

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041525\
 Data File : BM049933.D
 Acq On : 15 Apr 2025 13:56
 Operator : RC/JU
 Sample : Q1779-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 TP-22

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: BM049933.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.887	318	323	332	rVB	303824	432546	4.00%	0.518%
2	5.357	397	403	420	rBV	4196721	6070280	56.20%	7.273%
3	5.963	501	506	516	rVB	218293	331455	3.07%	0.397%
4	6.951	666	674	688	rVB	3668118	6010548	55.65%	7.201%
5	7.769	807	813	820	rBV	1546622	2379122	22.03%	2.850%
6	8.928	1002	1010	1028	rBV	2219899	3714298	34.39%	4.450%
7	10.563	1279	1288	1301	rBV	1785248	2970568	27.50%	3.559%
8	13.033	1701	1708	1720	rBV	5851364	8411233	77.87%	10.077%
9	14.416	1931	1943	1951	rBV	2468191	3700499	34.26%	4.433%
10	15.774	2168	2174	2182	rBV	466514	673896	6.24%	0.807%
11	15.904	2189	2196	2219	rBV	4569227	6563144	60.76%	7.863%
12	17.157	2403	2409	2414	rBV2	2564718	3764347	34.85%	4.510%
13	17.198	2414	2416	2423	rVV	436514	573294	5.31%	0.687%
14	17.292	2423	2432	2439	rVB	114340	228362	2.11%	0.274%
15	18.062	2555	2563	2587	rBV	3100209	7384351	68.37%	8.847%
16	19.145	2744	2747	2752	rVB	121969	133023	1.23%	0.159%
17	19.215	2754	2759	2768	rBV	785348	1249615	11.57%	1.497%
18	19.345	2774	2781	2804	rBV	5639625	10800948	100.00%	12.940%
19	19.580	2817	2821	2830	rVB	738477	1076814	9.97%	1.290%
20	19.786	2850	2856	2861	rBV	7681551	9124172	84.48%	10.931%
21	21.397	3123	3130	3135	rBV2	2628251	4199911	38.88%	5.032%
22	24.397	3633	3640	3649	rVB	1581314	3675605	34.03%	4.404%

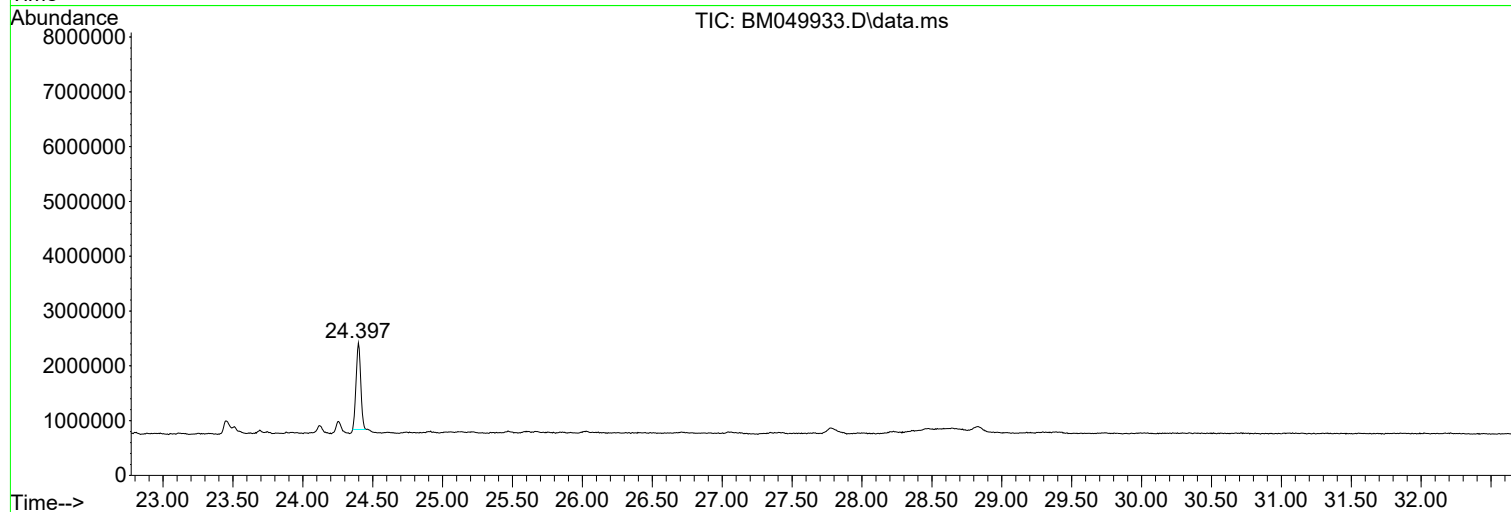
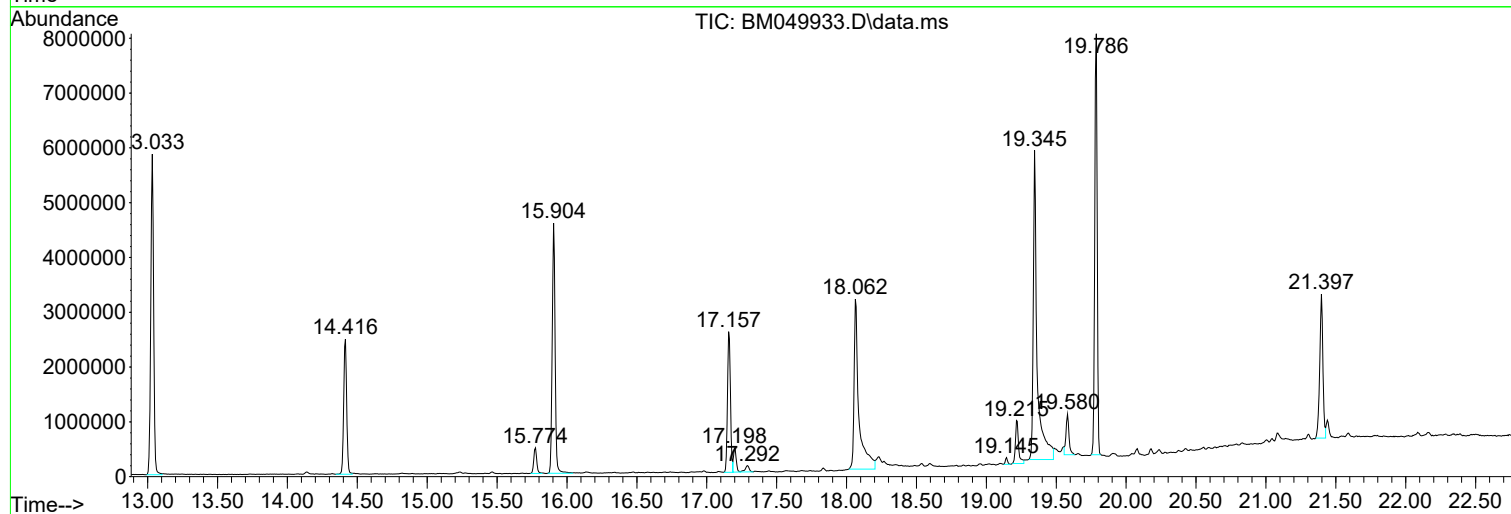
