

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052022\
 Data File : BM035181.D
 Acq On : 20 May 2022 17:58
 Operator : CG/JU
 Sample : N2872-18
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 P022-SS002-0006-02

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-BM042722.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM035181.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.016	323	328	334	rBV	61136	90771	1.09%	0.225%
2	5.481	400	407	426	rBV	2415181	3540729	42.48%	8.763%
3	7.075	669	678	694	rBV	2381578	3815817	45.78%	9.444%
4	7.410	727	735	753	rBV2	25657	138110	1.66%	0.342%
5	7.904	811	819	828	rBV	425900	674341	8.09%	1.669%
6	9.063	1006	1016	1025	rBV	1444482	2376604	28.51%	5.882%
7	9.510	1087	1092	1099	rBV	91496	142844	1.71%	0.354%
8	10.704	1289	1295	1305	rVB	544247	912260	10.94%	2.258%
9	11.063	1349	1356	1369	rBV	53137	108104	1.30%	0.268%
10	13.169	1704	1714	1724	rBV	3658395	5292719	63.50%	13.099%
11	14.539	1941	1947	1955	rBV	816543	1204263	14.45%	2.980%
12	15.363	2081	2087	2096	rBV	60643	100331	1.20%	0.248%
13	16.027	2193	2200	2217	rBV	2988158	4257307	51.08%	10.537%
14	17.286	2407	2414	2420	rBV	999019	1423894	17.08%	3.524%
15	18.186	2562	2567	2576	rBV	513168	797195	9.56%	1.973%
16	18.257	2576	2579	2585	rVB	51888	84832	1.02%	0.210%
17	19.345	2761	2764	2772	rVB3	58090	99675	1.20%	0.247%
18	19.468	2780	2785	2803	rBV	785232	1251084	15.01%	3.096%
19	19.909	2854	2860	2868	rBV	6916931	8335196	100.00%	20.629%
20	21.186	3073	3077	3086	rBV	306378	445238	5.34%	1.102%
21	21.468	3120	3125	3136	rBV	1437917	1901244	22.81%	4.705%
22	21.603	3144	3148	3152	rBV	631093	752471	9.03%	1.862%
23	21.774	3174	3177	3182	rBV	197675	249264	2.99%	0.617%
24	22.003	3213	3216	3224	rVB	136773	180518	2.17%	0.447%
25	22.174	3241	3245	3249	rVB	294250	362073	4.34%	0.896%
26	23.856	3525	3531	3543	rVB2	914194	1867913	22.41%	4.623%

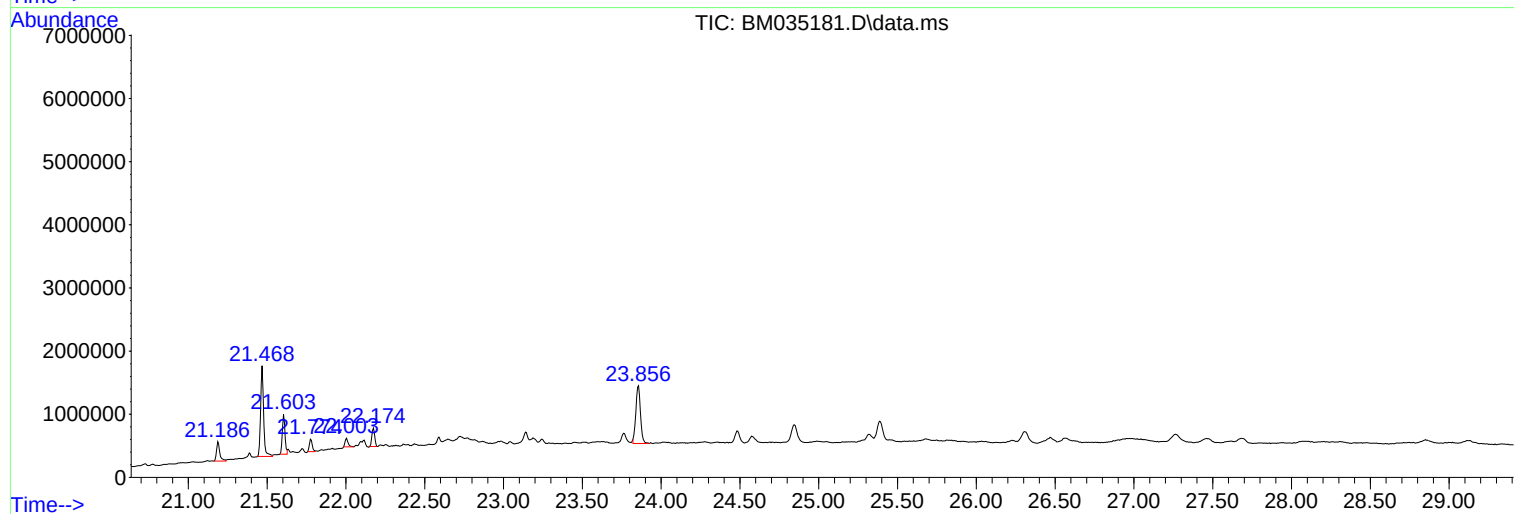
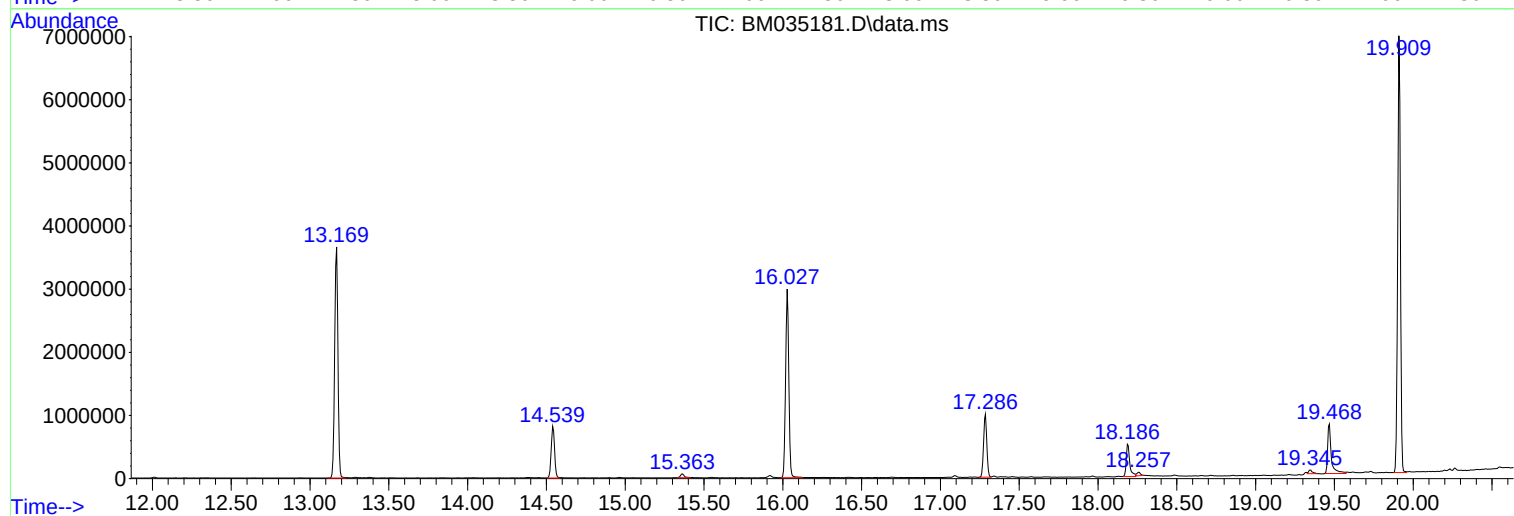
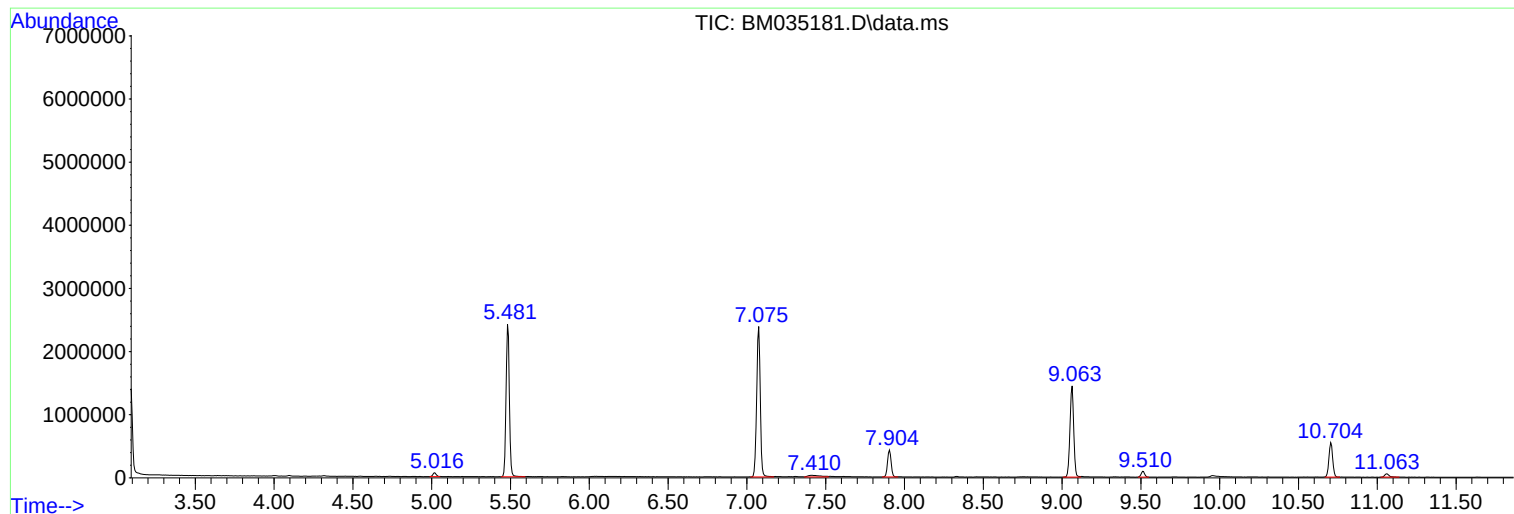
Sum of corrected areas: 40404797

