

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052523\
 Data File : BG057575.D
 Acq On : 26 May 2023 2:46
 Operator : CG/JU
 Sample : 02938-01 2X
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SU-04-052423

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-BG042723.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057575.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	309	314	319	rBV2	9168	14466	2.19%	0.262%
2	5.871	391	397	405	rBV	139048	235232	35.68%	4.259%
3	7.499	667	674	685	rBV	155251	273587	41.50%	4.954%
4	8.350	812	819	828	rVB	103521	177989	27.00%	3.223%
5	9.531	1012	1020	1031	rVB	93925	169454	25.70%	3.068%
6	11.188	1295	1302	1309	rVB	139668	250102	37.94%	4.529%
7	13.590	1705	1711	1717	rBV	279464	422229	64.04%	7.645%
8	14.812	1914	1919	1924	rVB3	6932	9667	1.47%	0.175%
9	14.965	1939	1945	1952	rVB	228054	347658	52.73%	6.295%
10	15.752	2073	2079	2084	rBV2	10888	14522	2.20%	0.263%
11	16.157	2142	2148	2152	rBV5	5159	8572	1.30%	0.155%
12	16.298	2167	2172	2178	rBV	37475	55268	8.38%	1.001%
13	16.451	2192	2198	2204	rBV	197935	304526	46.19%	5.514%
14	16.610	2221	2225	2228	rBV3	13929	19716	2.99%	0.357%
15	17.403	2354	2360	2364	rBV	16573	22029	3.34%	0.399%
16	17.450	2364	2368	2374	rVB5	6260	9861	1.50%	0.179%
17	17.708	2405	2412	2418	rBV	271105	423006	64.16%	7.659%
18	18.137	2482	2485	2492	rVB2	14614	17921	2.72%	0.324%
19	18.313	2510	2515	2521	rVB	119419	144803	21.96%	2.622%
20	18.542	2549	2554	2563	rBV	43725	75848	11.50%	1.373%
21	18.819	2598	2601	2605	rBV	13189	14163	2.15%	0.256%
22	19.271	2676	2678	2682	rBV5	5078	7814	1.19%	0.141%
23	19.441	2702	2707	2709	rBV	557744	659287	100.00%	11.938%
24	19.471	2709	2712	2722	rVB2	275251	398267	60.41%	7.211%
25	19.594	2729	2733	2737	rBV	62663	72800	11.04%	1.318%
26	19.653	2740	2743	2753	rVV	17824	44418	6.74%	0.804%
27	19.741	2754	2758	2762	rVV	17262	28364	4.30%	0.514%
28	19.794	2764	2767	2775	rVB9	13849	26304	3.99%	0.476%
29	20.099	2816	2819	2826	rVB	20916	31590	4.79%	0.572%
30	20.275	2844	2849	2853	rBV	434255	554371	84.09%	10.038%
31	22.014	3139	3145	3152	rVB2	222348	396590	60.15%	7.181%
32	25.527	3736	3743	3753	rVB	103430	292321	44.34%	5.293%

