

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM073123\
 Data File : BM041191.D
 Acq On : 31 Jul 2023 16:11
 Operator : MA/JU
 Sample : 03742-02
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 B-P32A

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-BM072823.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM041191.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.669	246	252	264	rBV4	16845	69712	1.19%	0.190%
2	5.369	365	371	384	rBV	1972291	2764997	47.10%	7.553%
3	6.975	637	644	665	rBV	1820932	2918992	49.73%	7.973%
4	7.798	777	784	791	rBV	641026	988712	16.84%	2.701%
5	8.975	975	984	1001	rBV	1093348	1804566	30.74%	4.929%
6	10.604	1250	1261	1277	rBV	809105	1387147	23.63%	3.789%
7	12.022	1493	1502	1507	rBV	63311	95753	1.63%	0.262%
8	12.980	1660	1665	1670	rVB	47697	65831	1.12%	0.180%
9	13.080	1675	1682	1696	rBV	2699394	3822958	65.13%	10.443%
10	13.269	1708	1714	1720	rBV	71621	107917	1.84%	0.295%
11	13.927	1821	1826	1831	rBV	102189	135373	2.31%	0.370%
12	14.463	1903	1917	1923	rBV	1244026	1952186	33.26%	5.332%
13	15.963	2165	2172	2186	rBV	2385337	3198891	54.50%	8.738%
14	17.221	2380	2386	2391	rBV	1531746	2080835	35.45%	5.684%
15	17.263	2391	2393	2398	rVB	86861	108218	1.84%	0.296%
16	18.121	2534	2539	2550	rBV2	346620	575234	9.80%	1.571%
17	19.168	2713	2717	2724	rBV5	33958	68105	1.16%	0.186%
18	19.245	2724	2730	2733	rBV	253673	342594	5.84%	0.936%
19	19.286	2733	2737	2750	rVV	260610	510373	8.69%	1.394%
20	19.404	2754	2757	2771	rVB	151250	265027	4.51%	0.724%
21	19.651	2796	2799	2808	rVB	175236	248360	4.23%	0.678%
22	19.857	2829	2834	2845	rBV	5061300	5870020	100.00%	16.034%
23	21.139	3048	3052	3059	rVB3	185380	329073	5.61%	0.899%
24	21.421	3095	3100	3105	rBV	1952245	2526457	43.04%	6.901%
25	23.056	3374	3378	3386	rBV3	241991	456978	7.78%	1.248%
26	23.792	3497	3503	3519	rVB	1288330	2570047	43.78%	7.020%
27	24.368	3596	3601	3612	rVB	688542	1345232	22.92%	3.675%

