

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081425\
 Data File : BF143389.D
 Acq On : 14 Aug 2025 18:56
 Operator : RC/JU
 Sample : Q2814-11
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TW-38M-S

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-BF081225.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF143389.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.269	4	13	24	rBV	2676032	4501205	85.59%	13.600%
2	5.163	498	505	525	rVB	284628	424661	8.08%	1.283%
3	5.569	568	574	595	rBV	2108798	2805065	53.34%	8.475%
4	6.187	673	679	686	rBV	41847	57802	1.10%	0.175%
5	6.563	737	743	761	rBV	1567276	2152821	40.94%	6.505%
6	6.934	801	806	813	rVB	724540	891255	16.95%	2.693%
7	7.492	894	901	906	rBV	2231081	3127968	59.48%	9.451%
8	7.804	950	954	965	rVB2	31412	53020	1.01%	0.160%
9	8.210	1018	1023	1039	rBV	882896	1238175	23.54%	3.741%
10	8.328	1039	1043	1056	rVB	106955	141613	2.69%	0.428%
11	8.804	1118	1124	1129	rBV2	110083	176128	3.35%	0.532%
12	9.286	1200	1206	1217	rBV	3895635	5258829	100.00%	15.889%
13	9.969	1316	1322	1330	rBV	1046329	1323442	25.17%	3.999%
14	10.681	1438	1443	1450	rBV	354400	443199	8.43%	1.339%
15	10.757	1450	1456	1473	rBV	2258310	3111263	59.16%	9.401%
16	11.457	1569	1575	1582	rBV	932030	1217295	23.15%	3.678%
17	11.980	1658	1664	1678	rBV3	76755	167391	3.18%	0.506%
18	13.039	1838	1844	1849	rBV	3402126	4419877	84.05%	13.355%
19	13.945	1992	1998	2009	rBV2	25004	73592	1.40%	0.222%
20	14.098	2015	2024	2034	rBV	532282	749495	14.25%	2.265%
21	15.592	2272	2278	2287	rBV	464173	762157	14.49%	2.303%

