

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072121\
 Data File : BF124677.D
 Acq On : 22 Jul 2021 1:11
 Operator : JU/CG
 Sample : M3076-03
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 20210534-COM-7

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-BF070721.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124680.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.175	12	15	19	rBB	9859	11947	6.02%	0.953%
2	5.122	513	516	518	rBB	2392	2459	1.24%	0.196%
3	5.504	576	581	584	rBB	161439	147040	74.06%	11.728%
4	6.510	747	752	755	rBV	147633	154724	77.93%	12.341%
5	6.886	813	816	819	rBB	48932	35035	17.65%	2.794%
6	7.451	907	912	914	rBB	112986	100661	50.70%	8.029%
7	8.069	1014	1017	1019	rBB	9236	6428	3.24%	0.513%
8	8.169	1031	1034	1037	rBB	64350	50318	25.34%	4.013%
9	9.251	1213	1218	1220	rBV	207593	198545	100.00%	15.836%
10	9.927	1329	1333	1336	rBB	81301	61828	31.14%	4.931%
11	10.716	1463	1467	1470	rBB	154058	129657	65.30%	10.341%
12	11.416	1582	1586	1589	rBB	82208	62599	31.53%	4.993%
13	11.933	1672	1674	1677	rBB	14992	9597	4.83%	0.765%
14	12.716	1805	1807	1810	rBB	4302	3426	1.73%	0.273%
15	13.004	1852	1856	1859	rVB	229118	194344	97.88%	15.501%
16	13.892	2005	2007	2013	rBB	4501	5113	2.58%	0.408%
17	14.051	2031	2034	2037	rBB	51393	41676	20.99%	3.324%
18	15.533	2281	2286	2291	rBB	32363	38358	19.32%	3.059%

