

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040523\
 Data File : BG056997.D
 Acq On : 5 Apr 2023 19:20
 Operator : CG/JU
 Sample : 02104-02
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 B-37-SB02

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-BG033023.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG056997.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.440	317	324	332	rVB	99001	154800	19.18%	2.640%
2	5.922	399	406	414	rBV	259487	417718	51.75%	7.124%
3	7.543	674	682	690	rBV	278872	483243	59.87%	8.242%
4	8.413	823	830	836	rBV	52462	86534	10.72%	1.476%
5	9.588	1022	1030	1037	rBV	161189	288576	35.75%	4.922%
6	11.256	1305	1314	1321	rBV2	69752	126079	15.62%	2.150%
7	13.653	1715	1722	1729	rBV	433733	657340	81.44%	11.211%
8	15.021	1949	1955	1962	rVV	124392	196301	24.32%	3.348%
9	16.361	2176	2183	2190	rBV	28139	42939	5.32%	0.732%
10	16.502	2200	2207	2219	rBV	405447	631998	78.30%	10.779%
11	17.765	2415	2422	2426	rBV	175282	256723	31.81%	4.378%
12	17.806	2426	2429	2436	rVB	39399	54792	6.79%	0.934%
13	17.900	2441	2445	2449	rVB	9527	12752	1.58%	0.217%
14	18.605	2557	2565	2574	rBV7	24230	69220	8.58%	1.181%
15	18.675	2574	2577	2585	rVB5	8883	18577	2.30%	0.317%
16	18.822	2597	2602	2610	rVB6	6849	15227	1.89%	0.260%
17	19.016	2631	2635	2640	rVB3	16051	16346	2.03%	0.279%
18	19.510	2716	2719	2726	rBV6	5099	9692	1.20%	0.165%
19	19.791	2762	2767	2772	rBV	58946	81876	10.14%	1.396%
20	19.856	2772	2778	2791	rBV4	48728	140126	17.36%	2.390%
21	20.120	2819	2823	2824	rBV3	10592	12268	1.52%	0.209%
22	20.156	2824	2829	2835	rVB	43364	65170	8.07%	1.111%
23	20.332	2853	2859	2865	rBV	638299	807135	100.00%	13.766%
24	20.602	2898	2905	2908	rBV8	11716	22135	2.74%	0.378%
25	20.632	2908	2910	2915	rVB5	9871	12039	1.49%	0.205%
26	20.778	2932	2935	2941	rVB6	7057	12092	1.50%	0.206%
27	21.113	2988	2992	2997	rVB6	8476	12245	1.52%	0.209%
28	21.307	3020	3025	3033	rVB7	25228	40603	5.03%	0.692%
29	21.648	3077	3083	3093	rBV2	89543	169917	21.05%	2.898%
30	21.748	3096	3100	3106	rVB2	39373	58926	7.30%	1.005%
31	21.918	3126	3129	3136	rVB6	10055	15897	1.97%	0.271%
32	22.083	3149	3157	3163	rBV	140721	277700	34.41%	4.736%
33	22.241	3180	3184	3189	rBV8	8453	18434	2.28%	0.314%
34	22.505	3225	3229	3235	rBV9	9695	20043	2.48%	0.342%
35	22.934	3296	3302	3314	rVB6	70256	209235	25.92%	3.569%
36	23.040	3317	3320	3327	rVB7	16602	31033	3.84%	0.529%

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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-BG033023.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	23.322	3364	3368	3373	rVB8	4411	8919	1.11%	0.152%
38	24.491	3563	3567	3571	rBV4	7067	14858	1.84%	0.253%
39	24.626	3584	3590	3602	rVB6	29403	82211	10.19%	1.402%
40	25.631	3752	3761	3772	rBV2	73433	211656	26.22%	3.610%

