

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011821\
 Data File : BF123007.D
 Acq On : 19 Jan 2021 1:47
 Operator : JU/CG
 Sample : M1157-01
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-1

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-BF011621.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123007.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.210	14	21	27	rVB	1248361	1612688	31.10%	5.904%
2	5.510	577	582	585	rBV	969764	924268	17.82%	3.384%
3	6.504	747	751	757	rBV2	643253	888937	17.14%	3.254%
4	6.716	783	787	790	rBV	160413	124268	2.40%	0.455%
5	6.892	813	817	821	rBV	577803	513063	9.89%	1.878%
6	7.451	906	912	915	rBV	1331232	1417361	27.33%	5.189%
7	8.181	1031	1036	1038	rBV	777960	855060	16.49%	3.130%
8	8.198	1038	1039	1042	rVB	157904	81763	1.58%	0.299%
9	8.722	1121	1128	1133	rVB	87515	86956	1.68%	0.318%
10	9.257	1213	1219	1222	rBV	3976768	4214313	81.27%	15.429%
11	9.369	1233	1238	1242	rVB	1034768	905946	17.47%	3.317%
12	9.645	1281	1285	1288	rBV	284743	260565	5.02%	0.954%
13	9.933	1327	1334	1338	rBV	1621867	1495369	28.84%	5.475%
14	10.516	1429	1433	1440	rBV	148210	142358	2.75%	0.521%
15	10.722	1462	1468	1471	rBV	2933673	2764123	53.30%	10.120%
16	11.422	1582	1587	1590	rBV	1327409	1201296	23.17%	4.398%
17	11.945	1669	1676	1680	rBV	286296	264437	5.10%	0.968%
18	11.980	1680	1682	1692	rVB2	36948	69082	1.33%	0.253%
19	12.404	1751	1754	1758	rBV	70523	74471	1.44%	0.273%
20	12.474	1762	1766	1770	rVV	146319	178011	3.43%	0.652%
21	12.516	1770	1773	1778	rVB	87220	86727	1.67%	0.318%
22	12.669	1794	1799	1803	rVB2	103345	123085	2.37%	0.451%
23	12.733	1806	1810	1816	rBV	158104	226036	4.36%	0.828%
24	12.886	1834	1836	1839	rBV	126662	104966	2.02%	0.384%
25	13.016	1852	1858	1861	rBV	5227809	5185537	100.00%	18.985%
26	13.245	1891	1897	1900	rBV	131002	140341	2.71%	0.514%
27	13.586	1952	1955	1959	rVB2	65314	60744	1.17%	0.222%
28	13.910	2007	2010	2020	rBV	477036	573542	11.06%	2.100%
29	14.063	2032	2036	2040	rBV	1442349	1305539	25.18%	4.780%
30	14.539	2115	2117	2128	rVB5	41862	70303	1.36%	0.257%
31	15.539	2281	2287	2293	rBV2	972817	1266738	24.43%	4.638%
32	16.086	2375	2380	2388	rBV5	42232	96410	1.86%	0.353%