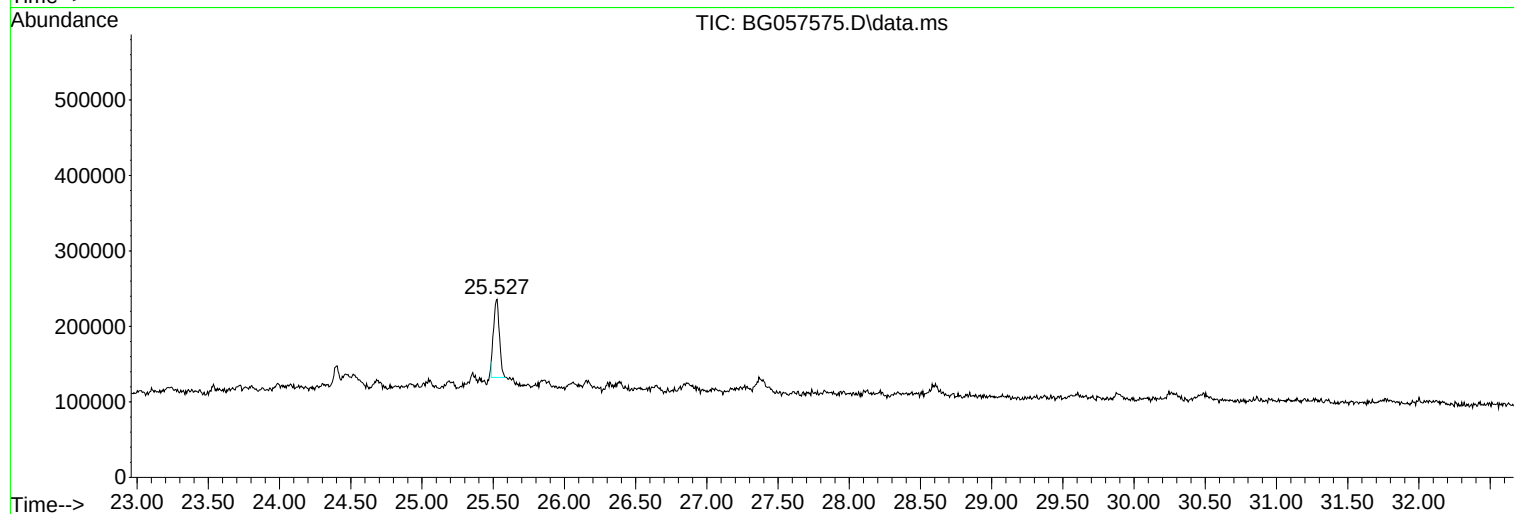
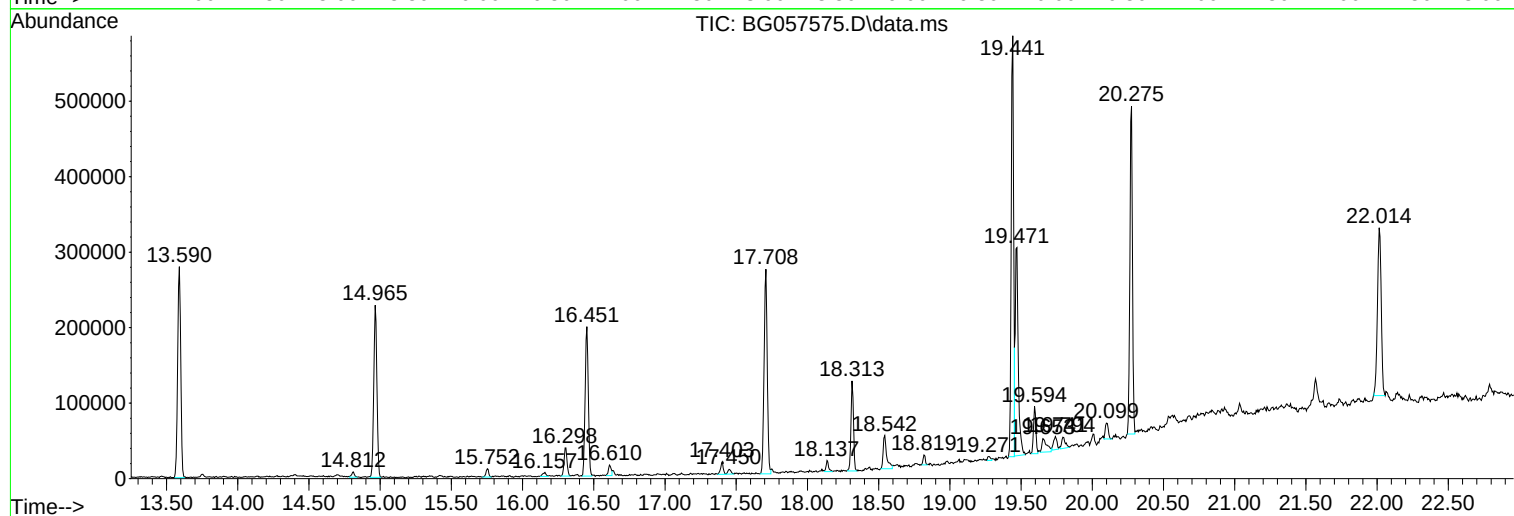
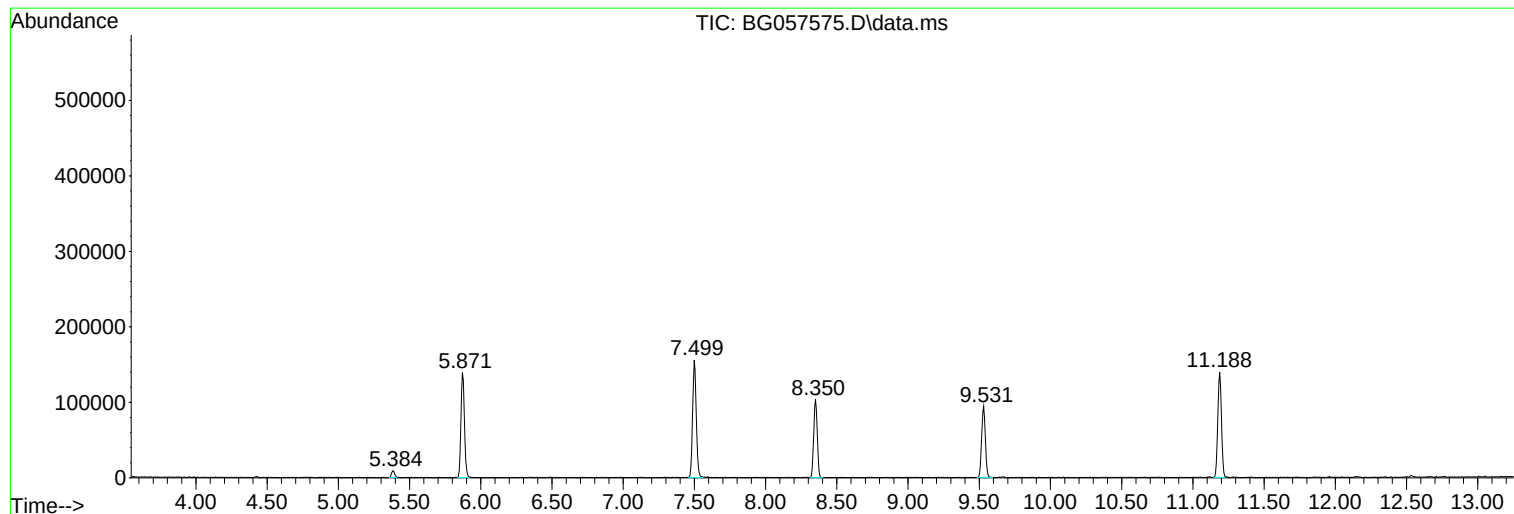
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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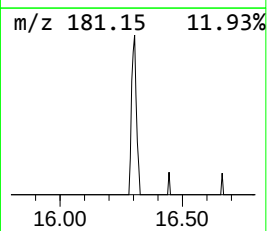
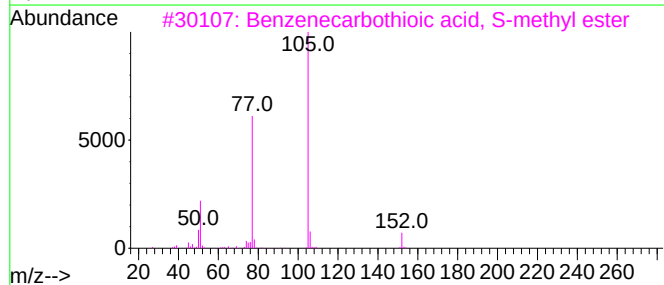
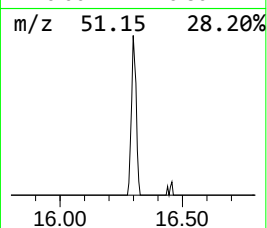
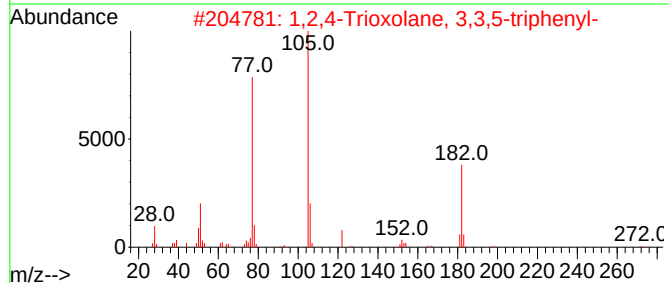
