

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021722\
 Data File : BF126938.D
 Acq On : 17 Feb 2022 20:44
 Operator : CG\JU
 Sample : N1573-04
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-26R

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-BF021622.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126938.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.457	365	369	376	rVB	336585	365596	8.19%	1.502%
2	5.157	484	488	495	rBV	128861	142502	3.19%	0.585%
3	5.545	549	554	557	rBV	1918563	1681278	37.68%	6.906%
4	6.539	720	723	729	rVB	1186774	1087972	24.38%	4.469%
5	6.722	751	754	756	rBV	263305	191117	4.28%	0.785%
6	6.751	756	759	762	rVB	266545	206281	4.62%	0.847%
7	6.845	771	775	778	rBV	369669	329453	7.38%	1.353%
8	6.928	785	789	792	rBV	802531	605777	13.57%	2.488%
9	6.981	795	798	807	rVB	190553	170094	3.81%	0.699%
10	7.492	880	885	888	rVB	2362359	2459131	55.11%	10.102%
11	7.563	894	897	901	rBV	58798	73606	1.65%	0.302%
12	7.922	954	958	962	rBV3	40761	47181	1.06%	0.194%
13	8.110	986	990	996	rBV3	71184	96432	2.16%	0.396%
14	8.210	1003	1007	1010	rBV	1070098	835472	18.72%	3.432%
15	8.357	1029	1032	1040	rBV	65104	67050	1.50%	0.275%
16	8.539	1060	1063	1069	rVB2	93270	93781	2.10%	0.385%
17	8.610	1072	1075	1082	rVB	49338	64143	1.44%	0.263%
18	9.157	1164	1168	1173	rBV	212339	223291	5.00%	0.917%
19	9.286	1183	1190	1193	rBV	4584590	4462462	100.00%	18.331%
20	9.380	1202	1206	1216	rVB	1047999	805889	18.06%	3.310%
21	9.969	1302	1306	1309	rVB	1116493	899979	20.17%	3.697%
22	10.274	1354	1358	1361	rBV2	49994	45978	1.03%	0.189%
23	10.380	1372	1376	1379	rVB	170358	137042	3.07%	0.563%
24	10.669	1422	1425	1427	rBV	174914	132695	2.97%	0.545%
25	10.763	1436	1441	1444	rBV	2975267	2837198	63.58%	11.655%
26	11.457	1555	1559	1562	rBV	1202810	939485	21.05%	3.859%
27	11.833	1620	1623	1626	rVB	165697	120369	2.70%	0.494%
28	13.051	1824	1830	1833	rBV	4066992	4167010	93.38%	17.117%
29	14.098	2004	2008	2012	rBV	642578	527085	11.81%	2.165%
30	15.604	2258	2264	2271	rBV	425776	528542	11.84%	2.171%

