

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG073123\
 Data File : BG058550.D
 Acq On : 31 Jul 2023 19:32
 Operator : MA/JU
 Sample : 03742-05
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 B-P33B

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: BG058550.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.384	385	391	404	rBV	534744	845115	42.67%	6.617%
2	6.983	655	663	679	rBV	540970	938329	47.37%	7.347%
3	7.811	797	804	812	rBV	180545	307430	15.52%	2.407%
4	8.974	994	1002	1021	rBV	284868	531160	26.82%	4.159%
5	10.614	1272	1281	1295	rBV	245105	449576	22.70%	3.520%
6	13.081	1694	1701	1717	rBV	780471	1266027	63.92%	9.913%
7	14.327	1905	1913	1922	rBV3	15755	31090	1.57%	0.243%
8	14.462	1929	1936	1945	rVB	407787	648503	32.74%	5.078%
9	15.196	2055	2061	2067	rBV	178586	250688	12.66%	1.963%
10	15.948	2183	2189	2211	rBV	650071	1036999	52.35%	8.120%
11	17.206	2396	2403	2415	rBV	518386	799435	40.36%	6.260%
12	18.093	2550	2554	2565	rBV2	68117	126107	6.37%	0.987%
13	19.004	2705	2709	2716	rBV	71562	99912	5.04%	0.782%
14	19.262	2745	2753	2758	rBV	171530	249741	12.61%	1.955%
15	19.380	2768	2773	2781	rBV3	41537	75896	3.83%	0.594%
16	19.503	2789	2794	2803	rBV	486614	586265	29.60%	4.590%
17	19.597	2806	2810	2814	rBV	40115	58449	2.95%	0.458%
18	19.820	2843	2848	2858	rVB	1451283	1980747	100.00%	15.509%
19	20.126	2897	2900	2904	rVB2	19800	20375	1.03%	0.160%
20	20.619	2981	2984	2987	rVV	19931	23309	1.18%	0.183%
21	20.996	3046	3048	3055	rVB3	26876	34641	1.75%	0.271%
22	21.330	3101	3105	3112	rVB	153548	209507	10.58%	1.640%
23	21.442	3118	3124	3136	rBV2	489964	835845	42.20%	6.545%
24	22.194	3250	3252	3259	rVB3	20518	29811	1.51%	0.233%
25	22.553	3308	3313	3321	rVB	113454	191684	9.68%	1.501%
26	23.610	3489	3493	3500	rVB3	37393	69105	3.49%	0.541%
27	24.515	3637	3647	3662	rVB	337286	954689	48.20%	7.475%
28	25.567	3820	3826	3834	rVB3	44018	120915	6.10%	0.947%

