

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041621\
 Data File : BF123601.D
 Acq On : 16 Apr 2021 20:12
 Operator : JU/CG
 Sample : M2046-02
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WC-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-BF041521.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123601.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.163	3	13	19	rBV	2695884	3510567	57.57%	6.853%
2	5.093	507	511	517	rVB	78165	99057	1.62%	0.193%
3	5.498	576	580	584	rBV	6575514	5789747	94.95%	11.302%
4	6.510	747	752	759	rBV	5959896	5899987	96.76%	11.517%
5	6.869	809	813	816	rBV	2053072	1597504	26.20%	3.118%
6	7.428	903	908	911	rBV	4035519	3963351	65.00%	7.737%
7	8.151	1027	1031	1034	rBV	2526274	2055273	33.71%	4.012%
8	9.234	1210	1215	1218	rBV	7429984	6097521	100.00%	11.903%
9	9.316	1223	1229	1232	rBV	69809	72040	1.18%	0.141%
10	9.622	1278	1281	1285	rBV	332822	299522	4.91%	0.585%
11	9.916	1327	1331	1334	rVB	2471397	2126270	34.87%	4.151%
12	10.116	1360	1365	1373	rBV3	58218	71746	1.18%	0.140%
13	10.704	1460	1465	1468	rBV	4648275	3920301	64.29%	7.653%
14	11.404	1580	1584	1586	rBV	2395555	2086497	34.22%	4.073%
15	11.422	1586	1587	1590	rVB	332361	245059	4.02%	0.478%
16	11.622	1618	1621	1625	rBV3	48236	77500	1.27%	0.151%
17	11.933	1671	1674	1685	rBV	1533313	1477988	24.24%	2.885%
18	12.222	1721	1723	1726	rVB2	83141	71692	1.18%	0.140%
19	12.616	1787	1790	1793	rBV	563137	484683	7.95%	0.946%
20	12.722	1804	1808	1814	rBV	637233	634938	10.41%	1.239%
21	12.845	1825	1829	1832	rBV	398827	337604	5.54%	0.659%
22	12.992	1850	1854	1858	rVB	4694664	4355787	71.44%	8.503%
23	13.227	1889	1894	1895	rBV3	81322	116309	1.91%	0.227%
24	13.686	1969	1972	1975	rVB3	100031	105777	1.73%	0.206%
25	13.904	2005	2009	2016	rBV2	662313	809288	13.27%	1.580%
26	14.051	2029	2034	2036	rBV2	1228044	1335605	21.90%	2.607%
27	14.074	2036	2038	2042	rVB	242746	198837	3.26%	0.388%
28	14.439	2098	2100	2102	rVB	122143	92513	1.52%	0.181%
29	14.468	2103	2105	2109	rVV2	111186	104471	1.71%	0.204%
30	14.545	2112	2118	2123	rVV3	207785	431681	7.08%	0.843%
31	14.816	2162	2164	2166	rBV3	81555	89104	1.46%	0.174%
32	15.098	2208	2212	2216	rBV	200664	342080	5.61%	0.668%
33	15.186	2224	2227	2230	rBV	243484	250917	4.12%	0.490%
34	15.410	2262	2265	2270	rVB	164031	208054	3.41%	0.406%
35	15.468	2272	2275	2279	rVB	164211	191795	3.15%	0.374%
36	15.539	2282	2287	2291	rBV	929109	1160847	19.04%	2.266%

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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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37	15.786	2326	2329	2332	rVB3	114479	140017	2.30%	0.273%
38	16.027	2367	2370	2375	rVB2	189793	274752	4.51%	0.536%
39	17.021	2536	2539	2543	rBV2	68903	100277	1.64%	0.196%

