

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121022\
 Data File : BF131584.D
 Acq On : 10 Dec 2022 11:57
 Operator : CG\JU
 Sample : PB149515BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB149515BL

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-BF120822.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131584.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.216	15	22	28	rVB	44951	56780	1.60%	0.316%
2	5.134	513	518	530	rBB	290881	405511	11.42%	2.257%
3	5.534	580	586	589	rBV	2162737	2074643	58.43%	11.547%
4	6.540	751	757	760	rBV	1816709	2132339	60.05%	11.868%
5	6.910	816	820	823	rBB	489448	394356	11.11%	2.195%
6	7.481	911	917	920	rBV	1313049	1384482	38.99%	7.705%
7	8.198	1034	1039	1042	rBV	596789	498100	14.03%	2.772%
8	9.281	1217	1223	1226	rBV	3264678	2750620	77.47%	15.309%
9	9.963	1334	1339	1342	rBV	761873	630340	17.75%	3.508%
10	10.757	1469	1474	1477	rBV	2296840	1990239	56.05%	11.077%
11	11.457	1589	1593	1596	rBV	865104	701593	19.76%	3.905%
12	12.863	1828	1832	1835	rBV	43227	38188	1.08%	0.213%
13	13.057	1859	1865	1867	rBV	3492271	3550709	100.00%	19.762%
14	14.104	2040	2043	2047	rBV	608152	570620	16.07%	3.176%
15	15.239	2233	2236	2241	rVB	32573	37091	1.04%	0.206%
16	15.621	2295	2301	2313	rBV	301588	438761	12.36%	2.442%
17	16.104	2377	2383	2389	rBV2	35823	58926	1.66%	0.328%
18	16.639	2467	2474	2481	rBV3	36880	71816	2.02%	0.400%
19	17.262	2574	2580	2591	rBV3	24676	64228	1.81%	0.357%
20	17.609	2628	2639	2648	rBV7	16455	64992	1.83%	0.362%
21	18.015	2702	2708	2716	rVB3	22429	53159	1.50%	0.296%

