

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF011819\
 Data File : BF112120.D
 Acq On : 18 Jan 2019 11:58
 Operator : JU/SJ
 Sample : K1157-13
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WC-07-011519

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	2.152	7	11	17	rVB	131362	176978	2.93%	0.331%
2	5.075	503	508	519	rVB	248348	288855	4.77%	0.540%
3	5.493	575	579	591	rBV	4895985	4482687	74.10%	8.387%
4	6.498	746	750	766	rBV	4614429	4903152	81.05%	9.174%
5	6.634	768	773	776	rBV	5407028	4936808	81.60%	9.237%
6	6.857	807	811	819	rBV	1928118	1610629	26.62%	3.014%
7	7.016	833	838	841	rBV	4206585	4006664	66.23%	7.497%
8	7.416	901	906	909	rBV	3338477	2985264	49.34%	5.586%
9	8.139	1024	1029	1032	rBV	2264827	2094011	34.61%	3.918%
10	9.210	1207	1211	1215	rBV	6453684	6049846	100.00%	11.320%
11	9.604	1274	1278	1282	rVB	355590	300661	4.97%	0.563%
12	9.804	1307	1312	1318	rVB6	29165	62410	1.03%	0.117%
13	9.892	1323	1327	1331	rBV	2773030	2340784	38.69%	4.380%
14	10.680	1457	1461	1474	rBV	3553017	3316639	54.82%	6.206%
15	11.380	1576	1580	1583	rBV	2478821	2234923	36.94%	4.182%
16	11.404	1583	1584	1587	rVB	136220	68053	1.12%	0.127%
17	11.904	1666	1669	1673	rBV2	119654	115494	1.91%	0.216%
18	12.592	1783	1786	1790	rVB	185174	156924	2.59%	0.294%
19	12.822	1820	1825	1831	rBV	162204	179286	2.96%	0.335%
20	12.963	1845	1849	1852	rBV	5361577	4669608	77.19%	8.737%
21	13.533	1944	1946	1954	rVB3	70198	98120	1.62%	0.184%
22	13.851	1997	2000	2007	rVB3	329440	401030	6.63%	0.750%
23	13.992	2021	2024	2025	rBV	73566	66538	1.10%	0.124%
