

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091125\
 Data File : BF143710.D
 Acq On : 11 Sep 2025 17:00
 Operator : RC/JU
 Sample : Q3066-03
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 VNJ-242

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-BF091025.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF143710.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.110	487	496	502	rBB2	35095	56295	8.49%	1.081%
2	5.504	557	563	568	rBV	430456	557165	84.06%	10.701%
3	6.510	728	734	739	rBV	400595	543152	81.94%	10.432%
4	6.893	794	799	804	rBB	152883	182379	27.51%	3.503%
5	7.451	888	894	899	rBV	271807	344657	52.00%	6.620%
6	8.104	1001	1005	1012	rVB	50502	65120	9.82%	1.251%
7	8.175	1012	1017	1022	rBV	193620	235076	35.47%	4.515%
8	8.351	1041	1047	1051	rBV	22782	28370	4.28%	0.545%
9	8.416	1054	1058	1062	rBV	28137	34684	5.23%	0.666%
10	9.251	1194	1200	1205	rBV	533218	662836	100.00%	12.731%
11	9.887	1298	1308	1312	rBV	119268	157918	23.82%	3.033%
12	9.928	1312	1315	1324	rVB	194369	248377	37.47%	4.771%
13	10.134	1345	1350	1354	rVB	70816	85780	12.94%	1.648%
14	10.275	1367	1374	1376	rBV4	5017	7241	1.09%	0.139%
15	10.304	1376	1379	1382	rVB	6993	8349	1.26%	0.160%
16	10.581	1422	1426	1432	rBV2	4717	6910	1.04%	0.133%
17	10.639	1432	1436	1444	rVB	37684	48489	7.32%	0.931%
18	10.716	1444	1449	1454	rBV	273069	338397	51.05%	6.500%
19	10.845	1465	1471	1479	rBV3	12034	21003	3.17%	0.403%
20	11.192	1526	1530	1533	rBV	10866	13013	1.96%	0.250%
21	11.281	1541	1545	1548	rBV	10586	15528	2.34%	0.298%
22	11.316	1548	1551	1556	rVB	14960	19539	2.95%	0.375%
23	11.369	1556	1560	1564	rBV	16192	24379	3.68%	0.468%
24	11.416	1564	1568	1576	rVV	167707	236046	35.61%	4.534%
25	11.481	1576	1579	1586	rVB4	7739	12989	1.96%	0.249%
26	11.710	1615	1618	1623	rVB	8094	9510	1.43%	0.183%
27	11.798	1630	1633	1639	rVB7	5070	6809	1.03%	0.131%
28	11.939	1652	1657	1662	rBV2	79102	109706	16.55%	2.107%
29	12.116	1684	1687	1692	rBV	9038	11288	1.70%	0.217%
30	12.398	1732	1735	1740	rBV	9665	14717	2.22%	0.283%
31	12.504	1750	1753	1758	rVB3	11290	15365	2.32%	0.295%
32	12.628	1770	1774	1784	rBV	37494	72286	10.91%	1.388%
33	12.728	1787	1791	1797	rBV3	28932	53741	8.11%	1.032%
34	12.857	1810	1813	1820	rBV2	34832	57382	8.66%	1.102%
35	13.004	1833	1838	1846	rBV	471193	623616	94.08%	11.978%
36	14.057	2013	2017	2025	rBV	186596	278360	42.00%	5.346%

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091125\
Data File : BF143710.D
Acq On : 11 Sep 2025 17:00
Operator : RC/JU
Sample : Q3066-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-242

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-BF091025.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