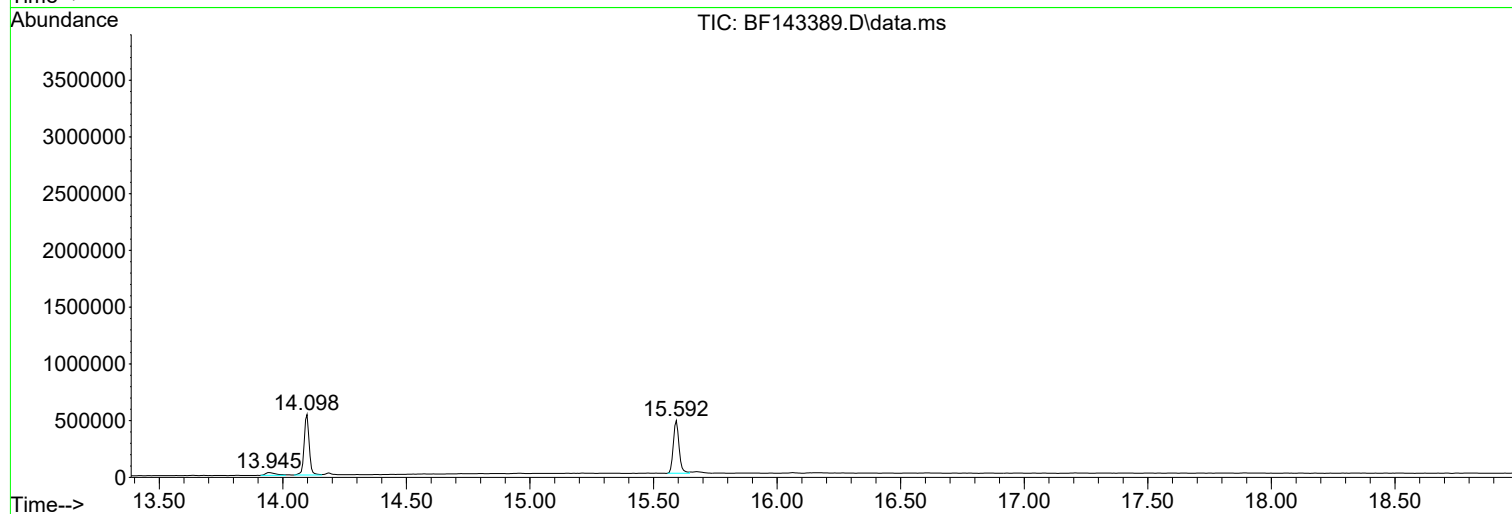
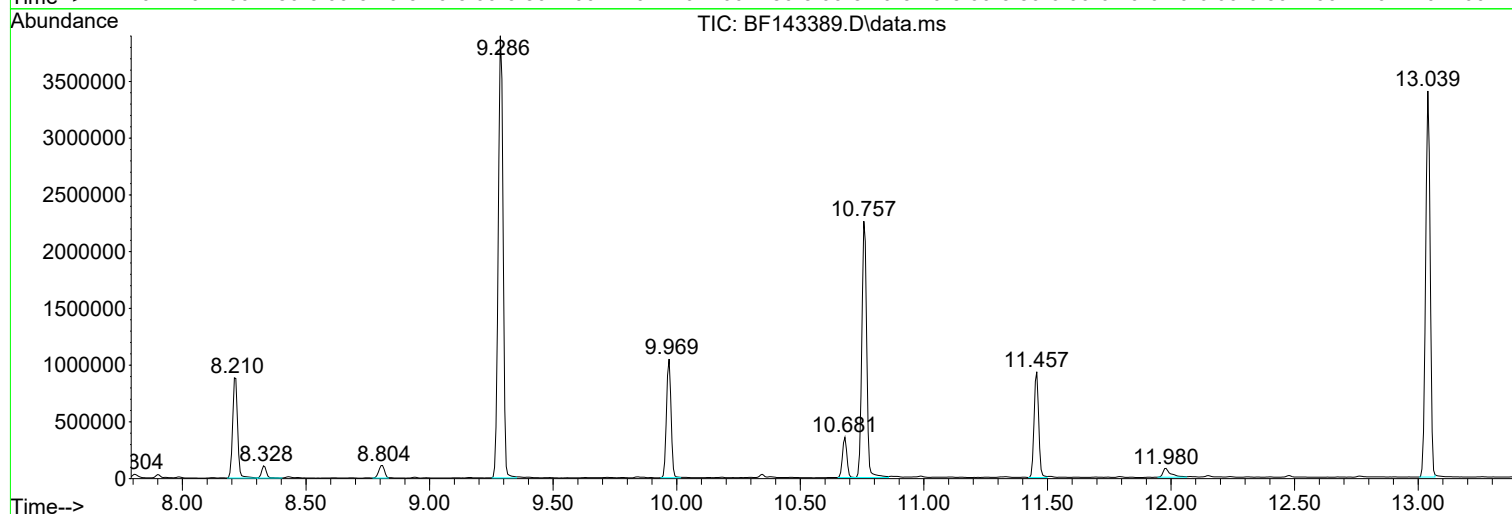
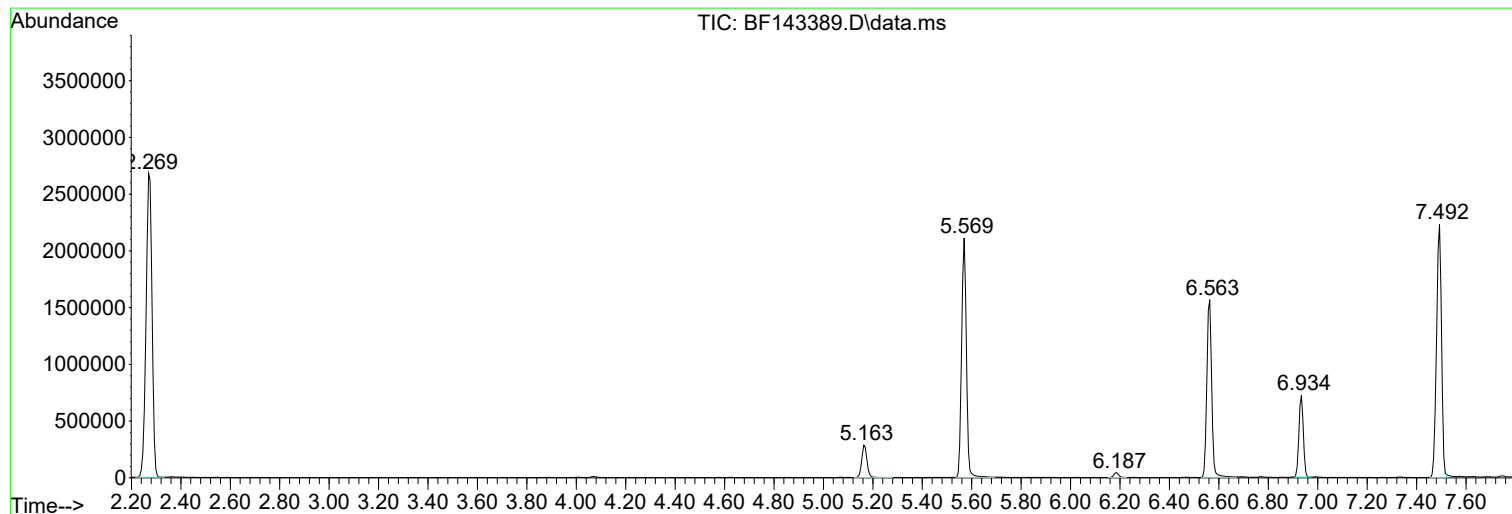
Sum of corrected areas: 33096253

