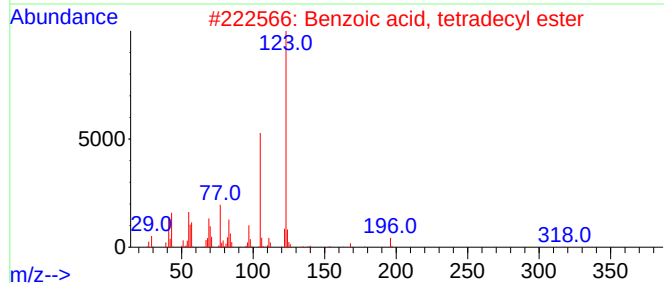
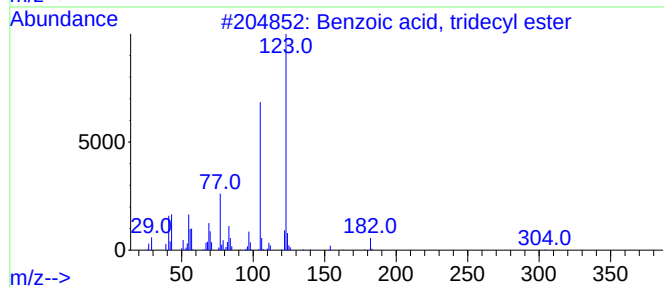
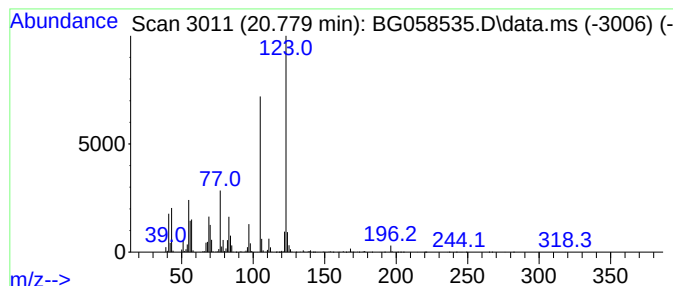
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 Benzoic acid, tetradecyl ester Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.779	26.51 ng	1634200	Chrysene-d12	21.448

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, tridecyl ester	304	C20H32O2	1010340-22-6	91
2			Benzoic acid, tetradecyl ester	318	C21H34O2	1000340-22-7	91
3			Benzoic acid, octadecyl ester	374	C25H42O2	010578-34-4	90
4			Benzoic acid, nonadecyl ester	388	C26H44O2	1000340-23-2	90
5			Benzoic acid, heptadecyl ester	360	C24H40O2	1000340-23-0	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072823\
Data File : BG058535.D
Acq On : 29 Jul 2023 2:36
Operator : MA/JU
Sample : 03642-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
EFF-WW