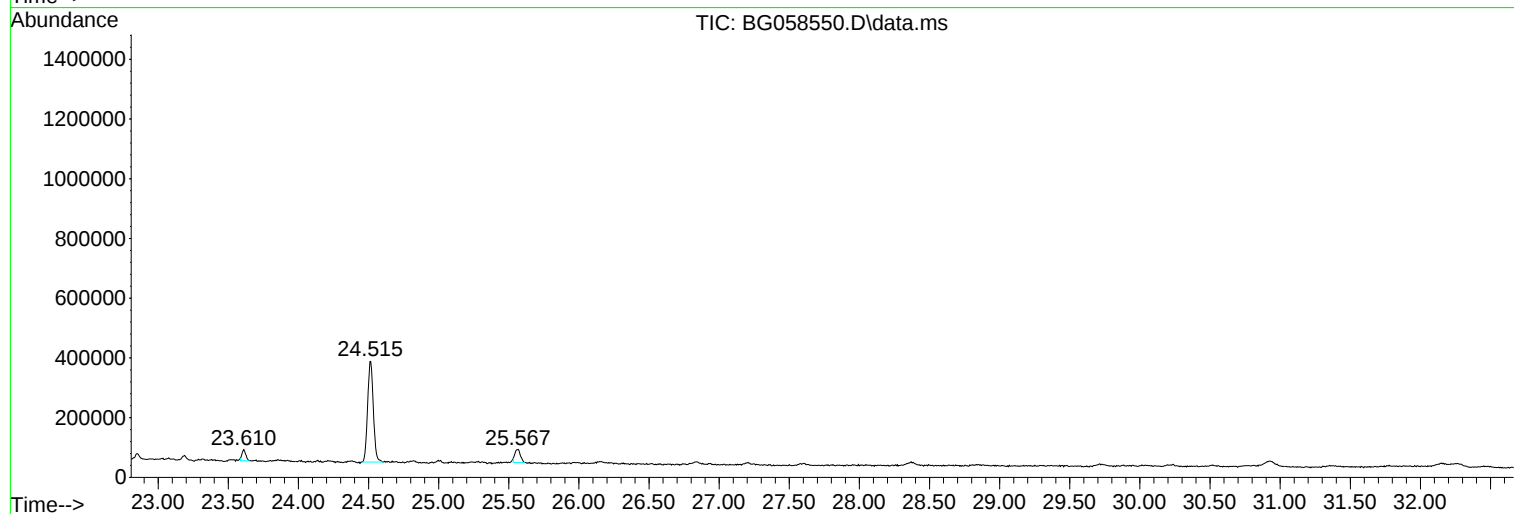
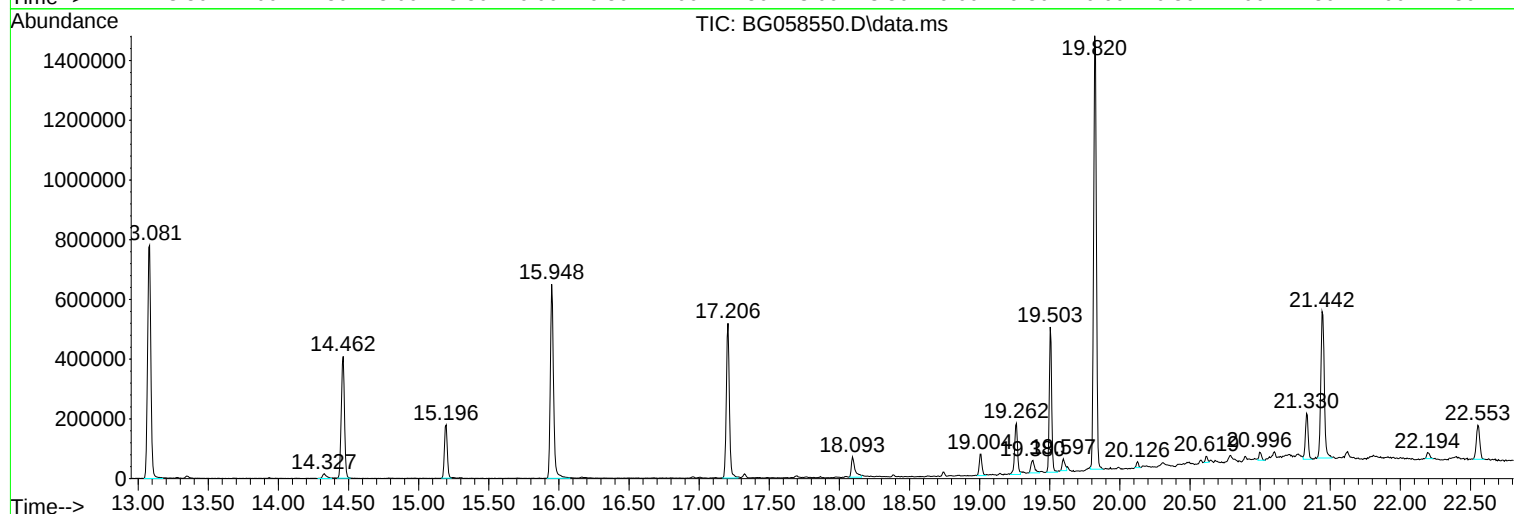
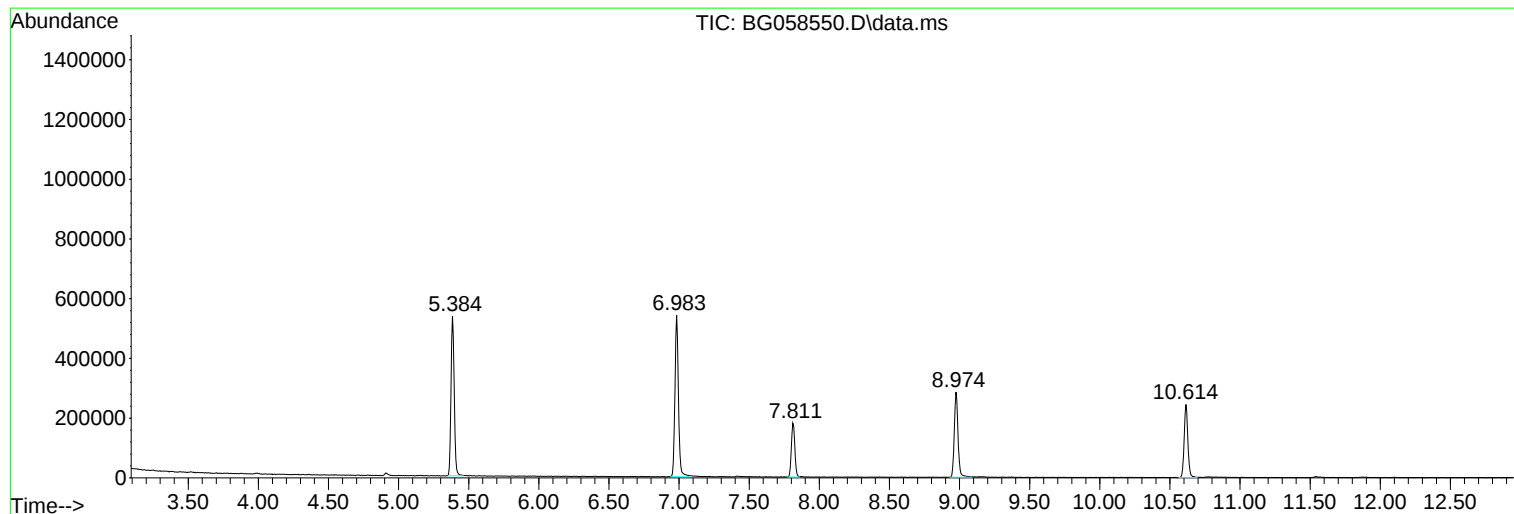
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Instrument :
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ClientSampleId :
B-P33B

