

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041423\
 Data File : BM039435.D
 Acq On : 14 Apr 2023 15:56
 Operator : CG/JU
 Sample : 02347-05
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 20230331-COMP-9

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-BM032923.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM039435.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.940	292	298	318	rVB	828541	1149479	11.84%	2.054%
2	5.428	374	381	397	rBV	3496651	5422599	55.87%	9.688%
3	7.051	649	657	676	rBV	3170606	5465829	56.31%	9.765%
4	7.851	786	793	803	rBV	566024	936623	9.65%	1.673%
5	9.022	983	992	1008	rBV	1904611	3421009	35.25%	6.112%
6	10.663	1263	1271	1282	rBV	670655	1254048	12.92%	2.241%
7	13.127	1683	1690	1712	rBV	4691072	7134934	73.51%	12.747%
8	14.510	1918	1925	1938	rBV	1003643	1583322	16.31%	2.829%
9	15.868	2150	2156	2169	rBV	586631	876230	9.03%	1.565%
10	16.004	2172	2179	2197	rBV	3714449	5541300	57.09%	9.900%
11	17.256	2386	2392	2408	rBV	1174117	1806959	18.62%	3.228%
12	18.162	2540	2546	2555	rBV	2060252	3408798	35.12%	6.090%
13	19.439	2758	2763	2784	rBV	1737227	3265844	33.65%	5.835%
14	19.886	2834	2839	2857	rBV	7313337	9705976	100.00%	17.341%
15	21.150	3050	3054	3062	rBV	685950	1009456	10.40%	1.804%
16	21.450	3100	3105	3118	rVB	1453969	1976659	20.37%	3.532%
17	23.833	3505	3510	3524	rVB2	984947	2012482	20.73%	3.596%

