

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080123\
 Data File : BG058561.D
 Acq On : 1 Aug 2023 13:58
 Operator : MA/JU
 Sample : 03769-10
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 B-P40B

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: BG058561.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.386	384	391	403	rBV	637925	1021858	43.16%	6.652%
2	6.984	655	663	675	rBV	643624	1106163	46.72%	7.201%
3	7.812	797	804	813	rBV	201931	337325	14.25%	2.196%
4	8.976	994	1002	1020	rBV	356983	656632	27.74%	4.275%
5	10.615	1272	1281	1291	rBV	274267	506141	21.38%	3.295%
6	13.083	1690	1701	1711	rBV	998400	1612963	68.13%	10.500%
7	13.911	1836	1842	1852	rBV	75946	119625	5.05%	0.779%
8	14.463	1929	1936	1946	rVB	454159	726076	30.67%	4.727%
9	15.198	2055	2061	2066	rBV	49992	67115	2.83%	0.437%
10	15.950	2182	2189	2208	rBV	924708	1461619	61.74%	9.515%
11	16.954	2355	2360	2364	rBV	30055	39330	1.66%	0.256%
12	17.007	2364	2369	2374	rVB2	18347	29906	1.26%	0.195%
13	17.207	2396	2403	2409	rBV	566098	863578	36.48%	5.622%
14	17.695	2481	2486	2493	rVB	40338	49399	2.09%	0.322%
15	18.094	2549	2554	2569	rBV	263963	461231	19.48%	3.003%
16	18.388	2599	2604	2609	rBV	37971	54948	2.32%	0.358%
17	19.017	2706	2711	2716	rBV2	46637	67385	2.85%	0.439%
18	19.258	2745	2752	2759	rBV2	77760	148251	6.26%	0.965%
19	19.369	2767	2771	2782	rBV2	89209	155047	6.55%	1.009%
20	19.504	2790	2794	2800	rVB	148195	171352	7.24%	1.115%
21	19.593	2806	2809	2813	rBV2	41853	53930	2.28%	0.351%
22	19.628	2813	2815	2820	rVB3	22914	27639	1.17%	0.180%
23	19.828	2843	2849	2857	rVB	1737235	2367399	100.00%	15.412%
24	20.127	2896	2900	2905	rVB	45401	47980	2.03%	0.312%
25	20.615	2980	2983	2987	rBV2	35694	41002	1.73%	0.267%
26	21.108	3062	3067	3088	rVB3	103821	448875	18.96%	2.922%
27	21.332	3101	3105	3111	rVB	184774	250159	10.57%	1.629%
28	21.443	3118	3124	3139	rVB	521226	918855	38.81%	5.982%
29	22.201	3248	3253	3257	rBV	50190	76456	3.23%	0.498%
30	22.554	3309	3313	3324	rVB	130910	220415	9.31%	1.435%
31	23.611	3489	3493	3502	rVB2	54246	110782	4.68%	0.721%
32	24.516	3638	3647	3659	rVB	368721	1024619	43.28%	6.670%
33	25.568	3821	3826	3836	rVB4	42949	117105	4.95%	0.762%

