

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF033120\
 Data File : BF119656.D
 Acq On : 31 Mar 2020 17:14
 Operator : MA/SJ
 Sample : L2042-02
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-02-1.0-1.5

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

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-BF031820.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.210	17	21	30	rVB2	101762	154597	1.93%	0.239%
2	5.045	490	503	510	rBV2	137642	262890	3.28%	0.407%
3	5.445	563	571	574	rBV	7344714	7387380	92.18%	11.440%
4	6.457	737	743	746	rBV	6232206	7194387	89.78%	11.141%
5	6.828	802	806	812	rVB	2310754	1849557	23.08%	2.864%
6	6.987	829	833	836	rBV	6771458	5879372	73.37%	9.105%
7	7.392	892	902	905	rBV	4965679	4848610	60.50%	7.509%
8	8.116	1020	1025	1028	rBV	2696671	2343564	29.24%	3.629%
9	9.198	1203	1209	1212	rBV	9170173	8013736	100.00%	12.410%
10	9.586	1272	1275	1279	rVB	905280	697902	8.71%	1.081%
11	9.875	1317	1324	1328	rBV	2961949	2519737	31.44%	3.902%
12	10.669	1454	1459	1462	rBV	4486026	4364072	54.46%	6.758%
13	10.880	1492	1495	1498	rVB2	81967	94154	1.17%	0.146%
14	11.027	1517	1520	1524	rVB3	97275	105094	1.31%	0.163%
15	11.069	1524	1527	1529	rBV	91315	87242	1.09%	0.135%
16	11.363	1573	1577	1580	rBV	2525740	2283850	28.50%	3.537%
17	11.386	1580	1581	1584	rVV	462929	297430	3.71%	0.461%
18	11.439	1584	1590	1593	rVB	127343	131989	1.65%	0.204%
19	11.863	1658	1662	1664	rBV2	100311	123640	1.54%	0.191%
20	11.898	1664	1668	1679	rVV	1520812	1505725	18.79%	2.332%
21	12.580	1778	1784	1787	rBV	677330	713700	8.91%	1.105%
22	12.686	1798	1802	1813	rBV2	613153	794758	9.92%	1.231%
23	12.810	1817	1823	1825	rVV	491508	498895	6.23%	0.773%
24	12.957	1844	1848	1851	rBV	6332589	5985261	74.69%	9.269%
25	13.192	1885	1888	1893	rBV2	133074	189130	2.36%	0.293%
26	13.533	1944	1946	1953	rVB	118463	145537	1.82%	0.225%
27	13.868	2000	2003	2010	rBV	812007	1102985	13.76%	1.708%
28	14.010	2022	2027	2030	rBV2	1732562	1783076	22.25%	2.761%
29	14.033	2030	2031	2036	rVB	212817	160847	2.01%	0.249%
30	14.115	2043	2045	2048	rVB2	138340	126201	1.57%	0.195%
31	14.180	2054	2056	2059	rBV	163606	155972	1.95%	0.242%
32	14.486	2106	2108	2111	rBV	255175	244659	3.05%	0.379%
33	14.521	2111	2114	2121	rVV4	164459	298724	3.73%	0.463%
34	14.798	2158	2161	2164	rVB	246163	238016	2.97%	0.369%

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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

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35	15.139	2216	2219	2225	rVB2	296210	357727	4.46%	0.554%
36	15.480	2273	2277	2280	rBV	1040903	1232276	15.38%	1.908%
37	15.957	2355	2358	2367	rVB	266426	401893	5.02%	0.622%

