

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG032024\
 Data File : BG060695.D
 Acq On : 20 Mar 2024 17:18
 Operator : MA/JU
 Sample : P1804-03 2X
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 JC-03-03192024-B

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-BG031324.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG060695.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.788	400	408	415	rBV	669054	1102520	37.86%	4.645%
2	7.410	676	684	699	rVB	701846	1209609	41.54%	5.096%
3	8.297	828	835	844	rBV	404156	691636	23.75%	2.914%
4	9.490	1026	1038	1047	rBV	432994	803344	27.59%	3.385%
5	10.277	1165	1172	1177	rBV9	16331	36922	1.27%	0.156%
6	11.011	1292	1297	1302	rBV2	26233	41293	1.42%	0.174%
7	11.141	1311	1319	1325	rBV	553874	990969	34.03%	4.175%
8	12.445	1538	1541	1546	rBV2	28776	43207	1.48%	0.182%
9	12.991	1628	1634	1641	rBV8	27187	52595	1.81%	0.222%
10	13.250	1672	1678	1684	rBV8	17833	32939	1.13%	0.139%
11	13.549	1722	1729	1735	rBV	1109288	1707569	58.64%	7.194%
12	13.673	1745	1750	1755	rBV2	52805	76670	2.63%	0.323%
13	13.755	1759	1764	1769	rVB4	21936	39751	1.37%	0.167%
14	14.319	1855	1860	1863	rVB6	28378	40578	1.39%	0.171%
15	14.736	1928	1931	1936	rVB	52299	64030	2.20%	0.270%
16	14.924	1956	1963	1969	rBV	847254	1277679	43.88%	5.383%
17	15.688	2088	2093	2097	rVB	71458	93144	3.20%	0.392%
18	16.088	2153	2161	2166	rBV3	42022	90969	3.12%	0.383%
19	16.235	2184	2186	2194	rVB9	15501	29340	1.01%	0.124%
20	16.405	2209	2215	2227	rBV	787093	1236729	42.47%	5.211%
21	16.552	2235	2240	2245	rBV	85237	156430	5.37%	0.659%
22	17.339	2371	2374	2378	rBV	67070	80607	2.77%	0.340%
23	17.386	2378	2382	2387	rVB3	43277	62383	2.14%	0.263%
24	17.674	2425	2431	2436	rBV	971929	1468066	50.42%	6.185%
25	17.715	2436	2438	2443	rVB	117363	145939	5.01%	0.615%
26	17.809	2451	2454	2460	rBV2	34051	53376	1.83%	0.225%
27	18.085	2497	2501	2505	rVB	83674	109693	3.77%	0.462%
28	18.273	2528	2533	2540	rVB	463922	580581	19.94%	2.446%
29	18.497	2566	2571	2576	rBV	293342	424166	14.57%	1.787%
30	18.773	2615	2618	2622	rVB	113144	123013	4.22%	0.518%
31	19.407	2721	2726	2728	rBV	2375761	2911815	100.00%	12.268%
32	19.437	2728	2731	2742	rVB2	1282972	1919945	65.94%	8.089%
33	19.560	2748	2752	2755	rBV	280400	318426	10.94%	1.342%
34	19.613	2759	2761	2771	rVV7	112628	247648	8.50%	1.043%
35	19.707	2773	2777	2782	rVV	454932	670182	23.02%	2.824%
36	19.754	2782	2785	2789	rVV2	115369	137111	4.71%	0.578%

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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-BG031324.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	20.071	2835	2839	2844	rVB	464060	669983	23.01%	2.823%
38	20.253	2865	2870	2876	rBV	1783529	2290003	78.65%	9.648%
39	21.993	3159	3166	3171	rBV2	857524	1703940	58.52%	7.179%