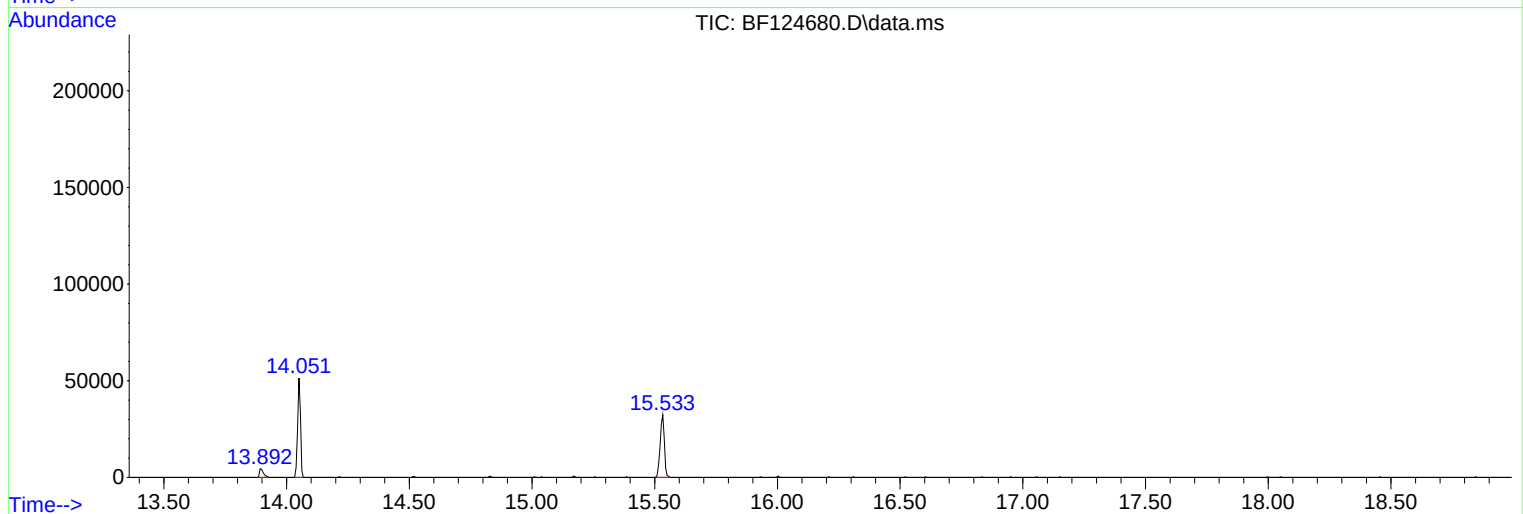
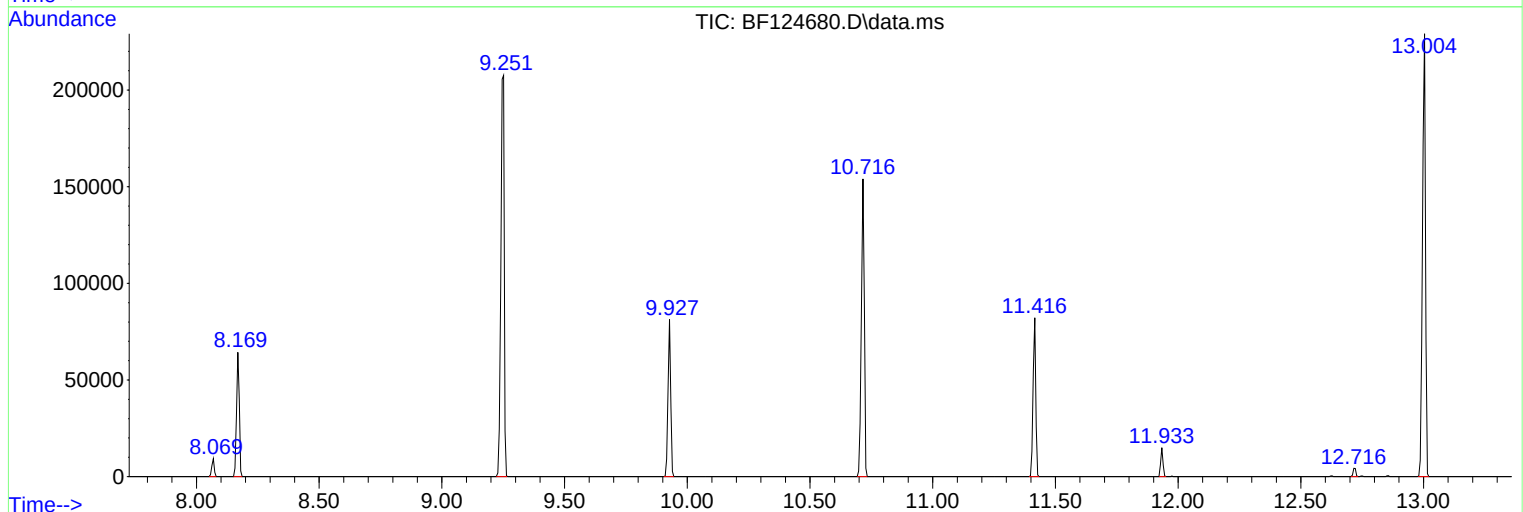