24	14.021	2025	2029	2032	rVV	1820983	1719059	28.41%	3.216%
25	14.180	2052	2056	2059	rBV	227527	221800	3.67%	0.415%
26	14.480	2103	2107	2113	rVB	477979	475744	7.86%	0.890%
27	14.786	2156	2159	2164	rBV	566873	535245	8.85%	1.001%
28	15.063	2203	2206	2213	rVB	77247	119312	1.97%	0.223%
29	15.127	2213	2217	2227	rBV	603081	720436	11.91%	1.348%
30	15.363	2254	2257	2264	rVB	60769	90387	1.49%	0.169%
31	15.427	2265	2268	2274	rVB	52815	77294	1.28%	0.145%
32	15.492	2274	2279	2291	rBV3	1536832	2517515	41.61%	4.710%
33	15.945	2351	2356	2361	rVB	493756	697787	11.53%	1.306%
34	16.451	2436	2442	2452	rVB	262931	464783	7.68%	0.870%

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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 >
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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	17.039	2538	2542	2550	rVB2	128223	261445	4.32%	0.489%
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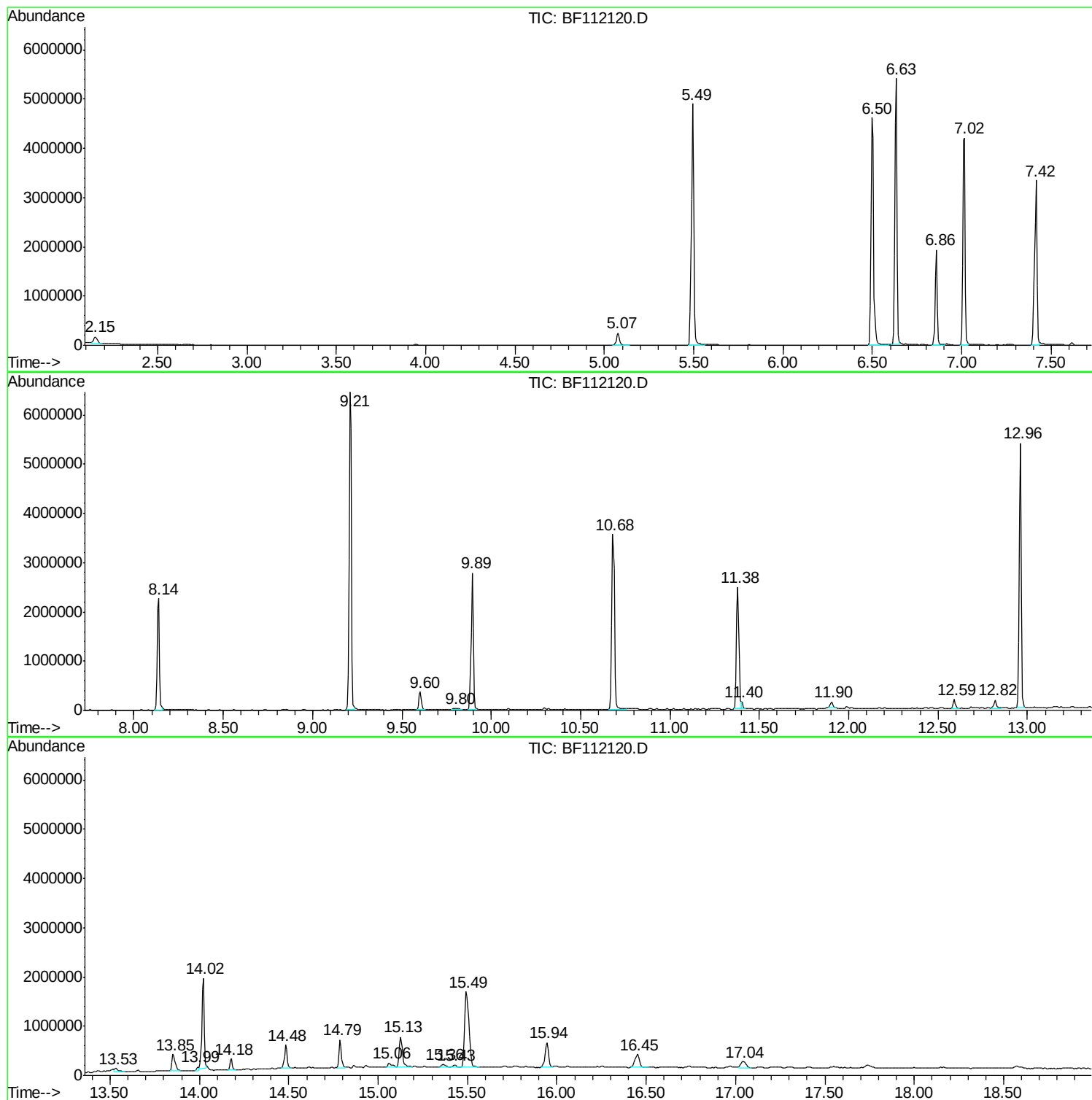
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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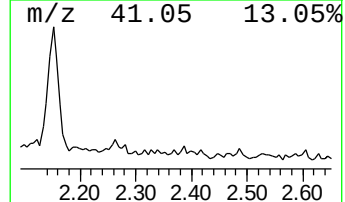
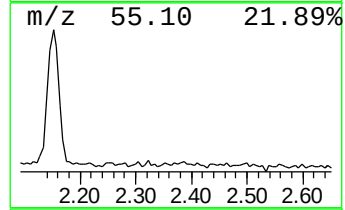
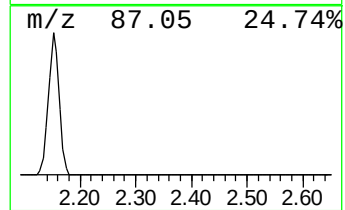
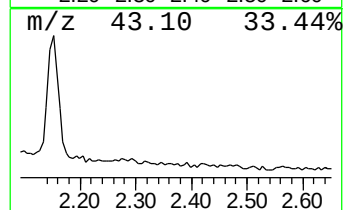
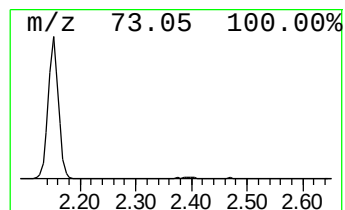
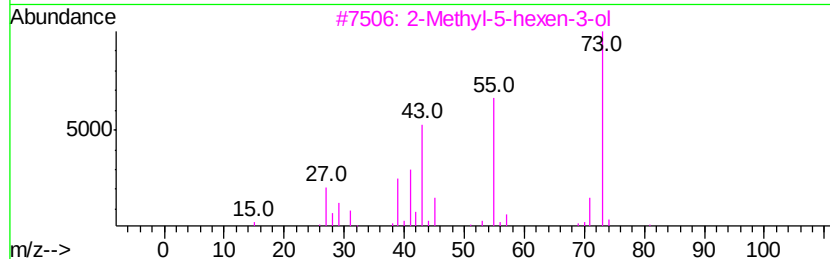
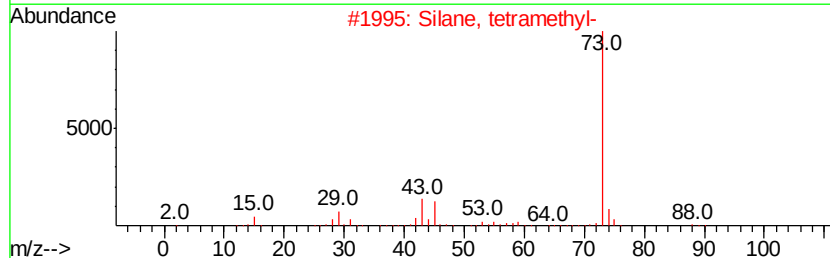
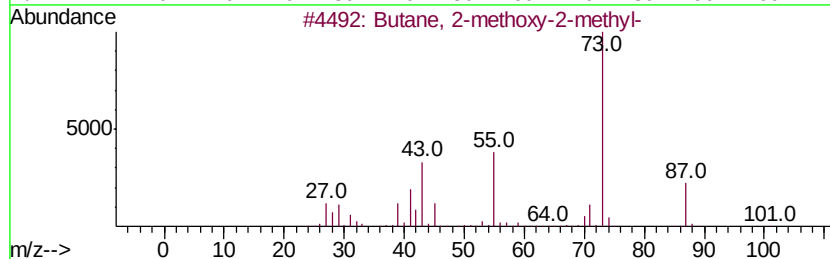
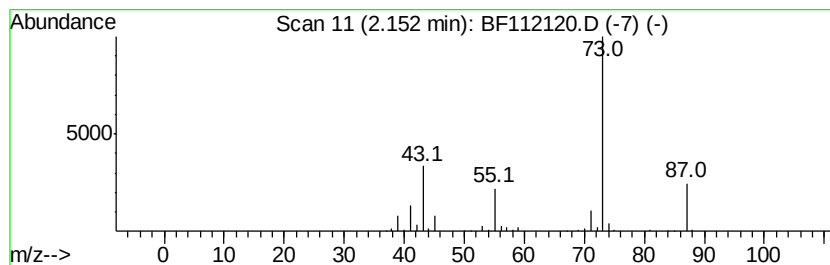
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.		