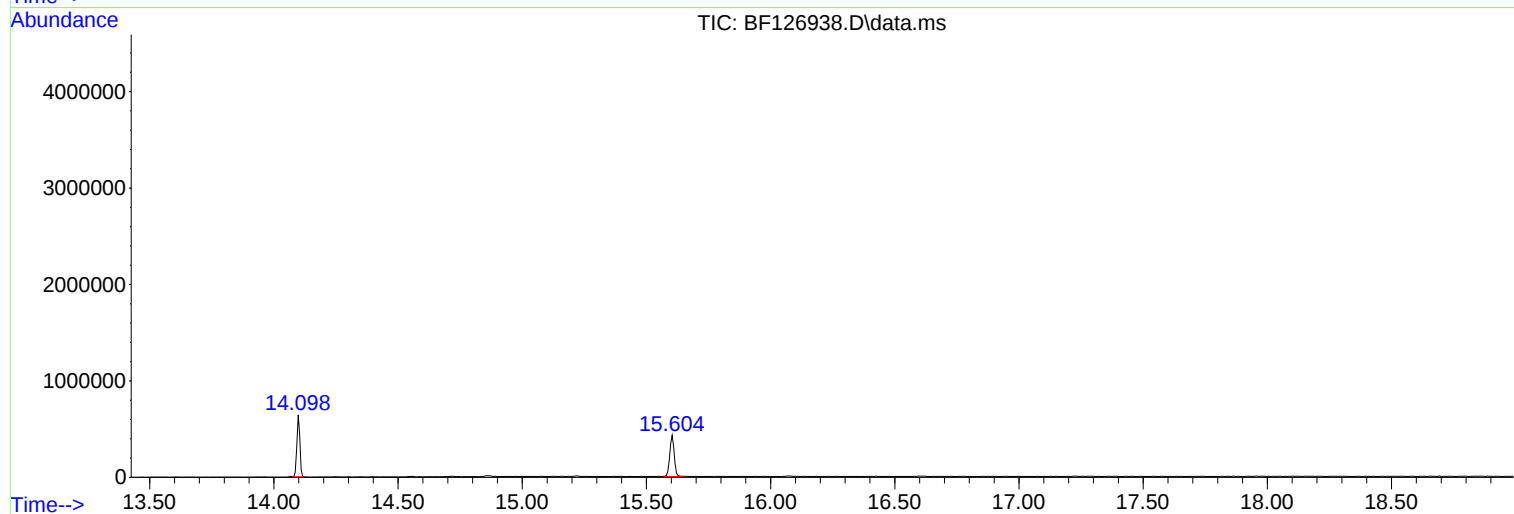
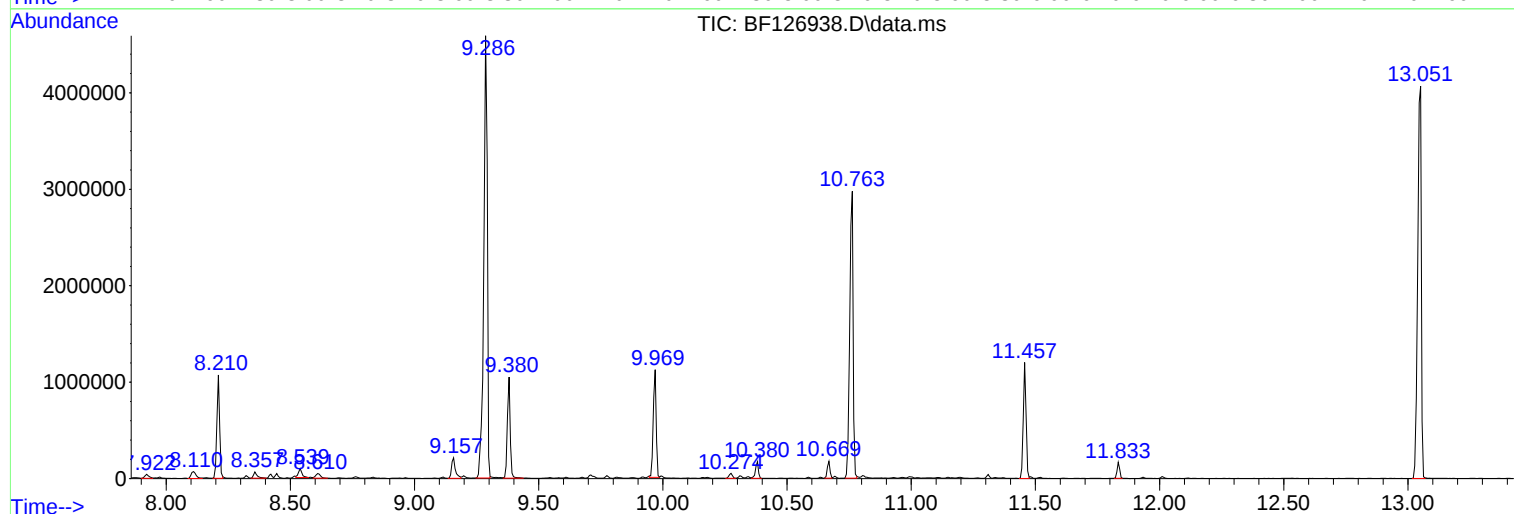
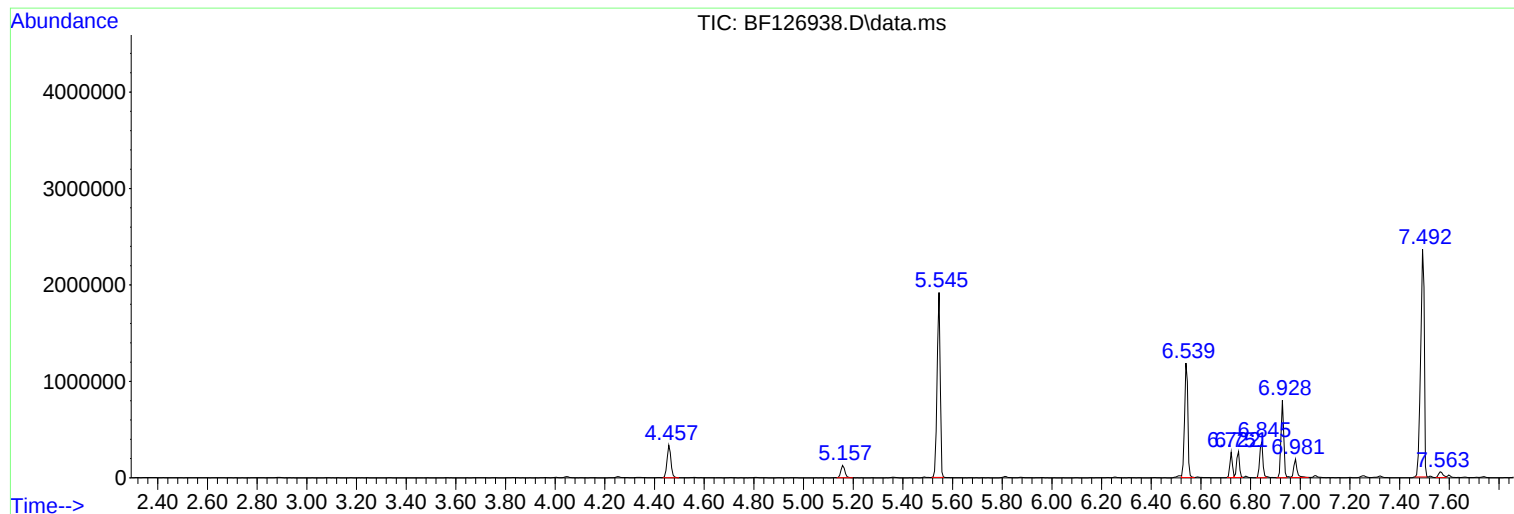
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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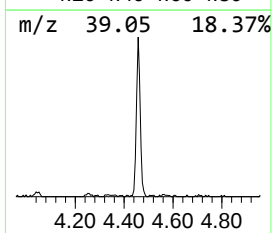
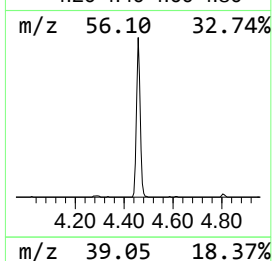
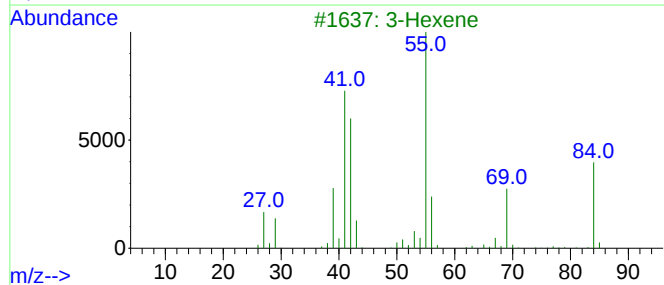
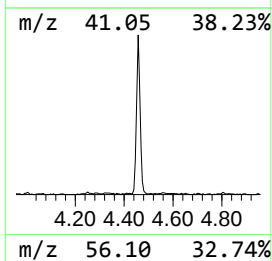
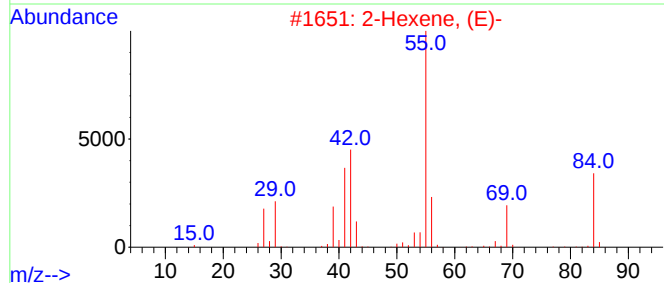
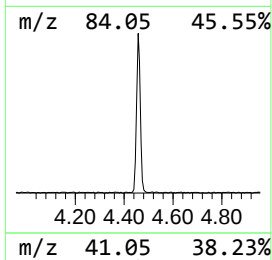
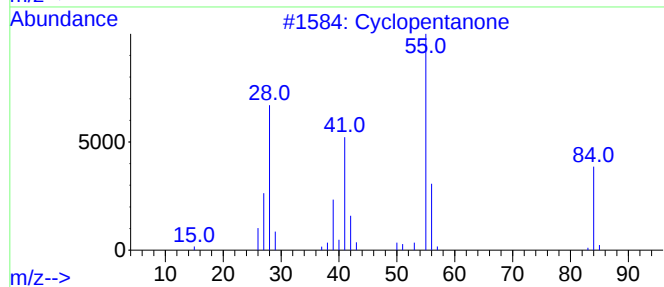
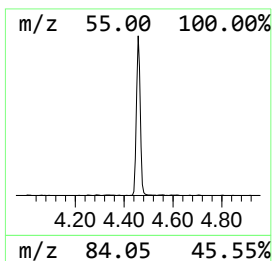
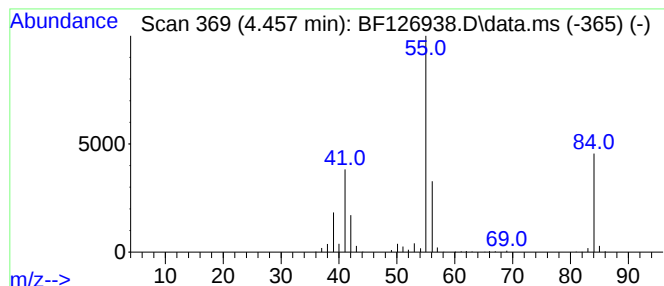
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Cyclopentanone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.457	12.07 ng	365596	1,4-Dichlorobenzene-d4	6.928

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentanone	84	C5H8O	000120-92-3	90
2			2-Hexene, (E)-	84	C6H12	004050-45-7	64
3			3-Hexene	84	C6H12	000592-47-2	64
4			2-Hexene	84	C6H12	000592-43-8	64
5			3-Hexene, (Z)-	84	C6H12	007642-09-3	50



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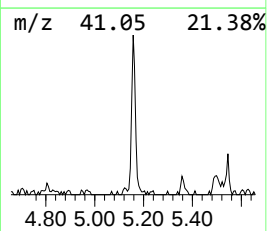
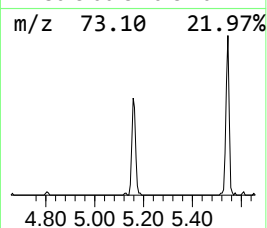
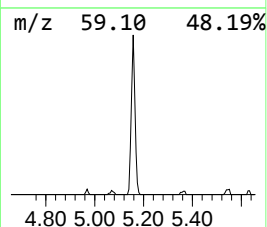
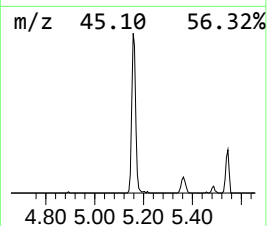
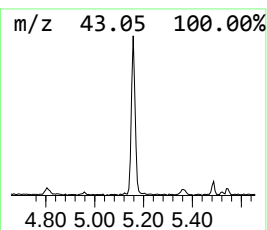
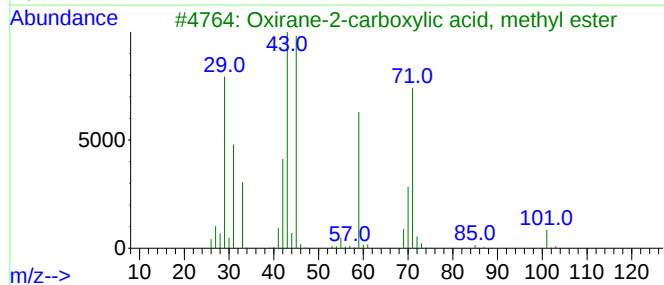
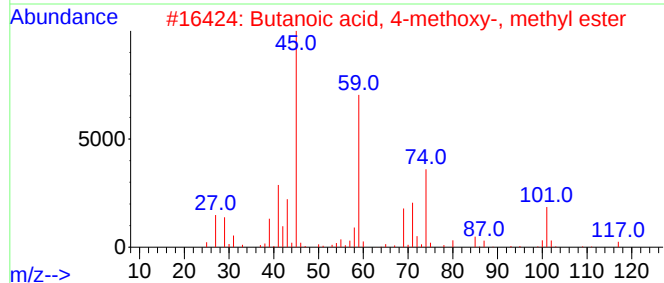
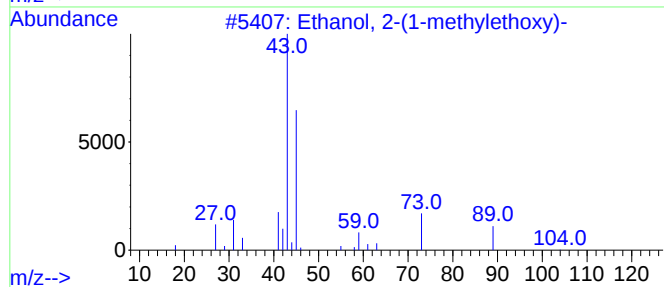
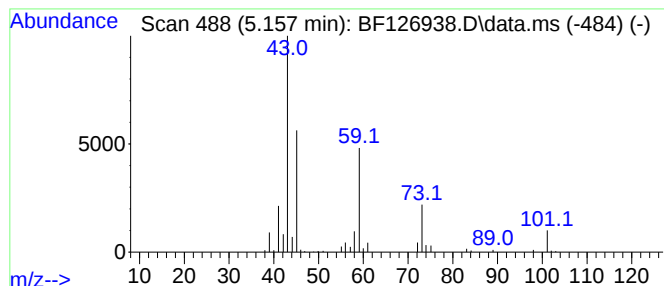
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Ethanol, 2-(1-methylethoxy)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.157	4.70 ng	142502	1,4-Dichlorobenzene-d4	6.928

