

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
 Data File : BF139119.D
 Acq On : 22 Aug 2024 13:22
 Operator : RC/JU
 Sample : P3641-02
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S-907-K1-0.5-1.0-081524

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-BF082024.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139119.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.228	15	23	30	rVB	1257539	1987442	97.82%	11.744%
2	3.422	217	226	243	rBV	18729	44636	2.20%	0.264%
3	5.122	505	515	522	rBV	84933	133082	6.55%	0.786%
4	5.516	576	582	587	rBV	1487621	1953052	96.13%	11.541%
5	6.181	691	695	701	rBV	17744	21783	1.07%	0.129%
6	6.516	745	752	757	rBV	1488525	2031765	100.00%	12.006%
7	6.716	778	786	791	rBV	19139	27415	1.35%	0.162%
8	6.898	811	817	822	rBV	512072	630309	31.02%	3.725%
9	7.051	838	843	848	rBV	93725	115778	5.70%	0.684%
10	7.457	905	912	917	rBV	1009880	1299961	63.98%	7.681%
11	7.710	949	955	960	rVB	18607	22047	1.09%	0.130%
12	8.181	1029	1035	1040	rBV	630592	792085	38.99%	4.680%
13	8.486	1082	1087	1096	rBV	83206	105537	5.19%	0.624%
14	9.251	1212	1217	1222	rBV	1489686	1874004	92.24%	11.074%
15	9.933	1324	1333	1338	rBV	715182	912644	44.92%	5.393%
16	10.027	1343	1349	1357	rBV2	38584	63623	3.13%	0.376%
17	10.716	1461	1466	1472	rBV	952605	1211213	59.61%	7.157%
18	11.416	1576	1585	1592	rBV	623603	798386	39.30%	4.718%
19	11.533	1600	1605	1609	rBV5	18574	27705	1.36%	0.164%
20	11.851	1655	1659	1665	rBV4	24997	37172	1.83%	0.220%
21	11.939	1668	1674	1679	rBV3	76072	127467	6.27%	0.753%
22	12.627	1787	1791	1798	rBV	23813	35854	1.76%	0.212%
23	12.727	1804	1808	1817	rBV	16097	24073	1.18%	0.142%
24	12.857	1822	1830	1845	rBV2	21863	67519	3.32%	0.399%
25	13.004	1850	1855	1860	rVB	934750	1136948	55.96%	6.718%
26	13.686	1963	1971	1981	rVV	23944	103422	5.09%	0.611%
27	13.768	1981	1985	1989	rVB	36304	46454	2.29%	0.274%
28	13.910	2004	2009	2022	rBV3	42446	89530	4.41%	0.529%
29	14.057	2028	2034	2043	rBV	427336	584344	28.76%	3.453%
30	14.551	2113	2118	2129	rVB6	19346	48385	2.38%	0.286%
31	15.098	2208	2211	2220	rVB	16874	38348	1.89%	0.227%
32	15.533	2279	2285	2297	rVB	344033	531306	26.15%	3.139%

