

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072821\
 Data File : BF124833.D
 Acq On : 28 Jul 2021 18:15
 Operator : JU/CG
 Sample : M3205-02
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 VNJ-209

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-BF072221.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124833.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.134	4	8	12	rBB	12737	14349	6.63%	1.051%
2	5.092	508	511	516	rBB	6300	6394	2.96%	0.468%
3	5.487	574	578	581	rBV	163914	150196	69.44%	11.005%
4	6.498	745	750	753	rBV	158188	153399	70.92%	11.240%
5	6.869	810	813	816	rBB	42958	29381	13.58%	2.153%
6	7.433	904	909	912	rBB	118335	104321	48.23%	7.644%
7	8.051	1012	1014	1019	rBB	6014	4962	2.29%	0.364%
8	8.151	1028	1031	1034	rBB	54802	41373	19.13%	3.031%
9	9.227	1210	1214	1217	rBV	241179	212109	98.06%	15.541%
10	9.910	1326	1330	1333	rBB	59624	50517	23.36%	3.701%
11	10.698	1460	1464	1467	rBV	171151	136144	62.94%	9.975%
12	11.398	1579	1583	1585	rBV	61607	53553	24.76%	3.924%
13	11.416	1585	1586	1589	rVB	12242	7699	3.56%	0.564%
14	11.915	1669	1671	1674	rBB2	12967	9972	4.61%	0.731%
15	12.004	1684	1686	1689	rBV2	2806	2628	1.21%	0.193%
16	12.604	1785	1788	1791	rBB	18403	15695	7.26%	1.150%
17	12.833	1822	1827	1831	rBB	17281	16383	7.57%	1.200%
18	12.986	1848	1853	1856	rVB	232058	216297	100.00%	15.848%
19	13.880	2003	2005	2015	rBB3	4971	11004	5.09%	0.806%
20	14.033	2027	2031	2034	rBV2	42528	40011	18.50%	2.932%
21	14.057	2034	2035	2038	rVB	7281	4183	1.93%	0.306%
22	14.527	2112	2115	2121	rBB3	3191	5721	2.64%	0.419%
23	14.786	2156	2159	2165	rBB2	7477	7731	3.57%	0.566%
24	15.074	2205	2208	2211	rBV	5322	6021	2.78%	0.441%
25	15.145	2217	2220	2223	rBB	9037	8306	3.84%	0.609%
26	15.380	2257	2260	2263	rBB	3004	2493	1.15%	0.183%
27	15.445	2267	2271	2274	rBB	4279	4132	1.91%	0.303%
28	15.509	2277	2282	2286	rBV	25461	30401	14.06%	2.227%
29	15.733	2317	2320	2323	rBB	4771	5075	2.35%	0.372%
30	15.968	2356	2360	2362	rBB2	2484	2490	1.15%	0.182%
31	16.774	2493	2497	2502	rBB2	7527	11876	5.49%	0.870%

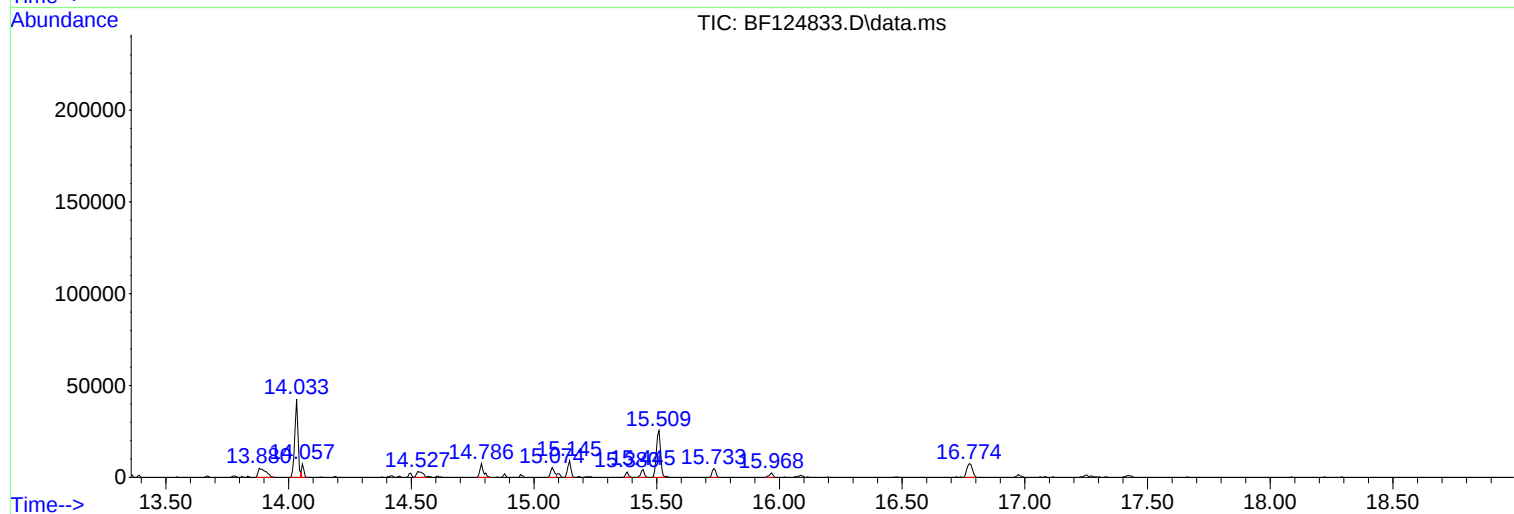
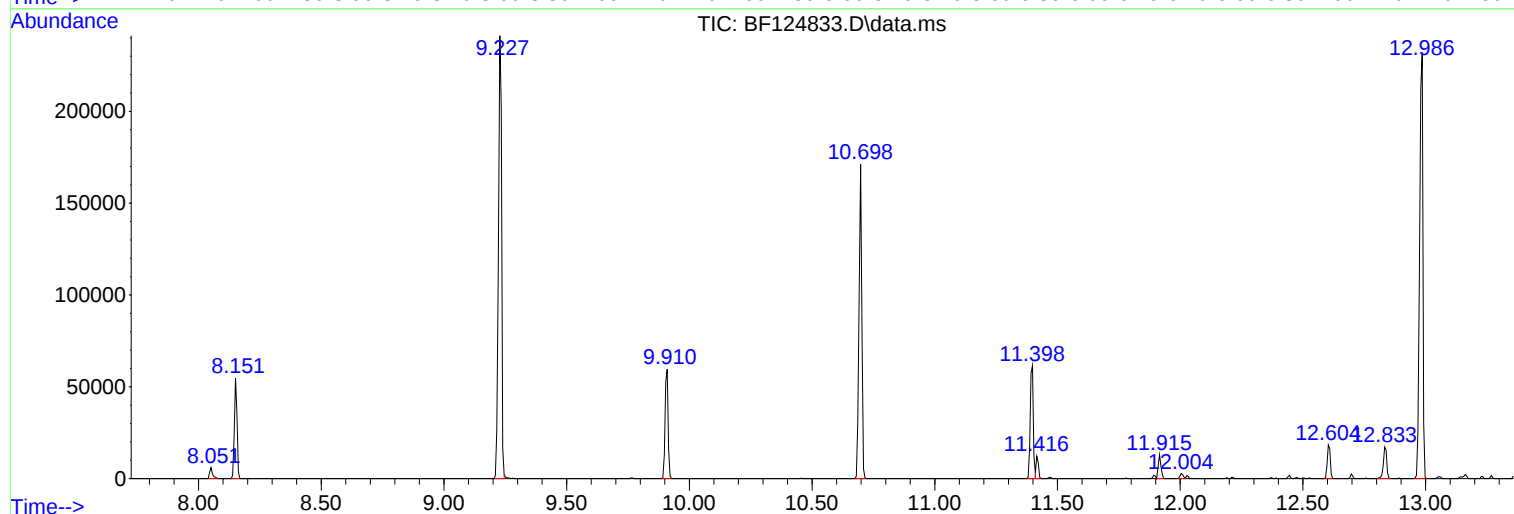
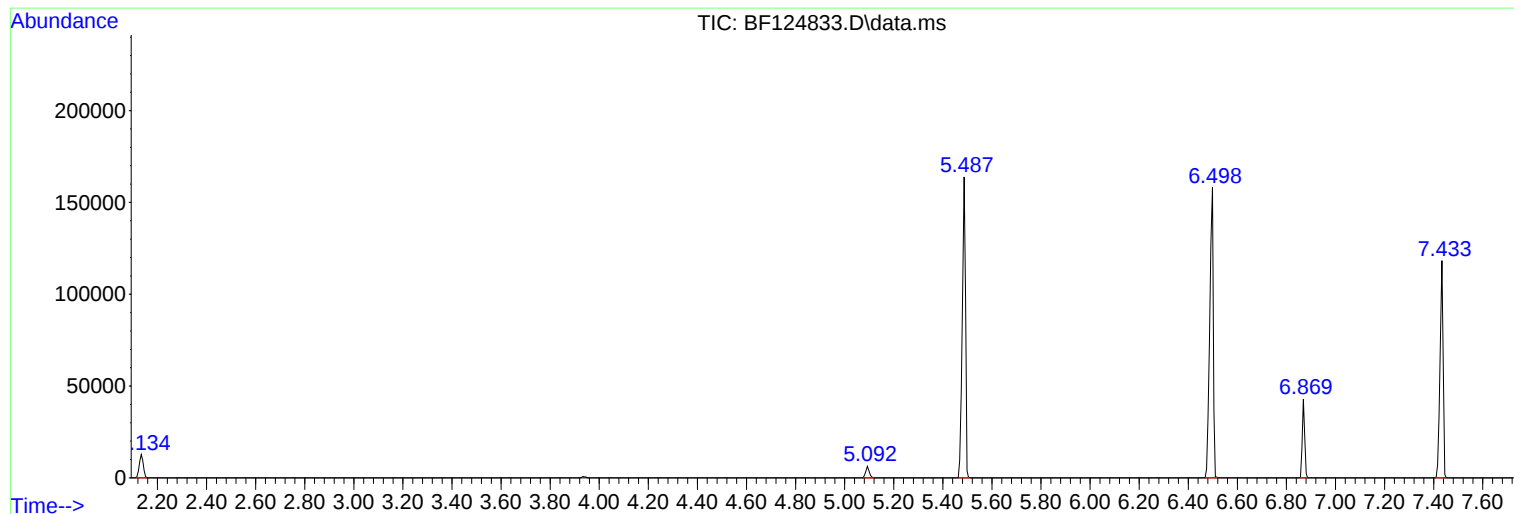
Sum of corrected areas: 1364816