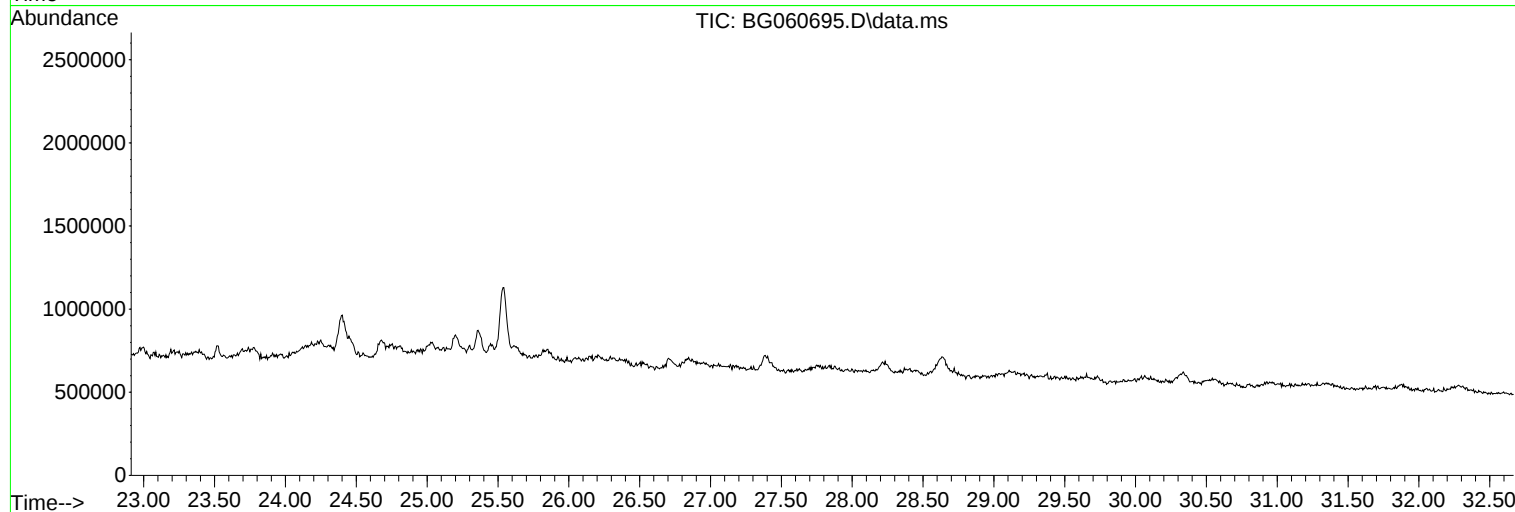
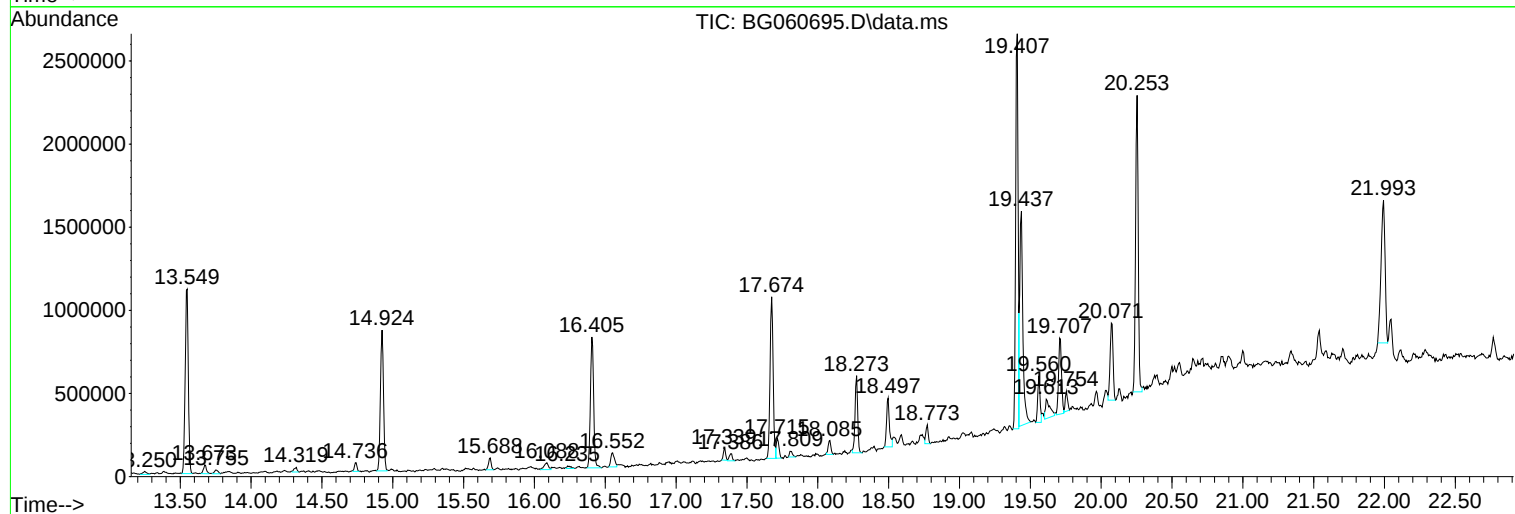
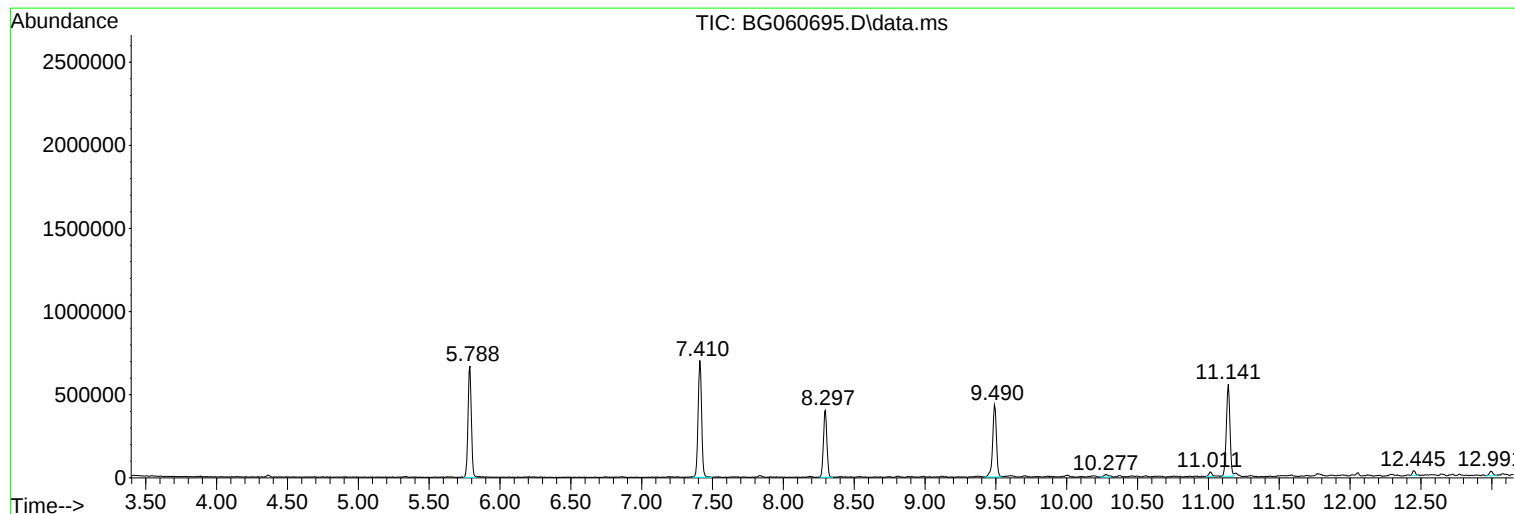
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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JC-03-03192024-B

