

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102523\
 Data File : BM042436.D
 Acq On : 25 Oct 2023 14:09
 Operator : MA/JU
 Sample : 04919-03
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 LSS-B5-COMP-101723

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-BM102123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM042436.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.069	316	320	327	rVB	249340	337815	5.40%	0.742%
2	5.522	390	397	407	rBV	2301917	3402643	54.36%	7.476%
3	7.145	664	673	686	rBV	2239303	3563234	56.93%	7.829%
4	7.992	810	817	828	rBV	525366	842509	13.46%	1.851%
5	9.187	1010	1020	1036	rBV	1399630	2319264	37.05%	5.096%
6	10.810	1287	1296	1310	rVB	671113	1112520	17.77%	2.444%
7	13.257	1705	1712	1722	rBV	3246143	4495155	71.82%	9.876%
8	13.480	1744	1750	1756	rVB	38152	67636	1.08%	0.149%
9	14.633	1940	1946	1955	rVB	969260	1354870	21.65%	2.977%
10	15.010	2004	2010	2017	rBV	47343	80780	1.29%	0.177%
11	16.127	2193	2200	2210	rBV	2657966	3743396	59.81%	8.224%
12	17.386	2408	2414	2428	rBV	1164489	1622124	25.92%	3.564%
13	18.233	2548	2558	2583	rBV	2231595	4058241	64.84%	8.916%
14	19.368	2747	2751	2752	rBV	85802	96069	1.53%	0.211%
15	19.392	2752	2755	2757	rVV2	102719	126554	2.02%	0.278%
16	19.509	2769	2775	2796	rVV	3488222	5325951	85.09%	11.701%
17	19.651	2797	2799	2803	rVB	81128	80027	1.28%	0.176%
18	19.998	2853	2858	2868	rVB	5265251	6259093	100.00%	13.752%
19	20.592	2954	2959	2965	rVB2	135255	283126	4.52%	0.622%
20	20.715	2977	2980	2983	rVB	155512	160266	2.56%	0.352%
21	21.227	3062	3067	3078	rBV	373855	624871	9.98%	1.373%
22	21.374	3089	3092	3096	rVB	95743	106683	1.70%	0.234%
23	21.562	3120	3124	3130	rVB	1365430	1789697	28.59%	3.932%
24	21.921	3181	3185	3191	rBV	171978	233579	3.73%	0.513%
25	22.497	3280	3283	3289	rVB	275071	382257	6.11%	0.840%
26	23.144	3389	3393	3404	rVB2	318642	647373	10.34%	1.422%
27	23.886	3515	3519	3527	rVB	328622	667390	10.66%	1.466%
28	24.027	3537	3543	3550	rVB	849066	1732079	27.67%	3.805%