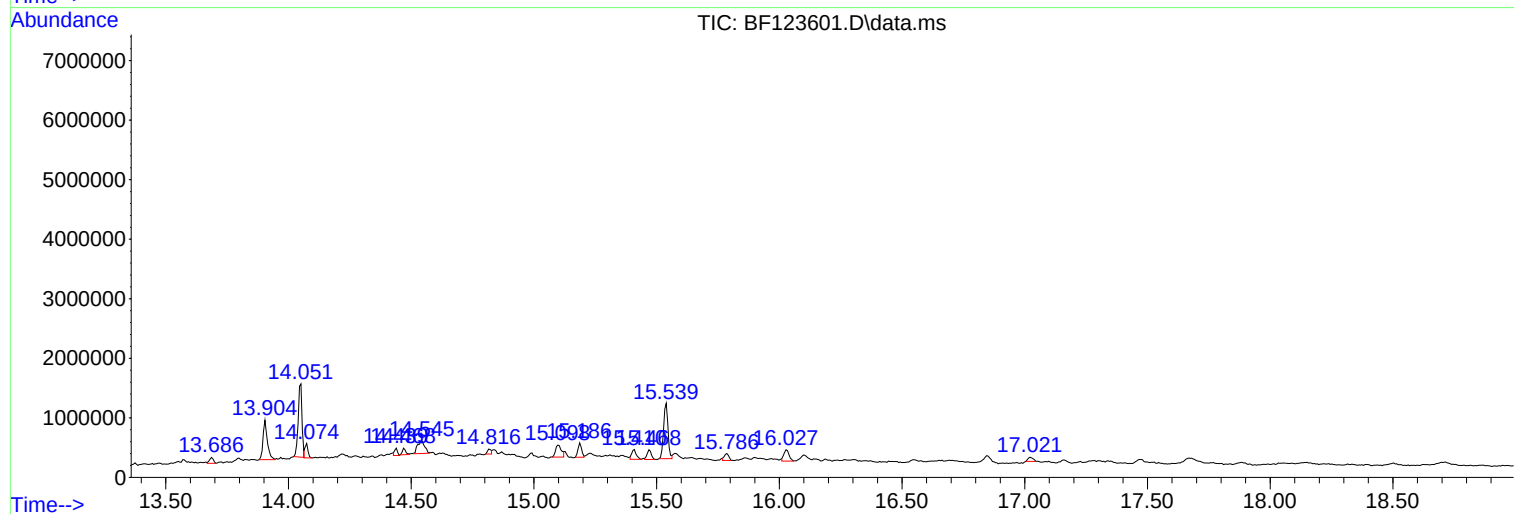
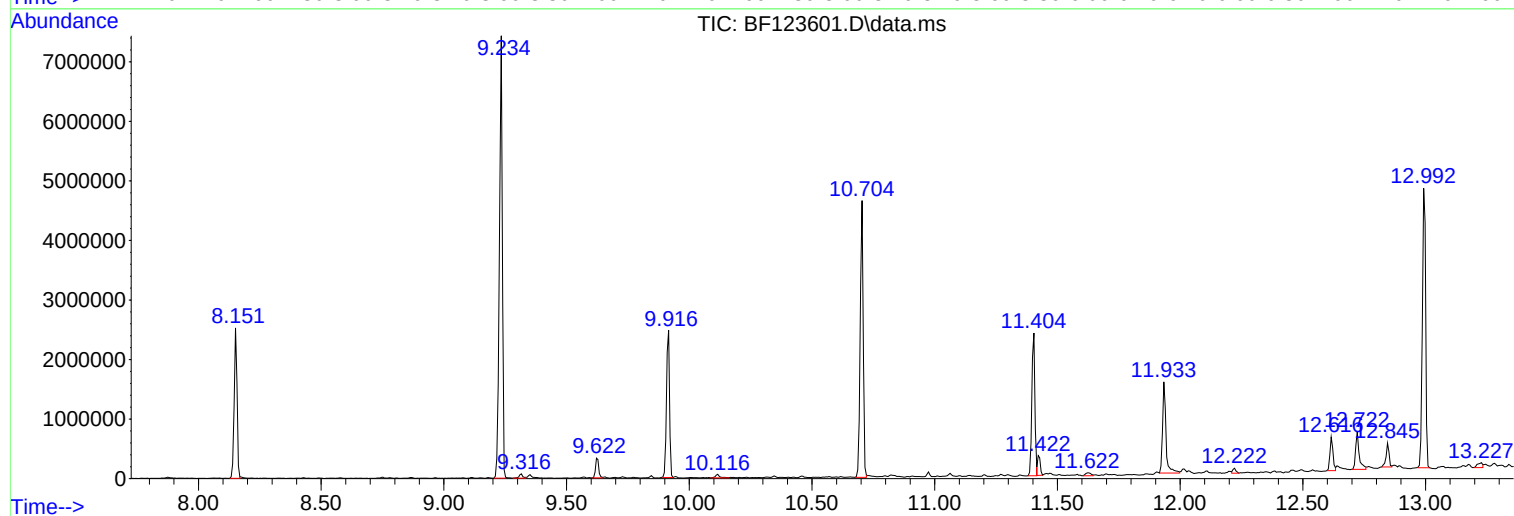
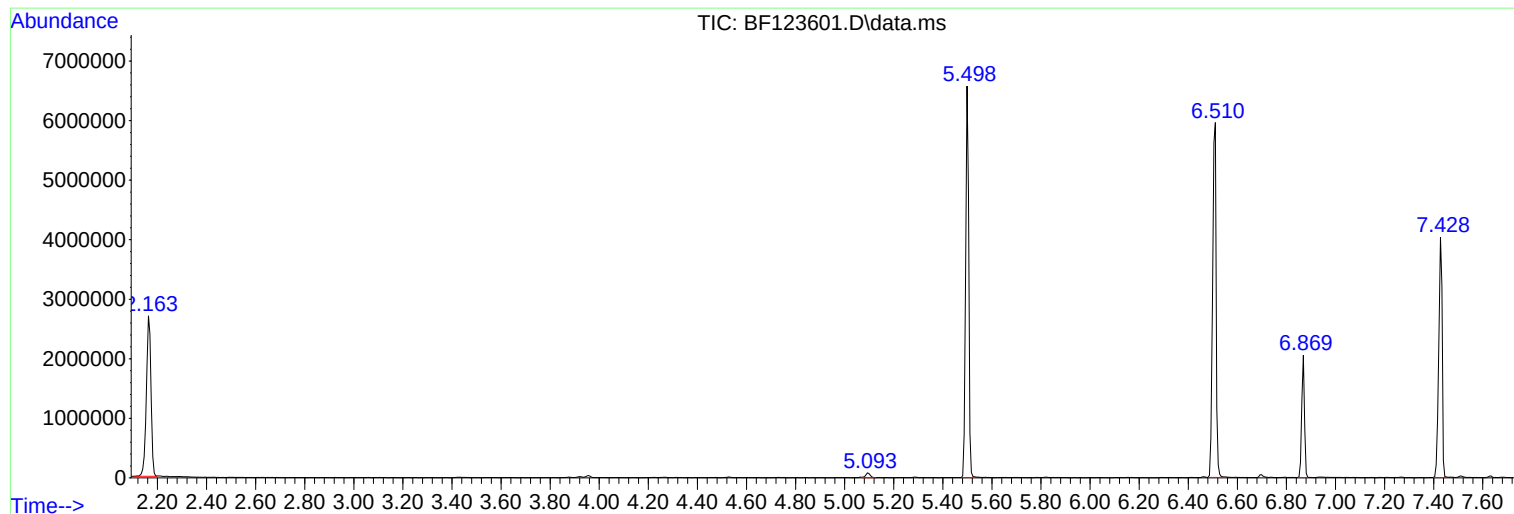
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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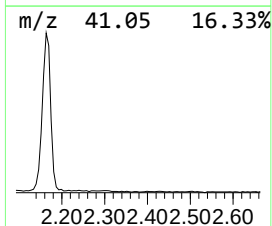
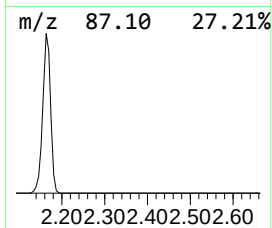
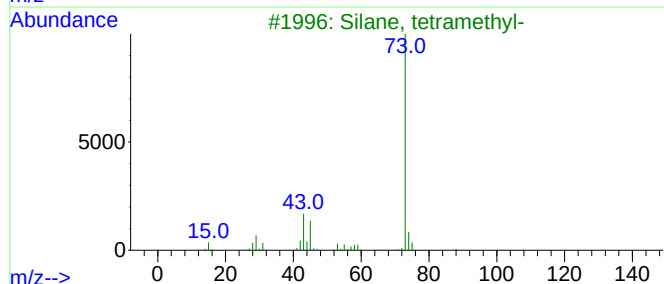
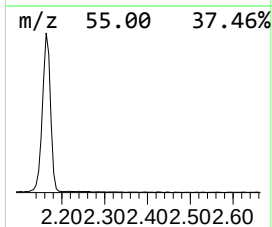
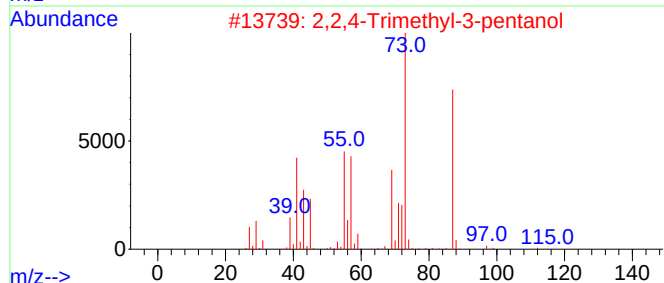
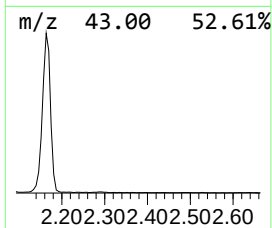
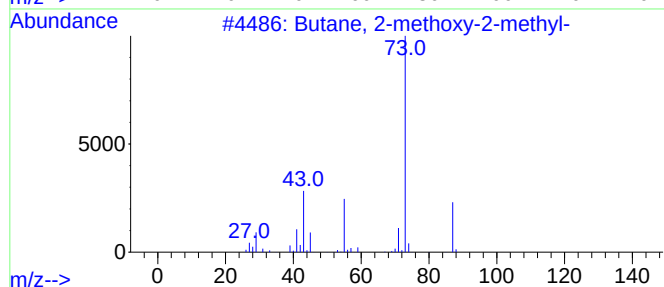
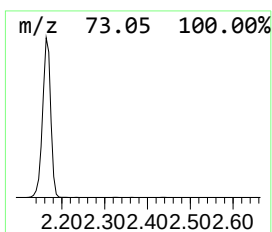
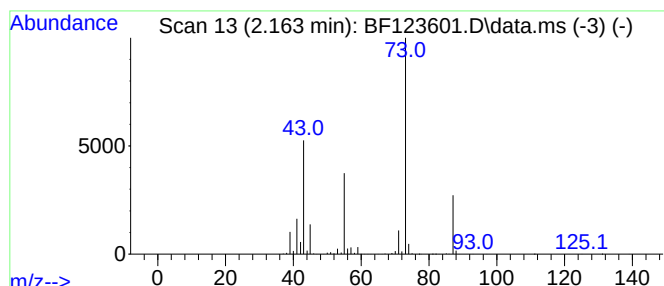
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.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.
2.163	43.95 ng	3510570	1,4-Dichlorobenzene-d4	6.869