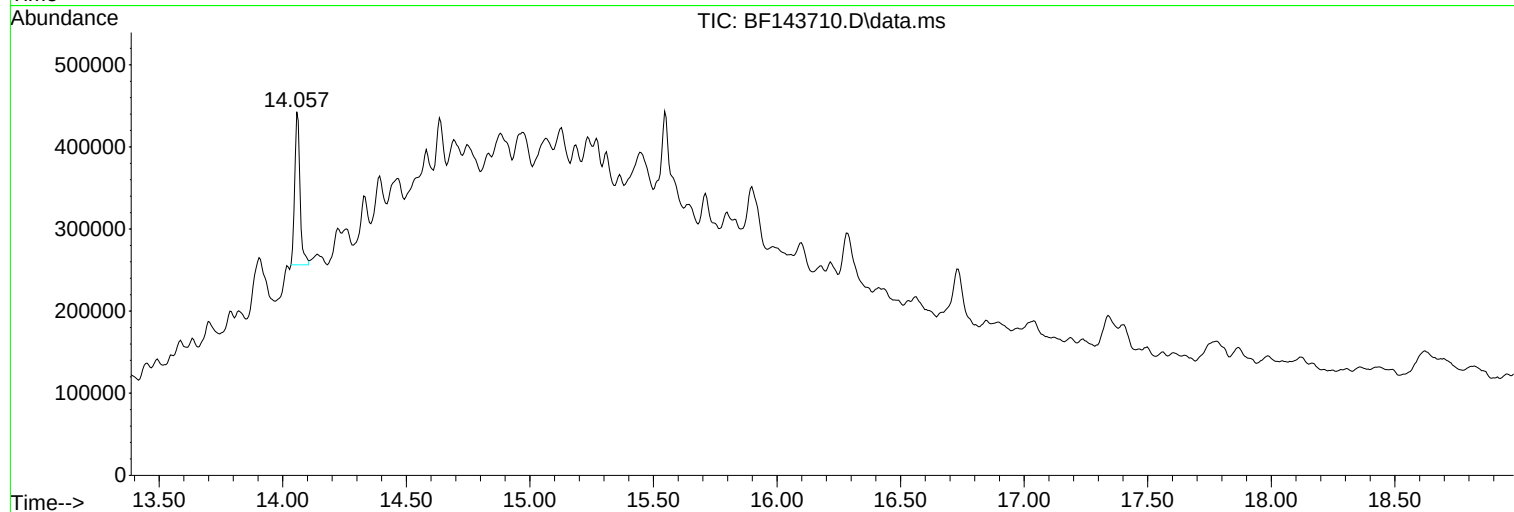
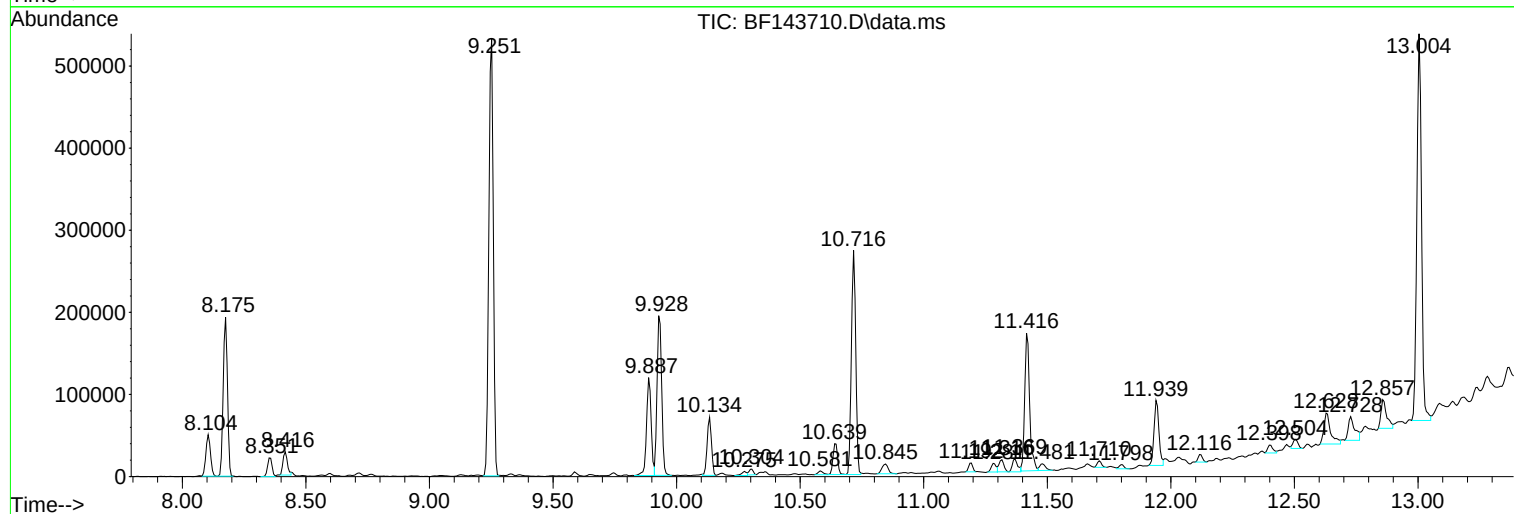
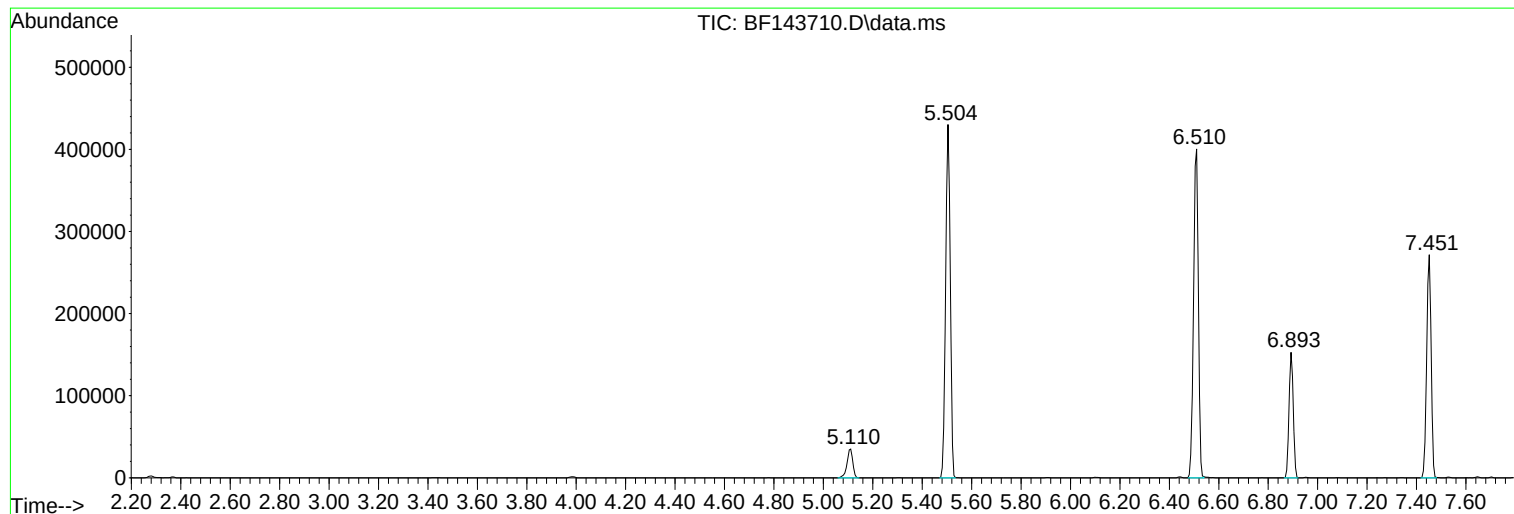
Sum of corrected areas: 5206472

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091125\
Data File : BF143710.D
Acq On : 11 Sep 2025 17:00
Operator : RC/JU
Sample : Q3066-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-242

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091025.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\BF091125\
Data File : BF143710.D
Acq On : 11 Sep 2025 17:00
Operator : RC/JU
Sample : Q3066-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-242