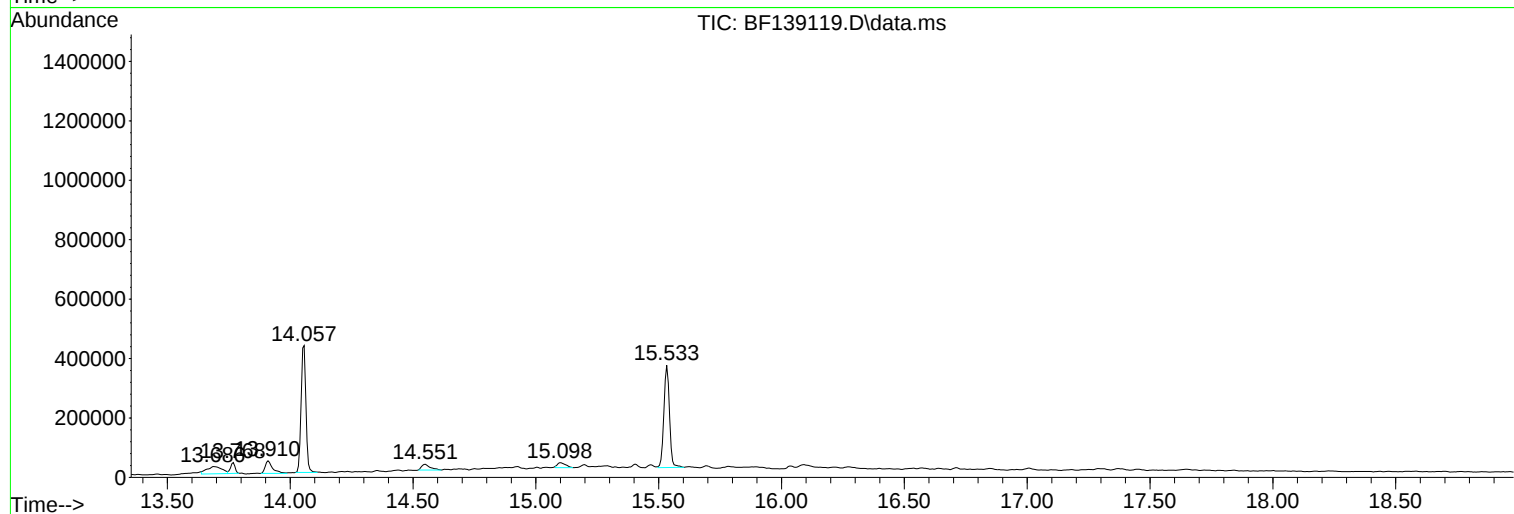
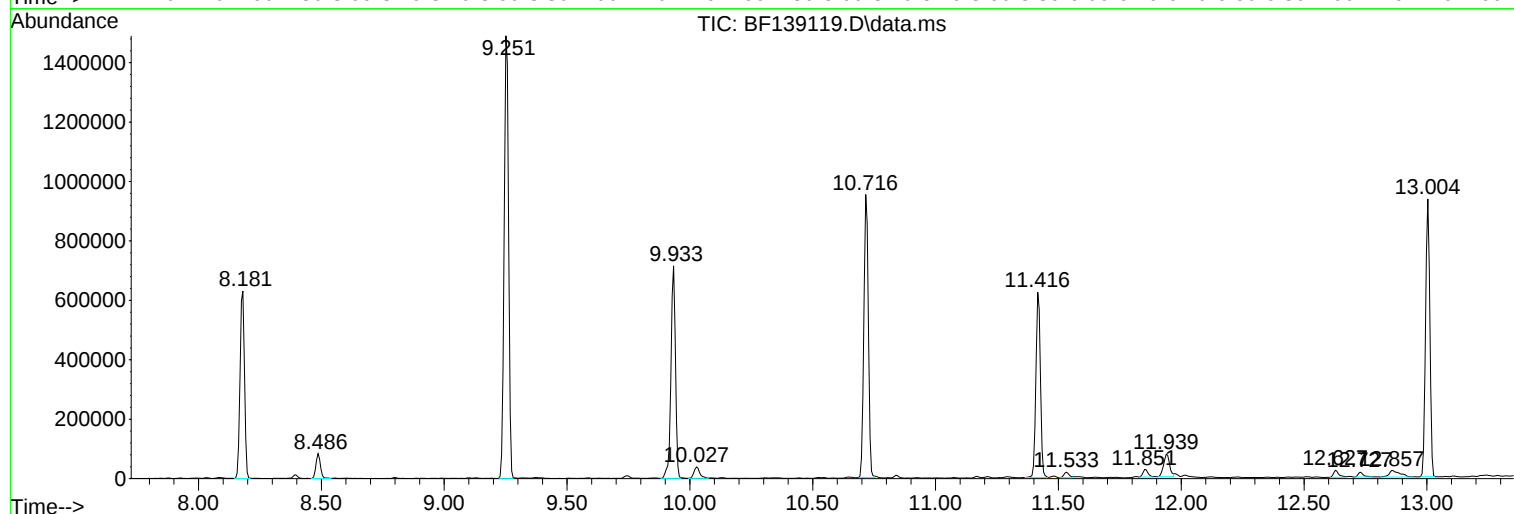
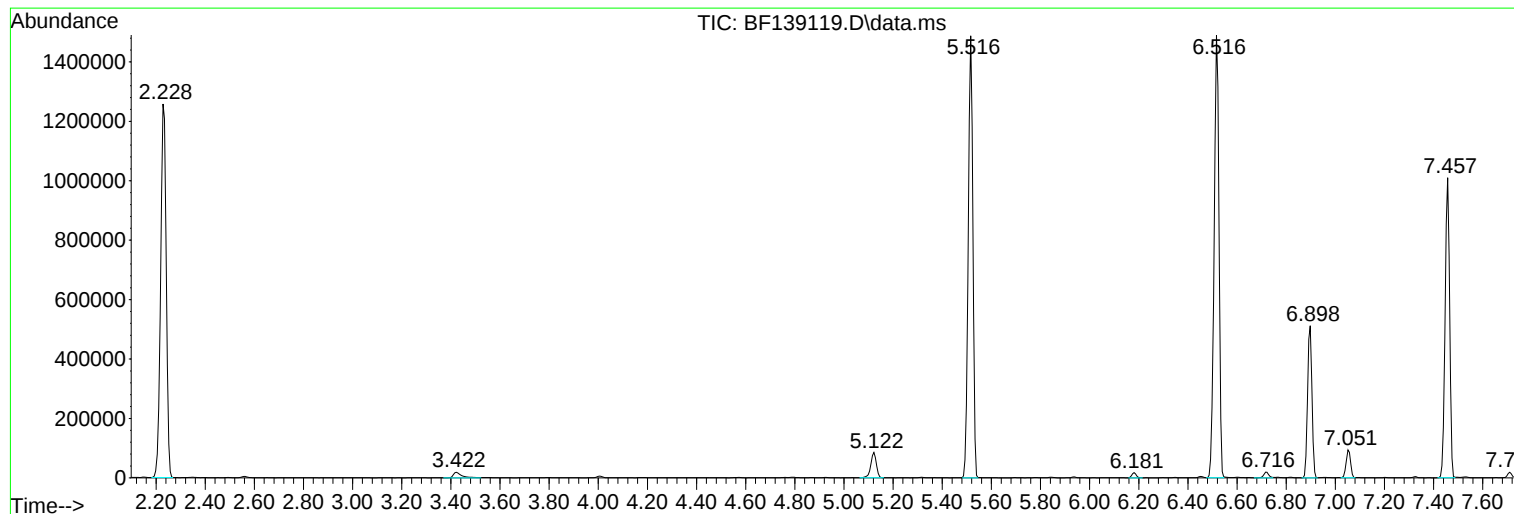
Sum of corrected areas: 16923289