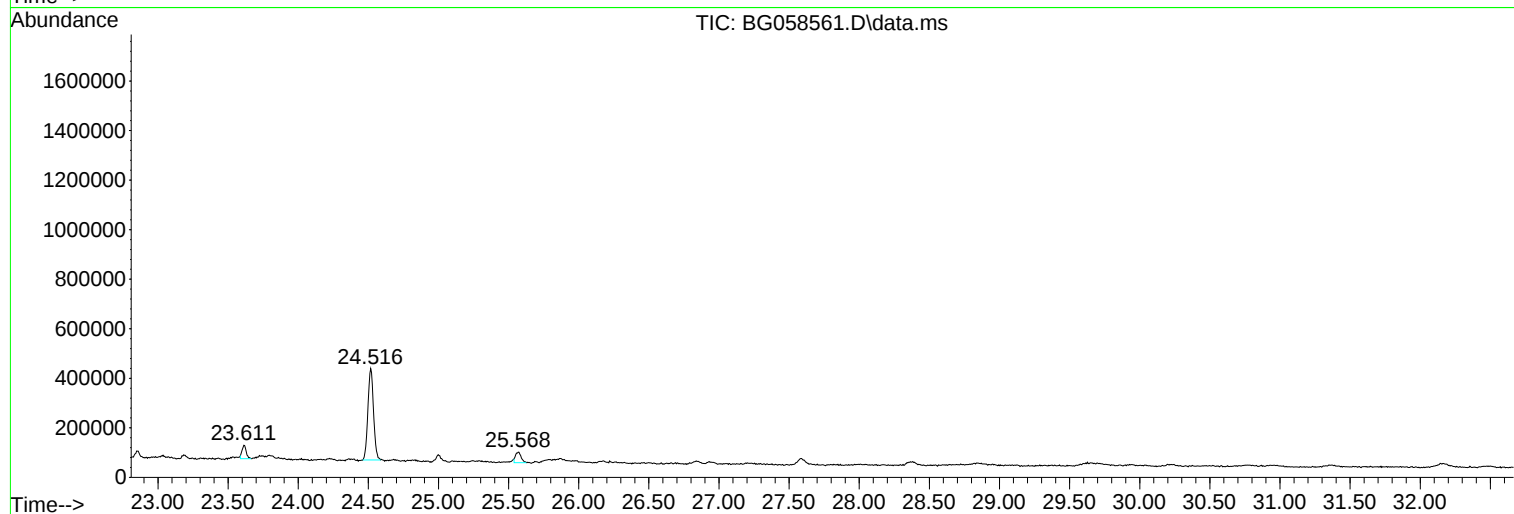
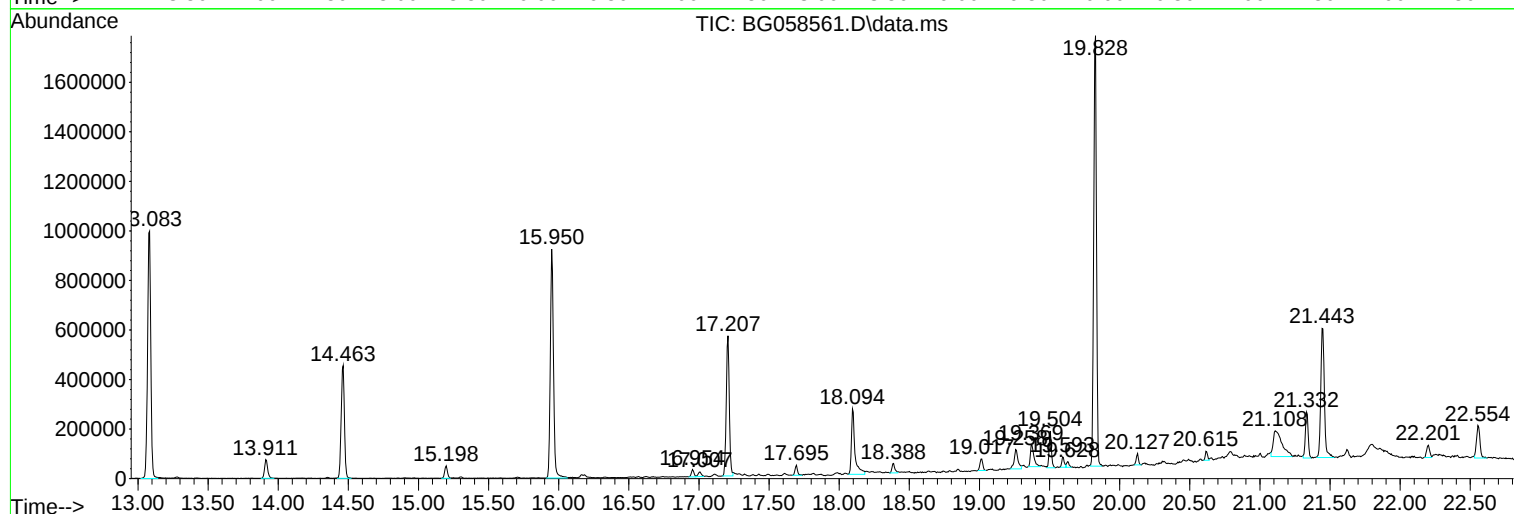
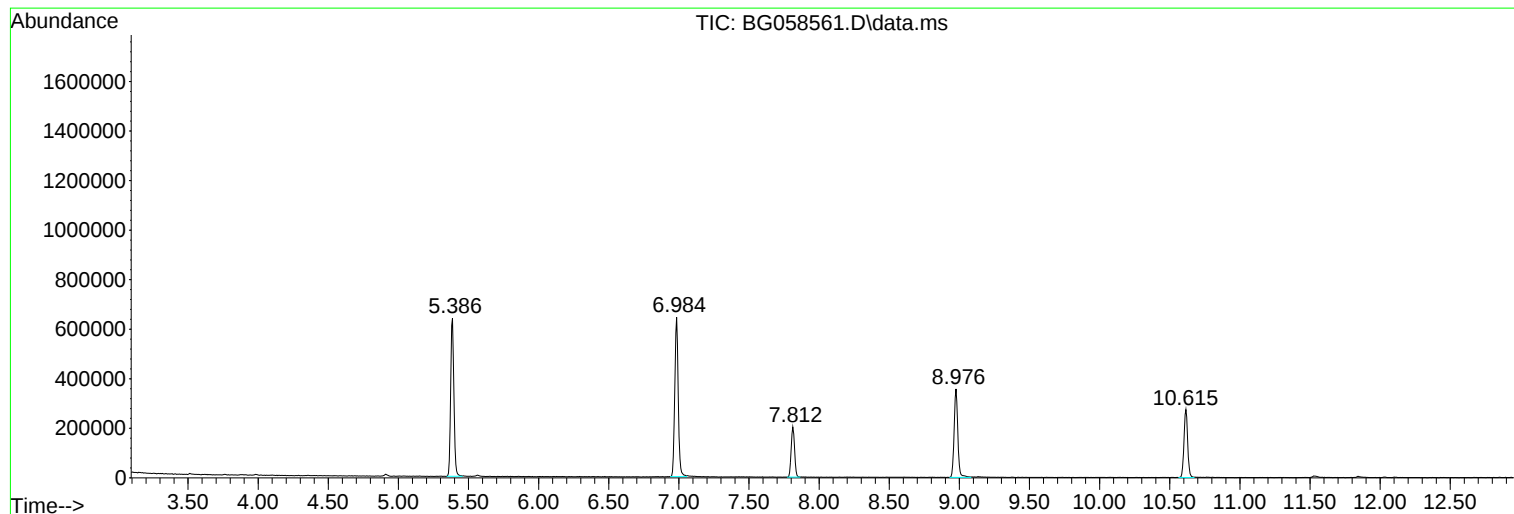
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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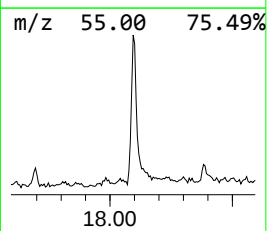
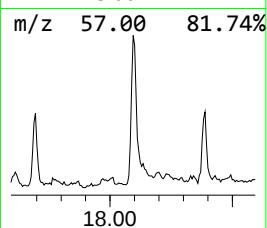
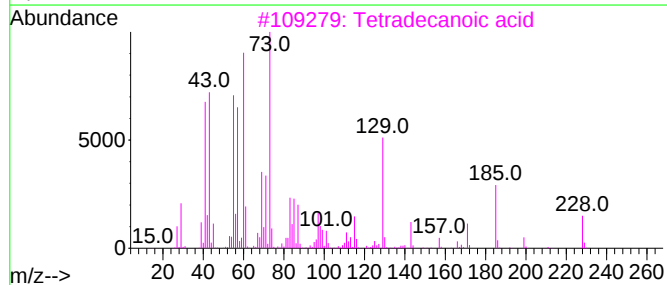
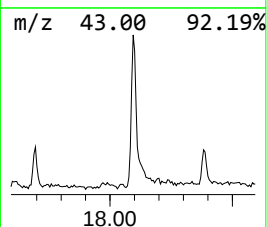
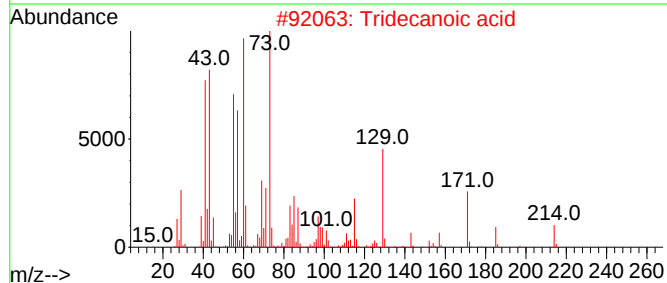
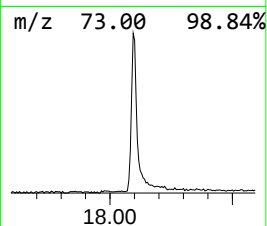
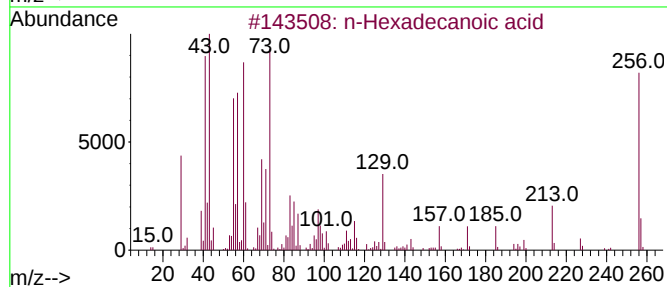
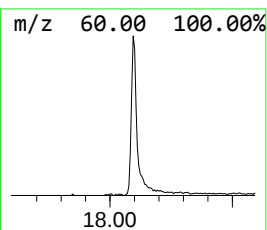
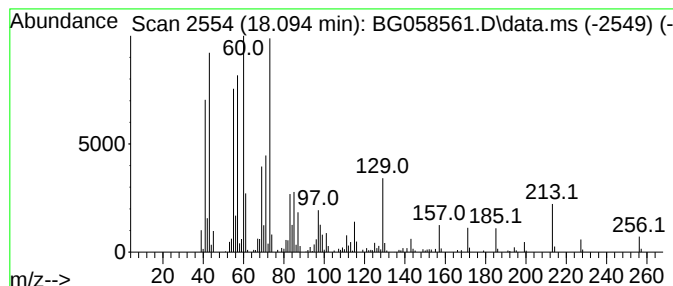
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.094	10.68 ng	461231	Phenanthrene-d10	17.207

