

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021722\
 Data File : BF126936.D
 Acq On : 17 Feb 2022 19:45
 Operator : CG\JU
 Sample : N1573-02
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-13R

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: BF126936.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.463	365	370	380	rVB	332258	380578	7.67%	1.439%
2	5.163	484	489	496	rVB	125600	145163	2.93%	0.549%
3	5.545	549	554	557	rBV	2105006	2025959	40.83%	7.662%
4	6.545	719	724	727	rBV	1625660	1424540	28.71%	5.388%
5	6.722	751	754	756	rBV	253707	185704	3.74%	0.702%
6	6.751	756	759	762	rVB	274356	197160	3.97%	0.746%
7	6.845	771	775	785	rBV	358555	320754	6.46%	1.213%
8	6.928	785	789	792	rBV	795428	612963	12.35%	2.318%
9	6.981	795	798	802	rBV	169529	133079	2.68%	0.503%
10	7.498	880	886	888	rBV	2477375	2695907	54.34%	10.196%
11	7.563	893	897	901	rBV	69689	85860	1.73%	0.325%
12	8.110	986	990	997	rBV3	71867	101206	2.04%	0.383%
13	8.210	1003	1007	1010	rBV	1085062	858215	17.30%	3.246%
14	8.357	1029	1032	1040	rBV	71973	75195	1.52%	0.284%
15	8.539	1056	1063	1069	rBV4	64899	106761	2.15%	0.404%
16	9.157	1164	1168	1173	rBV	228128	233570	4.71%	0.883%
17	9.286	1184	1190	1193	rBV	4627810	4961486	100.00%	18.765%
18	9.380	1202	1206	1209	rBV	1095379	862390	17.38%	3.262%
19	9.710	1258	1262	1267	rBV4	36534	49763	1.00%	0.188%
20	9.969	1303	1306	1309	rVB	1153153	897549	18.09%	3.395%
21	10.274	1354	1358	1361	rVB2	54784	50317	1.01%	0.190%
22	10.380	1372	1376	1379	rVB	255786	199580	4.02%	0.755%
23	10.669	1422	1425	1427	rBV	244186	175963	3.55%	0.666%
24	10.763	1436	1441	1444	rBV	3333411	3122891	62.94%	11.811%
25	11.310	1531	1534	1537	rBV	66539	49995	1.01%	0.189%
26	11.457	1555	1559	1562	rBV	1187283	923622	18.62%	3.493%
27	11.833	1620	1623	1626	rBV	180926	141209	2.85%	0.534%
28	13.051	1824	1830	1833	rBV	4689575	4375651	88.19%	16.549%
29	14.098	2004	2008	2012	rBV	590999	511482	10.31%	1.934%
30	15.604	2258	2264	2271	rBV	428611	535636	10.80%	2.026%