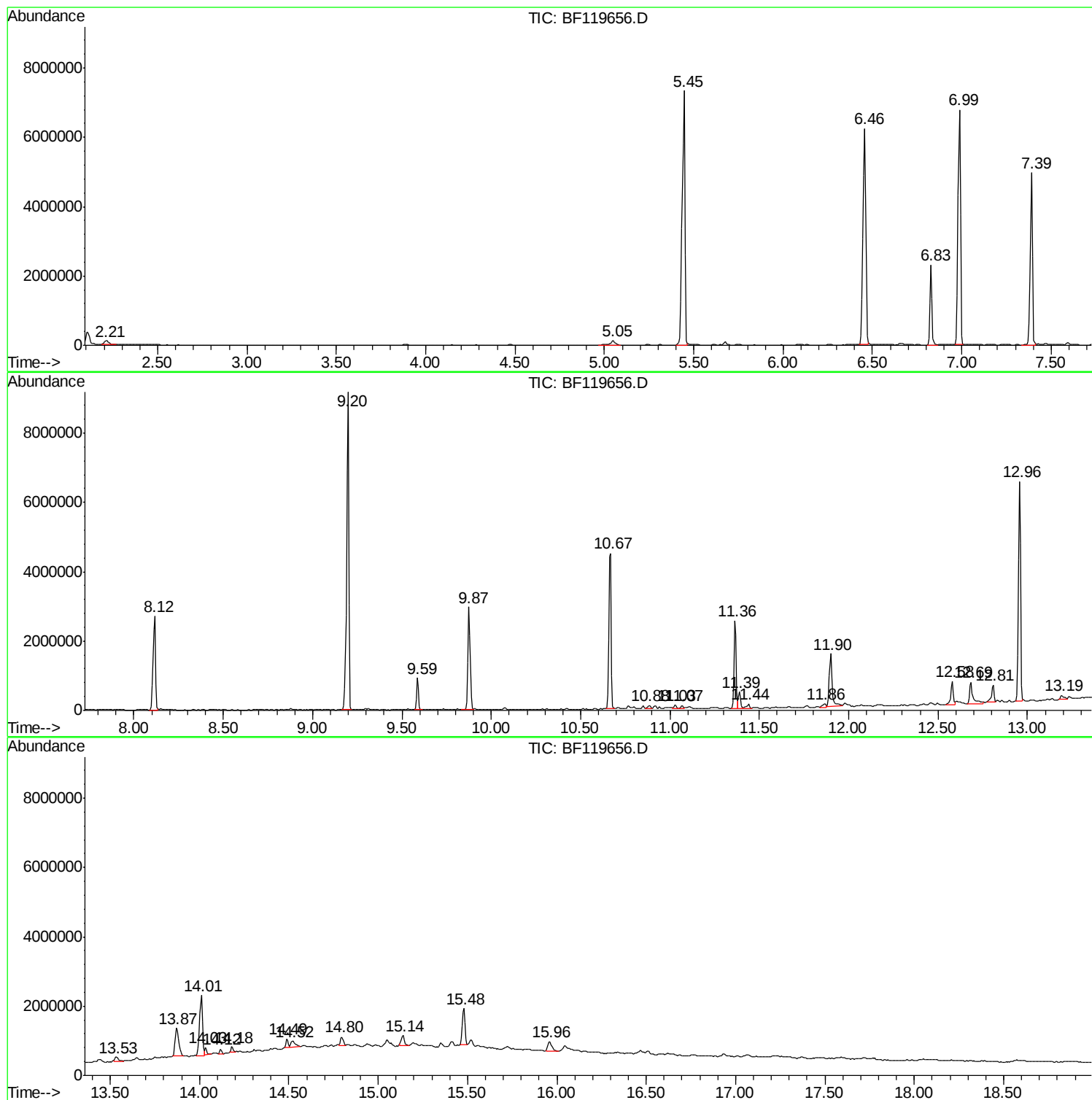
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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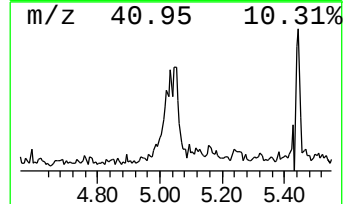
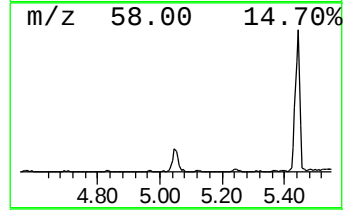
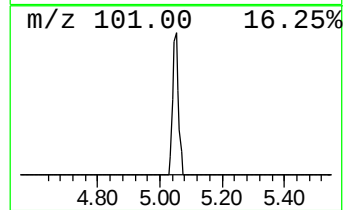
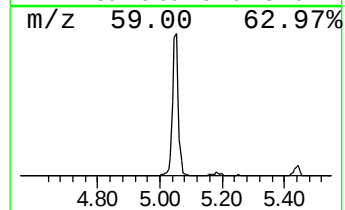
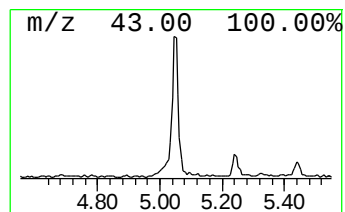
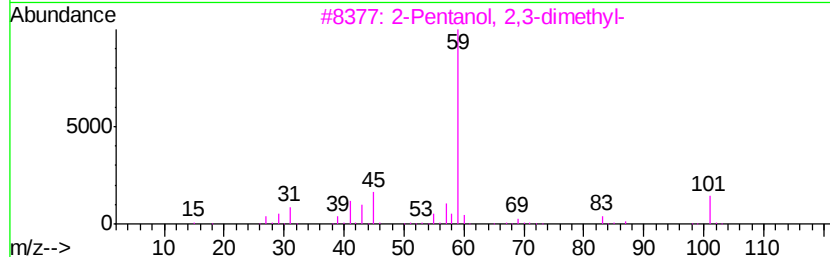
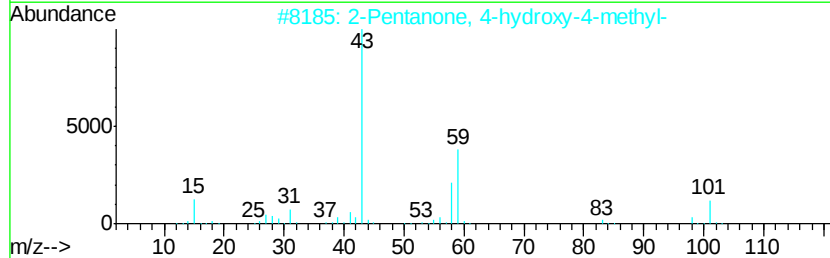
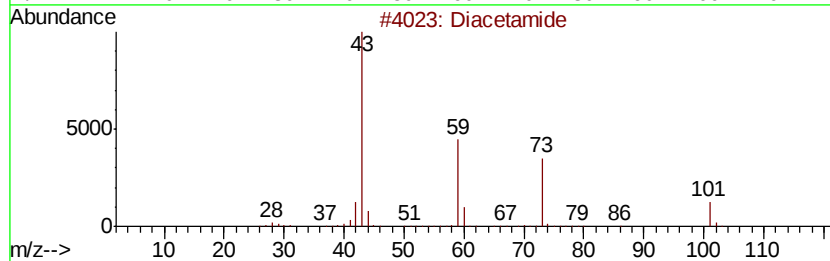
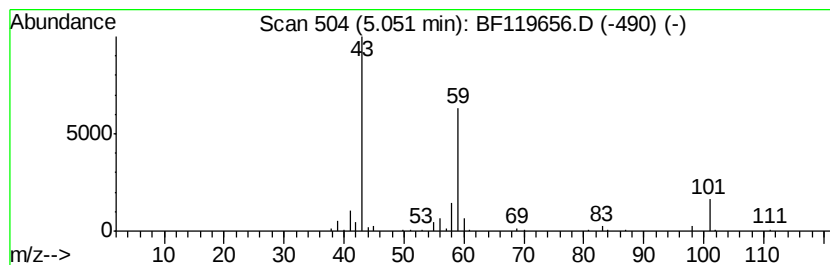
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown5.05 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	2.84 ng	262890	1,4-Dichlorobenzene-d4	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Diacetamide	101	C4H7NO2	000625-77-4	45
2		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
3		2-Pentanol, 2,3-dimethyl-	116	C7H16O	004911-70-0	25
4		1,1-Dimethyl-2-[2-(methoxycarbon...	160	C7H16N2O2	097812-30-1	25
5		1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	10



