

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM062123\
 Data File : BM040341.D
 Acq On : 21 Jun 2023 19:05
 Operator : MA/JU
 Sample : 03016-08
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 B-45(OW)

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-BM061323.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM040341.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.434	190	195	209	rVB	584433	800090	6.63%	1.305%
2	5.046	293	299	312	rBV	2876084	3882528	32.20%	6.331%
3	5.516	372	379	391	rBV	1861216	2793146	23.16%	4.554%
4	6.134	477	484	495	rBV	322547	484918	4.02%	0.791%
5	7.122	643	652	666	rBV	1148110	1838043	15.24%	2.997%
6	7.957	787	794	802	rBV	1159967	1856771	15.40%	3.028%
7	9.128	985	993	1010	rBV	3811939	6215490	51.54%	10.135%
8	10.769	1264	1272	1284	rBV	1457128	2487961	20.63%	4.057%
9	13.227	1682	1690	1704	rBV	8522934	11906242	98.74%	19.414%
10	14.598	1915	1923	1934	rBV	1835550	2623124	21.75%	4.277%
11	15.951	2149	2153	2160	rVB	101995	148754	1.23%	0.243%
12	16.086	2169	2176	2191	rBV	3443797	4850894	40.23%	7.910%
13	17.339	2383	2389	2400	rBV	1808793	2600739	21.57%	4.241%
14	18.233	2537	2541	2552	rBV	179071	356793	2.96%	0.582%
15	19.509	2754	2758	2766	rBV	167733	298919	2.48%	0.487%
16	19.962	2829	2835	2845	rBV	10116411	12058667	100.00%	19.662%
17	21.521	3095	3100	3109	rBV	2184969	2828353	23.45%	4.612%
18	23.939	3505	3511	3524	rVB	1629941	3297432	27.34%	5.377%

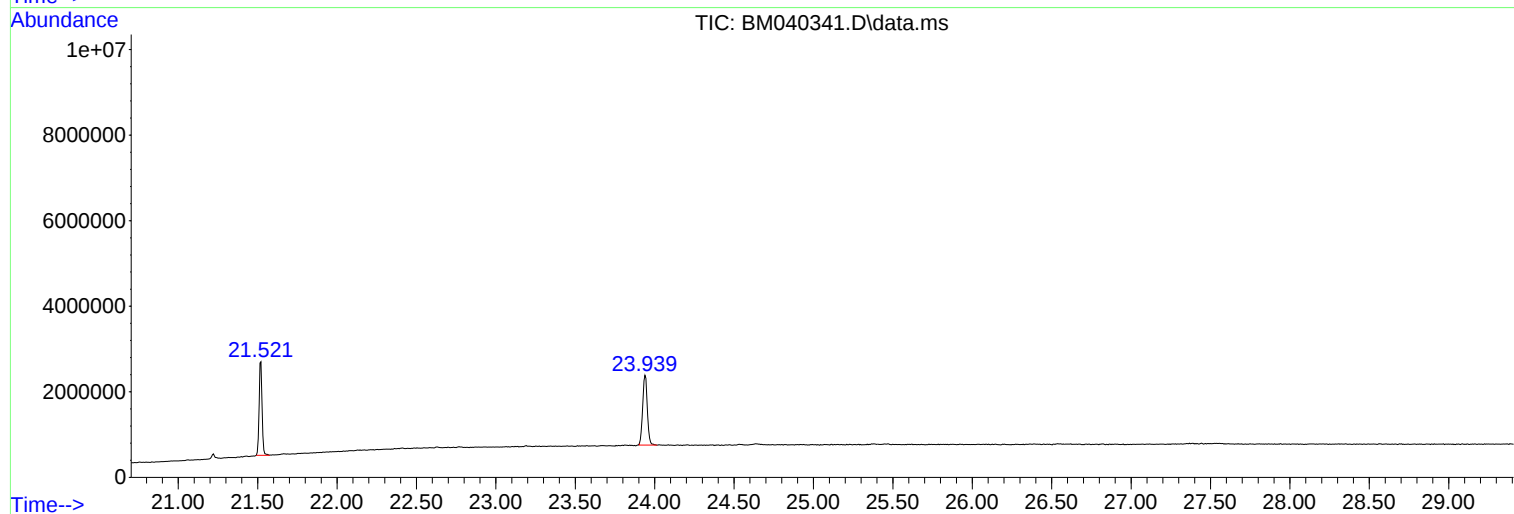
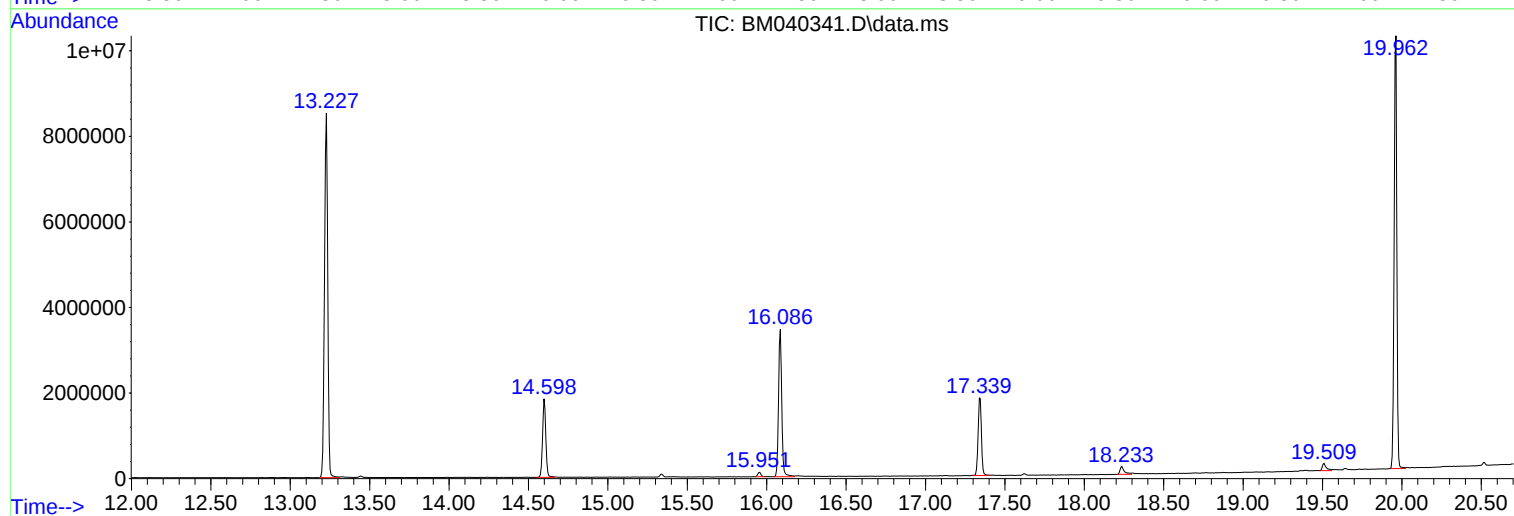
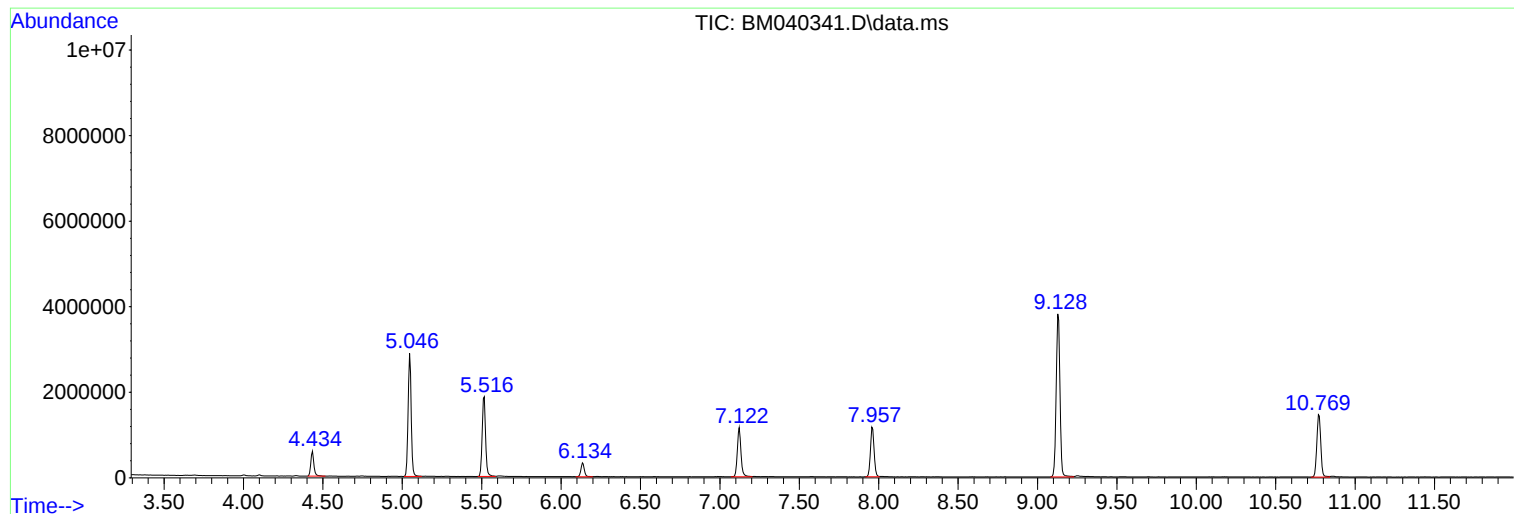
Sum of corrected areas: 61328864

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM062123\
Data File : BM040341.D
Acq On : 21 Jun 2023 19:05
Operator : MA/JU
Sample : 03016-08
