

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041621\
 Data File : BF123603.D
 Acq On : 16 Apr 2021 21:17
 Operator : JU/CG
 Sample : M2048-12
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-04-14.5-15.0

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: BF123603.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.181	8	16	23	rVB	3520262	4653755	51.60%	6.685%
2	3.010	150	157	164	rVB	102507	174530	1.94%	0.251%
3	5.104	510	513	522	rVB	226753	308974	3.43%	0.444%
4	5.504	576	581	584	rBV	9453422	8601909	95.38%	12.356%
5	6.510	747	752	755	rBV	8613770	8974727	99.51%	12.892%
6	6.869	809	813	816	rBV	2130475	1679116	18.62%	2.412%
7	7.433	903	909	912	rBV	5947901	5948993	65.96%	8.545%
8	8.151	1026	1031	1035	rBV	2615241	2258865	25.05%	3.245%
9	9.233	1209	1215	1218	rBV	9457957	9018751	100.00%	12.955%
10	9.622	1278	1281	1285	rBV	338879	283326	3.14%	0.407%
11	9.916	1326	1331	1334	rVB	2696390	2353705	26.10%	3.381%
12	10.710	1460	1466	1469	rBV	6091015	6295112	69.80%	9.043%
13	11.404	1580	1584	1586	rBV	2811818	2350204	26.06%	3.376%
14	11.427	1586	1588	1591	rVB	178746	143923	1.60%	0.207%
15	11.933	1671	1674	1684	rBV	995691	948006	10.51%	1.362%
16	12.615	1785	1790	1794	rBV	253724	239507	2.66%	0.344%
17	12.721	1804	1808	1814	rBV2	176208	183897	2.04%	0.264%
18	12.845	1826	1829	1832	rVB	199472	159451	1.77%	0.229%
19	12.998	1850	1855	1858	rBV	7976570	7615220	84.44%	10.939%
20	13.227	1889	1894	1900	rBV4	153926	218263	2.42%	0.314%
21	13.686	1969	1972	1977	rVB	111995	109646	1.22%	0.158%
22	13.904	2005	2009	2024	rBV	1096312	1676933	18.59%	2.409%
23	14.051	2029	2034	2037	rBV	1597799	1485673	16.47%	2.134%
24	14.221	2060	2063	2064	rBV	108194	96107	1.07%	0.138%
25	14.545	2112	2118	2131	rBV	726599	1358417	15.06%	1.951%
26	14.839	2165	2168	2171	rVB	97002	90399	1.00%	0.130%
27	14.874	2171	2174	2178	rBV6	64330	103679	1.15%	0.149%
28	15.098	2209	2212	2221	rVB2	60529	116307	1.29%	0.167%
29	15.186	2223	2227	2231	rBV	150207	170113	1.89%	0.244%
30	15.239	2231	2236	2240	rBV4	138296	263153	2.92%	0.378%
31	15.539	2281	2287	2291	rBV	997860	1244422	13.80%	1.788%
32	15.580	2291	2294	2299	rVB2	102202	143475	1.59%	0.206%
33	16.027	2366	2370	2375	rBV	148677	211035	2.34%	0.303%
34	16.103	2380	2383	2389	rBV5	73574	136806	1.52%	0.197%

Sum of corrected areas: 69616399

Instrument :

BNA_F

ClientSampleId :

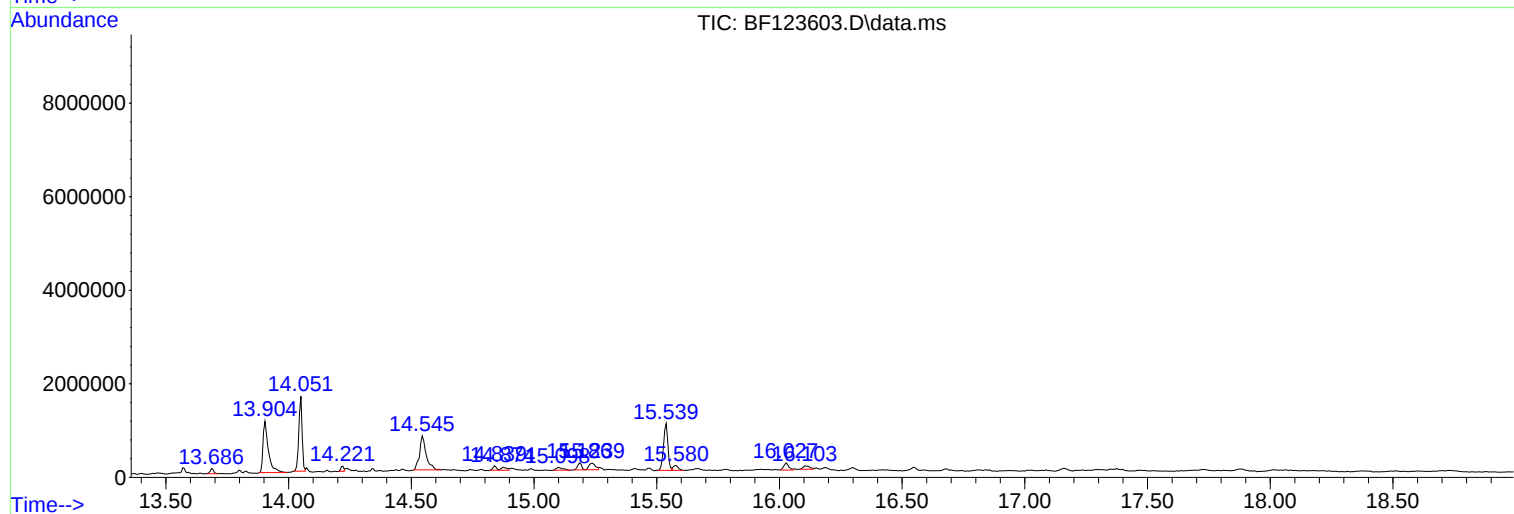
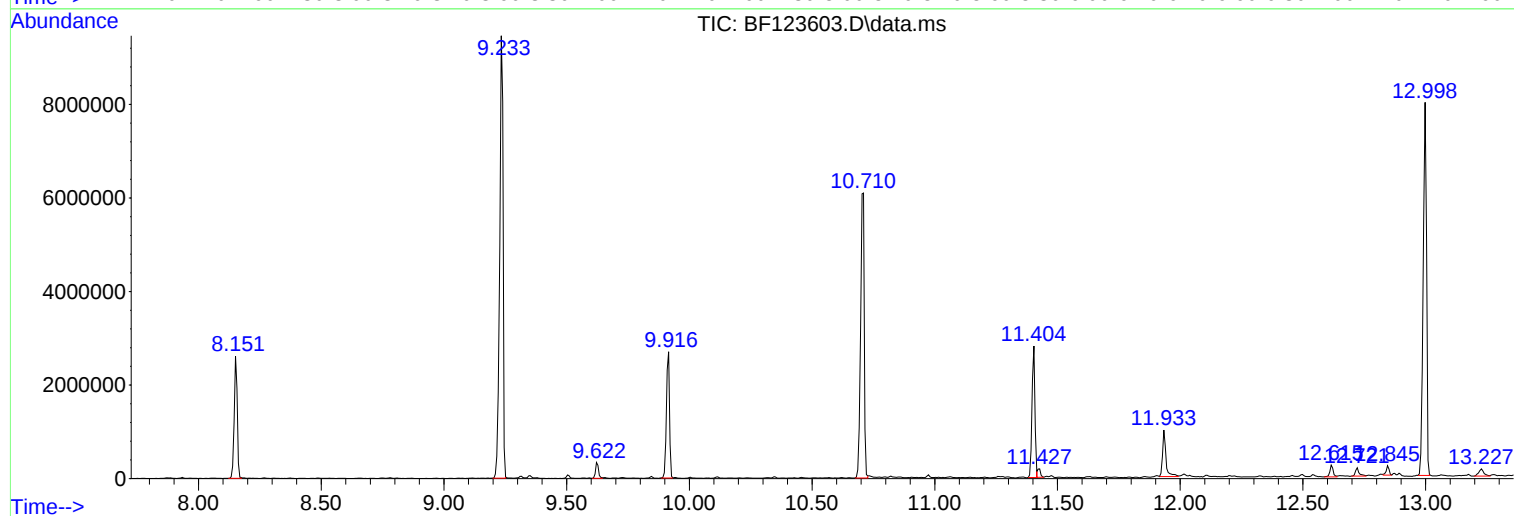
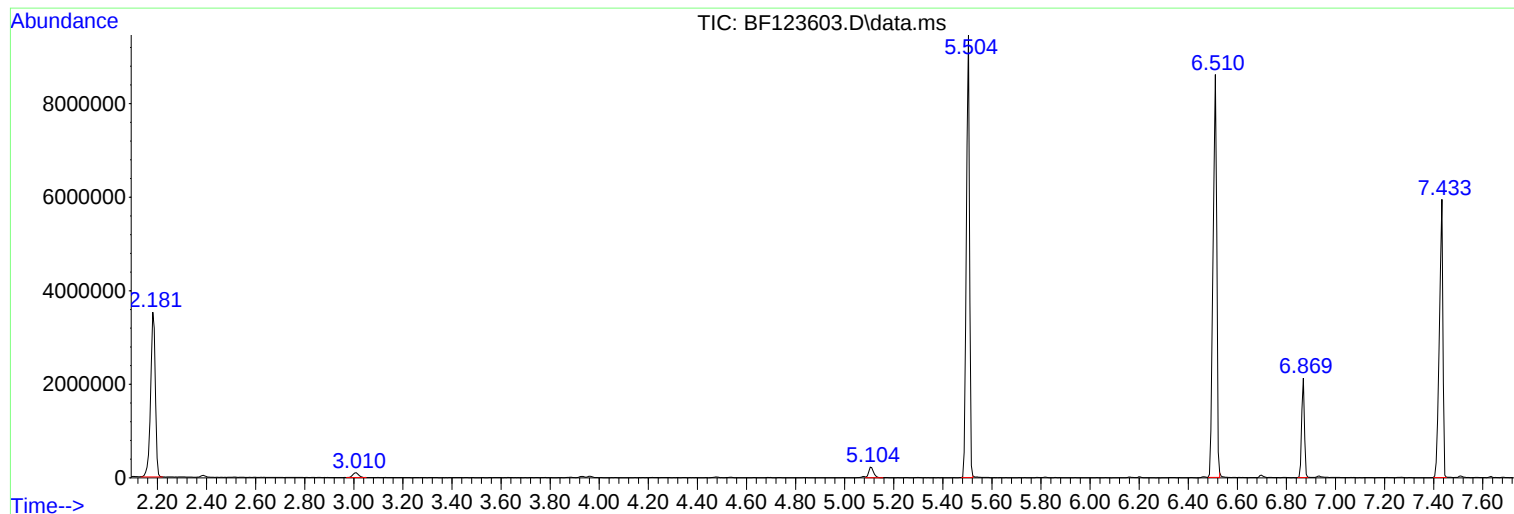
SB-04-14.5-15.0