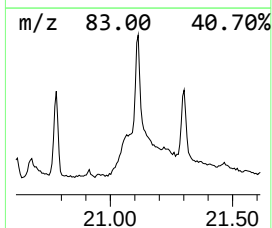
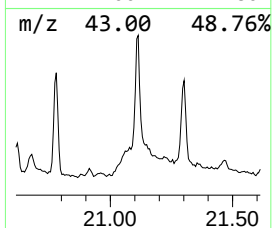
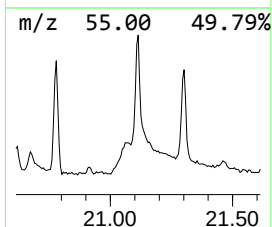
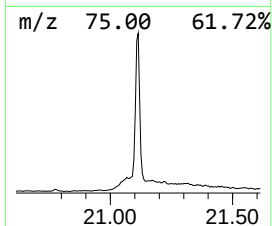
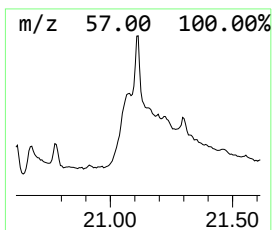
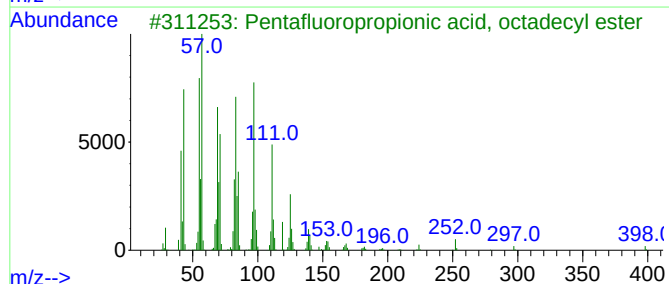
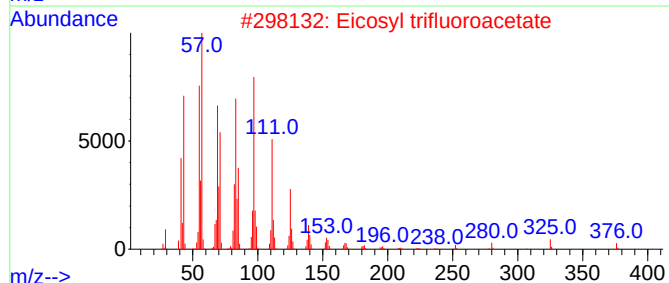
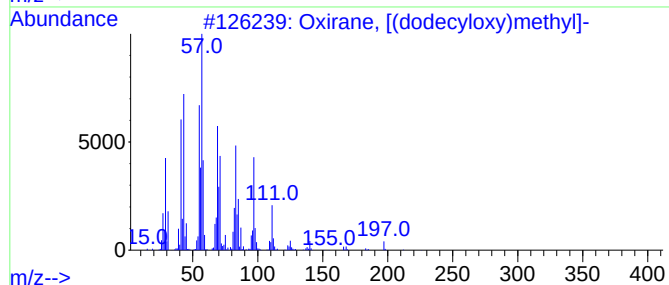
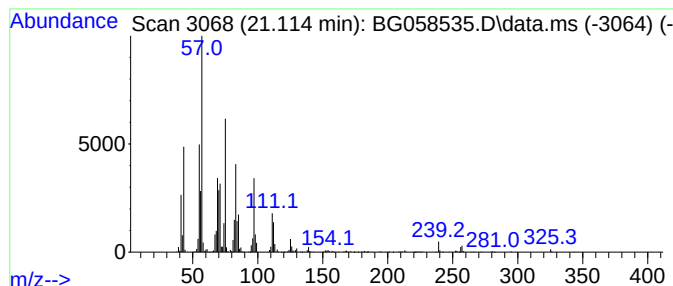
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 Oxirane, [(dodecyloxy)methyl]- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.114	44.87 ng	2766290	Chrysene-d12	21.448

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxirane, [(dodecyloxy)methyl]-	242	C15H30O2	002461-18-9	68
2			Eicosyl trifluoroacetate	394	C22H41F3O2	1000351-75-2	58
3			Pentafluoropropionic acid, octadecyl ester	416	C21H37F5O2	959261-25-7	52
4			3-Chloropropionic acid, heptadecyl ester	346	C20H39ClO2	1000283-05-1	52
5			Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	52



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072823\
Data File : BG058535.D
Acq On : 29 Jul 2023 2:36
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Sample : 03642-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