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-45(OW)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM061323.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\BM062123\
Data File : BM040341.D
Acq On : 21 Jun 2023 19:05
Operator : MA/JU
Sample : 03016-08
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-45(OW)

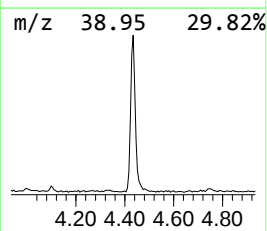
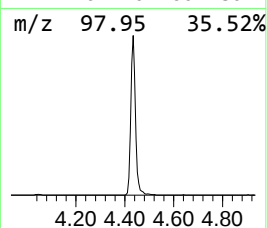
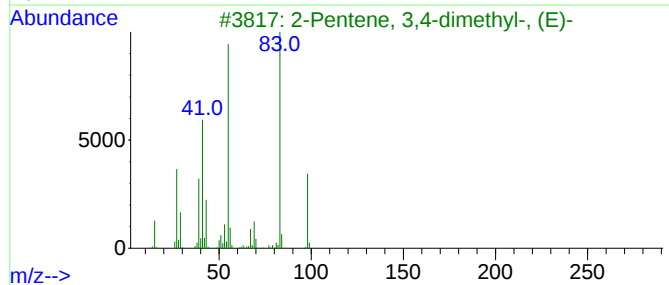
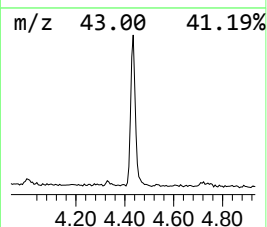
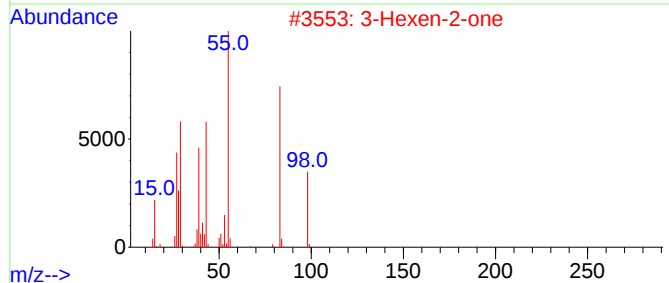
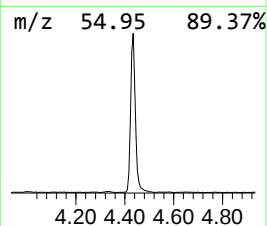
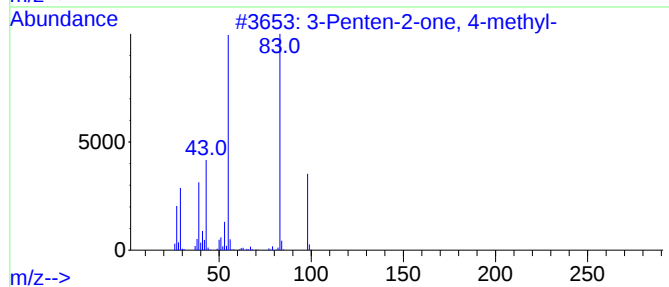
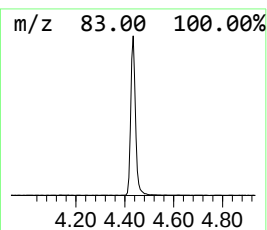
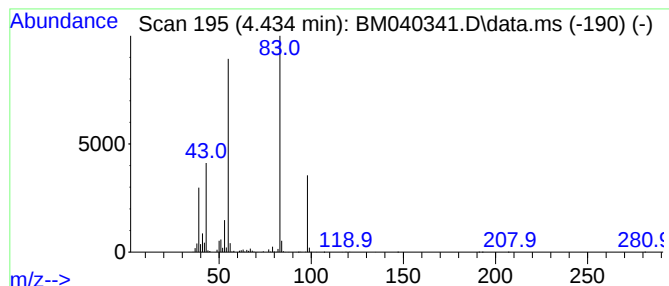
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM061323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.434	8.62 ng	800090	1,4-Dichlorobenzene-d4	7.957

