

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100818\
 Data File : BF109682.D
 Acq On : 9 Oct 2018 7:56
 Operator : JU/SJ
 Sample : J5309-03
 Misc :
 ALS Vial : 31 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S-11

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-BF100818.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	4.899	475	478	489	rBV	37878	49931	3.01%	0.335%
2	5.322	546	550	577	rBV	1009908	1353471	81.70%	9.089%
3	6.345	721	724	741	rBV	964061	1460512	88.16%	9.807%
4	6.469	741	745	770	rVB	1438997	1656578	100.00%	11.124%
5	6.698	780	784	795	rBV	378520	510418	30.81%	3.427%
6	6.851	806	810	830	rBV	1208628	1236265	74.63%	8.302%
7	7.257	876	879	915	rBV	692875	1020703	61.62%	6.854%
8	7.975	998	1001	1028	rBV	528083	661892	39.96%	4.445%
9	9.051	1180	1184	1202	rBV	1499876	1569943	94.77%	10.542%
10	9.357	1233	1236	1239	rBV	26717	22596	1.36%	0.152%
11	9.445	1244	1251	1262	rBV	69127	81080	4.89%	0.544%
12	9.722	1291	1298	1313	rBV	630074	664278	40.10%	4.461%
13	10.510	1428	1432	1448	rBV	630498	760022	45.88%	5.104%
14	11.204	1546	1550	1569	rBV	450835	558419	33.71%	3.750%
15	11.739	1637	1641	1651	rBV3	52502	73354	4.43%	0.493%
16	12.410	1751	1755	1759	rBV	15385	17743	1.07%	0.119%
17	12.780	1814	1818	1828	rBV	1197488	1172834	70.80%	7.876%
18	13.016	1856	1858	1863	rVB	20131	20031	1.21%	0.135%
19	13.204	1887	1890	1894	rBV	60447	61145	3.69%	0.411%
20	13.245	1894	1897	1904	rVB6	17584	30191	1.82%	0.203%
21	13.357	1912	1916	1919	rBV	25328	25020	1.51%	0.168%
22	13.680	1965	1971	1985	rBV2	117228	176485	10.65%	1.185%
23	13.827	1990	1996	2004	rVV	568095	600586	36.25%	4.033%
24	13.998	2022	2025	2029	rBV	46297	43920	2.65%	0.295%
25	14.304	2073	2077	2085	rBV3	69104	100313	6.06%	0.674%
26	14.598	2123	2127	2130	rBV	64139	62485	3.77%	0.420%
27	14.663	2135	2138	2144	rVV	43708	41824	2.52%	0.281%
28	14.904	2176	2179	2182	rBV	115195	114996	6.94%	0.772%
29	15.221	2229	2233	2237	rBV	308818	442778	26.73%	2.973%
30	15.433	2266	2269	2272	rBV5	18810	22278	1.34%	0.150%
31	15.651	2301	2306	2311	rBV	91603	121325	7.32%	0.815%
32	15.704	2312	2315	2320	rVB7	14621	25643	1.55%	0.172%
33	16.104	2379	2383	2387	rBV4	25045	40198	2.43%	0.270%
34	16.639	2470	2474	2480	rVB3	26984	47777	2.88%	0.321%