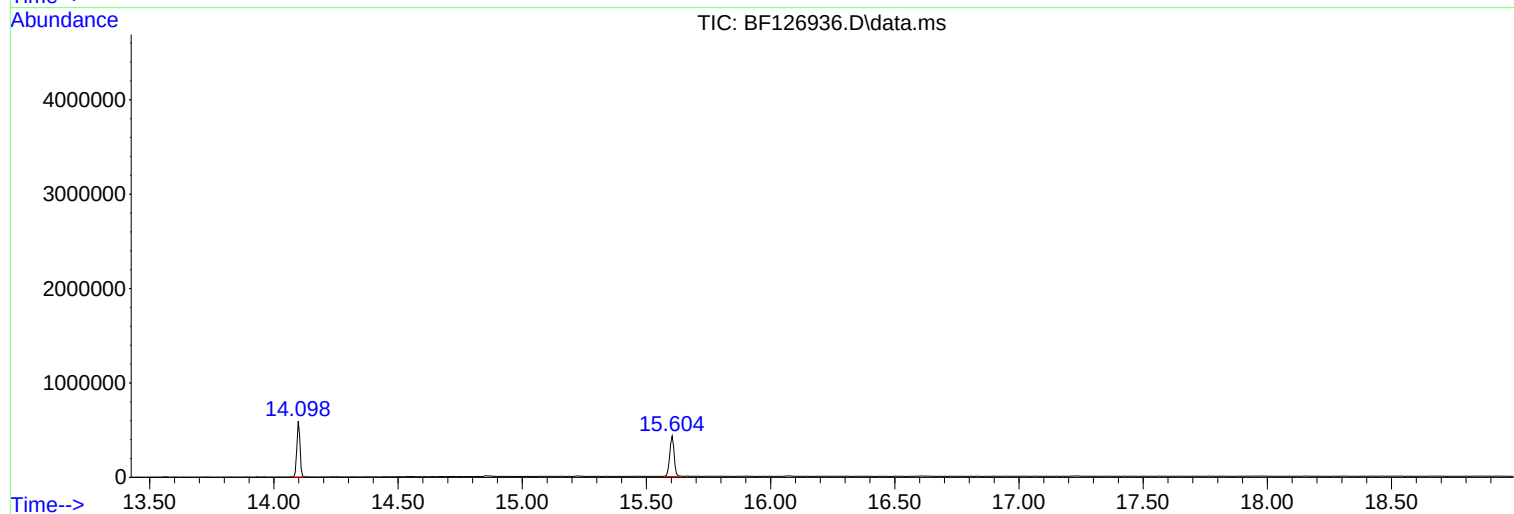
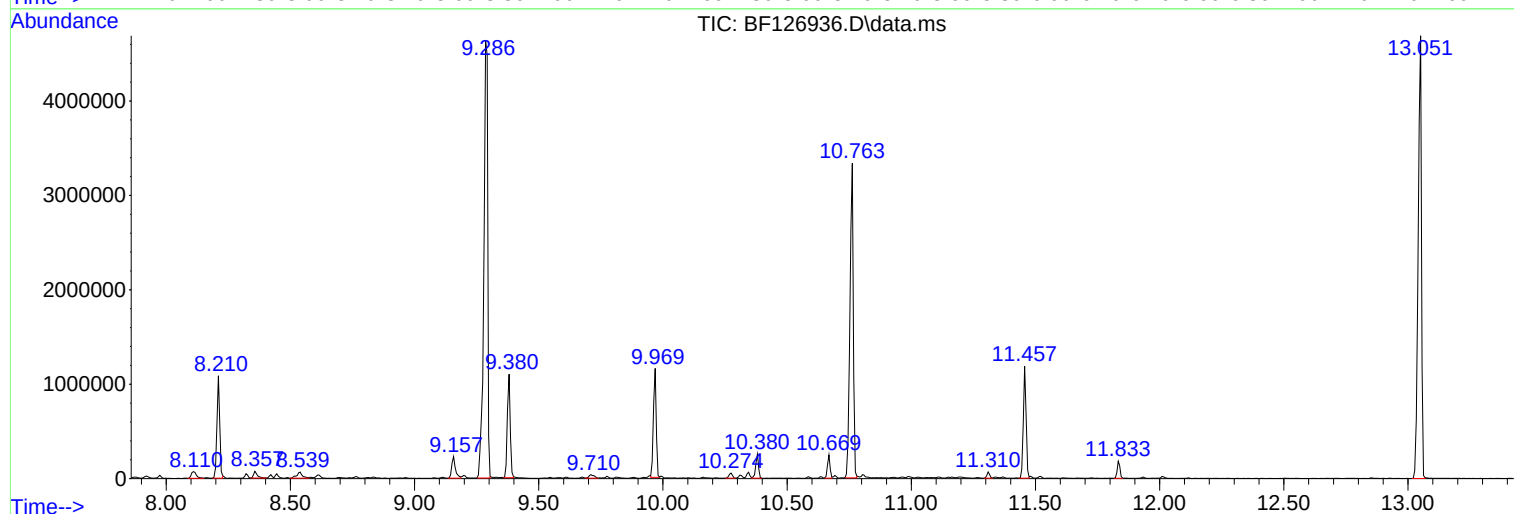
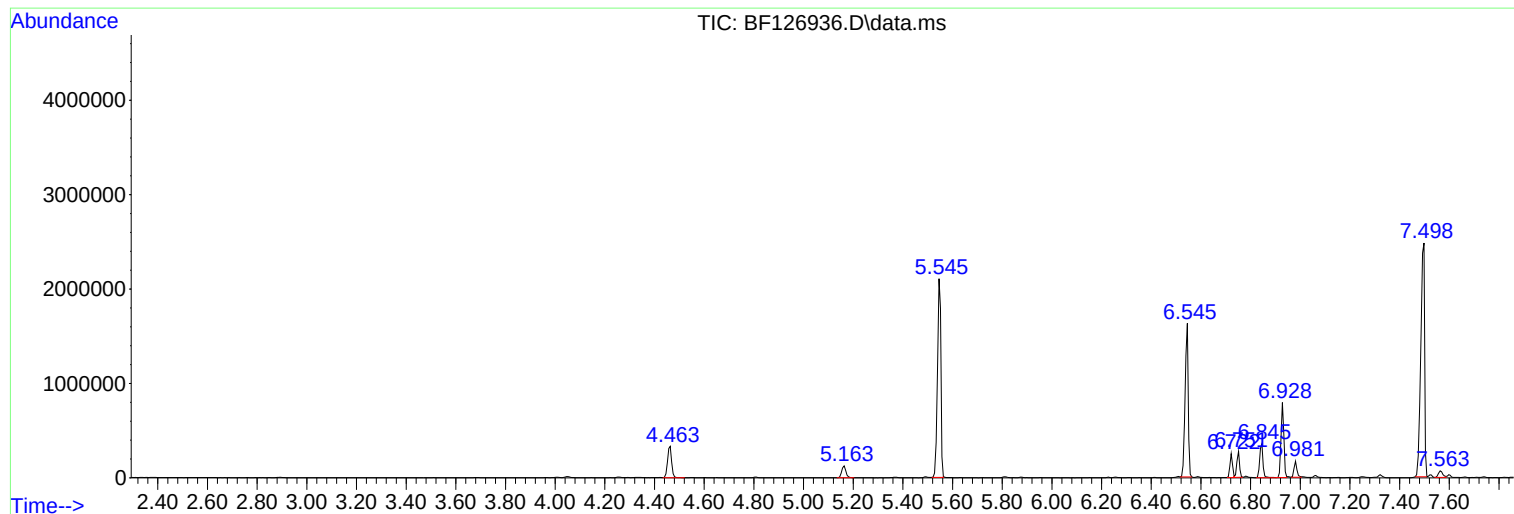
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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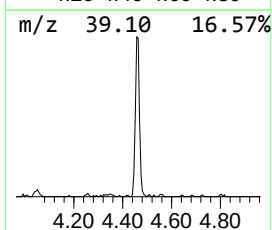
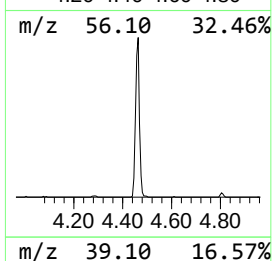
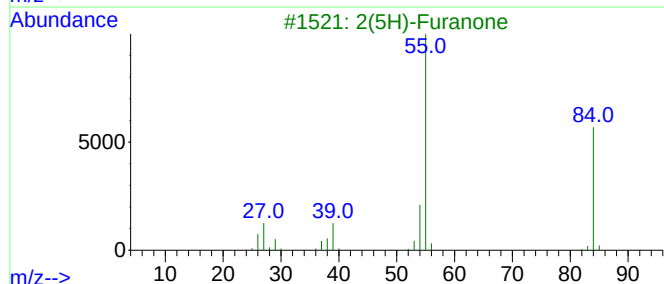
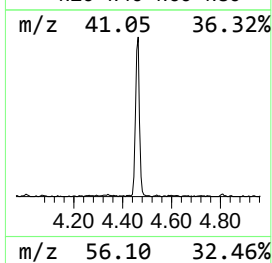
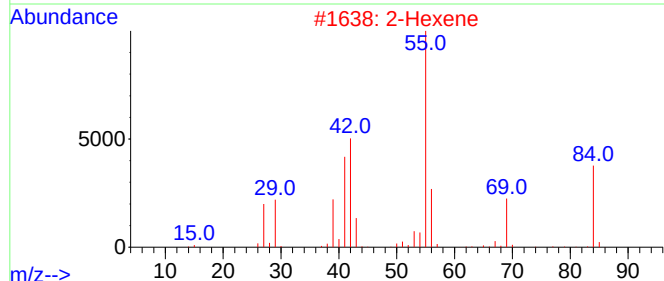
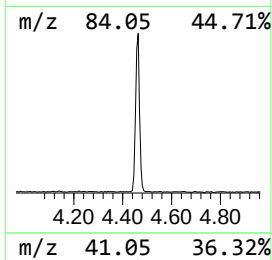
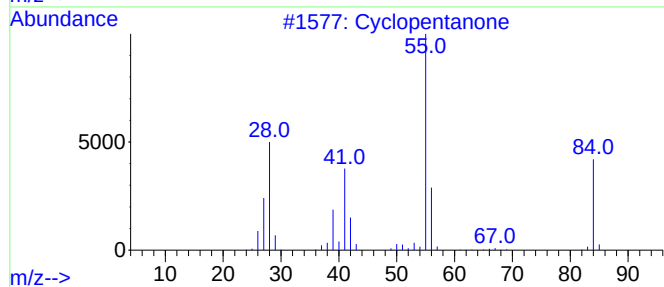
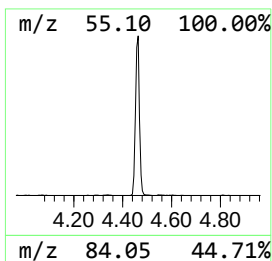
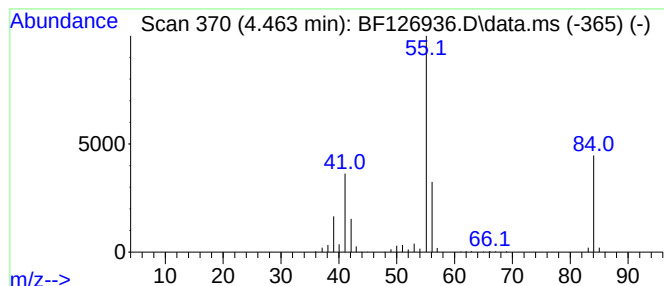
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.463	12.42 ng	380578	1,4-Dichlorobenzene-d4	6.928

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentanone	84	C5H8O	000120-92-3	91
2			2-Hexene	84	C6H12	000592-43-8	64
3			2(5H)-Furanone	84	C4H4O2	000497-23-4	53
4			2-Hexene, (E)-	84	C6H12	004050-45-7	45
5			2-Hexene, (Z)-	84	C6H12	007688-21-3	45