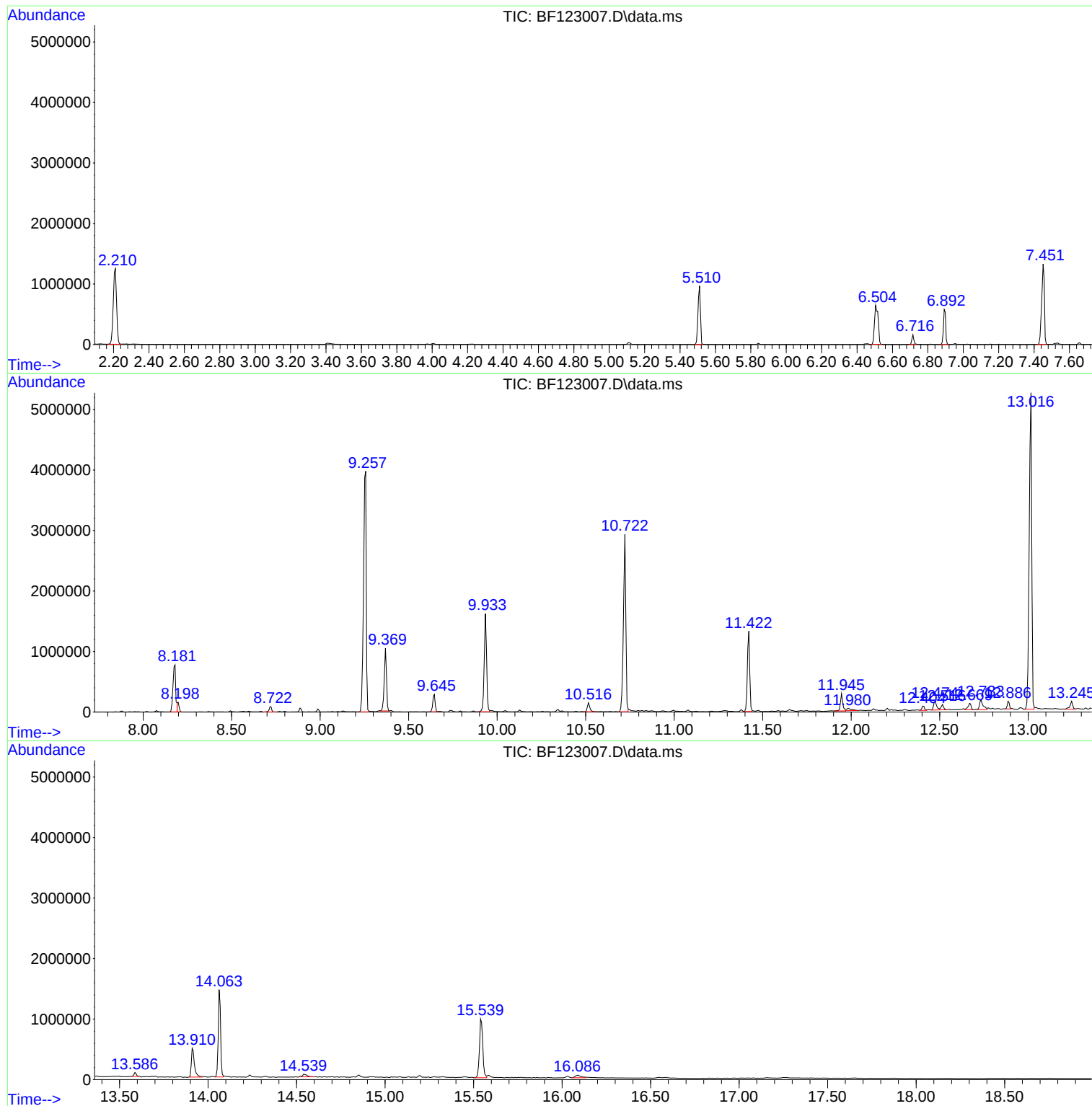
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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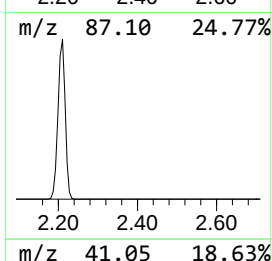
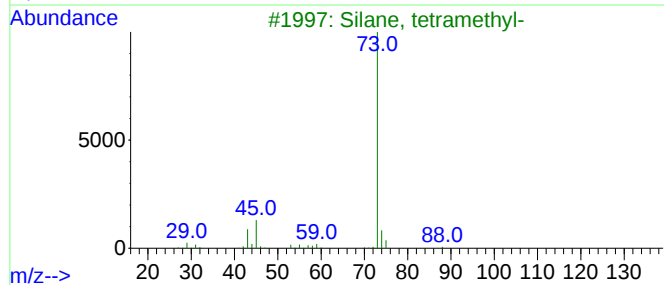
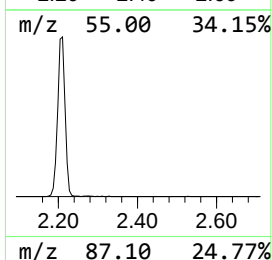
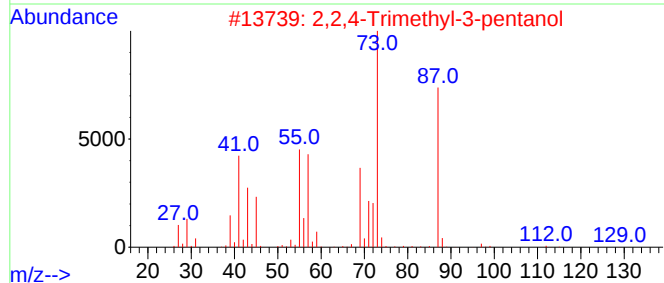
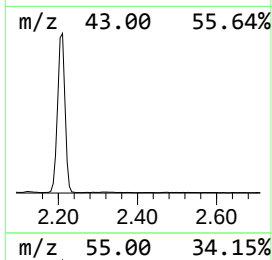
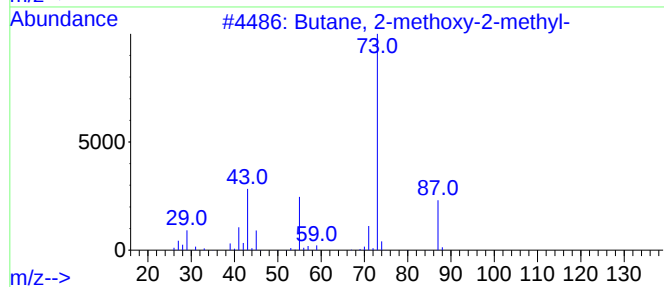
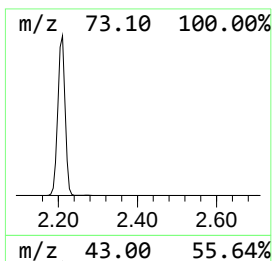
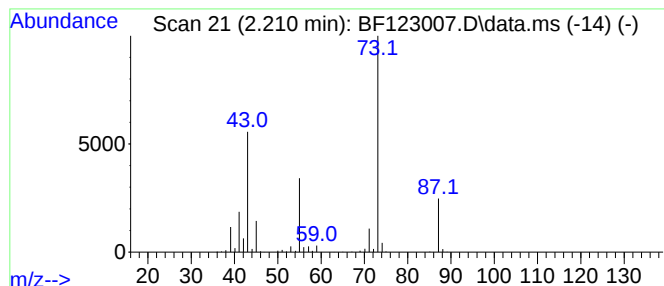
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.210	62.87 ng	1612690	1,4-Dichlorobenzene-d4	6.898