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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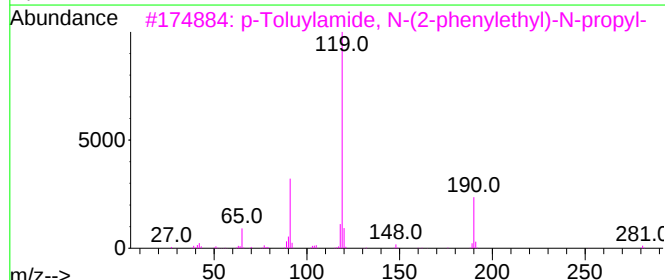
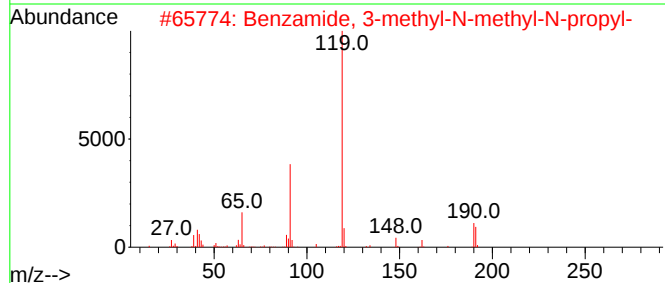
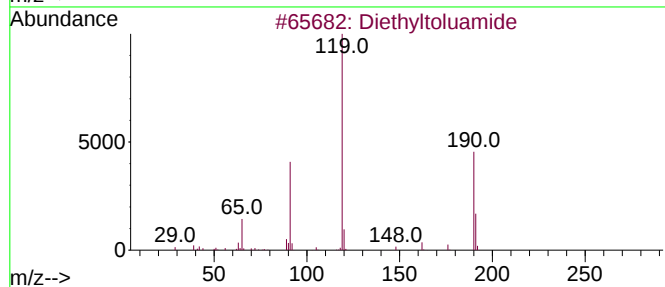
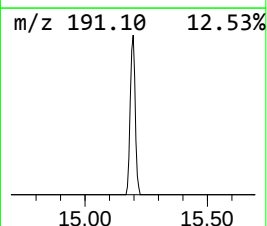
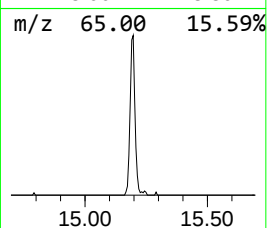
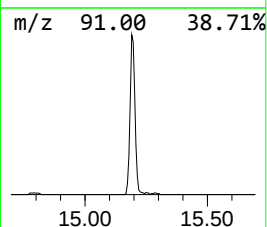
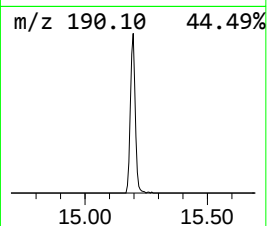
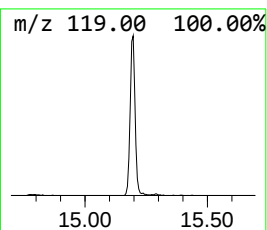
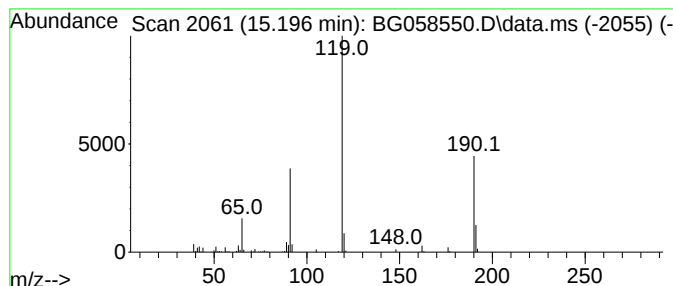
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Diethyltoluamide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.196	7.73 ng	250688	Acenaphthene-d10	14.462

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diethyltoluamide	191	C12H17NO	000134-62-3	96
2			Benzamide, 3-methyl-N-methyl-N-p...	191	C12H17NO	1000421-46-2	89
3			p-Toluyamide, N-(2-phenylethyl)...	281	C19H23NO	1000451-68-4	83
4			Benzamide, N,N-diethyl-4-methyl-	191	C12H17NO	002728-05-4	76
5			Benzamide, 3-methyl-N-butyl-	191	C12H17NO	1000407-41-1	76



