

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020122\
 Data File : BF126775.D
 Acq On : 01 Feb 2022 15:44
 Operator : CG/JU
 Sample : N1340-05
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-5(1-1.5)

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-BF011822.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126775.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.299	28	36	43	rVB	375503	496560	11.54%	1.622%
2	3.581	244	254	266	rBV	186806	456183	10.60%	1.490%
3	5.199	522	529	535	rBV	42550	49675	1.15%	0.162%
4	5.581	588	594	597	rBV	3116670	3128724	72.69%	10.222%
5	6.575	757	763	766	rBV	3121133	3291544	76.47%	10.754%
6	6.781	795	798	802	rBV	128023	99319	2.31%	0.324%
7	6.957	824	828	831	rVB	900342	741388	17.22%	2.422%
8	7.516	918	923	926	rBV	2191478	2252814	52.34%	7.360%
9	7.540	926	927	930	rVB	232455	116602	2.71%	0.381%
10	7.687	949	952	956	rBV	57126	44441	1.03%	0.145%
11	8.134	1025	1028	1034	rBV	41791	64978	1.51%	0.212%
12	8.210	1037	1041	1043	rBV	221420	204481	4.75%	0.668%
13	8.239	1043	1046	1048	rVV	1114680	880410	20.45%	2.876%
14	8.816	1140	1144	1149	rVB	255329	199142	4.63%	0.651%
15	8.951	1164	1167	1170	rVB	76207	64202	1.49%	0.210%
16	9.316	1223	1229	1232	rBV	3936962	3501963	81.36%	11.441%
17	9.381	1237	1240	1243	rBV	211022	182448	4.24%	0.596%
18	9.575	1270	1273	1277	rBV	33644	43304	1.01%	0.141%
19	9.916	1327	1331	1334	rVB	150432	118885	2.76%	0.388%
20	9.998	1341	1345	1348	rVB	1259131	1053632	24.48%	3.442%
21	10.416	1413	1416	1419	rVB2	108345	88132	2.05%	0.288%
22	10.492	1423	1429	1432	rBV	239209	275608	6.40%	0.900%
23	10.528	1432	1435	1446	rVB3	99378	187268	4.35%	0.612%
24	10.786	1475	1479	1485	rBV	2290703	2075934	48.23%	6.782%
25	10.892	1495	1497	1502	rVB2	65145	85629	1.99%	0.280%
26	11.339	1570	1573	1576	rBV	56259	47347	1.10%	0.155%
27	11.486	1595	1598	1601	rBV	1185937	1076622	25.01%	3.517%
28	11.510	1601	1602	1606	rVB	89043	64459	1.50%	0.211%
29	11.998	1680	1685	1687	rBV2	325408	326607	7.59%	1.067%
30	12.704	1802	1805	1810	rBV2	47703	47923	1.11%	0.157%
31	12.792	1816	1820	1828	rBV	312649	304063	7.06%	0.993%
32	13.080	1864	1869	1872	rBV	3533604	3165011	73.53%	10.340%
33	14.004	2022	2026	2040	rBV6	93376	273013	6.34%	0.892%
34	14.110	2040	2044	2047	rBV	4378346	4304344	100.00%	14.063%
35	14.139	2047	2049	2052	rVB	668500	543600	12.63%	1.776%
36	15.657	2302	2307	2319	rBV2	505936	699226	16.24%	2.284%

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SB-5(1-1.5)

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-BF011822.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	16.145	2384	2390	2395	rBV3	30249	52494	1.22%	0.172%
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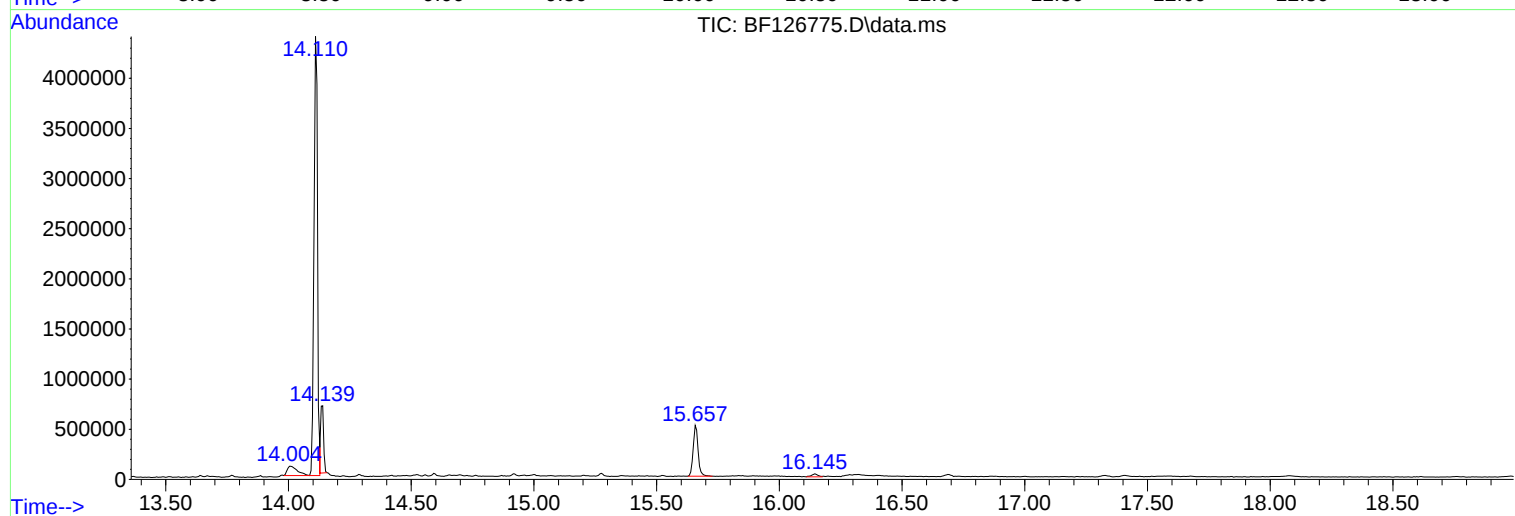
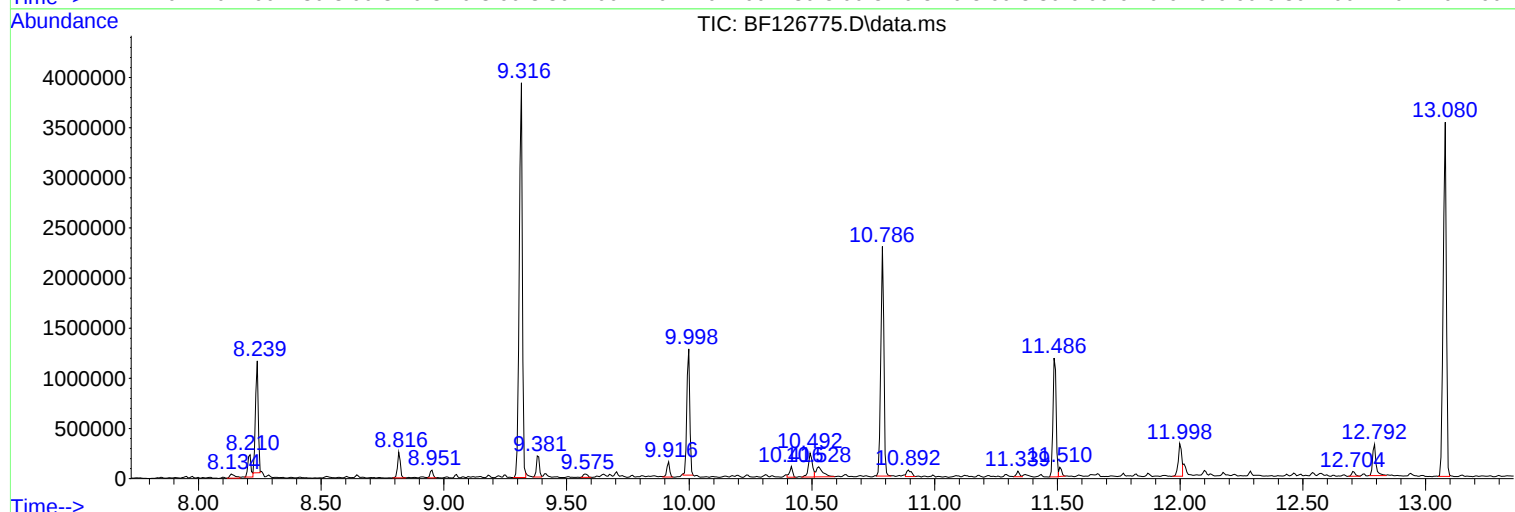
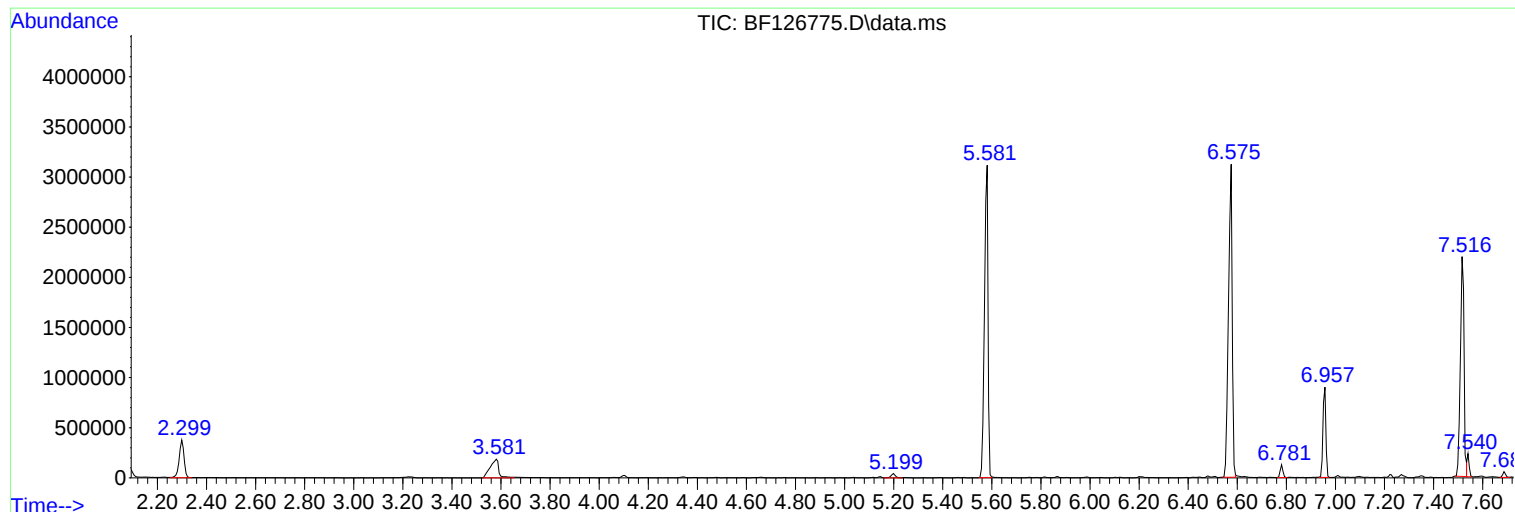
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
BNA_F
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SB-5(1-1.5)

