

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032223\
 Data File : BM039106.D
 Acq On : 22 Mar 2023 23:53
 Operator : CG/JU
 Sample : 02022-01
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 AU-05-32123

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_M\Methods\8270-BM030823.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM039106.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.446	192	197	201	rBV	127148	168559	1.52%	0.232%
2	5.057	295	301	308	rBV	2275726	3061861	27.60%	4.220%
3	5.522	373	380	389	rBV	4396004	6402392	57.71%	8.824%
4	7.128	642	653	661	rBV	4161013	6521690	58.79%	8.988%
5	7.969	786	796	804	rBV	1163069	1873212	16.89%	2.582%
6	9.075	975	984	988	rBV2	76623	154666	1.39%	0.213%
7	9.134	988	994	1002	rVV	2550942	4126825	37.20%	5.687%
8	9.957	1129	1134	1142	rBV5	42760	121421	1.09%	0.167%
9	10.780	1262	1274	1280	rBV	1438407	2612610	23.55%	3.601%
10	11.251	1349	1354	1362	rVB4	57745	128344	1.16%	0.177%
11	11.692	1423	1429	1436	rBV5	60925	122021	1.10%	0.168%
12	11.969	1467	1476	1483	rBV3	93275	192221	1.73%	0.265%
13	12.192	1505	1514	1519	rBV2	166134	289783	2.61%	0.399%
14	12.686	1587	1598	1603	rBV2	98136	199794	1.80%	0.275%
15	13.145	1672	1676	1682	rVB2	78622	139832	1.26%	0.193%
16	13.233	1682	1691	1701	rBV	6181126	8762142	78.98%	12.076%
17	13.427	1719	1724	1732	rVB	242793	367293	3.31%	0.506%
18	13.551	1737	1745	1750	rVB2	55654	122303	1.10%	0.169%
19	13.769	1773	1782	1787	rBV10	51468	141300	1.27%	0.195%
20	14.086	1829	1836	1839	rBV2	78921	141063	1.27%	0.194%
21	14.498	1902	1906	1914	rVB	269883	348169	3.14%	0.480%
22	14.604	1915	1924	1931	rBV	1995280	3016834	27.19%	4.158%
23	15.451	2063	2068	2072	rVB	228497	287656	2.59%	0.396%
24	15.963	2149	2155	2161	rBV	739198	1022828	9.22%	1.410%
25	16.092	2170	2177	2185	rBV	3712412	5219493	47.05%	7.193%
26	16.310	2210	2214	2217	rBV	230271	338475	3.05%	0.466%
27	17.104	2345	2349	2353	rBV	203080	238007	2.15%	0.328%
28	17.157	2355	2358	2370	rVB2	111889	197272	1.78%	0.272%
29	17.351	2385	2391	2395	rBV	2367894	3218271	29.01%	4.435%
30	17.392	2395	2398	2404	rVB	346169	471448	4.25%	0.650%
31	17.480	2410	2413	2418	rVB	97586	129517	1.17%	0.178%
32	17.845	2471	2475	2478	rBV	172743	206469	1.86%	0.285%
33	18.021	2501	2505	2509	rVB	310294	371710	3.35%	0.512%
34	18.245	2538	2543	2553	rBV2	602411	1131134	10.20%	1.559%
35	18.539	2589	2593	2597	rBV	176828	236585	2.13%	0.326%
36	19.156	2694	2698	2701	rBV2	1238467	1547458	13.95%	2.133%

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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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	19.192	2701	2704	2713	rVB2	820467	1079323	9.73%	1.487%
38	19.321	2723	2726	2731	rBV2	196776	267106	2.41%	0.368%
39	19.403	2736	2740	2747	rVB	724735	1058818	9.54%	1.459%
40	19.515	2757	2759	2764	rBV	218657	270746	2.44%	0.373%
41	19.768	2799	2802	2811	rVB	515651	822429	7.41%	1.133%
42	19.968	2831	2836	2842	rBV	9085218	11093547	100.00%	15.289%
43	21.233	3048	3051	3059	rBV2	796267	1025476	9.24%	1.413%
44	21.527	3097	3101	3105	rVB	2534889	3311462	29.85%	4.564%