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	89
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	76
5			Undecanoic acid	186	C11H22O2	000112-37-8	68



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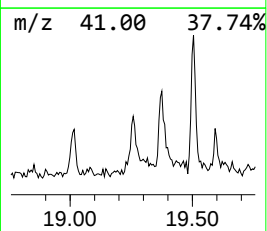
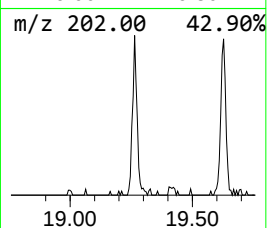
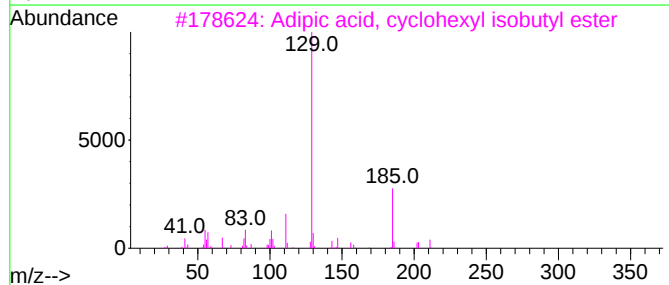
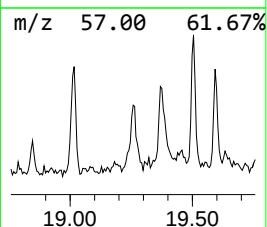
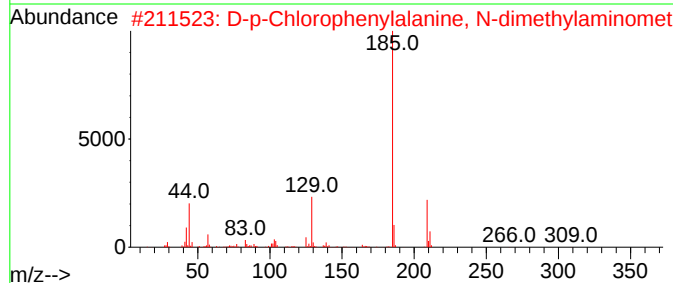
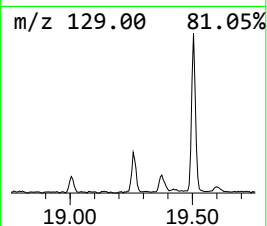
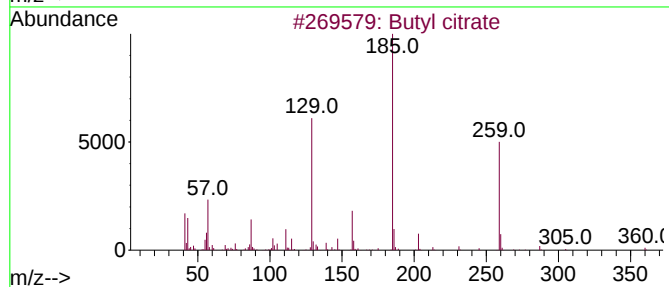
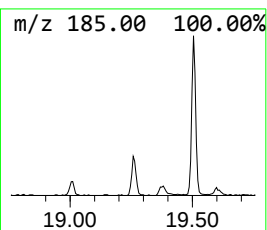
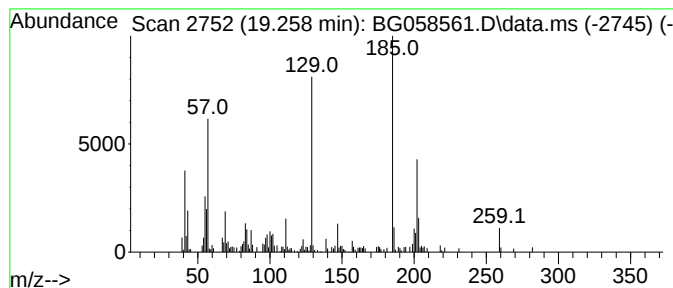
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Butyl citrate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.258	3.43 ng	148251	Phenanthrene-d10	17.207