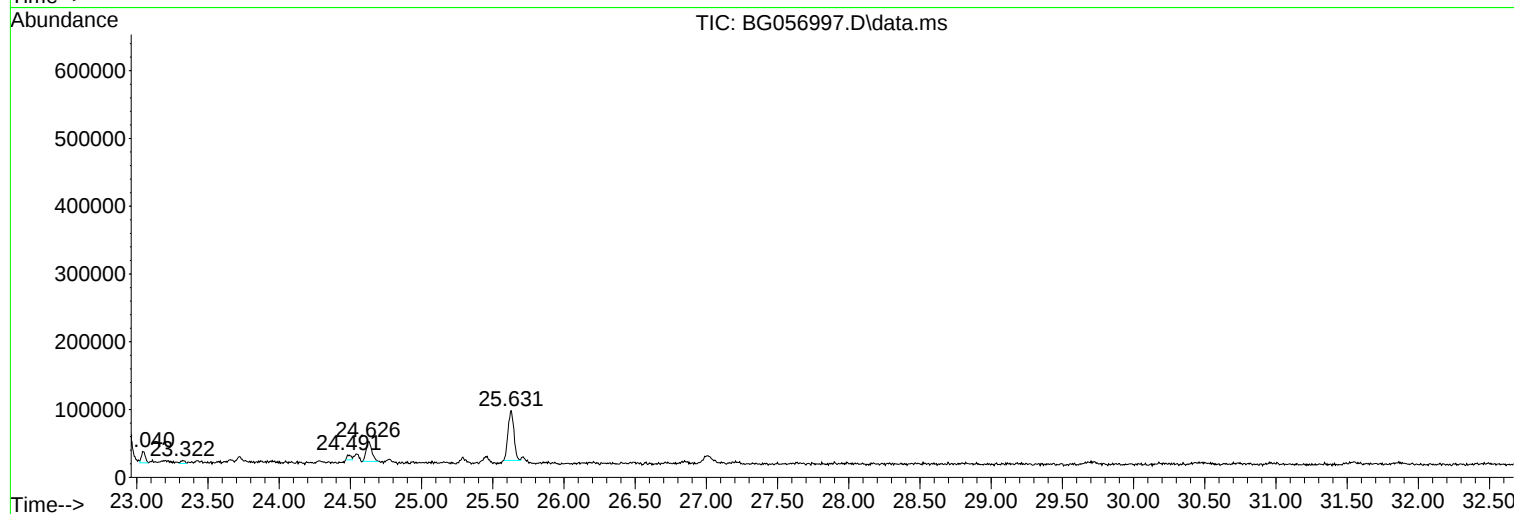
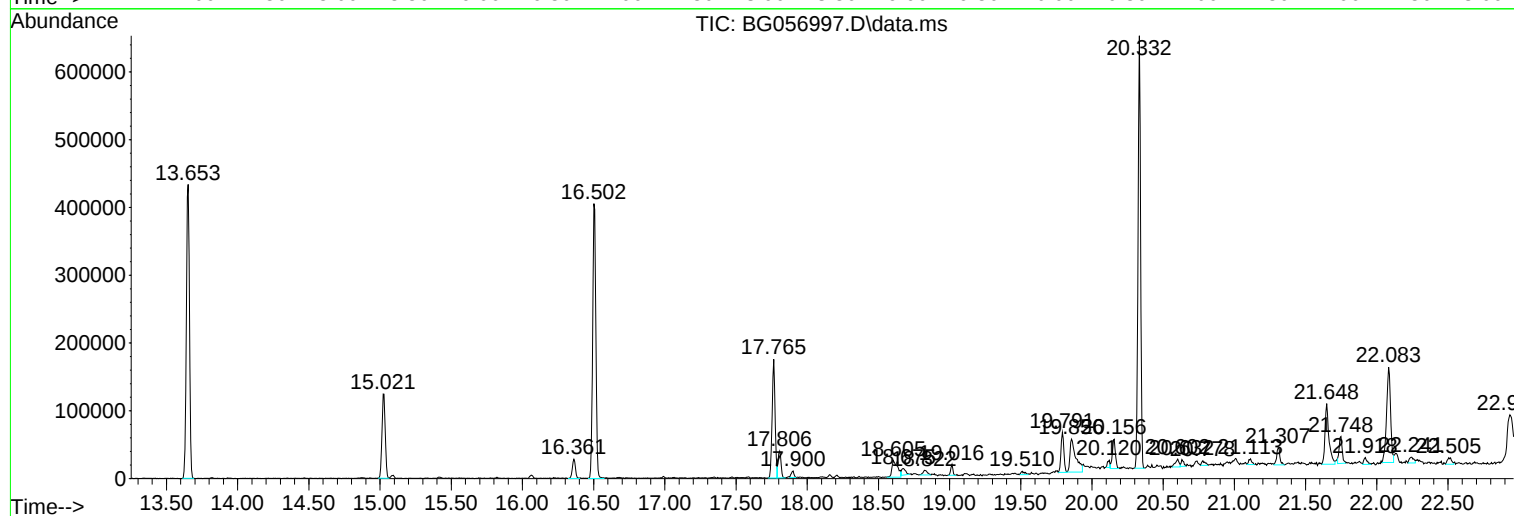
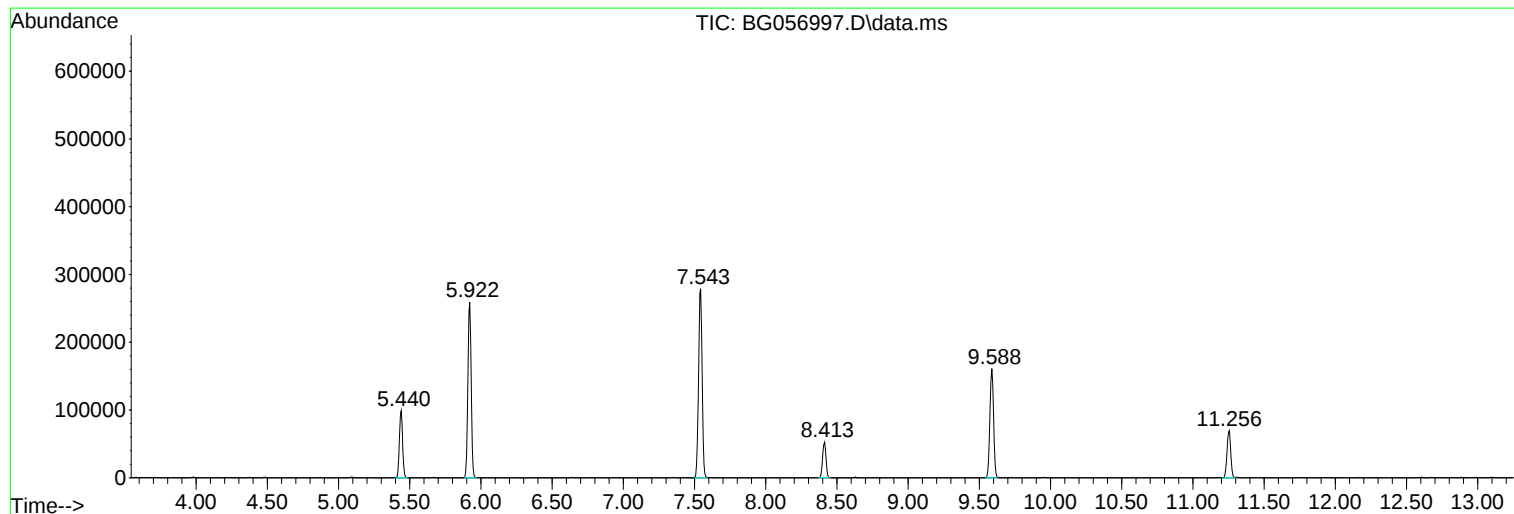
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Operator : CG/JU
Sample : 02104-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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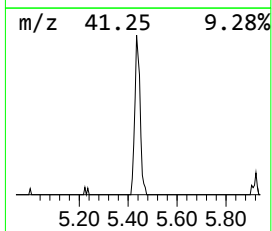
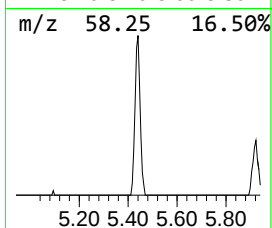
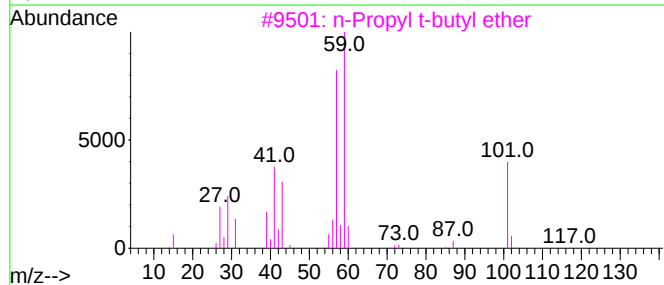
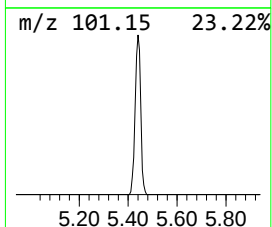
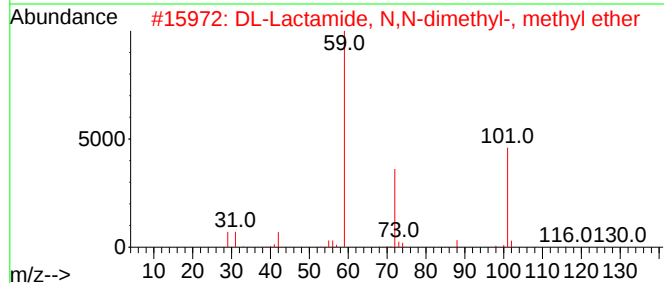
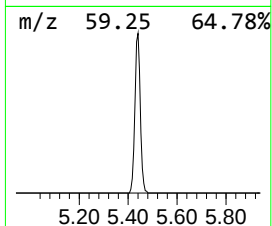
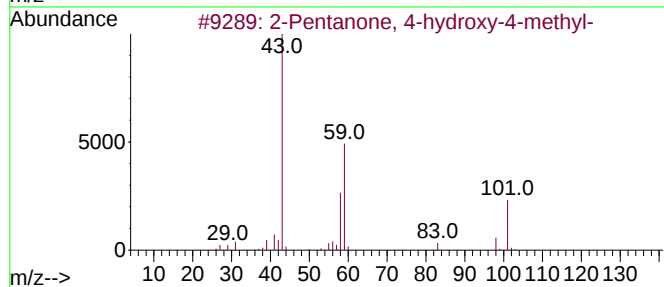
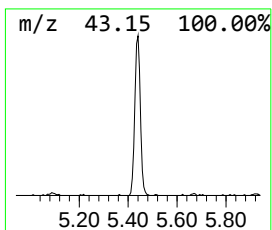
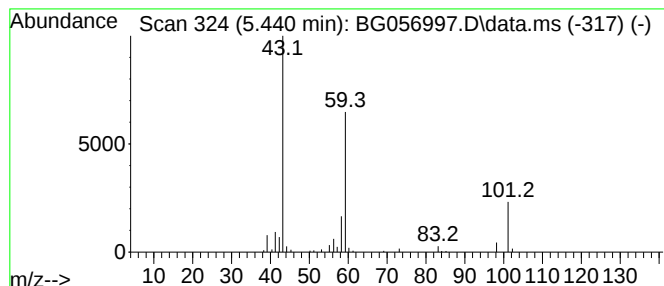
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.440	35.78 ng	154800	1,4-Dichlorobenzene-d4	8.413