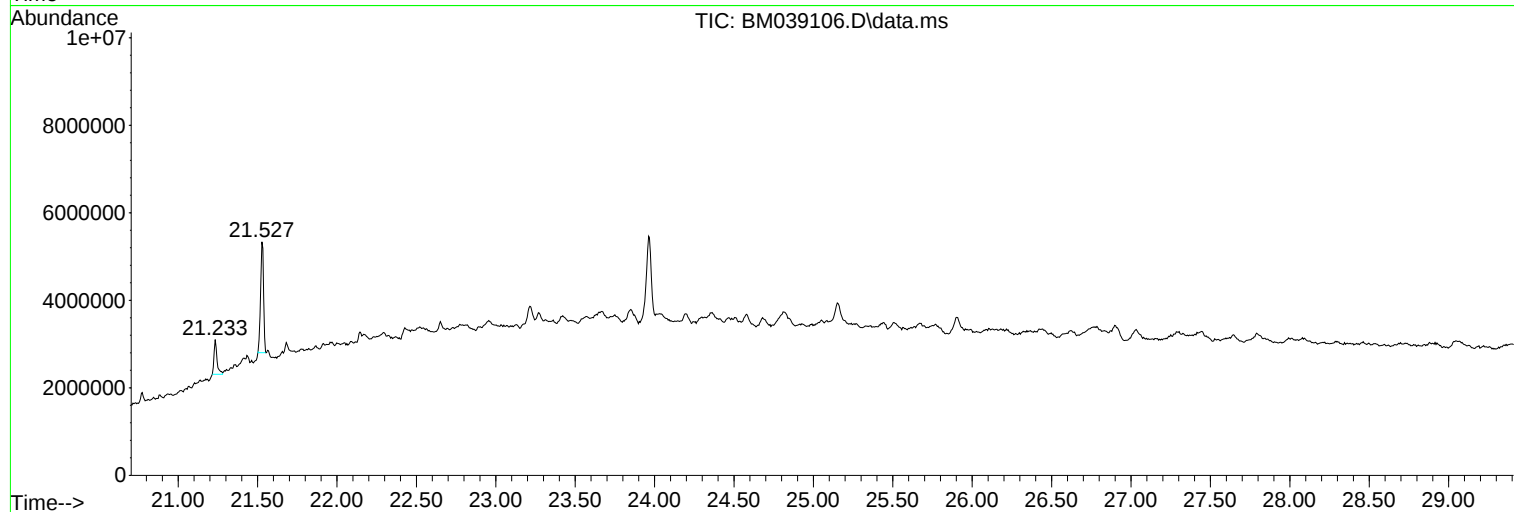
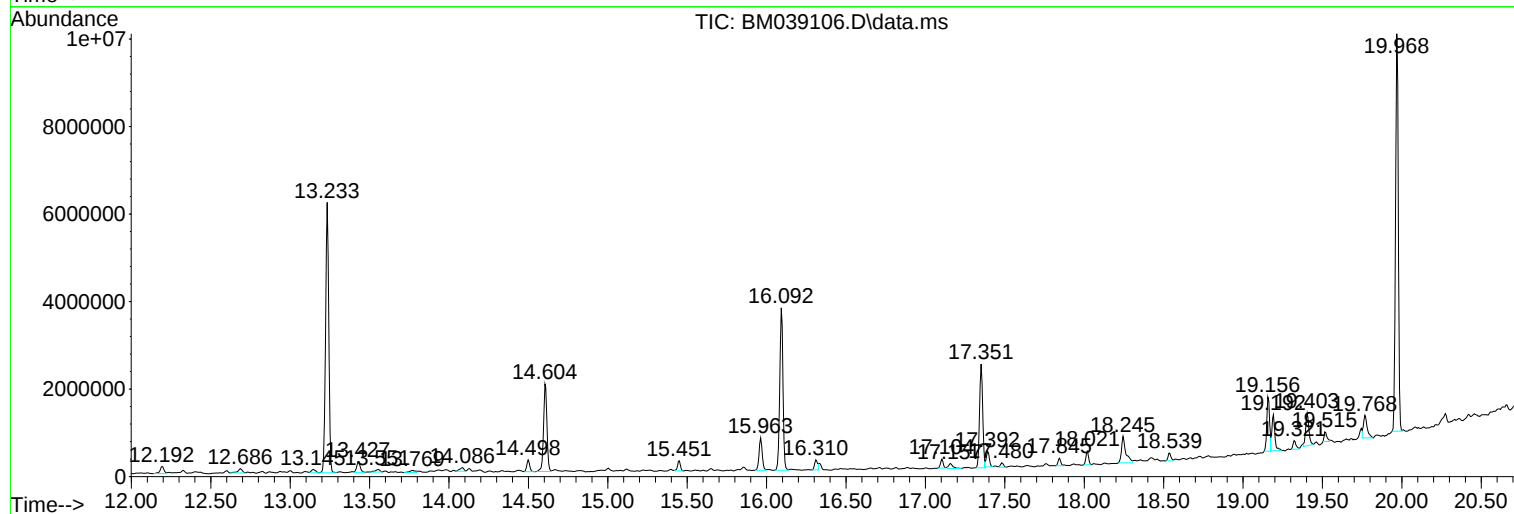
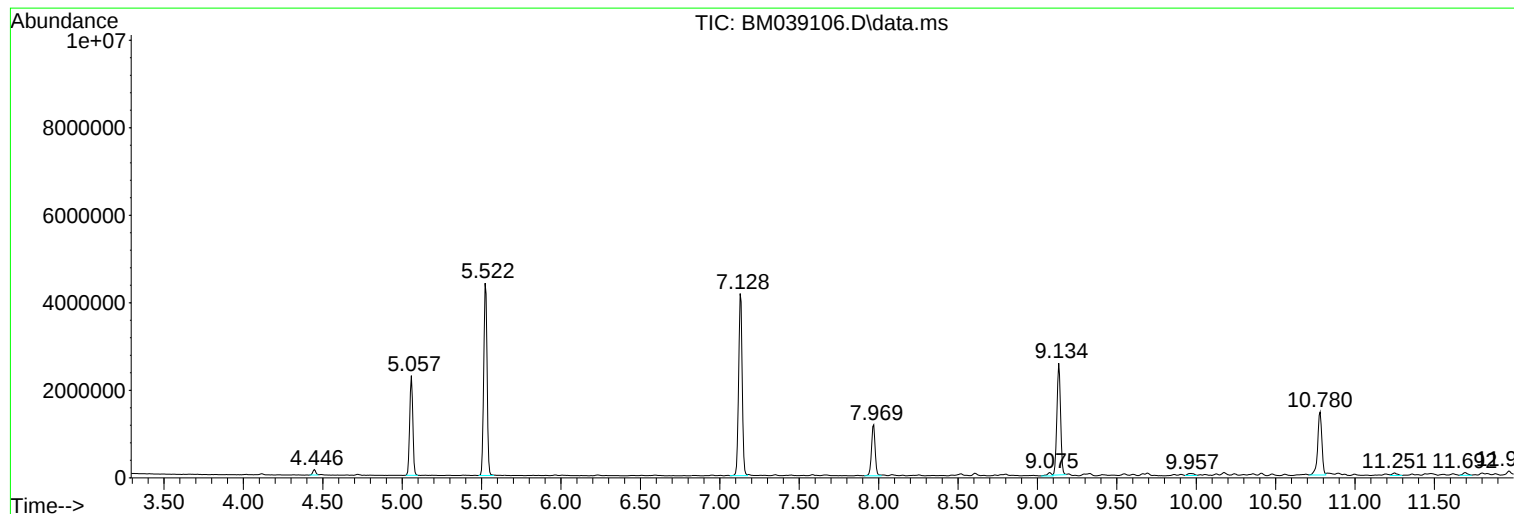
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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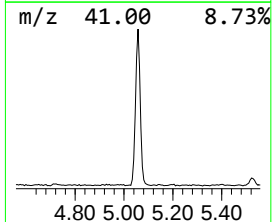
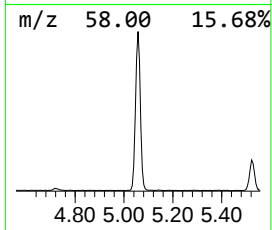
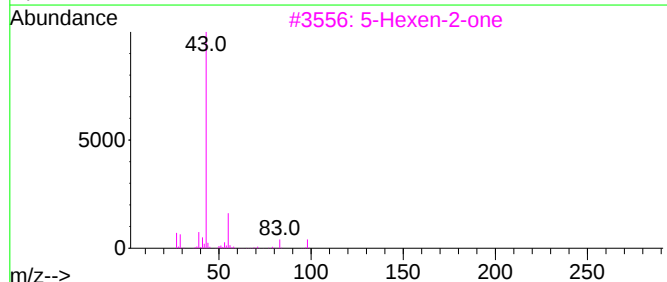
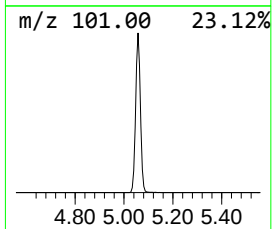
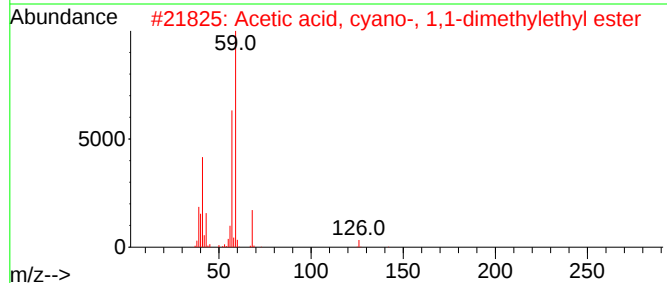
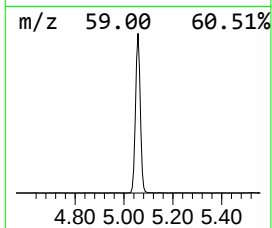
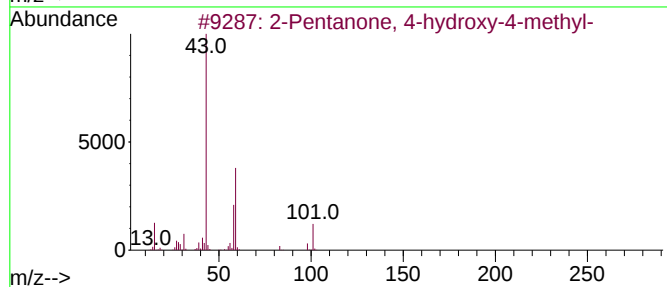
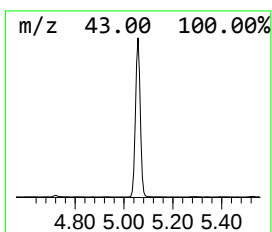
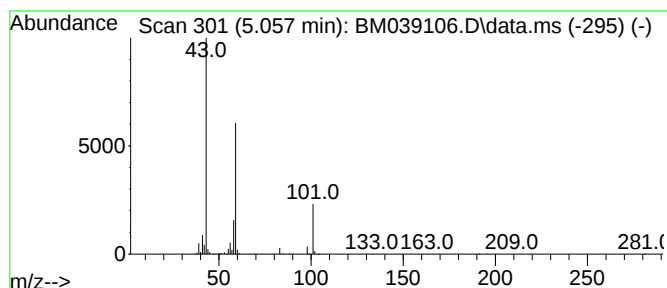
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.057	32.69 ng	3061860	1,4-Dichlorobenzene-d4	7.969