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
2		3-Hexen-2-one	98	C6H10O	000763-93-9	91
3		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM062123\
Data File : BM040341.D
Acq On : 21 Jun 2023 19:05
Operator : MA/JU
Sample : 03016-08
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-45(OW)

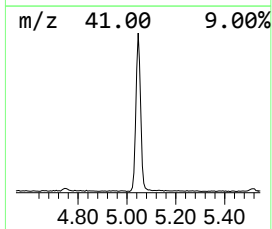
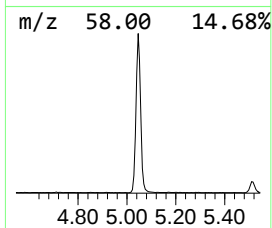
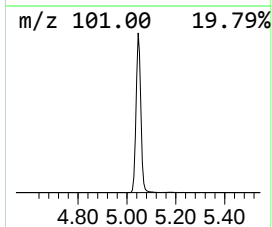
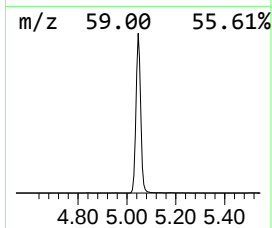
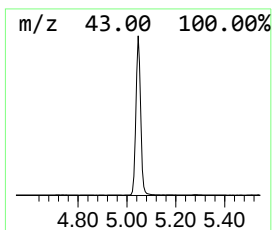
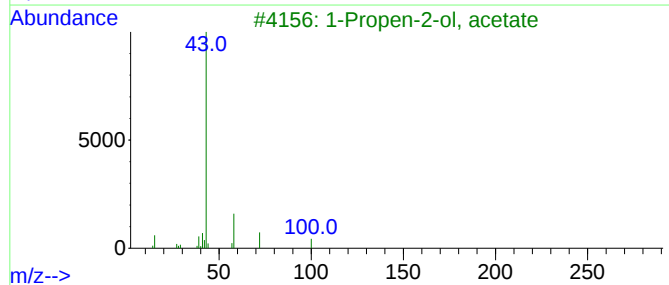
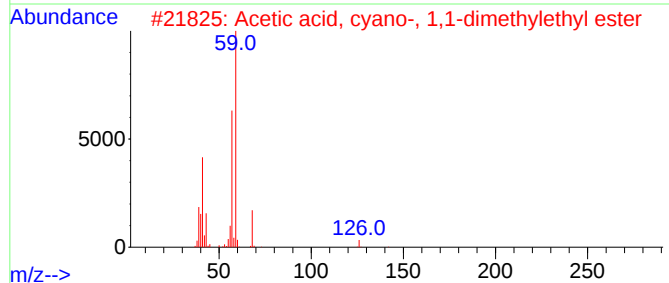
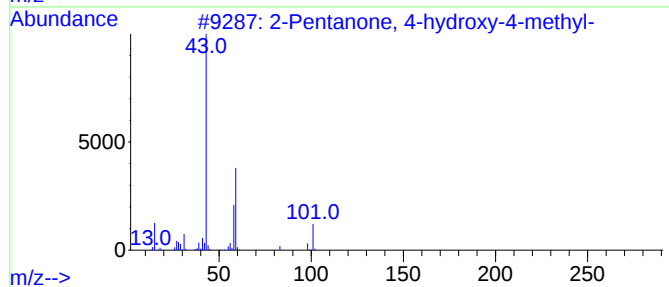
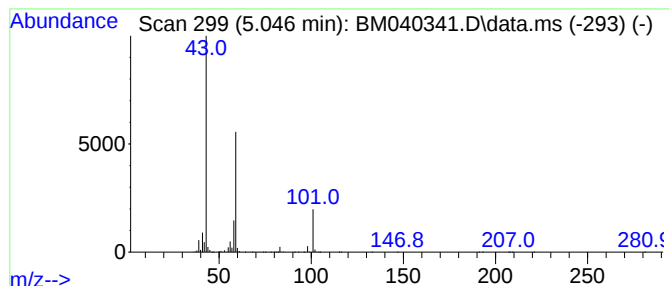
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM061323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.046	41.82 ng	3882530	1,4-Dichlorobenzene-d4	7.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9		