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052022\
Data File : BM035181.D
Acq On : 20 May 2022 17:58
Operator : CG/JU
Sample : N2872-18
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P022-SS002-0006-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042722.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\BM052022\
Data File : BM035181.D
Acq On : 20 May 2022 17:58
Operator : CG/JU
Sample : N2872-18
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P022-SS002-0006-02

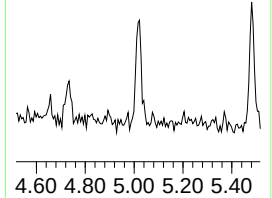
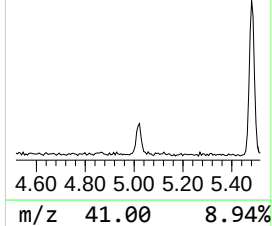
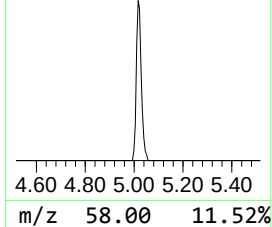
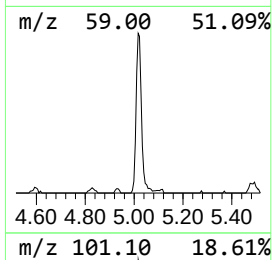
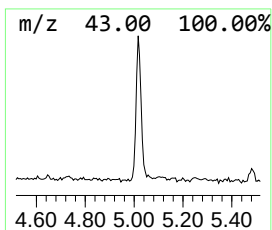
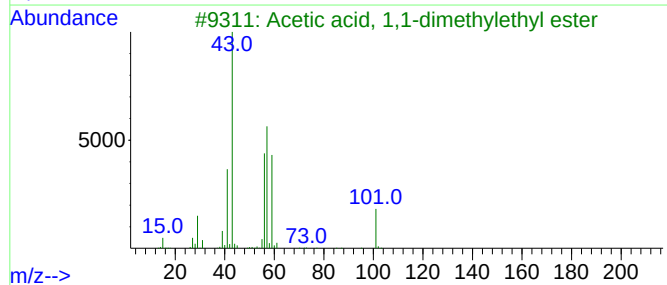
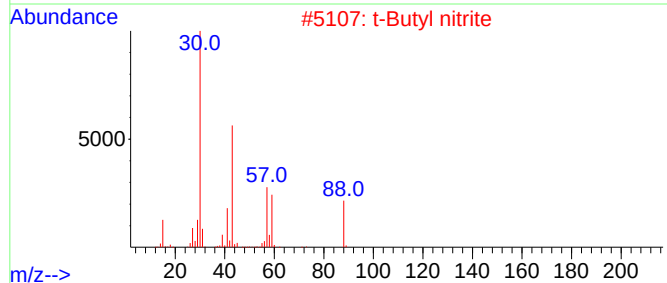
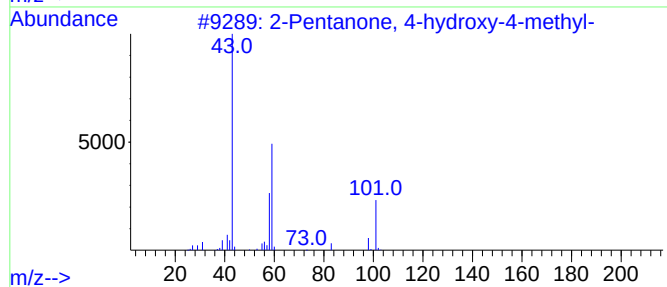
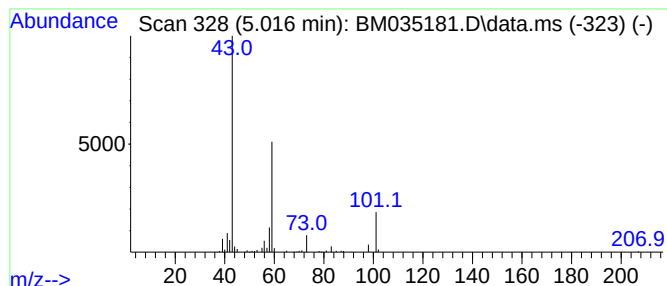
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.016	2.69 ng	90771	1,4-Dichlorobenzene-d4	7.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59		
2	t-Butyl nitrite	103	C4H9NO2	000540-80-7	38		
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	36		
4	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	25		
5	Hydrazine, (1-methylpropyl)-	88	C4H12N2	030924-14-2	23		