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			DL-Lactamide, N,N-dimethyl-, met...	131	C6H13NO2	1000452-57-0	33
3			n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	33
4			1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	25
5			1,2-Butanediol	90	C4H10O2	000584-03-2	17



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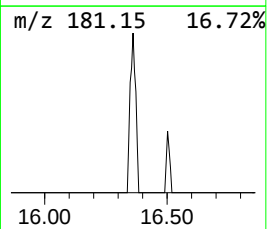
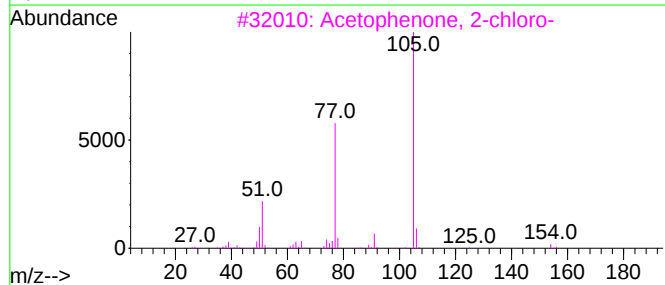
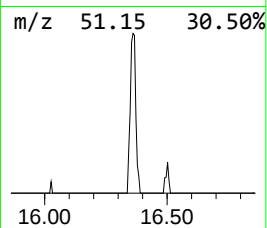
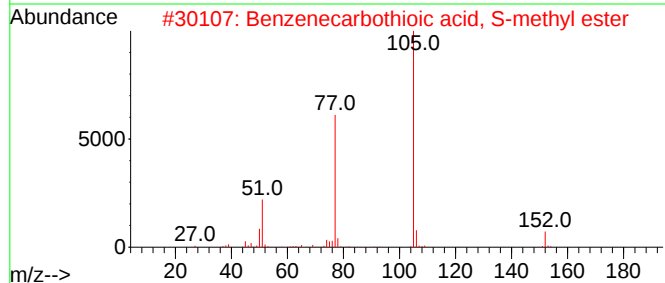
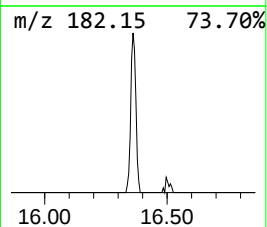
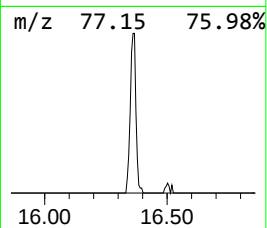
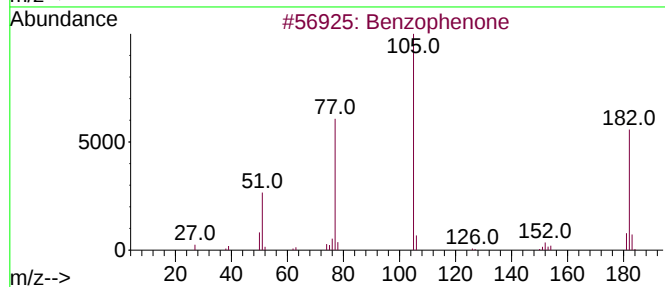
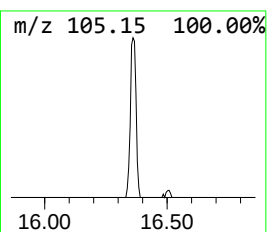
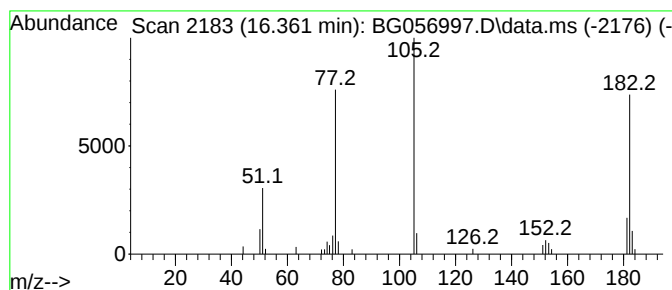
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Benzophenone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.361	4.37 ng	42939	Acenaphthene-d10	15.022

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	95
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	46
3			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	43
4			1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	38
5			2-Chloro-1-phenyl-1-propanone	168	C9H9ClO	006084-17-9	38