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
Data File : BF139119.D
Acq On : 22 Aug 2024 13:22
Operator : RC/JU
Sample : P3641-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-907-K1-0.5-1.0-081524

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.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\BF082224\
Data File : BF139119.D
Acq On : 22 Aug 2024 13:22
Operator : RC/JU
Sample : P3641-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-907-K1-0.5-1.0-081524

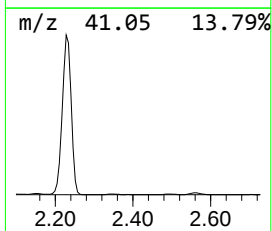
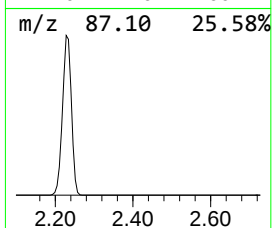
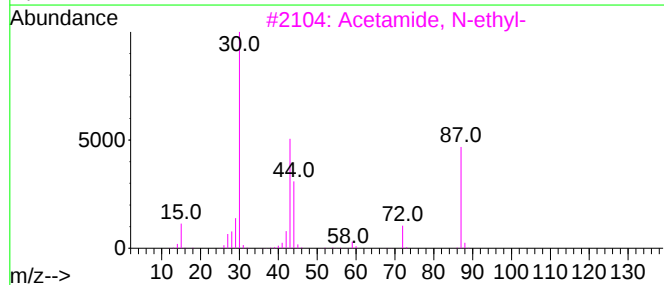
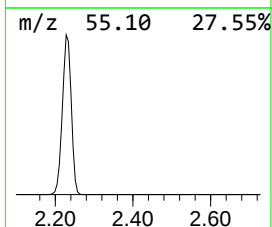
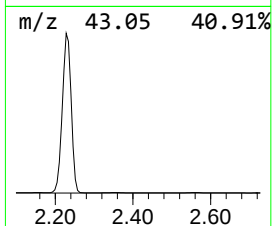
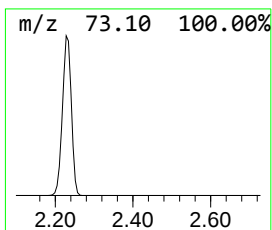
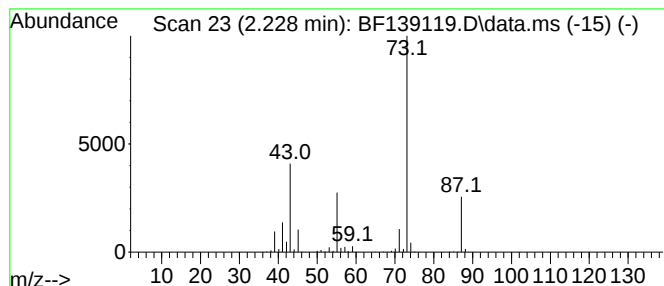
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.228	63.06 ng	1987440	1,4-Dichlorobenzene-d4	6.898

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			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
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\BF082224\
Data File : BF139119.D
Acq On : 22 Aug 2024 13:22
Operator : RC/JU
Sample : P3641-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-907-K1-0.5-1.0-081524

