

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060625\
 Data File : BF142653.D
 Acq On : 06 Jun 2025 18:31
 Operator : RC/JU
 Sample : Q2198-05
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B-202-GW01

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_F\Methods\8270-BF052025.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF142653.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.104	487	495	509	rBV	125824	189099	5.75%	0.976%
2	5.510	556	564	569	rBV	1223331	1589526	48.31%	8.203%
3	6.516	730	735	747	rVB	848923	1093184	33.22%	5.641%
4	6.892	794	799	804	rBV	590862	717647	21.81%	3.703%
5	6.951	804	809	815	rVB	25353	35396	1.08%	0.183%
6	7.457	885	895	900	rBV	1233105	1728822	52.54%	8.922%
7	7.663	924	930	932	rBV2	32935	51927	1.58%	0.268%
8	7.686	932	934	942	rVB	51537	59811	1.82%	0.309%
9	7.910	966	972	976	rBV2	38895	61477	1.87%	0.317%
10	8.175	1012	1017	1025	rBV	724431	1028314	31.25%	5.307%
11	9.251	1194	1200	1205	rBV	2568163	3290518	100.00%	16.981%
12	9.933	1311	1316	1321	rBV	844791	1041731	31.66%	5.376%
13	10.645	1432	1437	1444	rBV	281633	358707	10.90%	1.851%
14	10.722	1445	1450	1459	rBV	1416282	1854344	56.35%	9.570%
15	10.957	1486	1490	1495	rVB	75420	92136	2.80%	0.475%