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3			5-Hexen-2-one	98	C6H10O	000109-49-9	9
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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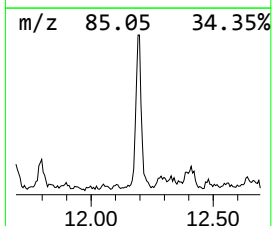
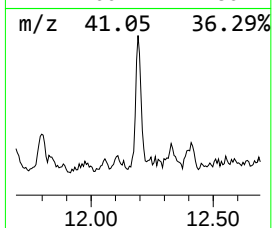
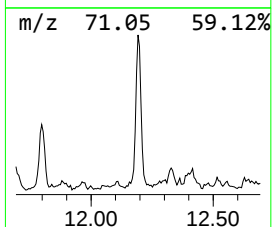
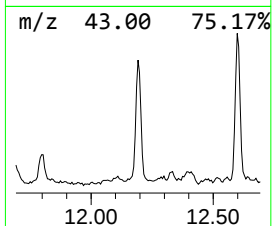
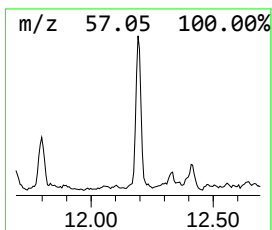
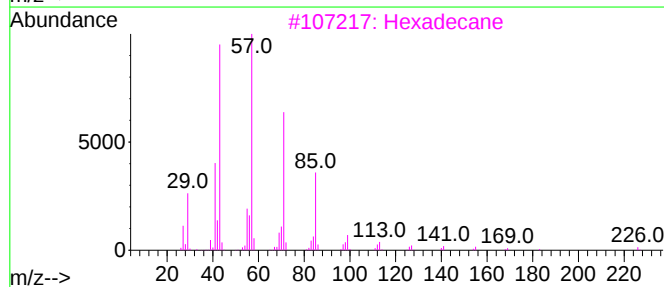
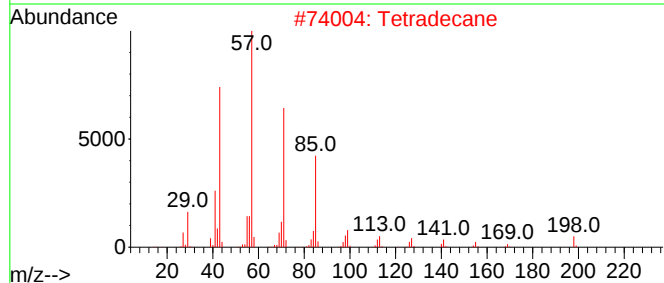
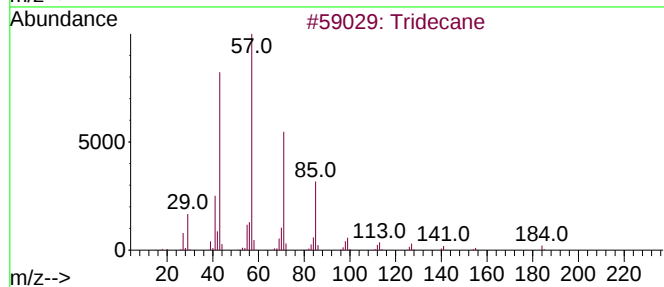
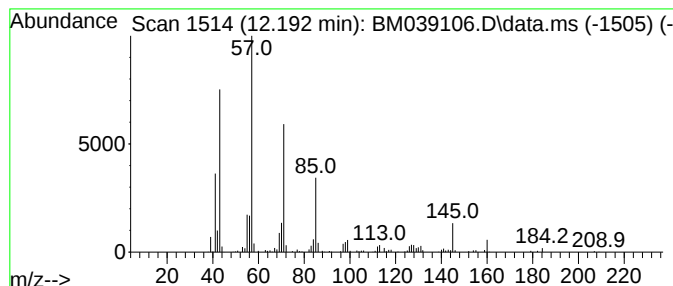
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Tridecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.192	2.22 ng	289783	Naphthalene-d8	10.781

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	94
2			Tetradecane	198	C14H30	000629-59-4	64
3			Hexadecane	226	C16H34	000544-76-3	64
4			Pentadecane	212	C15H32	000629-62-9	64
5			Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	58



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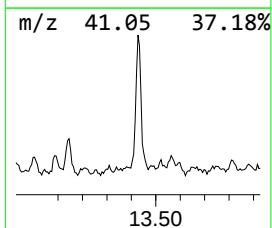
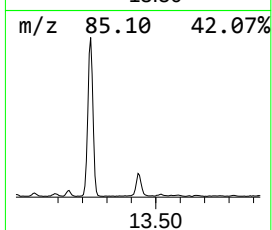
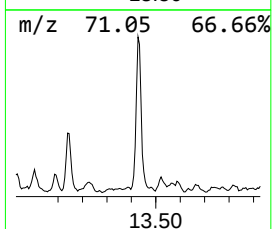
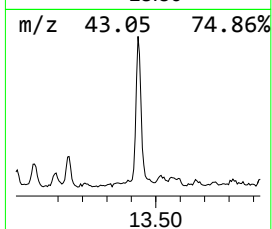
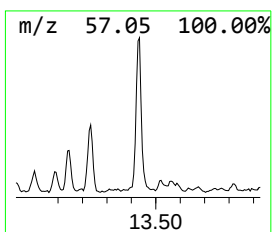
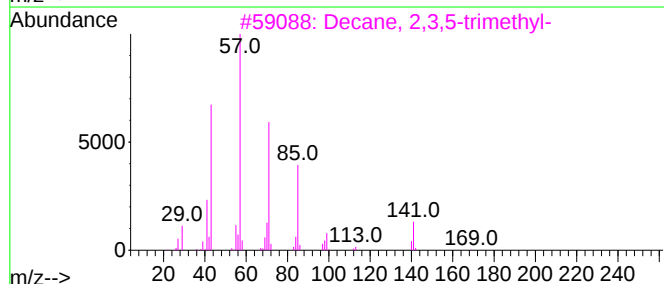
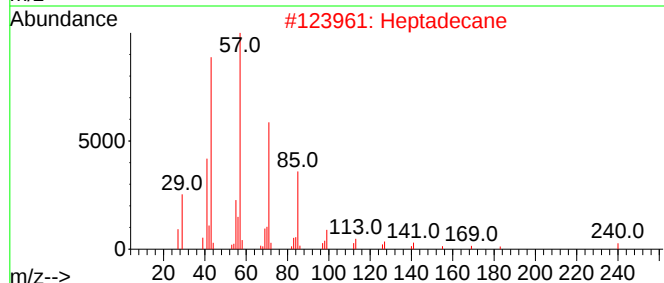
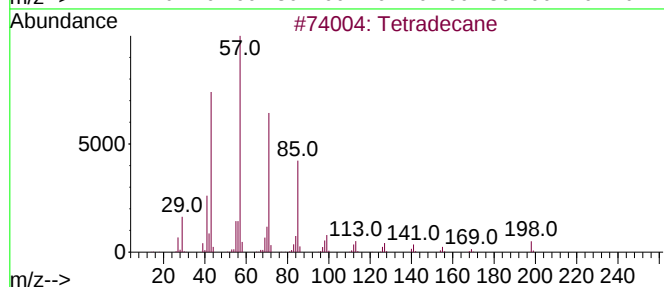
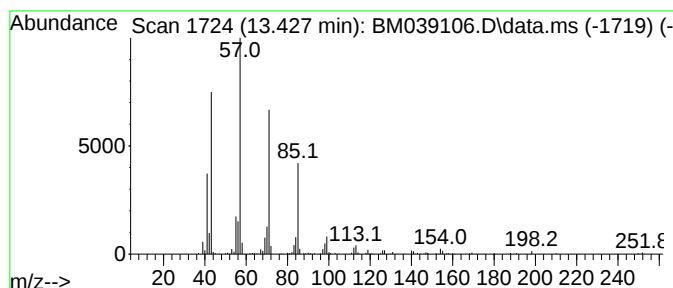
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Tetradecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.427	2.43 ng	367293	Acenaphthene-d10	14.604	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	94
2	Heptadecane	240	C17H36	000629-78-7	90
3	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	90
4	Decane, 2,3,6-trimethyl-	184	C13H28	062238-12-4	90
5	Tridecane	184	C13H28	000629-50-5	90



