

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111122\
 Data File : BF131155.D
 Acq On : 11 Nov 2022 15:08
 Operator : CG\JU
 Sample : N5531-12
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-28A

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-BF110922.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131155.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.210	7	21	27	rVB	218529	344340	13.16%	2.122%
2	2.316	34	39	45	rVB	27680	36071	1.38%	0.222%
3	2.416	51	56	63	rVB	22812	32008	1.22%	0.197%
4	3.040	156	162	168	rBV2	32960	53009	2.03%	0.327%
5	4.499	406	410	414	rBV	93097	103358	3.95%	0.637%
6	5.122	510	516	527	rVB	660868	911295	34.83%	5.617%
7	5.475	573	576	578	rBV	36915	33496	1.28%	0.206%
8	5.516	578	583	586	rVV	2134230	2155527	82.40%	13.286%
9	5.898	644	648	653	rBV	37491	31637	1.21%	0.195%
10	6.516	748	753	756	rBV	2026111	2230340	85.25%	13.747%
11	6.881	812	815	819	rBV	542154	420106	16.06%	2.589%
12	7.451	906	912	915	rVB	1616609	1589180	60.75%	9.795%
13	8.081	1012	1019	1029	rBV2	37452	89492	3.42%	0.552%
14	8.163	1029	1033	1037	rVB	495563	446671	17.07%	2.753%
15	9.245	1211	1217	1220	rBV	3037388	2616082	100.00%	16.125%
16	9.922	1328	1332	1336	rBV	566877	478094	18.28%	2.947%
17	10.716	1463	1467	1476	rBV	1439345	1306071	49.92%	8.050%
18	11.416	1582	1586	1589	rBV	467228	377932	14.45%	2.329%
19	12.633	1789	1793	1800	rVB	26607	32739	1.25%	0.202%
20	12.863	1827	1832	1835	rBV	35919	38749	1.48%	0.239%
21	13.004	1852	1856	1860	rVB	1783090	1681674	64.28%	10.365%
22	13.980	2015	2022	2029	rBV5	40970	119005	4.55%	0.734%
23	14.063	2032	2036	2039	rVV	396662	389777	14.90%	2.402%
24	14.092	2039	2041	2046	rVB	40958	37836	1.45%	0.233%
25	14.157	2047	2052	2057	rBV	114659	119761	4.58%	0.738%
26	14.216	2059	2062	2066	rBV	27789	38309	1.46%	0.236%
27	14.521	2110	2114	2117	rVB	42924	45071	1.72%	0.278%
28	14.833	2164	2167	2171	rVB	28220	30903	1.18%	0.190%
29	15.180	2222	2226	2231	rVB	69541	81419	3.11%	0.502%
30	15.557	2286	2290	2298	rVB	220679	295258	11.29%	1.820%
31	16.010	2364	2367	2373	rVB	40211	58788	2.25%	0.362%

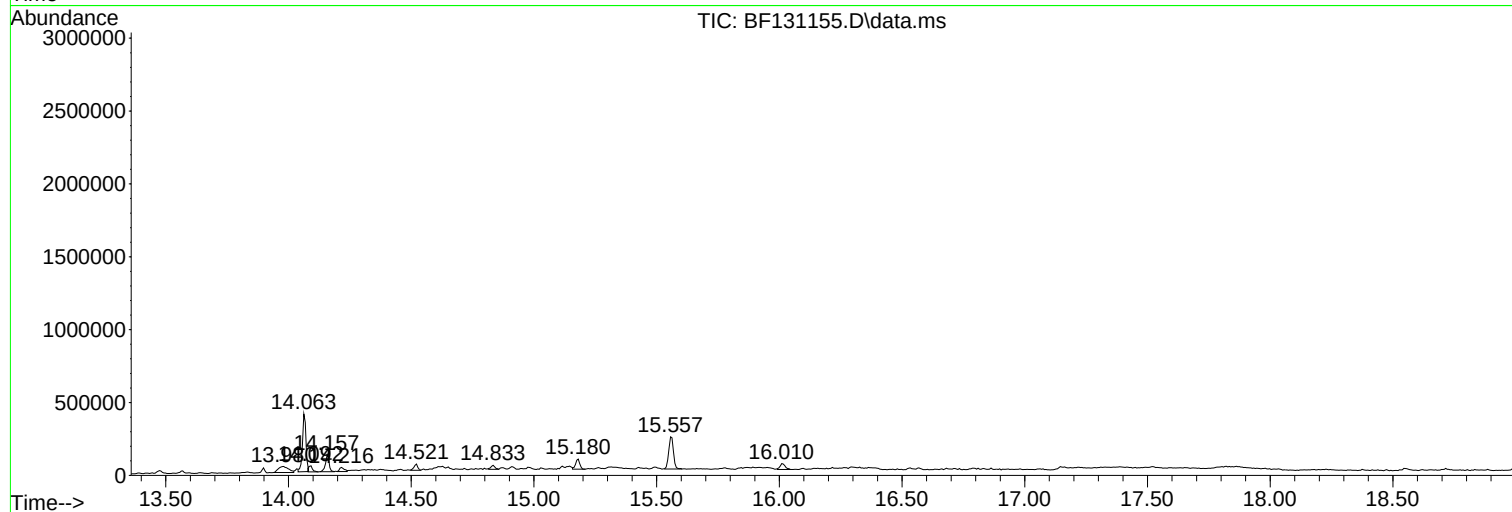
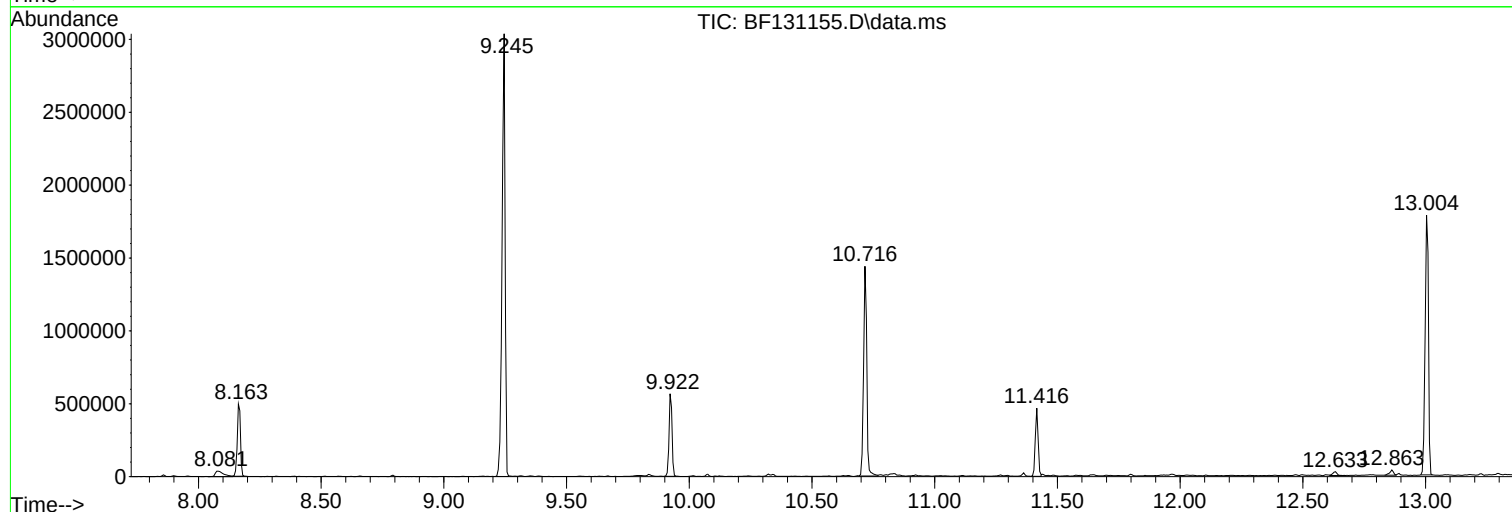
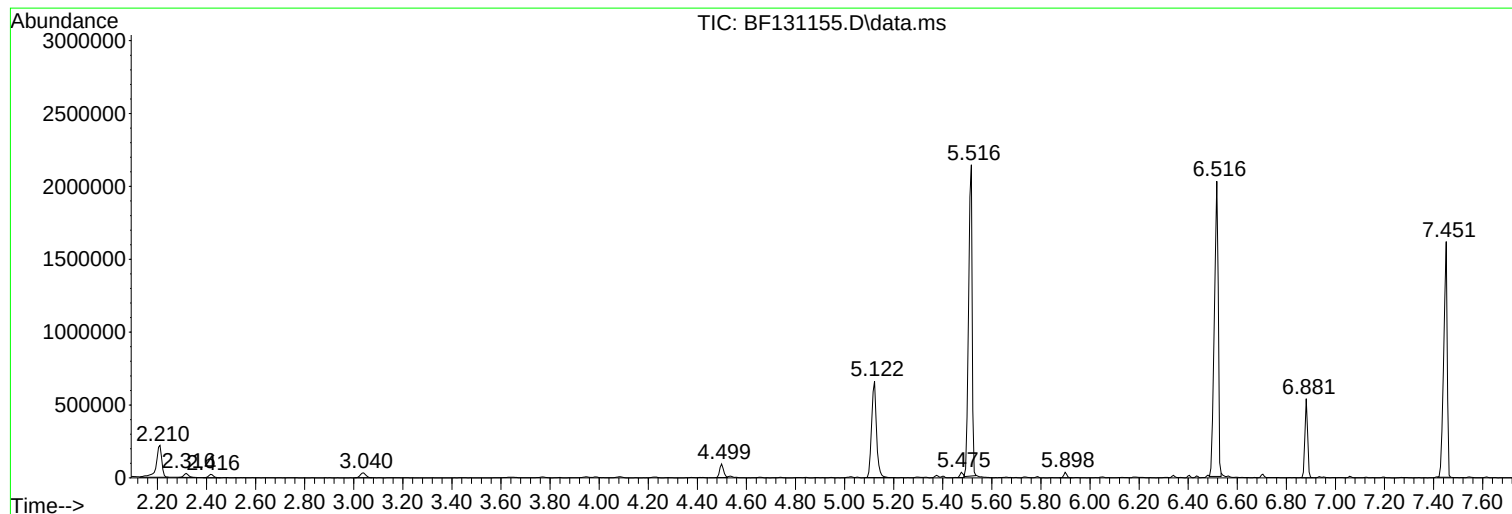
Sum of corrected areas: 16223998