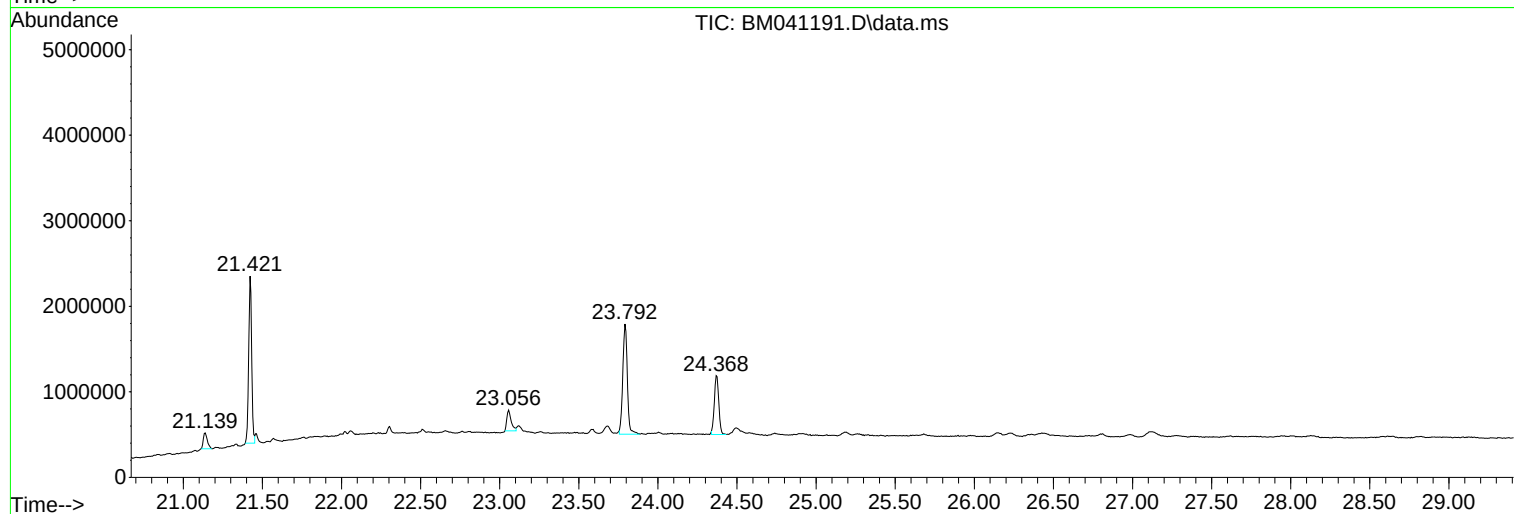
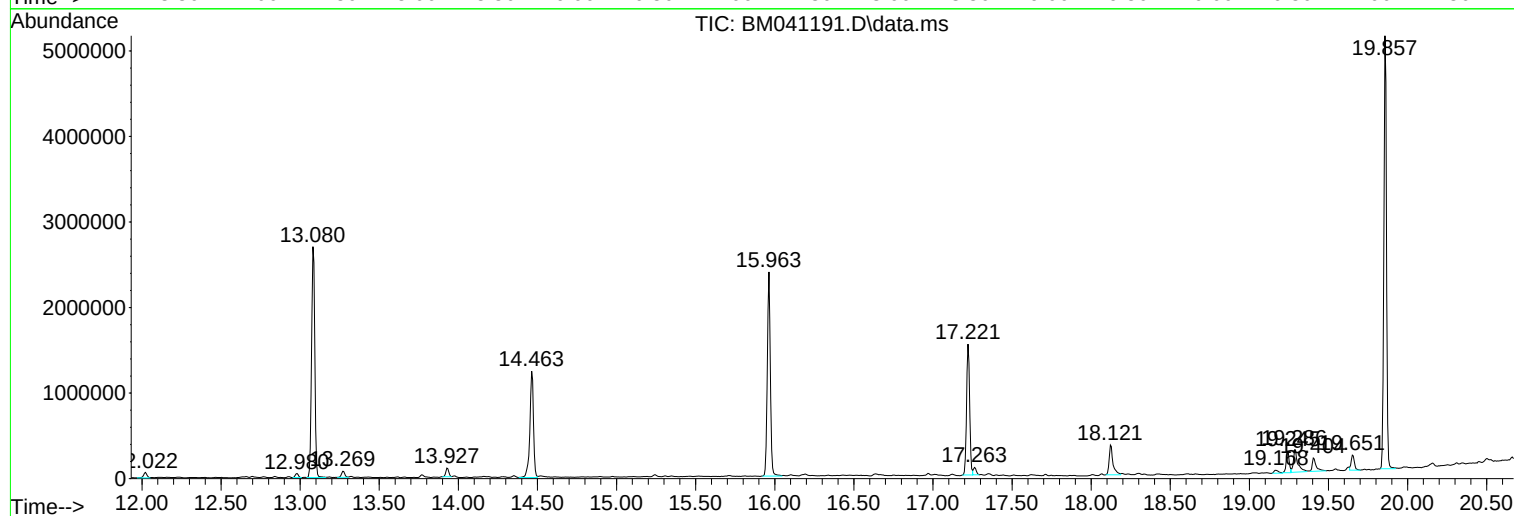
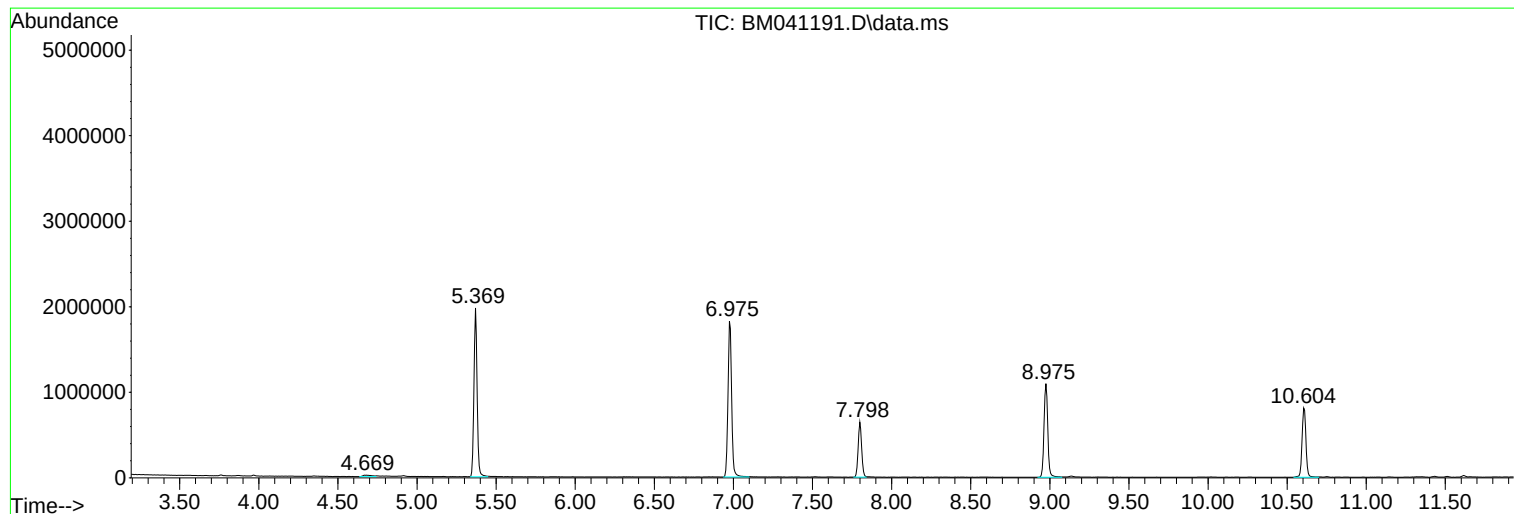
Sum of corrected areas: 36609588