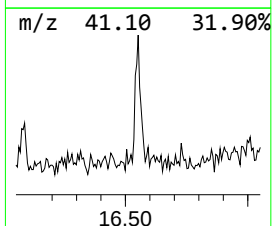
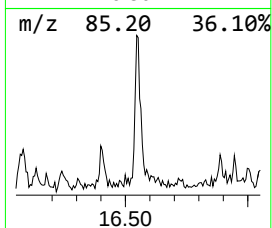
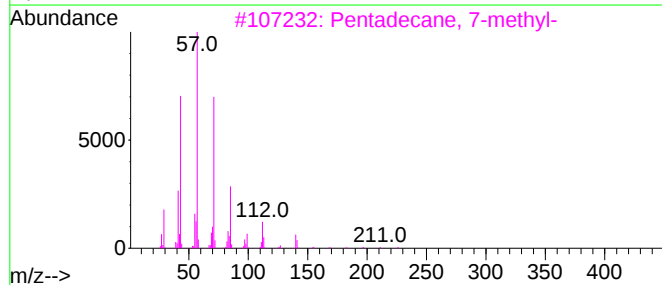
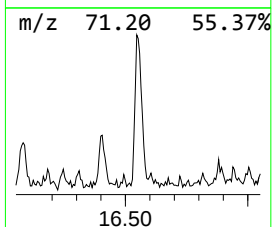
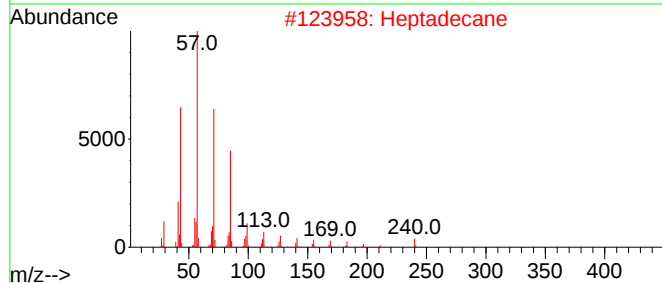
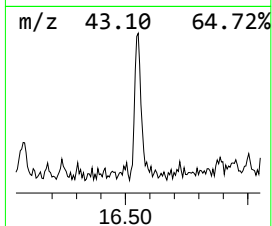
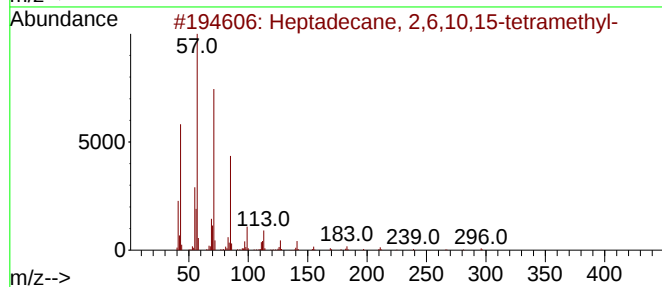
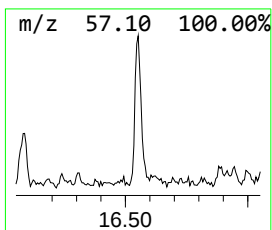
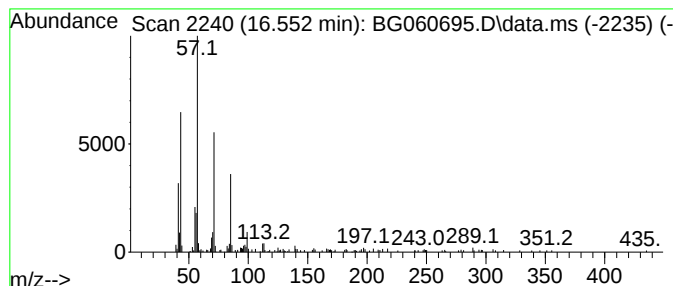
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Heptadecane, 2,6,10,15-tetr... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.552	2.13 ng	156430	Phenanthrene-d10	17.674

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	87
2		Heptadecane	240	C17H36	000629-78-7	87
3		Pentadecane, 7-methyl-	226	C16H34	006165-40-8	87
4		Heneicosane	296	C21H44	000629-94-7	87
5		Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	87