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111122\
Data File : BF131155.D
Acq On : 11 Nov 2022 15:08
Operator : CG\JU
Sample : N5531-12
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-28A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.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\BF111122\
Data File : BF131155.D
Acq On : 11 Nov 2022 15:08
Operator : CG\JU
Sample : N5531-12
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-28A

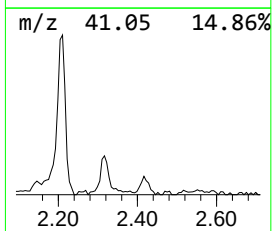
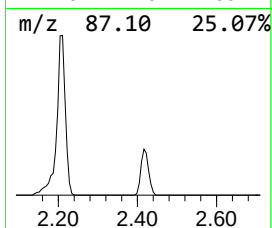
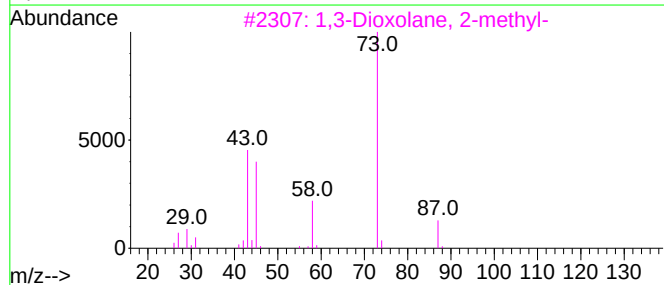
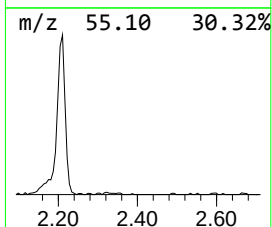
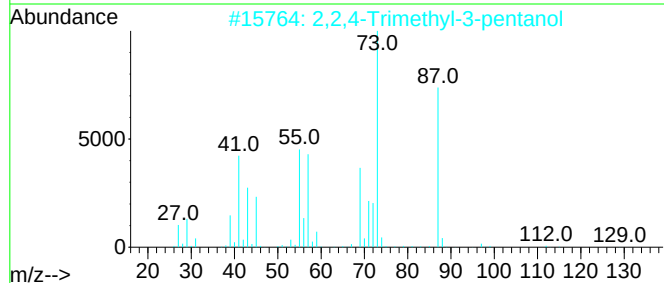
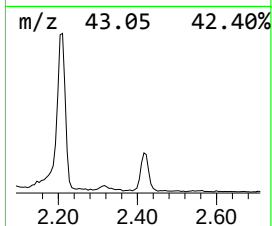
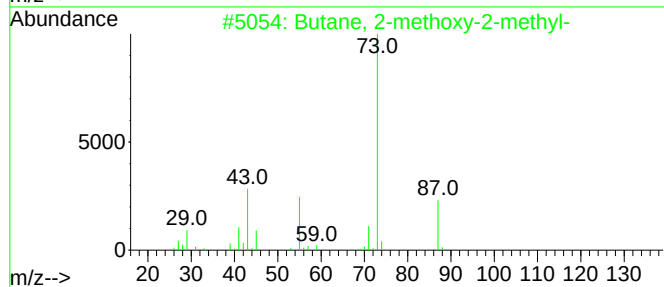
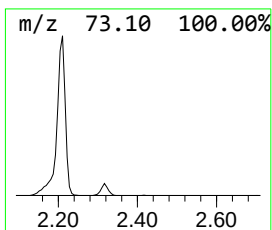
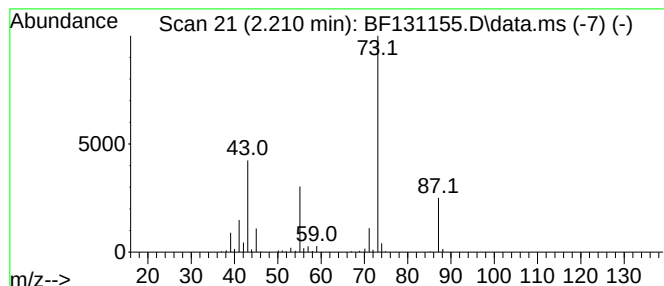
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.210	16.39 ng	344340	1,4-Dichlorobenzene-d4	6.881