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081425\
Data File : BF143389.D
Acq On : 14 Aug 2025 18:56
Operator : RC/JU
Sample : Q2814-11
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TW-38M-S

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081225.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\BF081425\
Data File : BF143389.D
Acq On : 14 Aug 2025 18:56
Operator : RC/JU
Sample : Q2814-11
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TW-38M-S

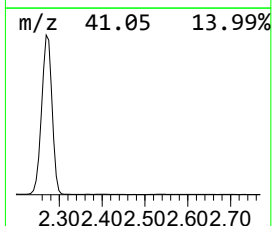
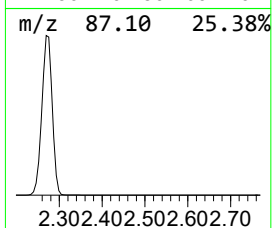
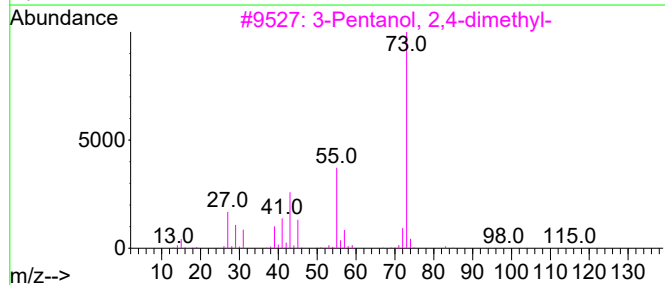
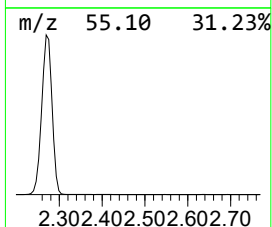
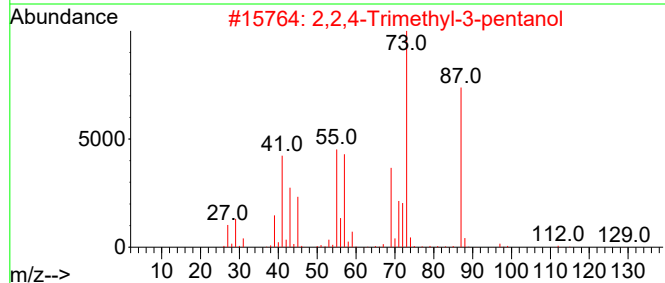
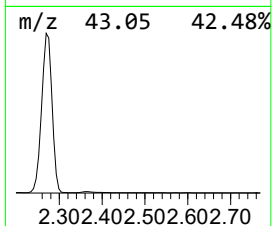
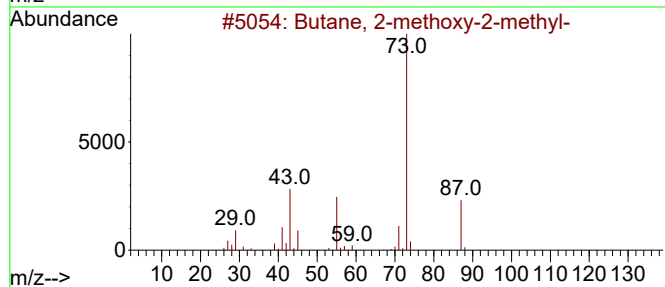
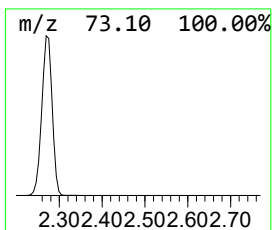
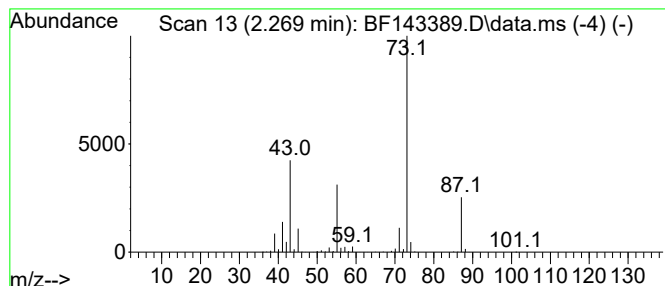
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081225.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.269	101.01 ng	4501210	1,4-Dichlorobenzene-d4	6.934