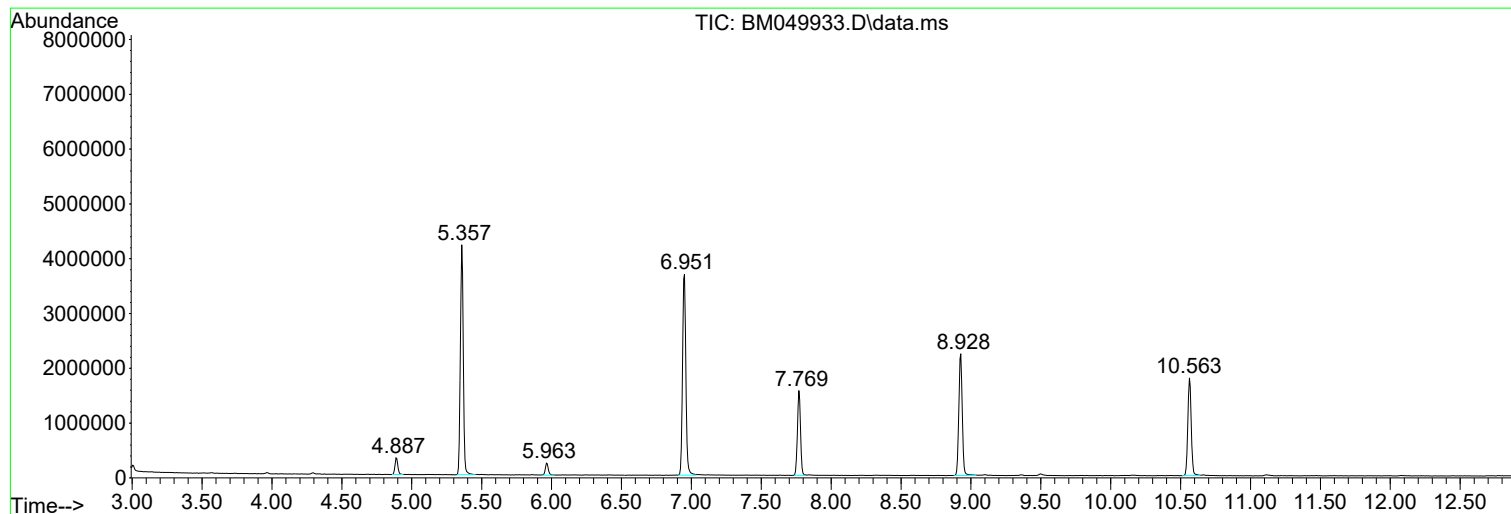
Sum of corrected areas: 83468031

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041525\
Data File : BM049933.D
Acq On : 15 Apr 2025 13:56
Operator : RC/JU
Sample : Q1779-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-22

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\BM041525\
Data File : BM049933.D
Acq On : 15 Apr 2025 13:56
Operator : RC/JU
Sample : Q1779-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-22

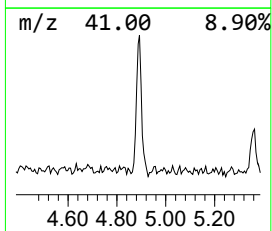
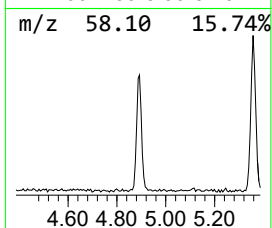
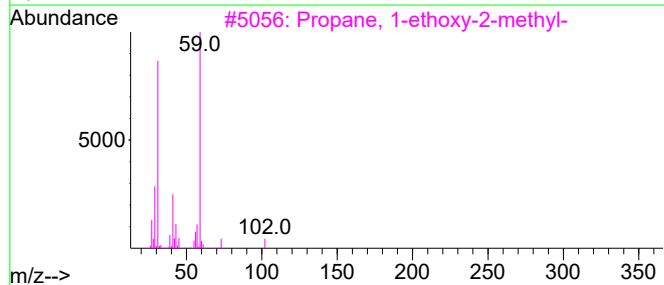
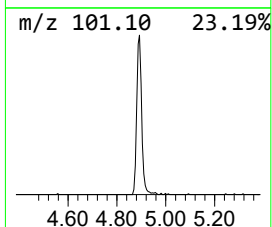
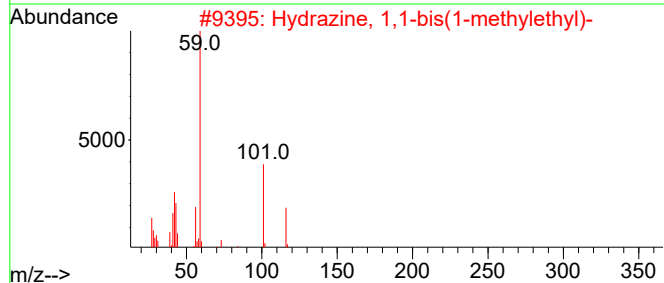
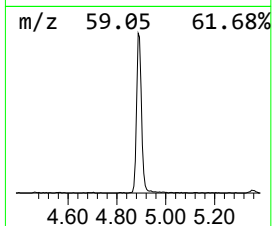
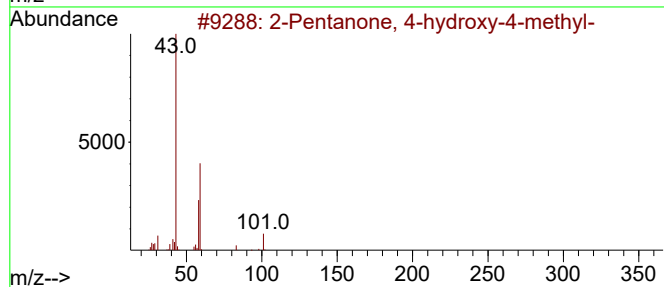
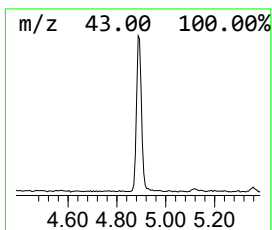
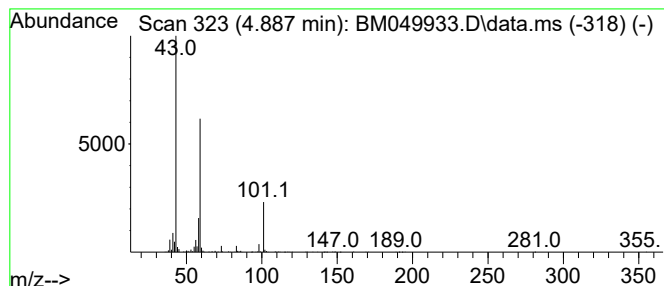