16	11.422	1564	1569	1576	rBV	708719	902365	27.42%	4.657%
17	11.945	1653	1658	1676	rBV	367636	575918	17.50%	2.972%
18	12.733	1787	1792	1802	rBV	88060	151823	4.61%	0.783%
19	12.816	1803	1806	1811	rVB	47724	58615	1.78%	0.302%
20	13.010	1833	1839	1852	rBV	1759914	2324588	70.65%	11.996%
21	13.904	1986	1991	2010	rVB	231262	390797	11.88%	2.017%
22	14.063	2013	2018	2024	rBV	469183	623712	18.95%	3.219%
23	14.539	2095	2099	2106	rVB	30874	50916	1.55%	0.263%
24	14.704	2122	2127	2144	rVB6	58508	228044	6.93%	1.177%
25	15.562	2266	2273	2286	rBV	456776	750222	22.80%	3.872%
26	16.086	2358	2362	2370	rBV6	15045	38387	1.17%	0.198%
27	17.403	2580	2586	2597	rVB3	38603	89528	2.72%	0.462%

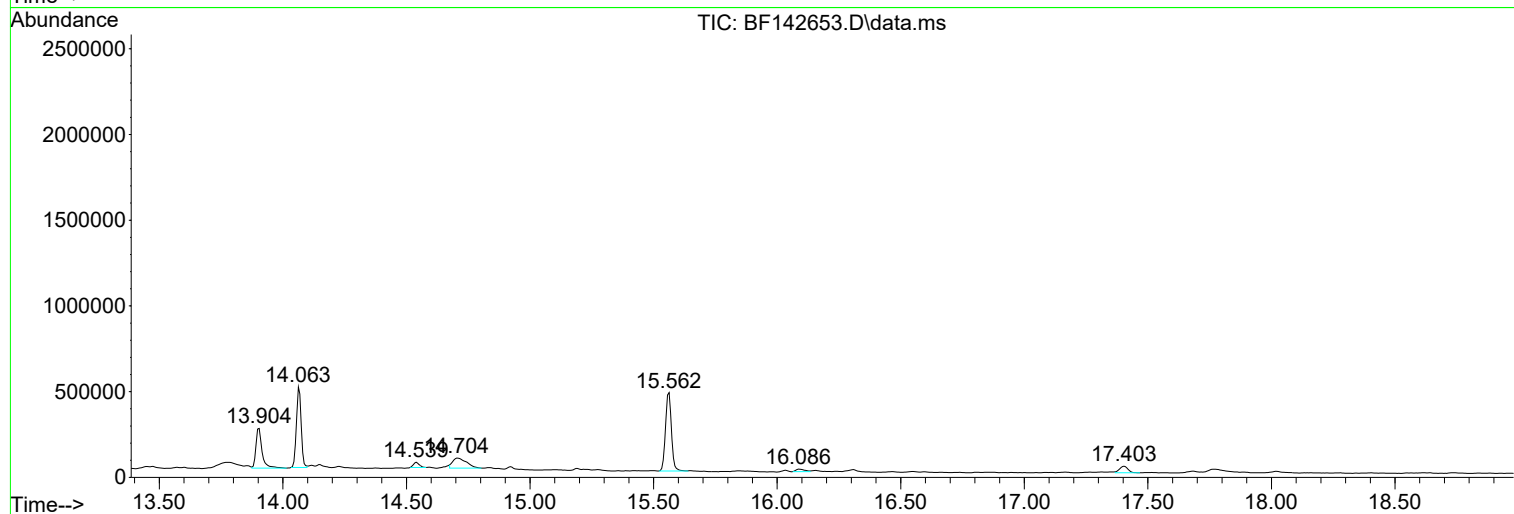
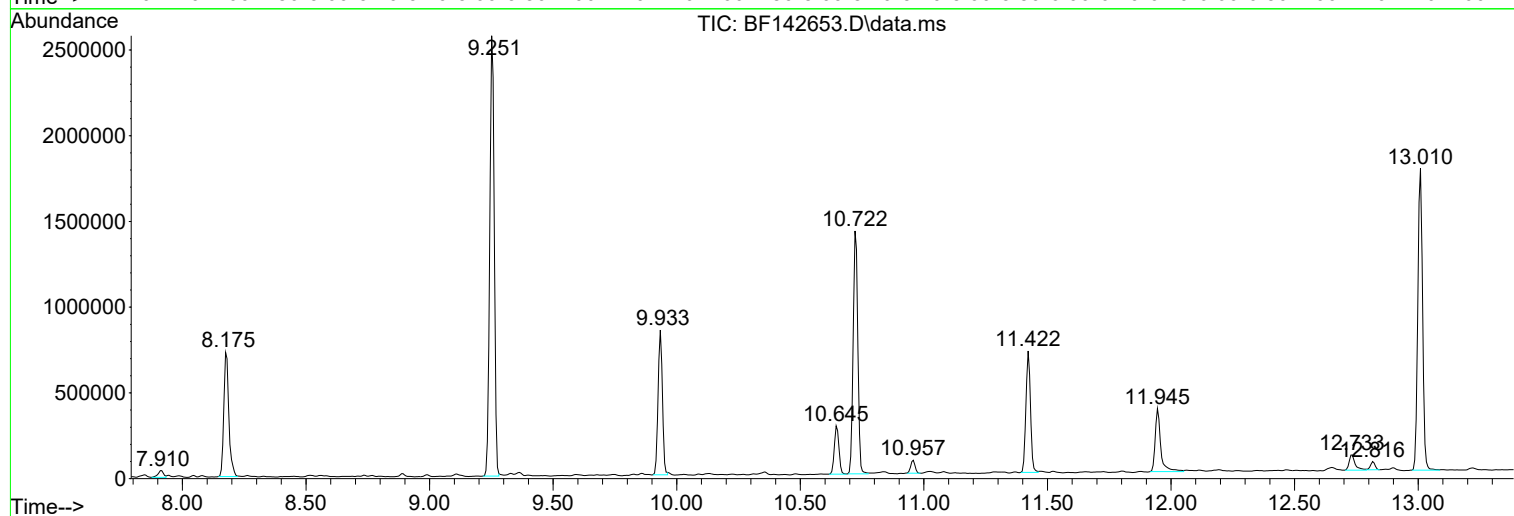
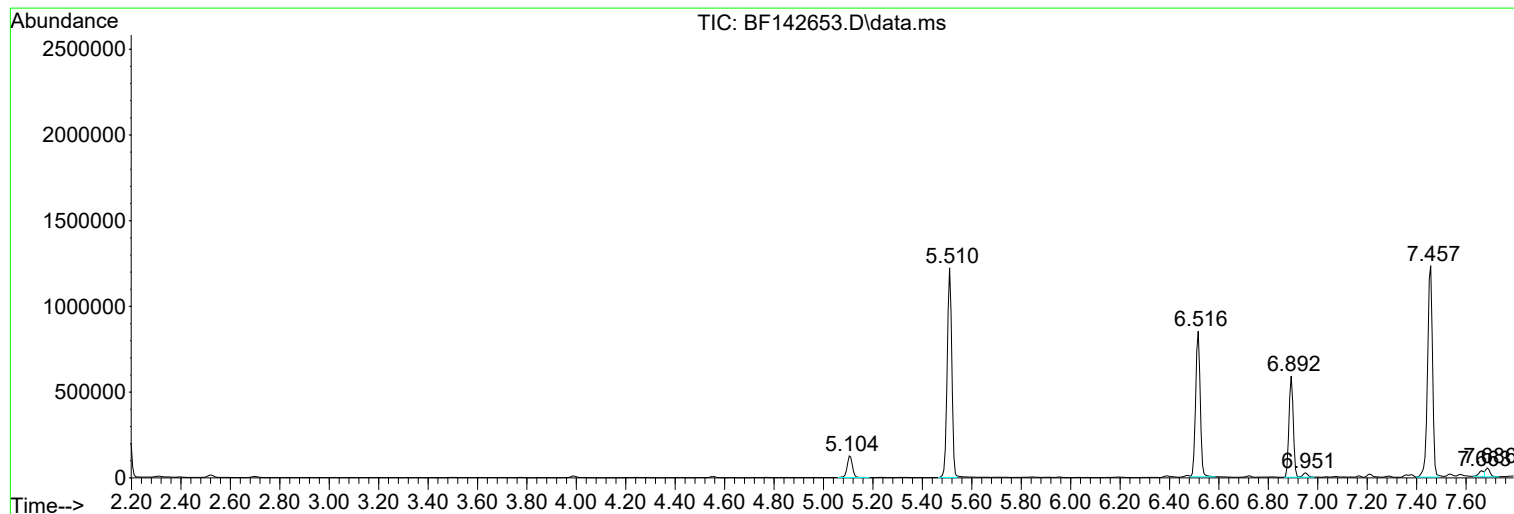
Sum of corrected areas: 19377554

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060625\
Data File : BF142653.D
Acq On : 06 Jun 2025 18:31
Operator : RC/JU
Sample : Q2198-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-202-GW01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052025.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_F\Data\BF060625\
Data File : BF142653.D
Acq On : 06 Jun 2025 18:31
Operator : RC/JU