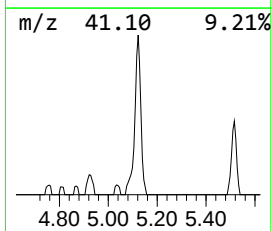
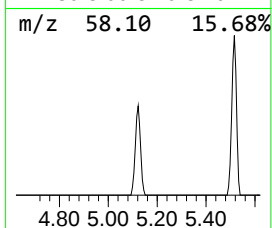
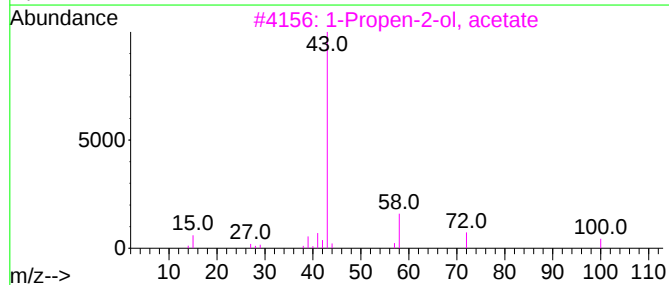
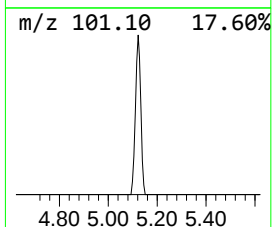
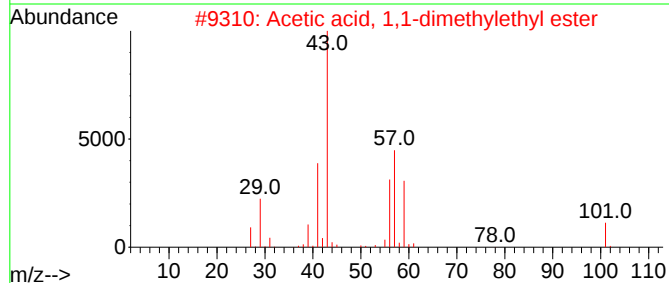
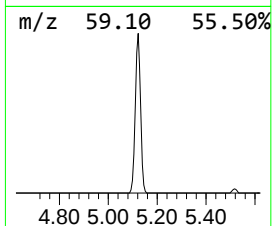
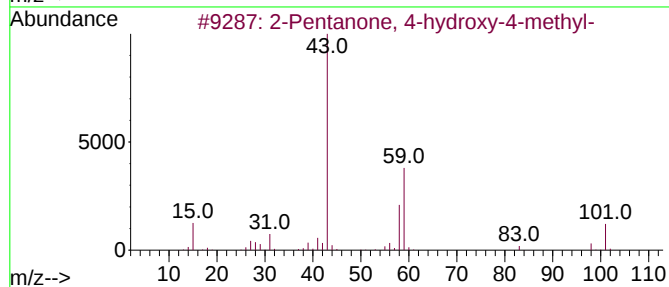
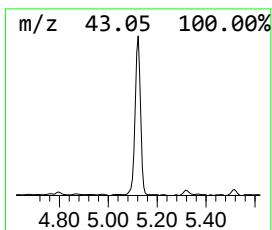
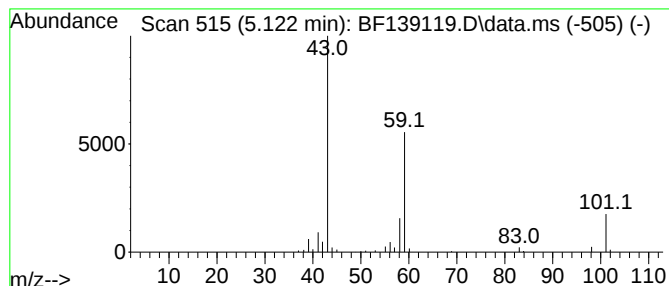
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.122	4.22 ng	133082	1,4-Dichlorobenzene-d4	6.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
Data File : BF139119.D
Acq On : 22 Aug 2024 13:22
Operator : RC/JU
Sample : P3641-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-907-K1-0.5-1.0-081524

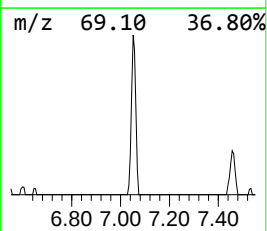
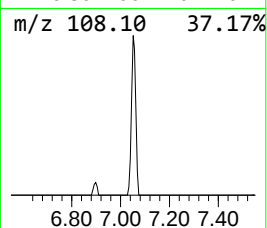
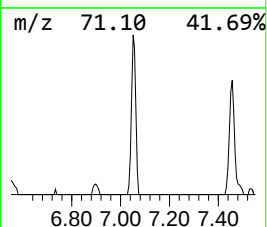
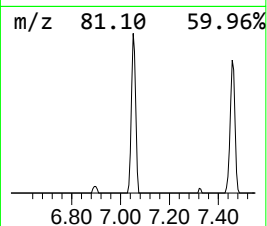
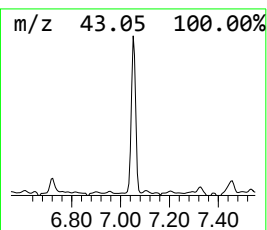
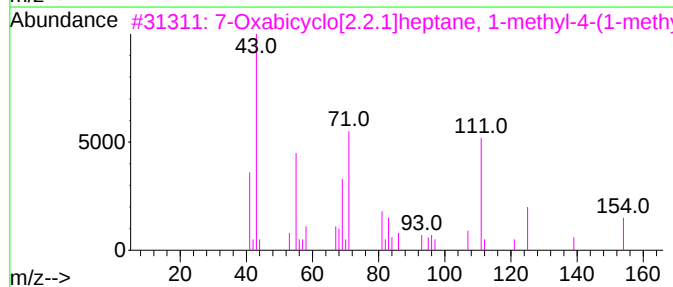
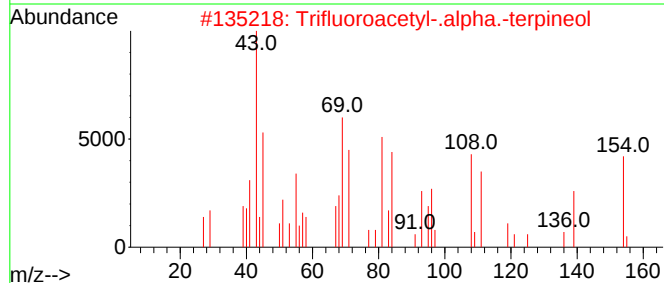
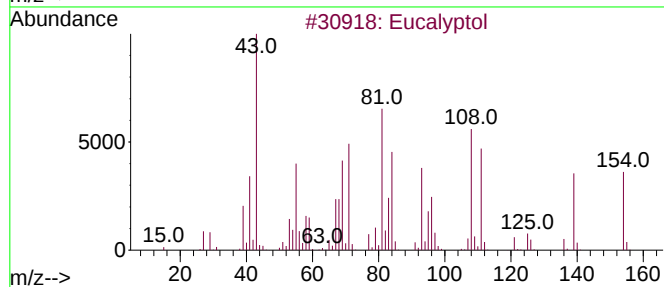
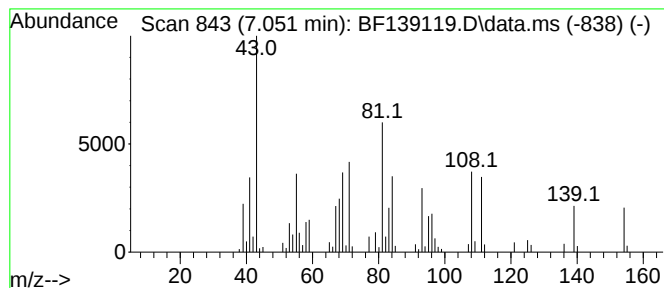
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Eucalyptol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.051	3.67 ng	115778	1,4-Dichlorobenzene-d4	6.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eucalyptol	154	C10H18O	000470-82-6	97
2			Trifluoroacetyl-.alpha.-terpineol	250	C12H17F3O2	1000058-17-6	40
3			7-Oxabicyclo[2.2.1]heptane, 1-me...	154	C10H18O	000470-67-7	37
4			7-Decen-2-one	154	C10H18O	035194-33-3	27
5			2-(3'-Oxo-butyl)-cyclopentanone	154	C9H14O2	1010143-37-2	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
Data File : BF139119.D
Acq On : 22 Aug 2024 13:22
Operator : RC/JU
Sample : P3641-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-907-K1-0.5-1.0-081524