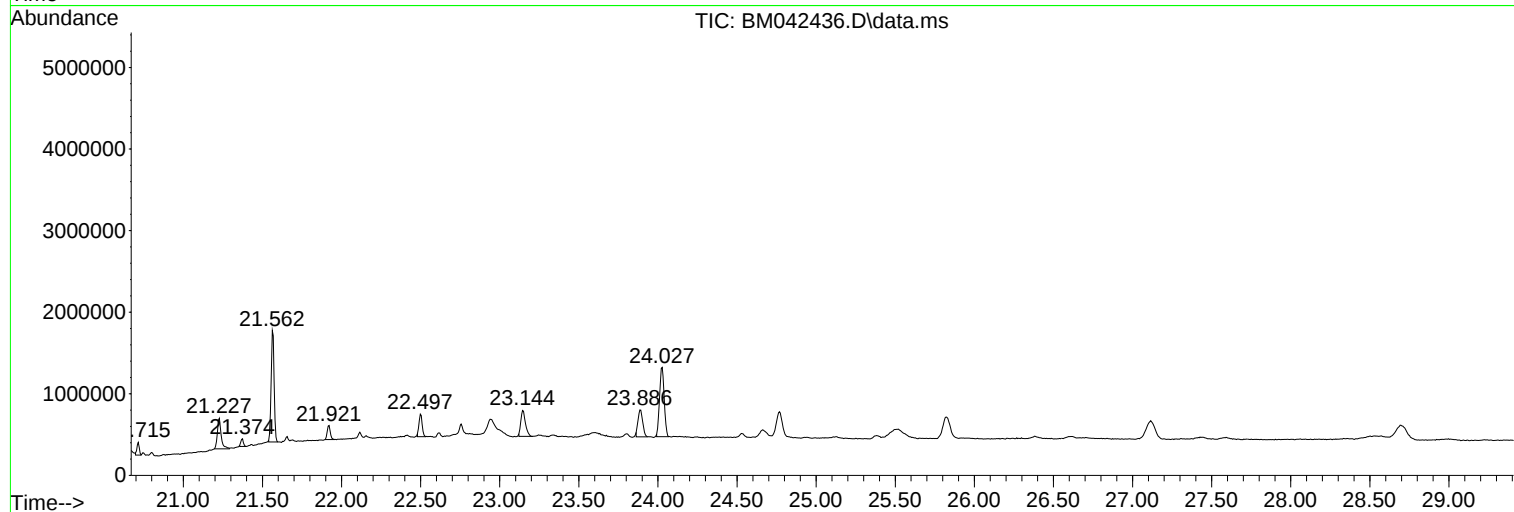
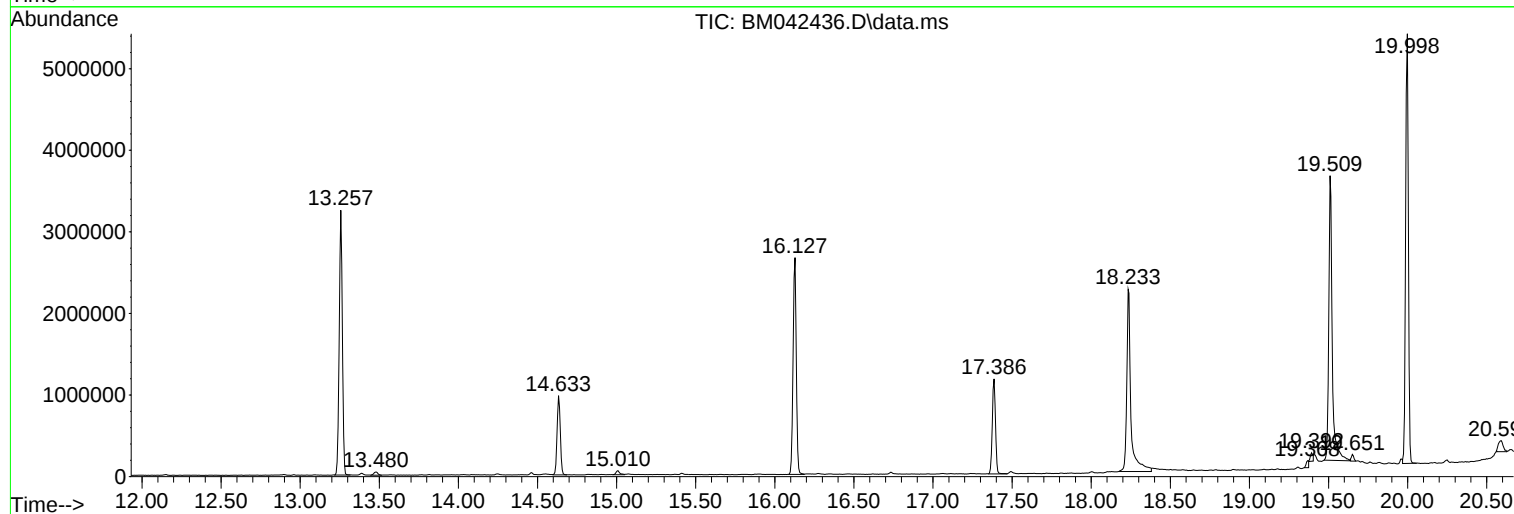
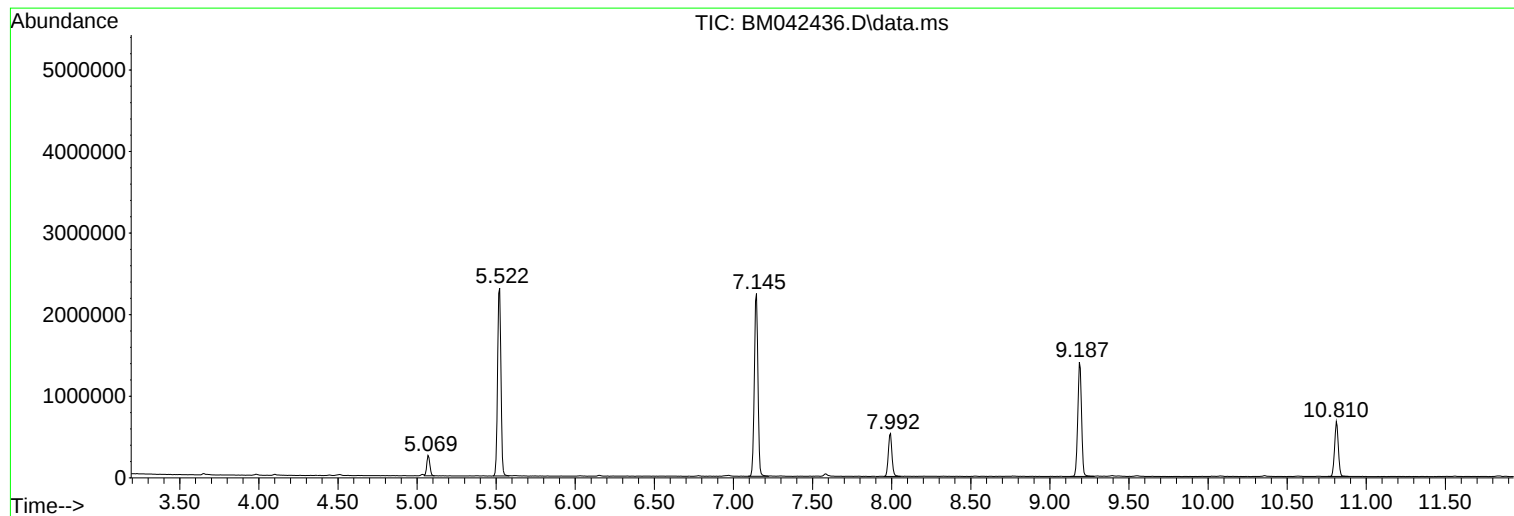
Sum of corrected areas: 45515202

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102523\
Data File : BM042436.D
Acq On : 25 Oct 2023 14:09
Operator : MA/JU
Sample : 04919-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
LSS-B5-COMP-101723

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102523\
Data File : BM042436.D
Acq On : 25 Oct 2023 14:09
Operator : MA/JU
Sample : 04919-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
LSS-B5-COMP-101723