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072821\
Data File : BF124833.D
Acq On : 28 Jul 2021 18:15
Operator : JU/CG
Sample : M3205-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-209

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.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\BF072821\
Data File : BF124833.D
Acq On : 28 Jul 2021 18:15
Operator : JU/CG
Sample : M3205-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-209

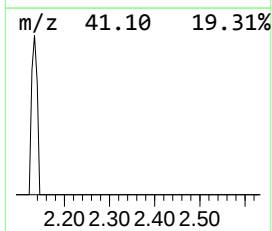
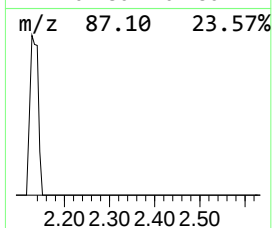
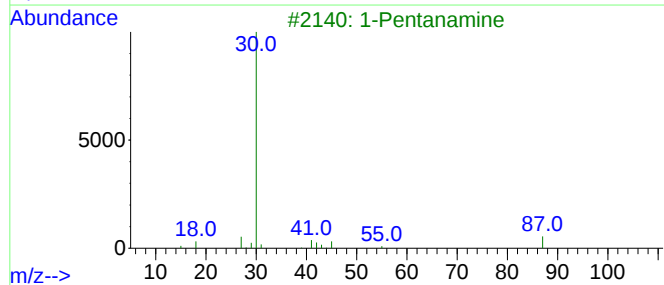
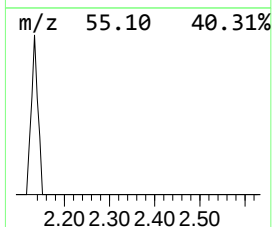
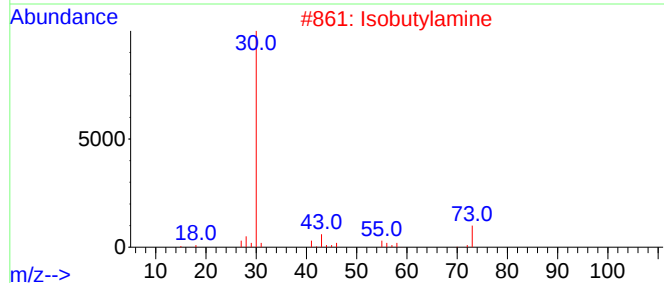
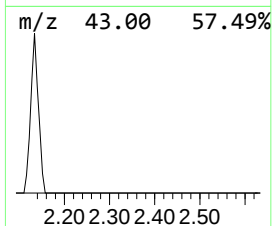
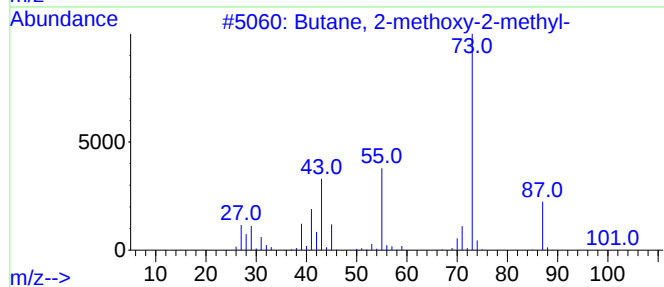
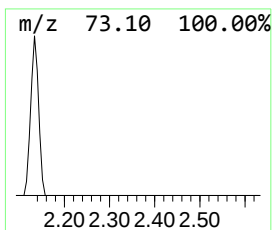
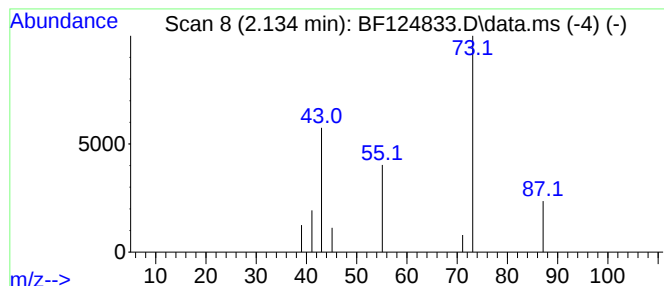
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.134	9.77 ng	14349	1,4-Dichlorobenzene-d4	6.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	64
2			Isobutylamine	73	C4H11N	000078-81-9	5
3			1-Pentanamine	87	C5H13N	000110-58-7	4
4			2-Butanone, 3-methoxy-3-methyl-	116	C6H12O2	036687-98-6	4
5			1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072821\
Data File : BF124833.D
Acq On : 28 Jul 2021 18:15
Operator : JU/CG
Sample : M3205-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-209