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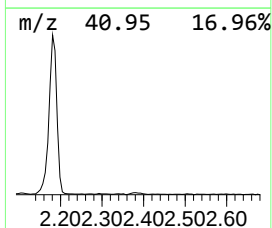
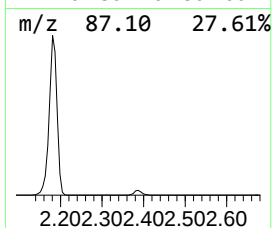
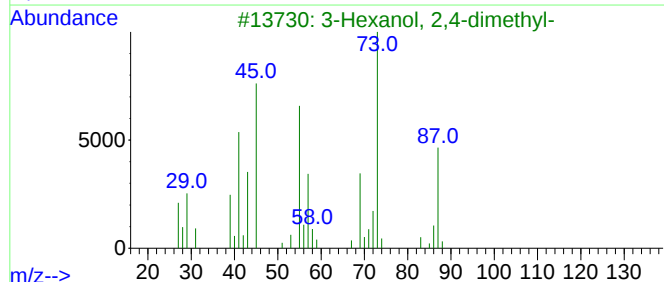
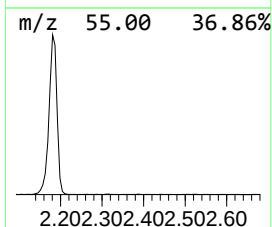
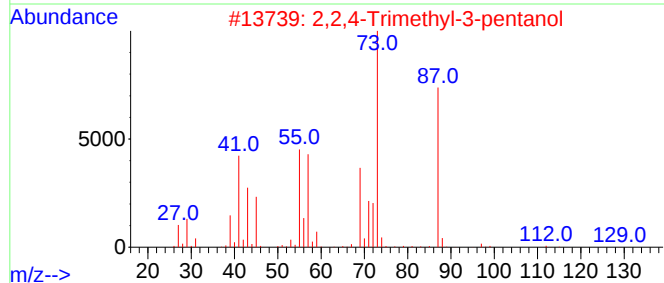
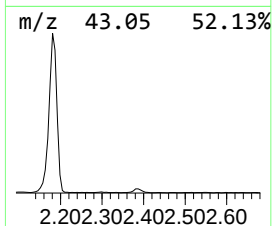
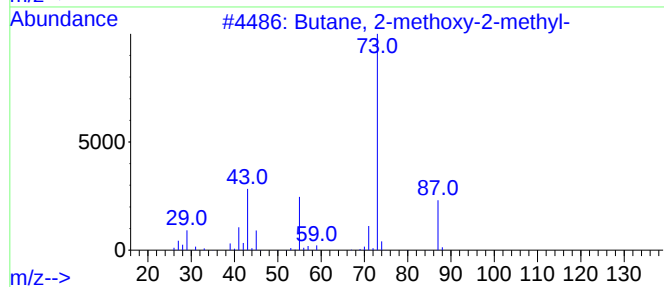
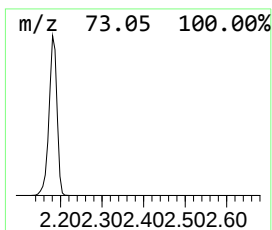
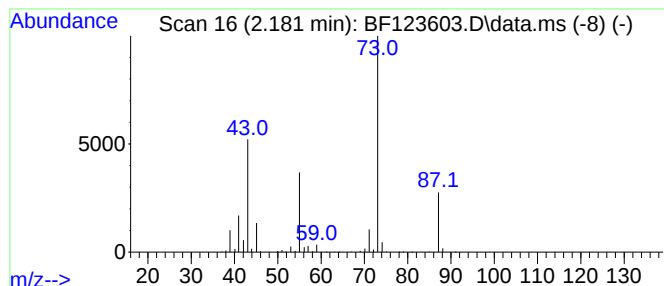
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.181	55.43 ng	4653760	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			3-Hexanol, 2,4-dimethyl-	130	C8H18O	013432-25-2	38
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9