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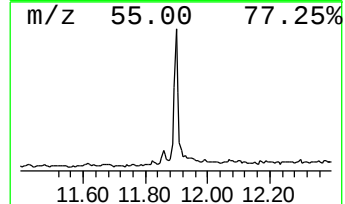
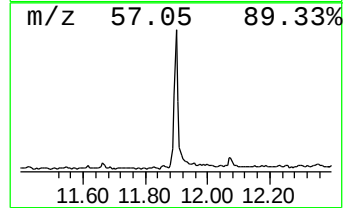
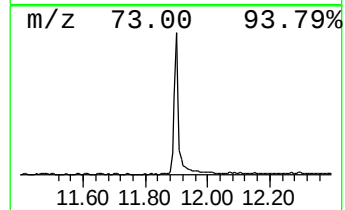
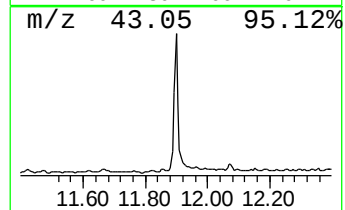
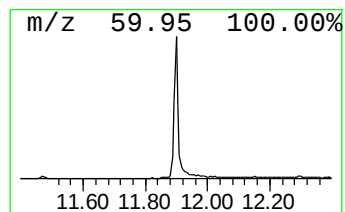
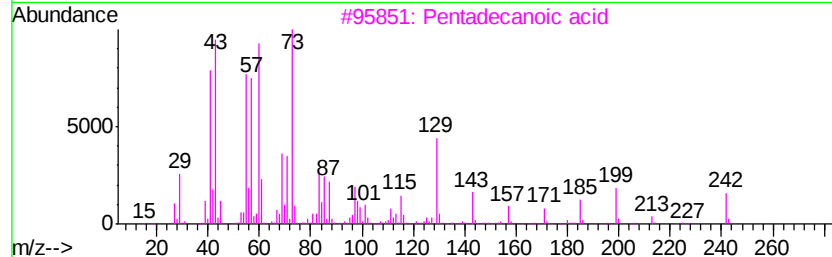
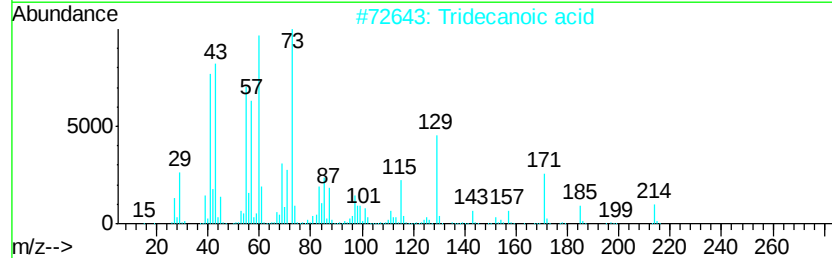
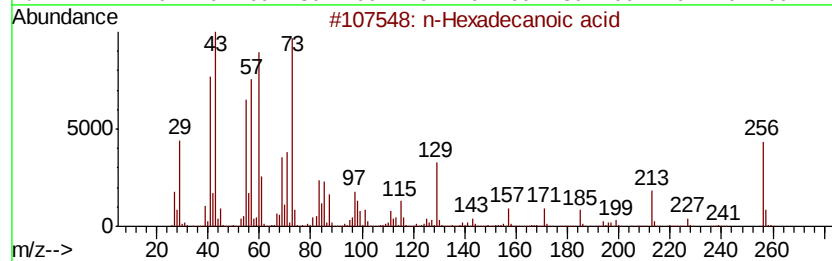
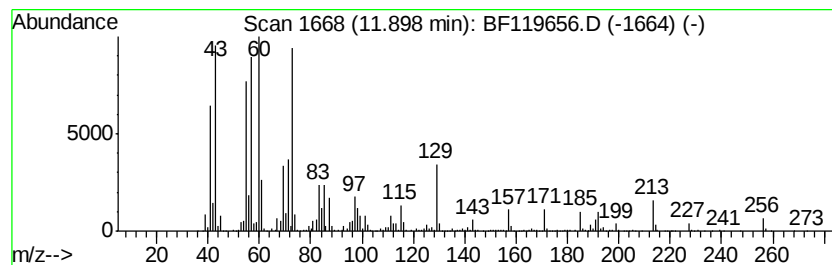
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.90	13.19 ng	1505730	Phenanthrene-d10		11.36	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	98
2	Tridecanoic acid		214	C13H26O2	000638-53-9	94
3	Pentadecanoic acid		242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid		228	C14H28O2	000544-63-8	72
5	n-Decanoic acid		172	C10H20O2	000334-48-5	47



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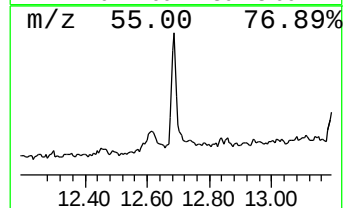
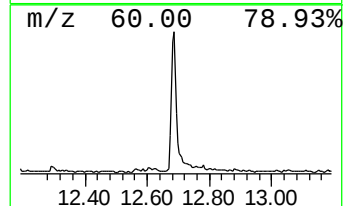
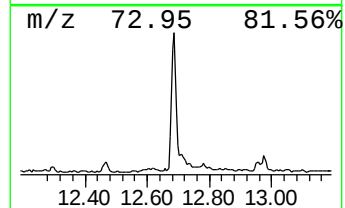
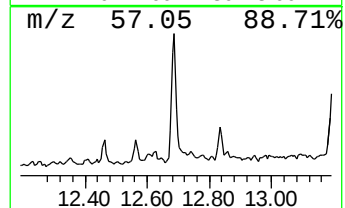
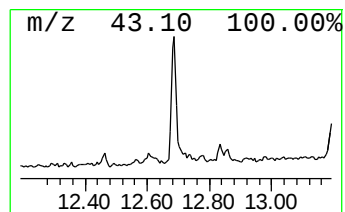
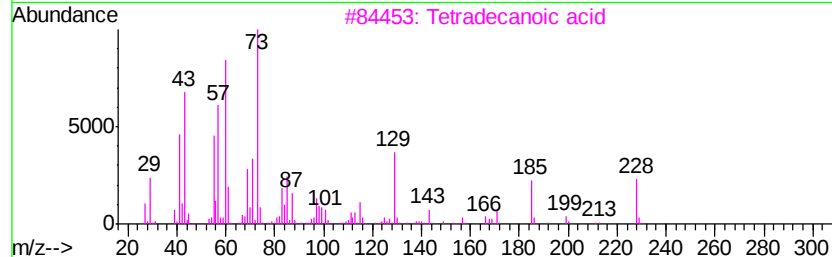
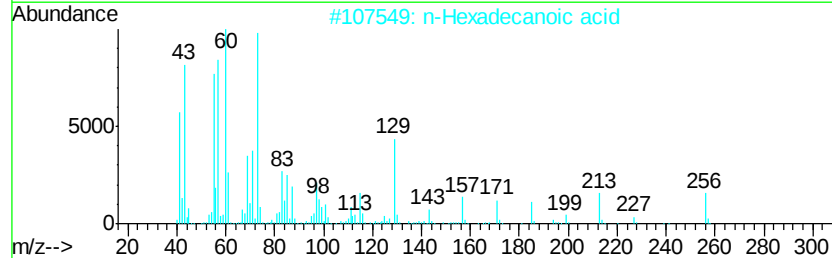
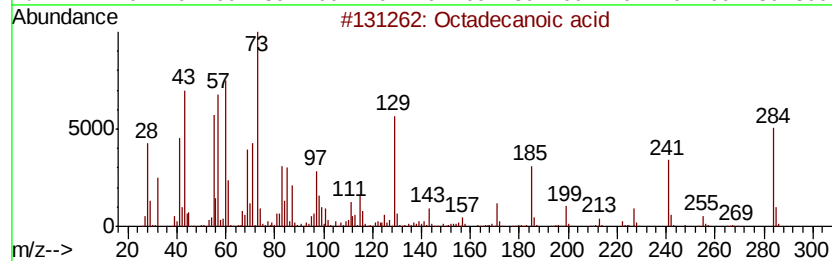
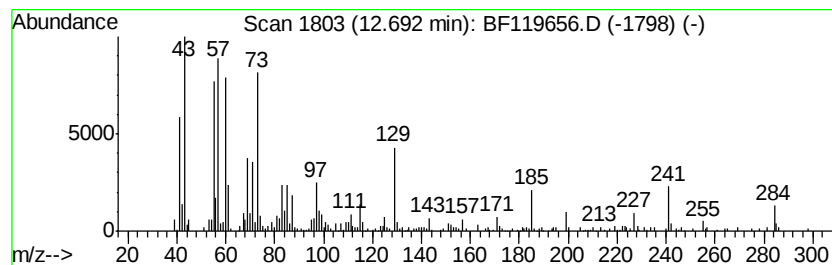
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.69	6.96 ng	794758	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4	Octadecanoic acid, 2-(2-hydroxyve...	372	C22H44O4	000106-11-6	58
5	Tridecanoic acid	214	C13H26O2	000638-53-9	58