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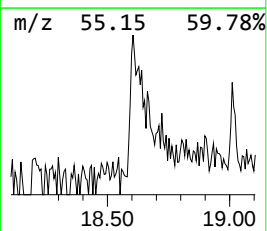
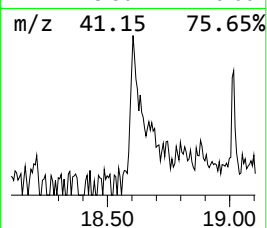
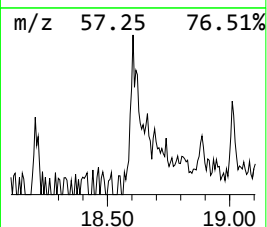
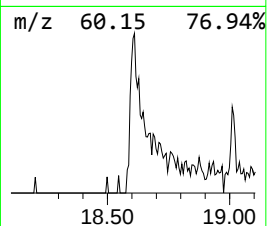
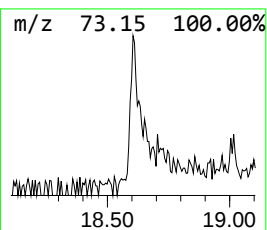
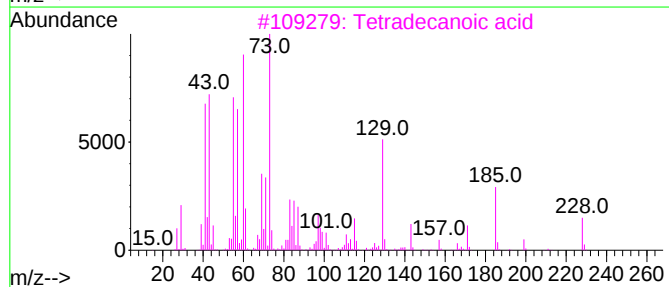
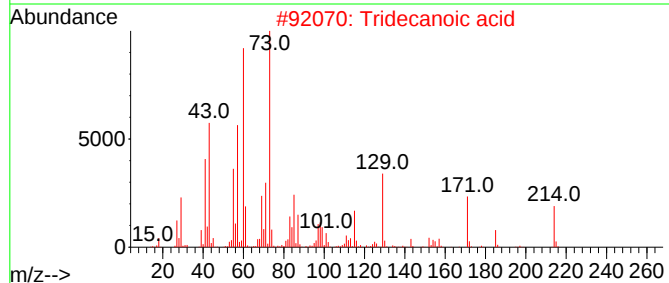
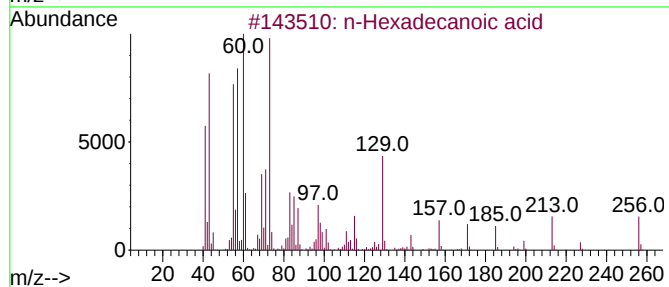
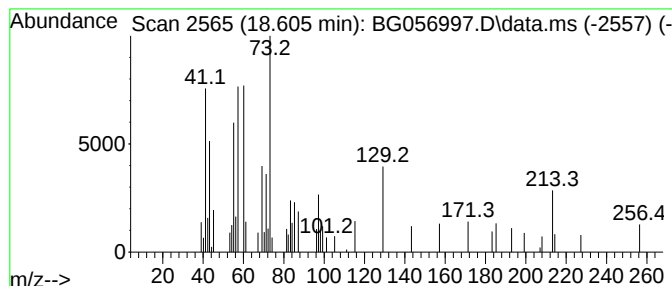
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.605	5.39 ng	69220	Phenanthrene-d10	17.765

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	76
2			Tridecanoic acid	214	C13H26O2	000638-53-9	70
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	62
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	58
5			n-Decanoic acid	172	C10H20O2	000334-48-5	47



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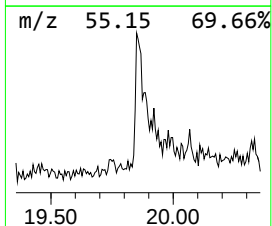
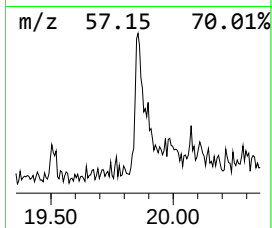
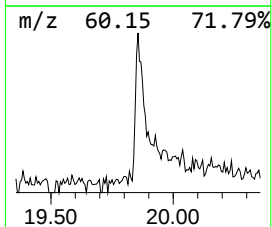
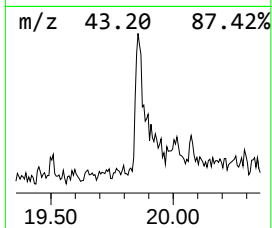
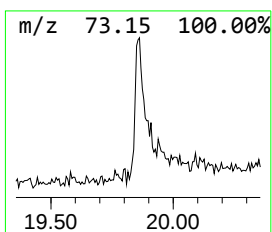
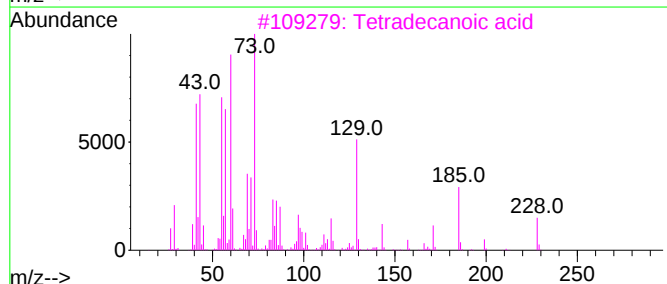
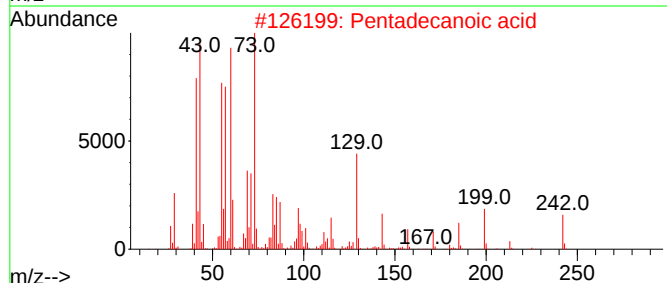
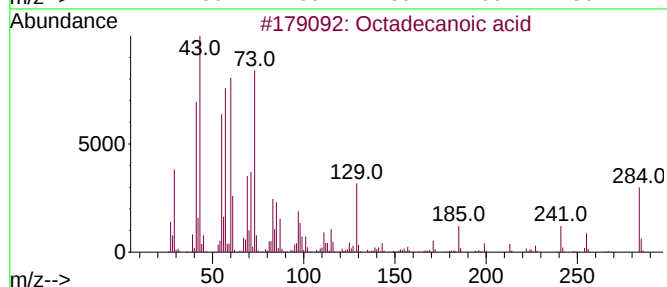
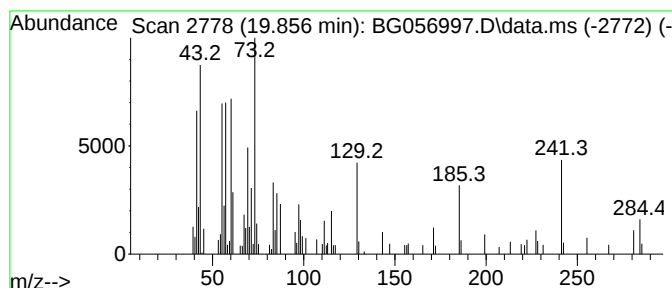
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
19.856	10.92 ng	140126	Phenanthrene-d10		17.765	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Octadecanoic acid		284	C18H36O2	000057-11-4	96
2	Pentadecanoic acid		242	C15H30O2	001002-84-2	62
3	Tetradecanoic acid		228	C14H28O2	000544-63-8	55
4	Tridecanoic acid		214	C13H26O2	000638-53-9	50
5	Dodecanoic acid		200	C12H24O2	000143-07-7	49