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			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4			Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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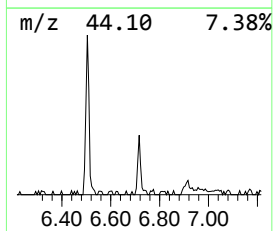
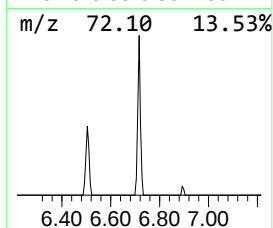
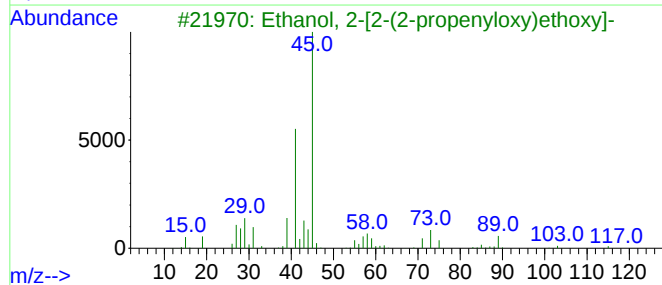
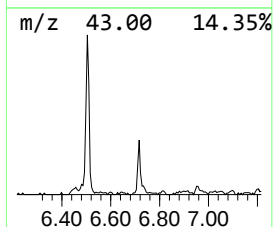
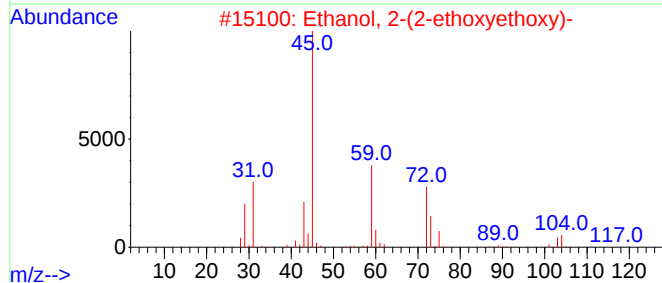
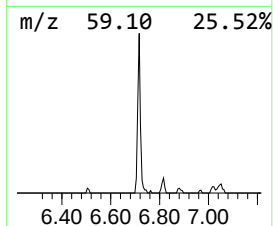
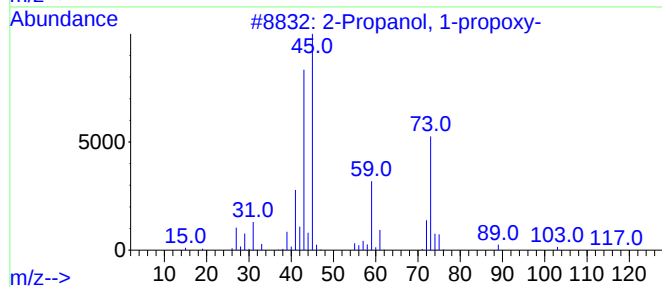
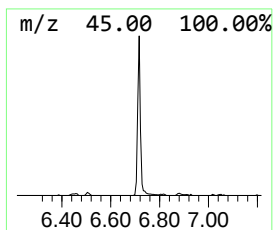
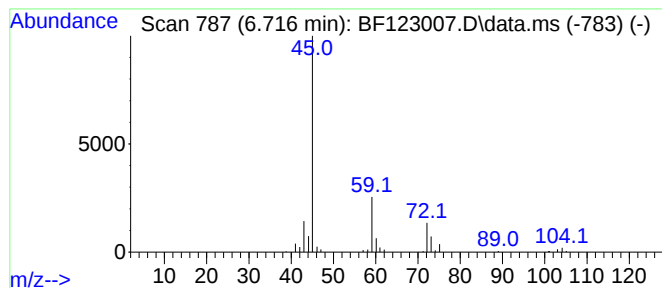
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.716 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.716	4.84 ng	124268	1,4-Dichlorobenzene-d4	6.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-propoxy-			118	C6H14O2	001569-01-3	40
2	Ethanol, 2-(2-ethoxyethoxy)-			134	C6H14O3	000111-90-0	40
3	Ethanol, 2-[2-(2-propenyloxy)etho...			146	C7H14O3	015075-50-0	38
4	2-Butanol			74	C4H10O	000078-92-2	38
5	Ethyl ether			74	C4H10O	000060-29-7	36



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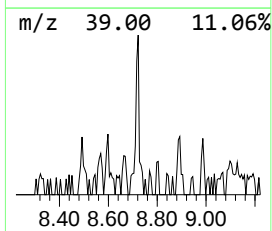
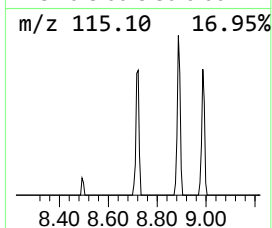
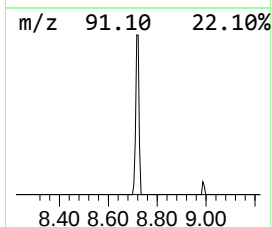
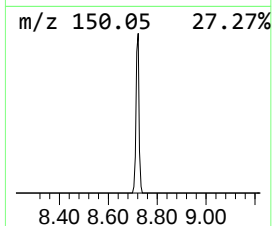
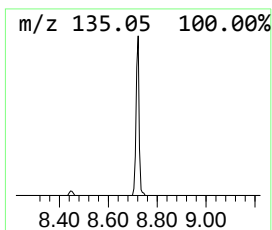
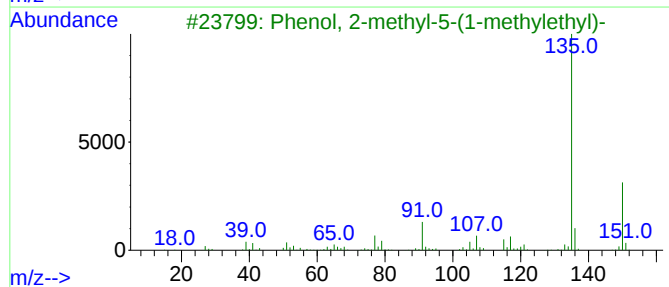
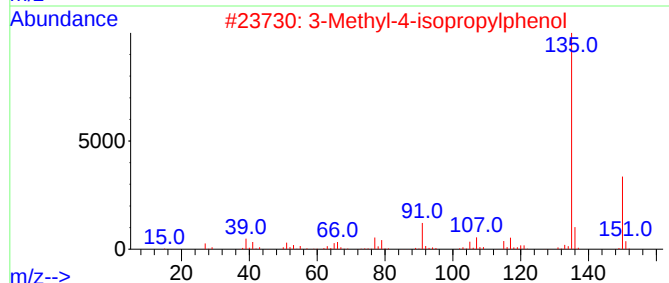
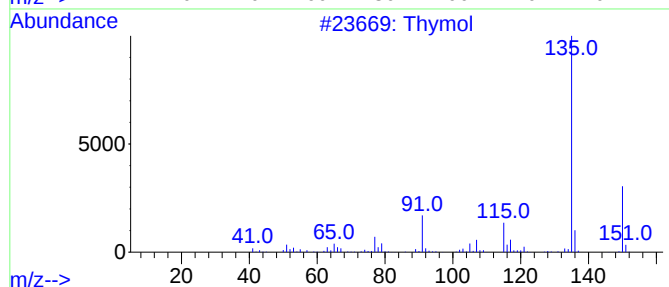
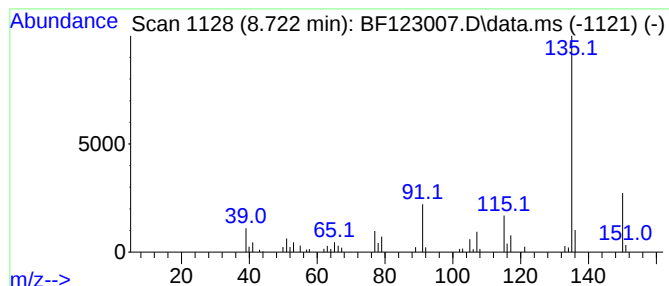
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Peak Number 3 Thymol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.722	2.03 ng	86956	Naphthalene-d8	8.181

