

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021722\
 Data File : BF126929.D
 Acq On : 17 Feb 2022 16:19
 Operator : CG\JU
 Sample : N1573-11
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 GES-1R

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: BF126929.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.469	366	371	380	rVB	346411	392240	7.19%	1.281%
2	5.169	485	490	496	rBV	146902	174894	3.21%	0.571%
3	5.551	550	555	558	rBV	2616345	2388603	43.80%	7.800%
4	6.545	719	724	727	rVB	1930646	1766516	32.39%	5.769%
5	6.722	751	754	756	rBV	297697	220690	4.05%	0.721%
6	6.751	756	759	762	rVB	318981	233334	4.28%	0.762%
7	6.845	771	775	785	rBV	446738	382873	7.02%	1.250%
8	6.928	785	789	792	rBV	864134	667419	12.24%	2.180%
9	6.981	795	798	807	rVB	267926	231208	4.24%	0.755%
10	7.498	877	886	888	rBV	2795753	3023060	55.43%	9.872%
11	7.563	893	897	906	rVB	75081	100893	1.85%	0.329%
12	7.922	954	958	962	rBV3	52715	56532	1.04%	0.185%
13	8.116	986	991	997	rBV2	89438	122114	2.24%	0.399%
14	8.210	1003	1007	1010	rBV	1115481	919172	16.85%	3.002%
15	8.357	1029	1032	1040	rVB	57236	66492	1.22%	0.217%
16	8.539	1057	1063	1069	rBV2	157189	197347	3.62%	0.644%
17	9.157	1165	1168	1174	rBV	241053	254234	4.66%	0.830%
18	9.292	1184	1191	1194	rBV	5208947	5453677	100.00%	17.810%
19	9.381	1202	1206	1209	rBV	1415993	1078748	19.78%	3.523%
20	9.945	1296	1302	1303	rBV2	85407	75721	1.39%	0.247%
21	9.969	1303	1306	1309	rVB	1258223	1011136	18.54%	3.302%
22	10.275	1354	1358	1361	rVB2	84903	70050	1.28%	0.229%
23	10.380	1372	1376	1379	rVB	230241	183767	3.37%	0.600%
24	10.669	1422	1425	1427	rBV	277741	195554	3.59%	0.639%
25	10.763	1436	1441	1444	rBV	3801444	3561622	65.31%	11.631%
26	11.457	1555	1559	1563	rBV	1321648	1071658	19.65%	3.500%
27	11.833	1620	1623	1626	rVB	206580	160436	2.94%	0.524%
28	13.051	1824	1830	1833	rBV	5567253	5398379	98.99%	17.629%
29	14.098	2005	2008	2012	rBV	719930	630206	11.56%	2.058%
30	15.604	2259	2264	2275	rBV	432868	533171	9.78%	1.741%