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Instrument :
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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	17.092	2548	2551	2562	rVB3	21238	44965	2.71%	0.302%
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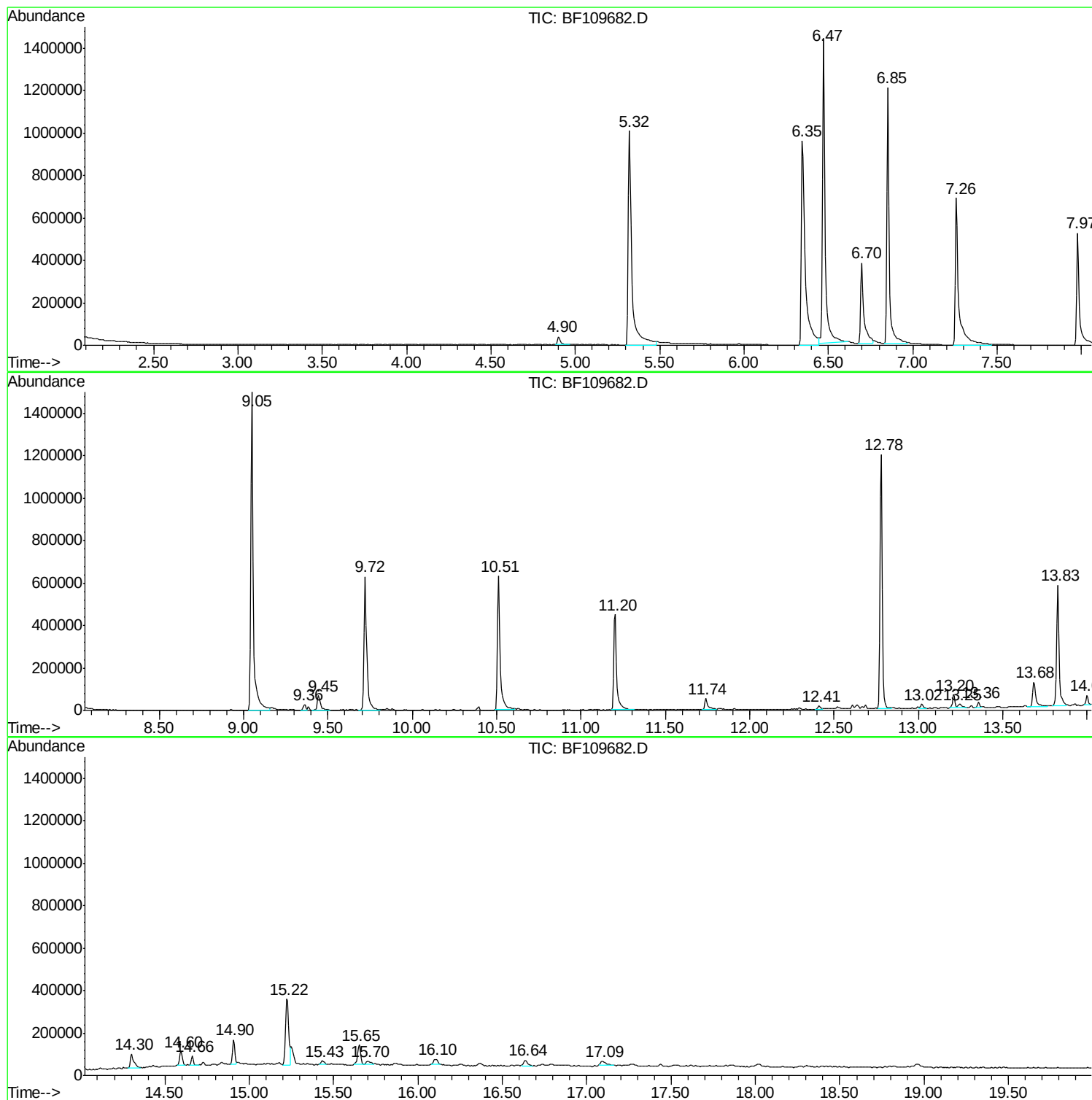
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF100818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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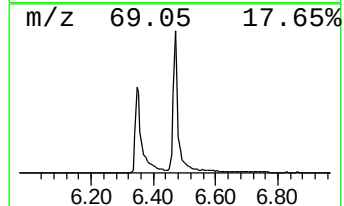
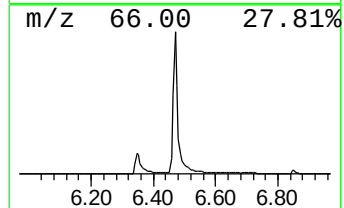
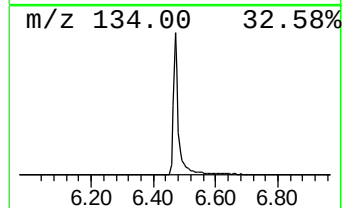
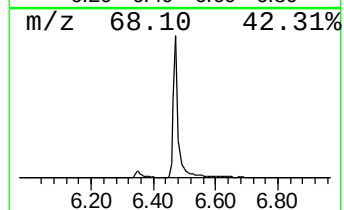
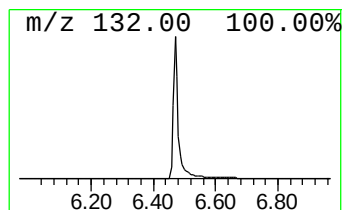
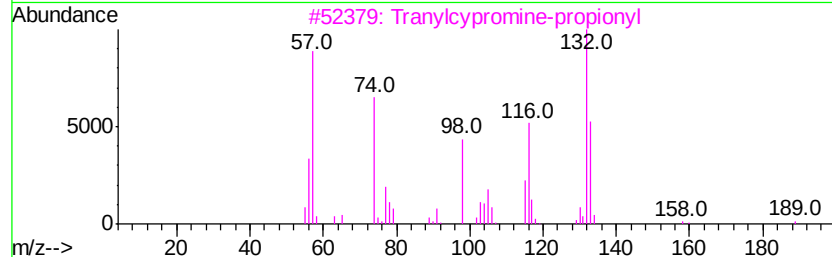
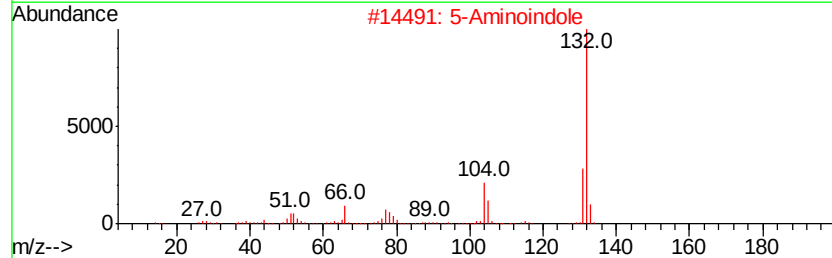
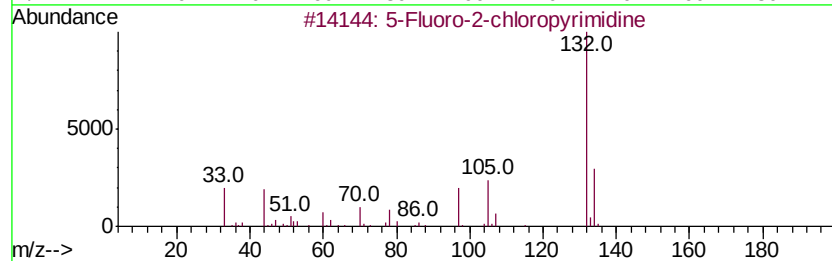
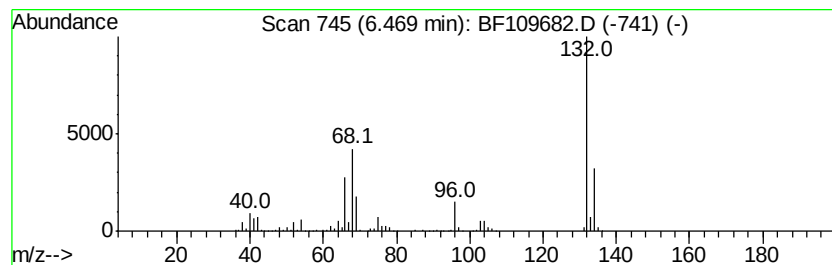
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown6.47 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	64.91 ng	1656580	1,4-Dichlorobenzene-d4	6.70