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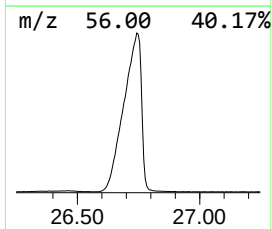
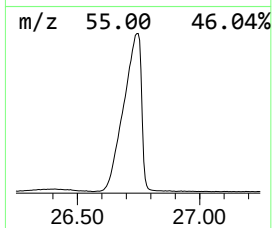
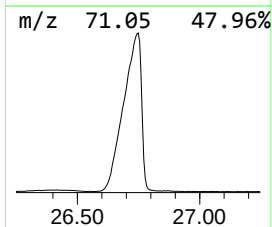
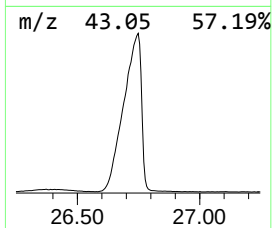
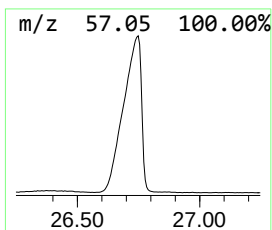
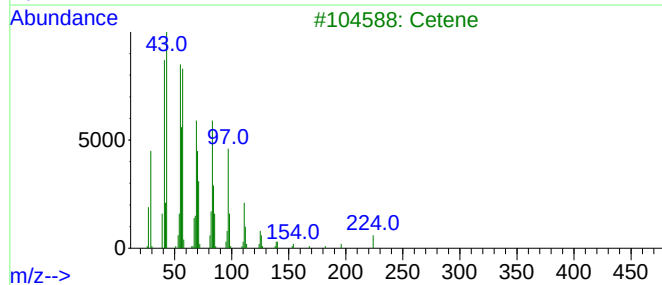
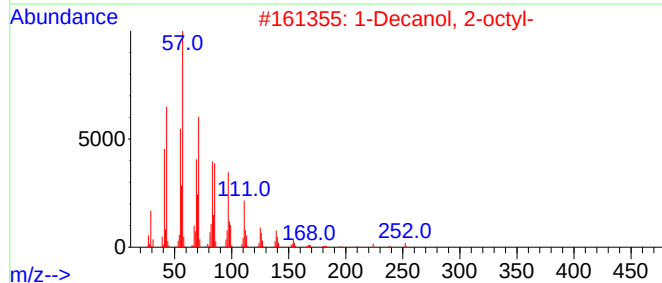
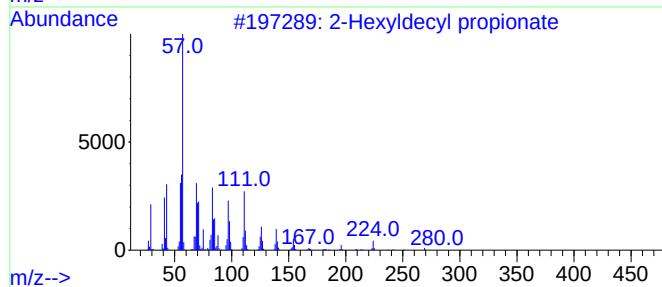
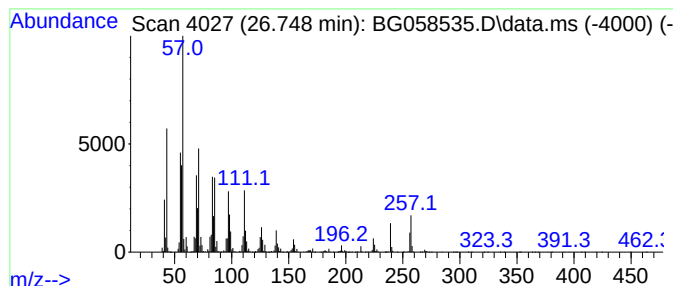
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 2-Hexyldecyl propionate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.748	653.32 ng	33687100	Perylene-d12	24.521

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Hexyldecyl propionate	298	C19H38O2	1072781-99-7	64
2			1-Decanol, 2-octyl-	270	C18H38O	045235-48-1	58
3			Cetene	224	C16H32	000629-73-2	53
4			1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	53
5			2-Hexyldecyl isobutyrate	312	C20H40O2	1000368-55-3	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072823\
Data File : BG058535.D
Acq On : 29 Jul 2023 2:36
Operator : MA/JU
Sample : 03642-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
EFF-WW

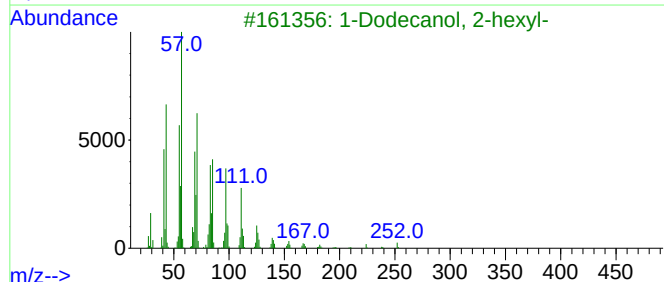
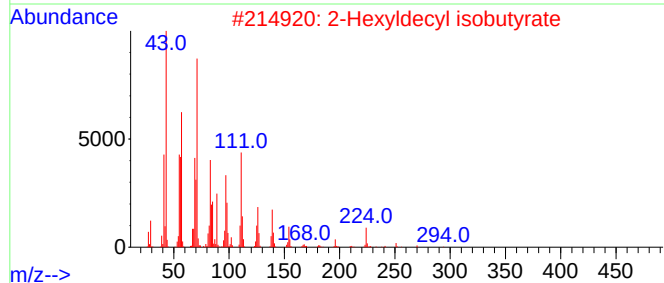
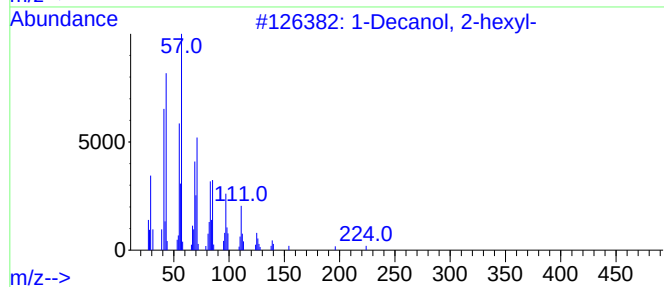
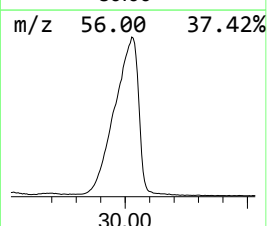
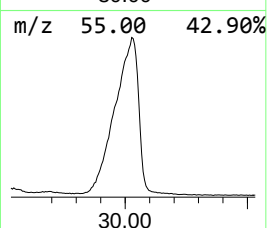
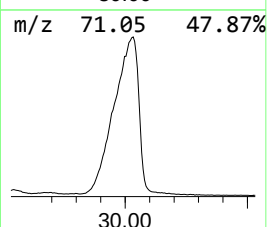
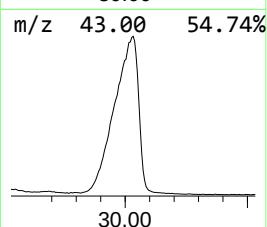
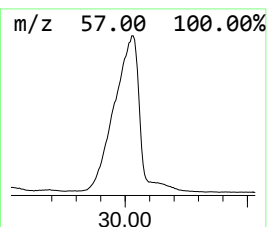
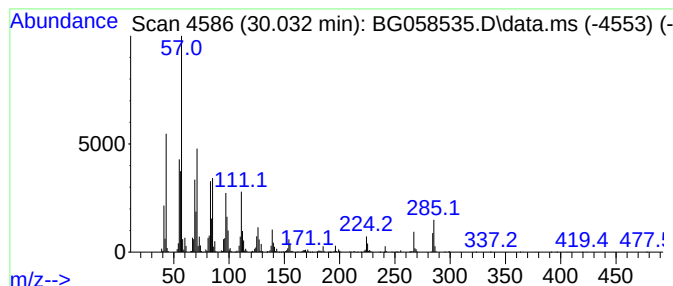
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 1-Decanol, 2-hexyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
30.032	602.78 ng	31081300	Perylene-d12	24.521

