

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070325\
 Data File : BF142999.D
 Acq On : 03 Jul 2025 16:29
 Operator : RC/JU
 Sample : Q2463-01
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TW-WTS-11

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-BF061925.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF142999.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.969	282	302	305	rBV2	12139	45526	2.11%	0.293%
2	4.816	375	446	454	rBV	91632	1026661	47.52%	6.598%
3	5.099	486	494	504	rBV	61347	93709	4.34%	0.602%
4	5.369	504	540	545	rBV4	97790	644294	29.82%	4.141%
5	5.498	556	562	567	rBV	693846	972731	45.02%	6.251%
6	5.798	595	613	618	rVB2	70807	307774	14.25%	1.978%
7	6.104	650	665	675	rBV4	14159	57508	2.66%	0.370%
8	6.228	675	686	690	rVV2	17798	42297	1.96%	0.272%
9	6.504	728	733	760	rBV2	464057	742162	34.35%	4.770%
10	6.734	760	772	780	rVB5	14377	40516	1.88%	0.260%
11	6.875	790	796	801	rBV	329500	415994	19.25%	2.673%
12	6.940	802	807	811	rVV	25617	40640	1.88%	0.261%
13	6.981	811	814	817	rVV	23611	30548	1.41%	0.196%
14	7.022	817	821	824	rVV	20027	31049	1.44%	0.200%
15	7.440	882	892	896	rBV	802232	1131045	52.35%	7.269%
16	7.551	904	911	917	rBV	44557	76680	3.55%	0.493%
17	7.904	964	971	988	rBV3	58475	118791	5.50%	0.763%
18	8.057	993	997	1007	rVB	26733	39299	1.82%	0.253%
19	8.157	1007	1014	1022	rBV	438858	579306	26.81%	3.723%
20	8.316	1033	1041	1048	rBV	12667	22895	1.06%	0.147%
21	8.416	1053	1058	1069	rBV2	42267	97905	4.53%	0.629%
22	8.587	1080	1087	1093	rVB5	9934	22139	1.02%	0.142%
23	8.669	1093	1101	1111	rBV	57487	158006	7.31%	1.015%
24	8.769	1111	1118	1119	rBV	100539	131678	6.09%	0.846%
25	8.792	1119	1122	1129	rVB2	120967	170796	7.91%	1.098%
26	8.857	1129	1133	1140	rBV2	31938	66050	3.06%	0.424%
27	9.069	1165	1169	1173	rBV	19340	25866	1.20%	0.166%
28	9.234	1191	1197	1202	rBV	1703101	2160466	100.00%	13.884%
29	9.375	1217	1221	1232	rVB	65121	93524	4.33%	0.601%
30	9.833	1292	1299	1304	rVB2	32859	46723	2.16%	0.300%
31	9.910	1307	1312	1317	rBV	468011	593736	27.48%	3.816%
32	10.304	1367	1379	1382	rBV3	22411	50361	2.33%	0.324%
33	10.628	1428	1434	1438	rBV	63340	83050	3.84%	0.534%
34	10.704	1442	1447	1457	rVV	908588	1160963	53.74%	7.461%
35	10.810	1461	1465	1474	rVB2	35056	50028	2.32%	0.322%
36	11.122	1512	1518	1534	rBV	16020	45658	2.11%	0.293%

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070325\
Data File : BF142999.D
Acq On : 03 Jul 2025 16:29
Operator : RC/JU
Sample : Q2463-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TW-WTS-11

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-BF061925.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	11.404	1560	1566	1577	rBV	420886	547787	25.36%	3.520%
38	11.927	1649	1655	1668	rBV	402967	666319	30.84%	4.282%
39	12.627	1768	1774	1778	rBV4	14275	33260	1.54%	0.214%
40	12.716	1783	1789	1802	rBV	234284	385057	17.82%	2.475%
41	12.874	1813	1816	1822	rVB	17973	25545	1.18%	0.164%
42	12.986	1830	1835	1841	rBV	1061891	1390958	64.38%	8.939%
43	13.216	1869	1874	1880	rVB4	18098	29320	1.36%	0.188%
44	13.886	1983	1988	2004	rVB3	30545	62273	2.88%	0.400%
45	14.051	2007	2016	2025	rBV	259010	354050	16.39%	2.275%
46	14.892	2154	2159	2168	rBV	119312	169744	7.86%	1.091%
47	15.545	2263	2270	2279	rVB	306944	479827	22.21%	3.084%

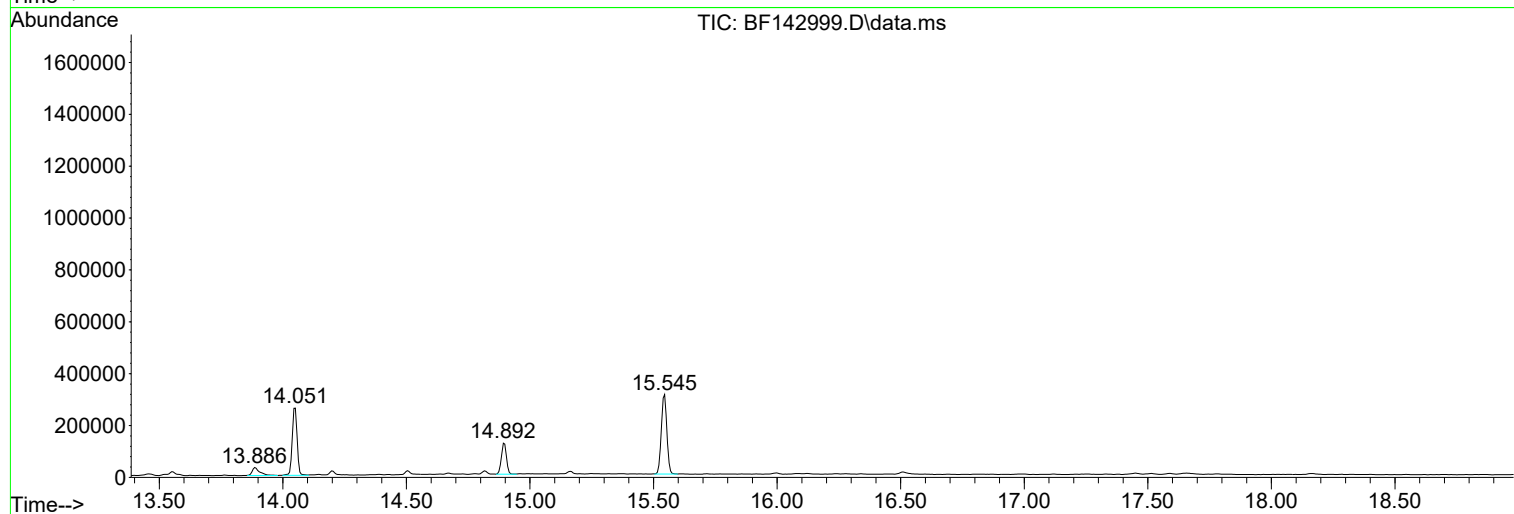
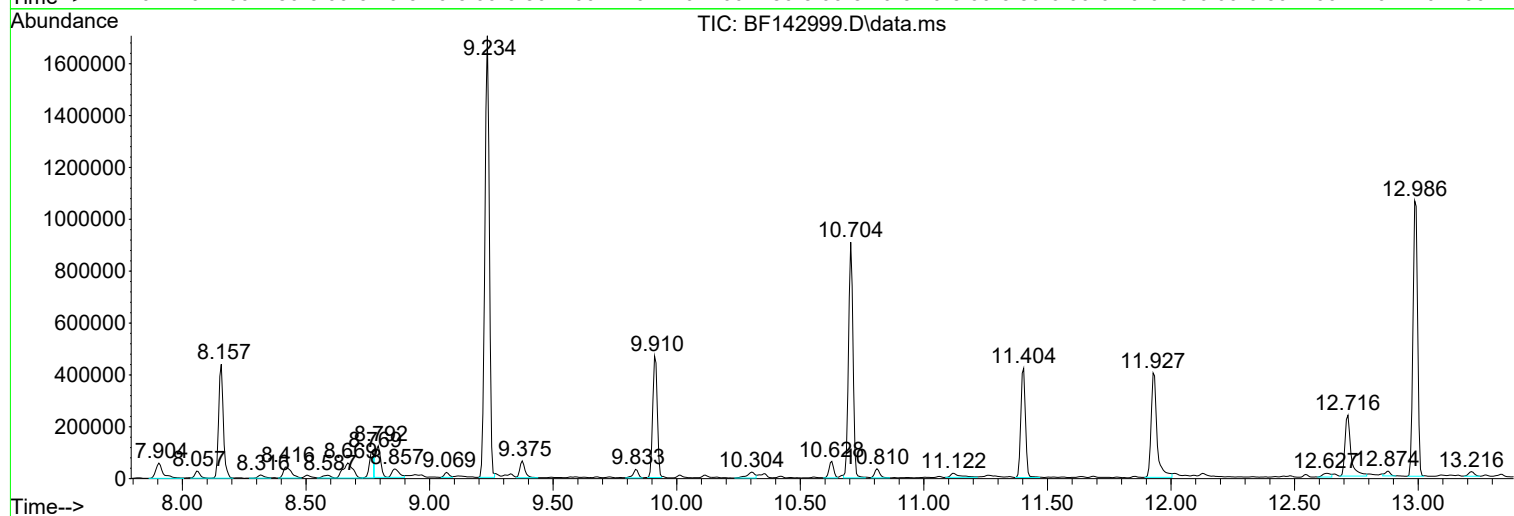
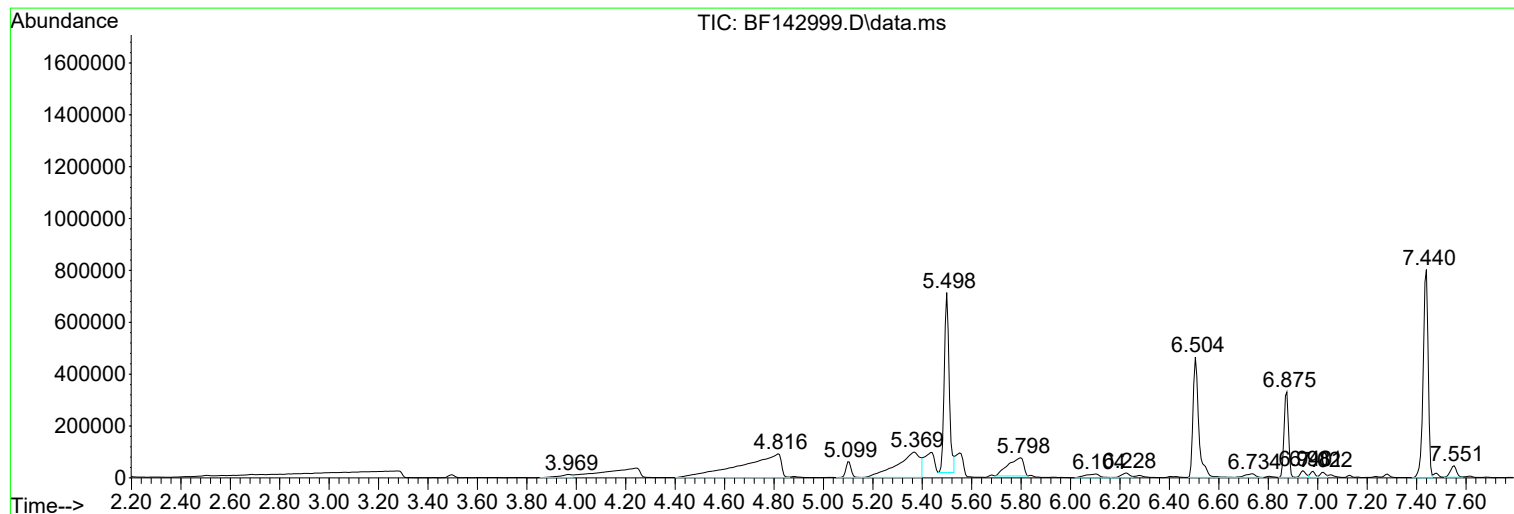
Sum of corrected areas: 15560514