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2			5-Aminoindole	132	C8H8N2	005192-03-0	12
3			Tranvlcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4			1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9
5			2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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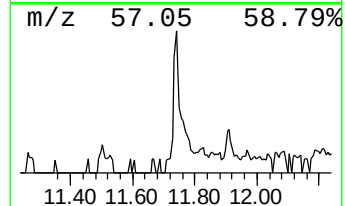
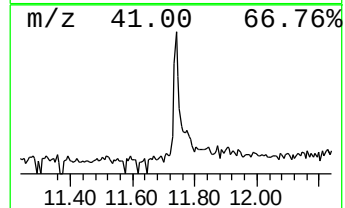
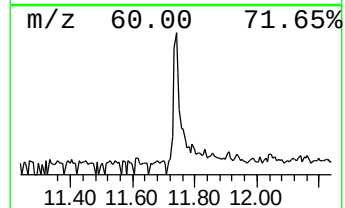
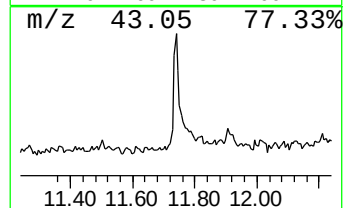
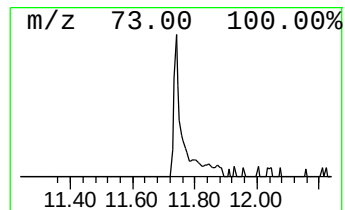
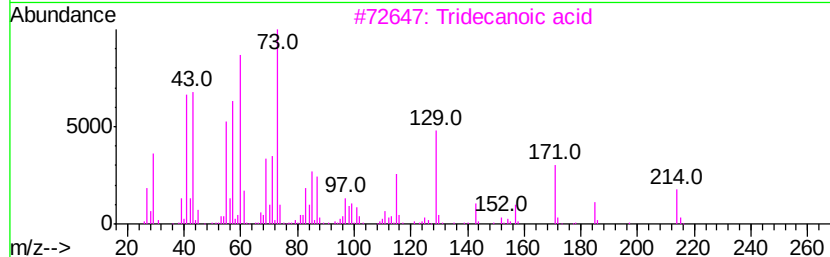
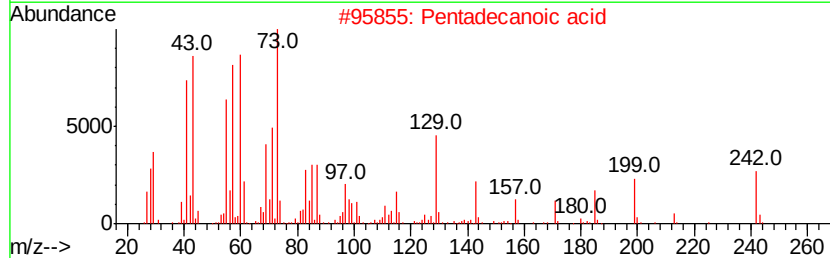
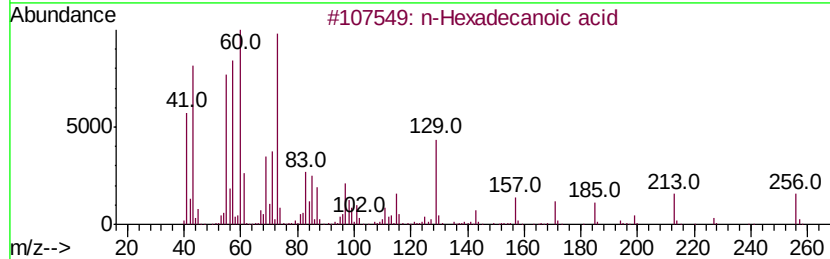
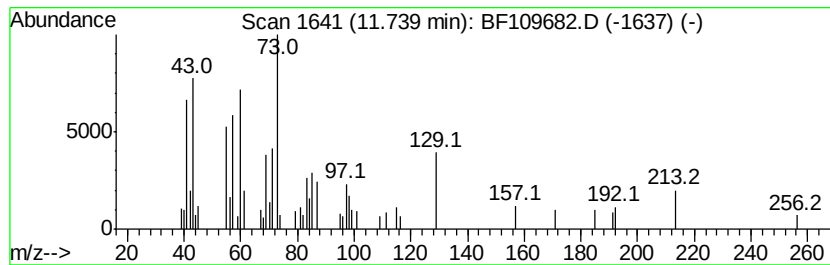
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.74	2.63 ng	73354	Phenanthrene-d10	11.20

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	92
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3		Tridecanoic acid	214	C13H26O2	000638-53-9	64
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	53
5		n-Decanoic acid	172	C10H20O2	000334-48-5	50