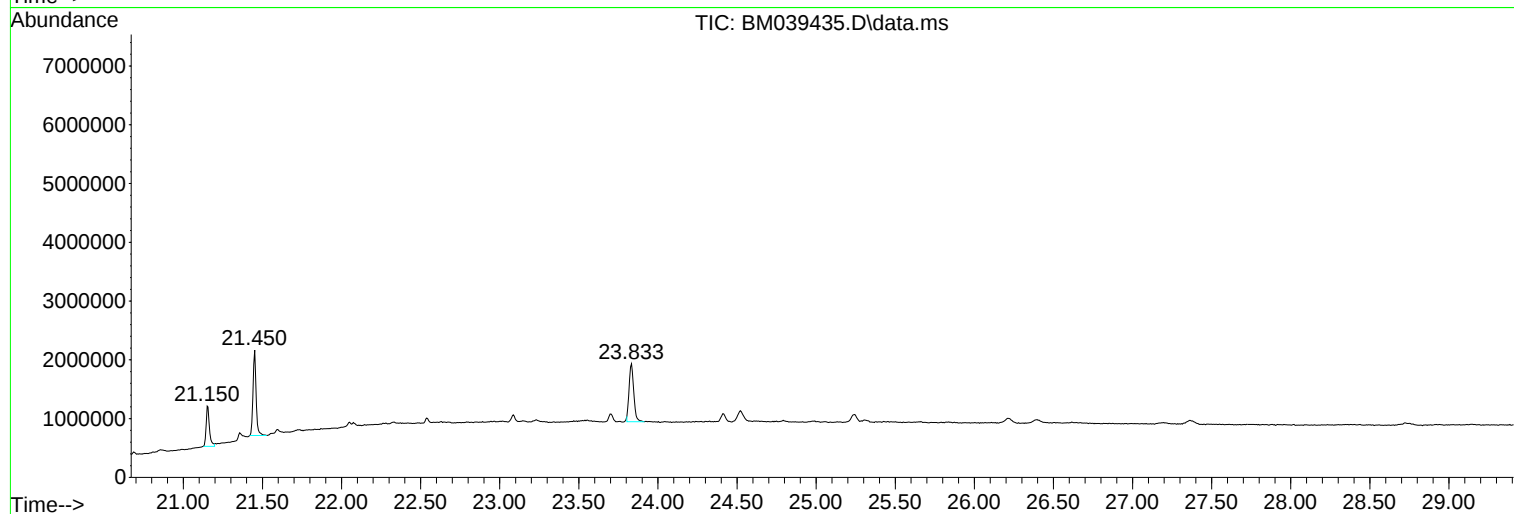
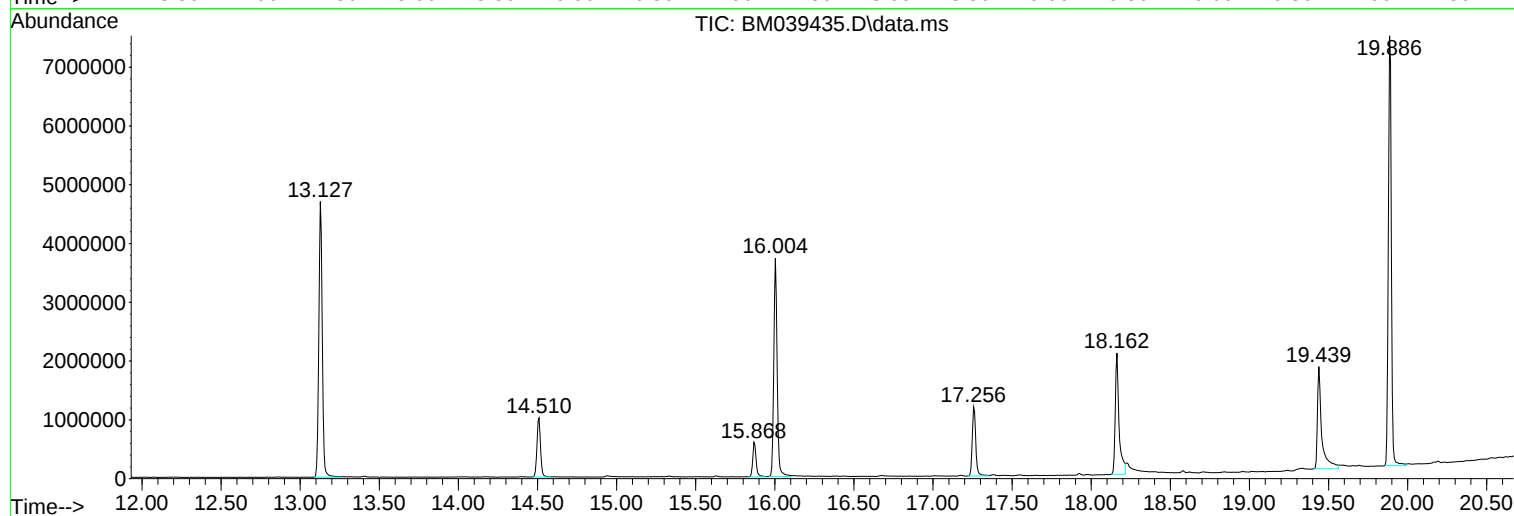
