

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG123022\
 Data File : BG056178.D
 Acq On : 30 Dec 2022 19:58
 Operator : CG/JU
 Sample : N6237-01
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TR-05-122922

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-BG122722.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG056178.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.370	7	14	24	rVB	61830	128368	4.08%	0.778%
2	5.385	350	357	363	rBV	81812	132285	4.20%	0.802%
3	5.861	431	438	447	rBV	374744	622042	19.75%	3.769%
4	7.471	704	712	721	rBV	379510	656159	20.83%	3.976%
5	8.340	852	860	867	rBV	168104	292736	9.29%	1.774%
6	9.510	1050	1059	1067	rBB	215137	387881	12.31%	2.350%
7	11.166	1333	1341	1350	rBV	223968	398121	12.64%	2.413%
8	13.569	1744	1750	1762	rVB	747550	1138947	36.16%	6.902%
9	14.944	1977	1984	1991	rVB	409045	625201	19.85%	3.789%
10	16.419	2228	2235	2244	rBV	548745	834407	26.49%	5.056%
11	17.676	2441	2449	2454	rBV	516872	788575	25.03%	4.779%
12	17.723	2454	2457	2464	rVB	75582	105105	3.34%	0.637%
13	18.305	2551	2556	2562	rBV	534217	649793	20.63%	3.938%
14	18.523	2587	2593	2601	rBV2	82928	145090	4.61%	0.879%
15	18.599	2601	2606	2612	rVB3	22580	40654	1.29%	0.246%
16	18.734	2624	2629	2634	rBV5	16457	36964	1.17%	0.224%
17	19.433	2742	2748	2751	rBV	2545229	3149949	100.00%	19.088%
18	19.463	2751	2753	2763	rVB2	1245772	1593002	50.57%	9.653%
19	19.586	2769	2774	2779	rBV	251414	297871	9.46%	1.805%
20	19.709	2790	2795	2800	rVB	184798	266212	8.45%	1.613%
21	20.033	2847	2850	2852	rBV2	25875	33749	1.07%	0.205%
22	20.068	2852	2856	2862	rVB	172166	243842	7.74%	1.478%
23	20.250	2882	2887	2892	rBV	1310396	1658560	52.65%	10.051%
24	20.667	2952	2958	2962	rBV4	26167	55541	1.76%	0.337%
25	21.331	3067	3071	3077	rVB	21633	36164	1.15%	0.219%
26	21.572	3108	3112	3116	rVB4	36937	56904	1.81%	0.345%
27	21.971	3172	3180	3186	rBV3	515331	1035871	32.89%	6.277%
28	22.024	3186	3189	3196	rVB2	80258	129413	4.11%	0.784%
29	25.262	3736	3740	3749	rVB2	43831	111052	3.53%	0.673%
30	25.432	3760	3769	3779	rVB2	286852	851707	27.04%	5.161%

