

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM060122\
 Data File : BM035352.D
 Acq On : 01 Jun 2022 18:17
 Operator : CG/JU
 Sample : N2953-08
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 P044-SS001-0612-02

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-BM052722.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM035352.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.451	396	402	414	rBV	1841619	2726610	48.51%	6.664%
2	7.051	666	674	689	rBV	1678427	2843862	50.59%	6.950%
3	7.863	805	812	821	rBV	474388	754429	13.42%	1.844%
4	9.022	1002	1009	1020	rBV	1039048	1757423	31.27%	4.295%
5	10.663	1280	1288	1299	rBV	522440	888368	15.80%	2.171%
6	12.333	1564	1572	1584	rBV	83808	174419	3.10%	0.426%
7	13.127	1700	1707	1724	rBV	2653899	3884162	69.10%	9.493%
8	14.504	1934	1941	1948	rBV	854790	1249720	22.23%	3.054%
9	15.992	2188	2194	2210	rBV	2030956	3068939	54.60%	7.501%
10	16.663	2303	2308	2316	rBV	79602	125991	2.24%	0.308%
11	16.757	2319	2324	2331	rVV	42990	67318	1.20%	0.165%
12	17.251	2401	2408	2414	rBV	1020215	1471573	26.18%	3.597%
13	18.039	2537	2542	2547	rBV4	33114	60600	1.08%	0.148%
14	18.168	2557	2564	2585	rBV	3361040	5447842	96.92%	13.315%
15	18.339	2588	2593	2604	rVB	420976	595431	10.59%	1.455%
16	18.821	2672	2675	2682	rBV	48863	67123	1.19%	0.164%
17	19.315	2755	2759	2775	rVB	1666980	2683586	47.74%	6.559%
18	19.439	2775	2780	2797	rBV	2548659	3427705	60.98%	8.377%
19	19.798	2838	2841	2846	rBV	76174	94769	1.69%	0.232%
20	19.874	2849	2854	2860	rBV	4629603	5620997	100.00%	13.738%
21	21.150	3068	3071	3077	rVB	245961	294367	5.24%	0.719%
22	21.433	3115	3119	3129	rBV	1328262	1808330	32.17%	4.420%
23	23.803	3517	3522	3530	rVB2	888887	1802481	32.07%	4.405%