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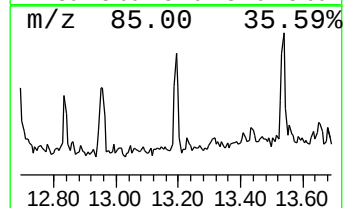
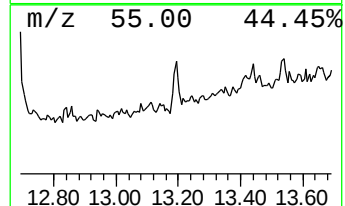
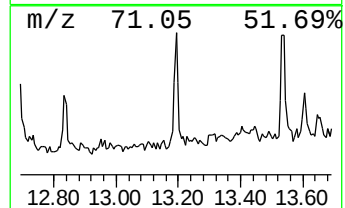
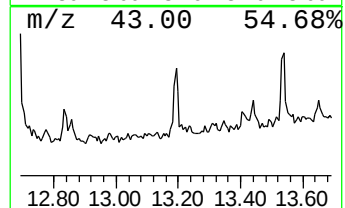
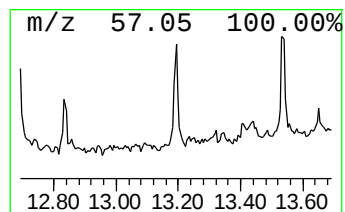
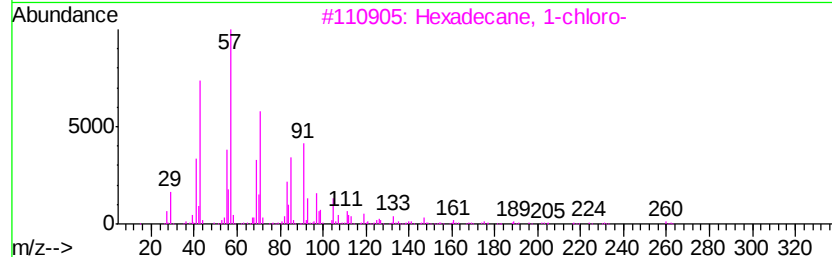
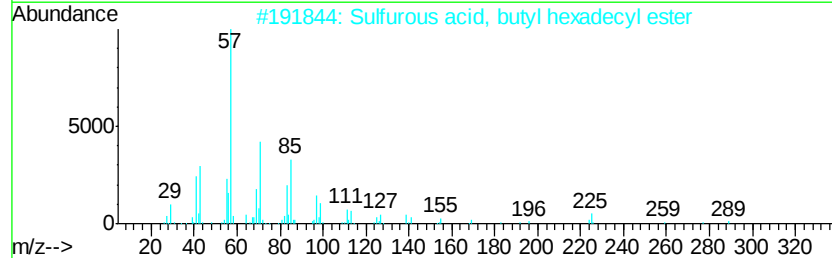
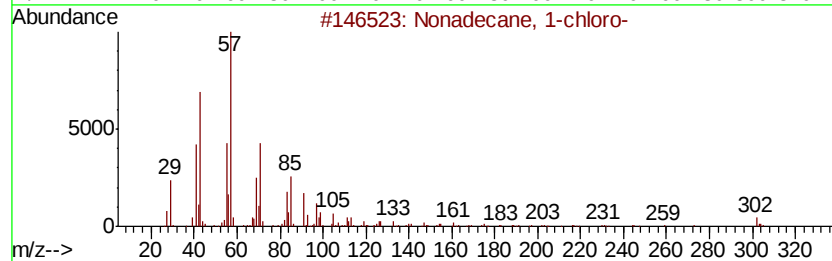
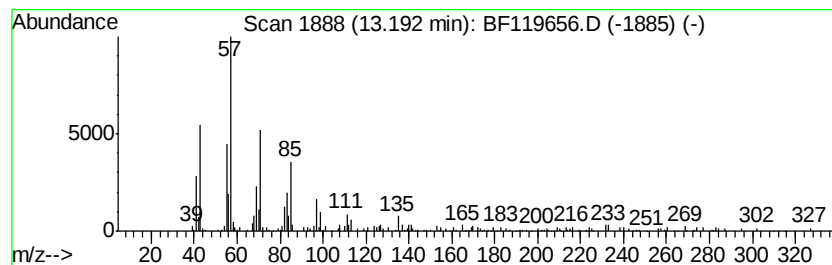
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Nonadecane, 1-chloro- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.19	2.12 ng	189130	Chrysene-d12	14.01
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Nonadecane, 1-chloro-	302 C19H39Cl	062016-76-6 94
2		Sulfurous acid, butyl hexadecyl ...	362 C20H42O3S	1000309-18-3 91
3		Hexadecane, 1-chloro-	260 C16H33Cl	004860-03-1 90
4		1-Chloroeicosane	316 C20H41Cl	042217-02-7 90
5		Heptadecane	240 C17H36	000629-78-7 89