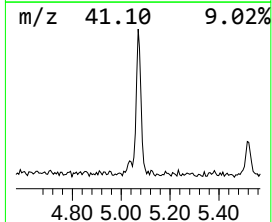
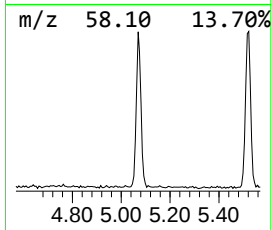
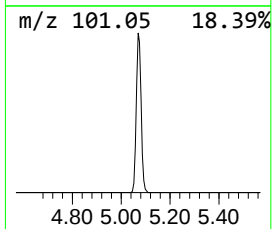
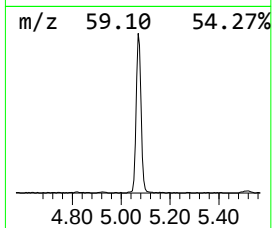
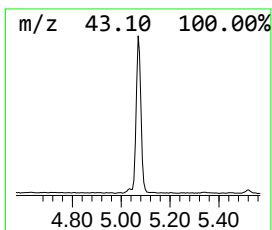
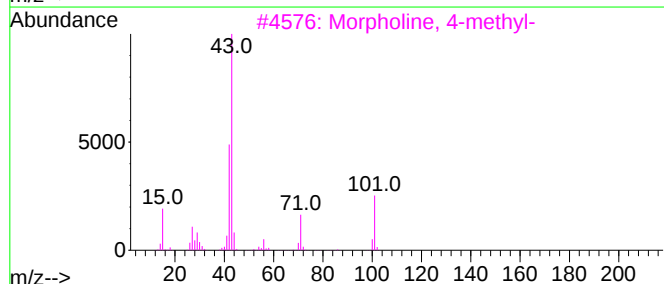
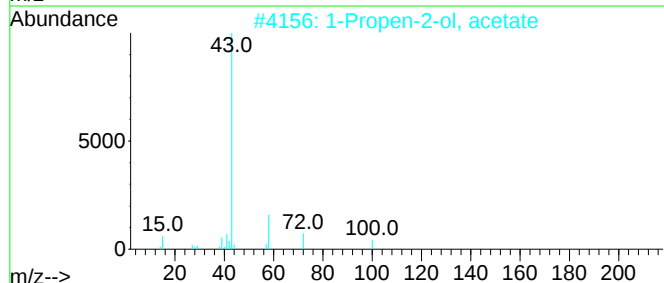
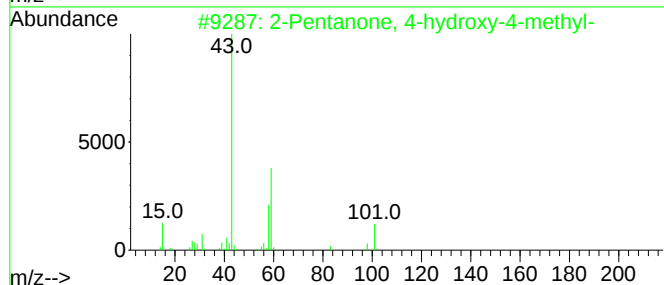
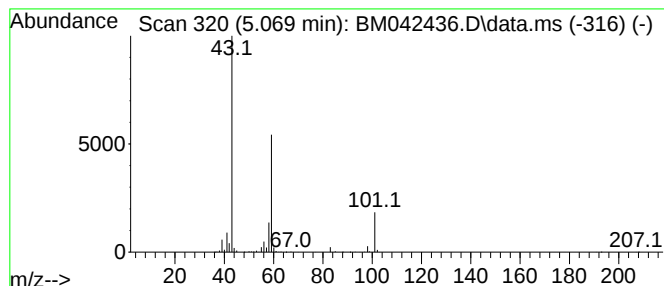
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.069	8.02 ng	337815	1,4-Dichlorobenzene-d4	7.992

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	9		



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102523\
Data File : BM042436.D
Acq On : 25 Oct 2023 14:09
Operator : MA/JU
Sample : 04919-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
LSS-B5-COMP-101723

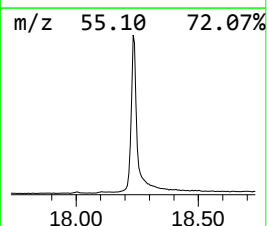
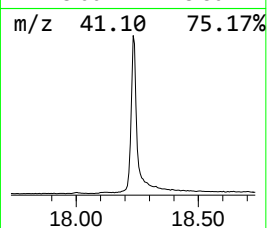
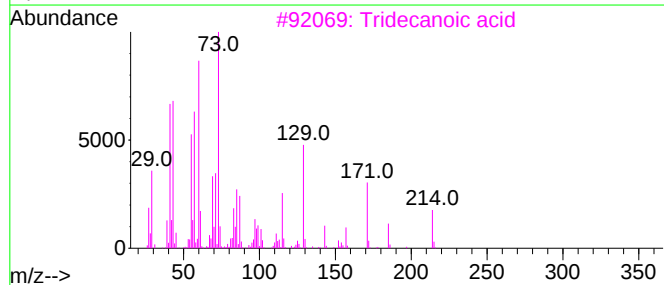
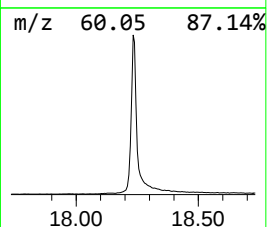
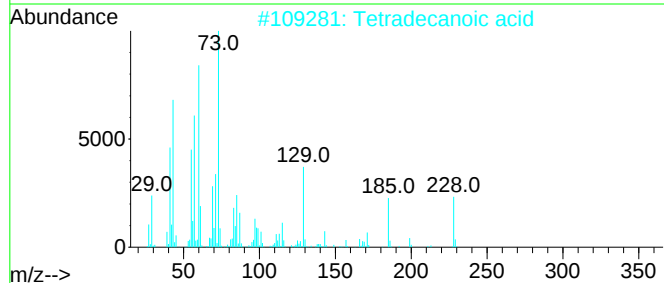
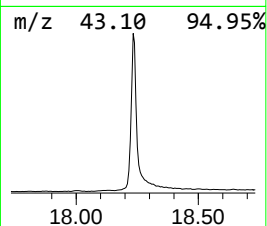
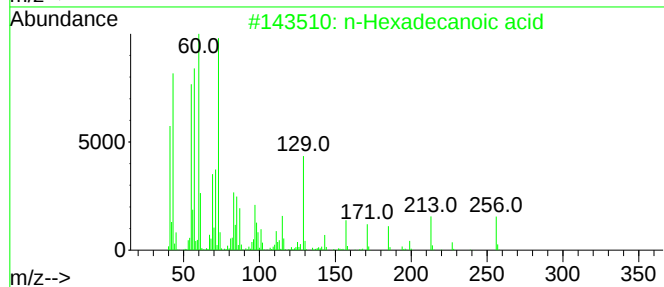
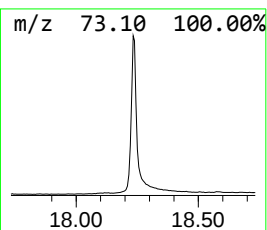
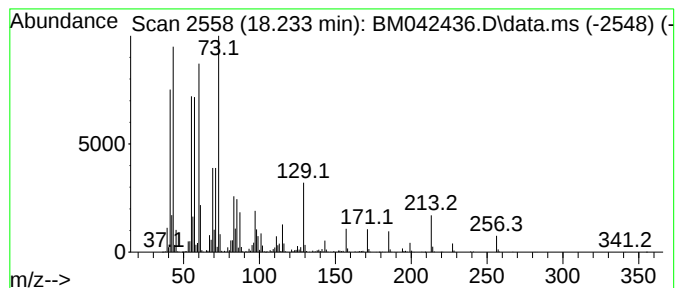
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.233	50.04 ng	4058240	Phenanthrene-d10	17.386