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081425\
Data File : BF143389.D
Acq On : 14 Aug 2025 18:56
Operator : RC/JU
Sample : Q2814-11
Misc :
ALS Vial : 14 Sample Multiplier: 1

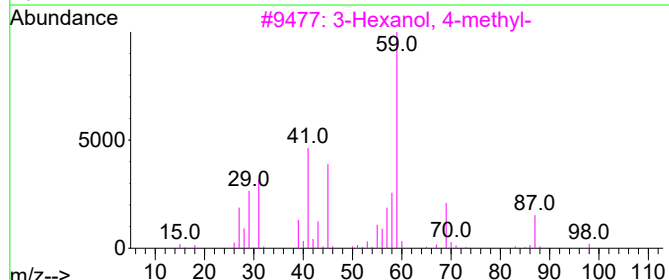
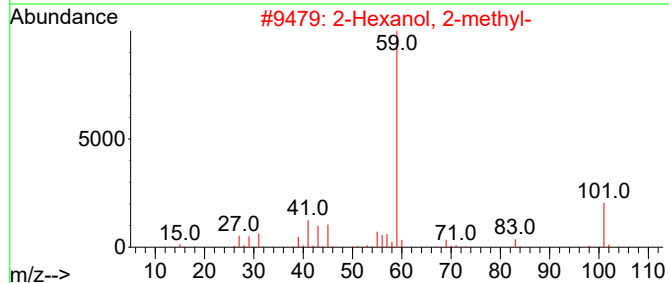
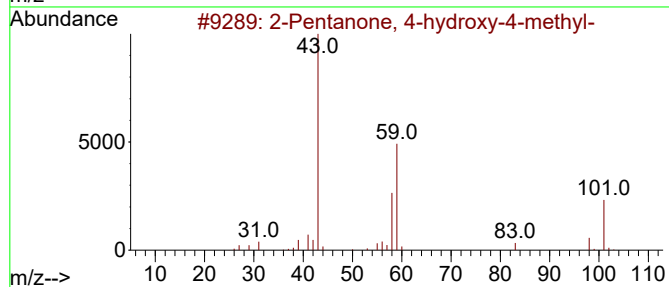
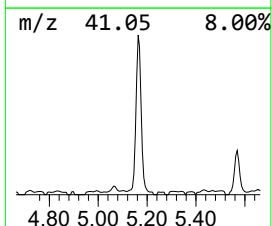
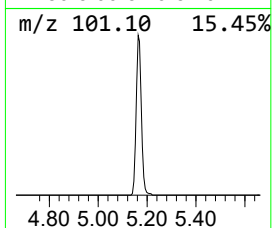
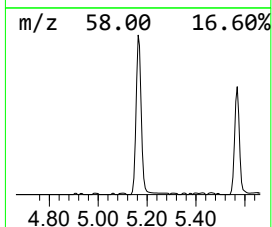
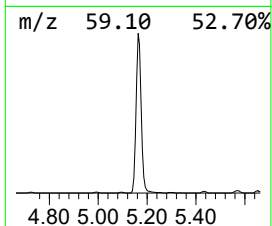
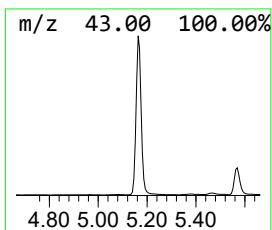
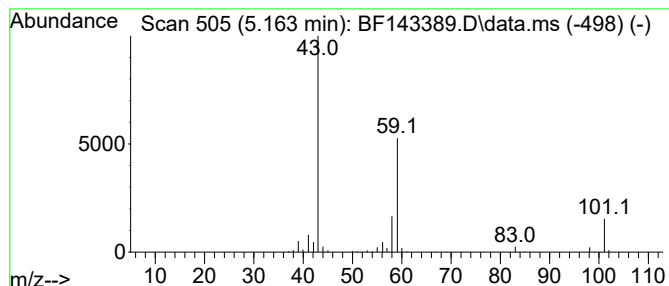
Instrument :
BNA_F
ClientSampleId :
TW-38M-S

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081225.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 2

R.T.	EstConc	Area	Relative to ISTD			R.T.
5.163	9.53 ng	424661	1,4-Dichlorobenzene-d4			6.934
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	64
2	2-Hexanol, 2-methyl-		116	C7H16O	000625-23-0	33
3	3-Hexanol, 4-methyl-		116	C7H16O	000615-29-2	33
4	Acetic acid, cyano-, 1,1-dimethy...		141	C7H11NO2	001116-98-9	25
5	1-Propen-2-ol, acetate		100	C5H8O2	000108-22-5	12



