

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040925\
 Data File : BM049864.D
 Acq On : 09 Apr 2025 12:29
 Operator : RC/JU
 Sample : Q1744-01
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 B-158-SB01

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-BM040825.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM049864.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.893	319	324	332	rBV	667512	930708	5.17%	1.135%
2	5.363	397	404	414	rBV	4891736	6962372	38.69%	8.493%
3	6.951	666	674	693	rBV	4648372	7222734	40.14%	8.811%
4	7.775	808	814	823	rVB	937433	1445836	8.03%	1.764%
5	8.934	1003	1011	1021	rBV	2706636	4449702	24.73%	5.428%
6	10.569	1282	1289	1300	rBV	1092686	1815835	10.09%	2.215%
7	13.039	1700	1709	1723	rBV	8016754	11115762	61.77%	13.560%
8	14.416	1936	1943	1952	rBV	1671923	2445087	13.59%	2.983%
9	15.774	2168	2174	2182	rBV	768888	994154	5.52%	1.213%
10	15.904	2189	2196	2212	rBV	6735718	9146088	50.83%	11.157%
11	17.163	2403	2410	2416	rBV2	1966681	2836889	15.77%	3.461%
12	18.062	2557	2563	2573	rBV	1700508	2699372	15.00%	3.293%
13	19.221	2753	2760	2765	rBV	138377	237214	1.32%	0.289%
14	19.345	2776	2781	2800	rBV	600872	1155316	6.42%	1.409%
15	19.580	2817	2821	2831	rVB	164594	261474	1.45%	0.319%
16	19.786	2851	2856	2865	rBV	16050903	17994548	100.00%	21.951%
17	21.080	3072	3076	3087	rBV3	374938	714671	3.97%	0.872%
18	21.303	3111	3114	3119	rBV	172272	213906	1.19%	0.261%
19	21.392	3123	3129	3134	rVV	2352052	3729378	20.73%	4.549%
20	21.439	3134	3137	3146	rVB	502292	792408	4.40%	0.967%
21	23.444	3473	3478	3484	rBV	370349	743115	4.13%	0.906%
22	23.503	3484	3488	3494	rVB	288013	552272	3.07%	0.674%
23	24.391	3631	3639	3652	rVB	1408334	3517688	19.55%	4.291%

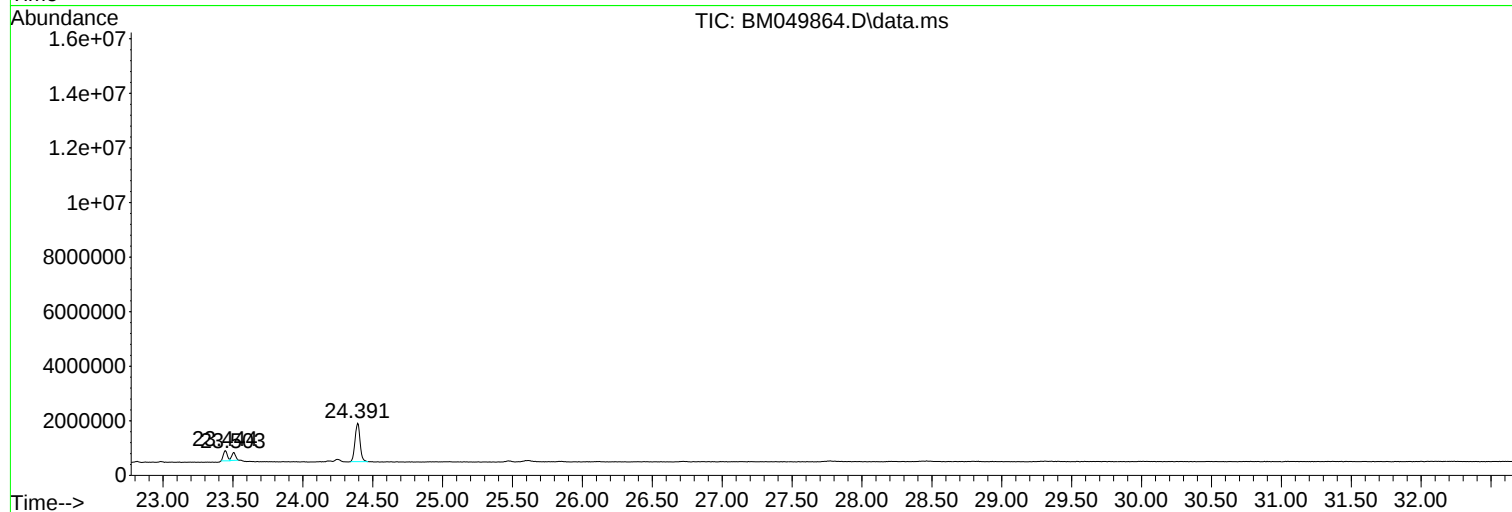
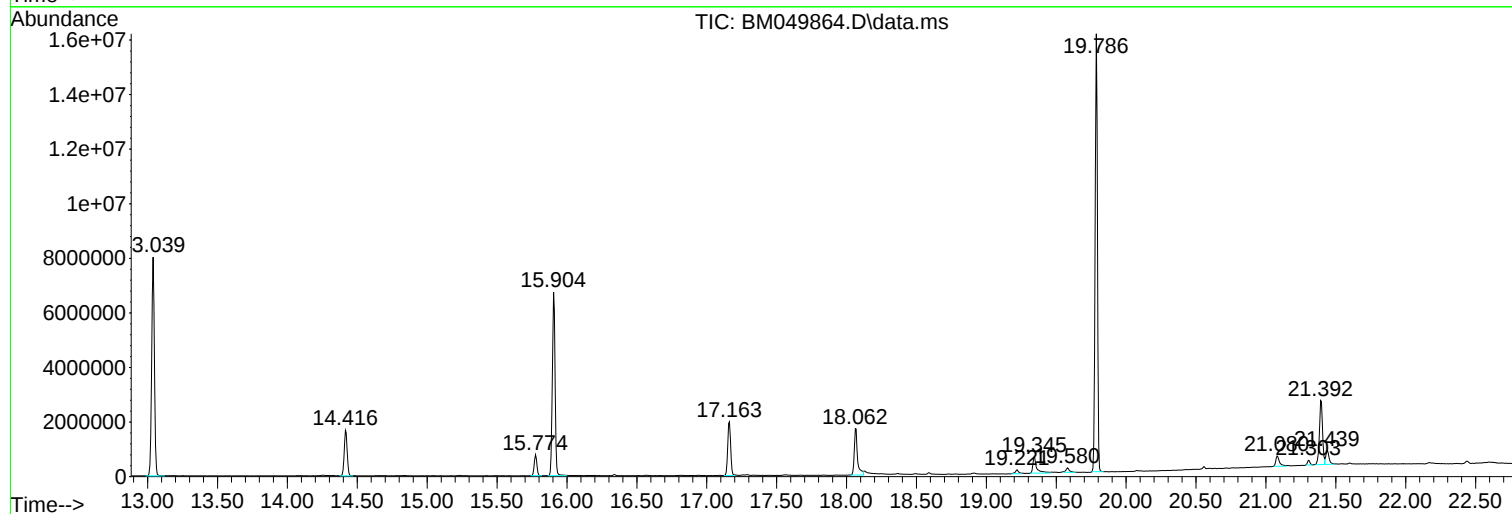