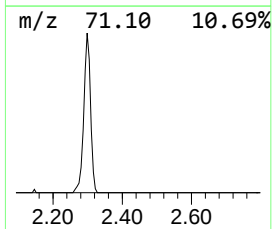
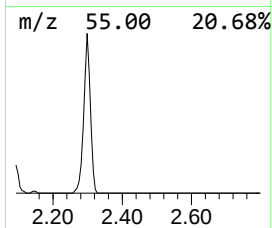
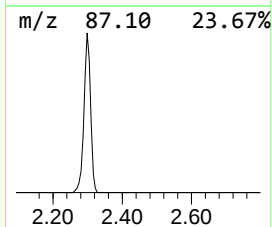
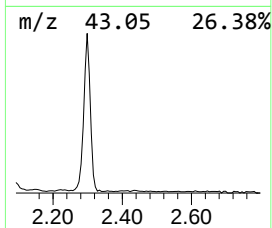
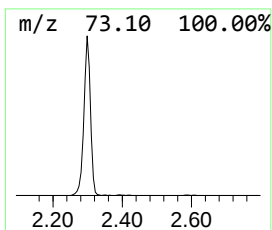
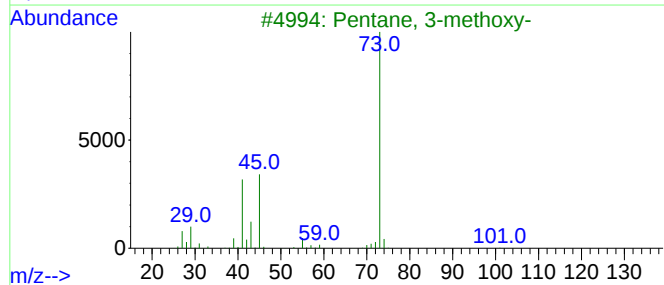
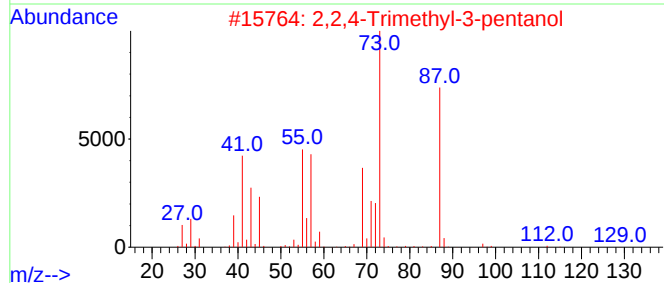
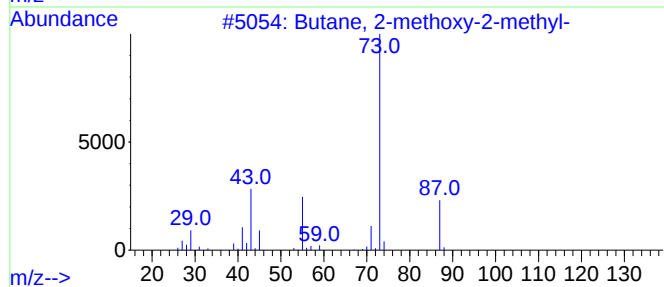
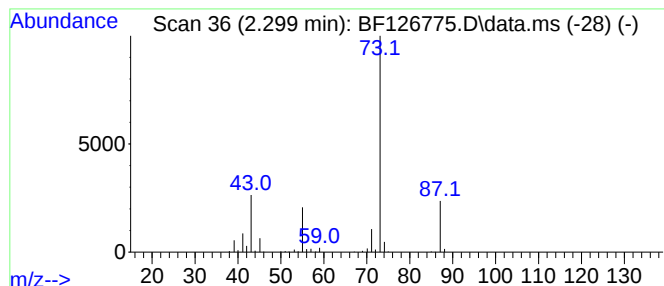
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.299	13.40 ng	496560	1,4-Dichlorobenzene-d4	6.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9