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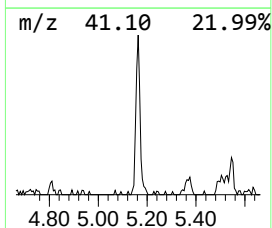
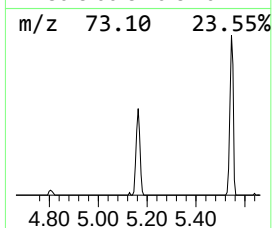
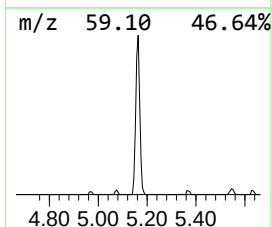
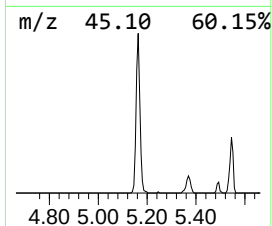
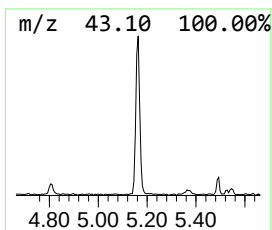
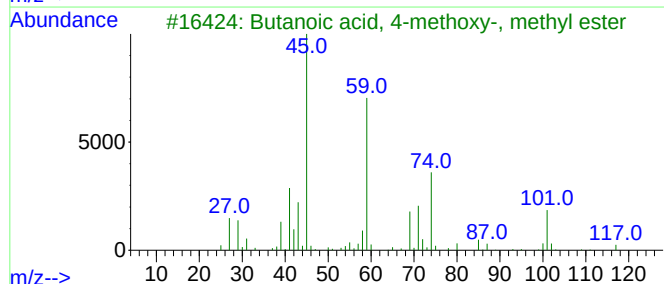
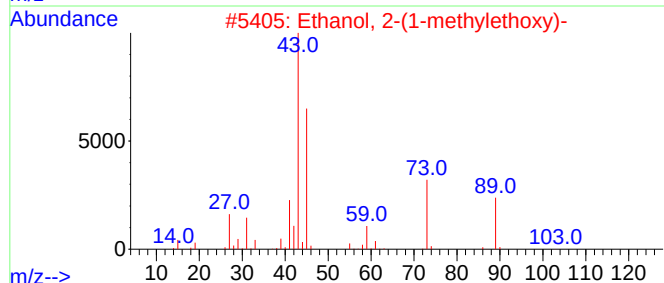
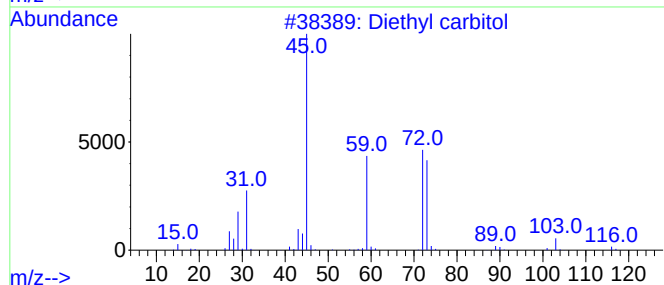
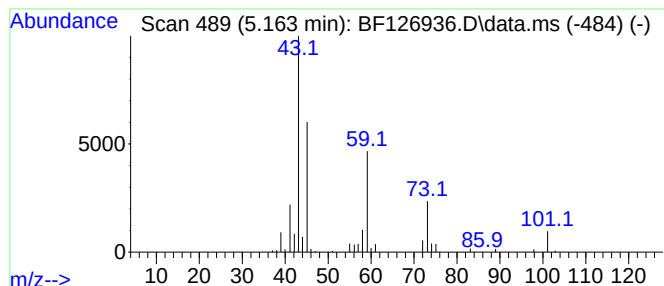
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Diethyl carbitol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.163	4.74 ng	145163	1,4-Dichlorobenzene-d4	6.928

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diethyl carbitol	162	C8H18O3	000112-36-7	50
2			Ethanol, 2-(1-methylethoxy)-	104	C5H12O2	000109-59-1	50
3			Butanoic acid, 4-methoxy-, methy...	132	C6H12O3	029006-01-7	42
4			Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	40
5			Butane, 1-(1-methylethoxy)-	116	C7H16O	001860-27-1	38



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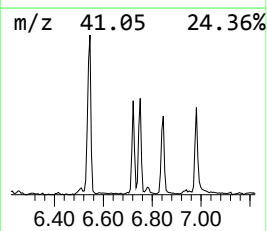
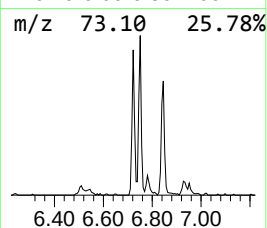
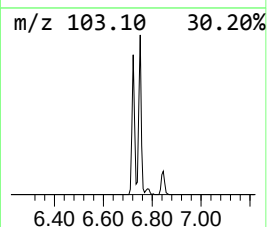
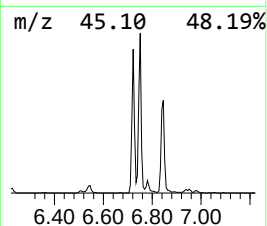
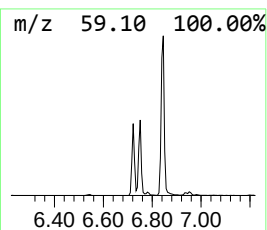
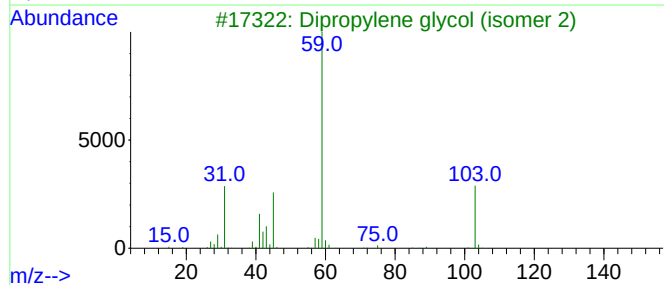
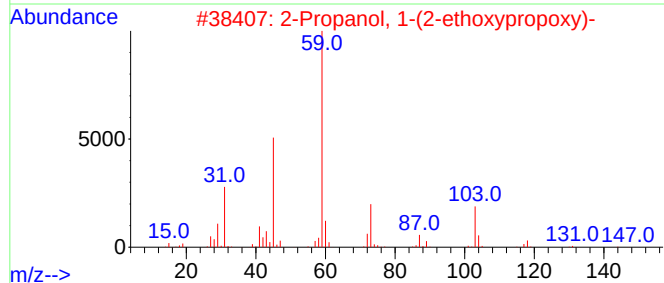
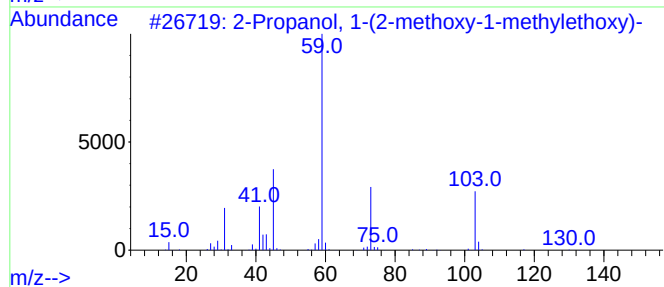
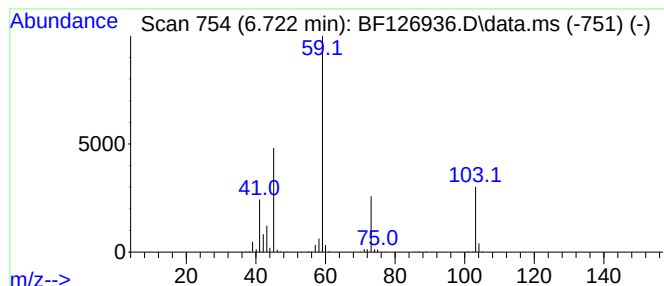
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.722	6.06 ng	185704	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	2-Propanol, 1-(2-ethoxypropoxy)-	162	C8H18O3	010143-32-5	64		
3	Dipropylene glycol (isomer 2)	134	C6H14O3	1000506-25-4	53		
4	Dipropylene glycol (isomer 3)	134	C6H14O3	1000506-25-5	53		
5	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	53		