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM073123\
Data File : BM041191.D
Acq On : 31 Jul 2023 16:11
Operator : MA/JU
Sample : 03742-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-P32A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.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\BM073123\
Data File : BM041191.D
Acq On : 31 Jul 2023 16:11
Operator : MA/JU
Sample : 03742-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-P32A

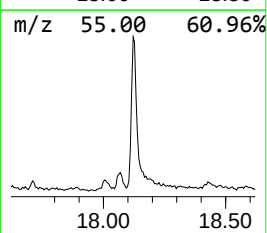
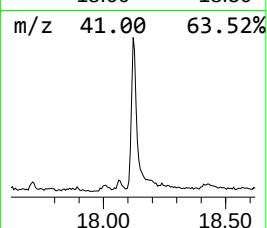
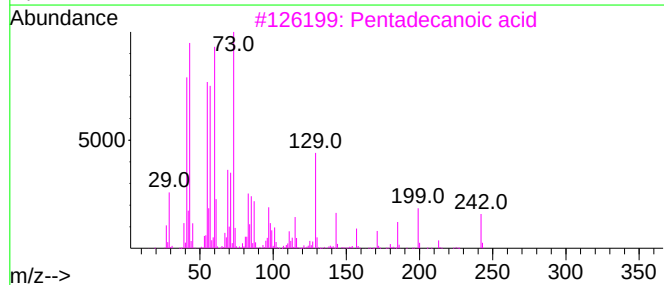
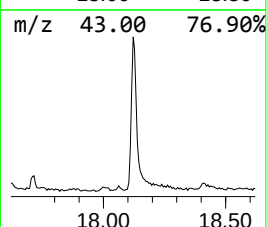
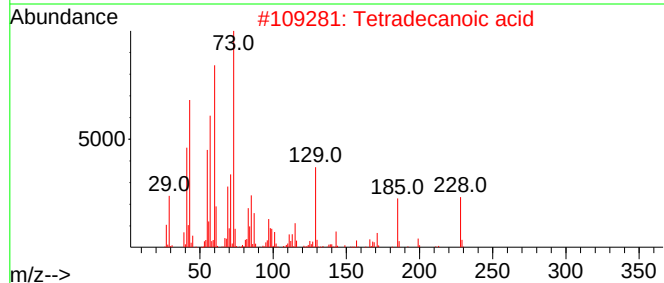
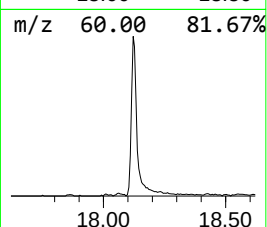
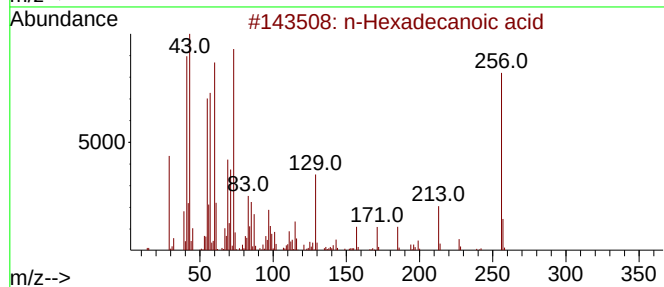
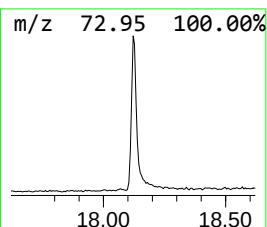
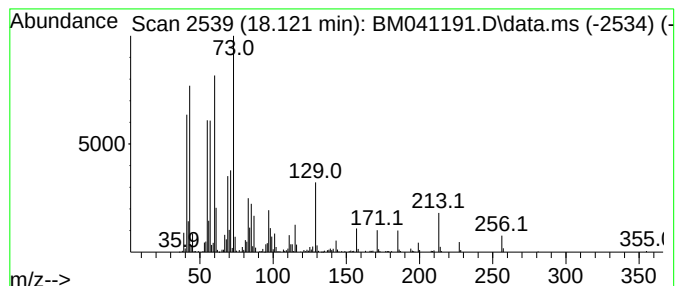
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.121	5.53 ng	575234	Phenanthrene-d10	17.221

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	94
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			Octadecanoic acid	284	C18H36O2	000057-11-4	83
5			Tridecanoic acid	214	C13H26O2	000638-53-9	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM073123\
Data File : BM041191.D
Acq On : 31 Jul 2023 16:11
Operator : MA/JU
Sample : 03742-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-P32A