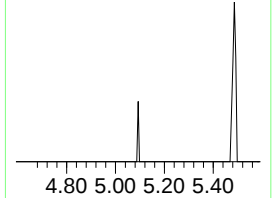
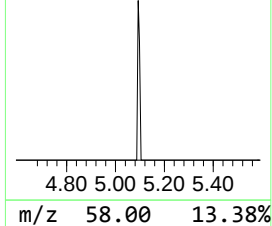
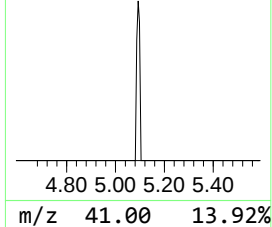
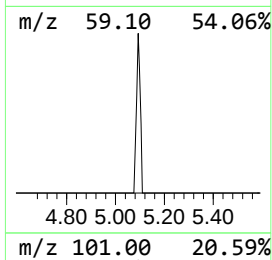
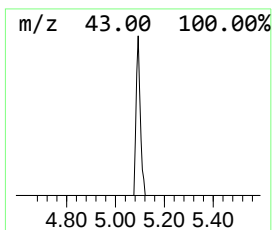
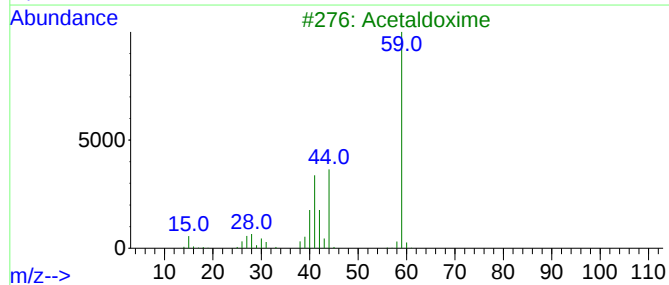
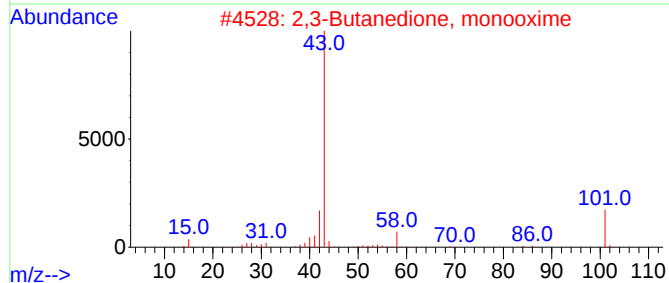
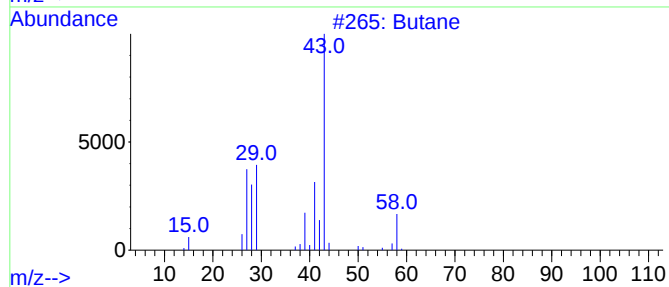
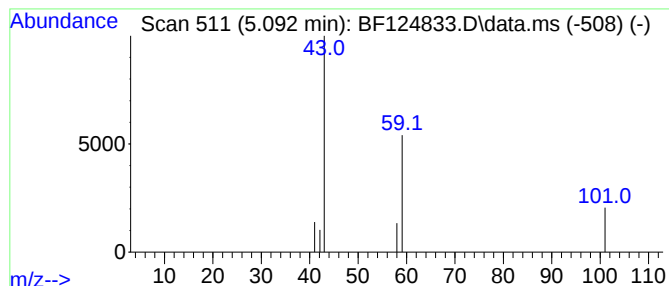
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown5.092 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.092	4.35 ng	6394	1,4-Dichlorobenzene-d4	6.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane	58	C4H10	000106-97-8	5
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	5
3			Acetaldoxime	59	C2H5NO	000107-29-9	4
4			N-(n-Propyl)acetamide	101	C5H11NO	005331-48-6	4
5			Diacetamide	101	C4H7NO2	000625-77-4	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072821\
Data File : BF124833.D
Acq On : 28 Jul 2021 18:15
Operator : JU/CG
Sample : M3205-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-209