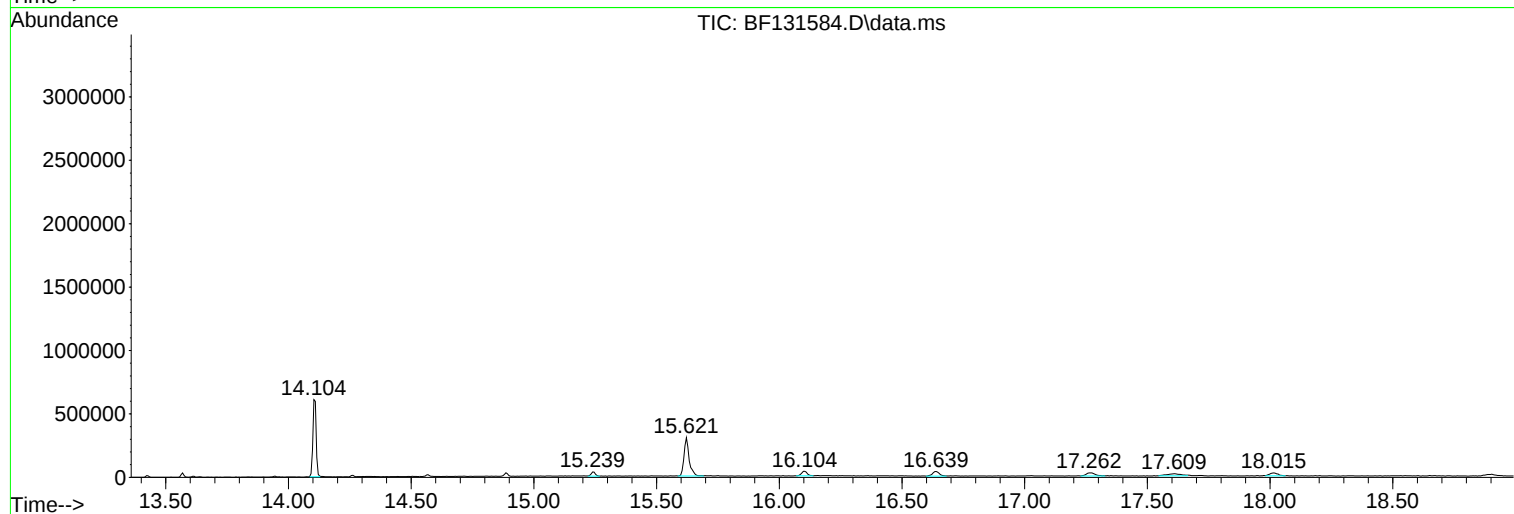
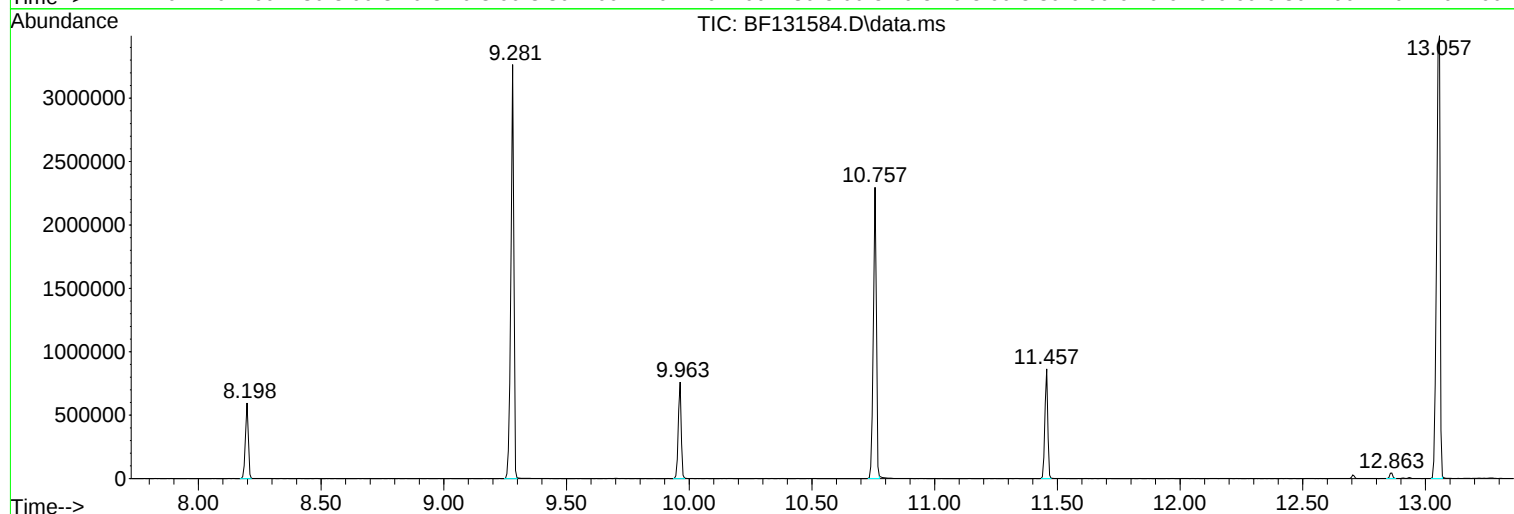
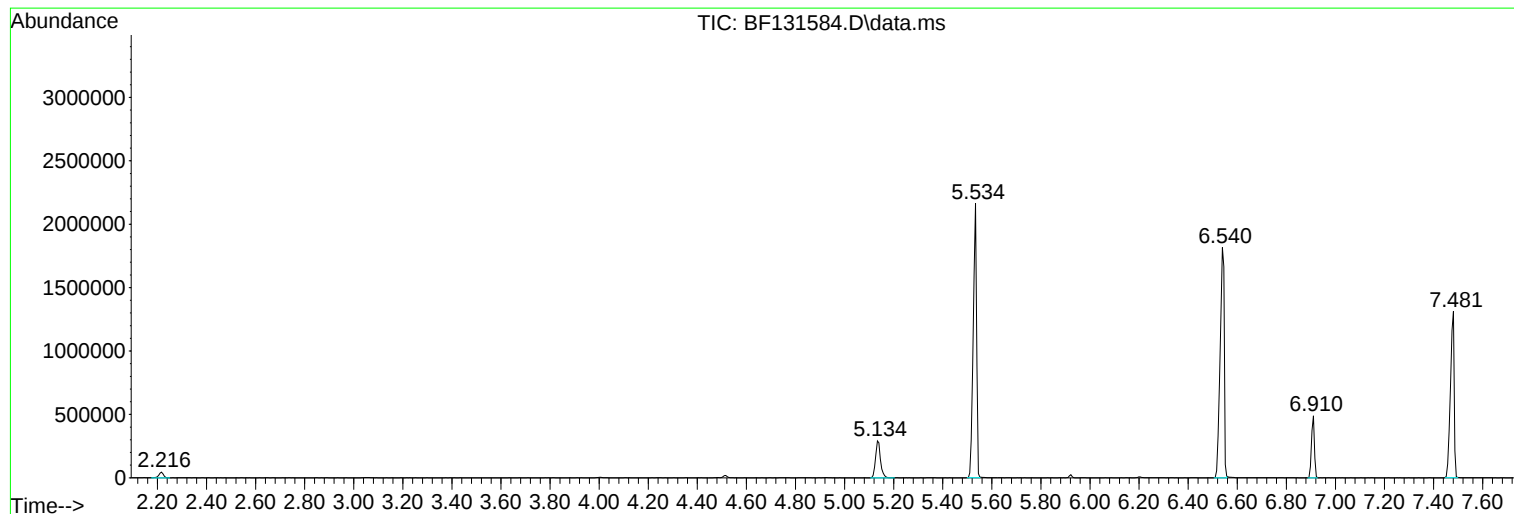
Sum of corrected areas: 17967493

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121022\
Data File : BF131584.D
Acq On : 10 Dec 2022 11:57
Operator : CG\JU
Sample : PB149515BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB149515BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.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\BF121022\
Data File : BF131584.D
Acq On : 10 Dec 2022 11:57
Operator : CG\JU
Sample : PB149515BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB149515BL

