

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110320\
 Data File : BF122246.D
 Acq On : 3 Nov 2020 18:03
 Operator : JU/CG
 Sample : L4607-05
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-01

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-BF101220.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF122246.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.345	551	554	588	rBV	447160	1006491	35.57%	5.776%
2	6.381	727	730	754	rBV	288119	711598	25.15%	4.083%
3	6.710	783	786	797	rVB	485070	491536	17.37%	2.821%
4	7.281	880	883	906	rBV	1542371	1707348	60.33%	9.798%
5	7.992	1001	1004	1023	rBV	614205	639822	22.61%	3.672%
6	9.069	1182	1187	1198	rBV	2668306	2829959	100.00%	16.240%
7	9.186	1203	1207	1223	rVB	433161	486668	17.20%	2.793%
8	9.469	1252	1255	1262	rBV	97754	109853	3.88%	0.630%
9	9.745	1298	1302	1316	rBV	725158	726874	25.68%	4.171%
10	10.333	1398	1402	1416	rBV	167578	312399	11.04%	1.793%
11	10.539	1433	1437	1452	rBV	1698403	1902779	67.24%	10.919%
12	11.233	1552	1555	1565	rBV	733157	723517	25.57%	4.152%
13	11.422	1583	1587	1594	rBV	30753	63964	2.26%	0.367%
14	11.769	1641	1646	1665	rBV	328774	458709	16.21%	2.632%
15	12.304	1732	1737	1748	rBV2	104302	216895	7.66%	1.245%
16	12.469	1761	1765	1768	rBV2	132980	115221	4.07%	0.661%
17	12.545	1775	1778	1788	rBV	84866	114374	4.04%	0.656%
18	12.816	1820	1824	1827	rBV	2865429	2560171	90.47%	14.691%
19	13.051	1858	1864	1873	rBV3	57163	144056	5.09%	0.827%
20	13.374	1916	1919	1922	rBV	42751	36883	1.30%	0.212%
21	13.704	1972	1975	1976	rBV	40002	32426	1.15%	0.186%
22	13.727	1976	1979	1991	rVV	180400	394895	13.95%	2.266%
23	13.839	1995	1998	2002	rVV	246933	210274	7.43%	1.207%
24	13.880	2002	2005	2014	rVV	487066	551946	19.50%	3.167%
25	14.021	2026	2029	2032	rVB	38938	32330	1.14%	0.186%
26	14.321	2077	2080	2085	rBV	43837	49157	1.74%	0.282%
27	14.621	2127	2131	2140	rBV2	49553	82881	2.93%	0.476%
28	14.939	2180	2185	2193	rBV2	46519	69342	2.45%	0.398%
29	15.286	2241	2244	2247	rBV3	29701	43174	1.53%	0.248%
30	15.321	2247	2250	2261	rVB	369117	524442	18.53%	3.009%
31	15.692	2310	2313	2317	rVB	25418	32054	1.13%	0.184%
32	16.392	2427	2432	2438	rVB4	22958	44310	1.57%	0.254%