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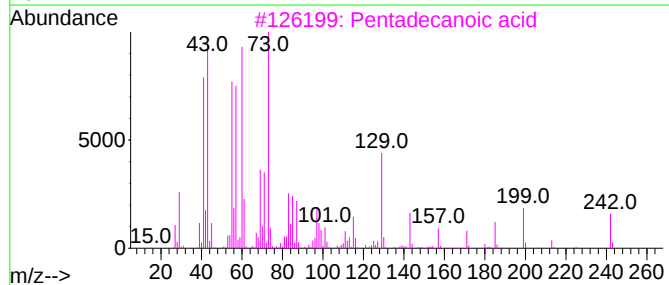
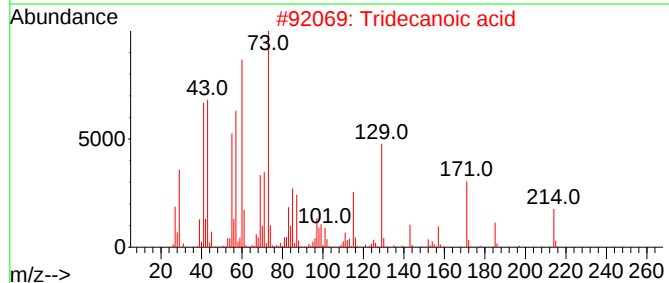
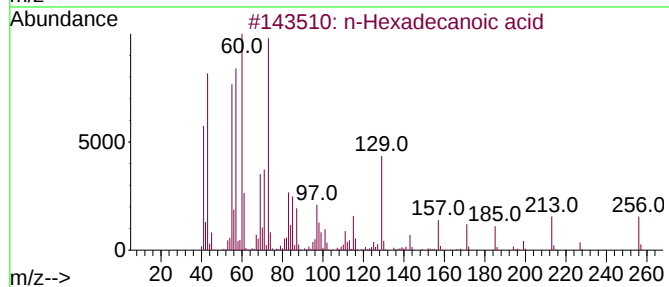
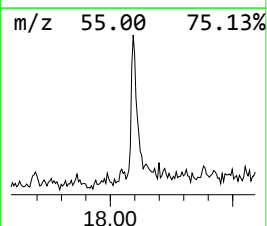
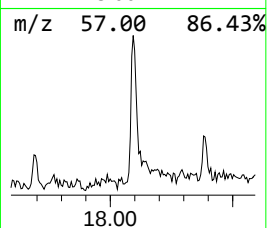
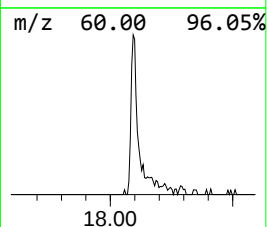
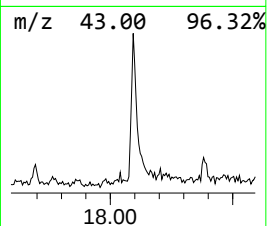
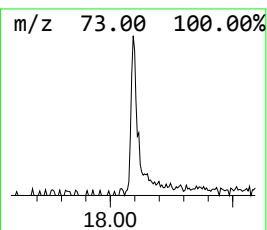
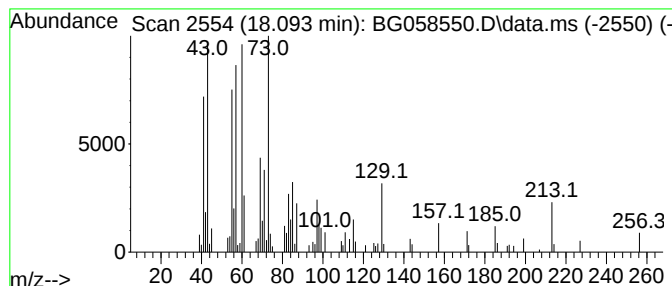
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.093	3.15 ng	126107	Phenanthrene-d10	17.206

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5			Undecanoic acid	186	C11H22O2	000112-37-8	62



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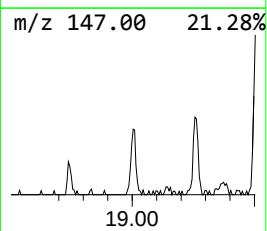
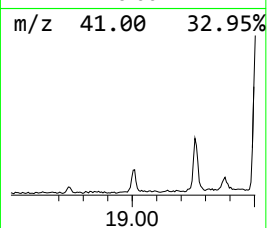
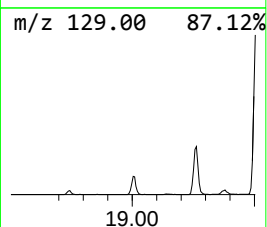
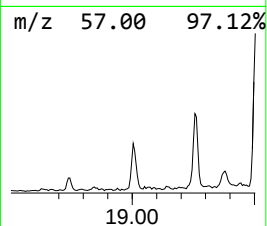
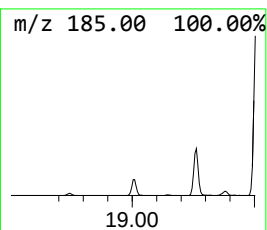
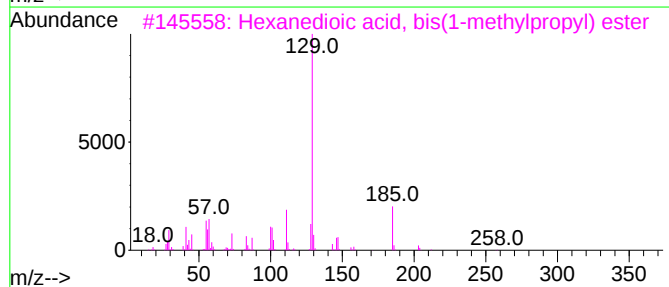
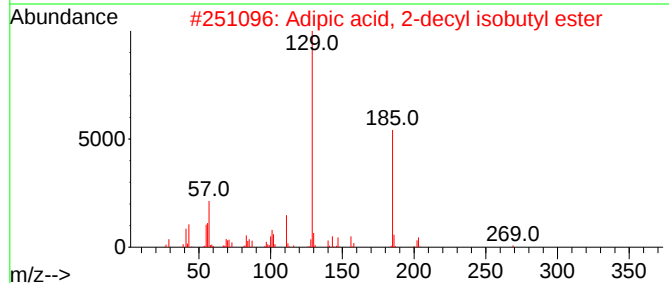
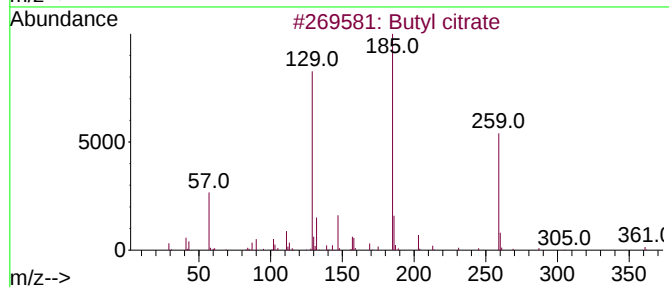
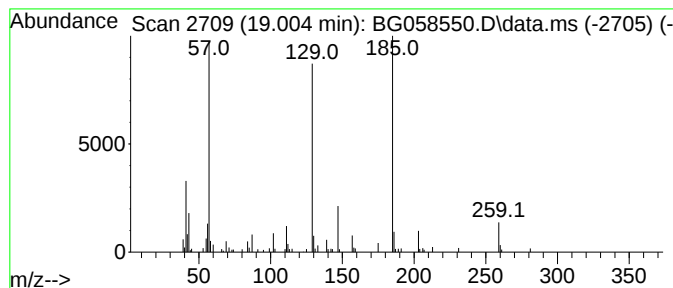
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Butyl citrate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.004	2.50 ng	99912	Phenanthrene-d10	17.206