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052022\
Data File : BM035181.D
Acq On : 20 May 2022 17:58
Operator : CG/JU
Sample : N2872-18
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P022-SS002-0006-02

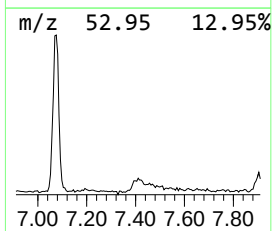
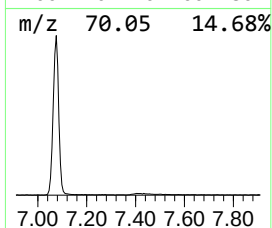
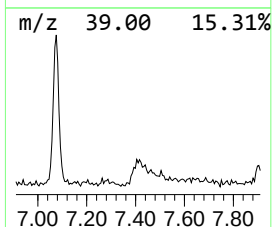
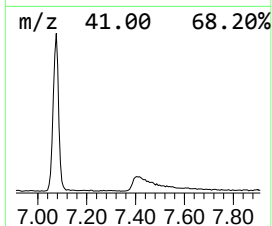
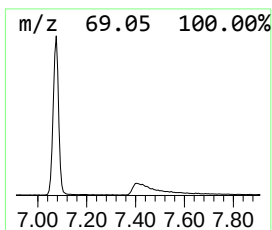
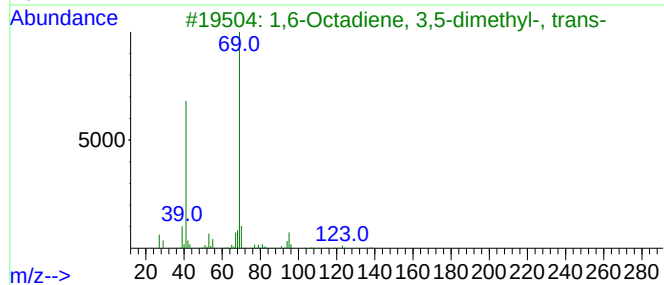
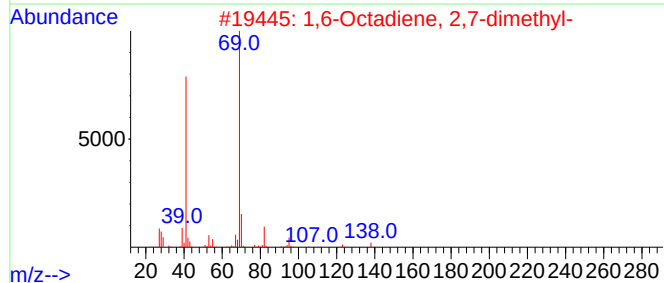
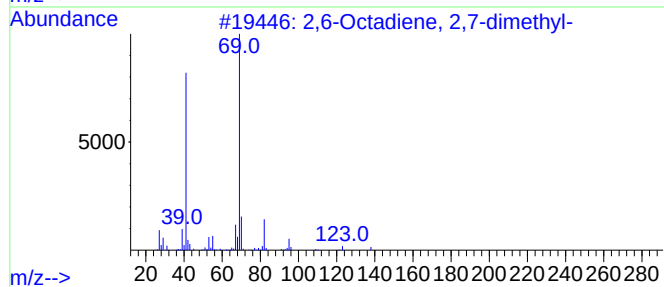
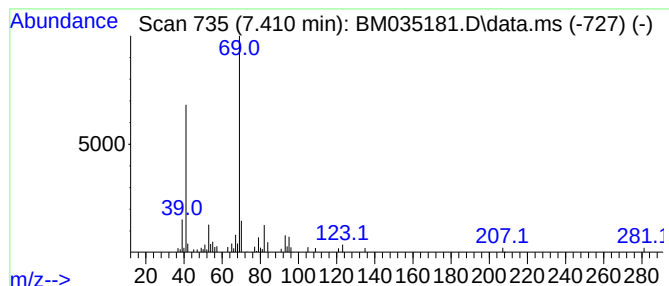
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2,6-Octadiene, 2,7-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.410	4.10 ng	138110	1,4-Dichlorobenzene-d4	7.904

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2,6-Octadiene, 2,7-dimethyl-	138	C10H18	016736-42-8	72
2		1,6-Octadiene, 2,7-dimethyl-	138	C10H18	040195-09-3	64
3		1,6-Octadiene, 3,5-dimethyl-, tr...	138	C10H18	074630-87-8	59
4		4-Methyl-1,5-Heptadiene	110	C8H14	000998-94-7	59
5		Cyclopropanecarboxylic acid, tr...	264	C17H28O2	1000299-38-2	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052022\
Data File : BM035181.D
Acq On : 20 May 2022 17:58
Operator : CG/JU
Sample : N2872-18
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P022-SS002-0006-02