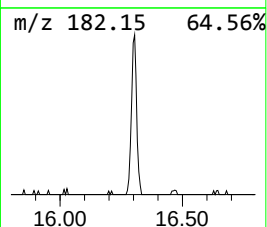
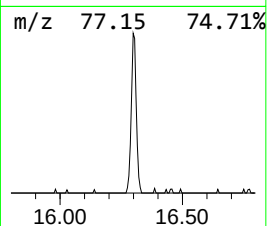
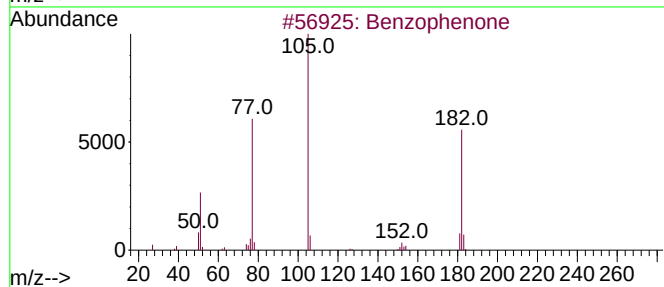
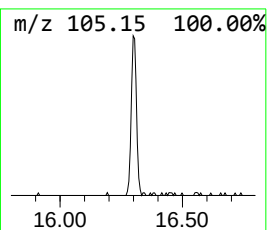
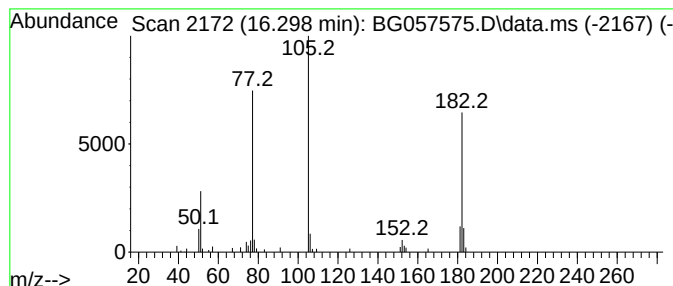
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Benzophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.299	3.18 ng	55268	Acenaphthene-d10	14.965