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	95
3			Tridecanoic acid	214	C13H26O2	000638-53-9	93
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	60



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102523\
Data File : BM042436.D
Acq On : 25 Oct 2023 14:09
Operator : MA/JU
Sample : 04919-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
LSS-B5-COMP-101723

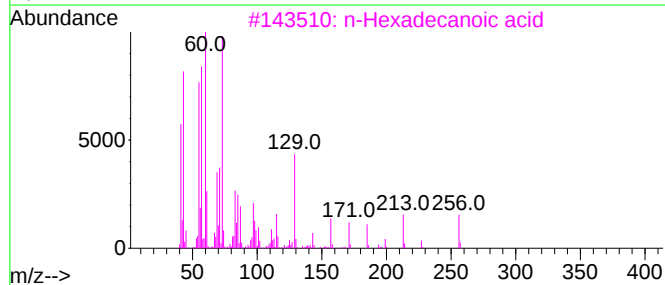
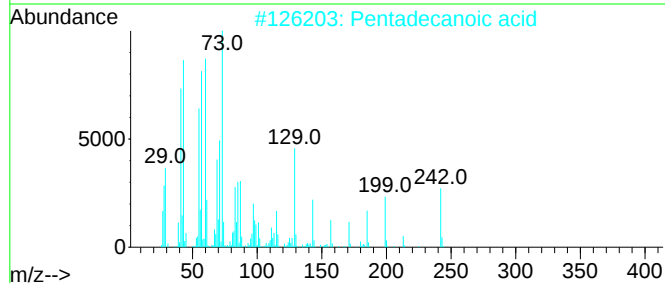
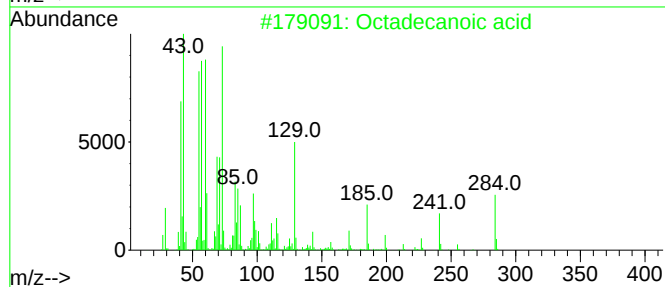
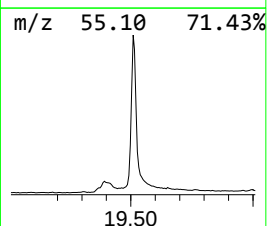
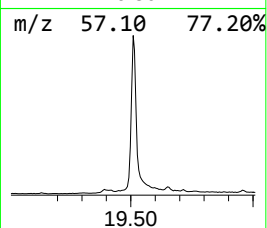
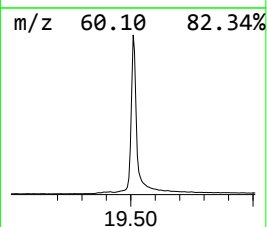
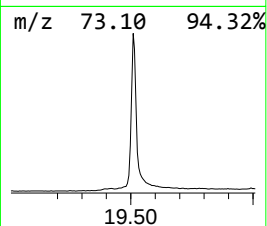
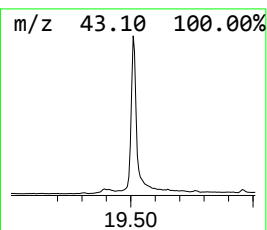
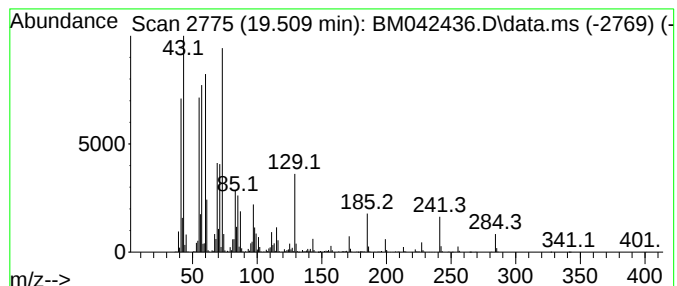
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.509	59.52 ng	5325950	Chrysene-d12	21.562

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	86
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	86
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102523\
Data File : BM042436.D
Acq On : 25 Oct 2023 14:09
Operator : MA/JU
Sample : 04919-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
LSS-B5-COMP-101723