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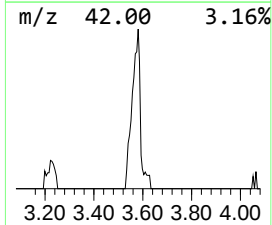
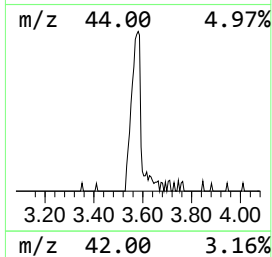
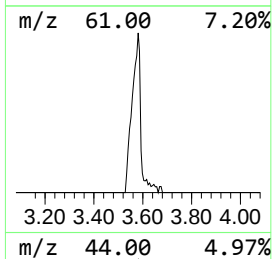
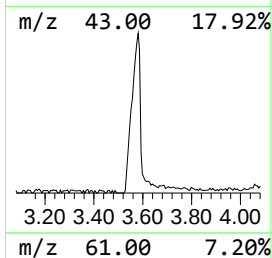
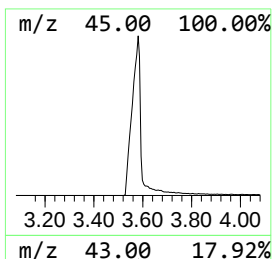
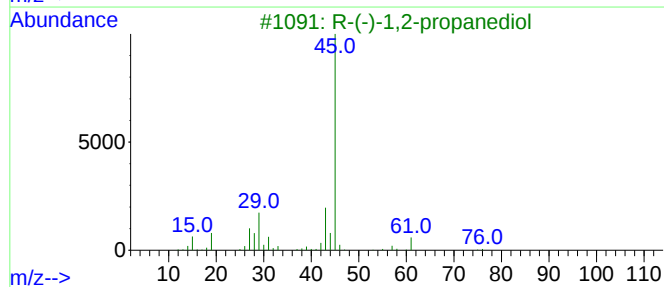
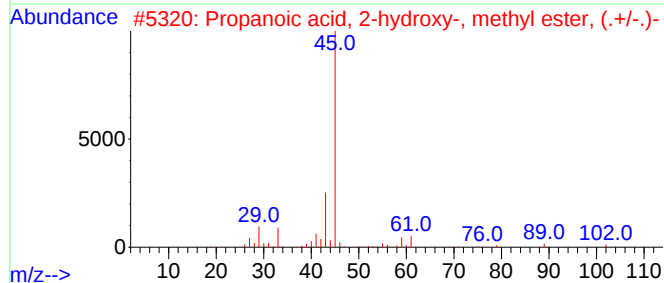
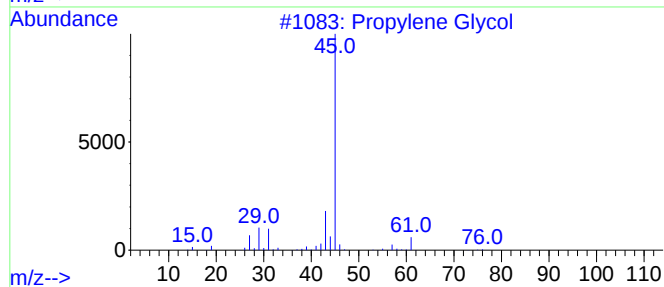
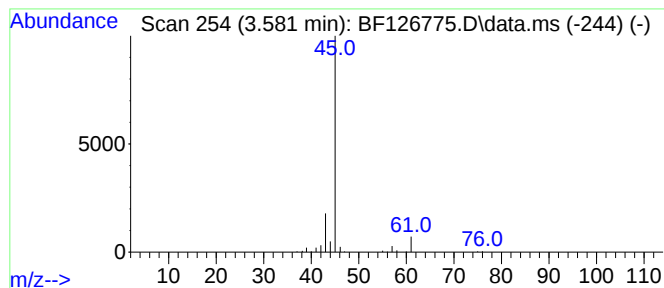
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Propylene Glycol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.581	12.31 ng	456183	1,4-Dichlorobenzene-d4	6.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propylene Glycol	76	C3H8O2	000057-55-6	86
2			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
3			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	37
4			Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5			(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	9



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Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-5(1-1.5)

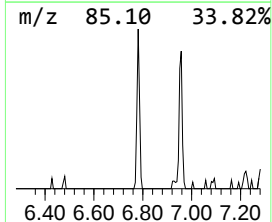
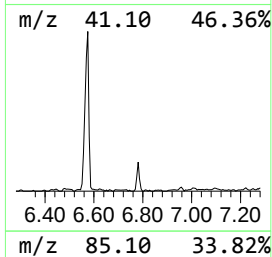
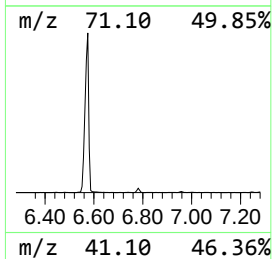
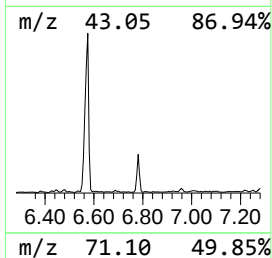
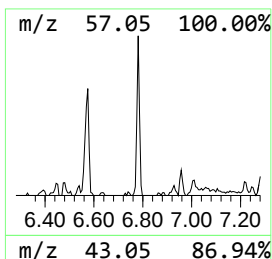
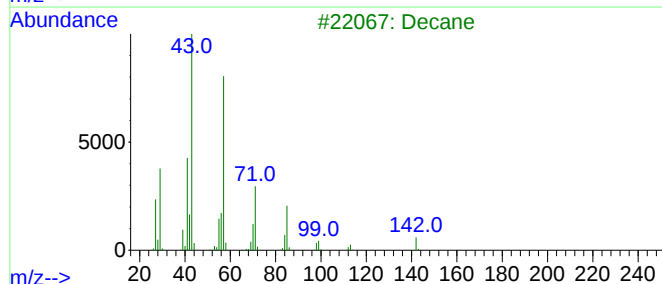
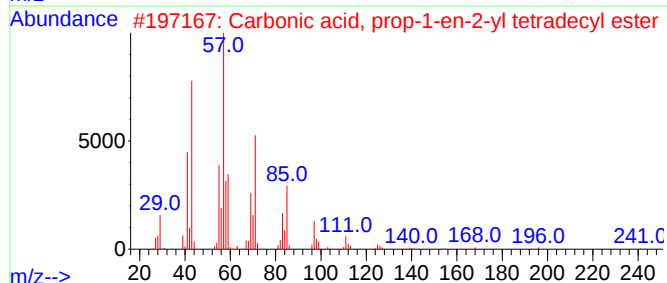
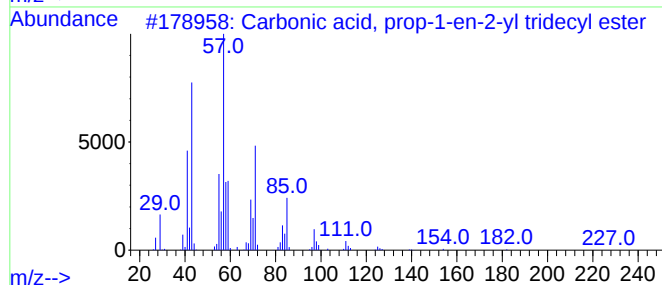
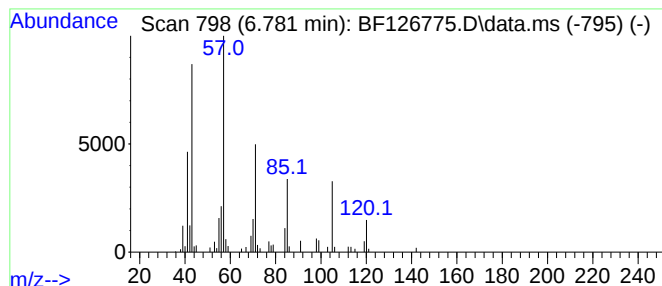
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Carbonic acid, prop-1-en-2-... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.781	2.68 ng	99319	1,4-Dichlorobenzene-d4	6.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, prop-1-en-2-yl tr...	284	C17H32O3	1000382-90-8	64
2			Carbonic acid, prop-1-en-2-yl te...	298	C18H34O3	1000382-90-9	64
3			Decane	142	C10H22	000124-18-5	64
4			Tetradecane	198	C14H30	000629-59-4	64
5			Undecane, 3,7-dimethyl-	184	C13H28	017301-29-0	59