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Decanol, 2-hexyl-		242	C16H34O	002425-77-6	74
2	2-Hexyldecyl isobutyrate		312	C20H40O2	1000368-55-3	70
3	1-Dodecanol, 2-hexyl-		270	C18H38O	110225-00-8	70
4	1-Decanol, 2-octyl-		270	C18H38O	045235-48-1	62
5	2-Hexyl-1-octanol		214	C14H30O	019780-79-1	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072823\
Data File : BG058535.D
Acq On : 29 Jul 2023 2:36
Operator : MA/JU
Sample : 03642-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
EFF-WW

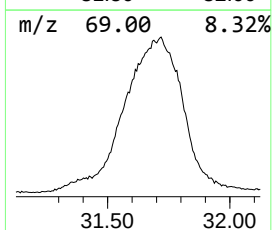
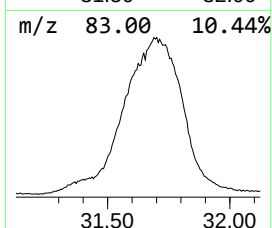
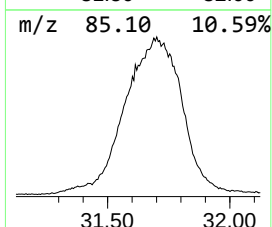
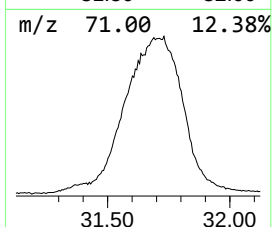
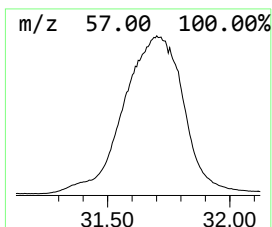
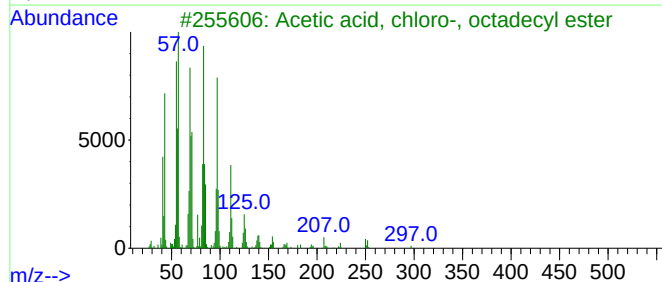
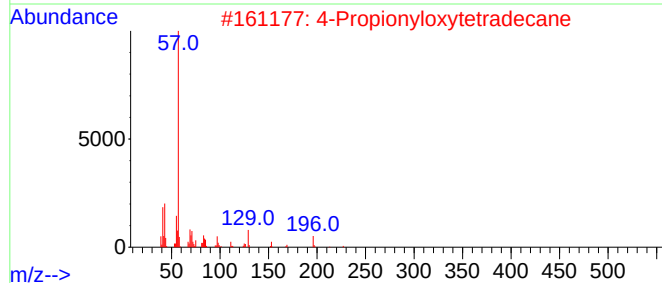
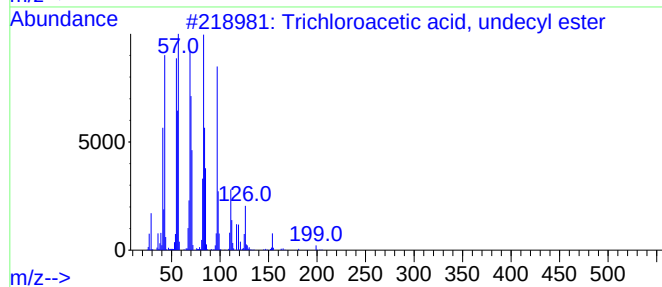
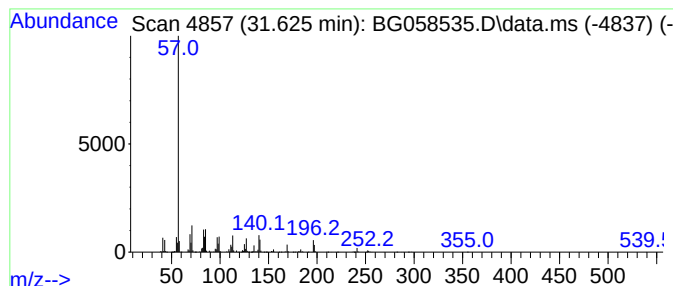
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 Trichloroacetic acid, undec... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
31.625	104.65 ng	5396190	Perylene-d12	24.521