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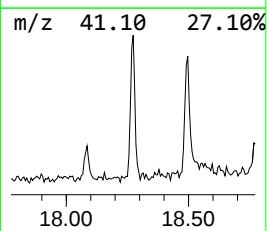
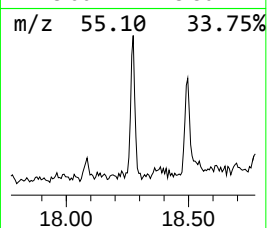
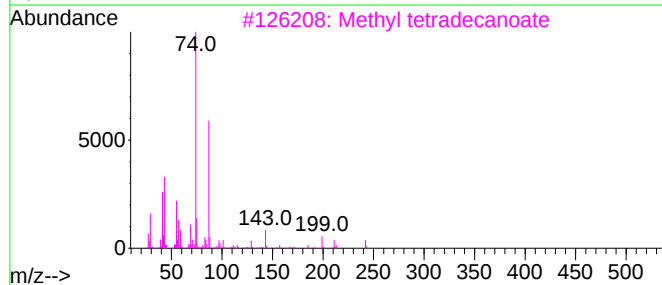
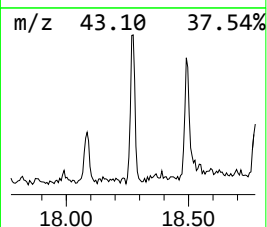
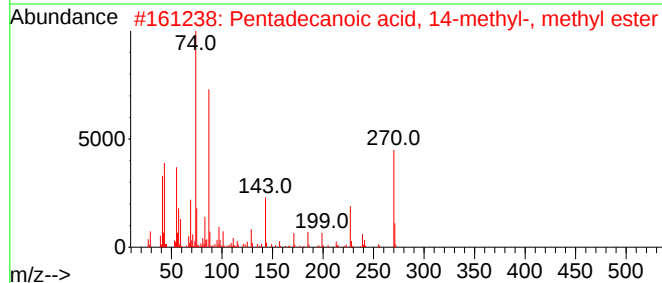
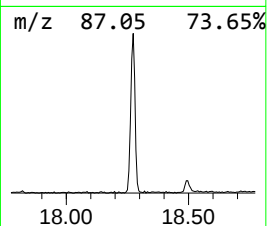
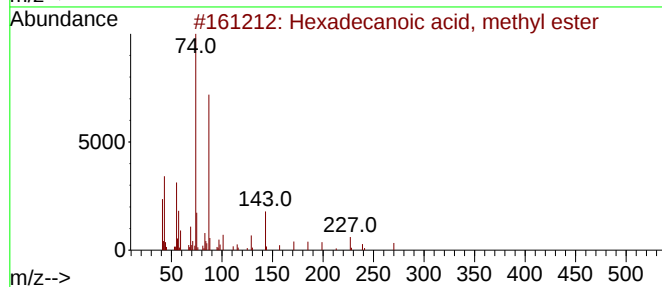
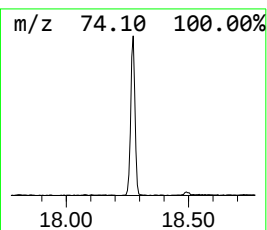
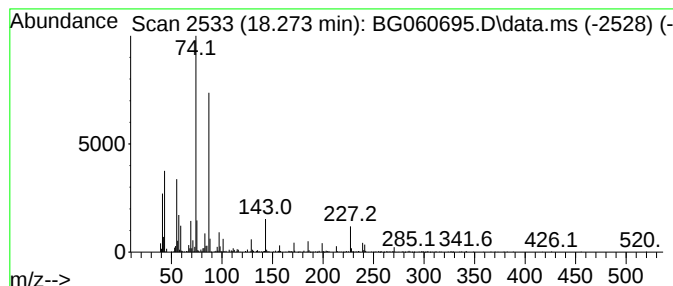
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Hexadecanoic acid, methyl e... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.273	7.91 ng	580581	Phenanthrene-d10	17.674

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	97
2			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	93
3			Methyl tetradecanoate	242	C15H30O2	000124-10-7	87
4			Methyl 11-methyl-dodecanoate	228	C14H28O2	1000336-45-1	83
5			Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	83