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.887	3.64 ng	432546	1,4-Dichlorobenzene-d4	7.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	25		
3	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	25		
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\BM041525\
Data File : BM049933.D
Acq On : 15 Apr 2025 13:56
Operator : RC/JU
Sample : Q1779-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-22

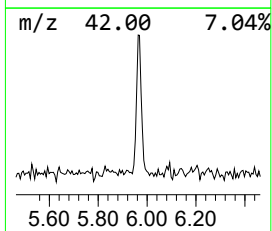
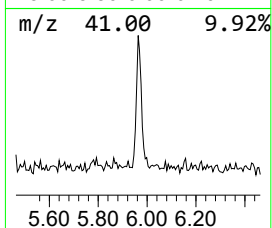
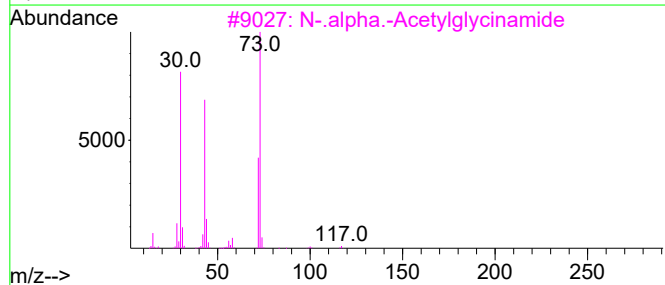
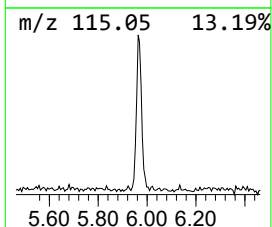
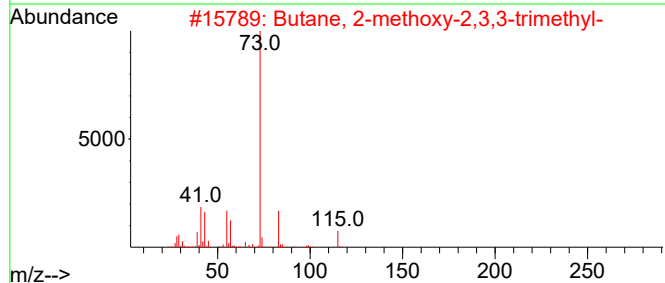
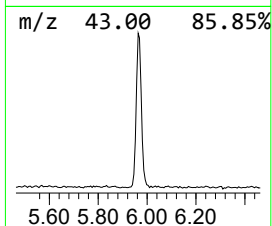
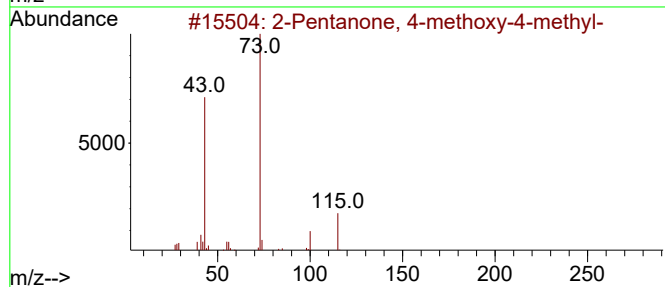
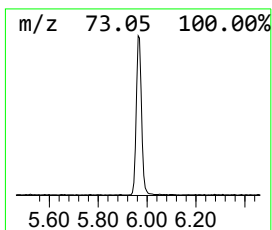
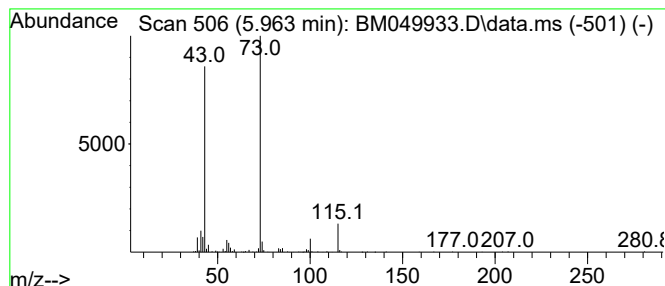