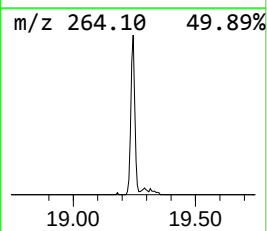
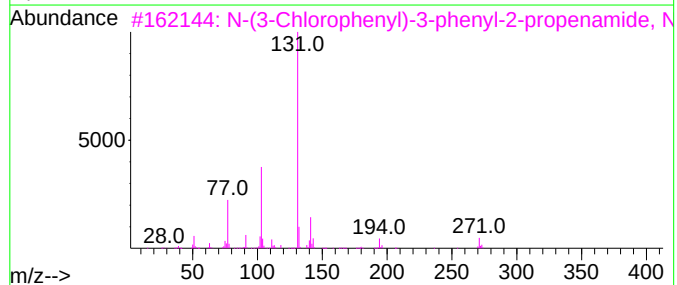
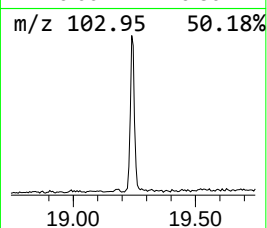
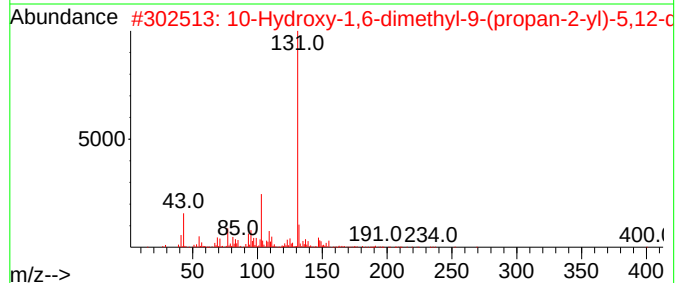
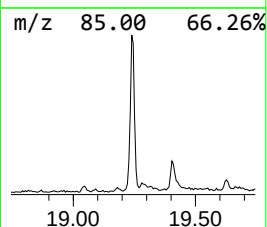
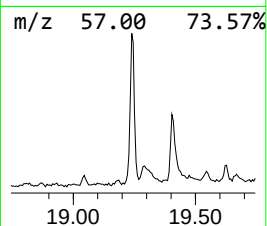
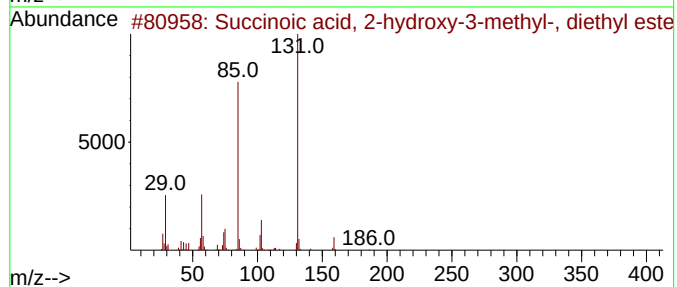
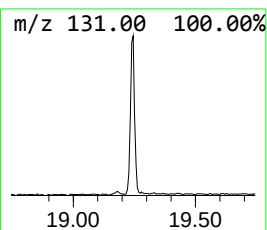
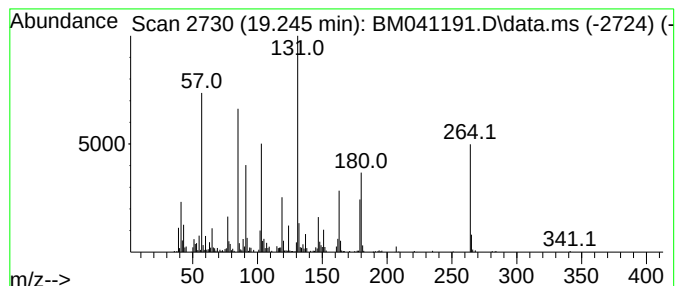
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown19.245 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.245	3.29 ng	342594	Phenanthrene-d10	17.221

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Succinic acid, 2-hydroxy-3-meth...	204	C9H16O5	1000196-85-6	35
2			10-Hydroxy-1,6-dimethyl-9-(propa...	400	C24H32O5	1000501-93-6	27
3			N-(3-Chlorophenyl)-3-phenyl-2-pr...	271	C16H14ClNO	1507357-48-3	27
4			trans-1-Cinnamoylimidazole	198	C12H10N2O	001138-15-4	27
5			p-Vinylbenzohydrazide	162	C9H10N2O	1000244-74-9	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM073123\
Data File : BM041191.D
Acq On : 31 Jul 2023 16:11
Operator : MA/JU
Sample : 03742-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