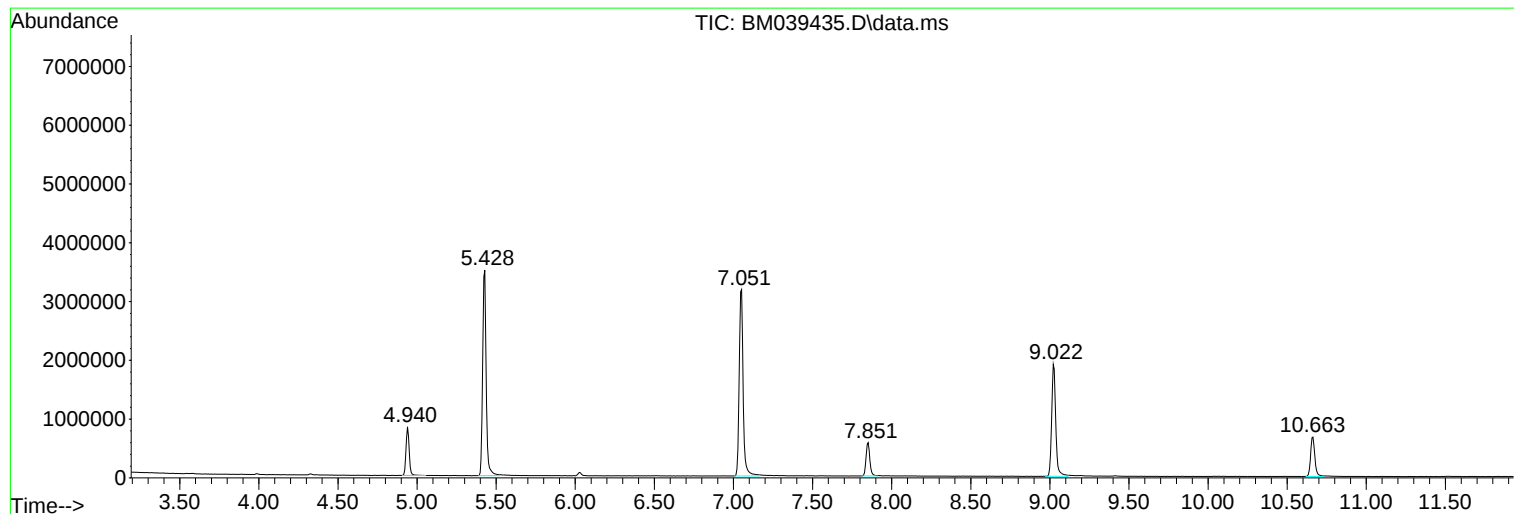
Sum of corrected areas: 55971547

