

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091719\
 Data File : BF117097.D
 Acq On : 17 Sep 2019 11:03
 Operator : HP/JU
 Sample : K4883-05
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW2-R2-1

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-BF091319.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	5.445	567	571	588	rBV	753964	833332	23.96%	2.211%
2	6.457	739	743	759	rBV	566312	593752	17.07%	1.575%
3	6.598	762	767	770	rBV	2002248	1820871	52.35%	4.831%
4	6.822	801	805	815	rBV	501276	432292	12.43%	1.147%
5	6.981	828	832	844	rBV	1986746	1779156	51.15%	4.721%
6	7.386	896	901	904	rBV	1366785	1338085	38.47%	3.550%
7	8.104	1018	1023	1039	rBV	549932	549766	15.81%	1.459%
8	9.175	1200	1205	1216	rBV	2775379	2717474	78.12%	7.210%
9	9.569	1269	1272	1276	rBV	47895	43015	1.24%	0.114%
10	9.851	1315	1320	1335	rBV	673727	643075	18.49%	1.706%
11	10.639	1450	1454	1468	rBV	1406043	1544121	44.39%	4.097%
12	11.333	1568	1572	1586	rBV	540619	599580	17.24%	1.591%
13	11.598	1596	1617	1618	rBV2	235539	813805	23.40%	2.159%
14	11.857	1655	1661	1669	rBV2	141197	200205	5.76%	0.531%
15	12.639	1789	1794	1808	rBV	146749	236165	6.79%	0.627%
16	12.863	1829	1832	1836	rVB	43469	40307	1.16%	0.107%
17	12.915	1836	1841	1844	rBV	2310420	2144771	61.66%	5.691%
18	13.080	1854	1869	1877	rBV	1010162	2929941	84.23%	7.774%
19	13.480	1931	1937	1940	rBV3	29522	38817	1.12%	0.103%
20	13.604	1952	1958	1961	rBV3	34937	72561	2.09%	0.193%
21	13.810	1988	1993	1997	rBV4	97264	161642	4.65%	0.429%
22	13.892	1997	2007	2013	rVV	1721934	3478411	100.00%	9.229%
23	13.968	2017	2020	2030	rVB	420318	460037	13.23%	1.221%
24	14.121	2041	2046	2050	rBV	216901	211723	6.09%	0.562%
25	14.268	2067	2071	2077	rVB	56423	92358	2.66%	0.245%
26	14.339	2078	2083	2090	rVB3	28809	53422	1.54%	0.142%
27	14.427	2093	2098	2102	rBV	531511	556821	16.01%	1.477%
28	14.492	2102	2109	2122	rVB	1811894	3080883	88.57%	8.175%
29	14.733	2144	2150	2155	rBV	935918	968902	27.85%	2.571%
30	14.804	2158	2162	2165	rBV	124354	154865	4.45%	0.411%
31	14.892	2174	2177	2181	rVB3	30755	43157	1.24%	0.115%
32	15.056	2195	2205	2217	rBV	1714004	3201758	92.05%	8.495%
33	15.427	2259	2268	2277	rBV2	1060330	1558194	44.80%	4.134%
34	15.680	2301	2311	2318	rBV2	404276	937217	26.94%	2.487%

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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

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35	15.851	2332	2340	2345	rBV	540226	838248	24.10%	2.224%
36	16.015	2362	2368	2374	rVB	139633	222321	6.39%	0.590%
37	16.145	2374	2390	2396	rBV10	45733	181781	5.23%	0.482%
38	16.333	2415	2422	2427	rBV	228138	417888	12.01%	1.109%
39	16.403	2427	2434	2444	rVB	172520	412945	11.87%	1.096%
40	16.903	2514	2519	2527	rVB2	62088	135630	3.90%	0.360%
41	17.056	2537	2545	2554	rVB2	230856	459737	13.22%	1.220%
42	17.245	2569	2577	2588	rBV4	69263	204753	5.89%	0.543%
43	18.250	2736	2748	2760	rBV5	41864	150814	4.34%	0.400%
44	18.480	2778	2787	2800	rVB3	115533	333438	9.59%	0.885%

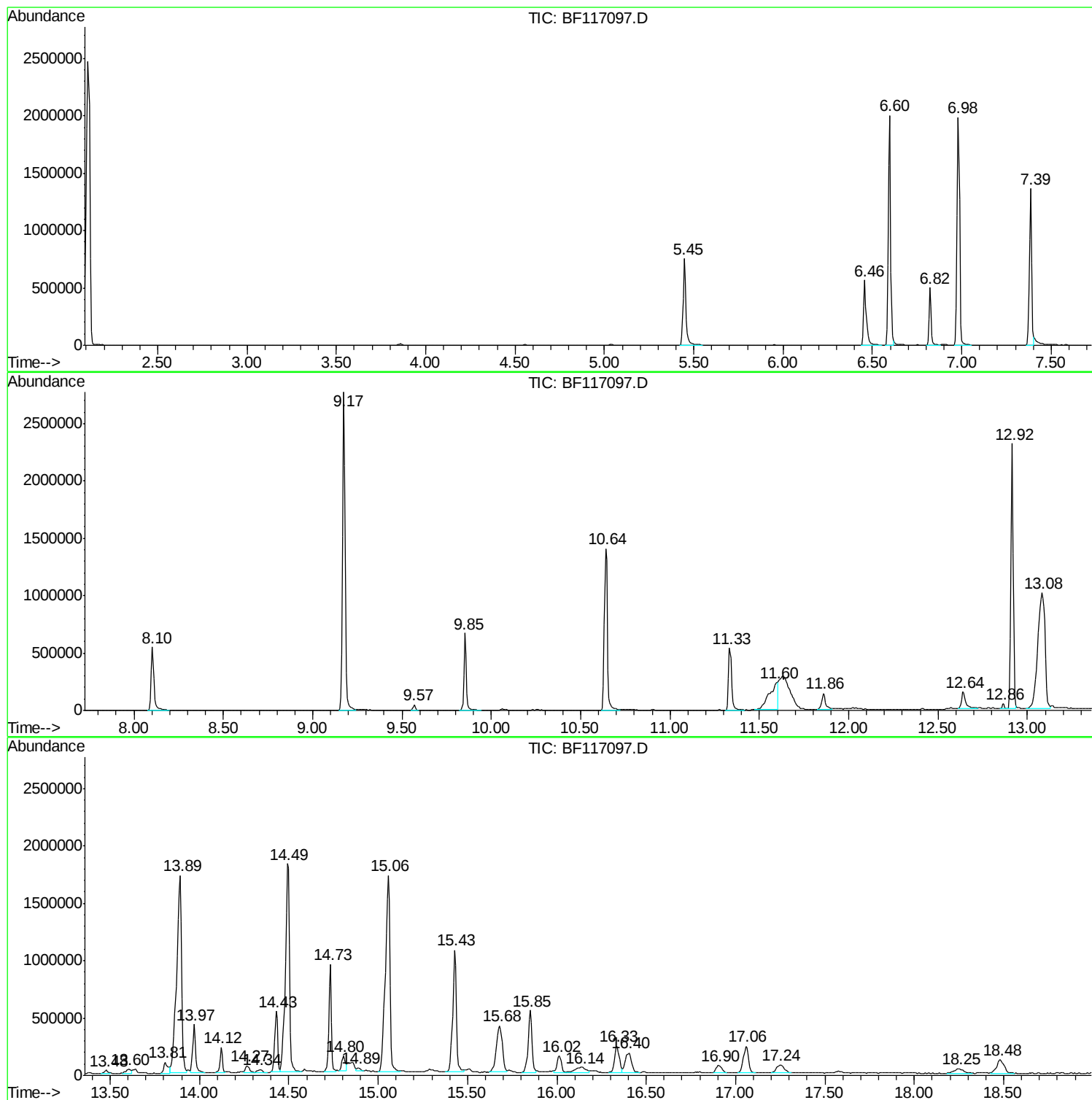
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Instrument :
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ClientSampled :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF091319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Sample : K4883-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW2-R2-1