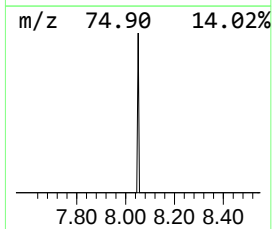
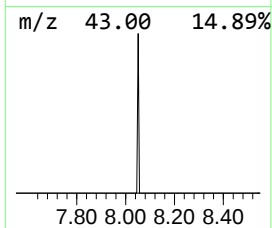
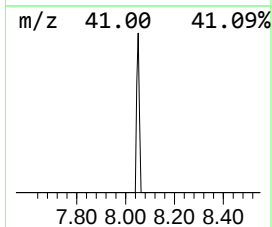
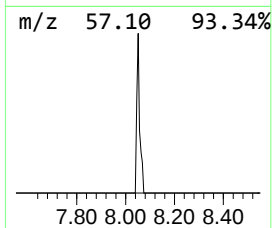
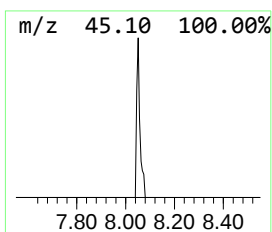
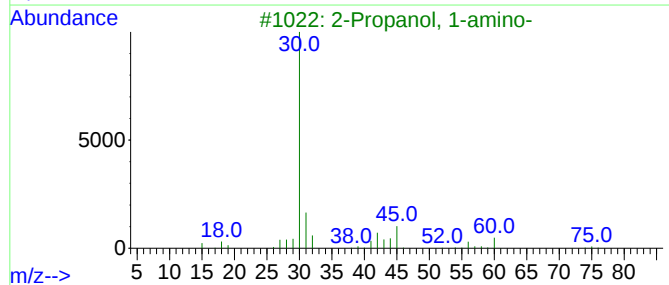
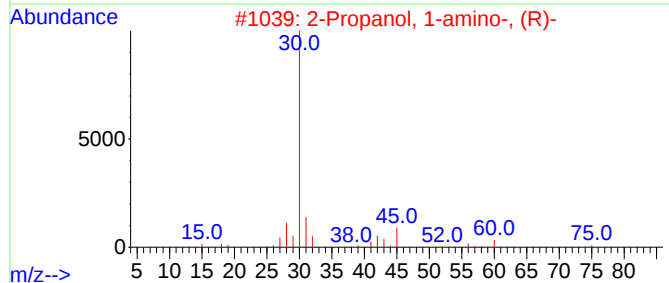
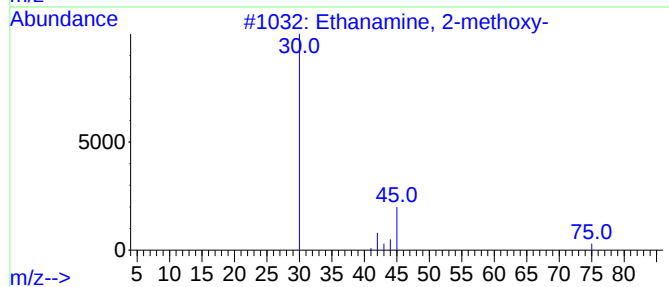
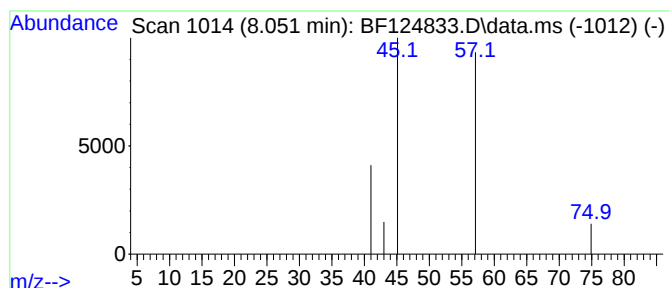
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown8.051 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.051	2.40 ng	4962	Naphthalene-d8	8.151

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanamine, 2-methoxy-	75	C3H9NO	000109-85-3	4
2			2-Propanol, 1-amino-, (R)-	75	C3H9NO	002799-16-8	3
3			2-Propanol, 1-amino-	75	C3H9NO	000078-96-6	3
4			Formamide	45	CH3NO	000075-12-7	3
5			Ethylamine	45	C2H7N	000075-04-7	3



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072821\
Data File : BF124833.D
Acq On : 28 Jul 2021 18:15
Operator : JU/CG
Sample : M3205-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-209

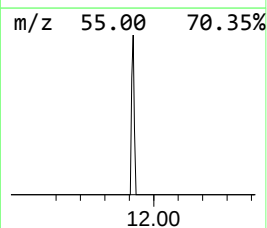
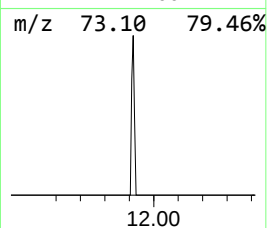
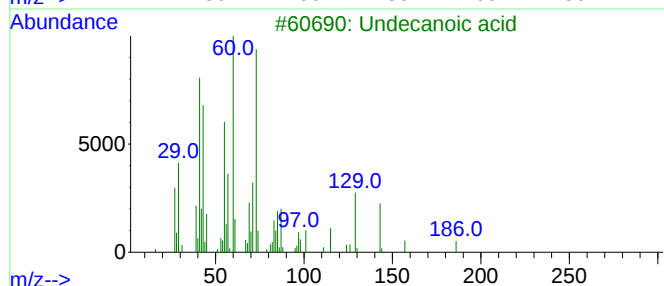
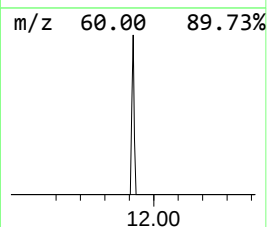
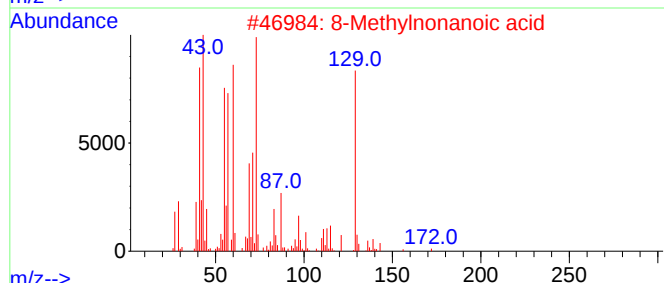
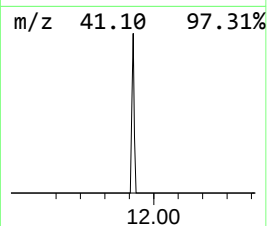
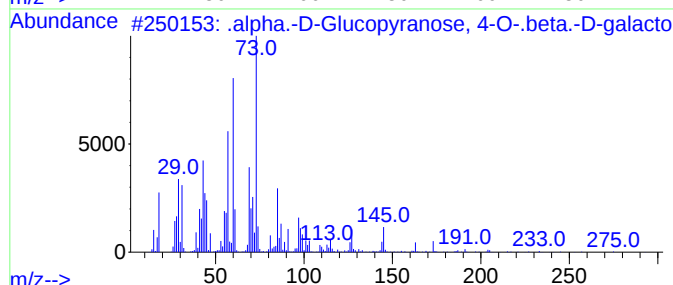
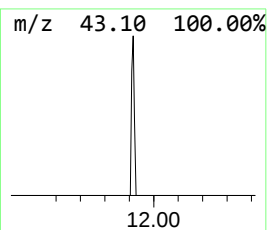
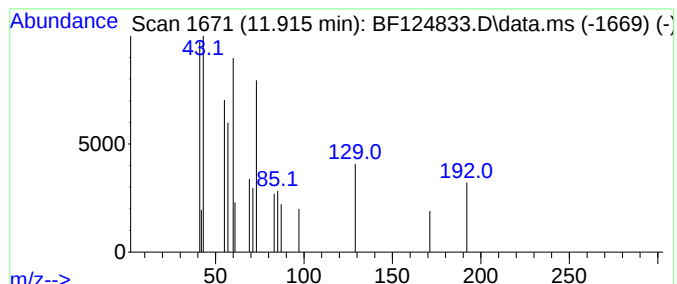
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 unknown11.916 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	3.72 ng	9972	Phenanthrene-d10	11.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	.		.alpha.-D-Glucopyranose, 4-O-.be...	342	C12H22O11	014641-93-1	47
2	8-Methylnonanoic acid			172	C10H20O2	005963-14-4	38
3	Undecanoic acid			186	C11H22O2	000112-37-8	38
4	8-Methylnonanoic acid, n-propyl ...			214	C13H26O2	1010452-00-5	33
5	n-Decanoic acid			172	C10H20O2	000334-48-5	28