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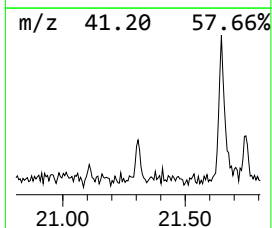
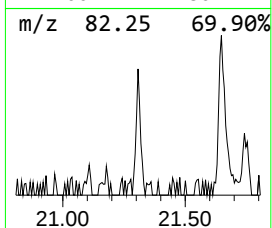
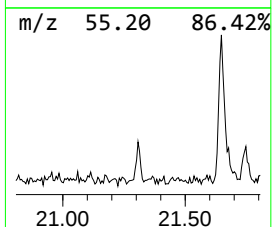
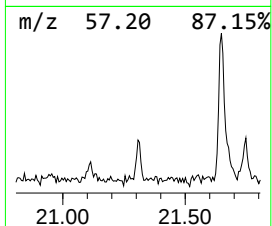
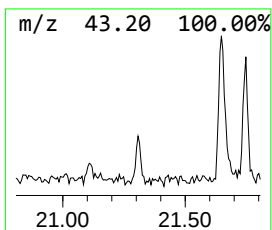
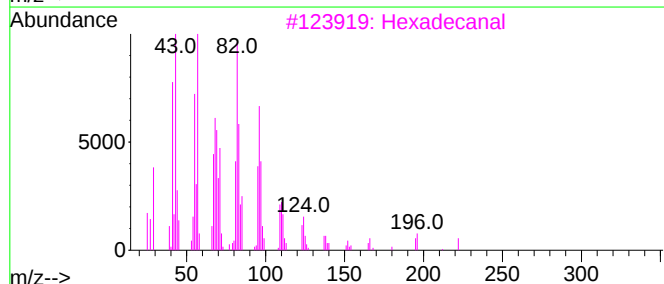
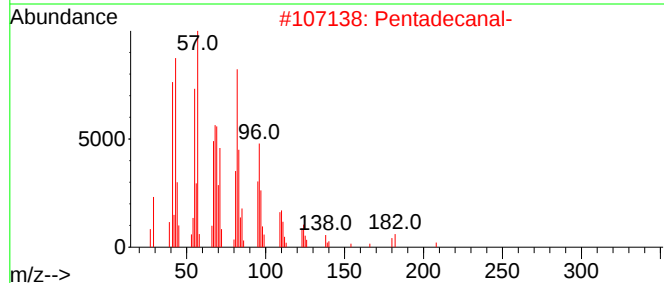
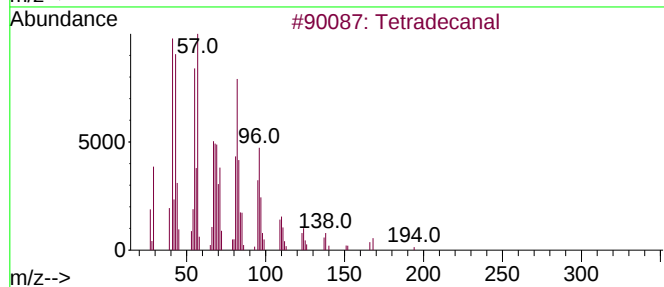
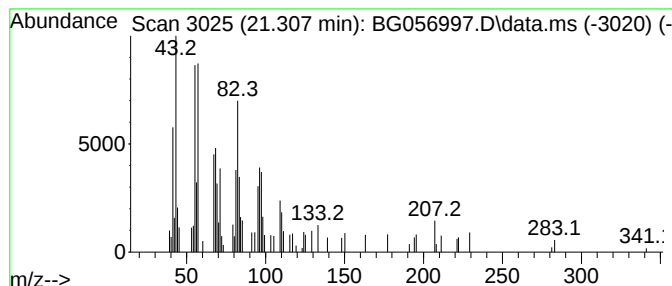
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Tetradecanal Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.307	2.92 ng	40603	Chrysene-d12	22.083

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecanal	212	C14H28O	000124-25-4	90
2			Pentadecanal-	226	C15H30O	002765-11-9	87
3			Hexadecanal	240	C16H32O	000629-80-1	87
4			E-2-Tetradecen-1-ol	212	C14H28O	1000130-83-7	86
5			Dodecanal	184	C12H24O	000112-54-9	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040523\
Data File : BG056997.D
Acq On : 5 Apr 2023 19:20
Operator : CG/JU
Sample : 02104-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
B-37-SB02

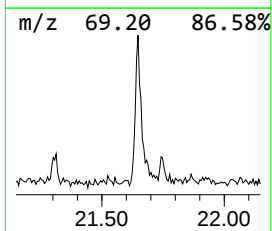
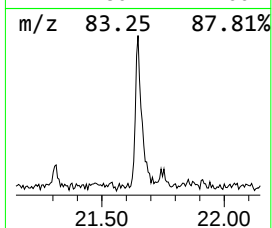
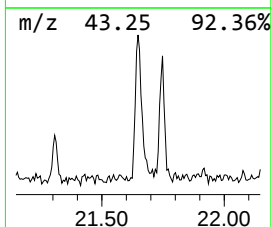
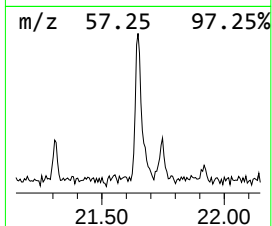
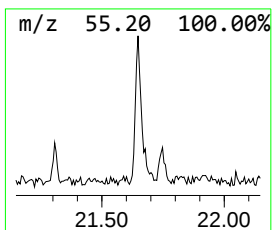
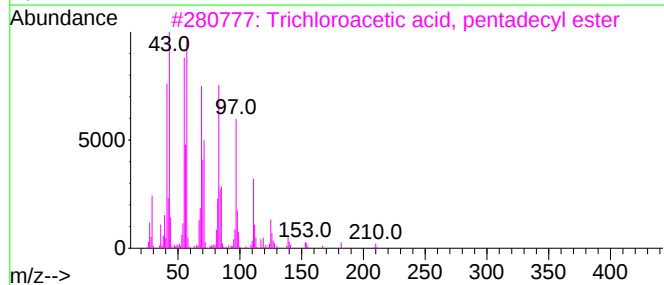
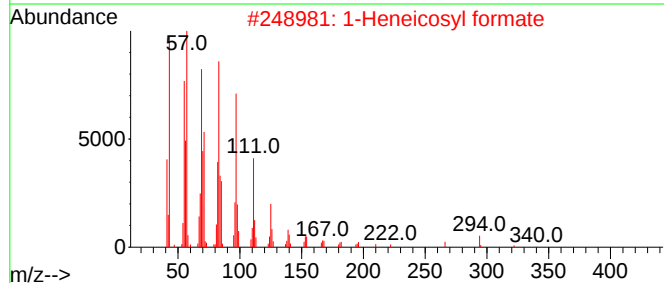
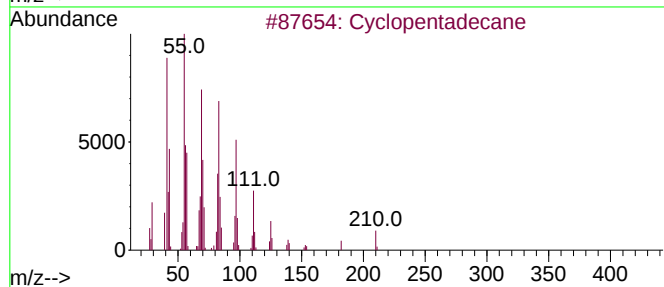
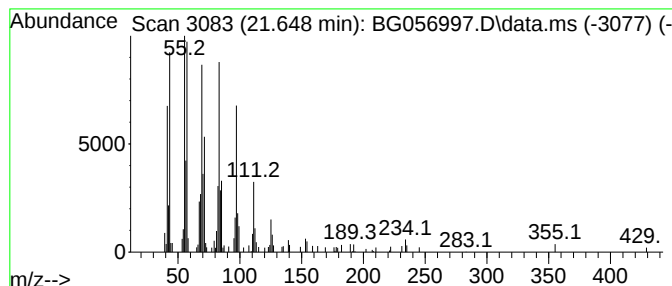
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Cyclopentadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.648	12.24 ng	169917	Chrysene-d12	22.083

