

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF011719\
 Data File : BF112079.D
 Acq On : 17 Jan 2019 10:26
 Operator : JU/SJ
 Sample : K1147-10
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-4

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-BF011619.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	2.163	8	13	21	rVB	162608	228408	2.62%	0.316%
2	5.087	505	510	518	rVB	313864	398776	4.58%	0.552%
3	5.498	576	580	601	rBV	6424309	6156496	70.65%	8.530%
4	6.504	746	751	769	rVB	5626732	6668588	76.52%	9.239%
5	6.639	769	774	777	rBV	6925168	6774266	77.73%	9.386%
6	6.686	779	782	788	rVB	94944	98490	1.13%	0.136%
7	6.857	808	811	815	rBV	1924315	1681514	19.30%	2.330%
8	7.016	834	838	842	rBV	5757656	5440672	62.43%	7.538%
9	7.422	901	907	910	rBV	4324268	4194068	48.13%	5.811%
10	8.139	1025	1029	1033	rBV	2430247	2208047	25.34%	3.059%
11	9.216	1207	1212	1216	rBV	8507225	8378617	96.14%	11.608%
12	9.604	1274	1278	1282	rBV	1887349	1651309	18.95%	2.288%
13	9.898	1323	1328	1332	rBV	2959201	2636108	30.25%	3.652%
14	10.692	1457	1463	1466	rBV	5257526	5539318	63.56%	7.675%
15	11.386	1576	1581	1584	rBV	2876424	2815145	32.30%	3.900%
16	11.910	1667	1670	1682	rBV2	321888	349553	4.01%	0.484%
17	12.421	1755	1757	1762	rBV2	83646	93946	1.08%	0.130%
18	12.968	1845	1850	1854	rBV	8169088	8714680	100.00%	12.074%
19	13.857	1998	2001	2009	rBV	333605	425630	4.88%	0.590%
20	14.021	2026	2029	2033	rBV	2158275	2071705	23.77%	2.870%
21	14.180	2053	2056	2062	rBV	133936	129366	1.48%	0.179%
22	14.486	2104	2108	2115	rBV2	263761	318560	3.66%	0.441%
23	14.698	2141	2144	2150	rVB3	95801	108340	1.24%	0.150%
24	14.792	2157	2160	2165	rVB	259473	248178	2.85%	0.344%
25	14.868	2170	2173	2176	rBV	283721	261934	3.01%	0.363%
26	15.133	2214	2218	2228	rVB	349661	407312	4.67%	0.564%
27	15.498	2275	2280	2289	rBV	1503029	2164090	24.83%	2.998%
28	15.951	2352	2357	2363	rVB	319628	455268	5.22%	0.631%
29	16.456	2438	2443	2450	rVB2	163850	272469	3.13%	0.377%
30	17.051	2539	2544	2552	rVB2	93938	202142	2.32%	0.280%
31	17.145	2553	2560	2569	rVV2	470078	911944	10.46%	1.263%
32	18.327	2757	2761	2769	rVB8	80617	173037	1.99%	0.240%

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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