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			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	17
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111122\
Data File : BF131155.D
Acq On : 11 Nov 2022 15:08
Operator : CG\JU
Sample : N5531-12
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-28A

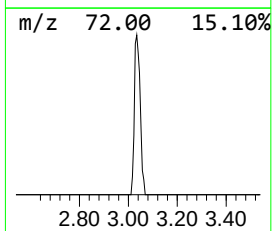
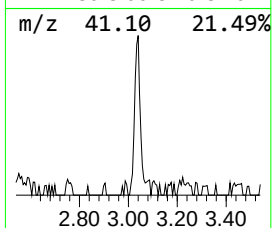
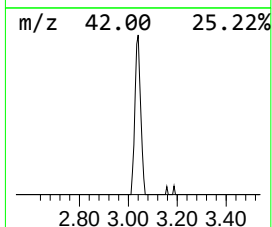
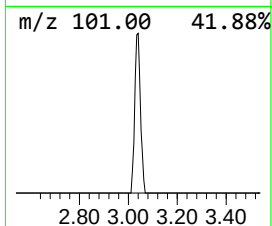
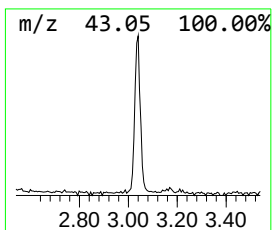
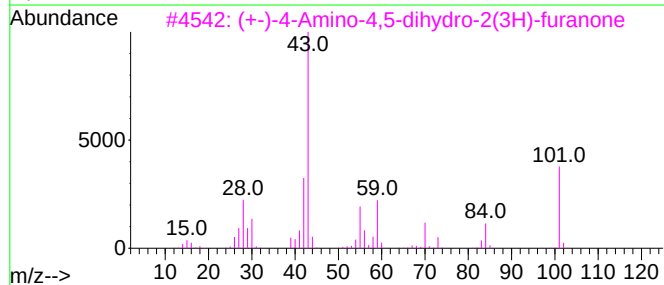
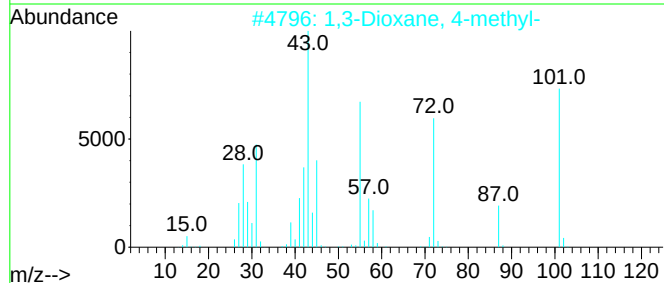
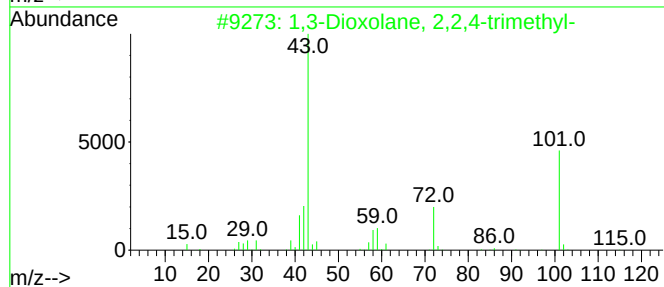
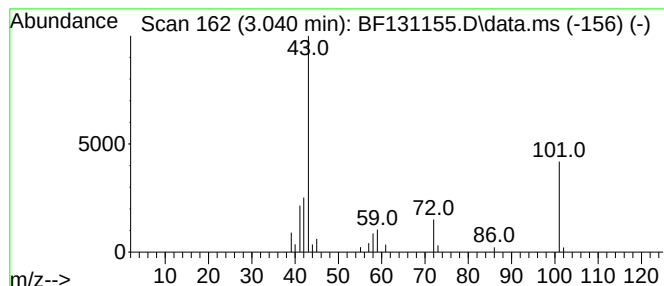
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 1,3-Dioxolane, 2,2,4-trimet... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.040	2.52 ng	53009	1,4-Dichlorobenzene-d4	6.881

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,3-Dioxolane, 2,2,4-trimethyl-	116	C6H12O2	001193-11-9	83
2		1,3-Dioxane, 4-methyl-	102	C5H10O2	001120-97-4	40
3		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	38
4		2-Butanone, 4-hydroxy-3-methyl-	102	C5H10O2	003393-64-4	9
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111122\
Data File : BF131155.D
Acq On : 11 Nov 2022 15:08
Operator : CG\JU
Sample : N5531-12
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-28A

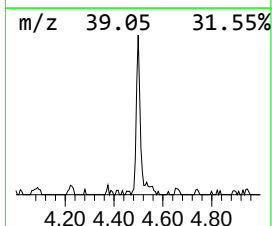
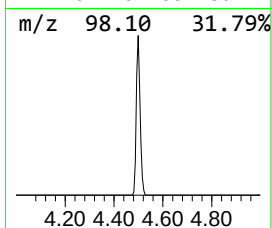
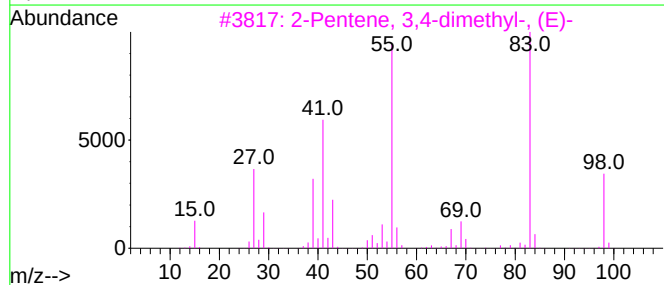
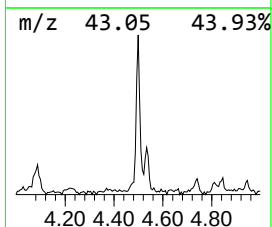
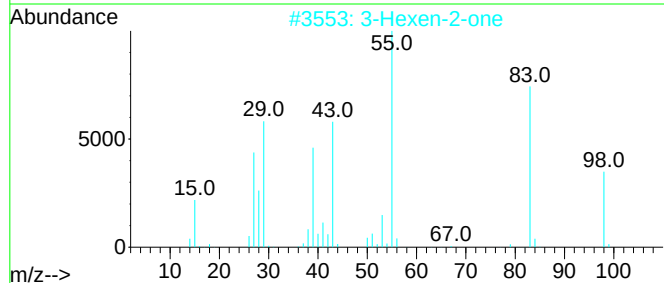
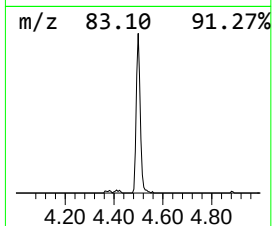
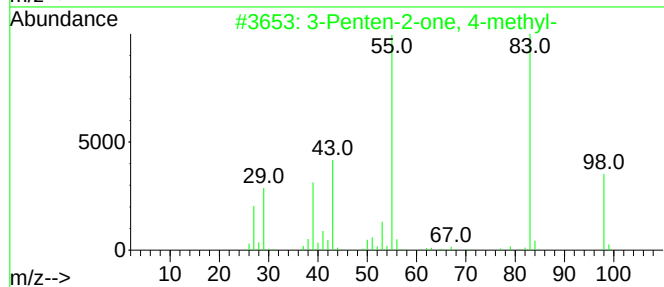
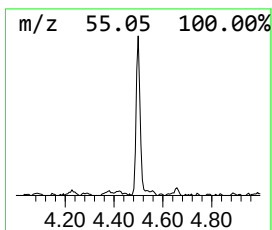
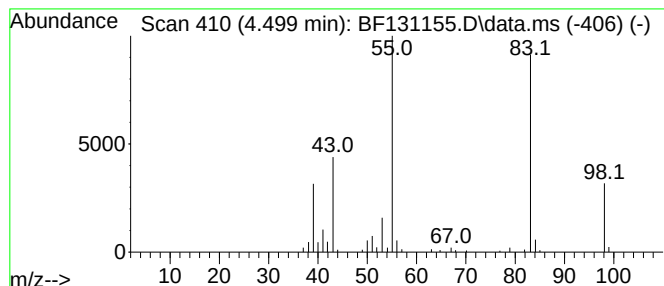
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 3-Penten-2-one, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.499	4.92 ng	103358	1,4-Dichlorobenzene-d4	6.881