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(1-methylethoxy)-	104	C5H12O2	000109-59-1	50
2			Butanoic acid, 4-methoxy-, methy...	132	C6H12O3	029006-01-7	42
3			Oxirane-2-carboxylic acid, methy...	102	C4H6O3	004538-50-5	36
4			Butanoic acid, 4-methoxy-	118	C5H10O3	029006-02-8	28
5			Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	28



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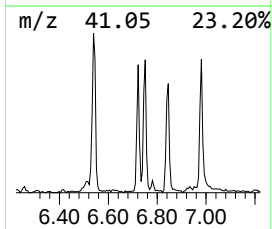
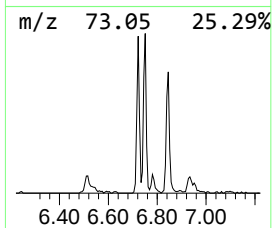
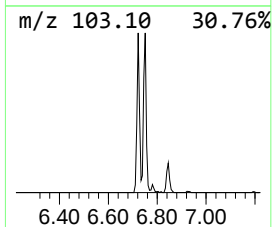
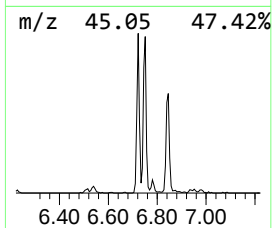
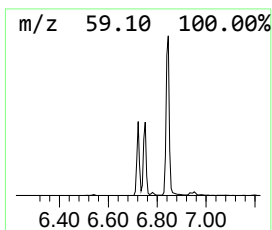
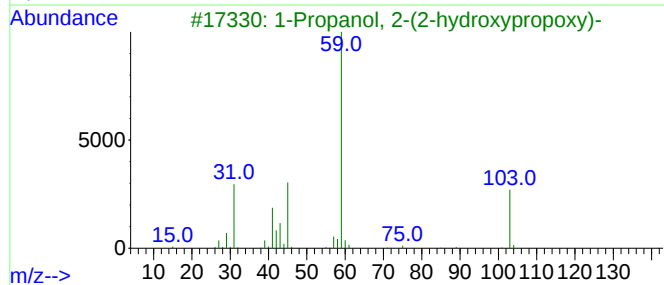
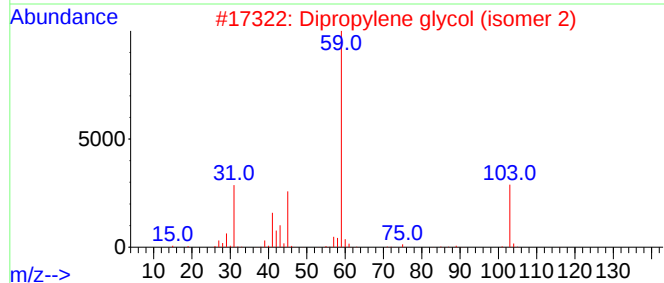
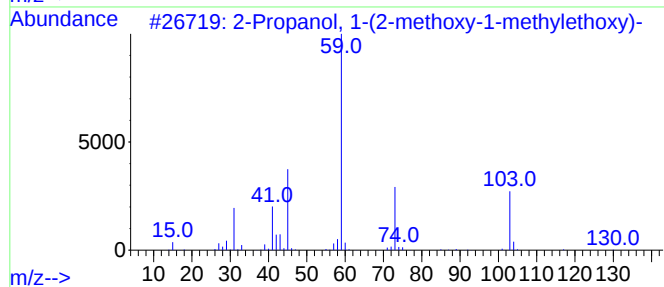
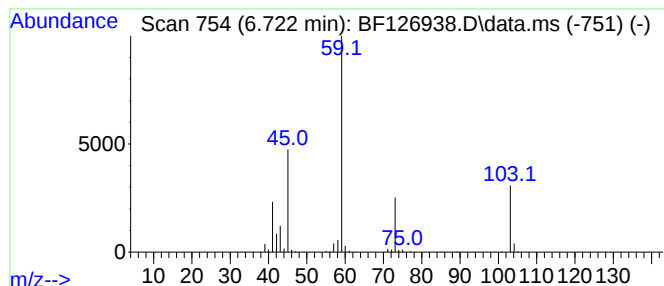
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Propanol, 1-(2-methoxy-1-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.722	6.31 ng	191117	1,4-Dichlorobenzene-d4	6.928

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	72
2			Dipropylene glycol (isomer 2)	134	C6H14O3	1000506-25-4	53
3			1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	50
4			Ethane, 1-ethoxy-1-methoxy-	104	C5H12O2	010471-14-4	50
5			1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	50



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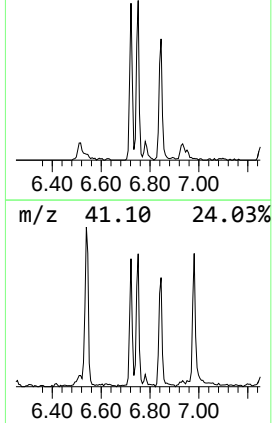
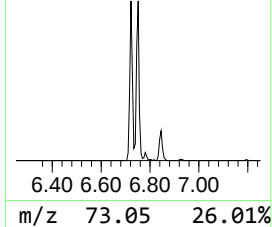
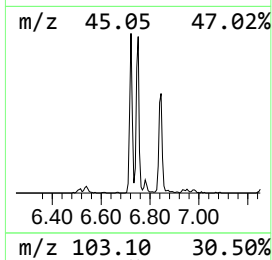
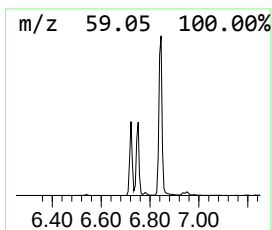
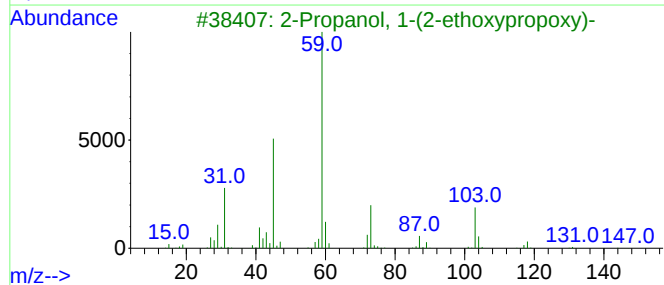
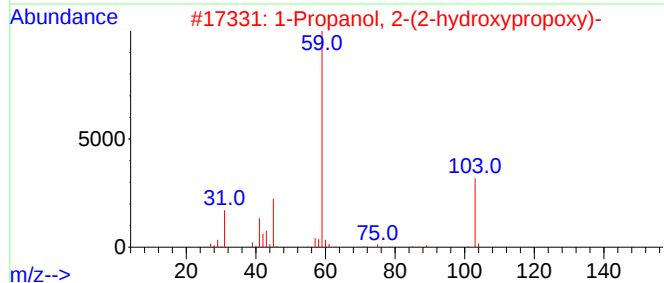
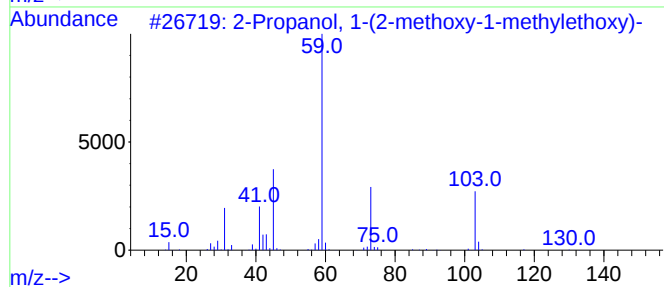
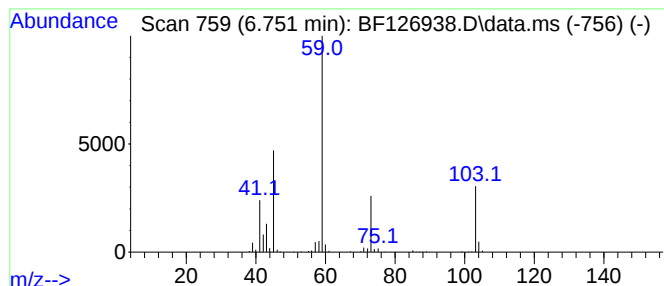
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Peak Number 4 1-Propanol, 2-(2-hydroxypro... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.751	6.81 ng	206281	1,4-Dichlorobenzene-d4	6.928