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070325\
Data File : BF142999.D
Acq On : 03 Jul 2025 16:29
Operator : RC/JU
Sample : Q2463-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TW-WTS-11

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061925.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\BF070325\
Data File : BF142999.D
Acq On : 03 Jul 2025 16:29
Operator : RC/JU
Sample : Q2463-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TW-WTS-11

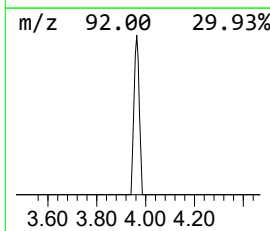
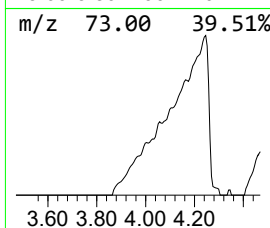
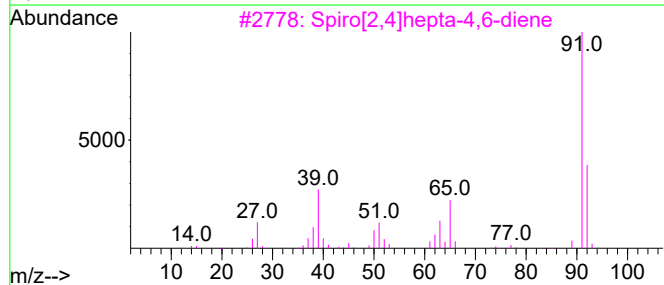
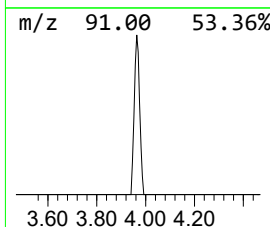
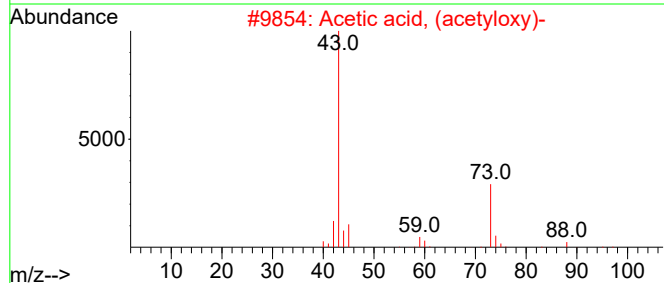
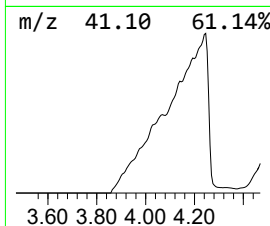
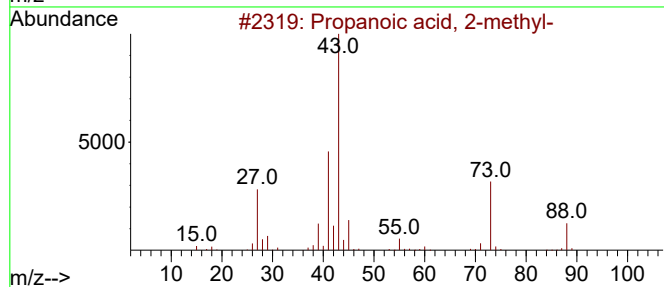
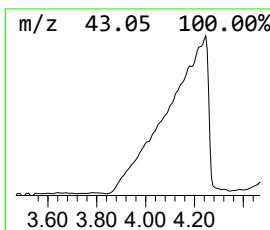
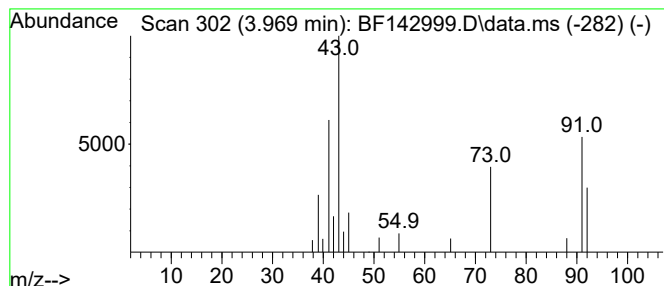
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061925.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propanoic acid, 2-methyl- Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.969	2.19 ng	45526	1,4-Dichlorobenzene-d4	6.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2-methyl-	88	C4H8O2	000079-31-2	50
2			Acetic acid, (acetyloxy)-	118	C4H6O4	013831-30-6	12
3			Spiro[2,4]hepta-4,6-diene	92	C7H8	000765-46-8	9
4			Propane, 2-(methylthio)-	90	C4H10S	001551-21-9	9
5			2-Propenoic acid, 2-methyl-, 2-a...	129	C6H11NO2	002420-94-2	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070325\
Data File : BF142999.D
Acq On : 03 Jul 2025 16:29
Operator : RC/JU
Sample : Q2463-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TW-WTS-11

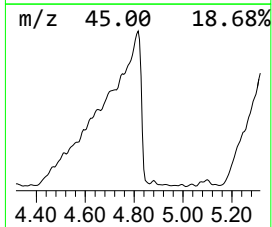
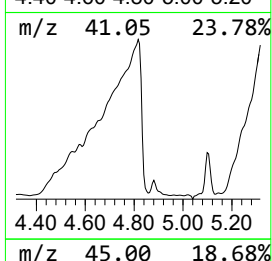
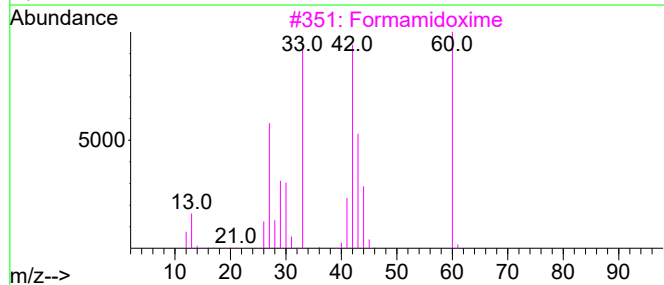
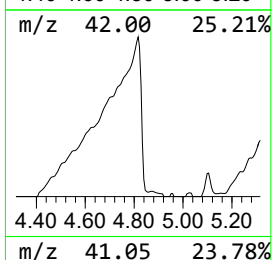
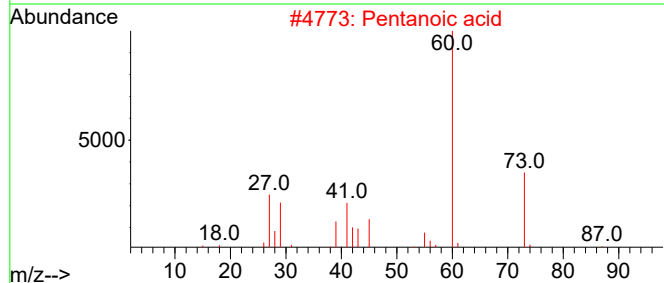
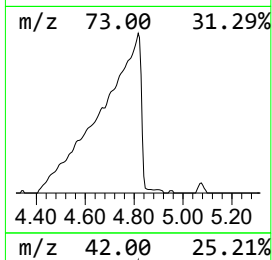
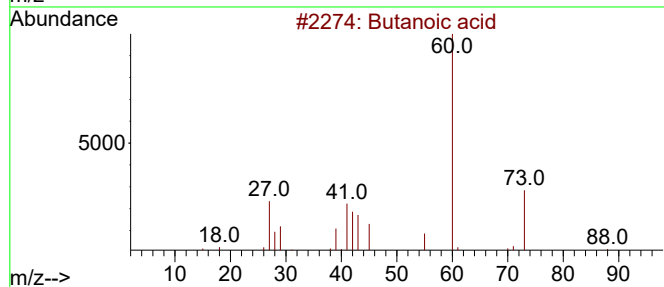
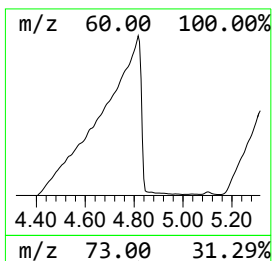
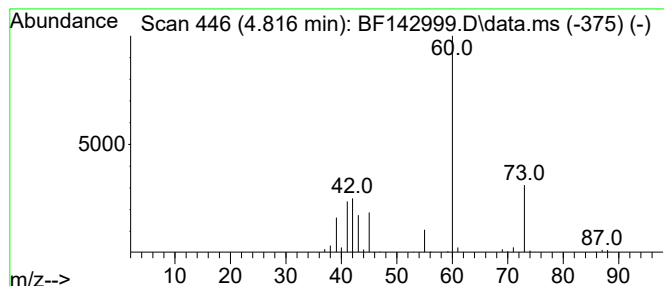
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061925.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Butanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.816	49.36 ng	1026660	1,4-Dichlorobenzene-d4	6.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid	88	C4H8O2	000107-92-6	91
2			Pentanoic acid	102	C5H10O2	000109-52-4	39
3			Formamidoxime	60	CH4N2O	000624-82-8	9
4			Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	9
5			4-Bromobutyric acid	166	C4H7BrO2	002623-87-2	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070325\
Data File : BF142999.D
Acq On : 03 Jul 2025 16:29
Operator : RC/JU
Sample : Q2463-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TW-WTS-11

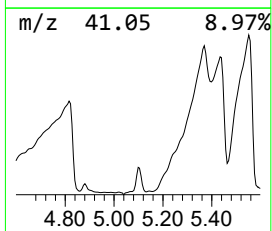
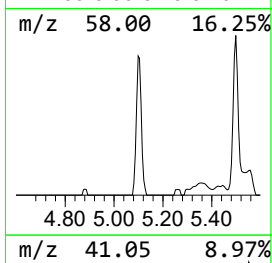
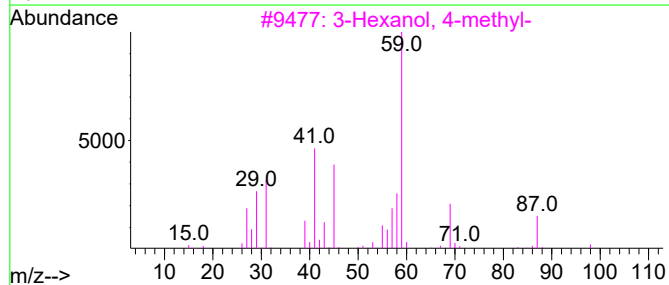
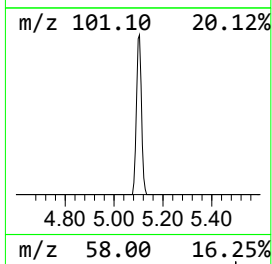
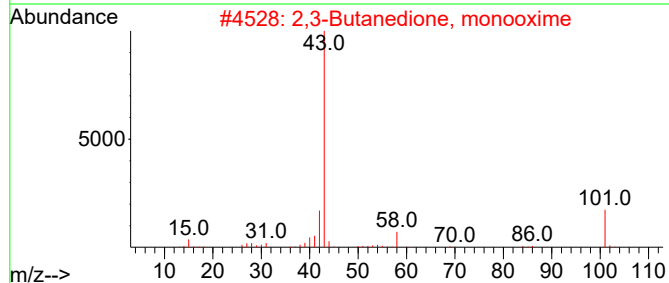
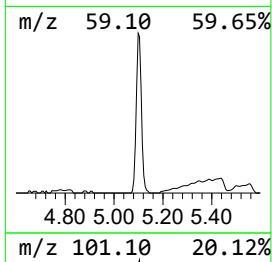
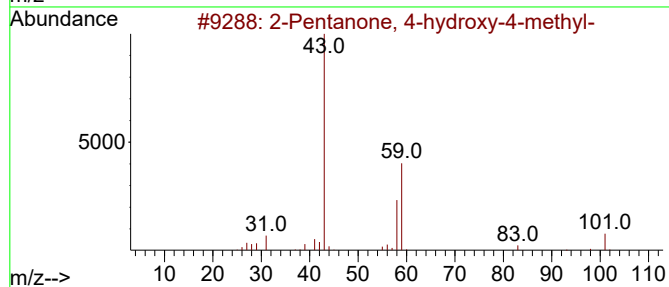
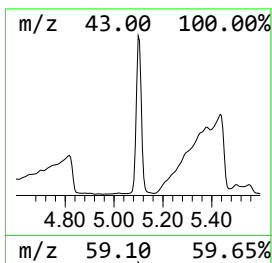
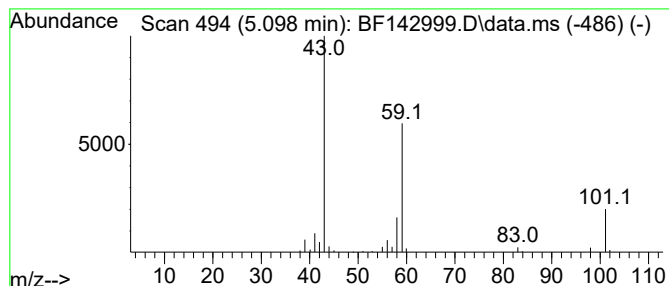
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061925.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.098	4.51 ng	93709	1,4-Dichlorobenzene-d4	6.875