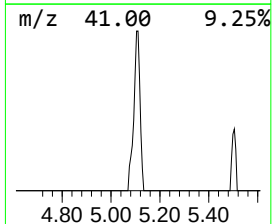
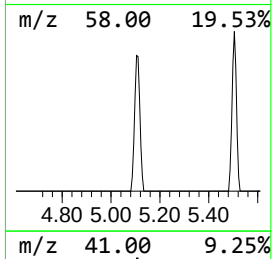
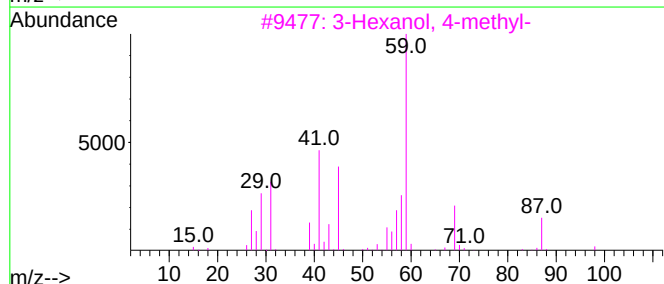
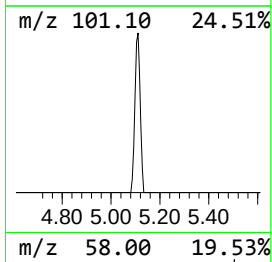
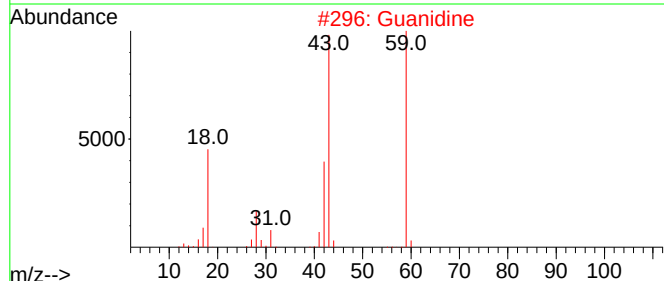
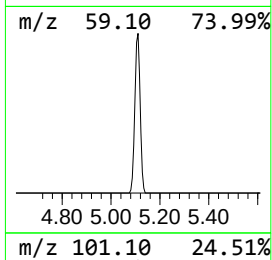
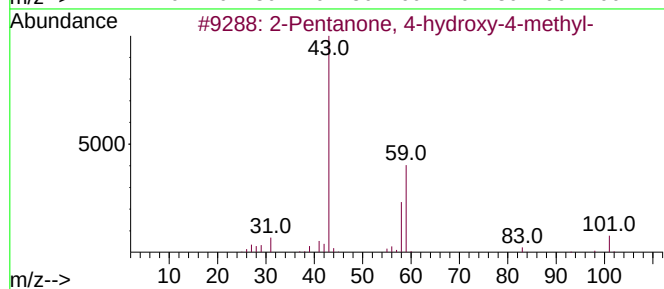
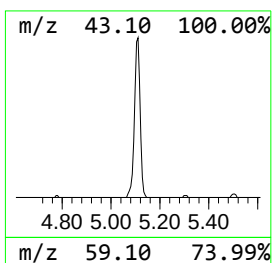
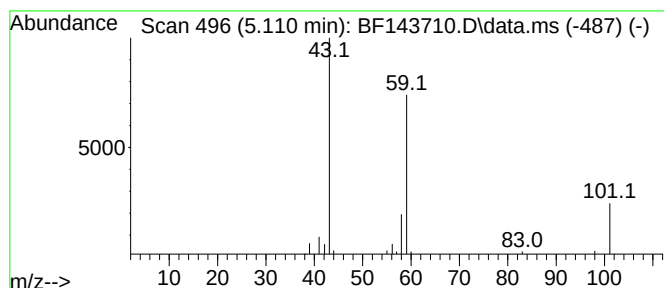
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.110	6.17 ng	56295	1,4-Dichlorobenzene-d4	6.893

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53		
2	Guanidine	59	CH5N3	000113-00-8	50		
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	36		
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10		
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091125\
Data File : BF143710.D
Acq On : 11 Sep 2025 17:00
Operator : RC/JU
Sample : Q3066-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-242

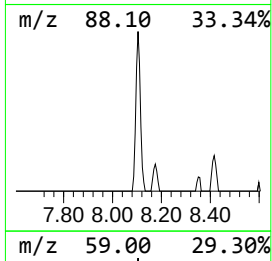
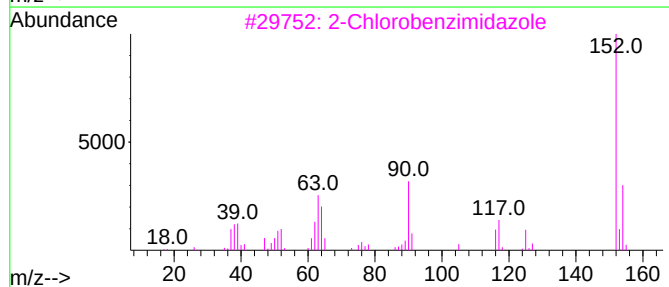
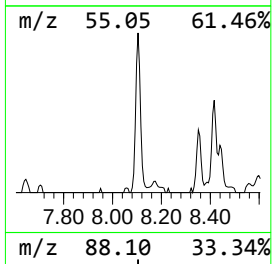
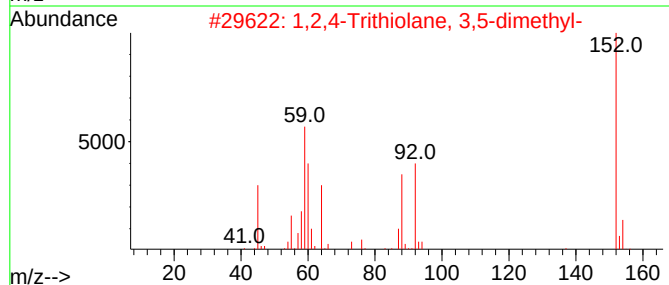
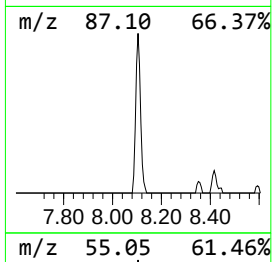
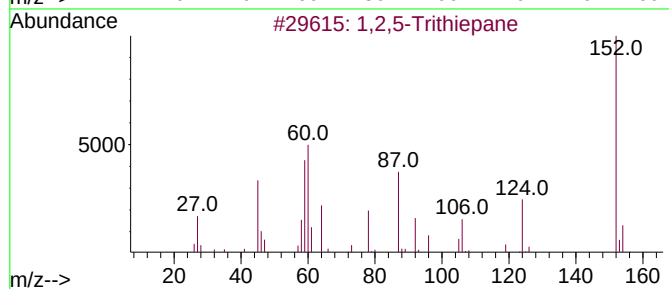
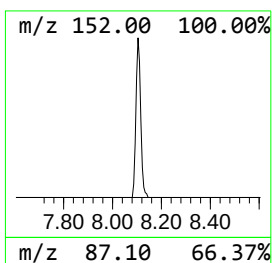
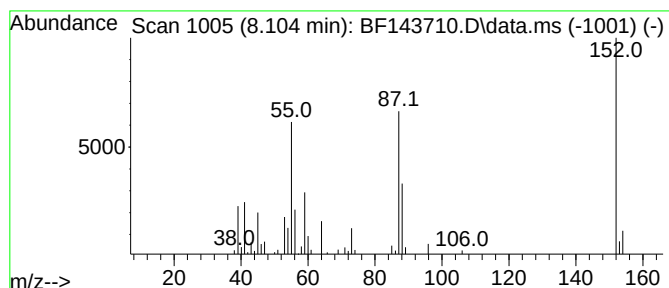
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown8.104 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.104	5.54 ng	65120	Naphthalene-d8	8.175

