

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF111919\
 Data File : BF117881.D
 Acq On : 20 Nov 2019 4:22
 Operator : JU
 Sample : K5908-04
 Misc :
 ALS Vial : 29 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B-8-3-(6-12)

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-BF111319.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	2.193	12	18	26	rVB	733070	941107	21.57%	2.376%
2	5.128	507	517	526	rBV	533142	636769	14.59%	1.608%
3	5.528	580	585	588	rBV	3528240	3264461	74.82%	8.243%
4	6.540	751	757	769	rVB	3538413	3971334	91.02%	10.028%
5	6.681	777	781	785	rBV	3890952	3688778	84.55%	9.314%
6	6.916	817	821	824	rBV	1332445	1057525	24.24%	2.670%
7	7.075	843	848	851	rBV	3326628	2884490	66.11%	7.284%
8	7.475	908	916	919	rBV	2522906	2290899	52.51%	5.785%
9	8.204	1036	1040	1043	rBV	1563052	1358101	31.13%	3.429%
10	9.281	1218	1223	1226	rBV	5199464	4362926	100.00%	11.017%
11	9.392	1238	1242	1246	rVB2	43912	53446	1.23%	0.135%
12	9.675	1286	1290	1294	rVB	619273	532147	12.20%	1.344%
13	9.963	1332	1339	1343	rBV	1669811	1462712	33.53%	3.693%
14	10.751	1469	1473	1477	rBV	2431698	2358585	54.06%	5.956%
15	10.880	1490	1495	1499	rVB2	46255	63220	1.45%	0.160%
16	11.457	1589	1593	1596	rBV	1466775	1225795	28.10%	3.095%
17	11.980	1673	1682	1692	rBV	834741	871374	19.97%	2.200%
18	12.674	1797	1800	1812	rVB	112730	185612	4.25%	0.469%
19	12.769	1812	1816	1824	rBV	623474	632079	14.49%	1.596%
20	12.904	1836	1839	1840	rBV	68428	55220	1.27%	0.139%
21	13.045	1859	1863	1867	rBV	4007065	3571967	81.87%	9.019%
22	13.274	1900	1902	1908	rBV3	63231	70173	1.61%	0.177%
23	13.621	1958	1961	1963	rBV	82038	71654	1.64%	0.181%
24	13.951	2014	2017	2018	rBV	172751	167208	3.83%	0.422%
25	14.080	2037	2039	2040	rBV	101585	83356	1.91%	0.210%
26	14.104	2040	2043	2046	rVB	1306152	1108172	25.40%	2.798%
27	14.263	2067	2070	2073	rBV	197165	194512	4.46%	0.491%
28	14.574	2119	2123	2127	rBV	256680	277063	6.35%	0.700%
29	14.868	2170	2173	2174	rBV	91192	88192	2.02%	0.223%
30	14.892	2174	2177	2181	rVB	244092	257598	5.90%	0.650%
31	15.245	2233	2237	2242	rVB	228071	265011	6.07%	0.669%
32	15.610	2295	2299	2303	rBV	689744	906810	20.78%	2.290%
33	15.645	2303	2305	2311	rVB	214891	250183	5.73%	0.632%
34	16.104	2379	2383	2390	rVB	142200	230658	5.29%	0.582%

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ALS Vial : 29 Sample Multiplier: 1

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ClientSampleId :
B-8-3-(6-12)

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 >
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35	17.339	2590	2593	2599	rVB6	95873	163869	3.76%	0.414%
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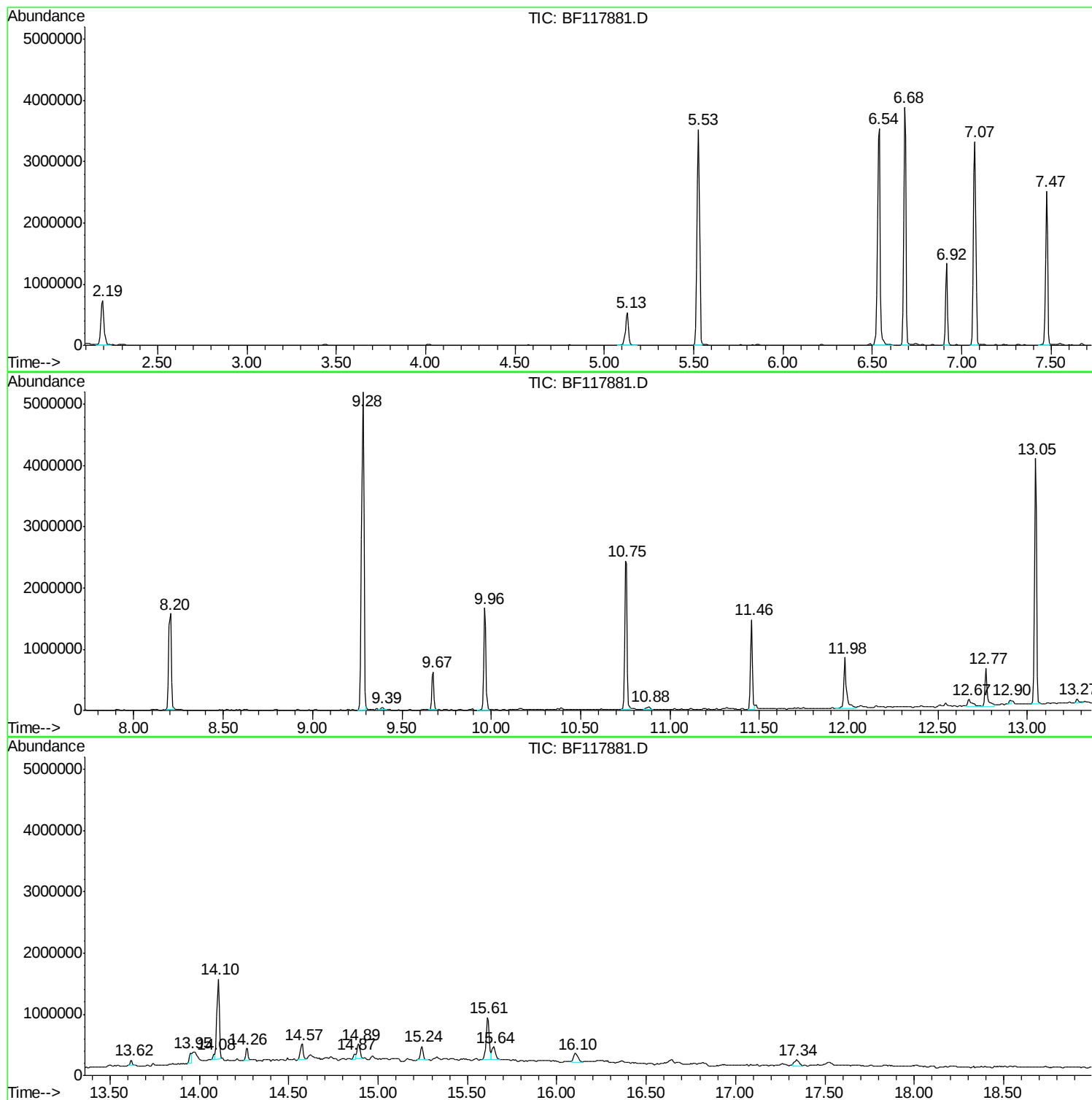
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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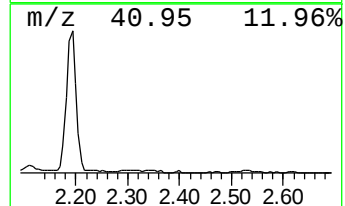
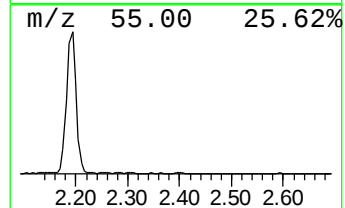
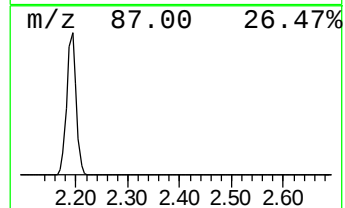
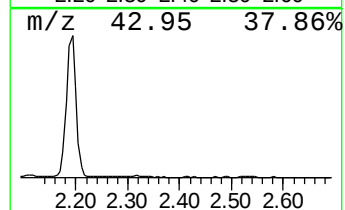
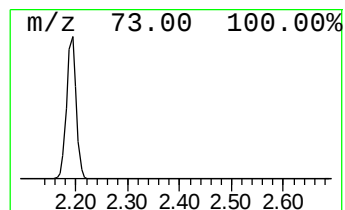
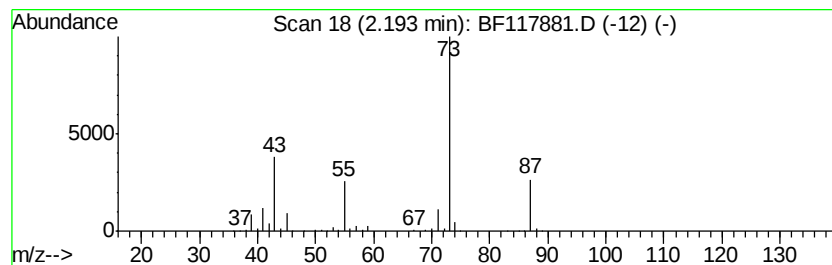
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.19	17.80 ng	941107	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5		N-Ethylformamide	73	C3H7NO	000627-45-2	9