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56	
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35	
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28	
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23	
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10	



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070325\
Data File : BF142999.D
Acq On : 03 Jul 2025 16:29
Operator : RC/JU
Sample : Q2463-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TW-WTS-11

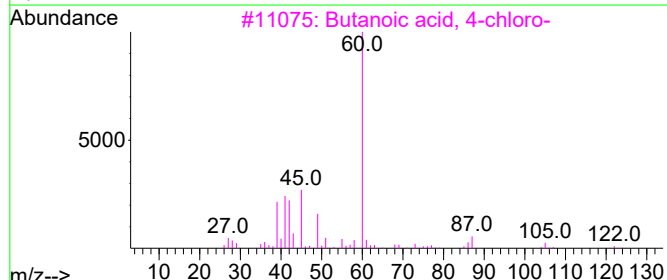
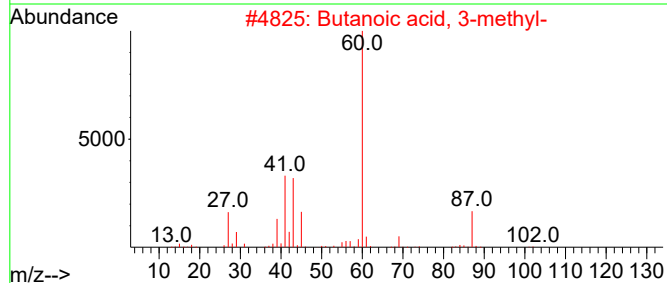
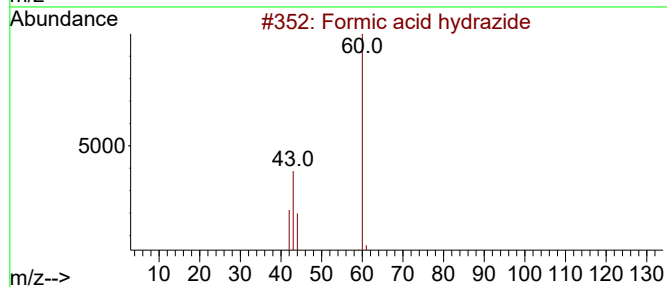
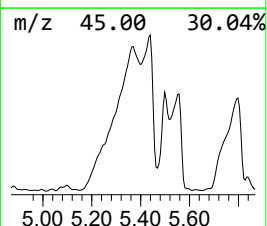
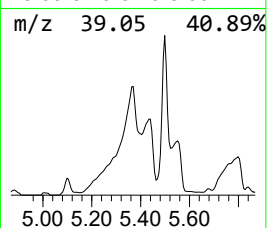
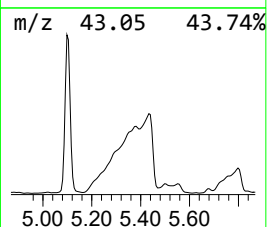
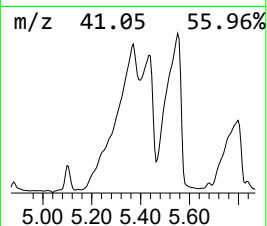
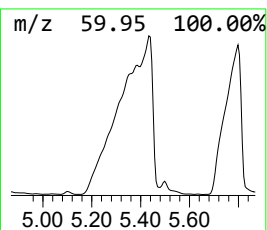
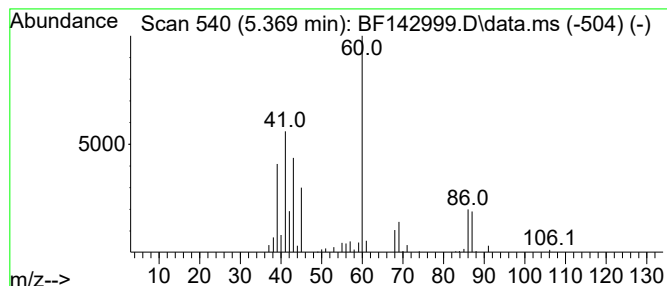
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061925.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 unknown5.369 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.369	30.98 ng	644294	1,4-Dichlorobenzene-d4	6.875

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Formic acid hydrazide	60	CH4N2O	000624-84-0	47
2		Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	43
3		Butanoic acid, 4-chloro-	122	C4H7ClO2	000627-00-9	38
4		1,2-Hydrazinedicarboxaldehyde	88	C2H4N2O2	000628-36-4	28
5		3-Butenoic acid	86	C4H6O2	000625-38-7	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070325\
Data File : BF142999.D
Acq On : 03 Jul 2025 16:29
Operator : RC/JU
Sample : Q2463-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TW-WTS-11

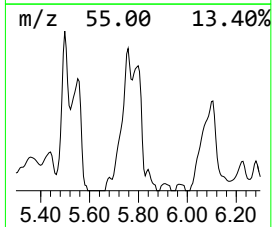
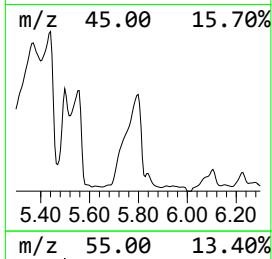
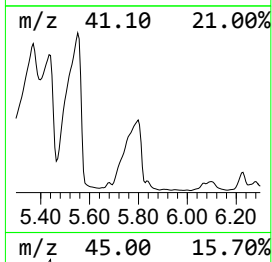
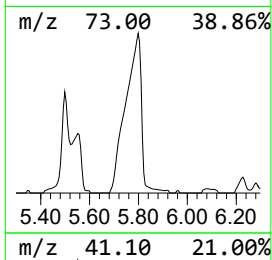
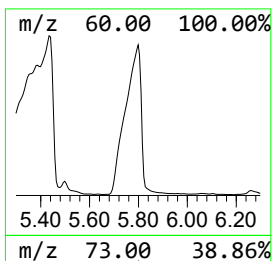
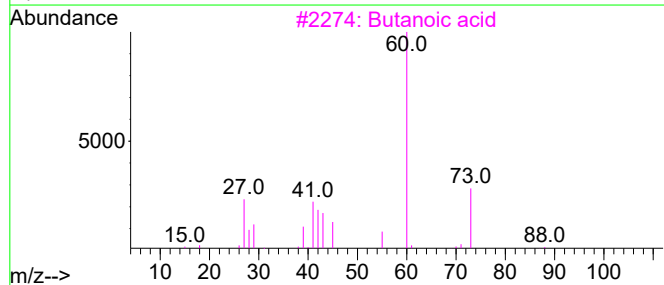
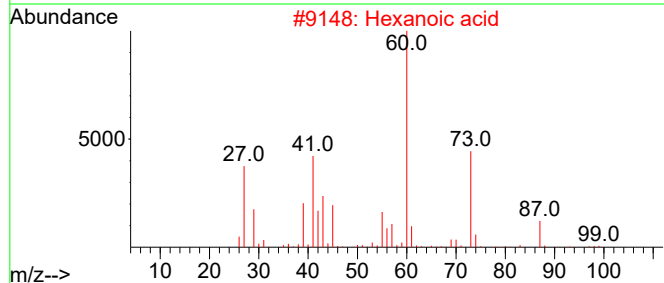
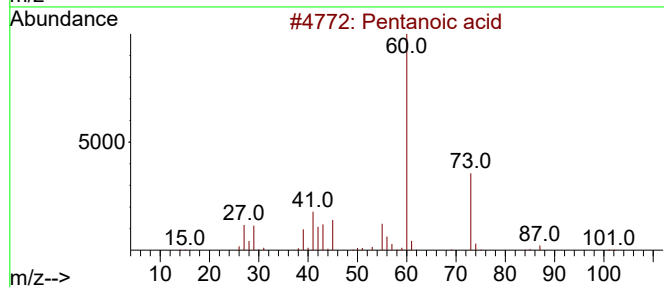
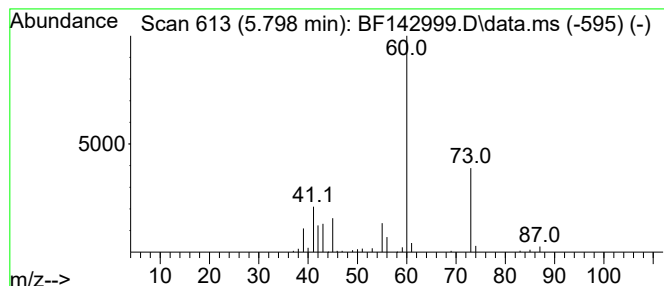
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061925.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Pentanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.798	14.80 ng	307774	1,4-Dichlorobenzene-d4	6.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentanoic acid	102	C5H10O2	000109-52-4	90
2			Hexanoic acid	116	C6H12O2	000142-62-1	64
3			Butanoic acid	88	C4H8O2	000107-92-6	64
4			Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	40
5			.beta.-Methyl xyloside	164	C6H12O5	007473-45-2	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070325\
Data File : BF142999.D
Acq On : 03 Jul 2025 16:29
Operator : RC/JU
Sample : Q2463-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TW-WTS-11

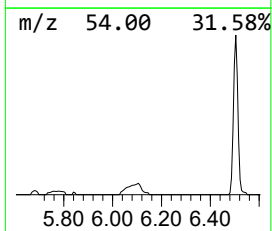
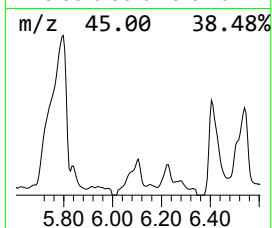
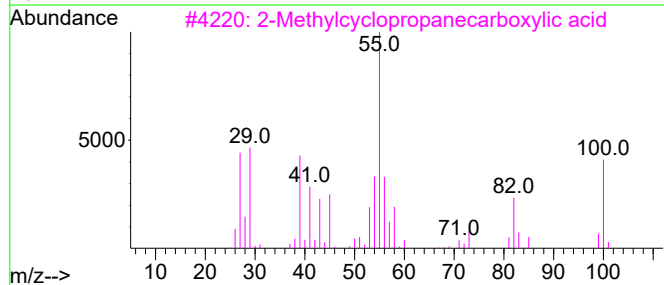
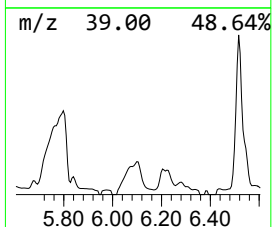
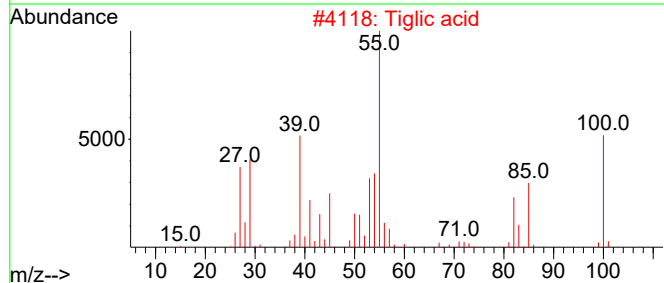
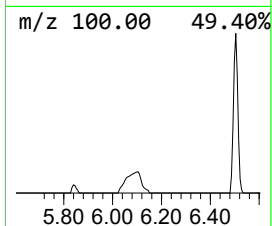
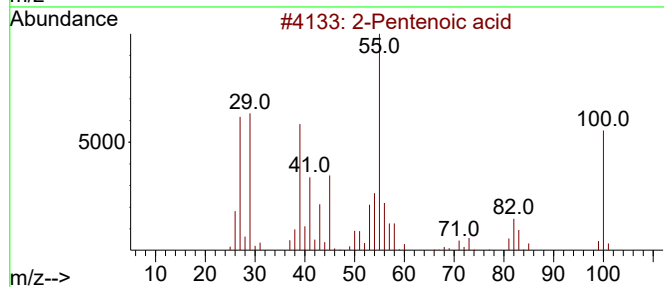
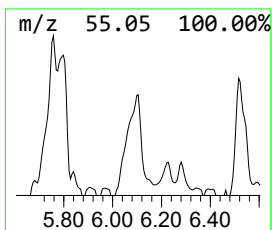
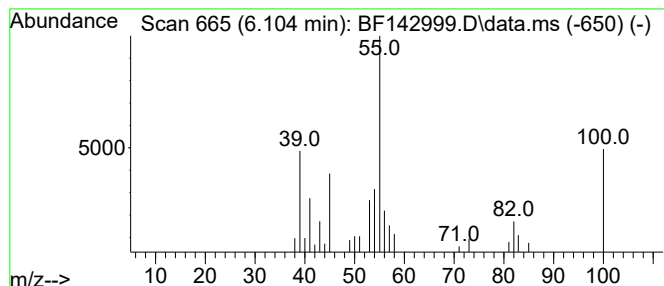
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061925.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 2-Pentenoic acid Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.104	2.76 ng	57508	1,4-Dichlorobenzene-d4	6.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentenoic acid	100	C5H8O2	000626-98-2	94
2			Tiglic acid	100	C5H8O2	000080-59-1	70
3			2-Methylcyclopropanecarboxylic acid	100	C5H8O2	029555-02-0	58
4			4-Pentenoic acid	100	C5H8O2	000591-80-0	38
5			2-Butenoic acid, 4-oxo-	100	C4H4O3	022418-77-5	37