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
2			3-Hexen-2-one	98	C6H10O	000763-93-9	91
3			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111122\
Data File : BF131155.D
Acq On : 11 Nov 2022 15:08
Operator : CG\JU
Sample : N5531-12
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-28A

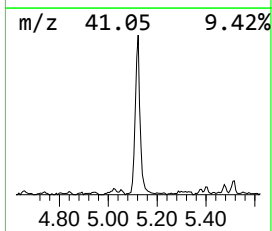
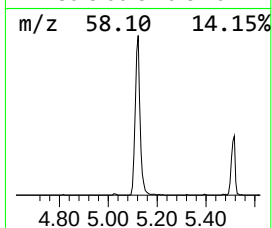
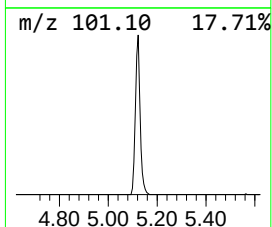
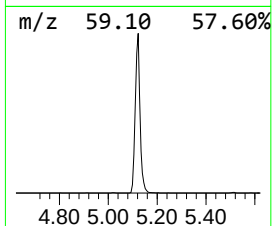
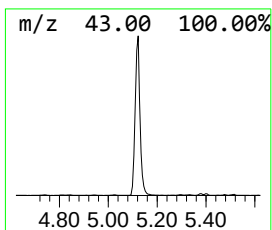
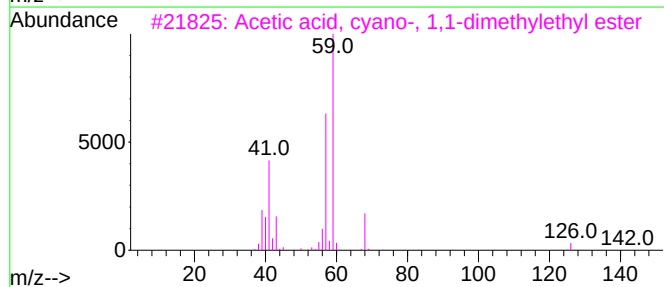
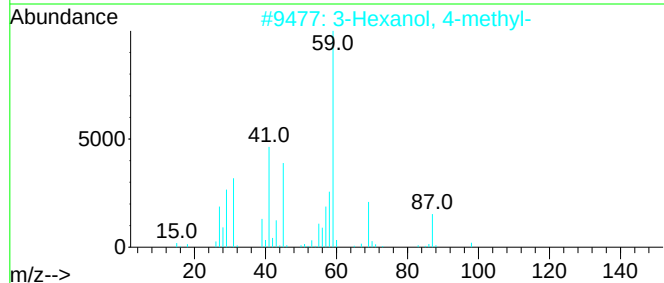
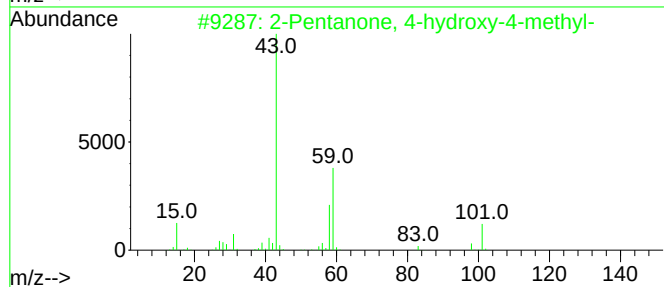
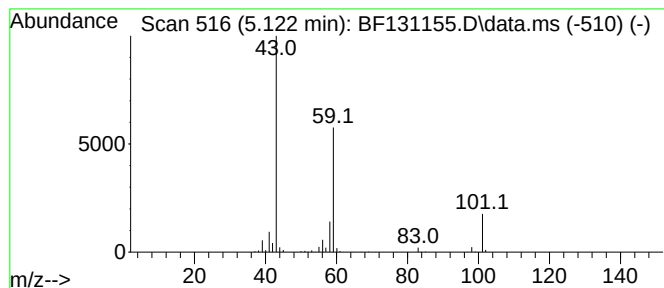
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.122	43.38 ng	911295	1,4-Dichlorobenzene-d4	6.881

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59		
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111122\
Data File : BF131155.D
Acq On : 11 Nov 2022 15:08
Operator : CG\JU
Sample : N5531-12
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-28A