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, undecyl ester	316	C13H23Cl3O2	074339-49-4	50
2			4-Propionyloxytetradecane	270	C17H34O2	1000245-62-9	47
3			Acetic acid, chloro-, octadecyl ...	346	C20H39ClO2	005348-82-3	46
4			Carbonic acid, decyl tetradecyl ...	398	C25H50O3	1010383-16-3	38
5			1-Nonen-3-ol	142	C9H18O	021964-44-3	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072823\
Data File : BG058535.D
Acq On : 29 Jul 2023 2:36
Operator : MA/JU
Sample : 03642-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
EFF-WW

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.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
Hexadecane	14.357	31.3	ng	1395860	3	14.463	890988	20.0
Tridecane, 5-pr...	14.803	111.3	ng	4960290	3	14.463	890988	20.0
Dodecanoic acid	15.121	1069.8	ng	47659400	3	14.463	890988	20.0
1-Octanol, 5,7,...	16.390	223.8	ng	9272830	4	17.212	828747	20.0
Hexanoic acid, ...	16.443	385.0	ng	15952100	4	17.212	828747	20.0
Carbonic acid, ...	16.490	317.6	ng	13161500	4	17.212	828747	20.0
Tetradecanoic acid	16.642	75.2	ng	3114690	4	17.212	828747	20.0
Heptafluorobuty...	16.730	28.9	ng	1196210	4	17.212	828747	20.0
1-Dodecanol, 2-...	16.983	317.5	ng	13156200	4	17.212	828747	20.0
n-Hexadecanoic ...	18.111	73.2	ng	3034220	4	17.212	828747	20.0
unknown19.022	19.022	46.0	ng	1905100	4	17.212	828747	20.0
Octadecanoic acid	19.386	35.9	ng	2211450	5	21.448	1232940	20.0
Benzoic acid, t...	19.715	26.9	ng	1656880	5	21.448	1232940	20.0
Benzoic acid, u...	20.267	29.3	ng	1807680	5	21.448	1232940	20.0
12-Hydroxystear...	20.479	39.6	ng	2442850	5	21.448	1232940	20.0
Benzoic acid, t...	20.779	26.5	ng	1634200	5	21.448	1232940	20.0
Oxirane, [(dode...	21.114	44.9	ng	2766290	5	21.448	1232940	20.0
2-Hexyldecyl pr...	26.748	653.3	ng	33687100	6	24.521	1031260	20.0
1-Decanol, 2-he...	30.032	602.8	ng	31081300	6	24.521	1031260	20.0
Trichloroacetic...	31.625	104.7	ng	5396190	6	24.521	1031260	20.0