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	12
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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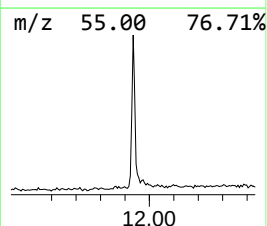
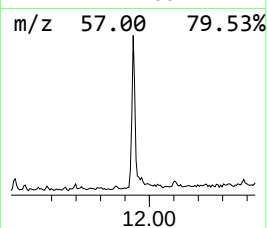
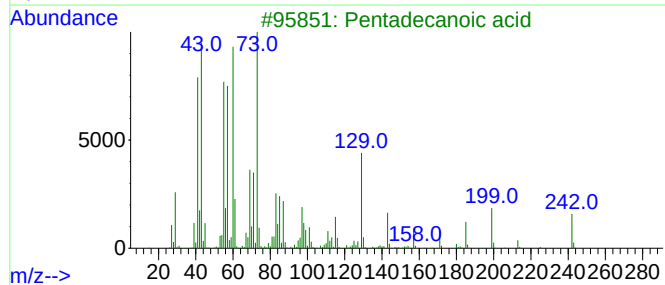
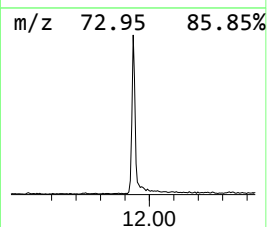
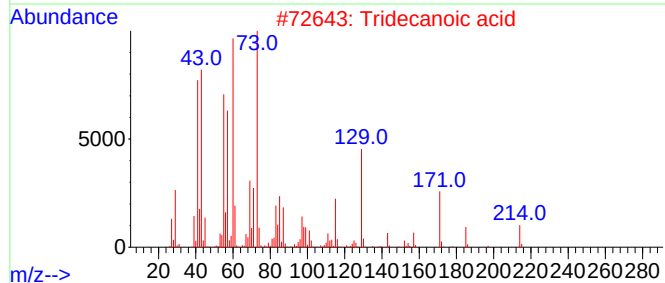
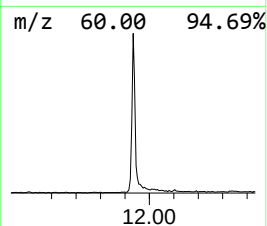
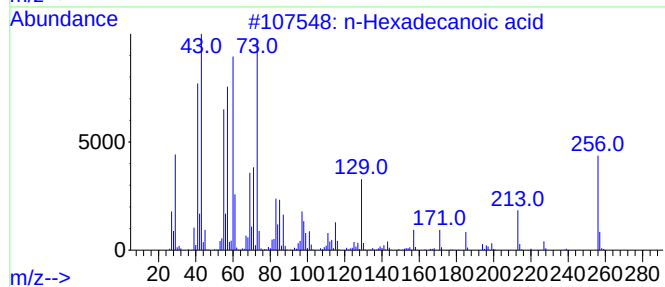
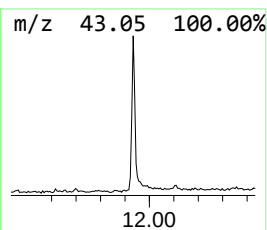
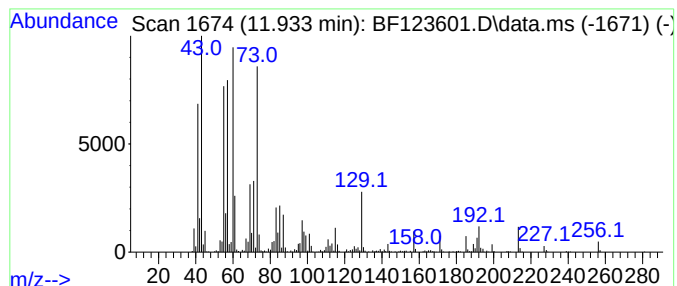
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	14.17 ng	1477990	Phenanthrene-d10	11.404