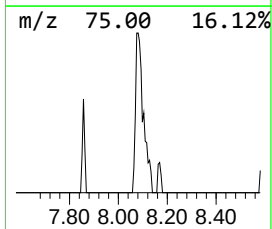
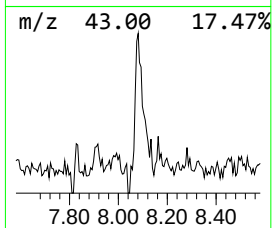
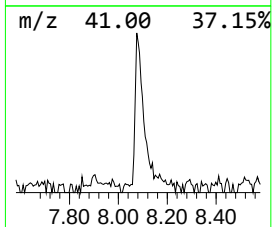
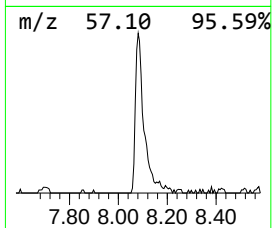
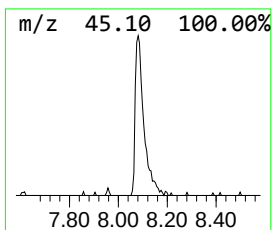
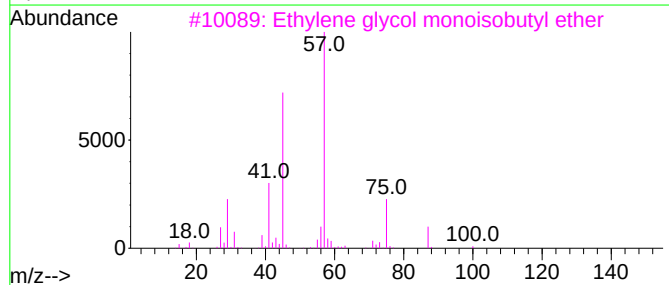
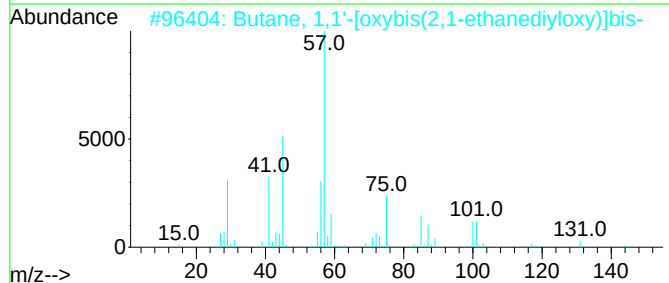
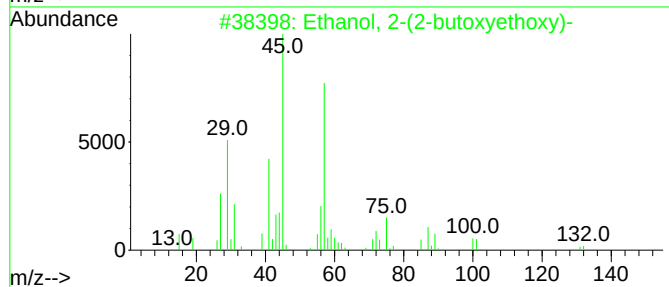
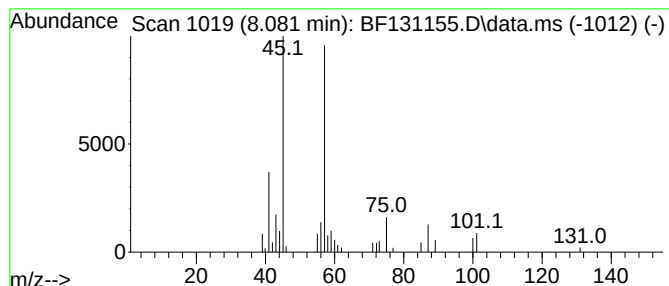
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.081	4.01 ng	89492	Naphthalene-d8	8.163

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	78
2			Butane, 1,1'-[oxybis(2,1-ethaned...	218	C12H26O3	000112-73-2	72
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
4			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
5			Di-sec-Butyl ether	130	C8H18O	006863-58-7	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111122\
Data File : BF131155.D
Acq On : 11 Nov 2022 15:08
Operator : CG\JU
Sample : N5531-12
Misc :
ALS Vial : 10 Sample Multiplier: 1

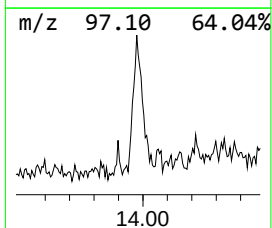
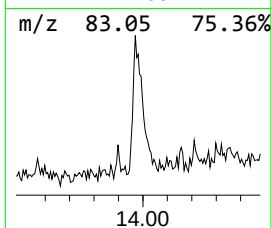
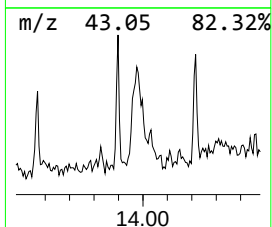
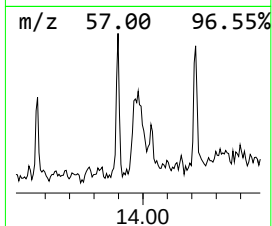
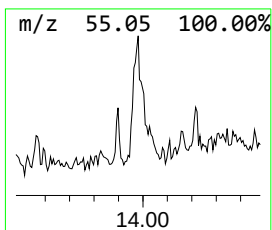
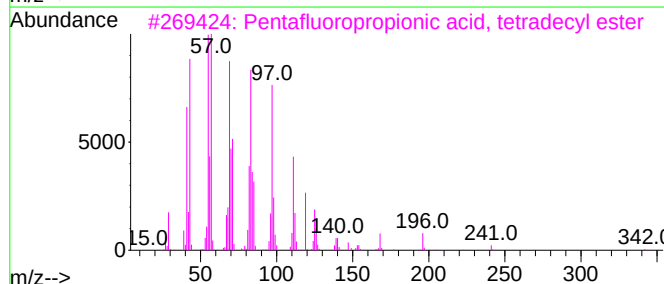
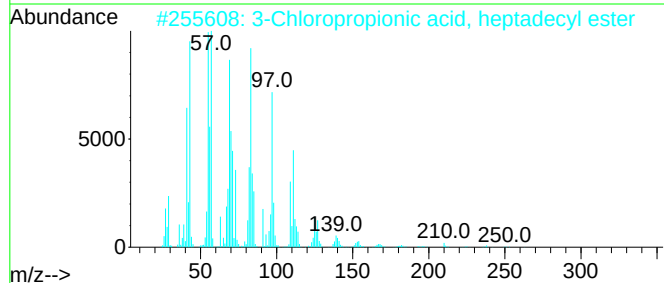
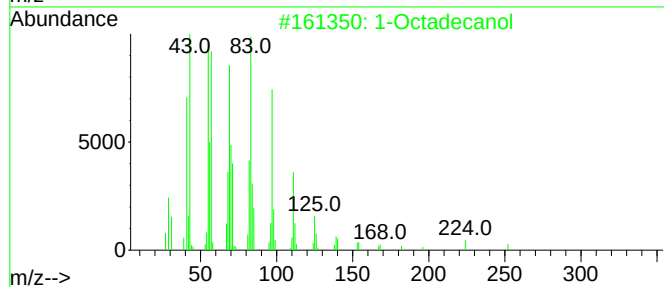
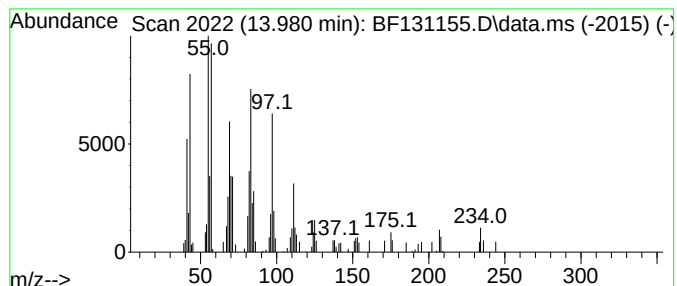
Instrument :
BNA_F
ClientSampleId :
SB-28A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.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-Octadecanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.980	6.11 ng	119005	Chrysene-d12	14.063	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecanol	270	C18H38O	000112-92-5	93
2	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	87
3	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	87
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	87
5	n-Heptadecanol-1	256	C17H36O	001454-85-9	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111122\
Data File : BF131155.D
Acq On : 11 Nov 2022 15:08
Operator : CG\JU
Sample : N5531-12
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-28A