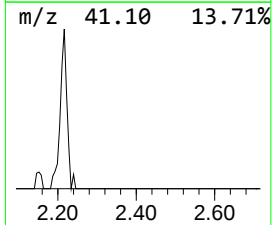
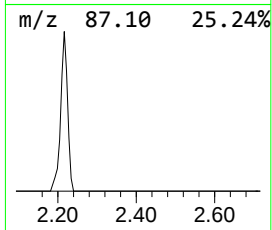
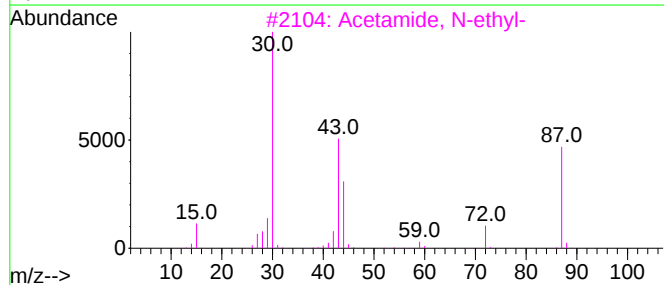
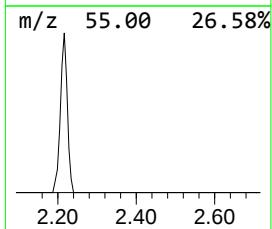
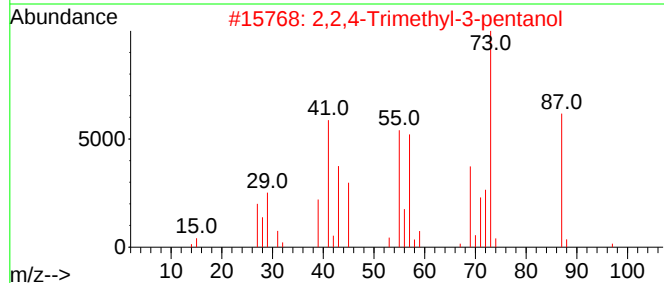
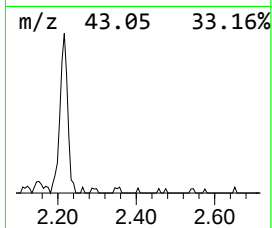
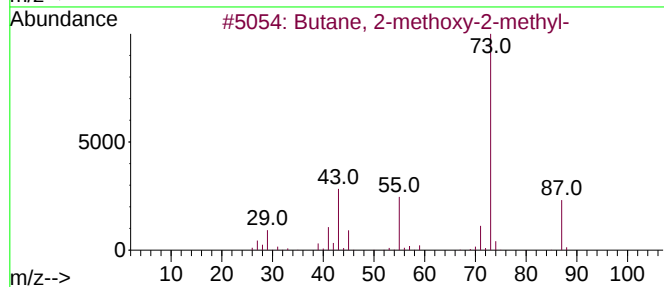
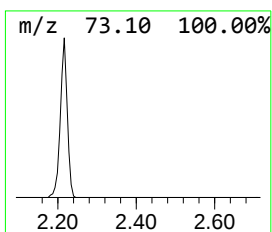
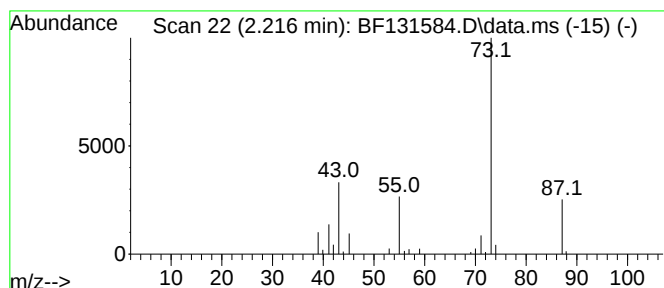
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.216	2.88 ng	56780	1,4-Dichlorobenzene-d4	6.910

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	12
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
5			Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121022\
Data File : BF131584.D
Acq On : 10 Dec 2022 11:57
Operator : CG\JU
Sample : PB149515BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB149515BL