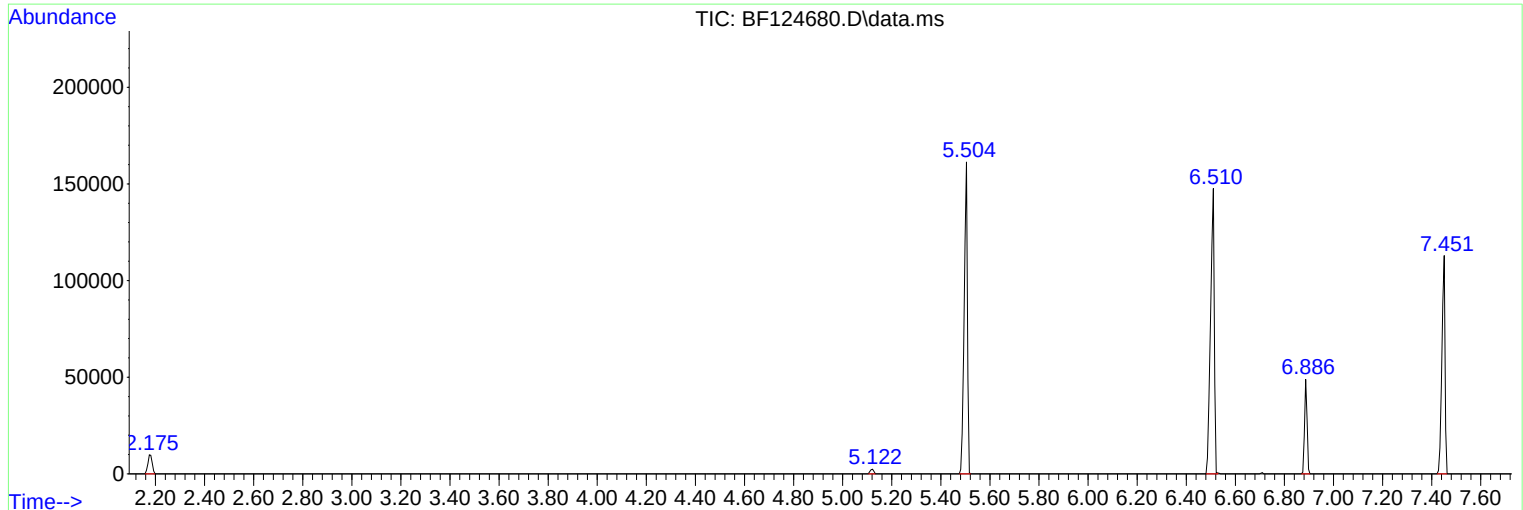
Sum of corrected areas: 1253755