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Misc :
ALS Vial : 10 Sample Multiplier: 1

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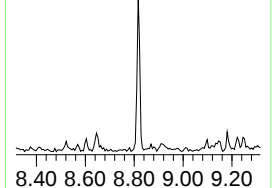
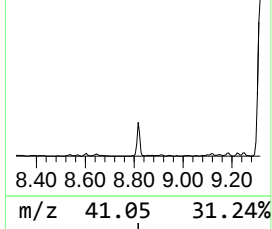
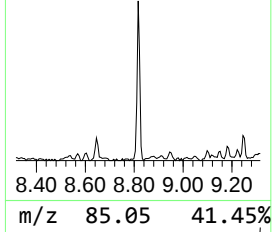
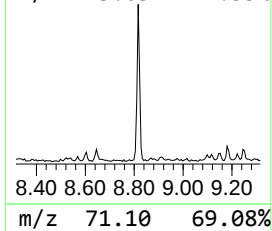
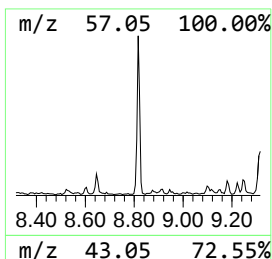
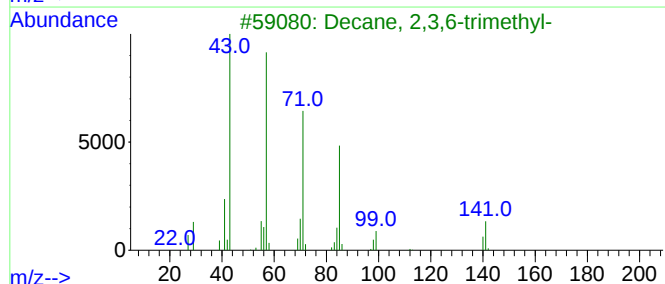
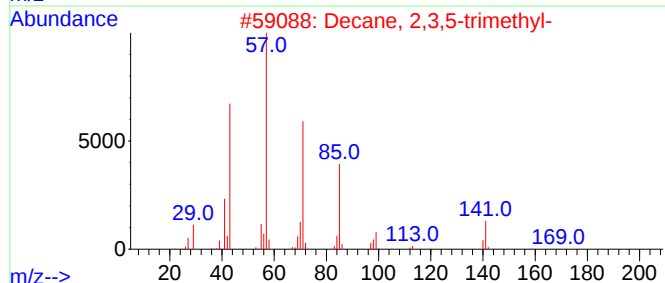
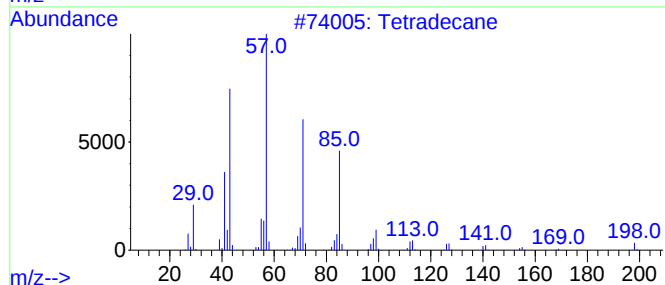
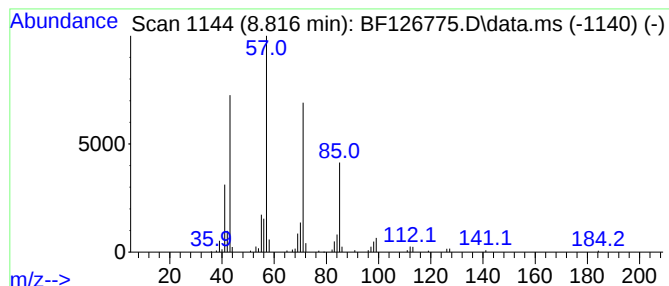
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Tetradecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.816	4.52 ng	199142	Naphthalene-d8	8.239

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecane	198	C14H30	000629-59-4	90
2			Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	86
3			Decane, 2,3,6-trimethyl-	184	C13H28	062238-12-4	78
4			Dodecane, 4-methyl-	184	C13H28	006117-97-1	74
5			Decane, 5-propyl-	184	C13H28	017312-62-8	74



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Misc :
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Instrument :
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ClientSampleId :
SB-5(1-1.5)