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011619.M
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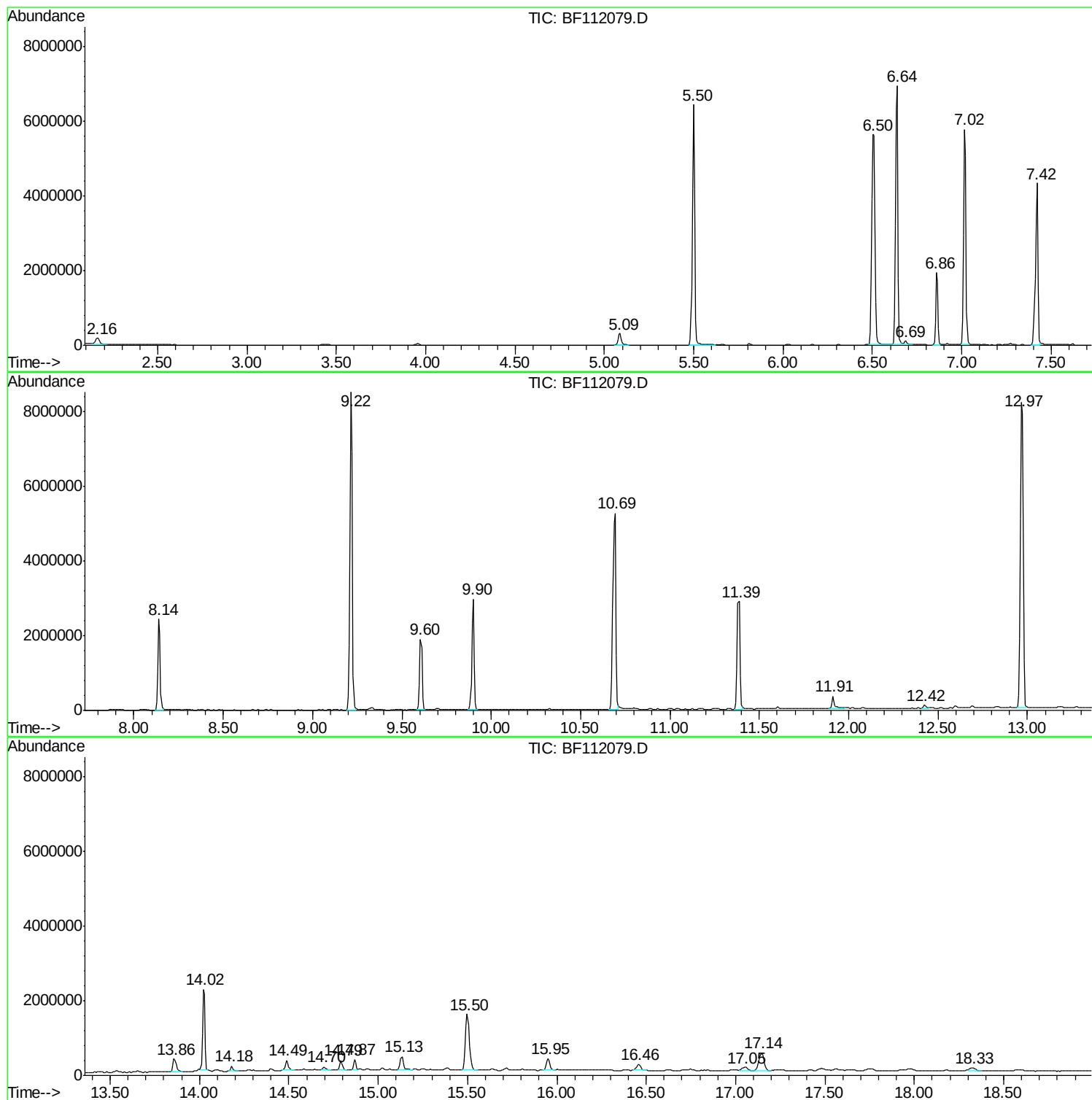
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF011619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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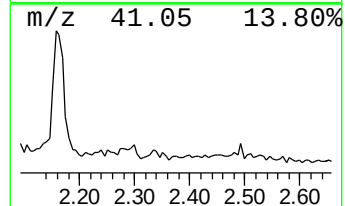
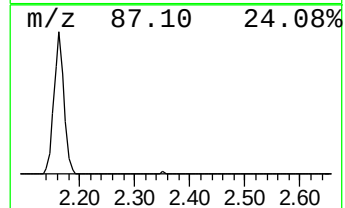
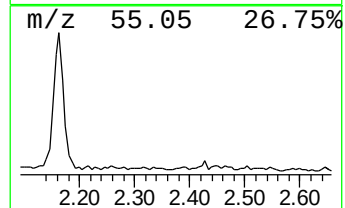
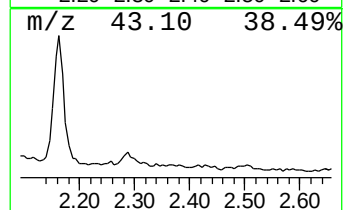
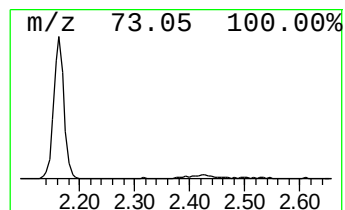
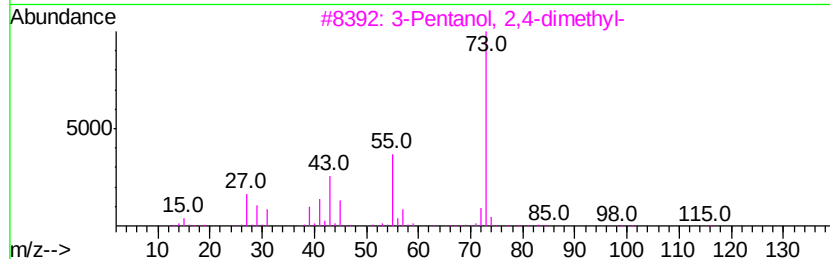
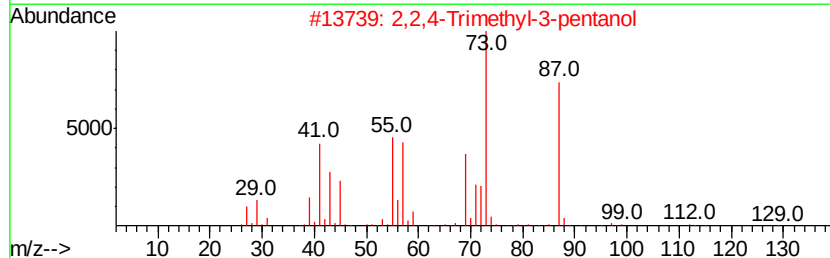
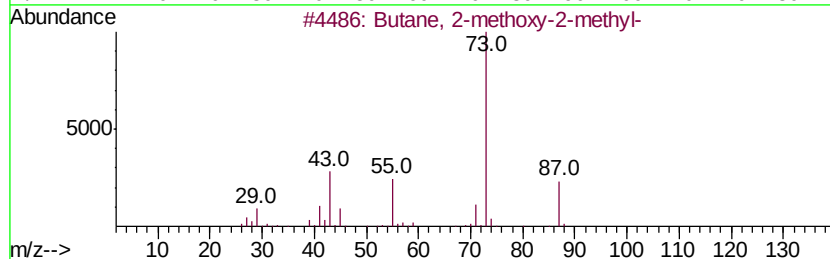
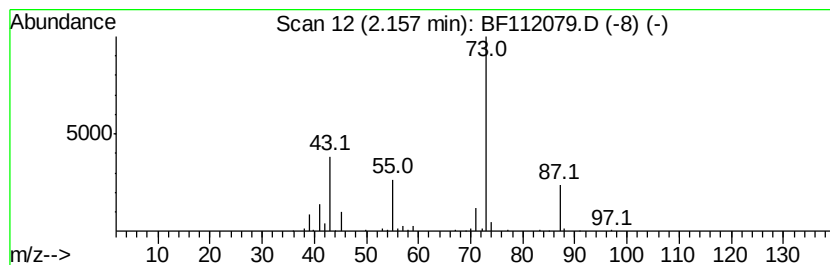
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.16	2.72 ng	228408	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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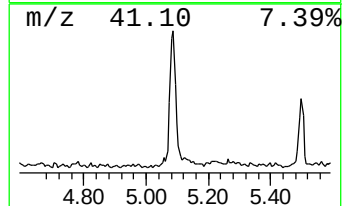
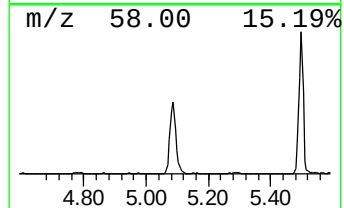
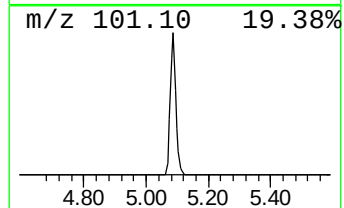
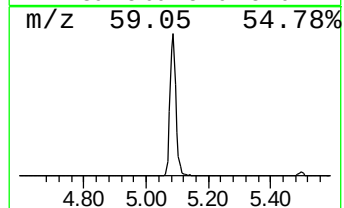
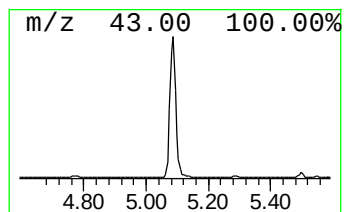
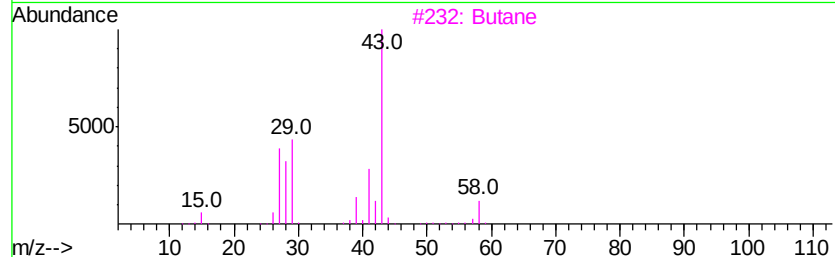
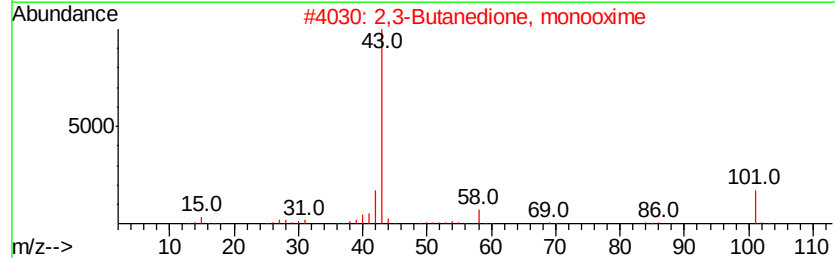
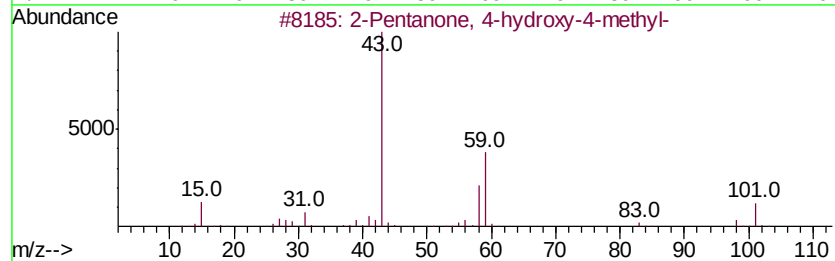
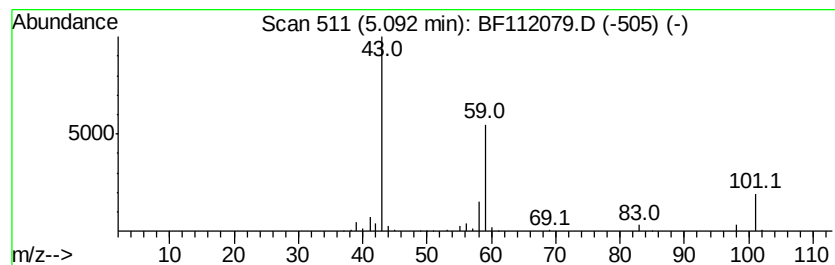
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	4.74 ng	398776	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	47
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
3		Butane	58	C4H10	000106-97-8	9
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		Allyl acetate	100	C5H8O2	000591-87-7	9