2.15	2.20 ng	176978	1,4-Dichlorobenzene-d4	6.86		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	64
2		Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
3		2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	25
4		Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9
5		N-Ethylformamide	73	C3H7NO	000627-45-2	9



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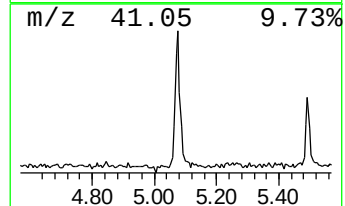
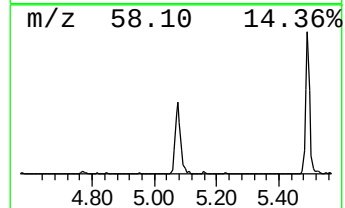
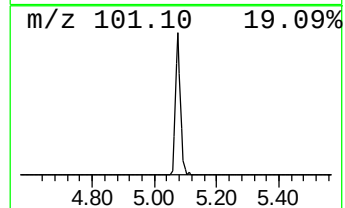
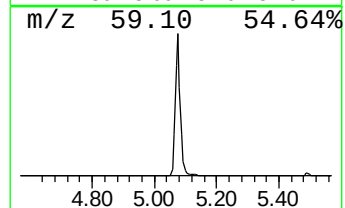
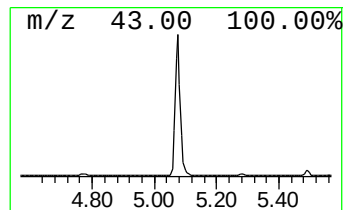
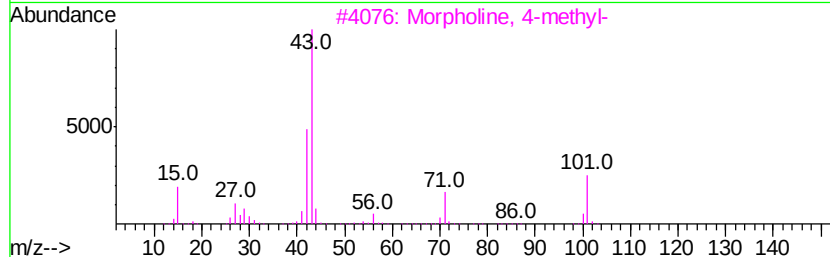
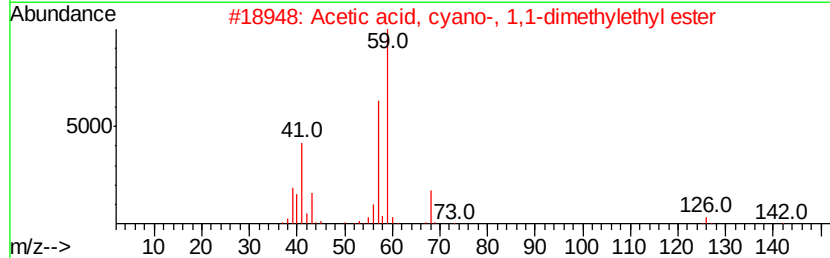
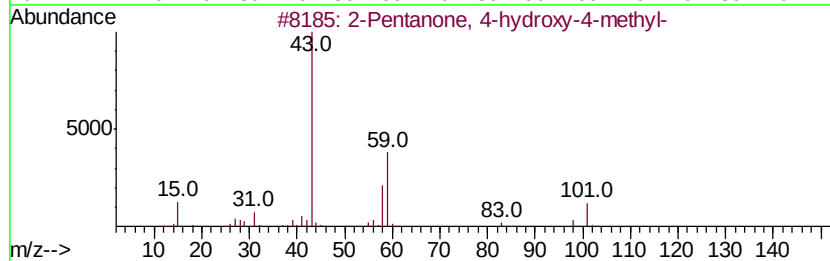
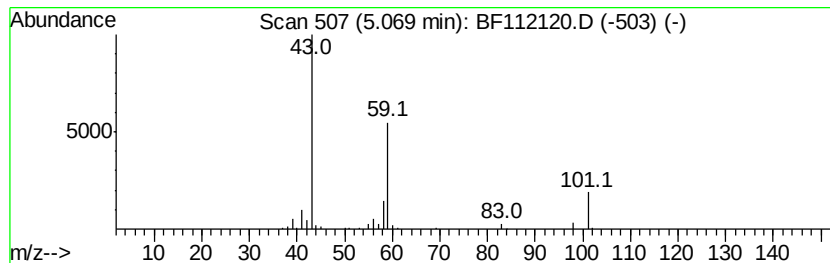
Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF011619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.07	3.59 ng	288855	1,4-Dichlorobenzene-d4	6.86	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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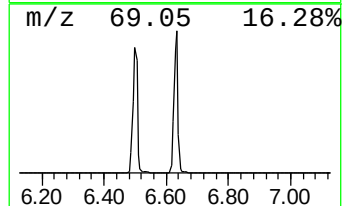