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081425\
Data File : BF143389.D
Acq On : 14 Aug 2025 18:56
Operator : RC/JU
Sample : Q2814-11
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TW-38M-S

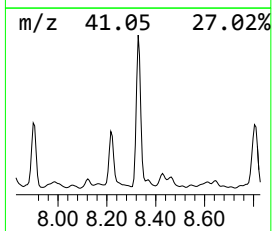
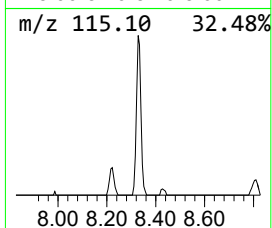
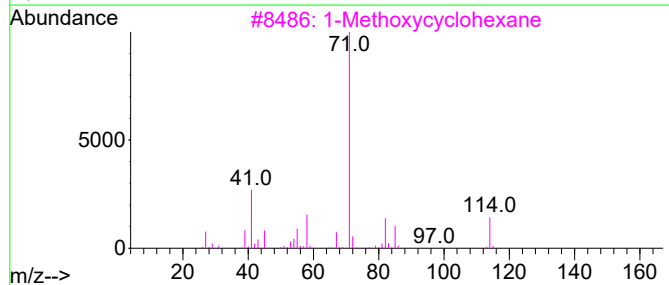
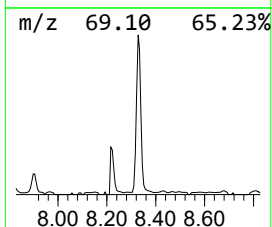
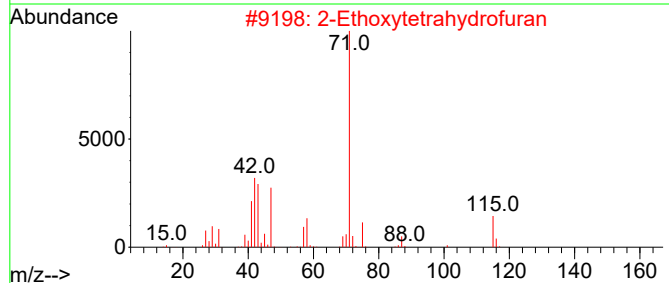
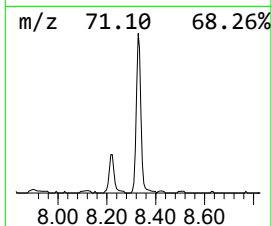
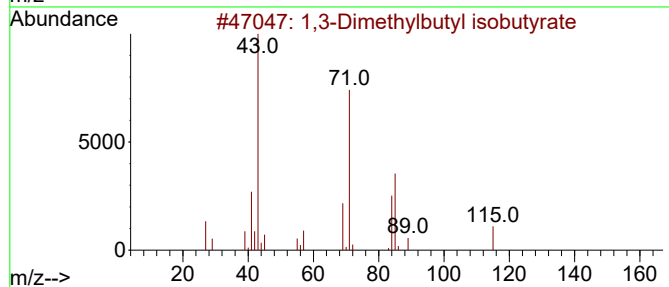
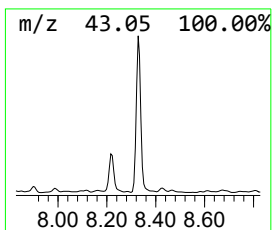
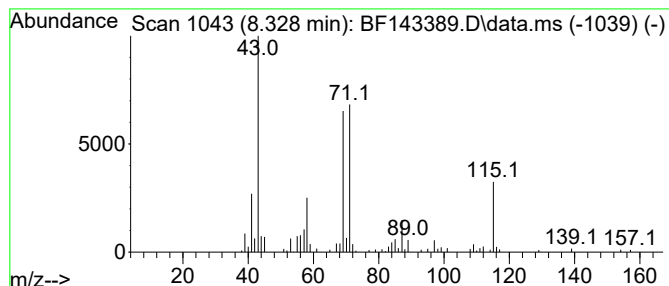
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081225.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown8.328 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.328	2.29 ng	141613	Naphthalene-d8	8.210

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,3-Dimethylbutyl isobutyrate	172	C10H20O2	1000429-31-6	35
2		2-Ethoxytetrahydrofuran	116	C6H12O2	013436-46-9	35
3		1-Methoxycyclohexane	114	C7H14O	000931-56-6	35
4		3,3-Dimethyl-2,4-pentane dione	128	C7H12O2	003142-58-3	35
5		trans-2,3-Epoxydecane	156	C10H20O	054125-39-2	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081425\
Data File : BF143389.D
Acq On : 14 Aug 2025 18:56
Operator : RC/JU
Sample : Q2814-11
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TW-38M-S