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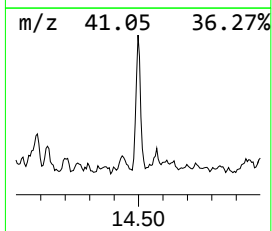
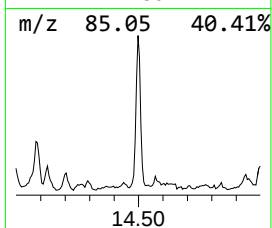
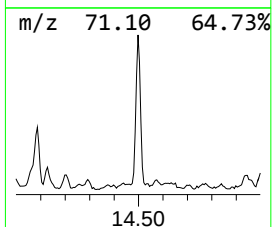
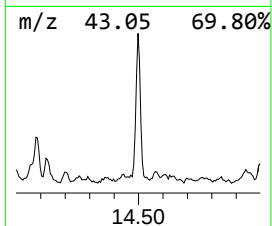
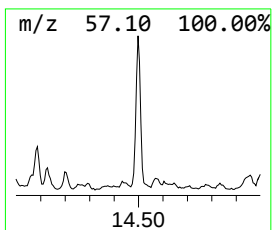
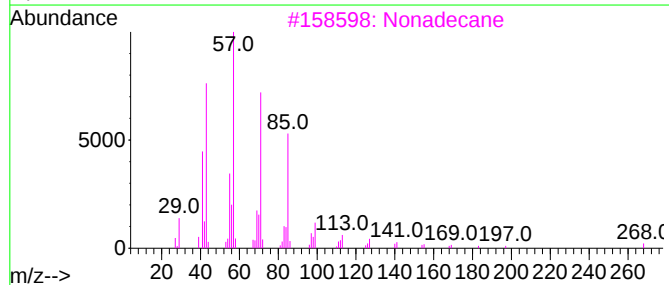
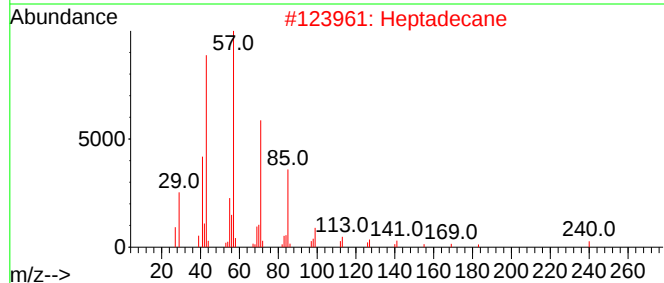
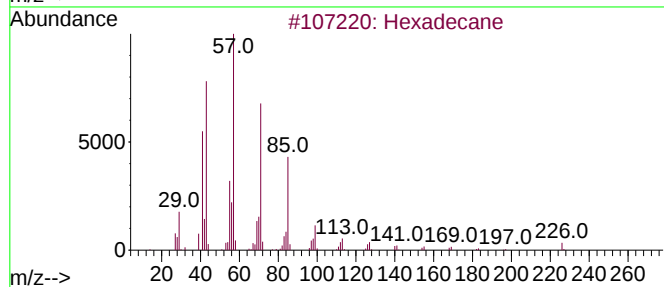
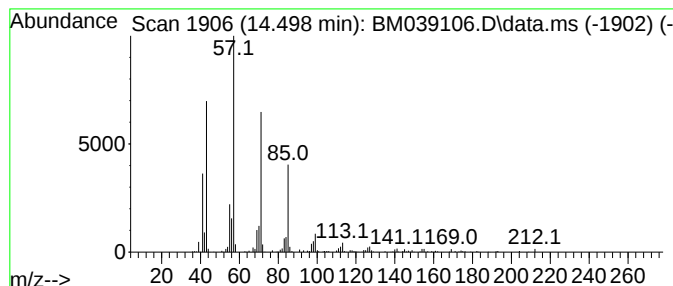
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Hexadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.498	2.31 ng	348169	Acenaphthene-d10	14.604

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane	226	C16H34	000544-76-3	87
2			Heptadecane	240	C17H36	000629-78-7	86
3			Nonadecane	268	C19H40	000629-92-5	86
4			Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	80
5			Tridecane	184	C13H28	000629-50-5	80