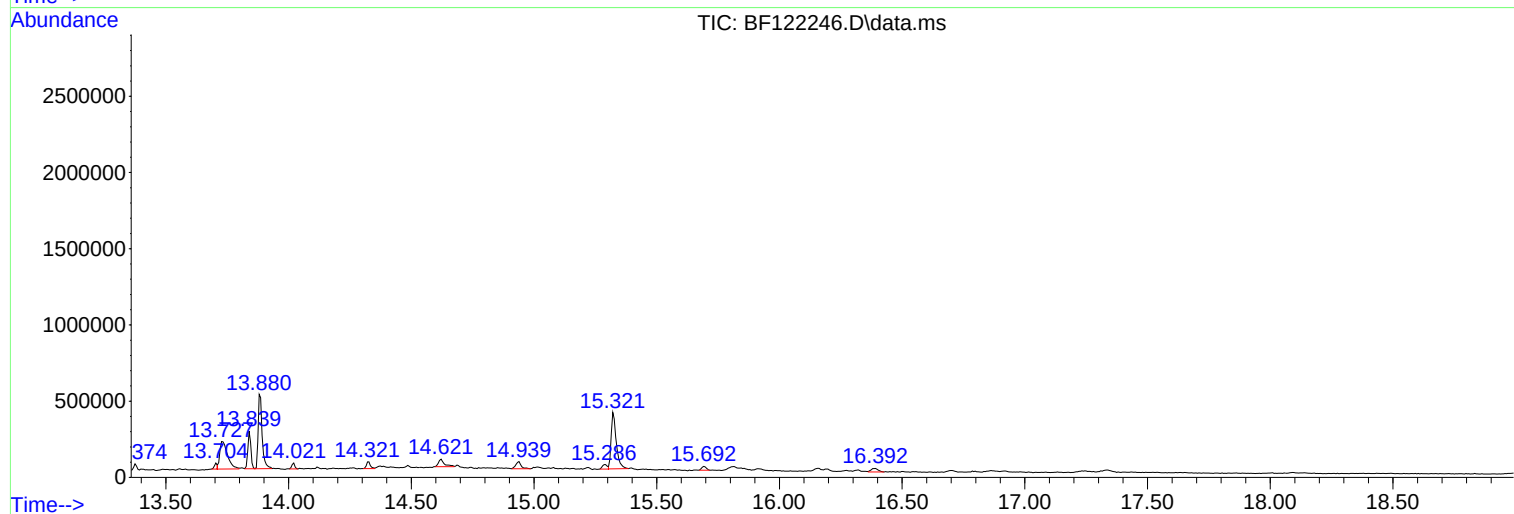
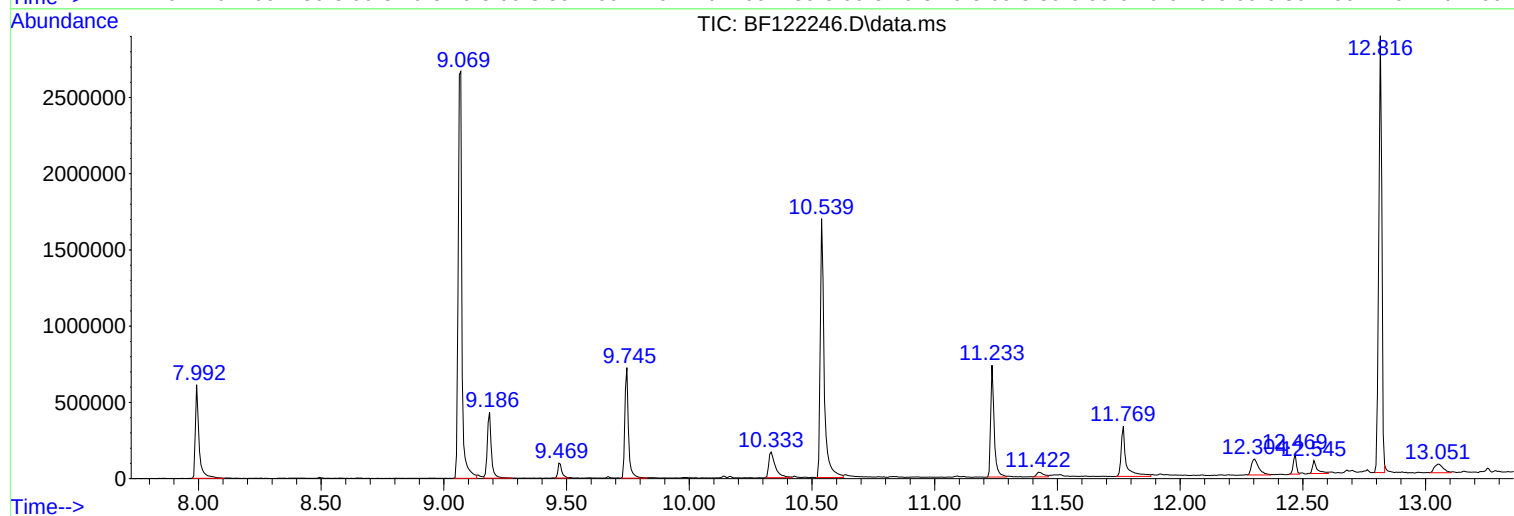
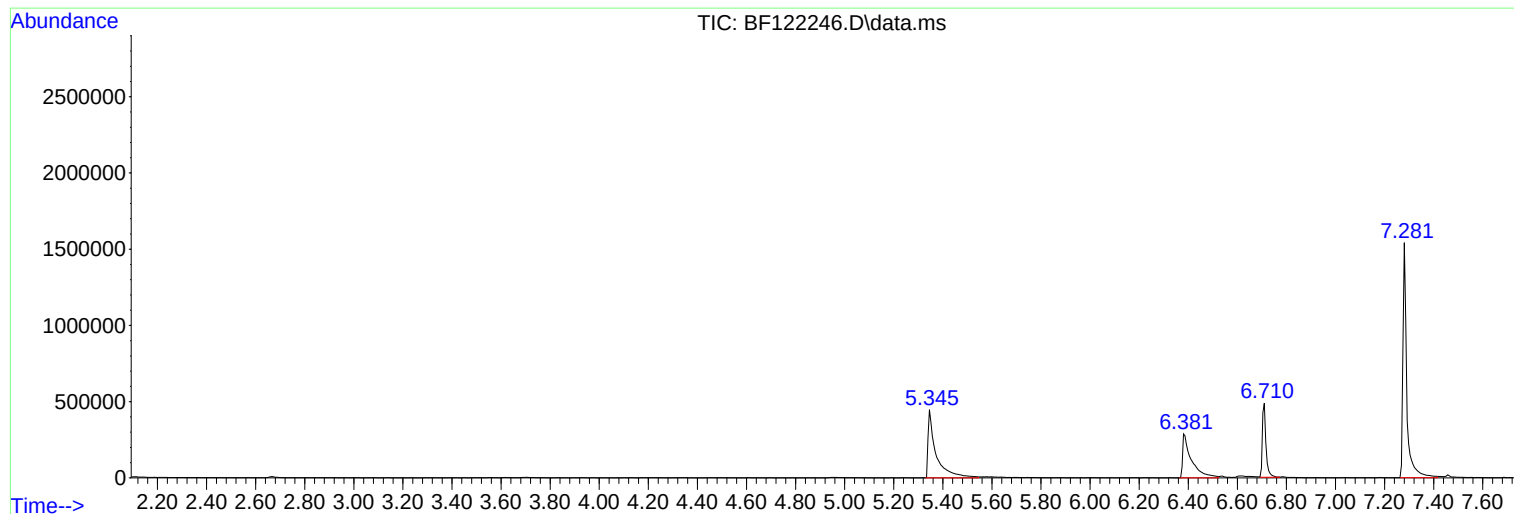
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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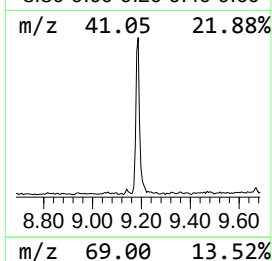
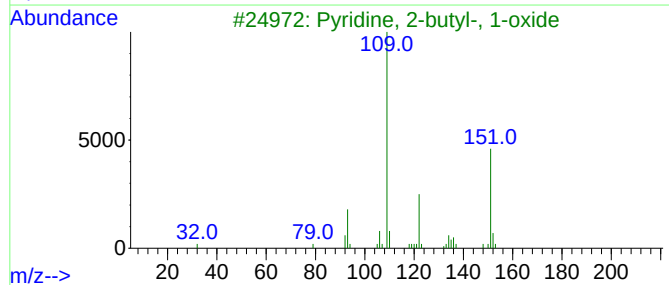
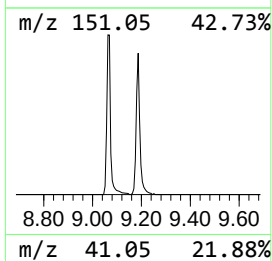
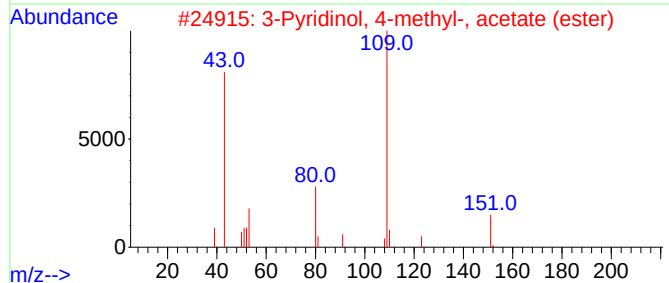
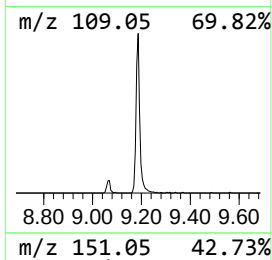
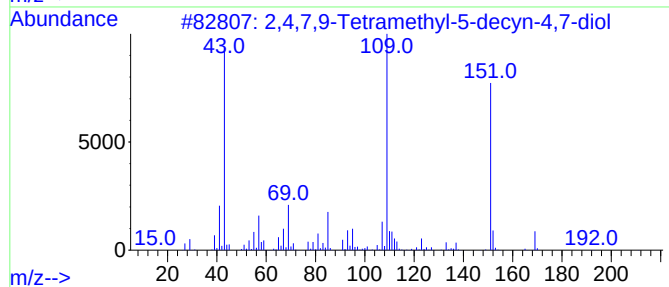
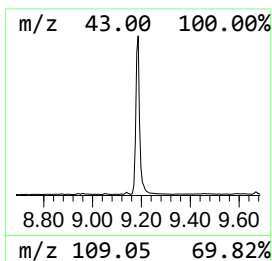
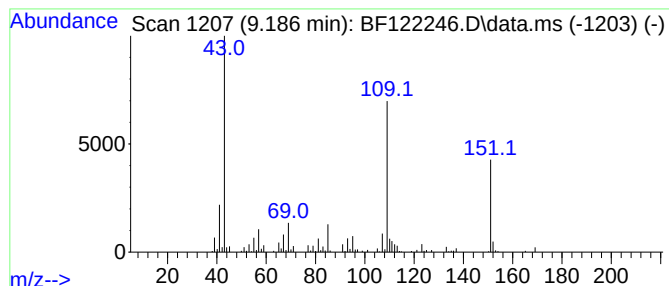
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Peak Number 1 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD			R.T.
9.186	13.39 ng	486668	Acenaphthene-d10			9.745
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...		226	C14H26O2	000126-86-3	91
2	3-Pyridinol, 4-methyl-, acetate ...		151	C8H9NO2	001006-96-8	53
3	Pyridine, 2-butyl-, 1-oxide		151	C9H13NO	031396-32-4	53
4	Metacetamol		151	C8H9NO2	000621-42-1	53
5	Cyclohexanol, 3,3,5-trimethyl-		142	C9H18O	000116-02-9	35