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM062123\
Data File : BM040341.D
Acq On : 21 Jun 2023 19:05
Operator : MA/JU
Sample : 03016-08
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-45(OW)

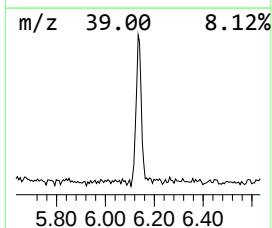
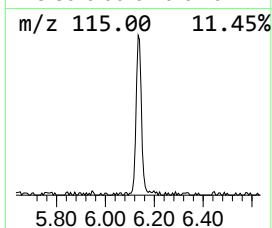
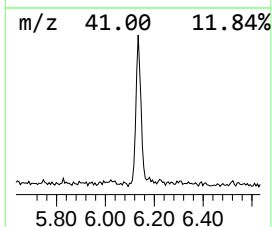
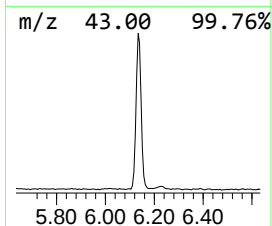
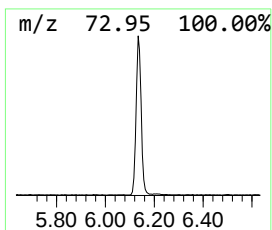
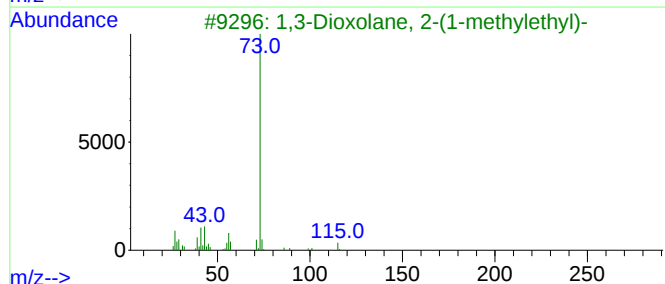
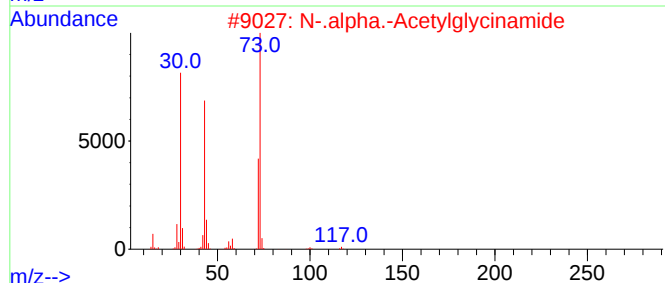
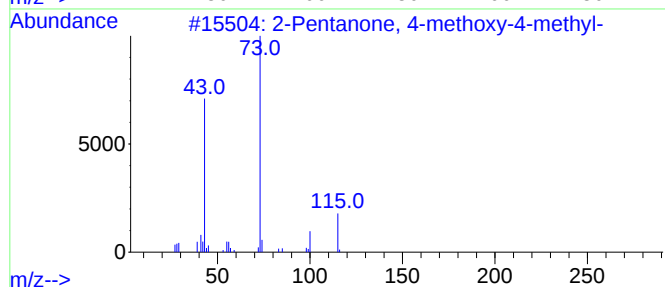
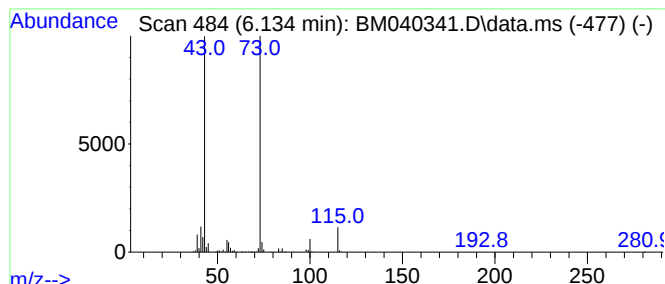
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM061323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.134	5.22 ng	484918	1,4-Dichlorobenzene-d4	7.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2			N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	38