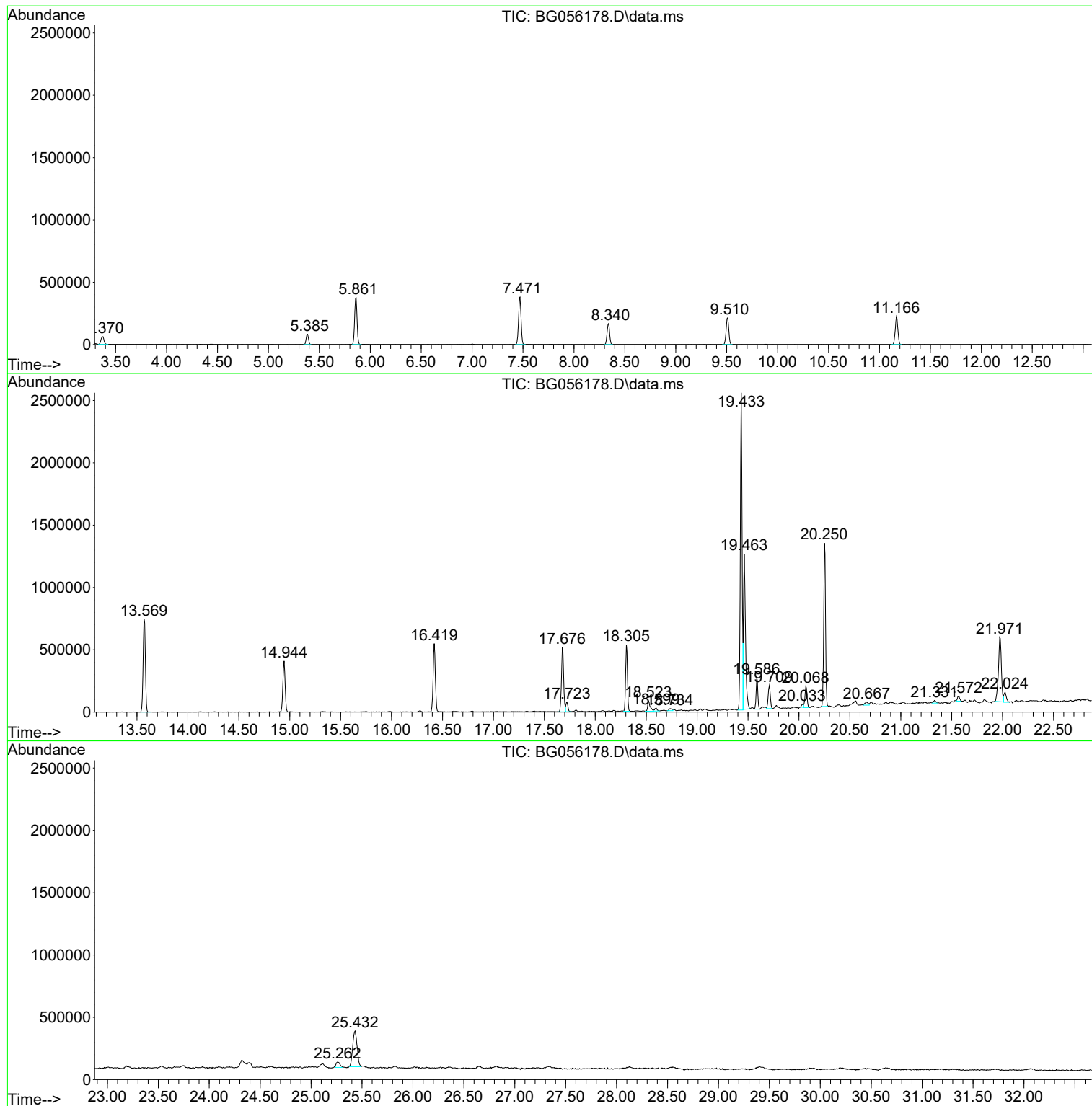
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Instrument :
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ClientSampleId :
TR-05-122922

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.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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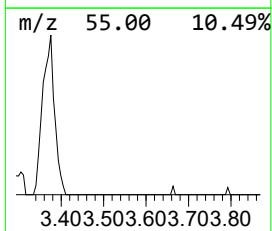
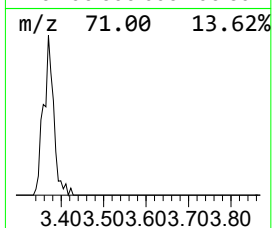
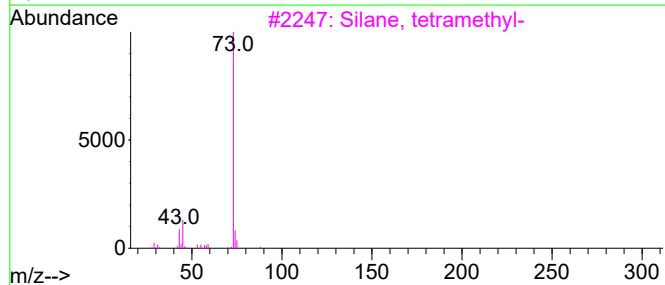
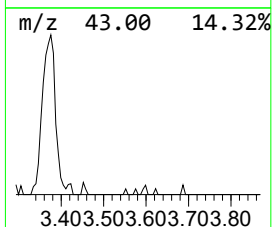
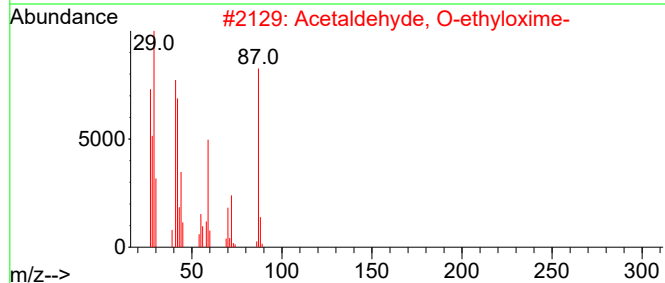
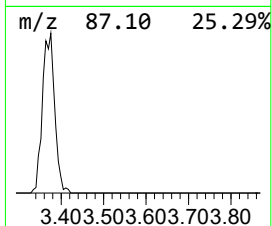
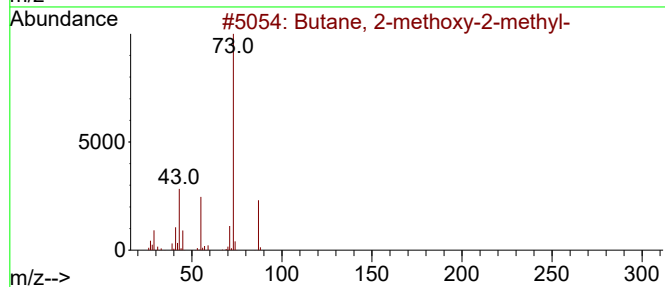
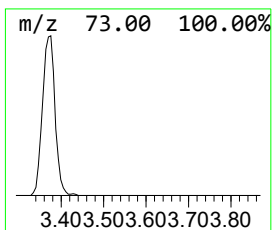
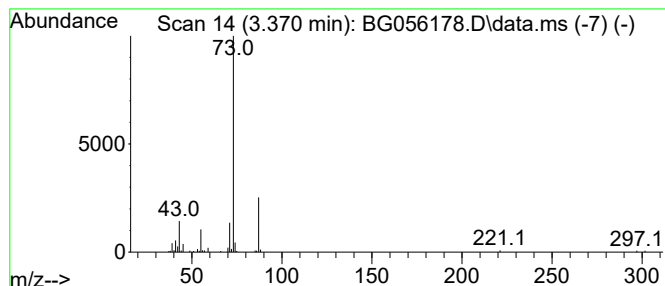
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.370	8.77 ng	128368	1,4-Dichlorobenzene-d4	8.340