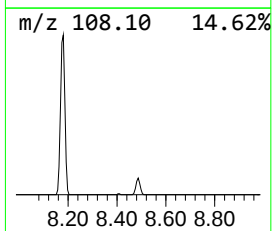
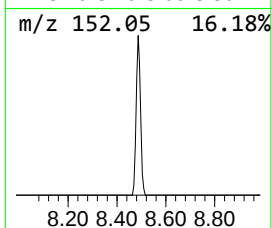
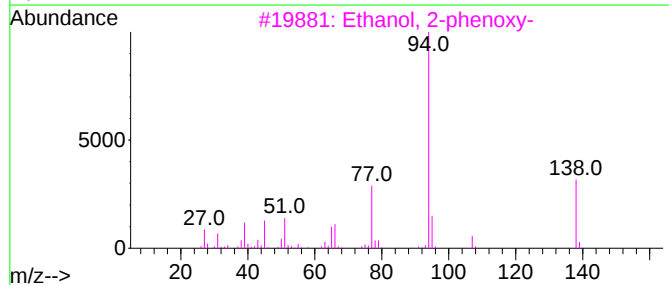
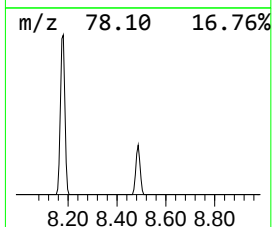
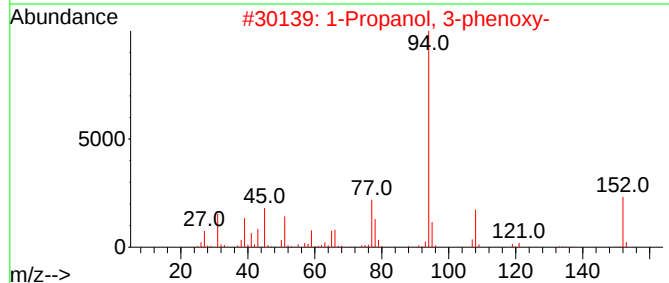
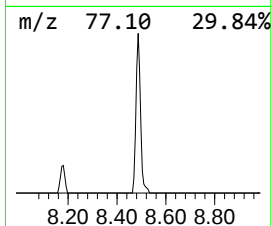
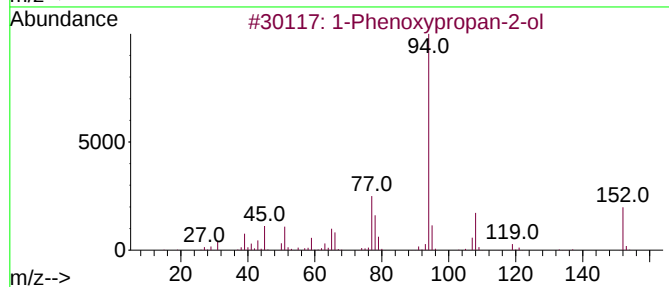
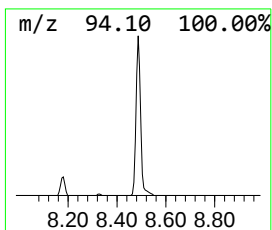
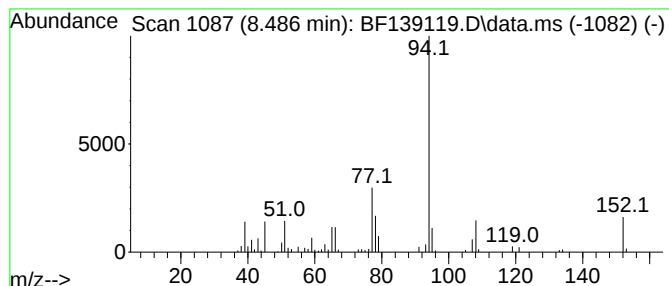
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 1-Phenoxypropan-2-ol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.486	2.66 ng	105537	Naphthalene-d8	8.181