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072821\
Data File : BF124833.D
Acq On : 28 Jul 2021 18:15
Operator : JU/CG
Sample : M3205-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-209

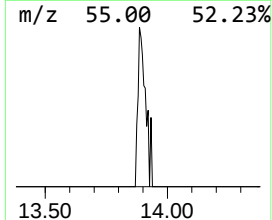
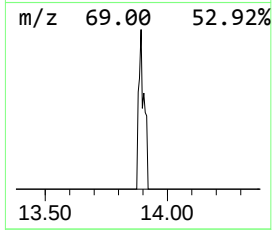
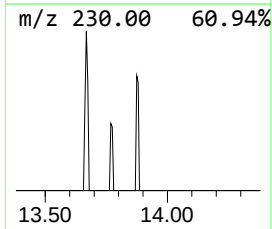
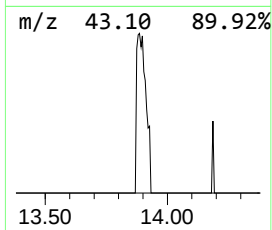
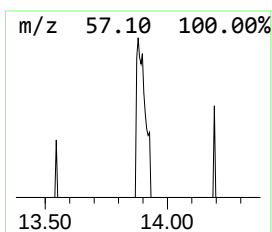
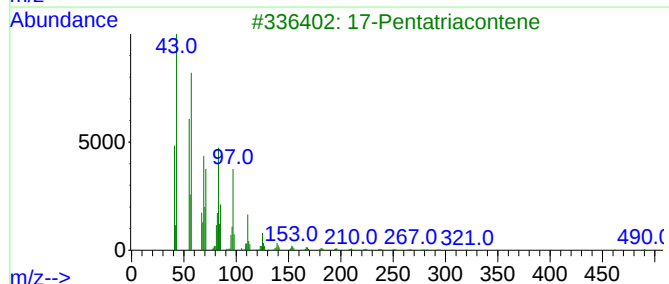
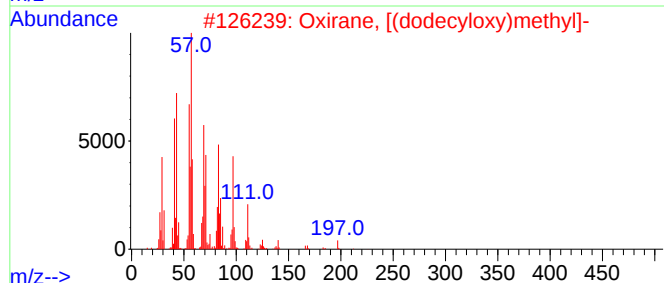
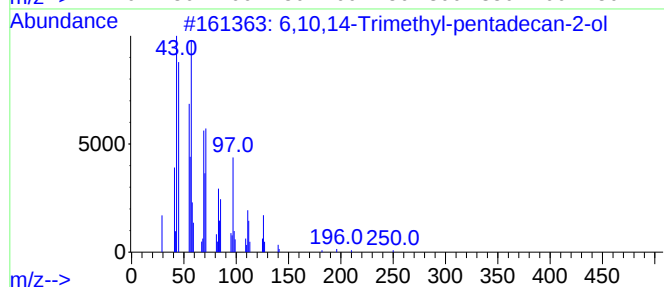
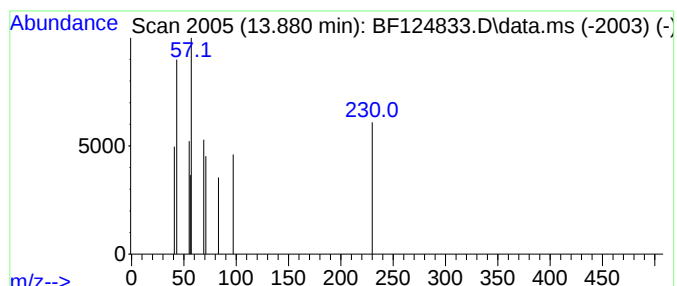
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown13.880 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.880	5.50 ng	11004	Chrysene-d12	14.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	6,10,14-Trimethyl-pentadecan-2-ol	270	C18H38O	069729-17-5	45		
2	Oxirane, [(dodecyloxy)methyl]-	242	C15H30O2	002461-18-9	45		
3	17-Pentatriacontene	491	C35H70	006971-40-0	40		
4	Vinyl lauryl ether	212	C14H28O	000765-14-0	38		
5	Dichloroacetic acid, tetradecyl ...	324	C16H30Cl2O2	083005-02-1	33		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072821\
Data File : BF124833.D
Acq On : 28 Jul 2021 18:15
Operator : JU/CG
Sample : M3205-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-209

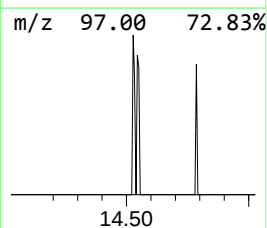
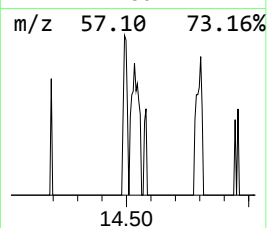
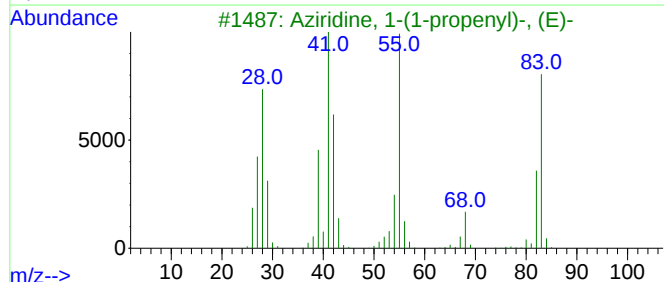
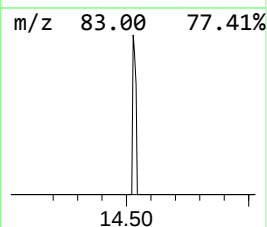
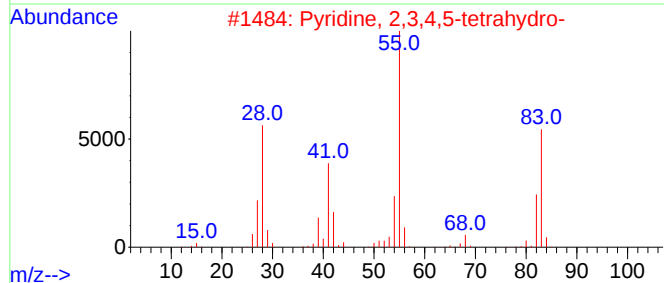
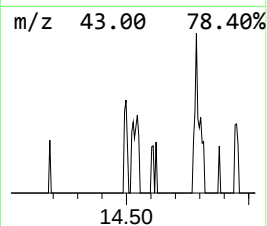
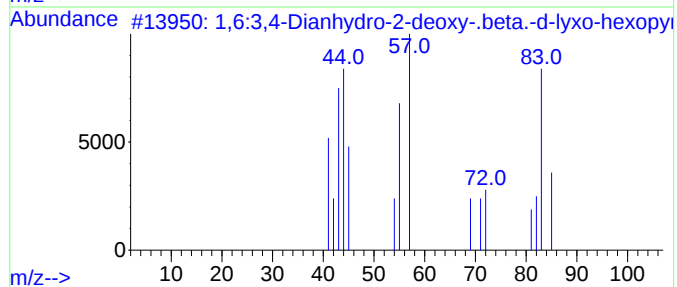
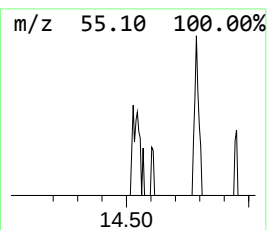
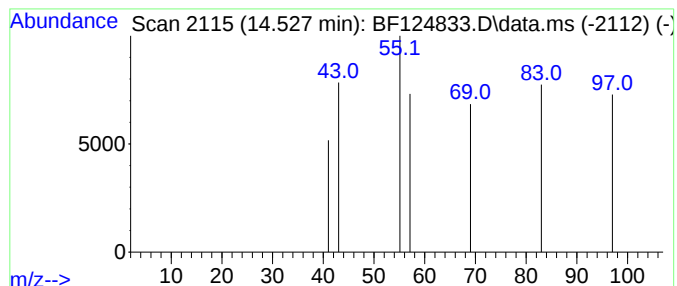
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown14.527 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.527	2.86 ng	5721	Chrysene-d12	14.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,6:3,4-Dianhydro-2-deoxy-.beta....	128	C6H8O3	050767-53-8	9		
2	Pyridine, 2,3,4,5-tetrahydro-	83	C5H9N	000505-18-0	7		
3	Aziridine, 1-(1-propenyl)-, (E)-	83	C5H9N	080839-91-4	4		
4	Isoxazole, 5-methyl-	83	C4H5N0	005765-44-6	4		
5	6-Methyloctyl acetate	186	C11H22O2	1000439-66-5	4		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072821\
Data File : BF124833.D
Acq On : 28 Jul 2021 18:15
Operator : JU/CG
Sample : M3205-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-209