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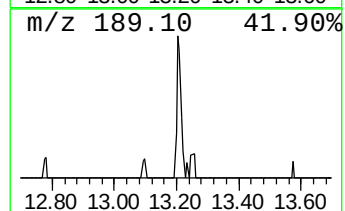
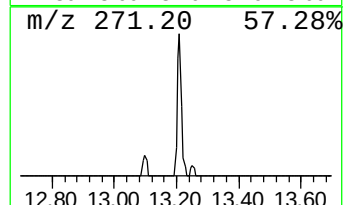
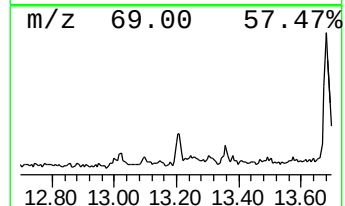
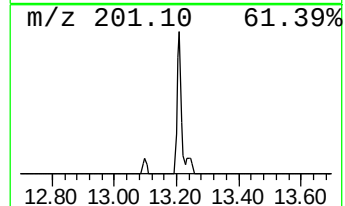
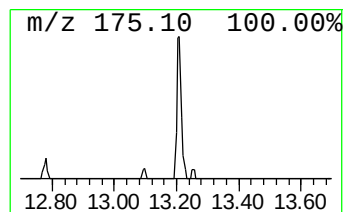
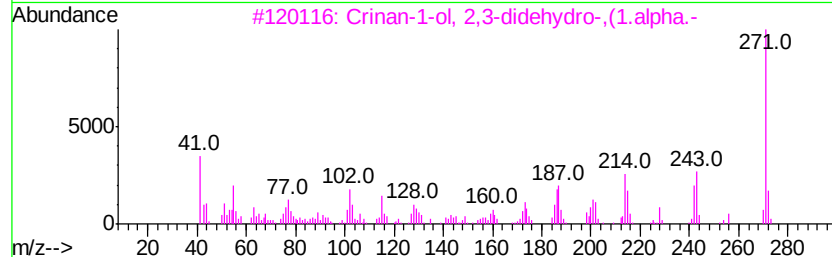
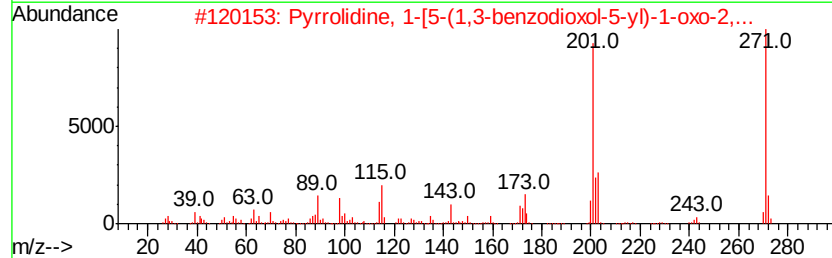
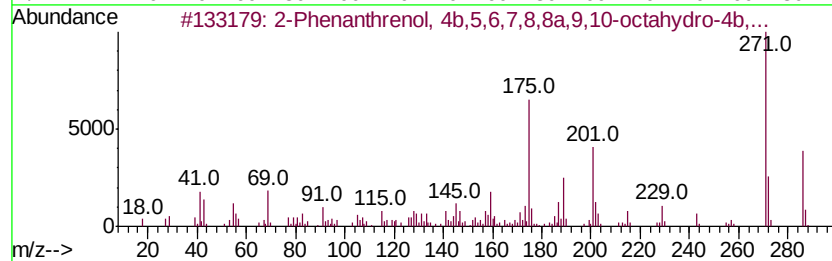
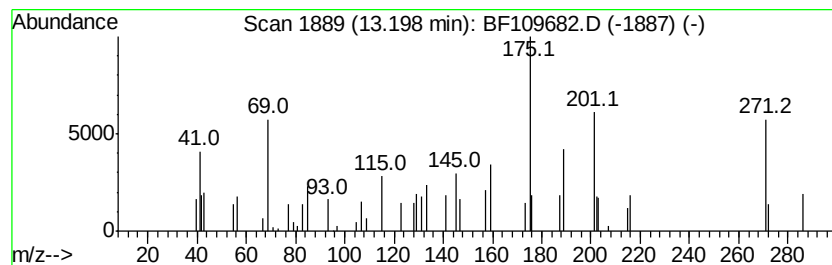
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Phenanthrenol, 4b,5,6,7,8... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.20	2.04 ng	61145	Chrysene-d12	13.83		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Phenanthrenol, 4b,5,6,7,8,8a,9...	286	C20H30O	000511-15-9	60	
2	Pyrrolidine, 1-[5-(1,3-benzodiox...	271	C16H17NO3	025924-78-1	46	
3	Crinan-1-ol, 2,3-didehydro-, (1.a...	271	C16H17NO3	1000111-31-3	22	
4	Quinuclidin-3-one, 2-(4-dimethyl...	271	C16H21N3O	1000266-14-6	22	
5	Oxazole, 2-(1-naphthalenyl)-5-ph...	271	C19H13NO	000846-63-9	14	