Sample : Q2198-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-202-GW01

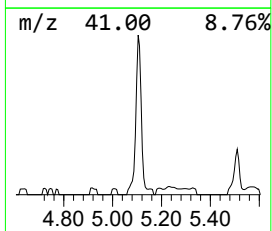
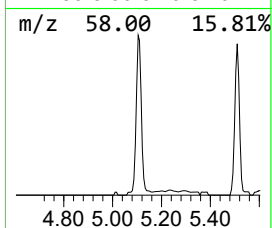
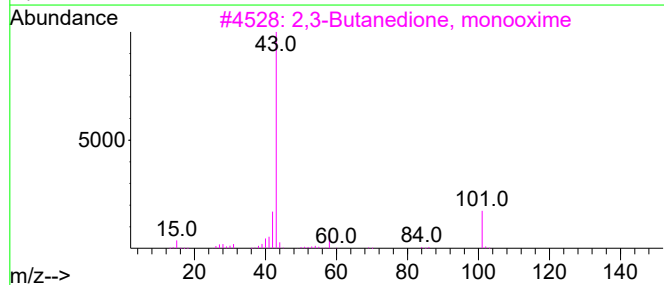
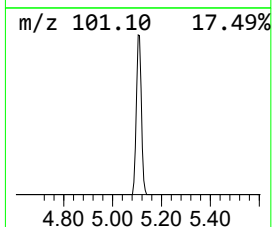
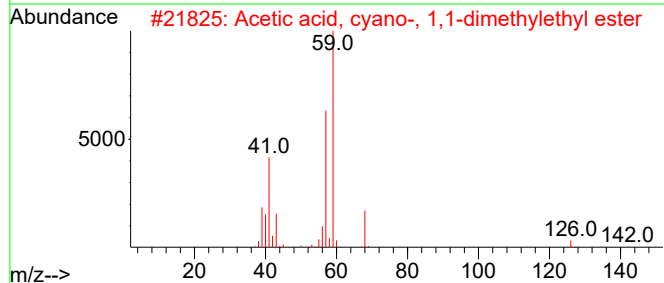
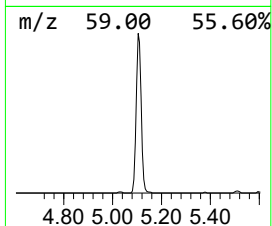
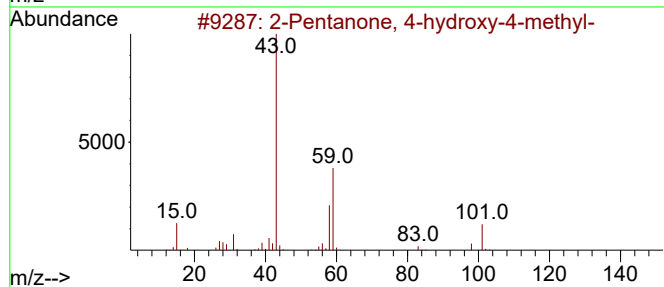
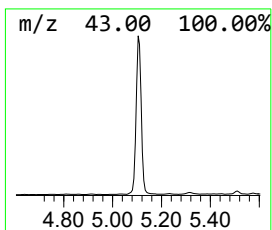
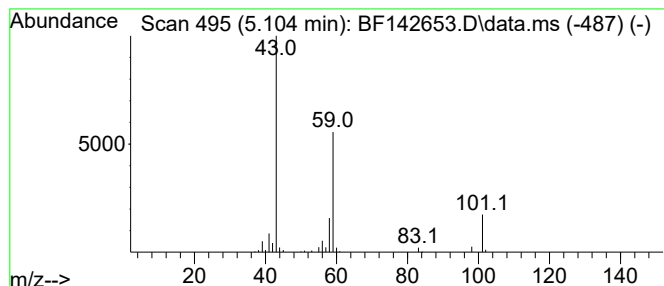
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.104	5.27 ng	189099	1,4-Dichlorobenzene-d4	6.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59		
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	37		
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060625\
Data File : BF142653.D
Acq On : 06 Jun 2025 18:31
Operator : RC/JU
Sample : Q2198-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-202-GW01

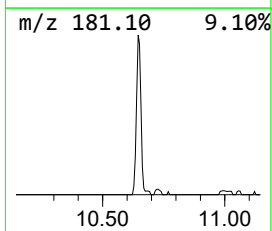
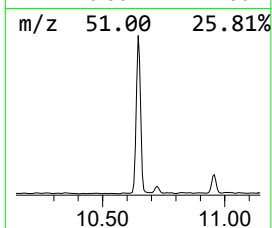
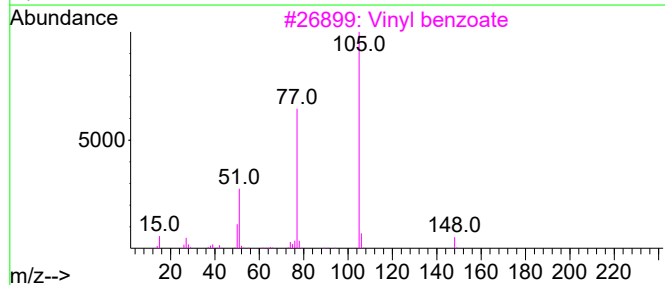
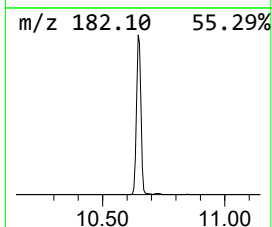
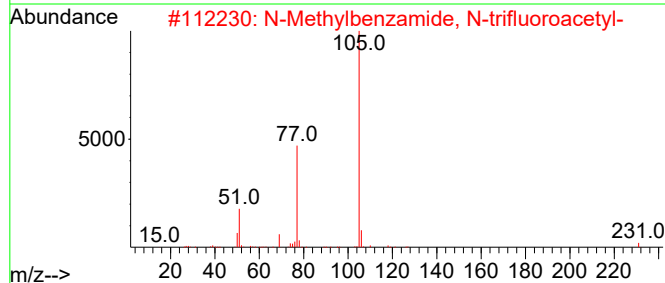
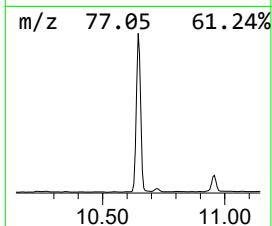
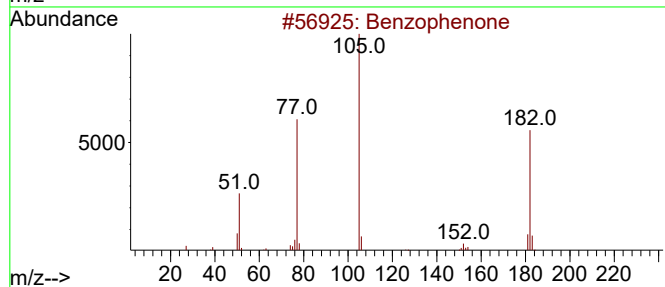
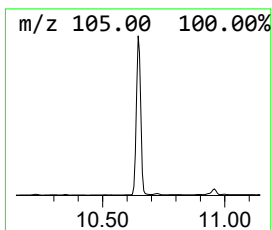
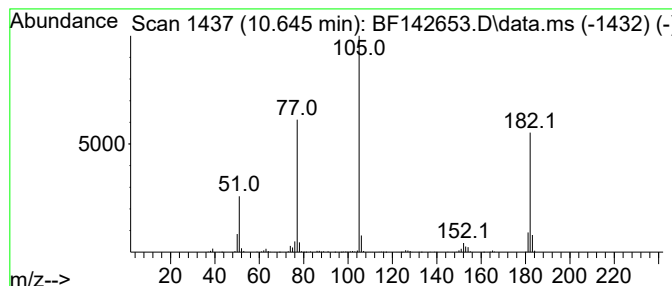
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