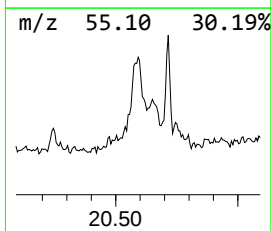
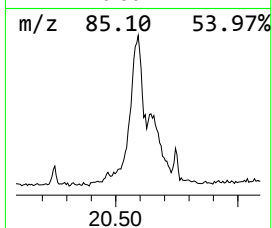
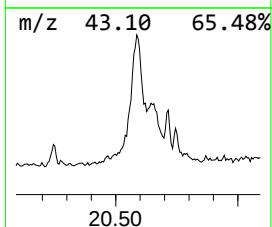
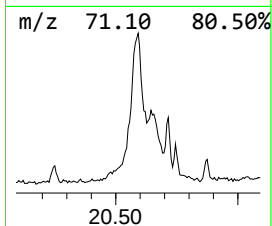
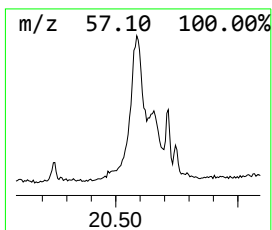
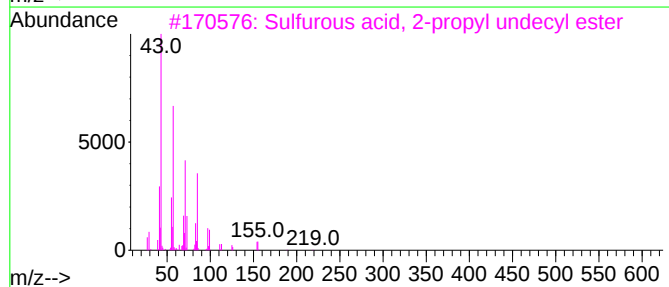
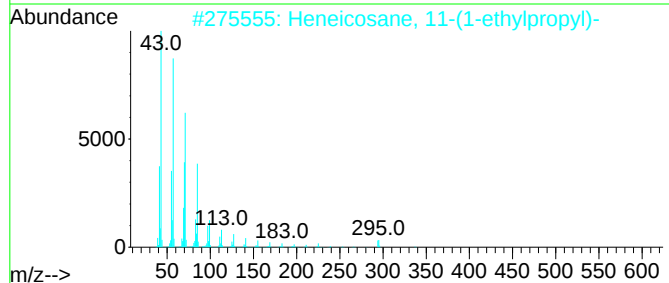
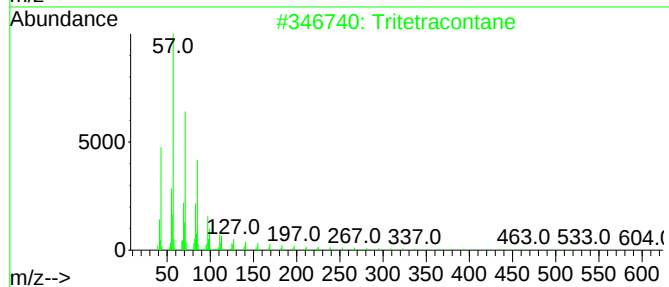
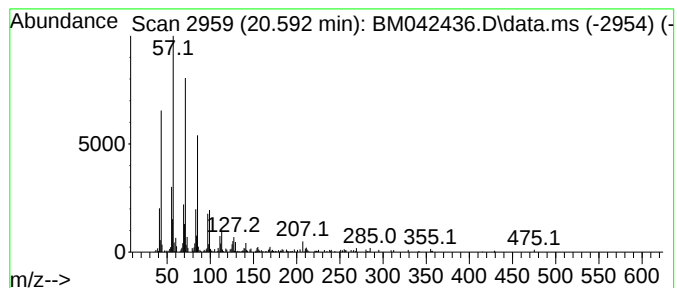
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Tritetracontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.592	3.16 ng	283126	Chrysene-d12	21.562

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tritetracontane	605	C43H88	007098-21-7	91
2			Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	90
3			Sulfurous acid, 2-propyl undecyl...	278	C14H30O3S	1000309-12-2	87
4			Hentriacontane	437	C31H64	000630-04-6	86
5			Heptadecane	240	C17H36	000629-78-7	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102523\
Data File : BM042436.D
Acq On : 25 Oct 2023 14:09
Operator : MA/JU
Sample : 04919-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

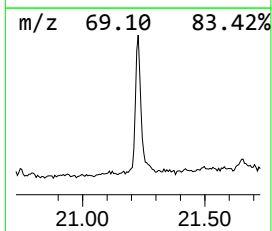
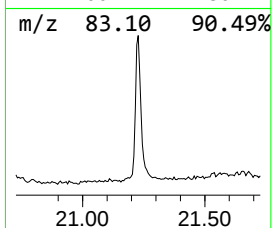
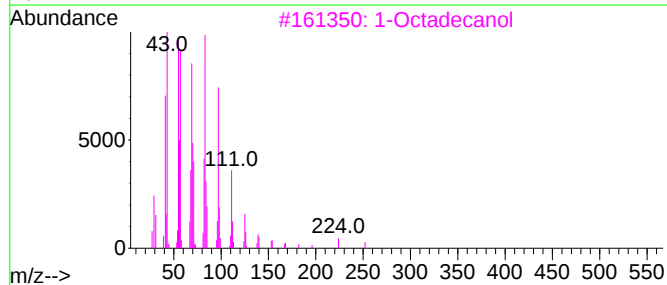
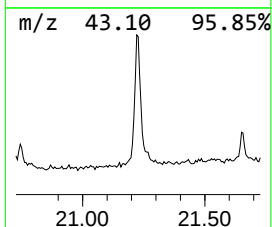
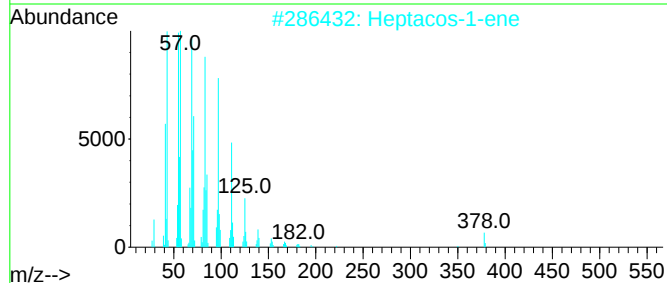
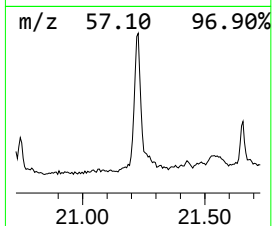
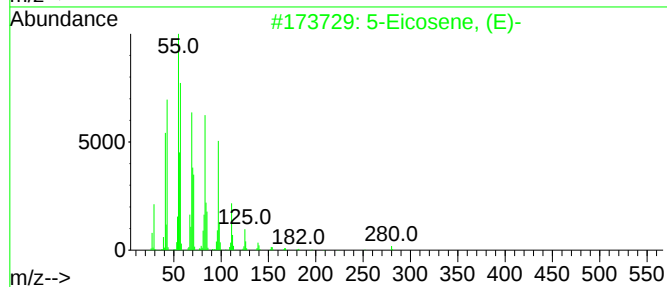
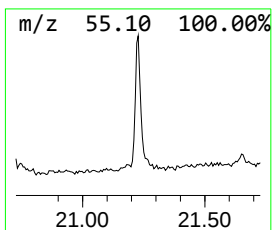
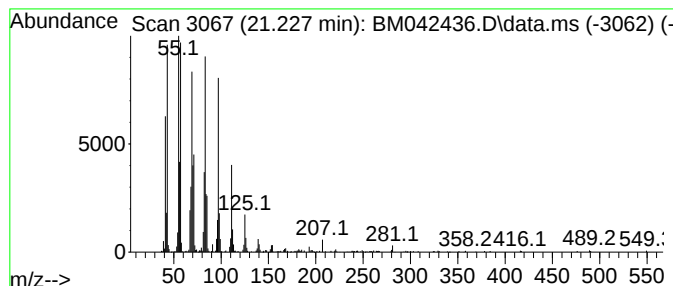
Instrument :
BNA_M
ClientSampleId :
LSS-B5-COMP-101723