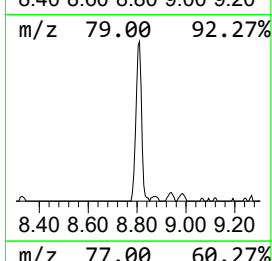
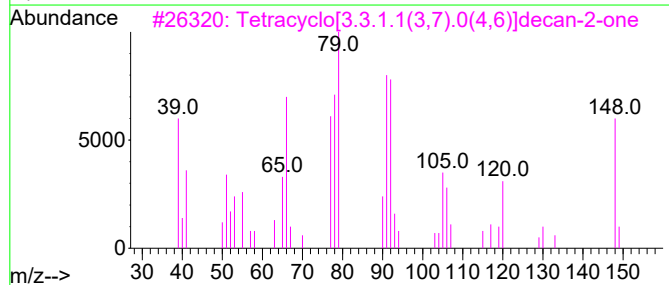
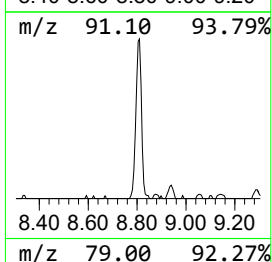
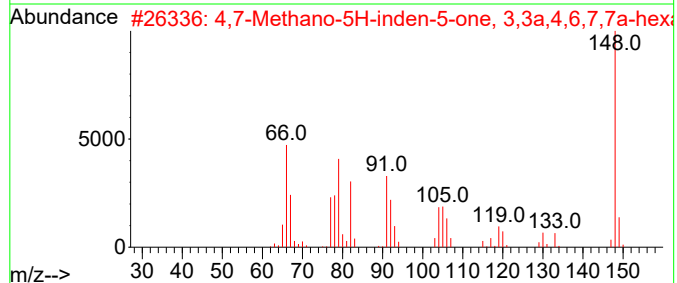
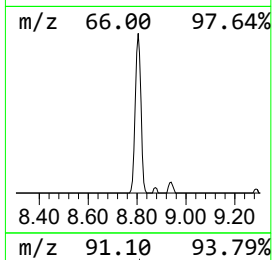
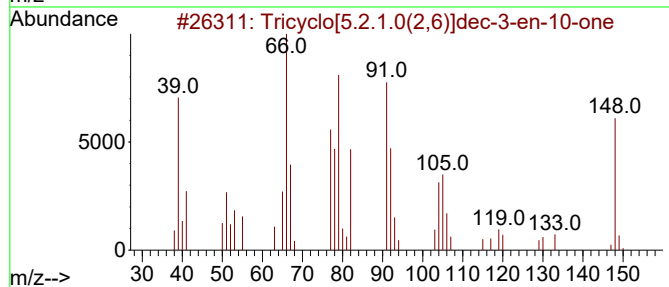
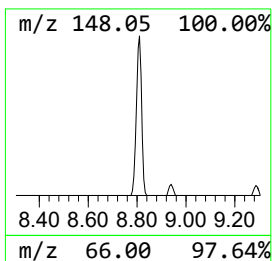
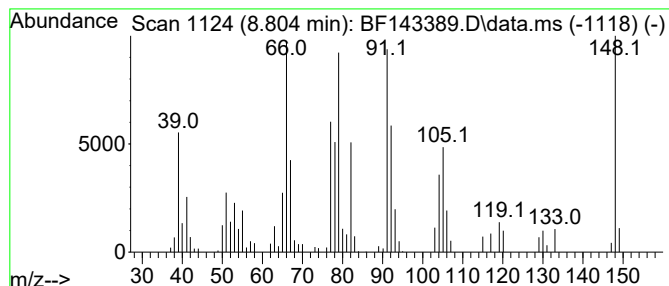
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081225.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Tricyclo[5.2.1.0(2,6)]dec-3... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.804	2.84 ng	176128	Naphthalene-d8	8.210

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tricyclo[5.2.1.0(2,6)]dec-3-en-1...	148	C10H12O	1000289-10-5	98
2			4,7-Methano-5H-inden-5-one, 3,3a...	148	C10H12O	014888-58-5	97
3			Tetracyclo[3.3.1.1(3,7).0(4,6)]d...	148	C10H12O	052750-53-5	72
4			1H-Indene, 3a,4,7,7a-tetrahydro-	120	C9H12	003048-65-5	50
5			1H-Indene, 3a,4,7,7a-tetrahydro-...	120	C9H12	066563-20-0	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081425\
Data File : BF143389.D
Acq On : 14 Aug 2025 18:56
Operator : RC/JU
Sample : Q2814-11
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TW-38M-S