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butyl citrate	360	C18H32O7	000077-94-1	59
2			D-p-Chlorophenylalanine, N-dimet...	310	C16H23ClN2O2	1000375-82-2	47
3			Adipic acid, cyclohexyl isobutyl...	284	C16H28O4	1000324-25-8	35
4			2-([Dimethylamino)methylene]ami...	382	C20H31ClN2O3	1000378-74-1	27
5			Adipic acid, 2-hexyl isobutyl ester	286	C16H30O4	1000353-70-9	27



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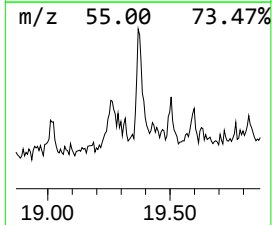
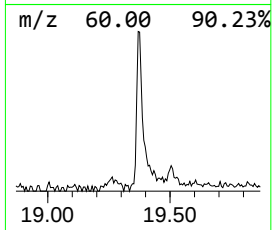
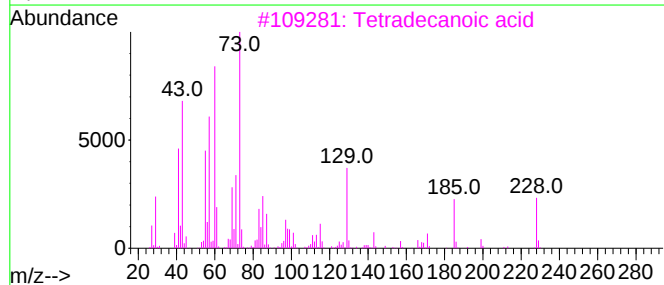
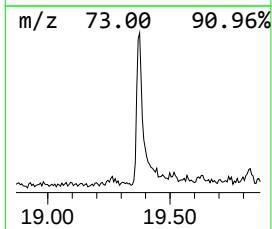
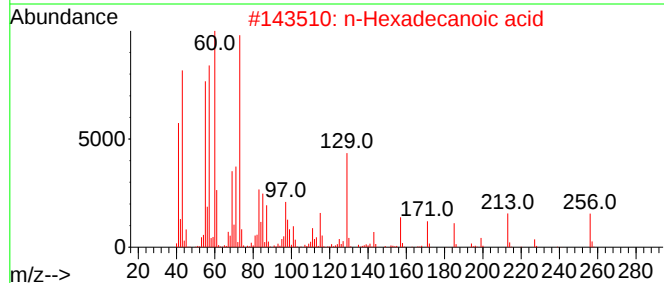
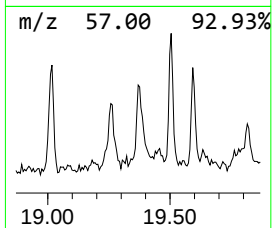
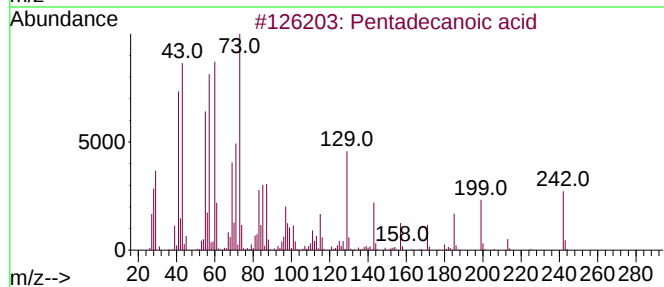
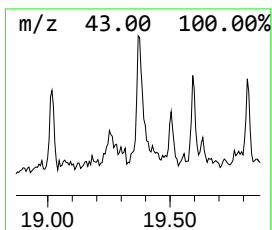
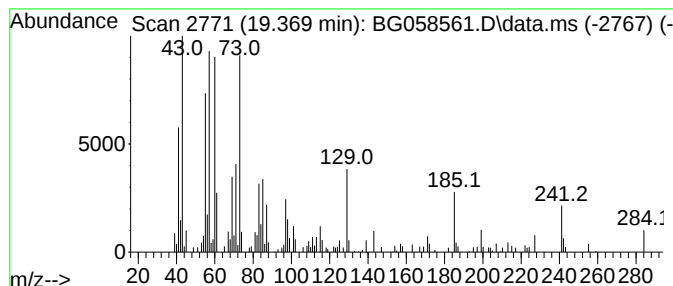
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Pentadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.369	3.37 ng	155047	Chrysene-d12	21.443