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thymol	150	C10H14O	000089-83-8	95
2			3-Methyl-4-isopropylphenol	150	C10H14O	003228-02-2	90
3			Phenol, 2-methyl-5-(1-methylethyl)-	150	C10H14O	000499-75-2	87
4			Phenol, 2,3,4,6-tetramethyl-	150	C10H14O	003238-38-8	80
5			Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	72



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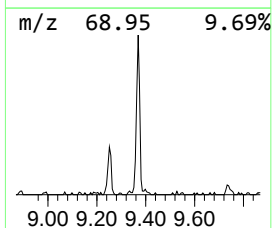
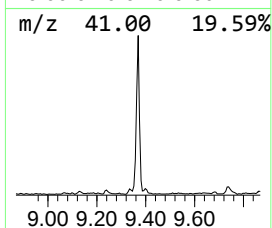
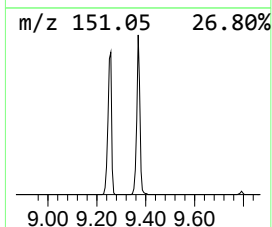
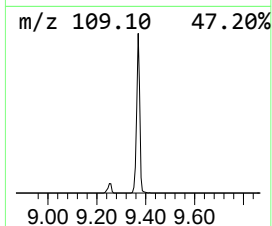
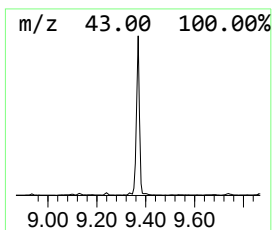
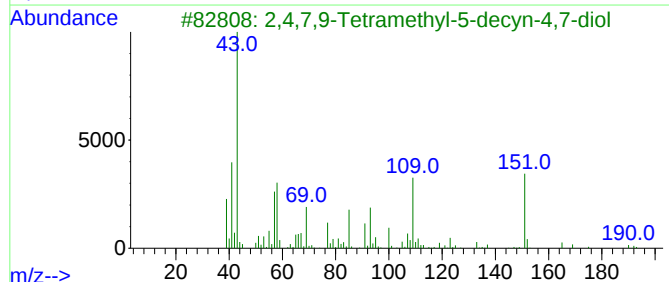
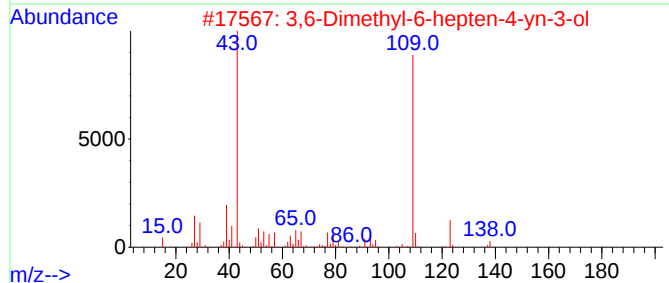
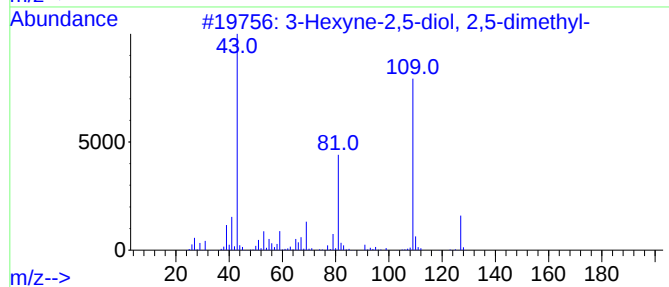
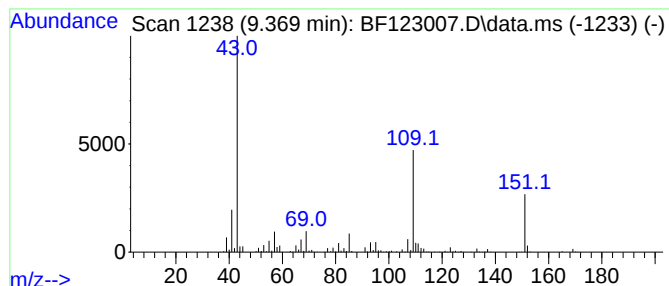
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Peak Number 4 unknown9.369 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.369	12.12 ng	905946	Acenaphthene-d10	9.933

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Hexyne-2,5-diol, 2,5-dimethyl-	142	C8H14O2	000142-30-3	28
2			3,6-Dimethyl-6-hepten-4-yn-3-ol	138	C9H14O	003601-67-0	17
3			2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	17
4			2,9-Decanedione	170	C10H18O2	016538-91-3	9
5			8-(2-Acetyloxiran-2-yl)-6,6-dime...	236	C14H20O3	091186-38-8	9