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072121\
Data File : BF124677.D
Acq On : 22 Jul 2021 1:11
Operator : JU/CG
Sample : M3076-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20210534-COM-7

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.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\BF072121\
Data File : BF124677.D
Acq On : 22 Jul 2021 1:11
Operator : JU/CG
Sample : M3076-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20210534-COM-7

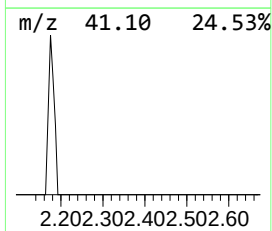
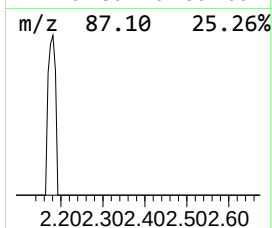
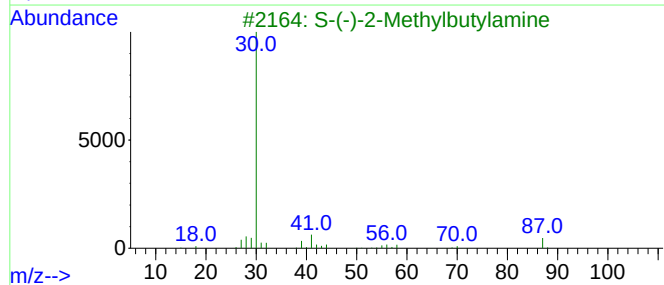
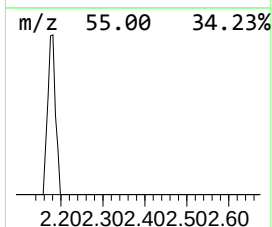
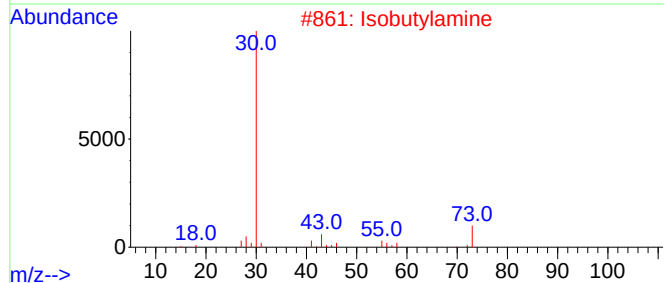
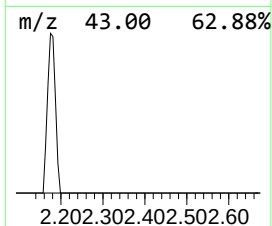
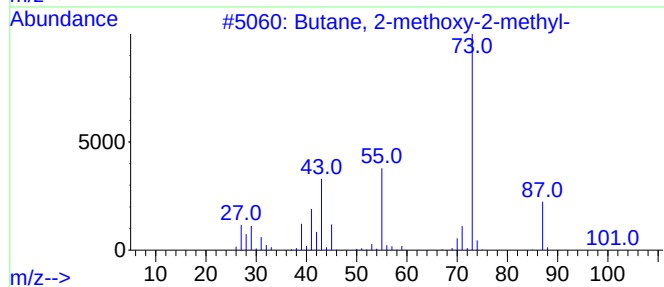
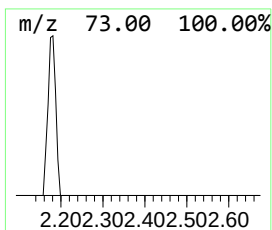
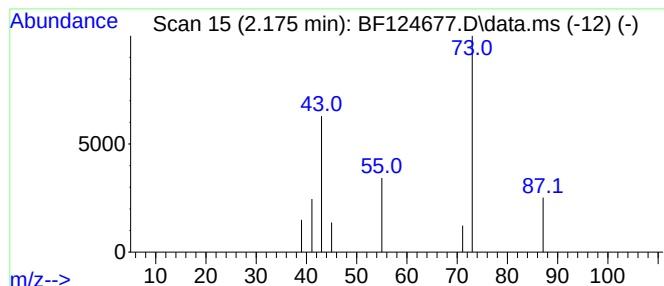
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.175	6.82 ng	11947	1,4-Dichlorobenzene-d4	6.886