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecanoic acid	242	C15H30O2	001002-84-2	89
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	80
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4			n-Decanoic acid	172	C10H20O2	000334-48-5	70
5			Dodecanoic acid	200	C12H24O2	000143-07-7	64



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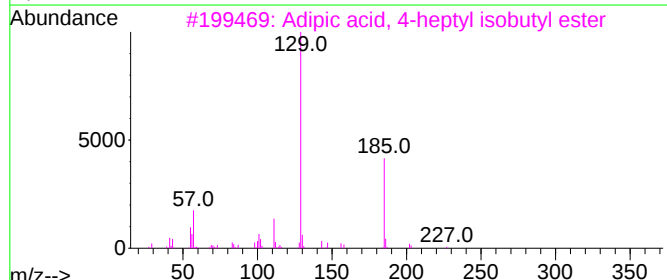
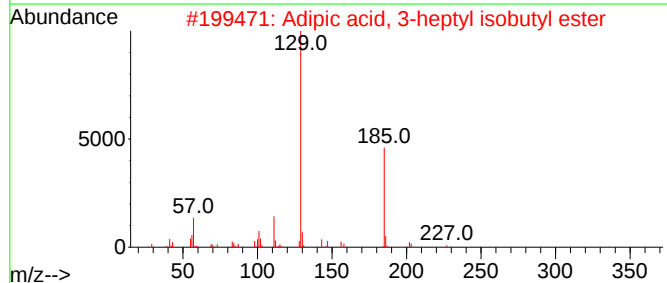
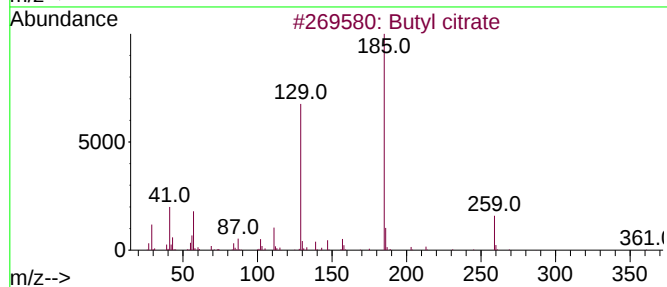
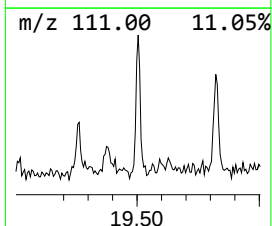
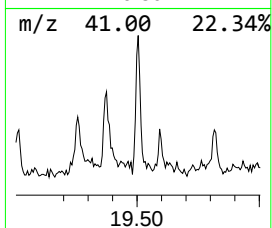
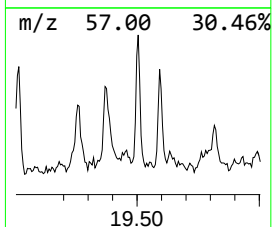
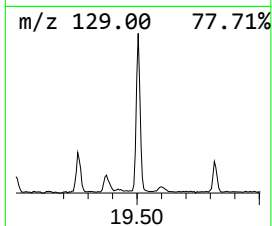
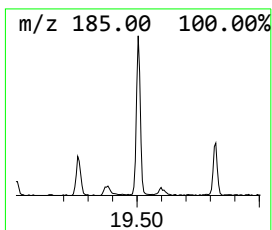
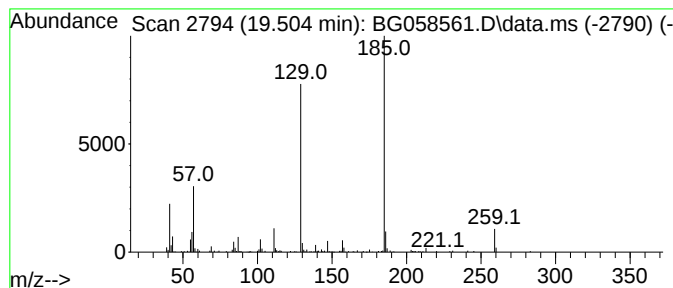
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Peak Number 4 Adipic acid, 3-heptyl isobu... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.504	3.73 ng	171352	Chrysene-d12	21.443

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butyl citrate	360	C18H32O7	000077-94-1	81
2			Adipic acid, 3-heptyl isobutyl e...	300	C17H32O4	1000353-64-8	78
3			Adipic acid, 4-heptyl isobutyl e...	300	C17H32O4	1000349-73-6	78
4			Adipic acid, 3,3-dimethylbut-2-y...	286	C16H30O4	1000353-66-7	64
5			Adipic acid, butyl 3-pentyl ester	272	C15H28O4	1000324-60-5	64