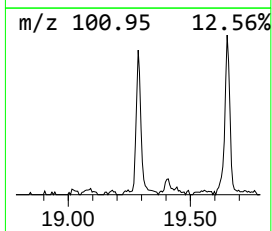
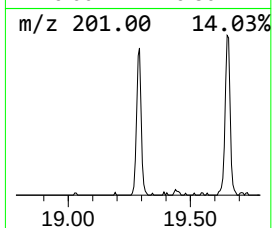
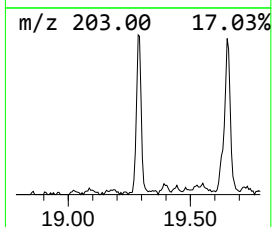
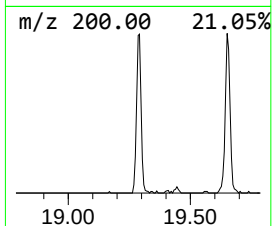
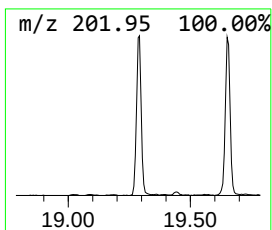
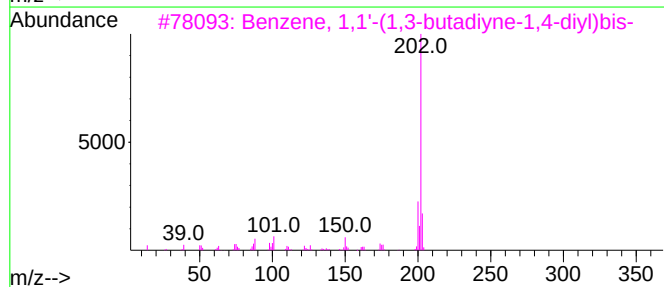
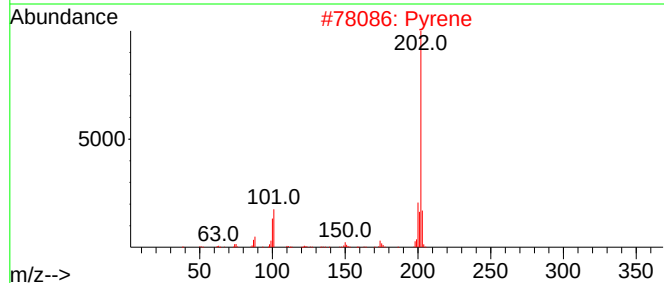
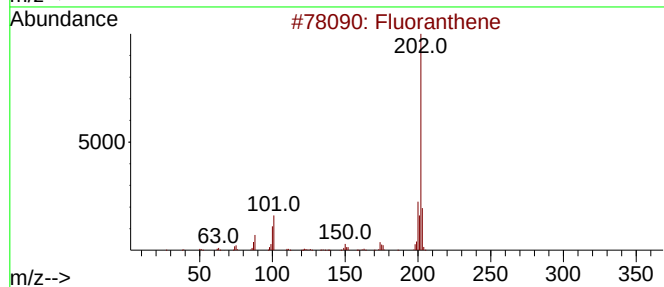
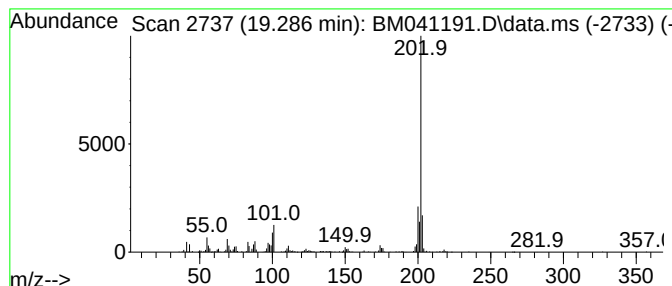
Instrument :
BNA_M
ClientSampleId :
B-P32A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Benzene, 1,1'-(1,3-butadiyn... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
19.286	4.91 ng	510373	Phenanthrene-d10		17.221	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Fluoranthene		202	C16H10	000206-44-0	98
2	Pyrene		202	C16H10	000129-00-0	96
3	Benzene, 1,1'-(1,3-butadiyne-1,4...		202	C16H10	000886-66-8	68
4	2,3-Dichlorobenzo[b]thiophene		202	C8H4Cl2S	1000298-87-9	47
5	Succinic acid, di(4-cyanophenyl)...		320	C18H12N2O4	1000360-71-2	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM073123\
Data File : BM041191.D
Acq On : 31 Jul 2023 16:11
Operator : MA/JU
Sample : 03742-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-P32A

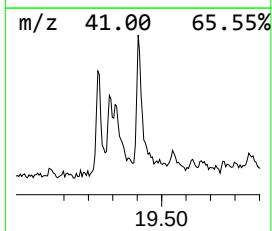
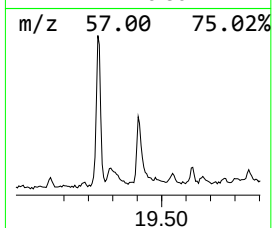
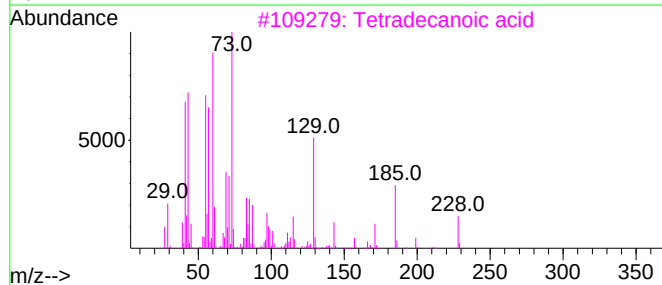
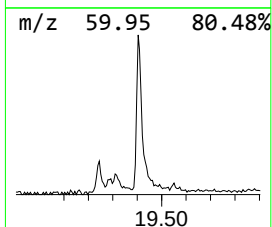
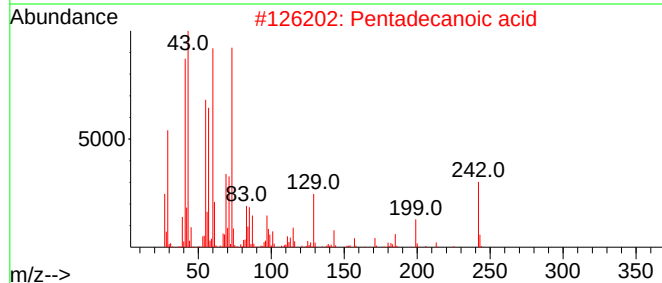
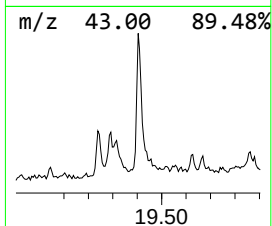
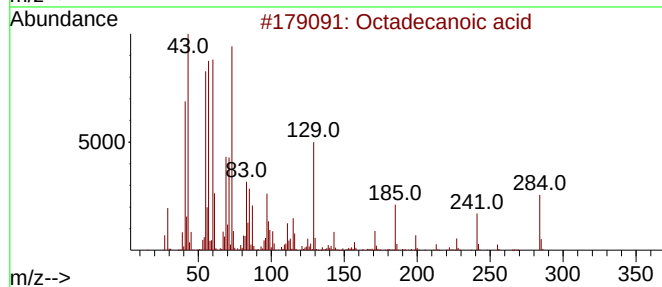
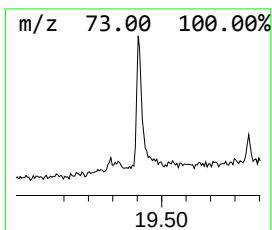
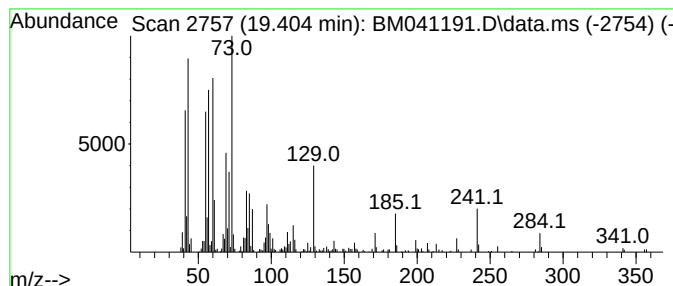
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.404	2.10 ng	265027	Chrysene-d12	21.421