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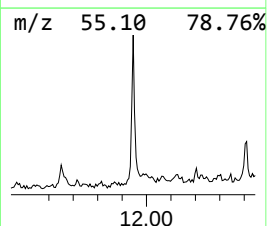
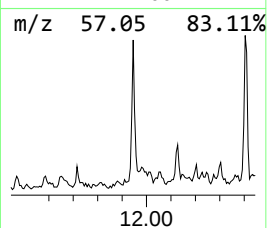
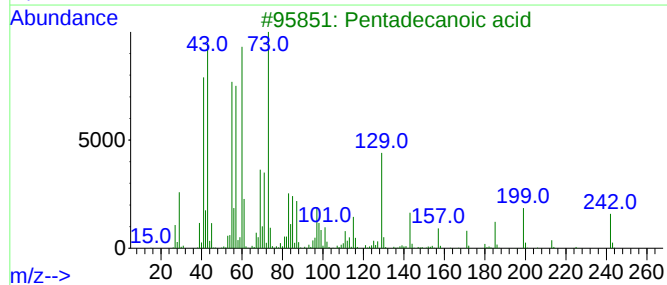
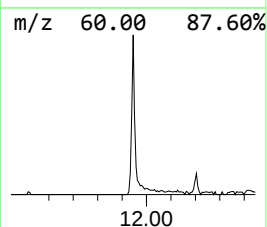
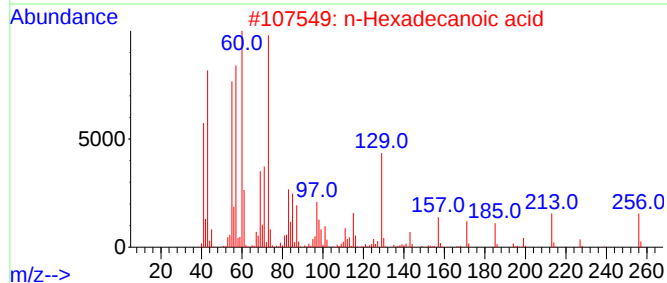
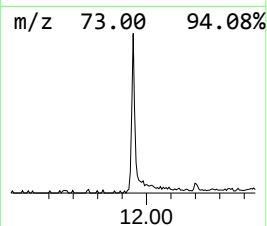
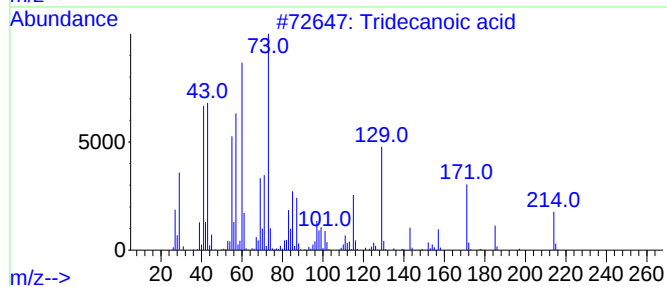
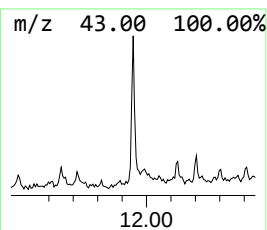
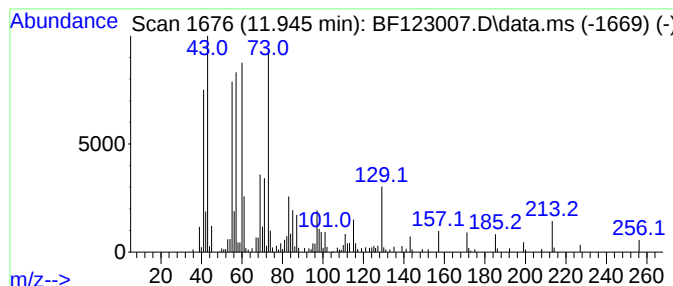
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Peak Number 5 Tridecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.945	4.40 ng	264437	Phenanthrene-d10	11.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid	214	C13H26O2	000638-53-9	95
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5			Dodecanoic acid	200	C12H24O2	000143-07-7	64



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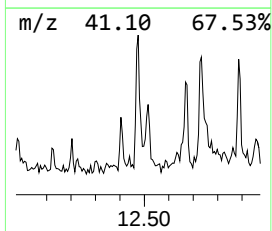
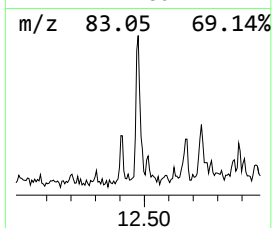
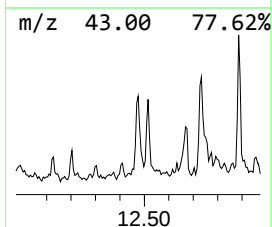
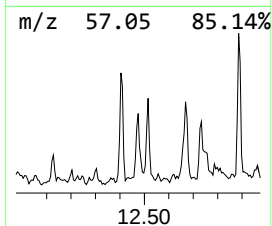
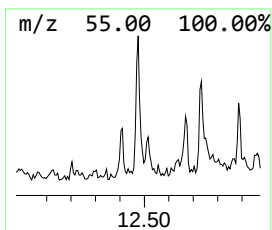
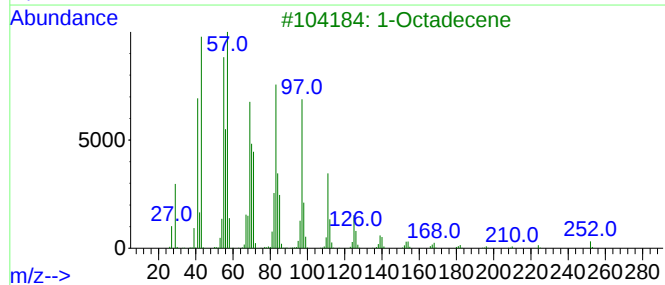
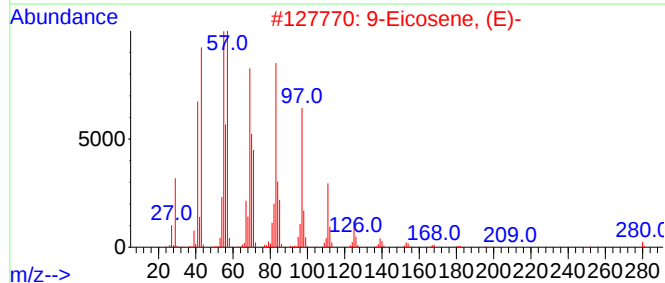
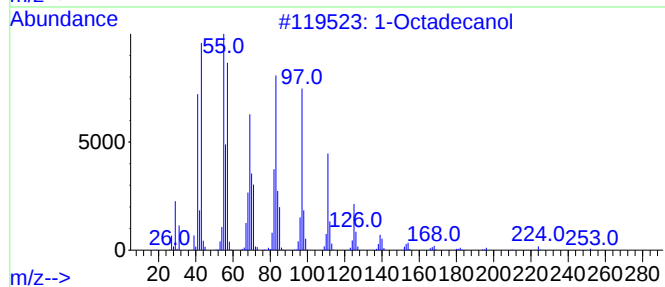
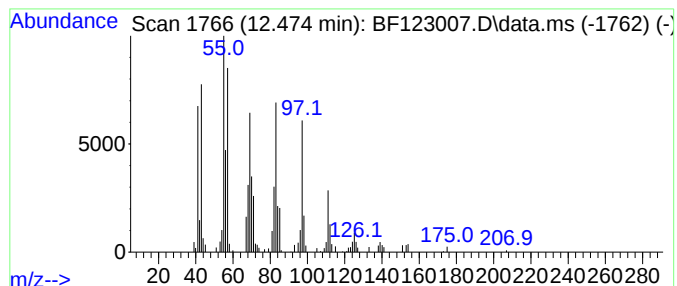
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 1-Octadecanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
12.475	2.96 ng	178011	Phenanthrene-d10		11.422