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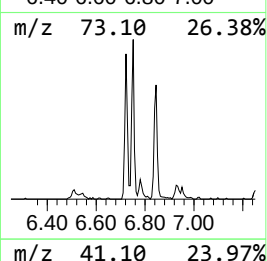
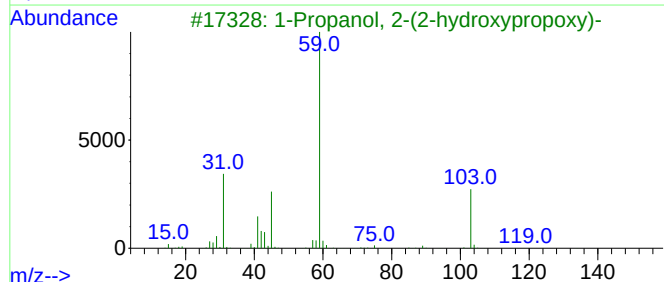
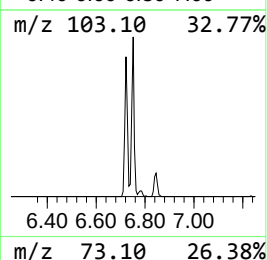
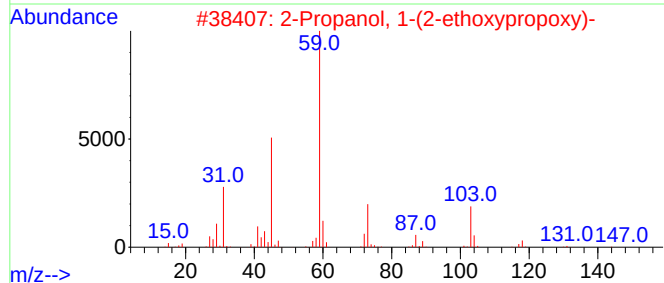
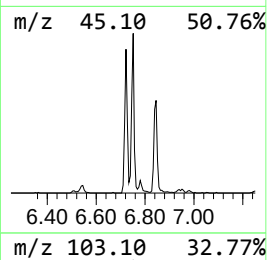
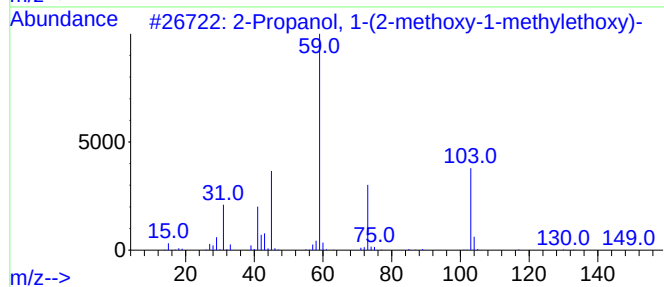
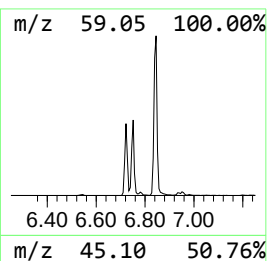
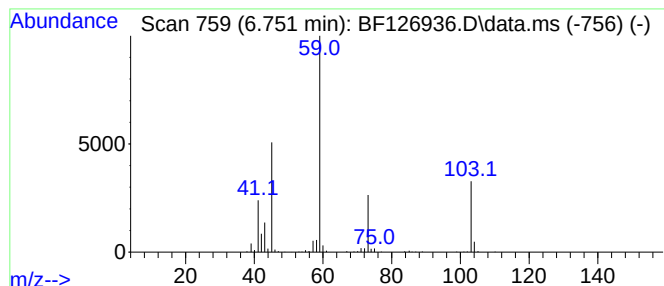
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 2-Propanol, 1-(2-ethoxyprop... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.751	6.43 ng	197160	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	2-Propanol, 1-(2-ethoxypropoxy)-	162	C8H18O3	010143-32-5	64		
3	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	59		
4	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	50		
5	Ethane, 1-ethoxy-1-methoxy-	104	C5H12O2	010471-14-4	50		



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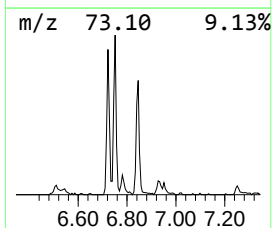
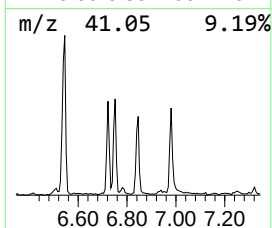
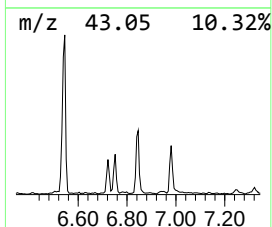
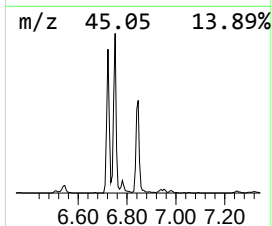
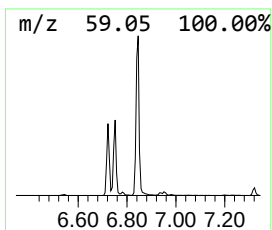
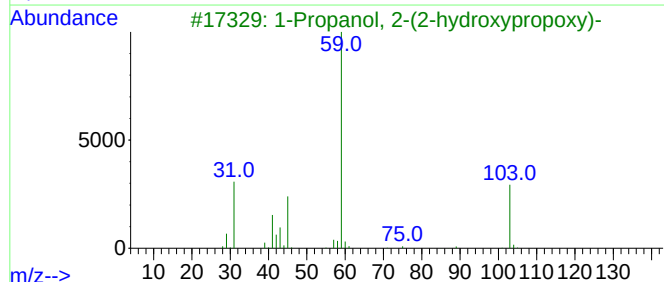
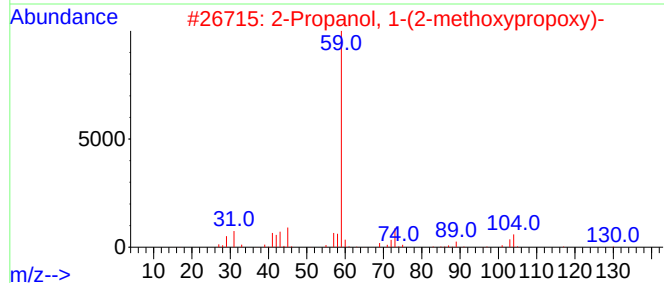
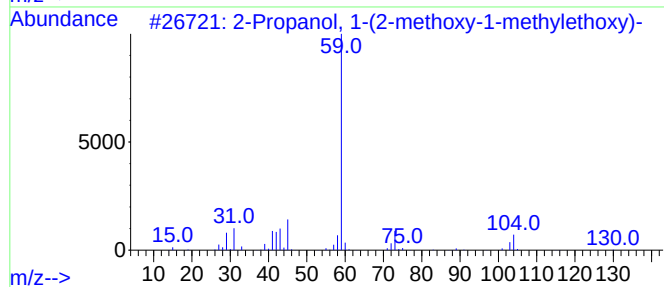
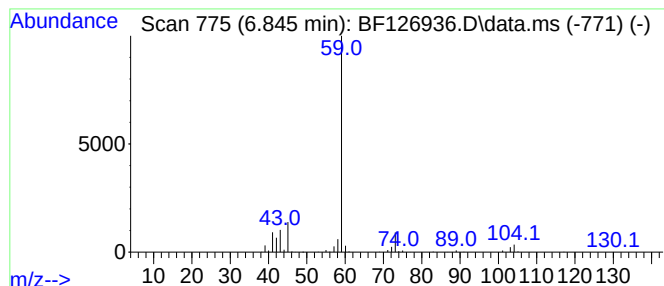
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 2-Propanol, 1-(2-methoxypro... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.845	10.47 ng	320754	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	50
4			2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	43
5			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	39



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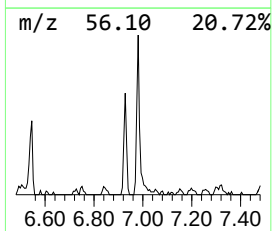
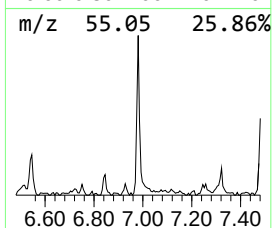
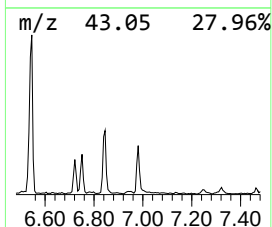
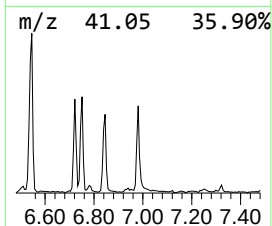
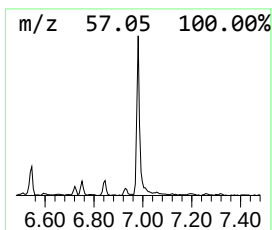
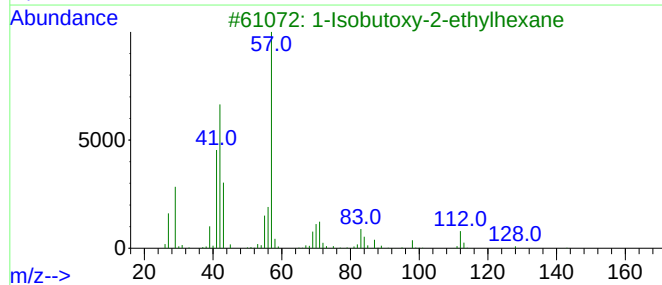
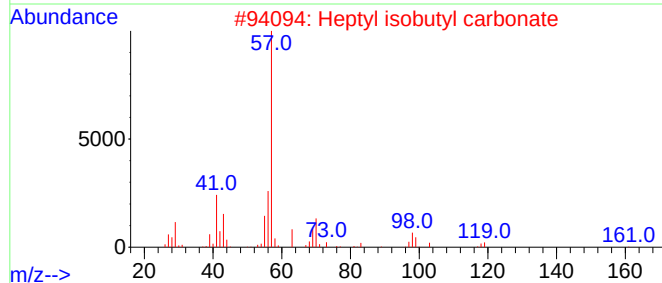
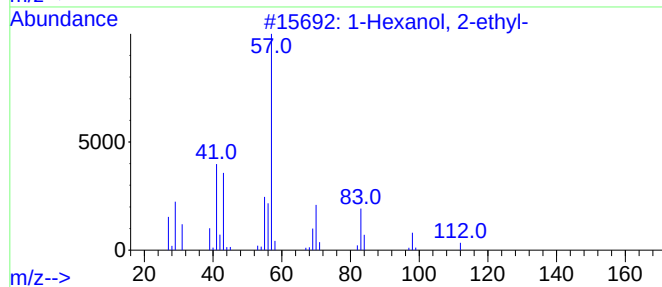
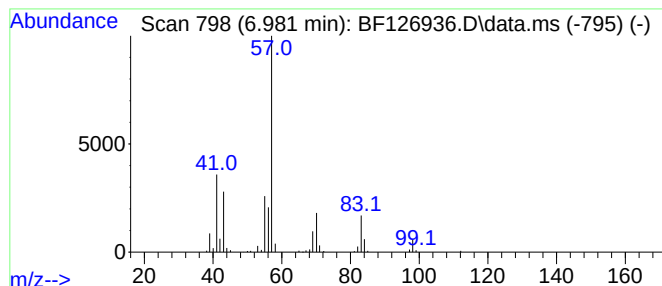
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Hexanol, 2-ethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.981	4.34 ng	133079	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	90
2		Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	59
3		1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	56
4		1-Hexene, 4-methyl-	98	C7H14	003769-23-1	47
5		2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021722\
Data File : BF126936.D
Acq On : 17 Feb 2022 19:45
Operator : CG\JU
Sample : N1573-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-13R