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentadecane	210	C15H30	000295-48-7	98
2			1-Heneicosyl formate	340	C22H44O2	077899-03-7	95
3			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	95
4			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
5			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	95



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040523\
Data File : BG056997.D
Acq On : 5 Apr 2023 19:20
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Sample : 02104-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

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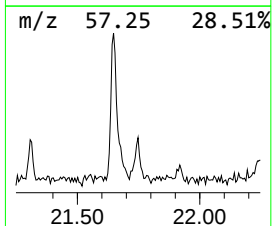
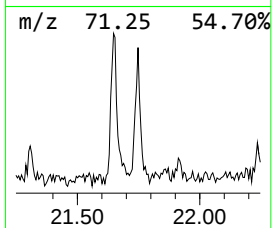
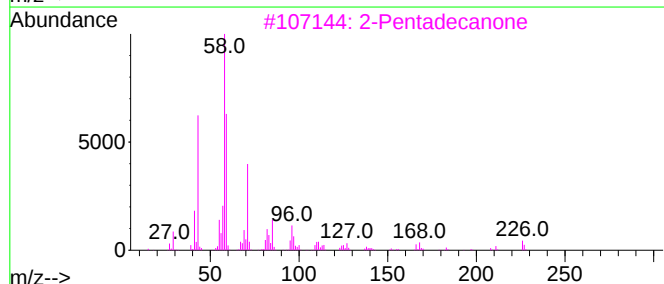
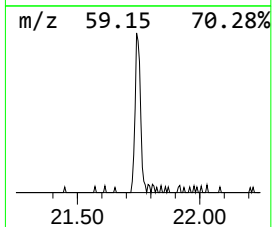
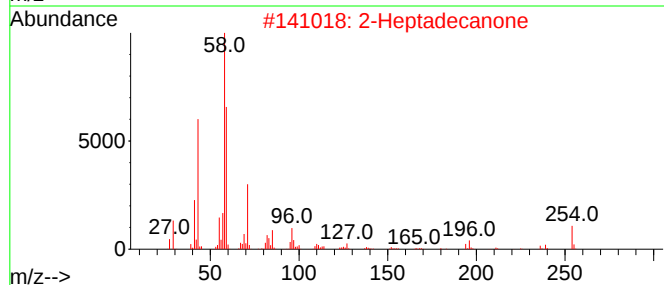
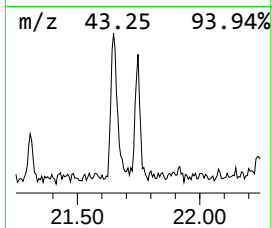
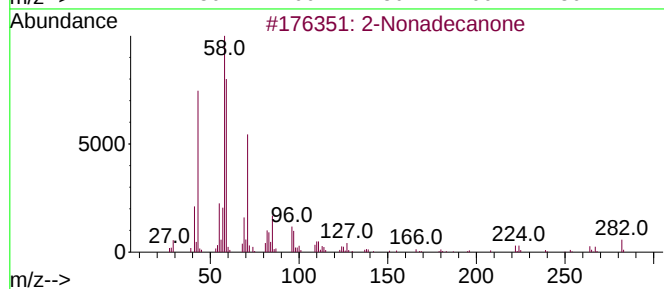
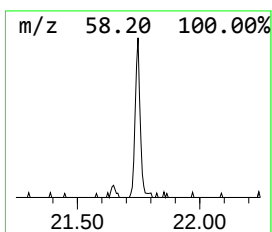
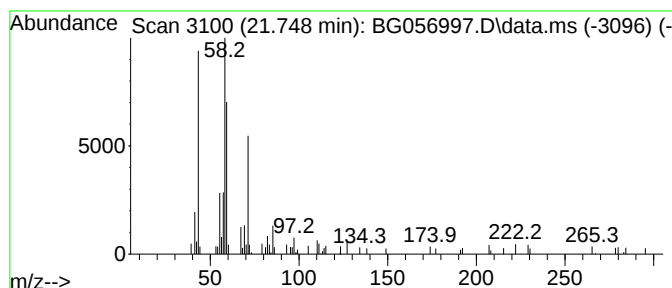
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 2-Nonadecanone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.748	4.24 ng	58926	Chrysene-d12	22.083

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Nonadecanone			282	C19H38O	000629-66-3	86
2	2-Heptadecanone			254	C17H34O	002922-51-2	78
3	2-Pentadecanone			226	C15H30O	002345-28-0	78
4	Methyl 3-oxohexadecanoate			284	C17H32O3	1010429-04-8	78
5	2-Undecanone			170	C11H22O	000112-12-9	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040523\
Data File : BG056997.D
Acq On : 5 Apr 2023 19:20
Operator : CG/JU
Sample : 02104-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