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.963	2.79 ng	331455	1,4-Dichlorobenzene-d4	7.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	78
2			Butane, 2-methoxy-2,3,3-trimethyl-	130	C8H18O	027705-21-1	37
3			N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	28
4			3-Hexanol, acetate	144	C8H16O2	040780-64-1	25
5			3-Heptanol, 3,5-dimethyl-	144	C9H20O	019549-74-7	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041525\
Data File : BM049933.D
Acq On : 15 Apr 2025 13:56
Operator : RC/JU
Sample : Q1779-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-22

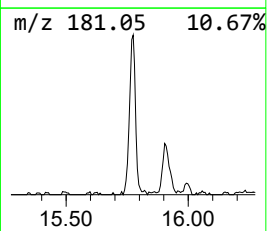
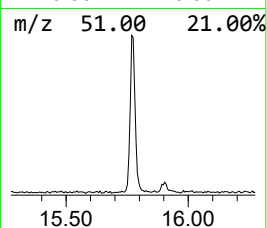
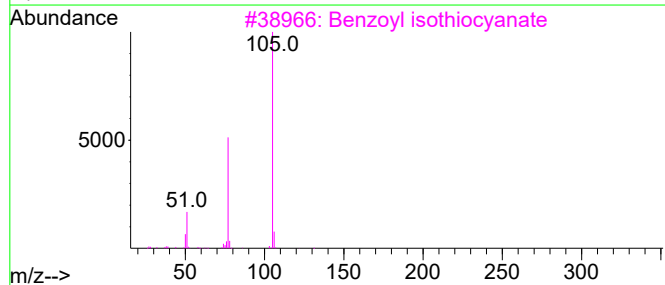
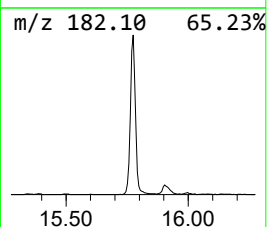
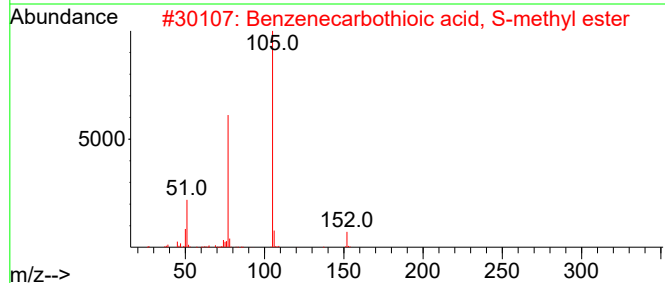
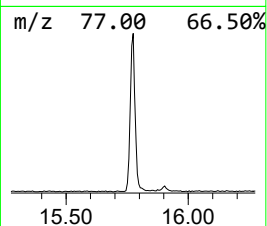
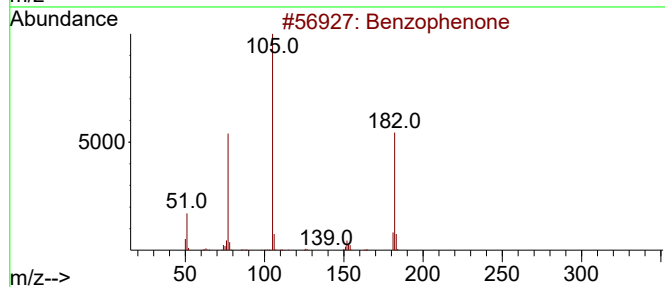