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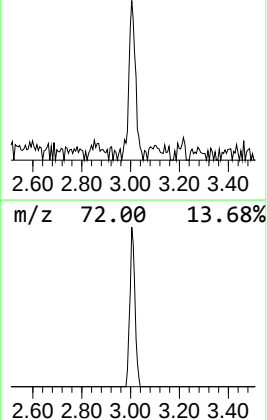
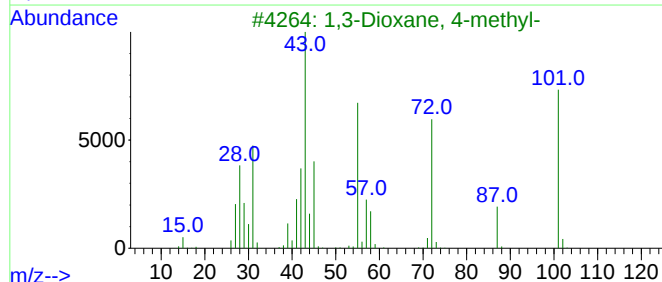
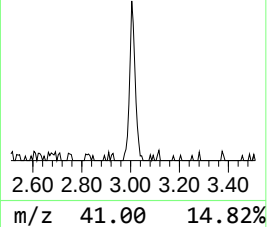
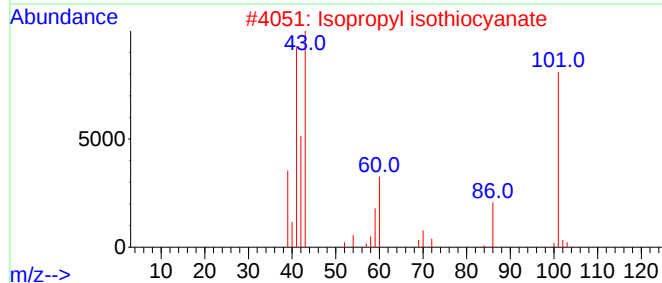
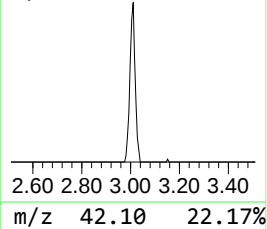
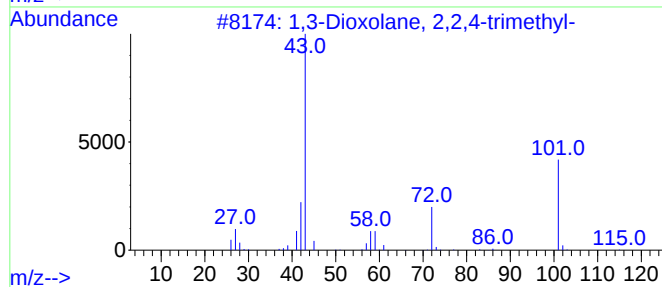
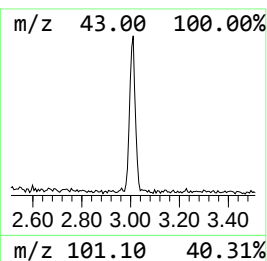
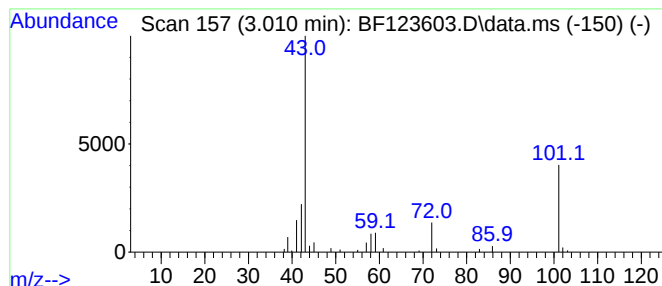
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 1,3-Dioxolane, 2,2,4-trimet... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.010	2.08 ng	174530	1,4-Dichlorobenzene-d4	6.869

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,3-Dioxolane, 2,2,4-trimethyl-	116	C6H12O2	001193-11-9	83
2		Isopropyl isothiocyanate	101	C4H7NS	002253-73-8	42
3		1,3-Dioxane, 4-methyl-	102	C5H10O2	001120-97-4	36
4		Thiocyanic acid, propyl ester	101	C4H7NS	004251-16-5	9
5		Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	9



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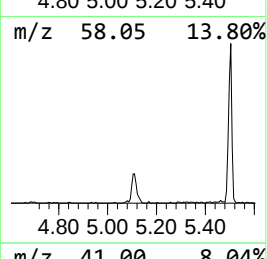
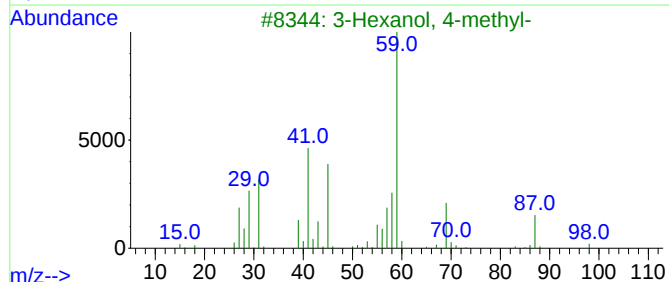
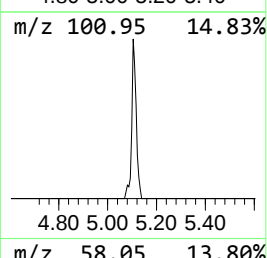
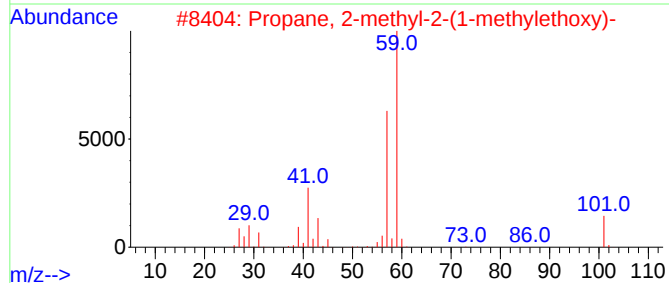
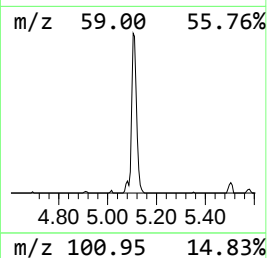
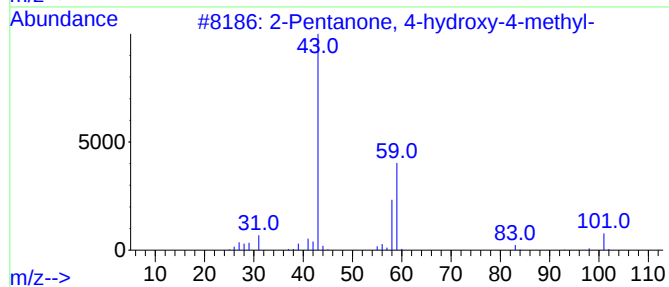
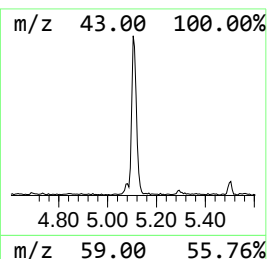
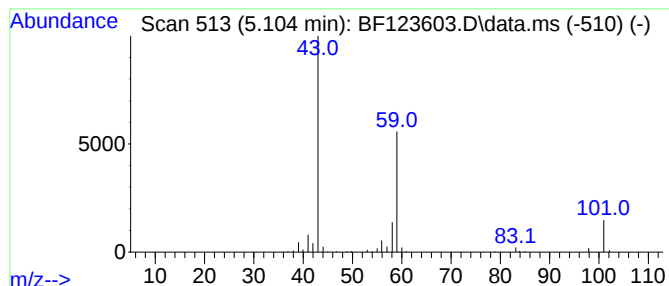
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.104	3.68 ng	308974	1,4-Dichlorobenzene-d4	6.869