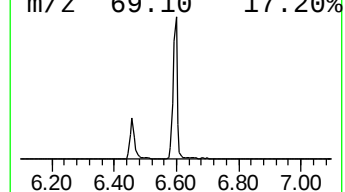
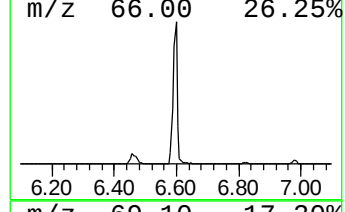
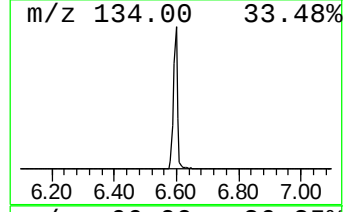
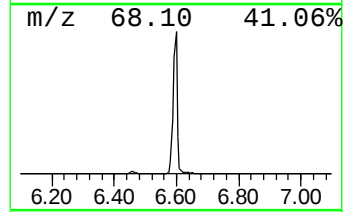
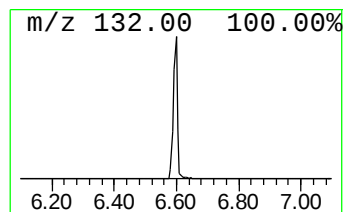
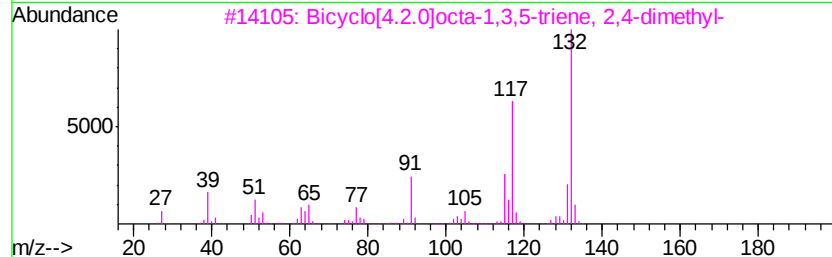
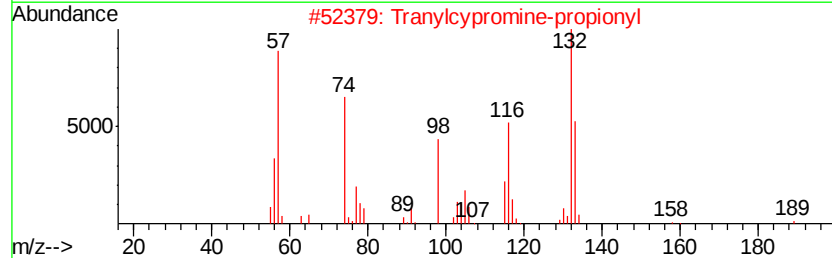
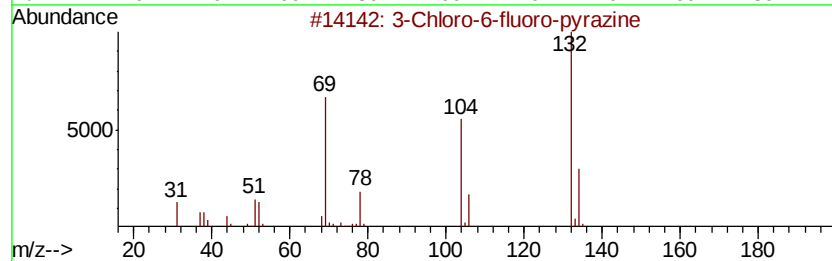
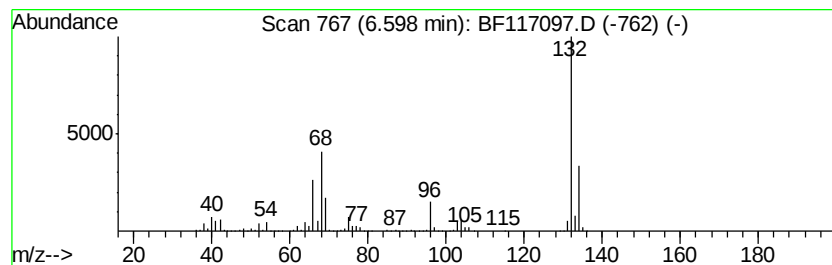
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF091319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown6.60 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	84.24 ng	1820870	1,4-Dichlorobenzene-d4	6.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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Instrument :
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ClientSampleId :
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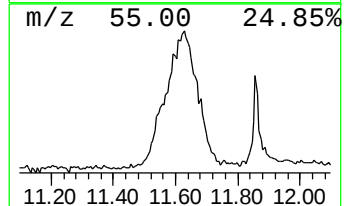
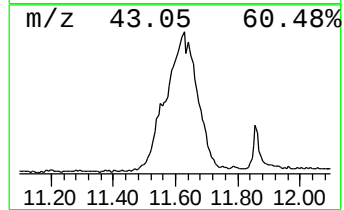
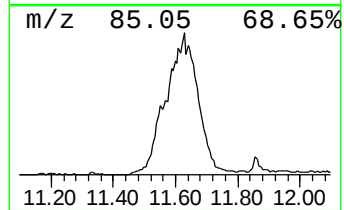
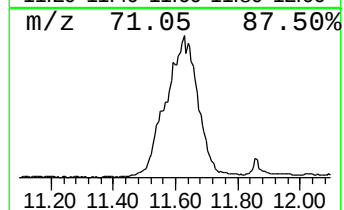
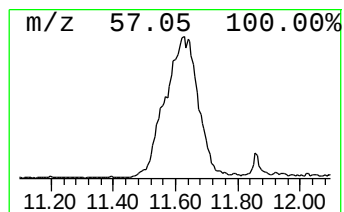
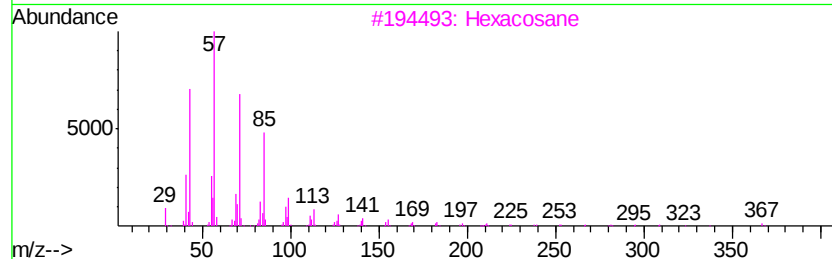
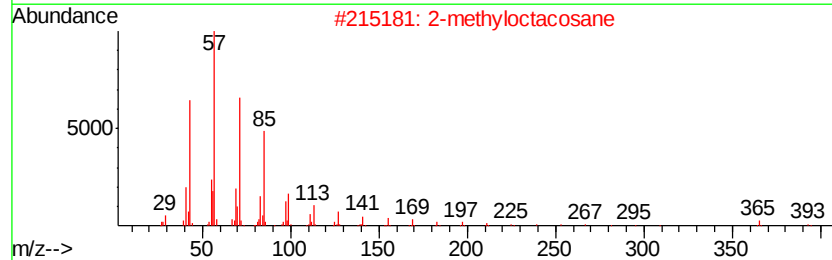
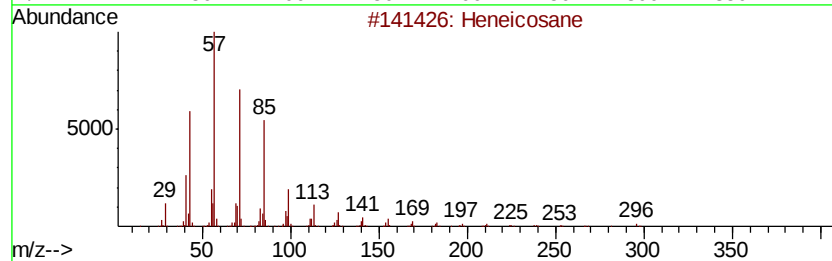
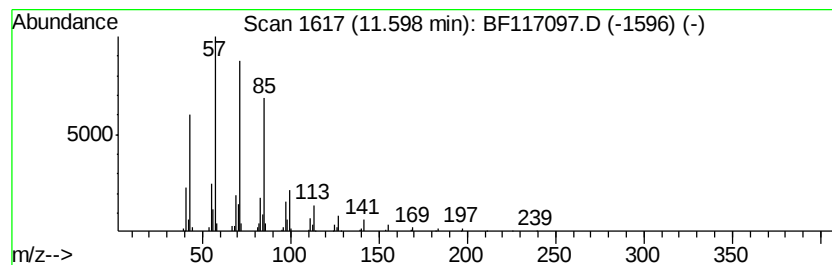
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.60	27.15 ng	813805	Phenanthrene-d10	11.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	91
2		2-methyloctacosane	408	C29H60	1000376-72-8	91
3		Hexacosane	366	C26H54	000630-01-3	91
4		Hentriacontane	437	C31H64	000630-04-6	91
5		Hexadecane	226	C16H34	000544-76-3	83