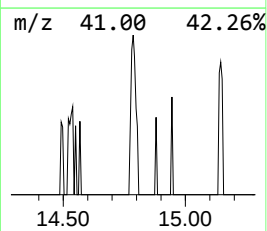
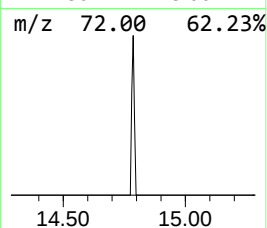
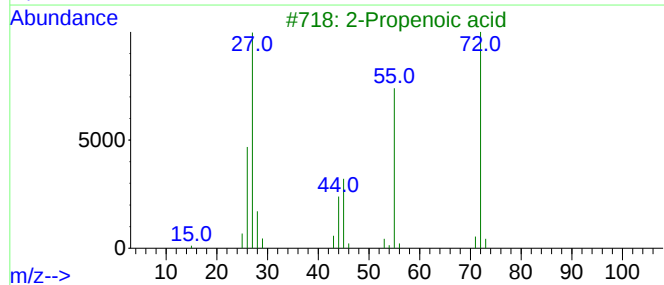
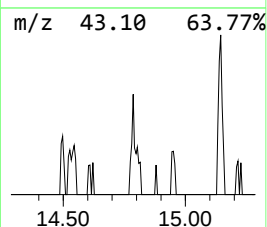
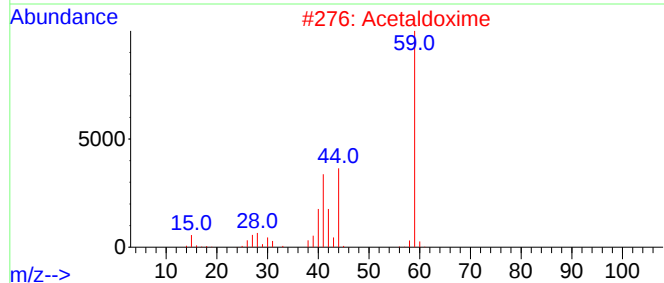
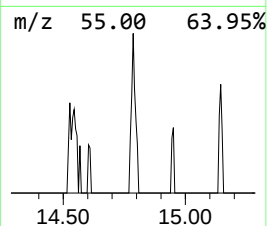
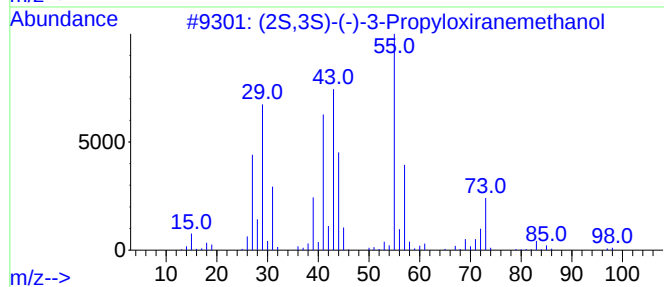
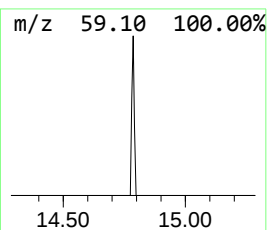
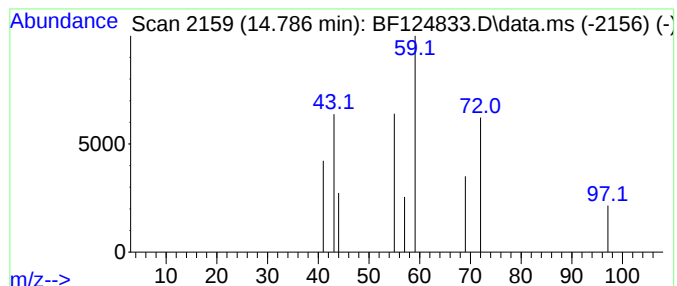
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown14.786 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.786	5.09 ng	7731	Perylene-d12	15.509

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(2S,3S)-(-)-3-Propyloxiranemethanol	116	C6H12O2	089321-71-1	9
2			Acetaldoxime	59	C2H5NO	000107-29-9	4
3			2-Propenoic acid	72	C3H4O2	000079-10-7	4
4			1-Propene, 1-methoxy-	72	C4H8O	007319-16-6	4
5			Guanidine	59	CH5N3	000113-00-8	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072821\
Data File : BF124833.D
Acq On : 28 Jul 2021 18:15
Operator : JU/CG
Sample : M3205-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-209