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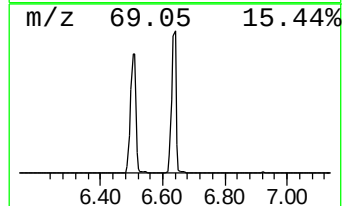
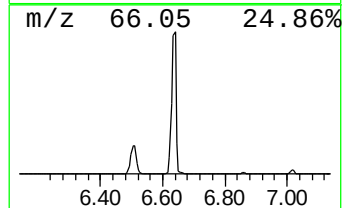
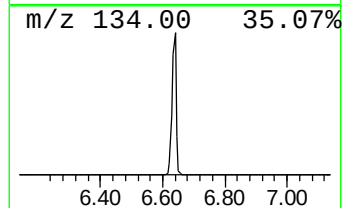
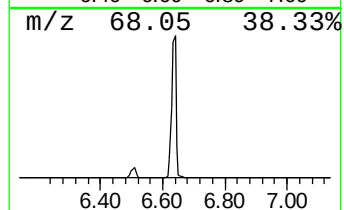
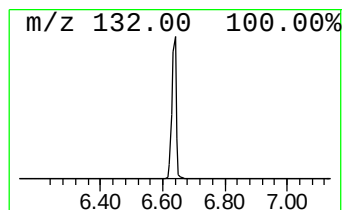
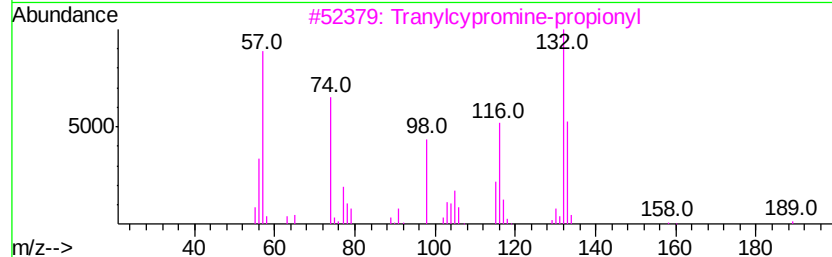
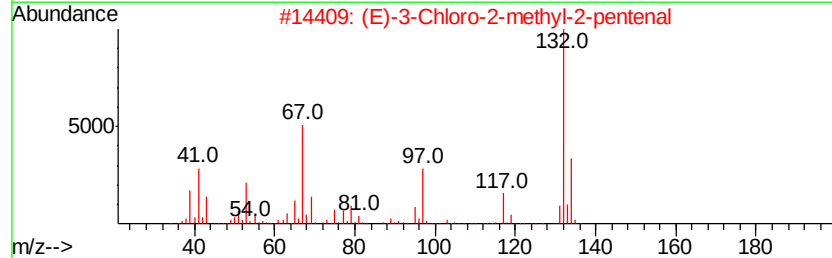
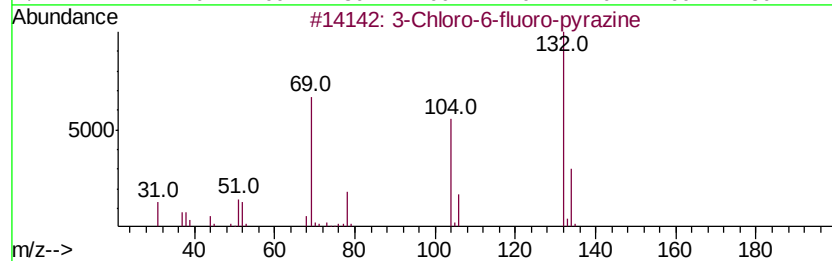
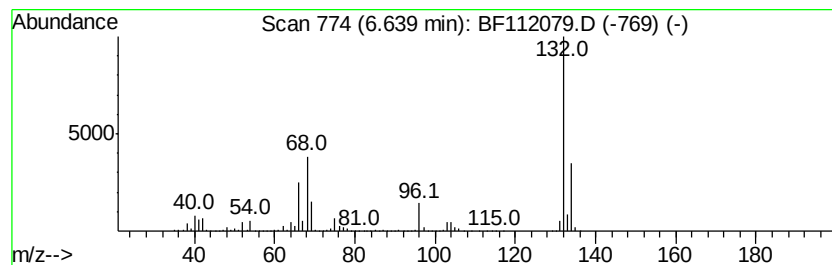
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.64 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.64	80.57 ng	6774270	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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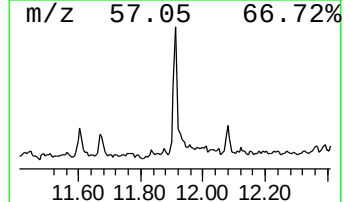
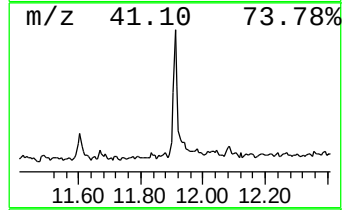
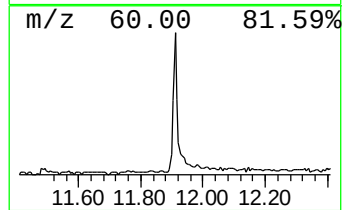
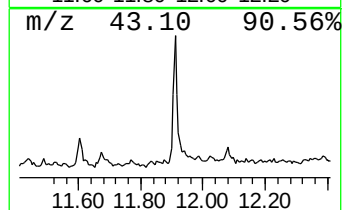
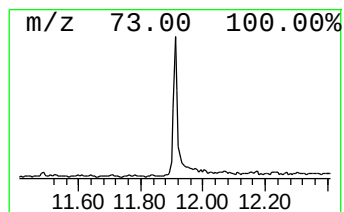
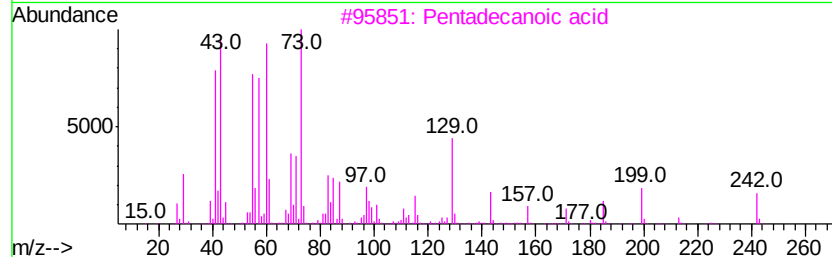
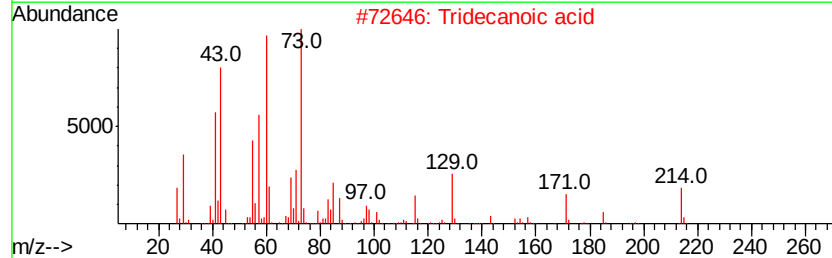
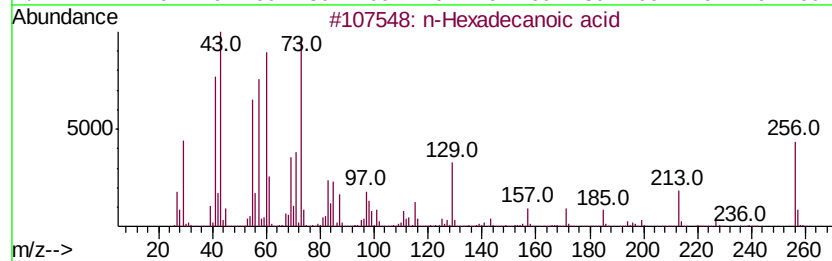
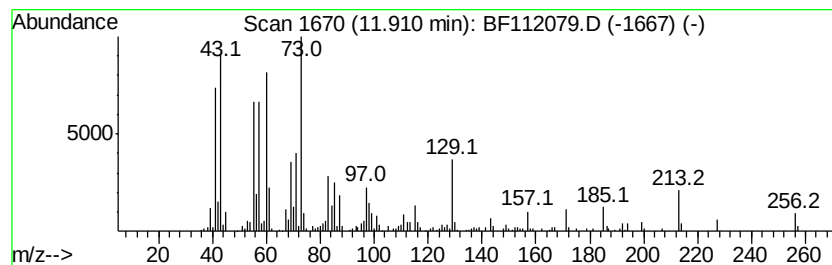
Instrument :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 n-Hexadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.91	2.48 ng	349553	Phenanthrene-d10		11.39
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	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5	n-Decanoic acid	172	C10H20O2	000334-48-5	49