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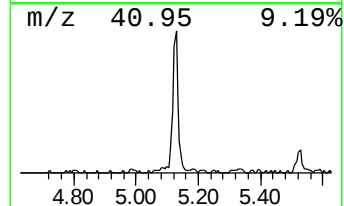
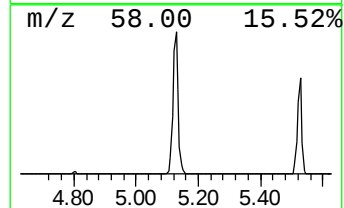
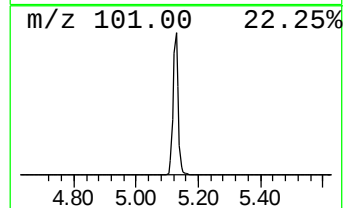
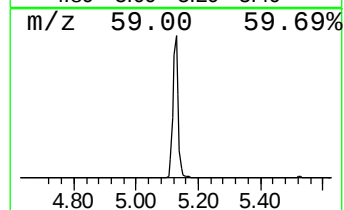
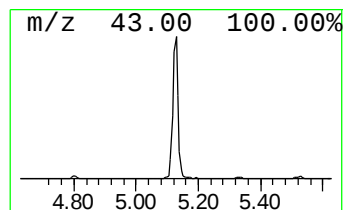
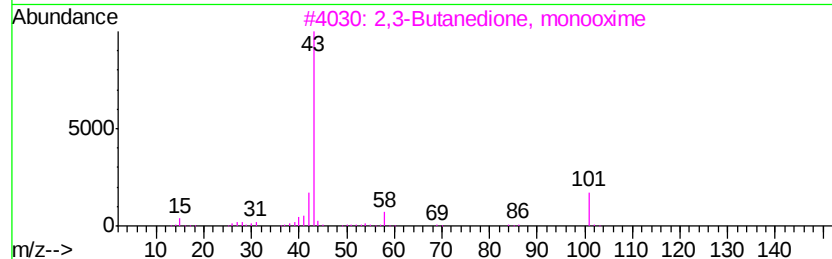
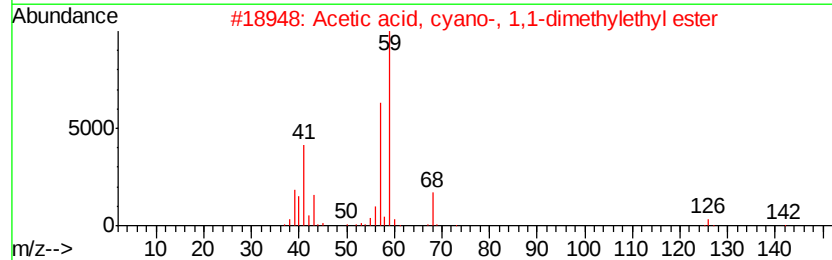
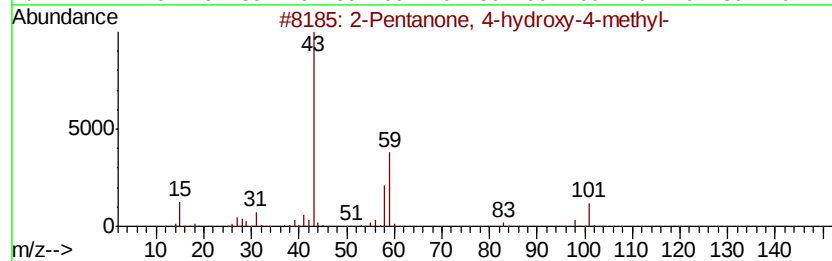
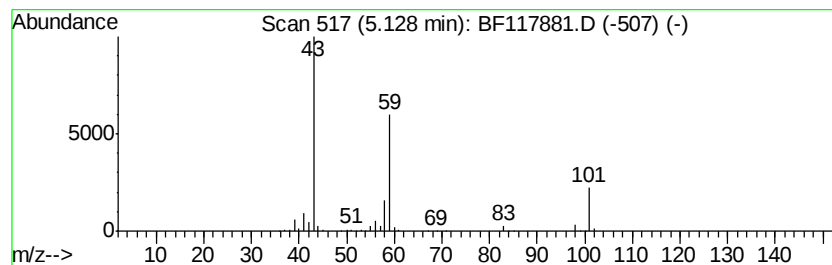
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	12.04 ng	636769	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	47
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		Allyl acetate	100	C5H8O2	000591-87-7	9