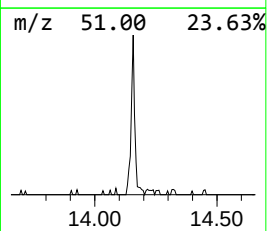
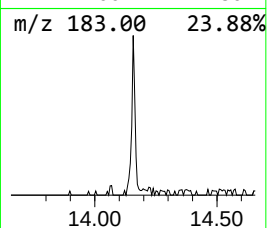
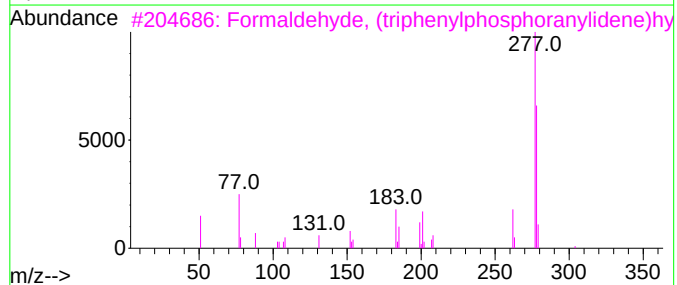
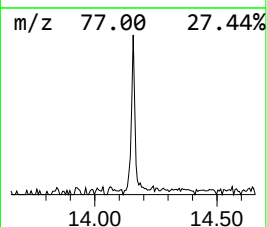
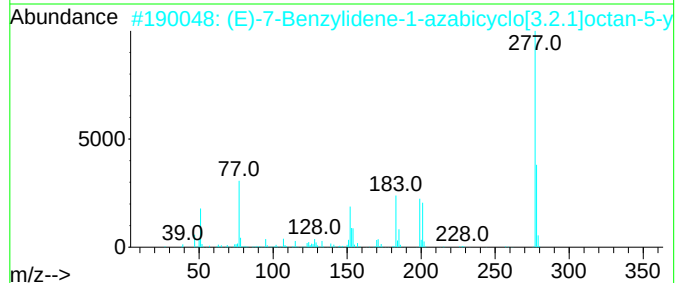
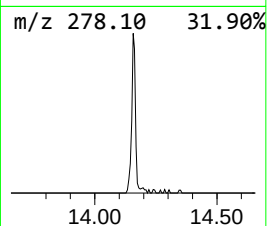
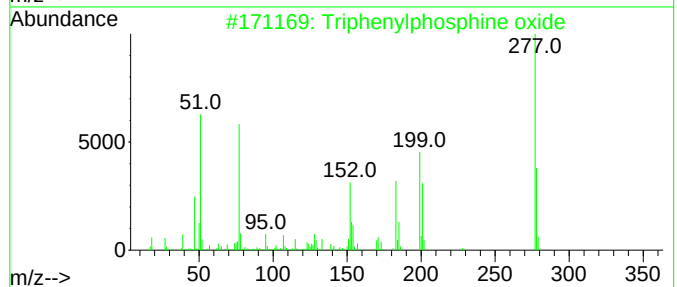
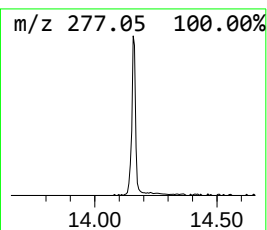
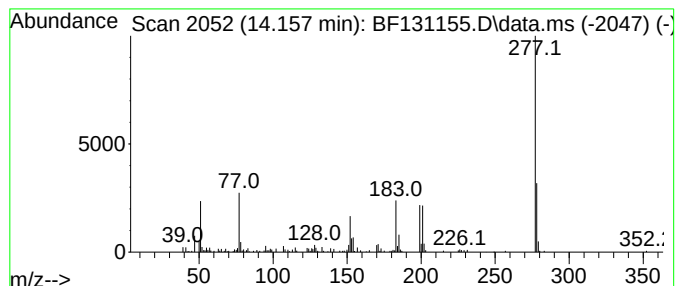
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Triphenylphosphine oxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.157	6.15 ng	119761	Chrysene-d12	14.063

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	97
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	93
3			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	50
4			Benzoic acid, 2-(diphenylphosphi...	306	C19H15O2P	017261-28-8	45
5			(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111122\
Data File : BF131155.D
Acq On : 11 Nov 2022 15:08
Operator : CG\JU
Sample : N5531-12
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-28A

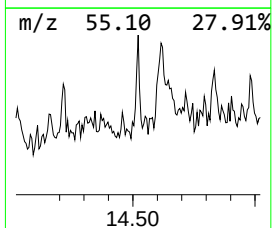
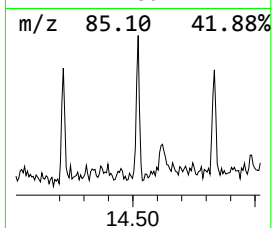
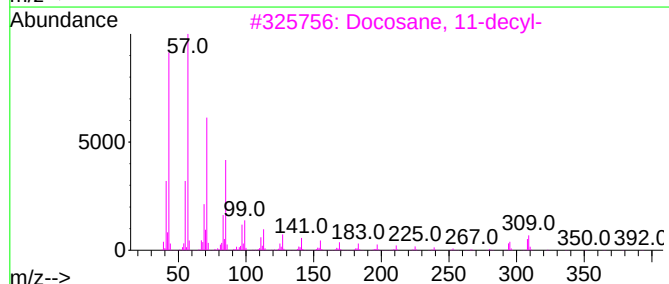
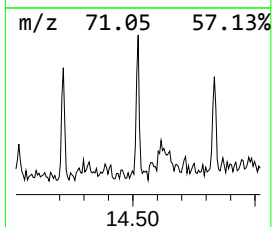
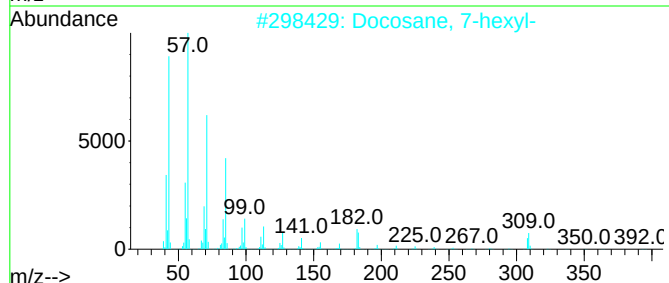
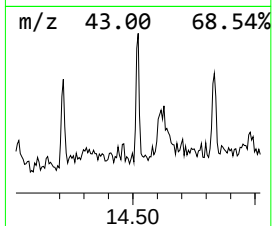
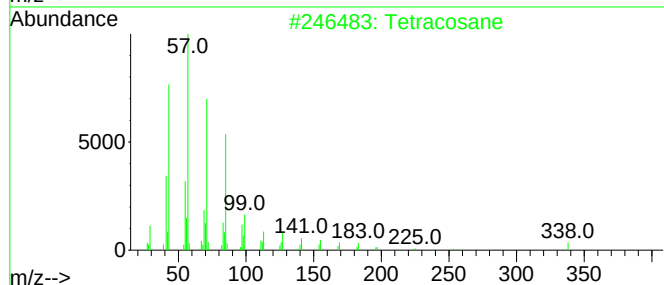
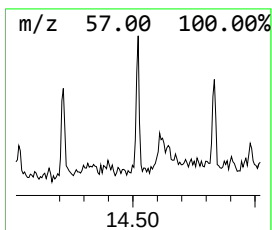
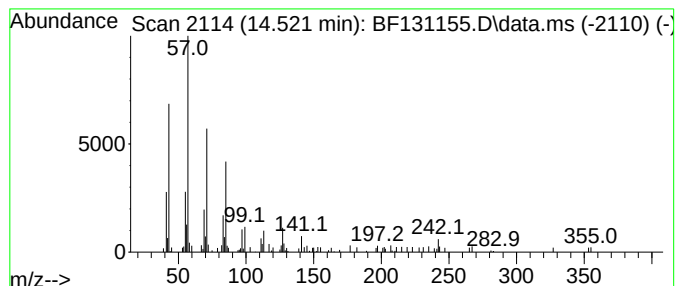
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tetracosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.521	2.31 ng	45071	Chrysene-d12	14.063