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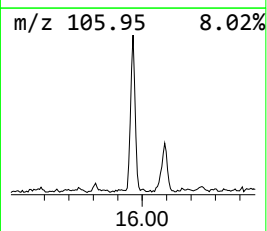
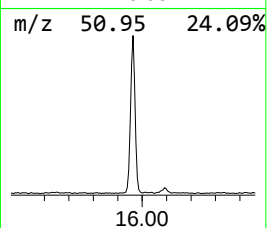
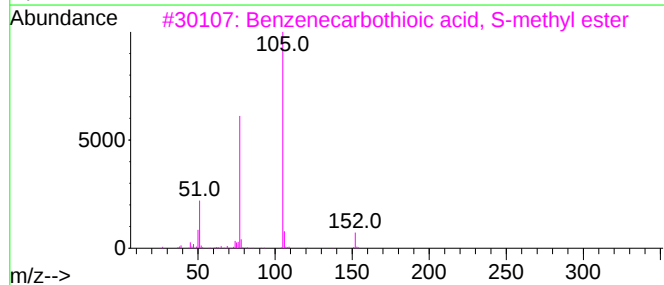
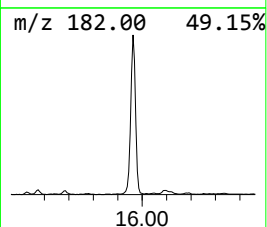
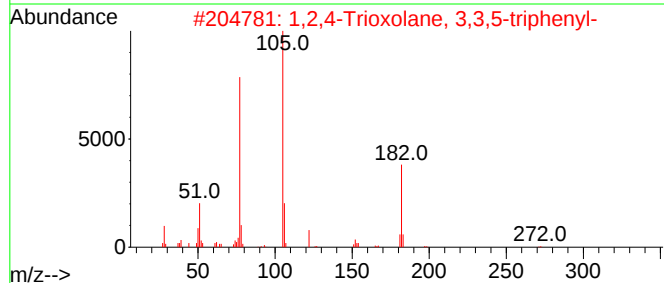
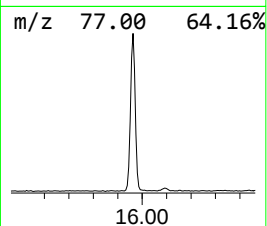
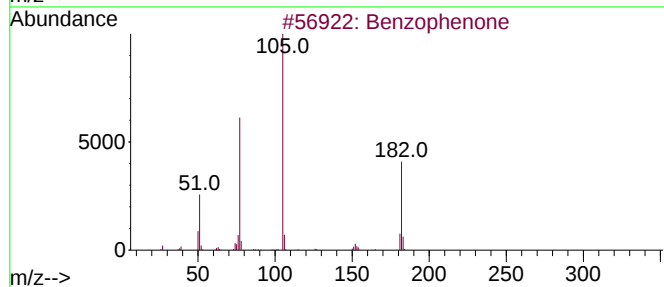
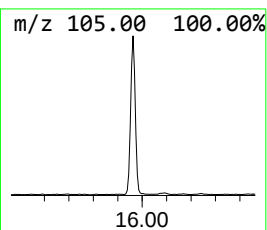
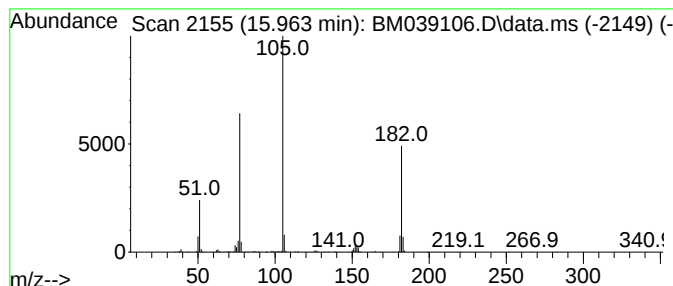
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.963	6.78 ng	1022830	Acenaphthene-d10	14.604

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			1,2,4-Trioxolane, 3,3,5-triphenyl-	304	C20H16O3	023246-12-0	64
3			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	50
4			N-Methylbenzamide, N-heptafluoro...	331	C12H8F7NO2	1000446-97-2	47
5			N-Methylbenzamide, N-trifluoroac...	231	C10H8F3NO2	1000446-91-5	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032223\
Data File : BM039106.D
Acq On : 22 Mar 2023 23:53
Operator : CG/JU
Sample : 02022-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
AU-05-32123

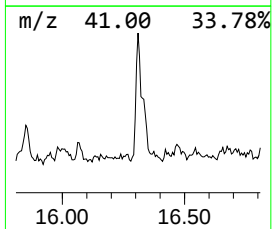
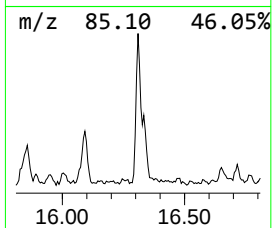
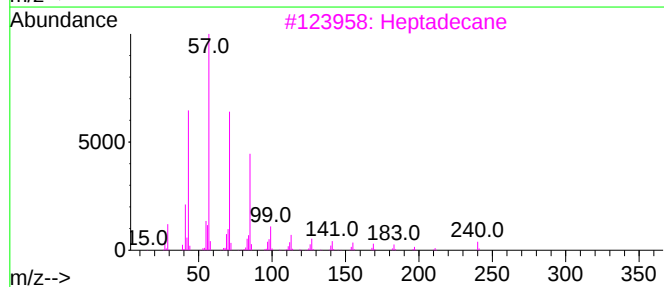
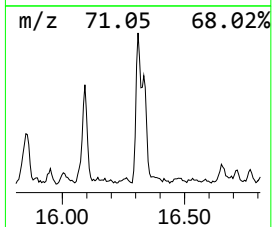
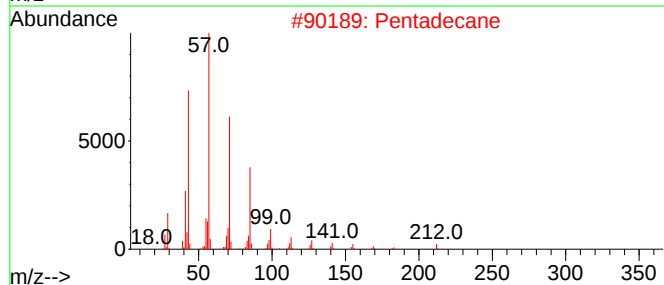
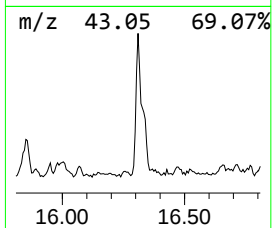
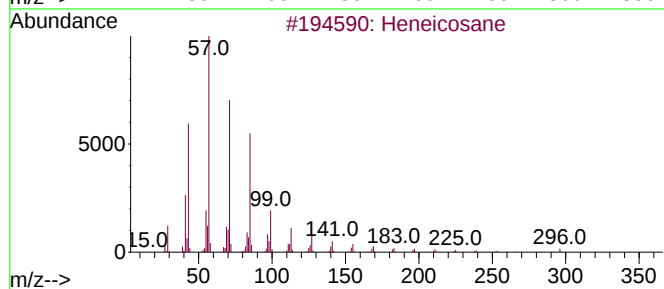
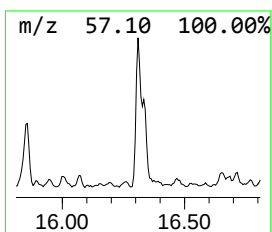
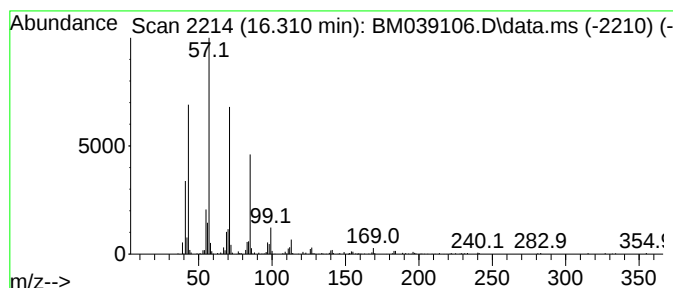
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heneicosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.310	2.10 ng	338475	Phenanthrene-d10	17.351

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	91
2			Pentadecane	212	C15H32	000629-62-9	90
3			Heptadecane	240	C17H36	000629-78-7	90
4			Octadecane	254	C18H38	000593-45-3	90
5			Nonadecane	268	C19H40	000629-92-5	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032223\
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Operator : CG/JU
Sample : 02022-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