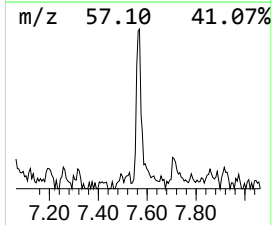
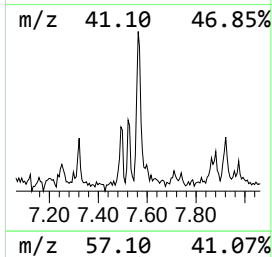
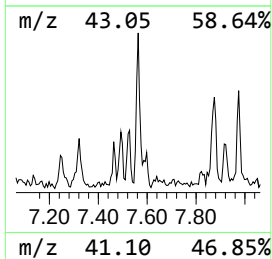
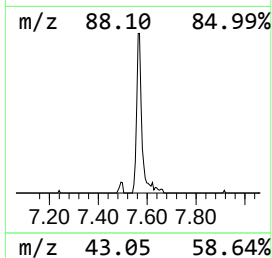
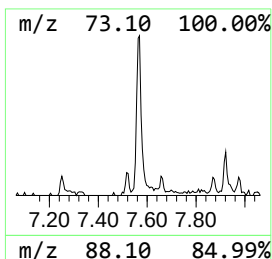
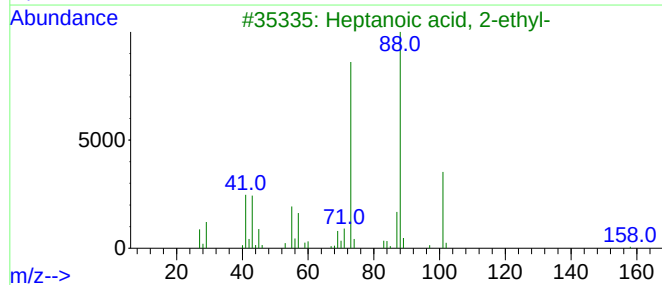
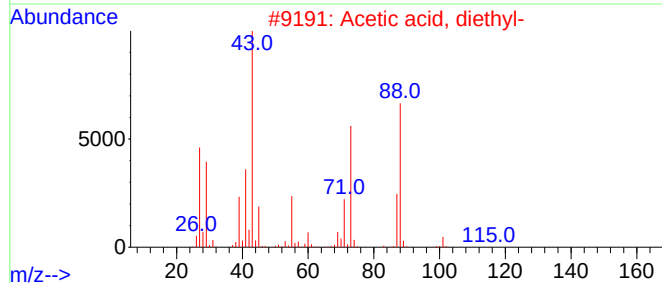
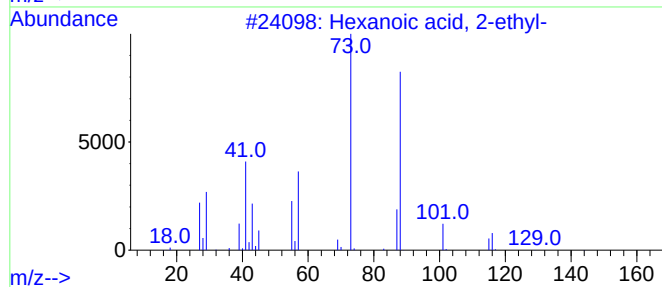
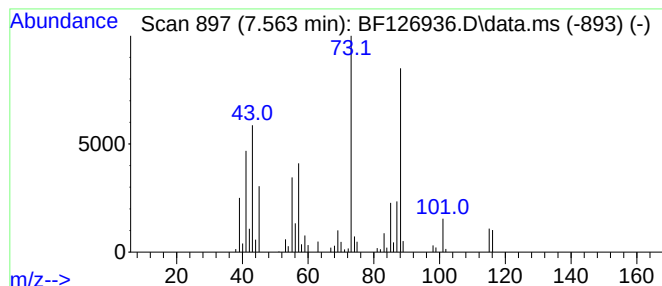
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	2.80 ng	85860	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	47
4			Butanoic acid, 2-methyl-, methyl...	116	C6H12O2	000868-57-5	47
5			Hydrazine, 1-methyl-1-(1-methyle...	88	C4H12N2	033668-54-1	37



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021722\
Data File : BF126936.D
Acq On : 17 Feb 2022 19:45
Operator : CG\JU
Sample : N1573-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

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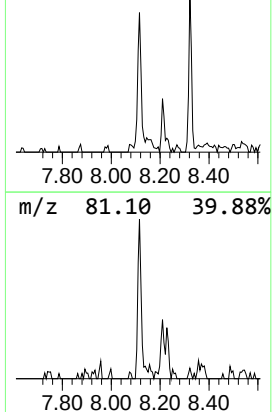
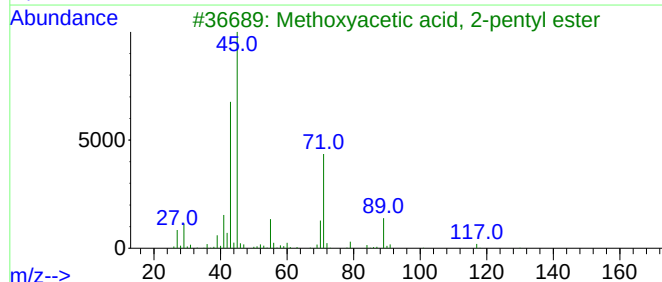
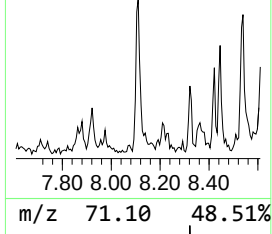
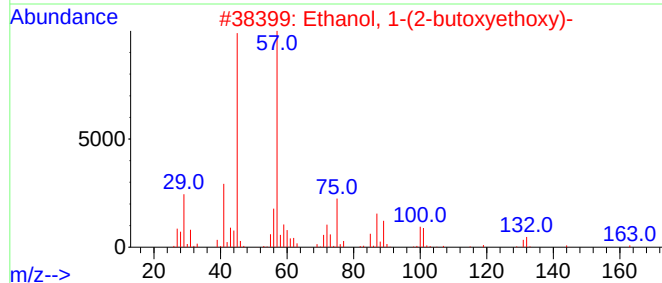
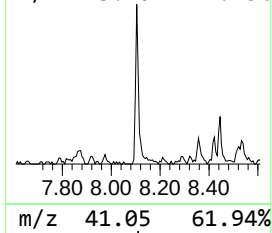
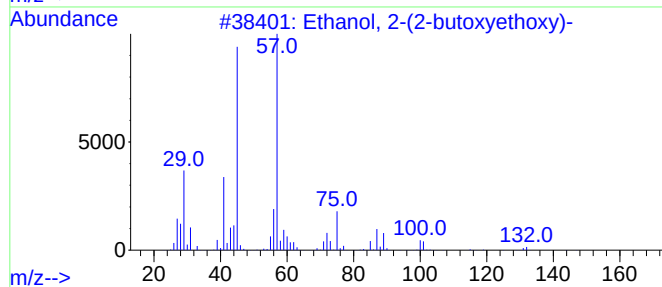
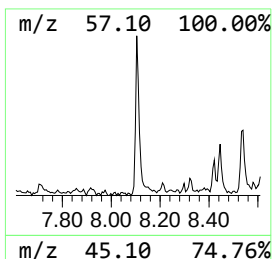
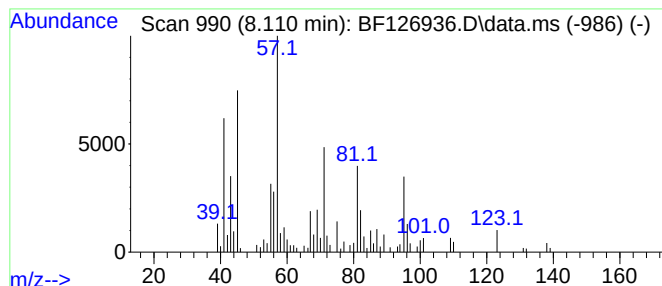
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown8.110 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.110	2.36 ng	101206	Naphthalene-d8	8.210