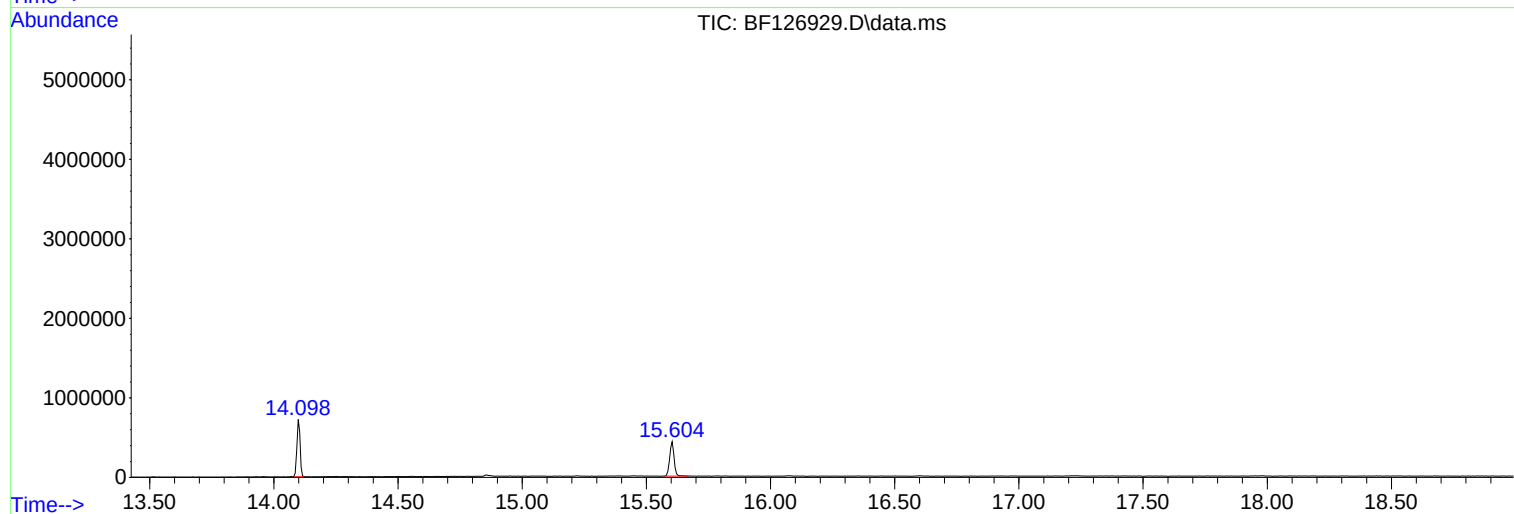
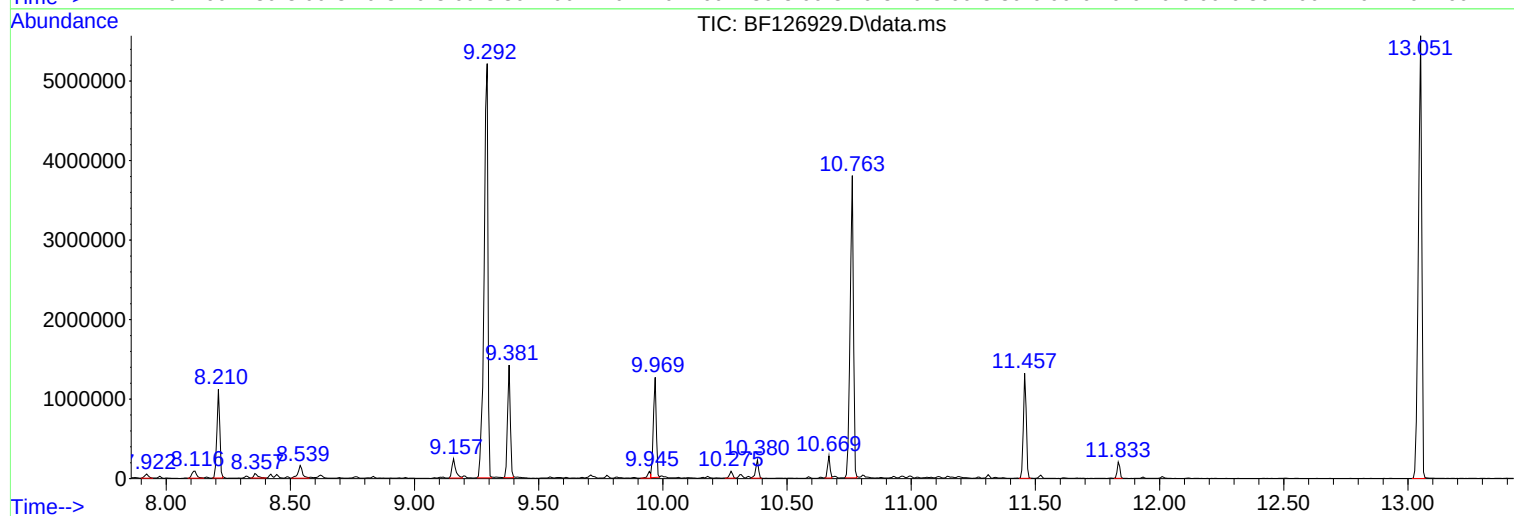
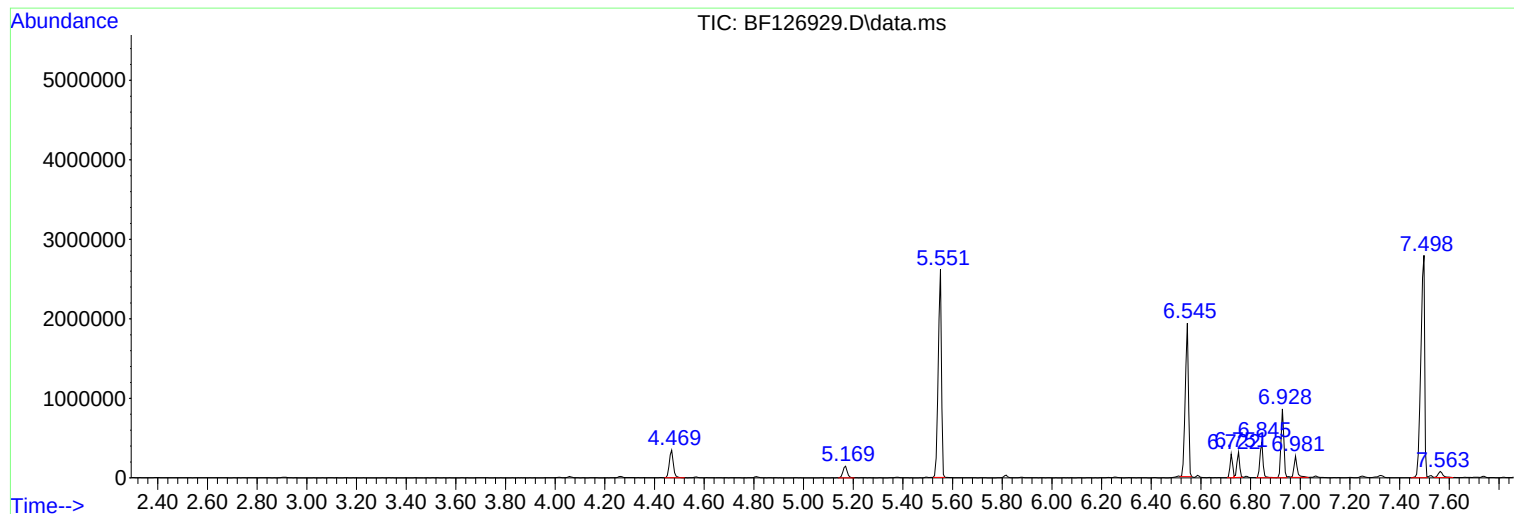
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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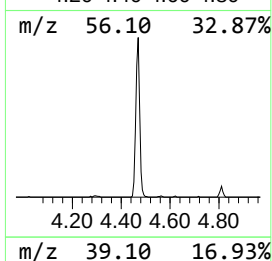
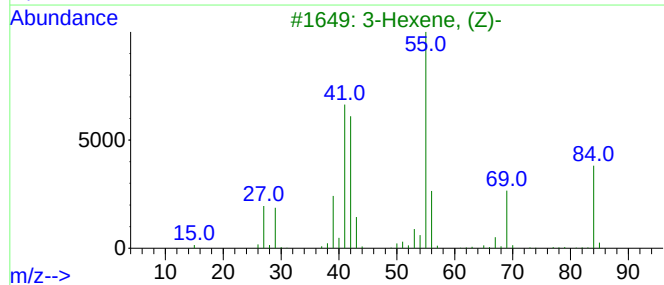
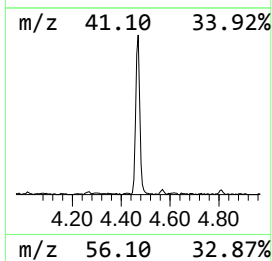
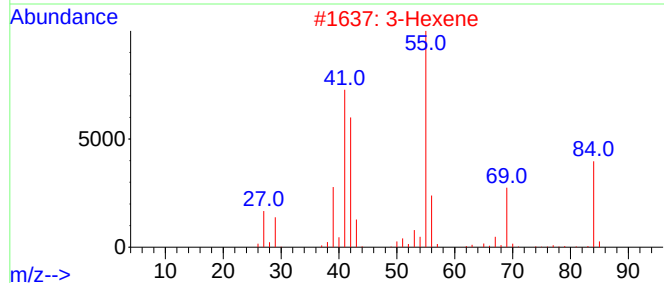
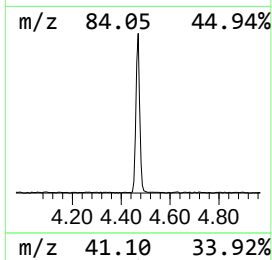
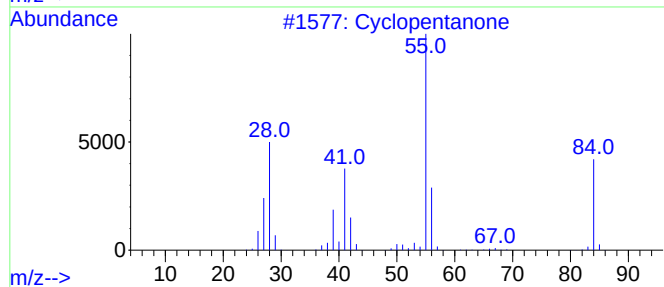
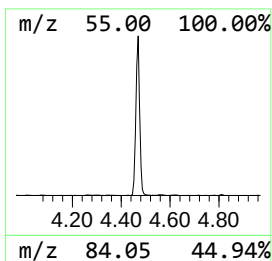
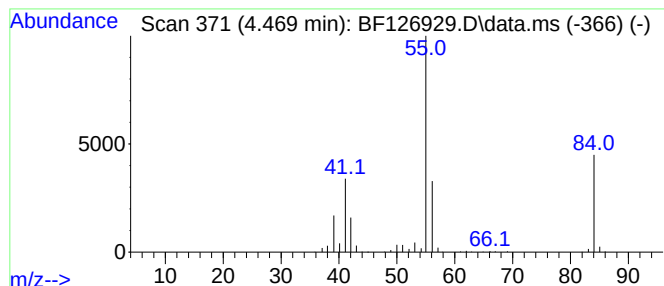
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Cyclopentanone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.469	11.75 ng	392240	1,4-Dichlorobenzene-d4	6.928

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentanone	84	C5H8O	000120-92-3	91
2			3-Hexene	84	C6H12	000592-47-2	64
3			3-Hexene, (Z)-	84	C6H12	007642-09-3	59
4			2-Hexene	84	C6H12	000592-43-8	59
5			2(5H)-Furanone	84	C4H4O2	000497-23-4	50



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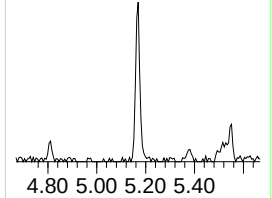
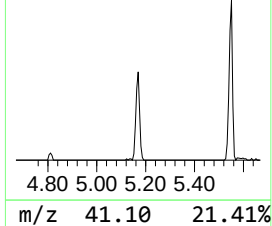
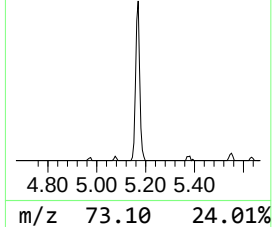
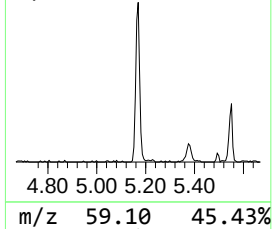
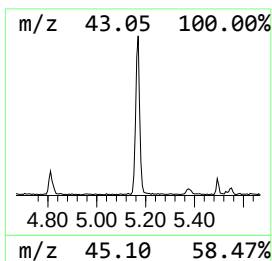
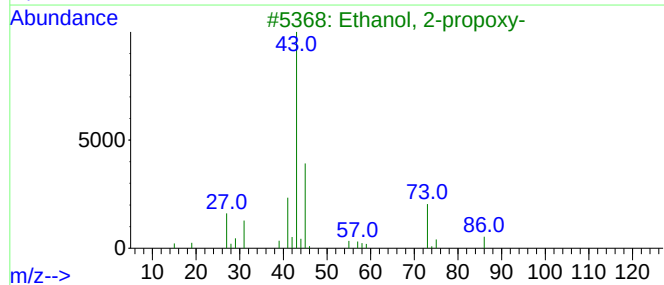
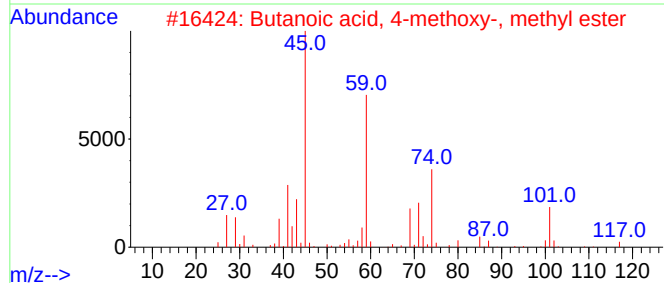
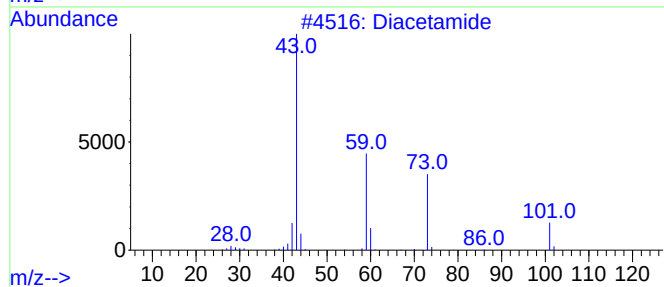
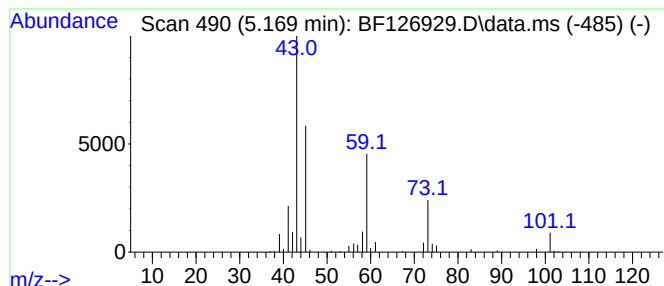
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 unknown5.169 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.169	5.24 ng	174894	1,4-Dichlorobenzene-d4	6.928