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	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4			Dodecanoic acid	200	C12H24O2	000143-07-7	76
5			Undecanoic acid	186	C11H22O2	000112-37-8	72



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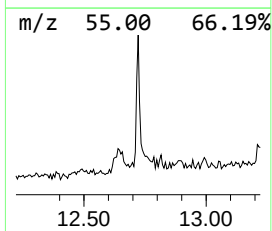
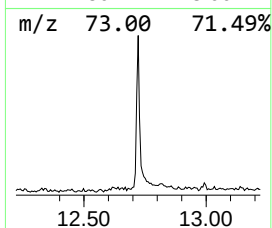
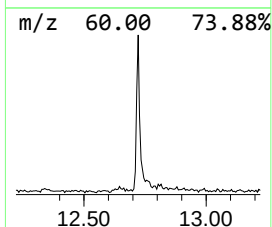
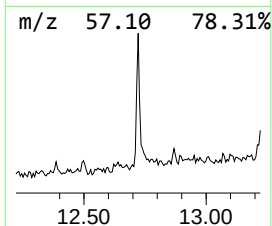
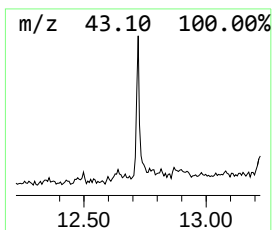
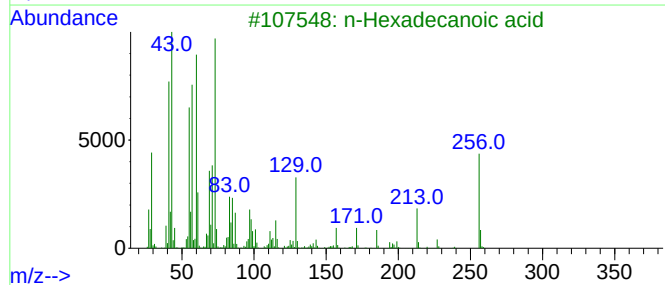
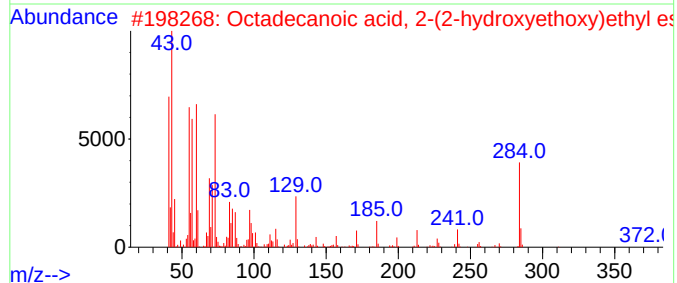
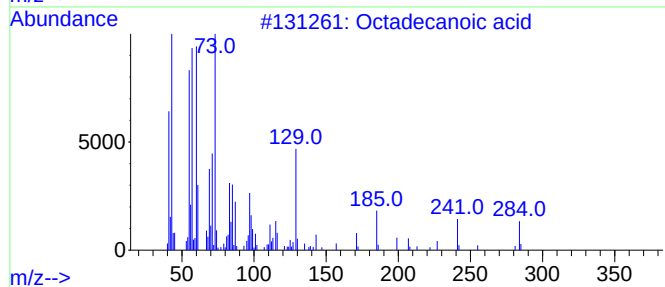
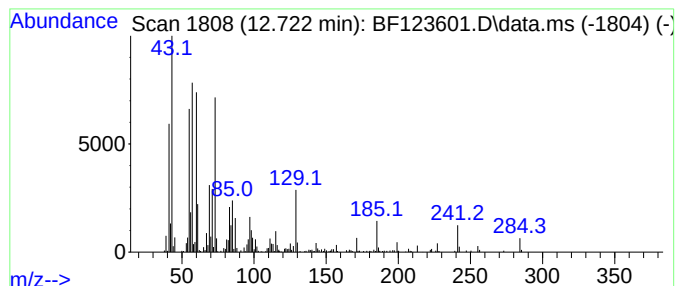
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.722	6.09 ng	634938	Phenanthrene-d10	11.404

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	95
2			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	91
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
4			Tridecanoic acid	214	C13H26O2	000638-53-9	80
5			Dodecanoic acid	200	C12H24O2	000143-07-7	74