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			1,2,4-Trioxolane, 3,3,5-triphenyl-	304	C20H16O3	023246-12-0	72
3			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	58
4			N-(1-Cyanovinyl)benzamide	172	C10H8N2O	1000186-19-1	50
5			N-Methylbenzamide, N-trifluoroac...	231	C10H8F3NO2	1000446-91-5	50



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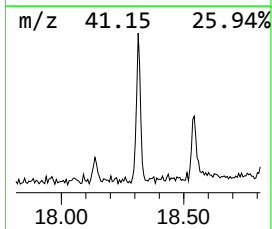
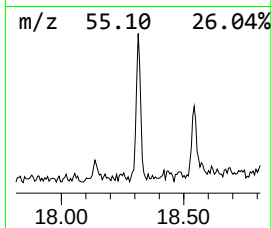
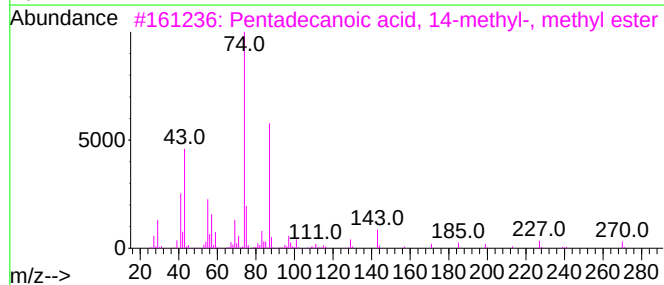
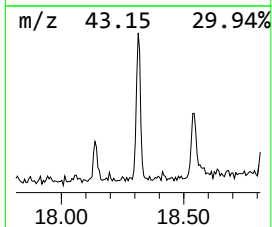
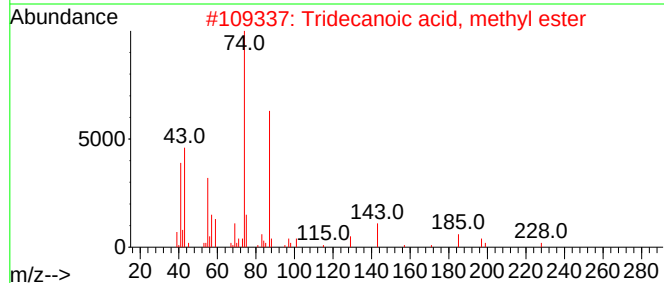
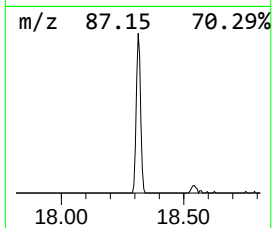
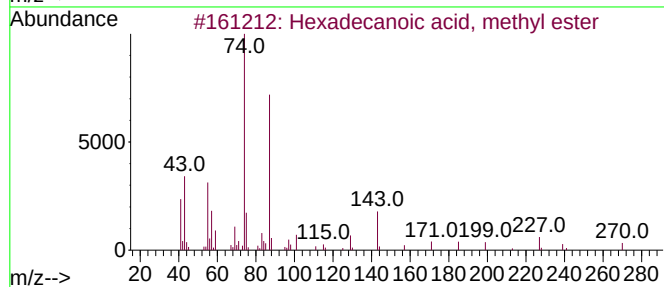
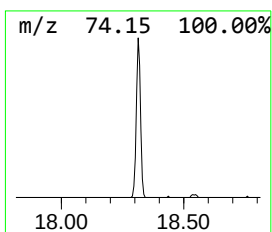
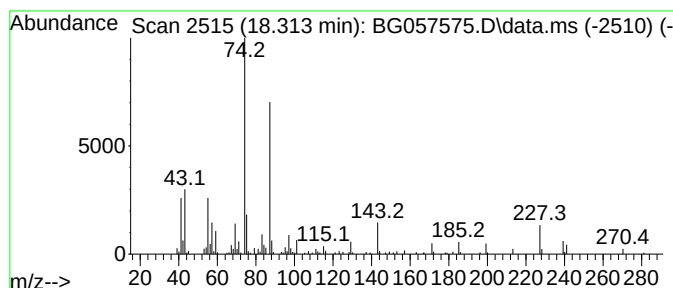
Instrument :
BNA_G
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 2 Hexadecanoic acid, methyl e... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.313	6.85 ng	144803	Phenanthrene-d10	17.708	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	97
2	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	94
3	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	94
4	Methyl tetradecanoate	242	C15H30O2	000124-10-7	83
5	Dodecanoic acid, 10-methyl-, met...	228	C14H28O2	005129-65-7	83