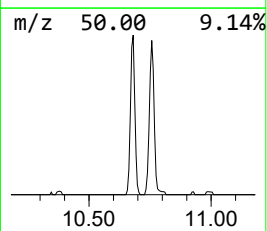
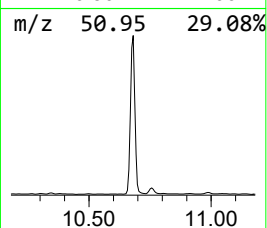
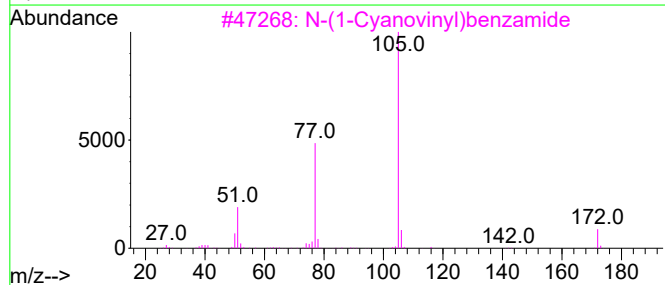
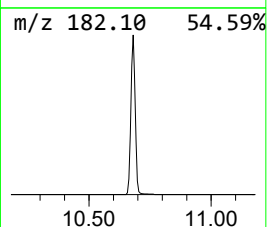
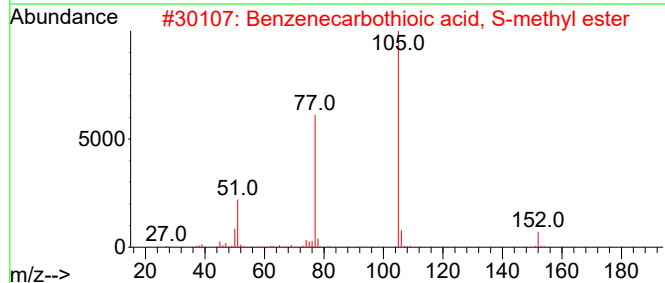
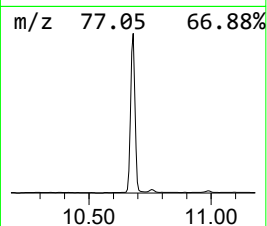
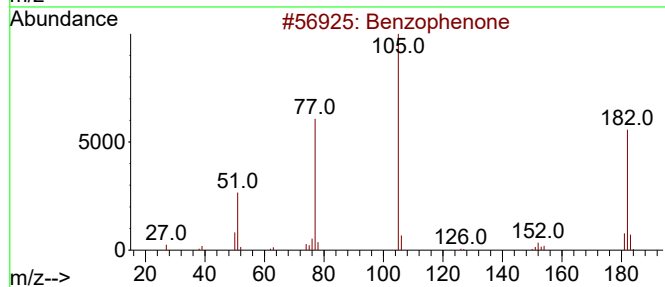
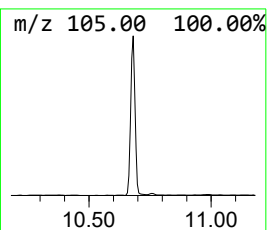
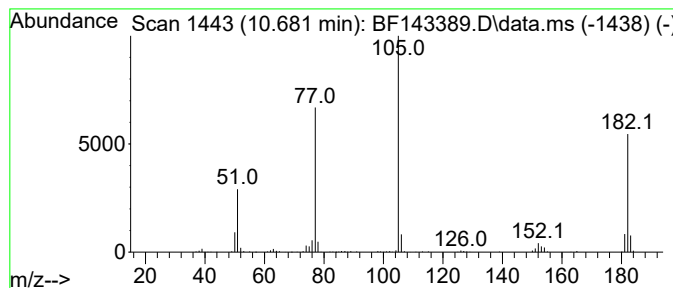
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081225.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.681	6.70 ng	443199	Acenaphthene-d10	9.969

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	52
3			N-(1-Cyanovinyl)benzamide	172	C10H8N2O	1000186-19-1	50
4			Benzenecarbothioic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	50
5			Benzoic acid, phenyl ester	198	C13H10O2	000093-99-2	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081425\
Data File : BF143389.D
Acq On : 14 Aug 2025 18:56
Operator : RC/JU
Sample : Q2814-11
Misc :
ALS Vial : 14 Sample Multiplier: 1