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	83		
2	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	59		
3	2-Propanol, 1-(2-ethoxypropoxy)-	162	C8H18O3	010143-32-5	56		
4	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	50		
5	Dipropylene glycol (isomer 3)	134	C6H14O3	1000506-25-5	50		



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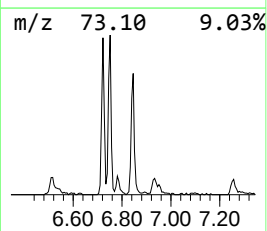
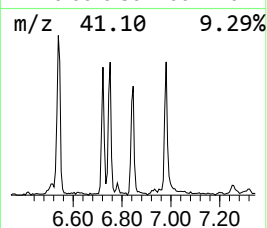
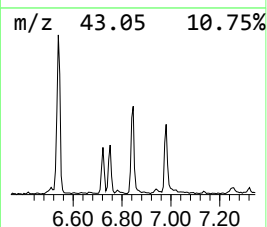
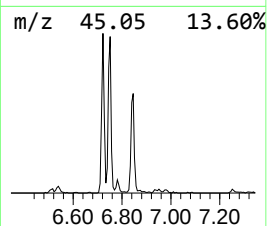
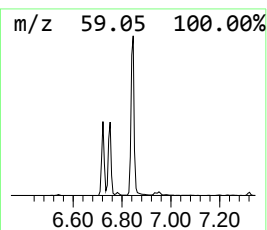
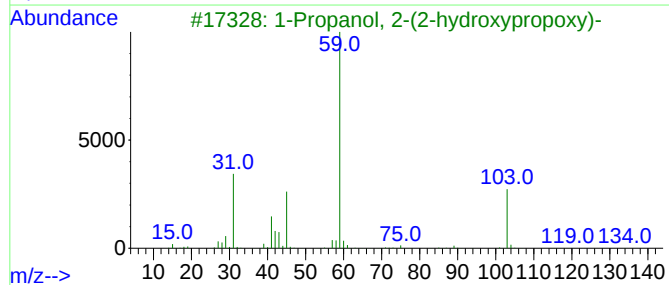
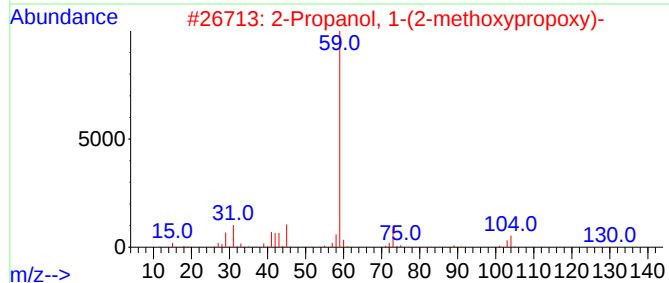
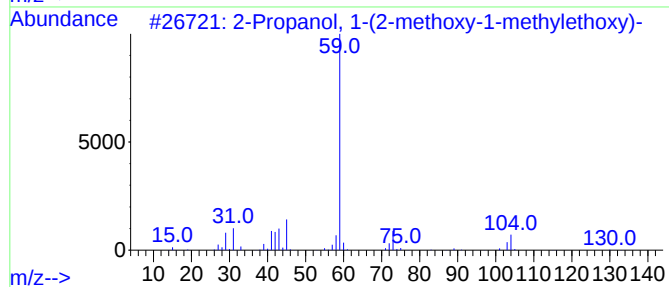
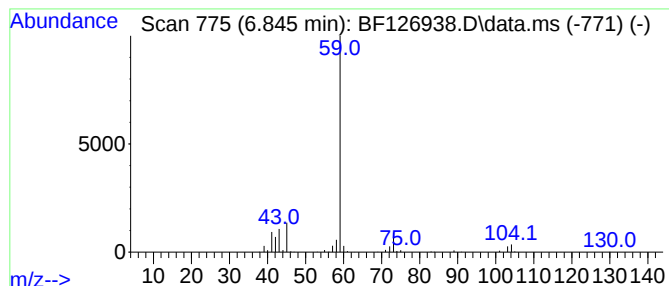
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Peak Number 5 2-Propanol, 1-(2-methoxypro... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.845	10.88 ng	329453	1,4-Dichlorobenzene-d4	6.928

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	83
2			2-Propanol, 1-(2-methoxypropoxy)-	148	C7H16O3	013429-07-7	74
3			1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	64
4			2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	64
5			Hexaethylene glycol dimethyl ether	310	C14H30O7	001072-40-8	50



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MW-26R

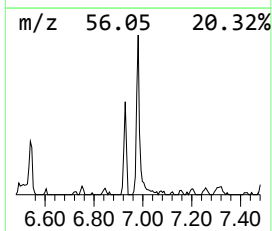
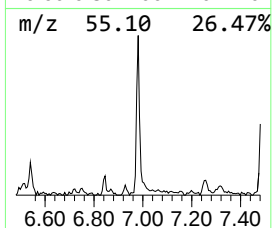
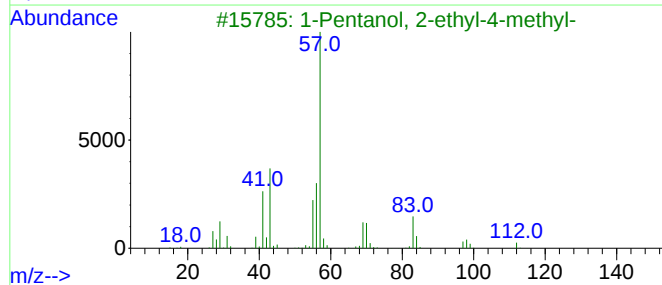
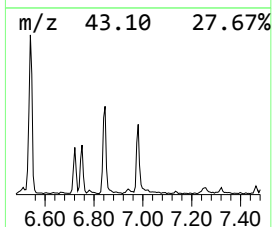
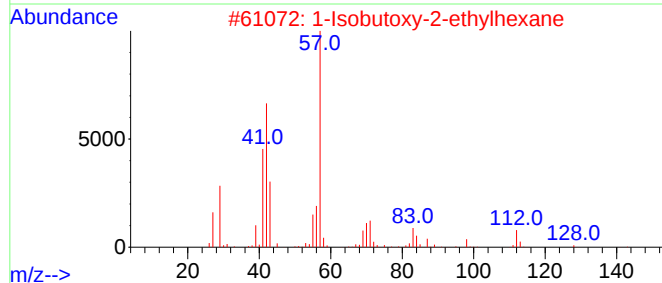
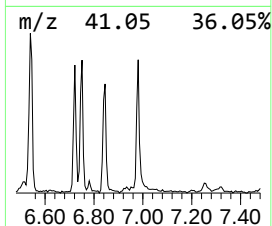
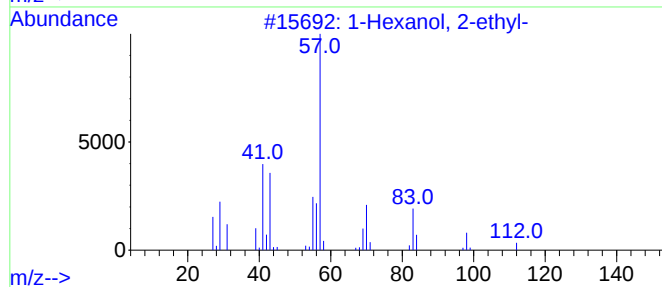
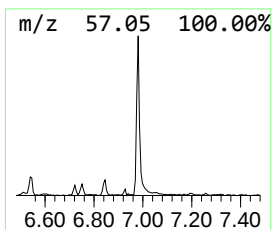
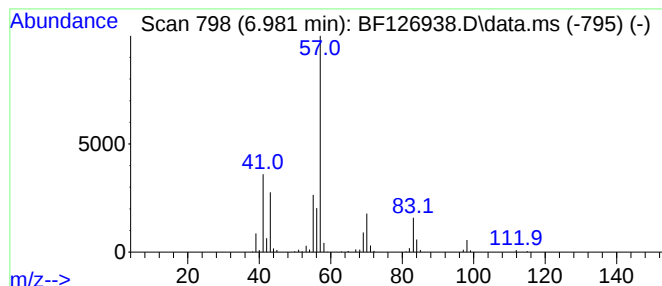
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Hexanol, 2-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.981	5.62 ng	170094	1,4-Dichlorobenzene-d4	6.928