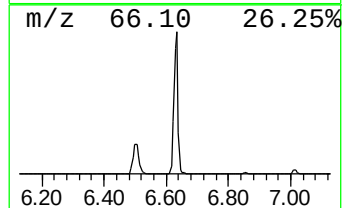
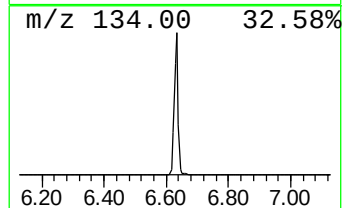
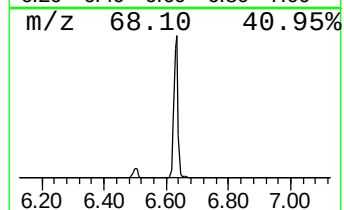
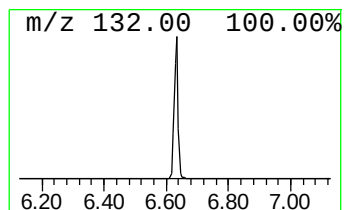
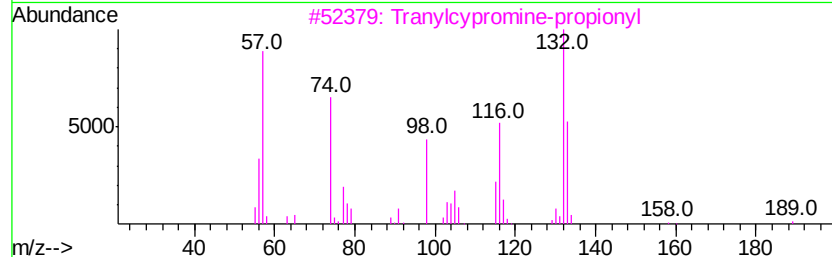
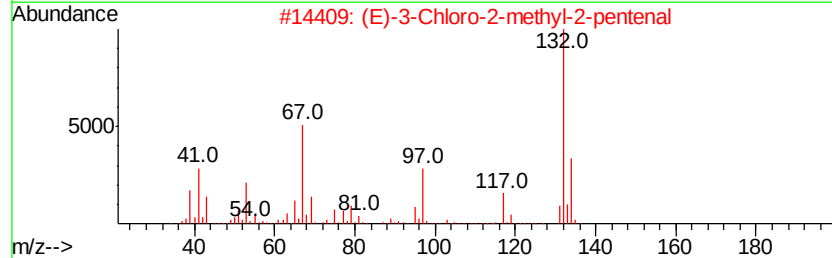
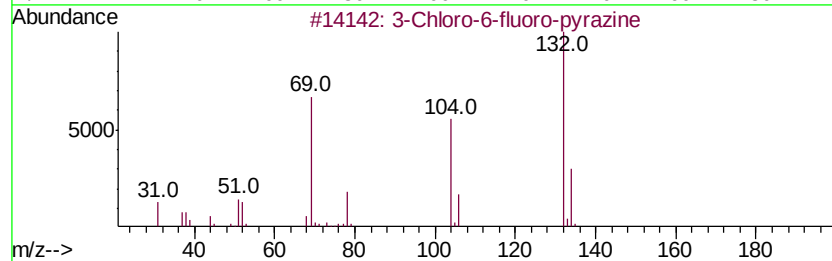
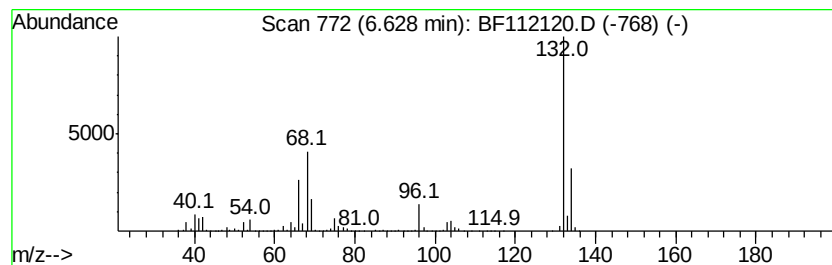
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	61.30 ng	4936810	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	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	16
4		Xenon	132	Xe	007440-63-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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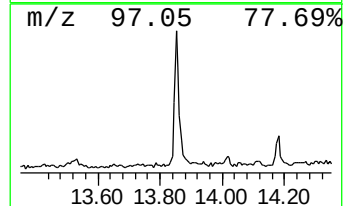
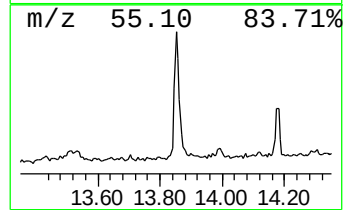
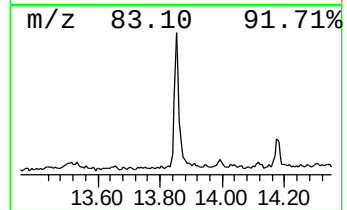
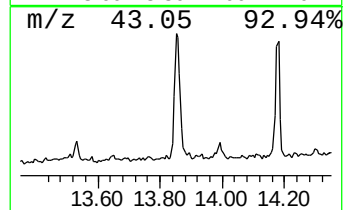
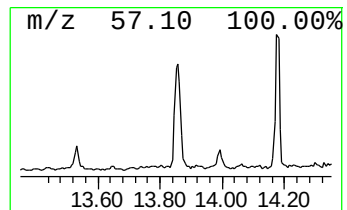