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecanol		270	C18H38O	000112-92-5	91
2	9-Eicosene, (E)-		280	C20H40	074685-29-3	91
3	1-Octadecene		252	C18H36	000112-88-9	91
4	n-Nonadecanol-1		284	C19H40O	001454-84-8	91
5	5-Eicosene, (E)-		280	C20H40	074685-30-6	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011821\
Data File : BF123007.D
Acq On : 19 Jan 2021 1:47
Operator : JU/CG
Sample : M1157-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-1

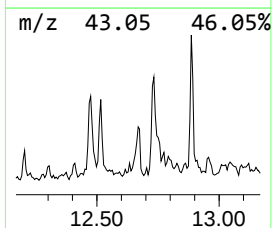
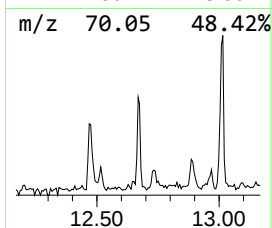
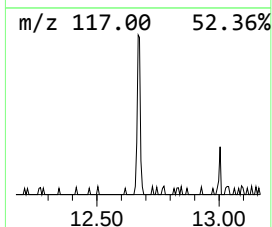
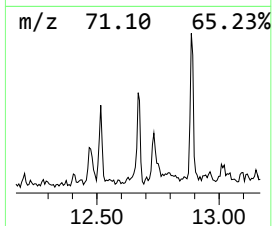
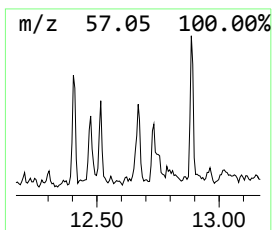
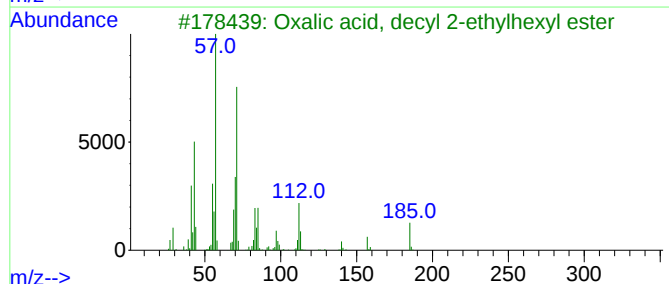
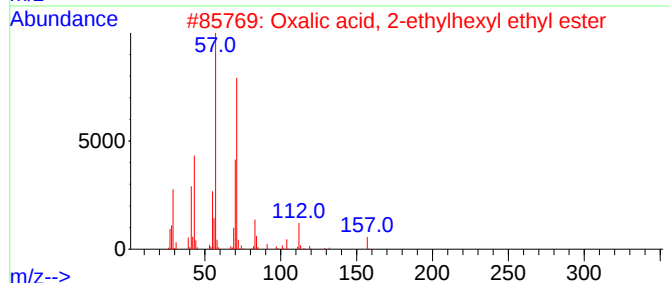
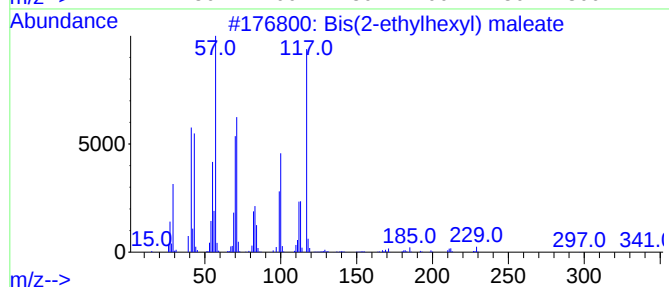
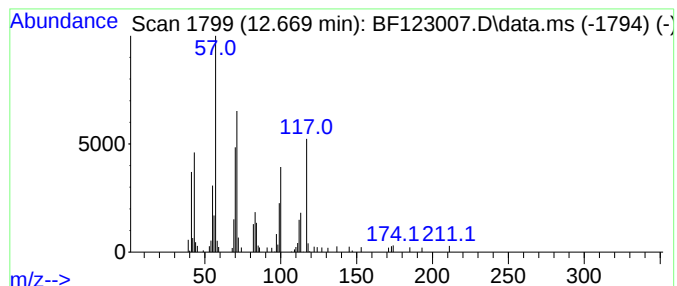
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Bis(2-ethylhexyl) maleate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.669	2.05 ng	123085	Phenanthrene-d10	11.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bis(2-ethylhexyl) maleate	340	C20H36O4	000142-16-5	90
2			Oxalic acid, 2-ethylhexyl ethyl ...	230	C12H22O4	1000309-38-4	38
3			Oxalic acid, decyl 2-ethylhexyl ...	342	C20H38O4	1000309-39-3	35
4			3-Hexanone	100	C6H12O	000589-38-8	30
5			Sulfurous acid, 2-ethylhexyl tet...	390	C22H46O3S	1000309-19-7	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011821\
Data File : BF123007.D
Acq On : 19 Jan 2021 1:47
Operator : JU/CG
Sample : M1157-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-1