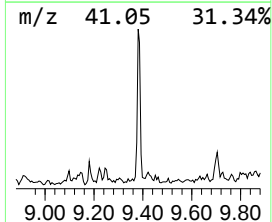
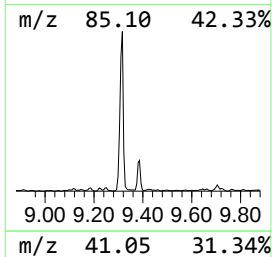
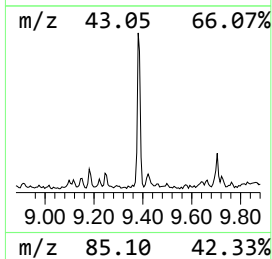
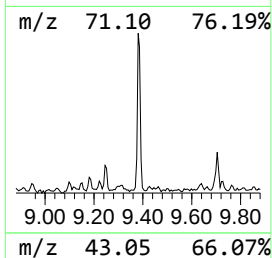
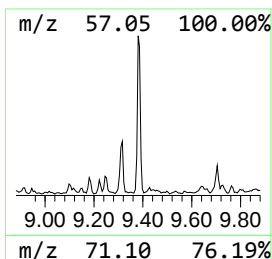
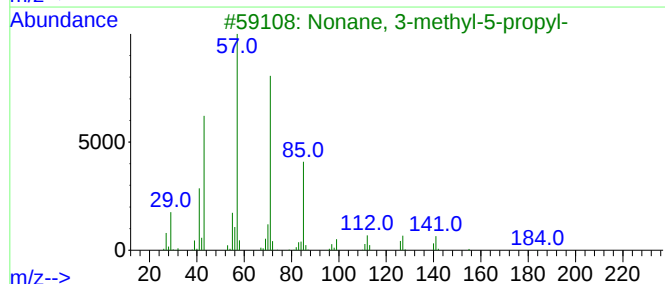
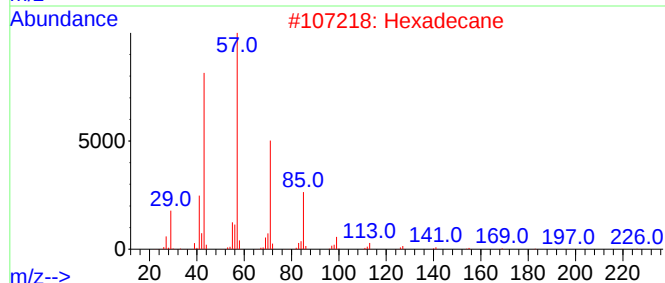
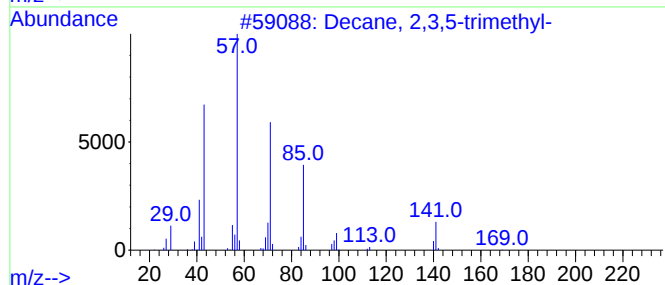
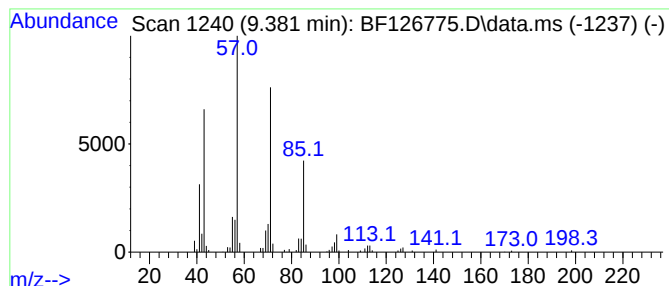
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Decane, 2,3,5-trimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.381	3.46 ng	182448	Acenaphthene-d10	9.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	90
2			Hexadecane	226	C16H34	000544-76-3	86
3			Nonane, 3-methyl-5-propyl-	184	C13H28	031081-18-2	78
4			Nonane, 5-methyl-5-propyl-	184	C13H28	017312-75-3	72
5			Tridecane, 7-methyl-	198	C14H30	026730-14-3	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020122\
Data File : BF126775.D
Acq On : 01 Feb 2022 15:44
Operator : CG/JU
Sample : N1340-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-5(1-1.5)

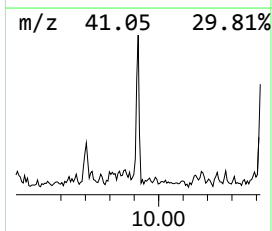
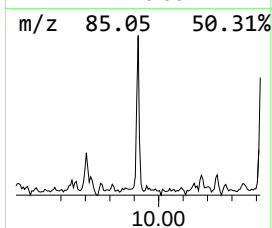
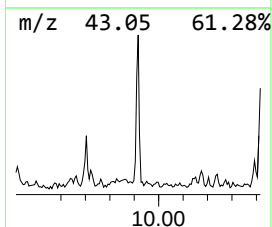
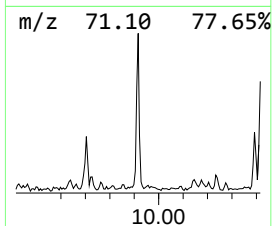
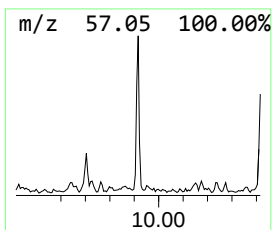
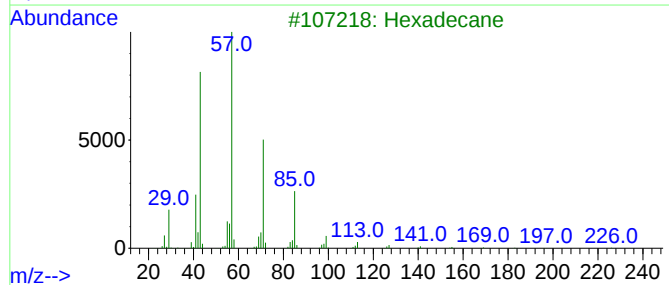
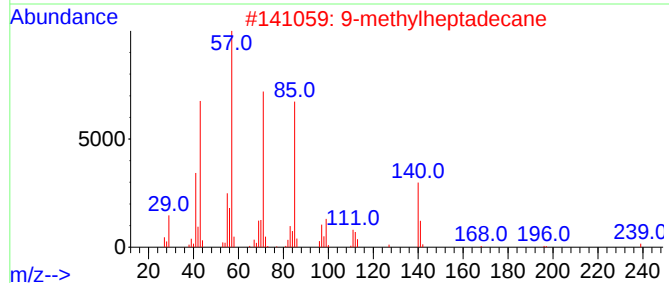
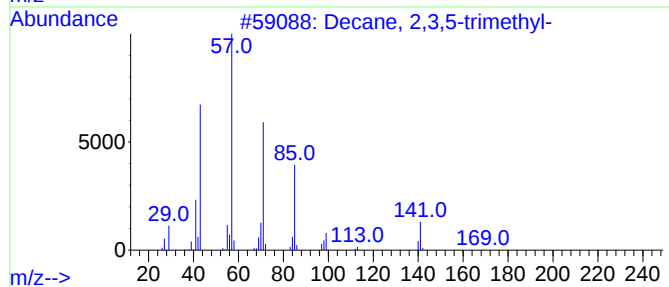
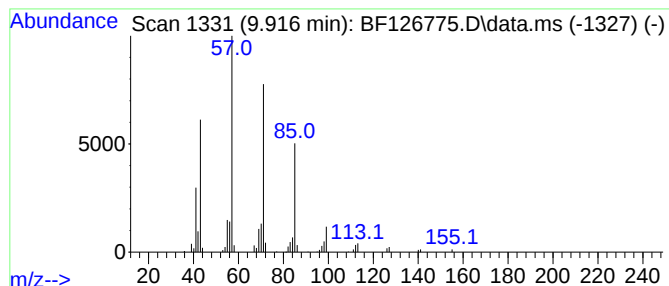
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 9-methylheptadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.916	2.26 ng	118885	Acenaphthene-d10	9.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	90
2			9-methylheptadecane	254	C18H38	026741-18-4	83
3			Hexadecane	226	C16H34	000544-76-3	78
4			Oxalic acid, bis(6-ethyloct-3-yl...)	370	C22H42O4	1000309-34-6	72
5			Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020122\
Data File : BF126775.D
Acq On : 01 Feb 2022 15:44
Operator : CG/JU
Sample : N1340-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-5(1-1.5)