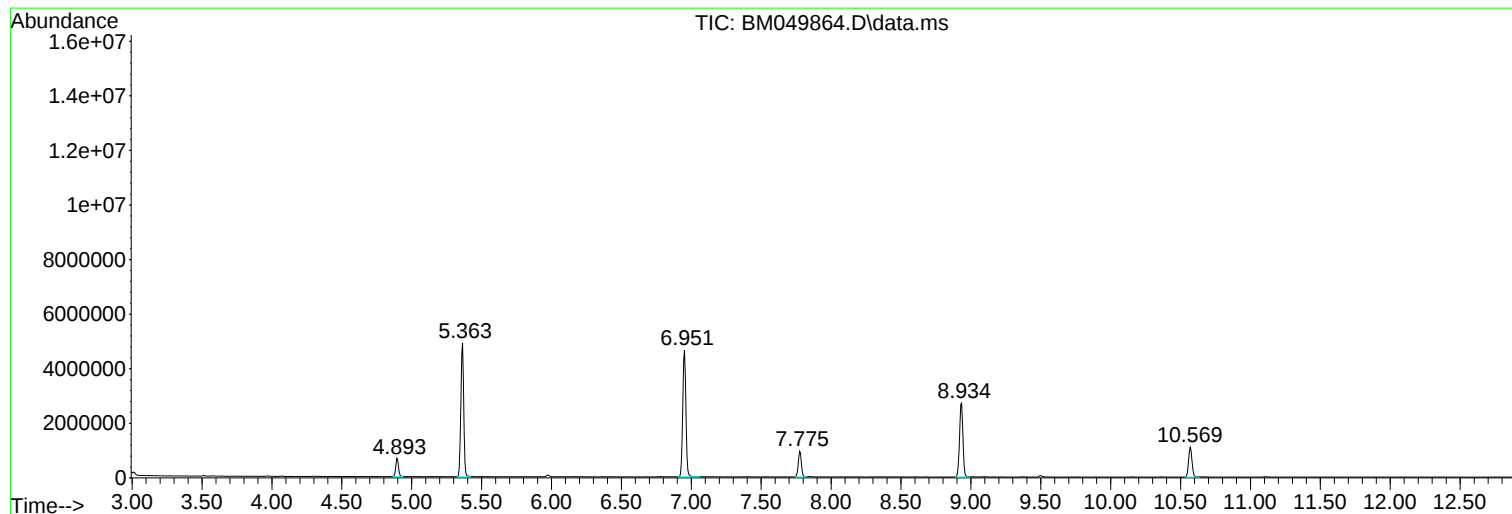
Sum of corrected areas: 81976529

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040925\
Data File : BM049864.D
Acq On : 09 Apr 2025 12:29
Operator : RC/JU
Sample : Q1744-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-158-SB01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.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\BM040925\
Data File : BM049864.D
Acq On : 09 Apr 2025 12:29
Operator : RC/JU
Sample : Q1744-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-158-SB01

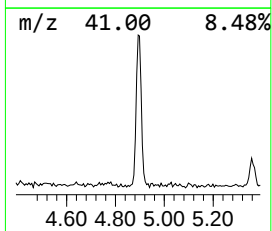
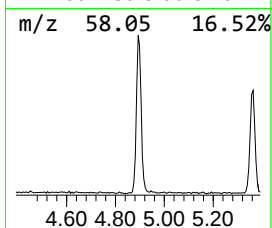
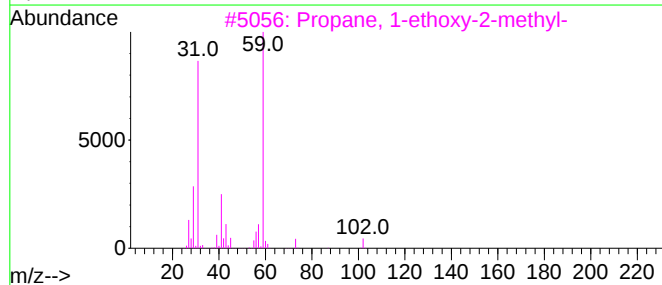
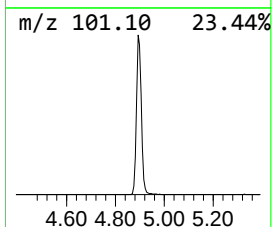
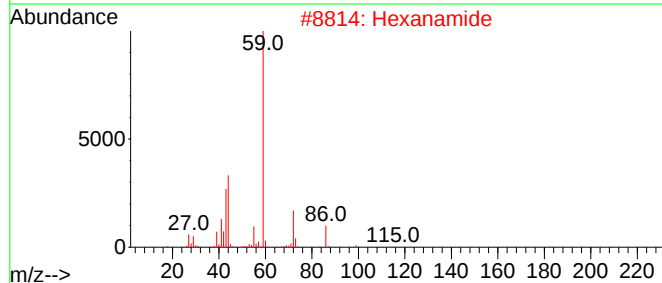
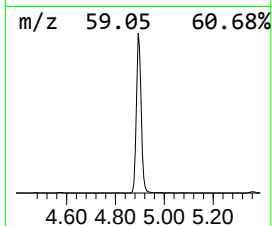
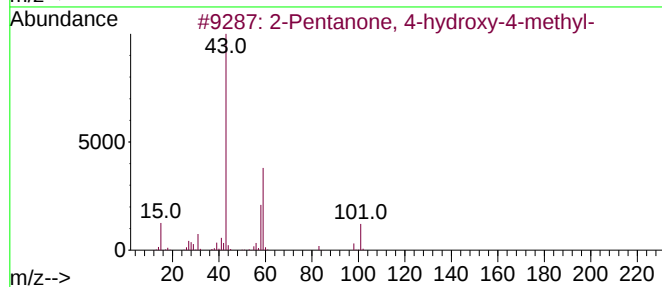
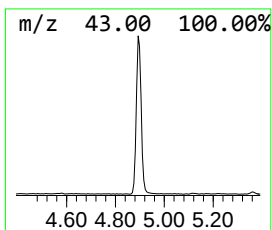
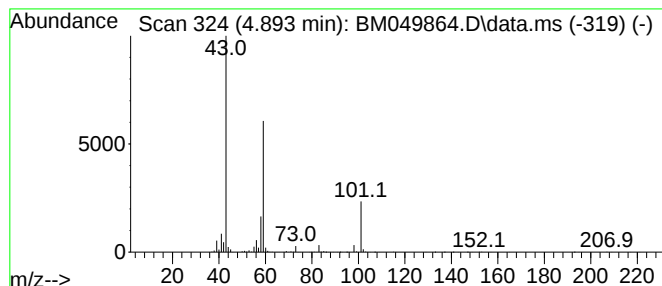