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butyl citrate	360	C18H32O7	000077-94-1	72
2			Adipic acid, 2-decyl isobutyl ester	342	C20H38O4	1000353-59-6	64
3			Hexanedioic acid, bis(1-methylpr...	258	C14H26O4	038447-22-2	64
4			Hexanedioic acid, bis(2-methylpr...	258	C14H26O4	000141-04-8	59
5			Adipic acid, butyl 2,4-dimethylp...	300	C17H32O4	1000349-77-7	53



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Misc :
ALS Vial : 15 Sample Multiplier: 1

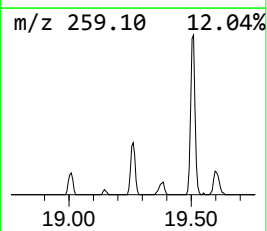
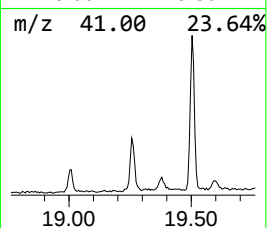
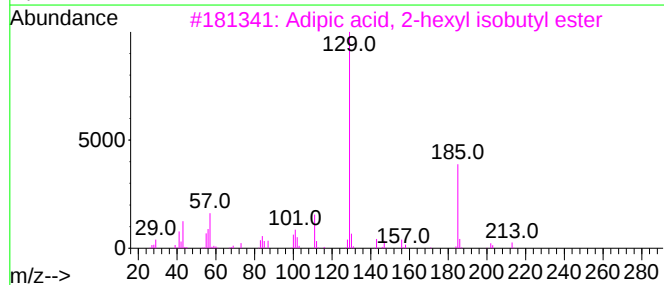
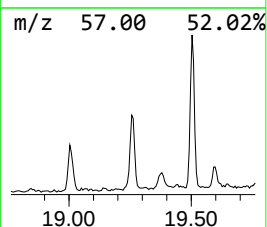
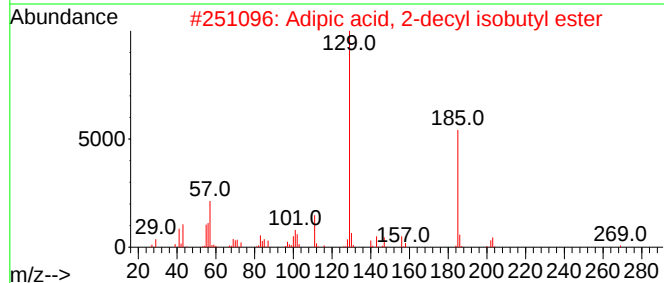
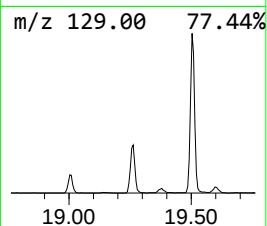
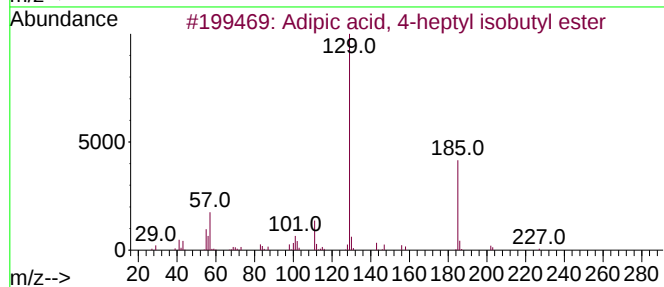
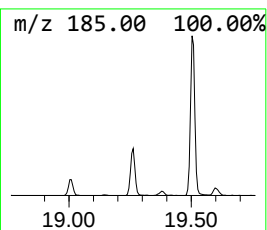
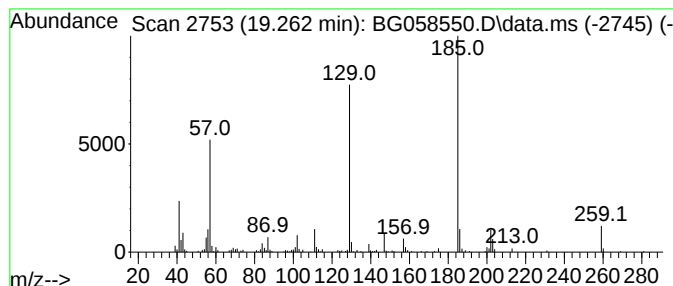
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Adipic acid, 4-heptyl isobu... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.262	6.25 ng	249741	Phenanthrene-d10	17.206	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Adipic acid, 4-heptyl isobutyl e...	300	C17H32O4	1000349-73-6	86
2	Adipic acid, 2-decyl isobutyl ester	342	C20H38O4	1000353-59-6	78
3	Adipic acid, 2-hexyl isobutyl ester	286	C16H30O4	1000353-70-9	78
4	Butyl citrate	360	C18H32O7	000077-94-1	68
5	Adipic acid, 2-heptyl isobutyl e...	300	C17H32O4	1000353-64-3	64