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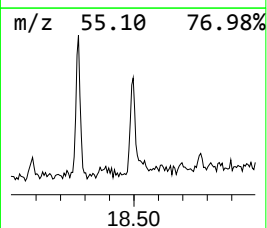
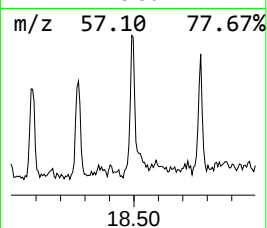
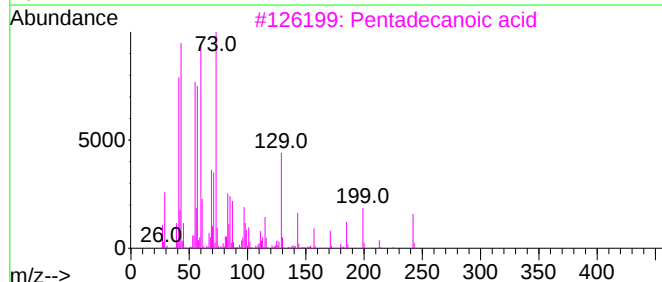
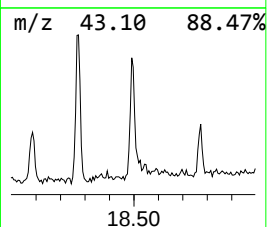
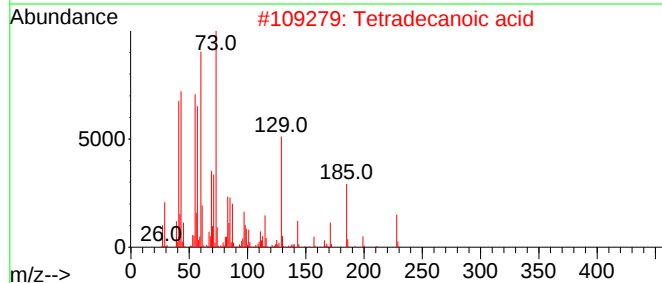
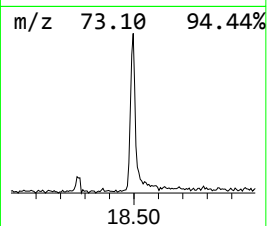
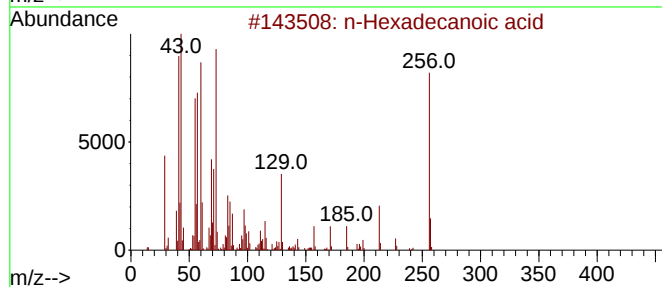
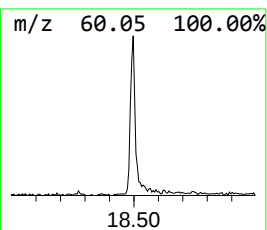
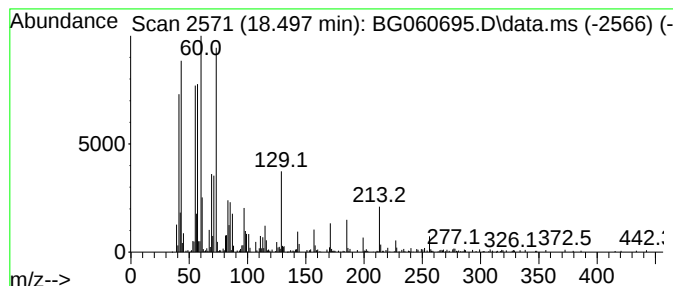
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031324.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.497	5.78 ng	424166	Phenanthrene-d10	17.674

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4			Octadecanoic acid	284	C18H36O2	000057-11-4	64
5			Dodecanoic acid	200	C12H24O2	000143-07-7	64



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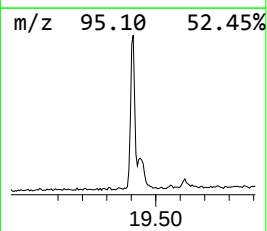
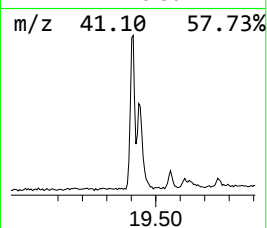
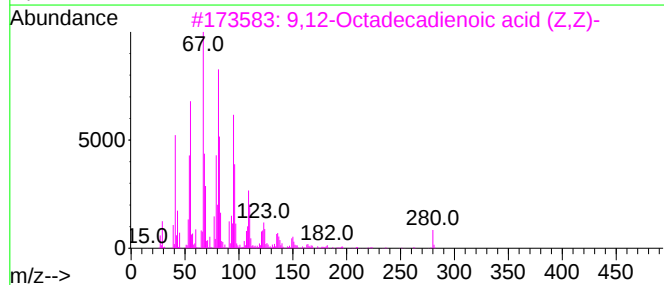
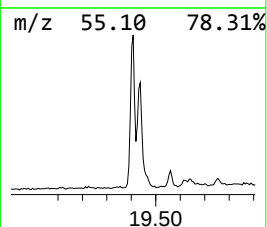
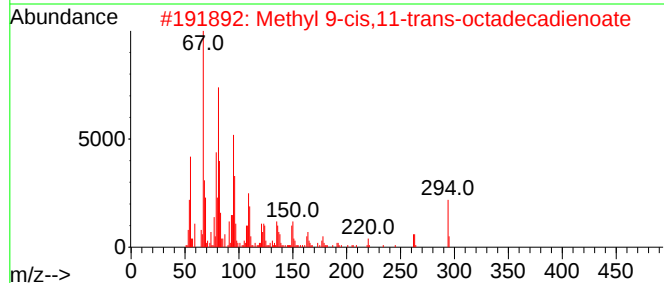
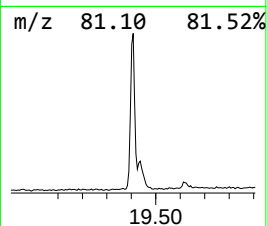
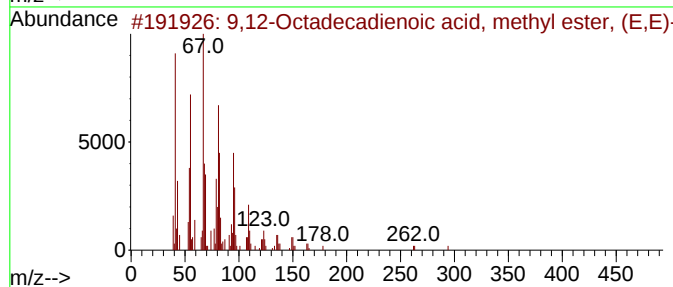
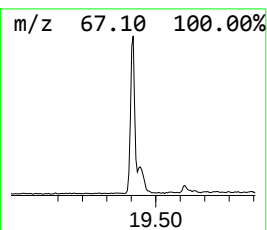
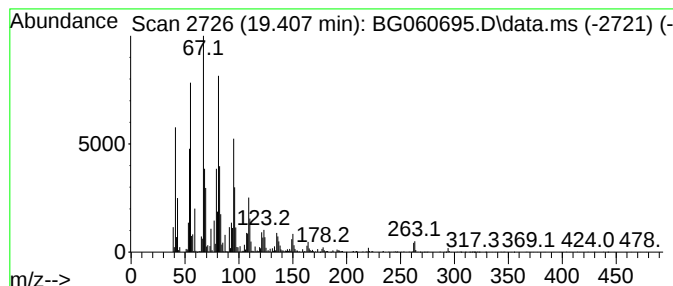
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Peak Number 4 9,12-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.407	39.67 ng	2911820	Phenanthrene-d10	17.674