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.893	12.87 ng	930708	1,4-Dichlorobenzene-d4	7.775

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	Hexanamide	115	C6H13NO	000628-02-4	35		
3	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	32		
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25		
5	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	17		



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040925\
Data File : BM049864.D
Acq On : 09 Apr 2025 12:29
Operator : RC/JU
Sample : Q1744-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-158-SB01

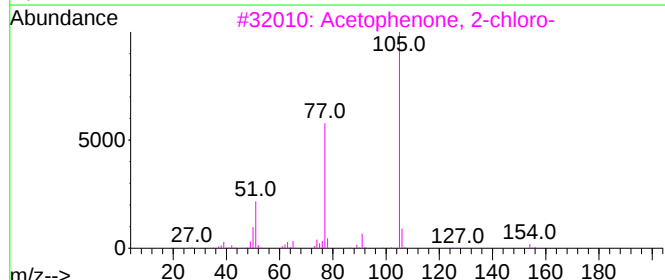
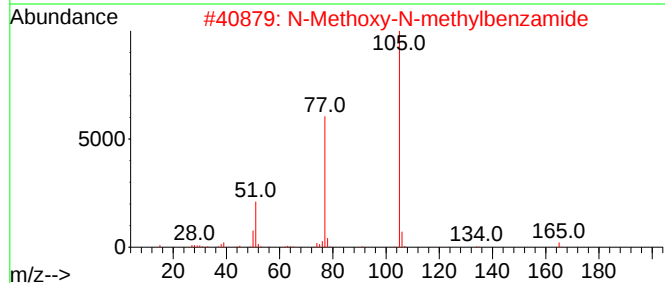
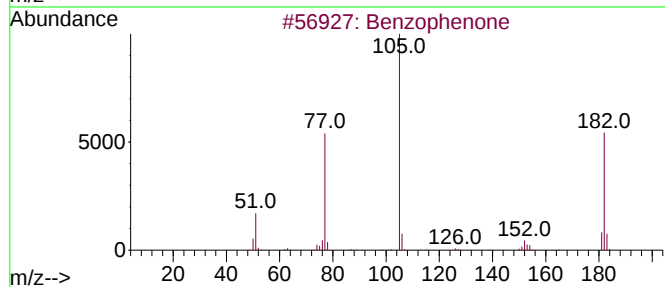
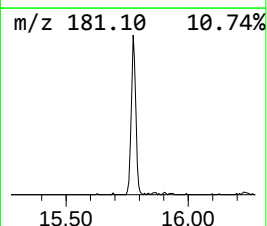
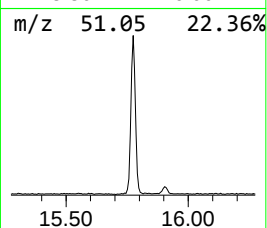
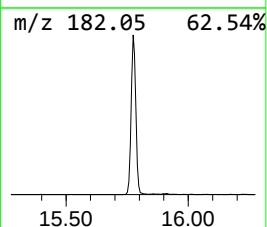
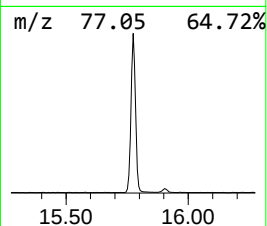