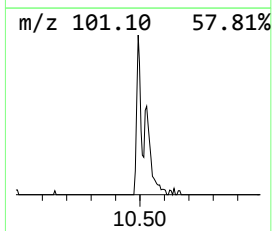
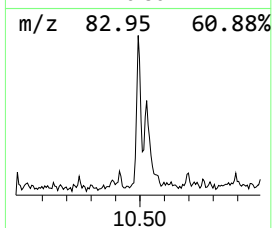
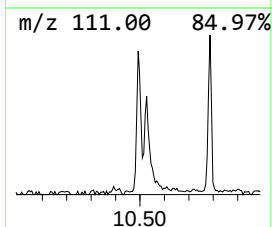
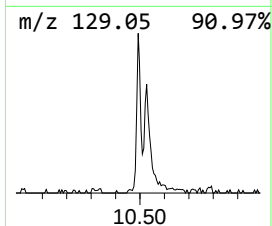
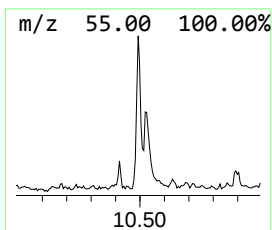
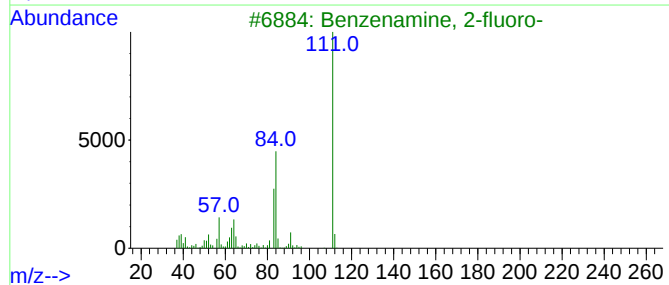
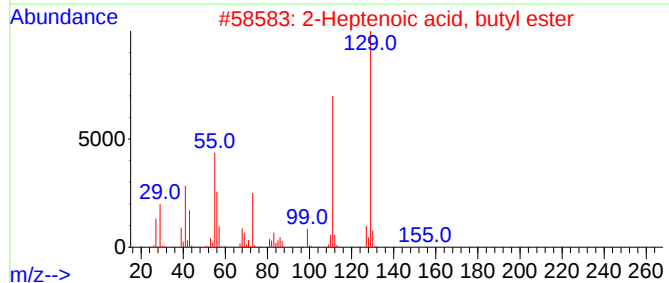
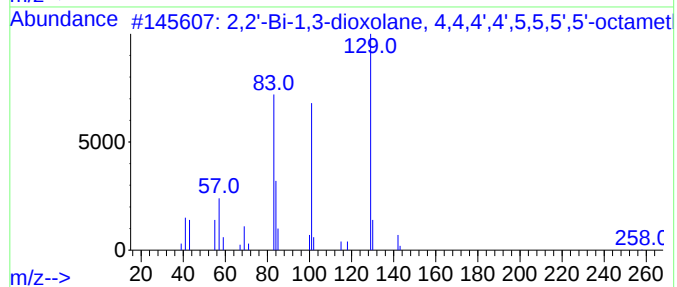
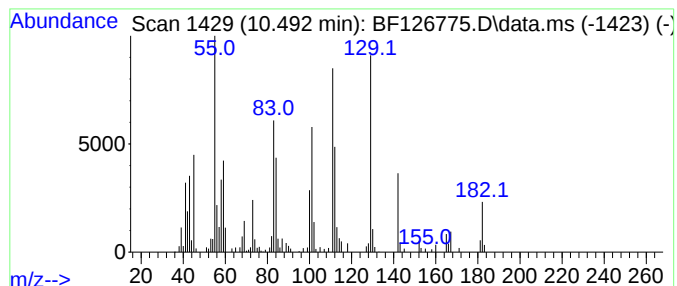
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown10.492 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.492	5.23 ng	275608	Acenaphthene-d10	9.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2'-Bi-1,3-dioxolane, 4,4,4',4'...	258	C14H26O4	035528-76-8	35		
2	2-Heptenoic acid, butyl ester	184	C11H20O2	1000406-08-9	27		
3	Benzenamine, 2-fluoro-	111	C6H6FN	000348-54-9	22		
4	Thiophene, 3,4-dimethyl-	112	C6H8S	000632-15-5	18		
5	Thiophene, 2,4-dimethyl-	112	C6H8S	000638-00-6	14		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020122\
Data File : BF126775.D
Acq On : 01 Feb 2022 15:44
Operator : CG/JU
Sample : N1340-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