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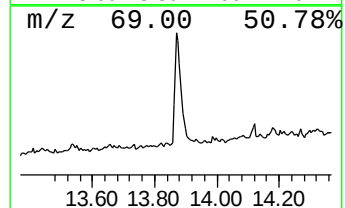
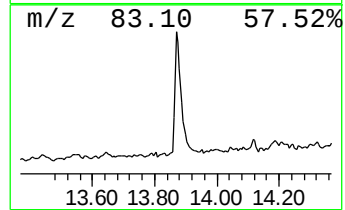
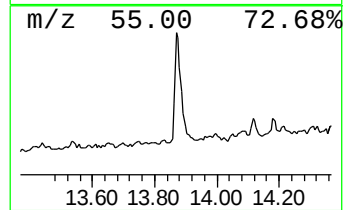
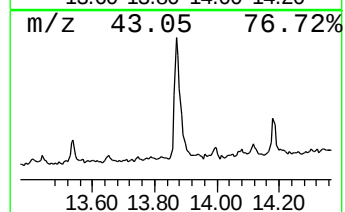
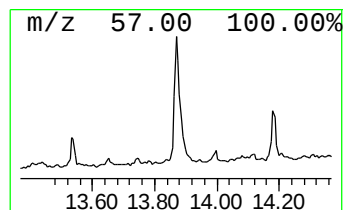
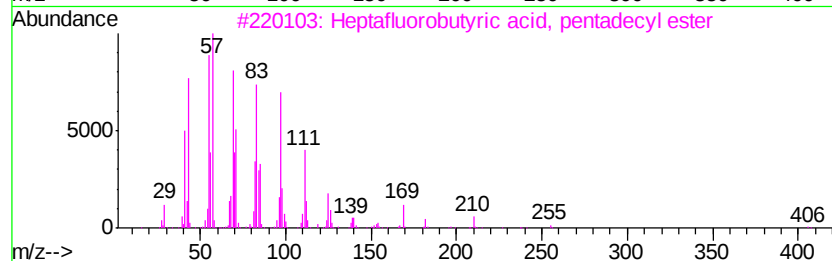
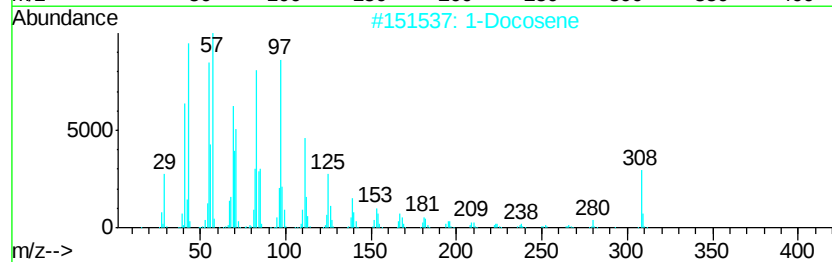
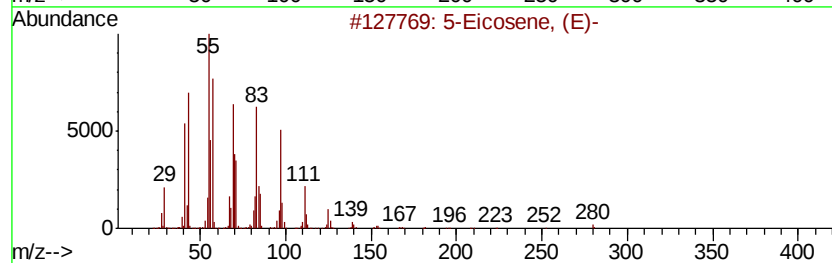
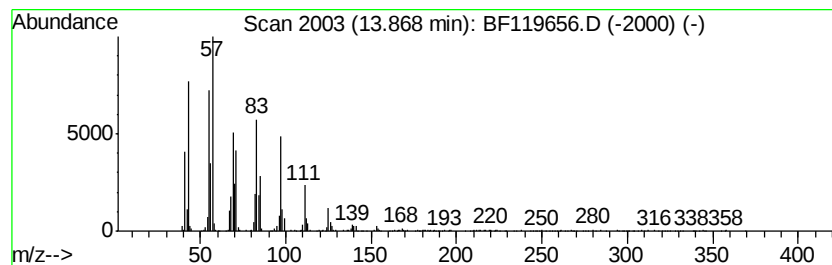
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 TIC Integration Parameters: LSCINT.P

 Peak Number 6 5-Eicosene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.87	12.37 ng	1102990	Chrysene-d12	14.01		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-		280	C20H40	074685-30-6	97
2	1-Docosene		308	C22H44	001599-67-3	97
3	Heptafluorobutvric acid, pentade...		424	C19H31F7O2	959261-23-5	91
4	Heptafluorobutvric acid, hexadec...		438	C20H33F7O2	006385-15-5	91
5	Octadecyl trifluoroacetate		366	C20H37F3O2	079392-43-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF033120\
Data File : BF119656.D
Acq On : 31 Mar 2020 17:14
Operator : MA/SJ
Sample : L2042-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

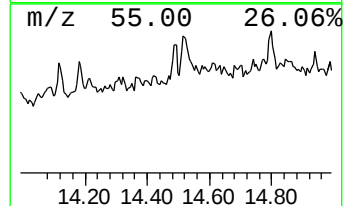
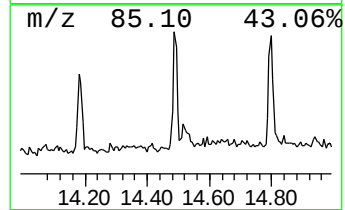
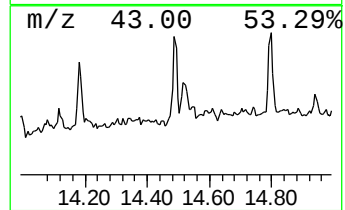
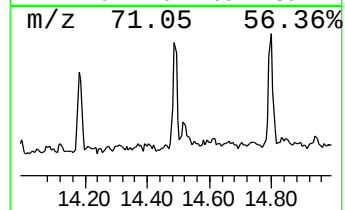
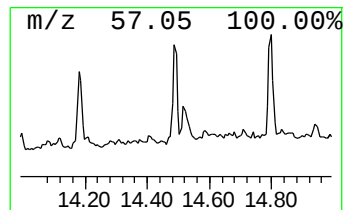
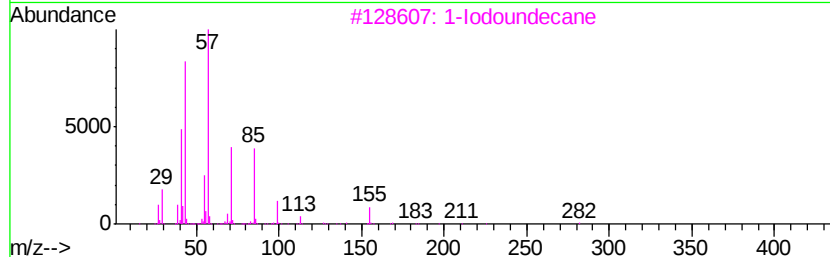
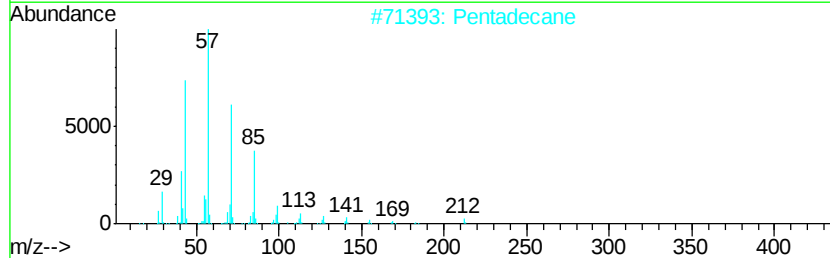
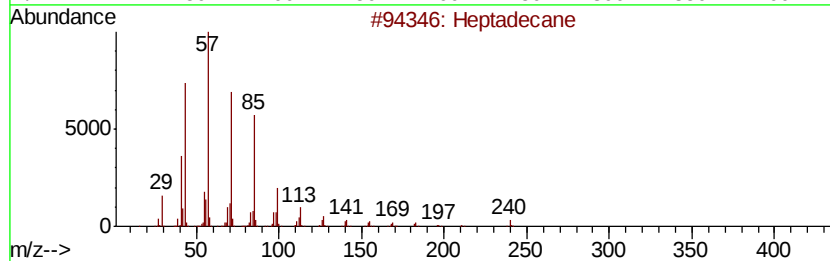
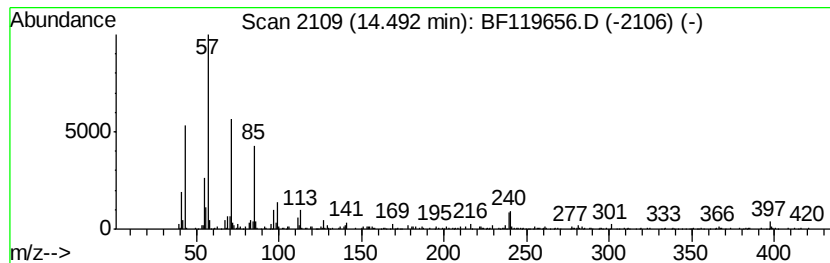
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ClientSampleId :
SB-02-1.0-1.5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF031820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.49	2.74 ng	244659	Chrysene-d12	14.01	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	90
2	Pentadecane	212	C15H32	000629-62-9	90
3	1-Iodoundecane	282	C11H23I	004282-44-4	81
4	Hexadecane	226	C16H34	000544-76-3	78
5	Octacosane	394	C28H58	000630-02-4	70