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,2,5-Trithiepane	152	C4H8S3	006576-93-8	38
2		1,2,4-Trithiolane, 3,5-dimethyl-	152	C4H8S3	023654-92-4	38
3		2-Chlorobenzimidazole	152	C7H5ClN2	004857-06-1	27
4		trans-O-Dithiane-4,5-diol	152	C4H8O2S2	014193-38-5	25
5		8-Azaguanine	152	C4H4N6O	000134-58-7	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091125\
Data File : BF143710.D
Acq On : 11 Sep 2025 17:00
Operator : RC/JU
Sample : Q3066-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-242

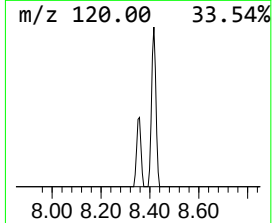
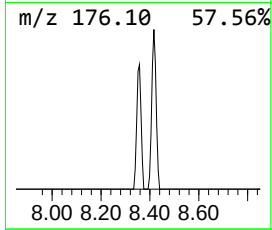
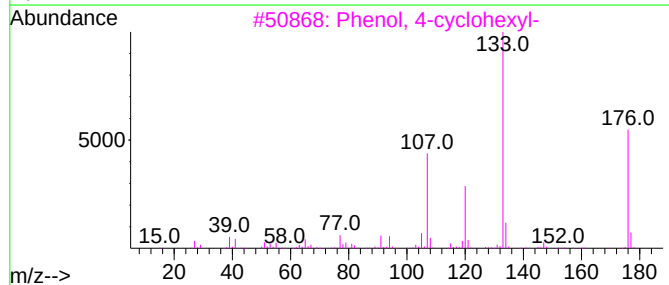
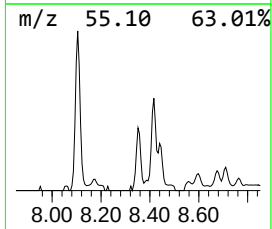
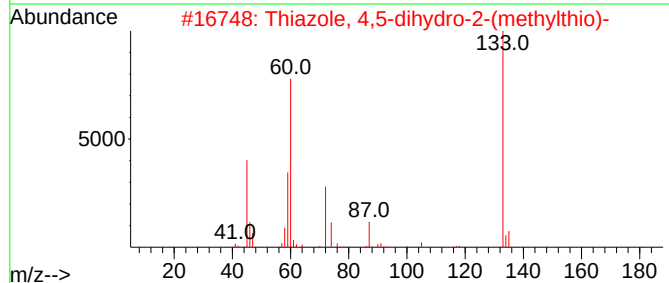
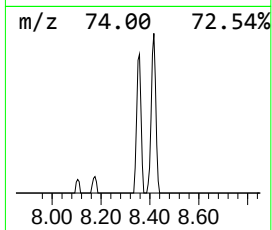
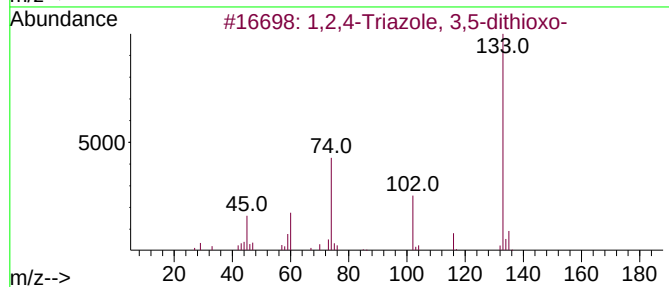
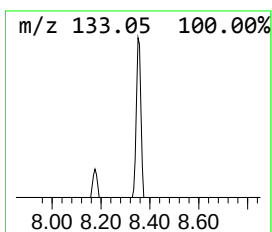
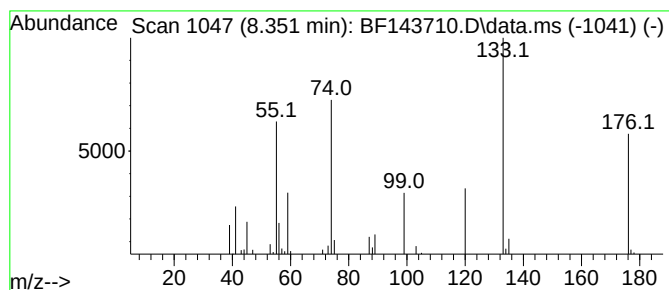
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown8.351 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.351	2.41 ng	28370	Naphthalene-d8	8.175