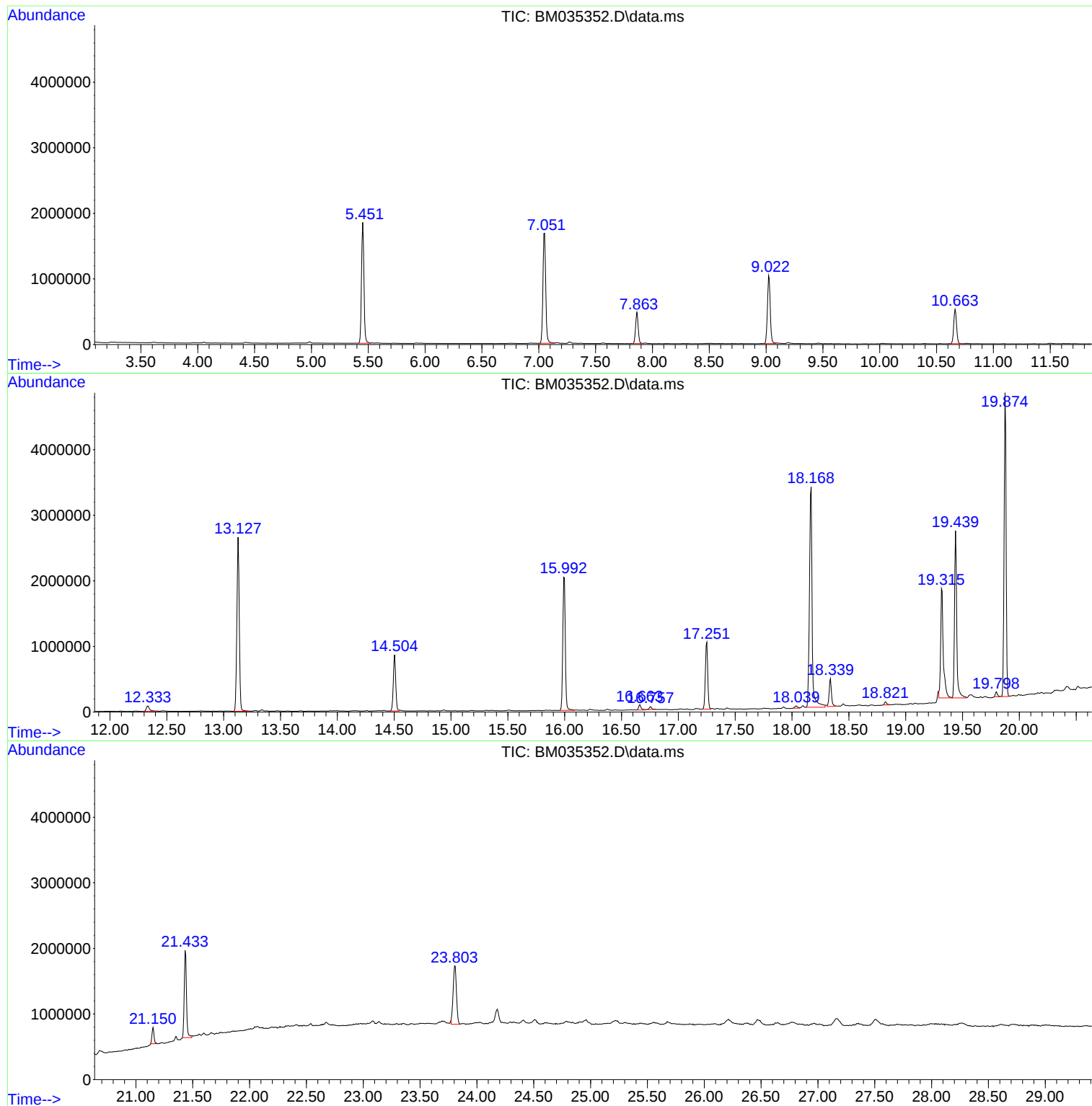
Sum of corrected areas: 40916045

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM060122\
Data File : BM035352.D
Acq On : 01 Jun 2022 18:17
Operator : CG/JU
Sample : N2953-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P044-SS001-0612-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052722.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\BM060122\
Data File : BM035352.D
Acq On : 01 Jun 2022 18:17
Operator : CG/JU
Sample : N2953-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P044-SS001-0612-02