10.645	6.89 ng	358707	Acenaphthene-d10	9.933

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			N-Methylbenzamide, N-trifluoroac...	231	C10H8F3NO2	1000446-91-5	47
3			Vinyl benzoate	148	C9H8O2	000769-78-8	47
4			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47
5			2-(2-Oxo-2-phenyl-ethyl)-malon...	184	C11H8N2O	1000296-76-9	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060625\
Data File : BF142653.D
Acq On : 06 Jun 2025 18:31
Operator : RC/JU
Sample : Q2198-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-202-GW01

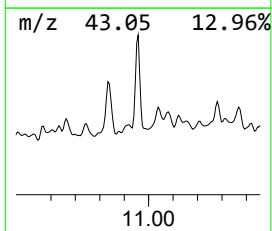
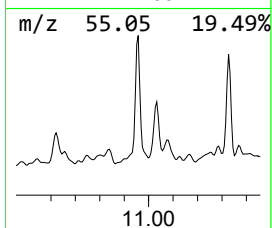
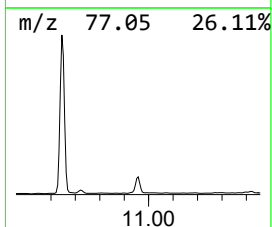
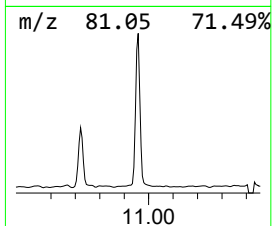
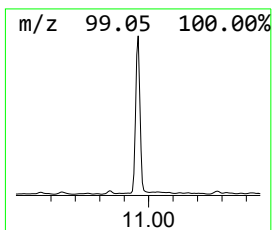
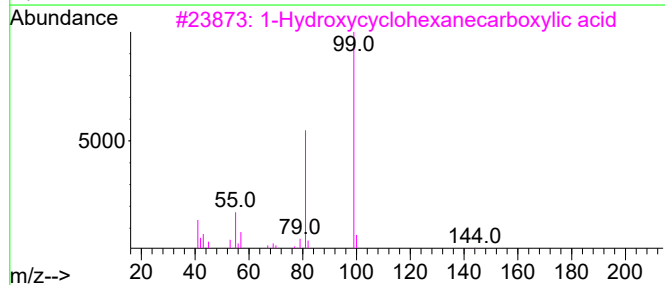
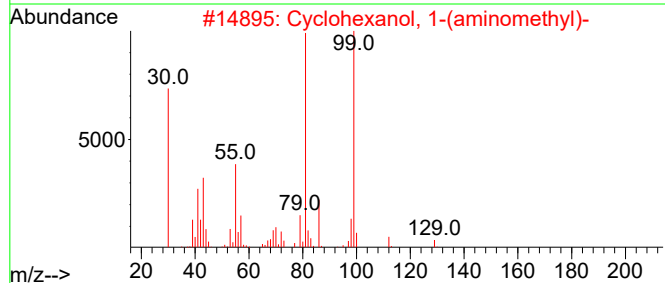
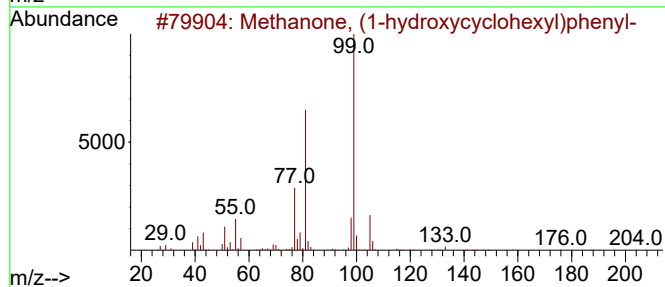
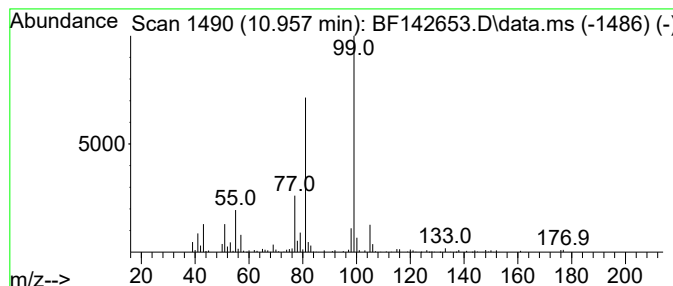
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Methanone, (1-hydroxycyclohexyl) Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.957	2.04 ng	92136	Phenanthrene-d10	11.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methanone, (1-hydroxycyclohexyl)...	204	C13H16O2	000947-19-3	90