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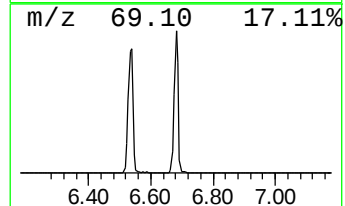
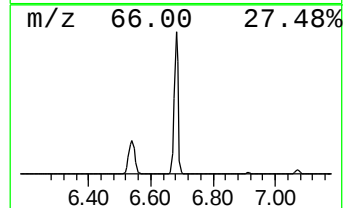
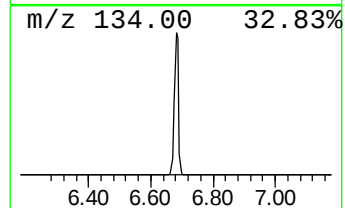
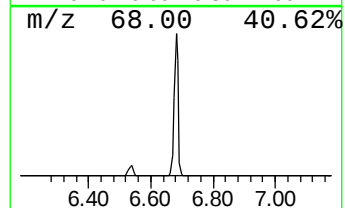
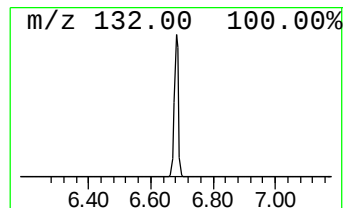
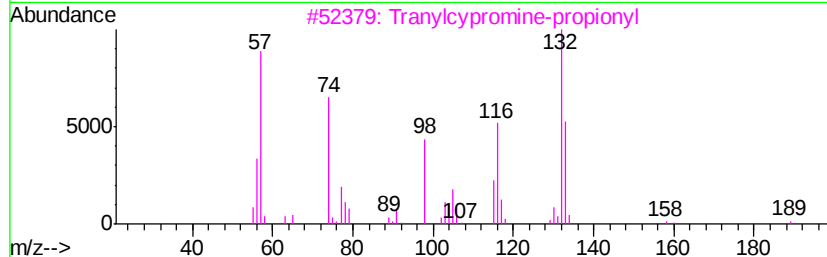
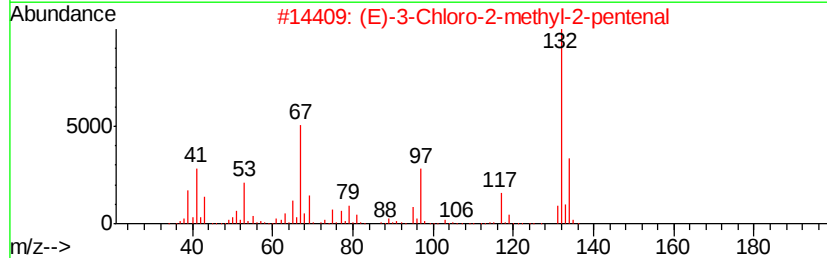
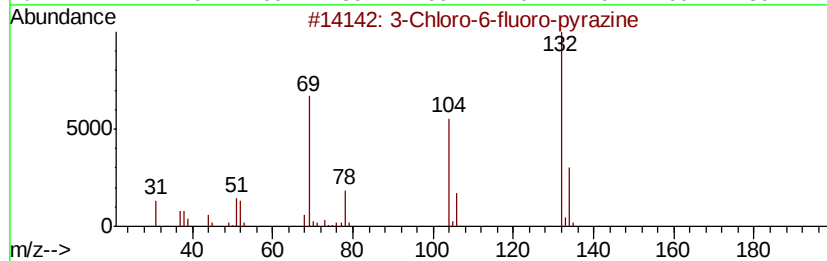
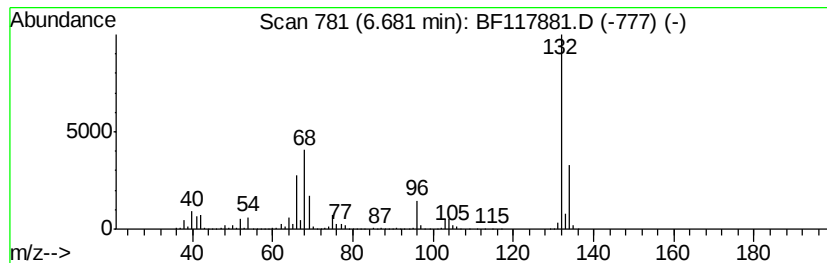
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.68 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.68	69.76 ng	3688780	1,4-Dichlorobenzene-d4	6.92

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	17
3		Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9



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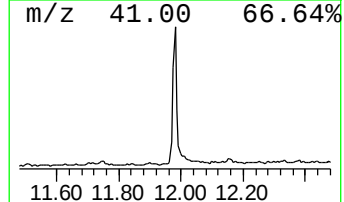
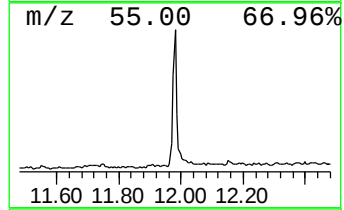
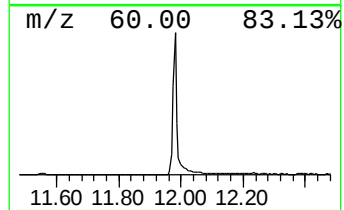
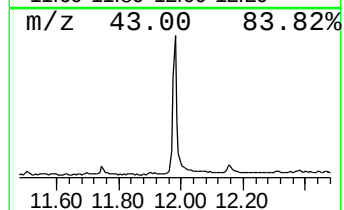
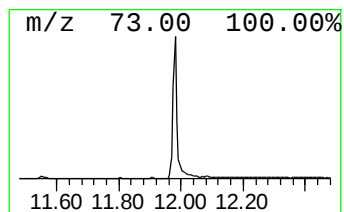
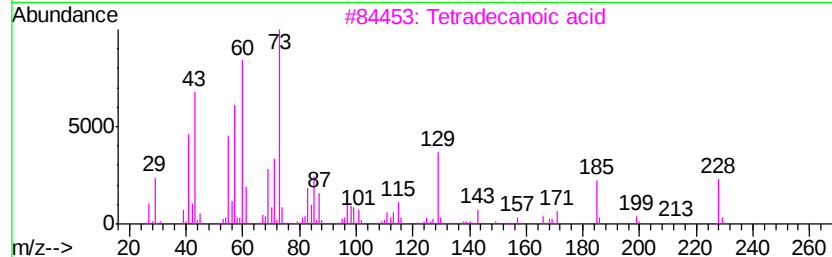
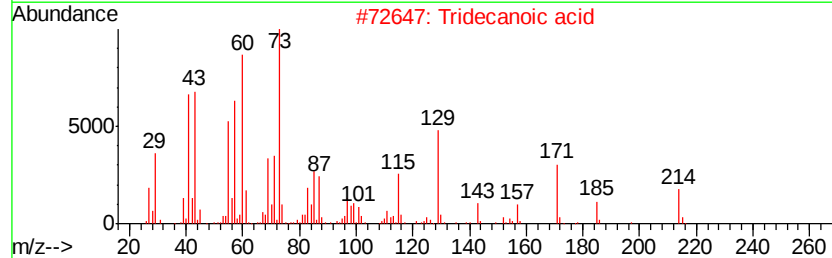
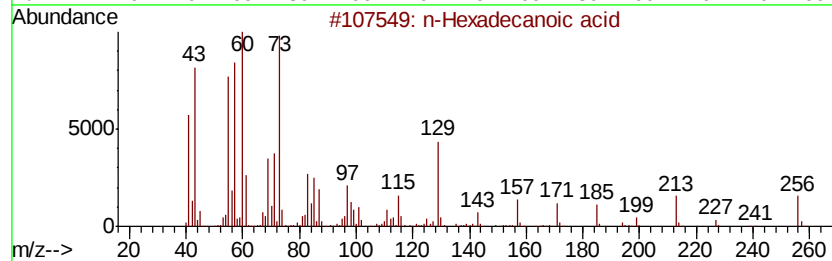
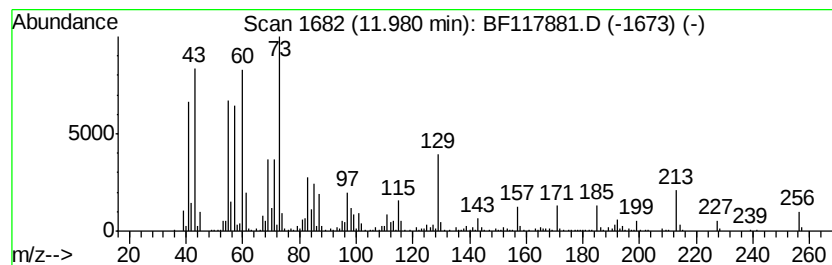
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.98	14.22 ng	871374	Phenanthrene-d10	11.46

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	95
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	91
5		Dodecanoic acid	200	C12H24O2	000143-07-7	72