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diacetamide	101	C4H7NO2	000625-77-4	49
2			Butanoic acid, 4-methoxy-, methy...	132	C6H12O3	029006-01-7	42
3			Ethanol, 2-propoxy-	104	C5H12O2	002807-30-9	38
4			2-Propanol, 1-propoxy-	118	C6H14O2	001569-01-3	37
5			1-(Methoxymethoxy)-3-methyl-3-hy...	148	C7H16O3	037587-78-3	33



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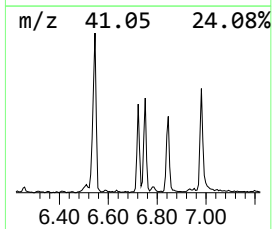
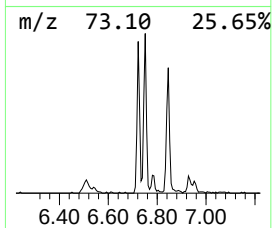
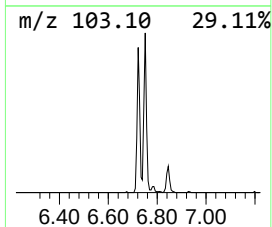
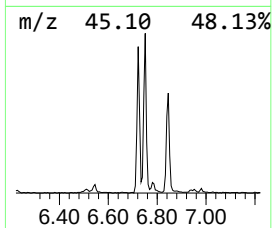
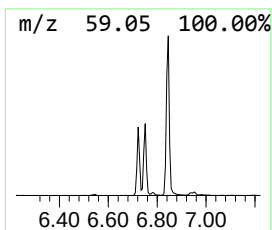
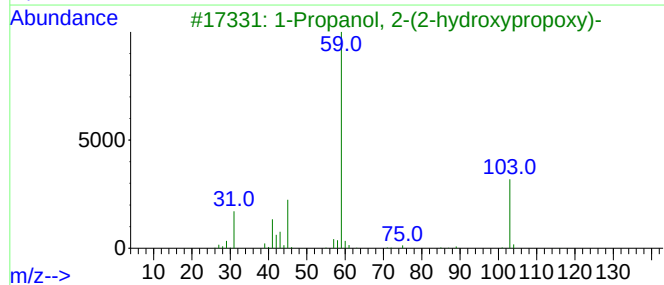
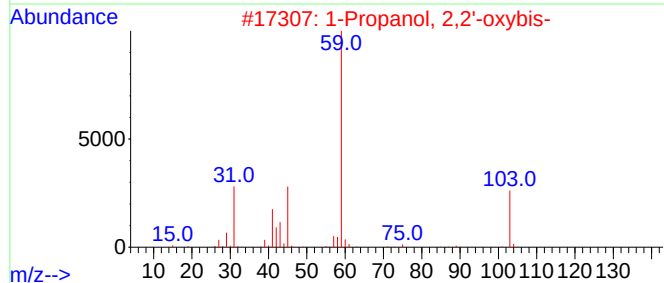
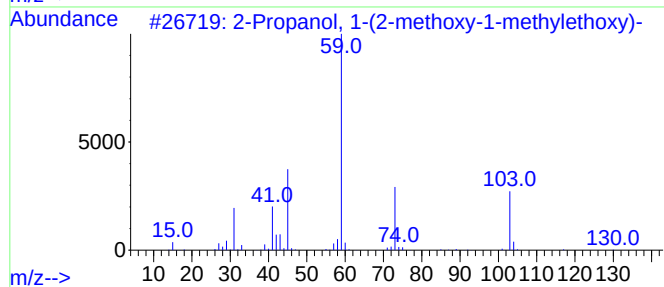
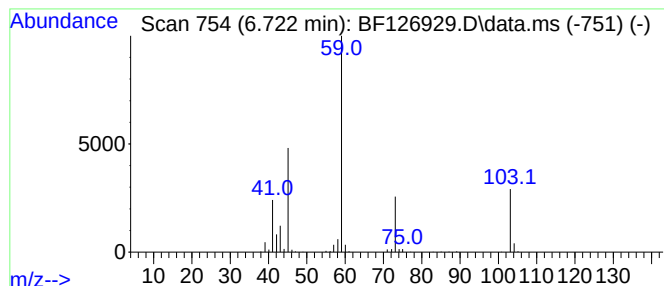
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Propanol, 1-(2-methoxy-1-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.722	6.61 ng	220690	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'-oxybis-	134	C6H14O3	000108-61-2	53		
3	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	50		
4	Dipropylene glycol (isomer 2)	134	C6H14O3	1000506-25-4	50		
5	Dipropylene glycol (isomer 3)	134	C6H14O3	1000506-25-5	50		



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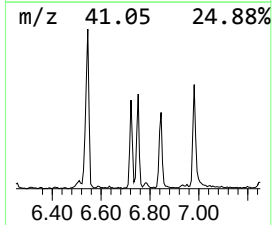
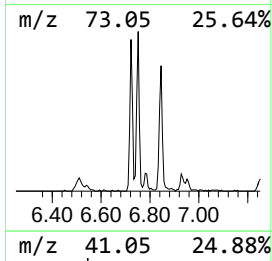
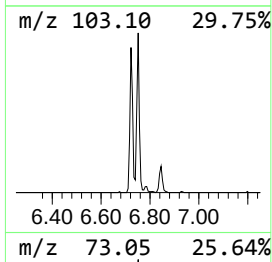
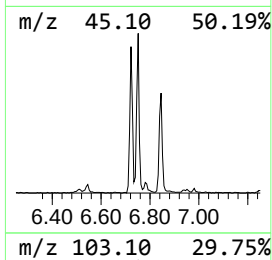
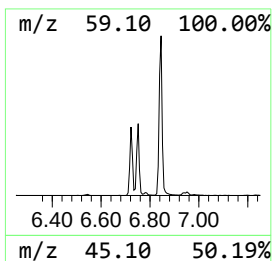
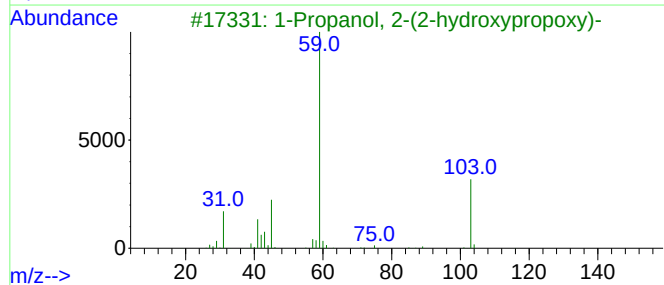
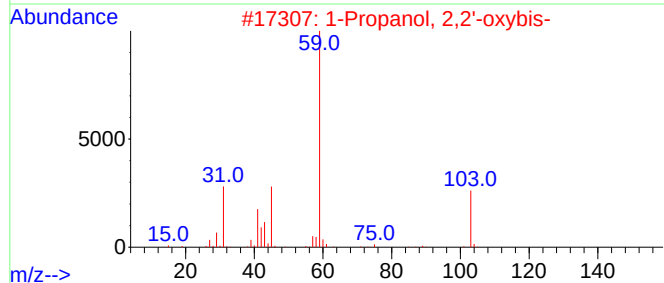
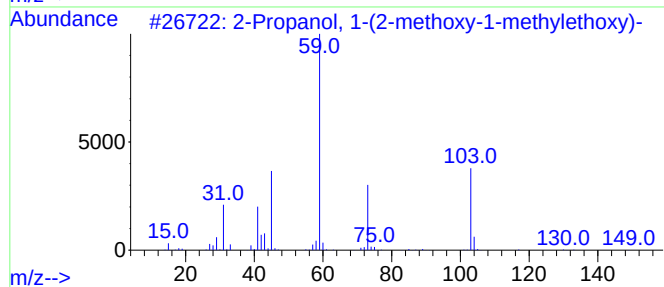
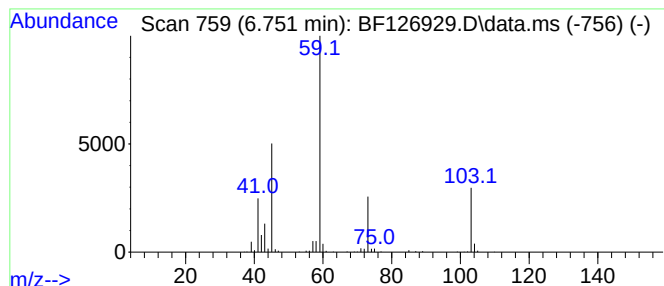
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Peak Number 4 1-Propanol, 2,2'-oxybis- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.751	6.99 ng	233334	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	80		
2	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	59		
3	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	59		
4	Dipropylene glycol (isomer 2)	134	C6H14O3	1000506-25-4	59		
5	2-Propanol, 1-(2-ethoxypropoxy)-	162	C8H18O3	010143-32-5	56		