2			Cyclohexanol, 1-(aminomethyl)-	129	C7H15NO	004000-72-0	53
3			1-Hydroxycyclohexanecarboxylic acid	144	C7H12O3	001123-28-0	52
4			3,5-Diamino-1,2,4-triazole	99	C2H5N5	001455-77-2	38
5			3-Methylcyclohexyl methylphospho...	194	C8H16FO2P	113548-86-0	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060625\
Data File : BF142653.D
Acq On : 06 Jun 2025 18:31
Operator : RC/JU
Sample : Q2198-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

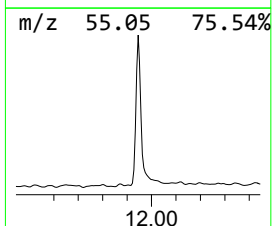
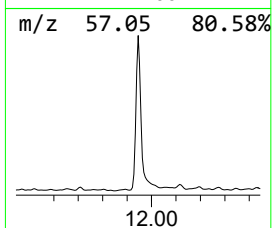
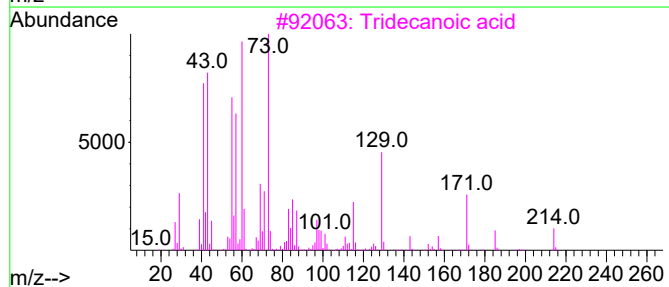
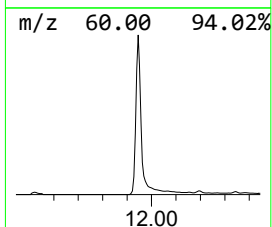
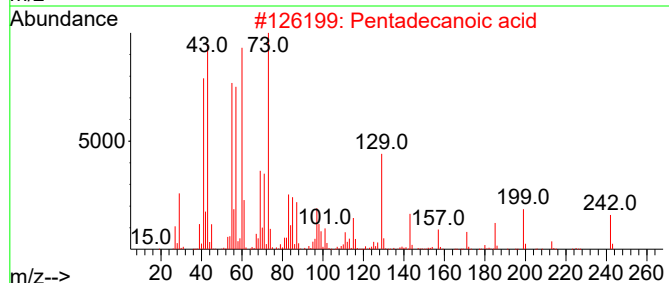
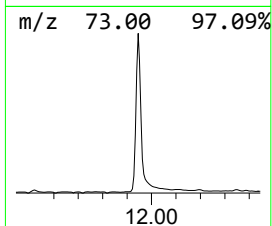
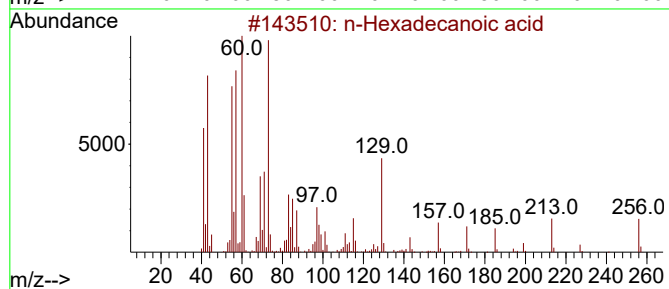
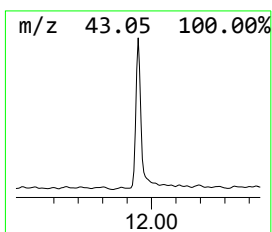
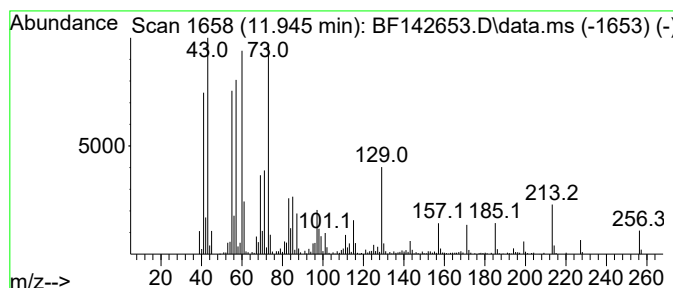
Instrument :
BNA_F
ClientSampleId :
B-202-GW01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052025.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 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.945	12.76 ng	575918	Phenanthrene-d10	11.422	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Tridecanoic acid	214	C13H26O2	000638-53-9	89
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060625\
Data File : BF142653.D