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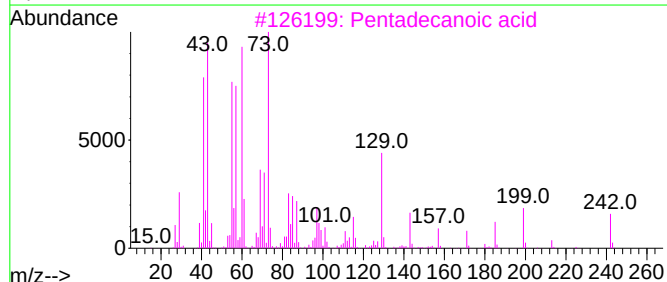
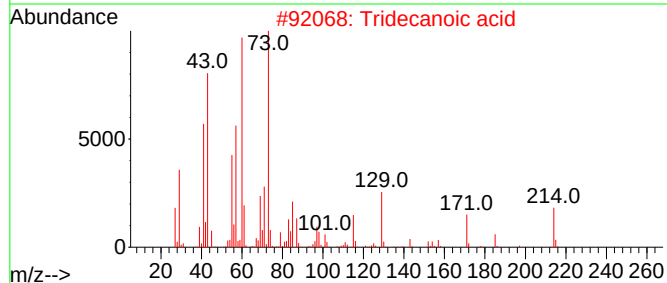
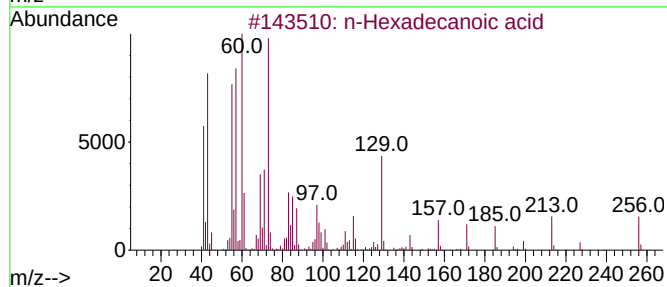
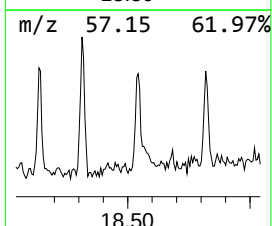
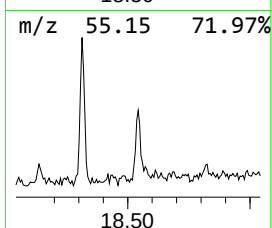
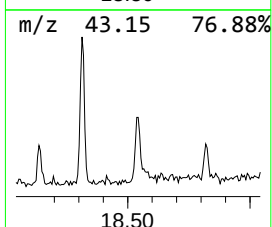
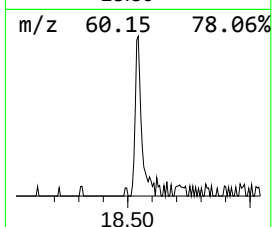
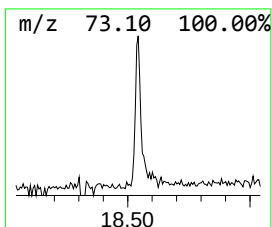
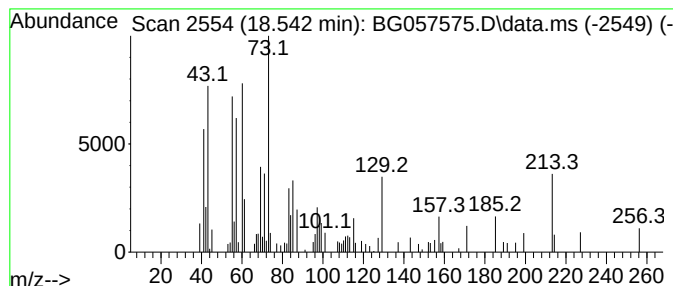
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.543	3.59 ng	75848	Phenanthrene-d10	17.708

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	76
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	59
5			Dodecanoic acid	200	C12H24O2	000143-07-7	50



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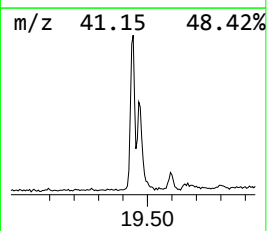
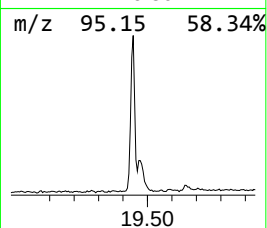
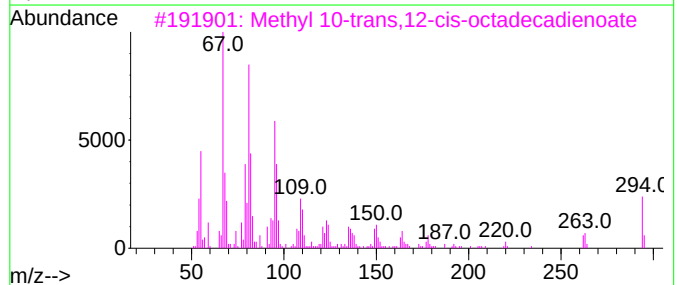
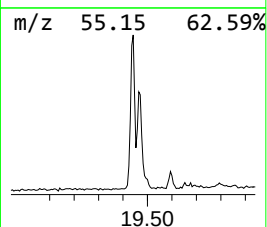
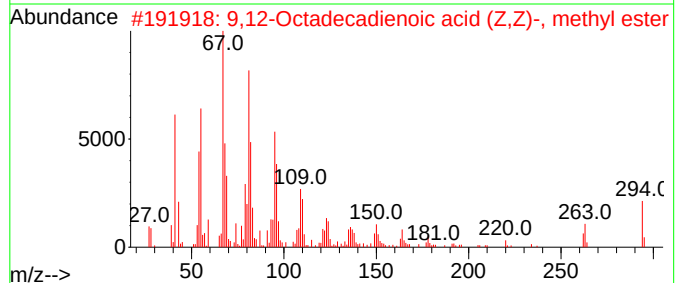
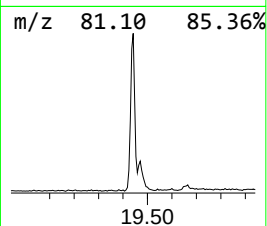
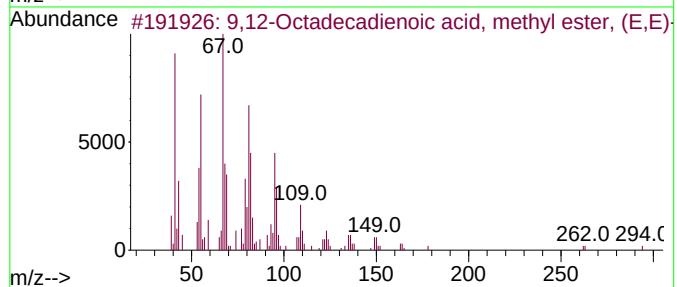
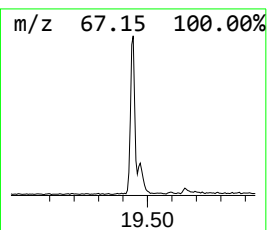
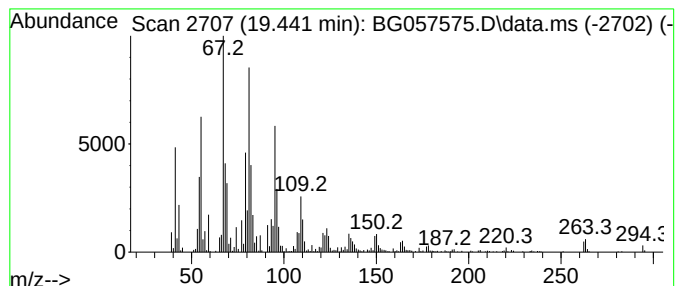
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Peak Number 4 9,12-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.441	31.17 ng	659287	Phenanthrene-d10	17.708