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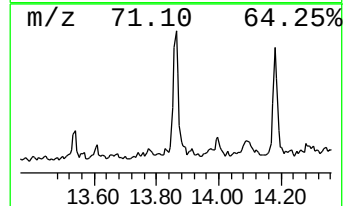
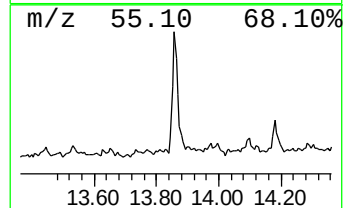
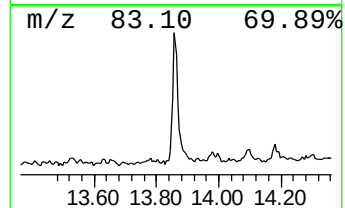
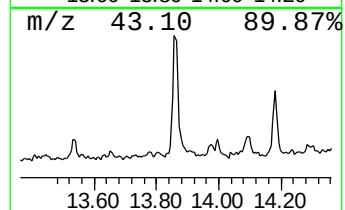
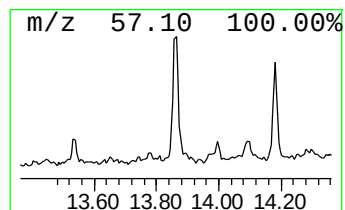
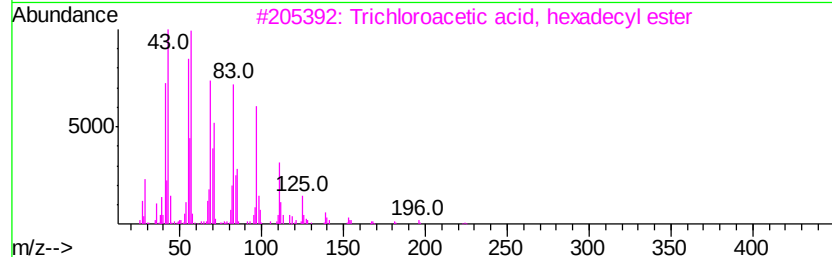
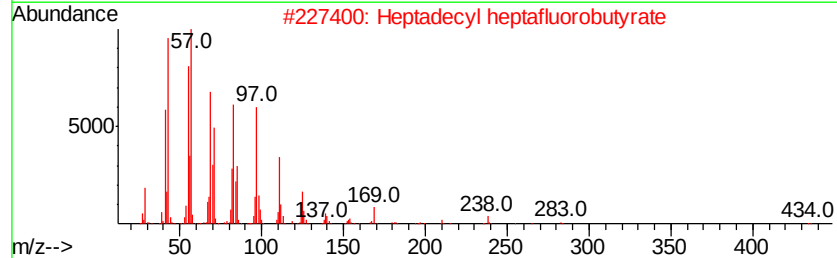
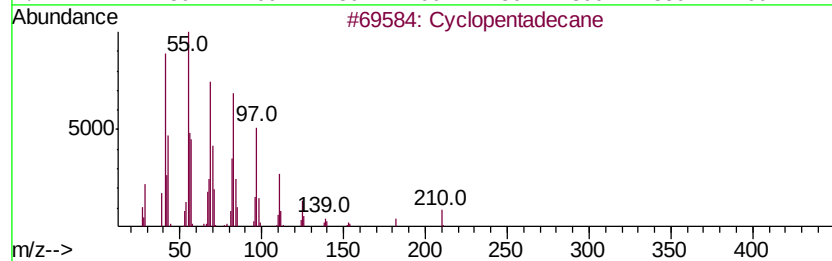
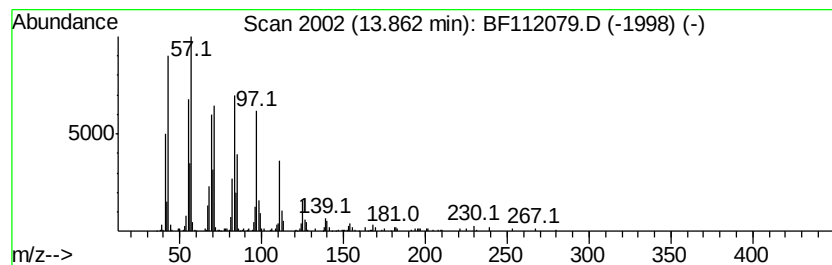
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Cyclopentadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.86	4.11 ng	425630	Chrysene-d12		14.02	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cvclopentadecane	210	C15H30	000295-48-7	94
2		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
4		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
5		Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94



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ALS Vial : 6 Sample Multiplier: 1

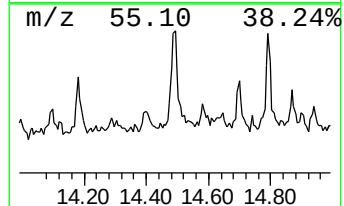
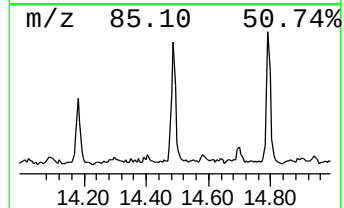
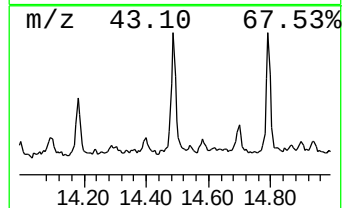
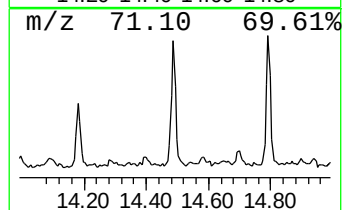
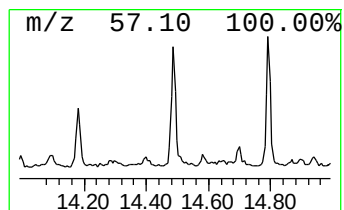
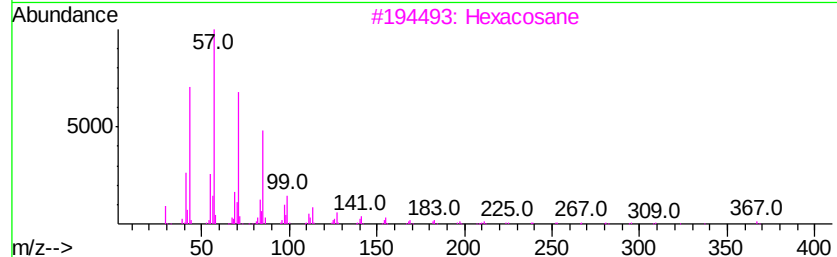
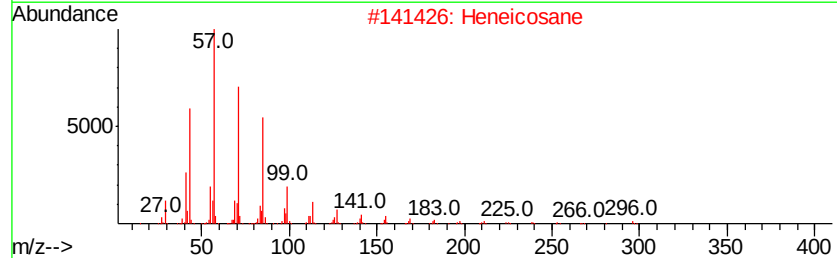
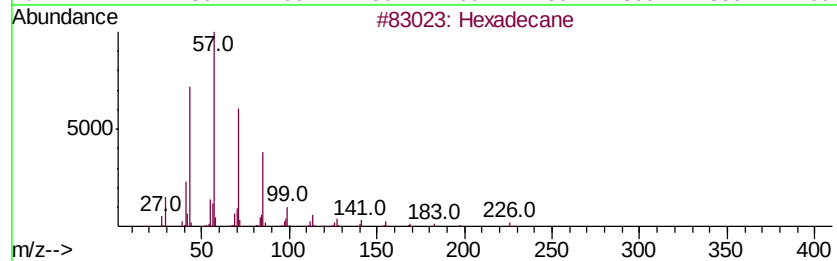
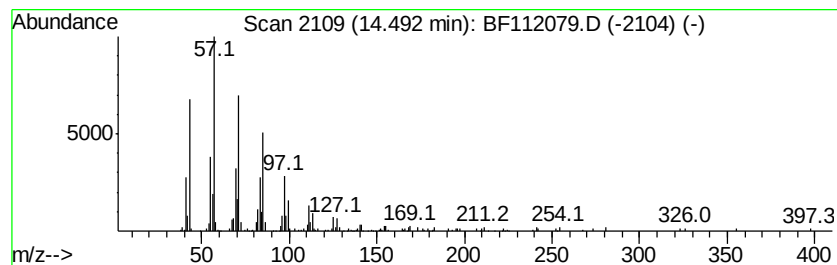
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF011619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.49	3.08 ng	318560	Chrysene-d12	14.02	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	93
2	Heneicosane	296	C21H44	000629-94-7	91
3	Hexacosane	366	C26H54	000630-01-3	91
4	Tritetracontane	605	C43H88	007098-21-7	91
5	Nonadecane	268	C19H40	000629-92-5	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF011719\
Data File : BF112079.D
Acq On : 17 Jan 2019 10:26
Operator : JU/SJ
Sample : K1147-10
Misc :
ALS Vial : 6 Sample Multiplier: 1