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	97
2			1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	87
3			Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4			1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	59
5			Benzene, propoxy-	136	C9H12O	000622-85-5	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
Data File : BF139119.D
Acq On : 22 Aug 2024 13:22
Operator : RC/JU
Sample : P3641-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-907-K1-0.5-1.0-081524

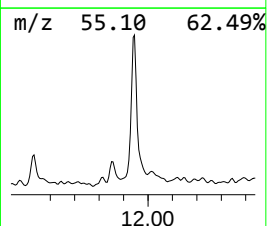
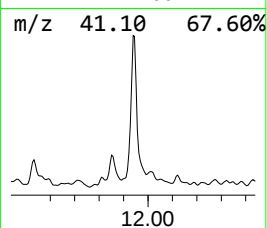
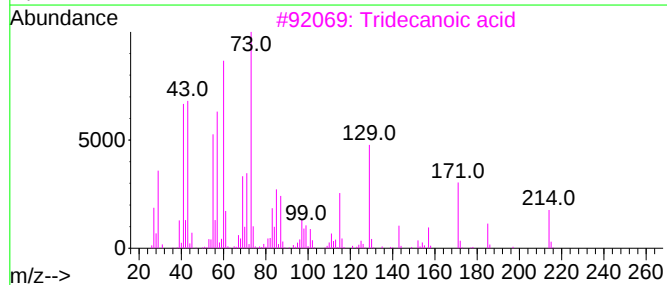
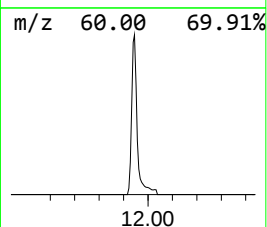
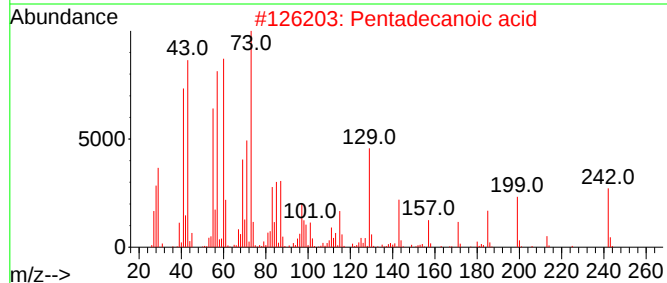
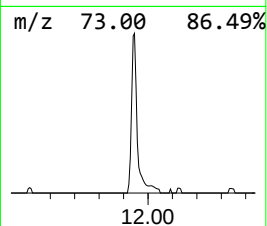
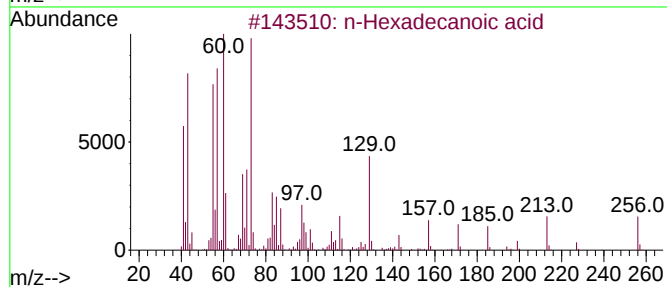
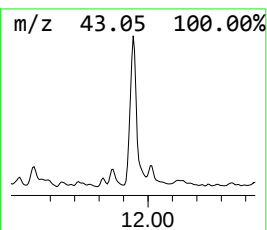
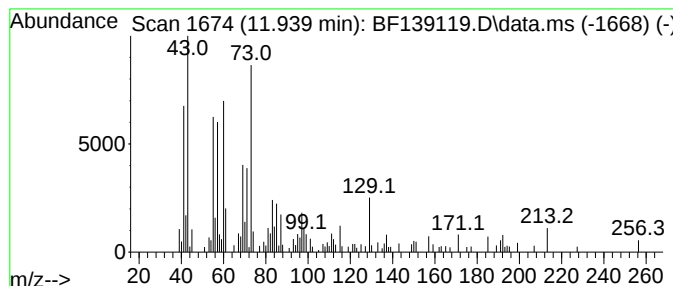
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.939	3.19 ng	127467	Phenanthrene-d10	11.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			Tridecanoic acid	214	C13H26O2	000638-53-9	58
4			n-Decanoic acid	172	C10H20O2	000334-48-5	38
5			Nonyl tetradecyl ether	340	C23H48O	1000406-37-6	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
Data File : BF139119.D
Acq On : 22 Aug 2024 13:22
Operator : RC/JU
Sample : P3641-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-907-K1-0.5-1.0-081524