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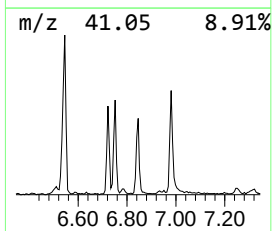
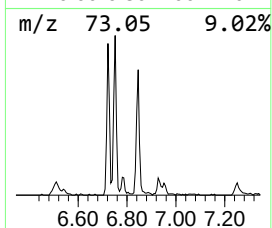
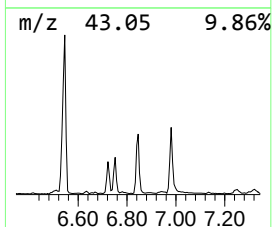
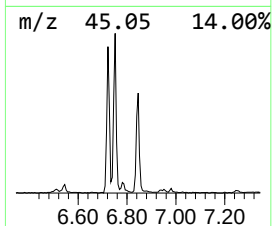
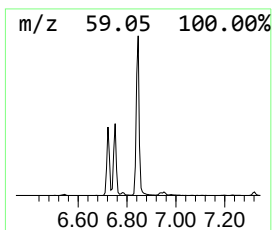
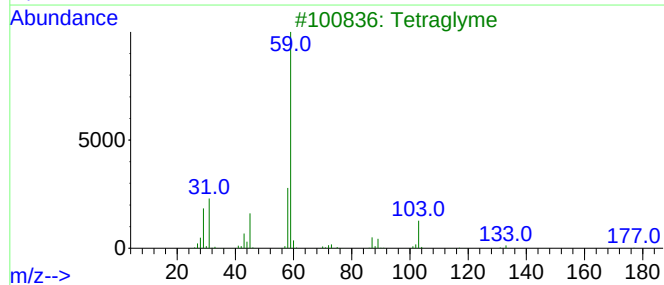
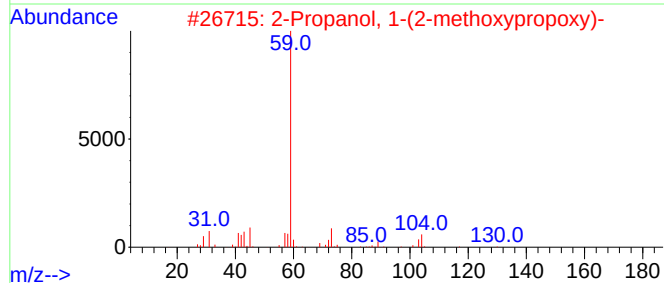
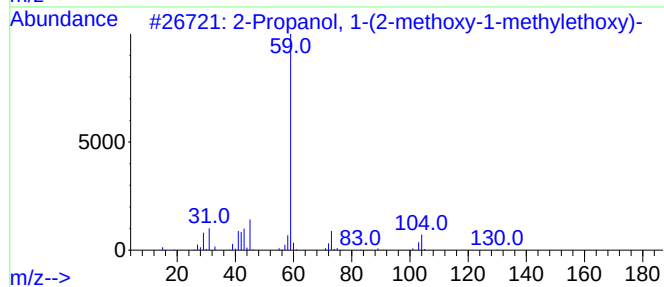
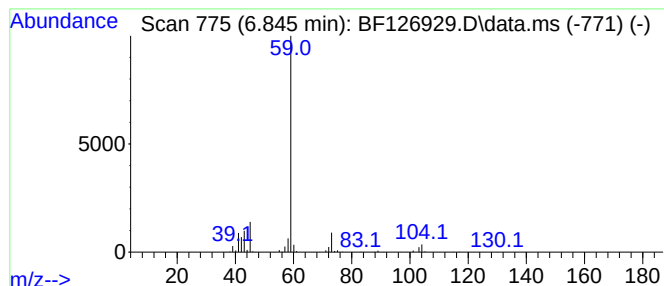
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Peak Number 5 2-Propanol, 1-(2-methoxypro... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.845	11.47 ng	382873	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	78		
3	Tetraglyme	222	C10H22O5	000143-24-8	50		
4	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	43		
5	2-Pentanol, 2,3-dimethyl-	116	C7H16O	004911-70-0	39		



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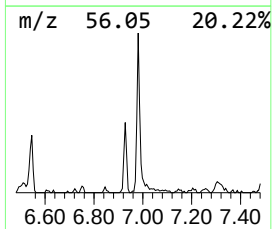
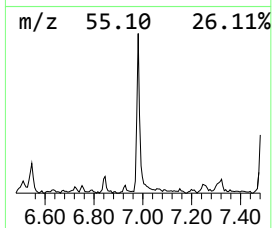
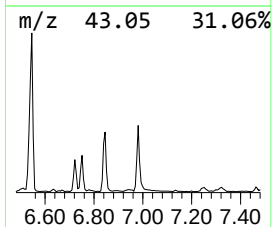
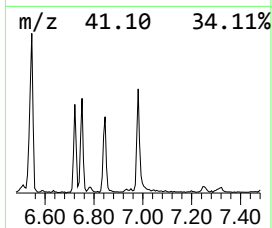
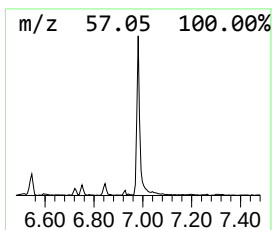
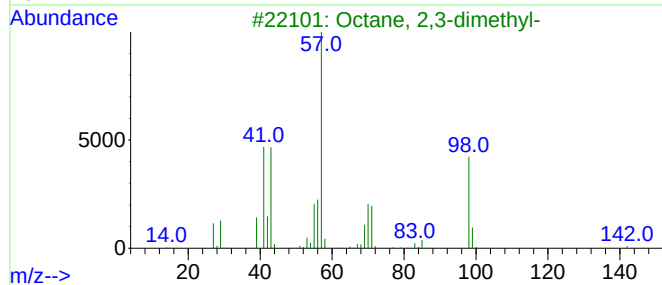
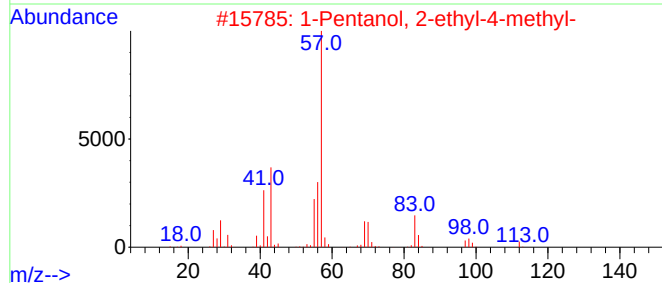
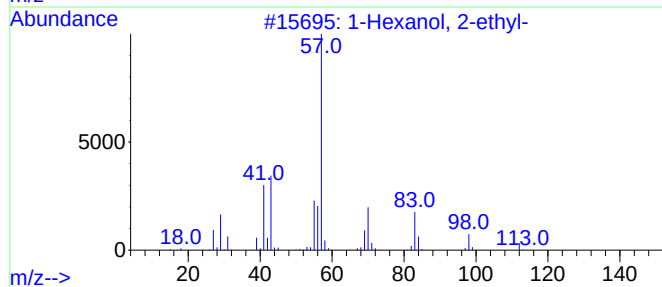
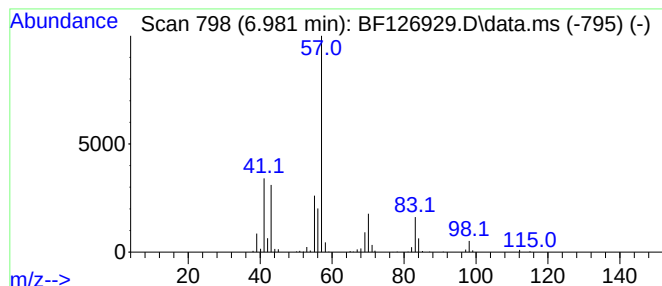
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Hexanol, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.981	6.93 ng	231208	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-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	74
3		Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	59
4		Carbonic acid, heptyl vinyl ester	186	C10H18O3	1010383-25-4	50
5		1-Hexene, 5,5-dimethyl-	112	C8H16	007116-86-1	45