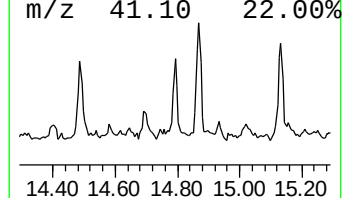
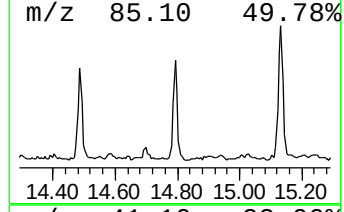
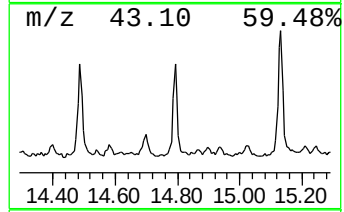
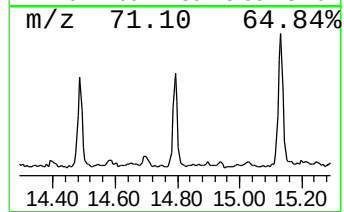
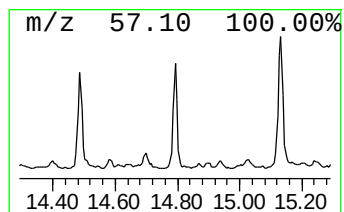
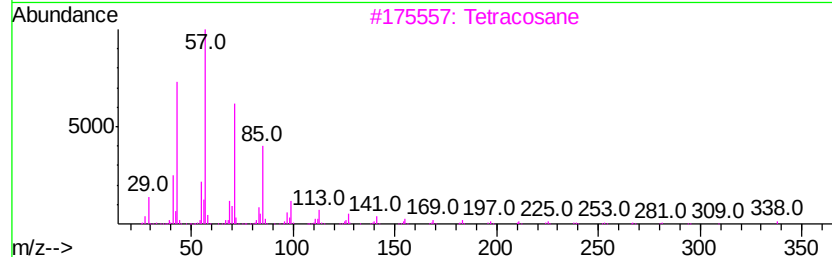
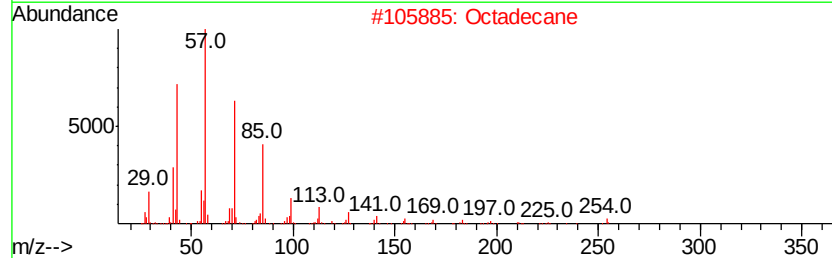
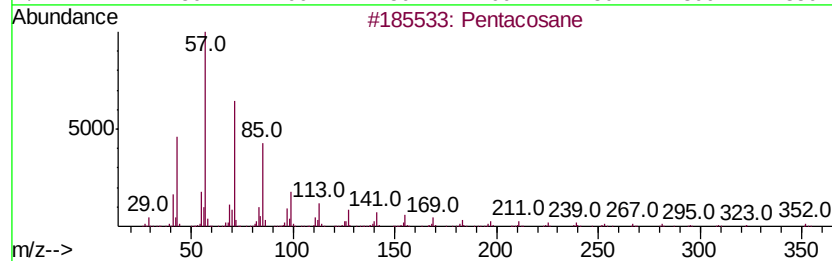
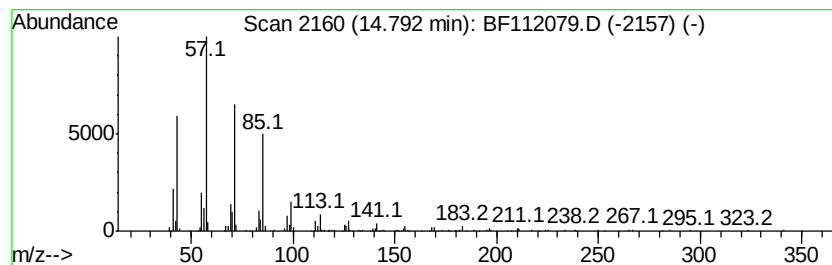
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Pentacosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.79	2.29 ng	248178	Perylene-d12	15.50
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Pentacosane	352 C25H52	000629-99-2	90
2	Octadecane	254 C18H38	000593-45-3	87
3	Tetracosane	338 C24H50	000646-31-1	87
4	Heneicosane	296 C21H44	000629-94-7	87
5	Heptadecane	240 C17H36	000629-78-7	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF011719\
Data File : BF112079.D
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Sample : K1147-10
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ALS Vial : 6 Sample Multiplier: 1