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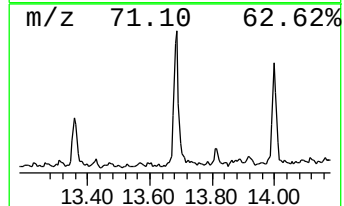
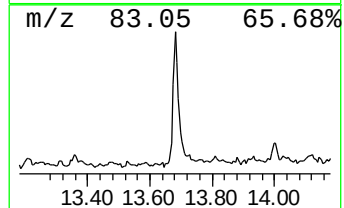
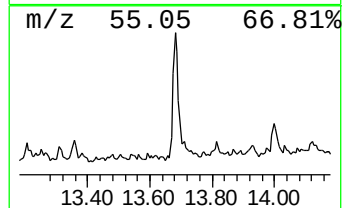
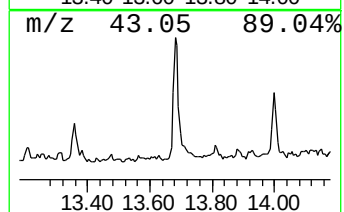
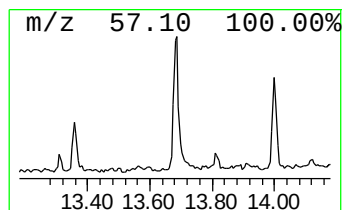
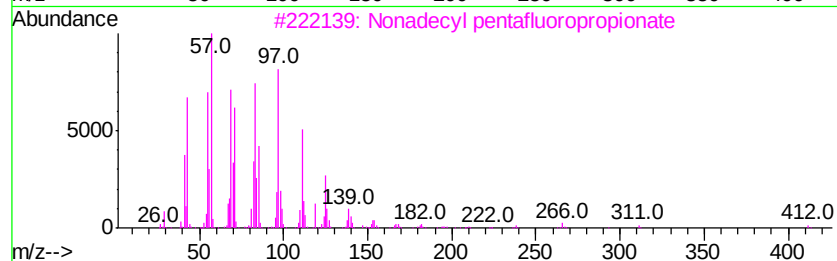
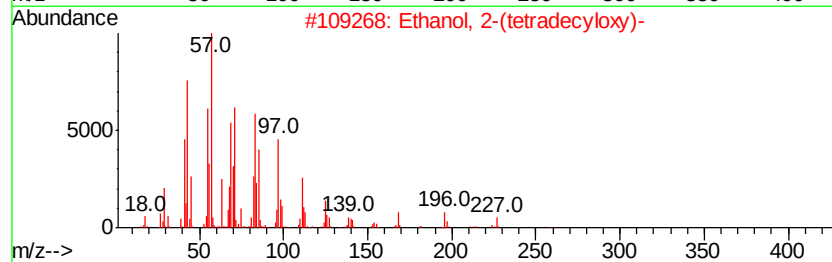
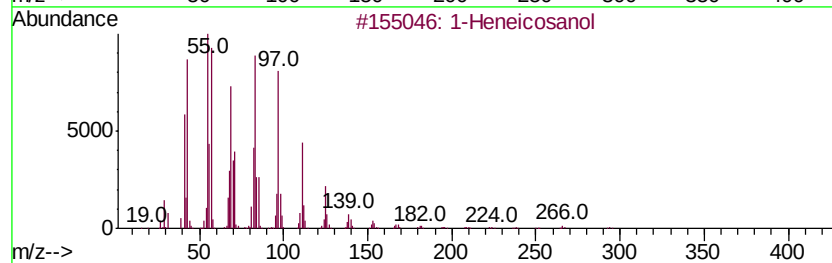
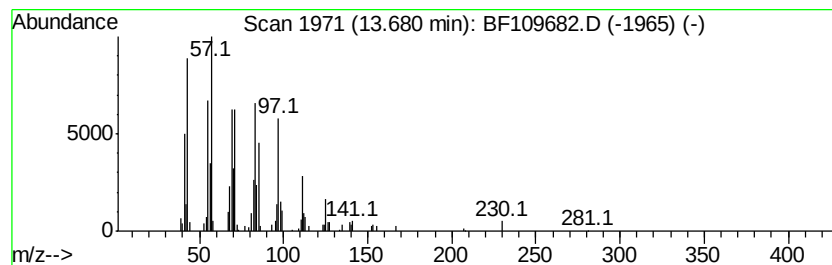
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.68	5.88 ng	176485	Chrysene-d12	13.83		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Heneicosanol	312	C21H44O	015594-90-8	92
2		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
3		Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	87
4		Carbonic acid, hexadecyl 2,2,2-t...	416	C19H35Cl3O3	1000314-56-2	81
5		Trifluoroacetic acid,n-tridecyl ...	296	C15H27F3O2	053800-02-5	76



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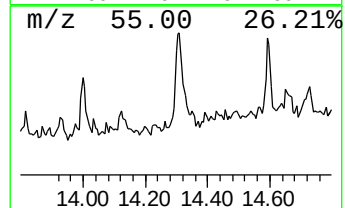
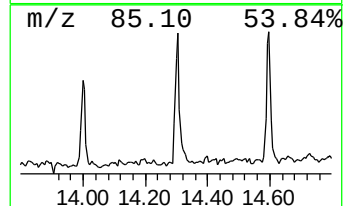
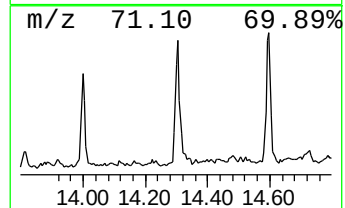
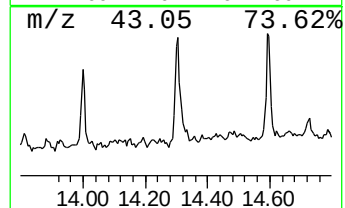
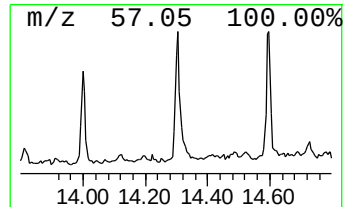
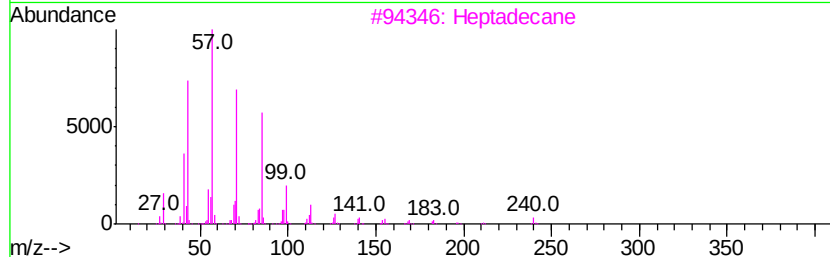
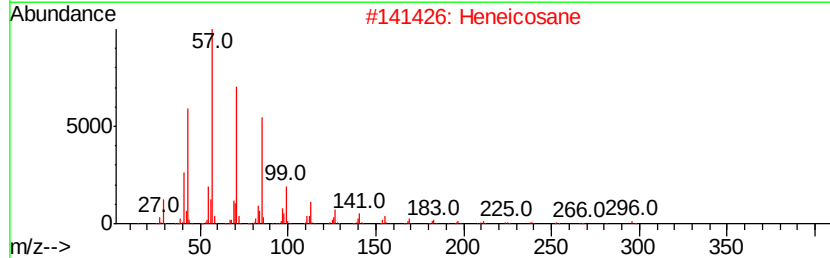
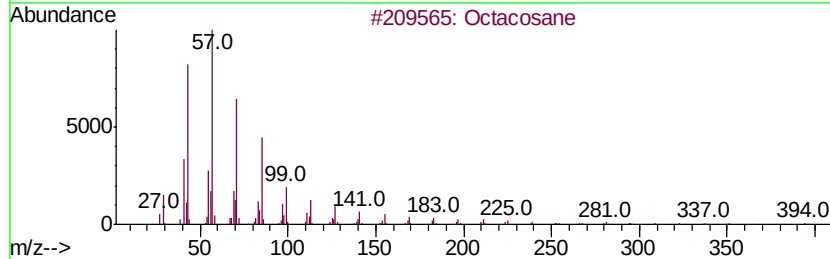
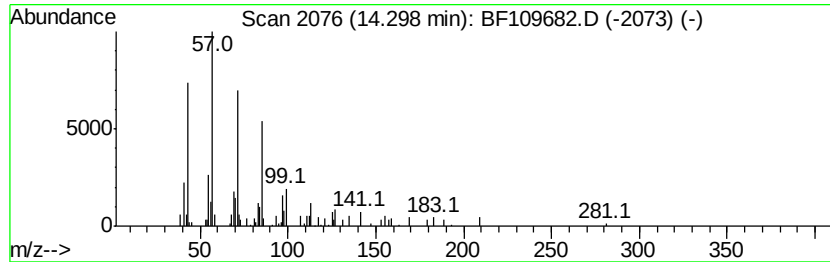
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Peak Number 6 Octacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.		
14.30	3.34 ng	100313	Chrysene-d12		13.83		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	90
2			Heneicosane	296	C21H44	000629-94-7	90
3			Heptadecane	240	C17H36	000629-78-7	87
4			2-methyloctacosane	408	C29H60	1000376-72-8	87
5			Hexacosane	366	C26H54	000630-01-3	86