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2,4-Triazole, 3,5-dithioxo-	133	C2H3N3S2	005650-03-3	43
2			Thiazole, 4,5-dihydro-2-(methylt...	133	C4H7NS2	019975-56-5	38
3			Phenol, 4-cyclohexyl-	176	C12H16O	001131-60-8	37
4			2H-1-Benzopyran-2-one, 7-methoxy-	176	C10H8O3	000531-59-9	32
5			2-Acetyl-5,6,7,8-tetrahydroquino...	176	C10H12N2O	086461-70-3	32



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091125\
Data File : BF143710.D
Acq On : 11 Sep 2025 17:00
Operator : RC/JU
Sample : Q3066-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-242

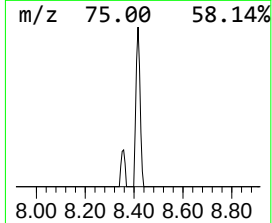
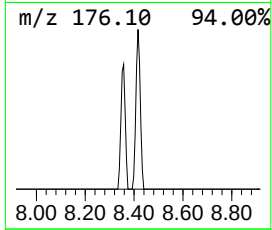
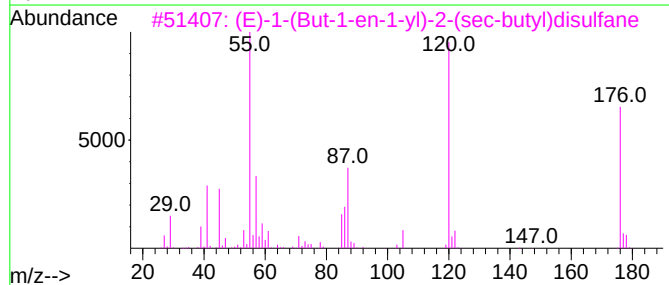
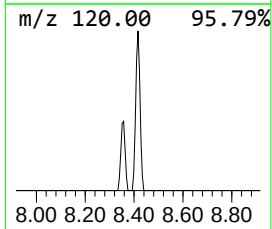
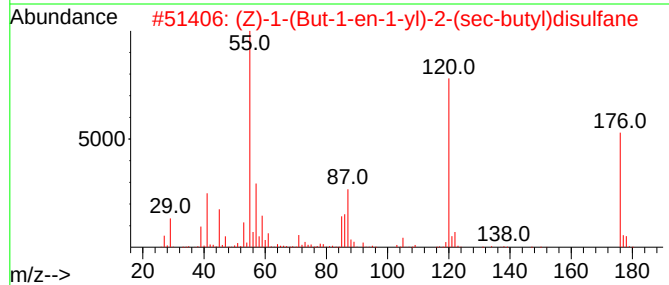
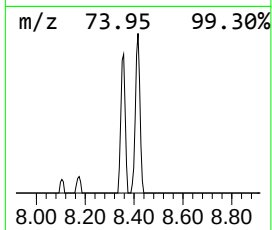
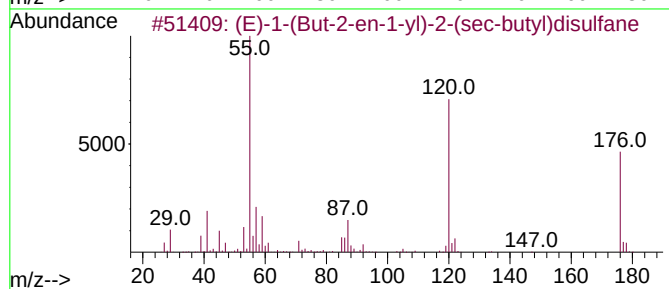
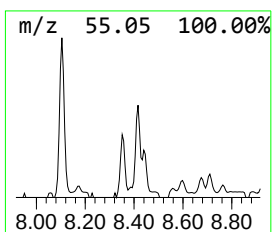
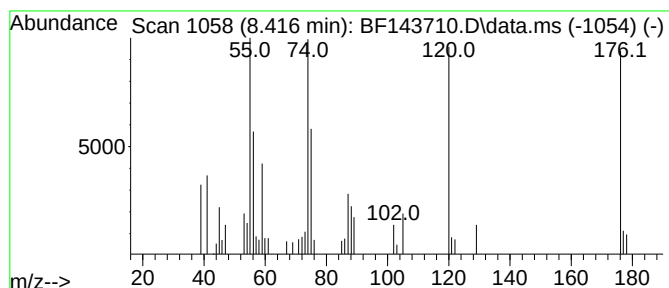
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 unknown8.416 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.416	2.95 ng	34684	Naphthalene-d8	8.175

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-1-(But-2-en-1-yl)-2-(sec-but...	176	C8H16S2	110690-24-9	46		
2	(Z)-1-(But-1-en-1-yl)-2-(sec-but...	176	C8H16S2	110690-21-6	45		
3	(E)-1-(But-1-en-1-yl)-2-(sec-but...	176	C8H16S2	110690-22-7	41		
4	(Z)-1-(But-2-en-1-yl)-2-(sec-but...	176	C8H16S2	110690-23-8	41		
5	7-Methoxy-1-tetralone	176	C11H12O2	006836-19-7	25		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091125\
Data File : BF143710.D
Acq On : 11 Sep 2025 17:00
Operator : RC/JU
Sample : Q3066-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-242