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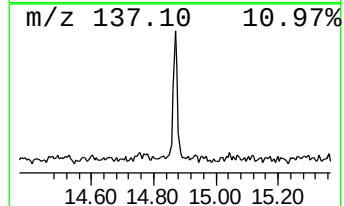
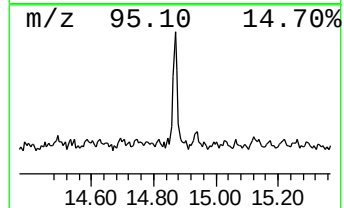
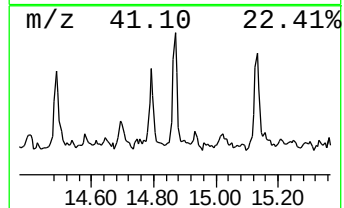
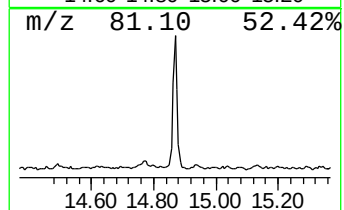
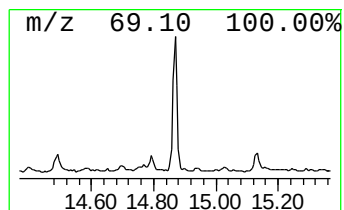
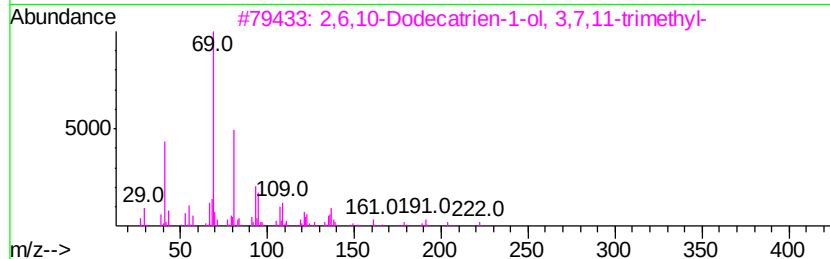
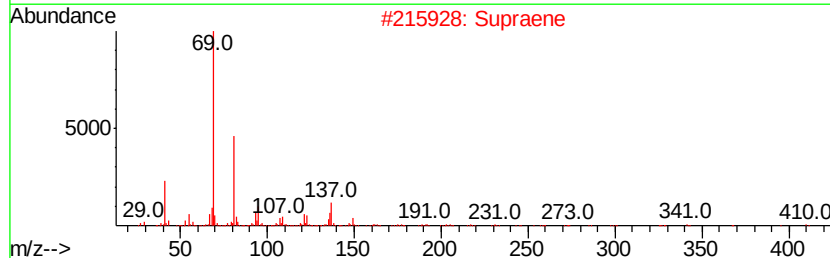
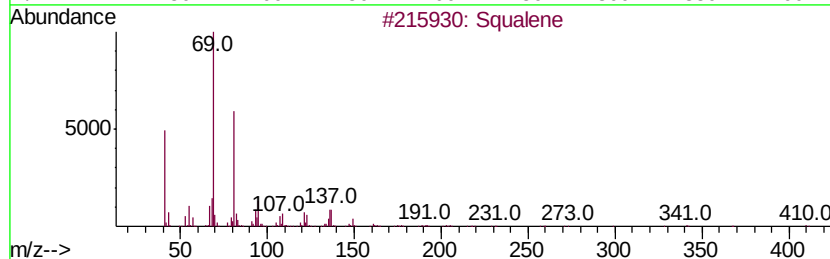
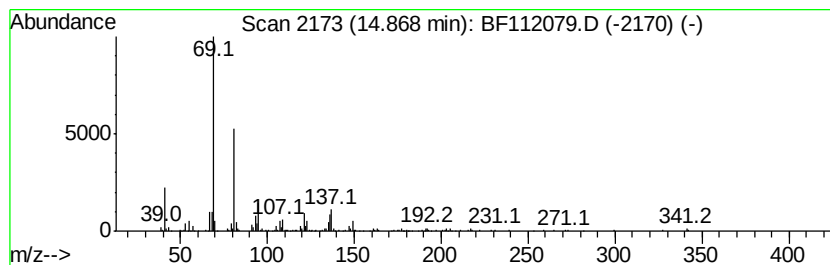
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Squalene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.87	2.42 ng	261934	Perylene-d12	15.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	91
2		Supraene	410	C30H50	007683-64-9	91
3		2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	78
4		1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	64
5		1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	50



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF011719\
 Data File : BF112079.D
 Acq On : 17 Jan 2019 10:26
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 Sample : K1147-10
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 ALS Vial : 6 Sample Multiplier: 1

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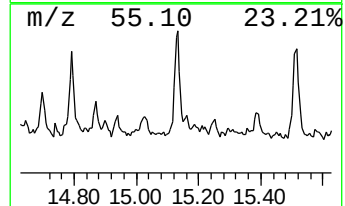
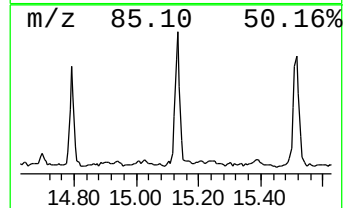
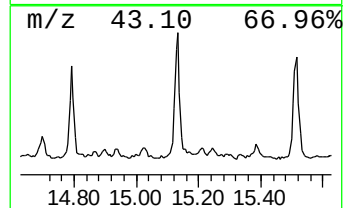
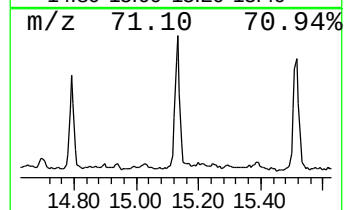
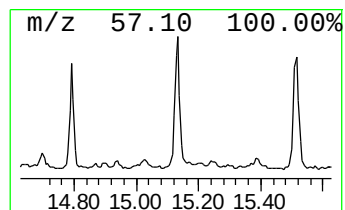
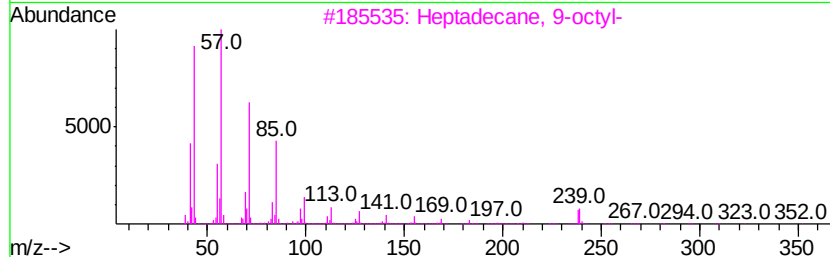
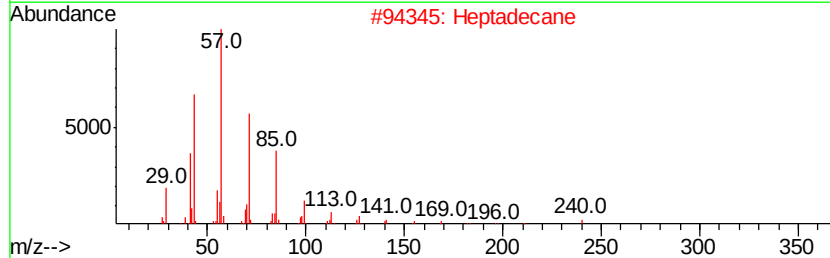
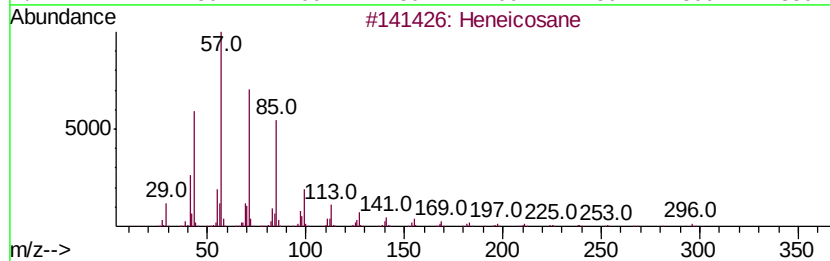
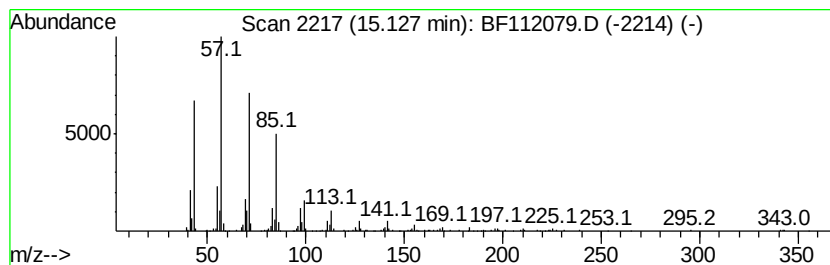
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 10 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.13	3.76 ng	407312	Perylene-d12	15.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	91
2		Heptadecane	240	C17H36	000629-78-7	91
3		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4		Eicosane	282	C20H42	000112-95-8	91
5		Tetracosane	338	C24H50	000646-31-1	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF011719\
Data File : BF112079.D
Acq On : 17 Jan 2019 10:26
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Sample : K1147-10
Misc :
ALS Vial : 6 Sample Multiplier: 1