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070325\
Data File : BF142999.D
Acq On : 03 Jul 2025 16:29
Operator : RC/JU
Sample : Q2463-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TW-WTS-11

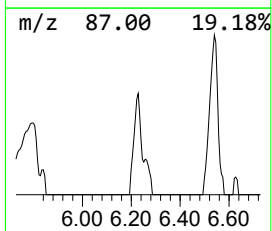
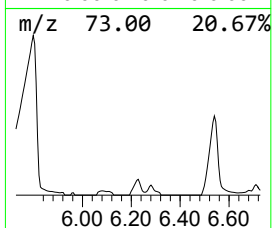
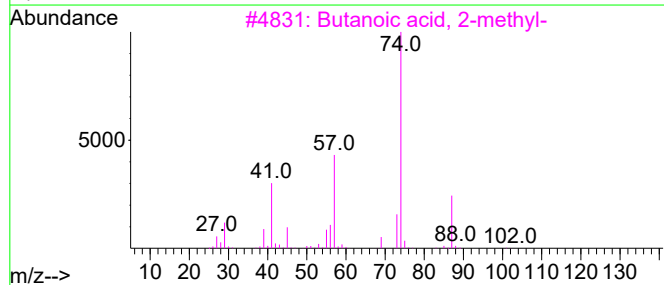
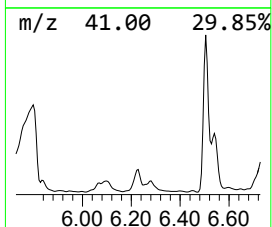
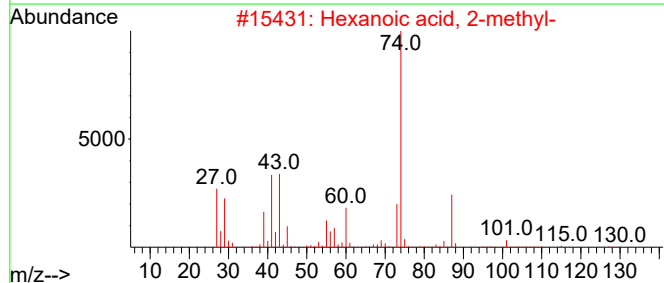
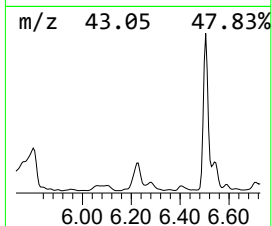
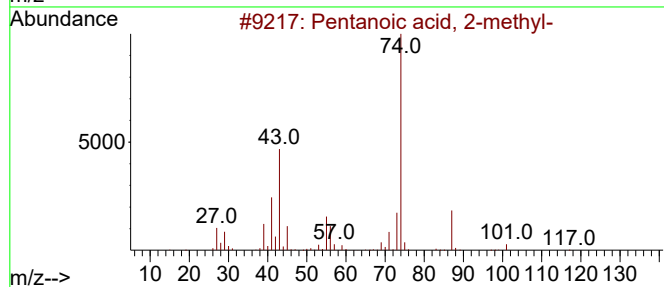
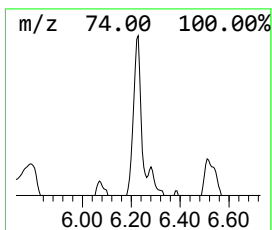
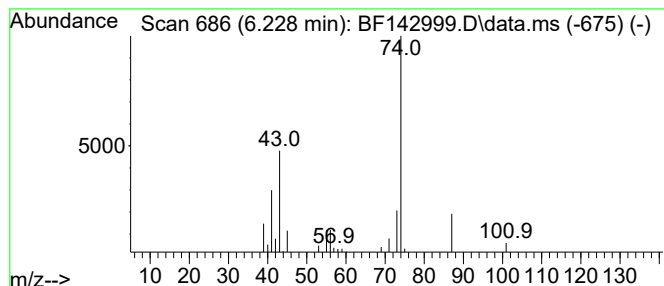
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061925.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Pentanoic acid, 2-methyl- Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.228	2.03 ng	42297	1,4-Dichlorobenzene-d4	6.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentanoic acid, 2-methyl-	116	C6H12O2	000097-61-0	83
2			Hexanoic acid, 2-methyl-	130	C7H14O2	004536-23-6	78
3			Butanoic acid, 2-methyl-	102	C5H10O2	000116-53-0	72
4			2-Methylheptanoic acid	144	C8H16O2	001188-02-9	45
5			Hexanoic acid, methyl ester	130	C7H14O2	000106-70-7	40



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070325\
Data File : BF142999.D
Acq On : 03 Jul 2025 16:29
Operator : RC/JU
Sample : Q2463-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TW-WTS-11

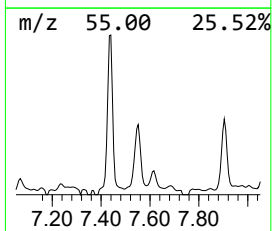
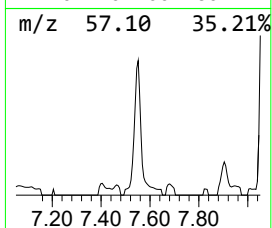
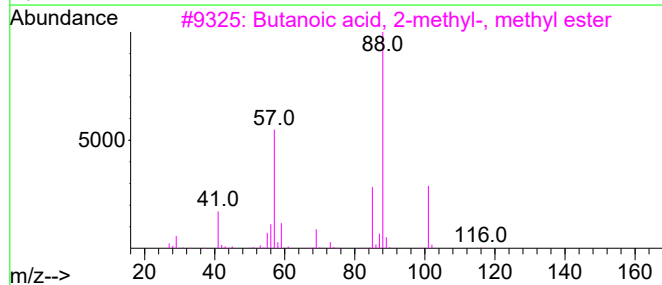
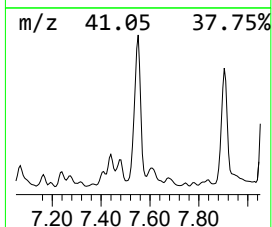
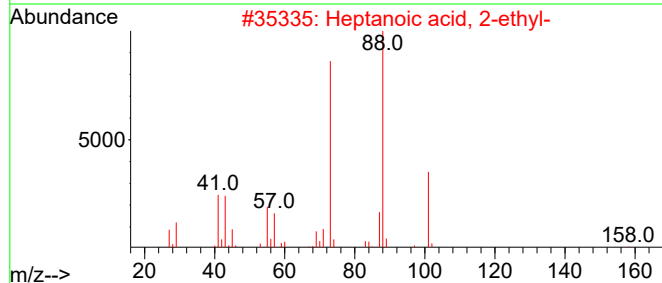
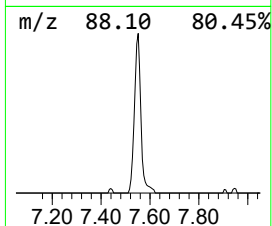
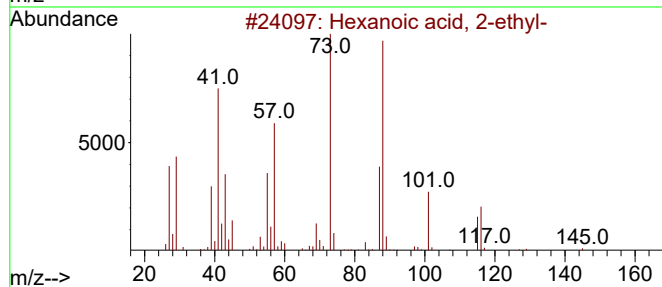
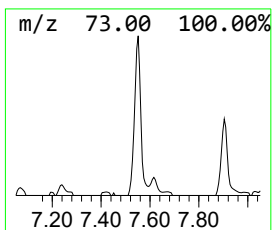
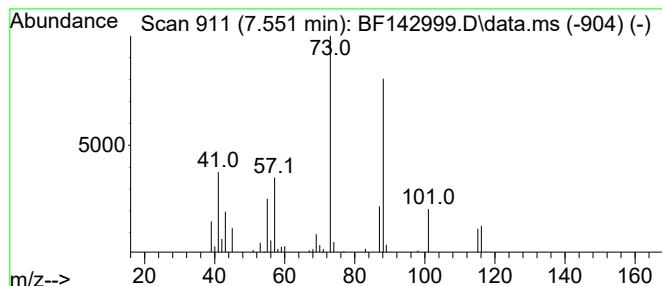
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061925.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexanoic acid, 2-ethyl- Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.551	2.65 ng	76680	Naphthalene-d8	8.157

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
2			Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	53
3			Butanoic acid, 2-methyl-, methyl...	116	C6H12O2	000868-57-5	50
4			2-Ethyl-4-methylpentanoic acid	144	C8H16O2	000108-81-6	45
5			Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	42



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070325\
Data File : BF142999.D
Acq On : 03 Jul 2025 16:29
Operator : RC/JU
Sample : Q2463-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TW-WTS-11