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021722\
Data File : BF126929.D
Acq On : 17 Feb 2022 16:19
Operator : CG\JU
Sample : N1573-11
Misc :
ALS Vial : 9 Sample Multiplier: 1

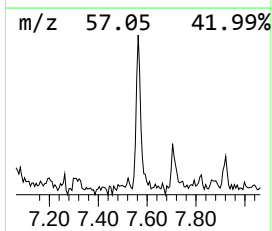
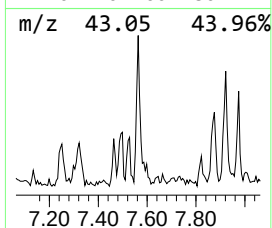
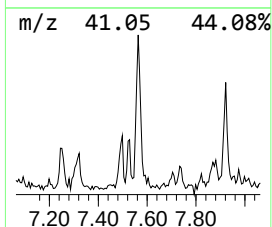
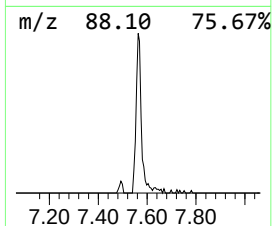
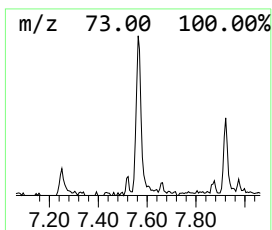
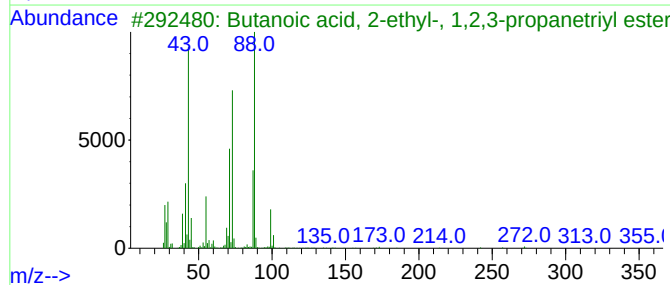
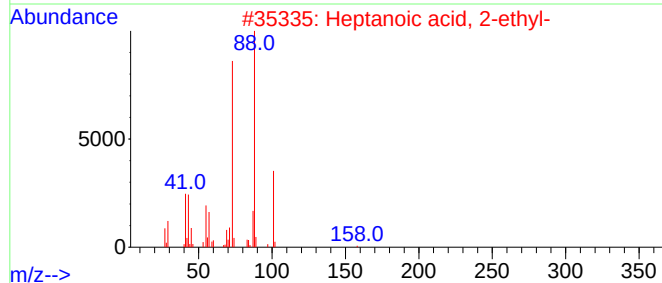
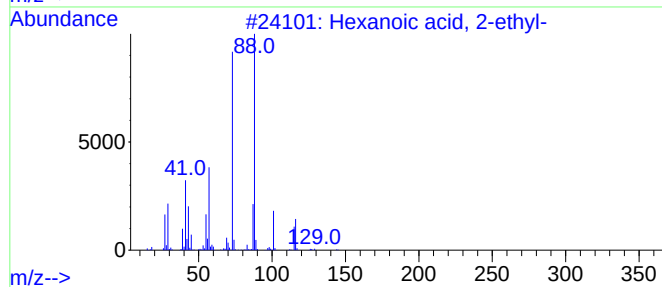
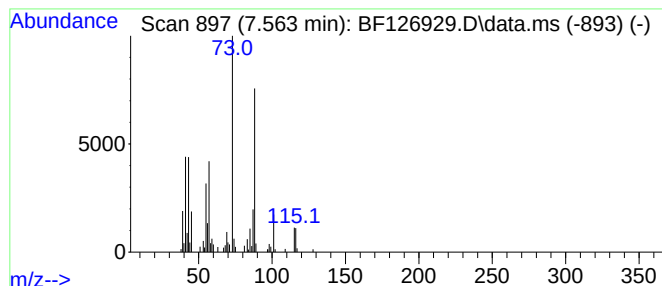
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	3.02 ng	100893	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	86
2	Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	53
3	Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	53
4	Acetic acid, diethyl-	116	C6H12O2	000088-09-5	53
5	2-Ethyl-4-methylpentanoic acid	144	C8H16O2	000108-81-6	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021722\
Data File : BF126929.D
Acq On : 17 Feb 2022 16:19
Operator : CG\JU
Sample : N1573-11
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GES-1R

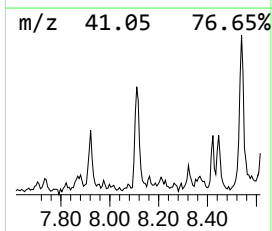
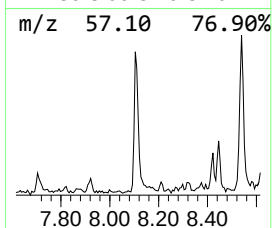
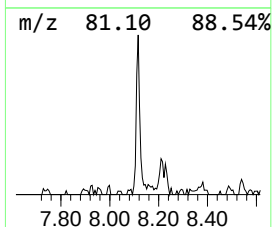
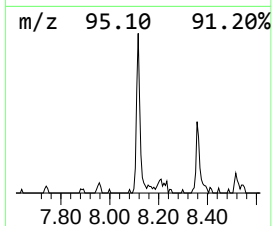
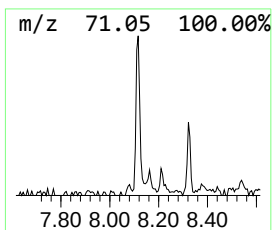
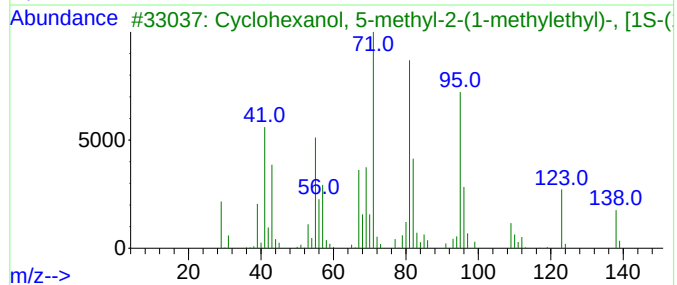
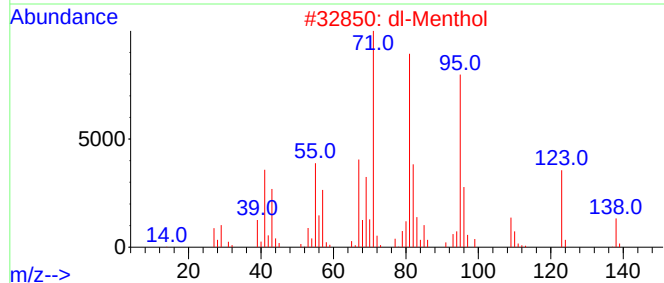
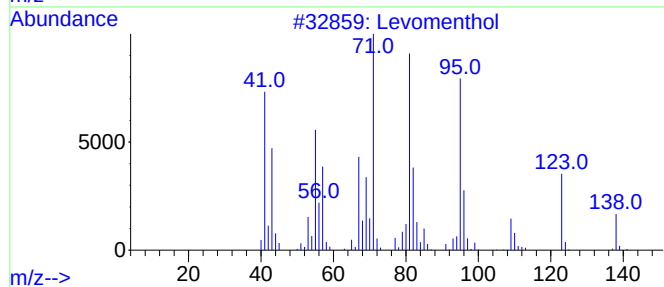
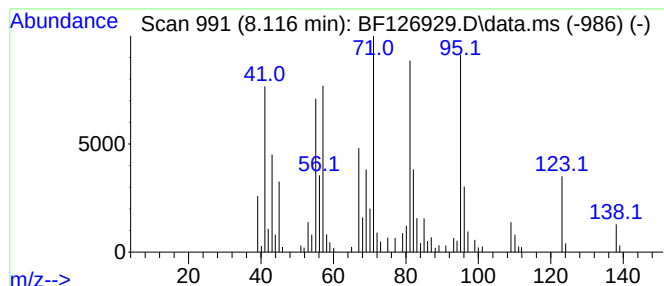
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Levomenthol Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.116	2.66 ng	122114	Naphthalene-d8	8.210