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	56
2		Acetaldehyde, O-ethyloxime-	87	C4H9NO	1000288-34-6	9
3		Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
4		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9



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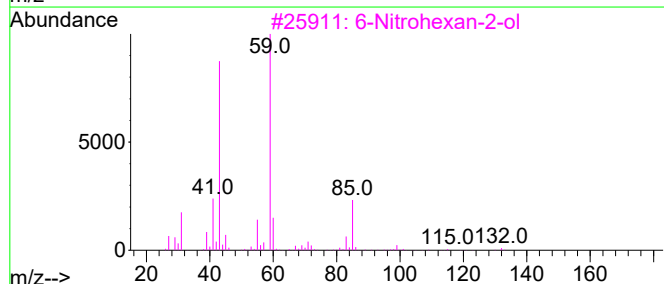
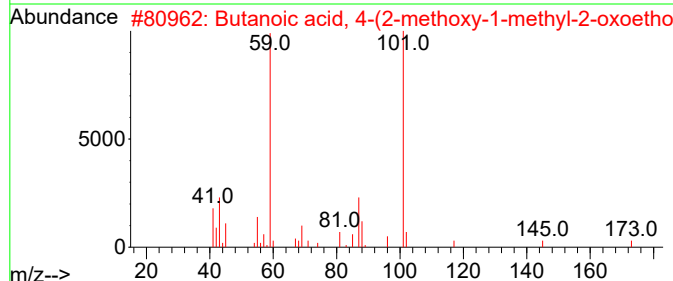
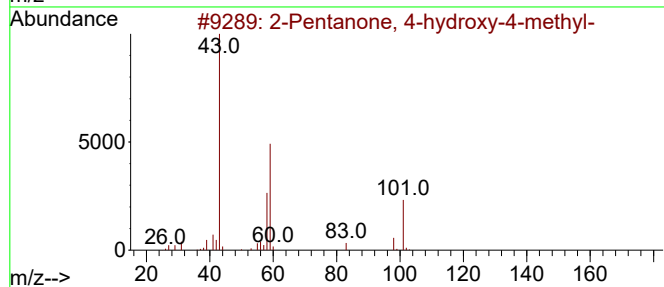
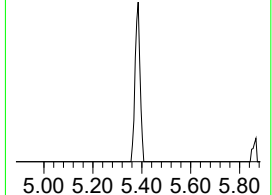
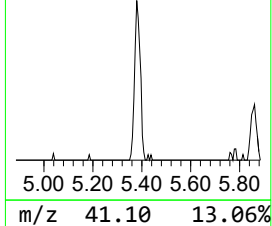
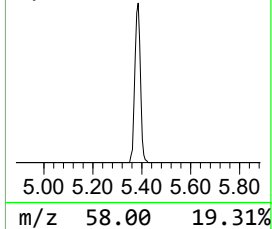
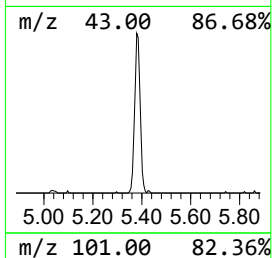
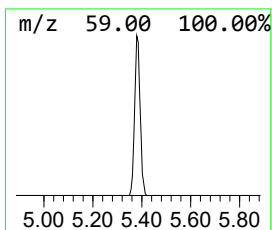
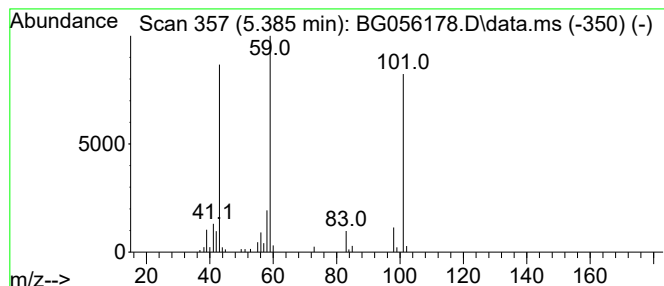
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.385	9.04 ng	132285	1,4-Dichlorobenzene-d4	8.340