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	7
3			S-(-)-2-Methylbutylamine	87	C5H13N	020626-52-2	4
4			3,4-Hexanediol, 2,5-dimethyl-	146	C8H18O2	022607-11-0	4
5			1-Butanamine, 2-methyl-	87	C5H13N	000096-15-1	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072121\
Data File : BF124677.D
Acq On : 22 Jul 2021 1:11
Operator : JU/CG
Sample : M3076-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20210534-COM-7

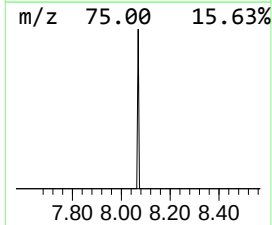
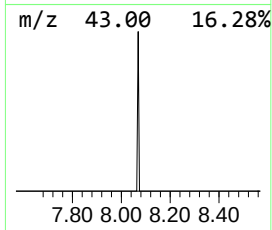
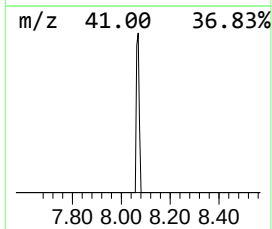
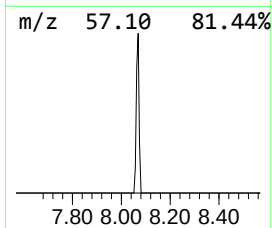
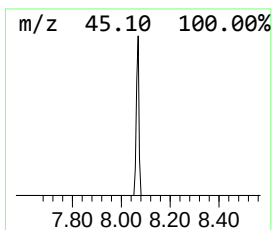
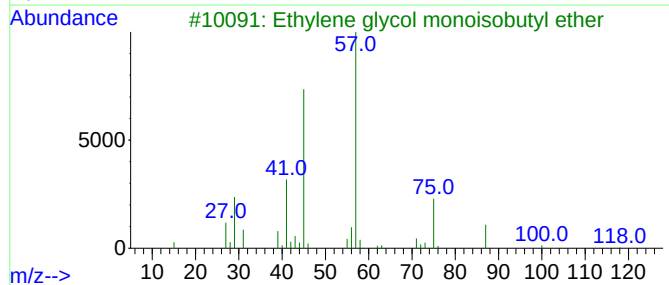
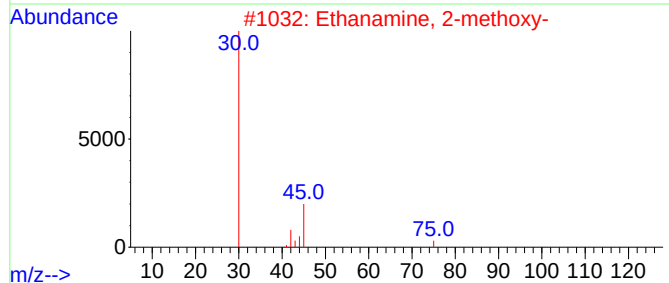
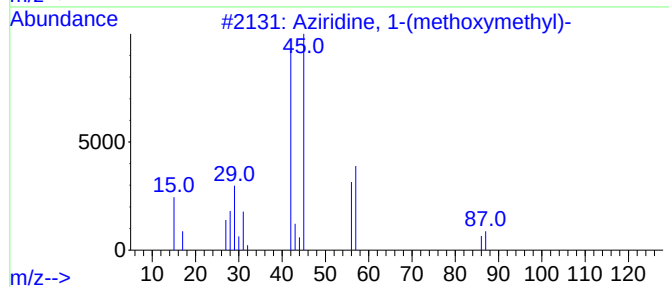
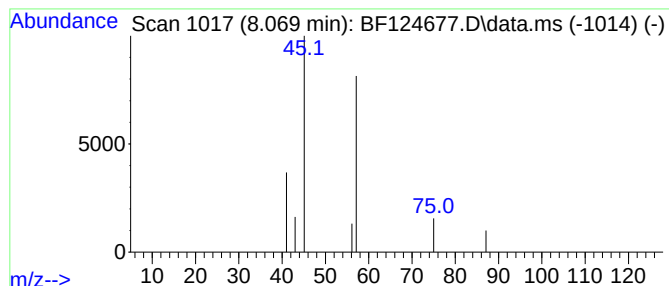
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown8.069 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.069	2.55 ng	6428	Naphthalene-d8	8.169

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Aziridine, 1-(methoxymethyl)-	87	C4H9NO	001497-83-2	5
2		Ethanamine, 2-methoxy-	75	C3H9NO	000109-85-3	4
3		Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	4
4		2-(Isobutoxymethyl)oxirane	130	C7H14O2	003814-55-9	4
5		Formamide	45	CH3NO	000075-12-7	3



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072121\
Data File : BF124677.D
Acq On : 22 Jul 2021 1:11
Operator : JU/CG
Sample : M3076-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20210534-COM-7