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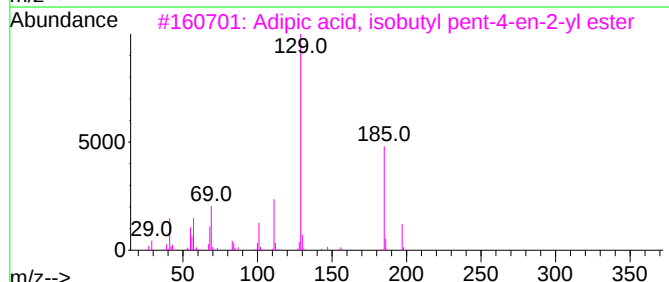
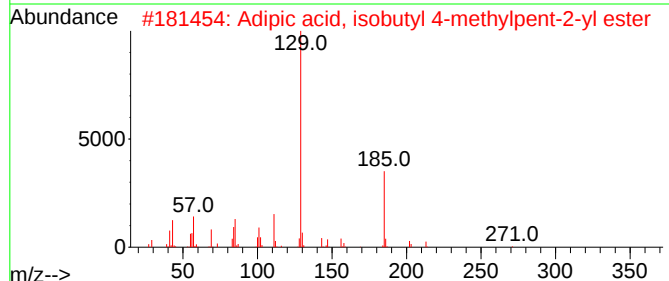
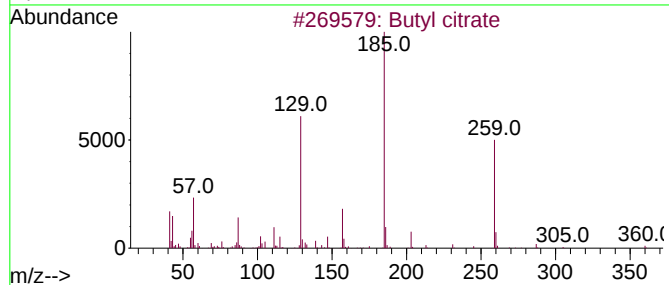
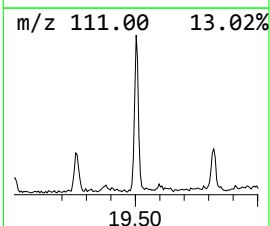
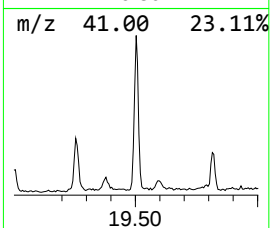
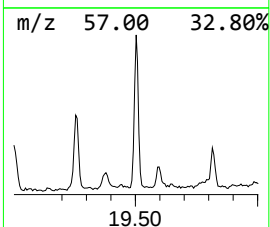
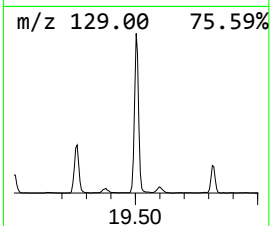
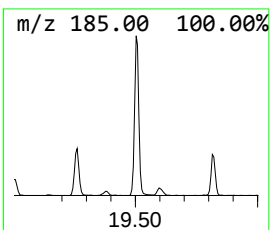
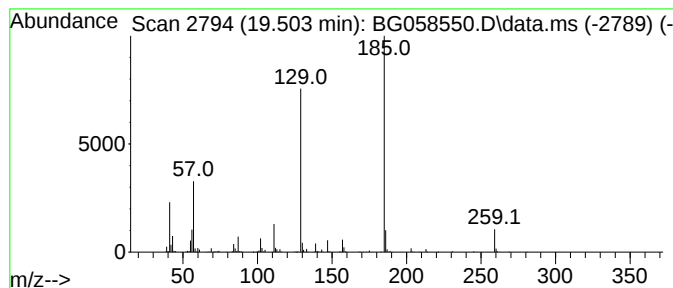
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Adipic acid, isobutyl 4-met... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.503	14.03 ng	586265	Chrysene-d12	21.442