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64	
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53	
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33	
4	Silane, dimethyl-	60	C2H8Si	001111-74-6	9	
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9	



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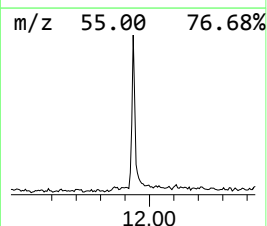
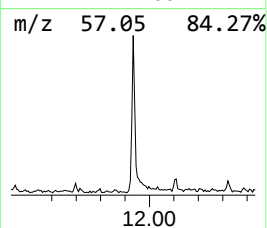
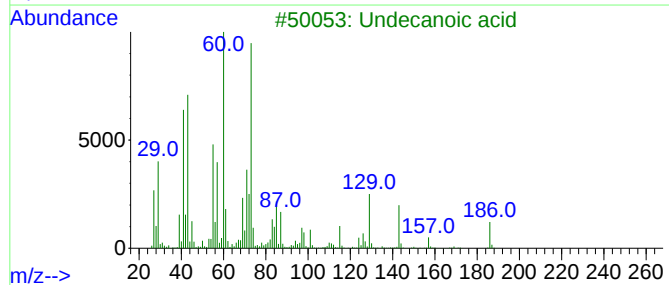
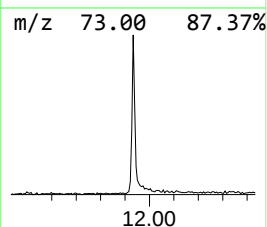
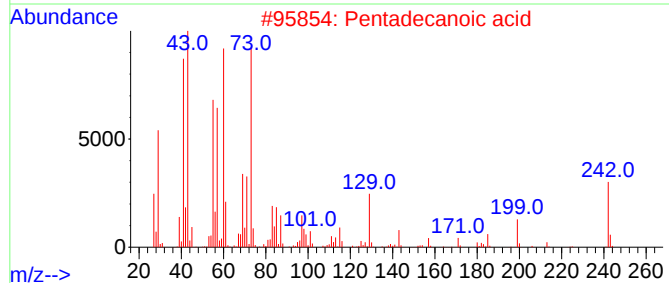
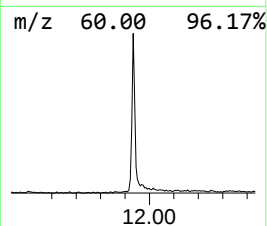
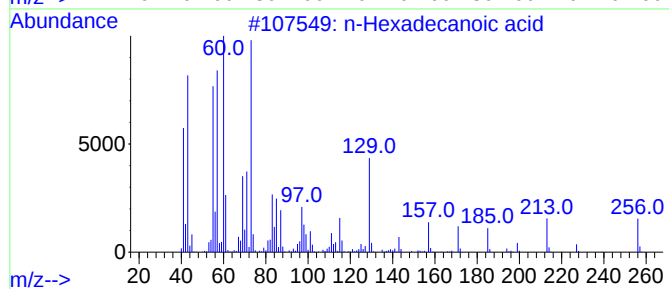
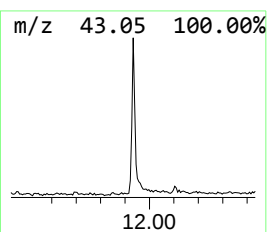
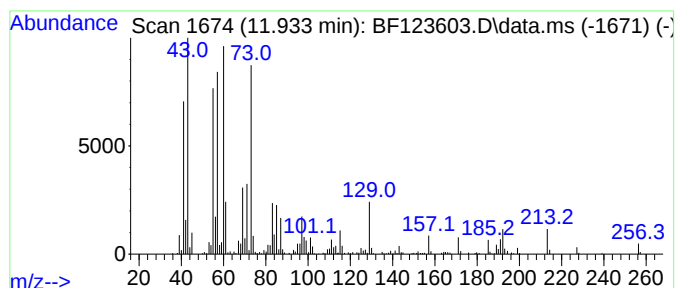
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	8.07 ng	948006	Phenanthrene-d10	11.404

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3			Undecanoic acid	186	C11H22O2	000112-37-8	86
4			Tridecanoic acid	214	C13H26O2	000638-53-9	81
5			Dodecanoic acid	200	C12H24O2	000143-07-7	81



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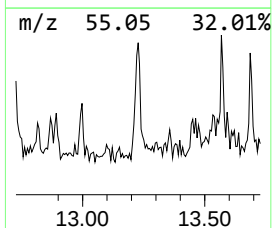
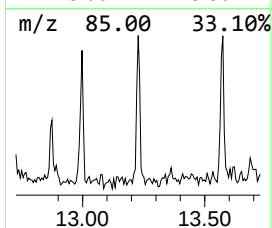
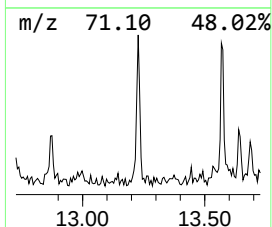
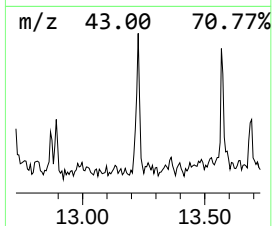
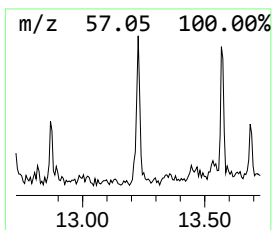
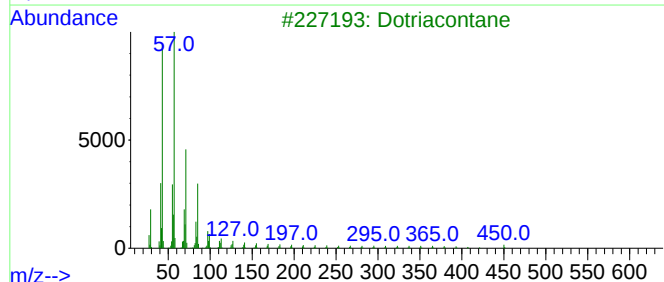
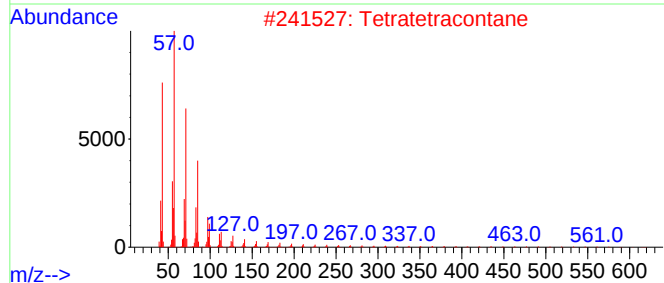
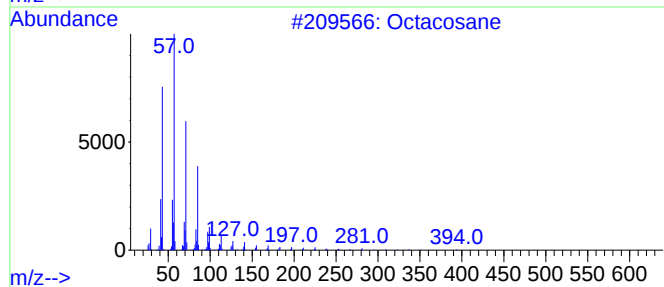
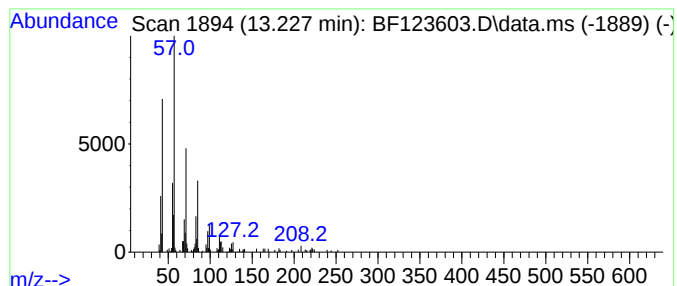
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Octacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.227	2.94 ng	218263	Chrysene-d12	14.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	83
2			Tetratetracontane	619	C44H90	007098-22-8	80
3			Dotriacontane	451	C32H66	000544-85-4	80
4			Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1000309-18-1	80
5			Sulfurous acid, 2-propyl tridecyl...	306	C16H34O3S	1000309-12-4	74