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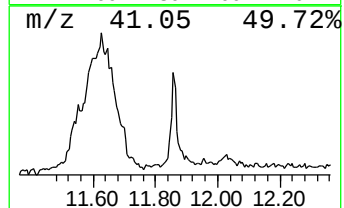
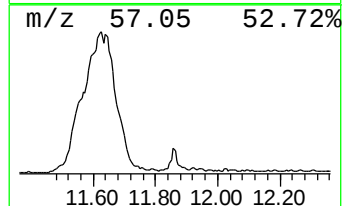
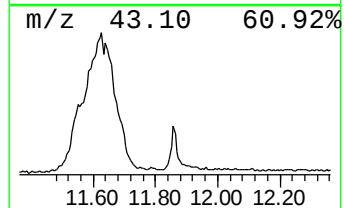
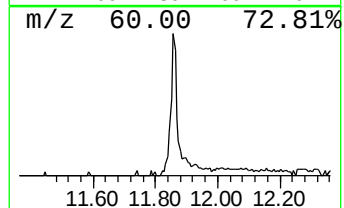
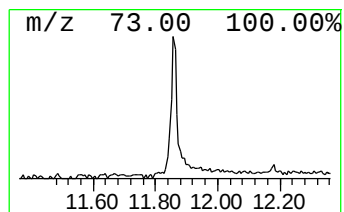
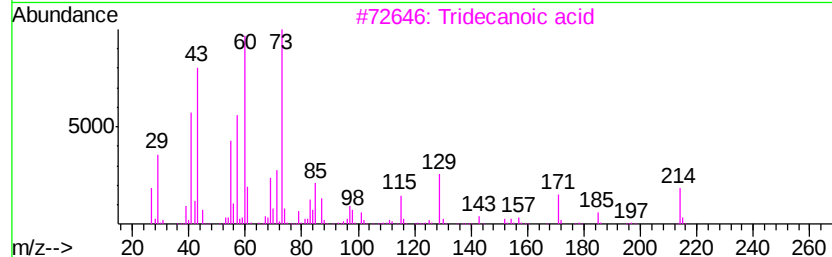
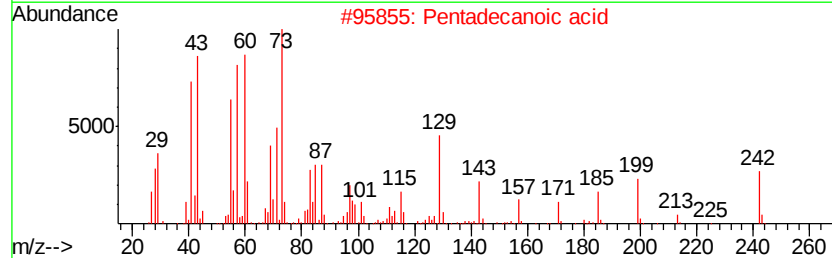
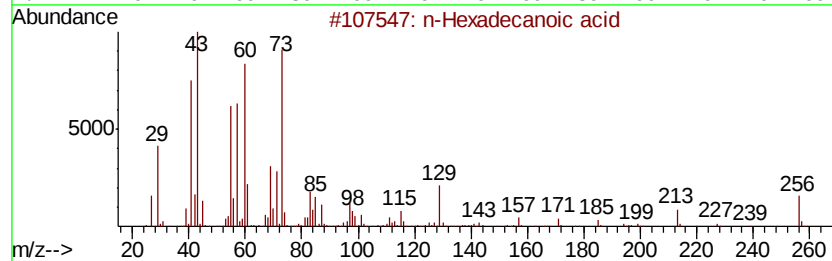
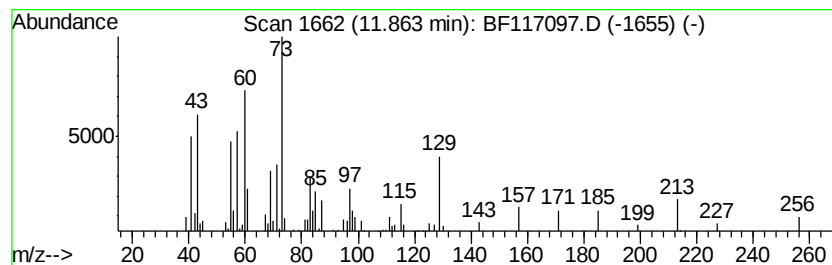
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.86	6.68 ng	200205	Phenanthrene-d10	11.33