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butyl citrate	360	C18H32O7	000077-94-1	83
2			Adipic acid, isobutyl 4-methylpe...	286	C16H30O4	1000353-50-1	64
3			Adipic acid, isobutyl pent-4-en-...	270	C15H26O4	1000354-11-8	56
4			Adipic acid, 3-heptyl isobutyl e...	300	C17H32O4	1000353-64-8	53
5			Adipic acid, butyl 2-octyl ester	314	C18H34O4	1010324-44-6	50



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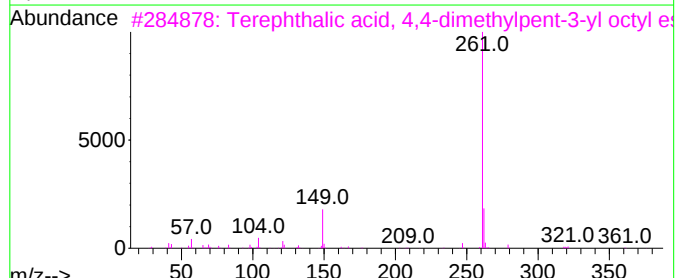
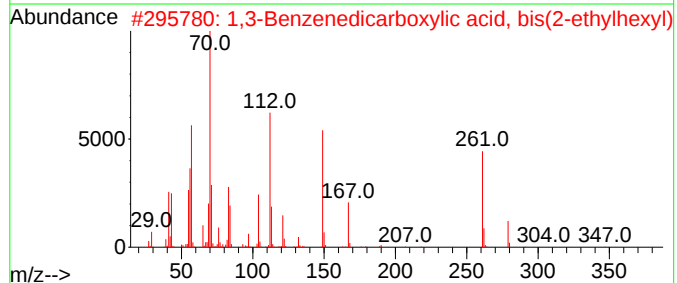
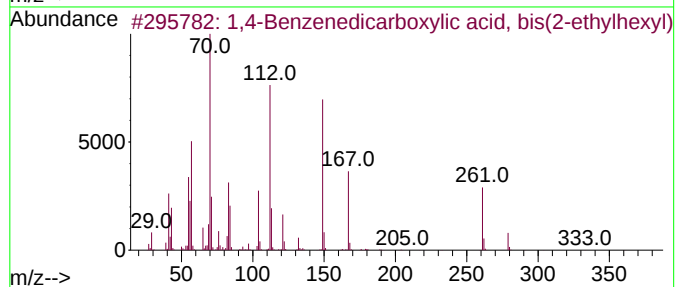
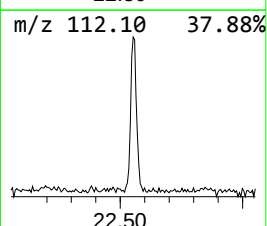
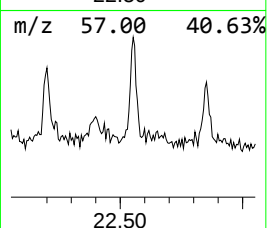
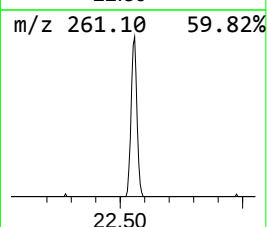
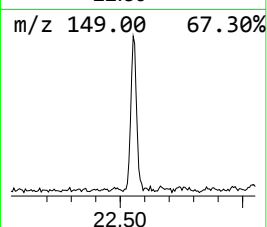
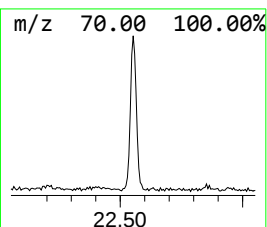
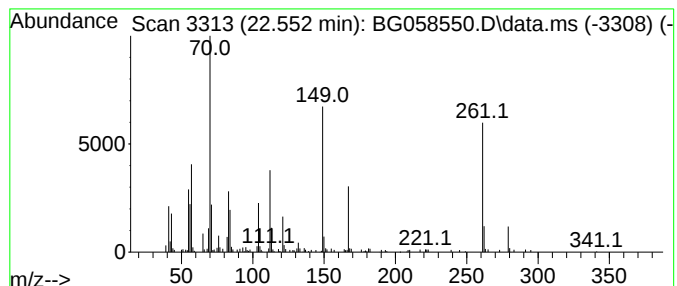
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1,4-Benzenedicarboxylic aci... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.552	4.59 ng	191684	Chrysene-d12	21.442

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	81
2			1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	49
3			Terephthalic acid, 4,4-dimethylp...	376	C23H36O4	1000415-97-1	35
4			Terephthalic acid, octyl 2,3,4-t...	408	C22H23F3O4	1010415-80-4	35
5			Terephthalic acid, 4-octyl octyl...	390	C24H38O4	1000323-73-7	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG073123\
Data File : BG058550.D
Acq On : 31 Jul 2023 19:32
Operator : MA/JU
Sample : 03742-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
B-P33B