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	90
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	90
5			Tridecanoic acid	214	C13H26O2	000638-53-9	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM073123\
Data File : BM041191.D
Acq On : 31 Jul 2023 16:11
Operator : MA/JU
Sample : 03742-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-P32A

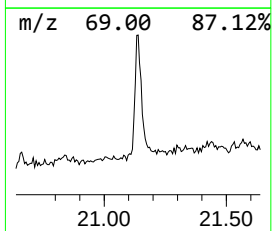
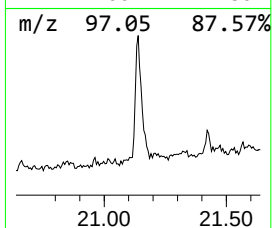
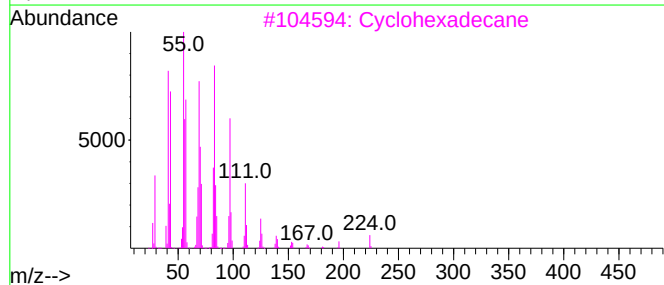
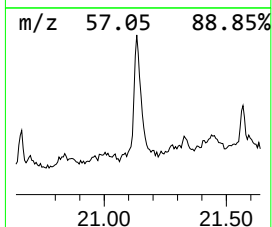
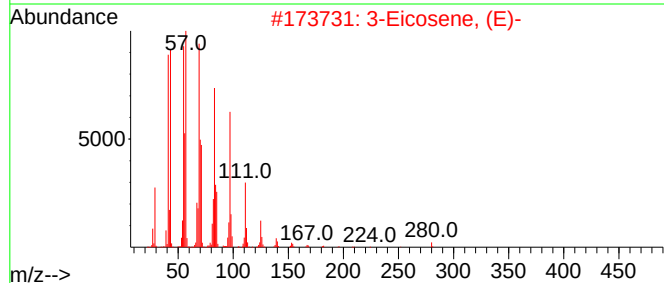
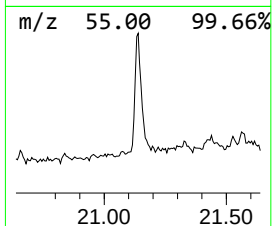
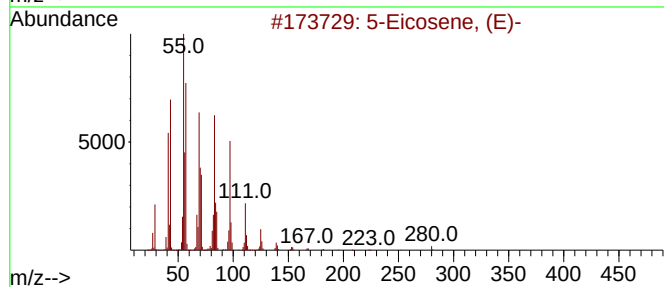
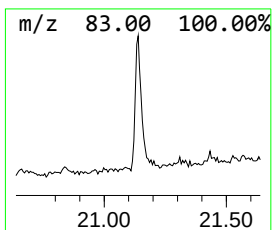
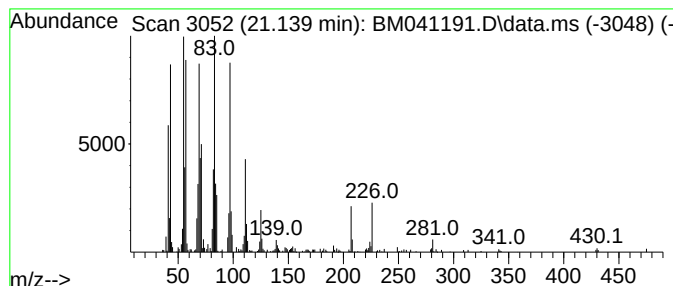
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
21.139	2.61 ng	329073	Chrysene-d12	21.421