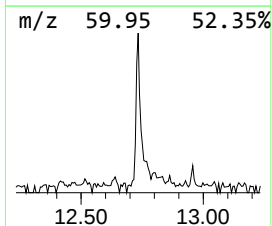
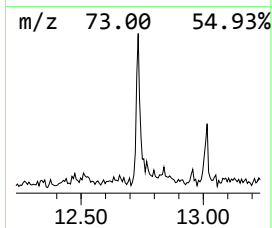
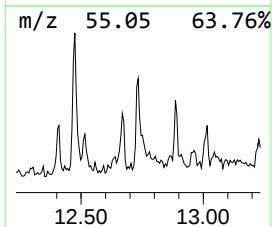
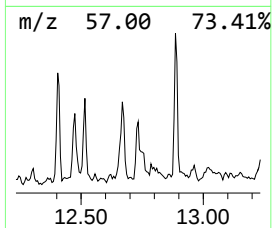
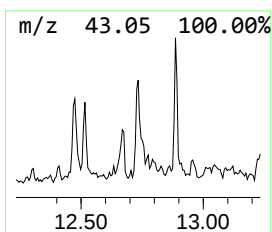
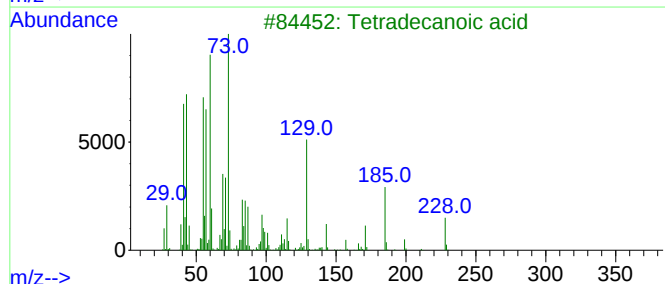
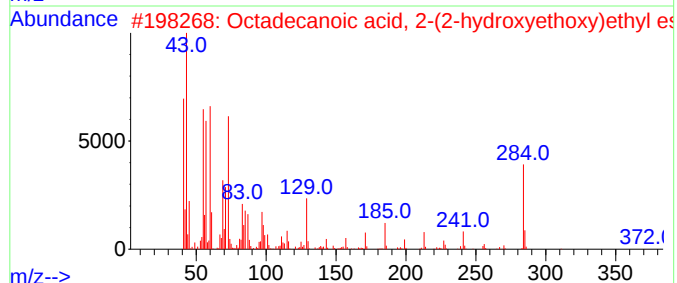
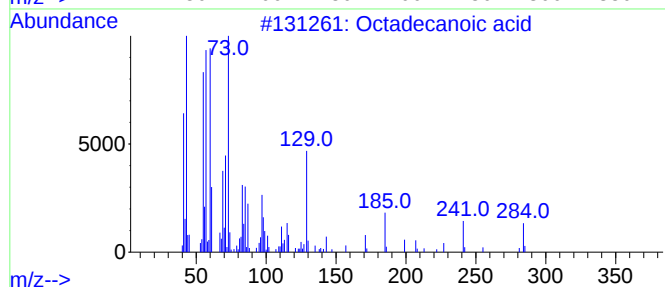
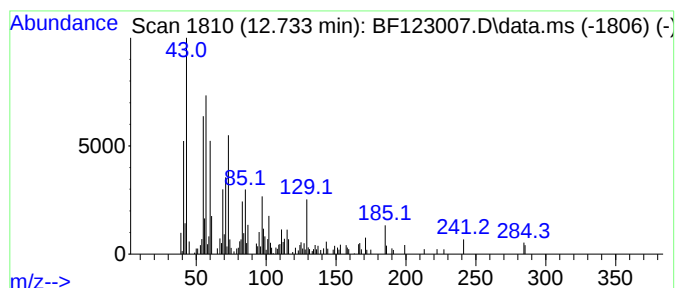
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.733	3.76 ng	226036	Phenanthrene-d10	11.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	98
2			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	52
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	49
4			Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	46
5			Undecanoic acid	186	C11H22O2	000112-37-8	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011821\
Data File : BF123007.D
Acq On : 19 Jan 2021 1:47
Operator : JU/CG
Sample : M1157-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-1

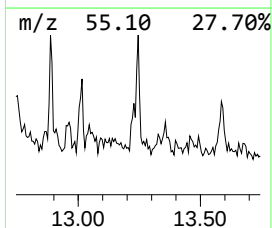
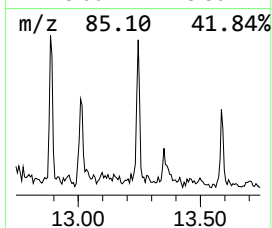
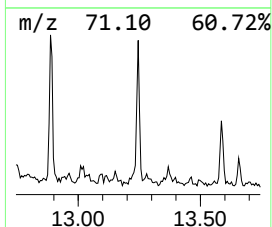
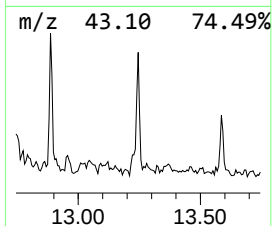
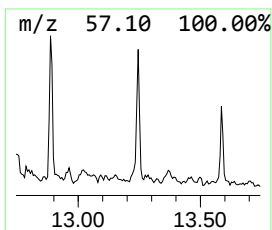
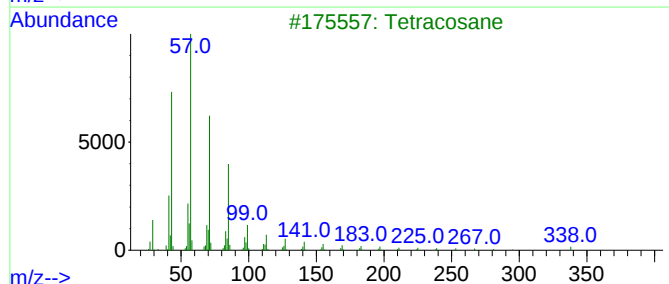
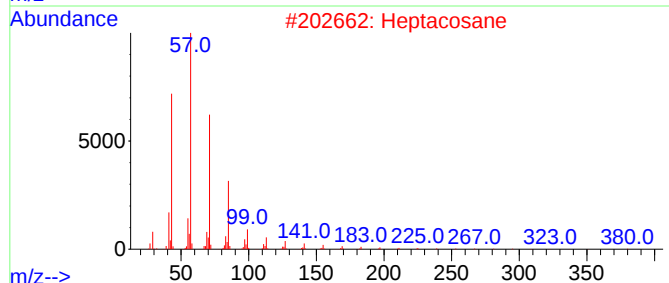
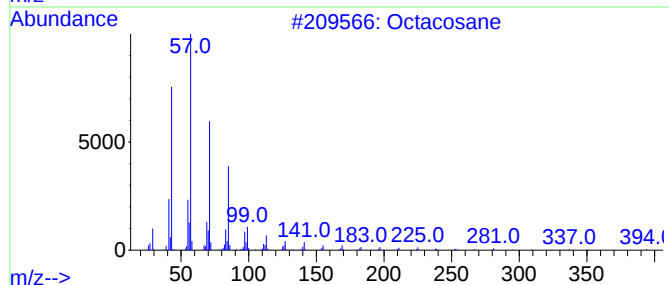
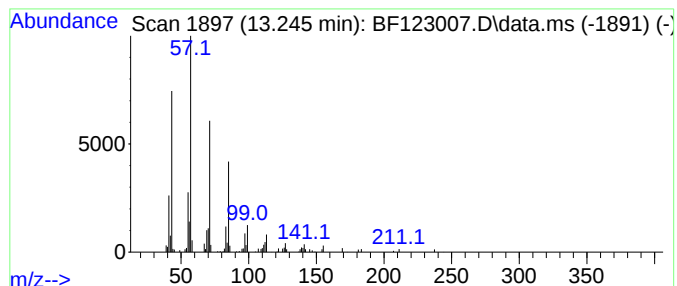
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Octacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.245	2.15 ng	140341	Chrysene-d12	14.063