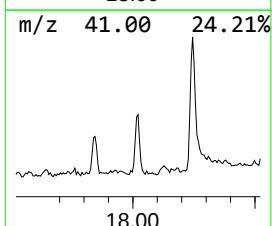
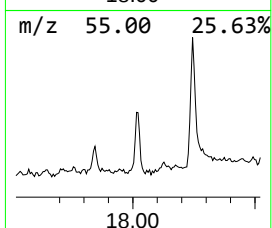
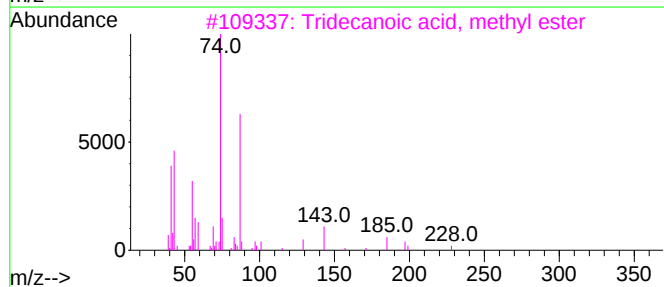
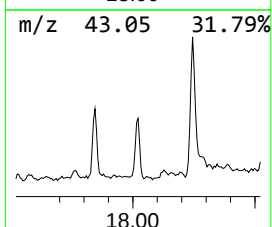
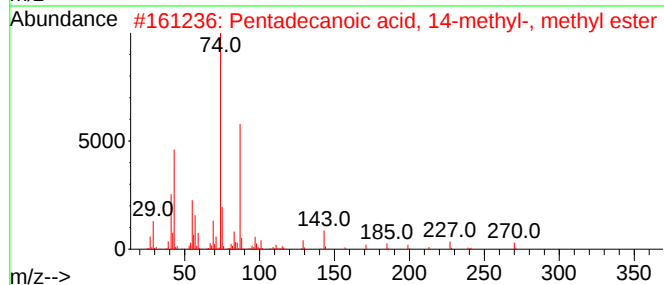
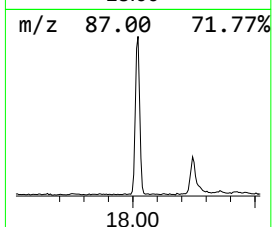
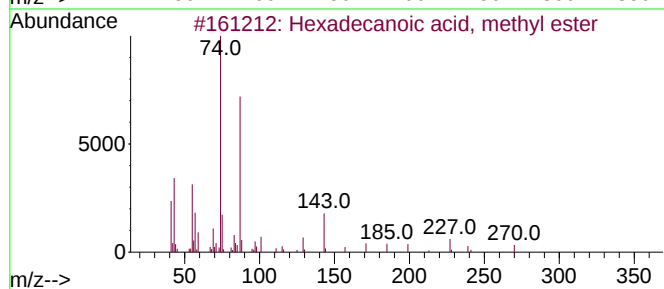
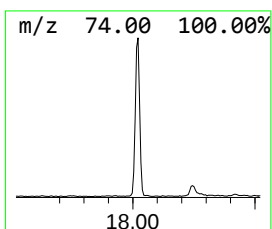
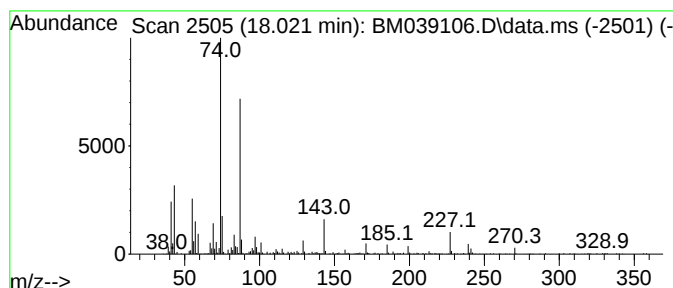
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ClientSampleId :
AU-05-32123