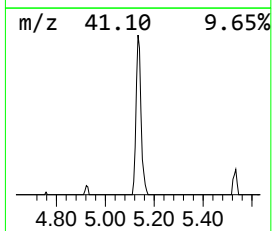
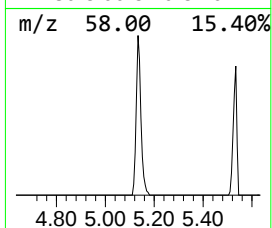
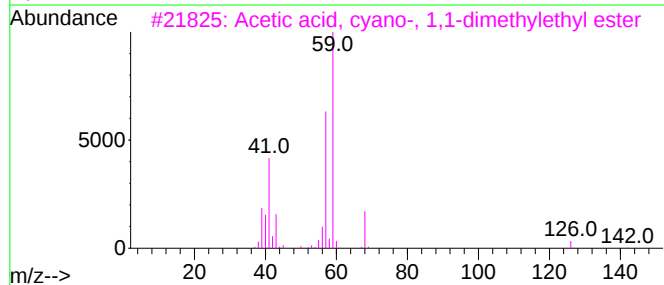
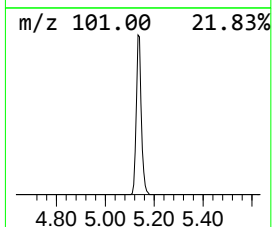
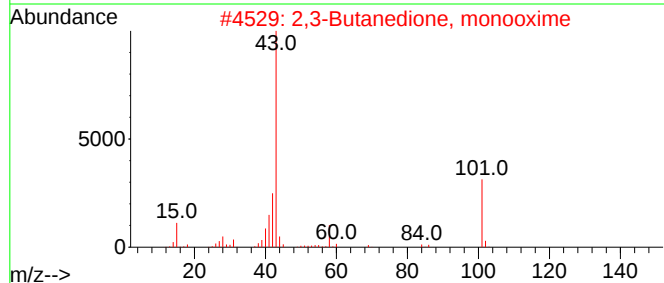
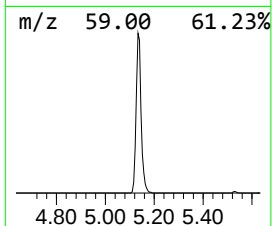
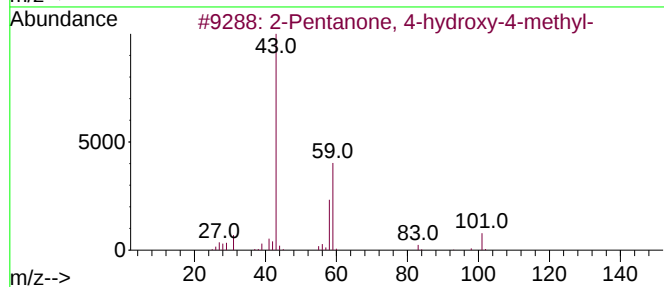
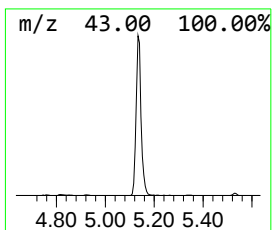
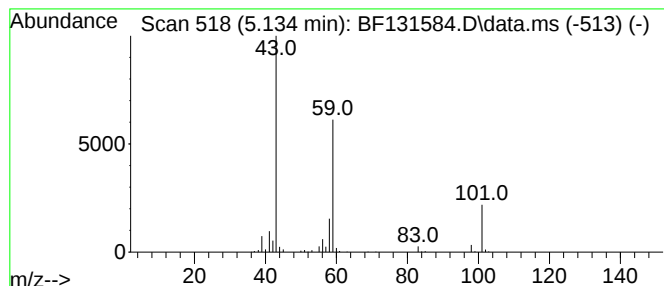
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.134	20.57 ng	405511	1,4-Dichlorobenzene-d4	6.910

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	25		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121022\
Data File : BF131584.D
Acq On : 10 Dec 2022 11:57
Operator : CG\JU
Sample : PB149515BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB149515BL

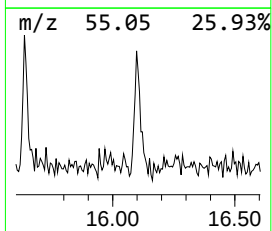
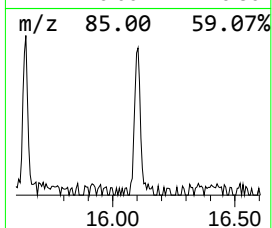
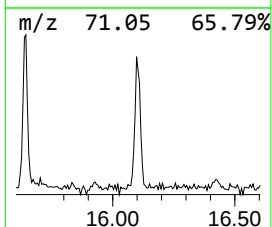
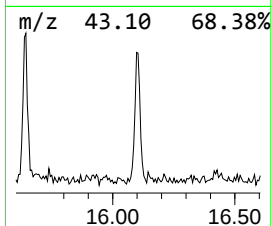
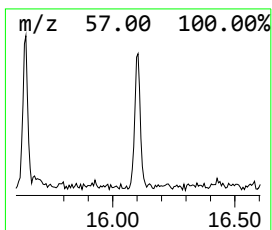
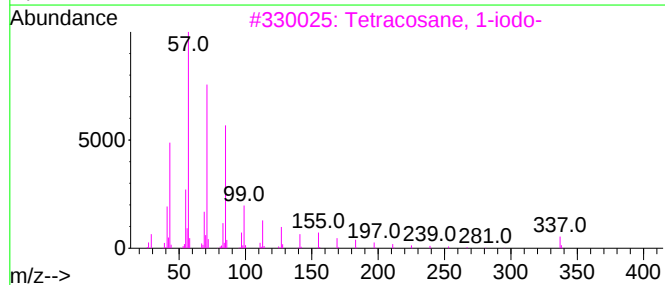
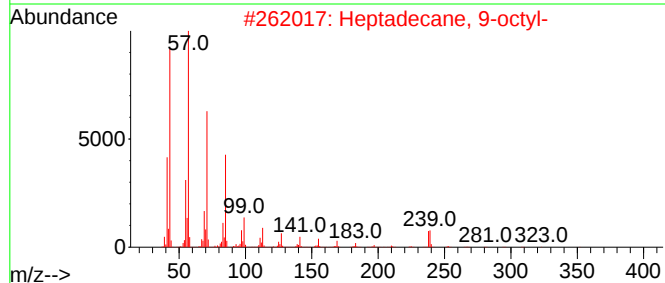
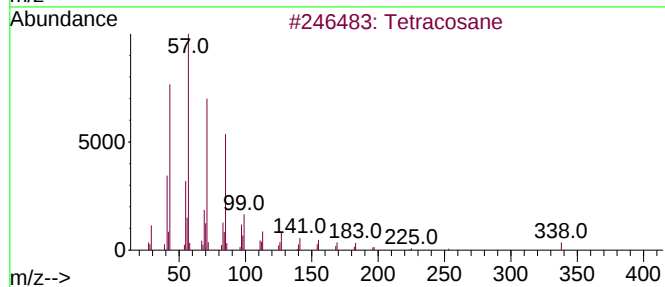
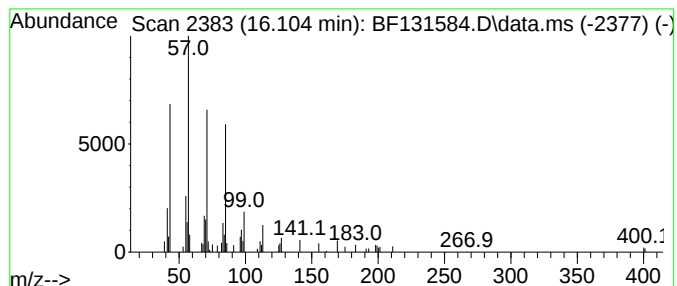
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Tetracosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.104	2.69 ng	58926	Perylene-d12	15.621