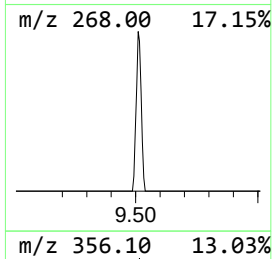
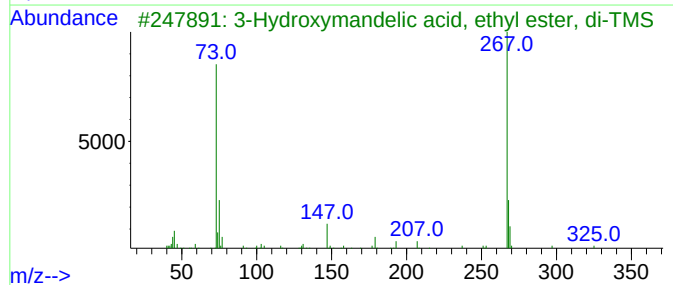
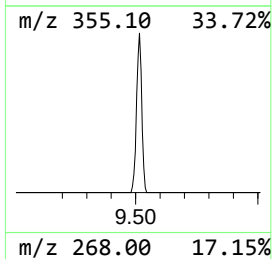
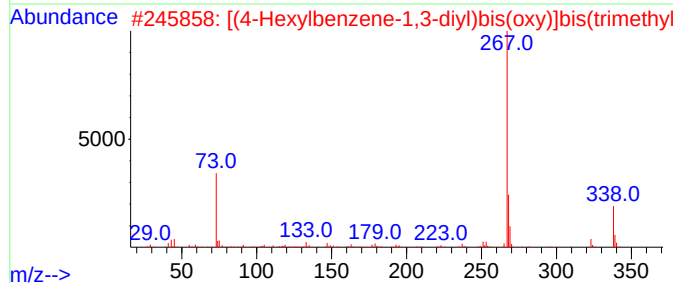
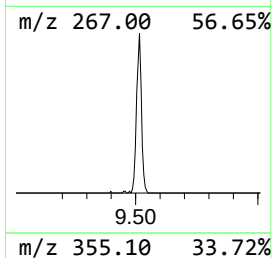
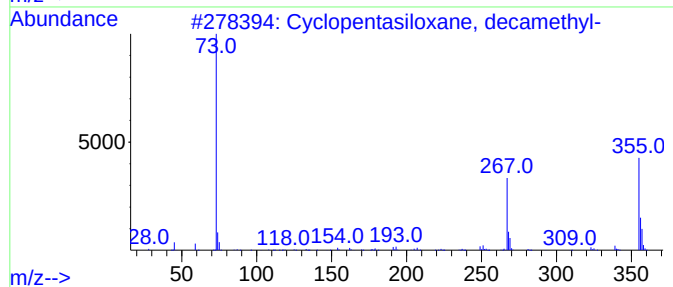
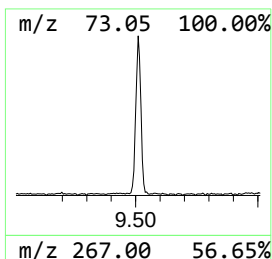
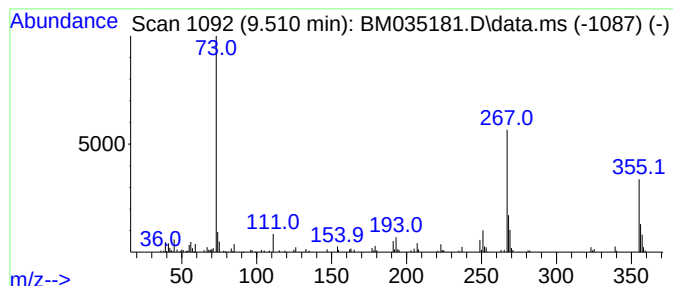
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Cyclopentasiloxane, decamet... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.510	3.13 ng	142844	Naphthalene-d8	10.704

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentasiloxane, decamethyl-	370	C10H30O5Si5	000541-02-6	90
2			[(4-Hexylbenzene-1,3-diyl)bis(ox...	338	C18H34O2Si2	134273-01-1	47
3			3-Hydroxymandelic acid, ethyl es...	340	C16H28O4Si2	1000071-88-9	47
4			Bamethan, 2TMS derivative	353	C18H35NO2Si2	040629-66-1	47
5			4-(4-Fluorophenyl)-2,3-dihydro-1...	267	C12H14FNOSSi	1010501-61-0	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052022\
Data File : BM035181.D
Acq On : 20 May 2022 17:58
Operator : CG/JU
Sample : N2872-18
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P022-SS002-0006-02

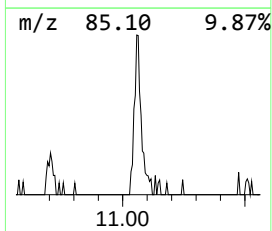
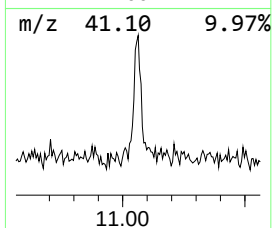
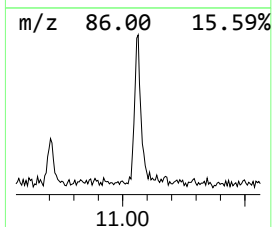
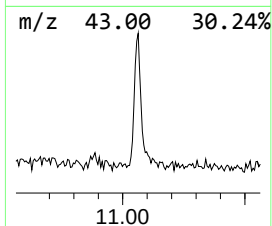
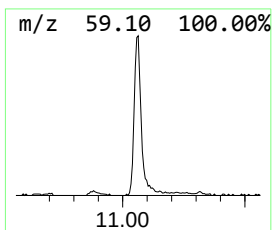
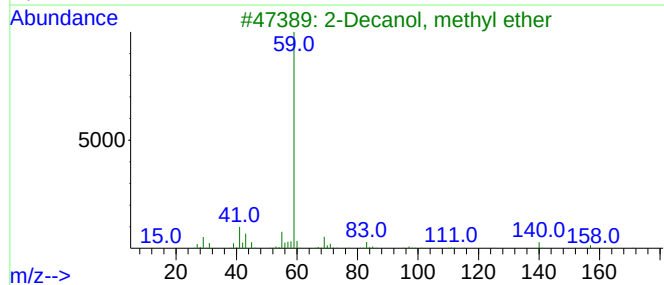
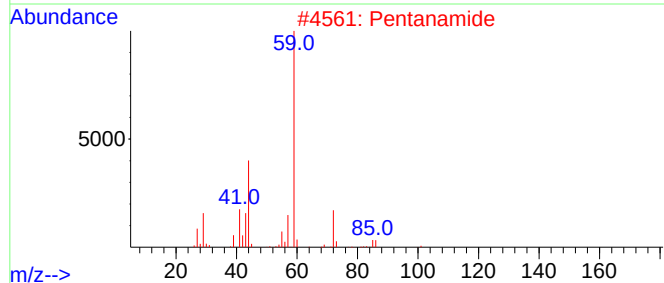
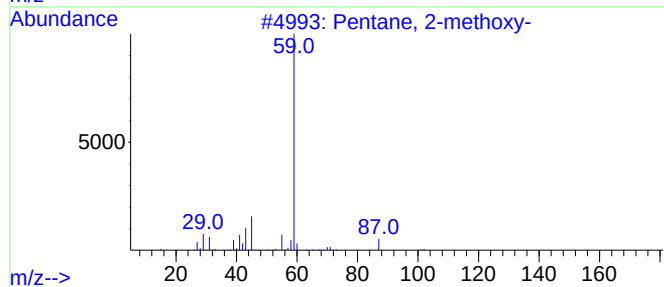
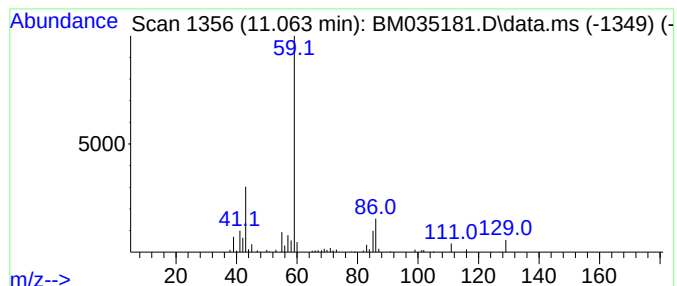
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Pentane, 2-methoxy- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.063	2.37 ng	108104	Naphthalene-d8	10.704