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	43
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	38
3			Methoxyacetic acid, 2-pentyl ester	160	C8H16O3	1000282-69-2	38
4			15-Crown-5	220	C10H20O5	033100-27-5	35
5			2-Pentanol, 4,4-dimethyl-	116	C7H16O	006144-93-0	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021722\
Data File : BF126936.D
Acq On : 17 Feb 2022 19:45
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Sample : N1573-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

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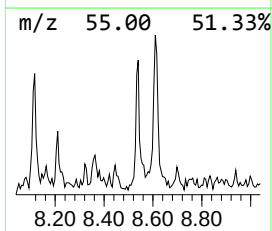
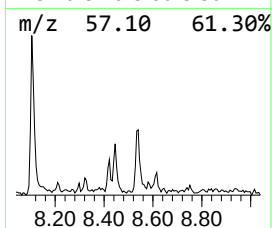
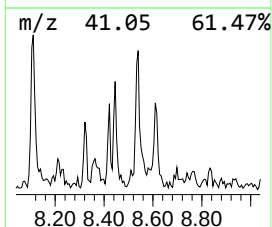
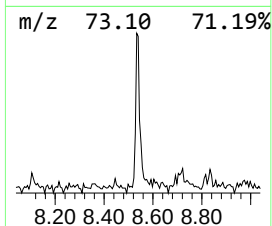
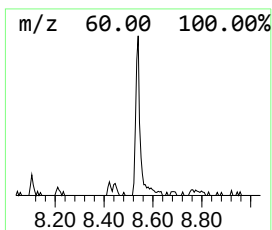
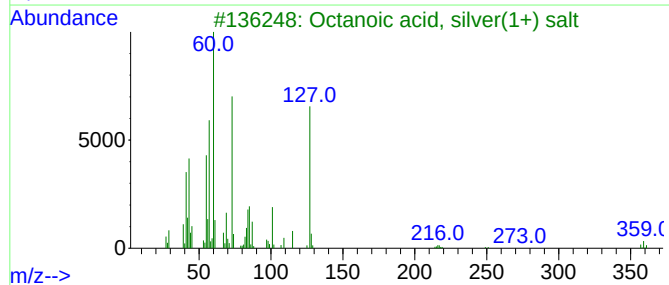
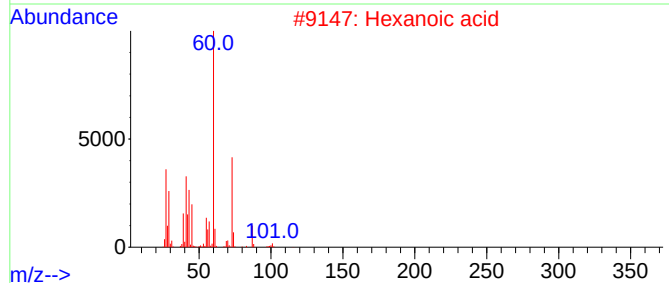
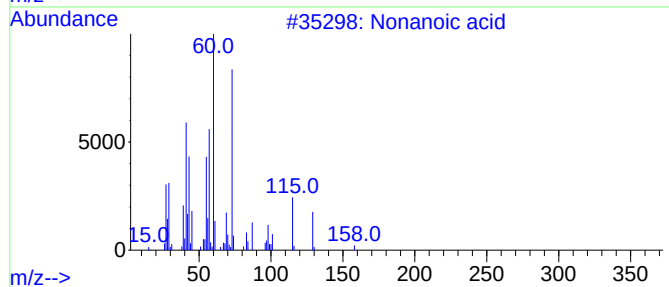
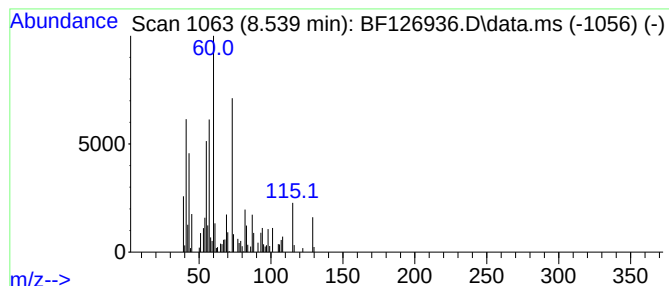
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Nonanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.539	2.49 ng	106761	Naphthalene-d8	8.210

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonanoic acid	158	C9H18O2	000112-05-0	80
2			Hexanoic acid	116	C6H12O2	000142-62-1	50
3			Octanoic acid, silver(1+) salt	250	C8H15AgO2	024927-67-1	47
4			Pentanoic acid, 3-methyl-	116	C6H12O2	000105-43-1	43
5			Octanoic acid	144	C8H16O2	000124-07-2	40



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021722\
Data File : BF126936.D
Acq On : 17 Feb 2022 19:45
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Sample : N1573-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

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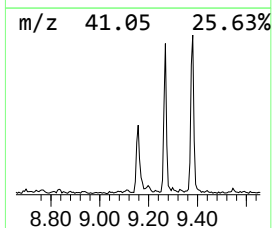
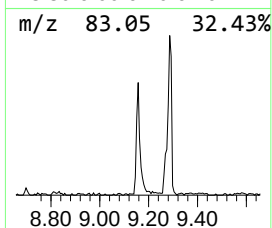
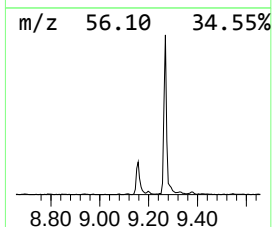
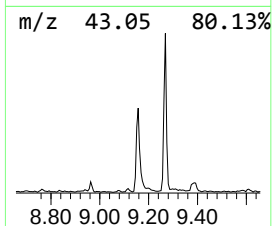
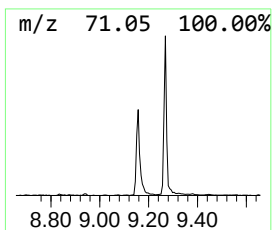
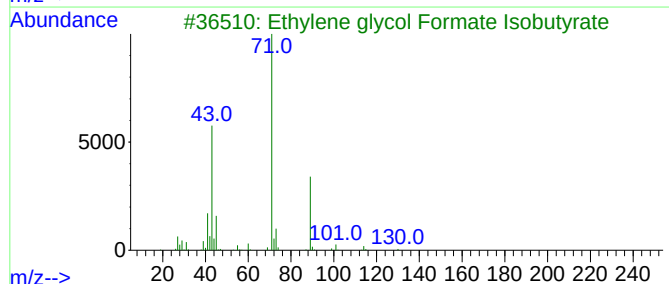
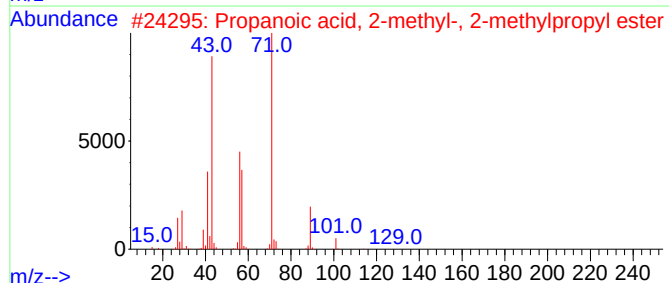
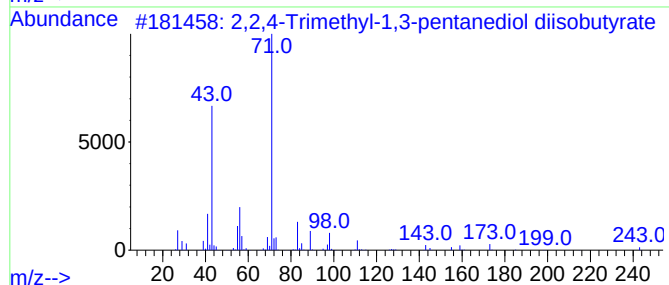
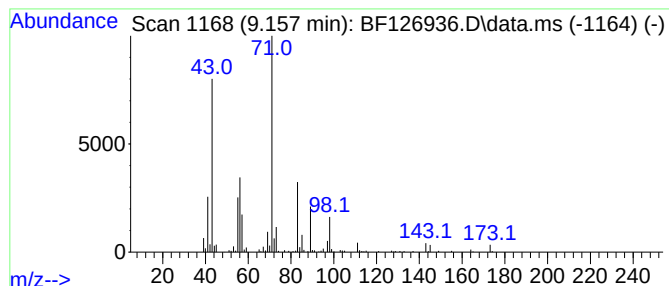
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 2,2,4-Trimethyl-1,3-pentane... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.157	5.20 ng	233570	Acenaphthene-d10	9.969