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF033120\
Data File : BF119656.D
Acq On : 31 Mar 2020 17:14
Operator : MA/SJ
Sample : L2042-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

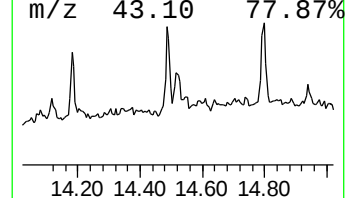
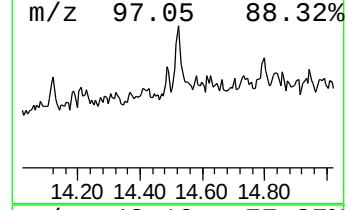
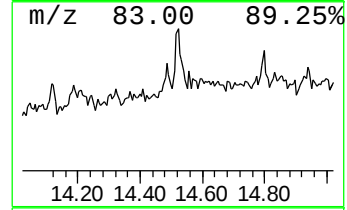
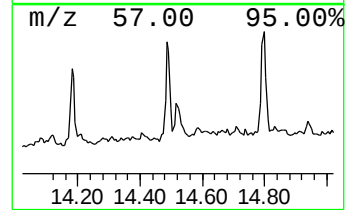
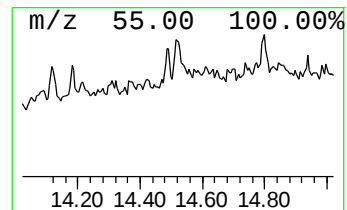
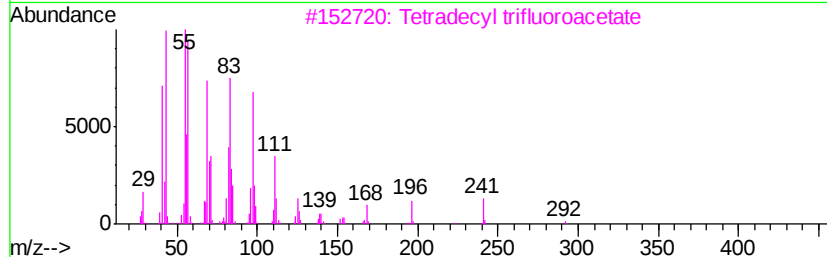
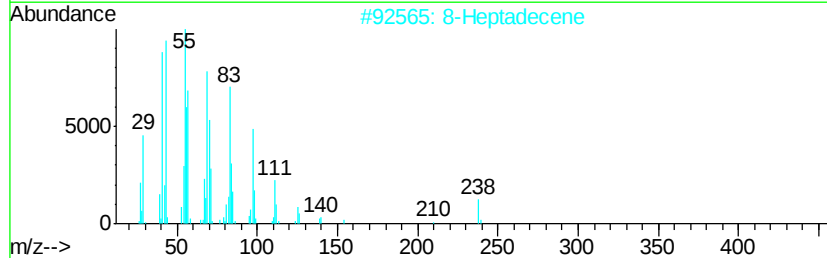
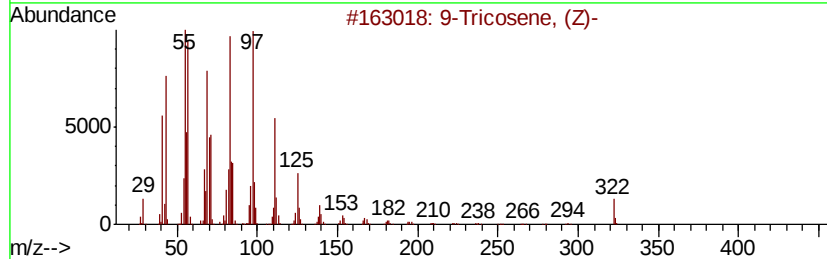
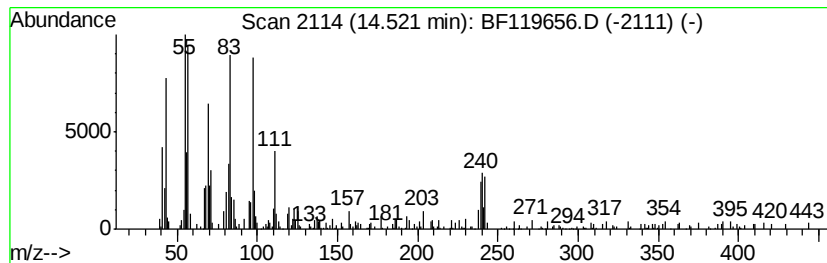
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 9-Tricosene, (Z)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.52	3.35 ng	298724	Chrysene-d12	14.01	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Tricosene, (Z)-	322	C23H46	027519-02-4	53
2	8-Heptadecene	238	C17H34	002579-04-6	49
3	Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	38
4	3-cyclohexylpropionic acid, 2,2,...	338	C13H17F7O2	1000376-61-3	35
5	2-Methyl-2-docosene	322	C23H46	1000131-16-9	35



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF033120\
Data File : BF119656.D
Acq On : 31 Mar 2020 17:14
Operator : MA/SJ
Sample : L2042-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-02-1.0-1.5