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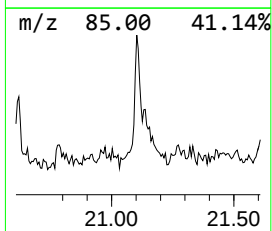
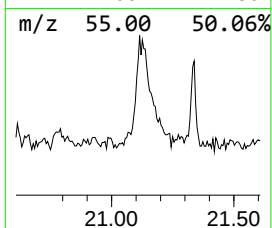
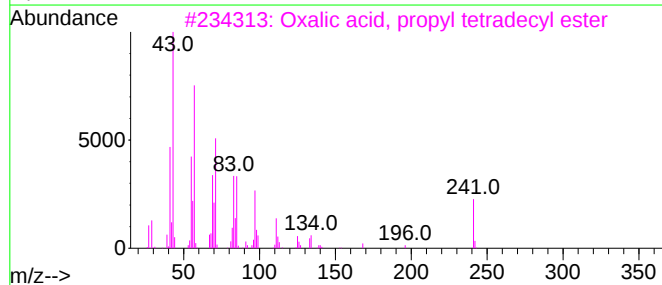
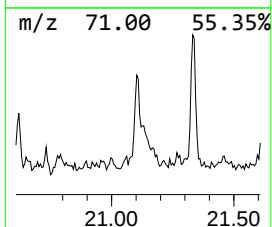
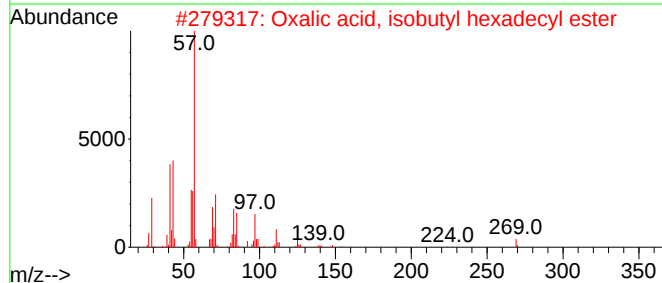
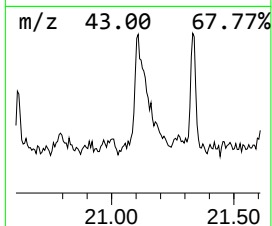
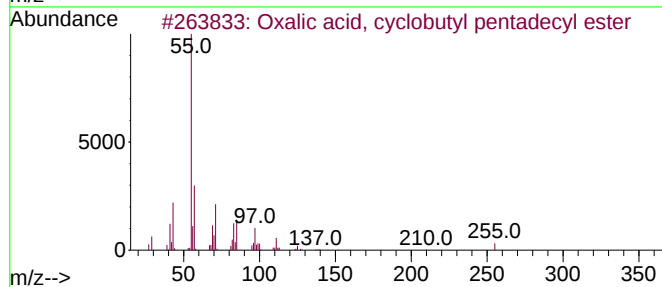
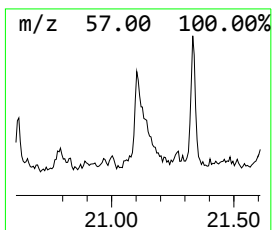
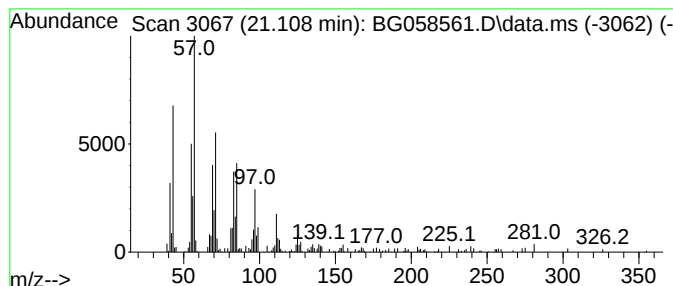
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Peak Number 5 Oxalic acid, cyclobutyl pen... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.108	9.77 ng	448875	Chrysene-d12	21.443

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxalic acid, cyclobutyl pentadec...	354	C21H38O4	1010309-70-5	91
2			Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	91
3			Oxalic acid, propyl tetradecyl e...	328	C19H36O4	1000309-26-7	91
4			Oxalic acid, isobutyl octadecyl ...	398	C24H46O4	1000309-38-3	91
5			Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	87



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ClientSampleId :
B-P40B

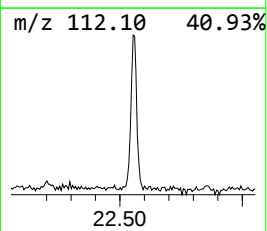
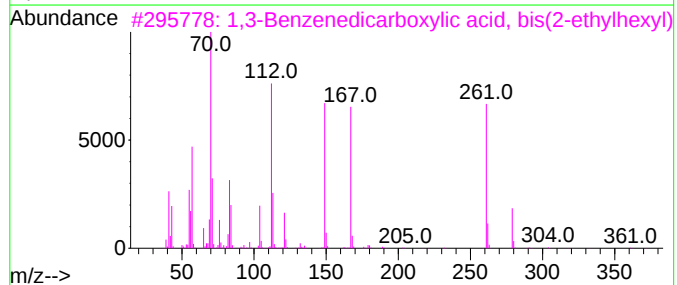
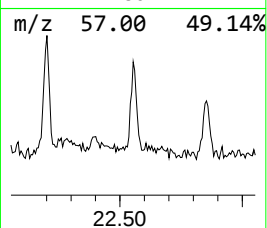
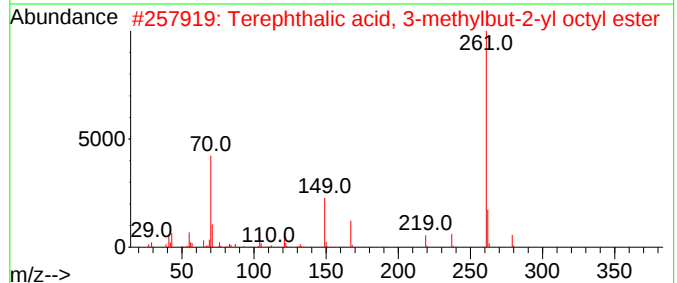
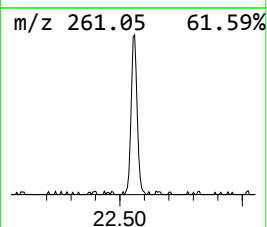
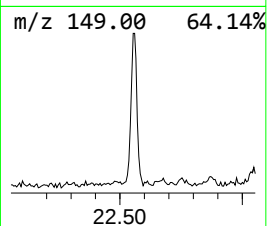
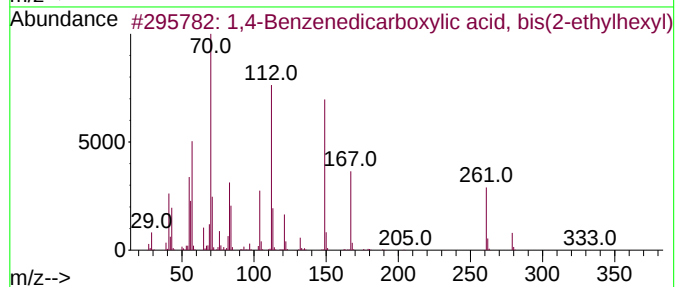
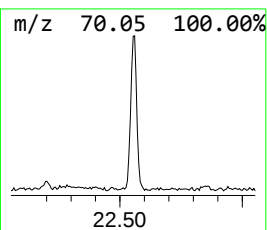
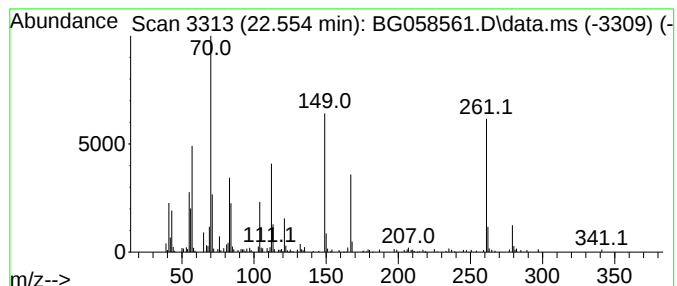
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1,4-Benzenedicarboxylic aci... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.554	4.80 ng	220415	Chrysene-d12	21.443