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	87
3		Tridecanoic acid	214	C13H26O2	000638-53-9	81
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5		Dodecanoic acid	200	C12H24O2	000143-07-7	64



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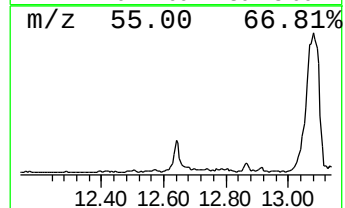
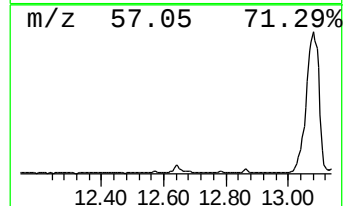
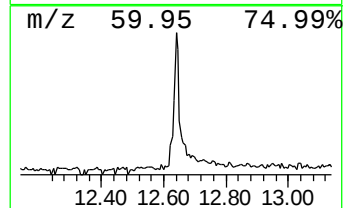
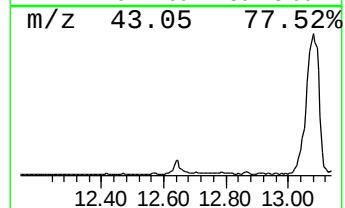
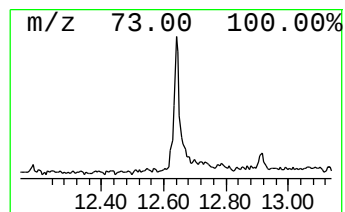
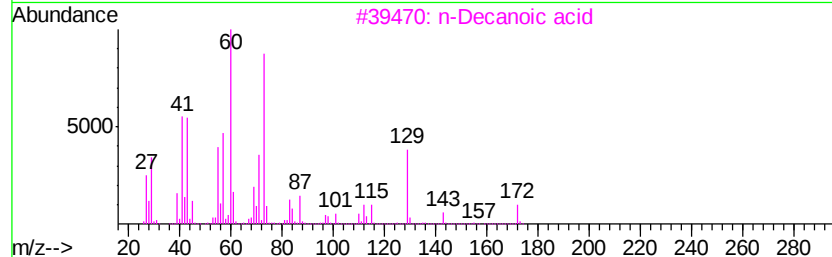
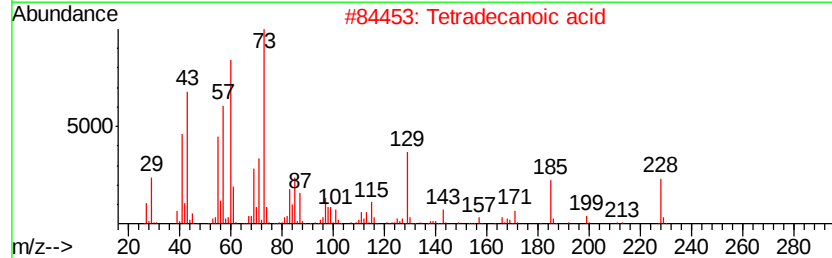
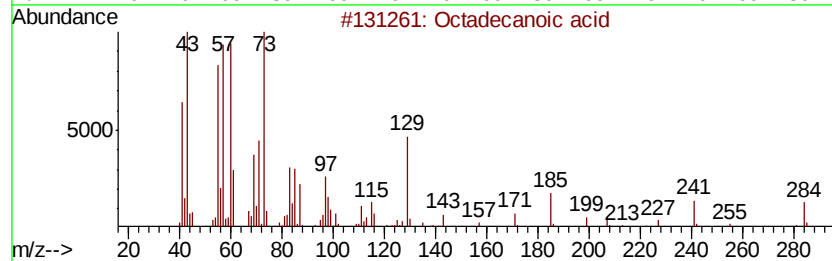
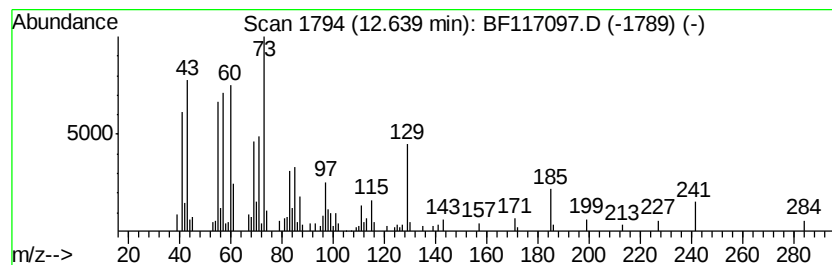
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octadecanoic acid Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD		R.T.
12.64	7.88 ng	236165	Phenanthrene-d10		11.33
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	97
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
3	n-Decanoic acid	172	C10H20O2	000334-48-5	62
4	Undecanoic acid	186	C11H22O2	000112-37-8	60
5	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	20