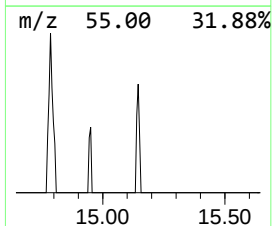
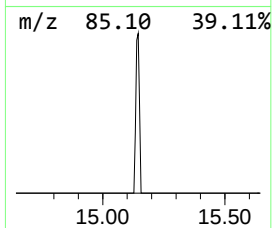
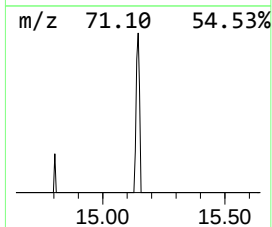
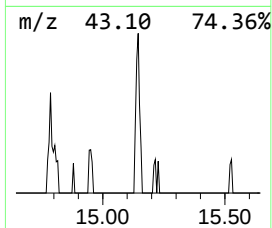
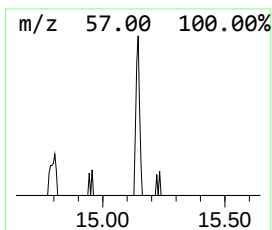
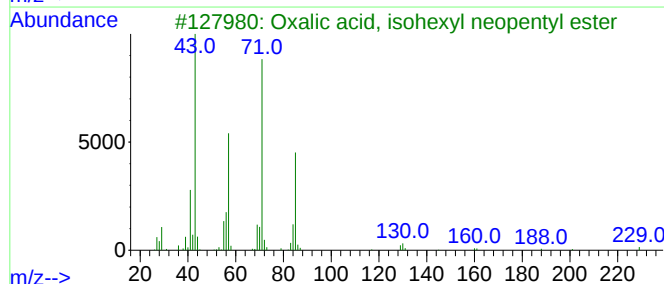
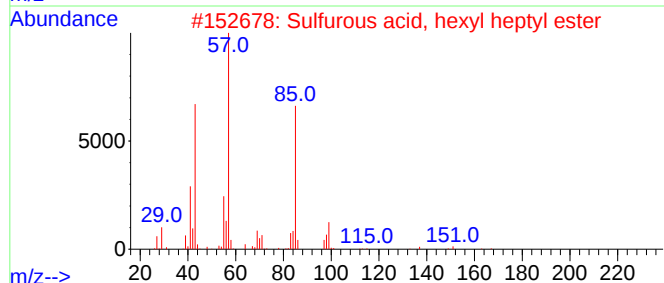
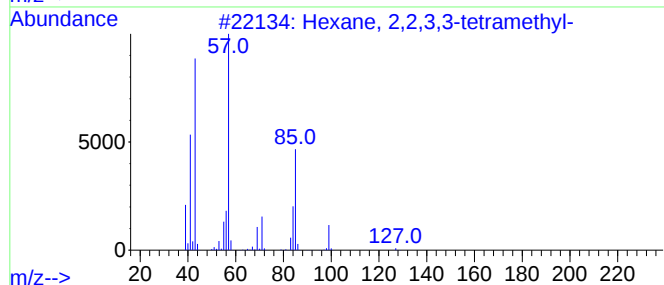
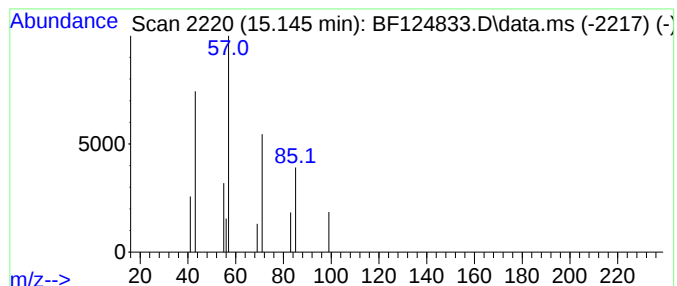
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown15.145 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.145	5.46 ng	8306	Perylene-d12	15.509

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 2,2,3,3-tetramethyl-	142	C10H22	013475-81-5	42
2			Sulfurous acid, hexyl heptyl ester	264	C13H28O3S	1000309-12-9	40
3			Oxalic acid, isohexyl neopentyl ...	244	C13H24O4	1000309-73-0	38
4			Hexane, 3-ethyl-3-methyl-	128	C9H20	003074-76-8	33
5			Hexane, 1-(hexyloxy)-5-methyl-	200	C13H28O	074421-19-5	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072821\
Data File : BF124833.D
Acq On : 28 Jul 2021 18:15
Operator : JU/CG
Sample : M3205-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-209

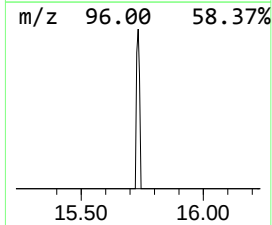
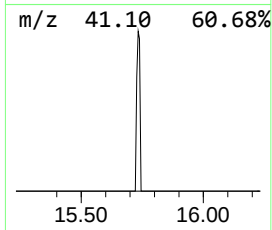
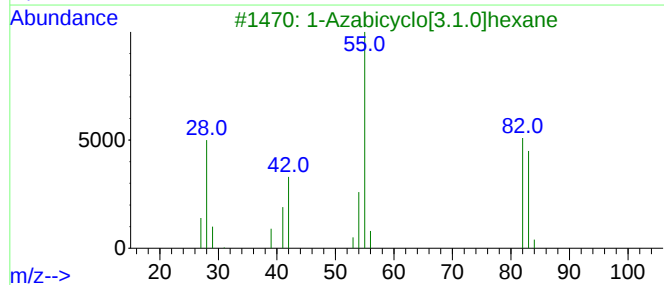
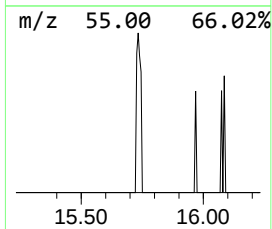
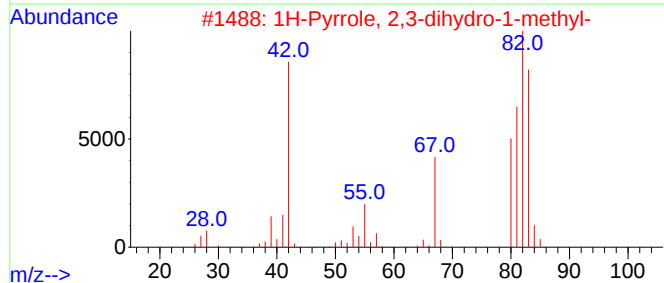
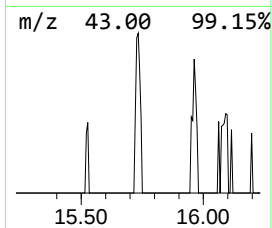
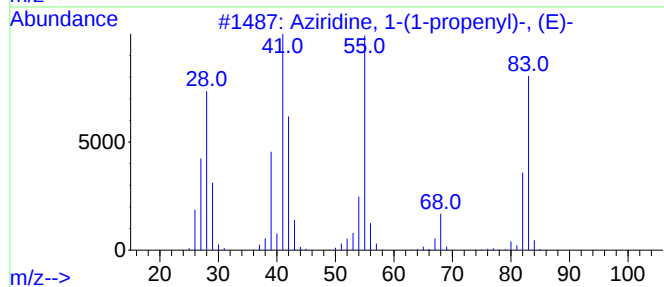
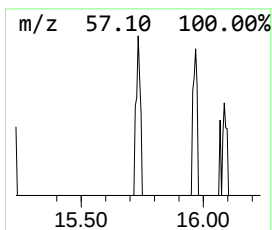
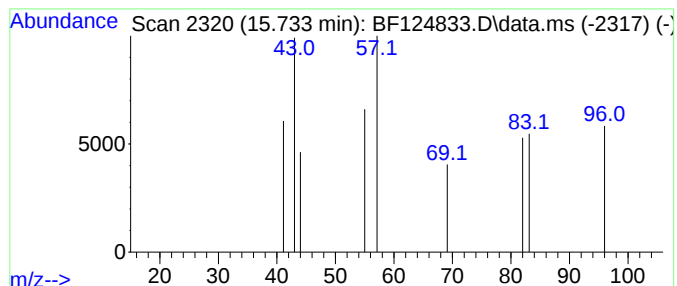
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown15.733 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.733	3.34 ng	5075	Perylene-d12	15.509