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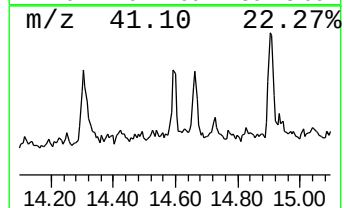
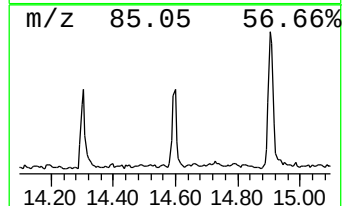
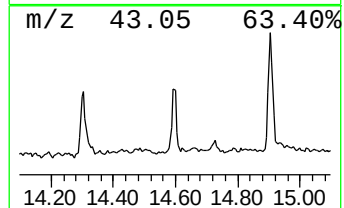
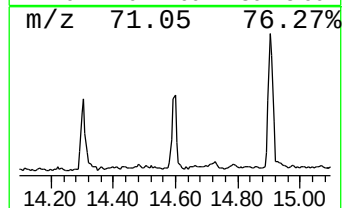
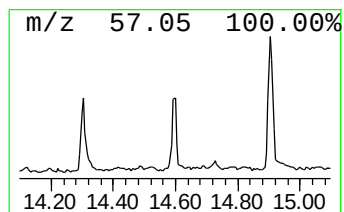
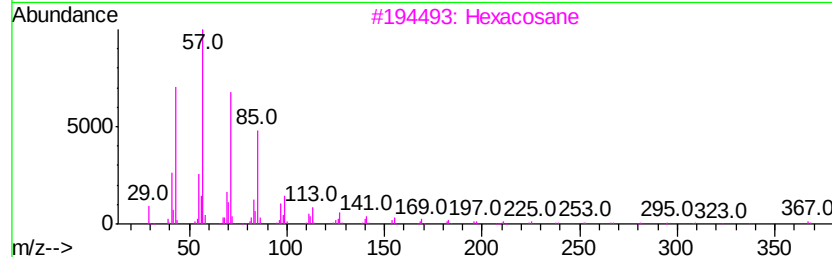
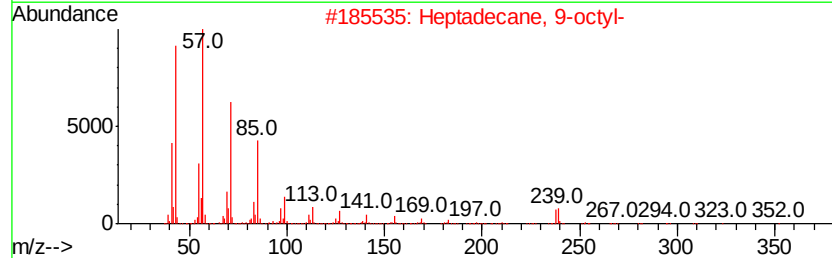
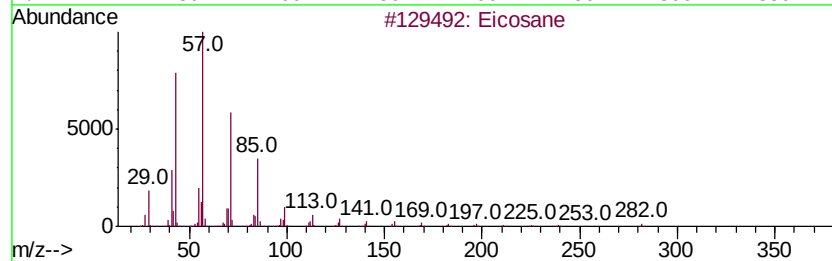
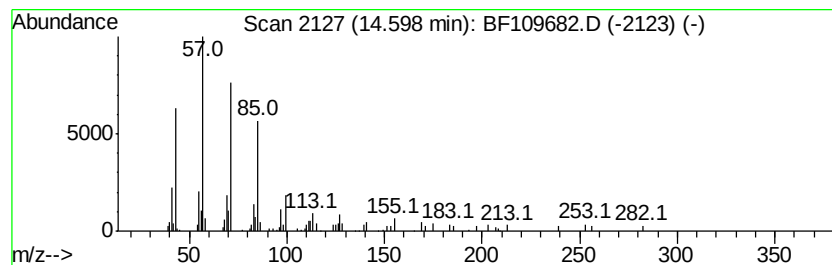
Instrument :
BNA_F
ClientSampleId :
S-11