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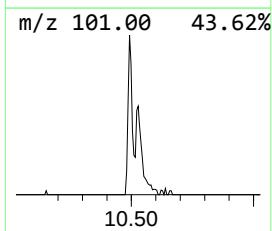
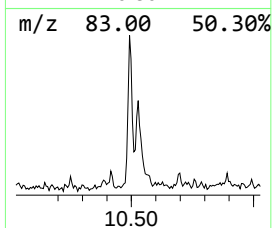
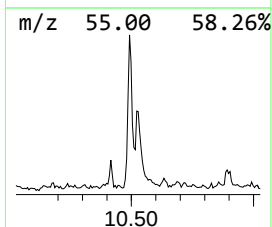
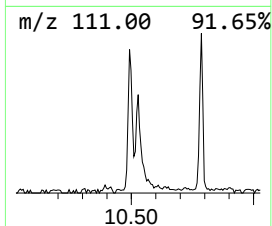
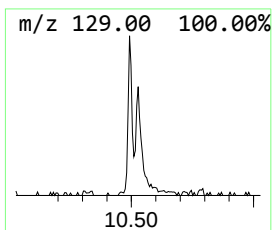
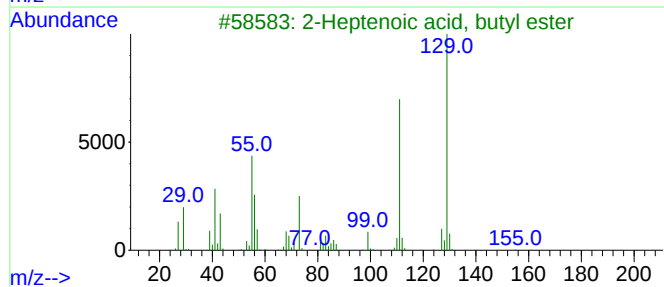
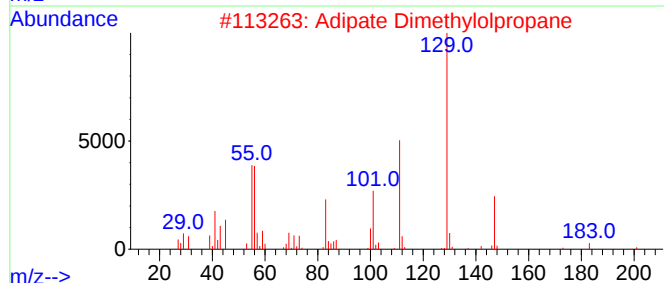
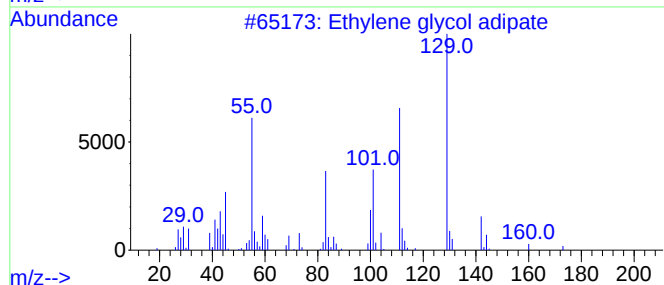
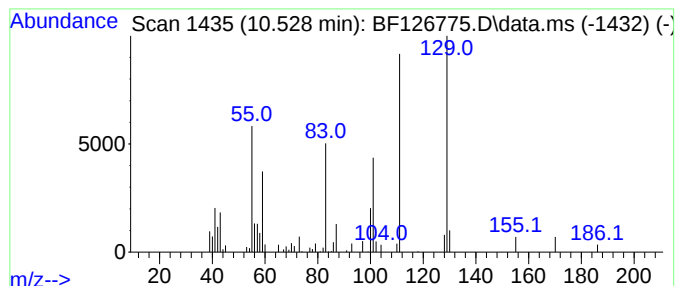
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Ethylene glycol adipate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.528	3.55 ng	187268	Acenaphthene-d10	9.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethylene glycol adipate	190	C8H14O5	1000445-97-3	64
2			Adipate Dimethylolpropane	232	C11H20O5	1000445-99-1	40
3			2-Heptenoic acid, butyl ester	184	C11H20O2	1000406-08-9	37
4			Diisopropyl adipate	230	C12H22O4	006938-94-9	37
5			Succinic acid, docosyl ethyl ester	454	C28H54O4	1000349-57-1	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020122\
Data File : BF126775.D
Acq On : 01 Feb 2022 15:44
Operator : CG/JU
Sample : N1340-05
Misc :
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Instrument :
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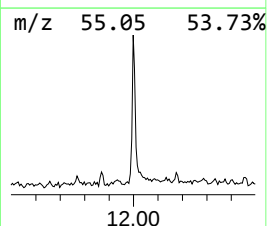
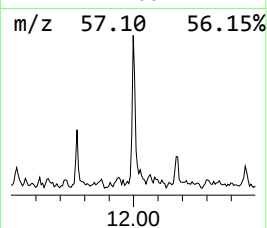
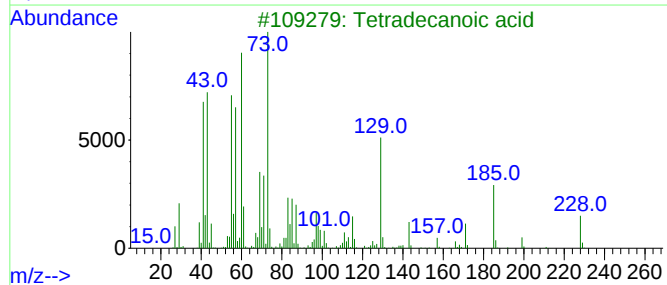
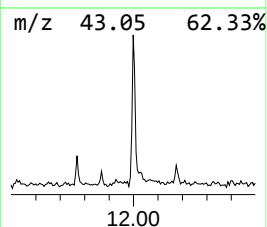
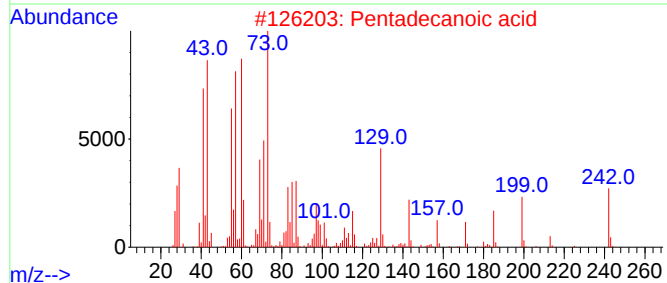
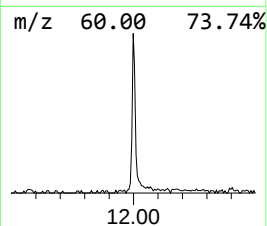
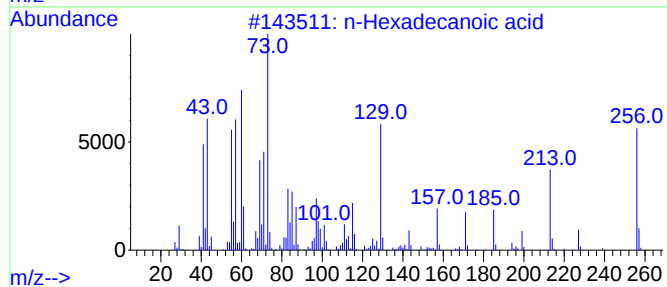
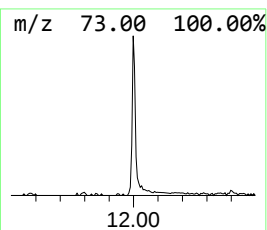
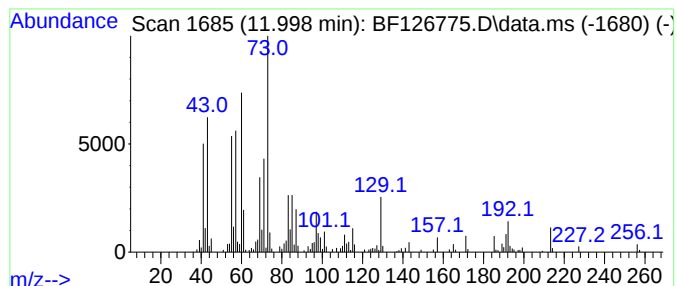
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.998	6.07 ng	326607	Phenanthrene-d10	11.486

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	58
4			Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	25
5			Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	15



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020122\
Data File : BF126775.D
Acq On : 01 Feb 2022 15:44
Operator : CG/JU
Sample : N1340-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-5(1-1.5)

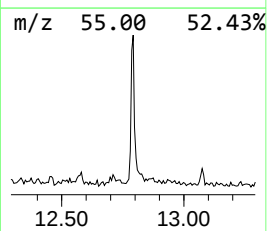
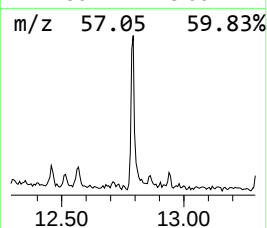
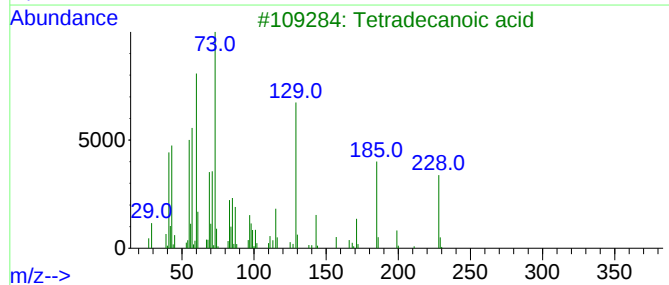
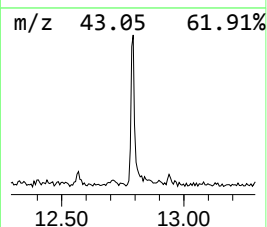
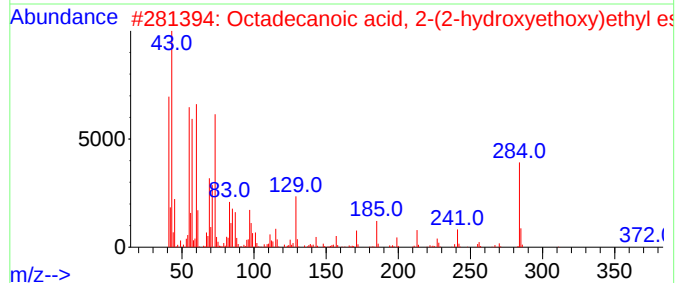
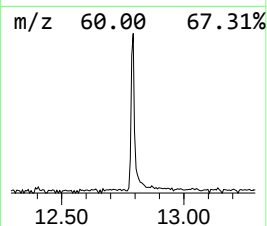
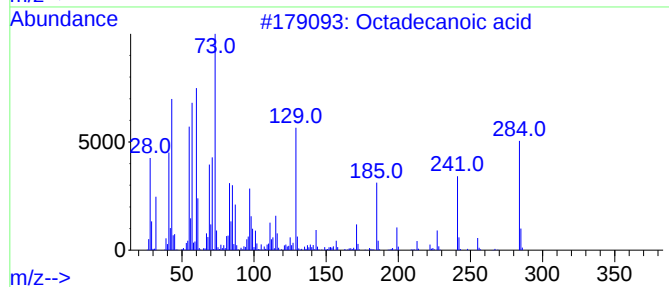
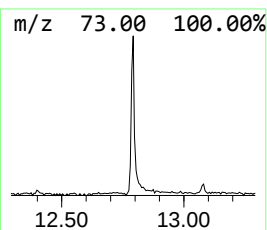
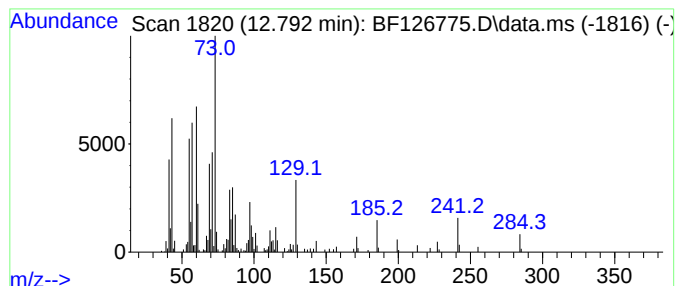
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.792	5.65 ng	304063	Phenanthrene-d10	11.486