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 5-Eicosene, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.227	6.98 ng	624871	Chrysene-d12	21.562	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	99
2	Heptacos-1-ene	378	C27H54	015306-27-1	96
3	1-Octadecanol	270	C18H38O	000112-92-5	95
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102523\
Data File : BM042436.D
Acq On : 25 Oct 2023 14:09
Operator : MA/JU
Sample : 04919-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
LSS-B5-COMP-101723

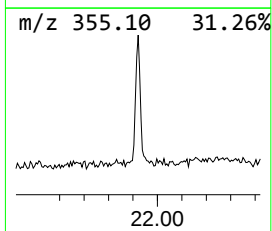
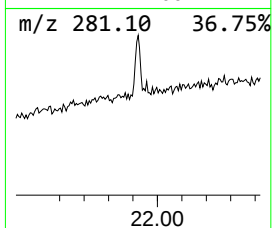
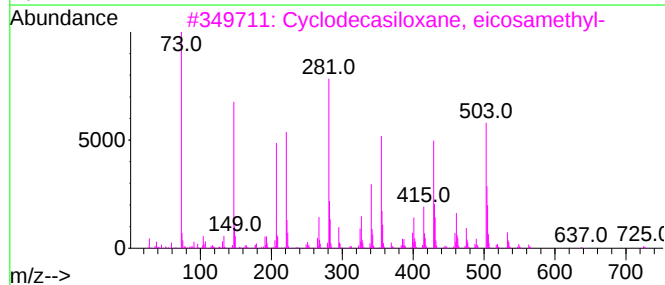
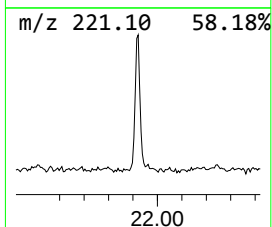
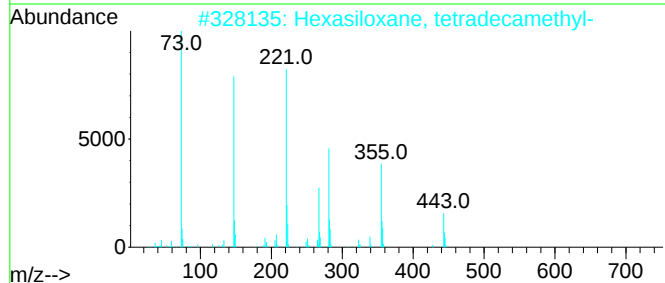
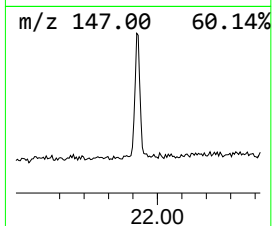
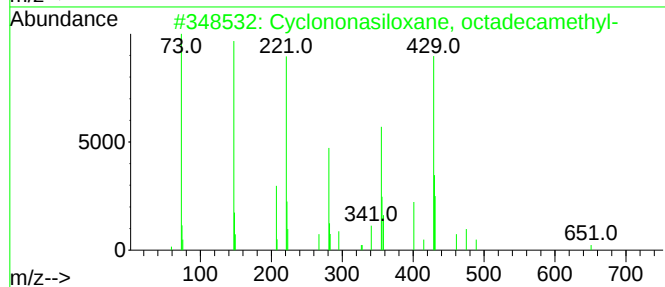
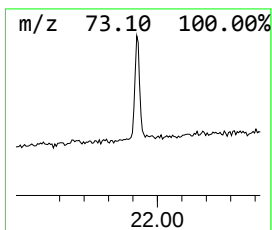
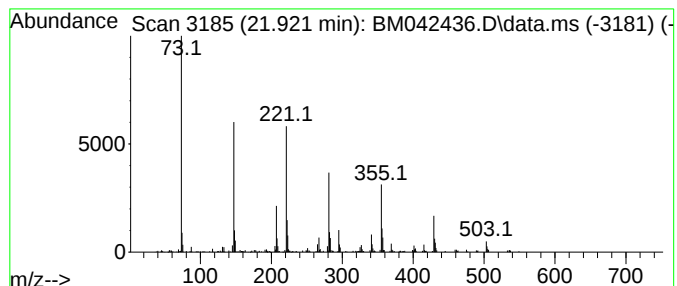
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Cyclononasiloxane, octadeca... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.921	2.61 ng	233579	Chrysene-d12	21.562

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	90
2			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	74
3			Cyclodecasiloxane, eicosamethyl-	740	C20H60O10Si10	018772-36-6	58
4			3,6-Dioxo-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	55
5			N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102523\
Data File : BM042436.D
Acq On : 25 Oct 2023 14:09
Operator : MA/JU
Sample : 04919-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
LSS-B5-COMP-101723