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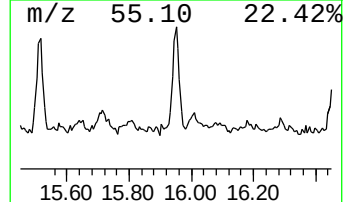
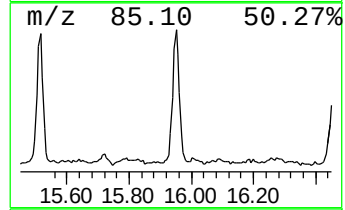
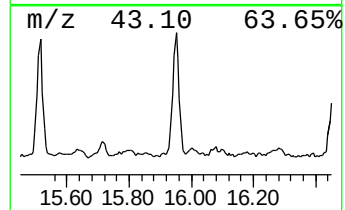
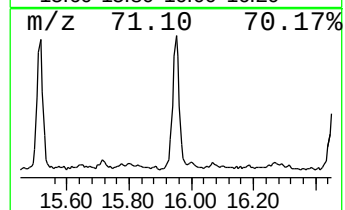
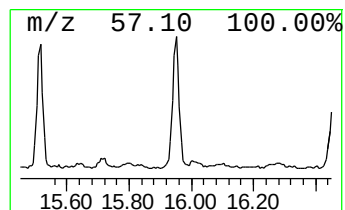
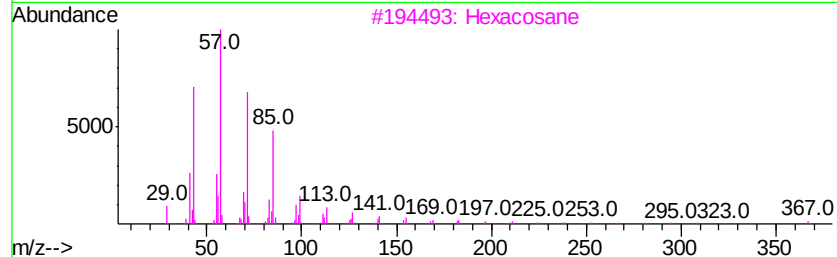
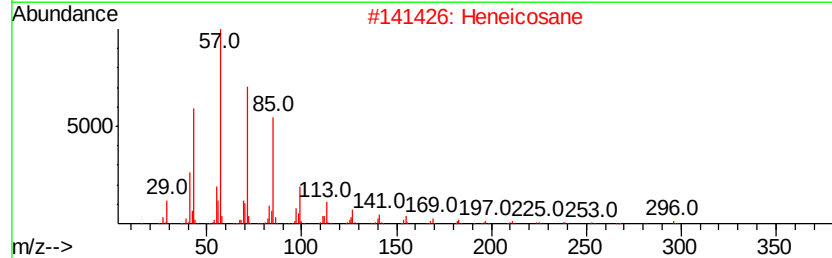
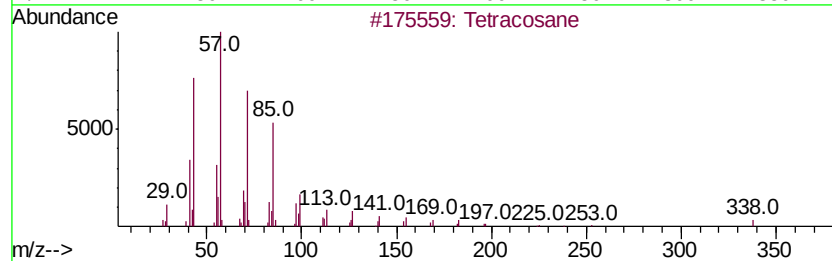
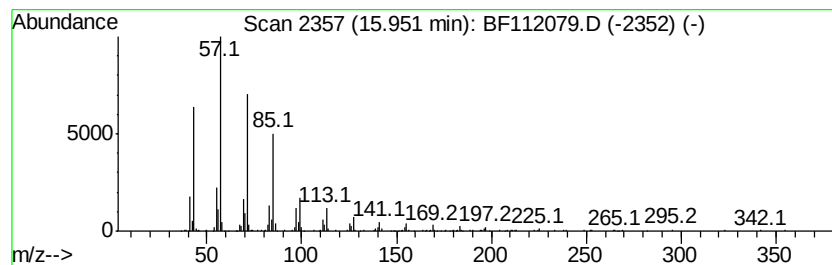
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Tetracosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.95	4.21 ng	455268	Perylene-d12	15.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetracosane	338	C24H50	000646-31-1	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Hexacosane	366	C26H54	000630-01-3	91
4		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5		Octadecane	254	C18H38	000593-45-3	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF011719\
Data File : BF112079.D
Acq On : 17 Jan 2019 10:26
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Sample : K1147-10
Misc :
ALS Vial : 6 Sample Multiplier: 1