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
2			Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	013058-52-1	97
3			9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	95
4			9,17-Octadecadienal, (Z)-	264	C18H32O	056554-35-9	94
5			Linoelaidic acid	280	C18H32O2	000506-21-8	94



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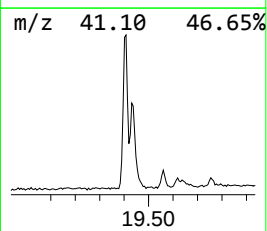
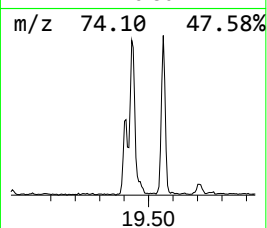
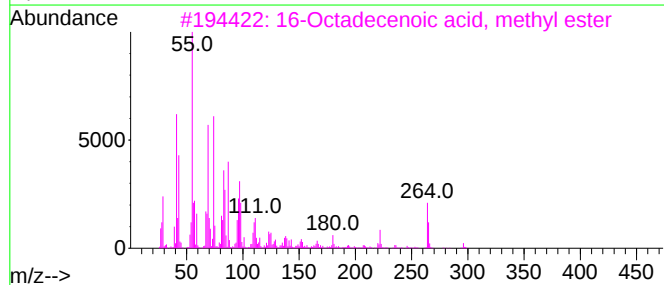
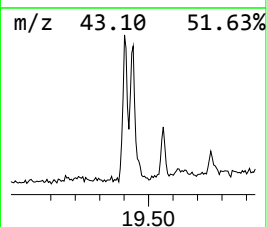
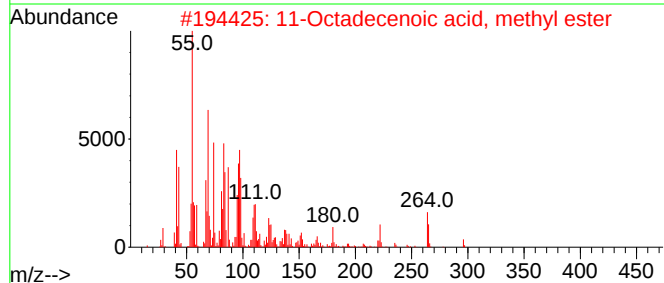
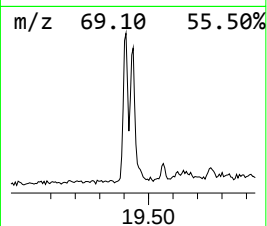
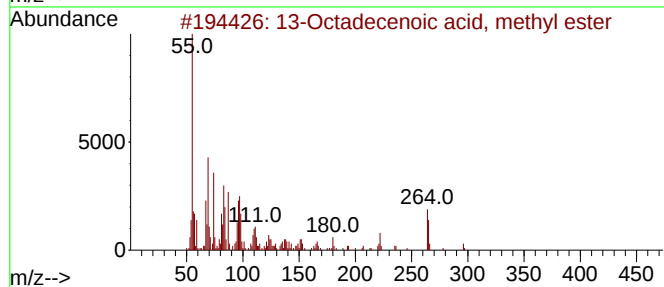
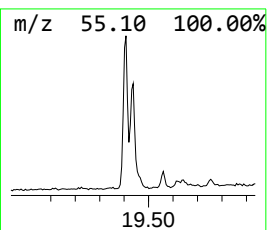
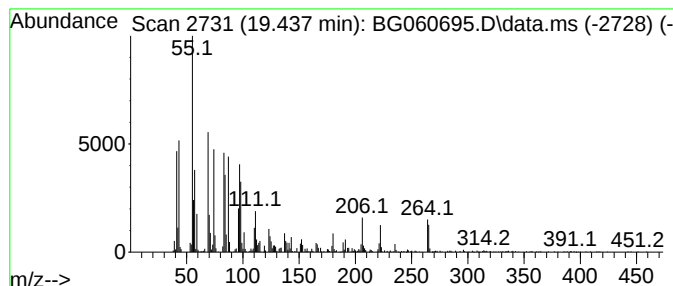
Instrument :
BNA_G
ClientSampleId :
JC-03-03192024-B