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	91
2			Docosane, 7-hexyl-	394	C28H58	055373-86-9	91
3			Docosane, 11-decyl-	451	C32H66	055401-55-3	91
4			Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	90
5			Tetracosane, 11-decyl-	479	C34H70	055429-84-0	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111122\
Data File : BF131155.D
Acq On : 11 Nov 2022 15:08
Operator : CG\JU
Sample : N5531-12
Misc :
ALS Vial : 10 Sample Multiplier: 1

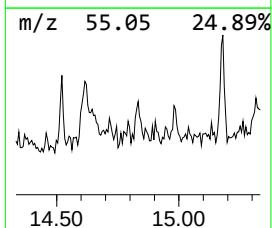
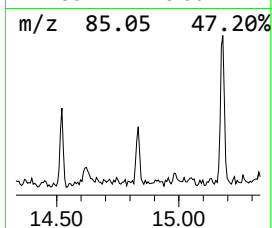
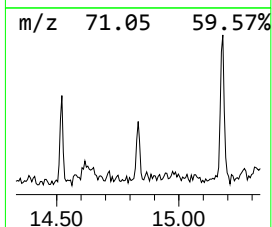
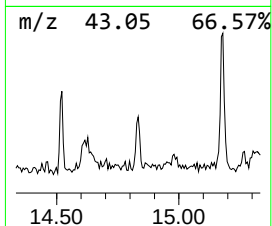
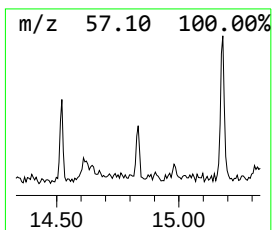
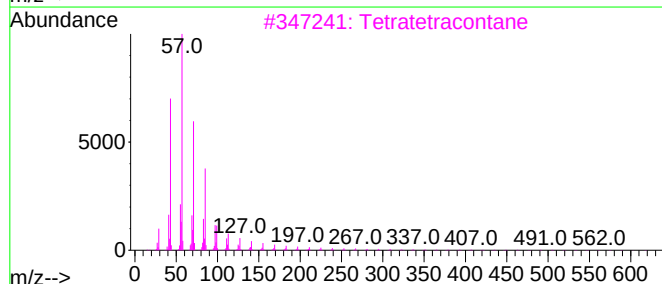
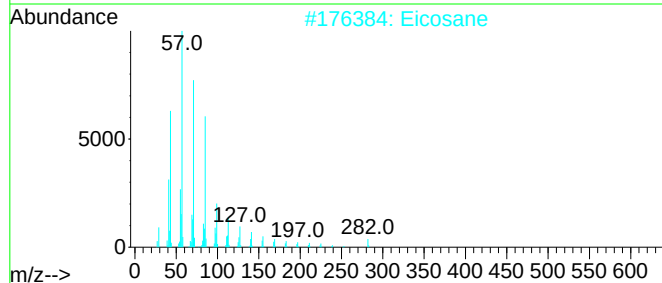
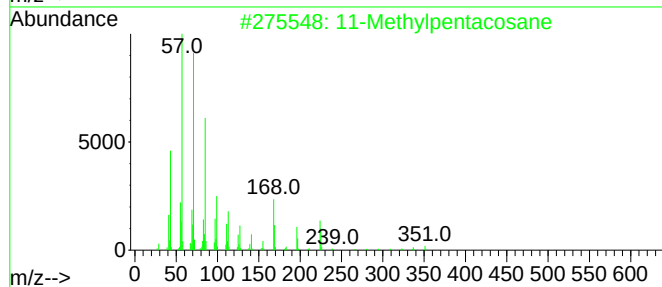
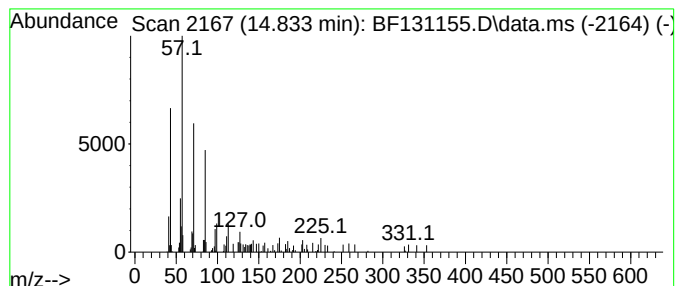
Instrument :
BNA_F
ClientSampleId :
SB-28A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 11-Methylpentacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.833	2.09 ng	30903	Perylene-d12	15.557	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11-Methylpentacosane	366	C26H54	015689-71-1	80
2	Eicosane	282	C20H42	000112-95-8	80
3	Tetratetracontane	619	C44H90	007098-22-8	80
4	Octacosane, 2-methyl-	408	C29H60	001560-98-1	80
5	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111122\
Data File : BF131155.D
Acq On : 11 Nov 2022 15:08
Operator : CG\JU
Sample : N5531-12
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-28A

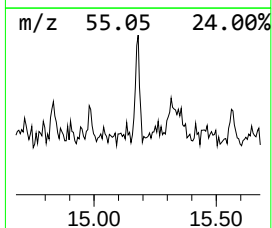
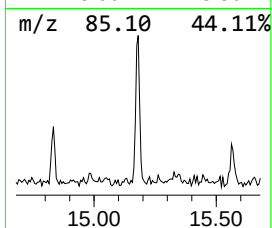
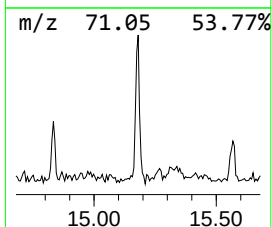
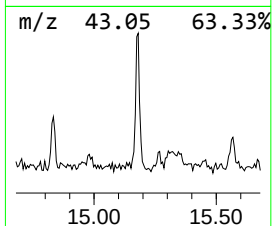
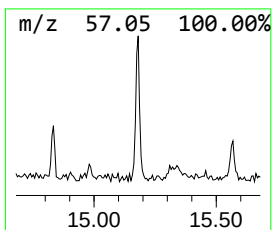
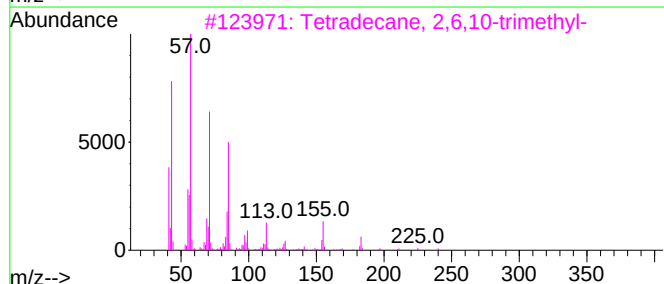
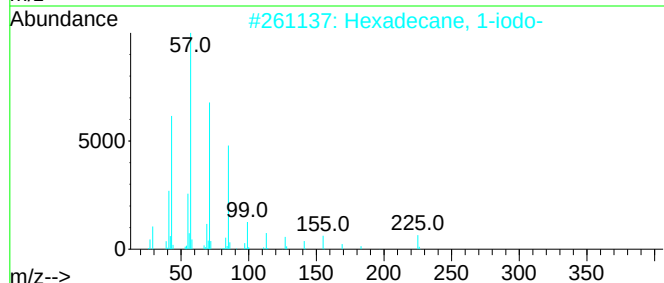
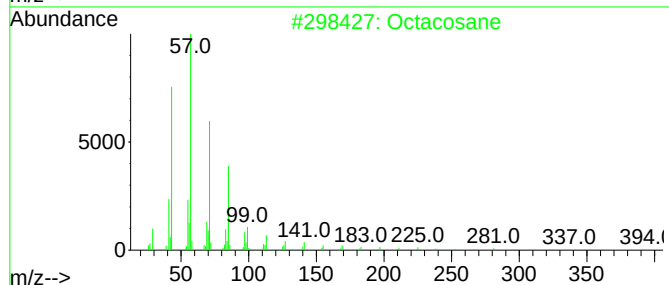
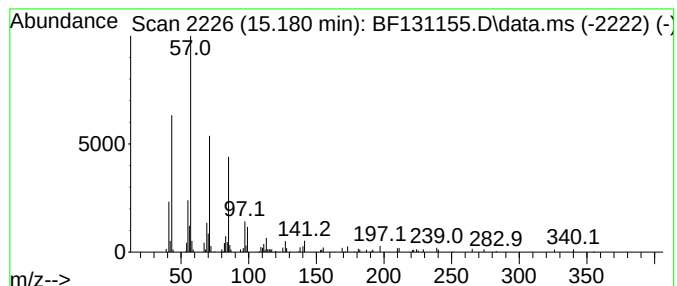
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.180	5.52 ng	81419	Perylene-d12	15.557