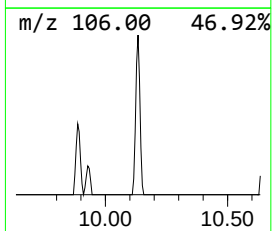
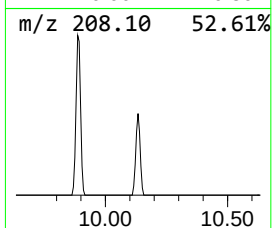
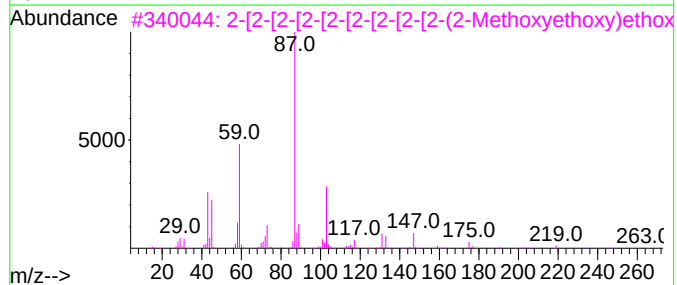
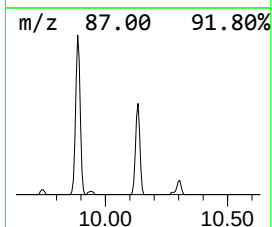
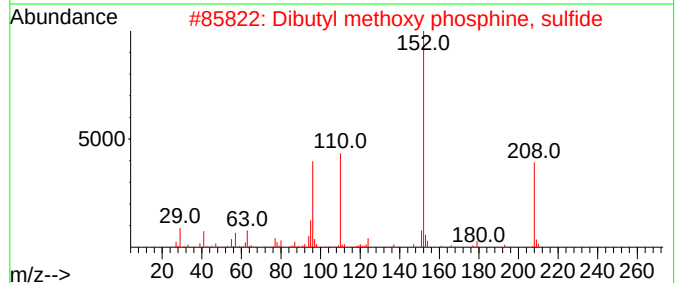
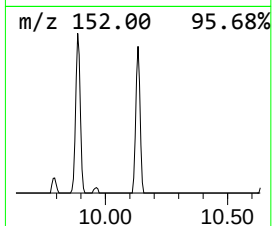
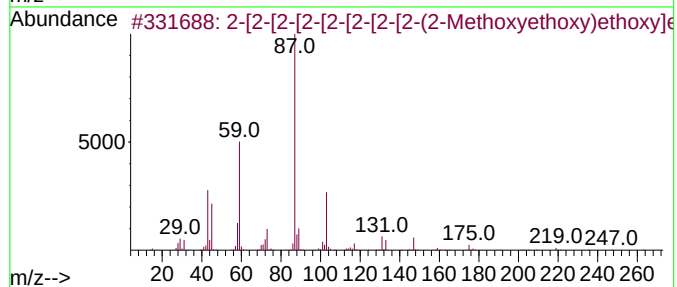
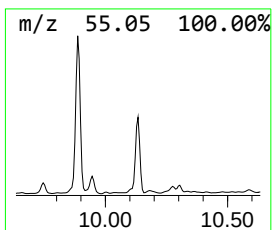
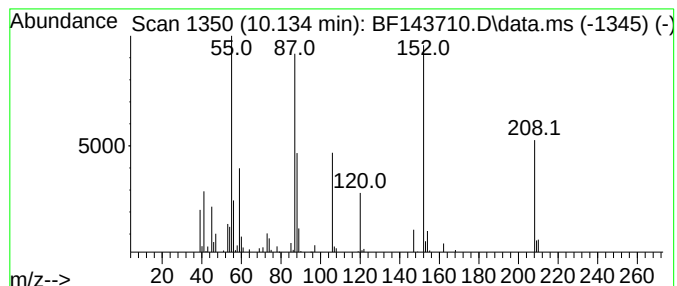
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown10.134 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.134	6.91 ng	85780	Acenaphthene-d10	9.928

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual					
1	2	-[2	-[2	-[2	-[2	-[2	-[2	(2-Methox...	470	C21H42O11	1000351-91-8	22
2	Dibutyl	methoxy	phosphine,	sulfide	208	C9H21OPS	098958-59-9	22				
3	2	-[2	-[2	-[2	-[2	-[2	-[2	(2-Met...	514	C23H46O12	1000351-89-8	22
4	Benzaldehyde,	2-hydroxy-3-methoxy-	152	C8H8O3	000148-53-8	14						
5	2-Methyl-6-nitroaniline	152	C7H8N2O2	000570-24-1	14							



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091125\
Data File : BF143710.D
Acq On : 11 Sep 2025 17:00
Operator : RC/JU
Sample : Q3066-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-242