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ClientSampled :
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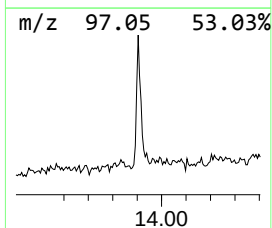
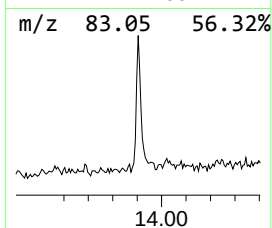
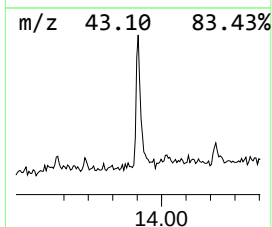
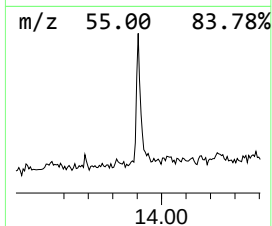
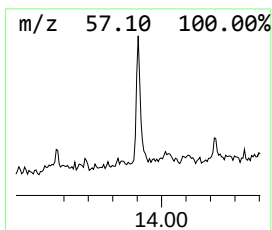
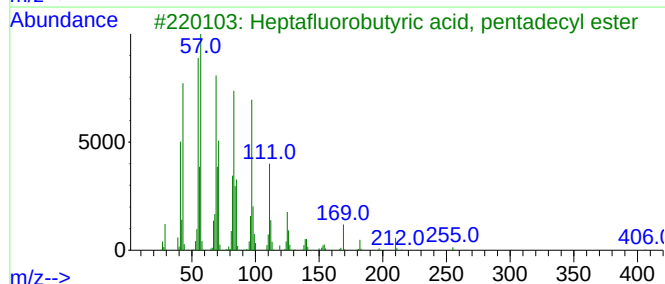
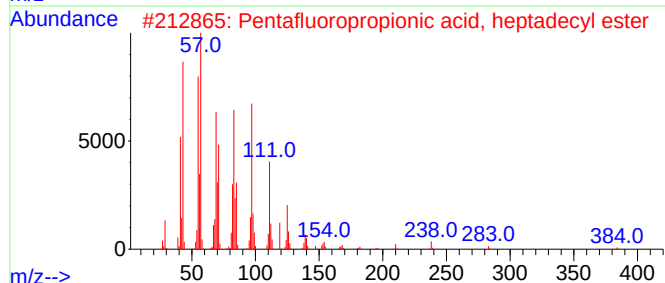
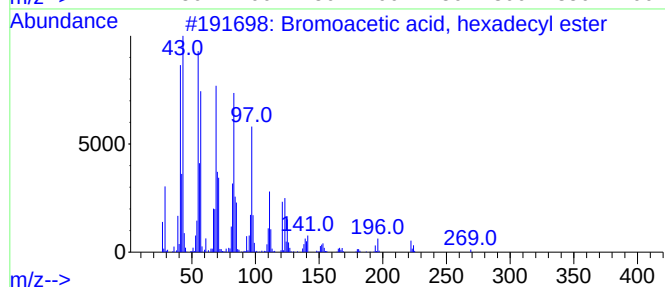
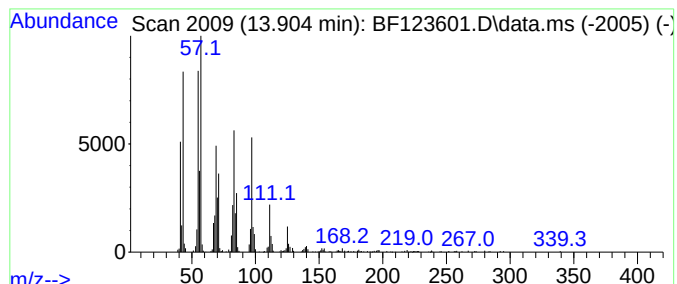
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Peak Number 4 Bromoacetic acid, hexadecyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.904	12.12 ng	809288	Chrysene-d12	14.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	91
2			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91
3			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91
4			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91
5			Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91



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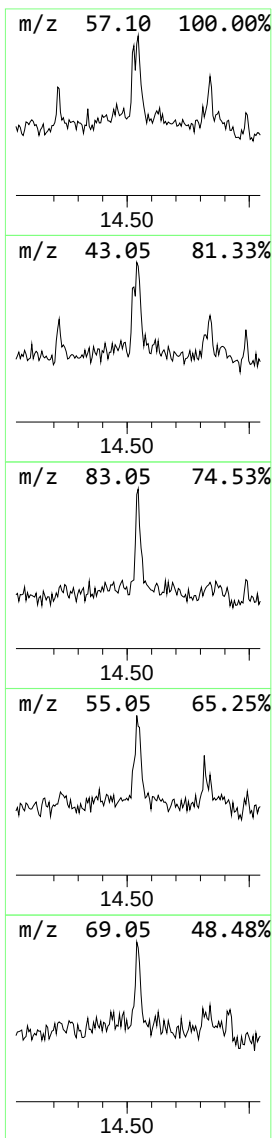
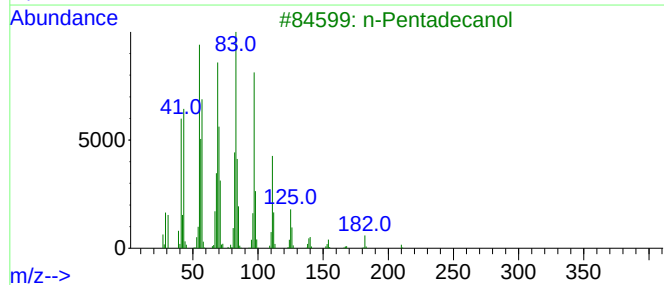
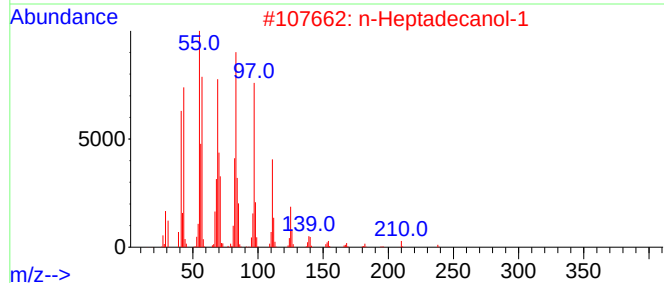
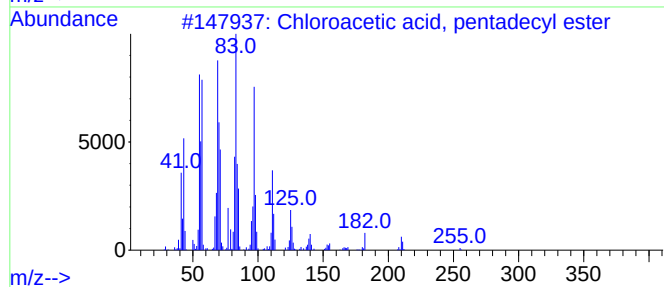
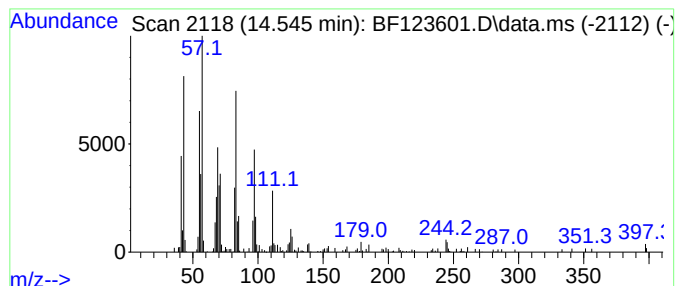
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Chloroacetic acid, pentadec... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.545	6.46 ng	431681	Chrysene-d12	14.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Chloroacetic acid, pentadecyl ester	304	C17H33ClO2	070301-47-2	87
2			n-Heptadecanol-1	256	C17H36O	001454-85-9	87
3			n-Pentadecanol	228	C15H32O	000629-76-5	86
4			1-Eicosanol	298	C20H42O	000629-96-9	86
5			1-Hexadecanethiol	258	C16H34S	002917-26-2	86