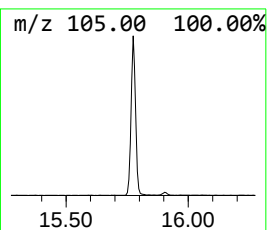
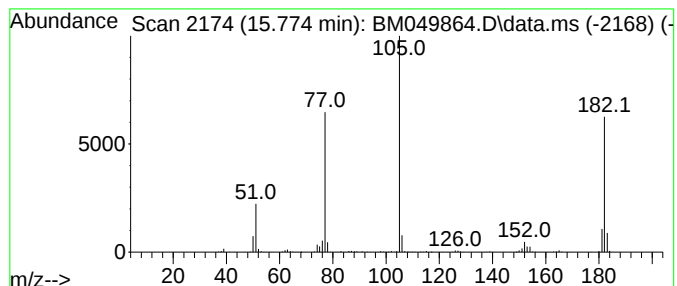
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.774	8.13 ng	994154	Acenaphthene-d10	14.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	53
3			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
4			Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	47
5			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040925\
Data File : BM049864.D
Acq On : 09 Apr 2025 12:29
Operator : RC/JU
Sample : Q1744-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-158-SB01

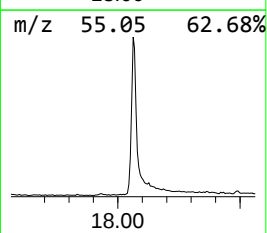
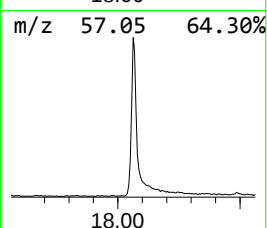
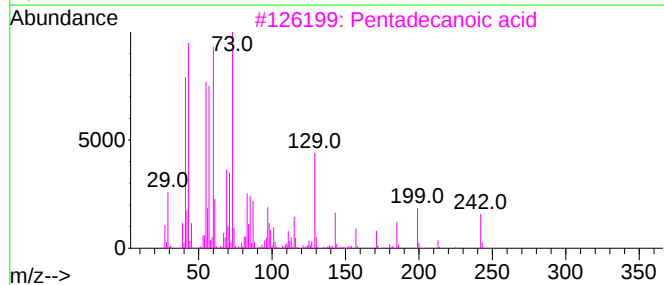
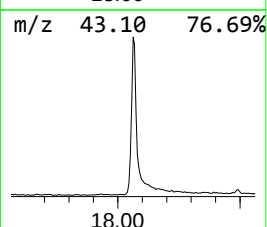
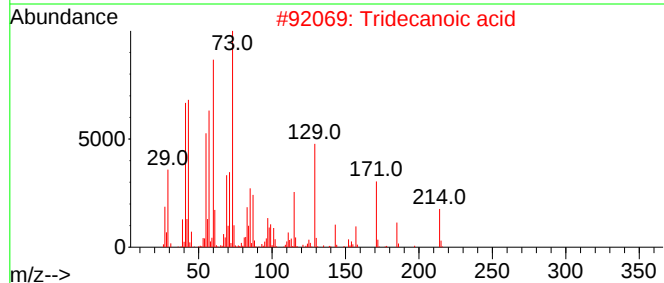
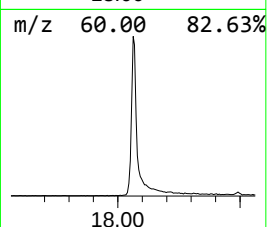
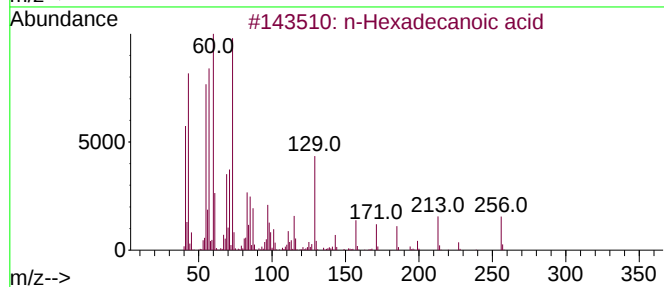
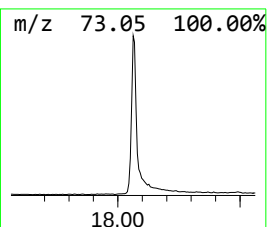