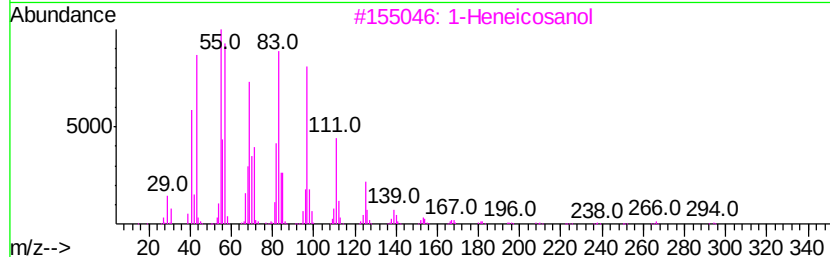
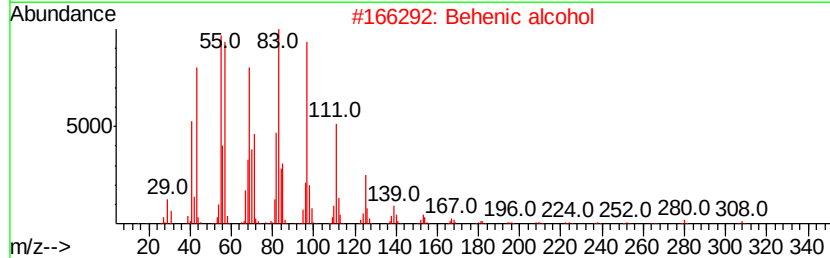
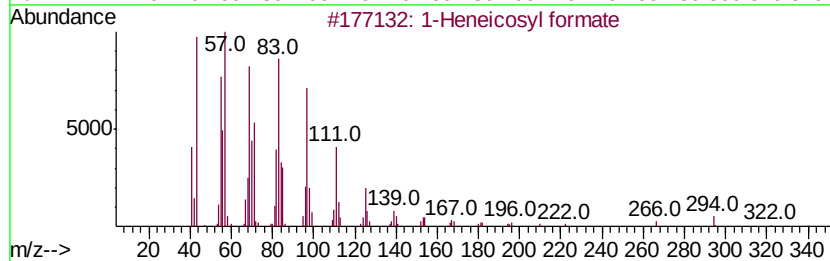
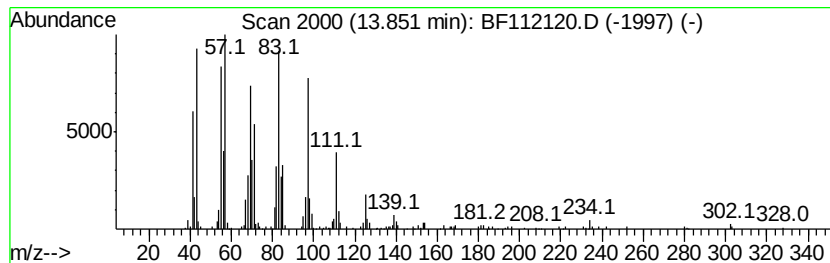
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 6 1-Heneicosyl formate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.85	4.67 ng	401030	Chrysene-d12	14.02	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosyl formate	340	C22H44O2	077899-03-7	95
2	Behenic alcohol	326	C22H46O	000661-19-8	93
3	1-Heneicosanol	312	C21H44O	015594-90-8	93
4	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	91
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	90



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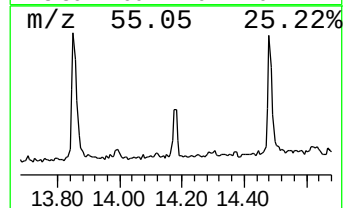
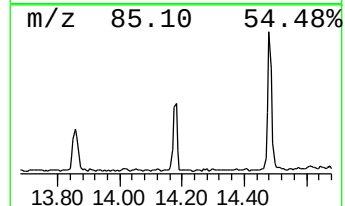
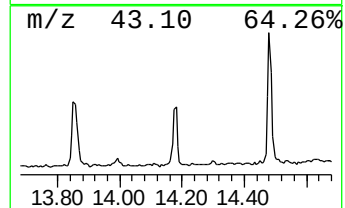
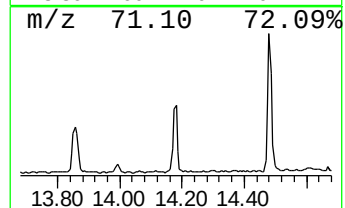
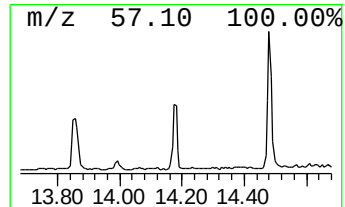
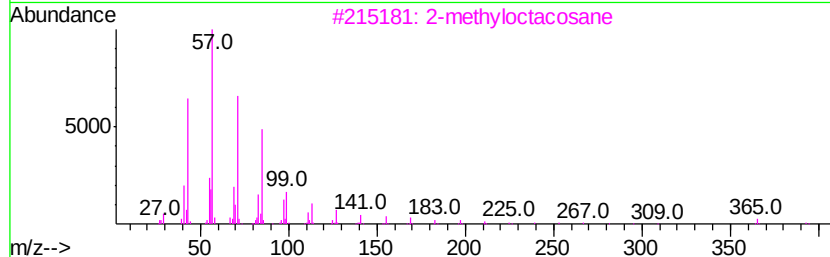
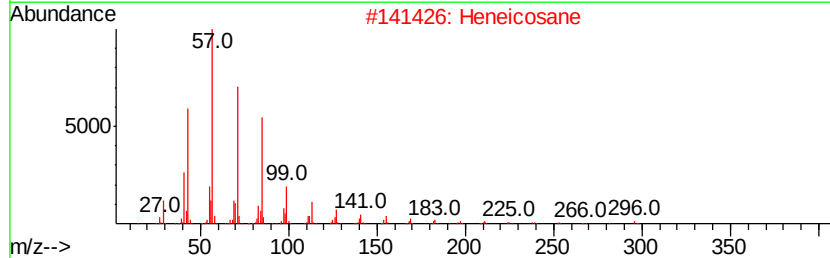