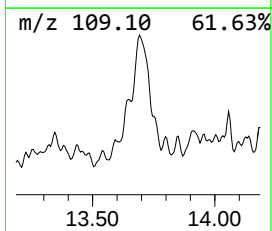
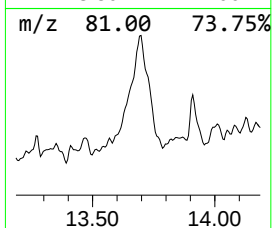
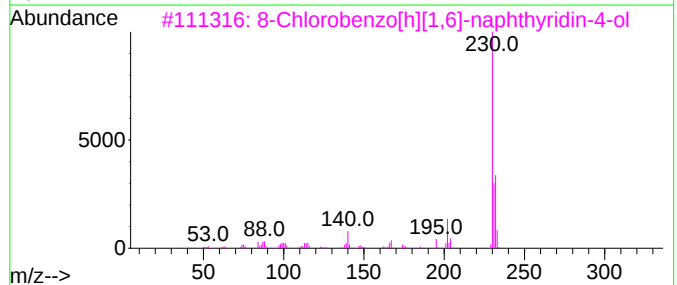
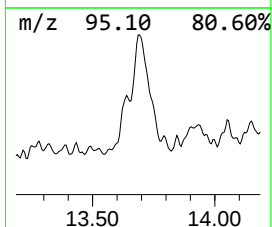
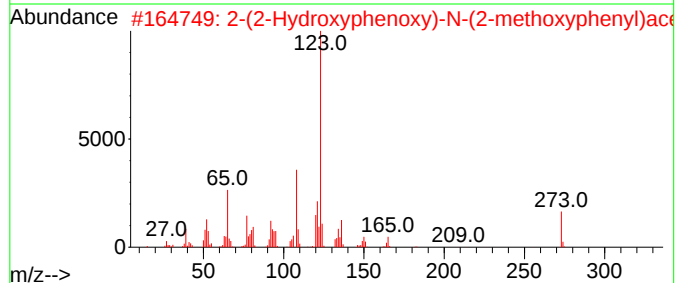
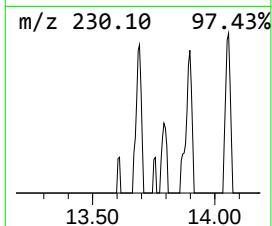
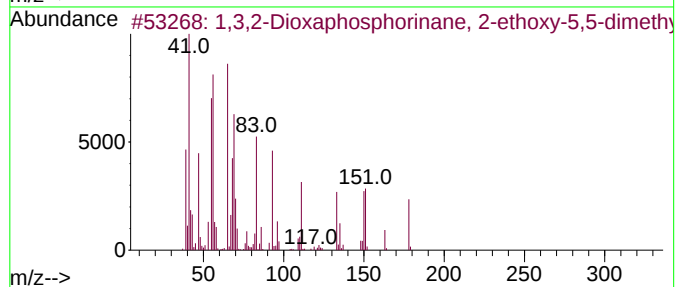
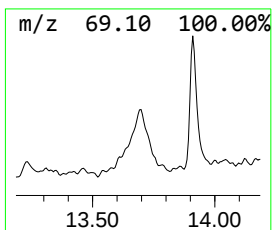
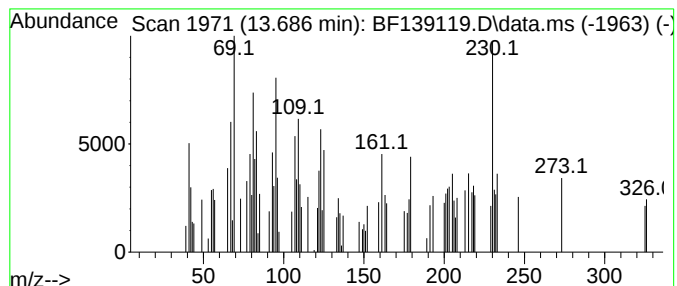
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown13.686 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.686	3.54 ng	103422	Chrysene-d12	14.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3,2-Dioxaphosphorinane, 2-etho...	178	C7H15O3P	001007-57-4	14
2			2-(2-Hydroxyphenoxy)-N-(2-methox...	273	C15H15NO4	092851-38-2	12
3			8-Chlorobenzo[h][1,6]-naphthyrid...	230	C12H7ClN2O	025100-26-9	11
4			1,6-Dihydropyridazine-3-carboxyl...	273	C13H8FN3O3	1000304-05-0	10
5			3-Chlorocatechol, cyclic phenylb...	230	C12H8BClO2	1000293-25-0	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
Data File : BF139119.D
Acq On : 22 Aug 2024 13:22
Operator : RC/JU
Sample : P3641-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-907-K1-0.5-1.0-081524