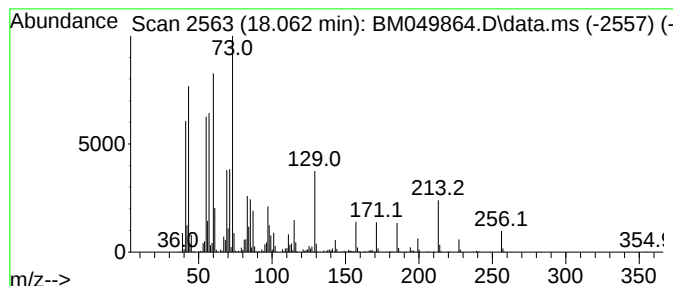
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
18.062	19.03 ng	2699370	Phenanthrene-d10	17.163

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	91
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	90
5			n-Decanoic acid	172	C10H20O2	000334-48-5	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040925\
Data File : BM049864.D
Acq On : 09 Apr 2025 12:29
Operator : RC/JU
Sample : Q1744-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-158-SB01

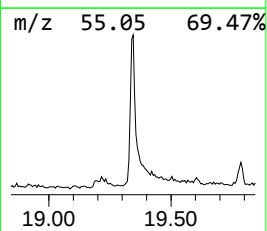
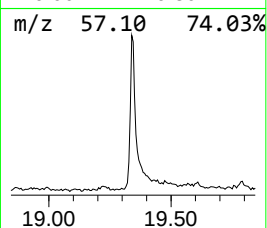
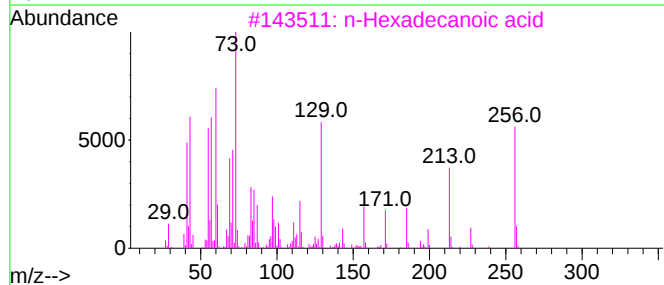
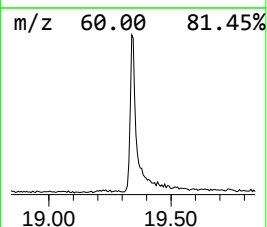
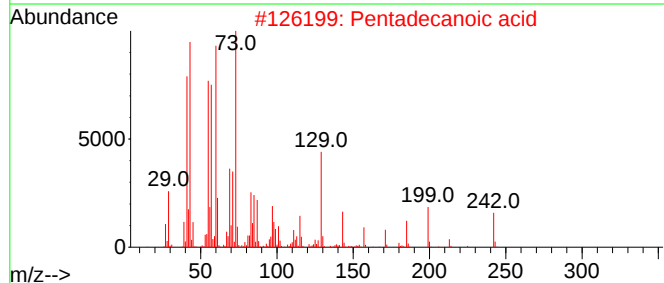
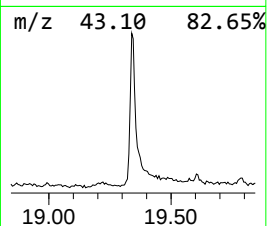
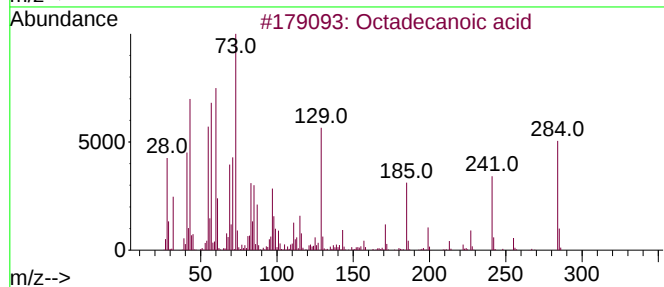
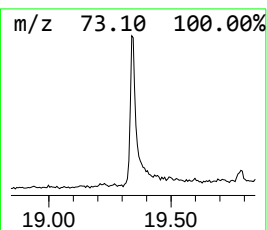
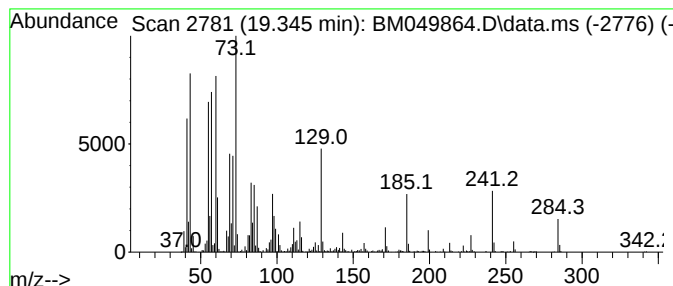