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2			1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	64
3			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	64
4			1-Hexene, 5,5-dimethyl-	112	C8H16	007116-86-1	53
5			Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021722\
Data File : BF126938.D
Acq On : 17 Feb 2022 20:44
Operator : CG\JU
Sample : N1573-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-26R

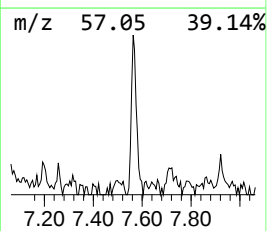
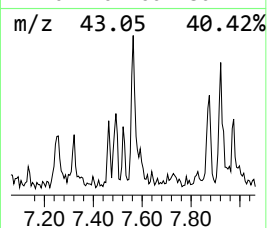
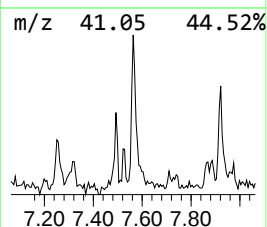
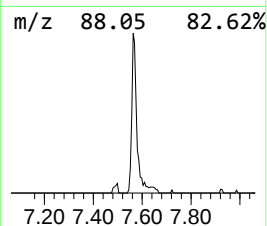
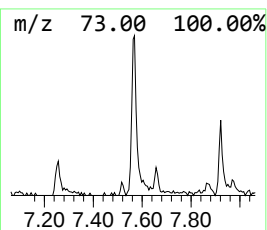
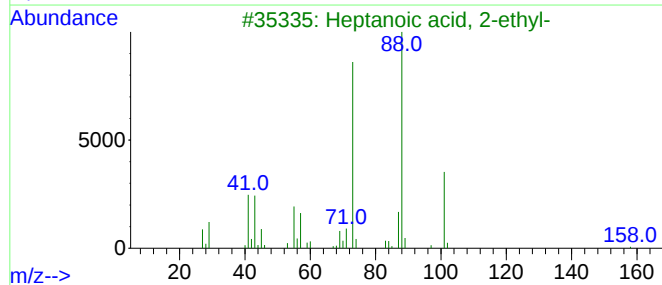
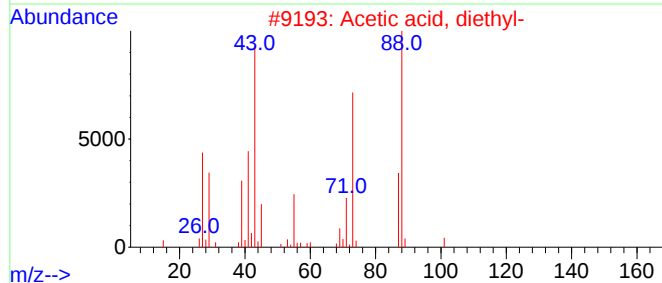
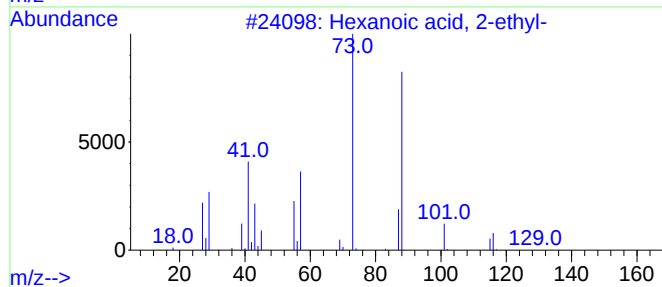
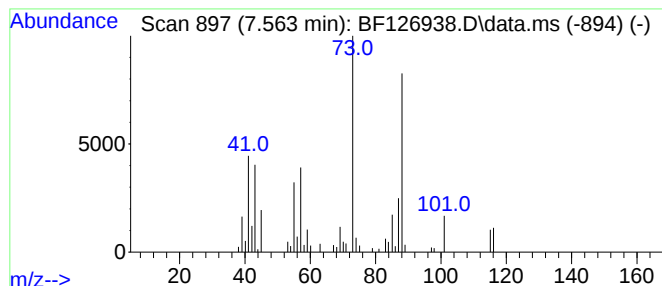
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexanoic acid, 2-ethyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.563	2.43 ng	73606	1,4-Dichlorobenzene-d4	6.928

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	64
2			Acetic acid, diethyl-	116	C6H12O2	000088-09-5	50
3			Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	50
4			Butanoic acid, 2-methyl-, methyl...	116	C6H12O2	000868-57-5	47
5			Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	40



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021722\
Data File : BF126938.D
Acq On : 17 Feb 2022 20:44
Operator : CG\JU
Sample : N1573-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-26R

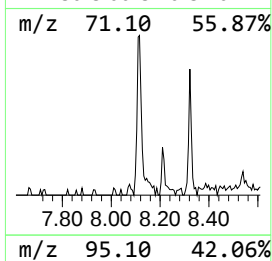
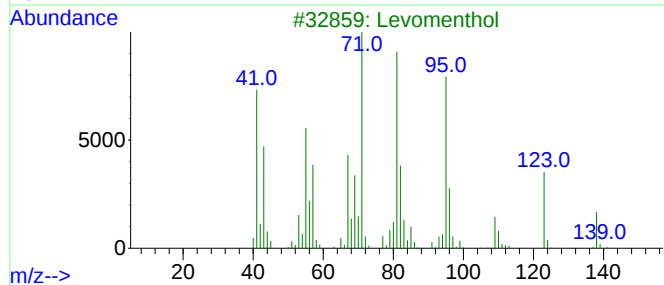
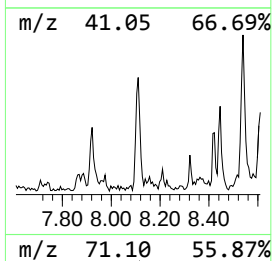
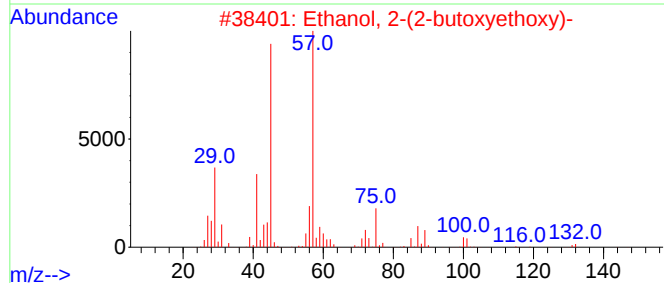
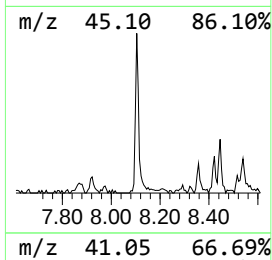
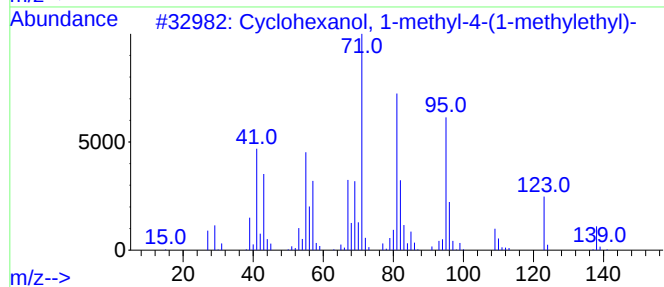
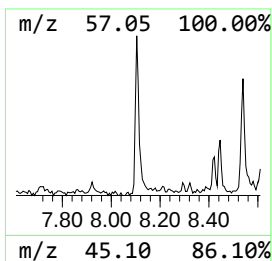
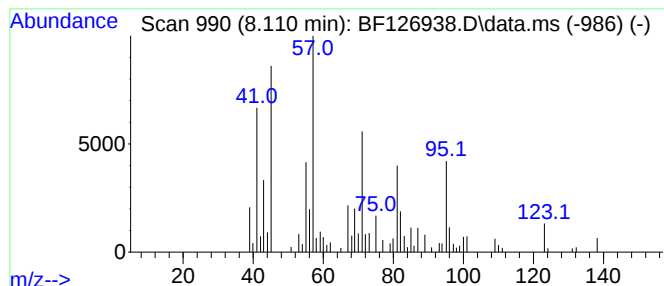
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown8.110 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.110	2.31 ng	96432	Naphthalene-d8	8.210