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	91
2			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
3			Tetracosane, 1-iodo-	464	C24H49I	1000406-32-0	91
4			Octacosane	394	C28H58	000630-02-4	91
5			Docosane, 1-iodo-	436	C22H45I	1000406-31-9	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121022\
Data File : BF131584.D
Acq On : 10 Dec 2022 11:57
Operator : CG\JU
Sample : PB149515BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB149515BL

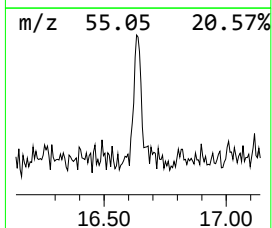
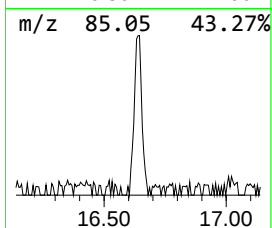
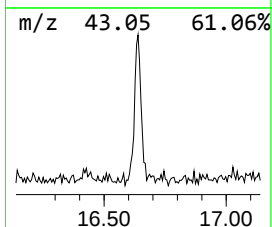
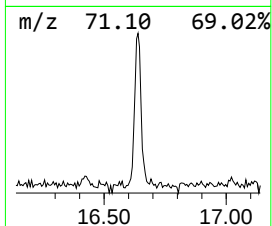
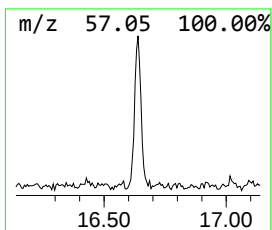
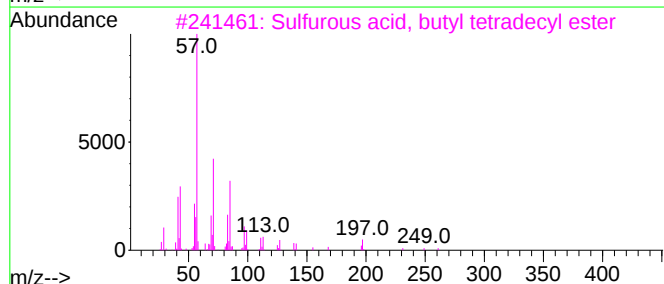
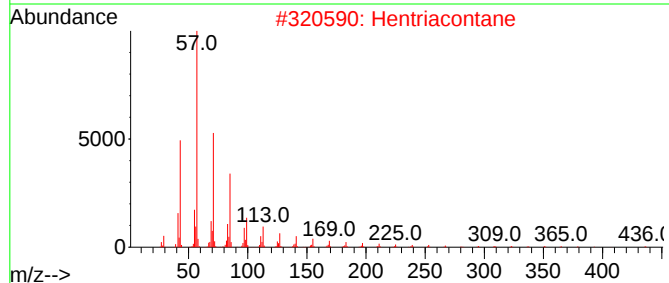
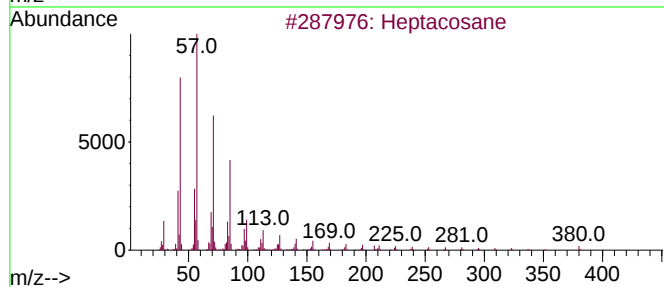
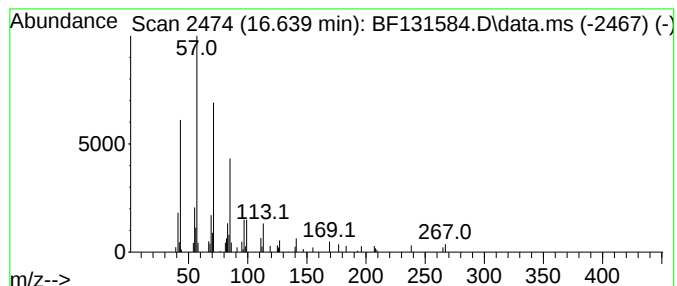
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Heptacosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.639	3.27 ng	71816	Perylene-d12	15.621