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	59
2			Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	59
3			1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	58
4			Terephthalic acid, monochloride,...	296	C16H21ClO3	1000324-22-9	47
5			Terephthalic acid, di(4-octyl) e...	390	C24H38O4	1000323-74-2	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080123\
Data File : BG058561.D
Acq On : 1 Aug 2023 13:58
Operator : MA/JU
Sample : 03769-10
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
B-P40B

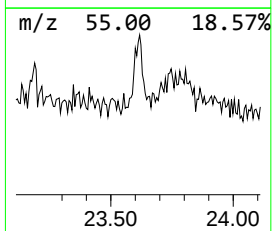
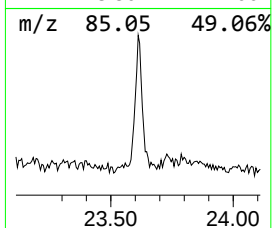
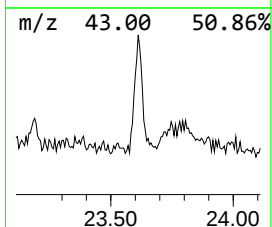
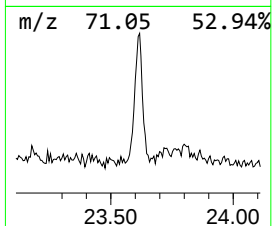
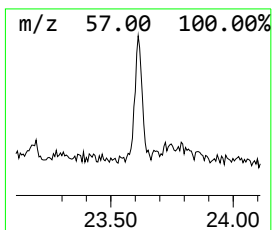
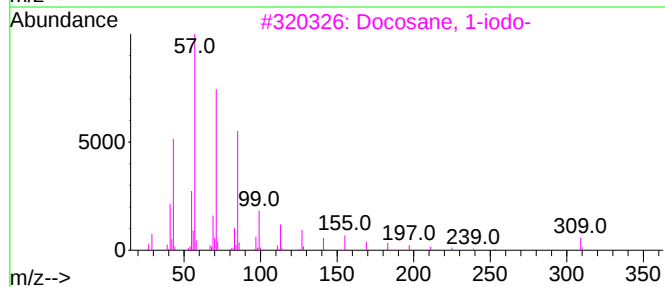
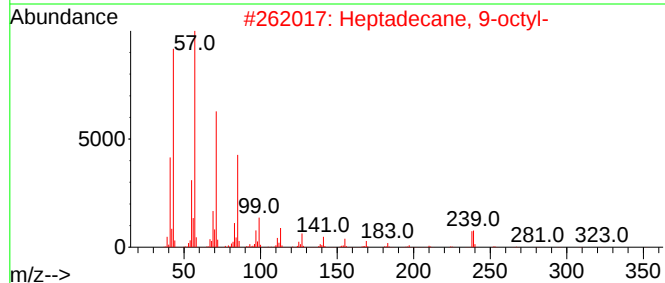
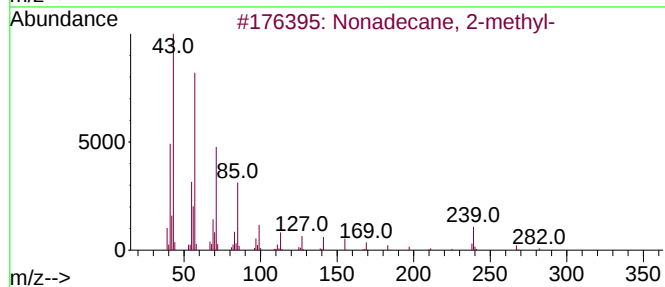
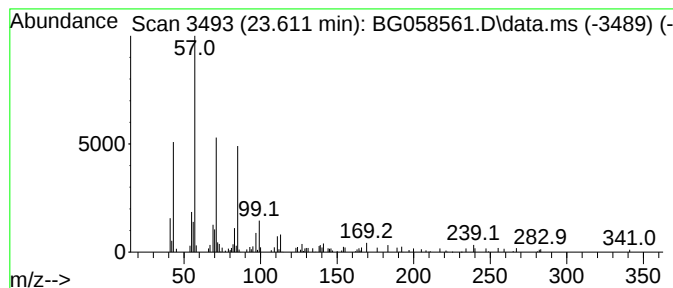
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Nonadecane, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.611	2.16 ng	110782	Perylene-d12	24.516