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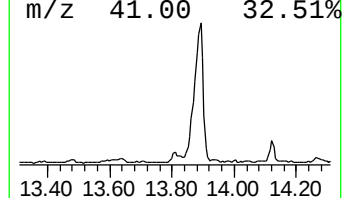
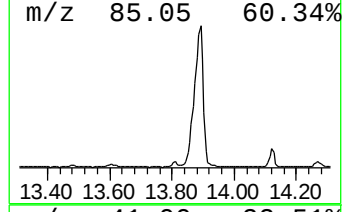
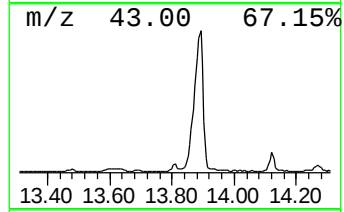
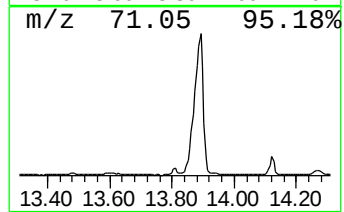
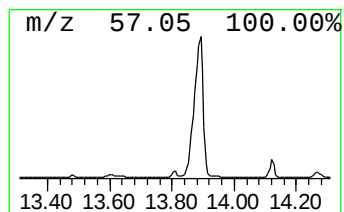
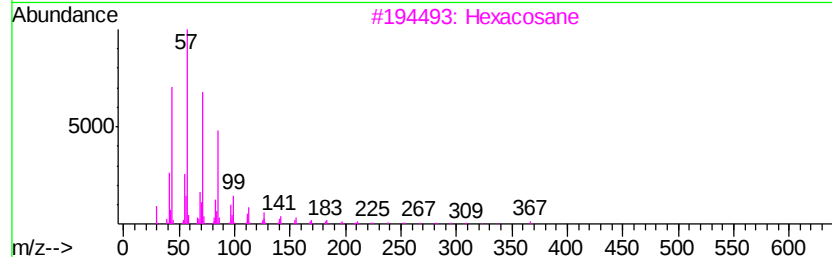
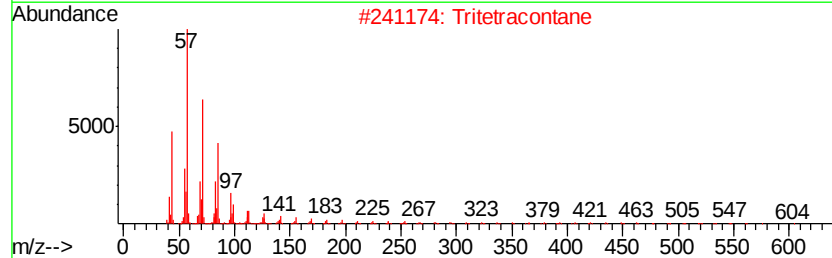
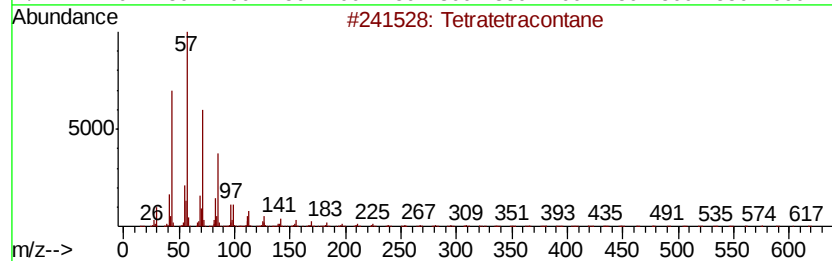
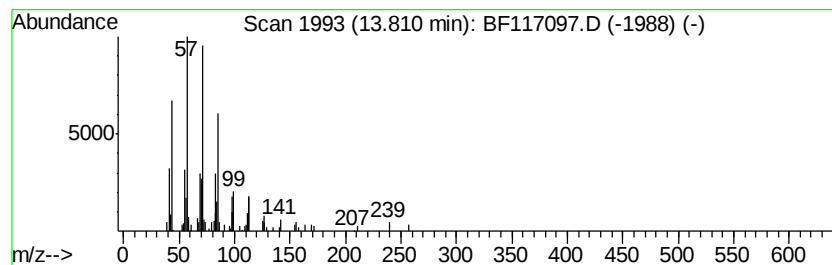
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Tetratetracontane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	7.03 ng	161642	Chrysene-d12	13.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetratetracontane	619	C44H90	007098-22-8	91
2		Tritetracontane	605	C43H88	007098-21-7	86
3		Hexacosane	366	C26H54	000630-01-3	86
4		Heneicosane	296	C21H44	000629-94-7	80
5		2-methyloctacosane	408	C29H60	1000376-72-8	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091719\
Data File : BF117097.D
Acq On : 17 Sep 2019 11:03
Operator : HP/JU
Sample : K4883-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW2-R2-1

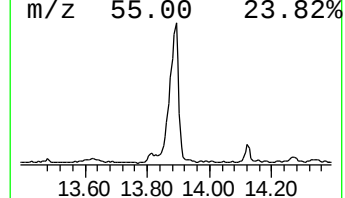
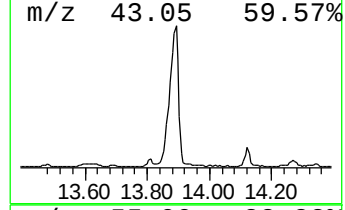
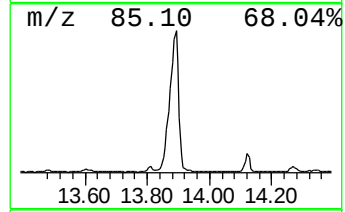
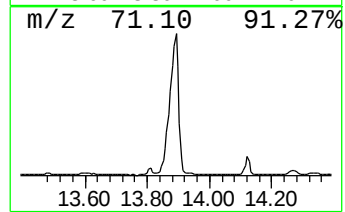
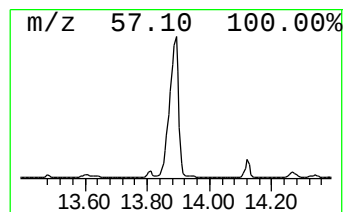
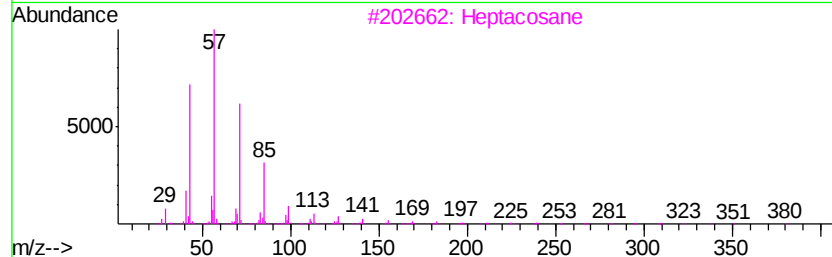
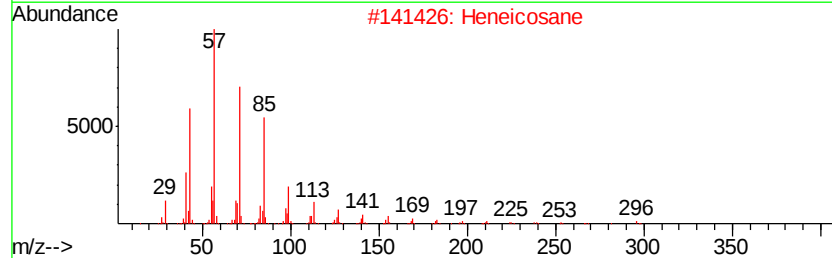
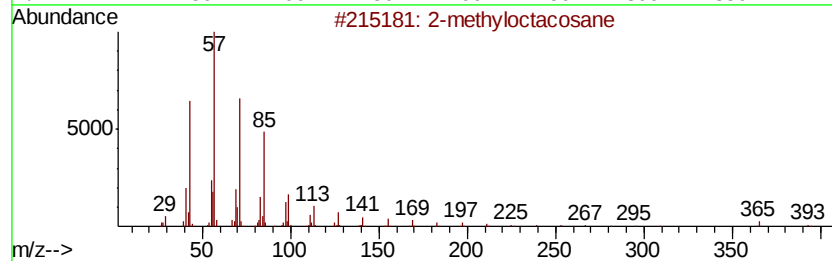
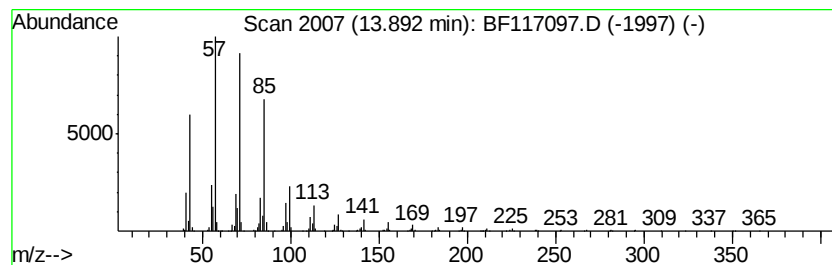
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 2-methyloctacosane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	151.22 ng	3478410	Chrysene-d12	13.97