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041423\
Data File : BM039435.D
Acq On : 14 Apr 2023 15:56
Operator : CG/JU
Sample : 02347-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
20230331-COMP-9

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.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\BM041423\
Data File : BM039435.D
Acq On : 14 Apr 2023 15:56
Operator : CG/JU
Sample : 02347-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
20230331-COMP-9

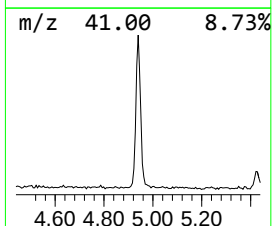
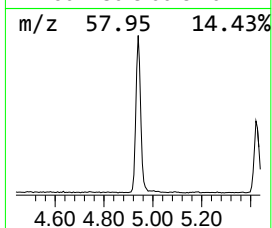
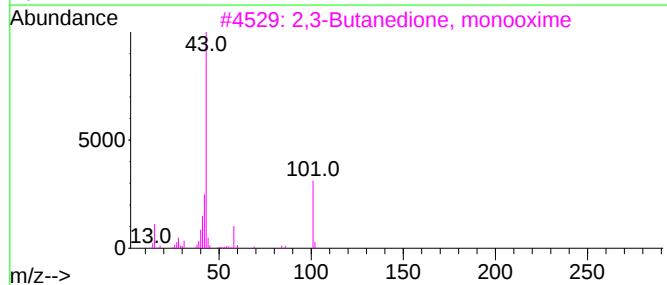
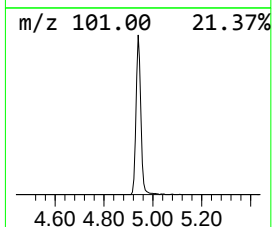
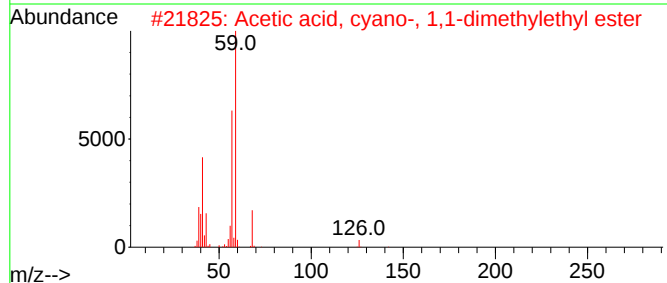
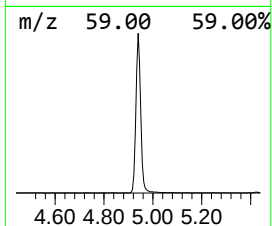
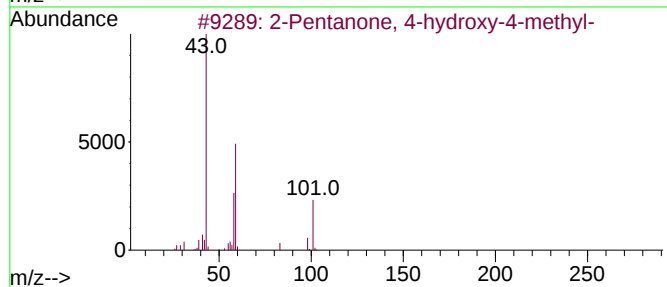
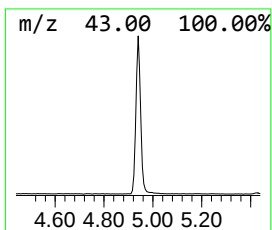
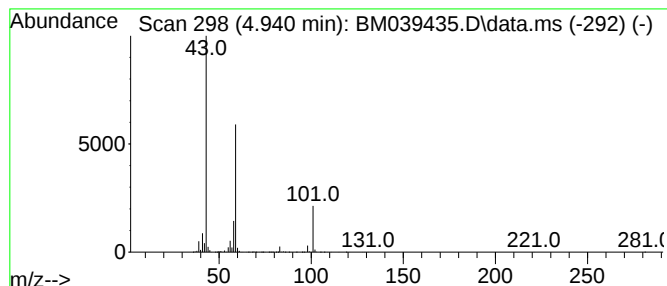
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.940	24.55 ng	1149480	1,4-Dichlorobenzene-d4	7.851

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041423\
Data File : BM039435.D
Acq On : 14 Apr 2023 15:56
Operator : CG/JU
Sample : 02347-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
20230331-COMP-9