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosane	380	C27H56	000593-49-7	87
2			Hentriacontane	437	C31H64	000630-04-6	87
3			Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1010309-18-1	86
4			Hexatriacontane	507	C36H74	000630-06-8	86
5			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121022\
Data File : BF131584.D
Acq On : 10 Dec 2022 11:57
Operator : CG\JU
Sample : PB149515BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB149515BL

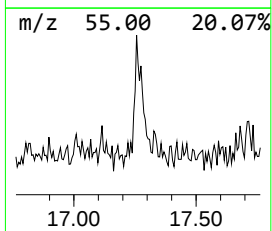
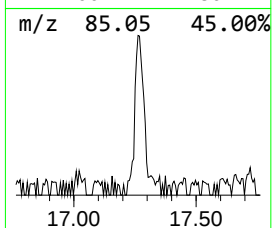
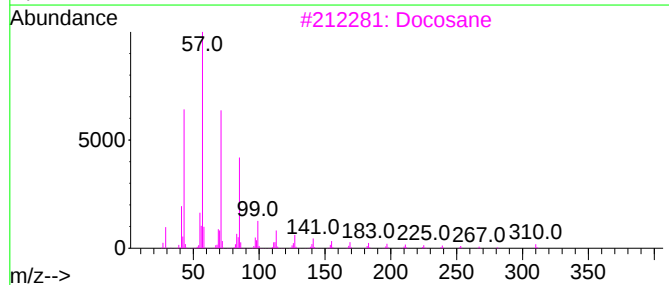
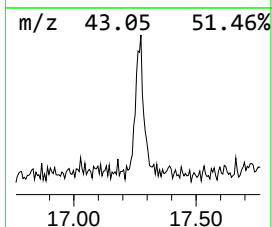
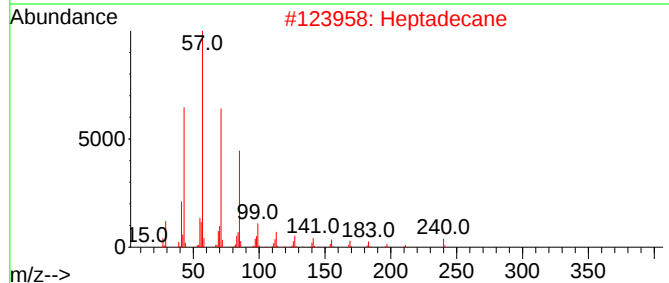
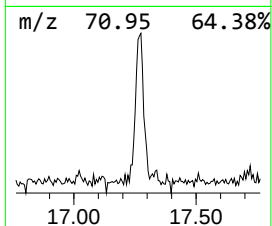
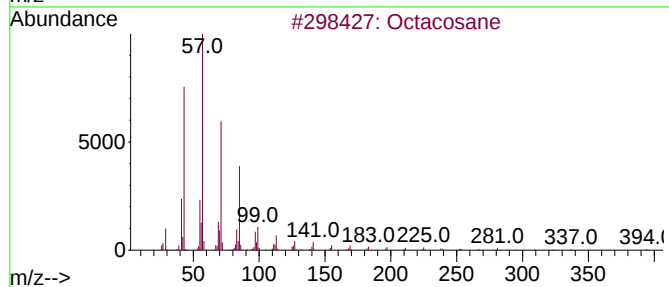
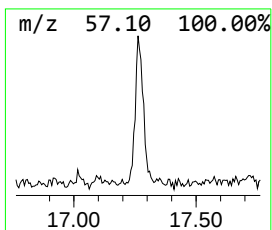
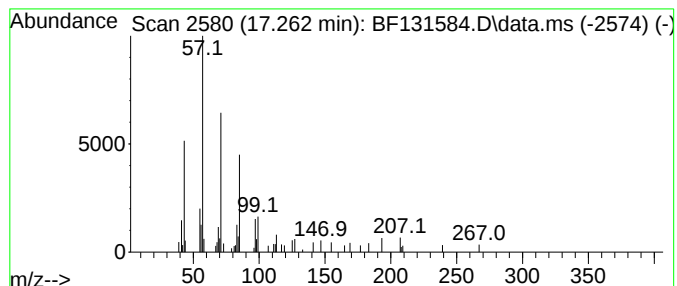
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Octacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.262	2.93 ng	64228	Perylene-d12	15.621