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexanol, 1-methyl-4-(1-meth...	156	C10H20O	021129-27-1	45
2			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	43
3			Levomenthol	156	C10H20O	002216-51-5	43
4			Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	023283-97-8	38
5			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021722\
Data File : BF126938.D
Acq On : 17 Feb 2022 20:44
Operator : CG\JU
Sample : N1573-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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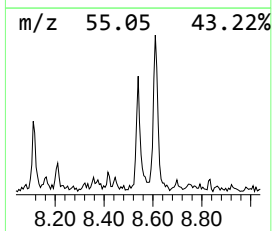
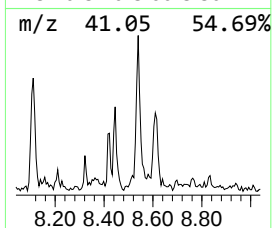
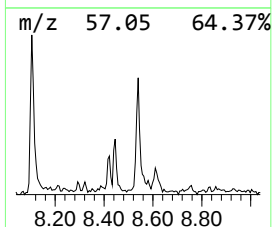
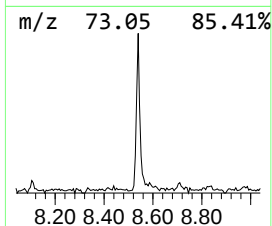
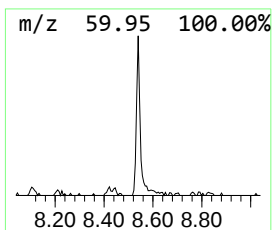
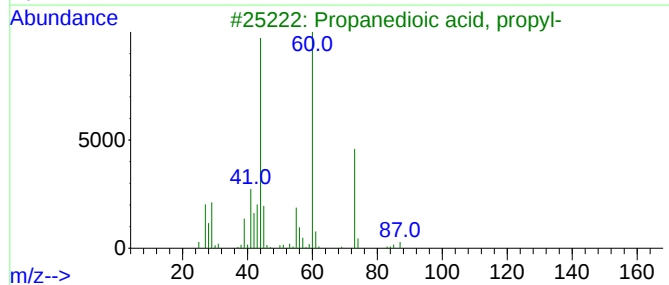
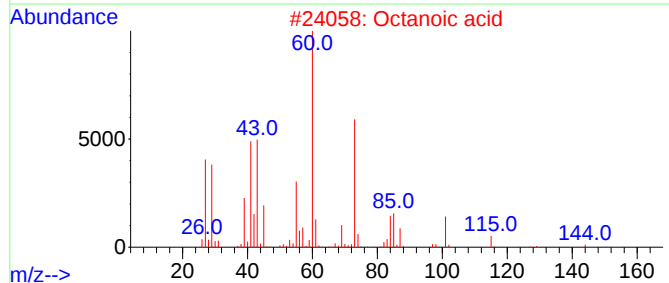
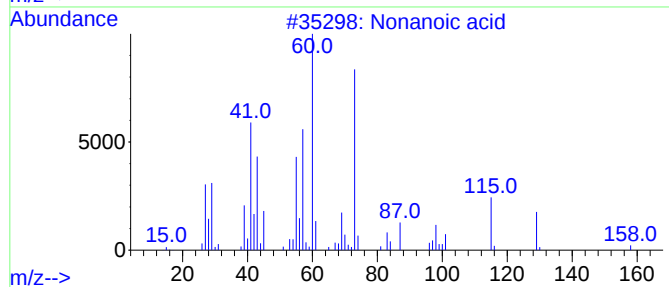
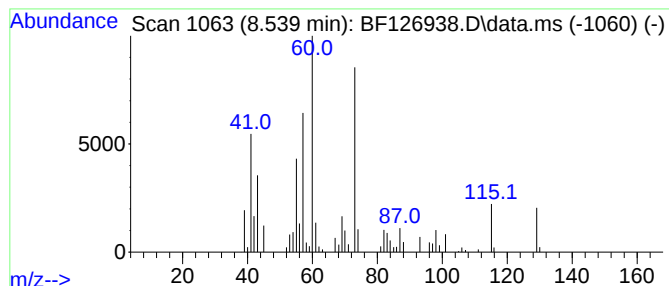
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Nonanoic acid Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.539	2.24 ng	93781	Naphthalene-d8	8.210

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonanoic acid	158	C9H18O2	000112-05-0	91
2			Octanoic acid	144	C8H16O2	000124-07-2	50
3			Propanedioic acid, propyl-	146	C6H10O4	000616-62-6	50
4			.beta.-D-Glucopyranose, 1,6-anhy...	162	C6H10O5	000498-07-7	50
5			Hexanoic acid	116	C6H12O2	000142-62-1	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021722\
Data File : BF126938.D
Acq On : 17 Feb 2022 20:44
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Sample : N1573-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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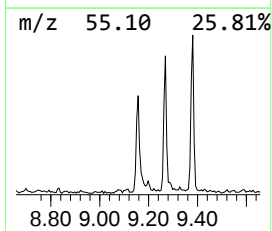
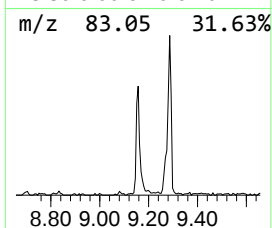
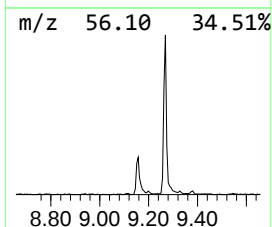
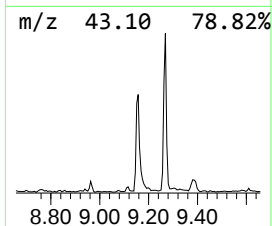
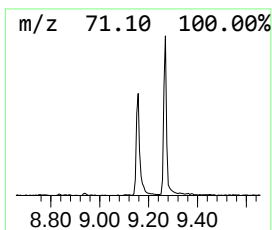
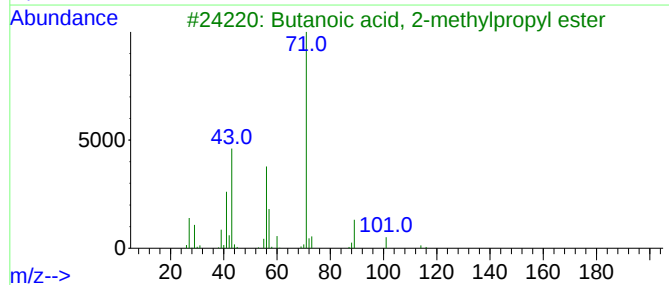
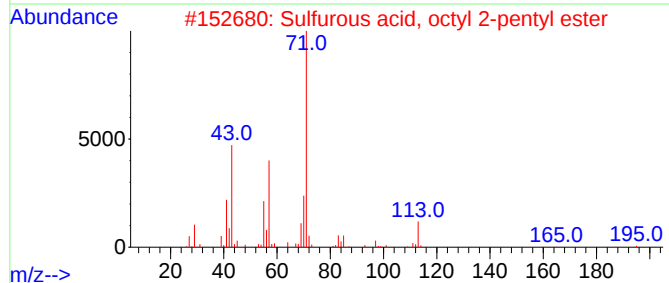
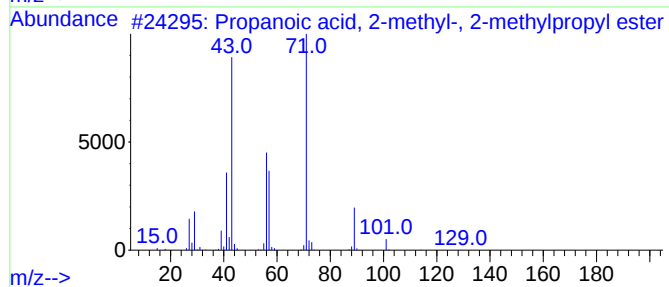
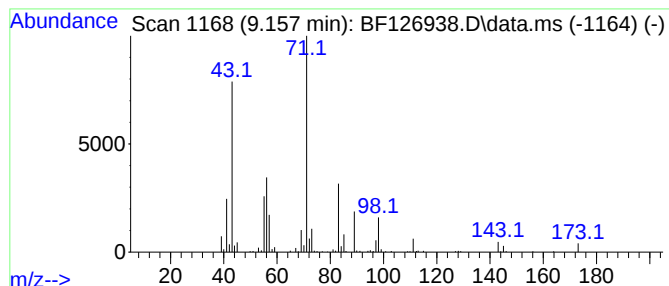
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Propanoic acid, 2-methyl-, ... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.157	4.96 ng	223291	Acenaphthene-d10	9.969