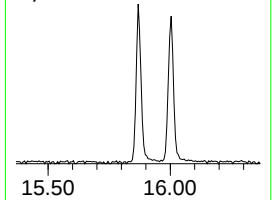
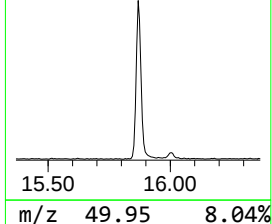
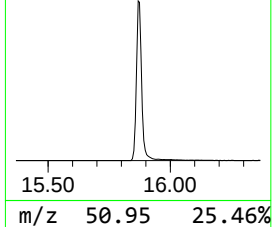
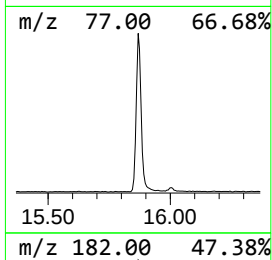
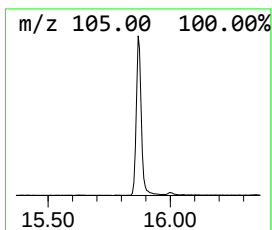
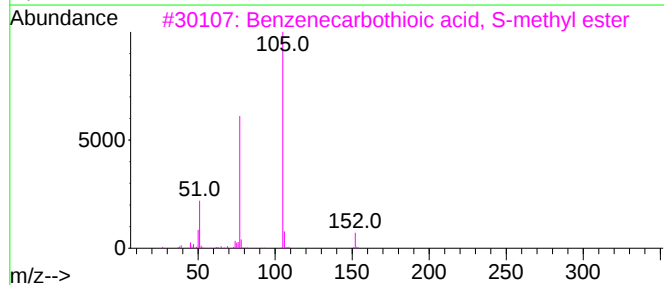
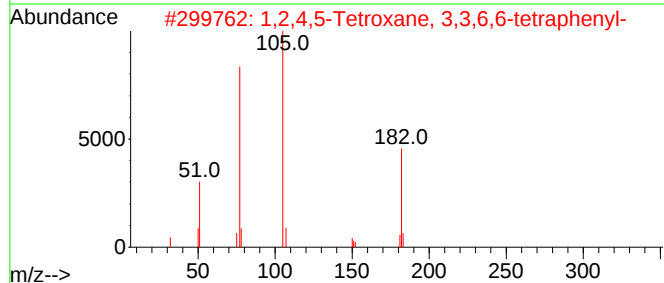
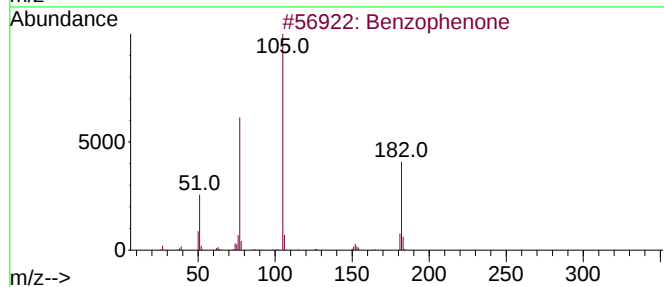
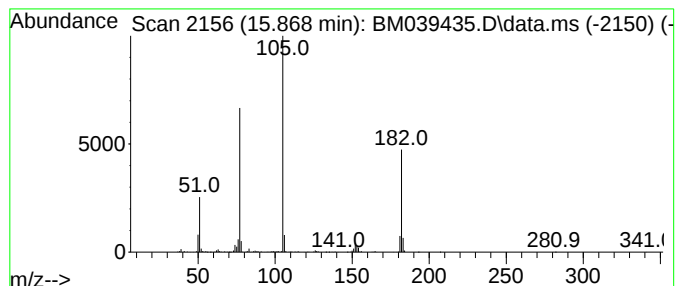
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.868	11.07 ng	876230	Acenaphthene-d10	14.510

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			1,2,4,5-Tetroxane, 3,3,6,6-tetra...	396	C26H20O4	016204-36-7	78
3			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	52
4			Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	49
5			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041423\
Data File : BM039435.D
Acq On : 14 Apr 2023 15:56
Operator : CG/JU
Sample : 02347-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
20230331-COMP-9