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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 Hexadecanoic acid, methyl e... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.021	2.31 ng	371710	Phenanthrene-d10	17.351	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	97
3	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	87
4	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	87
5	Methyl stearate	298	C19H38O2	000112-61-8	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032223\
Data File : BM039106.D
Acq On : 22 Mar 2023 23:53
Operator : CG/JU
Sample : 02022-01
Misc :
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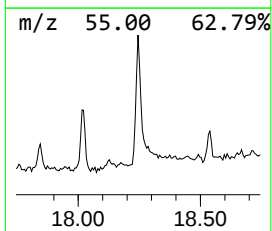
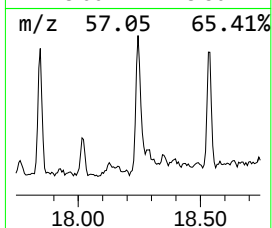
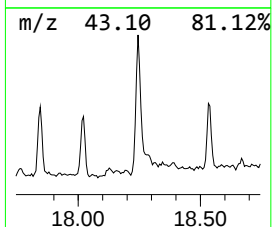
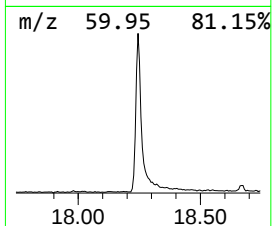
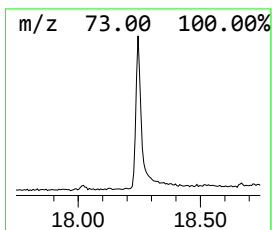
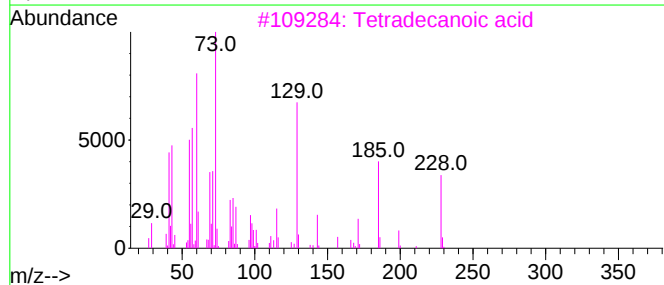
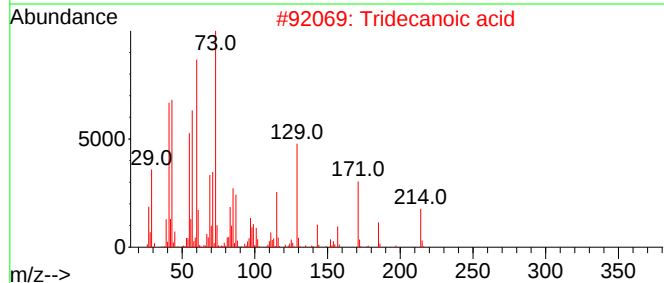
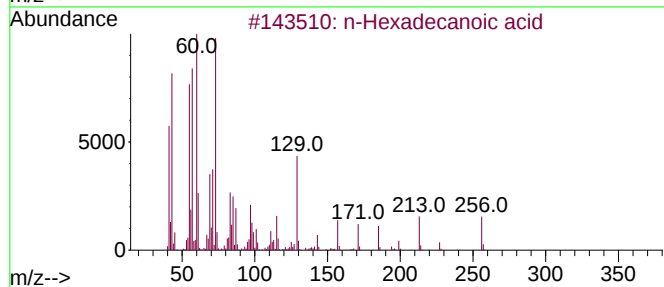
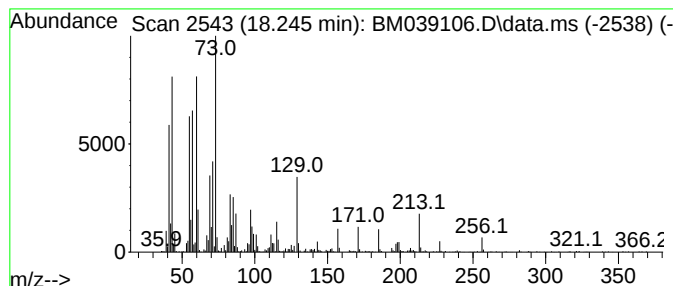
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.245	7.03 ng	1131130	Phenanthrene-d10	17.351	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
4	Octadecanoic acid	284	C18H36O2	000057-11-4	87
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032223\
Data File : BM039106.D
Acq On : 22 Mar 2023 23:53
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Sample : 02022-01
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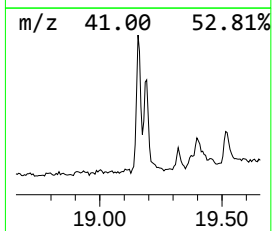
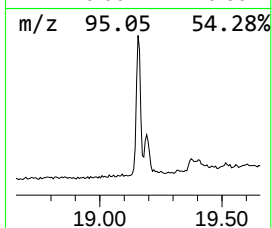
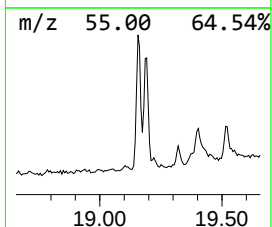
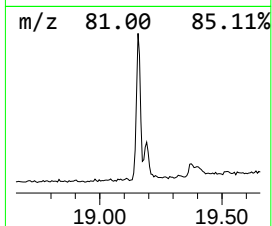
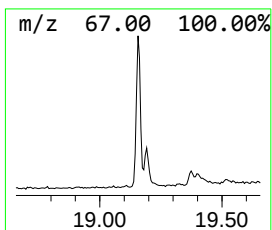
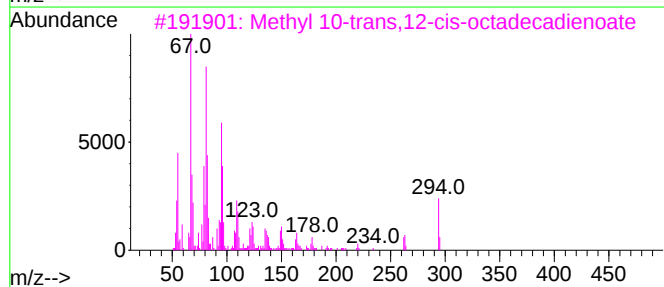
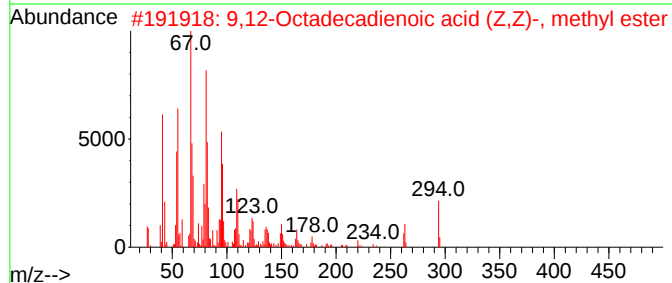
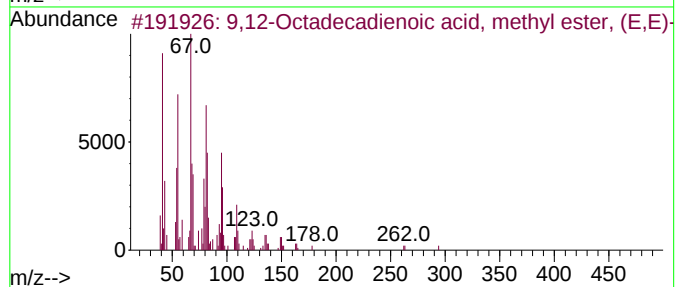
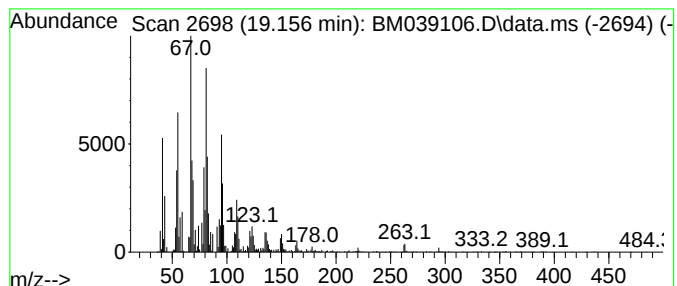
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 9,12-Octadecadienoic acid, ... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.156	9.62 ng	1547460	Phenanthrene-d10	17.351	
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	99
3	Methyl 10-trans,12-cis-octadecad...	294	C19H34O2	1000336-44-2	99
4	10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	98
5	9,11-Octadecadienoic acid, methy...	294	C19H34O2	013038-47-6	96