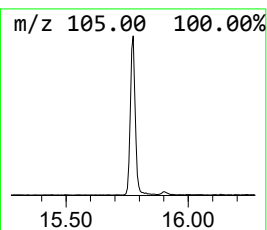
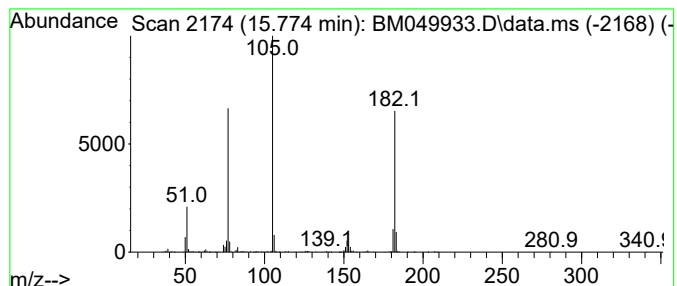
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.774	3.64 ng	673896	Acenaphthene-d10	14.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	46
3			Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	43
4			N-Methylbenzamide, N-trifluoroac...	231	C10H8F3NO2	1000446-91-5	43
5			Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041525\
Data File : BM049933.D
Acq On : 15 Apr 2025 13:56
Operator : RC/JU
Sample : Q1779-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-22

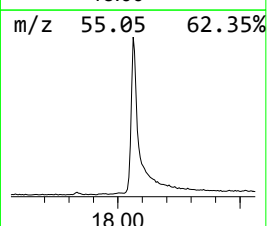
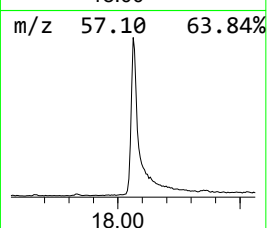
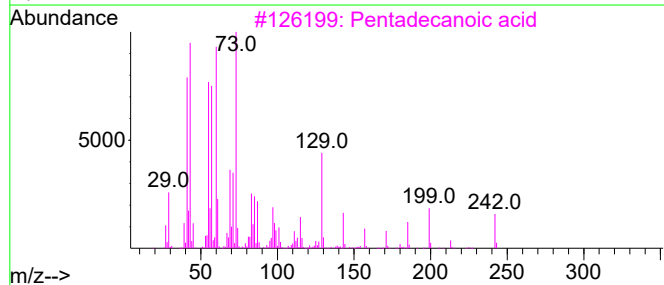
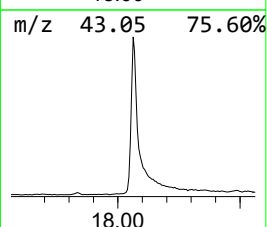
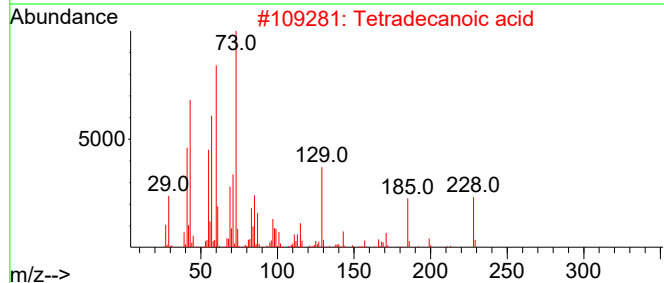
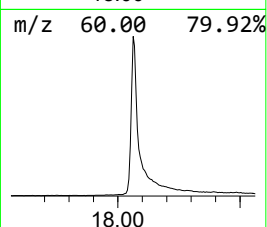