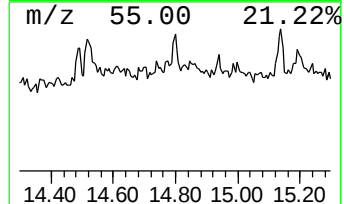
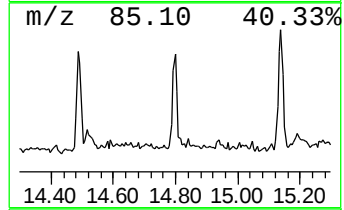
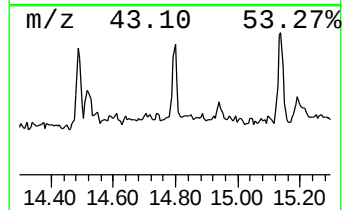
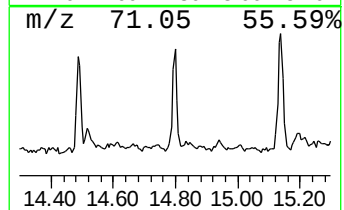
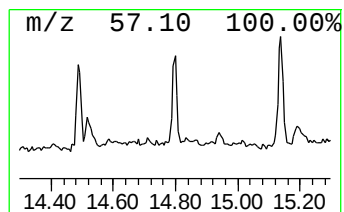
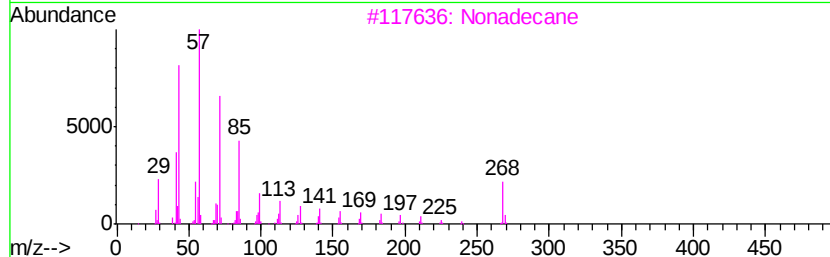
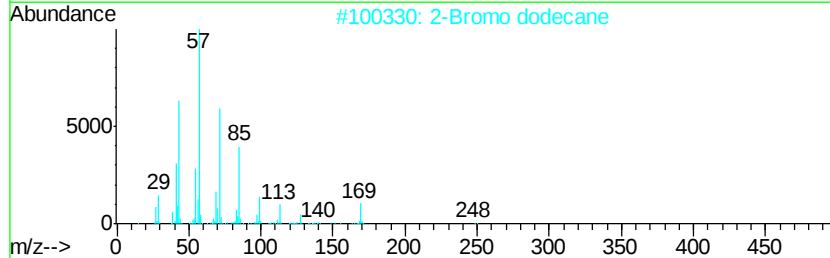
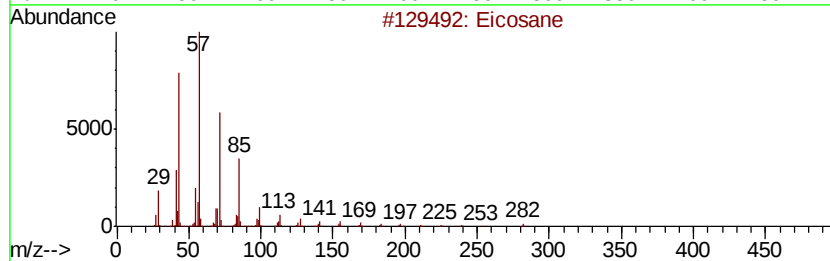
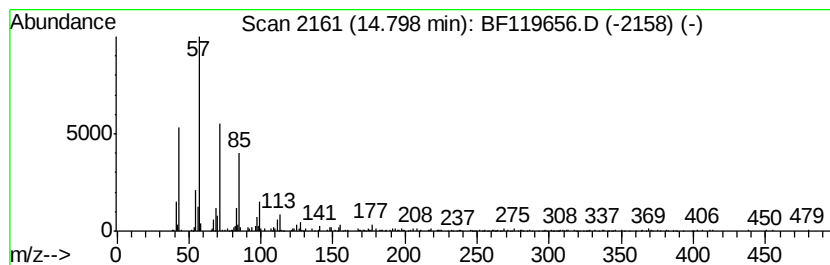
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.80	3.86 ng	238016	Perylene-d12	15.48

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	87
2	2-Bromo dodecane		248	C12H25Br	013187-99-0	87
3	Nonadecane		268	C19H40	000629-92-5	80
4	Tridecane, 2-methyl-		198	C14H30	001560-96-9	80
5	Tricosane, 2-methyl-		338	C24H50	001928-30-9	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF033120\
Data File : BF119656.D
Acq On : 31 Mar 2020 17:14
Operator : MA/SJ
Sample : L2042-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

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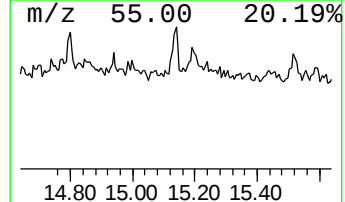
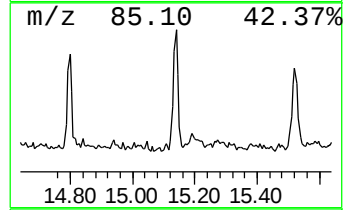
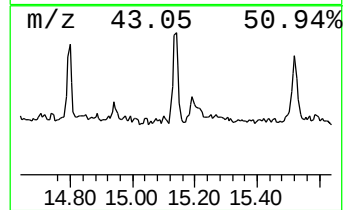
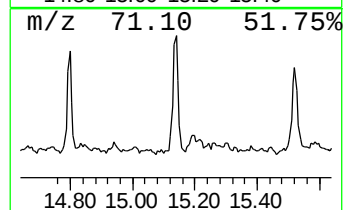
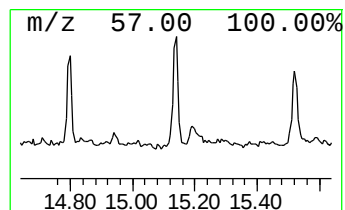
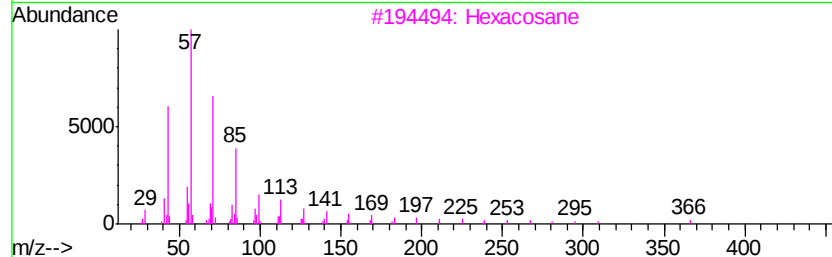
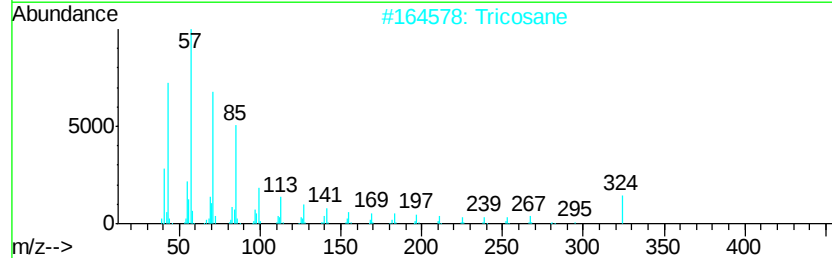
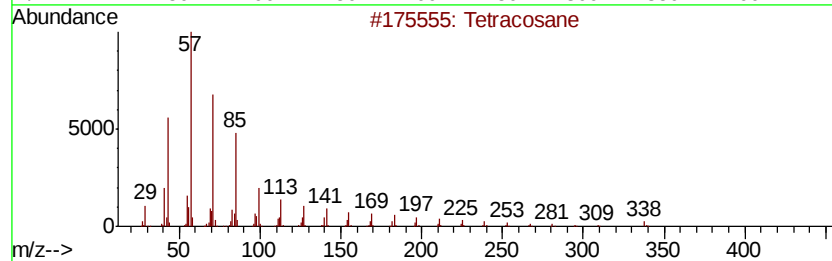
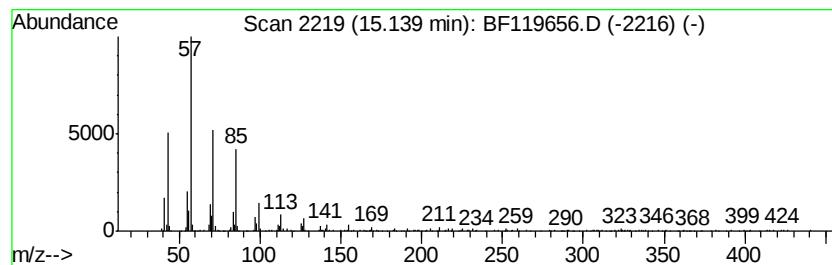
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Tetracosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.14	5.81 ng	357727	Perylene-d12	15.48