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
2			9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	98
3			Methyl 10-trans,12-cis-octadecad...	294	C19H34O2	1000336-44-2	98
4			9,11-Octadecadienoic acid, methy...	294	C19H34O2	013038-47-6	97
5			9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	97



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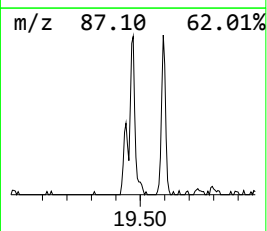
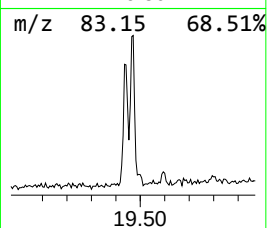
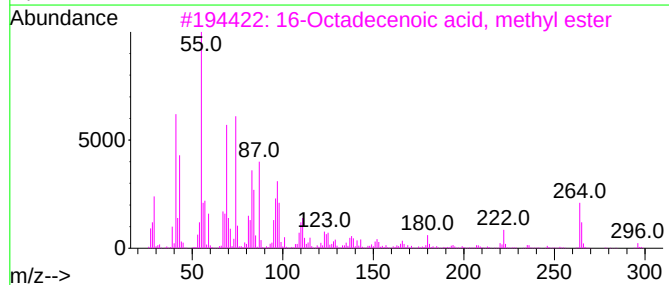
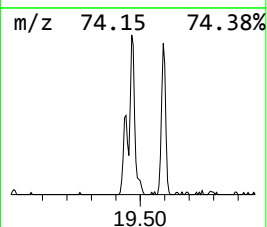
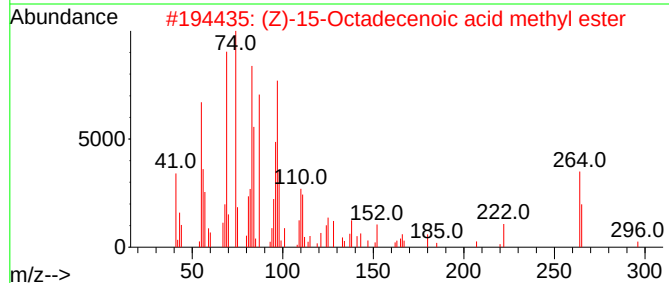
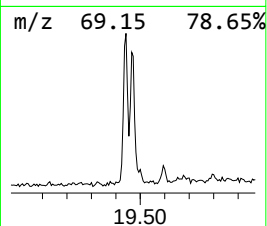
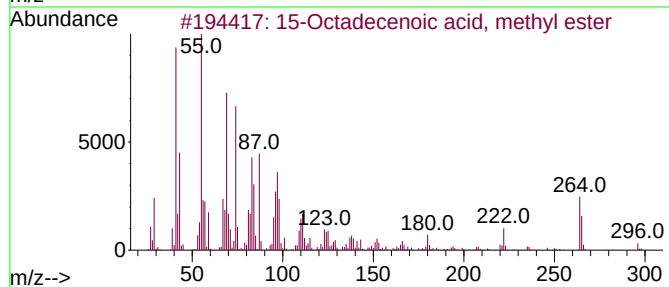
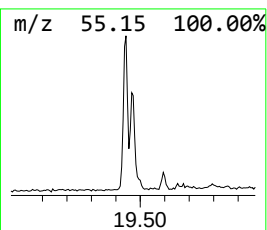
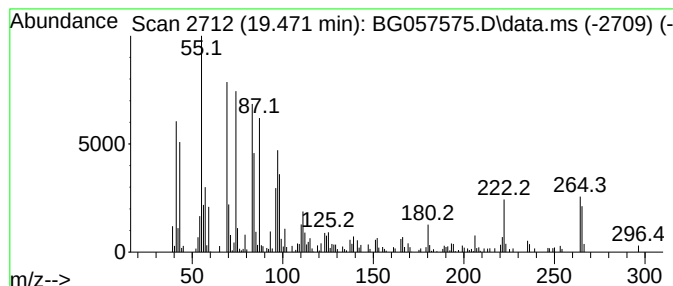
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Peak Number 5 15-Octadecenoic acid, methyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.471	18.83 ng	398267	Phenanthrene-d10	17.708