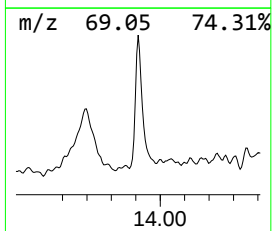
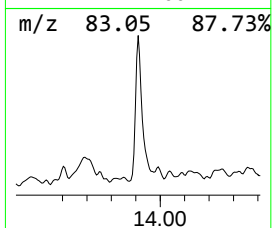
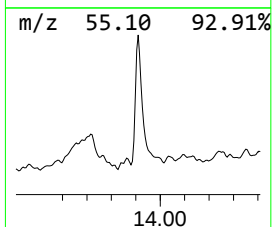
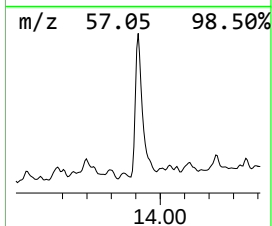
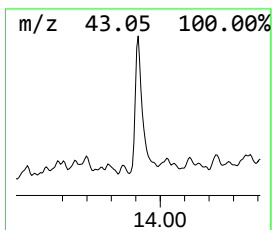
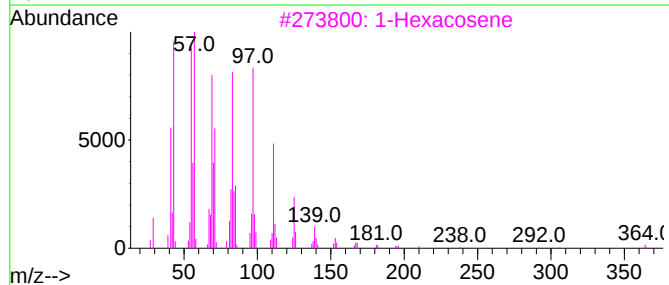
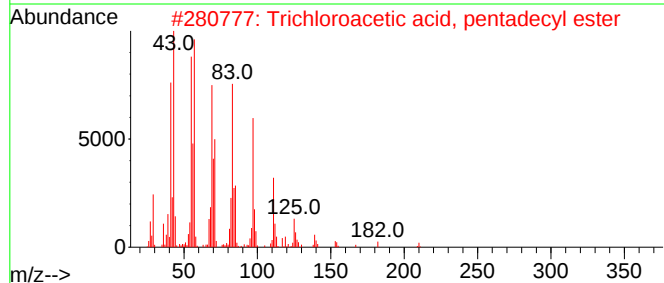
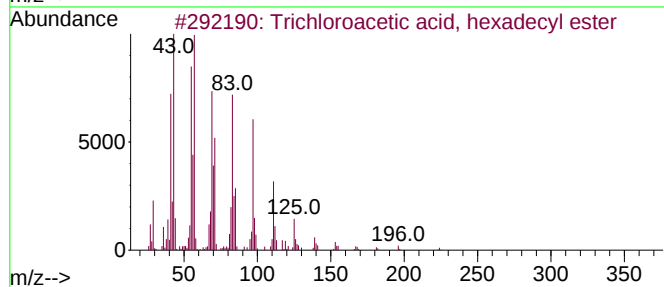
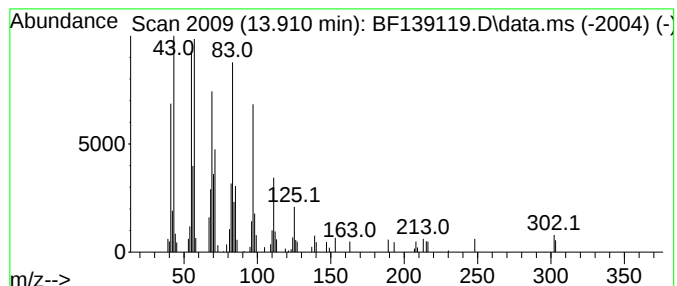
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Trichloroacetic acid, hexad... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.910	3.06 ng	89530	Chrysene-d12	14.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	95
2			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
3			1-Hexacosene	364	C26H52	018835-33-1	93
4			Behenic alcohol	326	C22H46O	000661-19-8	93
5			1-Heneicosanol	312	C21H44O	015594-90-8	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
Data File : BF139119.D
Acq On : 22 Aug 2024 13:22
Operator : RC/JU
Sample : P3641-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-907-K1-0.5-1.0-081524

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.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
Butane, 2-metho...	2.228	63.1	ng	1987440	1	6.898	630309	20.0
2-Pentanone, 4-...	5.122	4.2	ng	133082	1	6.898	630309	20.0
Eucalyptol	7.051	3.7	ng	115778	1	6.898	630309	20.0
1-Phenoxypropan...	8.486	2.7	ng	105537	2	8.181	792085	20.0
n-Hexadecanoic ...	11.939	3.2	ng	127467	4	11.416	798386	20.0
unknown13.686	13.686	3.5	ng	103422	5	14.057	584344	20.0
Trichloroacetic...	13.910	3.1	ng	89530	5	14.057	584344	20.0