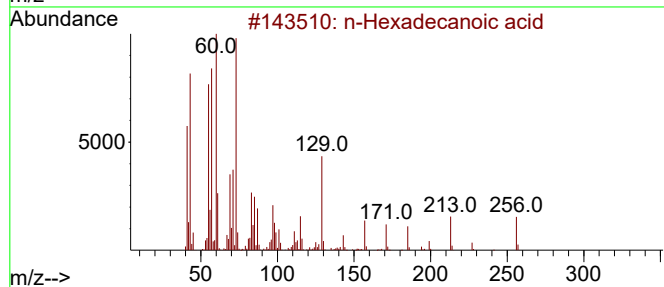
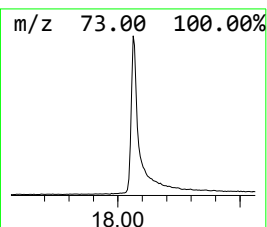
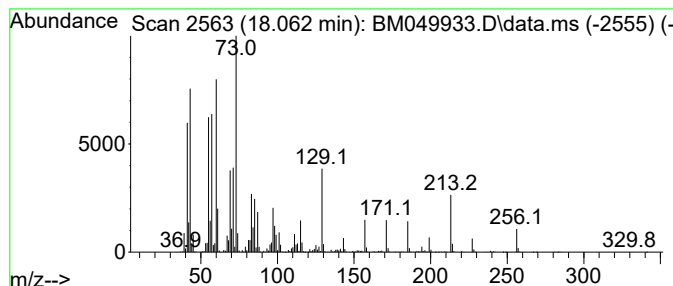
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.062	39.23 ng	7384350	Phenanthrene-d10	17.157

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	91
4		Tridecanoic acid	214	C13H26O2	000638-53-9	91
5		n-Decanoic acid	172	C10H20O2	000334-48-5	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041525\
Data File : BM049933.D
Acq On : 15 Apr 2025 13:56
Operator : RC/JU
Sample : Q1779-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-22

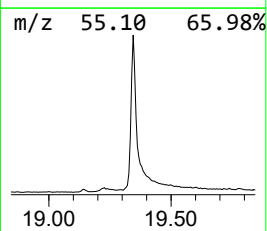
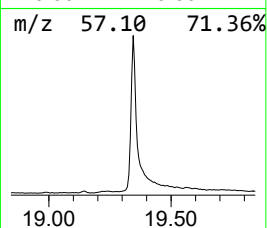
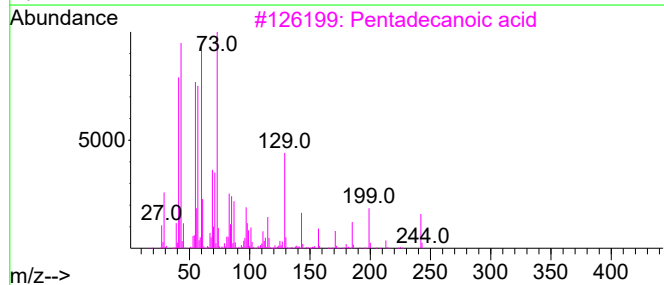
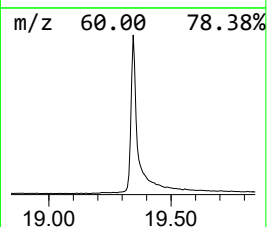
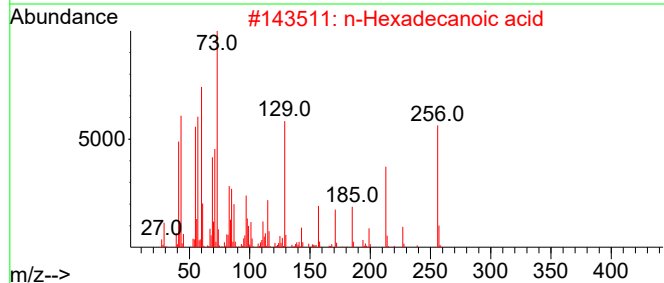
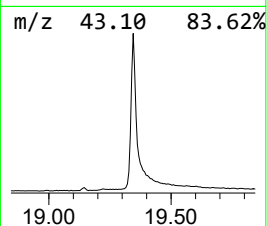
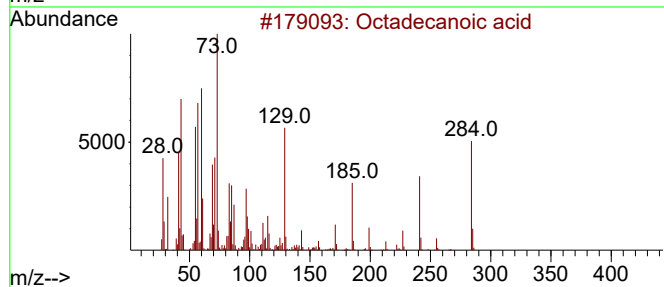