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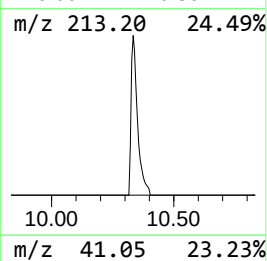
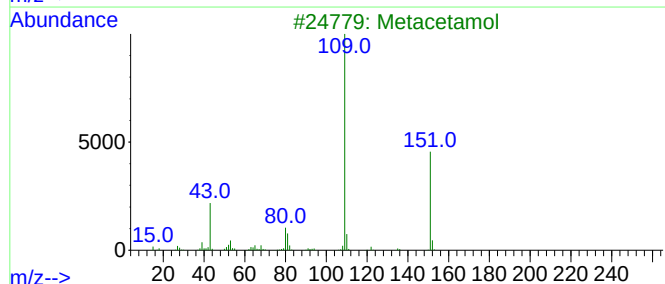
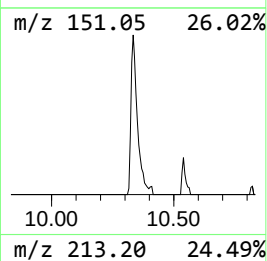
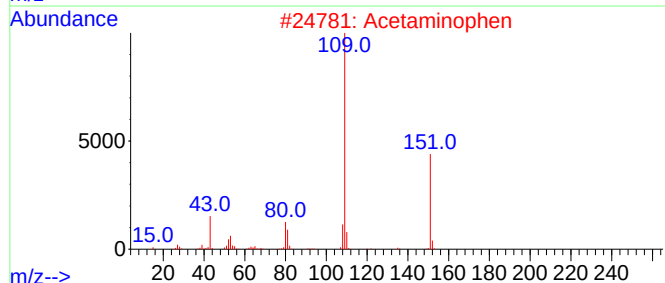
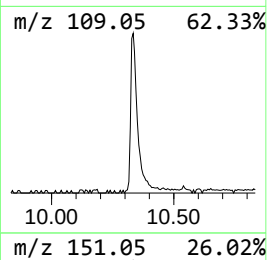
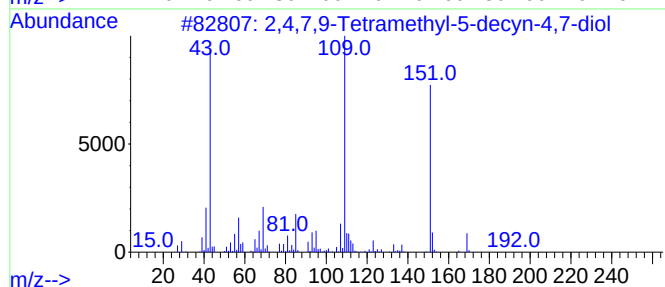
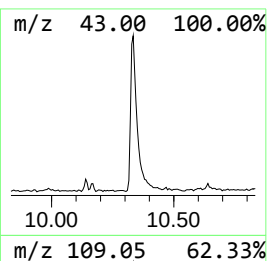
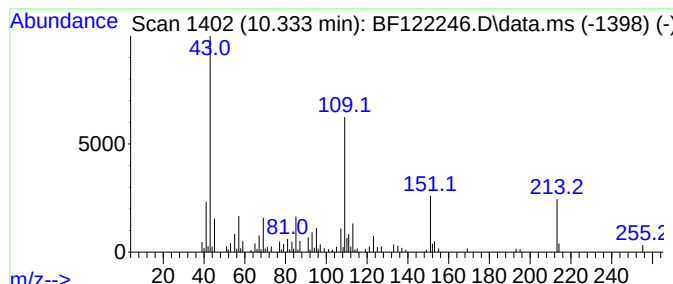
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown10.333 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.333	8.60 ng	312399	Acenaphthene-d10	9.745

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	53
2			Acetaminophen	151	C8H9NO2	000103-90-2	38
3			Metacetamol	151	C8H9NO2	000621-42-1	38
4			2-Propenal, 3-(2,2,6-trimethyl-7...	194	C12H18O2	055759-91-6	38
5			Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	38