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.345	6.20 ng	1155320	Chrysene-d12	21.398

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			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
4			n-Decanoic acid	172	C10H20O2	000334-48-5	91
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040925\
Data File : BM049864.D
Acq On : 09 Apr 2025 12:29
Operator : RC/JU
Sample : Q1744-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-158-SB01

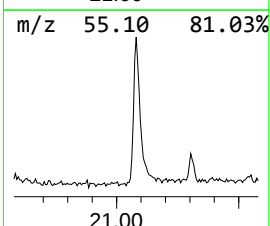
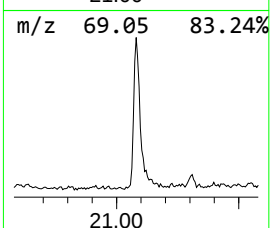
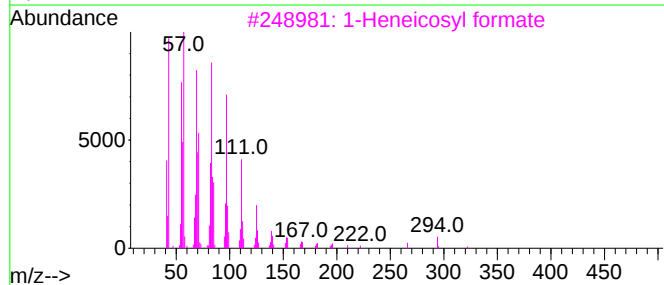
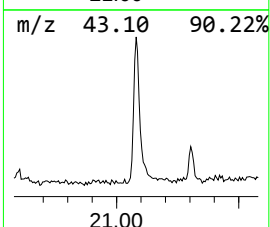
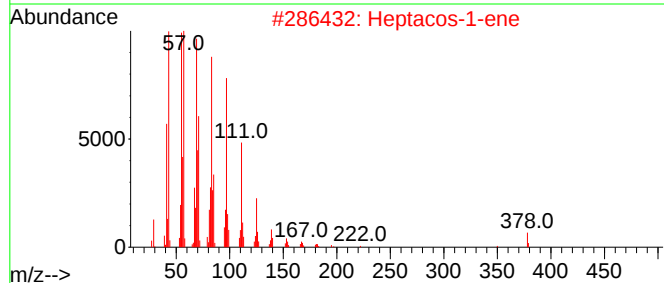
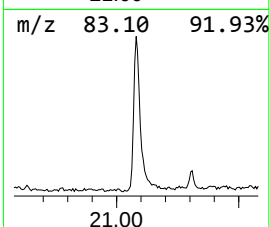
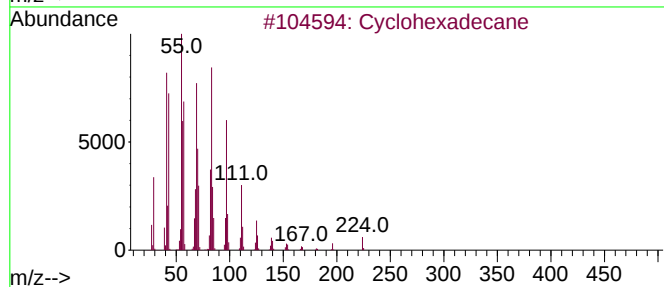
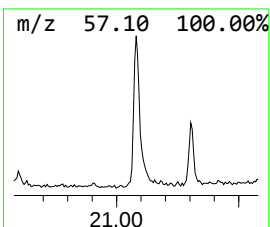
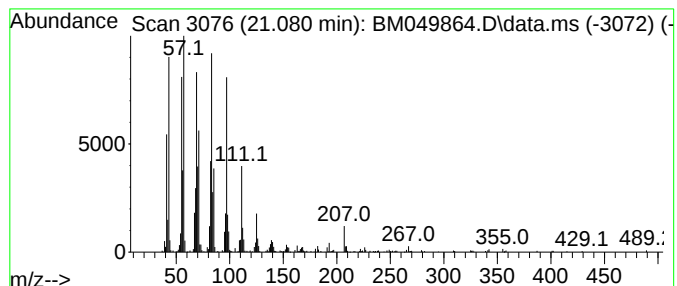
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Cyclohexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.080	3.83 ng	714671	Chrysene-d12	21.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexadecane	224	C16H32	000295-65-8	94
2			Heptacos-1-ene	378	C27H54	015306-27-1	93
3			1-Heneicosyl formate	340	C22H44O2	077899-03-7	93
4			Octacosanol	410	C28H58O	000557-61-9	91
5			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040925\
Data File : BM049864.D
Acq On : 09 Apr 2025 12:29
Operator : RC/JU
Sample : Q1744-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-158-SB01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.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-...	4.893	12.9	ng	930708	1	7.775	1445840	20.0
Benzophenone	15.774	8.1	ng	994154	3	14.416	2445090	20.0
n-Hexadecanoic ...	18.062	19.0	ng	2699370	4	17.163	2836890	20.0
Octadecanoic acid	19.345	6.2	ng	1155320	5	21.398	3729380	20.0
Cyclohexadecane	21.080	3.8	ng	714671	5	21.398	3729380	20.0