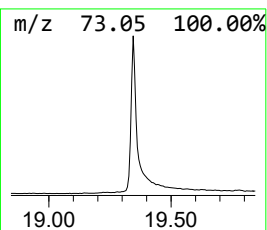
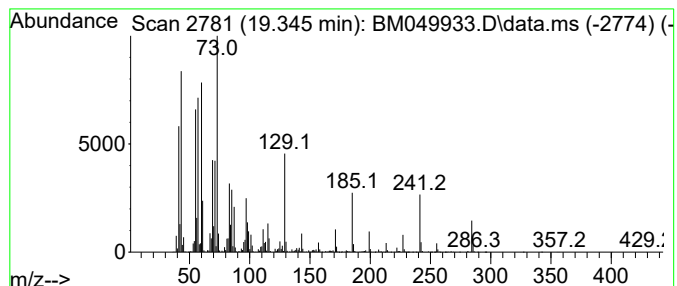
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.345	51.43 ng	10800900	Chrysene-d12	21.397

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5			Tridecanoic acid	214	C13H26O2	000638-53-9	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041525\
Data File : BM049933.D
Acq On : 15 Apr 2025 13:56
Operator : RC/JU
Sample : Q1779-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-22

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-...	4.887	3.6	ng	432546	1	7.769	2379120	20.0
2-Pentanone, 4-...	5.963	2.8	ng	331455	1	7.769	2379120	20.0
Benzophenone	15.774	3.6	ng	673896	3	14.416	3700500	20.0
n-Hexadecanoic ...	18.062	39.2	ng	7384350	4	17.157	3764350	20.0
Octadecanoic acid	19.345	51.4	ng	10800900	5	21.397	4199910	20.0