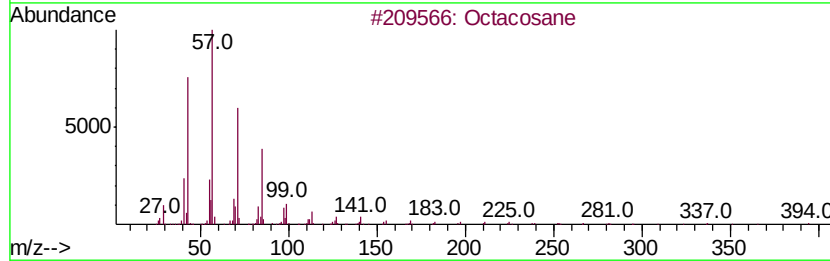
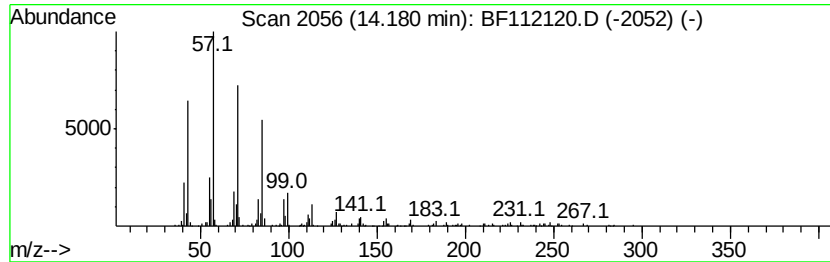
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Hexatriacontane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.18	2.58 ng	221800	Chrysene-d12	14.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	90
2		Heneicosane	296	C21H44	000629-94-7	90
3		2-methyloctacosane	408	C29H60	1000376-72-8	90
4		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
5		Hexatriacontane	507	C36H74	000630-06-8	90



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Misc :
ALS Vial : 8 Sample Multiplier: 1

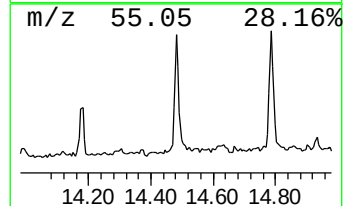
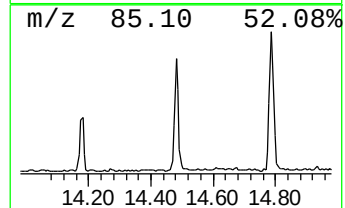
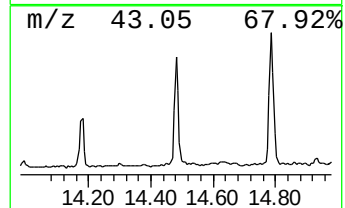
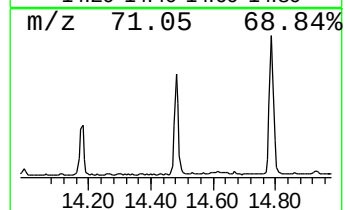
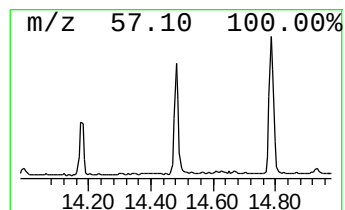
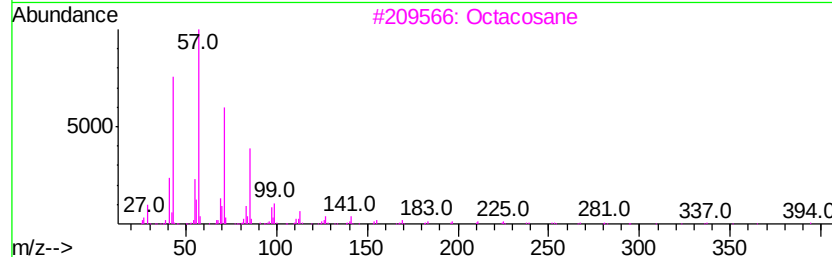
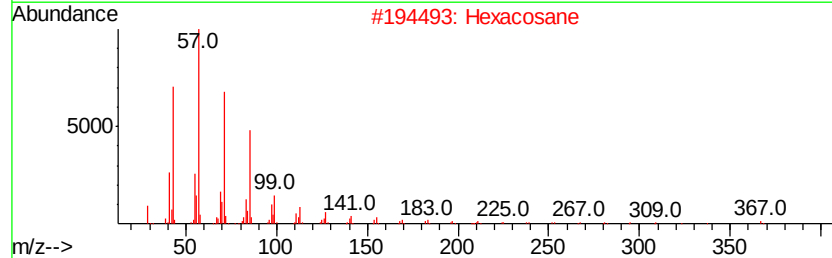
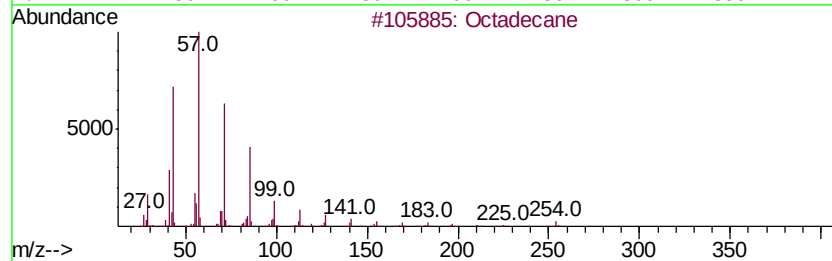
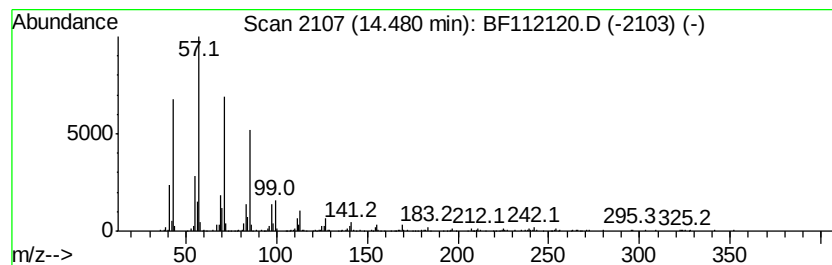