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octacosane	394	C28H58	000630-02-4	87
2		Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	83
3		Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	83
4		Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	80
5		Heneicosane	296	C21H44	000629-94-7	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111122\
Data File : BF131155.D
Acq On : 11 Nov 2022 15:08
Operator : CG\JU
Sample : N5531-12
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-28A

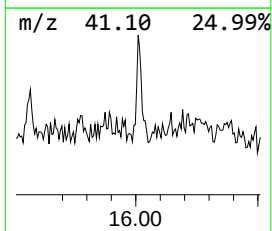
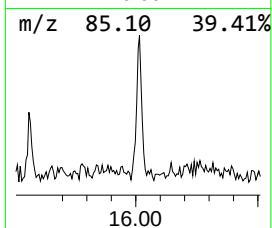
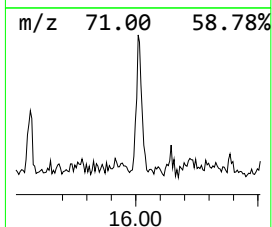
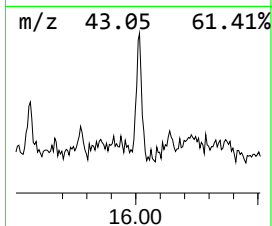
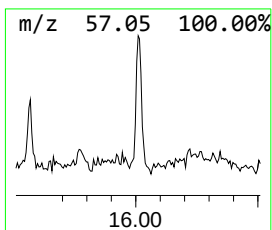
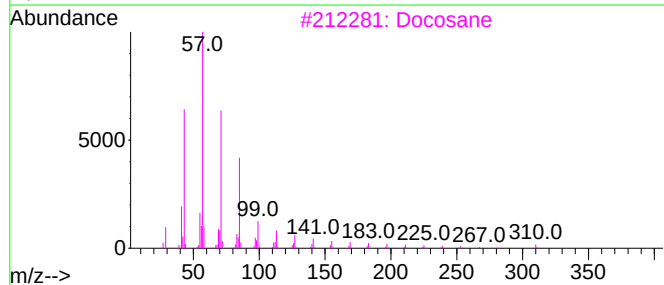
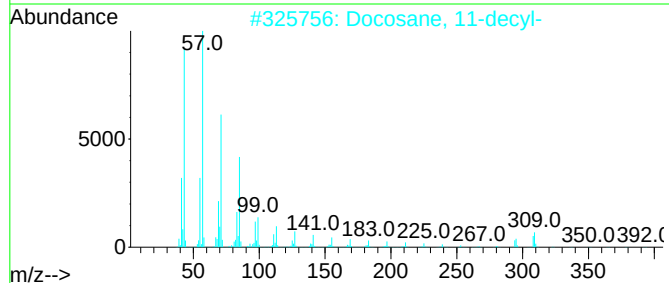
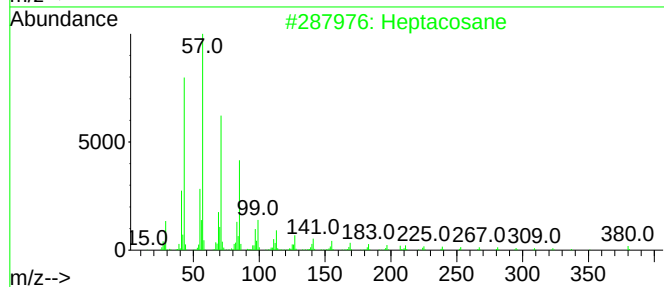
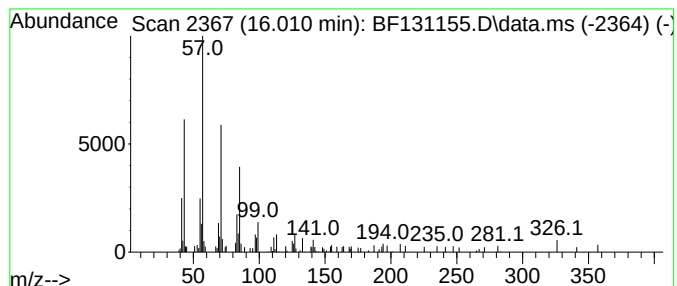
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Heptacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.010	3.98 ng	58788	Perylene-d12	15.557

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptacosane	380	C27H56	000593-49-7	81
2		Docosane, 11-decyl-	451	C32H66	055401-55-3	74
3		Docosane	310	C22H46	000629-97-0	74
4		Hentriacontane	437	C31H64	000630-04-6	74
5		Heneicosane	296	C21H44	000629-94-7	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111122\
Data File : BF131155.D
Acq On : 11 Nov 2022 15:08
Operator : CG\JU
Sample : N5531-12
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-28A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.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...	2.210	16.4	ng	344340	1	6.881	420106	20.0
1,3-Dioxolane, ...	3.040	2.5	ng	53009	1	6.881	420106	20.0
3-Penten-2-one,...	4.499	4.9	ng	103358	1	6.881	420106	20.0
2-Pentanone, 4-...	5.122	43.4	ng	911295	1	6.881	420106	20.0
Ethanol, 2-(2-b...	8.081	4.0	ng	89492	2	8.163	446671	20.0
1-Octadecanol	13.980	6.1	ng	119005	5	14.063	389777	20.0
Triphenylphosph...	14.157	6.2	ng	119761	5	14.063	389777	20.0
Tetracosane	14.521	2.3	ng	45071	5	14.063	389777	20.0
11-Methylpentac...	14.833	2.1	ng	30903	6	15.557	295258	20.0
Octacosane	15.180	5.5	ng	81419	6	15.557	295258	20.0
Heptacosane	16.010	4.0	ng	58788	6	15.557	295258	20.0