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Aziridine, 1-(1-propenyl)-, (E)-	83	C5H9N	080839-91-4	7
2			1H-Pyrrole, 2,3-dihydro-1-methyl-	83	C5H9N	033838-11-8	5
3			1-Azabicyclo[3.1.0]hexane	83	C5H9N	000285-76-7	4
4			(Z)-(Z)-Hex-3-en-1-yl 2-methylbu...	182	C11H18O2	084060-80-0	4
5			1,6:3,4-Dianhydro-2-deoxy-.beta....	128	C6H8O3	050767-53-8	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072821\
Data File : BF124833.D
Acq On : 28 Jul 2021 18:15
Operator : JU/CG
Sample : M3205-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-209

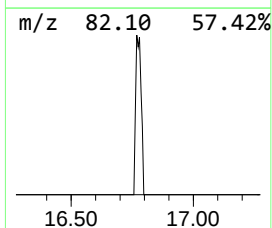
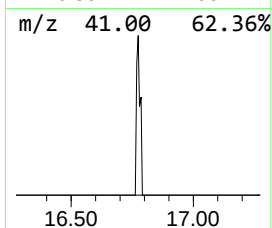
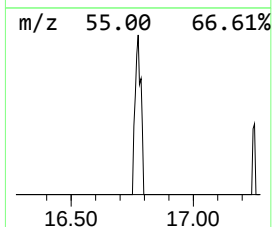
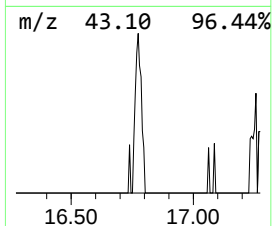
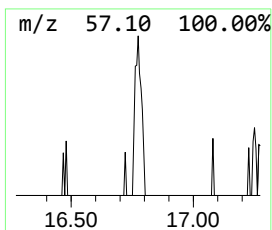
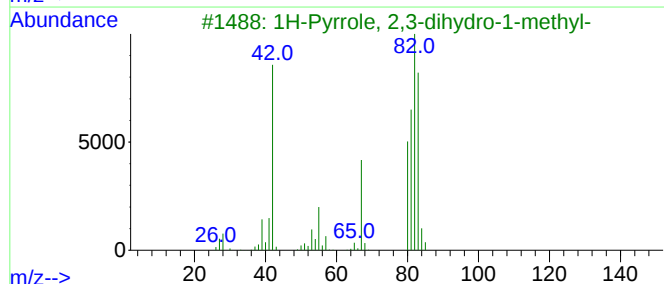
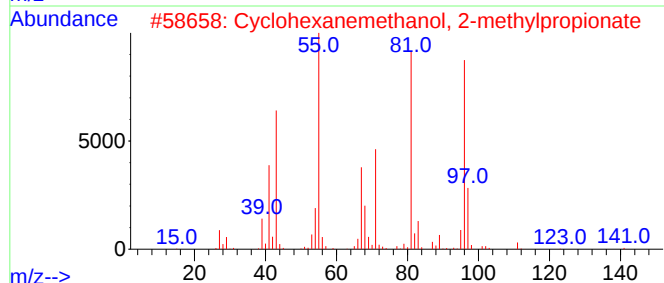
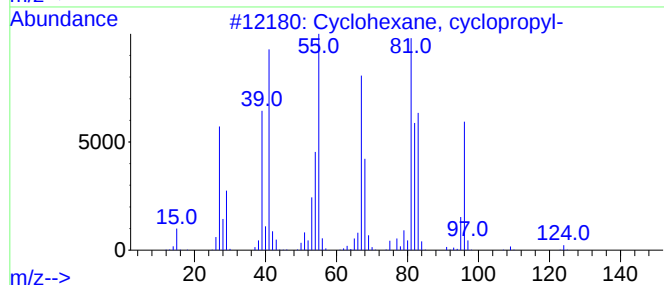
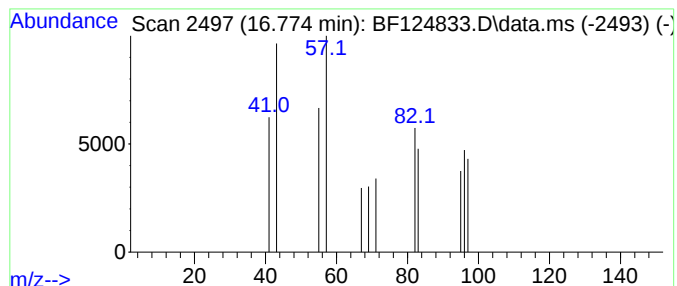
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown16.774 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.774	7.81 ng	11876	Perylene-d12	15.509

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, cyclopropyl-	124	C9H16	032669-86-6	25
2			Cyclohexanemethanol, 2-methylpro...	184	C11H20O2	1000447-33-9	12
3			1H-Pyrrole, 2,3-dihydro-1-methyl-	83	C5H9N	033838-11-8	9
4			1-Hexene, 6-bromo-	162	C6H11Br	002695-47-8	9
5			Aziridine, 1-(1-propenyl)-, (E)-	83	C5H9N	080839-91-4	7



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072821\
Data File : BF124833.D
Acq On : 28 Jul 2021 18:15
Operator : JU/CG
Sample : M3205-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-209

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.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...	2.134	9.8	ng	14349	1	6.869	29381	20.0
unknown5.092	5.092	4.3	ng	6394	1	6.869	29381	20.0
unknown8.051	8.051	2.4	ng	4962	2	8.151	41373	20.0
unknown11.916	11.916	3.7	ng	9972	4	11.398	53553	20.0
unknown13.880	13.880	5.5	ng	11004	5	14.033	40011	20.0
unknown14.527	14.527	2.9	ng	5721	5	14.033	40011	20.0
unknown14.786	14.786	5.1	ng	7731	6	15.509	30401	20.0
unknown15.145	15.145	5.5	ng	8306	6	15.509	30401	20.0
unknown15.733	15.733	3.3	ng	5075	6	15.509	30401	20.0
unknown16.774	16.774	7.8	ng	11876	6	15.509	30401	20.0