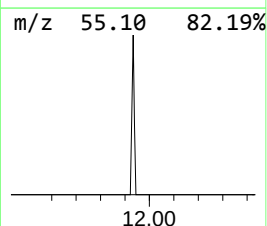
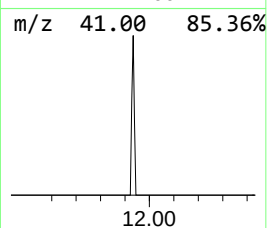
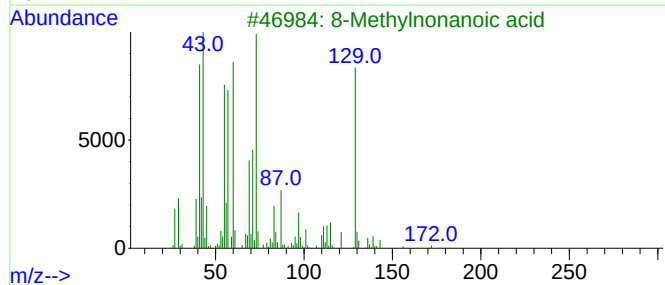
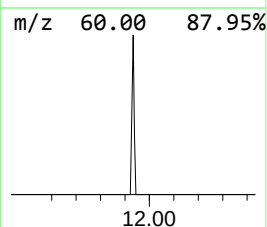
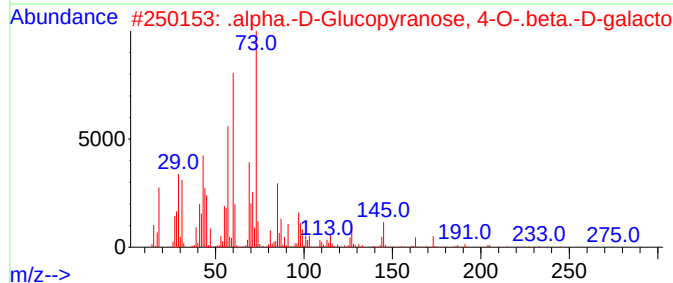
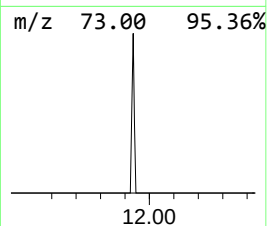
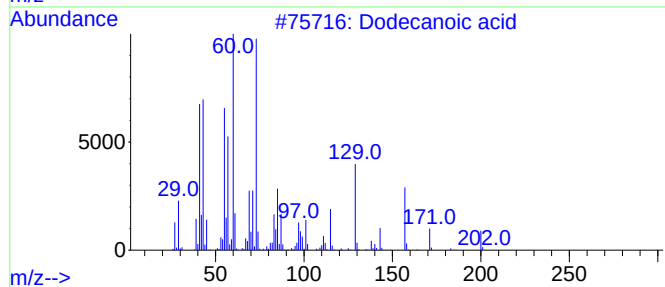
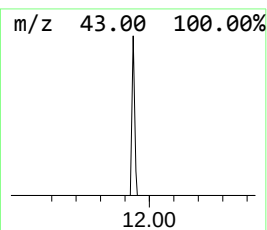
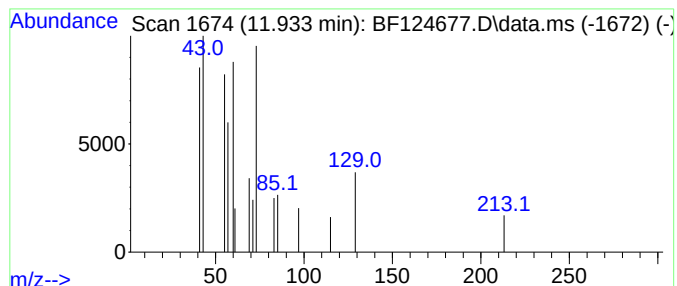
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Dodecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	3.07 ng	9597	Phenanthrene-d10	11.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecanoic acid	200	C12H24O2	000143-07-7	59
2			.alpha.-D-Glucopyranose, 4-O-.be...	342	C12H22O11	014641-93-1	42
3			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	38
4			Dodecanoic acid, 1-methylethyl e...	242	C15H30O2	010233-13-3	36
5			Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	33



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072121\
Data File : BF124677.D
Acq On : 22 Jul 2021 1:11
Operator : JU/CG
Sample : M3076-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20210534-COM-7