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	91
2			Heptacosane	380	C27H56	000593-49-7	91
3			Tetracosane	338	C24H50	000646-31-1	91
4			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	91
5			Hexacosane	366	C26H54	000630-01-3	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011821\
Data File : BF123007.D
Acq On : 19 Jan 2021 1:47
Operator : JU/CG
Sample : M1157-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

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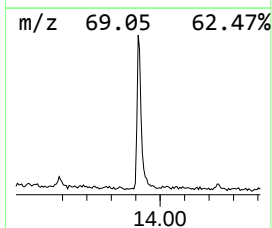
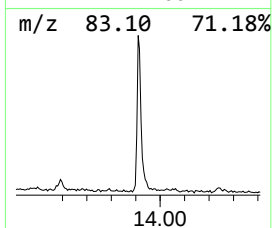
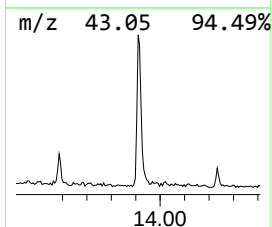
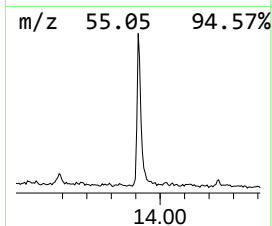
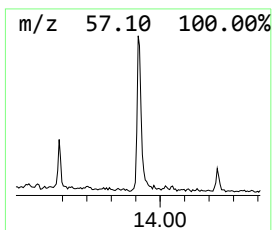
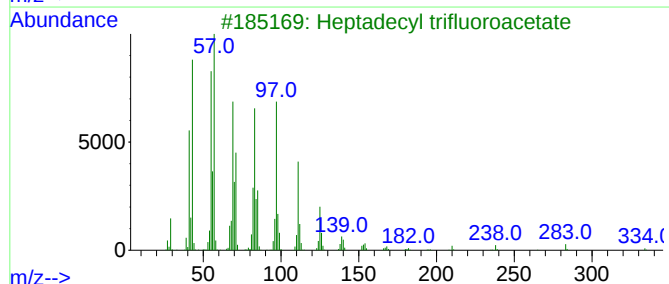
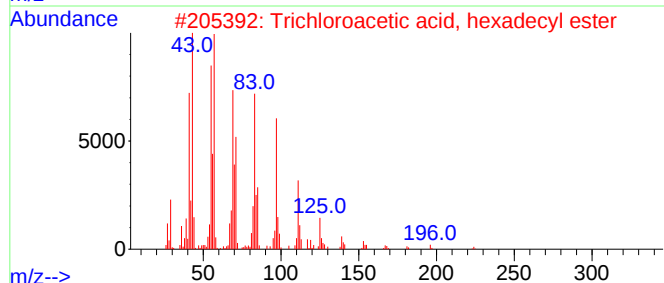
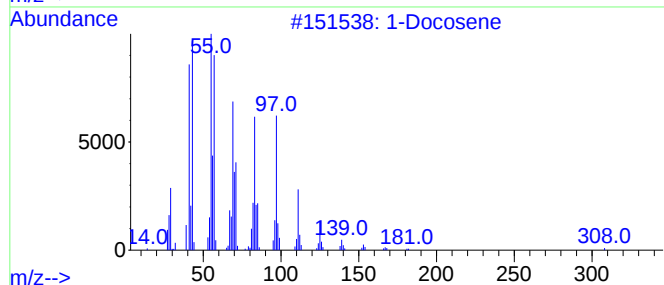
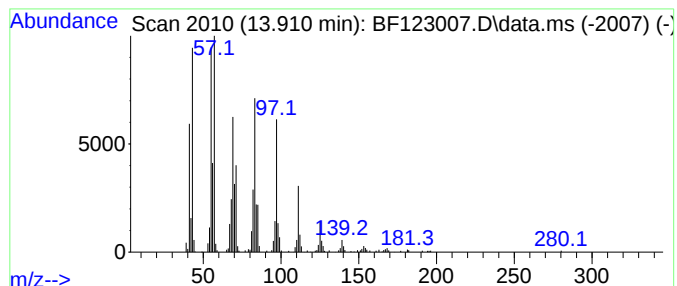
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 1-Docosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.910	8.79 ng	573542	Chrysene-d12	14.063

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene			308	C22H44	001599-67-3	95
2	Trichloroacetic acid, hexadecyl ...			386	C18H33Cl3O2	074339-54-1	94
3	Heptadecyl trifluoroacetate			352	C19H35F3O2	1000351-87-0	94
4	Pentafluoropropionic acid, hexadecyl ...			388	C19H33F5O2	006222-07-7	94
5	Heptafluorobutyric acid, hexadecyl ...			438	C20H33F7O2	006385-15-5	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011821\
Data File : BF123007.D
Acq On : 19 Jan 2021 1:47
Operator : JU/CG
Sample : M1157-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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unknown6.716	6.716	4.8	ng	124268	1	6.898	513063	20.0
Thymol	8.722	2.0	ng	86956	2	8.181	855060	20.0
unknown9.369	9.369	12.1	ng	905946	3	9.933	1495370	20.0
Tridecanoic acid	11.945	4.4	ng	264437	4	11.422	1201300	20.0
1-Octadecanol	12.475	3.0	ng	178011	4	11.422	1201300	20.0
Bis(2-ethylhexy...	12.669	2.0	ng	123085	4	11.422	1201300	20.0
Octadecanoic acid	12.733	3.8	ng	226036	4	11.422	1201300	20.0
Octacosane	13.245	2.1	ng	140341	5	14.063	1305540	20.0
1-Docosene	13.910	8.8	ng	573542	5	14.063	1305540	20.0