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Levomenthol	156	C10H20O	002216-51-5	91
2			dl-Menthol	156	C10H20O	000089-78-1	91
3			Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	002216-52-6	90
4			Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	001490-04-6	87
5			Cyclohexane, 1-methyl-4-(1-methy...	138	C10H18	001124-25-0	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021722\
Data File : BF126929.D
Acq On : 17 Feb 2022 16:19
Operator : CG\JU
Sample : N1573-11
Misc :
ALS Vial : 9 Sample Multiplier: 1

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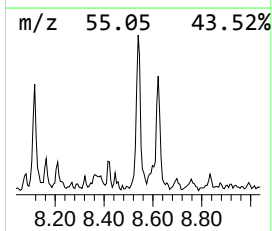
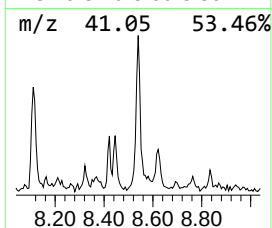
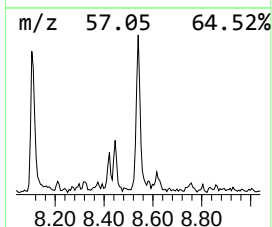
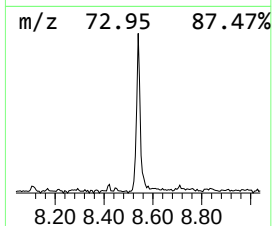
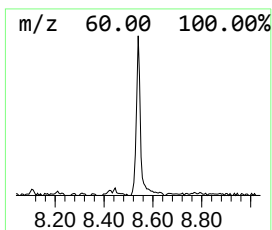
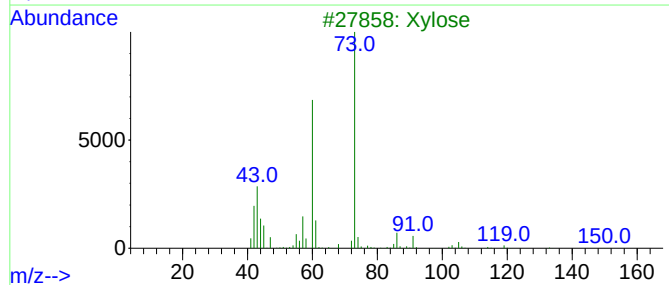
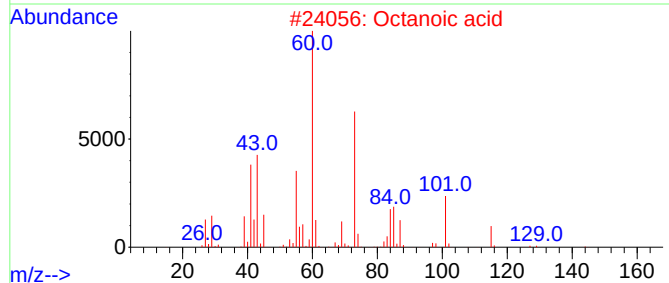
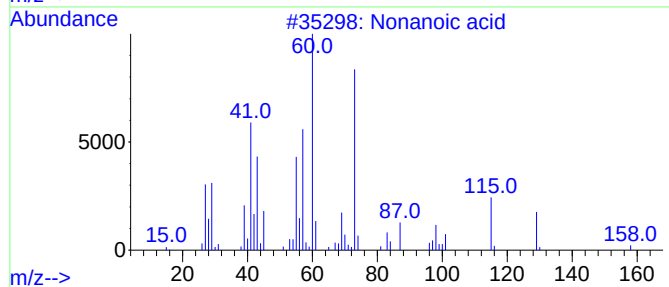
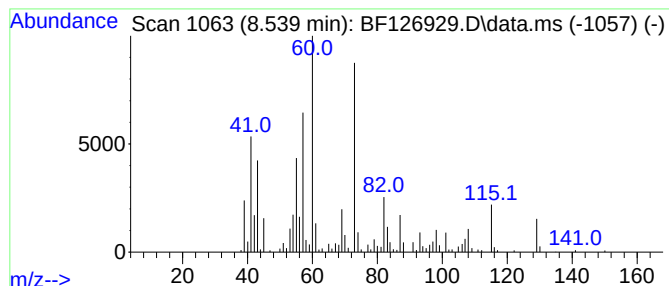
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Nonanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.539	4.29 ng	197347	Naphthalene-d8	8.210

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonanoic acid	158	C9H18O2	000112-05-0	80
2			Octanoic acid	144	C8H16O2	000124-07-2	47
3			Xylose	150	C5H10O5	000058-86-6	43
4			Butanoic acid	88	C4H8O2	000107-92-6	38
5			Pentanoic acid, 3-methyl-	116	C6H12O2	000105-43-1	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021722\
Data File : BF126929.D
Acq On : 17 Feb 2022 16:19
Operator : CG\JU
Sample : N1573-11
Misc :
ALS Vial : 9 Sample Multiplier: 1