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BNA_F
ClientSampleId :
WC-07-011519

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 8 Octadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
14.48	5.53 ng	475744	Chrysene-d12		14.02
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	95
2	Hexacosane	366	C26H54	000630-01-3	94
3	Octacosane	394	C28H58	000630-02-4	91
4	Tetratetracontane	619	C44H90	007098-22-8	91
5	Hexatriacontane	507	C36H74	000630-06-8	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF011819\
Data File : BF112120.D
Acq On : 18 Jan 2019 11:58
Operator : JU/SJ
Sample : K1157-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

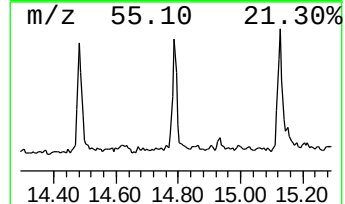
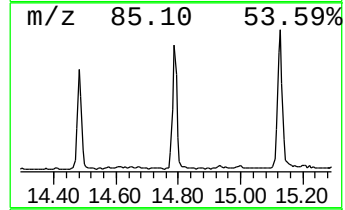
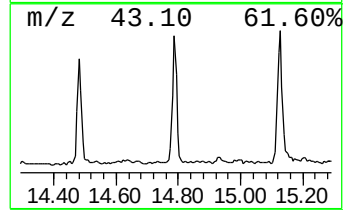
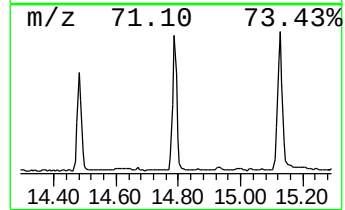
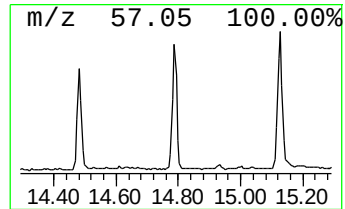
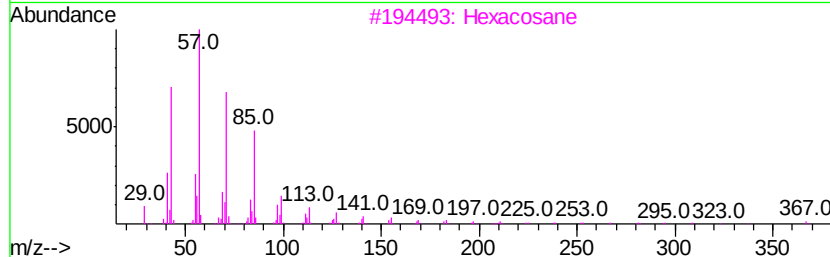
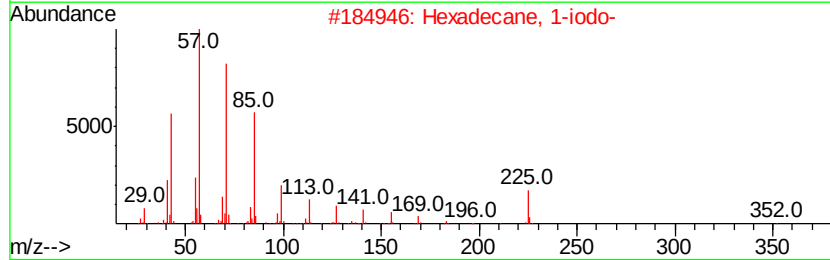