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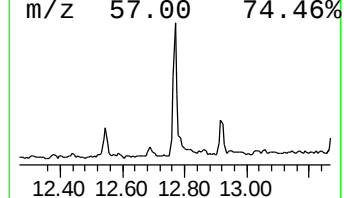
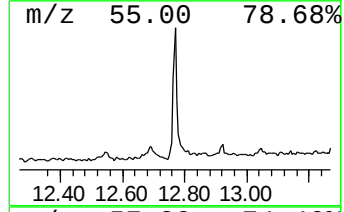
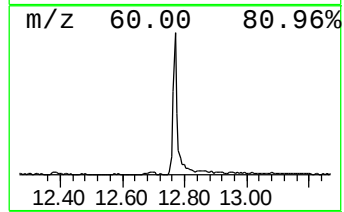
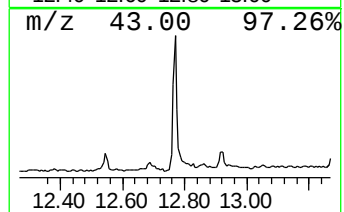
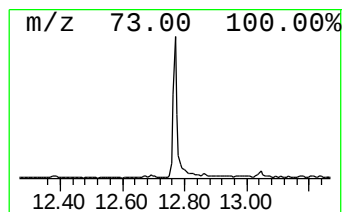
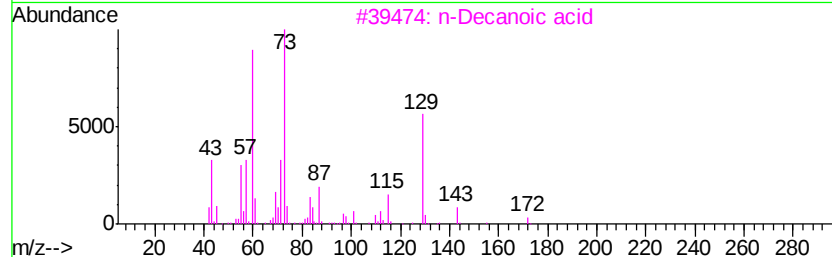
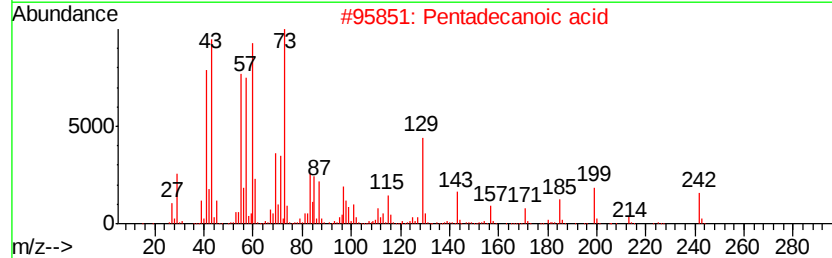
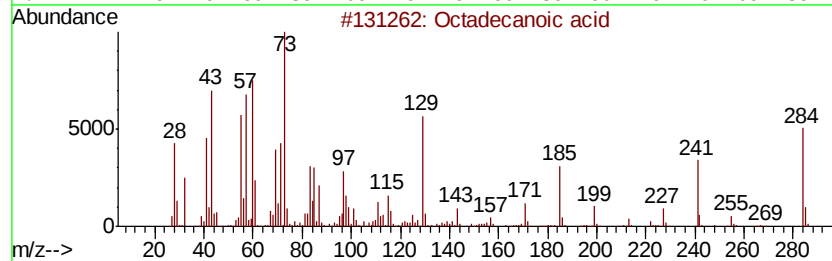
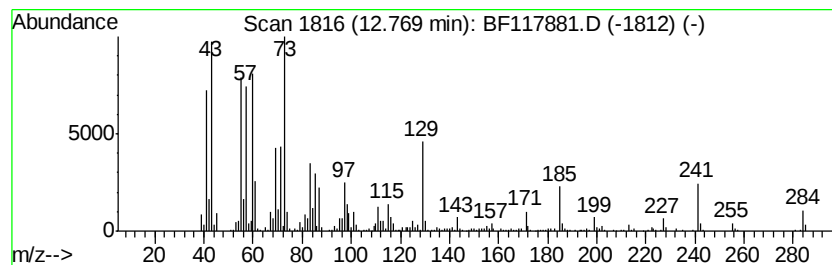
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 7 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.77	10.31 ng	632079	Phenanthrene-d10	11.46

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3		n-Decanoic acid	172	C10H20O2	000334-48-5	91
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87



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B-8-3-(6-12)

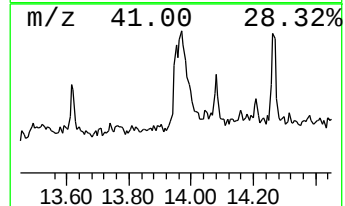
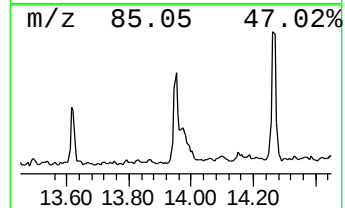
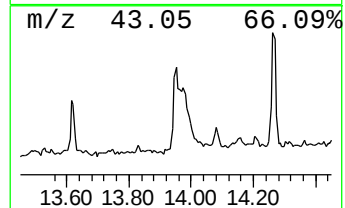
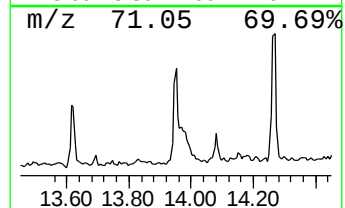
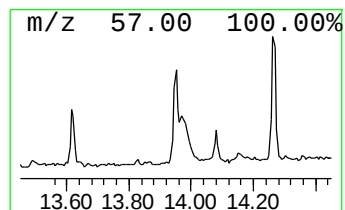
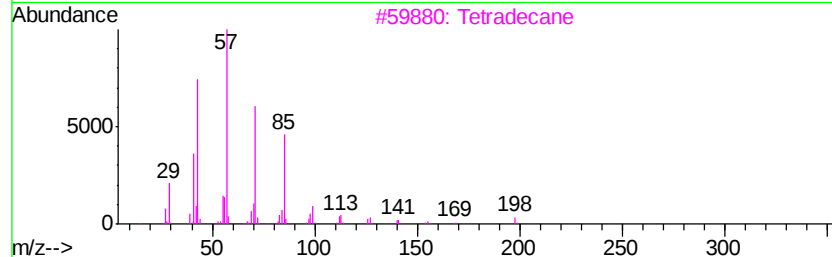
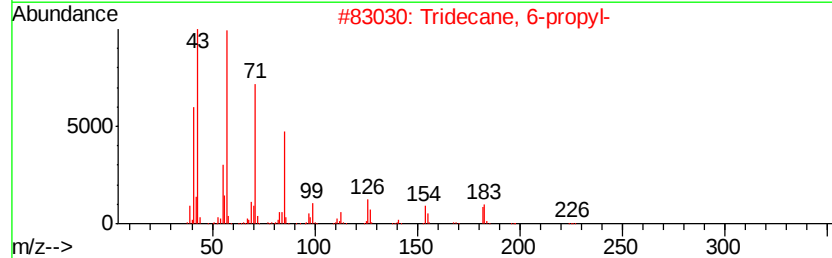
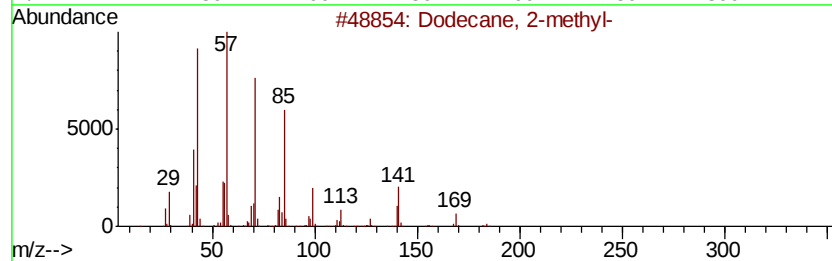
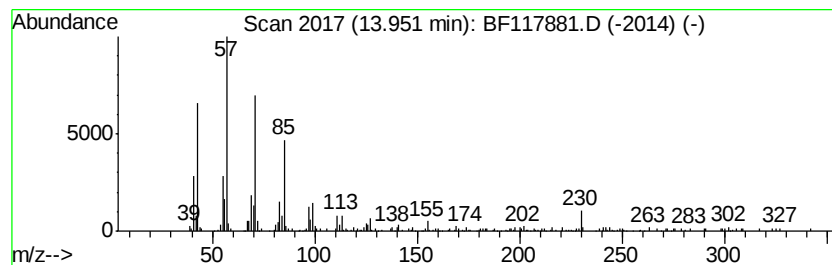
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Dodecane, 2-methyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.95	3.02 ng	167208	Chrysene-d12	14.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dodecane, 2-methyl-	184	C13H28	001560-97-0	90
2		Tridecane, 6-propyl-	226	C16H34	055045-10-8	90
3		Tetradecane	198	C14H30	000629-59-4	89
4		Pentadecane	212	C15H32	000629-62-9	89
5		Tetratetracontane	619	C44H90	007098-22-8	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111919\
Data File : BF117881.D
Acq On : 20 Nov 2019 4:22
Operator : JU
Sample : K5908-04
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-8-3-(6-12)