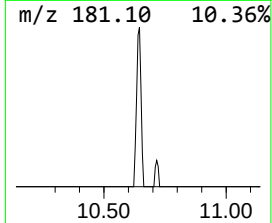
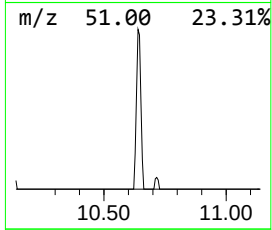
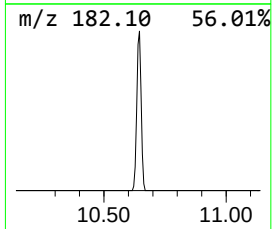
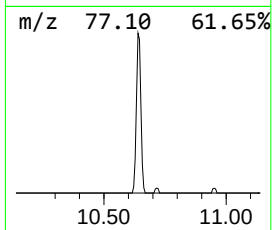
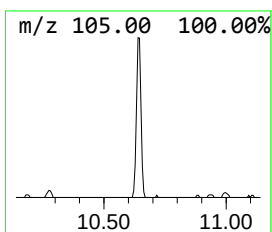
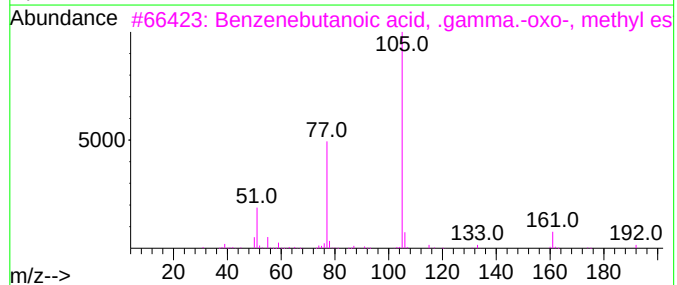
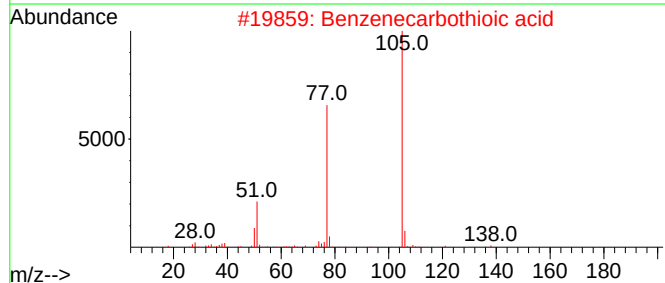
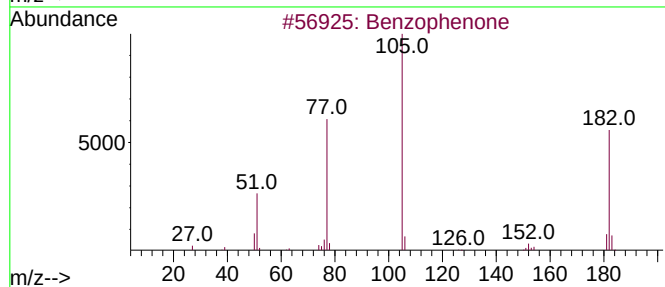
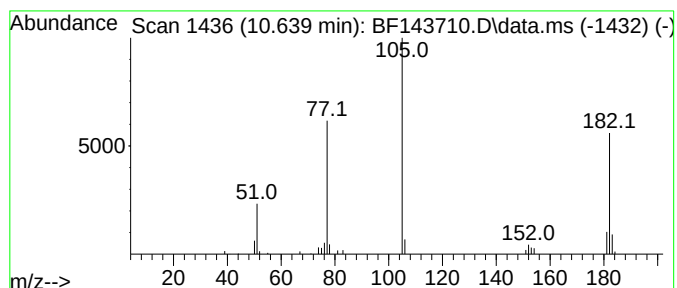
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Benzophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.639	3.90 ng	48489	Acenaphthene-d10	9.928

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Benzenecarbothioic acid	138	C7H6OS	000098-91-9	43
3			Benzenebutanoic acid, .gamma.-ox...	192	C11H12O3	025333-24-8	43
4			2-Benzoyl-4-bromo-5-methyl-1,2-o...	281	C11H8BrNO3	1000444-92-3	43
5			1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091125\
Data File : BF143710.D
Acq On : 11 Sep 2025 17:00
Operator : RC/JU
Sample : Q3066-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

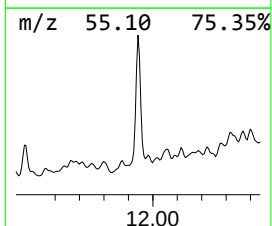
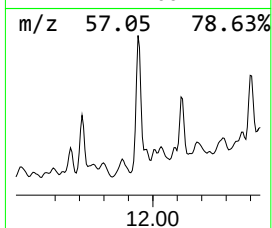
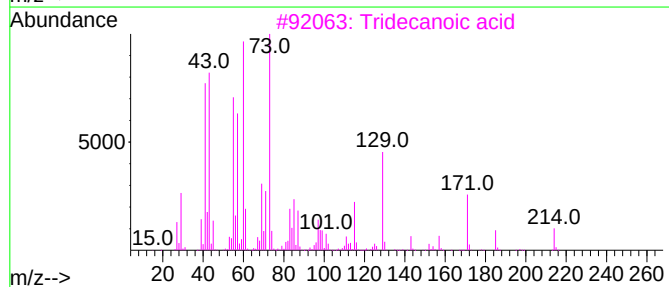
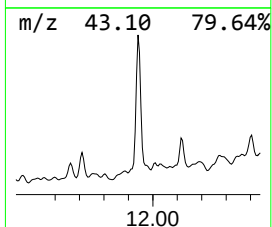
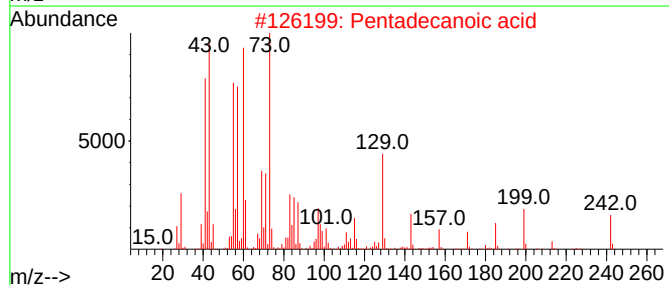
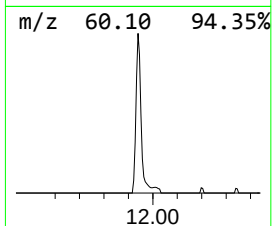
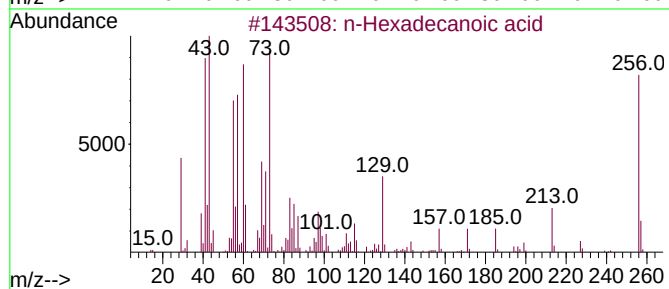
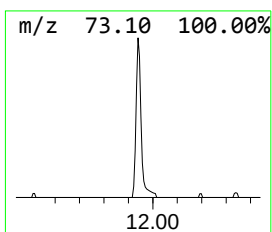
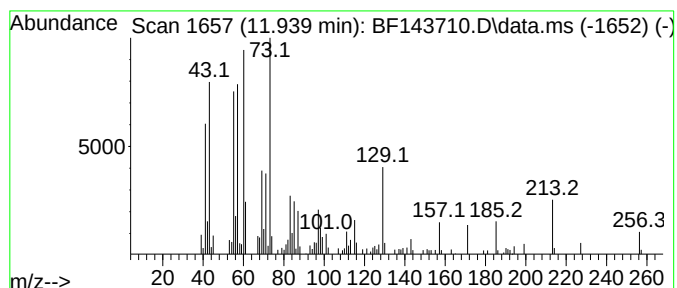
Instrument :
BNA_F
ClientSampleId :
VNJ-242