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ClientSampleId :
SB-04-14.5-15.0

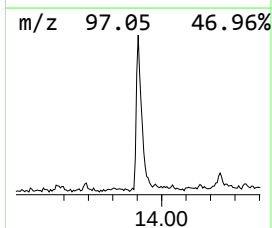
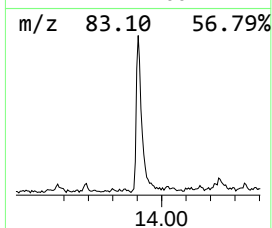
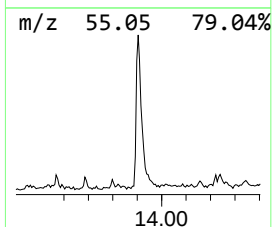
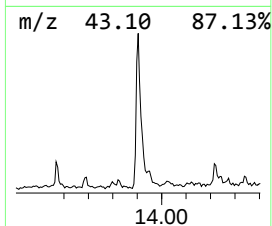
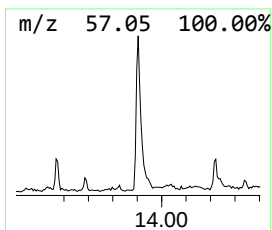
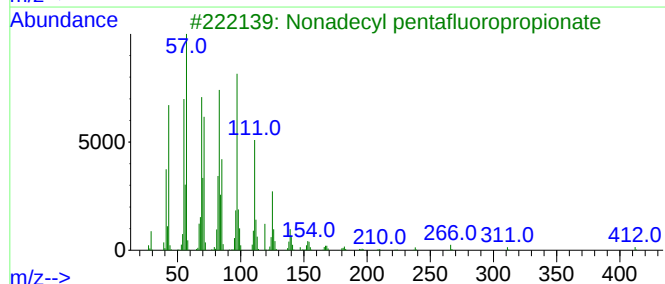
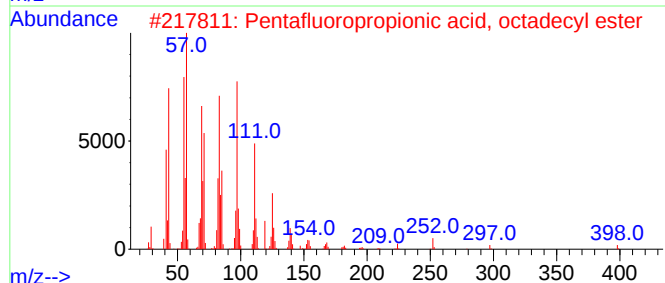
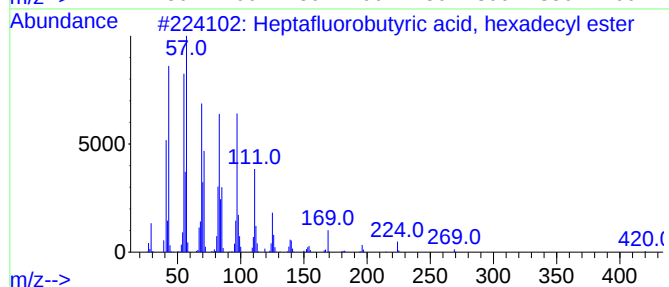
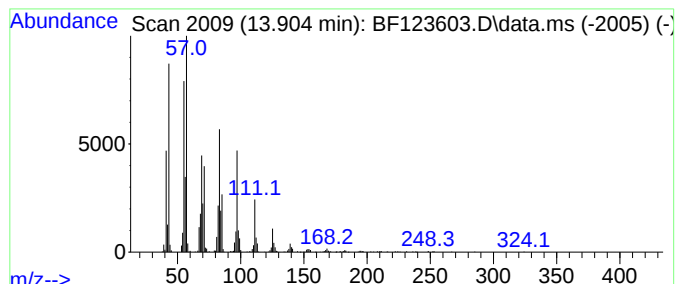
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptafluorobutyric acid, he... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.904	22.57 ng	1676930	Chrysene-d12	14.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
2			Pentafluoropropionic acid, octadec...	416	C21H37F5O2	959261-25-7	91
3			Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
4			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91
5			Eicosyl pentafluoropropionate	444	C23H41F5O2	1000351-80-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041621\
Data File : BF123603.D
Acq On : 16 Apr 2021 21:17
Operator : JU/CG
Sample : M2048-12
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-04-14.5-15.0