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Eicosene, (E)-	280	C20H40	074685-30-6	97
2			3-Eicosene, (E)-	280	C20H40	074685-33-9	95
3			Cyclohexadecane	224	C16H32	000295-65-8	93
4			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
5			Behenic alcohol	326	C22H46O	000661-19-8	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM073123\
Data File : BM041191.D
Acq On : 31 Jul 2023 16:11
Operator : MA/JU
Sample : 03742-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-P32A

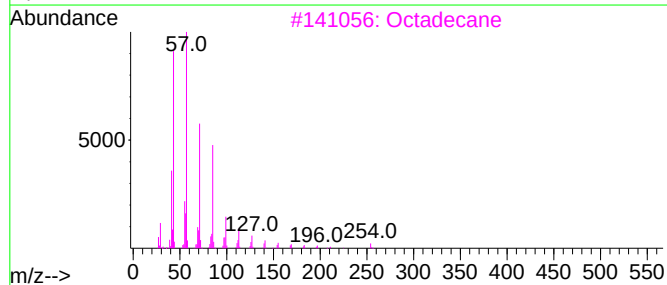
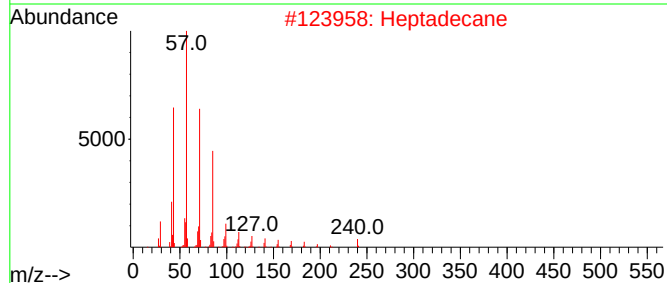
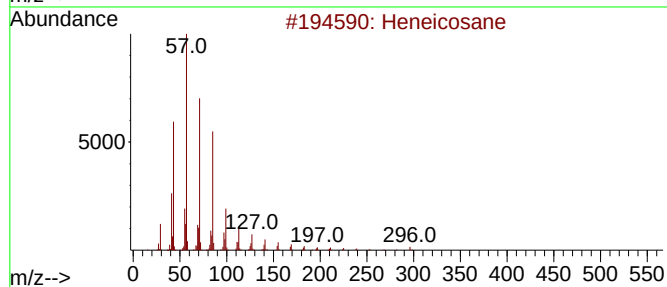
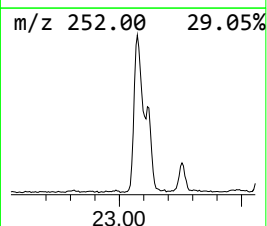
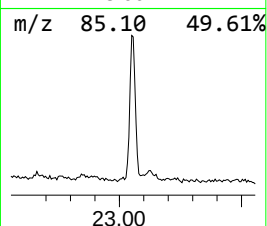
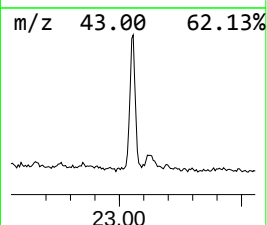
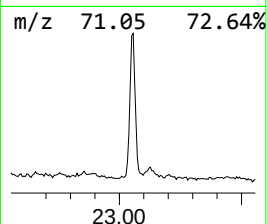
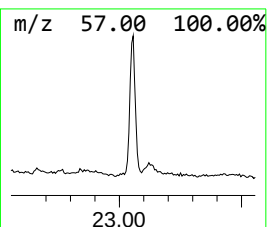
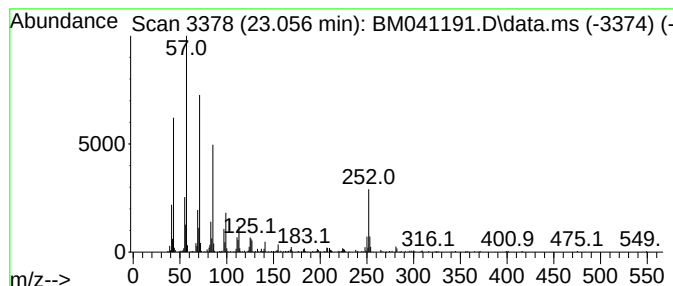
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.056	3.56 ng	456978	Perylene-d12	23.792

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	97
2			Heptadecane	240	C17H36	000629-78-7	94
3			Octadecane	254	C18H38	000593-45-3	92
4			Eicosane	282	C20H42	000112-95-8	90
5			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	89