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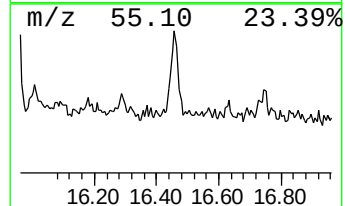
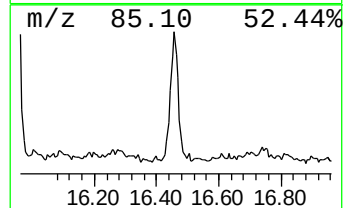
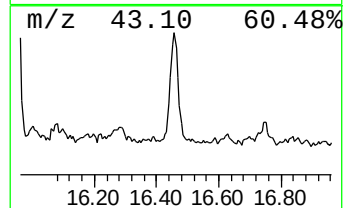
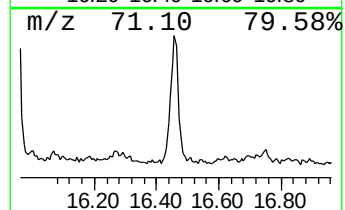
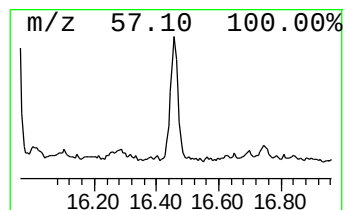
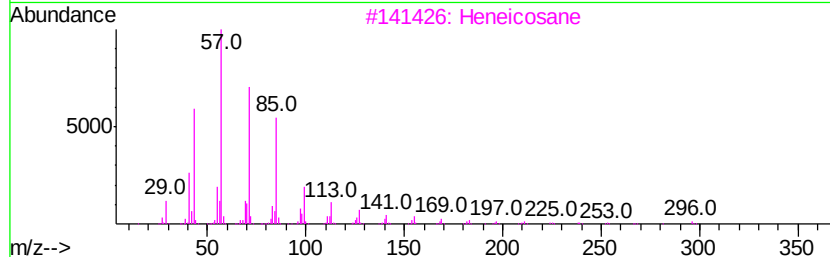
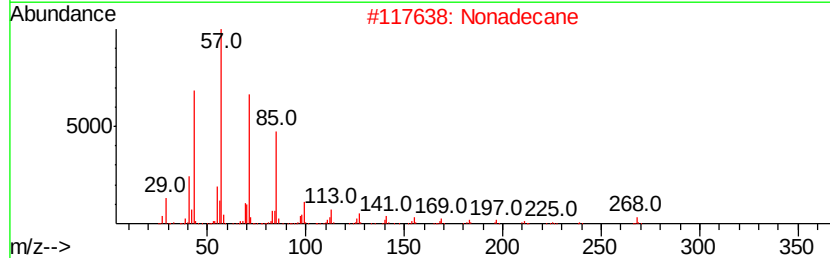
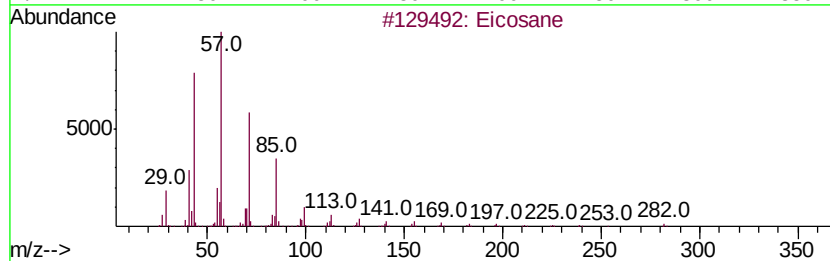
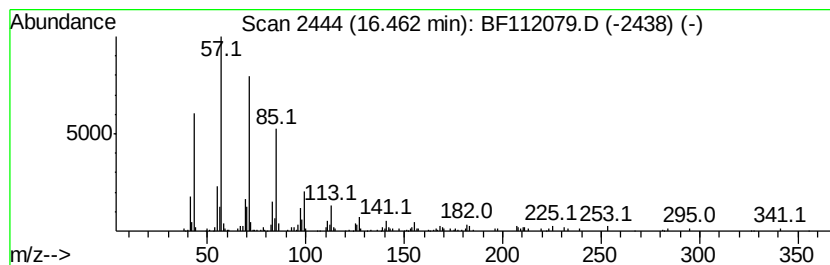
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Eicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.46	2.52 ng	272469	Perylene-d12	15.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	95
2		Nonadecane	268	C19H40	000629-92-5	93
3		Heneicosane	296	C21H44	000629-94-7	90
4		Octacosane	394	C28H58	000630-02-4	87
5		Pentacosane	352	C25H52	000629-99-2	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF011719\
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ClientSampled :
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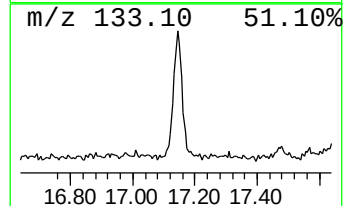
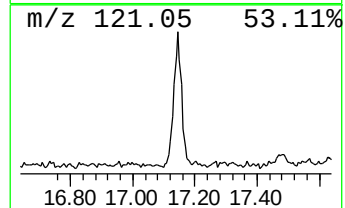
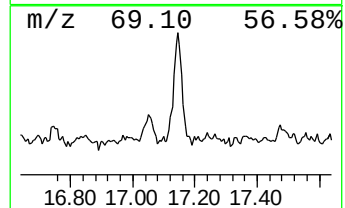
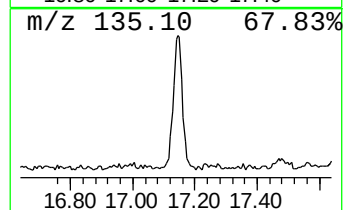
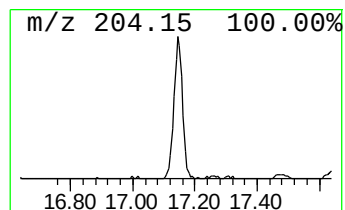
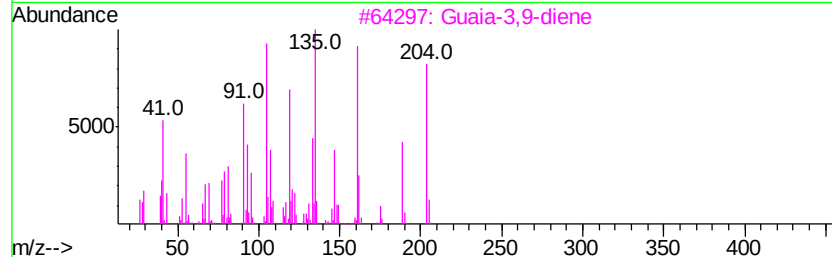
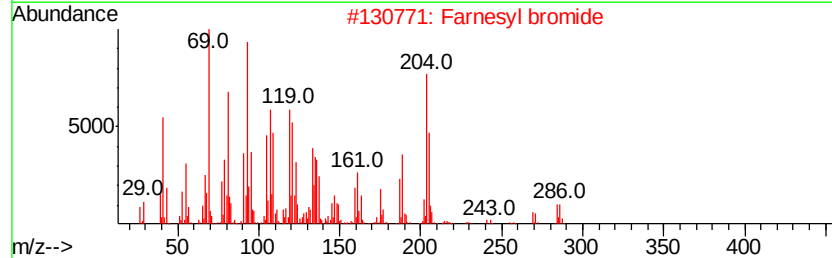
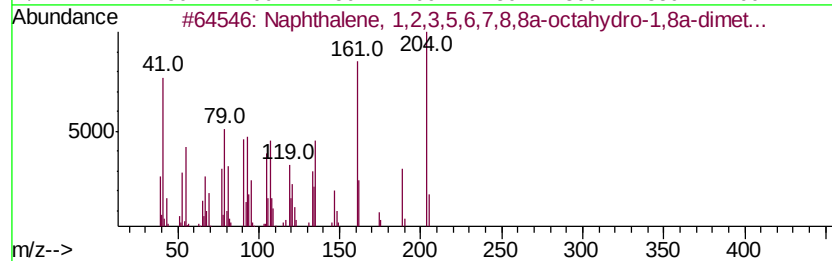
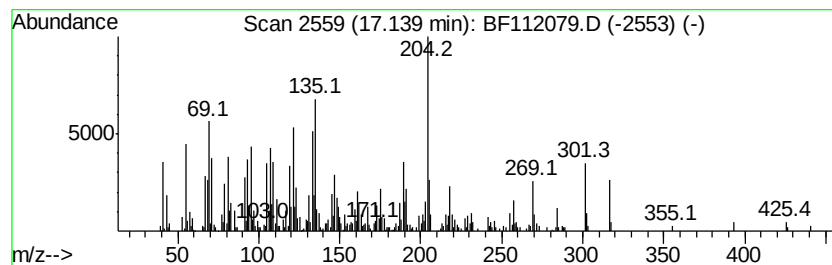
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Naphthalene, 1,2,3,5,6,7,8,... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.14	8.43 ng	911944	Perylene-d12	15.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Naphthalene, 1,2,3,5,6,7,8,8a-oc...	204	C15H24	004630-07-3	58
2		Farnesyl bromide	284	C15H25Br	006874-67-5	46
3		Guaia-3,9-diene	204	C15H24	000489-83-8	46
4		1,4-Dimethyl-8-isopropylidenetri...	204	C15H24	1000140-07-7	46
5		1,2,4,8-Tetramethylbicyclo[6.3.0...	204	C15H24	137235-51-9	45



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF011719\
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 Misc :
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Instrument :
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 ClientSampleId :
 TP-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011619.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-methoxy...	2.16	2.7	ng	228408	1	6.86	1681510	20.0
2-Pentanone, 4-hy...	5.09	4.7	ng	398776	1	6.86	1681510	20.0
unknown6.64	6.64	80.6	ng	6774270	1	6.86	1681510	20.0
n-Hexadecanoic acid	11.91	2.5	ng	349553	4	11.39	2815150	20.0
Cyclopentadecane	13.86	4.1	ng	425630	5	14.02	2071710	20.0
Hexadecane	14.49	3.1	ng	318560	5	14.02	2071710	20.0
Pentacosane	14.79	2.3	ng	248178	6	15.50	2164090	20.0
Squalene	14.87	2.4	ng	261934	6	15.50	2164090	20.0
Heneicosane	15.13	3.8	ng	407312	6	15.50	2164090	20.0
Tetracosane	15.95	4.2	ng	455268	6	15.50	2164090	20.0
Eicosane	16.46	2.5	ng	272469	6	15.50	2164090	20.0
Naphthalene, 1,2,...	17.14	8.4	ng	911944	6	15.50	2164090	20.0