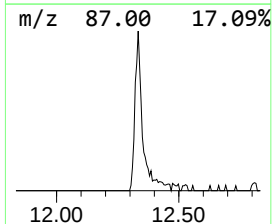
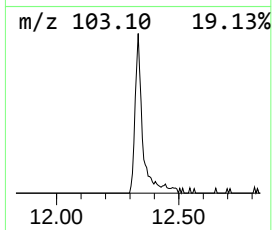
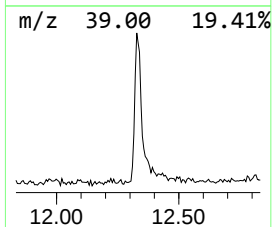
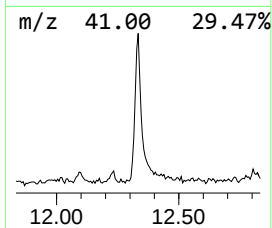
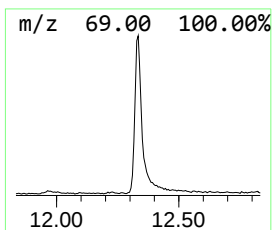
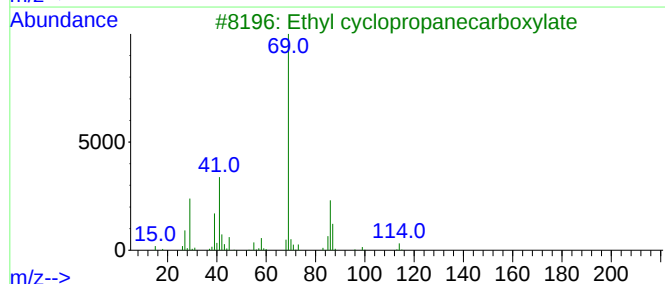
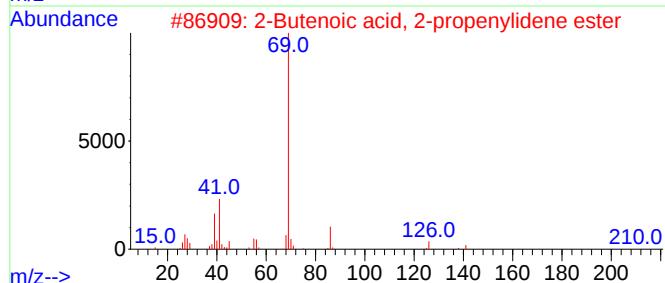
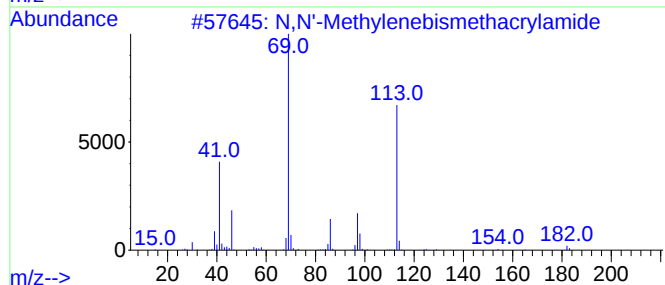
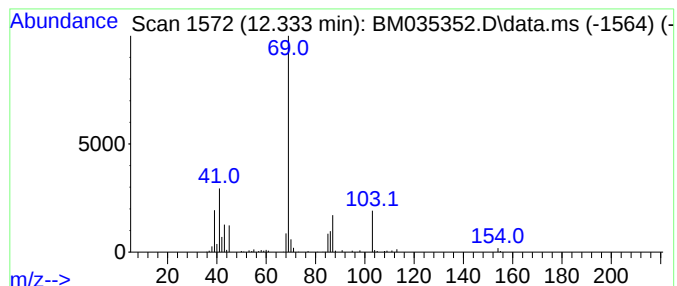
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown12.333 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.333	3.93 ng	174419	Naphthalene-d8	10.663

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			N,N'-Methylenebismethacrylamide	182	C9H14N2O2	002359-15-1	42
2			2-Butenoic acid, 2-propenylidene...	210	C11H14O4	055030-70-1	42
3			Ethyl cyclopropanecarboxylate	114	C6H10O2	004606-07-9	38
4			Cyclopropanecarboxylic acid, 3-m...	154	C9H14O2	1000299-37-4	38
5			Cyclopropanecarboxylic acid, buty...	142	C8H14O2	054947-39-6	36



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM060122\
Data File : BM035352.D
Acq On : 01 Jun 2022 18:17
Operator : CG/JU
Sample : N2953-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P044-SS001-0612-02