Acq On : 06 Jun 2025 18:31
Operator : RC/JU
Sample : Q2198-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

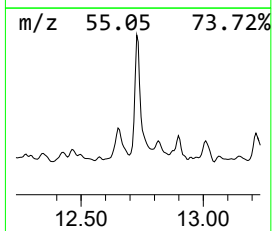
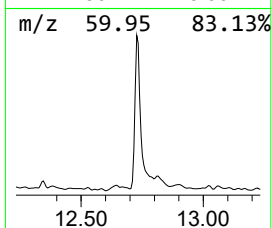
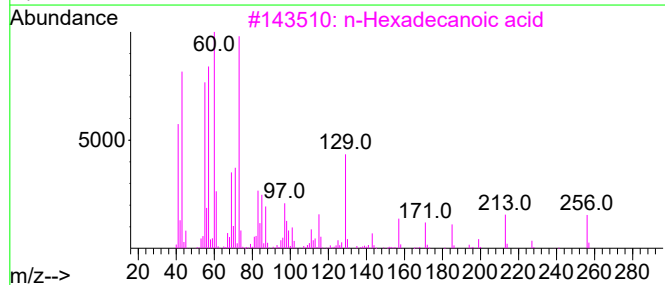
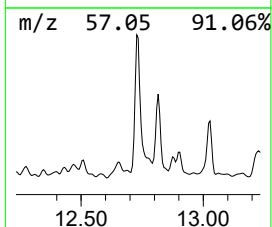
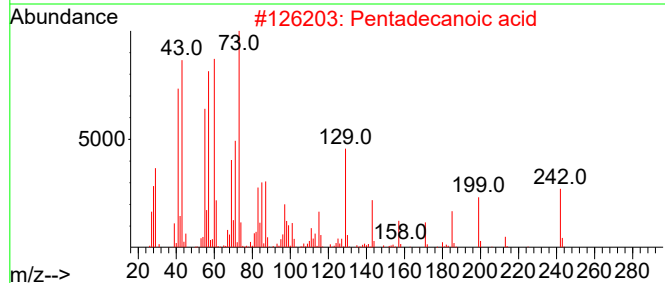
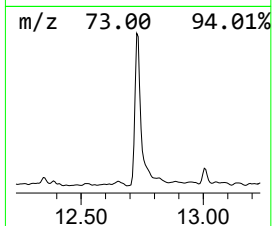
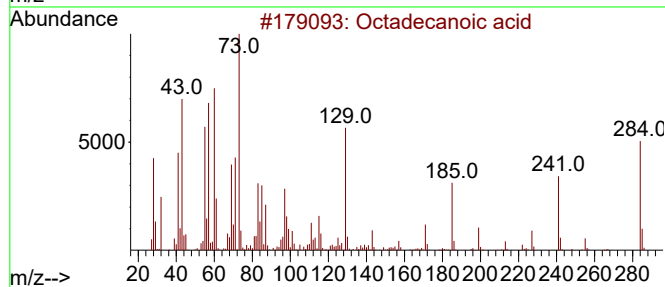
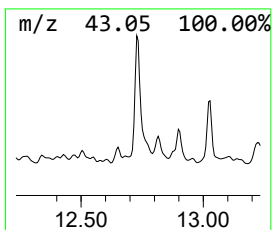
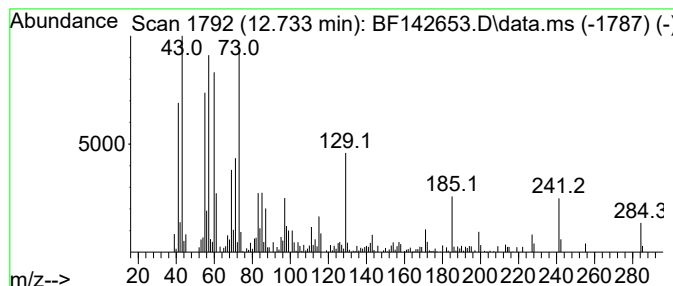
Instrument :
BNA_F
ClientSampleId :
B-202-GW01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052025.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 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.733	3.37 ng	151823	Phenanthrene-d10		11.422	
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	89
3	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	87
4	Tetradecanoic acid		228	C14H28O2	000544-63-8	83
5	Tridecanoic acid		214	C13H26O2	000638-53-9	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060625\
Data File : BF142653.D
Acq On : 06 Jun 2025 18:31
Operator : RC/JU
Sample : Q2198-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

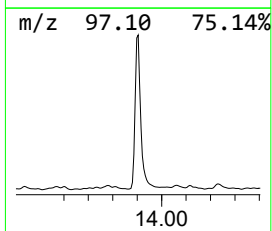
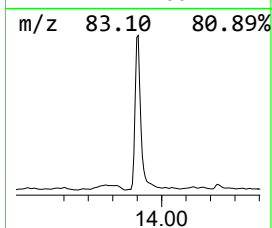