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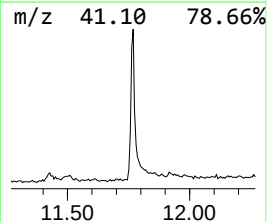
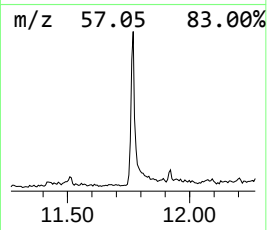
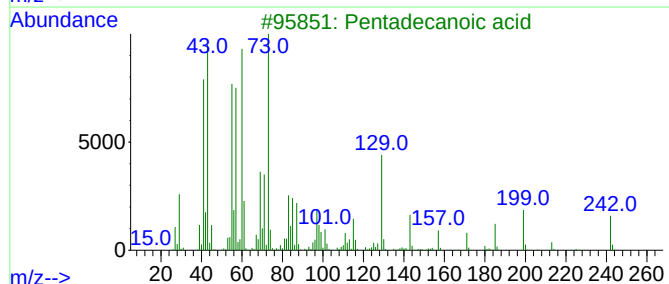
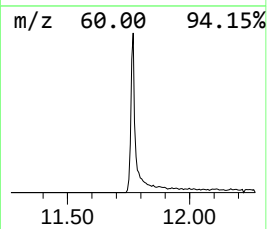
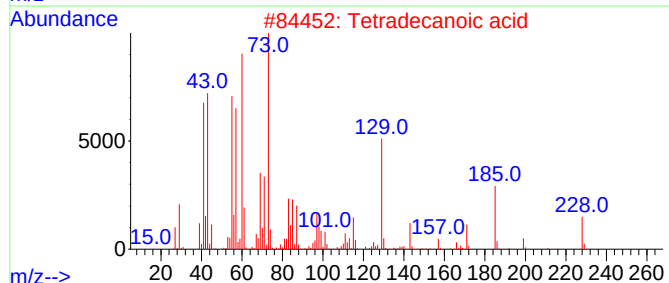
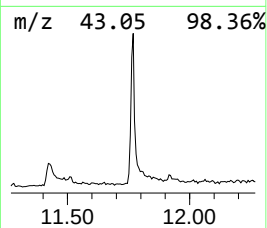
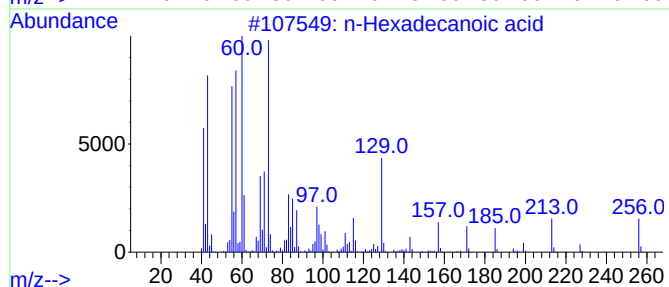
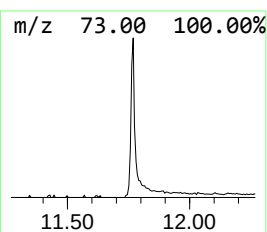
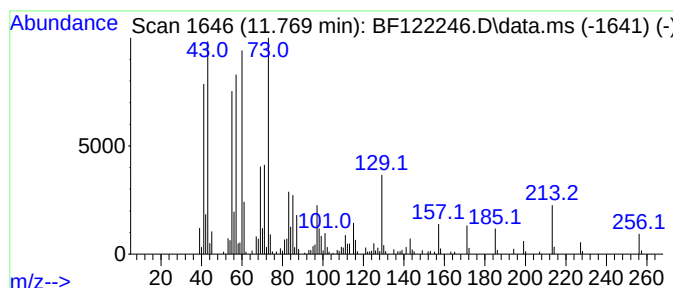
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.769	12.68 ng	458709	Phenanthrene-d10	11.233

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	95
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4			Tridecanoic acid	214	C13H26O2	000638-53-9	70
5			Undecanoic acid	186	C11H22O2	000112-37-8	68



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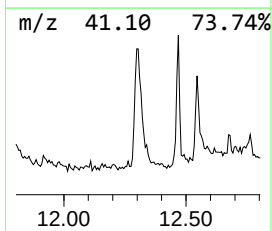
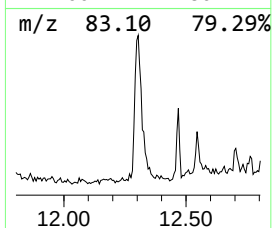
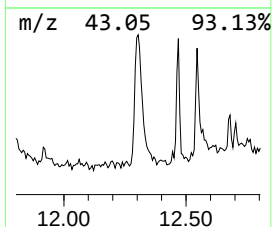
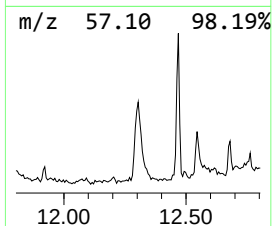
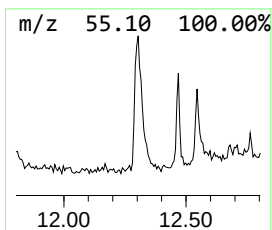
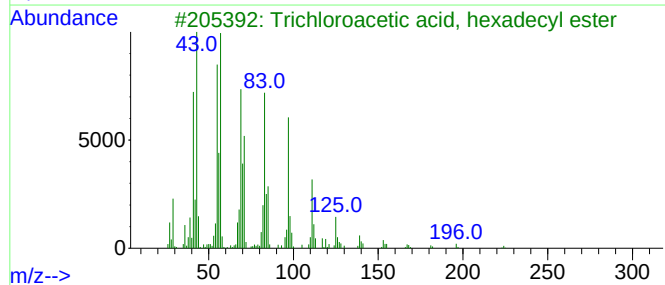
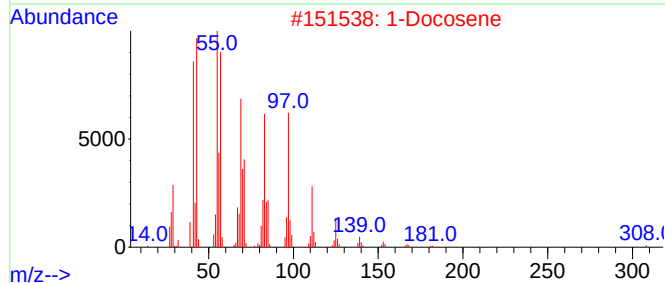
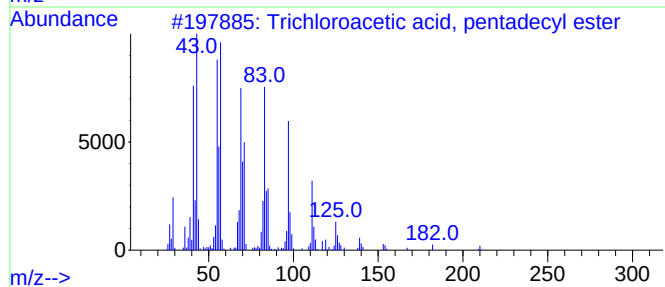
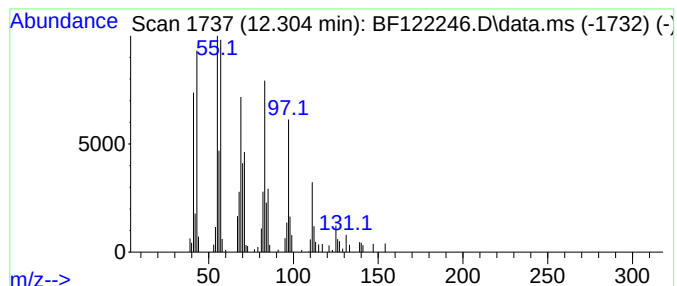
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Peak Number 4 Trichloroacetic acid, penta... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.304	6.00 ng	216895	Phenanthrene-d10	11.233