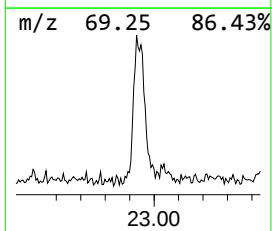
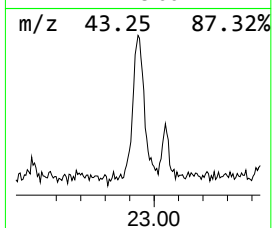
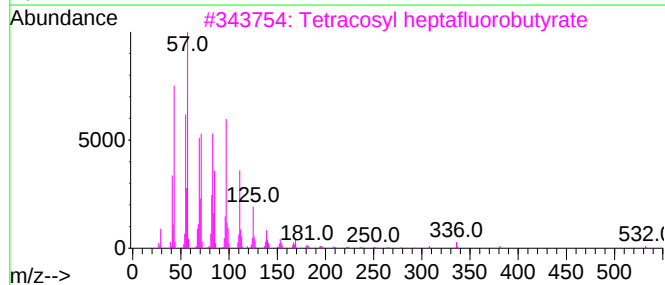
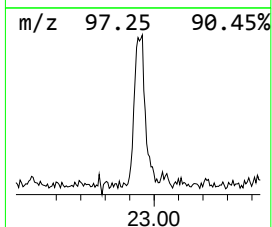
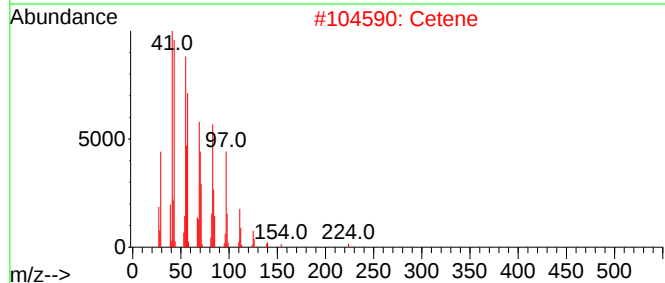
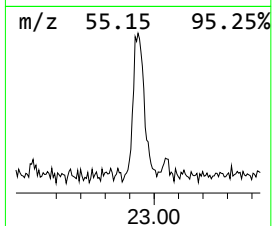
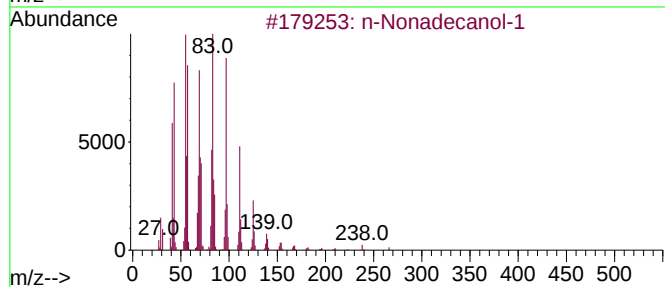
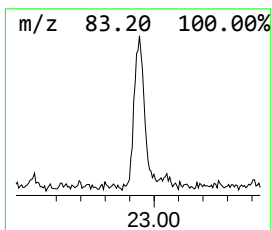
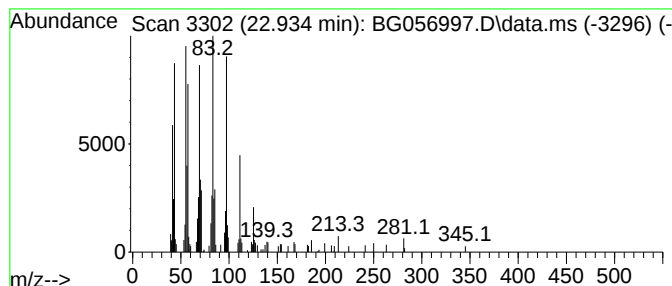
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 n-Nonadecanol-1 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
22.934	15.07 ng	209235	Chrysene-d12		22.083	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1		284	C19H40O	001454-84-8	90
2	Cetene		224	C16H32	000629-73-2	64
3	Tetracosyl heptafluorobutyrate		550	C28H49F7O2	1000351-83-7	49
4	Cyclohexane, 1,2,4-trimethyl-		126	C9H18	002234-75-5	45
5	4-Heptafluorobutyryloxyhexadecane		438	C20H33F7O2	1010282-97-2	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040523\
Data File : BG056997.D
Acq On : 5 Apr 2023 19:20
Operator : CG/JU
Sample : 02104-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
B-37-SB02

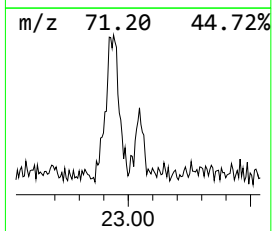
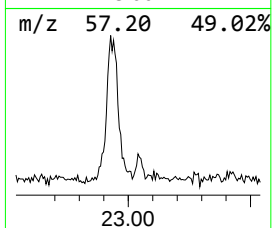
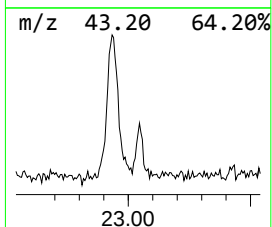
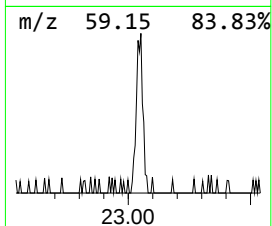
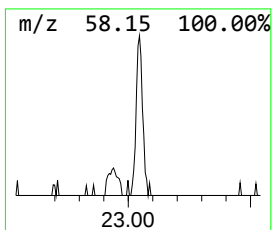
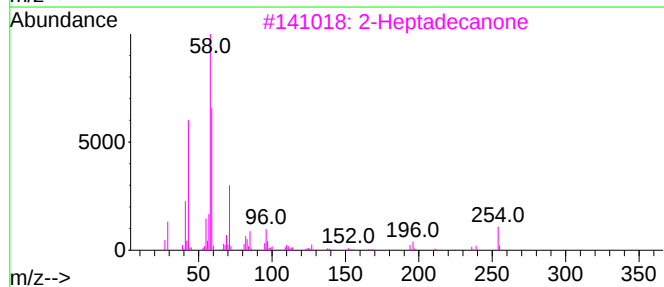
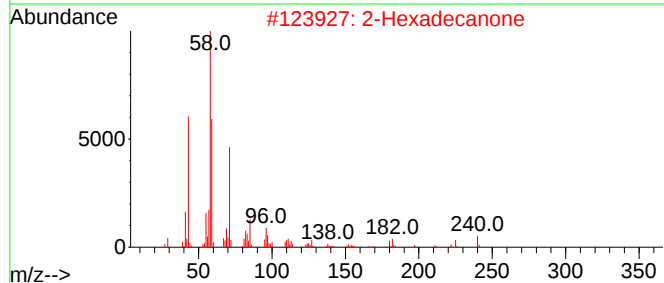
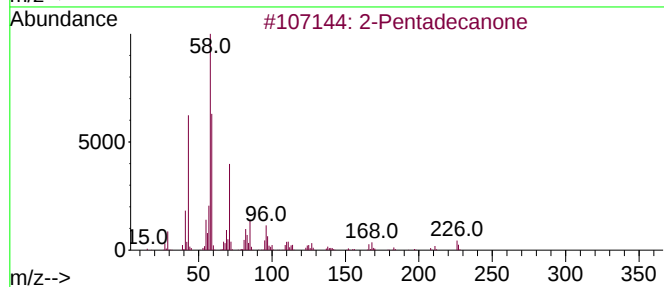
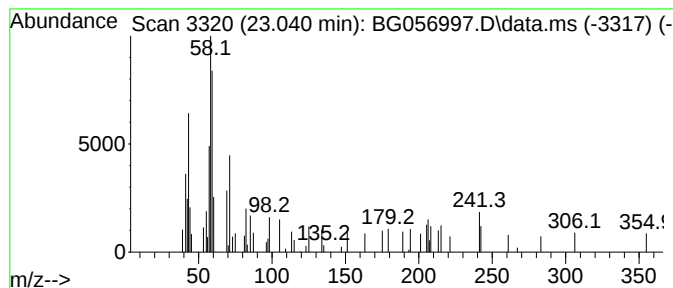
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown23.040 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.040	2.23 ng	31033	Chrysene-d12	22.083