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032223\
Data File : BM039106.D
Acq On : 22 Mar 2023 23:53
Operator : CG/JU
Sample : 02022-01
Misc :
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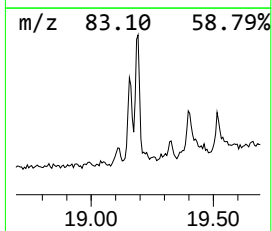
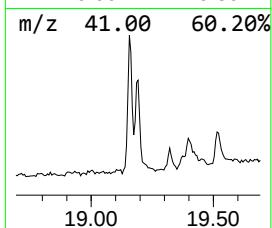
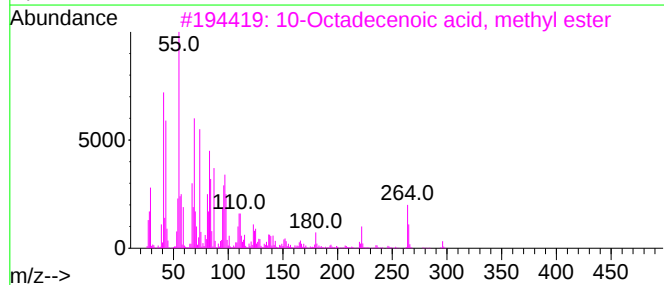
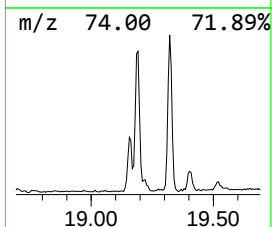
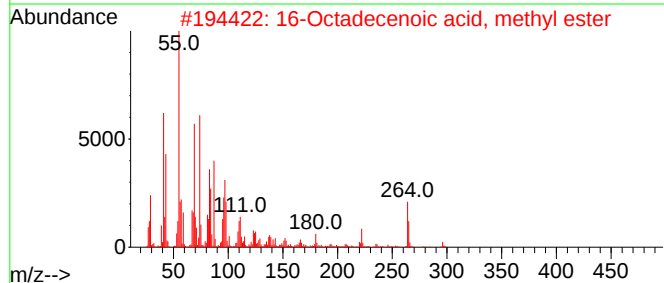
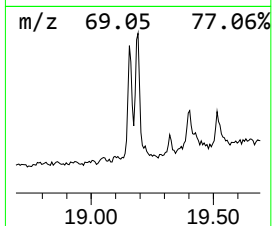
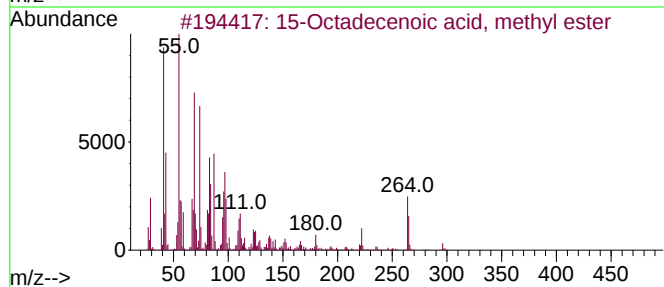
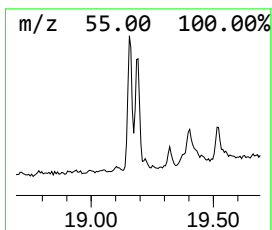
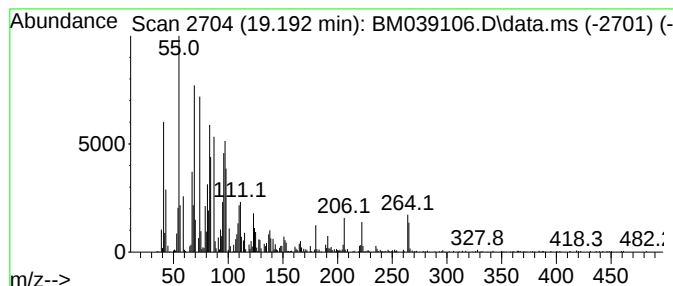
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 15-Octadecenoic acid, methy... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.192	6.71 ng	1079320	Phenanthrene-d10	17.351	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	99
2	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	99
3	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	99
4	10-Octadecenoic acid, methyl est...	296	C19H36O2	013038-45-4	99
5	9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	97



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032223\
Data File : BM039106.D
Acq On : 22 Mar 2023 23:53
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ALS Vial : 15 Sample Multiplier: 1

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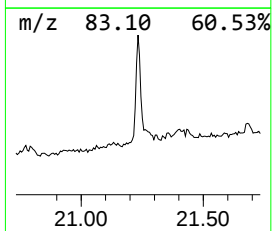
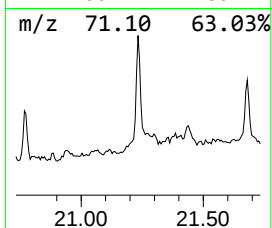
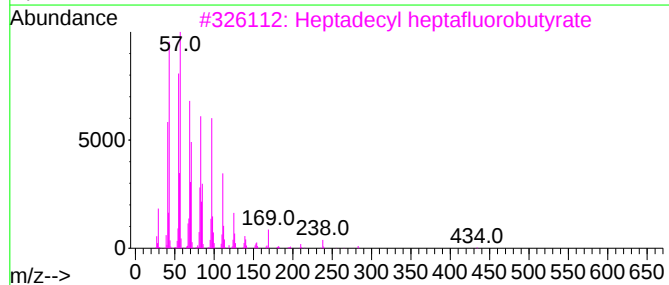
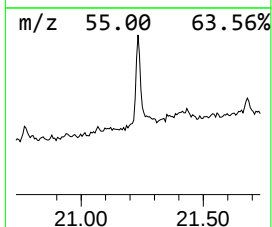
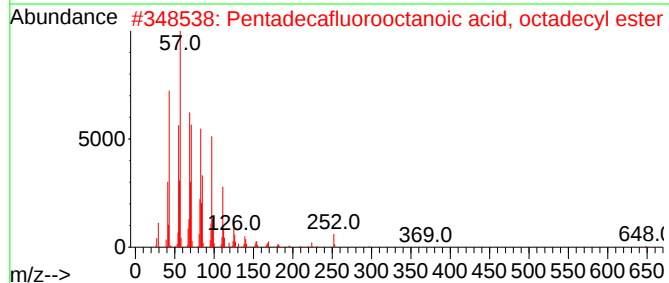
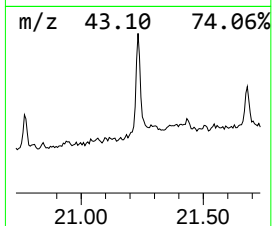
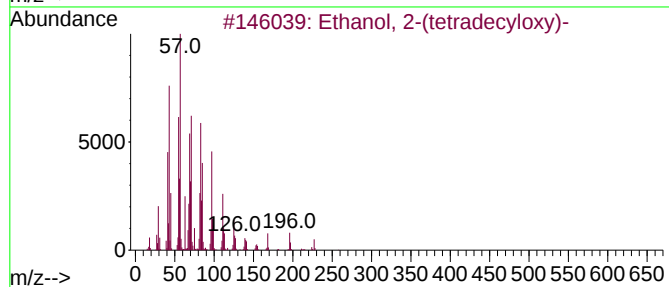
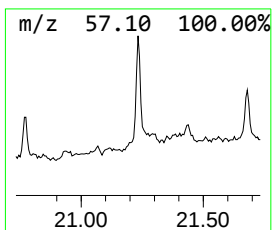
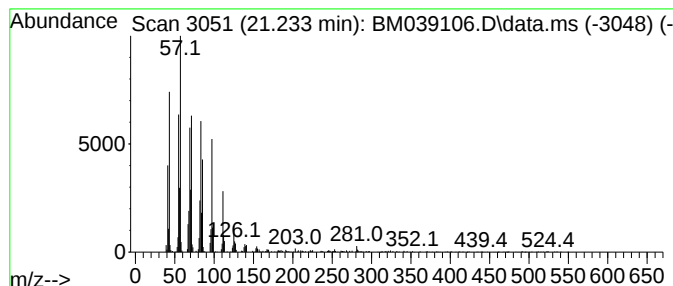
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Ethanol, 2-(tetradecyloxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.233	6.19 ng	1025480	Chrysene-d12	21.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	90
2			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	90
3			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	87
4			Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	87
5			Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032223\
Data File : BM039106.D
Acq On : 22 Mar 2023 23:53
Operator : CG/JU
Sample : 02022-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
AU-05-32123

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.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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Tridecane	12.192	2.2	ng	289783	2	10.781	2612610	20.0
Tetradecane	13.427	2.4	ng	367293	3	14.604	3016830	20.0
Hexadecane	14.498	2.3	ng	348169	3	14.604	3016830	20.0
Benzophenone	15.963	6.8	ng	1022830	3	14.604	3016830	20.0
Heneicosane	16.310	2.1	ng	338475	4	17.351	3218270	20.0
Hexadecanoic ac...	18.021	2.3	ng	371710	4	17.351	3218270	20.0
n-Hexadecanoic ...	18.245	7.0	ng	1131130	4	17.351	3218270	20.0
9,12-Octadecadi...	19.156	9.6	ng	1547460	4	17.351	3218270	20.0
15-Octadecenoic...	19.192	6.7	ng	1079320	4	17.351	3218270	20.0
Ethanol, 2-(tet...	21.233	6.2	ng	1025480	5	21.527	3311460	20.0