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane		408	C29H60	1000376-72-8	91
2	Heneicosane		296	C21H44	000629-94-7	91
3	Heptacosane		380	C27H56	000593-49-7	91
4	Triacontane		422	C30H62	000638-68-6	91
5	Octacosane		394	C28H58	000630-02-4	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091719\
 Data File : BF117097.D
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Instrument :
 BNA_F
 ClientSampleId :
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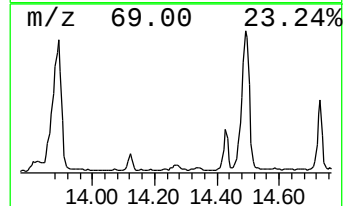
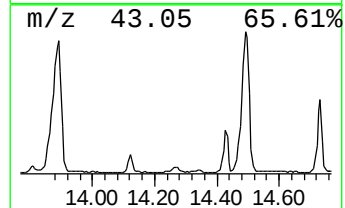
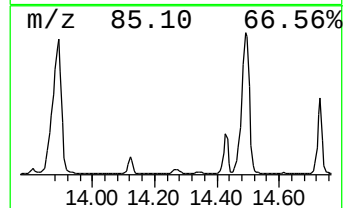
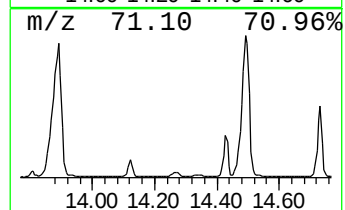
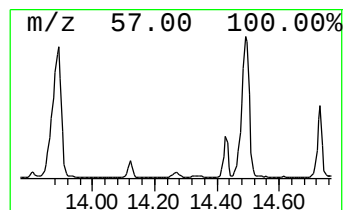
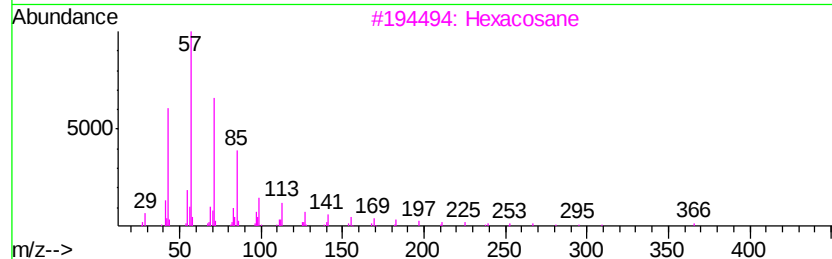
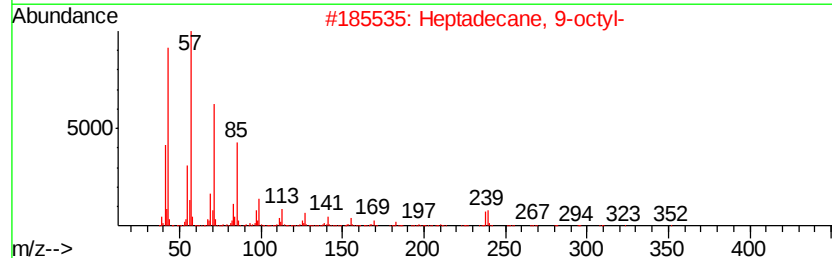
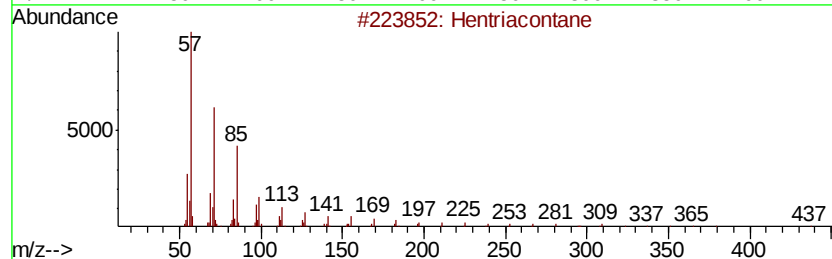
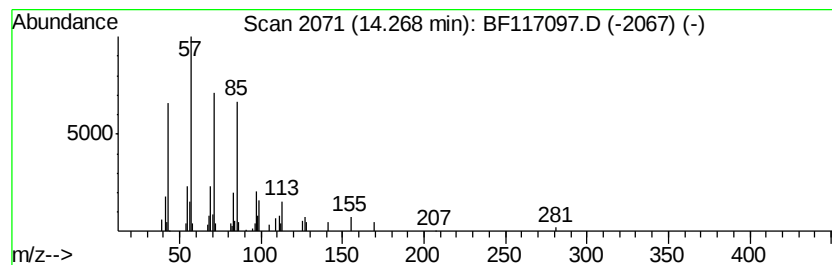
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 10 Hentriacontane Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.27	4.02 ng	92358	Chrysene-d12	13.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hentriacontane	437	C31H64	000630-04-6	91
2		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	80
3		Hexacosane	366	C26H54	000630-01-3	80
4		Tetratetracontane	619	C44H90	007098-22-8	72
5		Sulfurous acid, butyl decyl ester	278	C14H30O3S	1000309-17-7	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091719\
Data File : BF117097.D
Acq On : 17 Sep 2019 11:03
Operator : HP/JU
Sample : K4883-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
MW2-R2-1