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2-methoxy-	102	C6H14O	006795-88-6	53
2			Pentanamide	101	C5H11NO	000626-97-1	53
3			2-Decanol, methyl ether	172	C11H24O	1000333-83-9	50
4			3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	50
5			1-Butanol, 3-methoxy-, acetate	146	C7H14O3	004435-53-4	45



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052022\
Data File : BM035181.D
Acq On : 20 May 2022 17:58
Operator : CG/JU
Sample : N2872-18
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P022-SS002-0006-02

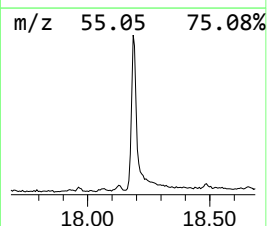
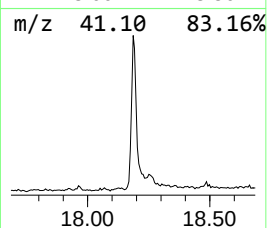
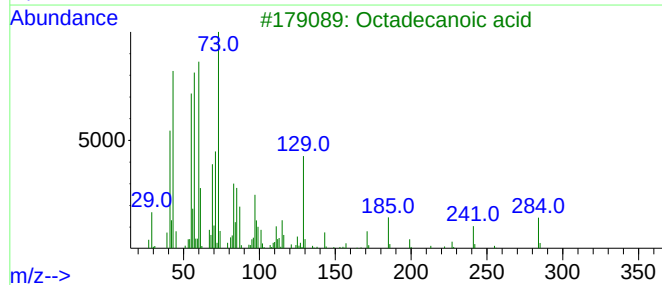
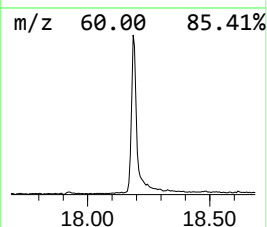
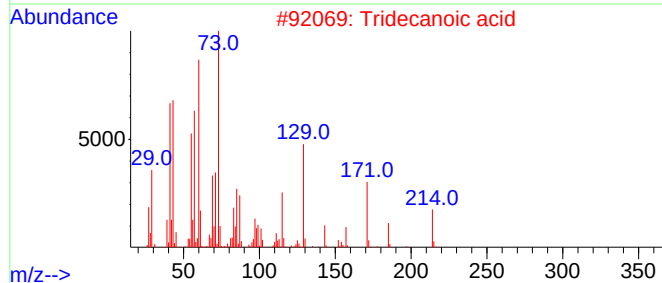
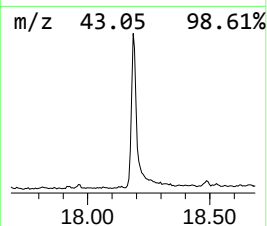
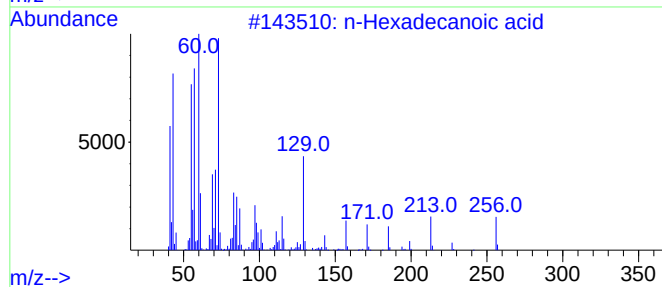
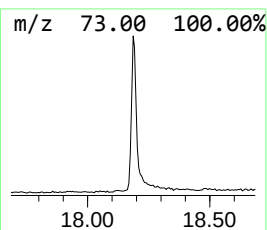
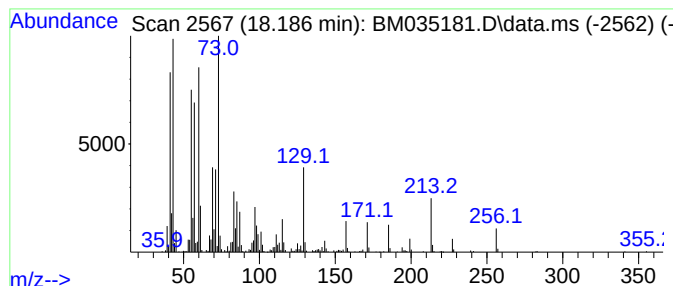
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.186	11.20 ng	797195	Phenanthrene-d10	17.286

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	95
3			Octadecanoic acid	284	C18H36O2	000057-11-4	93
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052022\
Data File : BM035181.D
Acq On : 20 May 2022 17:58
Operator : CG/JU
Sample : N2872-18
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P022-SS002-0006-02

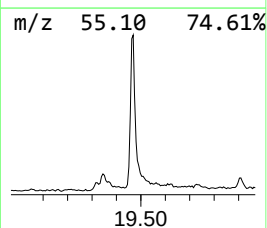
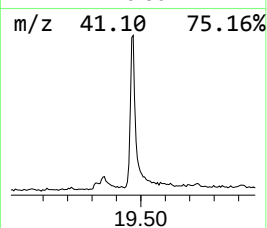
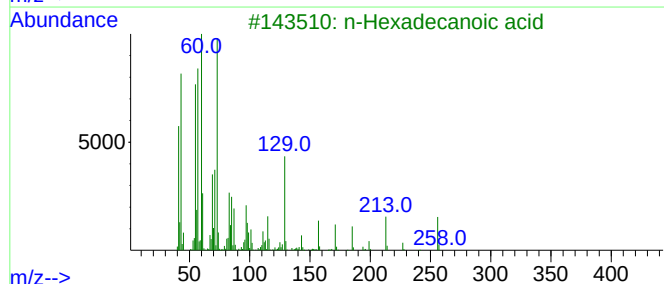
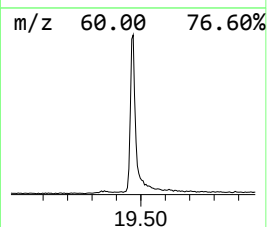
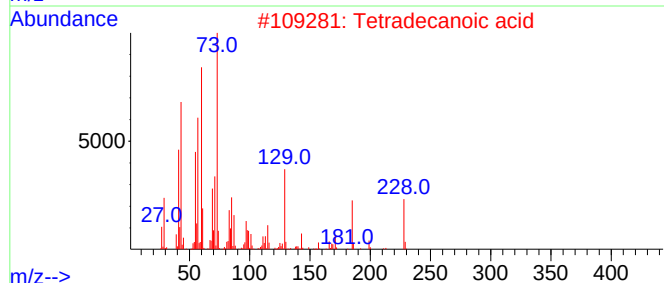
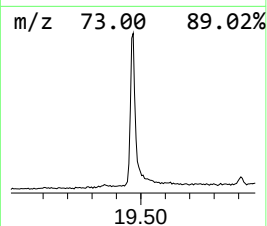
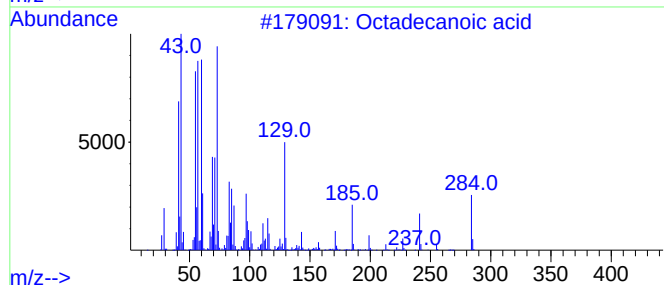
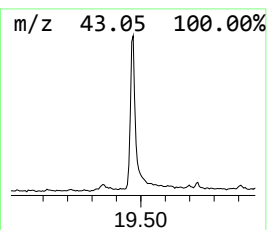
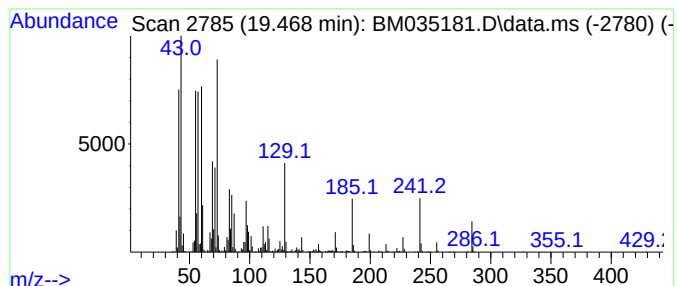
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.468	13.16 ng	1251080	Chrysene-d12	21.468