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,2,4-Trimethyl-1,3-pentenediol ...	286	C16H30O4	006846-50-0	72
2			Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	50
3			Ethylene glycol Formate Isobutyrate	160	C7H12O4	1000458-48-0	47
4			Sulfurous acid, octyl 2-pentyl e...	264	C13H28O3S	1000309-15-7	43
5			Isopropyl butyrate	130	C7H14O2	000638-11-9	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021722\
Data File : BF126936.D
Acq On : 17 Feb 2022 19:45
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Sample : N1573-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

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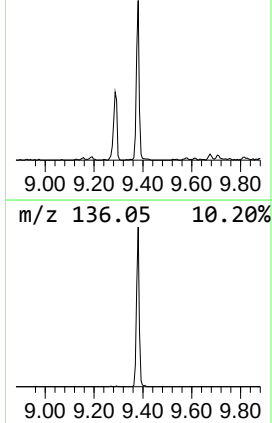
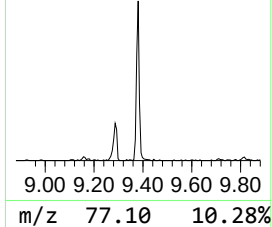
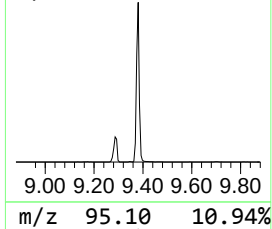
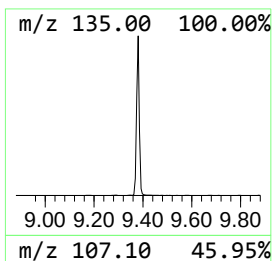
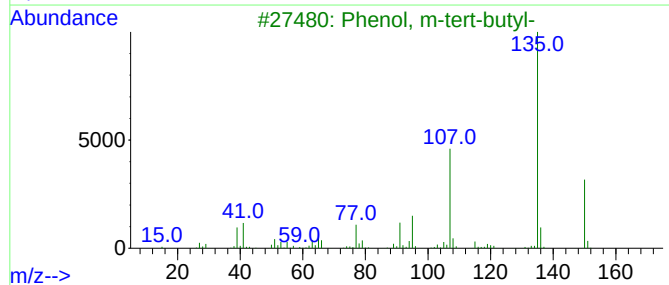
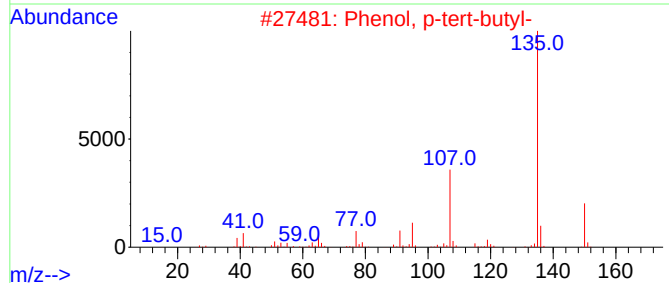
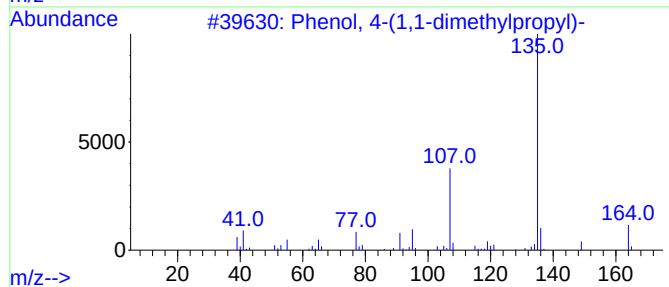
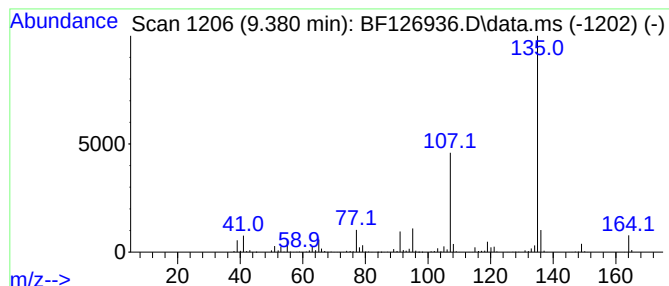
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	19.22 ng	862390	Acenaphthene-d10	9.969

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	91
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			Hexestrol, O-isopropylloxycarbonyl-	356	C22H28O4	1000487-68-4	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021722\
Data File : BF126936.D
Acq On : 17 Feb 2022 19:45
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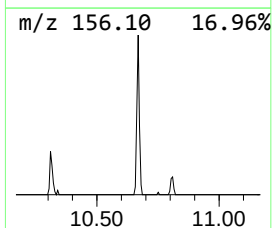
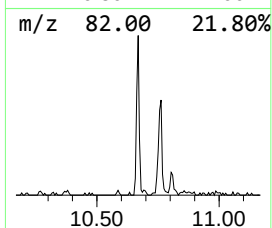
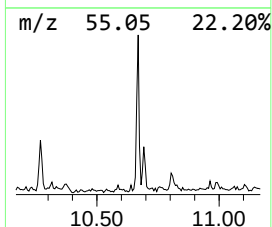
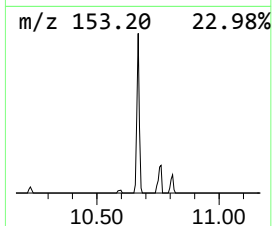
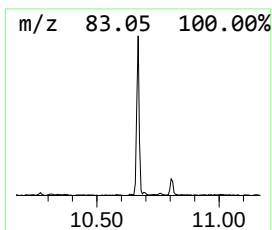
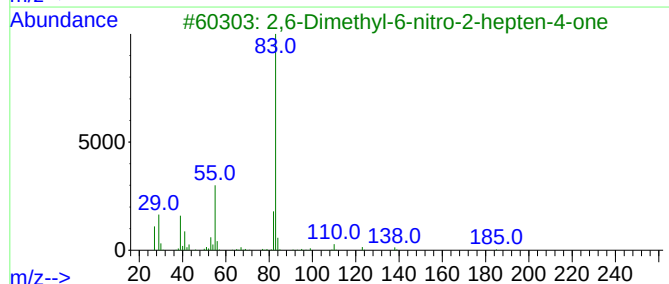
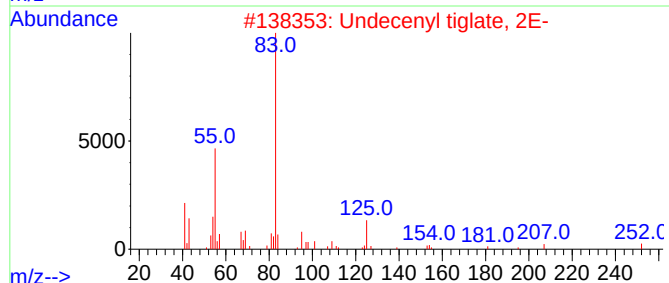
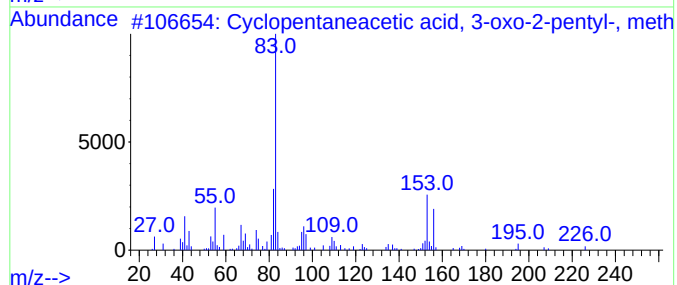
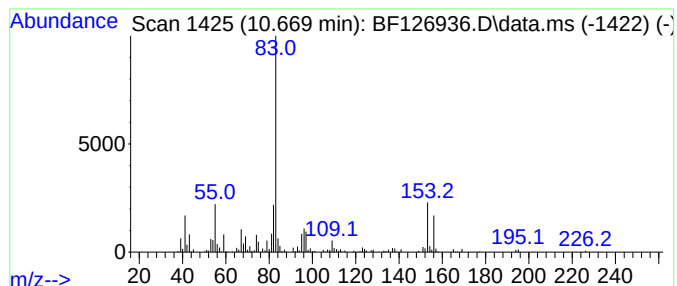
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	3.92 ng	175963	Acenaphthene-d10	9.969