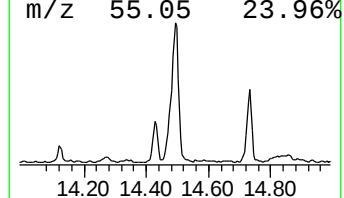
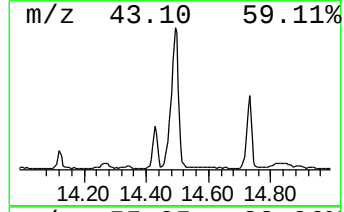
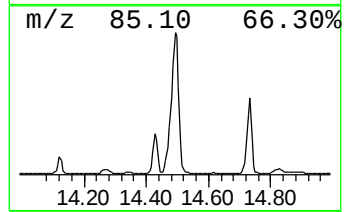
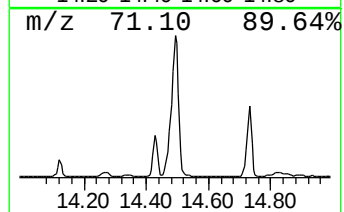
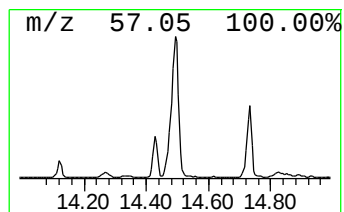
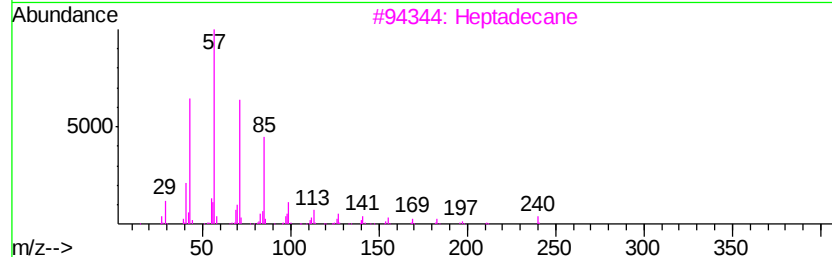
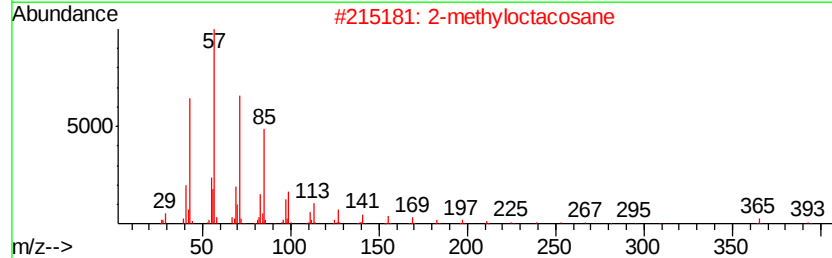
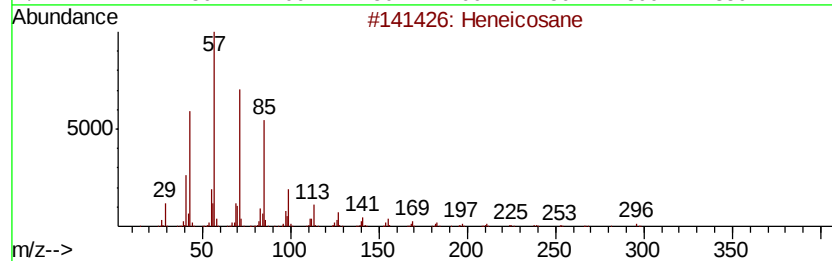
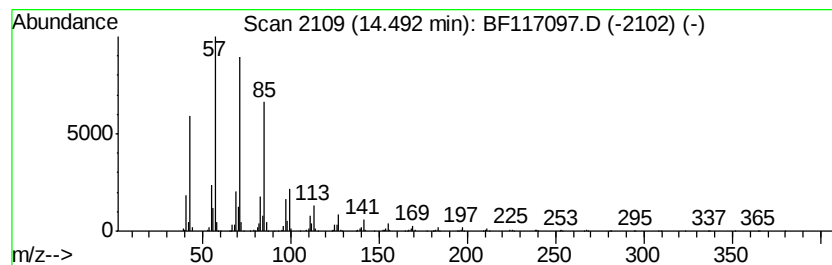
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Eicosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.49	133.94 ng	3080880	Chrysene-d12	13.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	91
2		2-methyloctacosane	408	C29H60	1000376-72-8	91
3		Heptadecane	240	C17H36	000629-78-7	86
4		Eicosane	282	C20H42	000112-95-8	86
5		Hexadecane	226	C16H34	000544-76-3	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091719\
Data File : BF117097.D
Acq On : 17 Sep 2019 11:03
Operator : HP/JU
Sample : K4883-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
MW2-R2-1

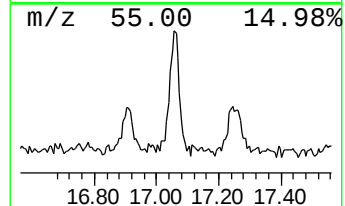
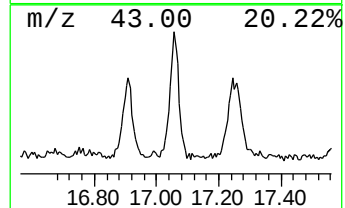
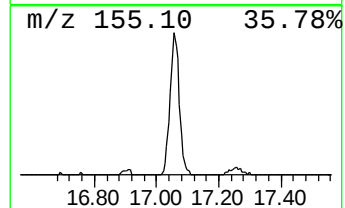
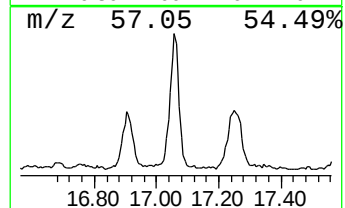
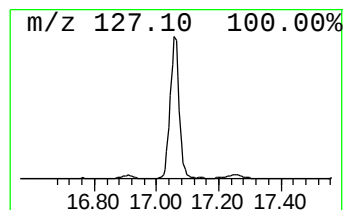
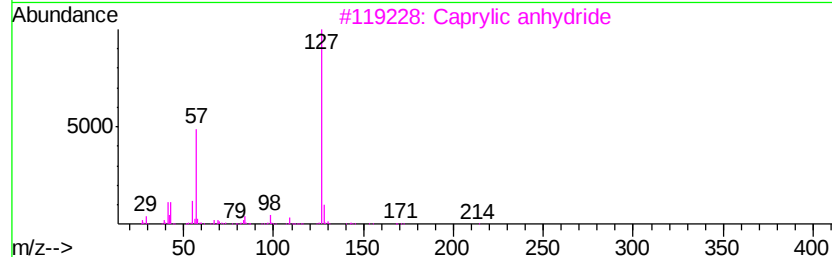
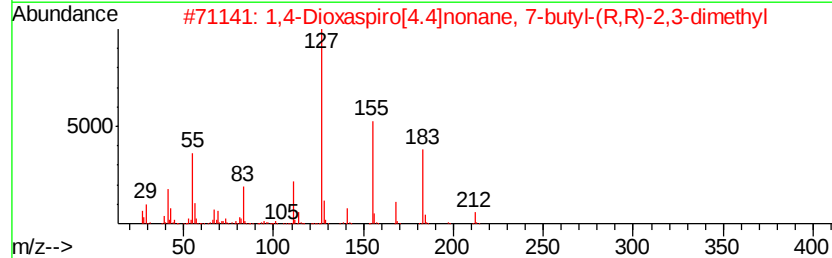
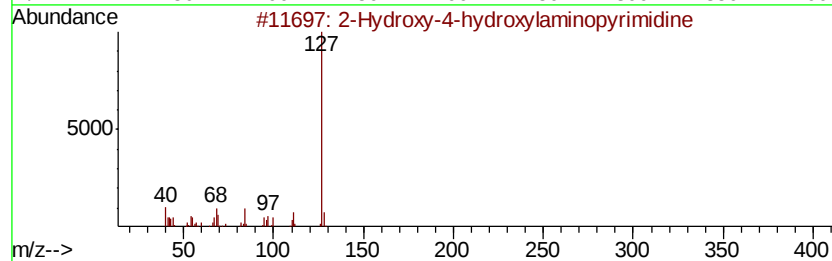
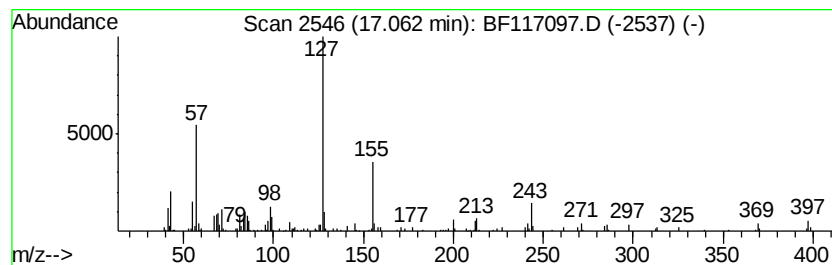
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 unknown17.06 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.06	5.90 ng	459737	Perylene-d12	15.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Hydroxy-4-hydroxylaminopyrimidine	127	C4H5N3O2	020555-88-8	46
2		1,4-Dioxaspiro[4.4]nonane, 7-but...	212	C13H24O2	104807-77-4	43
3		Caprylic anhydride	270	C16H30O3	000623-66-5	43
4		1H-Imidazole, 1-methyl-4-nitro-	127	C4H5N3O2	003034-41-1	43
5		5-Formyl-4-methylthiazole	127	C5H5NOS	082294-70-0	43