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
4			Tridecanoic acid	214	C13H26O2	000638-53-9	76
5			n-Decanoic acid	172	C10H20O2	000334-48-5	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052022\
Data File : BM035181.D
Acq On : 20 May 2022 17:58
Operator : CG/JU
Sample : N2872-18
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P022-SS002-0006-02

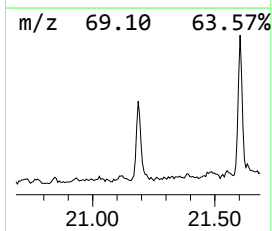
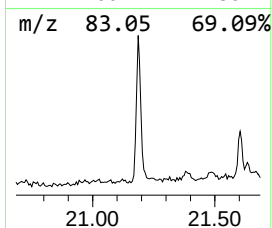
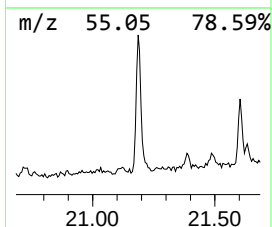
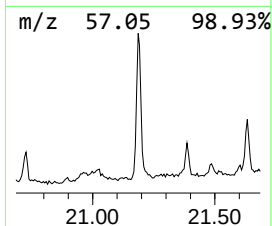
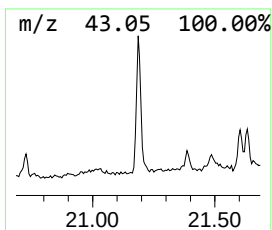
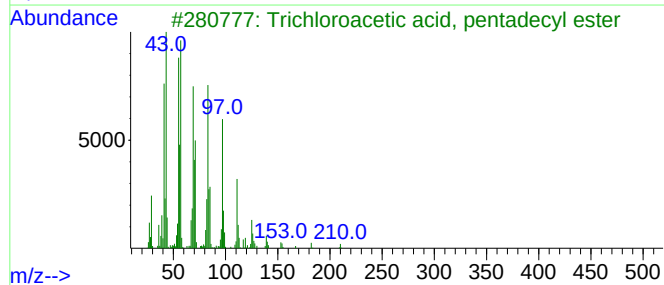
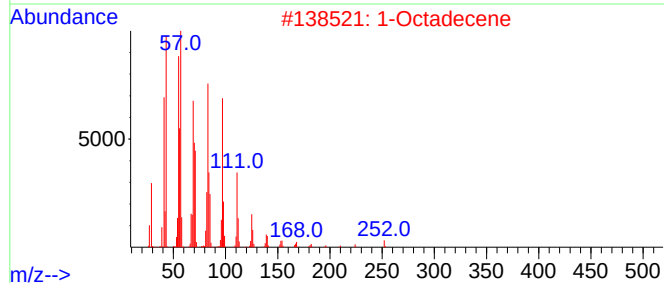
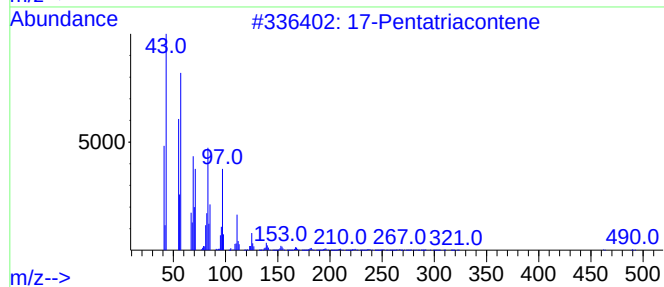
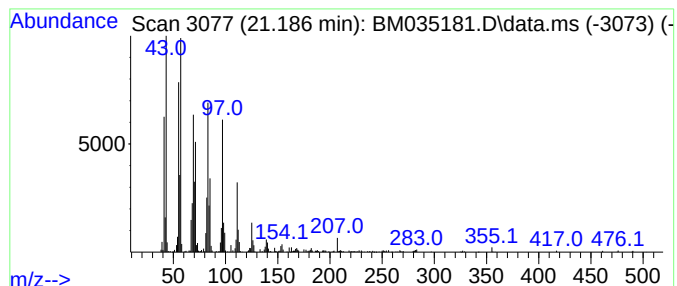
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 17-Pentatriacontene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.186	4.68 ng	445238	Chrysene-d12	21.468

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	17-Pentatriacontene			491	C35H70	006971-40-0	96
2	1-Octadecene			252	C18H36	000112-88-9	95
3	Trichloroacetic acid, pentadecyl...			372	C17H31Cl3O2	074339-53-0	94
4	Heptadecyl heptafluorobutyrate			452	C21H35F7O2	959085-66-6	94
5	Pentadecafluorooctanoic acid, oc...			666	C26H37F15O2	1000406-04-8	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052022\
Data File : BM035181.D
Acq On : 20 May 2022 17:58
Operator : CG/JU
Sample : N2872-18
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P022-SS002-0006-02