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	96
2			(Z)-15-Octadecenoic acid methyl ...	296	C19H36O2	1000427-69-3	93
3			16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	91
4			6-Octadecenoic acid, methyl ester	296	C19H36O2	052355-31-4	83
5			9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	72



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SU-04-052423

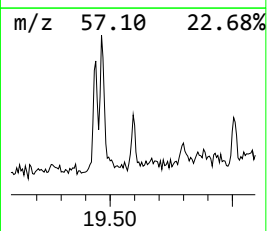
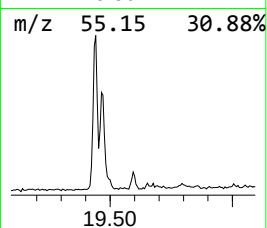
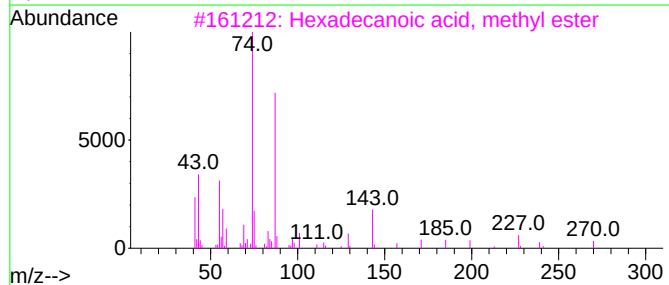
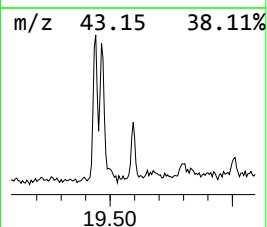
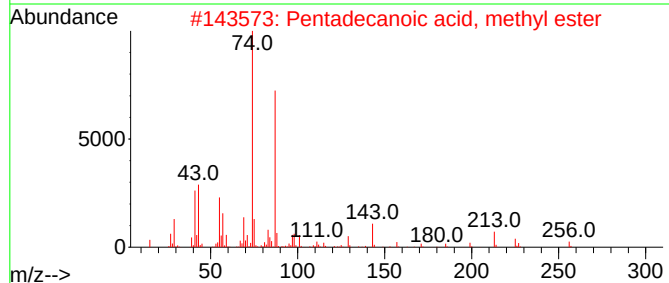
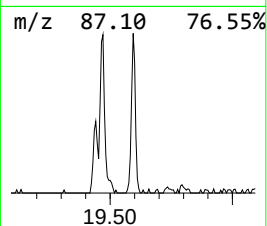
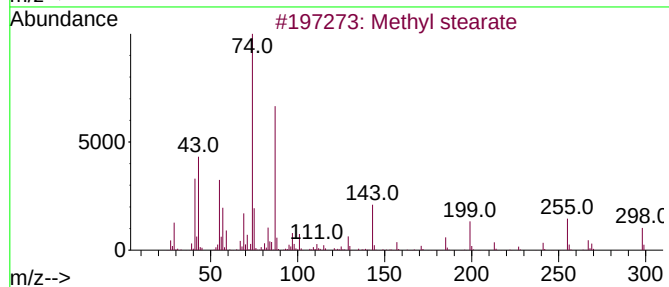
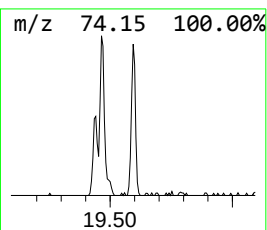
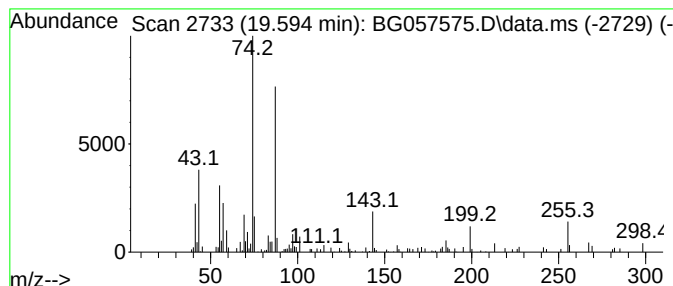
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Methyl stearate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.594	3.44 ng	72800	Phenanthrene-d10	17.708

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Methyl stearate	298	C19H38O2	000112-61-8	92
2		Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	87
3		Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	80
4		Methyl 9-methyltetradecanoate	256	C16H32O2	213617-69-7	80
5		Methyl tetradecanoate	242	C15H30O2	000124-10-7	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052523\
Data File : BG057575.D
Acq On : 26 May 2023 2:46
Operator : CG/JU
Sample : 02938-01 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SU-04-052423