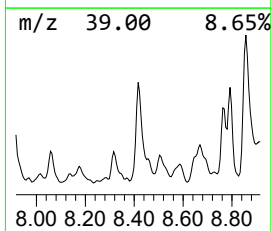
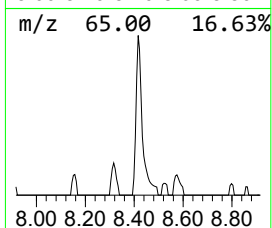
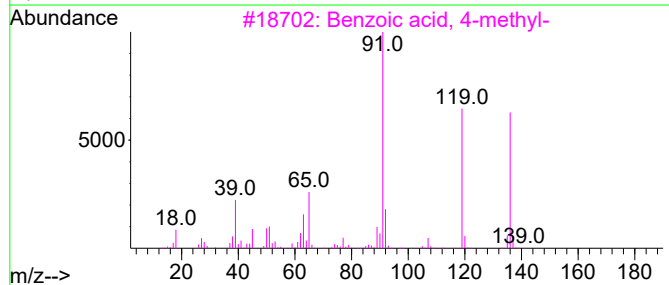
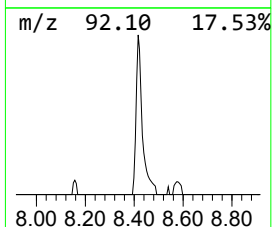
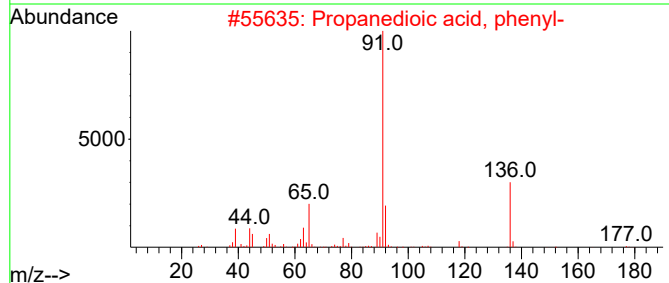
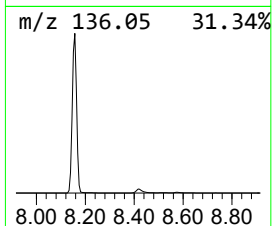
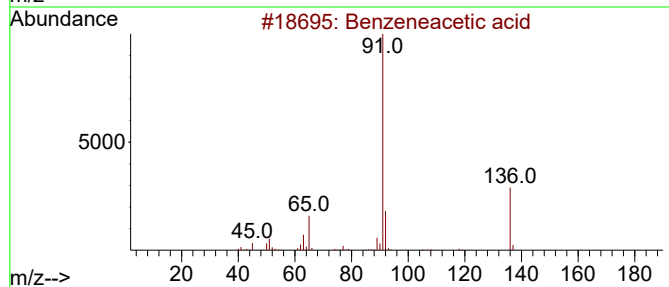
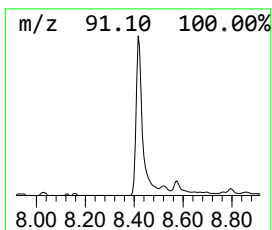
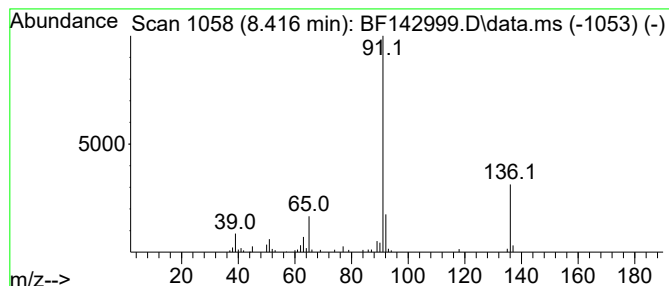
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061925.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Benzeneacetic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.416	3.38 ng	97905	Naphthalene-d8	8.157

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzeneacetic acid	136	C8H8O2	000103-82-2	93
2			Propanedioic acid, phenyl-	180	C9H8O4	002613-89-0	78
3			Benzoic acid, 4-methyl-	136	C8H8O2	000099-94-5	64
4			Benzene, (2-methoxyethyl)-	136	C9H12O	003558-60-9	59
5			3-Oxo-4-phenylbutyronitrile	159	C10H9NO	019212-27-2	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070325\
Data File : BF142999.D
Acq On : 03 Jul 2025 16:29
Operator : RC/JU
Sample : Q2463-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TW-WTS-11

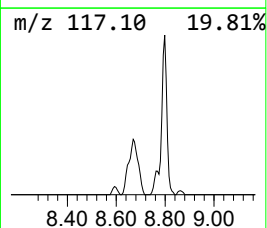
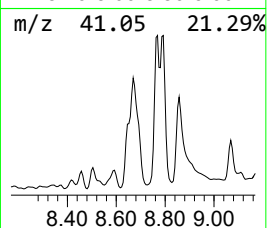
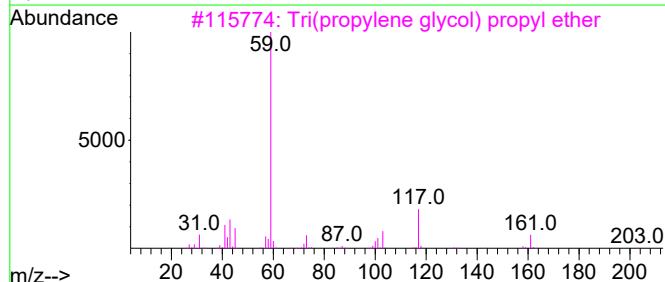
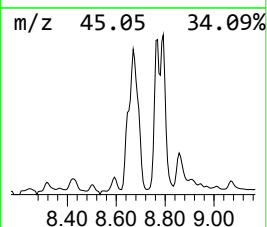
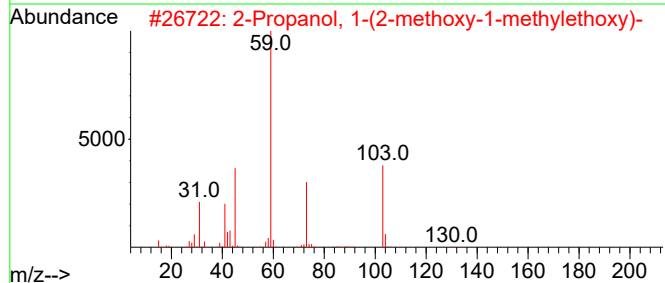
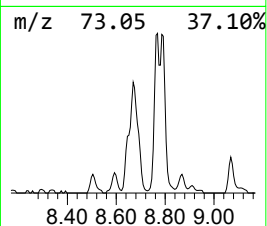
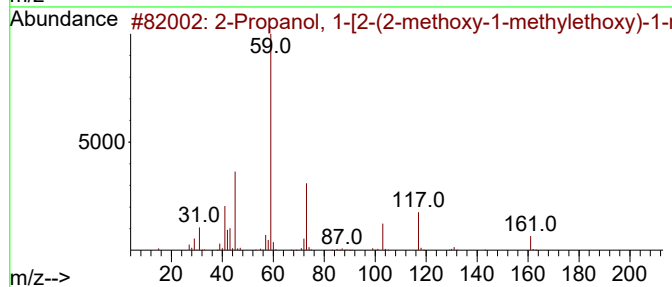
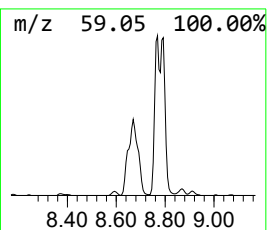
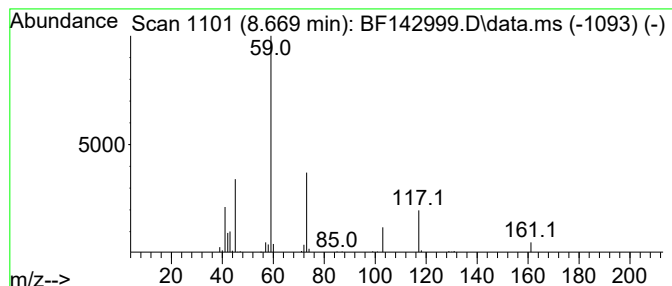
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061925.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 2-Propanol, 1-[2-(2-methoxy... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.669	5.46 ng	158006	Naphthalene-d8	8.157

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-[2-(2-methoxy-1-me...	206	C10H22O4	020324-33-8	90		
2	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	64		
3	Tri(propylene glycol) propyl ether	234	C12H26O4	096077-04-2	59		
4	Hydrazine, 1,1-dimethyl-2-pentyl-	130	C7H18N2	067398-36-1	52		
5	Dipropylene glycol (isomer 3)	134	C6H14O3	1000506-25-5	50		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070325\
Data File : BF142999.D
Acq On : 03 Jul 2025 16:29
Operator : RC/JU
Sample : Q2463-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TW-WTS-11

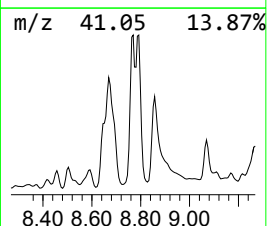
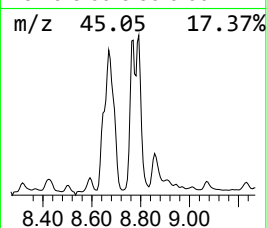
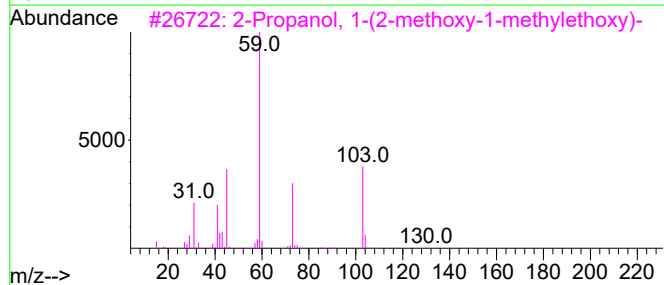
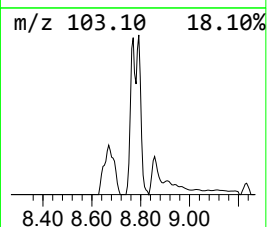
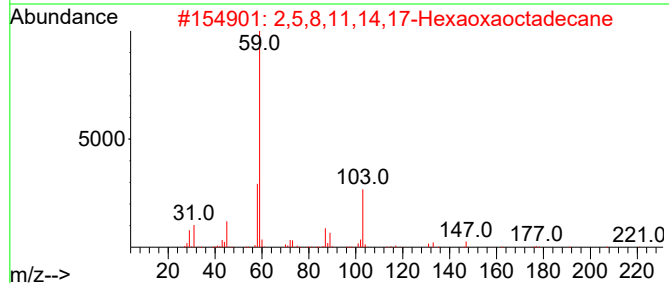
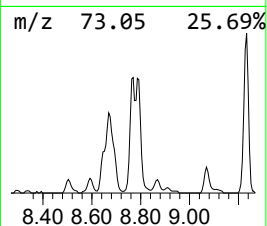
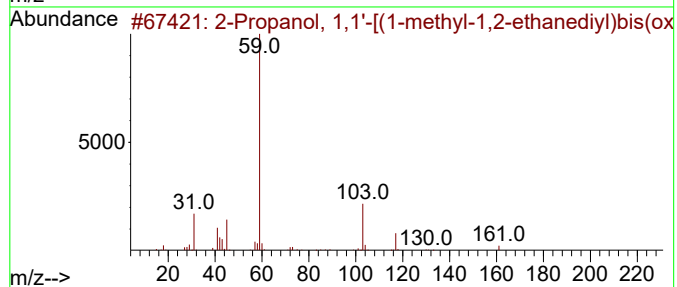
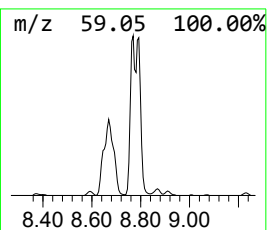
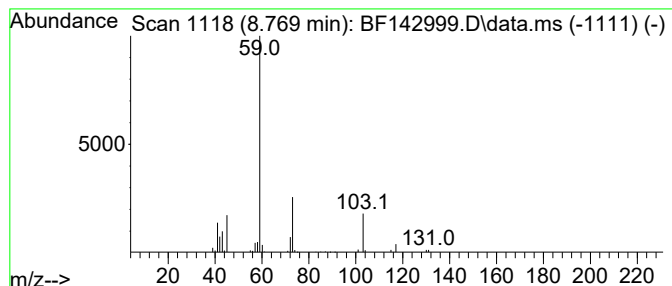
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061925.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 2-Propanol, 1,1'-[(1-methyl... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.769	4.55 ng	131678	Naphthalene-d8	8.157

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol,	1,1'-[(1-methyl-1,2-...	192	C9H20O4	001638-16-0	64
2	2,5,8,11,14,17-Hexaoxa	octadecane	266	C12H26O6	001191-87-3	64
3	2-Propanol,	1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	64
4	1,4,7-Trimethyl-3,6-dioxa	octane-...	192	C9H20O4	1000423-63-2	59
5	1-Propanol,	2,2'-oxybis-	134	C6H14O3	000108-61-2	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070325\
Data File : BF142999.D
Acq On : 03 Jul 2025 16:29
Operator : RC/JU
Sample : Q2463-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TW-WTS-11