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 13-Octadecenoic acid, methyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.437	26.16 ng	1919950	Phenanthrene-d10	17.674	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	93
2	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	87
3	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	86
4	9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	72
5	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG032024\
Data File : BG060695.D
Acq On : 20 Mar 2024 17:18
Operator : MA/JU
Sample : P1804-03 2X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
JC-03-03192024-B

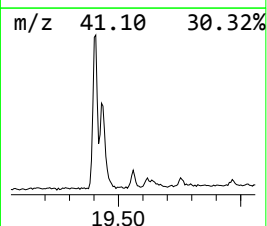
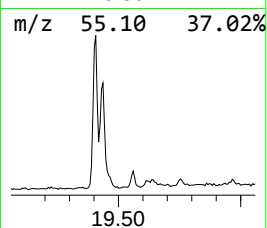
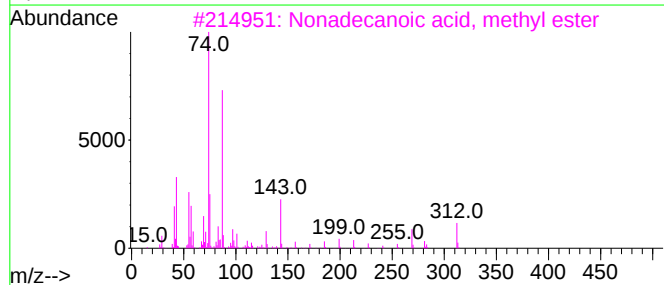
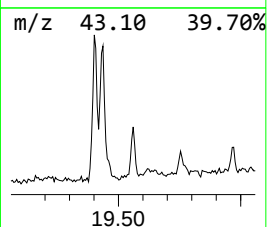
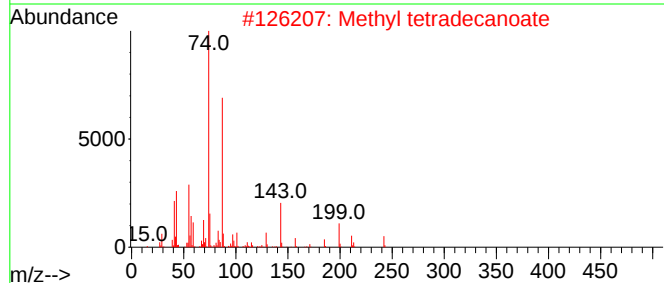
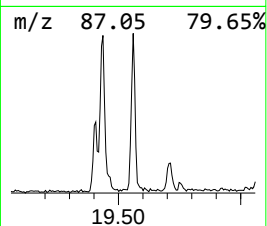
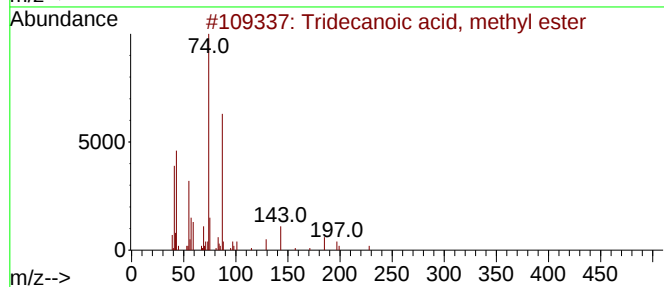
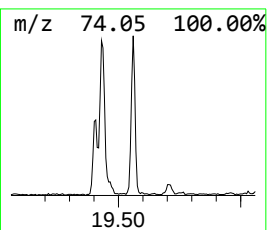
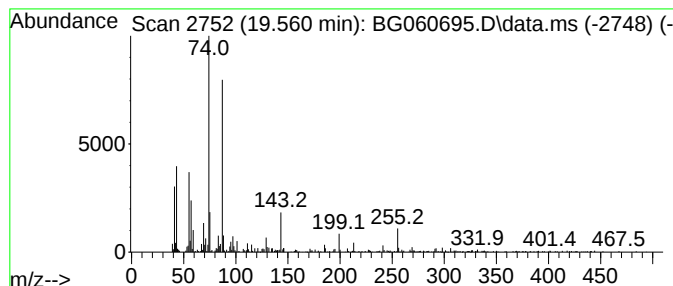
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Tridecanoic acid, methyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.560	4.34 ng	318426	Phenanthrene-d10	17.674

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	91
2			Methyl tetradecanoate	242	C15H30O2	000124-10-7	87
3			Nonadecanoic acid, methyl ester	312	C20H40O2	001731-94-8	87
4			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	87
5			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG032024\
Data File : BG060695.D
Acq On : 20 Mar 2024 17:18
Operator : MA/JU
Sample : P1804-03 2X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
JC-03-03192024-B