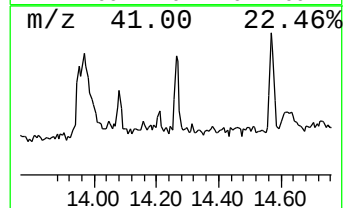
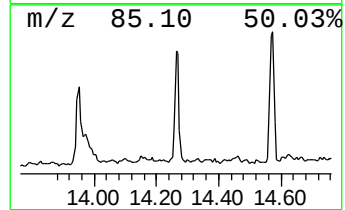
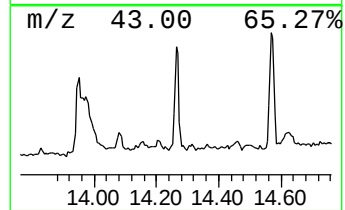
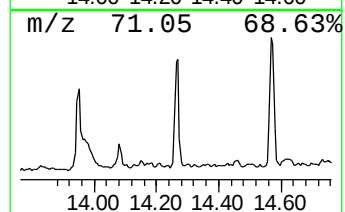
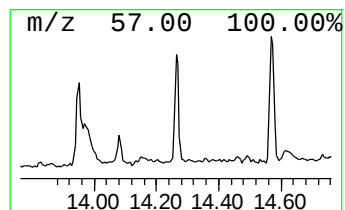
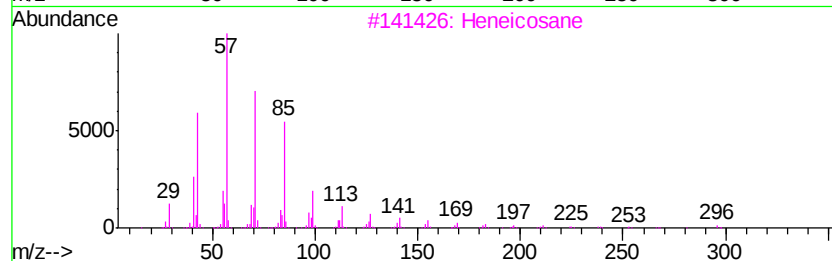
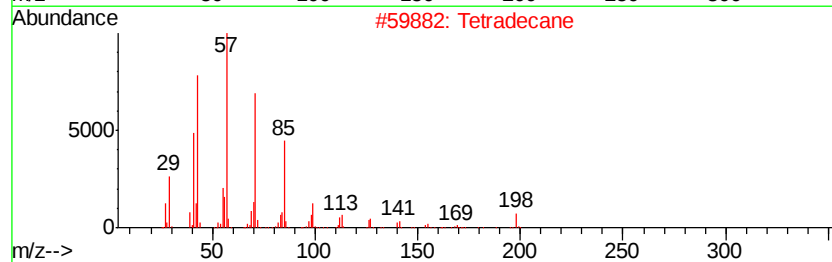
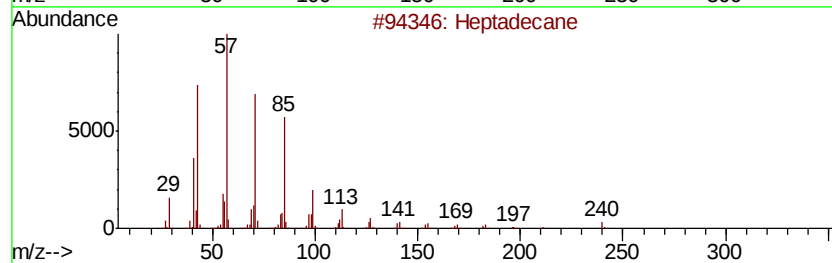
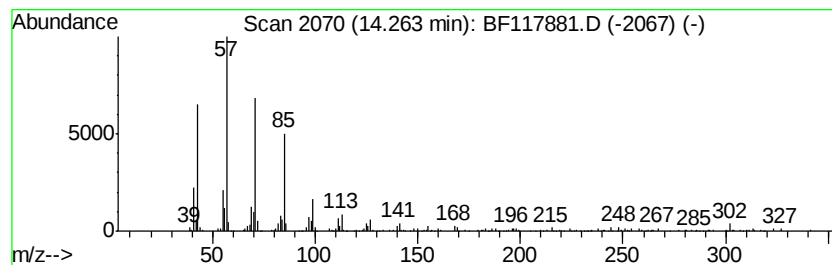
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heptadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.26	3.51 ng	194512	Chrysene-d12	14.10

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane		240	C17H36	000629-78-7	93
2	Tetradecane		198	C14H30	000629-59-4	87
3	Heneicosane		296	C21H44	000629-94-7	87
4	Tetracosane		338	C24H50	000646-31-1	83
5	Pentadecane		212	C15H32	000629-62-9	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111919\
Data File : BF117881.D
Acq On : 20 Nov 2019 4:22
Operator : JU
Sample : K5908-04
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
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ClientSampleId :
B-8-3-(6-12)