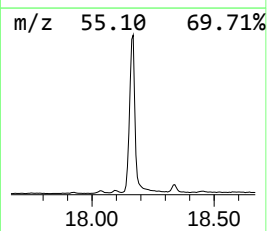
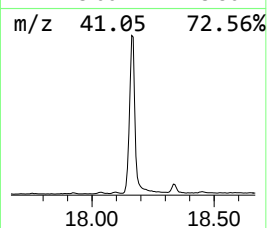
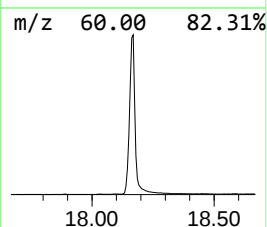
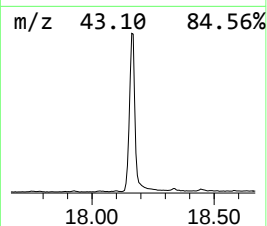
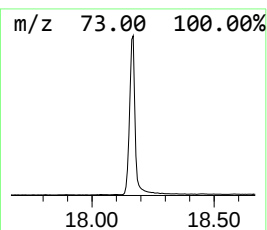
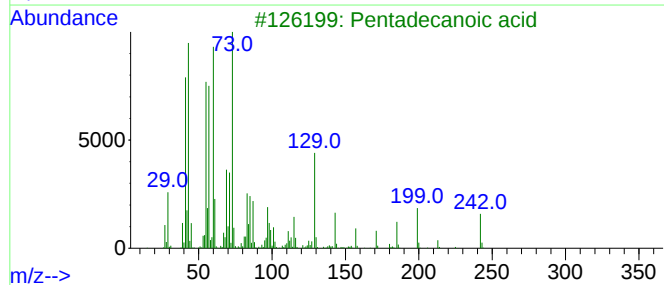
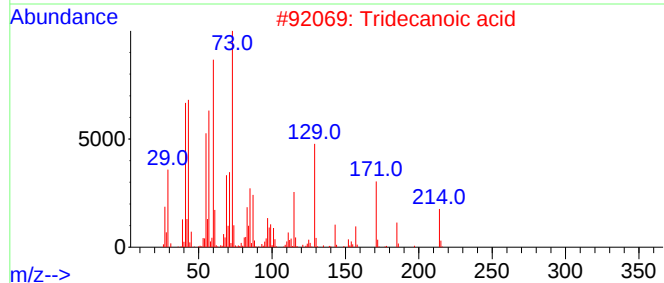
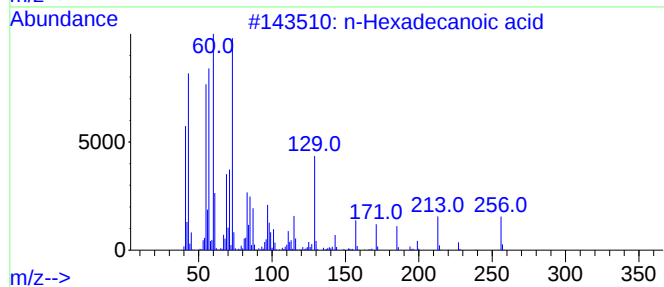
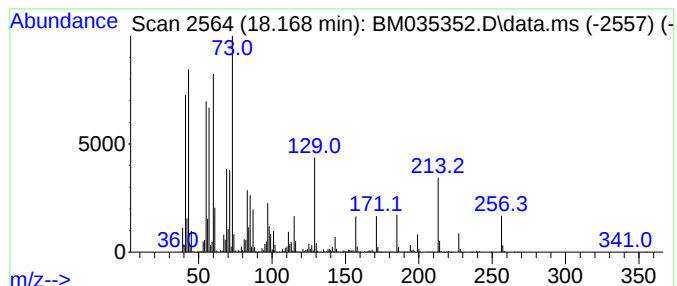
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.168	74.04 ng	5447840	Phenanthrene-d10	17.251

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	94
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Undecanoic acid	186	C11H22O2	000112-37-8	74
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM060122\
Data File : BM035352.D
Acq On : 01 Jun 2022 18:17
Operator : CG/JU
Sample : N2953-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P044-SS001-0612-02