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF100818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.60	2.82 ng	62485	Perylene-d12	15.22
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Eicosane	282 C20H42	000112-95-8	94
2	Heptadecane, 9-octyl-	352 C25H52	007225-64-1	91
3	Hexacosane	366 C26H54	000630-01-3	91
4	Heneicosane, 11-(1-ethylpropyl)-	366 C26H54	055282-11-6	90
5	Heptadecane	240 C17H36	000629-78-7	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100818\
Data File : BF109682.D
Acq On : 9 Oct 2018 7:56
Operator : JU/SJ
Sample : J5309-03
Misc :
ALS Vial : 31 Sample Multiplier: 1

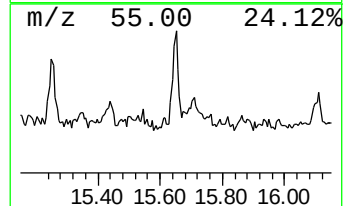
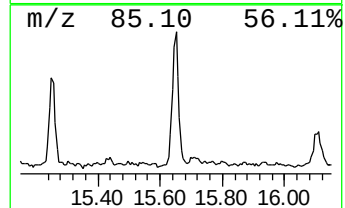
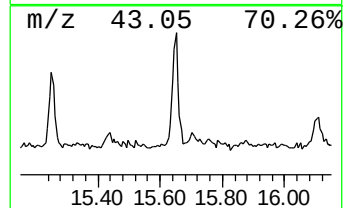
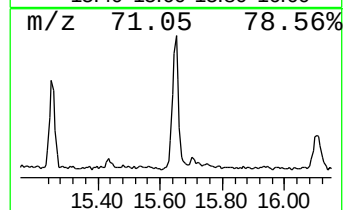
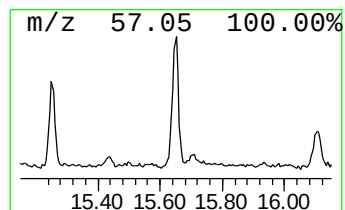
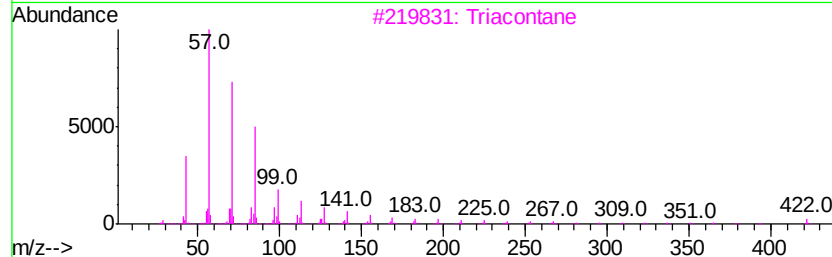
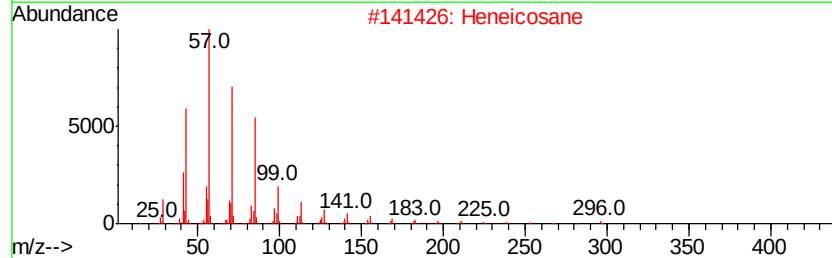
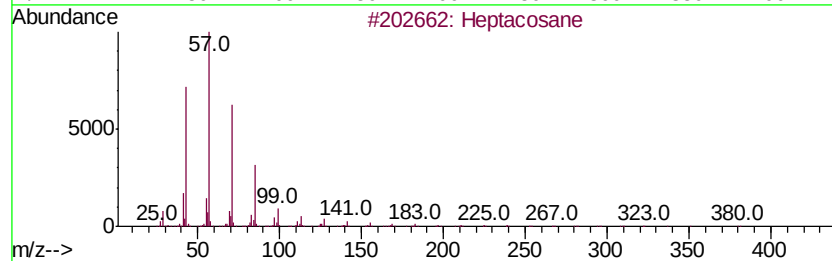
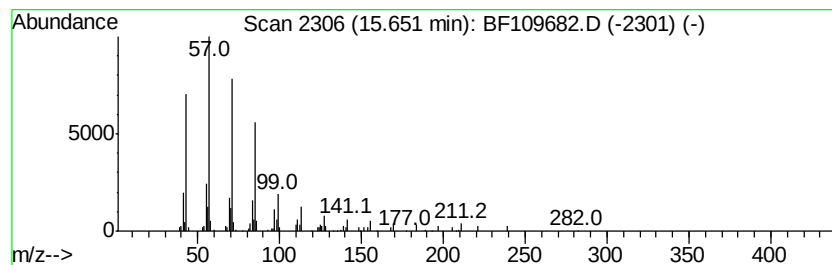
Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF100818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heptacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.65	5.48 ng	121325	Perylene-d12	15.22
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Heptacosane	380 C27H56	000593-49-7	91
2	Heneicosane	296 C21H44	000629-94-7	91
3	Triacontane	422 C30H62	000638-68-6	91
4	2-methyloctacosane	408 C29H60	1000376-72-8	91
5	Octacosane	394 C28H58	000630-02-4	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100818\
Data File : BF109682.D
Acq On : 9 Oct 2018 7:56
Operator : JU/SJ
Sample : J5309-03
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
S-11