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentadecanone	226	C15H30O	002345-28-0	45
2		2-Hexadecanone	240	C16H32O	018787-63-8	38
3		2-Heptadecanone	254	C17H34O	002922-51-2	38
4		Methylamine, N,N-dimethyl-	59	C3H9N	000075-50-3	38
5		Amonafide	283	C16H17N3O2	069408-81-7	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040523\
Data File : BG056997.D
Acq On : 5 Apr 2023 19:20
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Sample : 02104-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
B-37-SB02

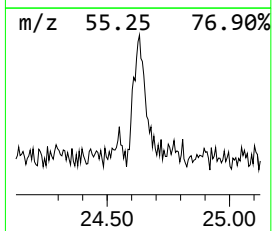
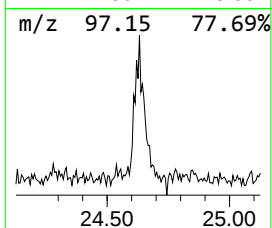
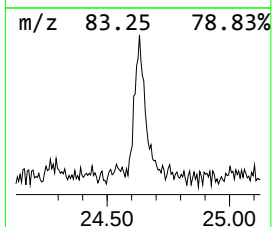
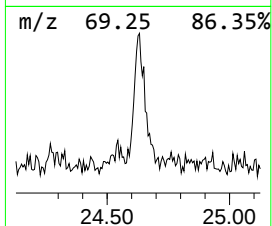
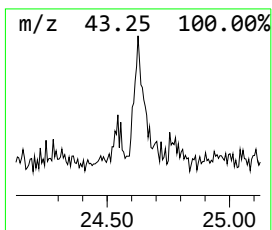
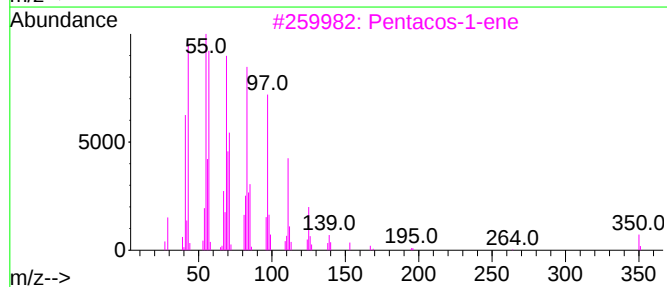
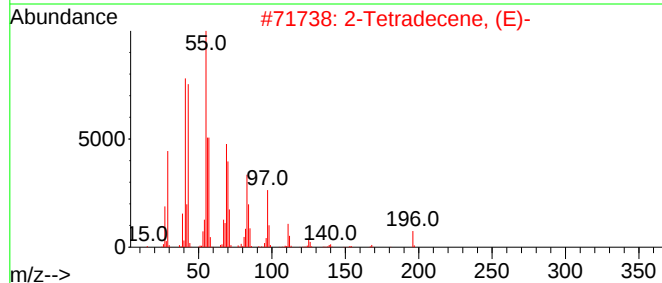
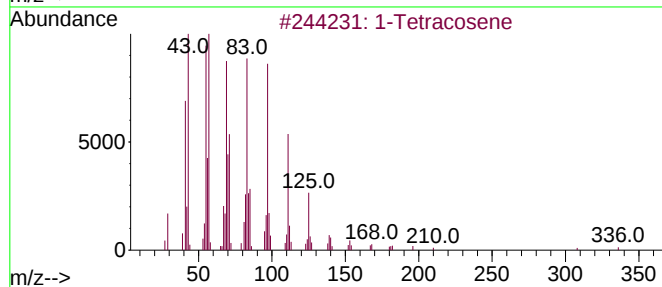
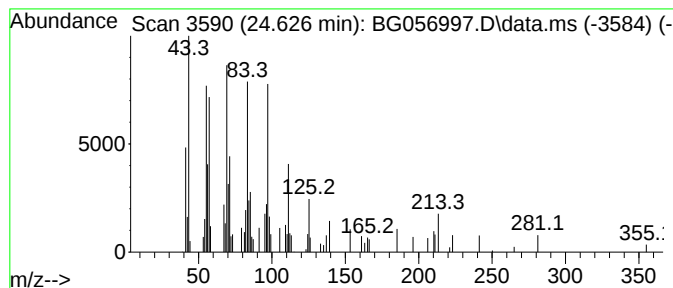
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1-Tetracosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.626	7.77 ng	82211	Perylene-d12	25.625

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Tetracosene	336	C24H48	010192-32-2	94
2		2-Tetradecene, (E)-	196	C14H28	035953-54-9	83
3		Pentacos-1-ene	350	C25H50	016980-85-1	81
4		Heptacosyl acetate	438	C29H58O2	1000351-78-2	76
5		1-Hexacosene	364	C26H52	018835-33-1	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040523\
Data File : BG056997.D
Acq On : 5 Apr 2023 19:20
Operator : CG/JU
Sample : 02104-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
B-37-SB02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.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
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Benzophenone	16.361	4.4	ng	42939	3	15.022	196301	20.0
n-Hexadecanoic ...	18.605	5.4	ng	69220	4	17.765	256723	20.0
Octadecanoic acid	19.856	10.9	ng	140126	4	17.765	256723	20.0
Tetradecanal	21.307	2.9	ng	40603	5	22.083	277700	20.0
Cyclopentadecane	21.648	12.2	ng	169917	5	22.083	277700	20.0
2-Nonadecanone	21.748	4.2	ng	58926	5	22.083	277700	20.0
n-Nonadecanol-1	22.934	15.1	ng	209235	5	22.083	277700	20.0
unknown23.040	23.040	2.2	ng	31033	5	22.083	277700	20.0
1-Tetracosene	24.626	7.8	ng	82211	6	25.625	211656	20.0