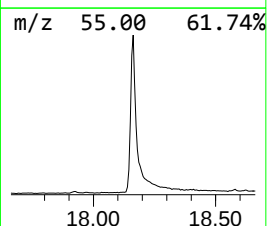
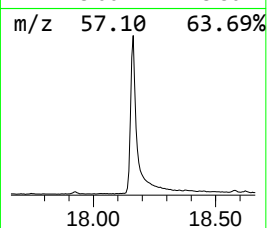
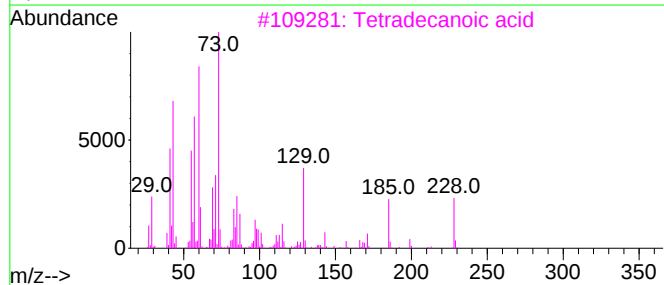
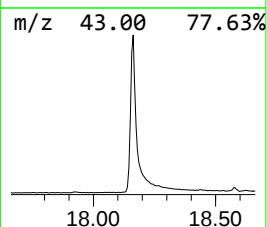
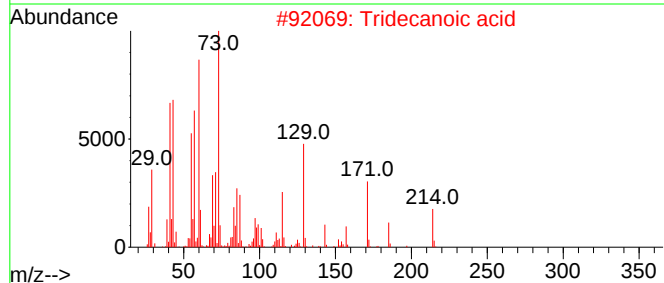
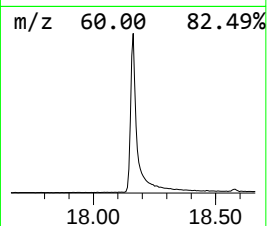
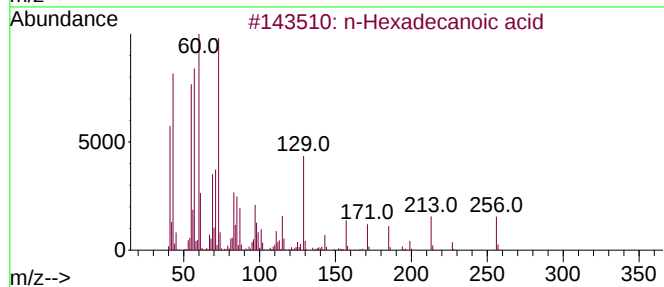
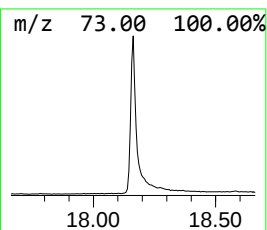
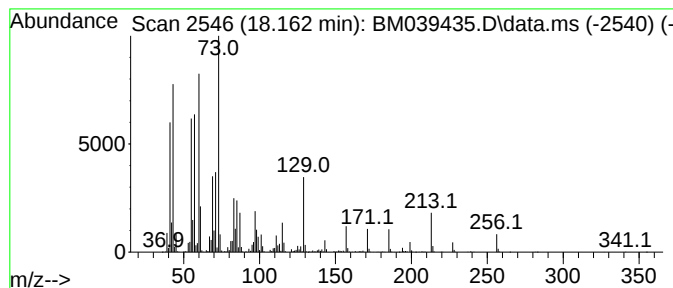
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.162	37.73 ng	3408800	Phenanthrene-d10	17.256

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			Tetradecanoic acid	228	C14H28O2	000544-63-8	94
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5			n-Decanoic acid	172	C10H20O2	000334-48-5	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041423\
Data File : BM039435.D
Acq On : 14 Apr 2023 15:56
Operator : CG/JU
Sample : 02347-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
20230331-COMP-9