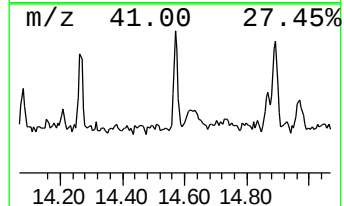
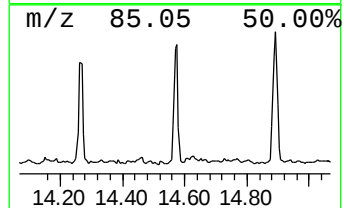
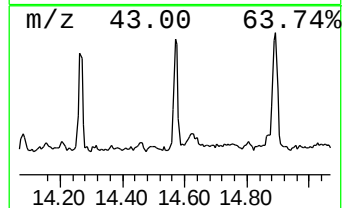
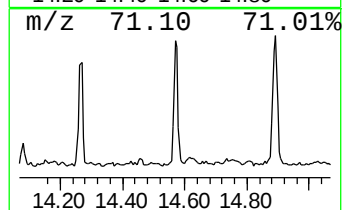
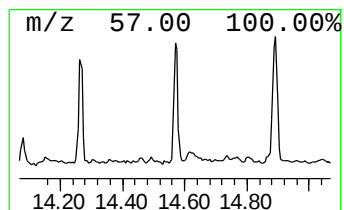
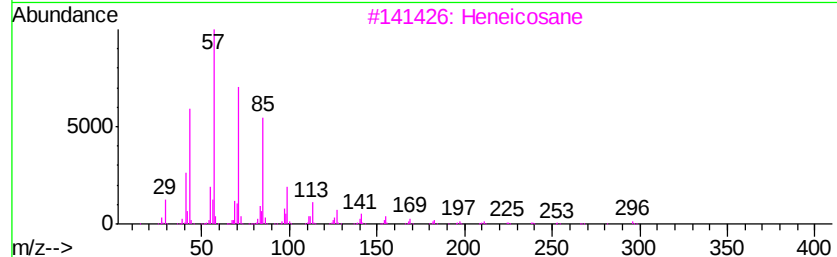
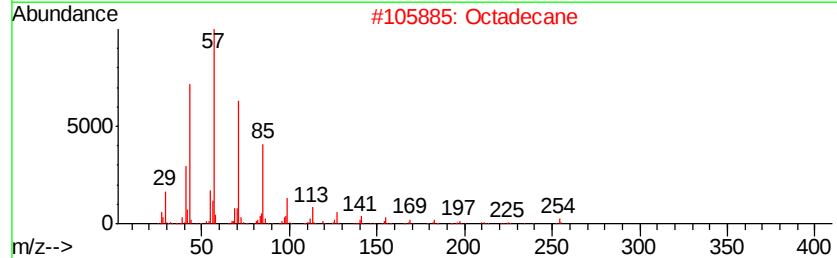
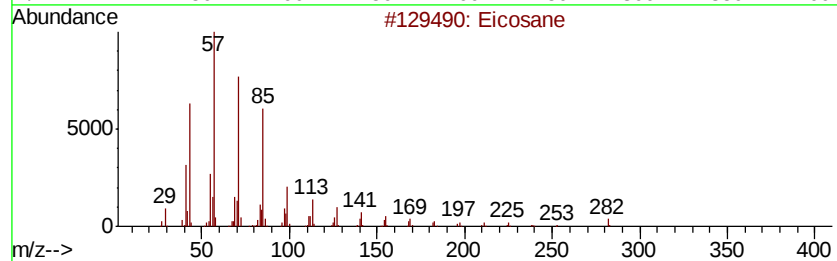
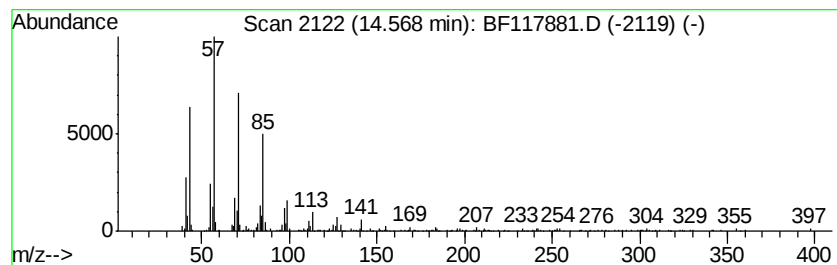
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Eicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.57	5.00 ng	277063	Chrysene-d12	14.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	97
2		Octadecane	254	C18H38	000593-45-3	97
3		Heneicosane	296	C21H44	000629-94-7	96
4		Nonadecane	268	C19H40	000629-92-5	93
5		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111919\
Data File : BF117881.D
Acq On : 20 Nov 2019 4:22
Operator : JU
Sample : K5908-04
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
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ClientSampleId :
B-8-3-(6-12)

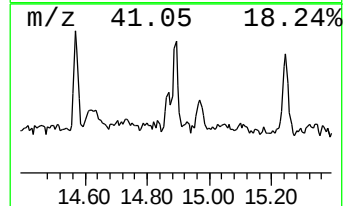
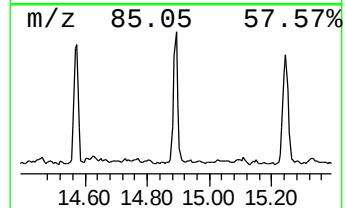
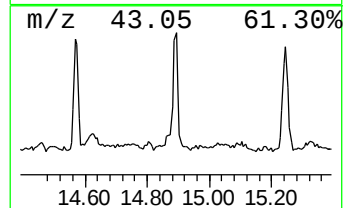
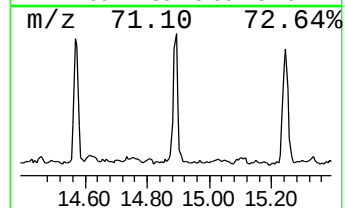
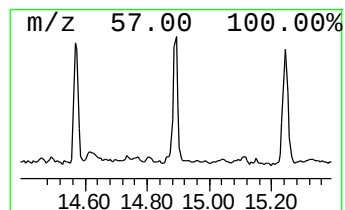
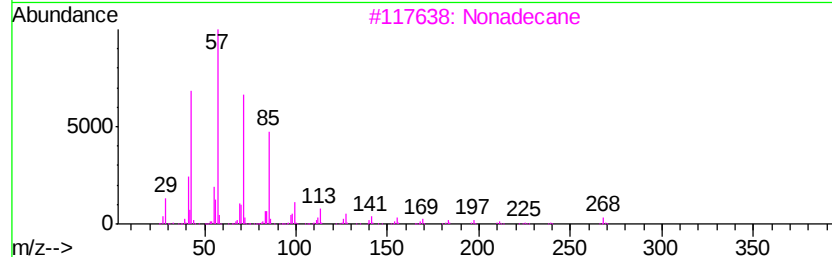
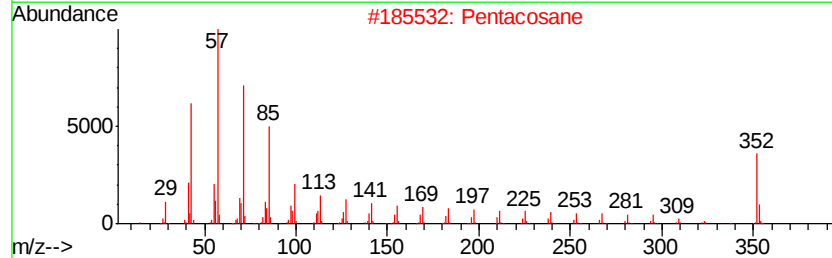
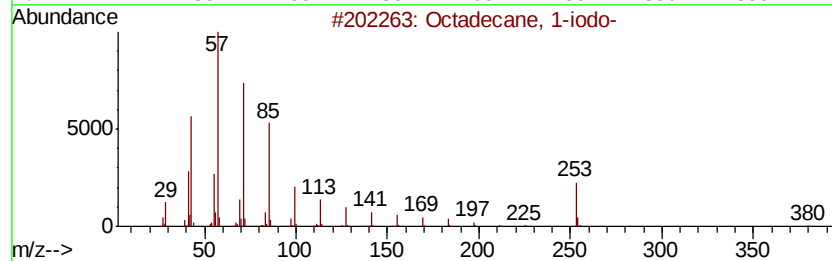
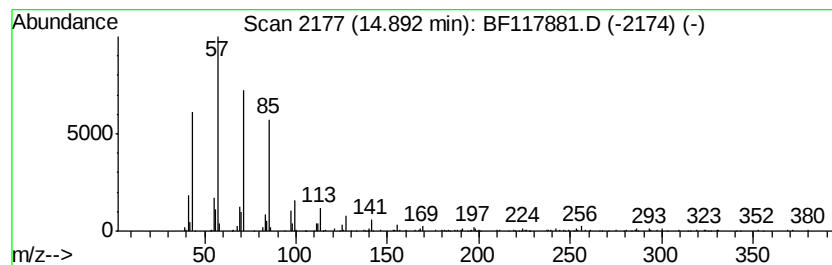
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Octadecane, 1-iodo- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.89	5.68 ng	257598	Perylene-d12	15.61