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetracosane	338	C24H50	000646-31-1	93
2		Tricosane	324	C23H48	000638-67-5	91
3		Hexacosane	366	C26H54	000630-01-3	91
4		Heneicosane	296	C21H44	000629-94-7	87
5		Tricosane, 2-methyl-	338	C24H50	001928-30-9	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF033120\
Data File : BF119656.D
Acq On : 31 Mar 2020 17:14
Operator : MA/SJ
Sample : L2042-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

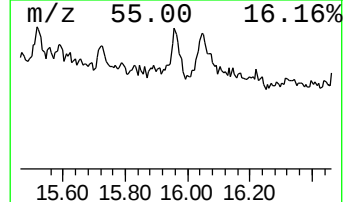
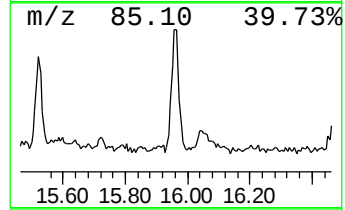
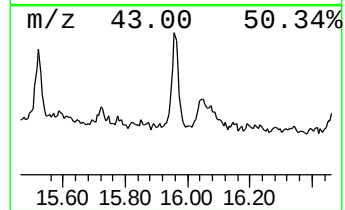
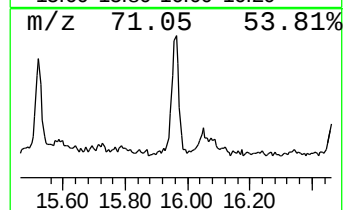
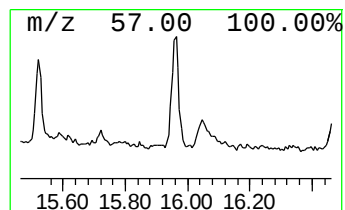
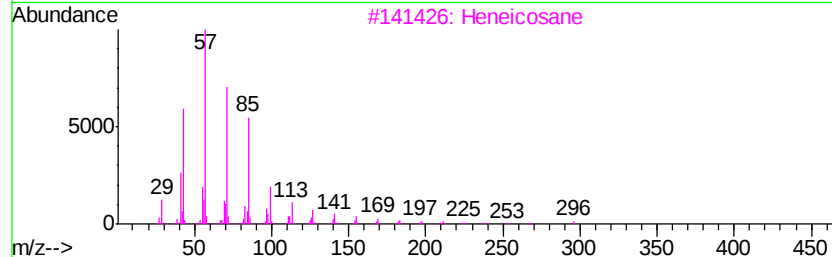
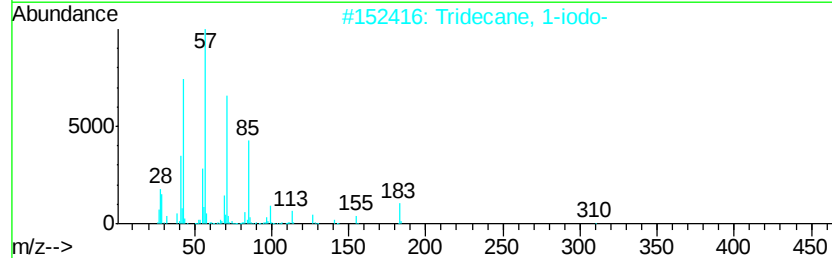
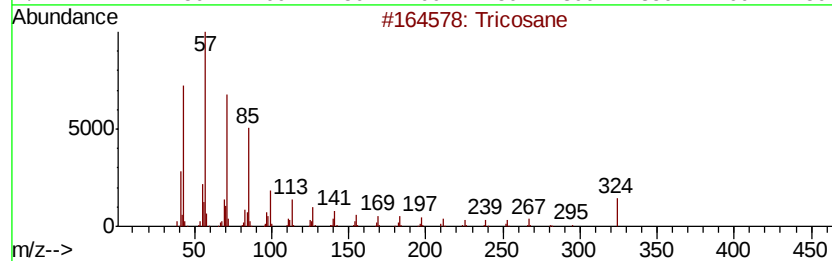
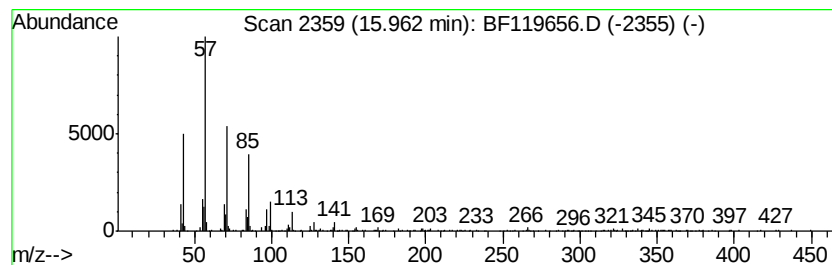
Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF031820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Tricosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.96	6.52 ng	401893	Perylene-d12	15.48	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricosane	324	C23H48	000638-67-5	91
2	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	87
3	Heneicosane	296	C21H44	000629-94-7	87
4	Octacosane	394	C28H58	000630-02-4	87
5	Heptadecane, 2-methyl-	254	C18H38	001560-89-0	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF033120\
 Data File : BF119656.D
 Acq On : 31 Mar 2020 17:14
 Operator : MA/SJ
 Sample : L2042-02
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-02-1.0-1.5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF031820.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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n-Hexadecanoic acid	11.90	13.2	ng	1505730	4	11.36	2283850	20.0
Octadecanoic acid	12.69	7.0	ng	794758	4	11.36	2283850	20.0
Nonadecane, 1-chl...	13.19	2.1	ng	189130	5	14.01	1783080	20.0
5-Eicosene, (E)-	13.87	12.4	ng	1102990	5	14.01	1783080	20.0
Heptadecane	14.49	2.7	ng	244659	5	14.01	1783080	20.0
9-Tricosene, (Z)-	14.52	3.4	ng	298724	5	14.01	1783080	20.0
Eicosane	14.80	3.9	ng	238016	6	15.48	1232280	20.0
Tetracosane	15.14	5.8	ng	357727	6	15.48	1232280	20.0
Tricosane	15.96	6.5	ng	401893	6	15.48	1232280	20.0