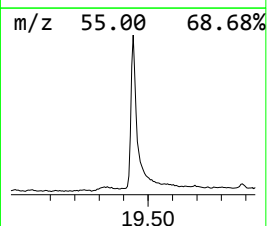
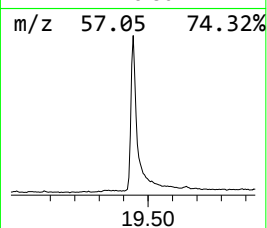
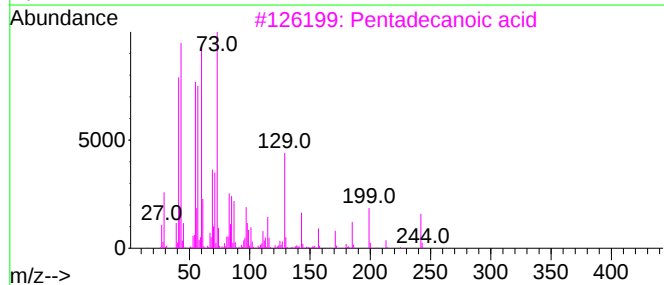
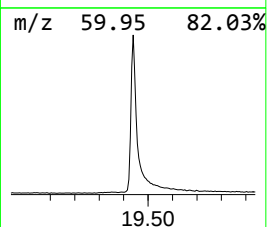
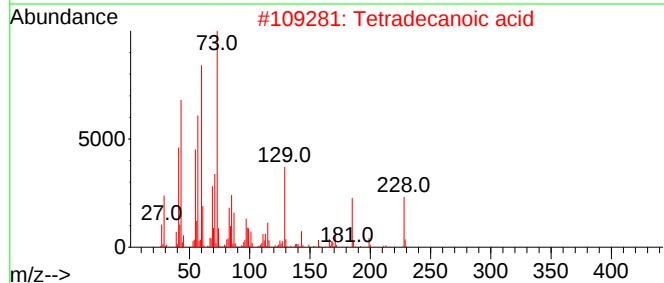
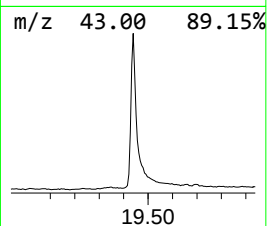
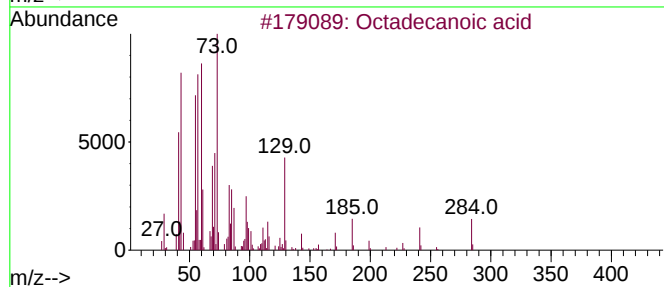
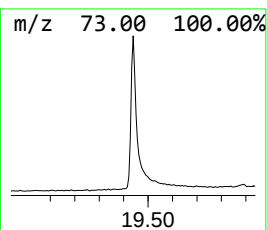
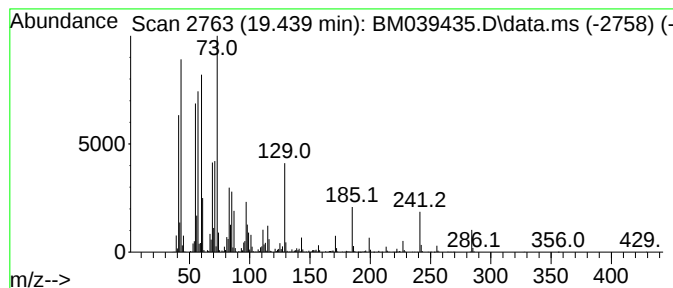
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.439	33.04 ng	3265840	Chrysene-d12	21.450

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	90
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			n-Decanoic acid	172	C10H20O2	000334-48-5	76
5			Tridecanoic acid	214	C13H26O2	000638-53-9	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041423\
Data File : BM039435.D
Acq On : 14 Apr 2023 15:56
Operator : CG/JU
Sample : 02347-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
20230331-COMP-9