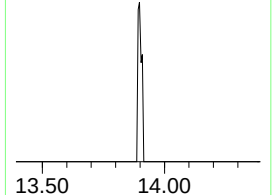
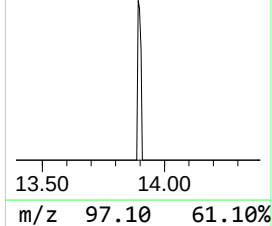
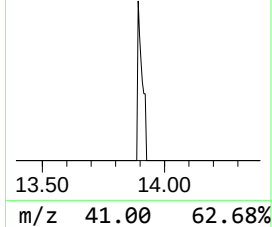
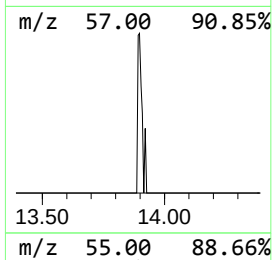
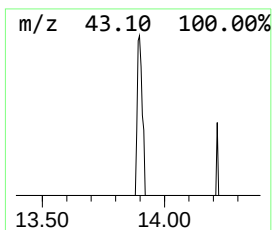
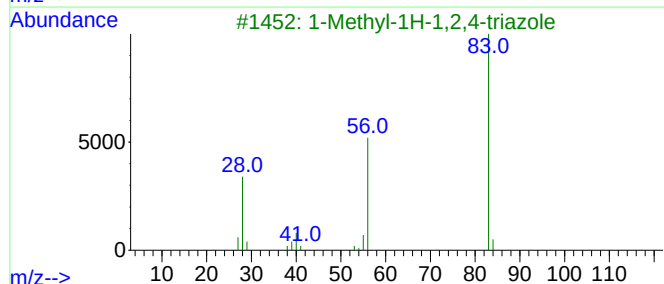
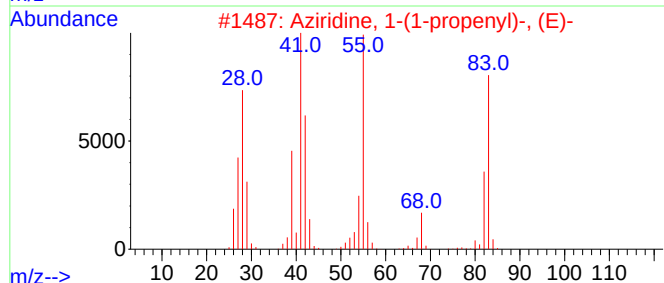
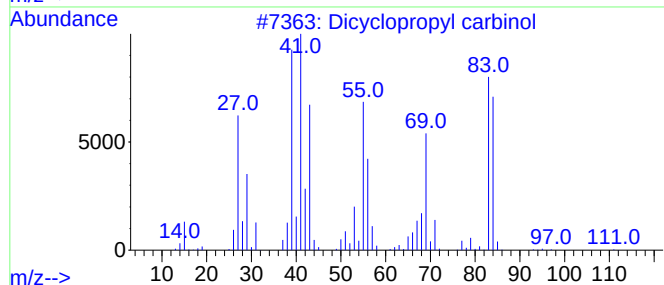
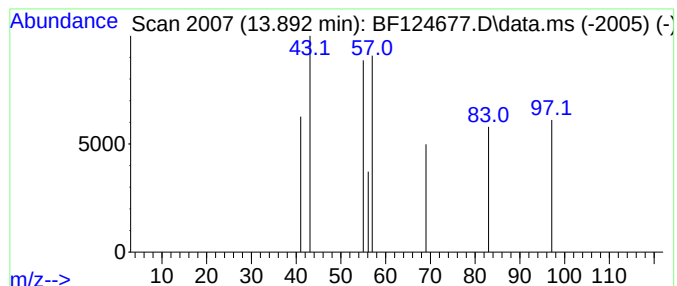
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 unknown13.892 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.892	2.45 ng	5113	Chrysene-d12	14.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dicyclopropyl carbinol	112	C7H12O	014300-33-5	9
2			Aziridine, 1-(1-propenyl)-, (E)-	83	C5H9N	080839-91-4	7
3			1-Methyl-1H-1,2,4-triazole	83	C3H5N3	006086-21-1	4
4			1H-1,2,4-Triazole, 3-methyl-	83	C3H5N3	007170-01-6	4
5			Aminoacetonitrile	56	C2H4N2	000540-61-4	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072121\
Data File : BF124677.D
Acq On : 22 Jul 2021 1:11
Operator : JU/CG
Sample : M3076-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20210534-COM-7

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.175	6.8	ng	11947	1	6.886	35035	20.0
unknown8.069	8.069	2.5	ng	6428	2	8.169	50318	20.0
Dodecanoic acid	11.933	3.1	ng	9597	4	11.416	62599	20.0
unknown13.892	13.892	2.5	ng	5113	5	14.051	41676	20.0