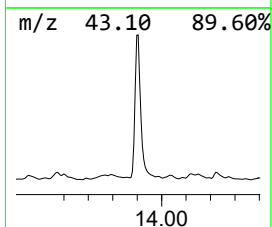
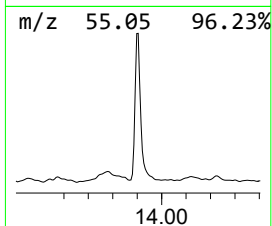
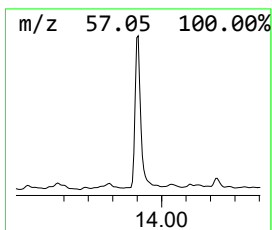
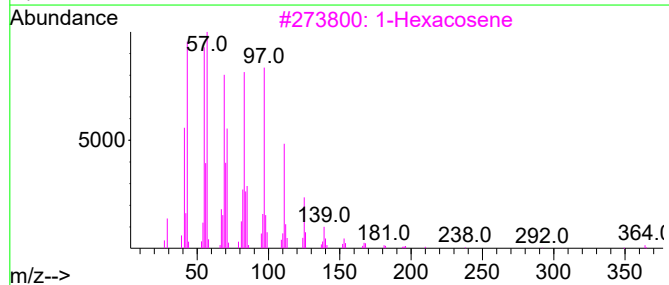
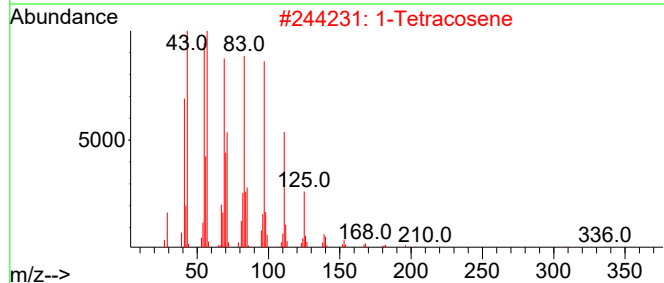
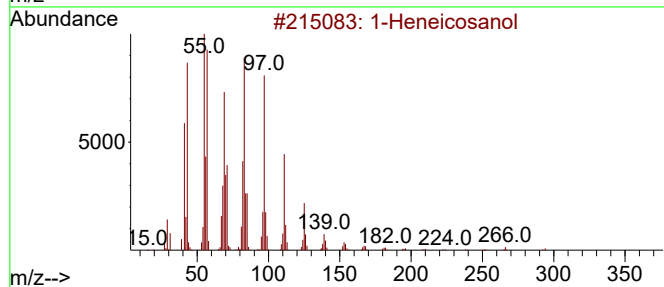
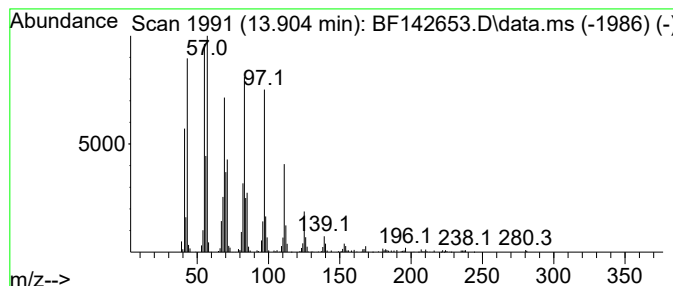
Instrument :
BNA_F
ClientSampleId :
B-202-GW01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Heneicosanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.904	12.53 ng	390797	Chrysene-d12	14.063	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	1-Tetracosene	336	C24H48	010192-32-2	95
3	1-Hexacosene	364	C26H52	018835-33-1	95
4	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	94
5	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060625\
Data File : BF142653.D
Acq On : 06 Jun 2025 18:31
Operator : RC/JU
Sample : Q2198-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-202-GW01

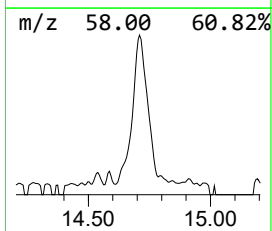
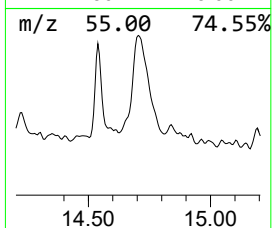
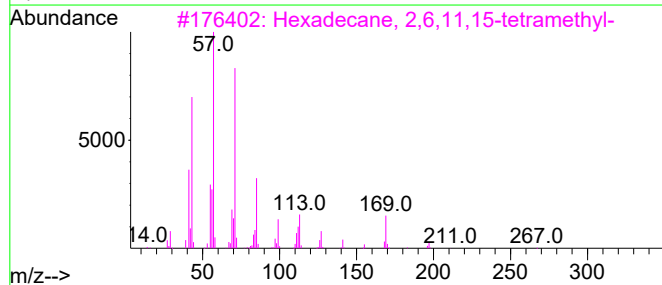
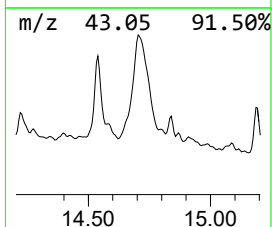
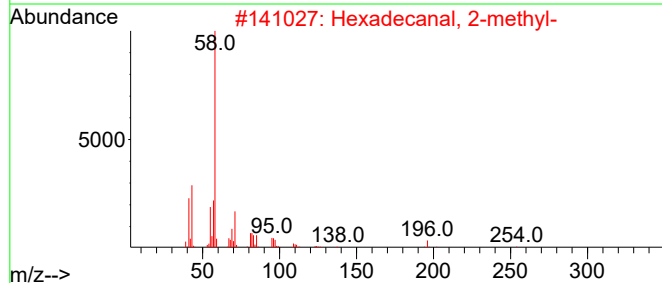
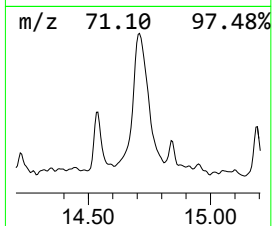
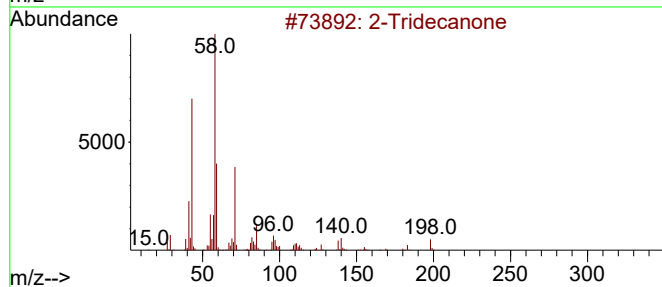
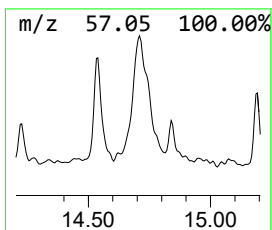
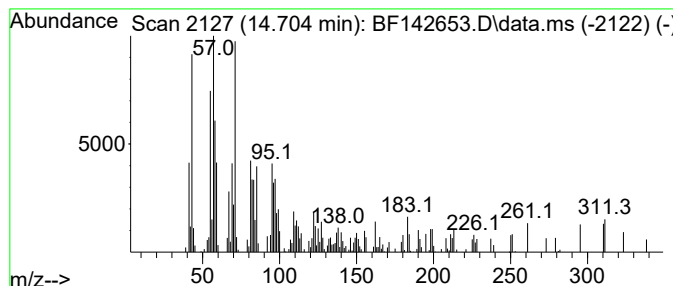