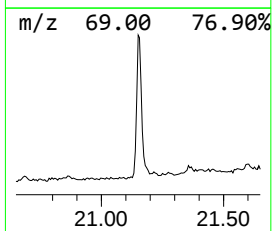
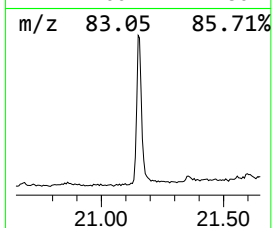
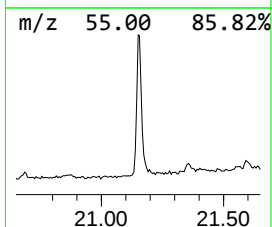
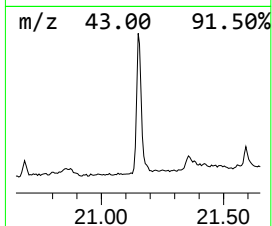
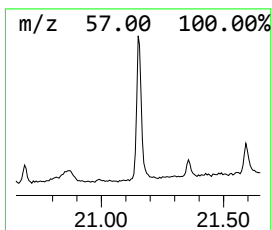
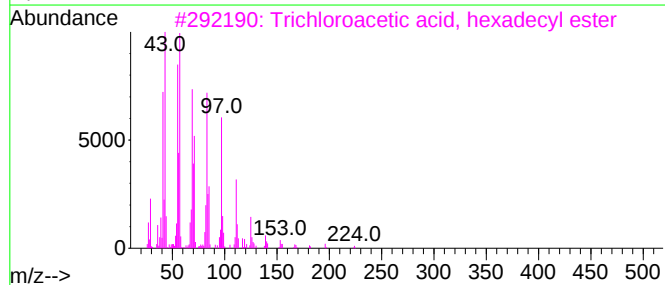
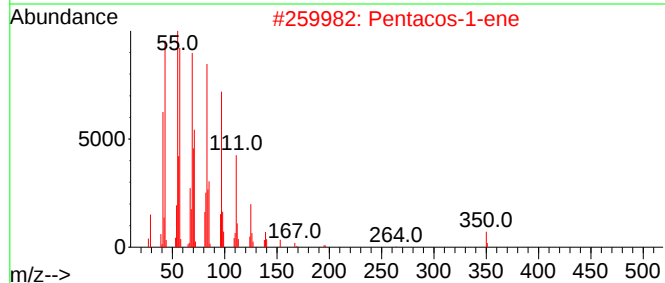
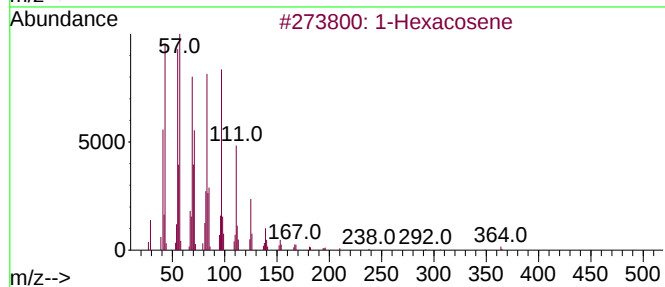
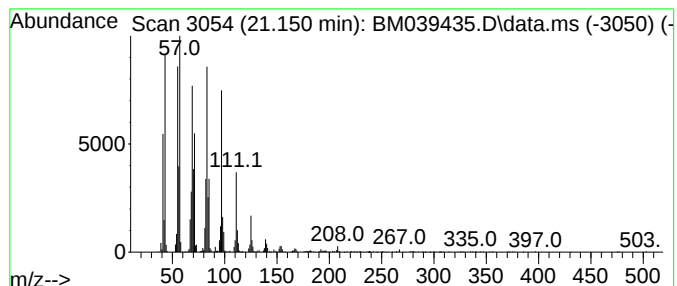
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 1-Hexacosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.150	10.21 ng	1009460	Chrysene-d12	21.450

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosene			364	C26H52	018835-33-1	94
2	Pentacos-1-ene			350	C25H50	016980-85-1	94
3	Trichloroacetic acid, hexadecyl ...			386	C18H33Cl3O2	074339-54-1	94
4	Bromoacetic acid, hexadecyl ester			362	C18H35BrO2	005454-48-8	91
5	1-Tetracosene			336	C24H48	010192-32-2	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041423\
Data File : BM039435.D
Acq On : 14 Apr 2023 15:56
Operator : CG/JU
Sample : 02347-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
20230331-COMP-9

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.940	24.6	ng	1149480	1	7.851	936623	20.0
Benzophenone	15.868	11.1	ng	876230	3	14.510	1583320	20.0
n-Hexadecanoic ...	18.162	37.7	ng	3408800	4	17.256	1806960	20.0
Octadecanoic acid	19.439	33.0	ng	3265840	5	21.450	1976660	20.0
1-Hexacosene	21.150	10.2	ng	1009460	5	21.450	1976660	20.0