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	80
2			Heptadecane	240	C17H36	000629-78-7	80
3			Docosane	310	C22H46	000629-97-0	80
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	72
5			Triacontane	422	C30H62	000638-68-6	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121022\
Data File : BF131584.D
Acq On : 10 Dec 2022 11:57
Operator : CG\JU
Sample : PB149515BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB149515BL

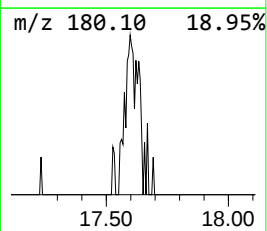
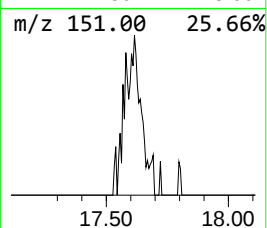
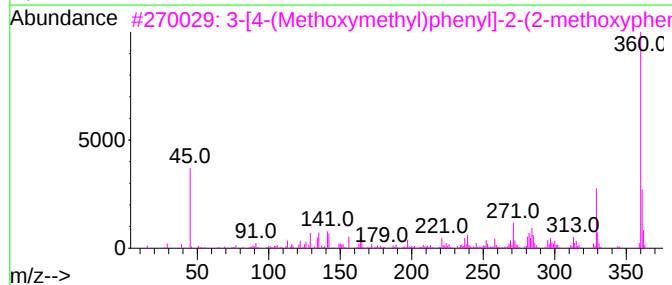
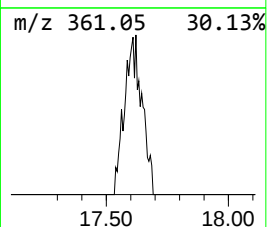
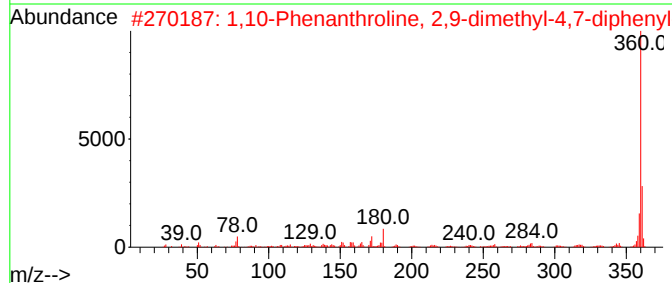
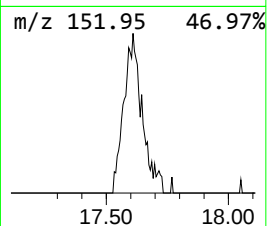
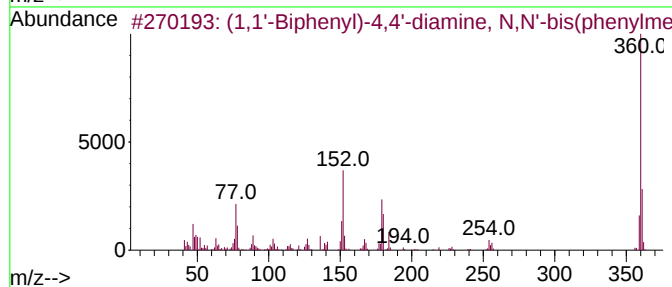
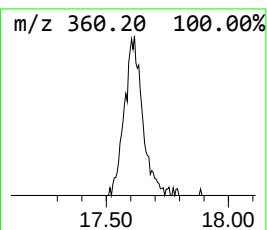
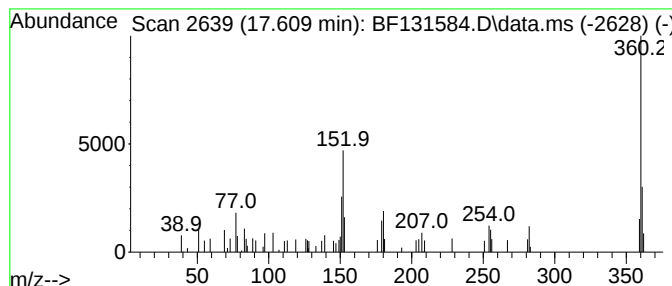
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 (1,1'-Biphenyl)-4,4'-diamin... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.609	2.96 ng	64992	Perylene-d12	15.621

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(1,1'-Biphenyl)-4,4'-diamine, N...	360	C26H20N2	006311-48-4	81
2			1,10-Phenanthroline, 2,9-dimethy...	360	C26H20N2	004733-39-5	43
3			3-[4-(Methoxymethyl)phenyl]-2-(2...	360	C23H20O2S	1000458-33-8	43
4			Ethene, 1-(anthracen-9-yl)-2-(4-...	360	C27H20O	1000163-55-1	43
5			1H-isindole-1,3(2H)-dione, 2-[5...	360	C21H16N2O4	1000398-48-8	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121022\
Data File : BF131584.D
Acq On : 10 Dec 2022 11:57
Operator : CG\JU
Sample : PB149515BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB149515BL