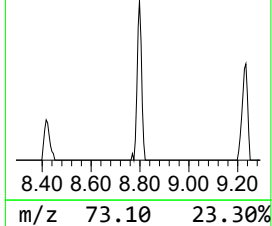
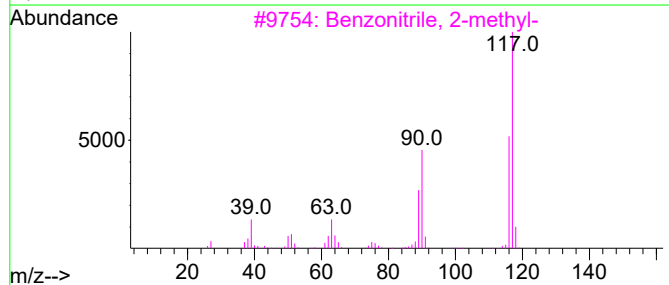
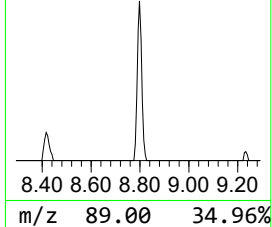
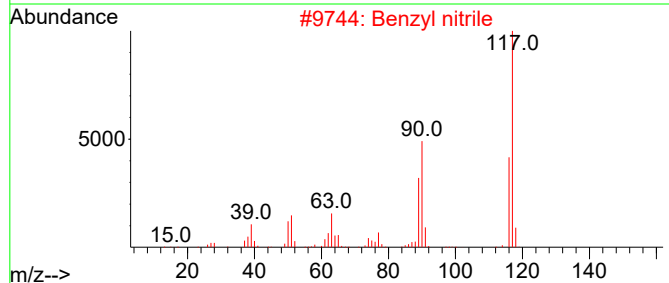
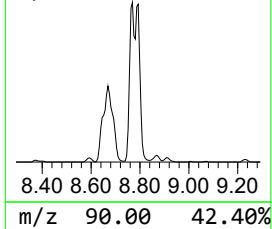
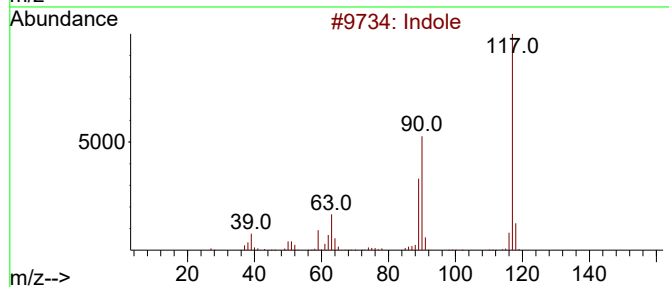
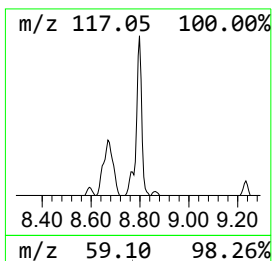
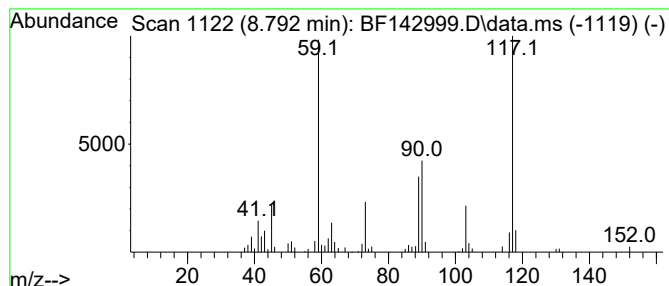
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061925.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Indole Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.792	5.90 ng	170796	Naphthalene-d8	8.157

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Indole	117	C8H7N	000120-72-9	90
2		Benzyl nitrile	117	C8H7N	000140-29-4	50
3		Benzonitrile, 2-methyl-	117	C8H7N	000529-19-1	50
4		Indolizine	117	C8H7N	000274-40-8	50
5		Benzonitrile, 3-methyl-	117	C8H7N	000620-22-4	45



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070325\
Data File : BF142999.D
Acq On : 03 Jul 2025 16:29
Operator : RC/JU
Sample : Q2463-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TW-WTS-11

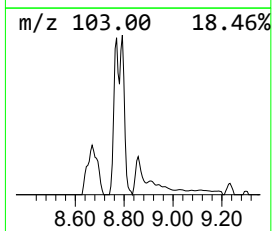
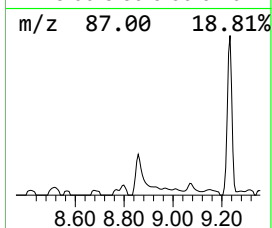
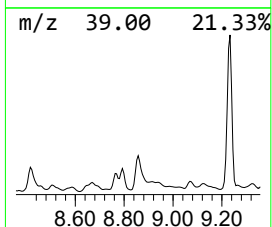
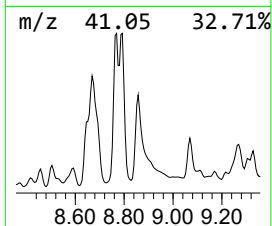
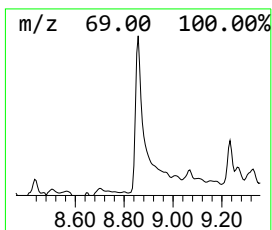
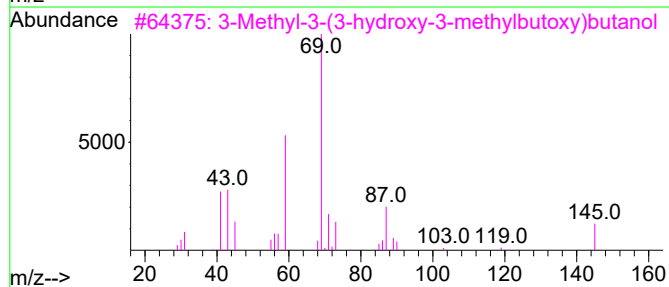
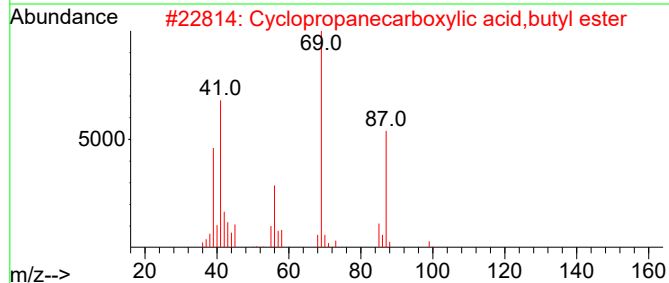
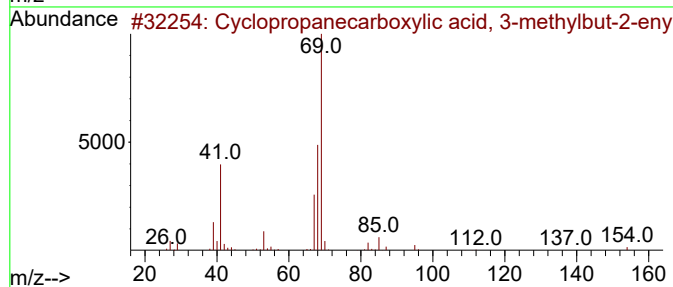
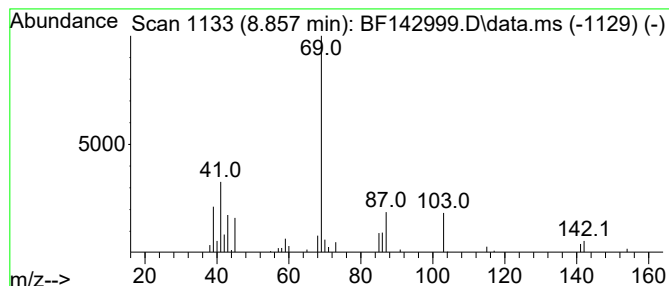
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061925.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown8.857 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.857	2.28 ng	66050	Naphthalene-d8	8.157

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropanecarboxylic acid, 3-m...	154	C9H14O2	1000299-37-4	47
2			Cyclopropanecarboxylic acid, buty...	142	C8H14O2	054947-39-6	45
3			3-Methyl-3-(3-hydroxy-3-methylbu...	190	C10H22O3	1000432-16-8	38
4			2-Butenoic acid, 2-propenylidene...	210	C11H14O4	055030-70-1	38
5			Ethyl cyclopropanecarboxylate	114	C6H10O2	004606-07-9	36



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070325\
Data File : BF142999.D
Acq On : 03 Jul 2025 16:29
Operator : RC/JU
Sample : Q2463-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TW-WTS-11

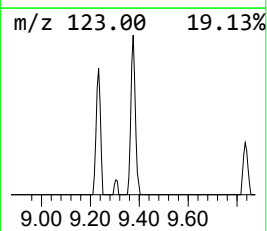
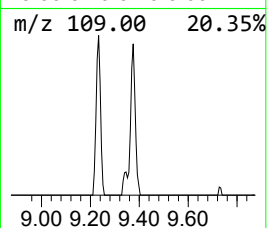
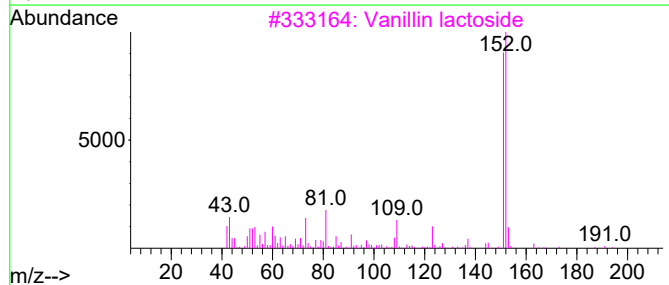
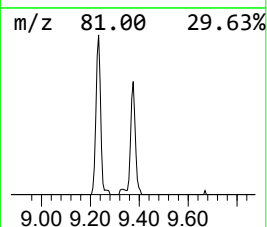
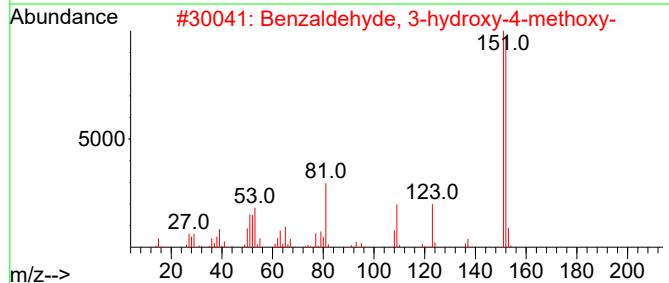
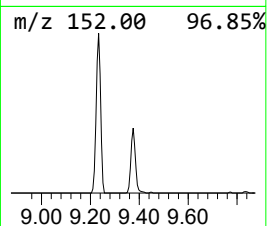
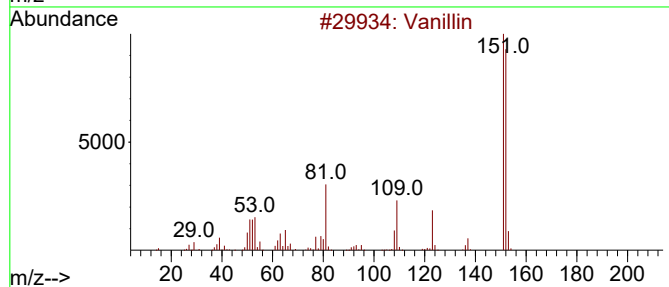
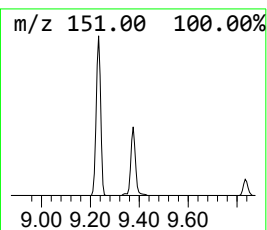
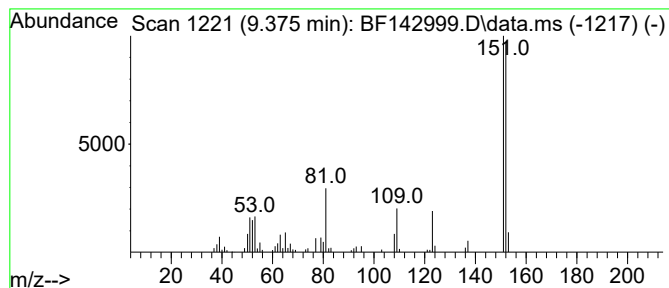
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061925.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Vanillin Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.375	3.15 ng	93524	Acenaphthene-d10	9.910