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Butanoic acid, 4-(2-methoxy-1-me...	204	C9H16O5	054966-46-0	36
3			6-Nitrohexan-2-ol	147	C6H13NO3	062224-53-7	17
4			3-Heptanol, 4-methyl-	130	C8H18O	014979-39-6	17
5			Oxirane, tetramethyl-	100	C6H12O	005076-20-0	16



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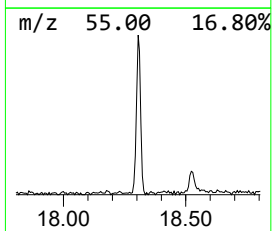
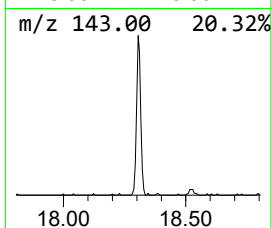
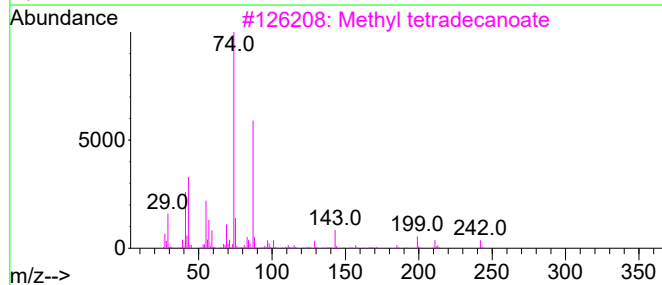
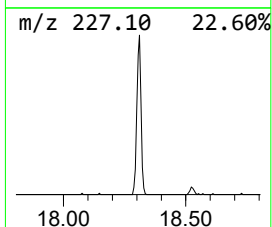
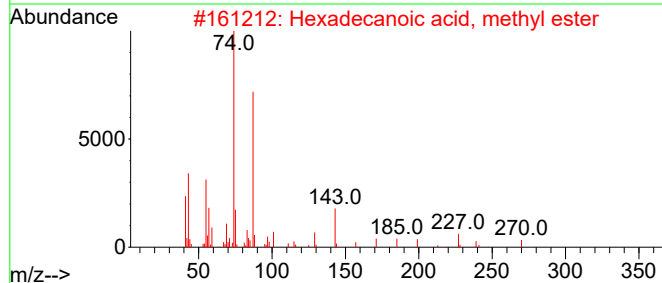
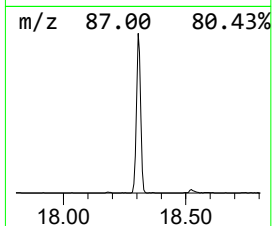
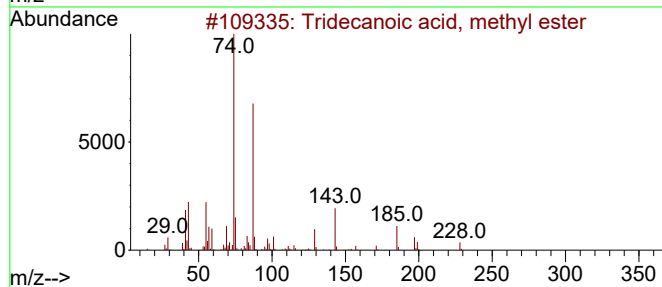
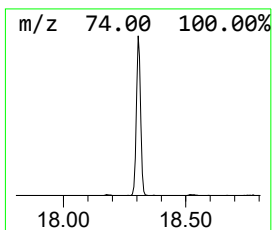
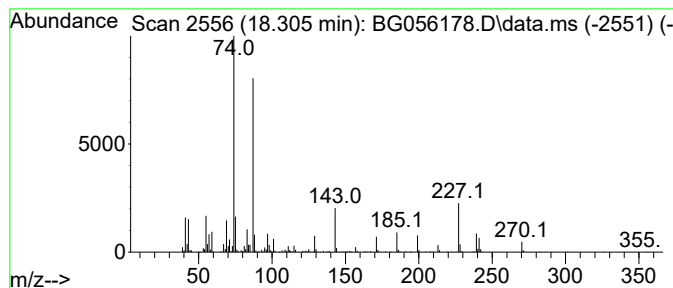
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Tridecanoic acid, methyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.305	16.48 ng	649793	Phenanthrene-d10	17.676