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.939	9.30 ng	109706	Phenanthrene-d10	11.416	
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	76
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5	Undecanoic acid	186	C11H22O2	000112-37-8	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091125\
Data File : BF143710.D
Acq On : 11 Sep 2025 17:00
Operator : RC/JU
Sample : Q3066-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-242

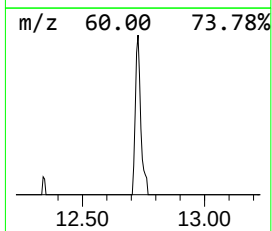
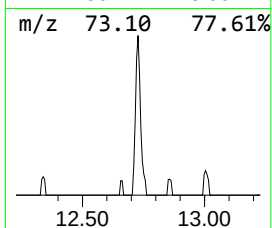
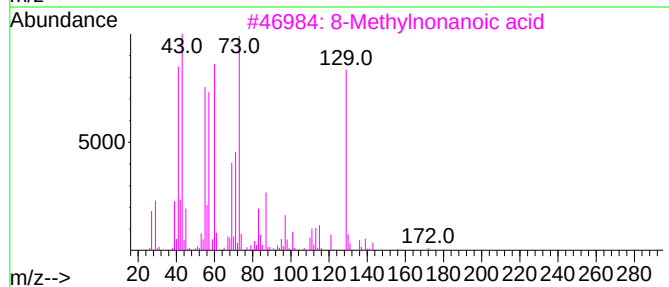
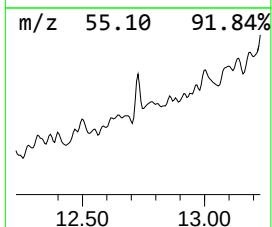
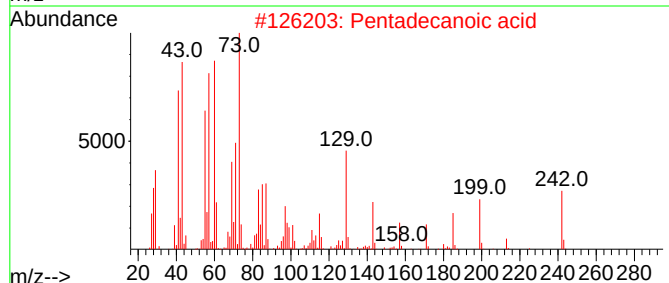
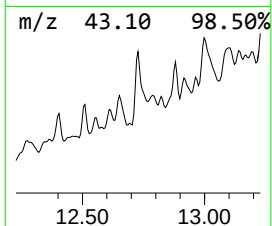
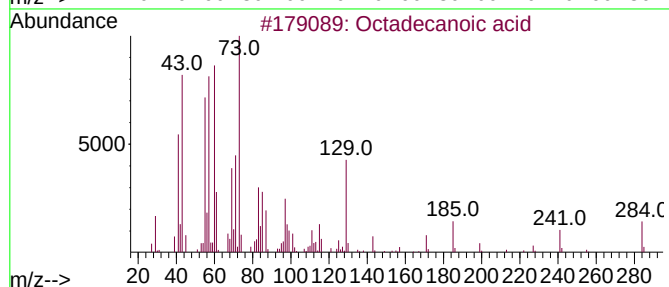
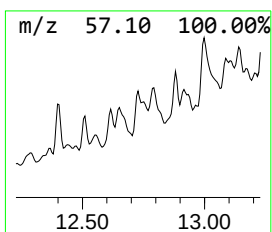
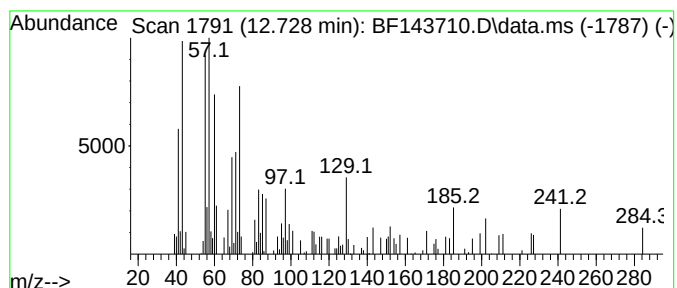
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.727	4.55 ng	53741	Phenanthrene-d10	11.416

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	93
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	64
3		8-Methylnonanoic acid	172	C10H20O2	005963-14-4	50
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	50
5		n-Decanoic acid	172	C10H20O2	000334-48-5	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091125\
Data File : BF143710.D
Acq On : 11 Sep 2025 17:00
Operator : RC/JU
Sample : Q3066-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-242

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091025.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-...	5.110	6.2	ng	56295	1	6.893	182379	20.0
unknown8.104	8.104	5.5	ng	65120	2	8.175	235076	20.0
unknown8.351	8.351	2.4	ng	28370	2	8.175	235076	20.0
unknown8.416	8.416	3.0	ng	34684	2	8.175	235076	20.0
unknown10.134	10.134	6.9	ng	85780	3	9.928	248377	20.0
Benzophenone	10.639	3.9	ng	48489	3	9.928	248377	20.0
n-Hexadecanoic ...	11.939	9.3	ng	109706	4	11.416	236046	20.0
Octadecanoic acid	12.727	4.5	ng	53741	4	11.416	236046	20.0