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentaneacetic acid, 3-oxo-2...	226	C13H22O3	024851-98-7	91
2			Undecenyl tiglate, 2E-	252	C16H28O2	1000383-56-5	47
3			2,6-Dimethyl-6-nitro-2-hepten-4-one	185	C9H15NO3	073583-56-9	47
4			Prop-2-ynyl (E)-2-methylbut-2-en...	138	C8H10O2	1000373-72-5	43
5			1,5-Dicyano-2,4-dimethyl-2,4-dia...	152	C7H12N4	1010289-23-5	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021722\
Data File : BF126936.D
Acq On : 17 Feb 2022 19:45
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Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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MW-13R

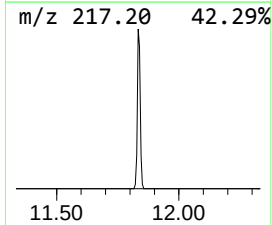
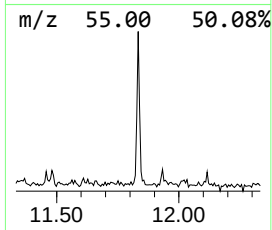
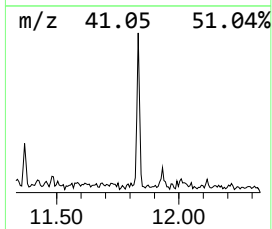
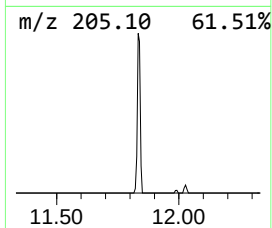
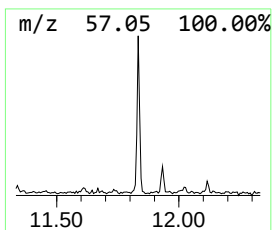
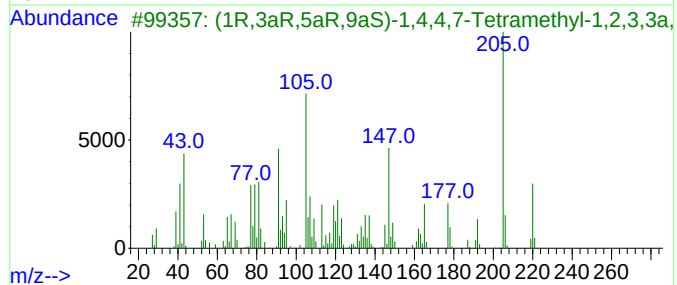
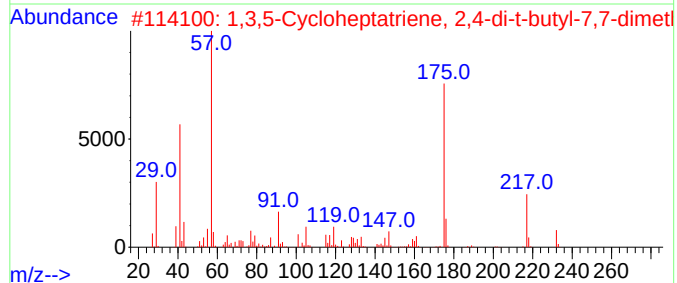
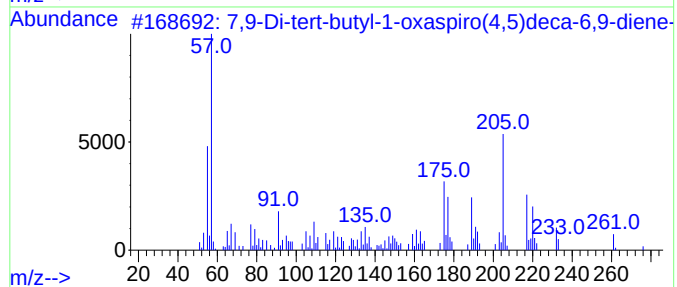
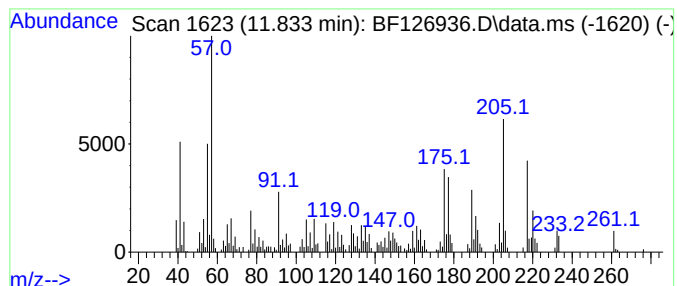
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	3.06 ng	141209	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	97		
2	1,3,5-Cycloheptatriene, 2,4-di-t...	232	C17H28	1000160-92-5	46		
3	(1R,3aR,5aR,9aS)-1,4,4,7-Tetrame...	220	C15H24O	104188-25-2	42		
4	1-(3-Amino-4,6-dimethylthieno[2,...	220	C11H12N2OS	052505-42-7	38		
5	Ethanone, 1-(5,6,7,8-tetrahydro...	220	C14H20O2	071596-88-8	30		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021722\
Data File : BF126936.D
Acq On : 17 Feb 2022 19:45
Operator : CG\JU
Sample : N1573-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-13R

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	4.463	12.4	ng	380578	1	6.928	612963	20.0
Diethyl carbitol	5.163	4.7	ng	145163	1	6.928	612963	20.0
2-Propanol, 1-(...	6.722	6.1	ng	185704	1	6.928	612963	20.0
2-Propanol, 1-(...	6.751	6.4	ng	197160	1	6.928	612963	20.0
2-Propanol, 1-(...	6.845	10.5	ng	320754	1	6.928	612963	20.0
1-Hexanol, 2-et...	6.981	4.3	ng	133079	1	6.928	612963	20.0
Hexanoic acid, ...	7.563	2.8	ng	85860	1	6.928	612963	20.0
unknown8.110	8.110	2.4	ng	101206	2	8.210	858215	20.0
Nonanoic acid	8.539	2.5	ng	106761	2	8.210	858215	20.0
2,2,4-Trimethyl...	9.157	5.2	ng	233570	3	9.969	897549	20.0
Phenol, 4-(1,1-...	9.380	19.2	ng	862390	3	9.969	897549	20.0
Cyclopentaneace...	10.669	3.9	ng	175963	3	9.969	897549	20.0
7,9-Di-tert-but...	11.833	3.1	ng	141209	4	11.457	923622	20.0