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	96
2			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	91
3			Methyl tetradecanoate	242	C15H30O2	000124-10-7	89
4			Hexadecanoic acid, 2-methyl-	270	C17H34O2	027147-71-3	83
5			Dodecanoic acid, 10-methyl-, met...	228	C14H28O2	005129-65-7	80



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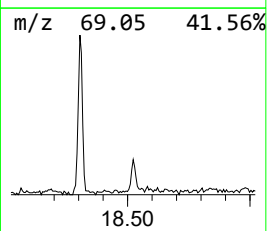
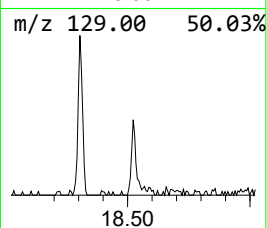
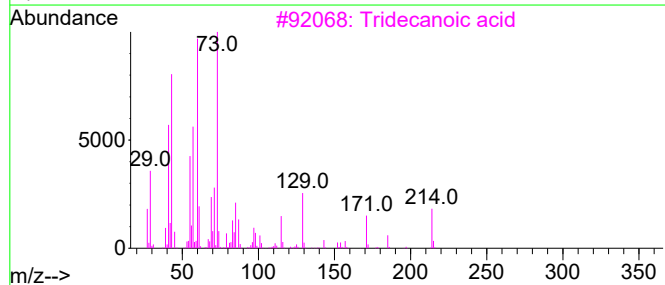
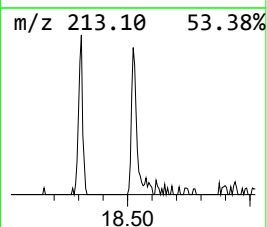
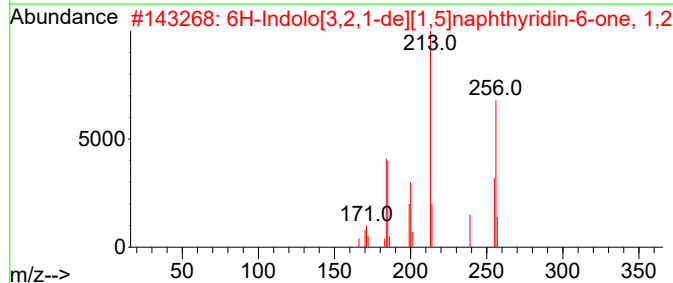
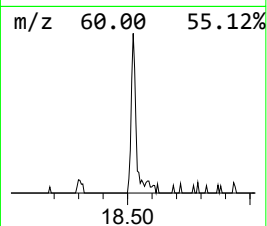
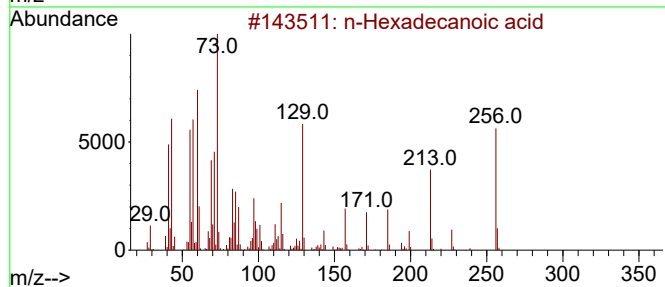
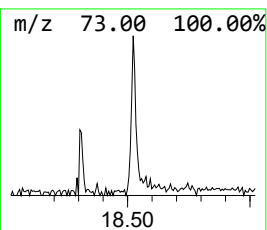
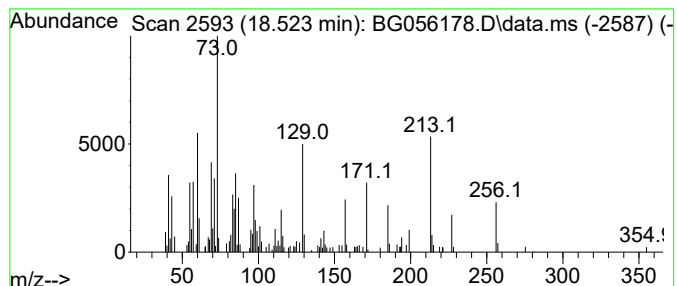
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.523	3.68 ng	145090	Phenanthrene-d10	17.676