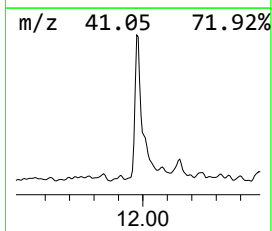
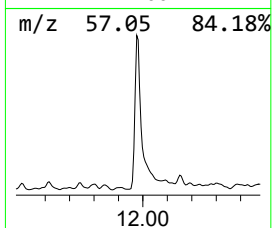
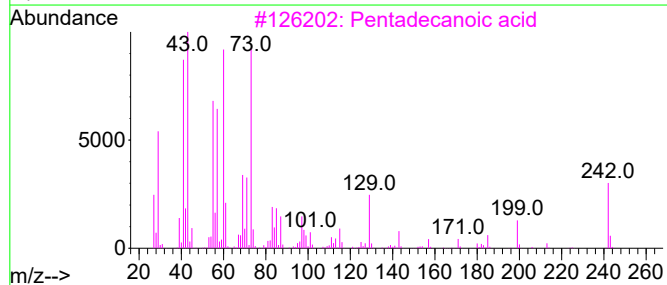
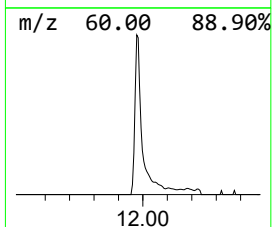
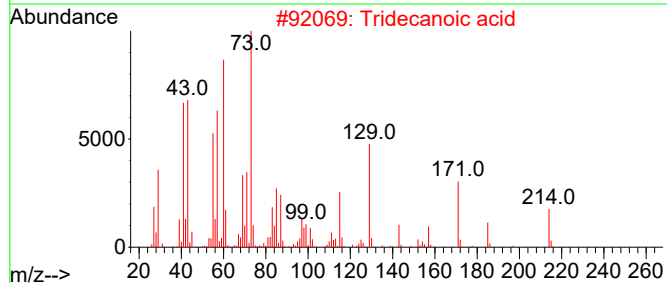
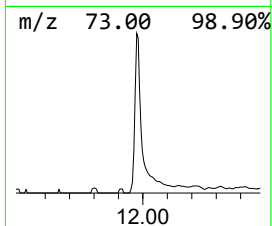
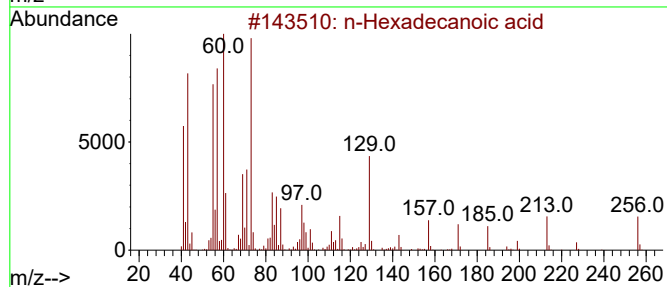
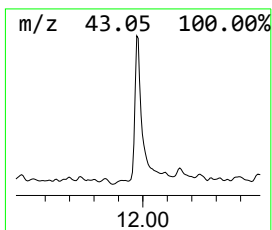
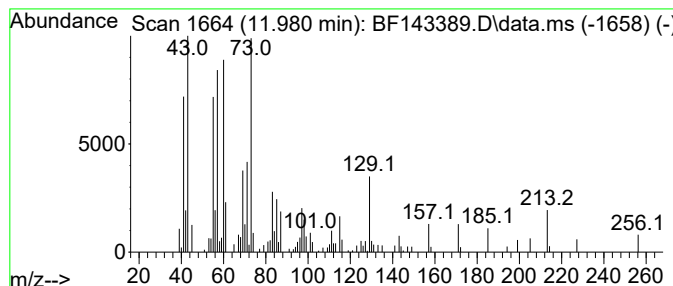
Instrument :
BNA_F
ClientSampleId :
TW-38M-S

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081225.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.980	2.75 ng	167391	Phenanthrene-d10	11.457	
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	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Oxalic acid, dodecyl propyl ester	300	C17H32O4	1000309-26-5	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081425\
Data File : BF143389.D
Acq On : 14 Aug 2025 18:56
Operator : RC/JU
Sample : Q2814-11
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TW-38M-S

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081225.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
Butane, 2-metho...	2.269	101.0	ng	4501210	1	6.934	891255	20.0
2-Pentanone, 4-...	5.163	9.5	ng	424661	1	6.934	891255	20.0
unknown8.328	8.328	2.3	ng	141613	2	8.210	1238180	20.0
Tricyclo[5.2.1....	8.804	2.8	ng	176128	2	8.210	1238180	20.0
Benzophenone	10.681	6.7	ng	443199	3	9.969	1323440	20.0
n-Hexadecanoic ...	11.980	2.8	ng	167391	4	11.457	1217300	20.0