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane, 1-iodo-	380	C18H37I	000629-93-6	93
2			Pentacosane	352	C25H52	000629-99-2	87
3			Nonadecane	268	C19H40	000629-92-5	86
4			Tetracosane	338	C24H50	000646-31-1	86
5			Hentriacontane	437	C31H64	000630-04-6	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111919\
Data File : BF117881.D
Acq On : 20 Nov 2019 4:22
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Sample : K5908-04
Misc :
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Instrument :
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ClientSampleId :
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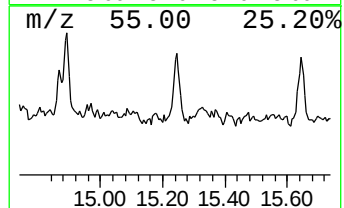
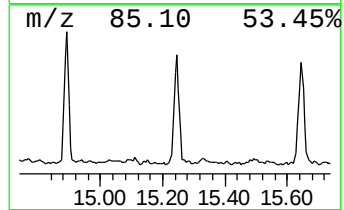
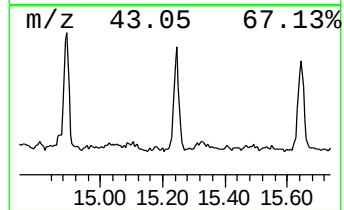
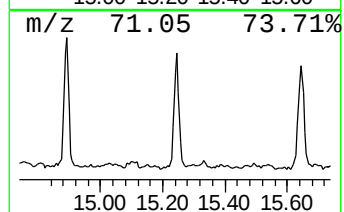
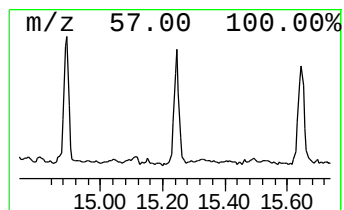
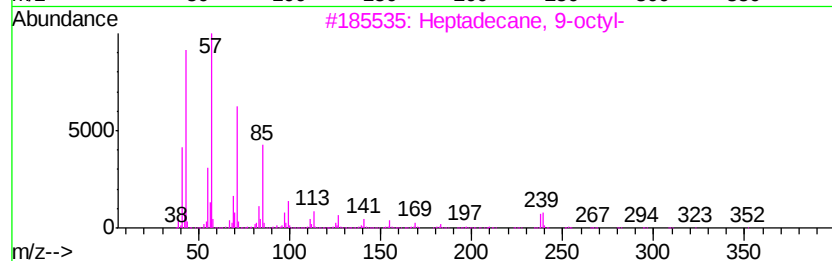
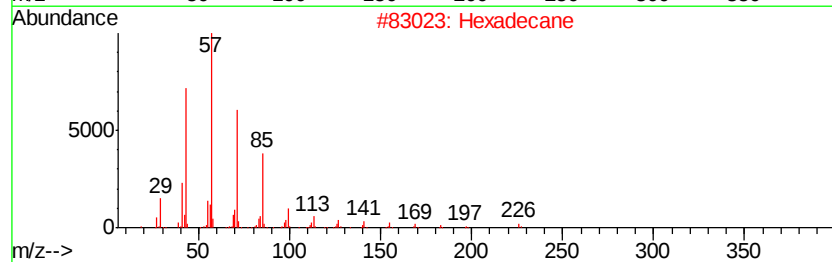
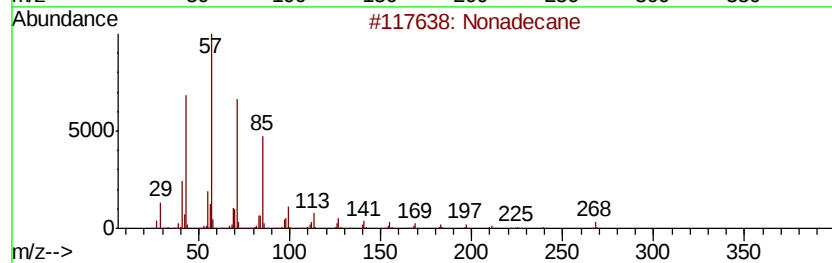
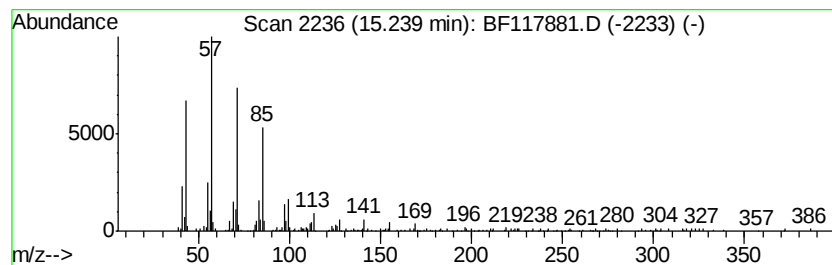
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Nonadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.24	5.84 ng	265011	Perylene-d12	15.61

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane		268	C19H40	000629-92-5	94
2	Hexadecane		226	C16H34	000544-76-3	91
3	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	90
4	Hexacosane		366	C26H54	000630-01-3	90
5	Heneicosane		296	C21H44	000629-94-7	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111919\
Data File : BF117881.D
Acq On : 20 Nov 2019 4:22
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Misc :
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Instrument :
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ClientSampleId :
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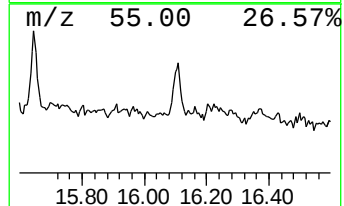
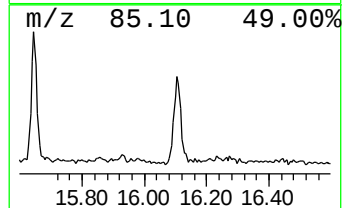
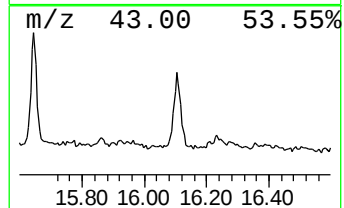
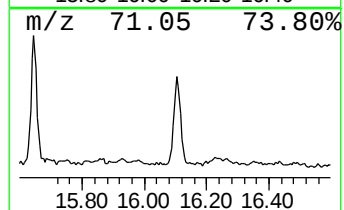
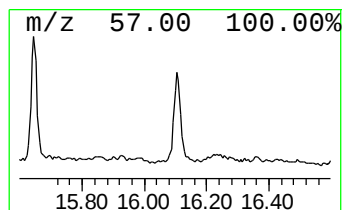
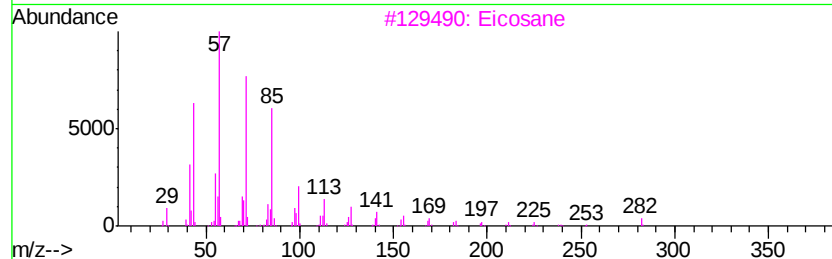
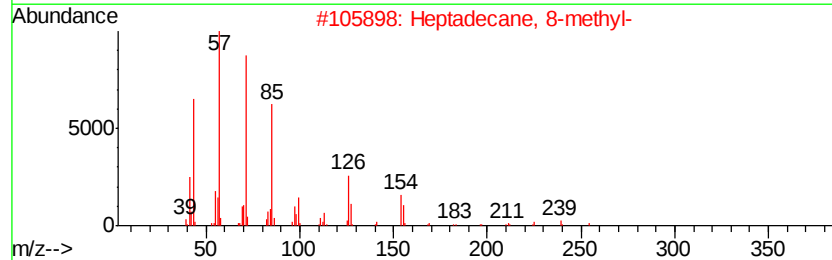
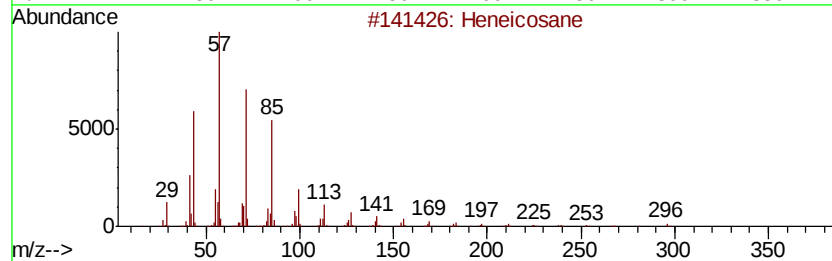
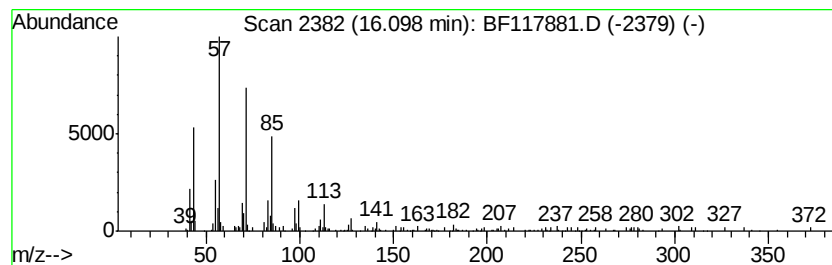
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.10	5.09 ng	230658	Perylene-d12	15.61