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2			6H-Indolo[3,2,1-de][1,5]naphthyr...	256	C15H16N2O2	050630-67-6	53
3			Tridecanoic acid	214	C13H26O2	000638-53-9	45
4			Dodecanoic acid	200	C12H24O2	000143-07-7	43
5			Octadecanoic acid	284	C18H36O2	000057-11-4	38



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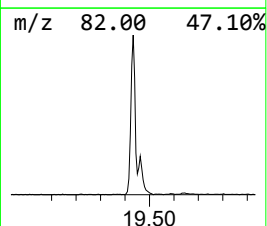
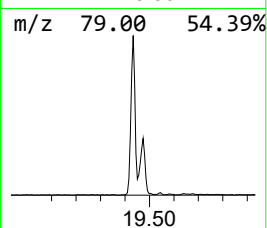
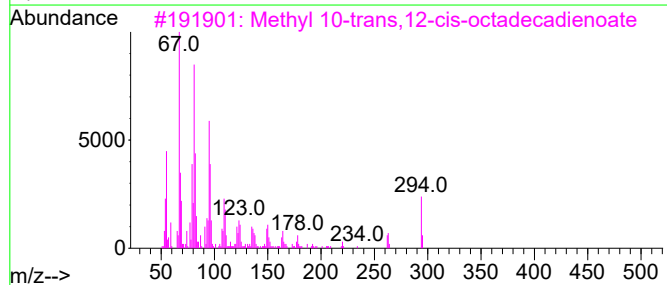
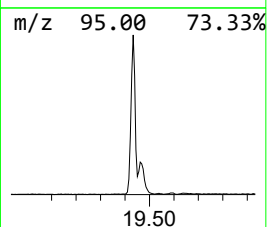
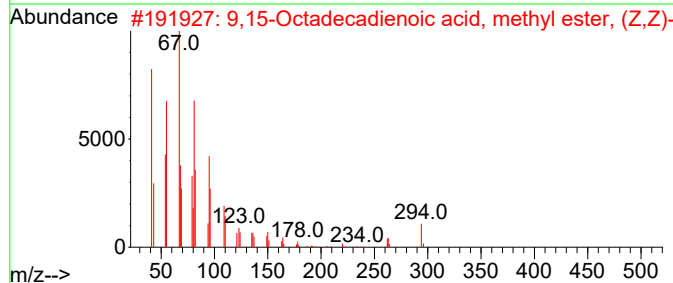
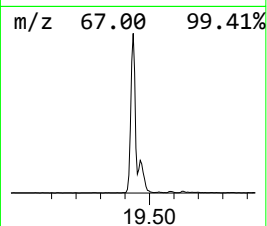
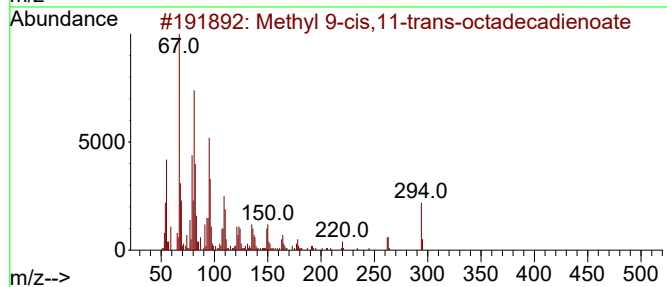
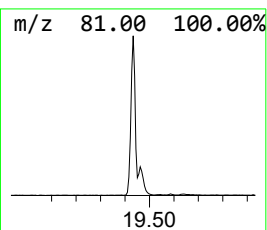
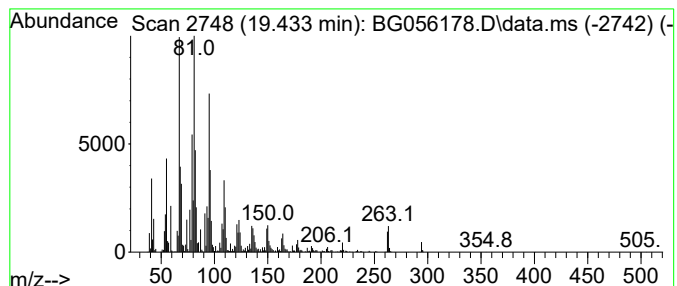
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Methyl 9-cis,11-trans-octad... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.	
19.433	79.89 ng	3149950	Phenanthrene-d10		17.676	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Methyl 9-cis,11-trans-octadecadi...		294	C19H34O2	013058-52-1	97
2	9,15-Octadecadienoic acid, methy...		294	C19H34O2	017309-05-6	97
3	Methyl 10-trans,12-cis-octadecad...		294	C19H34O2	1000336-44-2	94
4	9,12-Octadecadienoic acid, methy...		294	C19H34O2	002566-97-4	94
5	9,12-Octadecadienoic acid (Z,Z)-...		294	C19H34O2	000112-63-0	94