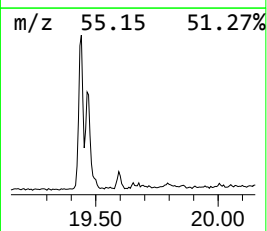
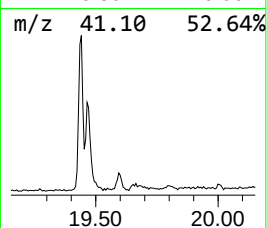
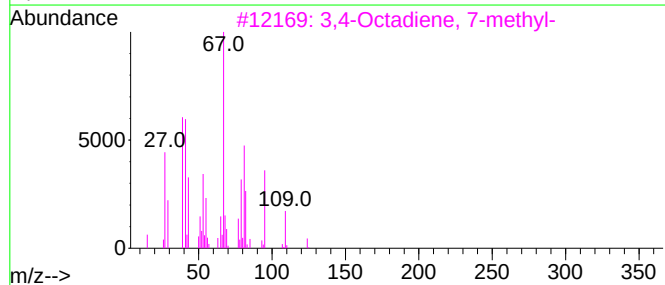
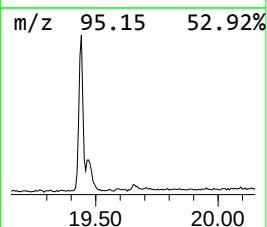
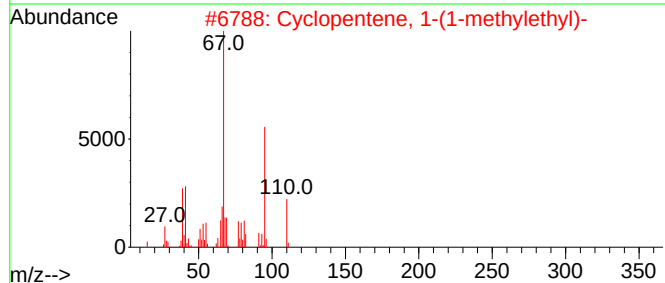
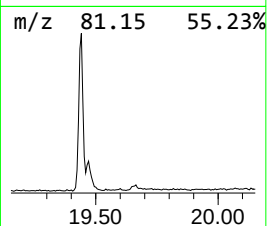
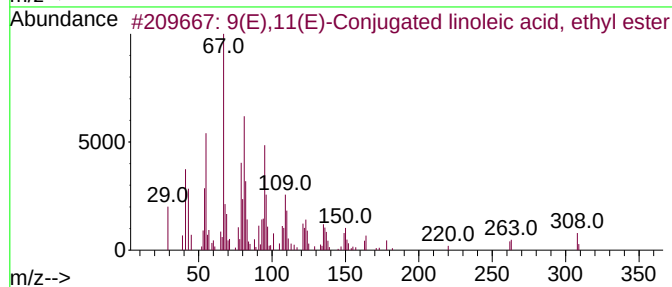
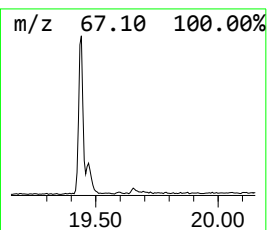
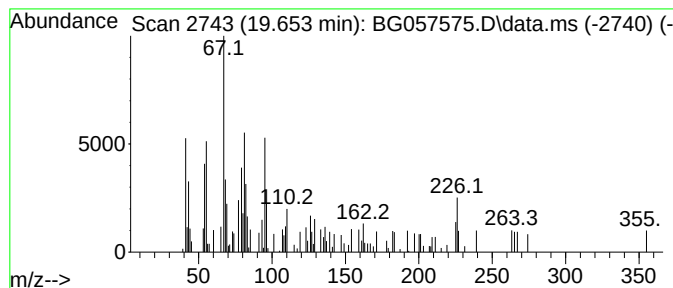
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 9(E),11(E)-Conjugated linol... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.653	2.10 ng	44418	Phenanthrene-d10	17.708

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9(E),11(E)-Conjugated linoleic a...	308	C20H36O2	1000452-08-1	59		
2	Cyclopentene, 1-(1-methylethyl)-	110	C8H14	001462-07-3	49		
3	3,4-Octadiene, 7-methyl-	124	C9H16	037050-05-8	47		
4	1,E-8,Z-10-Tetradecatatriene	192	C14H24	080625-31-6	47		
5	1,E-11,Z-13-Octadecatatriene	248	C18H32	080625-36-1	43		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052523\
Data File : BG057575.D
Acq On : 26 May 2023 2:46
Operator : CG/JU
Sample : 02938-01 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SU-04-052423

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.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
Benzophenone	16.299	3.2	ng	55268	3	14.965	347658	20.0
Hexadecanoic ac...	18.313	6.8	ng	144803	4	17.708	423006	20.0
n-Hexadecanoic ...	18.543	3.6	ng	75848	4	17.708	423006	20.0
9,12-Octadecadi...	19.441	31.2	ng	659287	4	17.708	423006	20.0
15-Octadecenoic...	19.471	18.8	ng	398267	4	17.708	423006	20.0
Methyl stearate	19.594	3.4	ng	72800	4	17.708	423006	20.0
9(E),11(E)-Conj...	19.653	2.1	ng	44418	4	17.708	423006	20.0