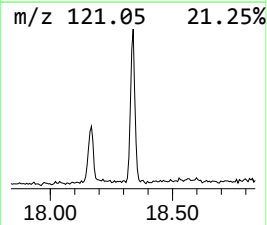
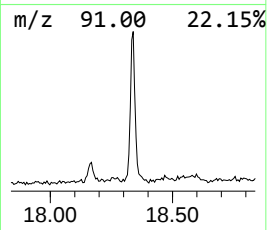
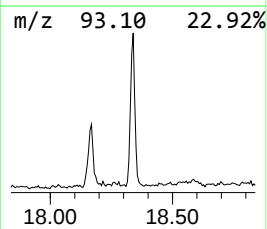
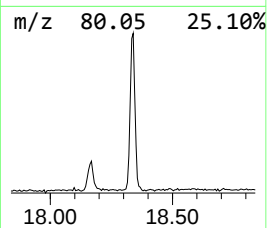
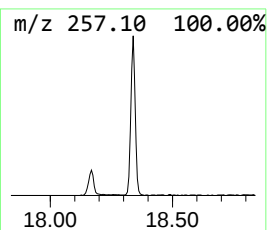
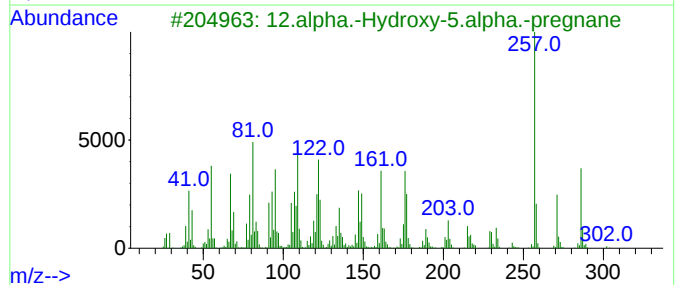
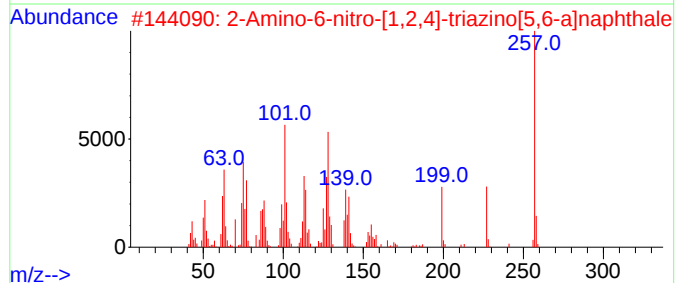
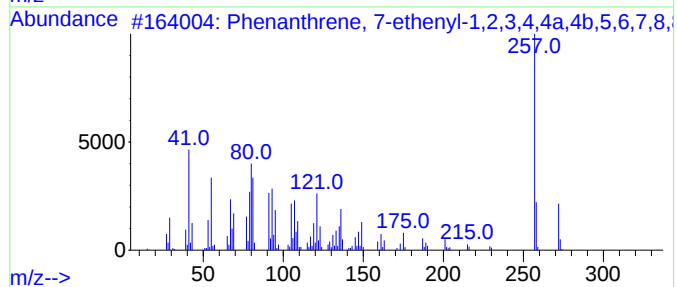
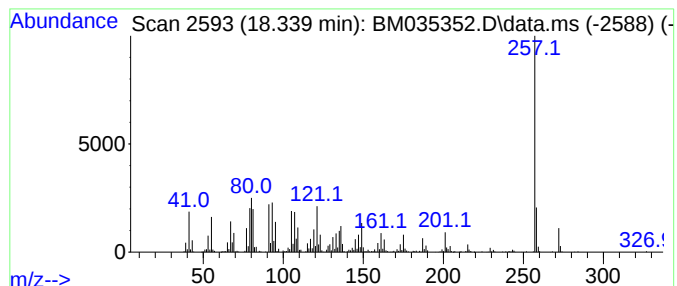
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Phenanthrene, 7-ethenyl-1,2... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.339	8.09 ng	595431	Phenanthrene-d10	17.251

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenanthrene, 7-ethenyl-1,2,3,4,...	272	C20H32	001686-67-5	93
2			2-Amino-6-nitro-[1,2,4]-triazino...	257	C11H7N5O3	020028-59-5	43
3			12.alpha.-Hydroxy-5.alpha.-pregnane	304	C21H36O	006908-29-8	40
4			Pyrrole, 1-methyl-2-phenyl-4-(ph...	257	C19H15N	066463-26-1	38
5			Acetamide, N-(3-methylphenyl)-2-...	257	C15H15NOS	1000307-20-6	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM060122\
Data File : BM035352.D
Acq On : 01 Jun 2022 18:17
Operator : CG/JU
Sample : N2953-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P044-SS001-0612-02