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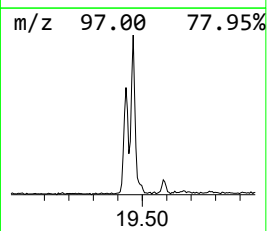
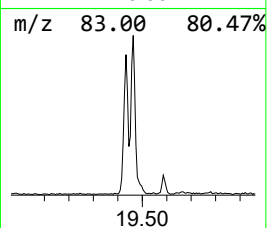
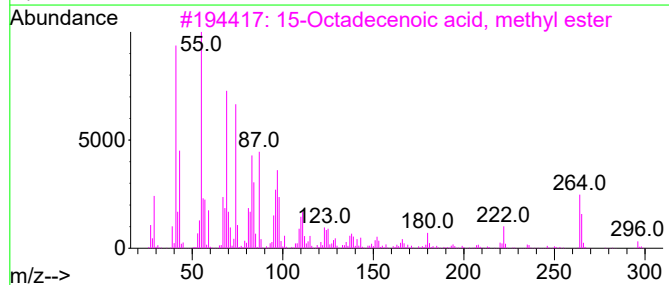
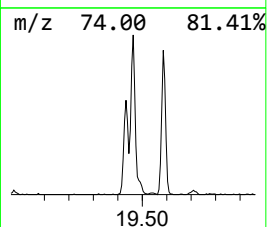
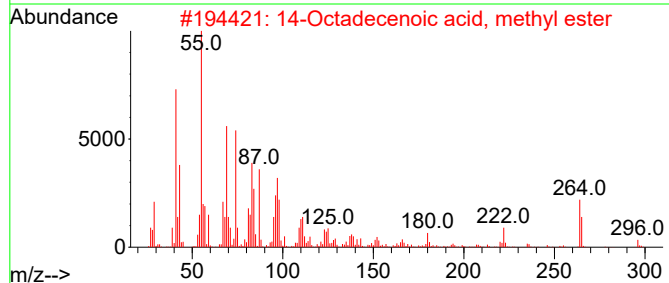
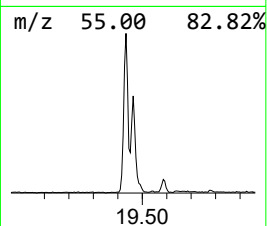
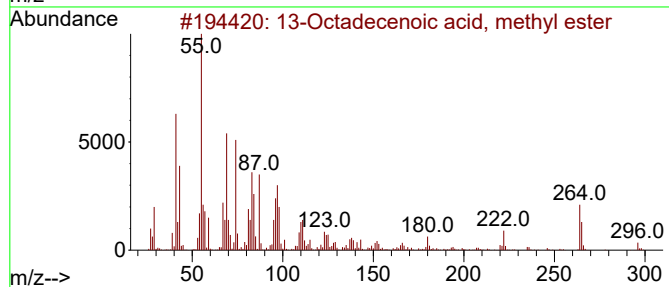
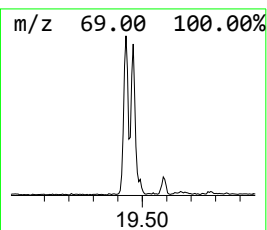
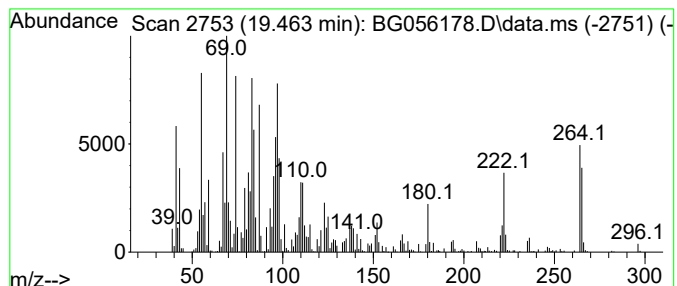
Instrument :
BNA_G
ClientSampleId :
TR-05-122922

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 13-Octadecenoic acid, methyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.463	40.40 ng	1593000	Phenanthrene-d10	17.676	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	99
2	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	99
3	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	99
4	12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	98
5	6-Octadecenoic acid, methyl este...	296	C19H36O2	002777-58-4	98



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG123022\
Data File : BG056178.D
Acq On : 30 Dec 2022 19:58
Operator : CG/JU
Sample : N6237-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TR-05-122922