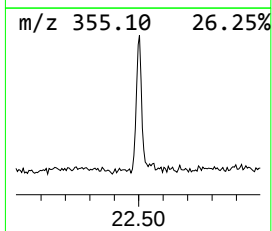
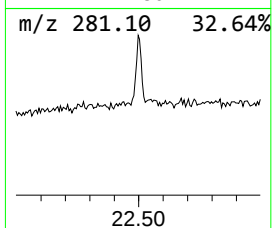
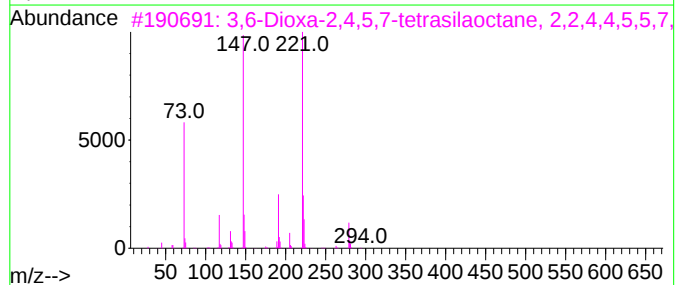
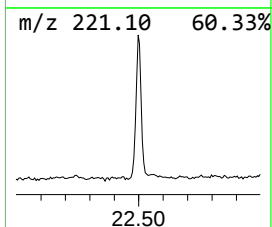
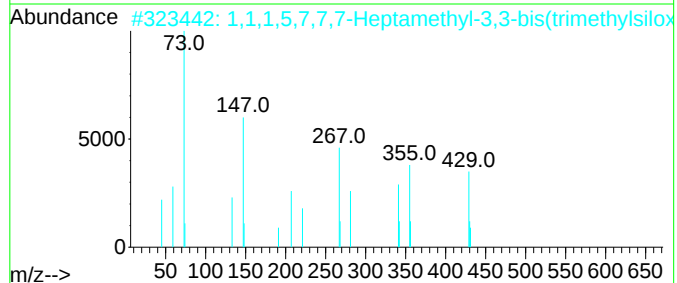
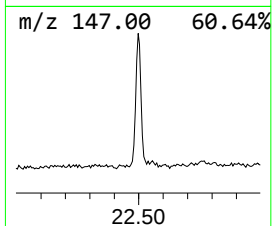
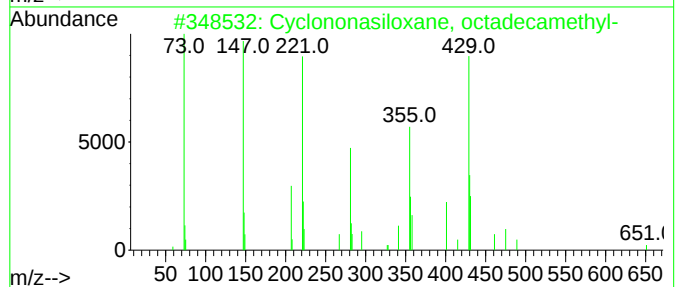
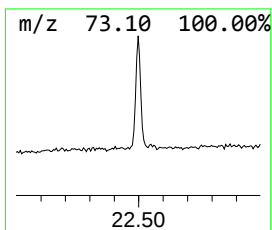
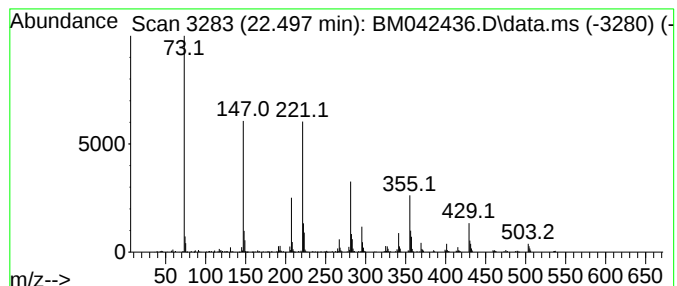
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1,1,1,5,7,7,7-Heptamethyl-3... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.497	4.27 ng	382257	Chrysene-d12	21.562

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	72
2			1,1,1,5,7,7,7-Heptamethyl-3,3-bi...	444	C13H40O5Si6	038147-00-1	50
3			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	49
4			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	35
5			N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102523\
Data File : BM042436.D
Acq On : 25 Oct 2023 14:09
Operator : MA/JU
Sample : 04919-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
LSS-B5-COMP-101723

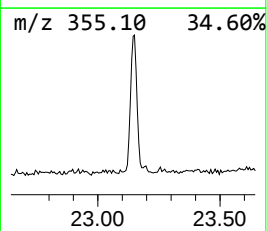
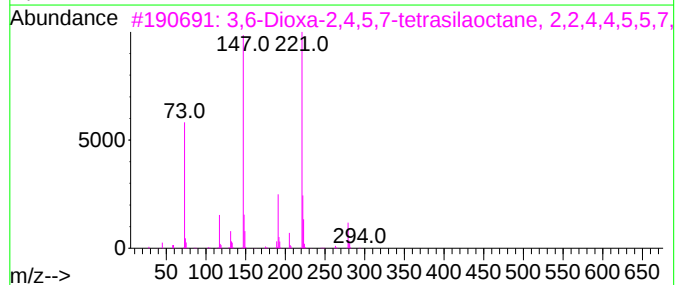
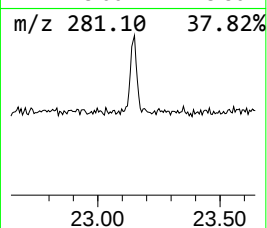
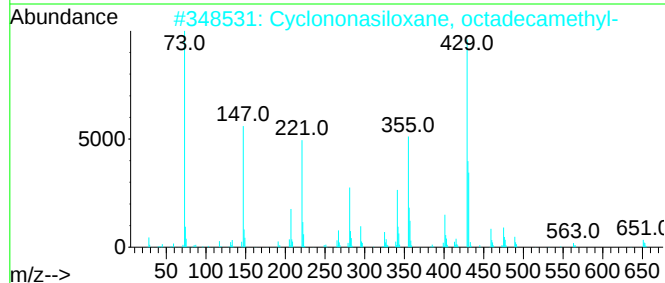
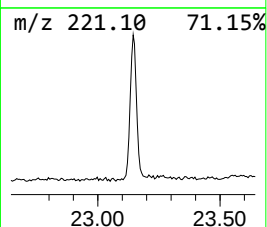
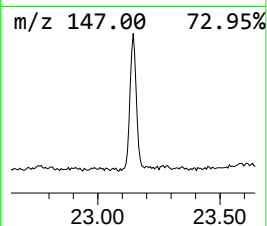
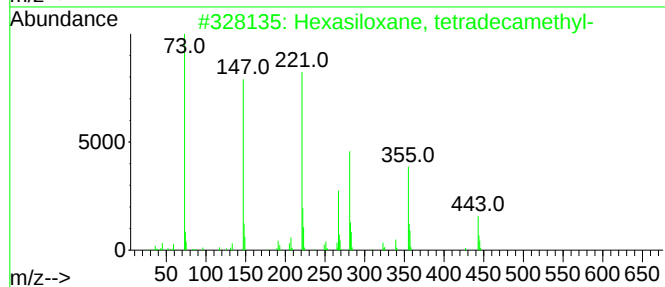
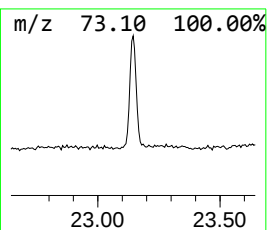
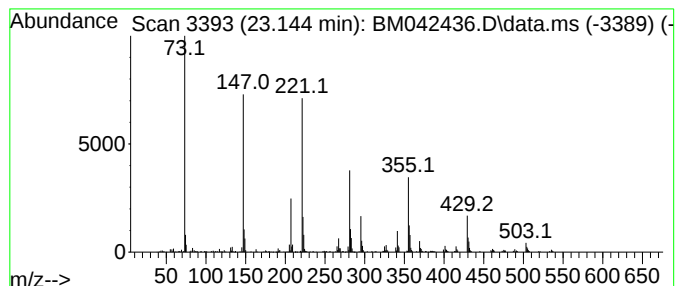
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexasiloxane, tetradecamethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.144	7.48 ng	647373	Perylene-d12	24.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	74
2			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	64
3			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	43
4			Mercaptoacetic acid, 2TMS deriva...	236	C8H20O2SSi2	006398-62-5	37
5			N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102523\
Data File : BM042436.D
Acq On : 25 Oct 2023 14:09
Operator : MA/JU
Sample : 04919-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
LSS-B5-COMP-101723