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Vanillin	152	C8H8O3	000121-33-5	97
2			Benzaldehyde, 3-hydroxy-4-methoxy-	152	C8H8O3	000621-59-0	96
3			Vanillin lactoside	476	C20H28O13	1000129-94-7	78
4			Benzaldehyde, 3-(chloroacetoxy)-...	228	C10H9ClO4	066267-38-7	59
5			2-Hydroxy-4-methoxybenzaldehyde,...	194	C10H10O4	1010352-92-0	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070325\
Data File : BF142999.D
Acq On : 03 Jul 2025 16:29
Operator : RC/JU
Sample : Q2463-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

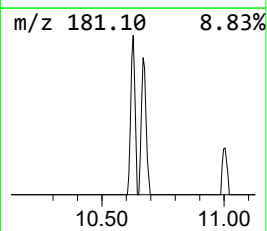
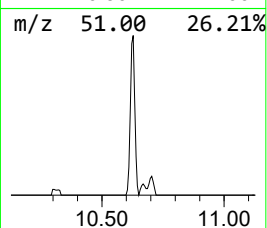
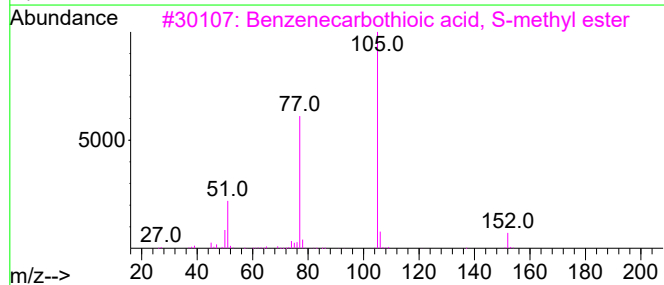
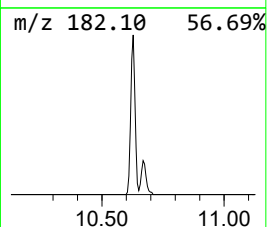
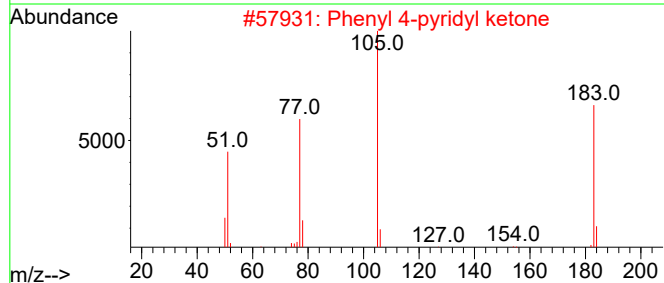
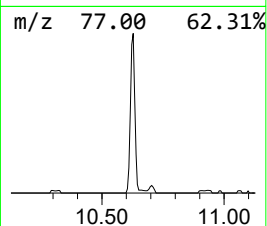
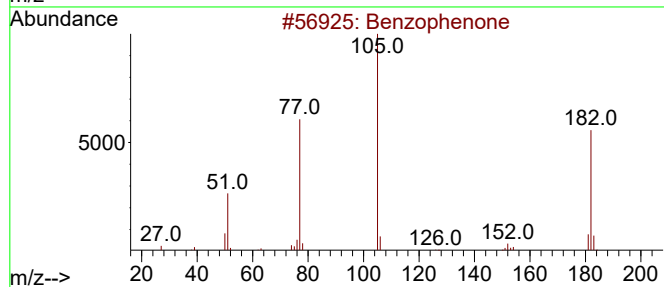
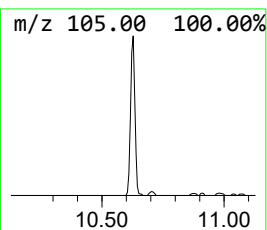
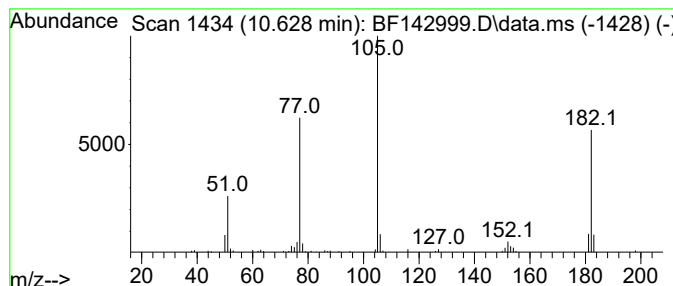
Instrument :
BNA_F
ClientSampleId :
TW-WTS-11

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061925.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 Benzophenone Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD		R.T.	
10.628	2.80 ng	83050	Acenaphthene-d10		9.910	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Benzophenone		182	C13H10O	000119-61-9	96
2	Phenyl 4-pyridyl ketone		183	C12H9NO	014548-46-0	58
3	Benzenecarbothioic acid, S-methy...		152	C8H8OS	005925-68-8	52
4	Ethanone, 2-bromo-1-phenyl-		198	C8H7BrO	000070-11-1	49
5	Benzenepropanenitrile, .beta.-oxo-		145	C9H7NO	000614-16-4	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070325\
Data File : BF142999.D
Acq On : 03 Jul 2025 16:29
Operator : RC/JU
Sample : Q2463-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

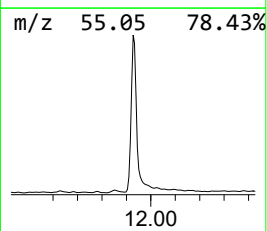
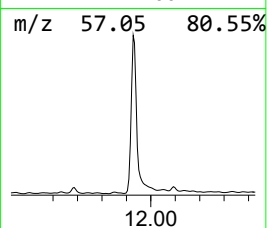
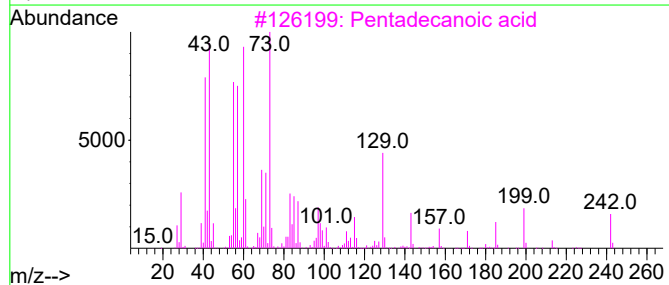
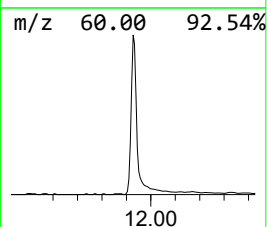
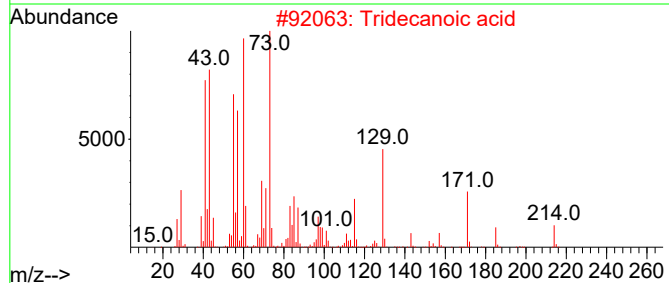
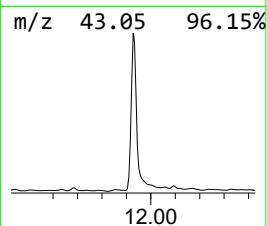
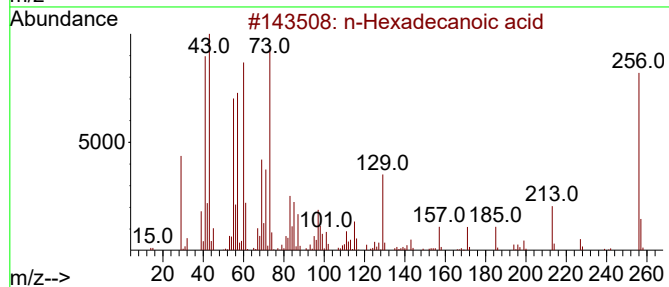
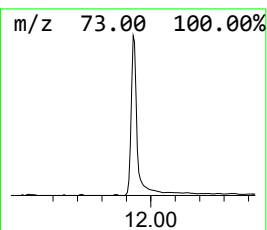
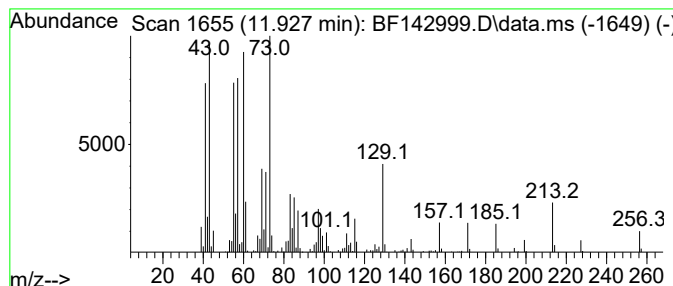
Instrument :
BNA_F
ClientSampleId :
TW-WTS-11

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061925.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.928	24.33 ng	666319	Phenanthrene-d10	11.404	
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	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Undecanoic acid	186	C11H22O2	000112-37-8	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070325\
Data File : BF142999.D
Acq On : 03 Jul 2025 16:29
Operator : RC/JU
Sample : Q2463-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TW-WTS-11

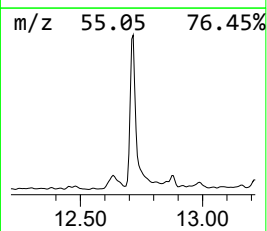
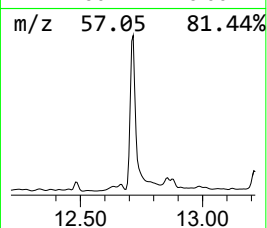
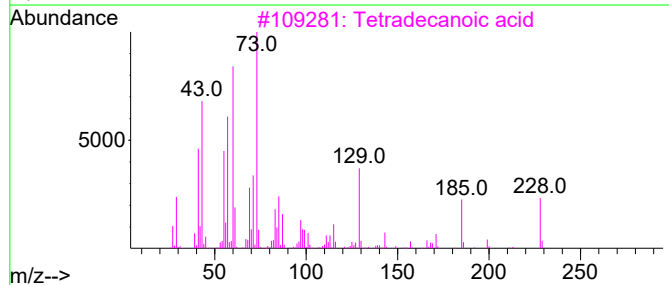
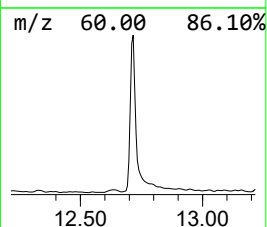
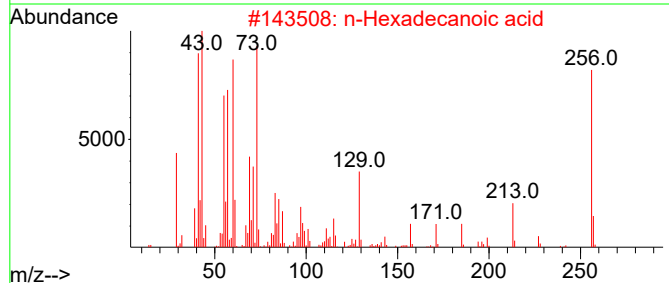
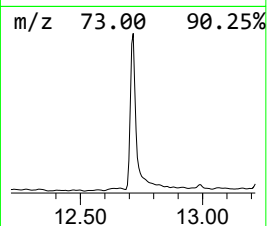
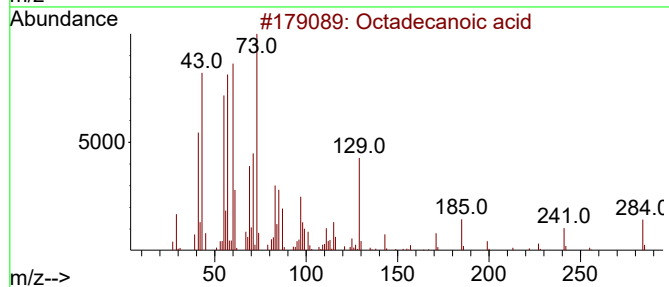
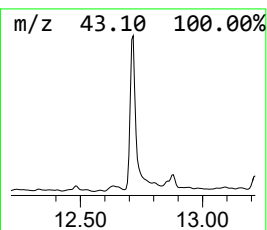
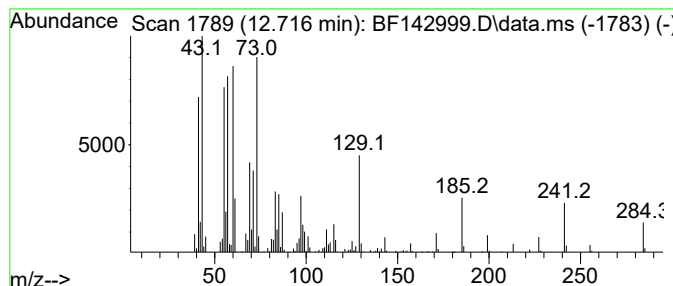
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061925.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.716	14.06 ng	385057	Phenanthrene-d10	11.404