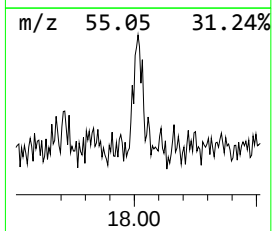
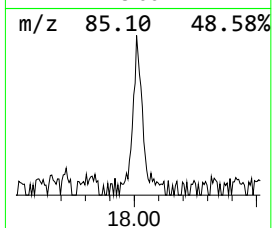
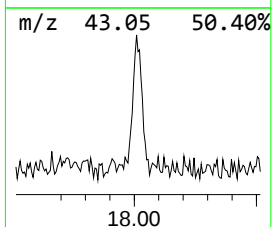
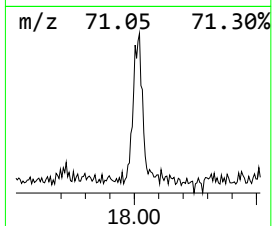
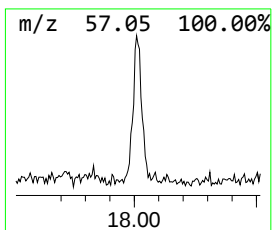
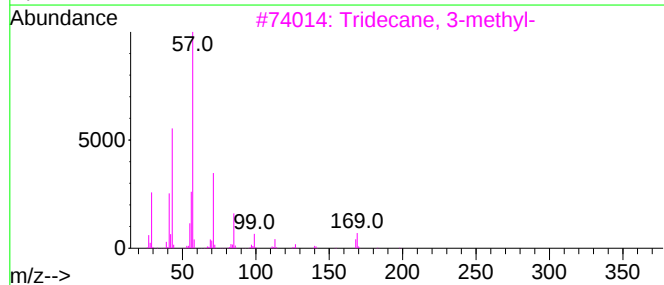
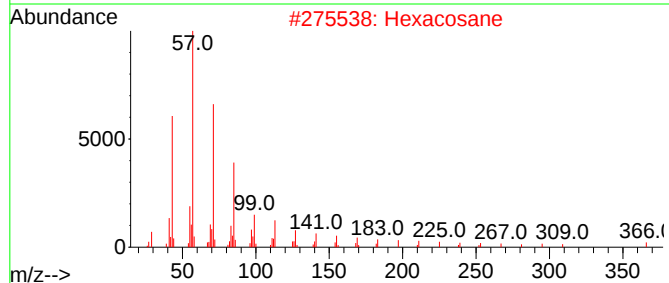
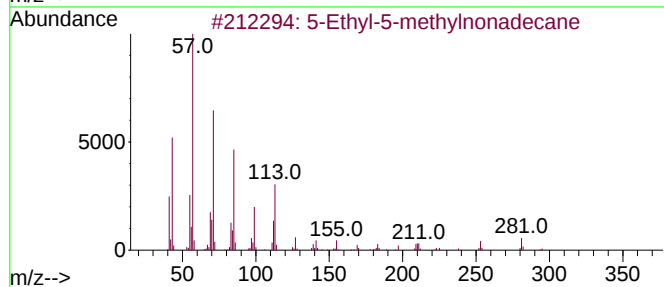
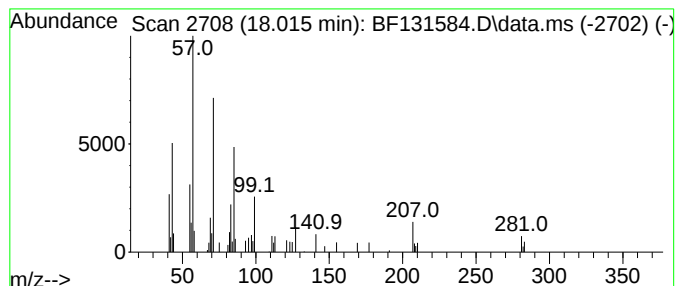
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 5-Ethyl-5-methylnonadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.015	2.42 ng	53159	Perylene-d12	15.621

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Ethyl-5-methylnonadecane	310	C22H46	1000360-42-7	83
2			Hexacosane	366	C26H54	000630-01-3	59
3			Tridecane, 3-methyl-	198	C14H30	006418-41-3	59
4			Nonadecane, 2-methyl-	282	C20H42	001560-86-7	59
5			Eicosane, 2-methyl-	296	C21H44	001560-84-5	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121022\
Data File : BF131584.D
Acq On : 10 Dec 2022 11:57
Operator : CG\JU
Sample : PB149515BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB149515BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.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...	2.216	2.9	ng	56780	1	6.910	394356	20.0
2-Pentanone, 4-...	5.134	20.6	ng	405511	1	6.910	394356	20.0
Tetracosane	16.104	2.7	ng	58926	6	15.621	438761	20.0
Heptacosane	16.639	3.3	ng	71816	6	15.621	438761	20.0
Octacosane	17.262	2.9	ng	64228	6	15.621	438761	20.0
(1,1'-Biphenyl)...	17.609	3.0	ng	64992	6	15.621	438761	20.0
5-Ethyl-5-methy...	18.015	2.4	ng	53159	6	15.621	438761	20.0