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	95
2			1-Docosene	308	C22H44	001599-67-3	95
3			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
4			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
5			5-Eicosene, (E)-	280	C20H40	074685-30-6	91



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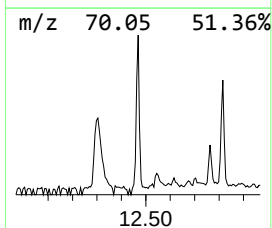
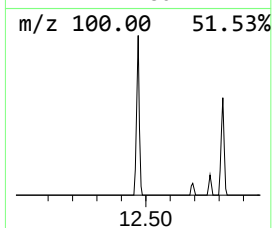
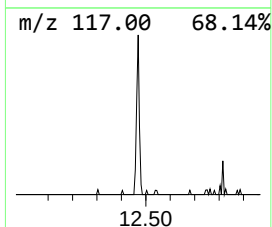
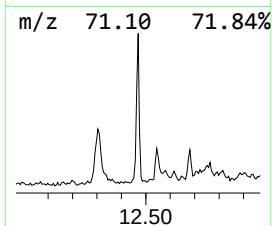
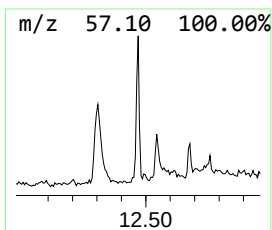
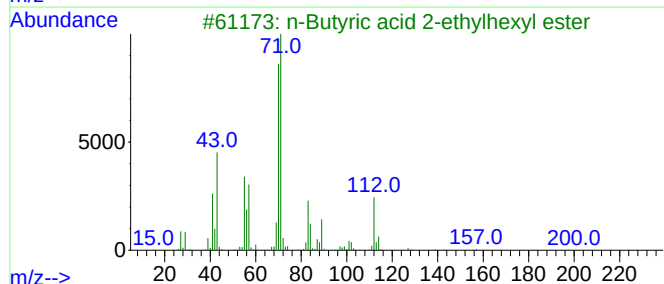
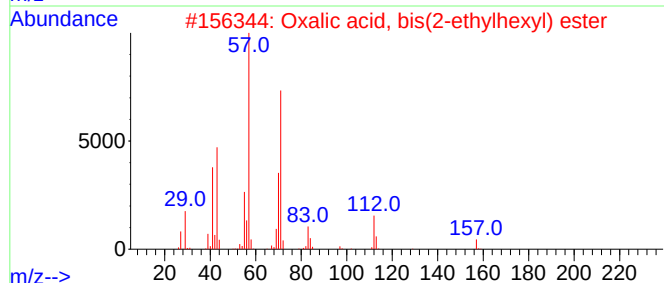
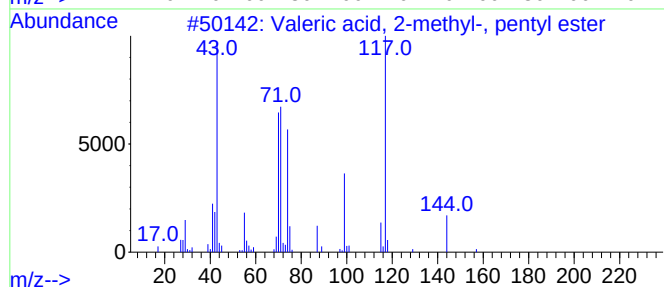
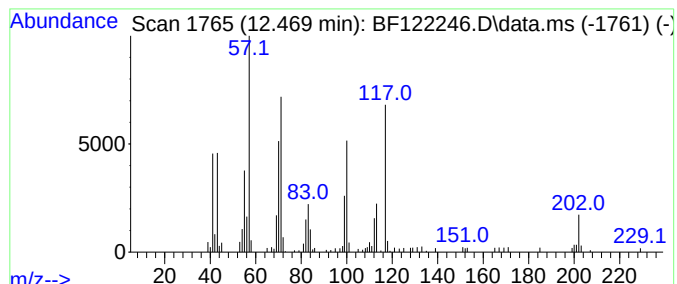
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Peak Number 5 unknown12.469 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.469	3.19 ng	115221	Phenanthrene-d10	11.233

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Valeric acid, 2-methyl-, pentyl ...	186	C11H22O2	006297-48-9	43
2			Oxalic acid, bis(2-ethylhexyl) e...	314	C18H34O4	1000309-39-0	38
3			n-Butyric acid 2-ethylhexyl ester	200	C12H24O2	025415-84-3	35
4			Carbonic acid, isobutyl 2-ethylh...	230	C13H26O3	1000357-82-9	27
5			2-Ethyl-1-hexanol, pentafluoropr...	276	C11H17F5O2	1000365-51-1	25



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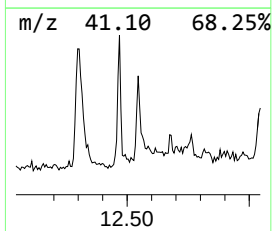
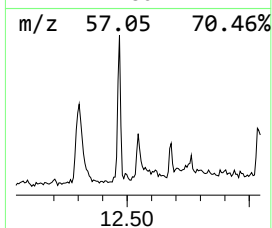
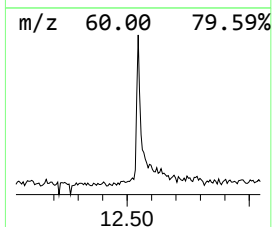
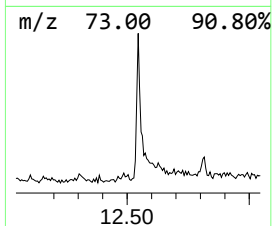
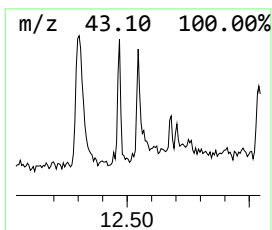
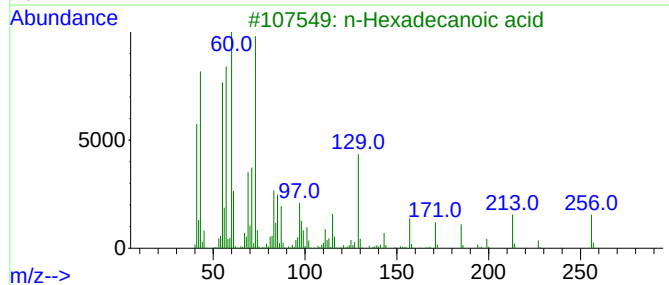
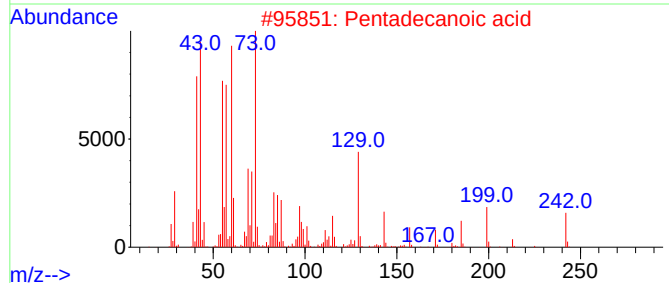
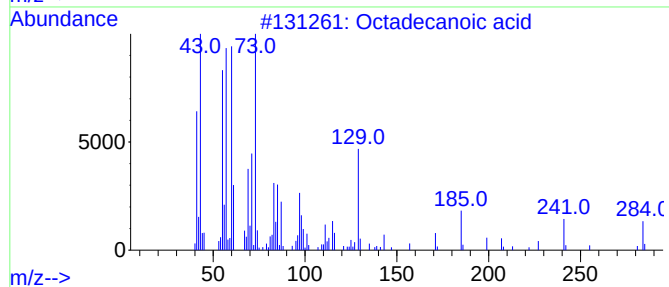
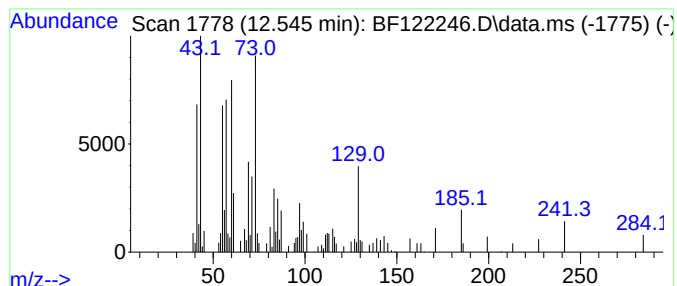
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.545	3.16 ng	114374	Phenanthrene-d10	11.233