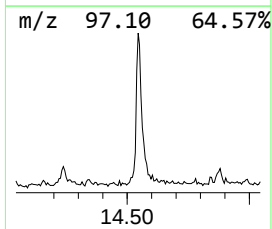
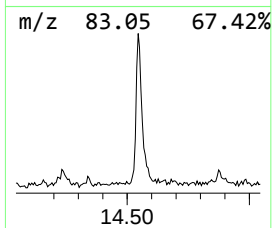
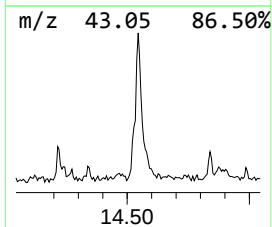
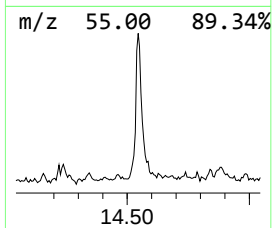
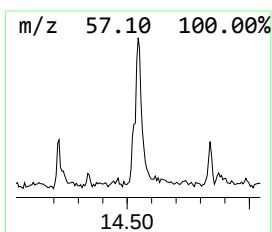
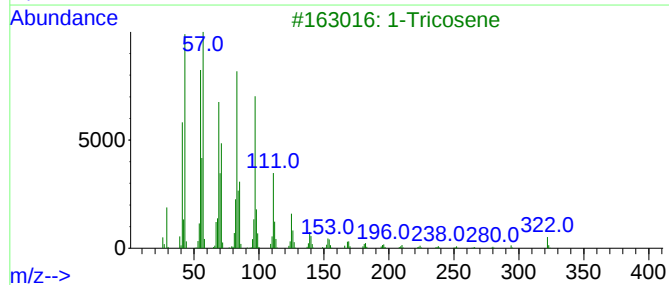
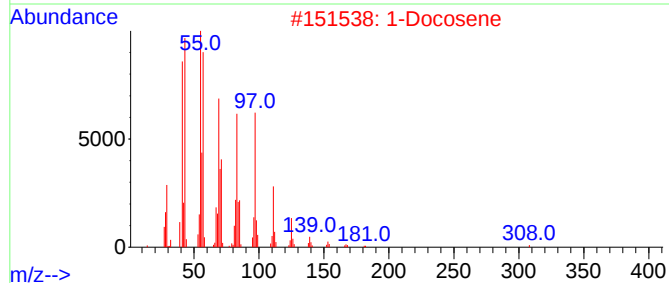
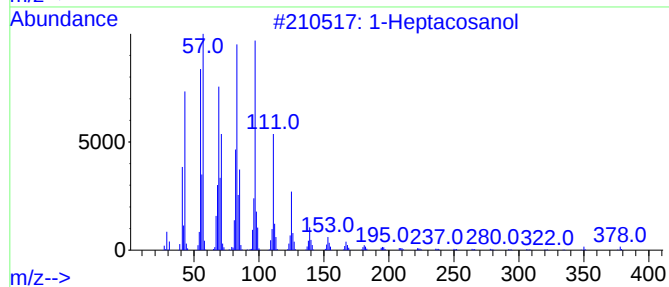
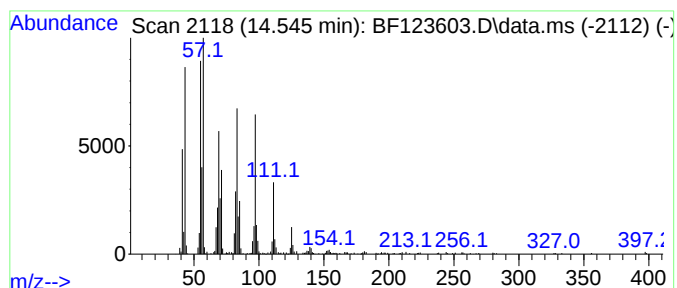
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Heptacosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.545	18.29 ng	1358420	Chrysene-d12	14.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heptacosanol	396	C27H56O	002004-39-9	91
2			1-Docosene	308	C22H44	001599-67-3	91
3			1-Tricosene	322	C23H46	018835-32-0	90
4			Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	87
5			Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041621\
Data File : BF123603.D
Acq On : 16 Apr 2021 21:17
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Sample : M2048-12
Misc :
ALS Vial : 11 Sample Multiplier: 1

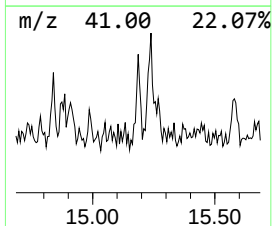
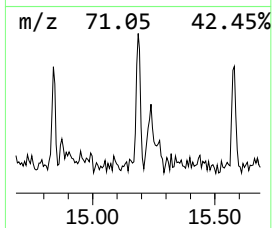
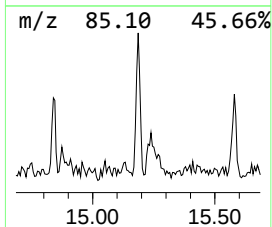
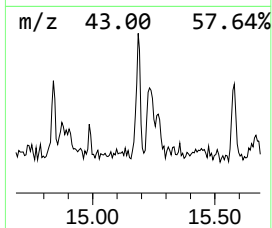
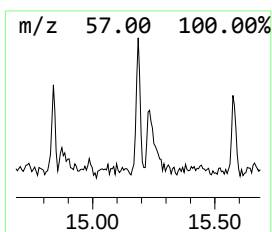
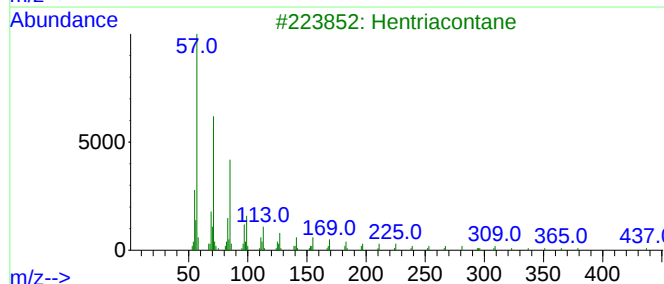
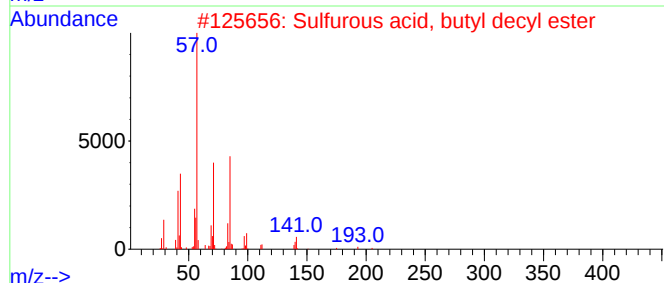
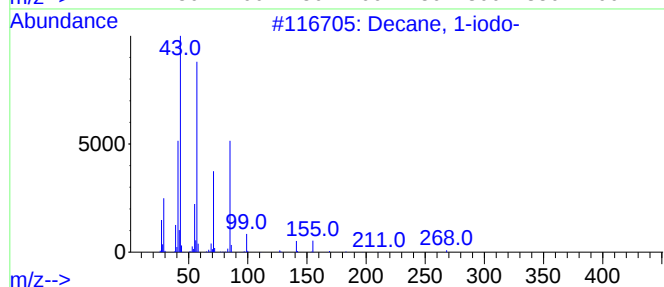
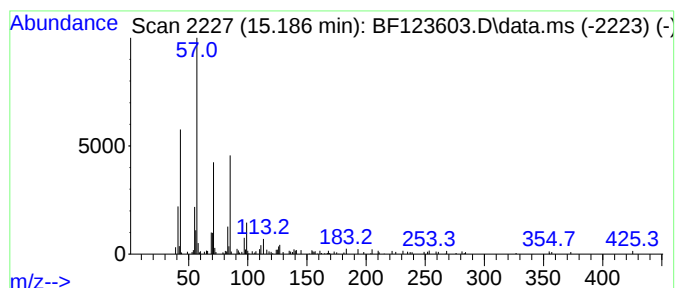
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ClientSampleId :
SB-04-14.5-15.0