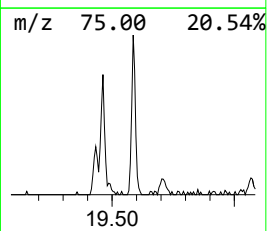
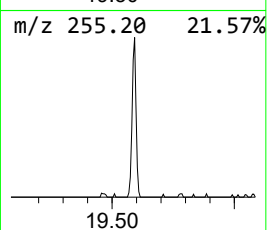
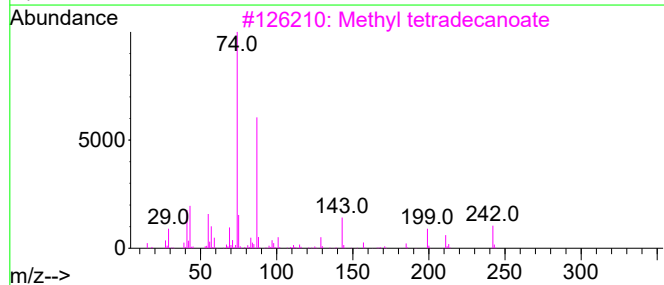
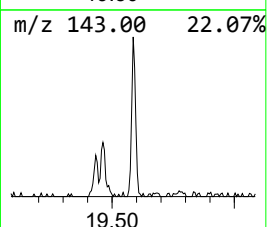
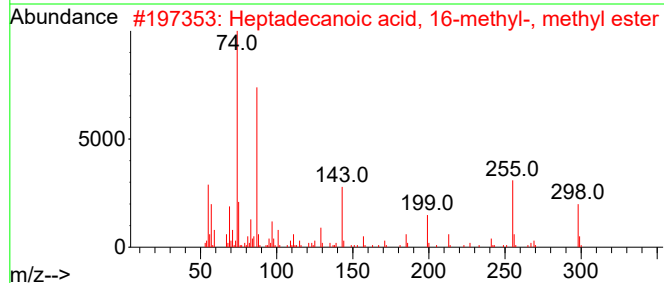
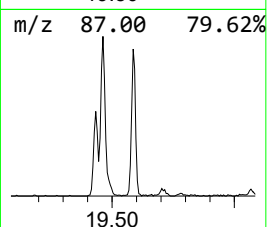
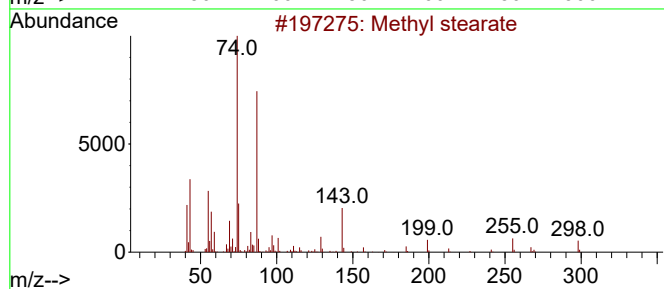
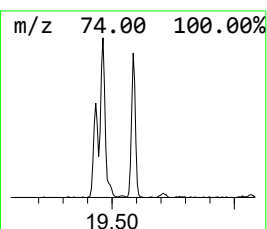
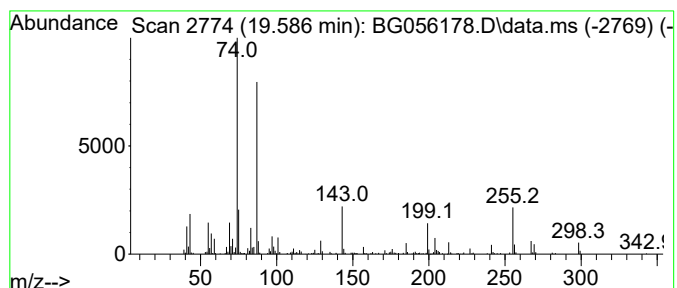
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Methyl stearate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.586	7.55 ng	297871	Phenanthrene-d10	17.676

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl stearate	298	C19H38O2	000112-61-8	91
2			Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	89
3			Methyl tetradecanoate	242	C15H30O2	000124-10-7	81
4			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	81
5			Nonadecanoic acid, methyl ester	312	C20H40O2	001731-94-8	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG123022\
Data File : BG056178.D
Acq On : 30 Dec 2022 19:58
Operator : CG/JU
Sample : N6237-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TR-05-122922

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.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
Butane, 2-metho...	3.370	8.8	ng	128368	1	8.340	292736	20.0
2-Pentanone, 4-...	5.385	9.0	ng	132285	1	8.340	292736	20.0
Tridecanoic aci...	18.305	16.5	ng	649793	4	17.676	788575	20.0
n-Hexadecanoic ...	18.523	3.7	ng	145090	4	17.676	788575	20.0
Methyl 9-cis,11...	19.433	79.9	ng	3149950	4	17.676	788575	20.0
13-Octadecenoic...	19.463	40.4	ng	1593000	4	17.676	788575	20.0
Methyl stearate	19.586	7.5	ng	297871	4	17.676	788575	20.0