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	97
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5			Tridecanoic acid	214	C13H26O2	000638-53-9	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110320\
Data File : BF122246.D
Acq On : 3 Nov 2020 18:03
Operator : JU/CG
Sample : L4607-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-01

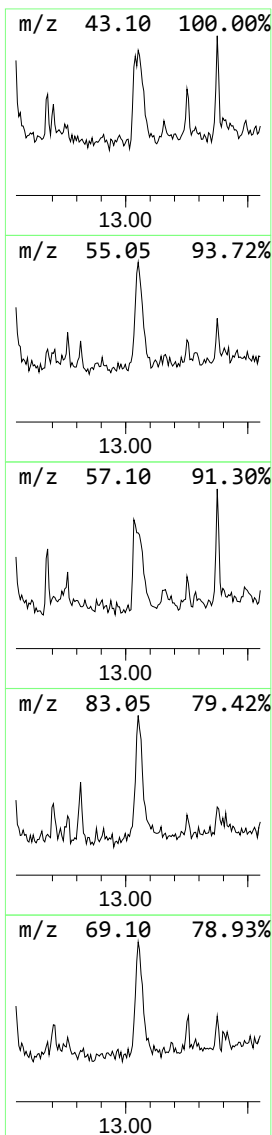
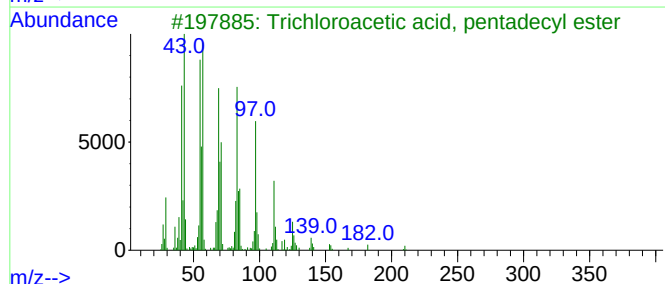
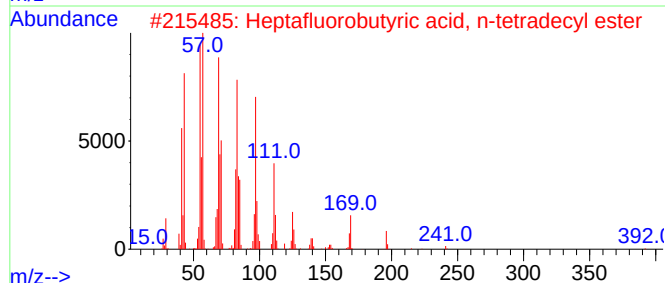
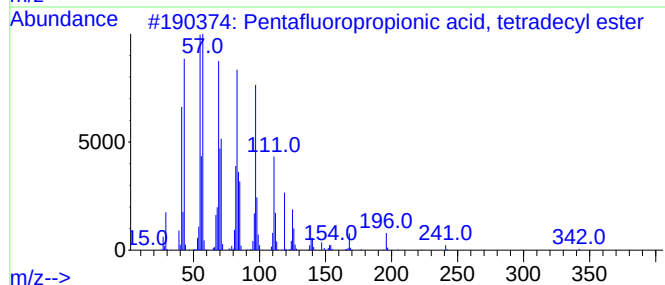
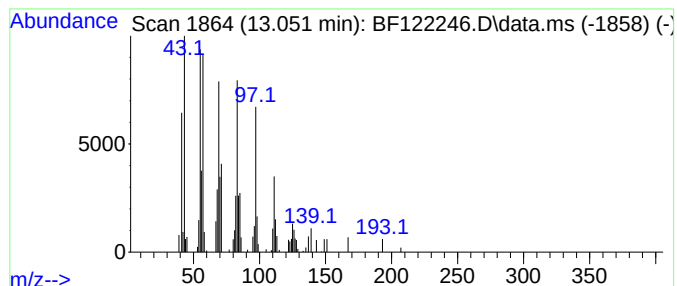
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Pentafluoropropionic acid, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.051	5.22 ng	144056	Chrysene-d12	13.880

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	95
2			Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	95
3			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
4			11-Tricosene	322	C23H46	052078-56-5	91
5			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110320\
Data File : BF122246.D
Acq On : 3 Nov 2020 18:03
Operator : JU/CG
Sample : L4607-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-01