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	95
2		Heptadecane, 8-methyl-	254	C18H38	013287-23-5	93
3		Eicosane	282	C20H42	000112-95-8	93
4		Tetratetracontane	619	C44H90	007098-22-8	90
5		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111919\
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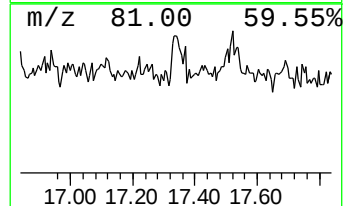
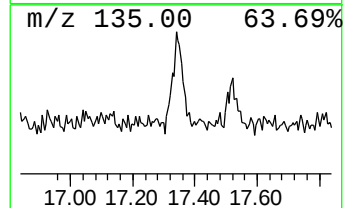
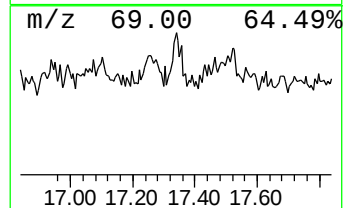
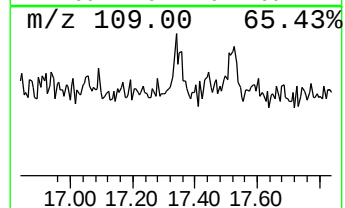
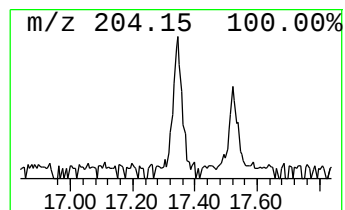
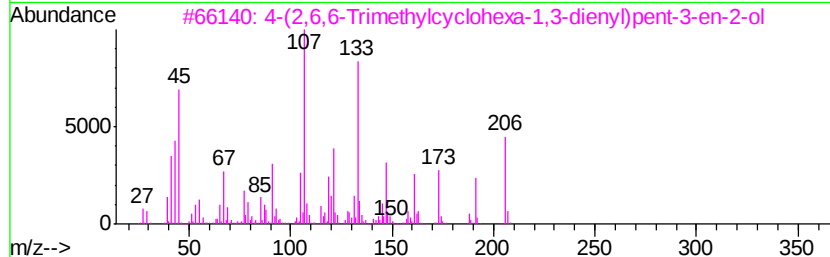
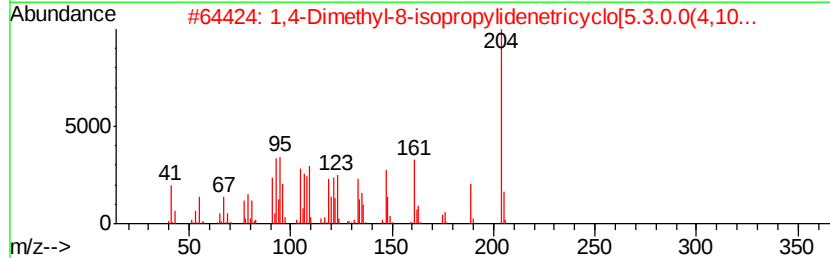
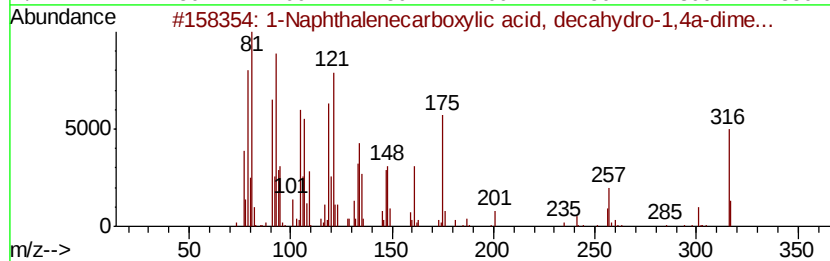
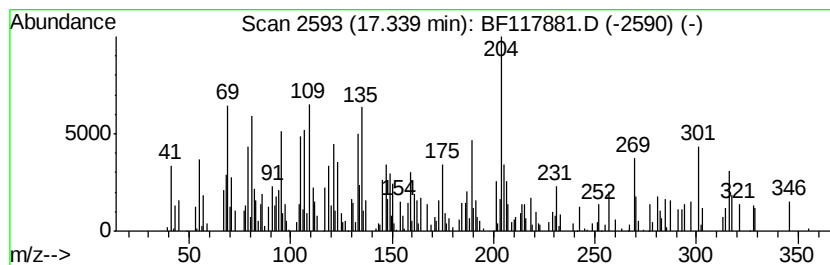
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 1-Naphthalenecarboxylic aci... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.34	3.61 ng	163869	Perylene-d12	15.61	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Naphthalenecarboxylic acid, de...	316	C21H32O2	015798-13-7	53
2	1,4-Dimethyl-8-isopropylidenetri...	204	C15H24	1000140-07-7	45
3	4-(2,6,6-Trimethylcyclohexa-1,3-...	206	C14H22O	1000195-14-8	44
4	Guaia-3,9-diene	204	C15H24	000489-83-8	43
5	Aciphyllene	204	C15H24	087745-31-1	38



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF111919\
Data File : BF117881.D
Acq On : 20 Nov 2019 4:22
Operator : JU
Sample : K5908-04
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-8-3-(6-12)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.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...	2.19	17.8	ng	941107	1	6.92	1057530	20.0
2-Pentanone, 4-hy...	5.13	12.0	ng	636769	1	6.92	1057530	20.0
unknown6.68	6.68	69.8	ng	3688780	1	6.92	1057530	20.0
n-Hexadecanoic acid	11.98	14.2	ng	871374	4	11.46	1225800	20.0
Octadecanoic acid	12.77	10.3	ng	632079	4	11.46	1225800	20.0
Dodecane, 2-methyl-	13.95	3.0	ng	167208	5	14.10	1108170	20.0
Heptadecane	14.26	3.5	ng	194512	5	14.10	1108170	20.0
Eicosane	14.57	5.0	ng	277063	5	14.10	1108170	20.0
Octadecane, 1-iodo-	14.89	5.7	ng	257598	6	15.61	906810	20.0
Nonadecane	15.24	5.8	ng	265011	6	15.61	906810	20.0
Heneicosane	16.10	5.1	ng	230658	6	15.61	906810	20.0
1-Naphthalenecarb...	17.34	3.6	ng	163869	6	15.61	906810	20.0