3			1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	10
4			2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	10
5			Morpholine, 2,6-dimethyl-	115	C6H13NO	000141-91-3	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM062123\
Data File : BM040341.D
Acq On : 21 Jun 2023 19:05
Operator : MA/JU
Sample : 03016-08
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-45(OW)

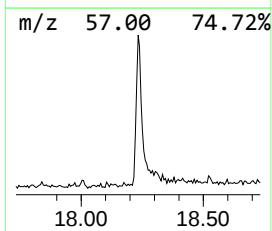
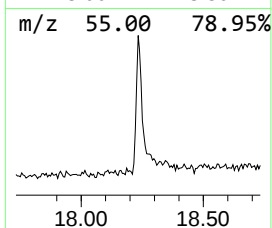
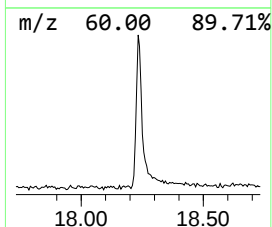
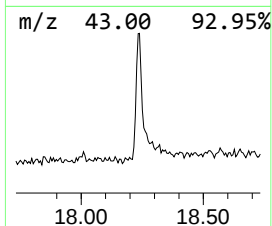
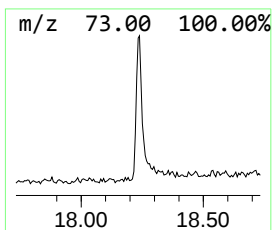
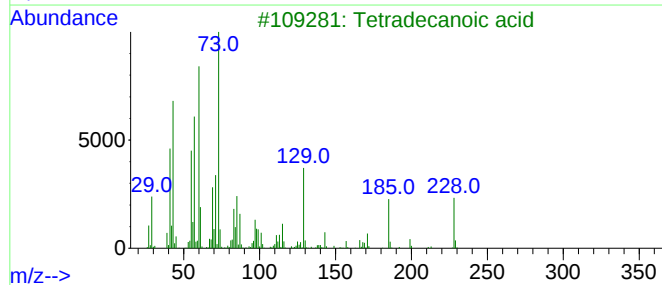
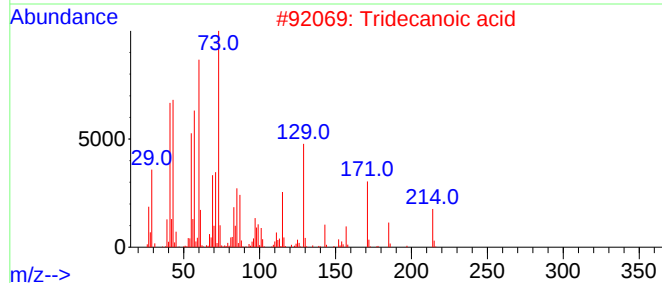
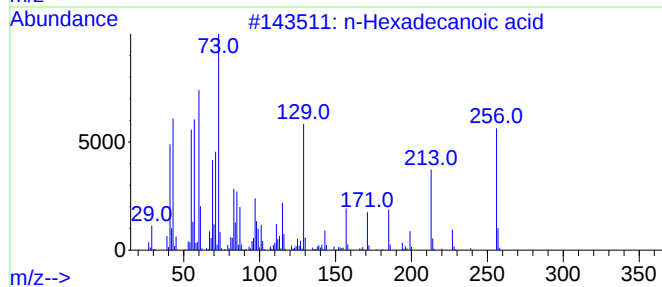
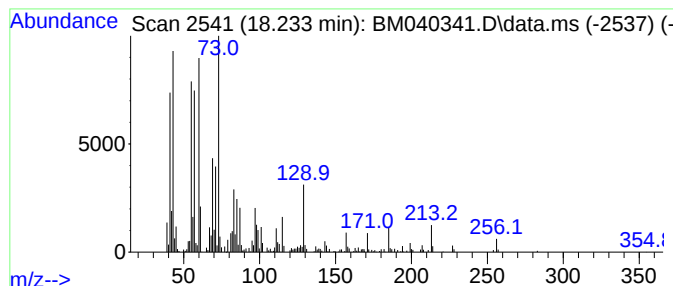