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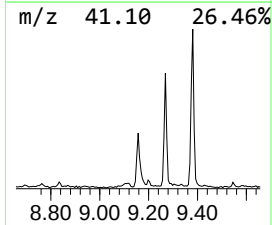
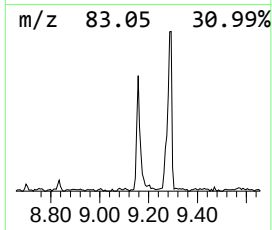
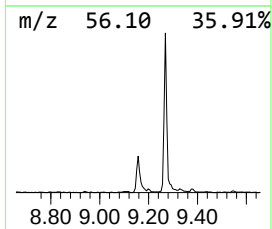
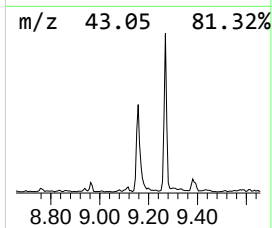
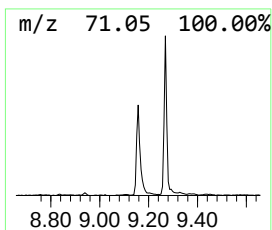
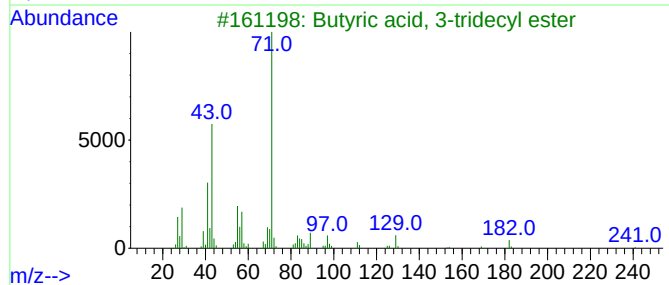
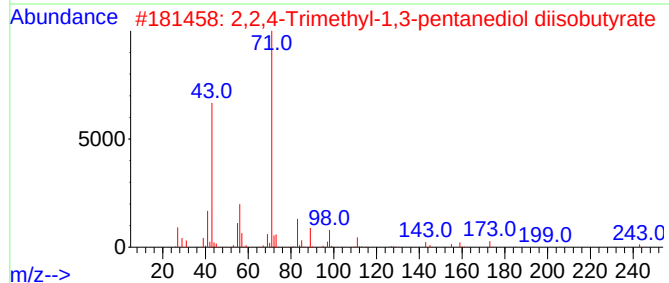
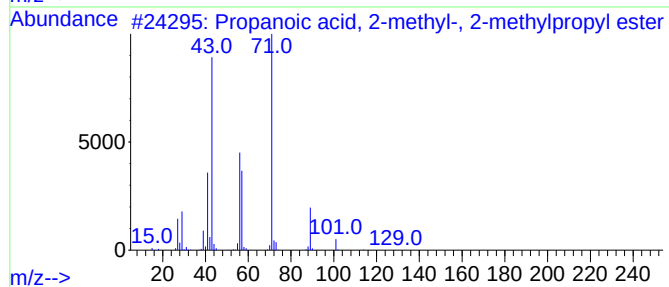
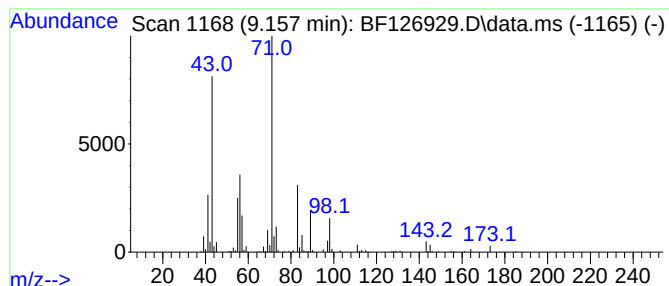
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Propanoic acid, 2-methyl-, ... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.157	5.03 ng	254234	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			2,2,4-Trimethyl-1,3-pentanediol ...	286	C16H30O4	006846-50-0	50
3			Butyric acid, 3-tridecyl ester	270	C17H34O2	1000280-56-8	43
4			Sulfurous acid, octyl 2-pentyl e...	264	C13H28O3S	1000309-15-7	43
5			Butanoic acid, 1-methylpropyl ester	144	C8H16O2	000819-97-6	42



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021722\
Data File : BF126929.D
Acq On : 17 Feb 2022 16:19
Operator : CG\JU
Sample : N1573-11
Misc :
ALS Vial : 9 Sample Multiplier: 1

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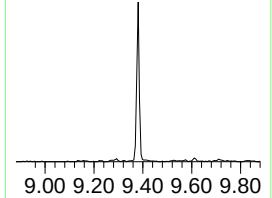
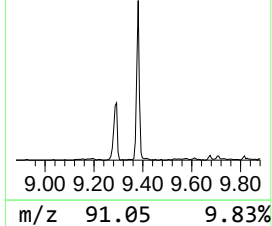
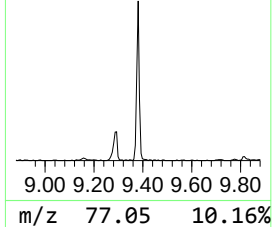
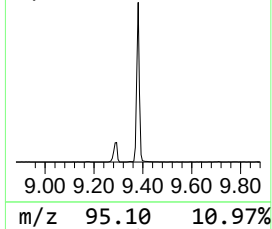
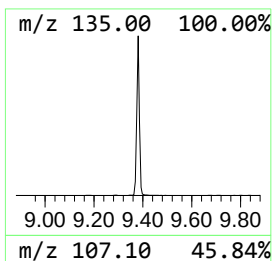
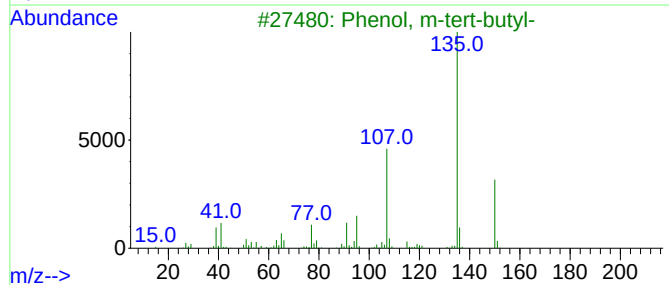
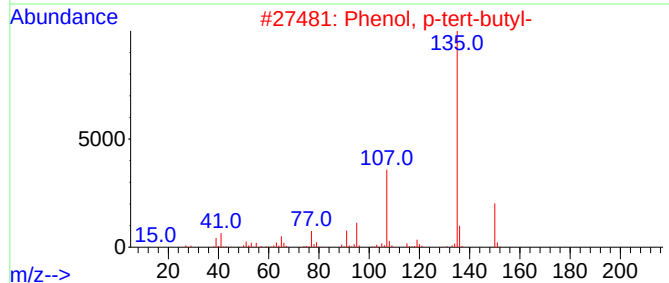
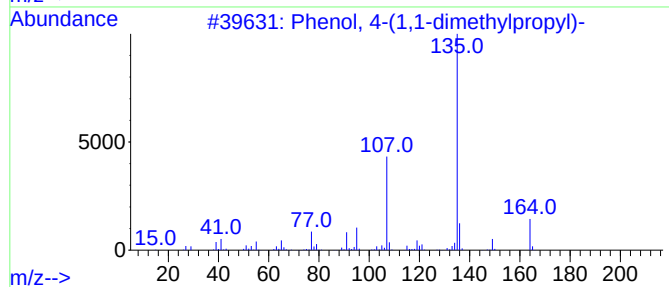
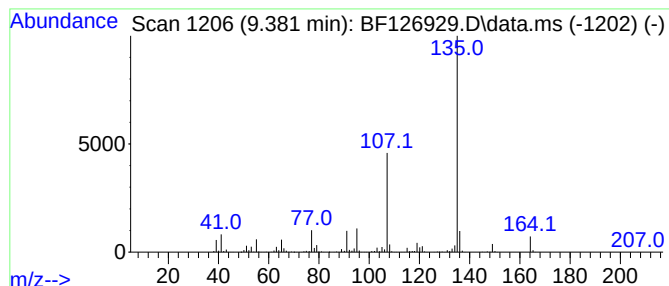
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.381	21.34 ng	1078750	Acenaphthene-d10	9.969

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	95
2		Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	90
3		Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	78
4		Hexestrol	270	C18H22O2	000084-16-2	64
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 : BF126929.D
Acq On : 17 Feb 2022 16:19
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ALS Vial : 9 Sample Multiplier: 1