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091719\
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Sample : K4883-05
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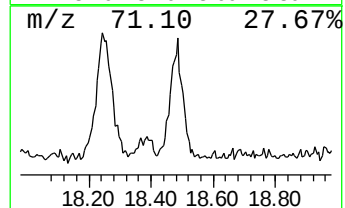
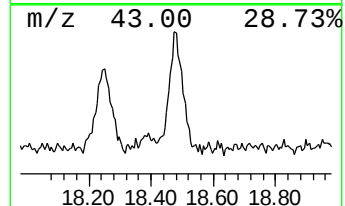
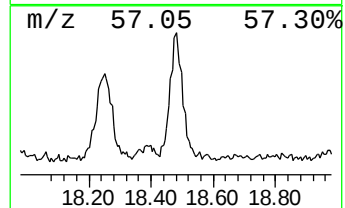
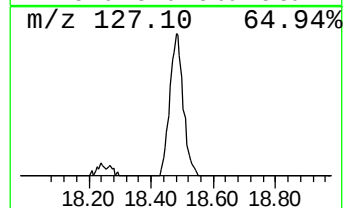
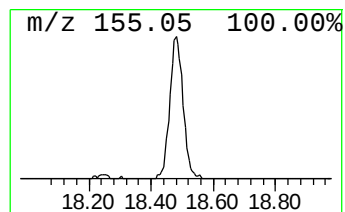
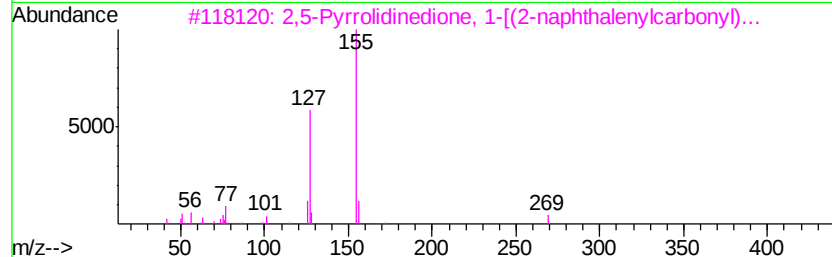
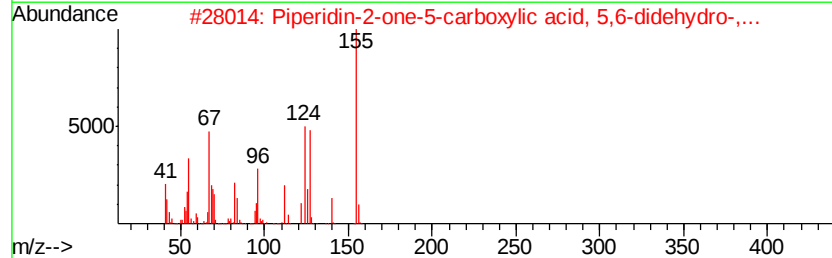
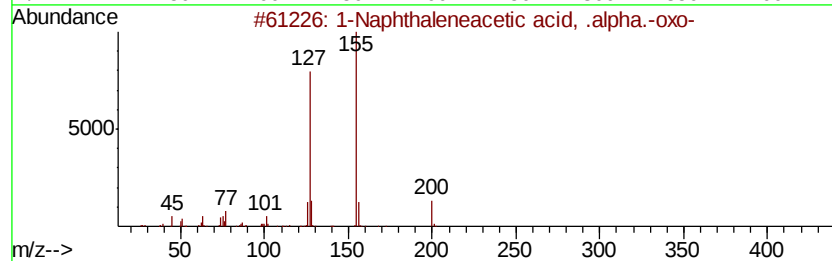
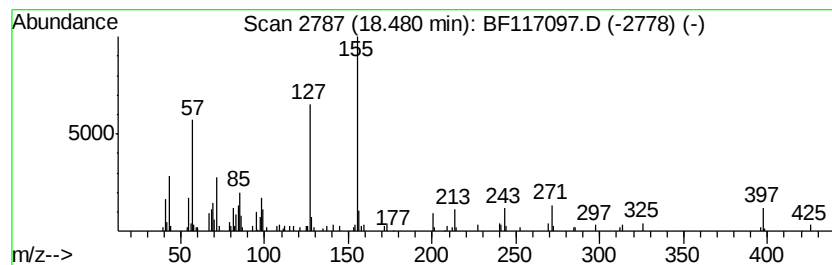
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF091319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 1-Naphthaleneacetic acid, Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.		
18.48	4.28 ng	333438	Perylene-d12	15.42		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Naphthaleneacetic acid, .alpha...	200	C12H8O3	026153-26-4	50	
2	Piperidin-2-one-5-carboxylic aci...	155	C7H9NO3	080658-33-9	50	
3	2,5-Pvrrolidinedione, 1-[f(2-naph...	269	C15H11NO4	056374-47-1	50	
4	2,5-Pvrrolidinedione, 1-[f(1-naph...	269	C15H11NO4	134676-06-5	50	
5	5-Oxazolidinone, 2-(1,1-dimethyl...	297	C18H19NO3	119215-56-4	49	



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF091719\
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 Acq On : 17 Sep 2019 11:03
 Operator : HP/JU
 Sample : K4883-05
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
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 ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Heneicosane	11.60	27.1	ng	813805	4	11.33	599580	20.0
n-Hexadecanoic acid	11.86	6.7	ng	200205	4	11.33	599580	20.0
Octadecanoic acid	12.64	7.9	ng	236165	4	11.33	599580	20.0
Tetratetracontane	13.81	7.0	ng	161642	5	13.97	460037	20.0
2-methyloctacosane	13.89	151.2	ng	3478410	5	13.97	460037	20.0
Hentriacontane	14.27	4.0	ng	92358	5	13.97	460037	20.0
Eicosane	14.49	133.9	ng	3080880	5	13.97	460037	20.0
unknown17.06	17.06	5.9	ng	459737	6	15.42	1558190	20.0
1-Naphthaleneacet...	18.48	4.3	ng	333438	6	15.42	1558190	20.0