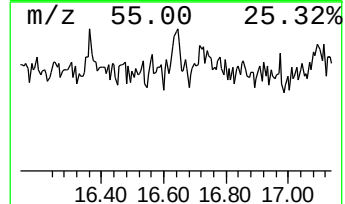
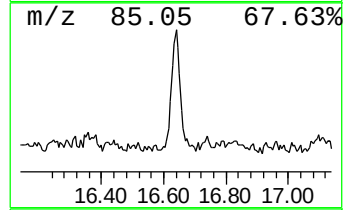
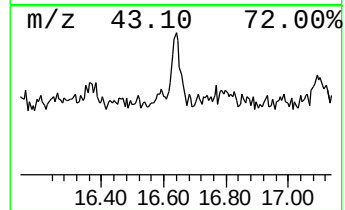
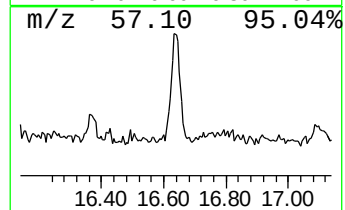
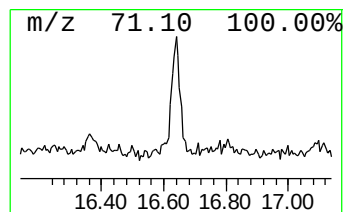
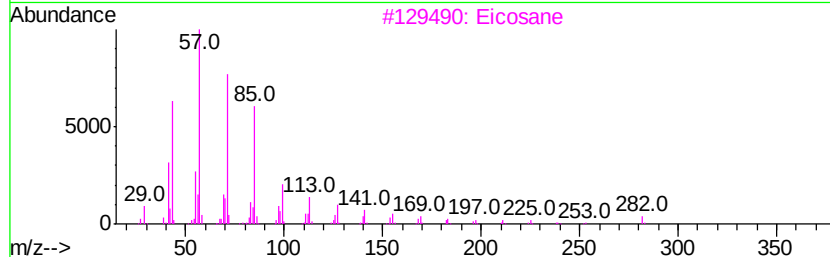
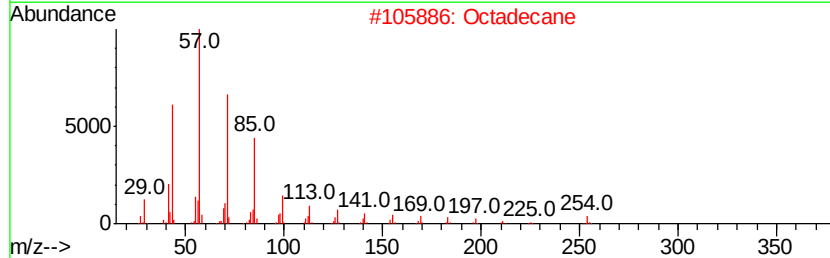
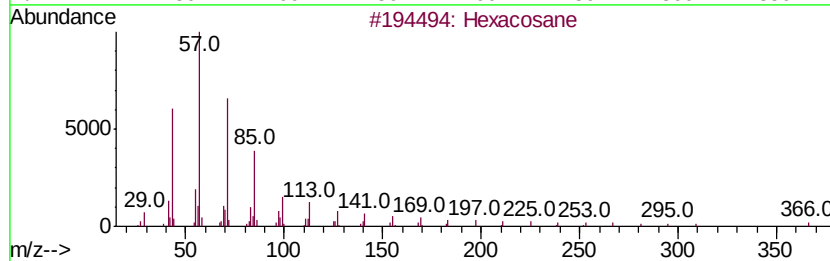
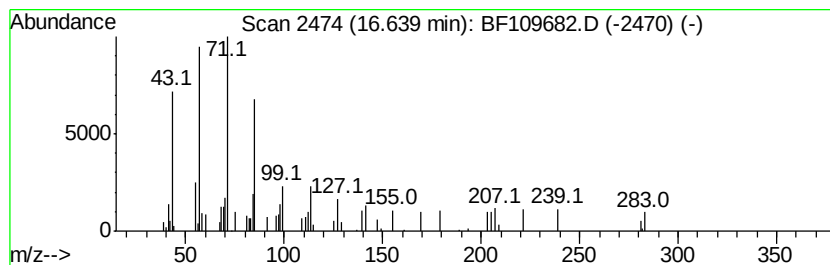
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hexacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.64	2.16 ng	47777	Perylene-d12	15.22

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	59
2		Octadecane	254	C18H38	000593-45-3	59
3		Eicosane	282	C20H42	000112-95-8	58
4		Tetracosane	338	C24H50	000646-31-1	53
5		Hexatriacontane	507	C36H74	000630-06-8	53



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF100818\
Data File : BF109682.D
Acq On : 9 Oct 2018 7:56
Operator : JU/SJ
Sample : J5309-03
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-11

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.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
unknown6.47	6.47	64.9	ng	1656580	1	6.70	510418	20.0
n-Hexadecanoic acid	11.74	2.6	ng	73354	4	11.20	558419	20.0
2-Phenanthrenol, ...	13.20	2.0	ng	61145	5	13.83	600586	20.0
1-Heneicosanol	13.68	5.9	ng	176485	5	13.83	600586	20.0
Octacosane	14.30	3.3	ng	100313	5	13.83	600586	20.0
Eicosane	14.60	2.8	ng	62485	6	15.22	442778	20.0
Heptacosane	15.65	5.5	ng	121325	6	15.22	442778	20.0
Hexacosane	16.64	2.2	ng	47777	6	15.22	442778	20.0