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	64
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	41
4			n-Decanoic acid	172	C10H20O2	000334-48-5	30
5			Sulfurous acid, 2-propyl tetra...	320	C17H36O3S	1010309-12-5	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020122\
Data File : BF126775.D
Acq On : 01 Feb 2022 15:44
Operator : CG/JU
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Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-5(1-1.5)

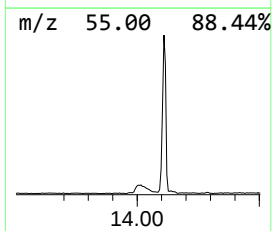
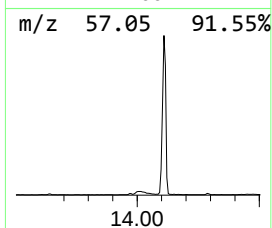
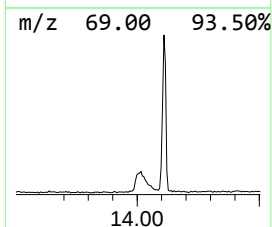
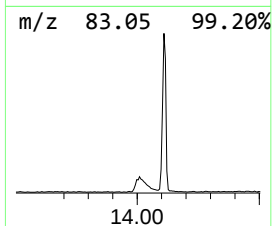
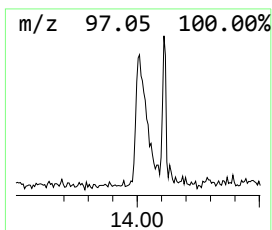
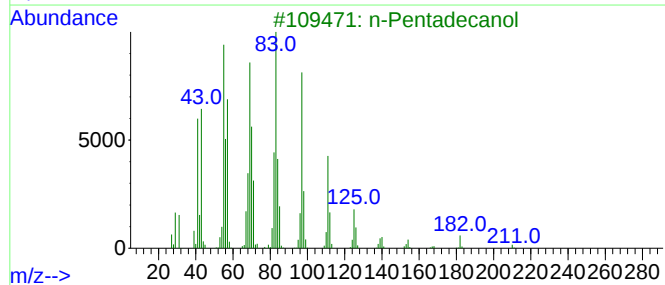
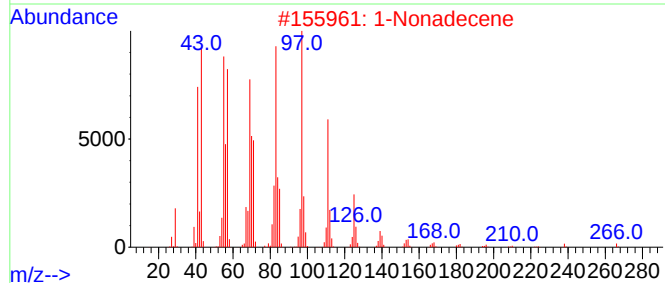
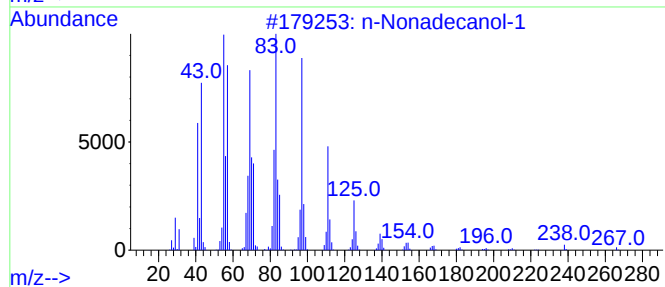
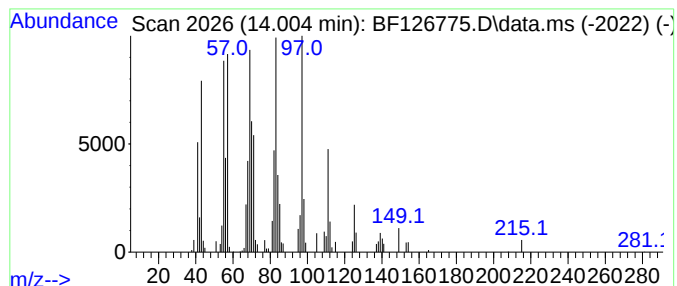
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 n-Nonadecanol-1 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.004	10.04 ng	273013	Chrysene-d12	14.139

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Nonadecanol-1	284	C19H40O	001454-84-8	95
2			1-Nonadecene	266	C19H38	018435-45-5	95
3			n-Pentadecanol	228	C15H32O	000629-76-5	94
4			1-Hexadecanol	242	C16H34O	036653-82-4	93
5			n-Heptadecanol-1	256	C17H36O	001454-85-9	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020122\
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Acq On : 01 Feb 2022 15:44
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Sample : N1340-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-5(1-1.5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.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
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Propylene Glycol	3.581	12.3	ng	456183	1	6.957	741388	20.0
Carbonic acid, ...	6.781	2.7	ng	99319	1	6.957	741388	20.0
Tetradecane	8.816	4.5	ng	199142	2	8.239	880410	20.0
Decane, 2,3,5-t...	9.381	3.5	ng	182448	3	9.998	1053630	20.0
9-methylheptade...	9.916	2.3	ng	118885	3	9.998	1053630	20.0
unknown10.492	10.492	5.2	ng	275608	3	9.998	1053630	20.0
Ethylene glycol...	10.528	3.5	ng	187268	3	9.998	1053630	20.0
n-Hexadecanoic ...	11.998	6.1	ng	326607	4	11.486	1076620	20.0
Octadecanoic acid	12.792	5.7	ng	304063	4	11.486	1076620	20.0
n-Nonadecanol-1	14.004	10.0	ng	273013	5	14.139	543600	20.0