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ClientSampleId :
WC-5

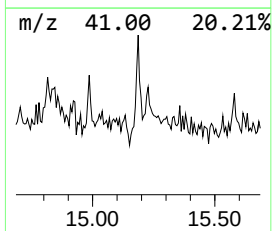
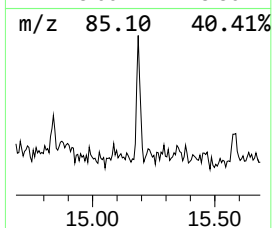
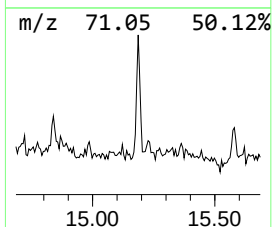
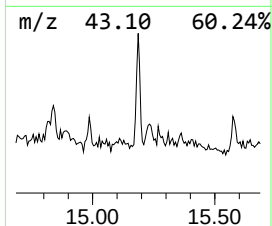
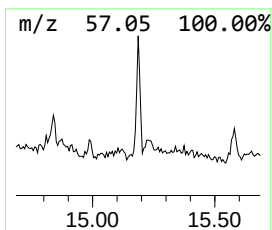
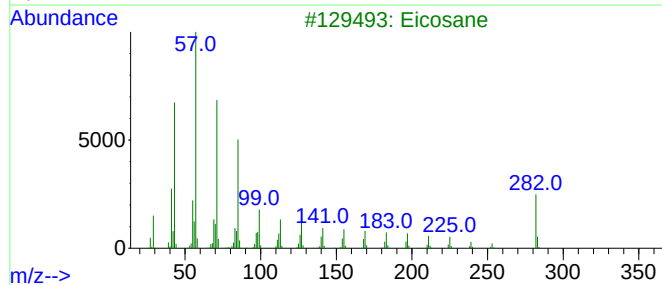
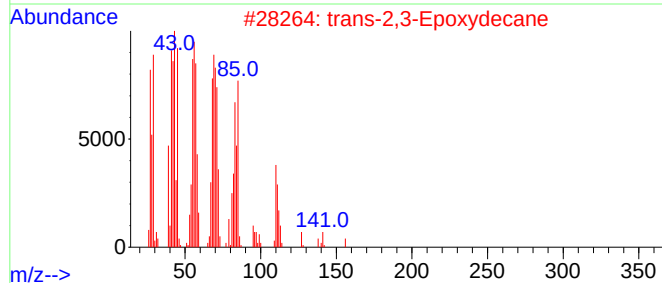
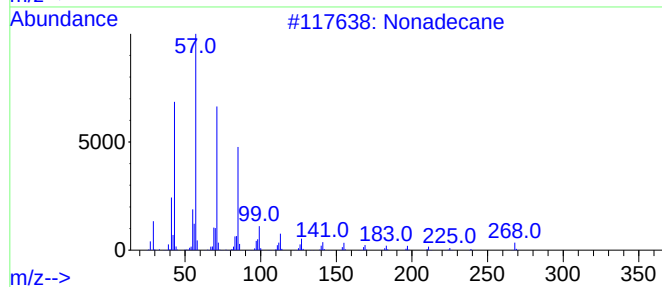
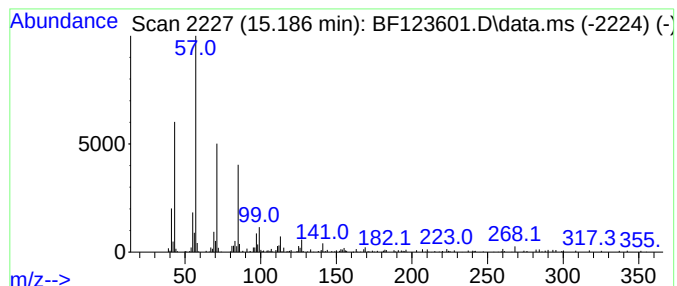
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Nonadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.186	4.32 ng	250917	Perylene-d12	15.539

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	93
2			trans-2,3-Epoxydecane	156	C10H20O	054125-39-2	90
3			Eicosane	282	C20H42	000112-95-8	86
4			Dodecane, 1-iodo-	296	C12H25I	004292-19-7	80
5			Hexadecane	226	C16H34	000544-76-3	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041621\
Data File : BF123601.D
Acq On : 16 Apr 2021 20:12
Operator : JU/CG
Sample : M2046-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-5