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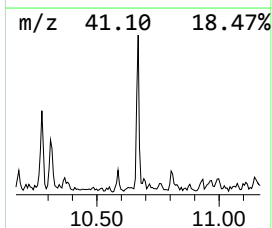
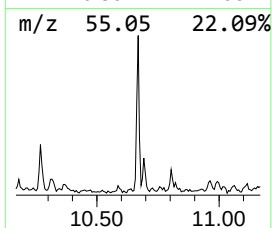
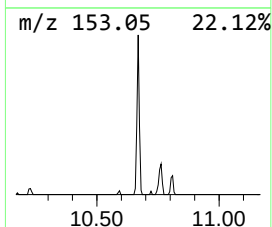
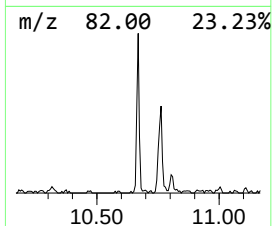
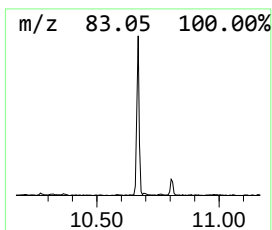
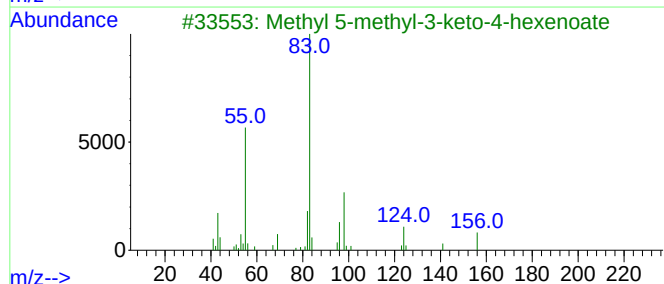
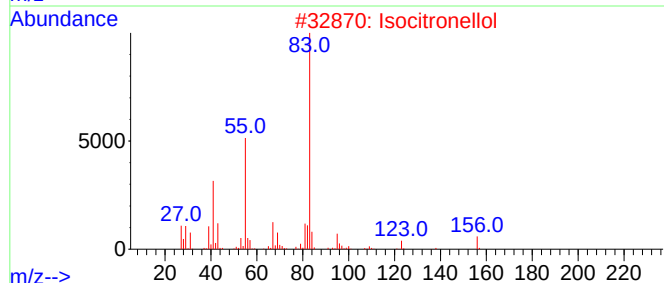
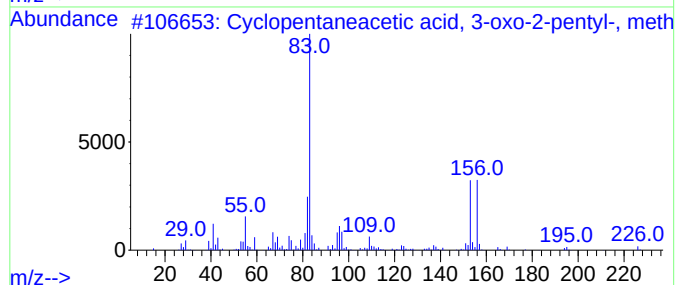
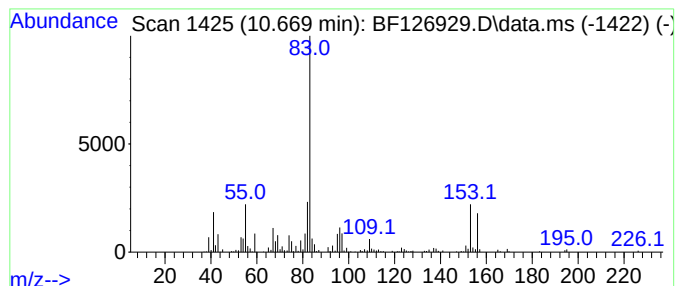
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Cyclopentaneacetic acid, 3-... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.669	3.87 ng	195554	Acenaphthene-d10	9.969

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopentaneacetic acid, 3-oxo-2...	226	C13H22O3	024851-98-7	97
2		Isocitronellol	156	C10H20O	018479-52-2	50
3		Methyl 5-methyl-3-keto-4-hexenoate	156	C8H12O3	1000427-08-8	45
4		Hexanal di-cis-3-hexenyl acetal	282	C18H34O2	1000430-94-7	43
5		Phomopsolide B, diacetate	380	C19H24O8	097533-95-4	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021722\
Data File : BF126929.D
Acq On : 17 Feb 2022 16:19
Operator : CG\JU
Sample : N1573-11
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GES-1R

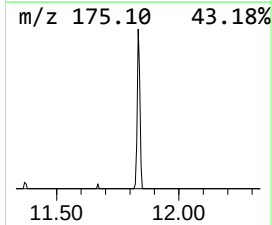
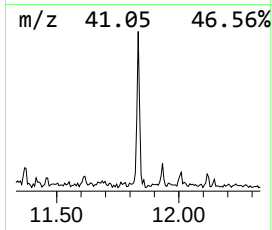
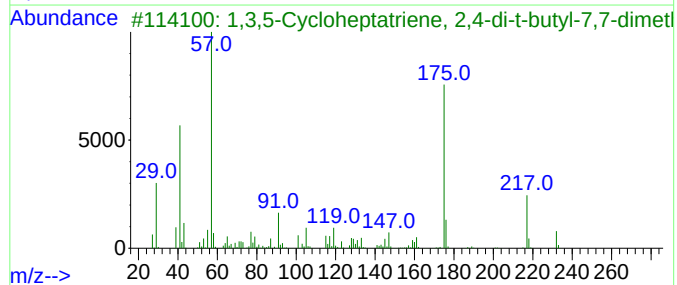
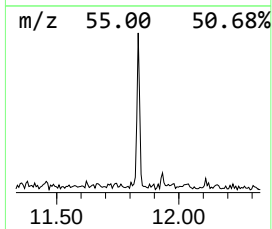
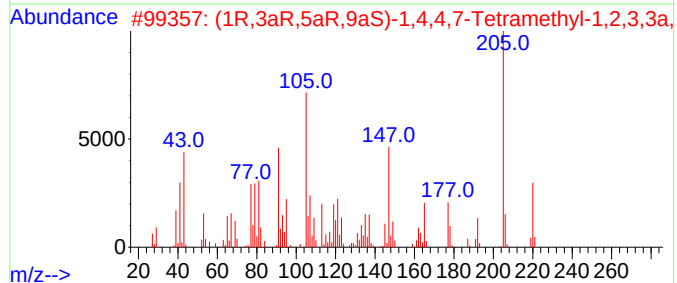
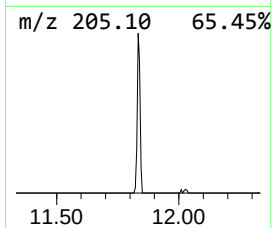
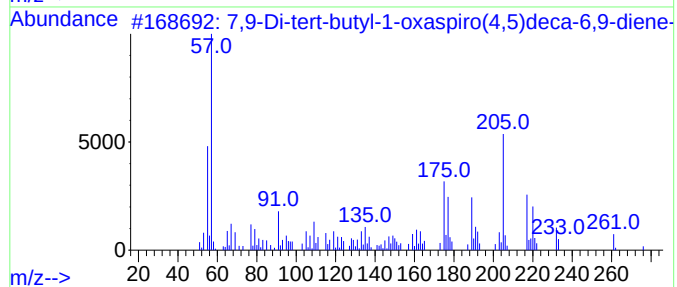
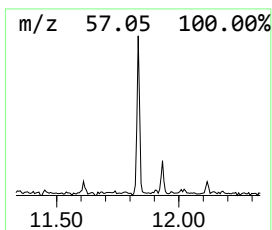
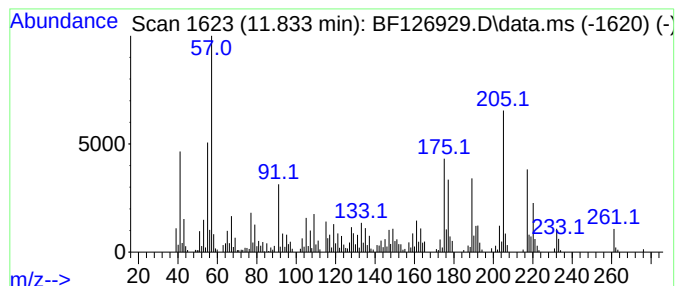
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 7,9-Di-tert-butyl-1-oxaspiro... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.833	2.99 ng	160436	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			(1R,3aR,5aR,9aS)-1,4,4,7-Tetrame...	220	C15H24O	104188-25-2	48
3			1,3,5-Cycloheptatriene, 2,4-di-t...	232	C17H28	1000160-92-5	46
4			1-(3-Amino-4,6-dimethylthieno[2,...	220	C11H12N2OS	052505-42-7	42
5			9-Acetylphenanthrene	220	C16H12O	002039-77-2	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021722\
 Data File : BF126929.D
 Acq On : 17 Feb 2022 16:19
 Operator : CG\JU
 Sample : N1573-11
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 GES-1R

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	4.469	11.8	ng	392240	1	6.928	667419	20.0
unknown5.169	5.169	5.2	ng	174894	1	6.928	667419	20.0
2-Propanol, 1-(...	6.722	6.6	ng	220690	1	6.928	667419	20.0
1-Propanol, 2,2...	6.751	7.0	ng	233334	1	6.928	667419	20.0
2-Propanol, 1-(...	6.845	11.5	ng	382873	1	6.928	667419	20.0
1-Hexanol, 2-et...	6.981	6.9	ng	231208	1	6.928	667419	20.0
Hexanoic acid, ...	7.563	3.0	ng	100893	1	6.928	667419	20.0
Levomenthol	8.116	2.7	ng	122114	2	8.210	919172	20.0
Nonanoic acid	8.539	4.3	ng	197347	2	8.210	919172	20.0
Propanoic acid,...	9.157	5.0	ng	254234	3	9.969	1011140	20.0
Phenol, 4-(1,1-...	9.381	21.3	ng	1078750	3	9.969	1011140	20.0
Cyclopentaneace...	10.669	3.9	ng	195554	3	9.969	1011140	20.0
7,9-Di-tert-but...	11.833	3.0	ng	160436	4	11.457	1071660	20.0