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane, 2-methyl-	282	C20H42	001560-86-7	87
2			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	86
3			Docosane, 1-iodo-	436	C22H45I	1000406-31-9	80
4			Dodecane, 1-iodo-	296	C12H25I	004292-19-7	80
5			Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080123\
Data File : BG058561.D
Acq On : 1 Aug 2023 13:58
Operator : MA/JU
Sample : 03769-10
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
B-P40B

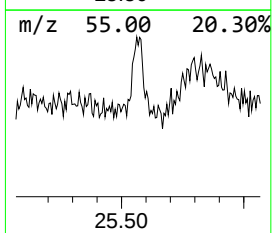
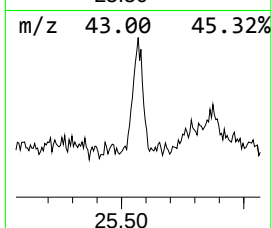
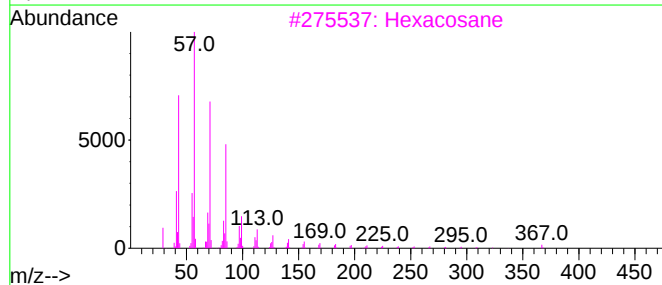
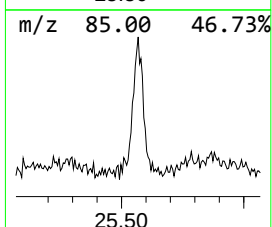
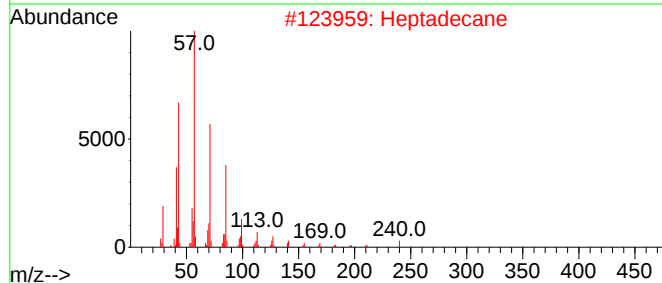
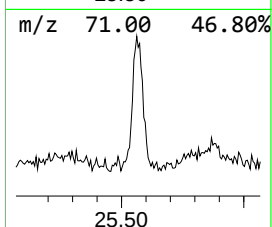
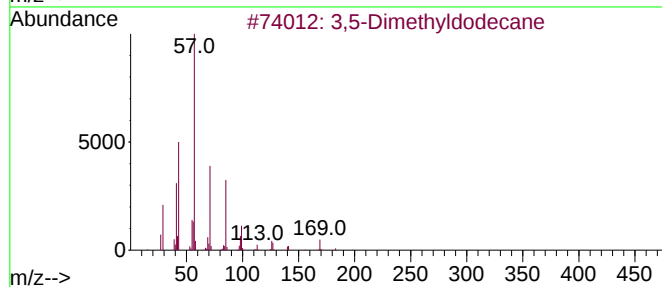
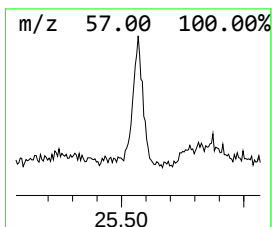
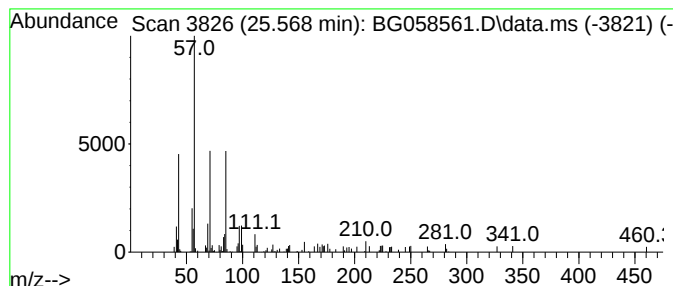
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 3,5-Dimethyldodecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.568	2.29 ng	117105	Perylene-d12	24.516

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,5-Dimethyldodecane		198	C14H30	107770-99-0	50
2	Heptadecane		240	C17H36	000629-78-7	50
3	Hexacosane		366	C26H54	000630-01-3	47
4	Hexadecane		226	C16H34	000544-76-3	47
5	Octane, 2,5-dimethyl-		142	C10H22	015869-89-3	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080123\
Data File : BG058561.D
Acq On : 1 Aug 2023 13:58
Operator : MA/JU
Sample : 03769-10
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
B-P40B

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
n-Hexadecanoic ...	18.094	10.7	ng	461231	4	17.207	863578	20.0
Butyl citrate	19.258	3.4	ng	148251	4	17.207	863578	20.0
Pentadecanoic acid	19.369	3.4	ng	155047	5	21.443	918855	20.0
Adipic acid, 3-...	19.504	3.7	ng	171352	5	21.443	918855	20.0
Oxalic acid, cy...	21.108	9.8	ng	448875	5	21.443	918855	20.0
1,4-Benzenedica...	22.554	4.8	ng	220415	5	21.443	918855	20.0
Nonadecane, 2-m...	23.611	2.2	ng	110782	6	24.516	1024620	20.0
3,5-Dimethyldod...	25.568	2.3	ng	117105	6	24.516	1024620	20.0