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	50
2			Sulfurous acid, octyl 2-pentyl e...	264	C13H28O3S	1000309-15-7	43
3			Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	42
4			2-Decanol, 2-methylpropionate	228	C14H28O2	1000447-30-4	40
5			Isopropyl butyrate	130	C7H14O2	000638-11-9	37



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021722\
Data File : BF126938.D
Acq On : 17 Feb 2022 20:44
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ClientSampleId :
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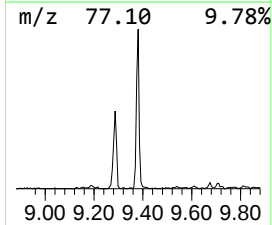
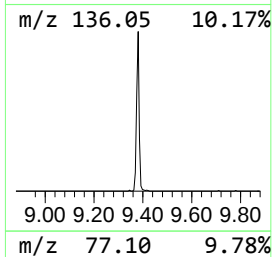
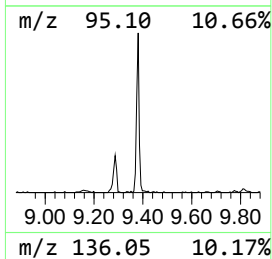
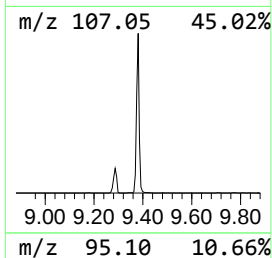
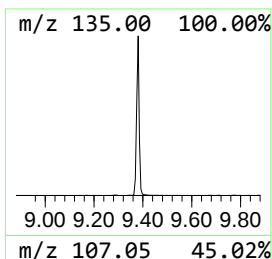
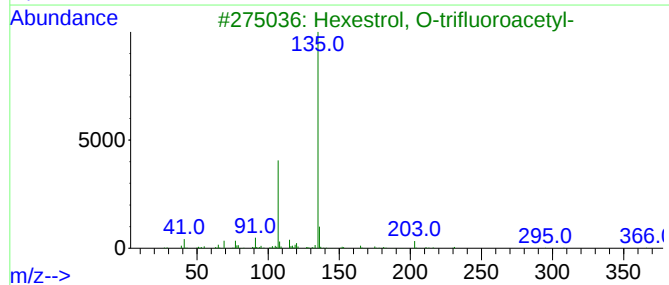
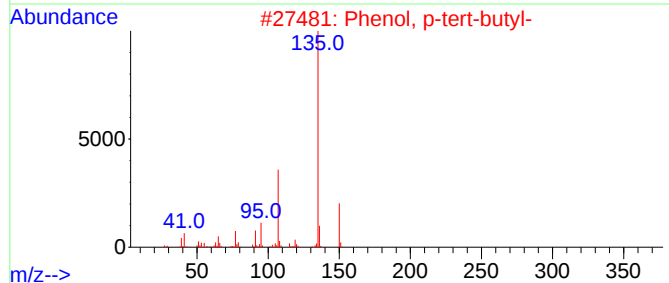
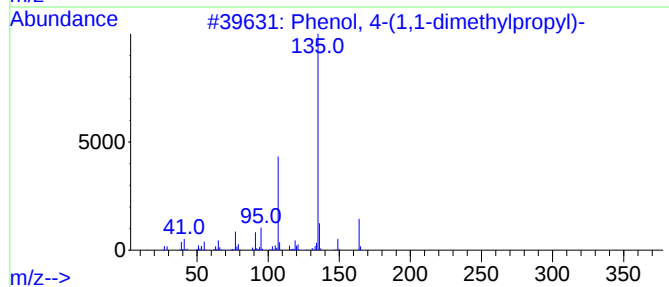
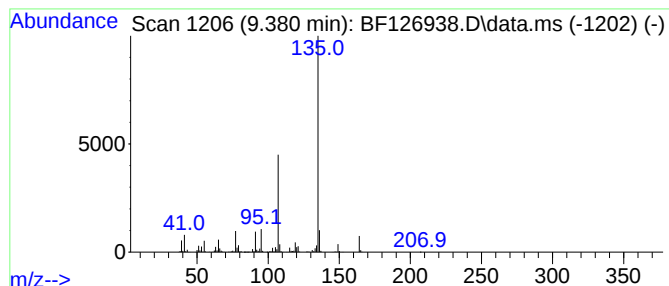
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Phenol, 4-(1,1-dimethylprop... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.380	17.91 ng	805889	Acenaphthene-d10	9.969

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	93
2			Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	90
3			Hexestrol, O-trifluoroacetyl-	366	C20H21F3O3	1000365-31-7	72
4			Hexestrol	270	C18H22O2	000084-16-2	72
5			Phenol, 4-(1,1,3,3-tetramethylbu...	206	C14H22O	000140-66-9	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021722\
Data File : BF126938.D
Acq On : 17 Feb 2022 20:44
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Sample : N1573-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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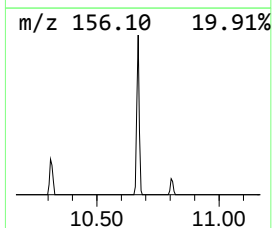
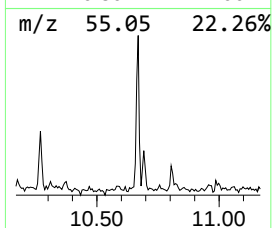
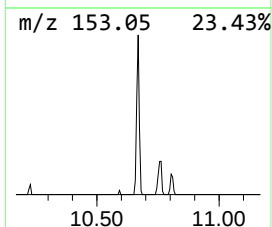
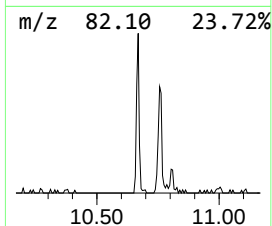
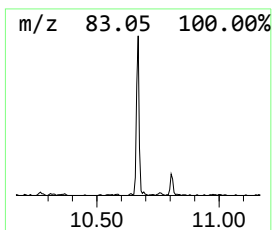
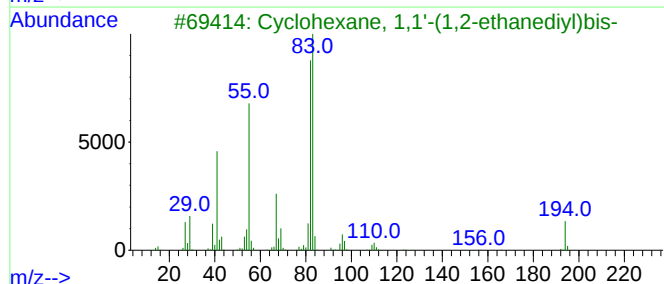
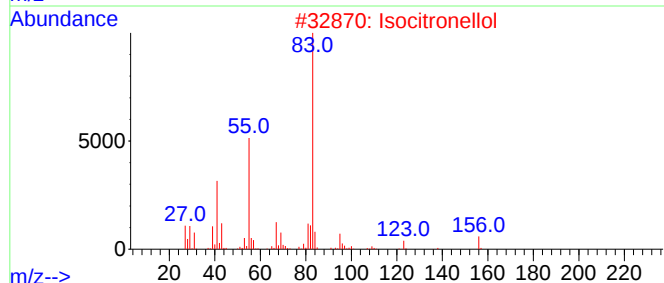
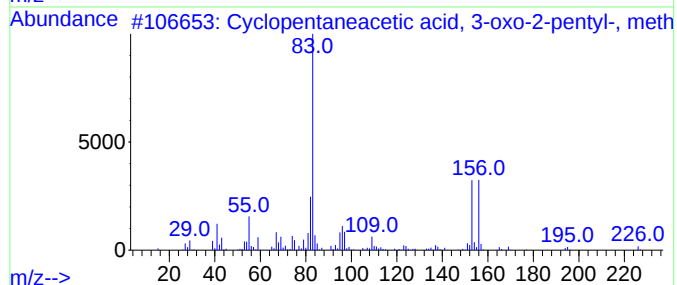
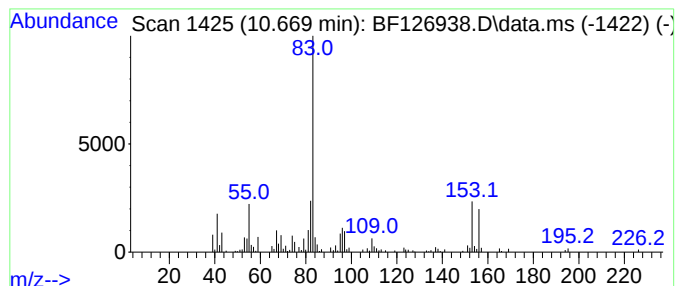
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Cyclopentaneacetic acid, 3-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.669	2.95 ng	132695	Acenaphthene-d10	9.969