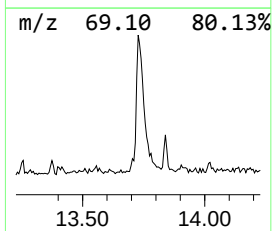
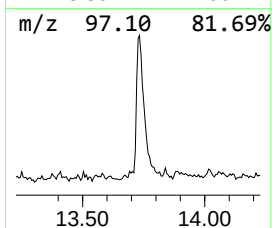
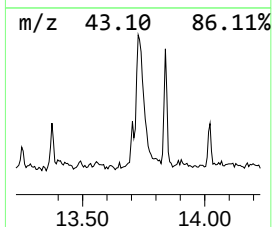
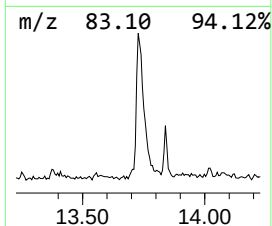
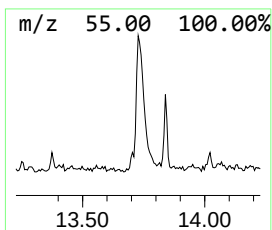
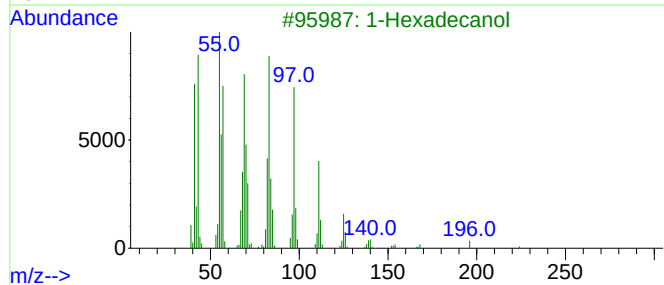
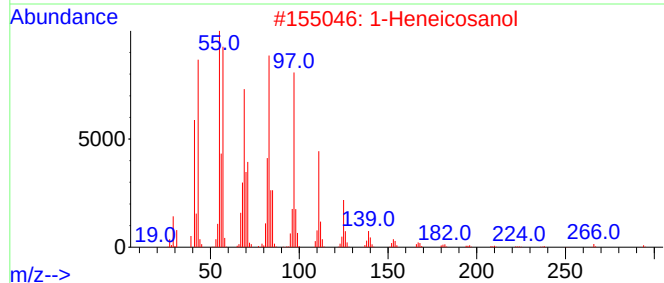
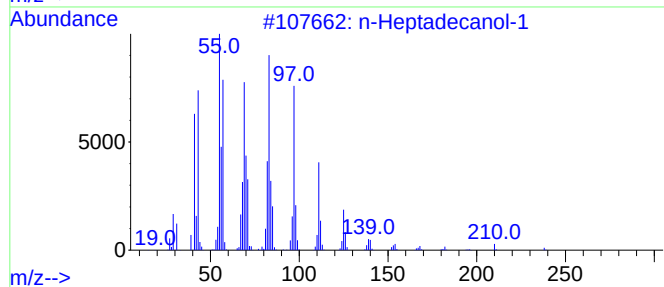
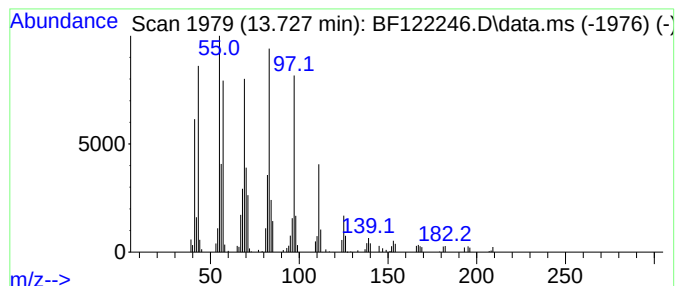
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 n-Heptadecanol-1 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.727	14.31 ng	394895	Chrysene-d12	13.880

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Heptadecanol-1	256	C17H36O	001454-85-9	93
2			1-Heneicosanol	312	C21H44O	015594-90-8	91
3			1-Hexadecanol	242	C16H34O	036653-82-4	91
4			n-Tetracosanol-1	354	C24H50O	000506-51-4	91
5			Behenic alcohol	326	C22H46O	000661-19-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110320\
Data File : BF122246.D
Acq On : 3 Nov 2020 18:03
Operator : JU/CG
Sample : L4607-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-01

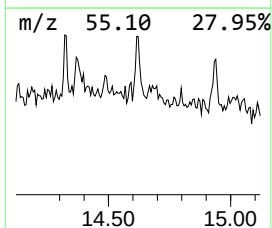
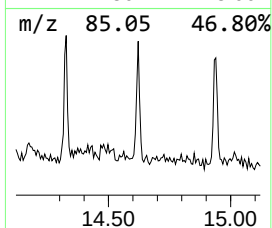
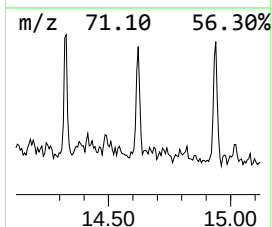
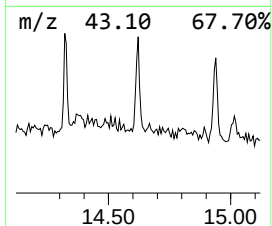
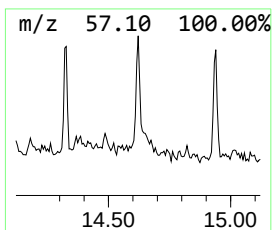
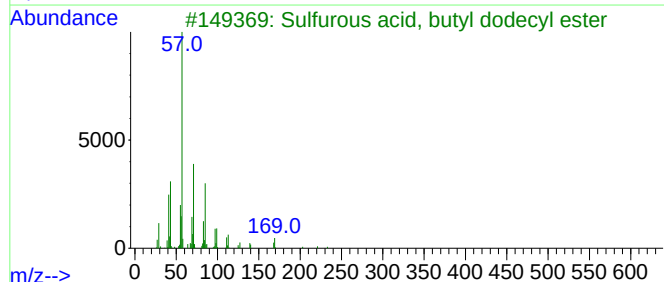
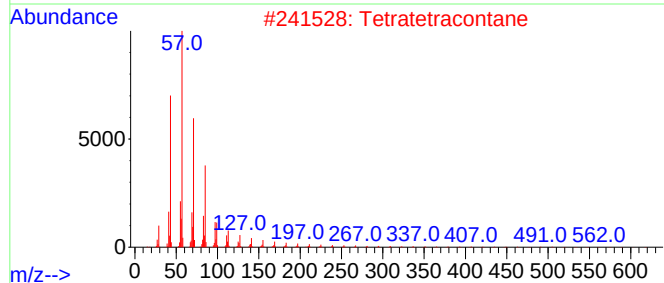
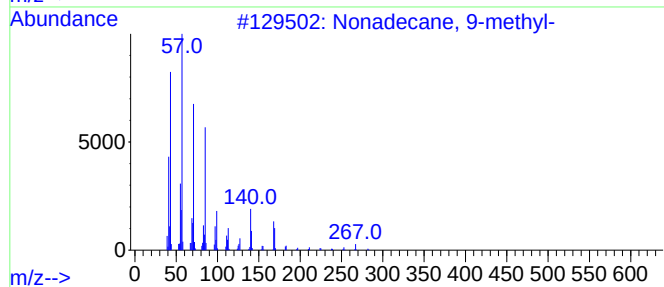
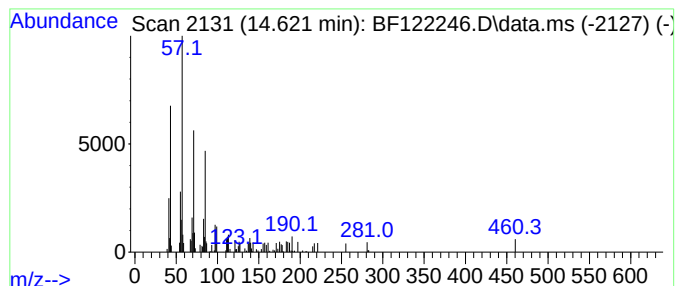
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Nonadecane, 9-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.621	3.16 ng	82881	Perylene-d12	15.321