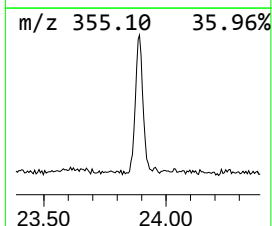
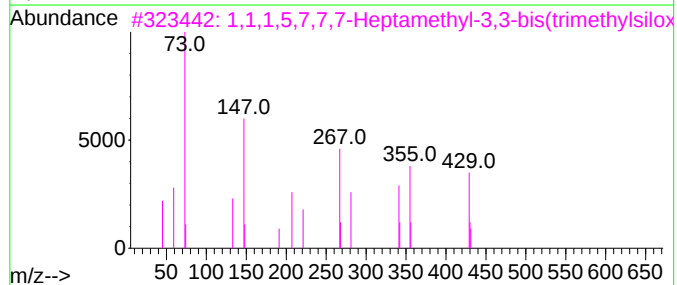
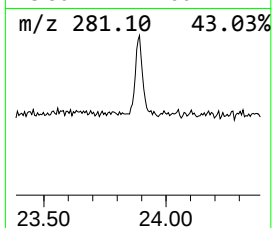
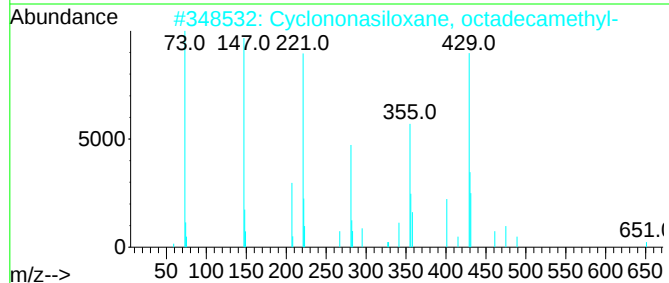
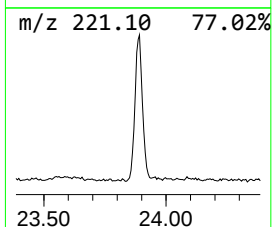
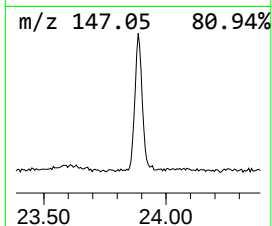
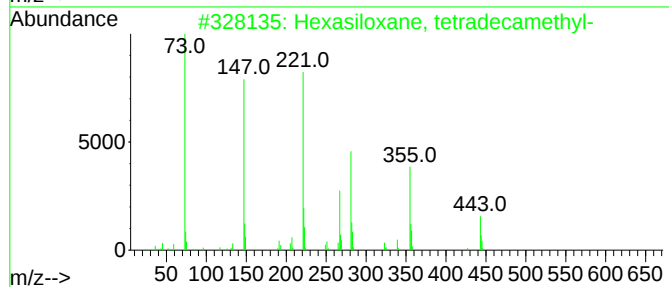
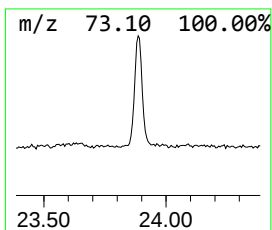
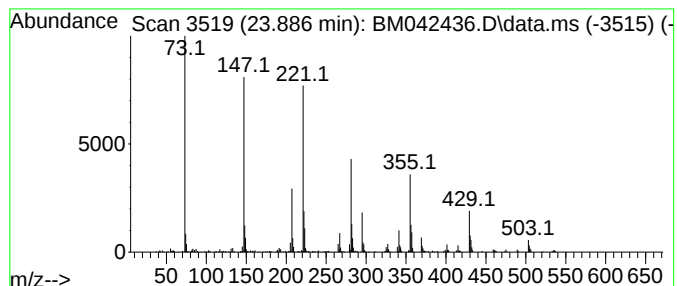
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 unknown23.886 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.886	7.71 ng	667390	Perylene-d12	24.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	87
2			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	83
3			1,1,1,5,7,7,7-Heptamethyl-3,3-bi...	444	C13H40O5Si6	038147-00-1	50
4			Mercaptoacetic acid, 2TMS deriva...	236	C8H20O2SSi2	006398-62-5	47
5			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102523\
Data File : BM042436.D
Acq On : 25 Oct 2023 14:09
Operator : MA/JU
Sample : 04919-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
LSS-B5-COMP-101723

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.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
2-Pentanone, 4-...	5.069	8.0	ng	337815	1	7.992	842509	20.0
n-Hexadecanoic ...	18.233	50.0	ng	4058240	4	17.386	1622120	20.0
Octadecanoic acid	19.509	59.5	ng	5325950	5	21.562	1789700	20.0
Tritetracontane	20.592	3.2	ng	283126	5	21.562	1789700	20.0
5-Eicosene, (E)-	21.227	7.0	ng	624871	5	21.562	1789700	20.0
Cyclononasiloxa...	21.921	2.6	ng	233579	5	21.562	1789700	20.0
1,1,1,5,7,7,7-H...	22.497	4.3	ng	382257	5	21.562	1789700	20.0
Hexasiloxane, t...	23.144	7.5	ng	647373	6	24.027	1732080	20.0
unknown23.886	23.886	7.7	ng	667390	6	24.027	1732080	20.0