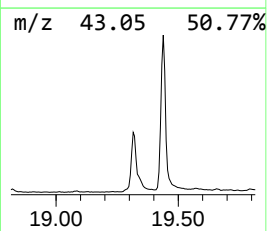
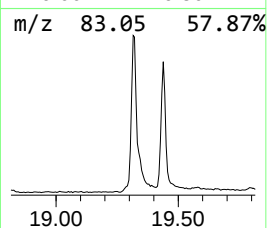
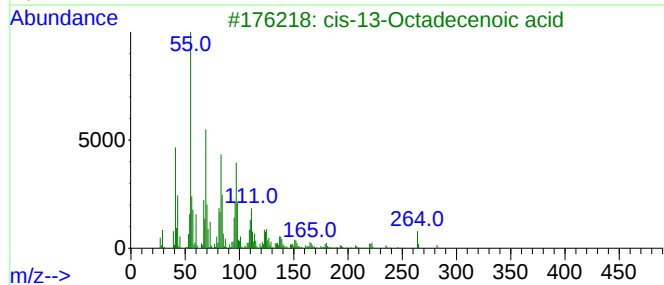
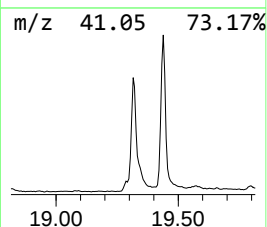
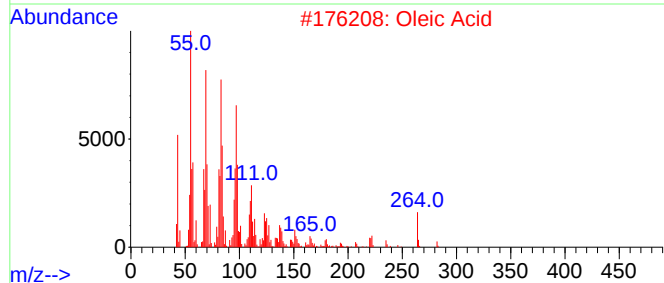
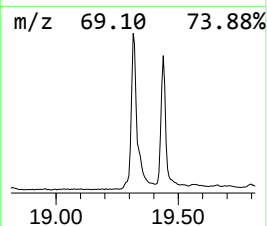
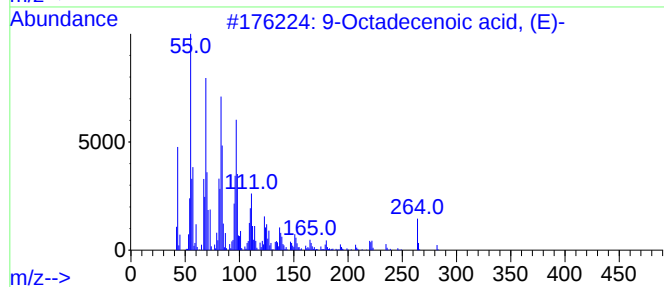
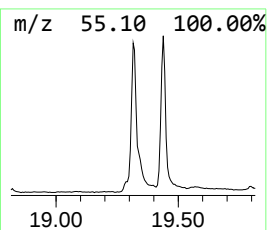
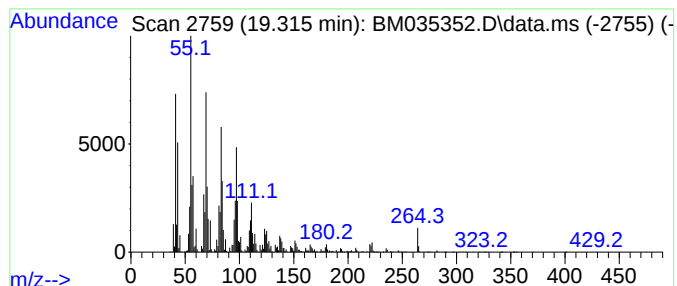
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 9-Octadecenoic acid, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.315	36.47 ng	2683590	Phenanthrene-d10	17.251

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	94
2			Oleic Acid	282	C18H34O2	000112-80-1	91
3			cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	86
4			cis-Vaccenic acid	282	C18H34O2	000506-17-2	83
5			trans-13-Octadecenoic acid	282	C18H34O2	000693-71-0	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM060122\
Data File : BM035352.D
Acq On : 01 Jun 2022 18:17
Operator : CG/JU
Sample : N2953-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P044-SS001-0612-02