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	93
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4		Undecanoic acid	186	C11H22O2	000112-37-8	70
5		n-Decanoic acid	172	C10H20O2	000334-48-5	60



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070325\
Data File : BF142999.D
Acq On : 03 Jul 2025 16:29
Operator : RC/JU
Sample : Q2463-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

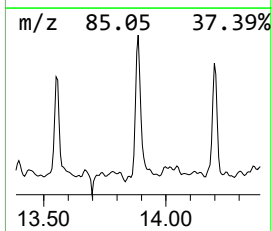
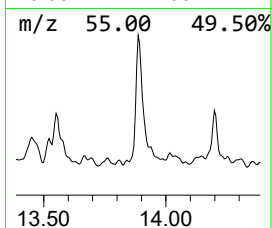
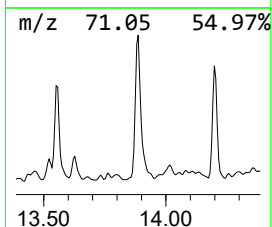
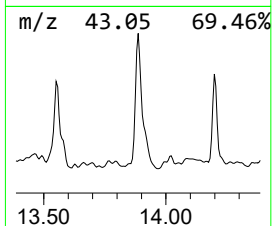
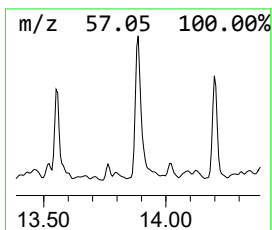
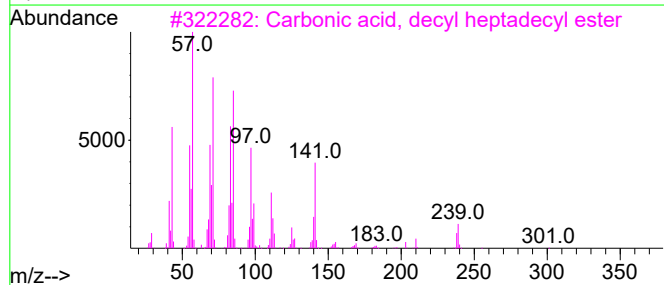
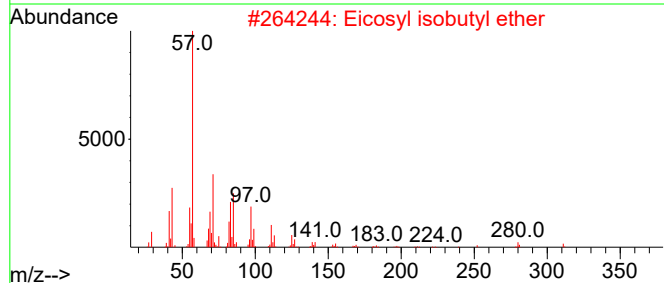
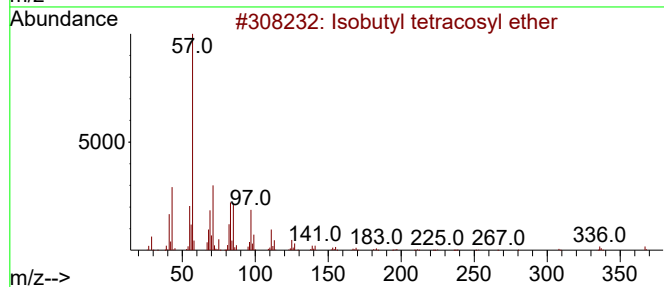
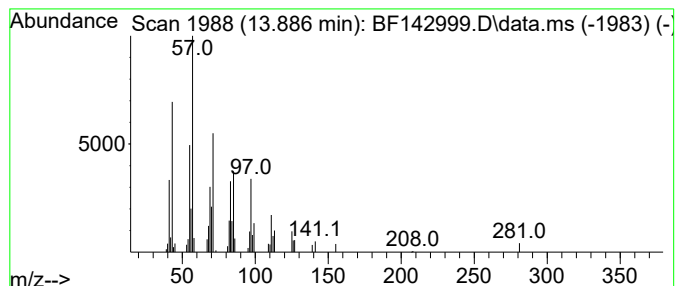
Instrument :
BNA_F
ClientSampleId :
TW-WTS-11

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061925.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 Isobutyl tetracosyl ether Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.886	3.52 ng	62273	Chrysene-d12	14.051	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutyl tetracosyl ether	410	C28H58O	1000406-33-2	91
2	Eicosyl isobutyl ether	354	C24H50O	1000406-33-0	91
3	Carbonic acid, decyl heptadecyl ...	440	C28H56O3	1000383-16-6	90
4	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	87
5	Docosyl isobutyl ether	382	C26H54O	1000406-33-1	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070325\
Data File : BF142999.D
Acq On : 03 Jul 2025 16:29
Operator : RC/JU
Sample : Q2463-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TW-WTS-11

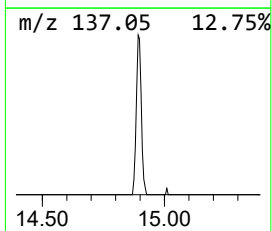
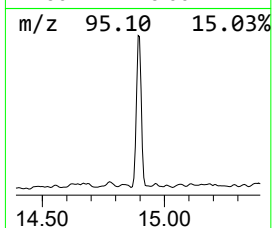
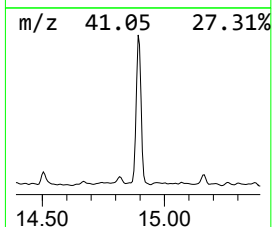
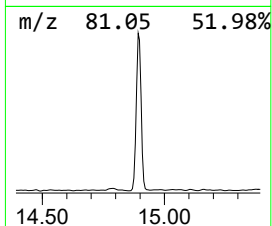
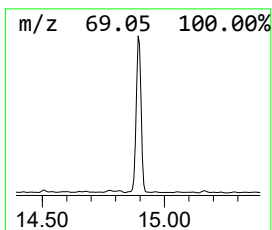
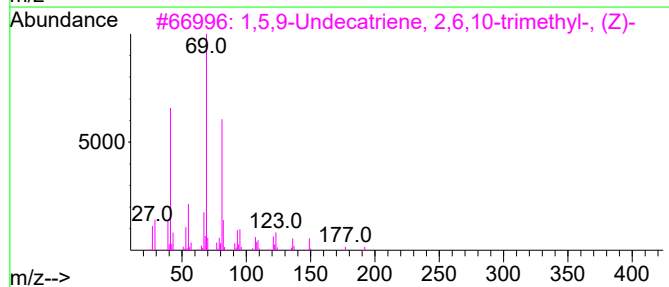
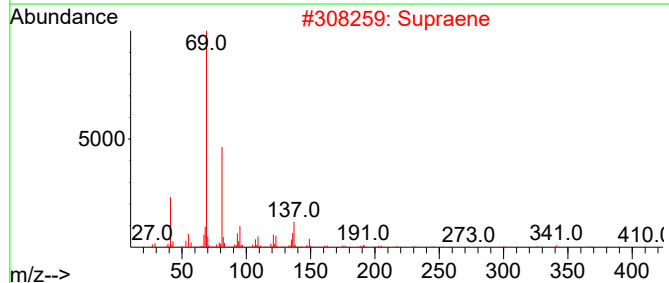
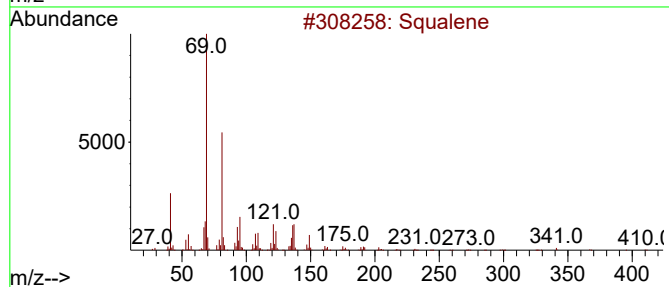
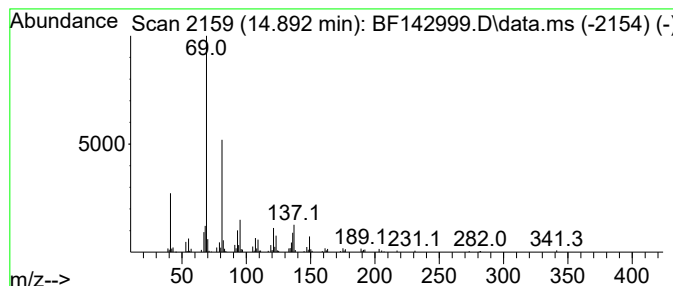
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061925.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.892	7.08 ng	169744	Perylene-d12	15.545

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	91
2			Supraene	410	C30H50	007683-64-9	91
3			1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	80
4			2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	72
5			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070325\
 Data File : BF142999.D
 Acq On : 03 Jul 2025 16:29
 Operator : RC/JU
 Sample : Q2463-01
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TW-WTS-11

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061925.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
Propanoic acid,...	3.969	2.2	ng	45526	1	6.875	415994	20.0
Butanoic acid	4.816	49.4	ng	1026660	1	6.875	415994	20.0
2-Pentanone, 4-...	5.098	4.5	ng	93709	1	6.875	415994	20.0
unknown5.369	5.369	31.0	ng	644294	1	6.875	415994	20.0
Pentanoic acid	5.798	14.8	ng	307774	1	6.875	415994	20.0
2-Pentenoic acid	6.104	2.8	ng	57508	1	6.875	415994	20.0
Pentanoic acid,...	6.228	2.0	ng	42297	1	6.875	415994	20.0
Hexanoic acid, ...	7.551	2.6	ng	76680	2	8.157	579306	20.0
Benzeneacetic acid	8.416	3.4	ng	97905	2	8.157	579306	20.0
2-Propanol, 1-[...	8.669	5.5	ng	158006	2	8.157	579306	20.0
2-Propanol, 1,1...	8.769	4.5	ng	131678	2	8.157	579306	20.0
Indole	8.792	5.9	ng	170796	2	8.157	579306	20.0
unknown8.857	8.857	2.3	ng	66050	2	8.157	579306	20.0
Vanillin	9.375	3.1	ng	93524	3	9.910	593736	20.0
Benzophenone	10.628	2.8	ng	83050	3	9.910	593736	20.0
n-Hexadecanoic ...	11.928	24.3	ng	666319	4	11.404	547787	20.0
Octadecanoic acid	12.716	14.1	ng	385057	4	11.404	547787	20.0
Isobutyl tetrac...	13.886	3.5	ng	62273	5	14.051	354050	20.0
Squalene	14.892	7.1	ng	169744	6	15.545	479827	20.0