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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 Decane, 1-iodo- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.186	2.73 ng	170113	Perylene-d12	15.539	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane, 1-iodo-	268	C10H21I	002050-77-3	86
2	Sulfurous acid, butyl decyl ester	278	C14H30O3S	1000309-17-7	72
3	Hentriacontane	437	C31H64	000630-04-6	58
4	Tridecane, 6-methyl-	198	C14H30	013287-21-3	52
5	Heptacosane	380	C27H56	000593-49-7	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041621\
Data File : BF123603.D
Acq On : 16 Apr 2021 21:17
Operator : JU/CG
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Misc :
ALS Vial : 11 Sample Multiplier: 1

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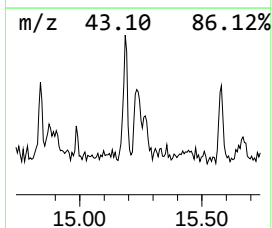
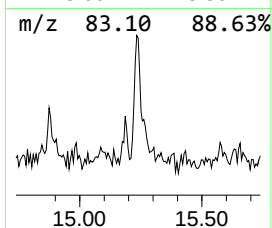
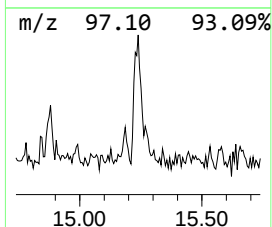
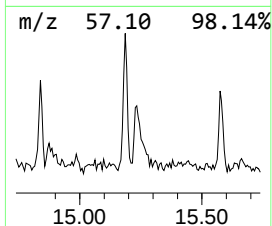
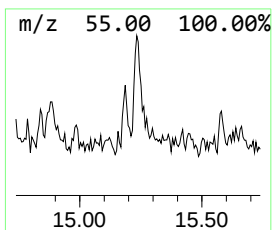
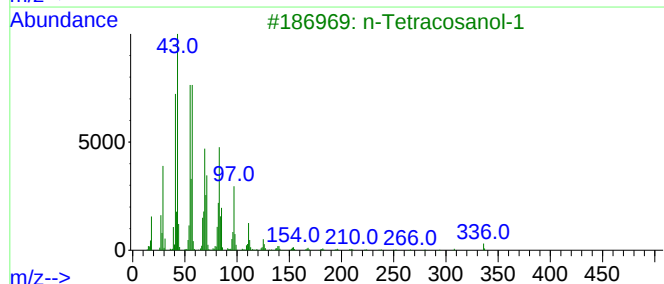
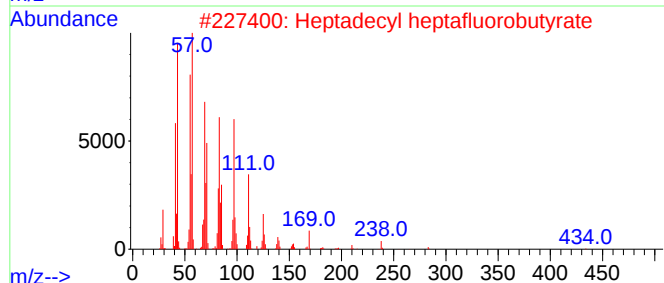
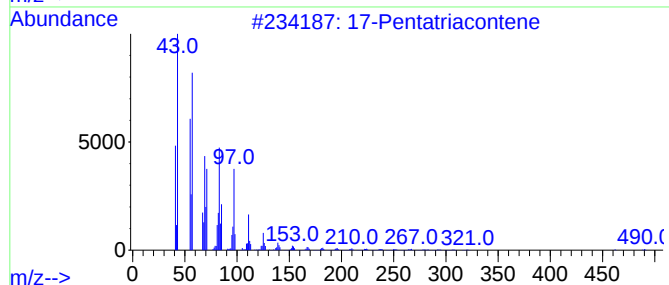
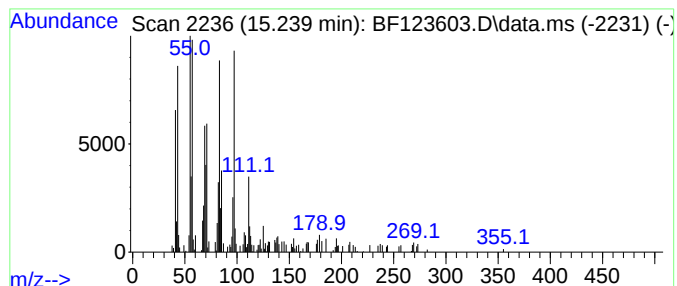
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 17-Pentatriacontene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.239	4.23 ng	263153	Perylene-d12	15.539

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	17-Pentatriacontene			491	C35H70	006971-40-0	72
2	Heptadecyl heptafluorobutyrate			452	C21H35F7O2	959085-66-6	62
3	n-Tetracosanol-1			354	C24H50O	000506-51-4	58
4	1-Dodecanol, 2-octyl-			298	C20H42O	005333-42-6	53
5	Tetracosyl heptafluorobutyrate			550	C28H49F7O2	1000351-83-7	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041621\
Data File : BF123603.D
Acq On : 16 Apr 2021 21:17
Operator : JU/CG
Sample : M2048-12
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-04-14.5-15.0

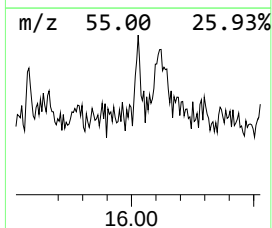
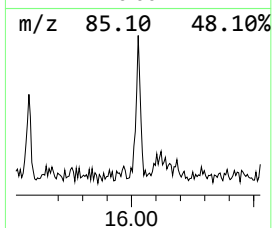
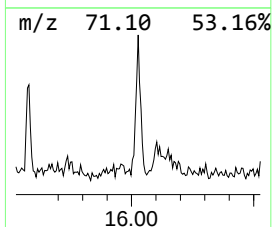
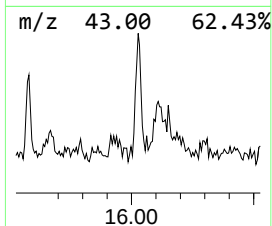
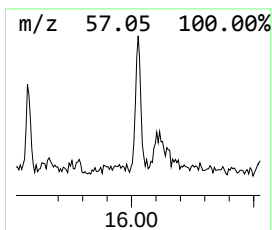
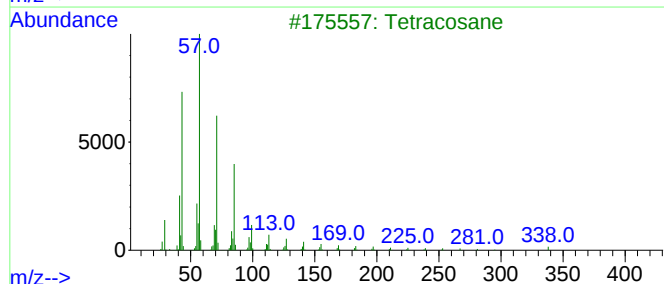
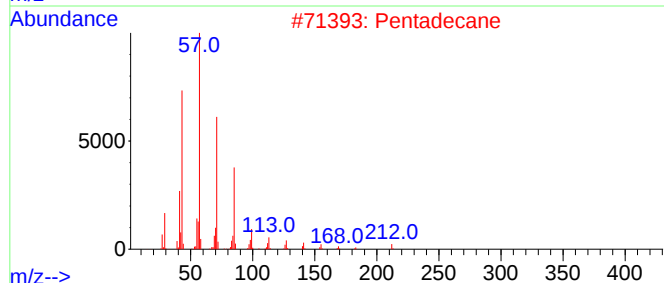
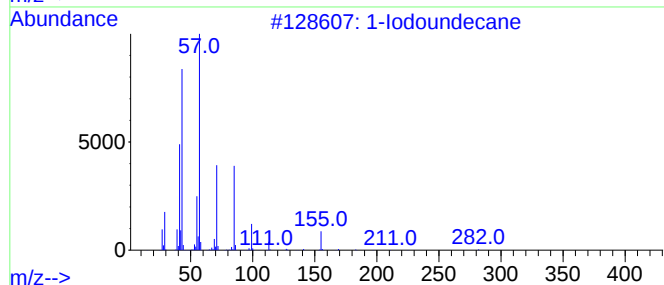
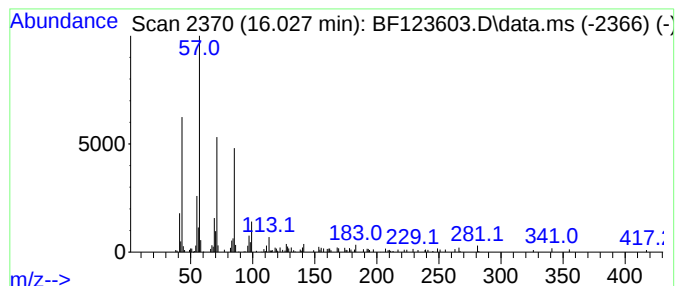
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 1-Iodoundecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.027	3.39 ng	211035	Perylene-d12	15.539