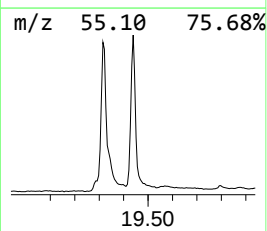
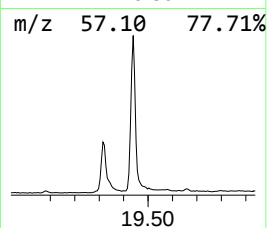
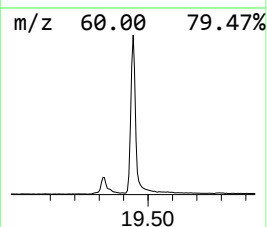
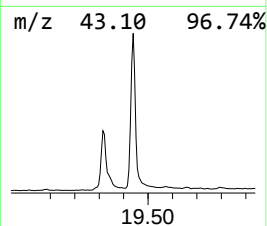
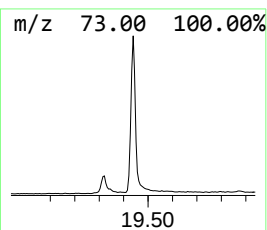
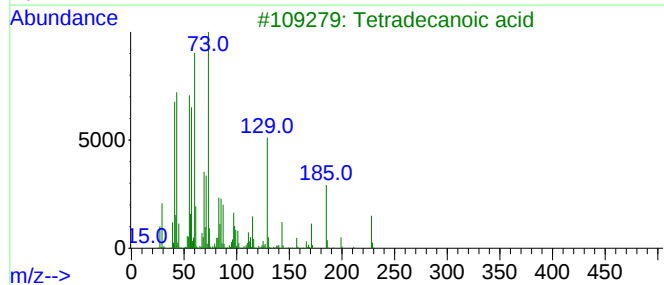
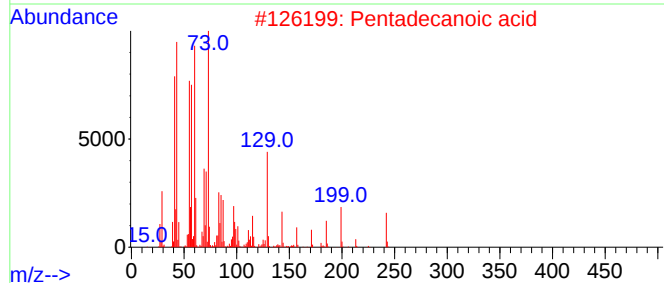
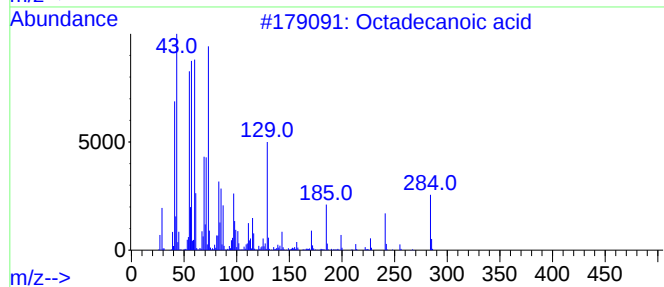
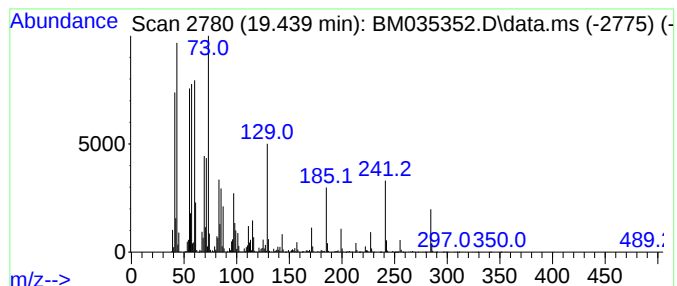
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.439	37.91 ng	3427710	Chrysene-d12	21.433

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	93
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	81
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	76
5			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM060122\
Data File : BM035352.D
Acq On : 01 Jun 2022 18:17
Operator : CG/JU
Sample : N2953-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P044-SS001-0612-02