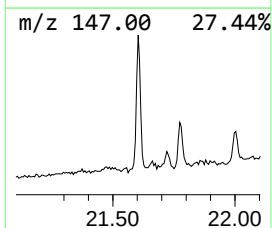
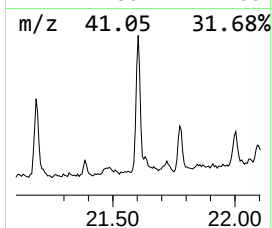
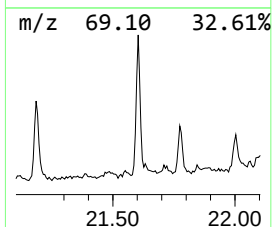
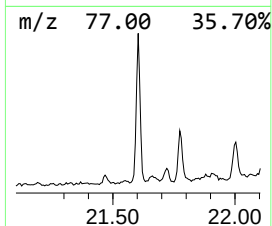
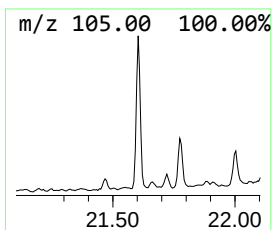
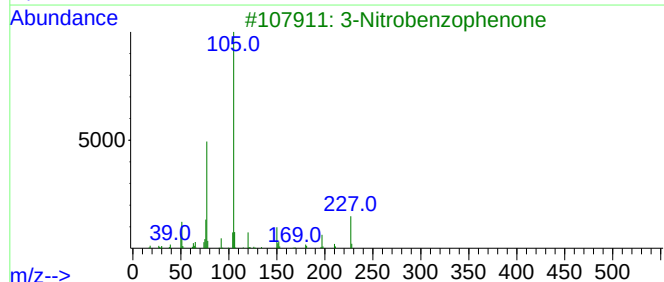
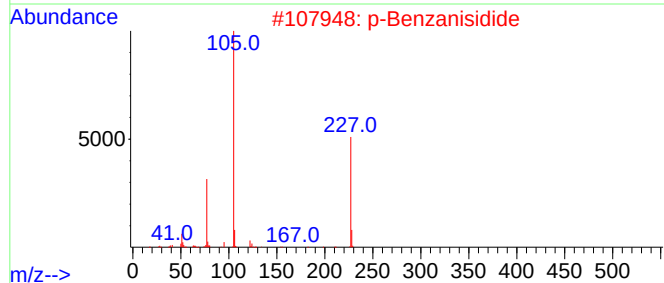
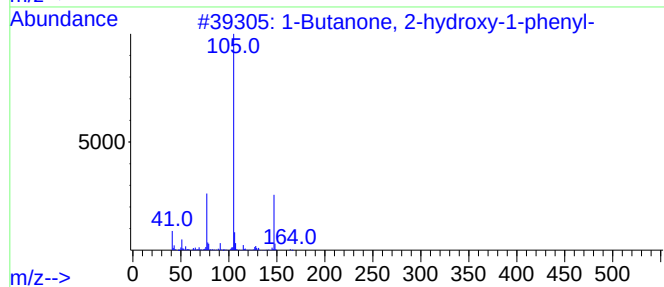
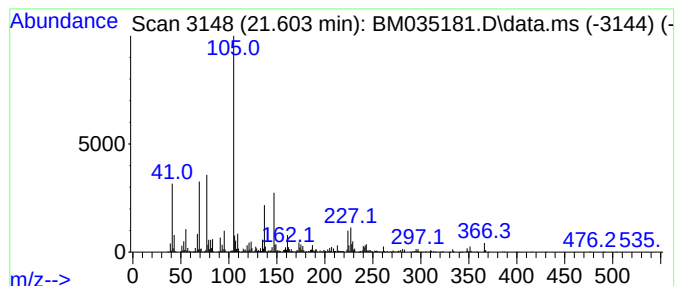
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown21.604 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.604	7.92 ng	752471	Chrysene-d12	21.468

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Butanone, 2-hydroxy-1-phenyl-	164	C10H12O2	016183-46-3	43
2			p-Benzanisidide	227	C14H13NO2	007472-54-0	27
3			3-Nitrobenzophenone	227	C13H9NO3	002243-80-3	27
4			3-(Benzoylthio)-2-methylpropanoi...	224	C11H12O3S	067714-34-5	27
5			acetic acid, 2-bromo-, 2-oxo-2-p...	256	C10H9BrO3	1000401-50-0	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052022\
Data File : BM035181.D
Acq On : 20 May 2022 17:58
Operator : CG/JU
Sample : N2872-18
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P022-SS002-0006-02

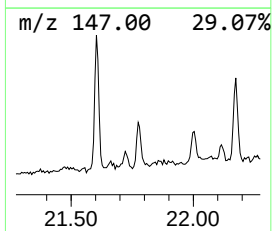
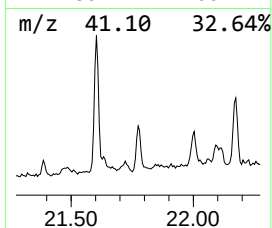
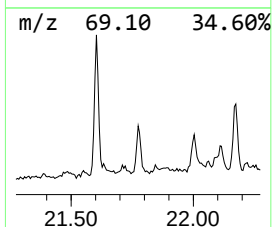
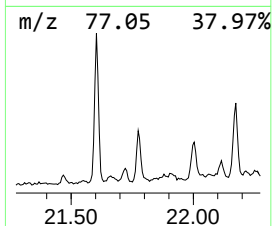
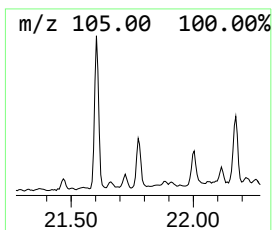
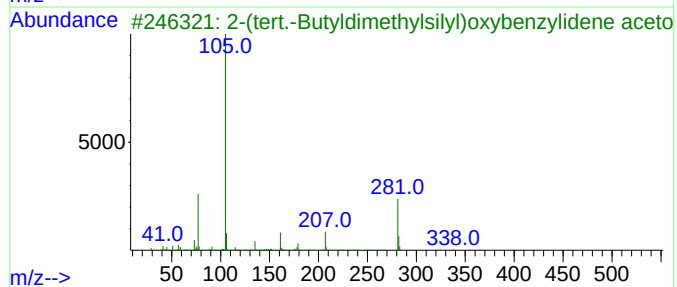
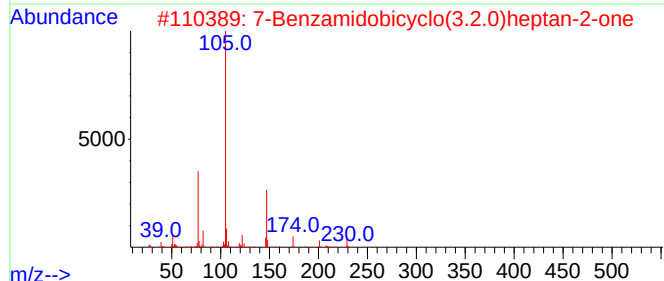
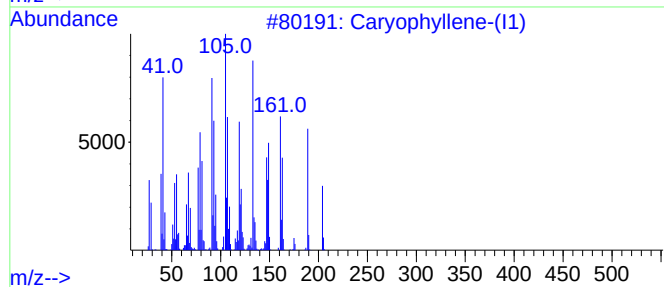
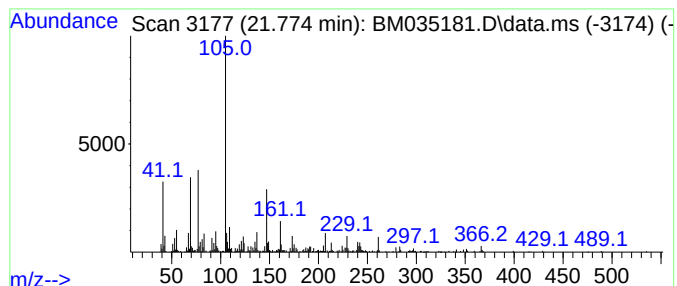
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown21.774 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.774	2.62 ng	249264	Chrysene-d12	21.468