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Iodoundecane			282	C11H23I	004282-44-4	87
2	Pentadecane			212	C15H32	000629-62-9	83
3	Tetracosane			338	C24H50	000646-31-1	80
4	Tetradecane			198	C14H30	000629-59-4	80
5	Tridecane, 1-iodo-			310	C13H27I	035599-77-0	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041621\
Data File : BF123603.D
Acq On : 16 Apr 2021 21:17
Operator : JU/CG
Sample : M2048-12
Misc :
ALS Vial : 11 Sample Multiplier: 1

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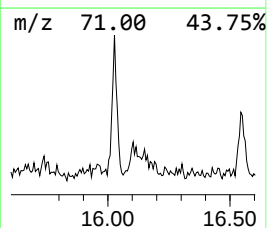
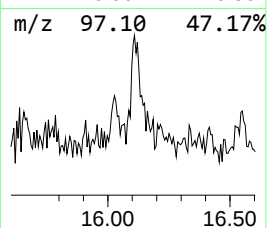
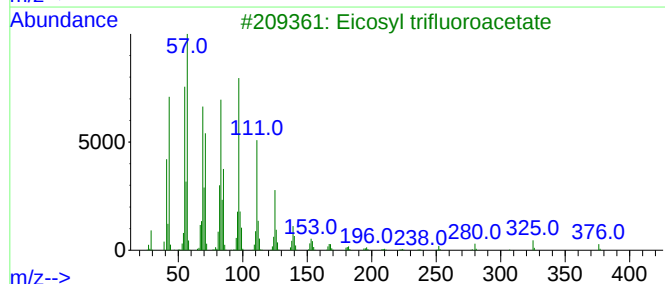
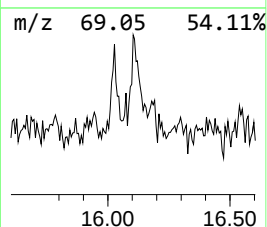
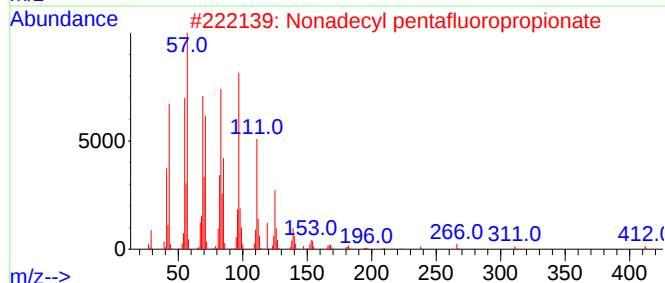
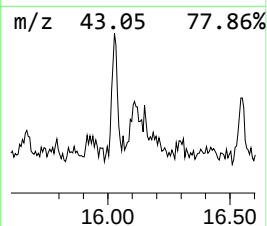
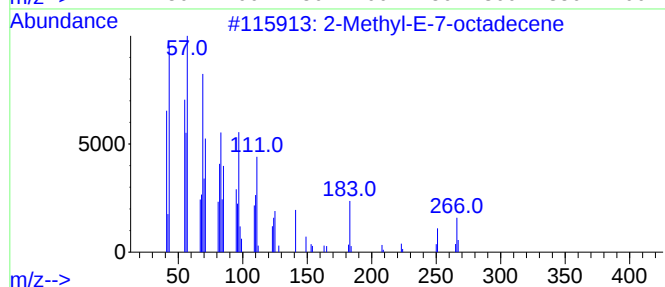
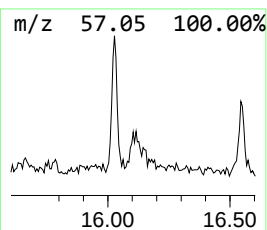
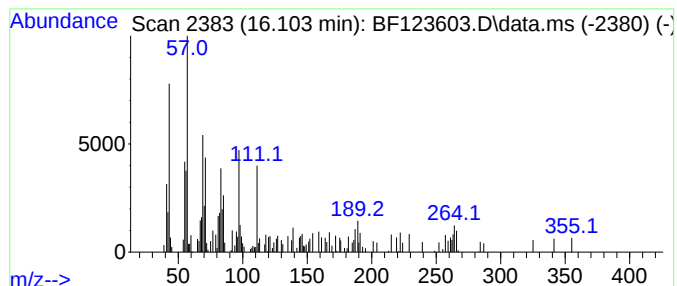
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 2-Methyl-E-7-octadecene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.104	2.20 ng	136806	Perylene-d12	15.539

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Methyl-E-7-octadecene	266	C19H38	1000130-92-3	90
2			Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	80
3			Eicosyl trifluoroacetate	394	C22H41F3O2	1000351-75-2	74
4			Eicosyl pentafluoropropionate	444	C23H41F5O2	1000351-80-8	72
5			Carbonic acid, isobutyl pentadec...	328	C20H40O3	1000314-61-2	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041621\
Data File : BF123603.D
Acq On : 16 Apr 2021 21:17
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Sample : M2048-12
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
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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...	2.181	55.4	ng	4653760	1	6.869	1679120	20.0
1,3-Dioxolane, ...	3.010	2.1	ng	174530	1	6.869	1679120	20.0
2-Pentanone, 4-...	5.104	3.7	ng	308974	1	6.869	1679120	20.0
n-Hexadecanoic ...	11.933	8.1	ng	948006	4	11.404	2350200	20.0
Octacosane	13.227	2.9	ng	218263	5	14.051	1485670	20.0
Heptafluorobuty...	13.904	22.6	ng	1676930	5	14.051	1485670	20.0
1-Heptacosanol	14.545	18.3	ng	1358420	5	14.051	1485670	20.0
Decane, 1-iodo-	15.186	2.7	ng	170113	6	15.539	1244420	20.0
17-Pentatriacon...	15.239	4.2	ng	263153	6	15.539	1244420	20.0
1-Iodoundecane	16.027	3.4	ng	211035	6	15.539	1244420	20.0
2-Methyl-E-7-oc...	16.104	2.2	ng	136806	6	15.539	1244420	20.0