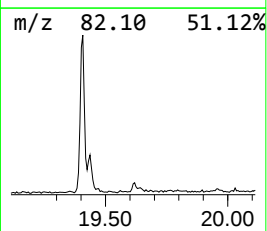
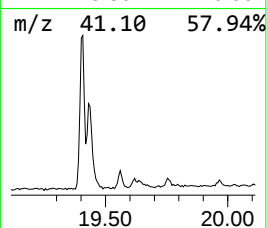
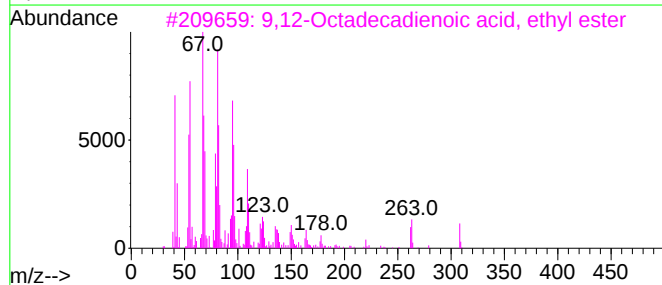
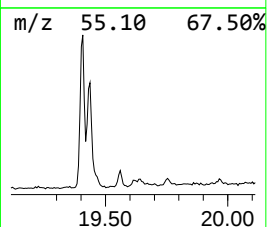
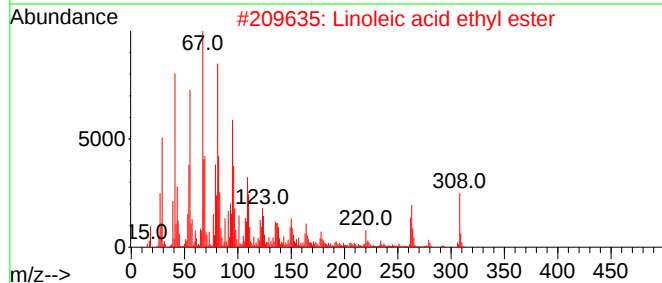
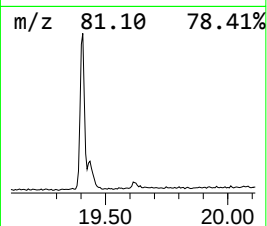
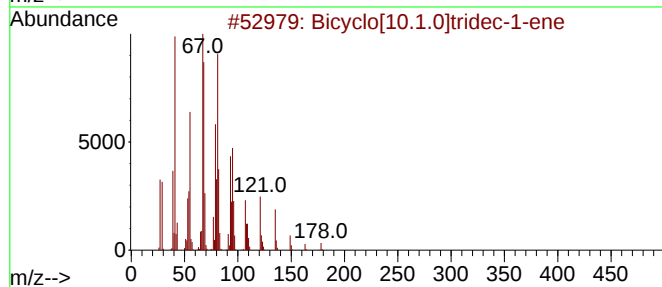
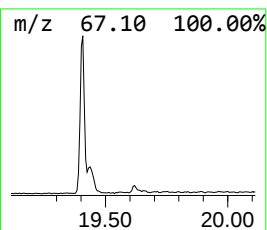
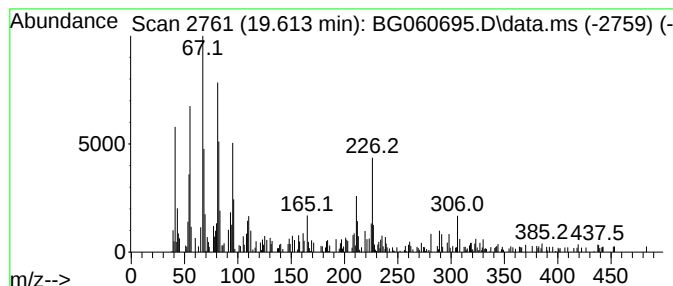
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Bicyclo[10.1.0]tridec-1-ene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.613	3.37 ng	247648	Phenanthrene-d10	17.674

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[10.1.0]tridec-1-ene	178	C13H22	054766-91-5	58
2			Linoleic acid ethyl ester	308	C20H36O2	000544-35-4	58
3			9,12-Octadecadienoic acid, ethyl...	308	C20H36O2	007619-08-1	58
4			3,9-Dodecadiene	166	C12H22	054764-65-7	58
5			9-Octadecynoic acid, methyl ester	294	C19H34O2	001120-32-7	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG032024\
Data File : BG060695.D
Acq On : 20 Mar 2024 17:18
Operator : MA/JU
Sample : P1804-03 2X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
JC-03-03192024-B

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031324.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
Heptadecane, 2,...	16.552	2.1	ng	156430	4	17.674	1468070	20.0
Hexadecanoic ac...	18.273	7.9	ng	580581	4	17.674	1468070	20.0
n-Hexadecanoic ...	18.497	5.8	ng	424166	4	17.674	1468070	20.0
9,12-Octadecadi...	19.407	39.7	ng	2911820	4	17.674	1468070	20.0
13-Octadecenoic...	19.437	26.2	ng	1919950	4	17.674	1468070	20.0
Tridecanoic aci...	19.560	4.3	ng	318426	4	17.674	1468070	20.0
Bicyclo[10.1.0]...	19.613	3.4	ng	247648	4	17.674	1468070	20.0