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane, 9-methyl-	282	C20H42	013287-24-6	89
2			Tetratetracontane	619	C44H90	007098-22-8	74
3			Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	74
4			Octacosane	394	C28H58	000630-02-4	74
5			Sulfurous acid, butyl decyl ester	278	C14H30O3S	1000309-17-7	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110320\
Data File : BF122246.D
Acq On : 3 Nov 2020 18:03
Operator : JU/CG
Sample : L4607-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-01

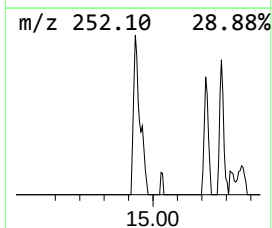
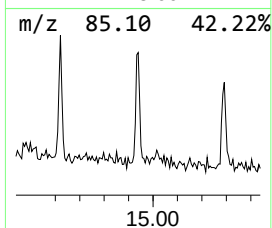
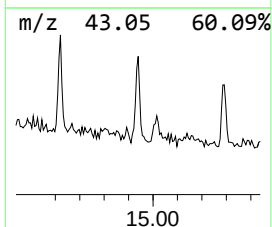
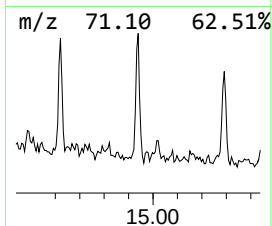
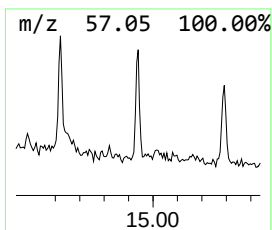
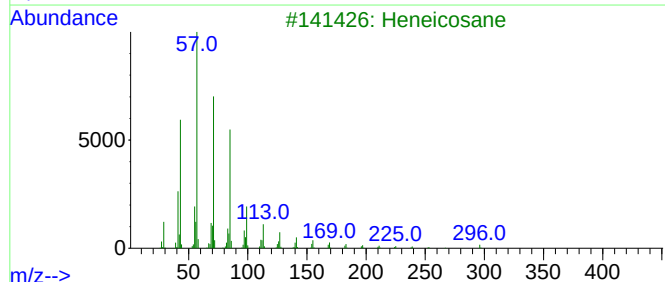
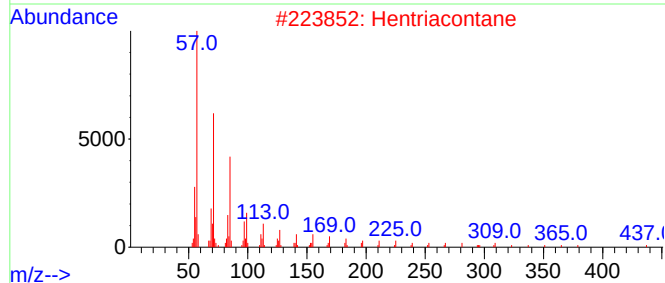
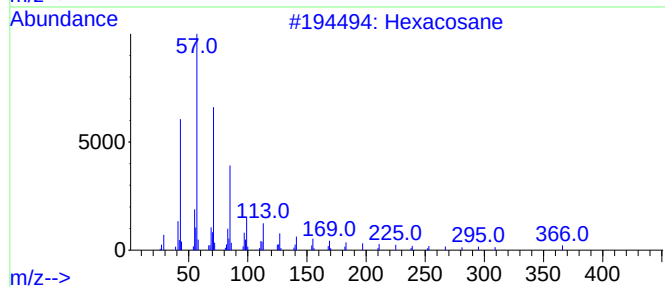
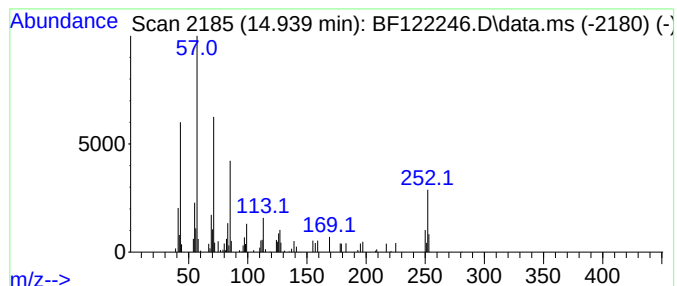
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hexacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.939	2.64 ng	69342	Perylene-d12	15.321

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexacosane	366	C26H54	000630-01-3	68
2		Hentriacontane	437	C31H64	000630-04-6	68
3		Heneicosane	296	C21H44	000629-94-7	68
4		Tetracosane	338	C24H50	000646-31-1	59
5		Tridecane, 1-iodo-	310	C13H27I	035599-77-0	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110320\
Data File : BF122246.D
Acq On : 3 Nov 2020 18:03
Operator : JU/CG
Sample : L4607-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.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
2,4,7,9-Tetrame...	9.186	13.4	ng	486668	3	9.745	726874	20.0
unknown10.333	10.333	8.6	ng	312399	3	9.745	726874	20.0
n-Hexadecanoic ...	11.769	12.7	ng	458709	4	11.233	723517	20.0
Trichloroacetic...	12.304	6.0	ng	216895	4	11.233	723517	20.0
unknown12.469	12.469	3.2	ng	115221	4	11.233	723517	20.0
Octadecanoic acid	12.545	3.2	ng	114374	4	11.233	723517	20.0
Pentafluoroprop...	13.051	5.2	ng	144056	5	13.880	551946	20.0
n-Heptadecanol-1	13.727	14.3	ng	394895	5	13.880	551946	20.0
Nonadecane, 9-m...	14.621	3.2	ng	82881	6	15.321	524442	20.0
Hexacosane	14.939	2.6	ng	69342	6	15.321	524442	20.0