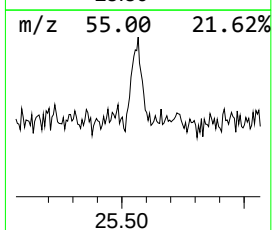
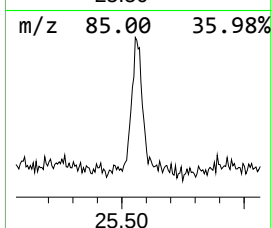
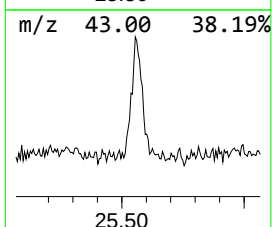
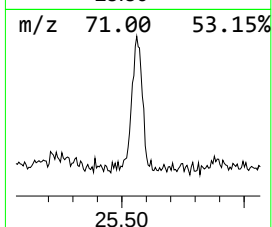
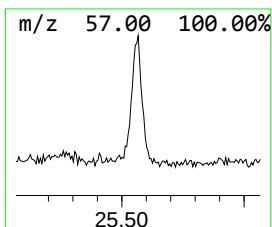
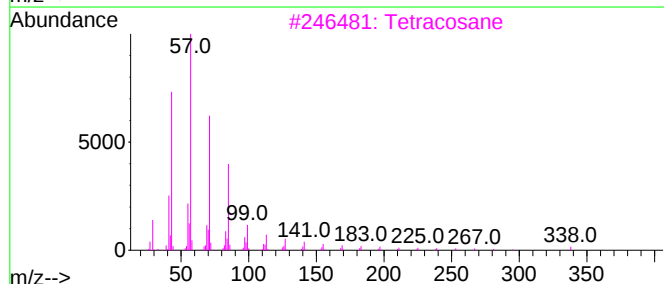
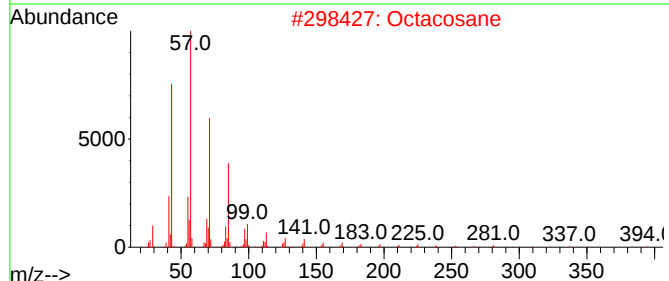
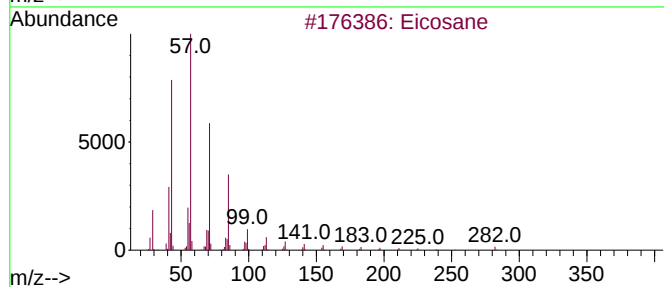
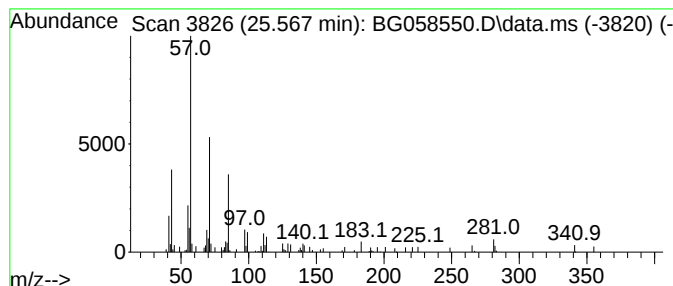
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.567	2.53 ng	120915	Perylene-d12	24.509

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane			282	C20H42	000112-95-8	83
2	Octacosane			394	C28H58	000630-02-4	80
3	Tetracosane			338	C24H50	000646-31-1	72
4	Hexadecane			226	C16H34	000544-76-3	64
5	triacontane			422	C30H62	000638-68-6	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG073123\
Data File : BG058550.D
Acq On : 31 Jul 2023 19:32
Operator : MA/JU
Sample : 03742-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
B-P33B

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
Diethyltoluamide	15.196	7.7	ng	250688	3	14.462	648503	20.0
n-Hexadecanoic ...	18.093	3.1	ng	126107	4	17.206	799435	20.0
Butyl citrate	19.004	2.5	ng	99912	4	17.206	799435	20.0
Adipic acid, 4-...	19.262	6.3	ng	249741	4	17.206	799435	20.0
Adipic acid, is...	19.503	14.0	ng	586265	5	21.442	835845	20.0
1,4-Benzenedica...	22.552	4.6	ng	191684	5	21.442	835845	20.0
Eicosane	25.567	2.5	ng	120915	6	24.509	954689	20.0