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM061323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.233	2.74 ng	356793	Phenanthrene-d10	17.345

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	93
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
5			Dodecanoic acid	200	C12H24O2	000143-07-7	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM062123\
Data File : BM040341.D
Acq On : 21 Jun 2023 19:05
Operator : MA/JU
Sample : 03016-08
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-45(OW)

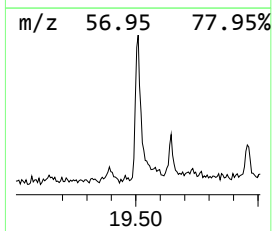
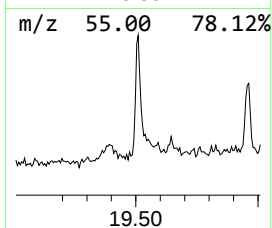
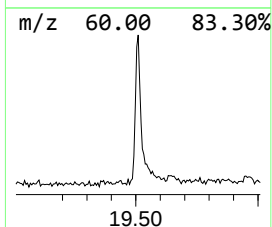
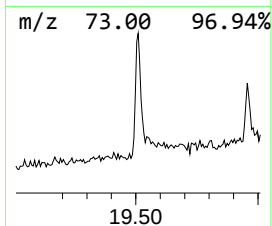
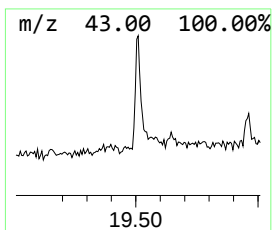
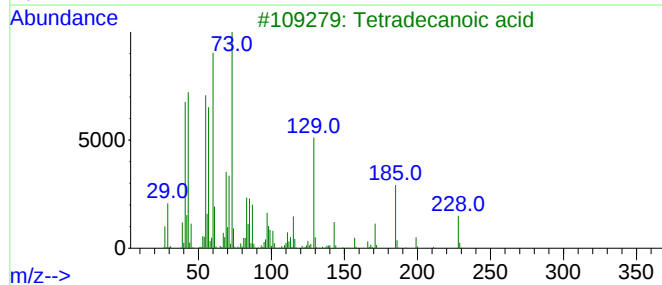
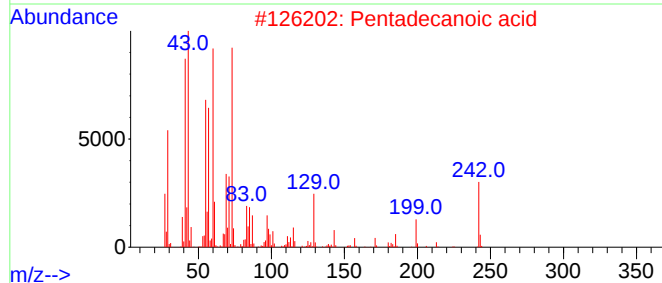
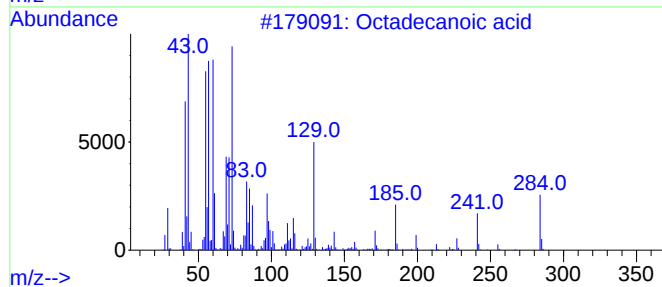
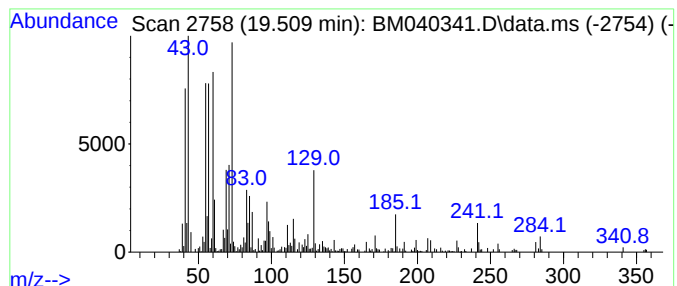
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM061323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.509	2.11 ng	298919	Chrysene-d12	21.521

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			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
5			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM062123\
Data File : BM040341.D
Acq On : 21 Jun 2023 19:05
Operator : MA/JU
Sample : 03016-08
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-45(OW)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM061323.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
3-Penten-2-one,...	4.434	8.6	ng	800090	1	7.957	1856770	20.0
2-Pentanone, 4-...	5.046	41.8	ng	3882530	1	7.957	1856770	20.0
2-Pentanone, 4-...	6.134	5.2	ng	484918	1	7.957	1856770	20.0
n-Hexadecanoic ...	18.233	2.7	ng	356793	4	17.345	2600740	20.0
Octadecanoic acid	19.509	2.1	ng	298919	5	21.521	2828350	20.0