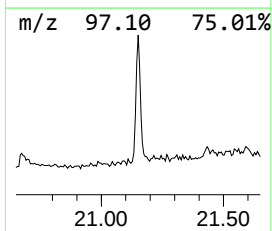
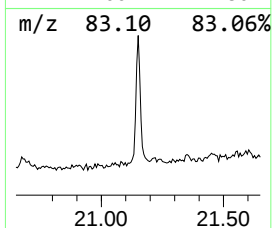
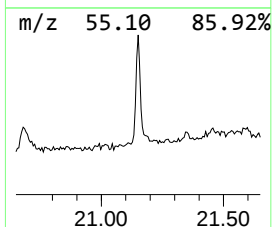
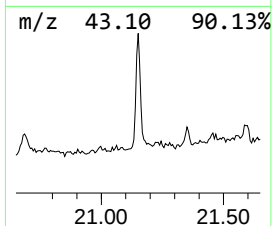
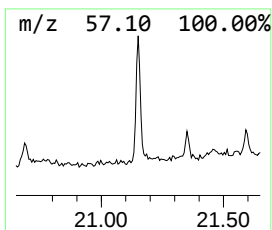
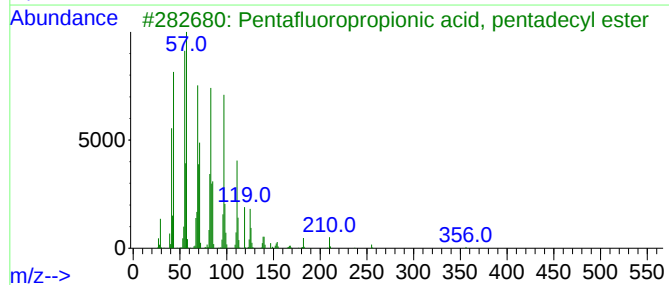
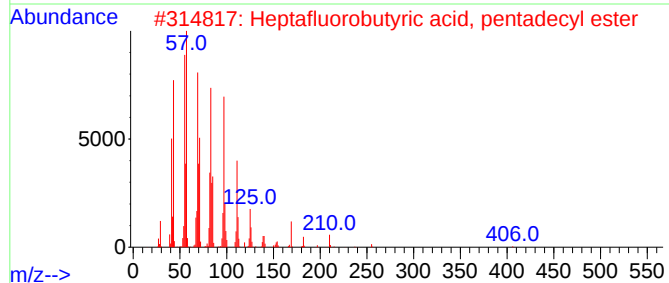
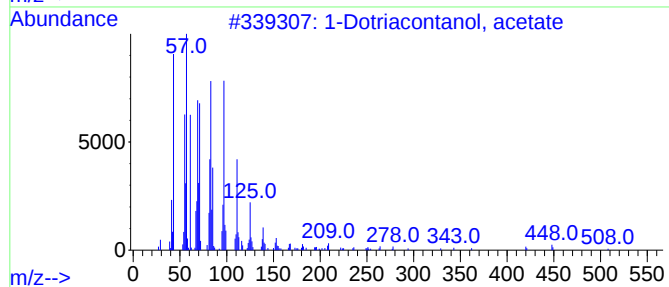
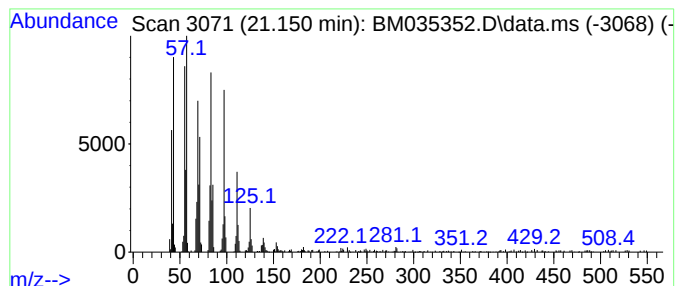
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Dotriacontanol, acetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.150	3.26 ng	294367	Chrysene-d12	21.433

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Dotriacontanol, acetate	509	C34H68O2	023811-94-1	94
2			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
3			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
4			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	94
5			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM060122\
Data File : BM035352.D
Acq On : 01 Jun 2022 18:17
Operator : CG/JU
Sample : N2953-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P044-SS001-0612-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052722.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
unknown12.333	12.333	3.9	ng	174419	2	10.663	888368	20.0
n-Hexadecanoic ...	18.168	74.0	ng	5447840	4	17.251	1471570	20.0
Phenanthrene, 7...	18.339	8.1	ng	595431	4	17.251	1471570	20.0
9-Octadecenoic ...	19.315	36.5	ng	2683590	4	17.251	1471570	20.0
Octadecanoic acid	19.439	37.9	ng	3427710	5	21.433	1808330	20.0
1-Dotriacontano...	21.150	3.3	ng	294367	5	21.433	1808330	20.0