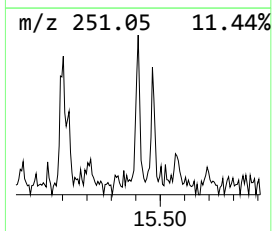
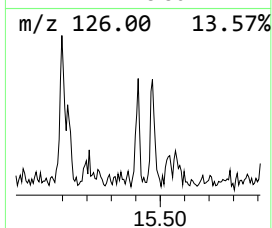
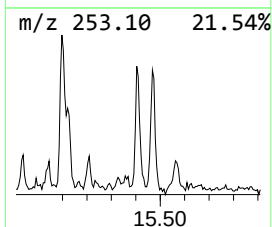
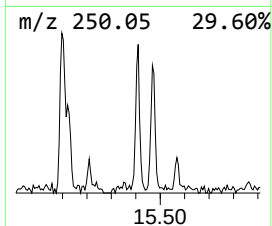
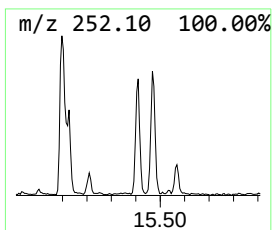
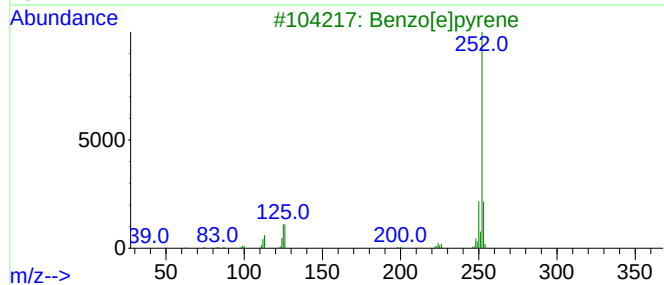
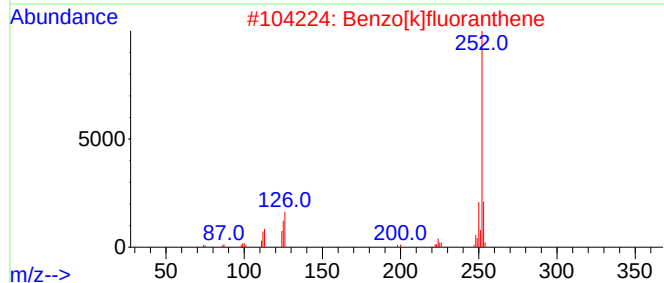
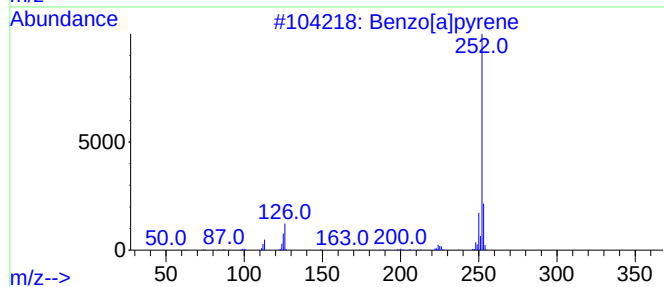
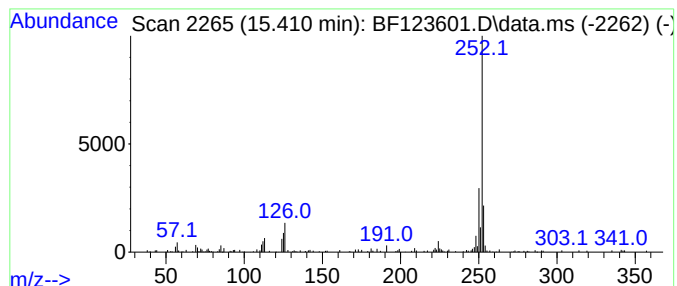
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzo[e]pyrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.410	3.58 ng	208054	Perylene-d12	15.539

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[a]pyrene	252	C20H12	000050-32-8	91
2			Benzo[k]fluoranthene	252	C20H12	000207-08-9	90
3			Benzo[e]pyrene	252	C20H12	000192-97-2	90
4			Perylene	252	C20H12	000198-55-0	81
5			(1-Cyclopentenyl)ferrocene	252	C15H16Fe	012260-67-2	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041621\
Data File : BF123601.D
Acq On : 16 Apr 2021 20:12
Operator : JU/CG
Sample : M2046-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-5

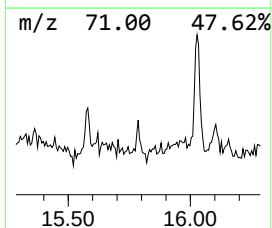
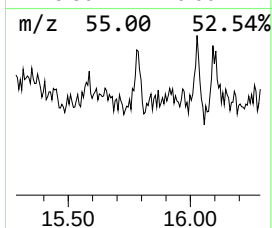
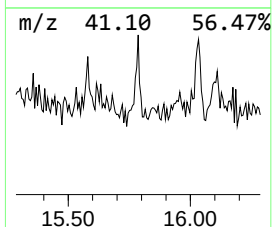
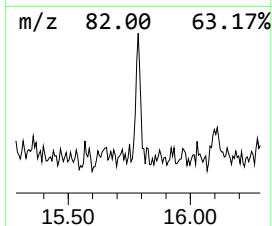
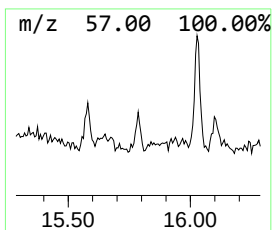
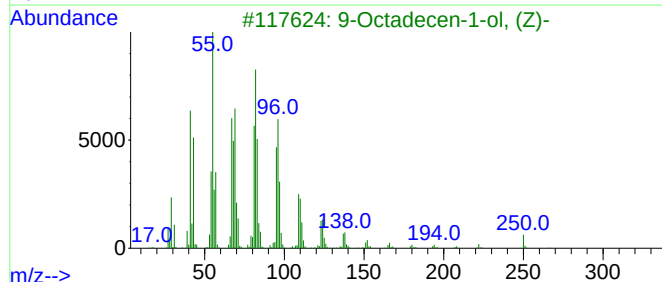
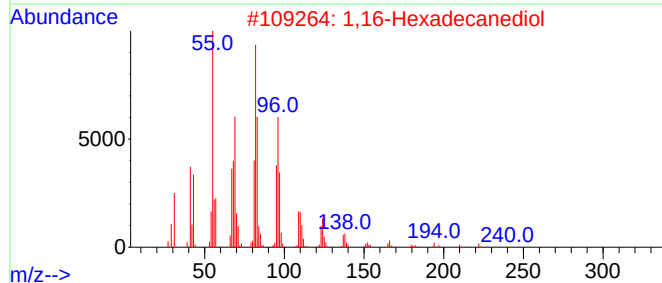
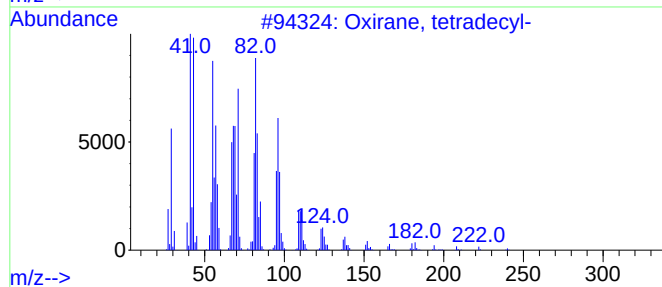
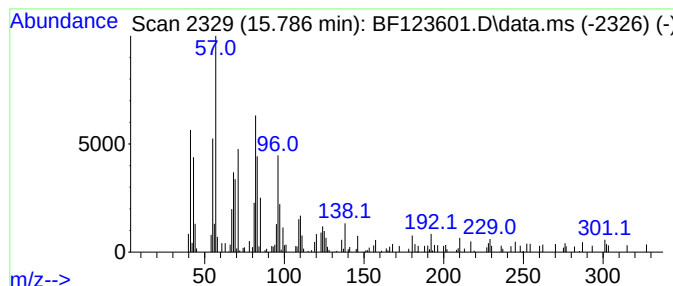
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Oxirane, tetradecyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.786	2.41 ng	140017	Perylene-d12	15.539