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentaneacetic acid, 3-oxo-2...	226	C13H22O3	024851-98-7	96
2			Isocitronellol	156	C10H20O	018479-52-2	50
3			Cyclohexane, 1,1'-(1,2-ethanediyl...	194	C14H26	003321-50-4	47
4			6-Hydroxy-10a-methyl-4,7-dimethy...	376	C20H24O7	1798297-60-5	43
5			2,6-Dimethyl-6-nitro-2-hepten-4-one	185	C9H15NO3	073583-56-9	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021722\
Data File : BF126938.D
Acq On : 17 Feb 2022 20:44
Operator : CG\JU
Sample : N1573-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-26R

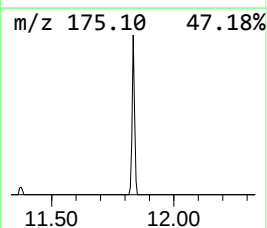
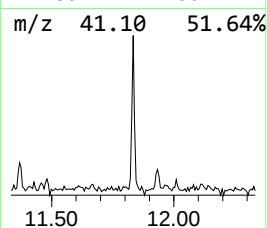
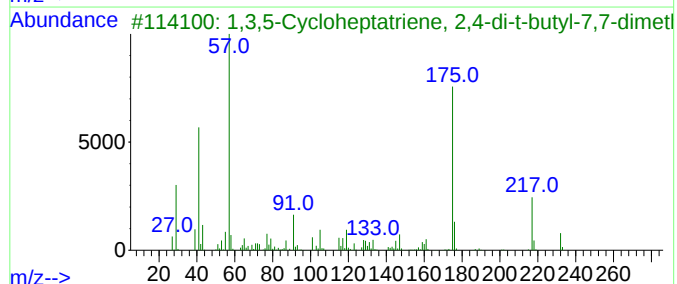
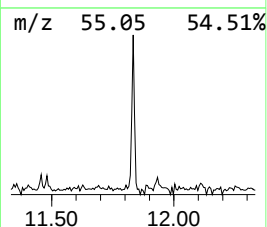
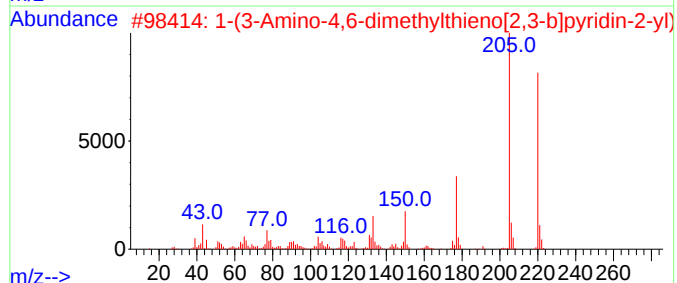
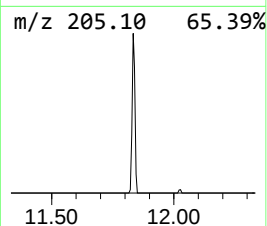
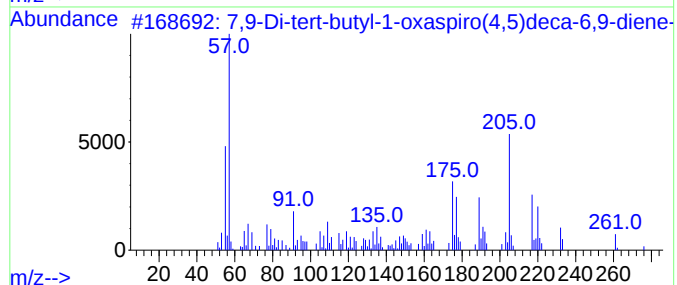
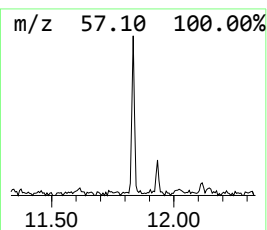
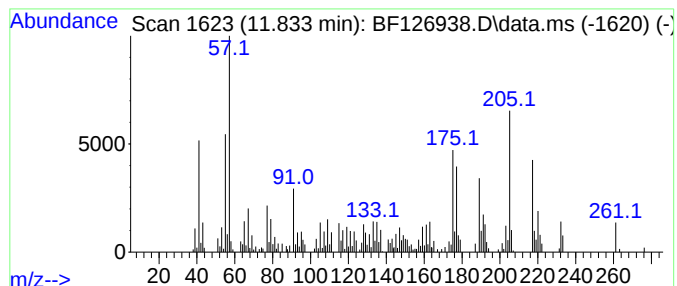
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 7,9-Di-tert-butyl-1-oxaspiro... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.833	2.56 ng	120369	Phenanthrene-d10	11.457

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	98		
2	1-(3-Amino-4,6-dimethylthieno[2,...	220	C11H12N2OS	052505-42-7	46		
3	1,3,5-Cycloheptatriene, 2,4-di-t...	232	C17H28	1000160-92-5	44		
4	(1R,3aR,5aR,9aS)-1,4,4,7-Tetrame...	220	C15H24O	104188-25-2	38		
5	Ethanone, 1-(5,6,7,8-tetrahydro-...	220	C14H20O2	071596-88-8	38		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021722\
Data File : BF126938.D
Acq On : 17 Feb 2022 20:44
Operator : CG\JU
Sample : N1573-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-26R

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.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
Cyclopentanone	4.457	12.1	ng	365596	1	6.928	605777	20.0
Ethanol, 2-(1-m...	5.157	4.7	ng	142502	1	6.928	605777	20.0
2-Propanol, 1-(...	6.722	6.3	ng	191117	1	6.928	605777	20.0
1-Propanol, 2-(...	6.751	6.8	ng	206281	1	6.928	605777	20.0
2-Propanol, 1-(...	6.845	10.9	ng	329453	1	6.928	605777	20.0
1-Hexanol, 2-et...	6.981	5.6	ng	170094	1	6.928	605777	20.0
Hexanoic acid, ...	7.563	2.4	ng	73606	1	6.928	605777	20.0
unknown8.110	8.110	2.3	ng	96432	2	8.210	835472	20.0
Nonanoic acid	8.539	2.2	ng	93781	2	8.210	835472	20.0
Propanoic acid,...	9.157	5.0	ng	223291	3	9.969	899979	20.0
Phenol, 4-(1,1-...	9.380	17.9	ng	805889	3	9.969	899979	20.0
Cyclopentaneace...	10.669	3.0	ng	132695	3	9.969	899979	20.0
7,9-Di-tert-but...	11.833	2.6	ng	120369	4	11.457	939485	20.0