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM073123\
Data File : BM041191.D
Acq On : 31 Jul 2023 16:11
Operator : MA/JU
Sample : 03742-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

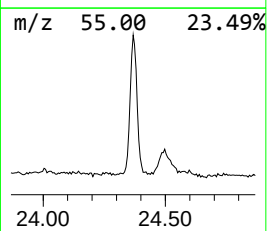
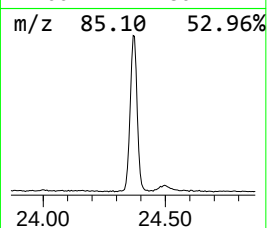
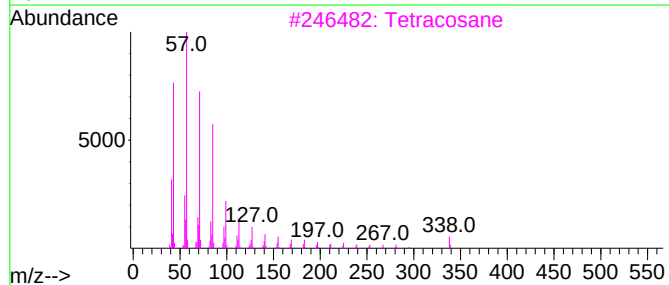
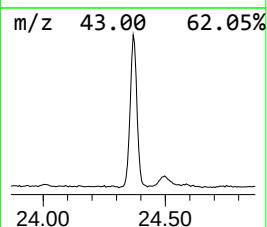
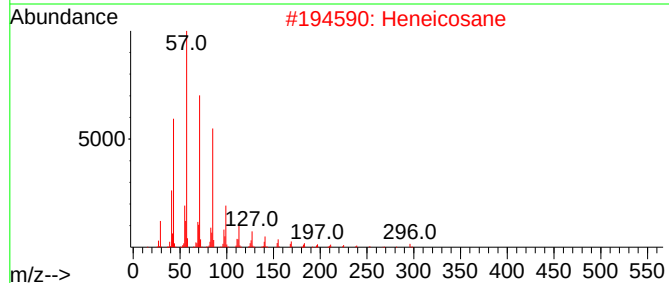
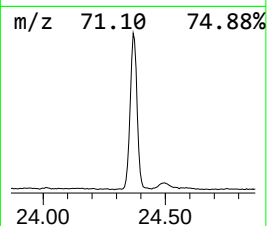
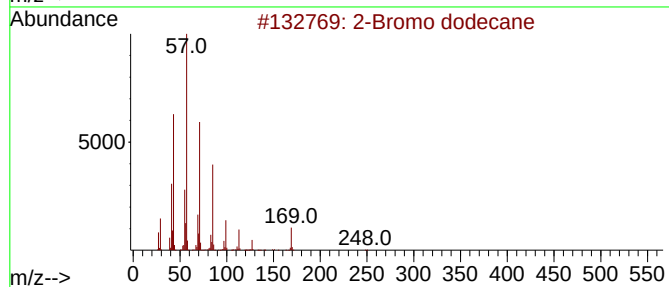
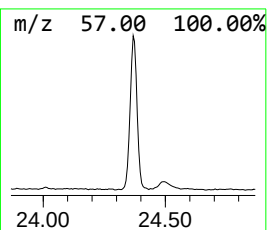
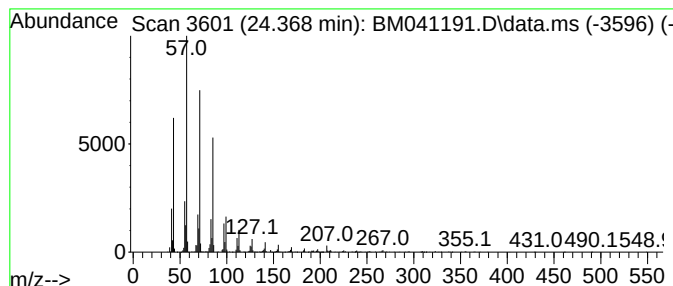
Instrument :
BNA_M
ClientSampleId :
B-P32A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 2-Bromo dodecane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
24.368	10.47 ng	1345230	Perylene-d12	23.792	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Bromo dodecane	248	C12H25Br	013187-99-0	93
2	Heneicosane	296	C21H44	000629-94-7	91
3	Tetracosane	338	C24H50	000646-31-1	91
4	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	91
5	Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM073123\
Data File : BM041191.D
Acq On : 31 Jul 2023 16:11
Operator : MA/JU
Sample : 03742-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-P32A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.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
n-Hexadecanoic ...	18.121	5.5	ng	575234	4	17.221	2080840	20.0
unknown19.245	19.245	3.3	ng	342594	4	17.221	2080840	20.0
Benzene, 1,1'-(...	19.286	4.9	ng	510373	4	17.221	2080840	20.0
Octadecanoic acid	19.404	2.1	ng	265027	5	21.421	2526460	20.0
5-Eicosene, (E)-	21.139	2.6	ng	329073	5	21.421	2526460	20.0
Heneicosane	23.056	3.6	ng	456978	6	23.792	2570050	20.0
2-Bromo dodecane	24.368	10.5	ng	1345230	6	23.792	2570050	20.0