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxirane, tetradecyl-	240	C16H32O	007320-37-8	72
2			1,16-Hexadecanediol	258	C16H34O2	007735-42-4	47
3			9-Octadecen-1-ol, (Z)-	268	C18H36O	000143-28-2	46
4			Z-11(13-Methyl)tetradecen-1-ol a...	268	C17H32O2	1000131-33-3	43
5			9-Octadecen-1-ol, (E)-	268	C18H36O	000506-42-3	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041621\
Data File : BF123601.D
Acq On : 16 Apr 2021 20:12
Operator : JU/CG
Sample : M2046-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-5

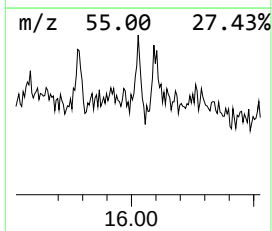
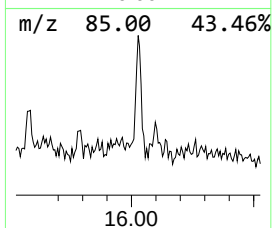
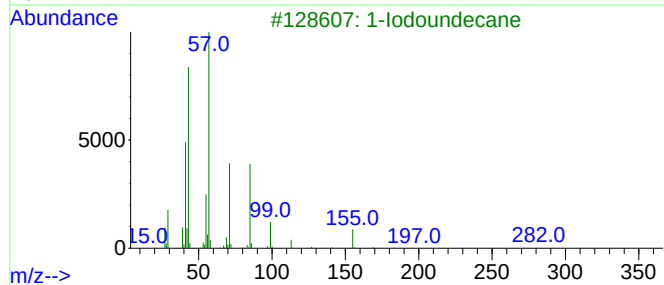
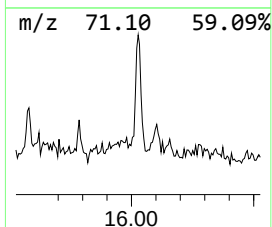
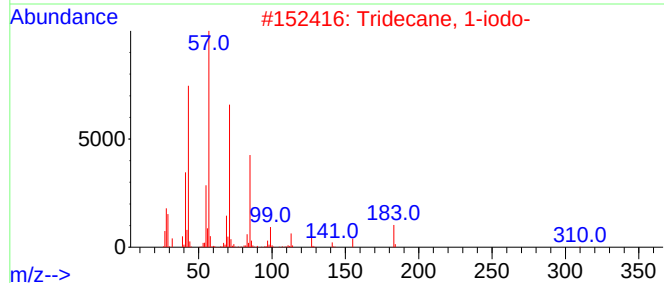
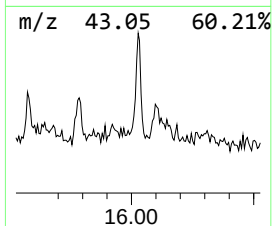
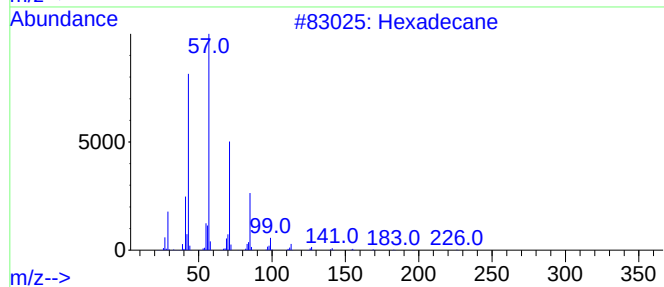
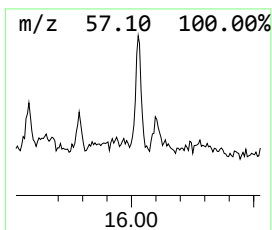
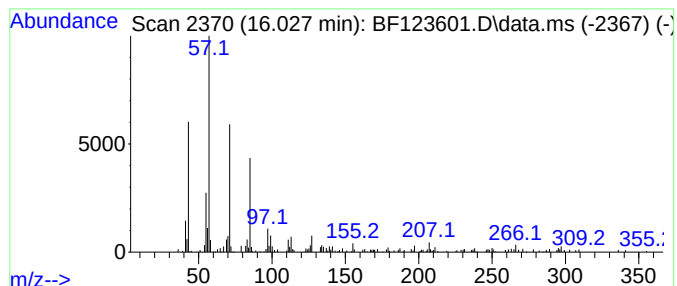
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.027	4.73 ng	274752	Perylene-d12	15.539

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane	226	C16H34	000544-76-3	90
2			Tridecane, 1-iodo-	310	C13H27I	035599-77-0	72
3			1-Iodoundecane	282	C11H23I	004282-44-4	64
4			5,5,7,7-Tetraethylundecane	268	C19H40	1000360-42-0	59
5			Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041621\
Data File : BF123601.D
Acq On : 16 Apr 2021 20:12
Operator : JU/CG
Sample : M2046-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.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
Butane, 2-metho...	2.163	44.0	ng	3510570	1	6.869	1597500	20.0
n-Hexadecanoic ...	11.933	14.2	ng	1477990	4	11.404	2086500	20.0
Octadecanoic acid	12.722	6.1	ng	634938	4	11.404	2086500	20.0
Bromoacetic aci...	13.904	12.1	ng	809288	5	14.051	1335610	20.0
Chloroacetic ac...	14.545	6.5	ng	431681	5	14.051	1335610	20.0
Nonadecane	15.186	4.3	ng	250917	6	15.539	1160850	20.0
Benzo[e]pyrene	15.410	3.6	ng	208054	6	15.539	1160850	20.0
Oxirane, tetrad...	15.786	2.4	ng	140017	6	15.539	1160850	20.0
Hexadecane	16.027	4.7	ng	274752	6	15.539	1160850	20.0