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Caryophyllene-(I1)	204	C15H24	1000158-18-5	43
2			7-Benzamidobicyclo(3.2.0)heptan-...	229	C14H15NO2	1000241-65-0	43
3			2-(tert.-Butyldimethylsilyl)oxyb...	338	C21H26O2Si	1000395-75-9	41
4			.beta.-Guaiene	204	C15H24	000088-84-6	38
5			Valerena-4,7(11)-diene	204	C15H24	351222-66-7	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052022\
Data File : BM035181.D
Acq On : 20 May 2022 17:58
Operator : CG/JU
Sample : N2872-18
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P022-SS002-0006-02

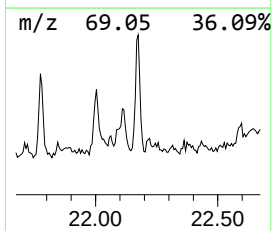
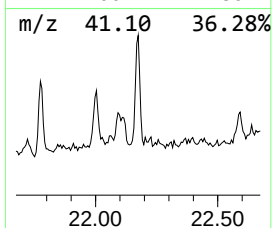
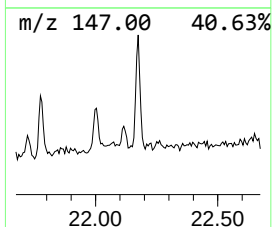
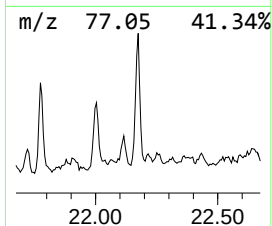
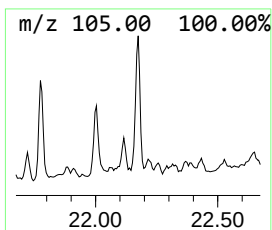
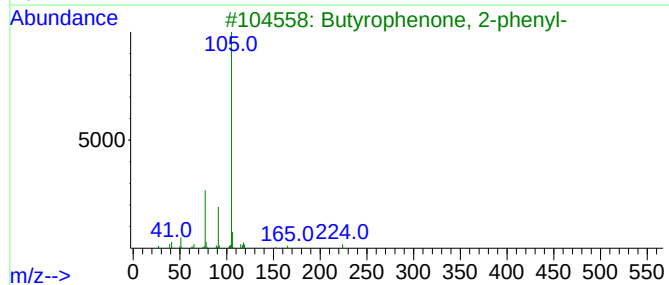
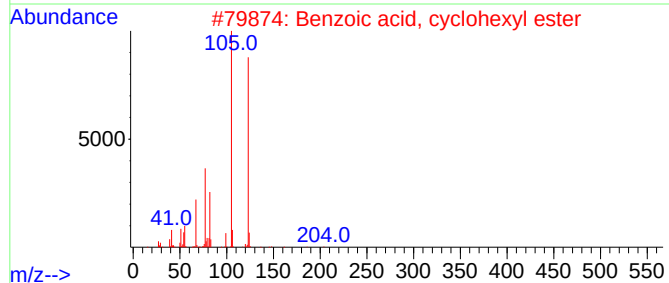
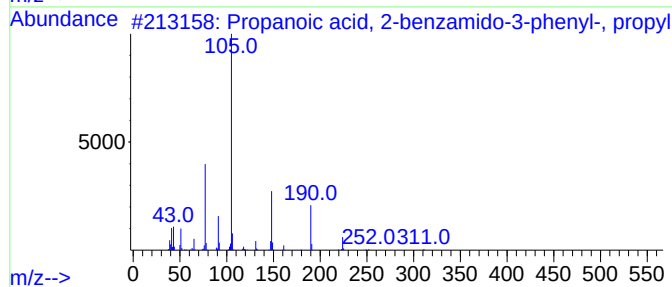
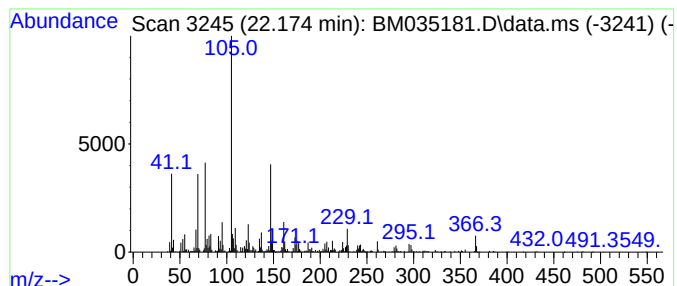
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown22.174 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.174	3.81 ng	362073	Chrysene-d12	21.468

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2-benzamido-3-ph...	311	C19H21NO3	1000261-32-6	25
2			Benzoic acid, cyclohexyl ester	204	C13H16O2	002412-73-9	22
3			Butyrophenone, 2-phenyl-	224	C16H16O	016282-16-9	18
4			Methyl tri-O-benzoyl-.beta.-d-ri...	476	C27H24O8	1000129-82-3	18
5			Benzoic acid, 2-isopropylphenyl ...	240	C16H16O2	1000368-96-0	15



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052022\
Data File : BM035181.D
Acq On : 20 May 2022 17:58
Operator : CG/JU
Sample : N2872-18
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P022-SS002-0006-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042722.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-...	5.016	2.7	ng	90771	1	7.904	674341	20.0
2,6-Octadiene, ...	7.410	4.1	ng	138110	1	7.904	674341	20.0
Cyclopentasilox...	9.510	3.1	ng	142844	2	10.704	912260	20.0
Pentane, 2-meth...	11.063	2.4	ng	108104	2	10.704	912260	20.0
n-Hexadecanoic ...	18.186	11.2	ng	797195	4	17.286	1423890	20.0
Octadecanoic acid	19.468	13.2	ng	1251080	5	21.468	1901240	20.0
17-Pentatriacon...	21.186	4.7	ng	445238	5	21.468	1901240	20.0
unknown21.604	21.604	7.9	ng	752471	5	21.468	1901240	20.0
unknown21.774	21.774	2.6	ng	249264	5	21.468	1901240	20.0
unknown22.174	22.174	3.8	ng	362073	5	21.468	1901240	20.0