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 2-Tridecanone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.704	7.31 ng	228044	Chrysene-d12	14.063

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Tridecanone			198	C13H26O	000593-08-8	70
2	Hexadecanal, 2-methyl-			254	C17H34O	055019-46-0	38
3	Hexadecane, 2,6,11,15-tetramethyl-			282	C20H42	000504-44-9	38
4	Docosane			310	C22H46	000629-97-0	30
5	Citronellol			156	C10H20O	000106-22-9	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060625\
Data File : BF142653.D
Acq On : 06 Jun 2025 18:31
Operator : RC/JU
Sample : Q2198-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-202-GW01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052025.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-...	5.104	5.3	ng	189099	1	6.892	717647	20.0
Benzophenone	10.645	6.9	ng	358707	3	9.933	1041730	20.0
Methanone, (1-h...	10.957	2.0	ng	92136	4	11.422	902365	20.0
n-Hexadecanoic ...	11.945	12.8	ng	575918	4	11.422	902365	20.0
Octadecanoic acid	12.733	3.4	ng	151823	4	11.422	902365	20.0
1-Heneicosanol	13.904	12.5	ng	390797	5	14.063	623712	20.0
2-Tridecanone	14.704	7.3	ng	228044	5	14.063	623712	20.0
unknown17.404	17.404	2.4	ng	89528	6	15.562	750222	20.0