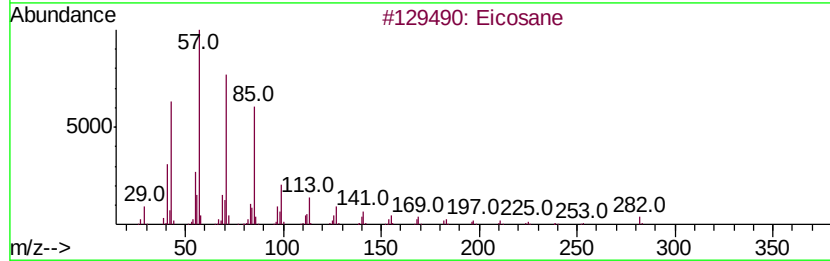
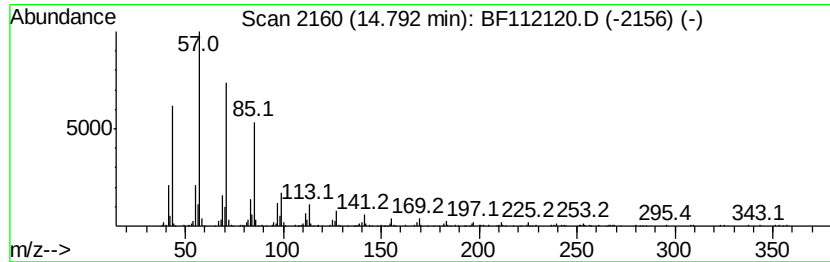
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
14.79	4.25 ng	535245	Perylene-d12		15.49
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	98
2	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	95
3	Hexacosane	366	C26H54	000630-01-3	94
4	Tetracosane	338	C24H50	000646-31-1	94
5	Nonadecane	268	C19H40	000629-92-5	93



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF011819\
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 Acq On : 18 Jan 2019 11:58
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 Sample : K1157-13
 Misc :
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Instrument :
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 ClientSampleId :
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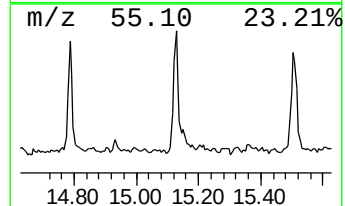
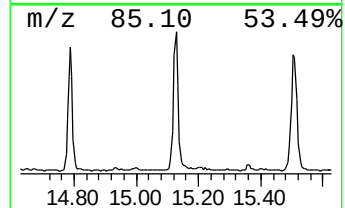
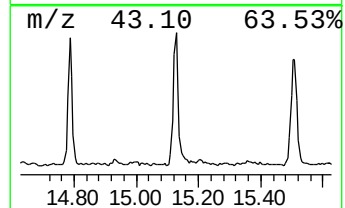
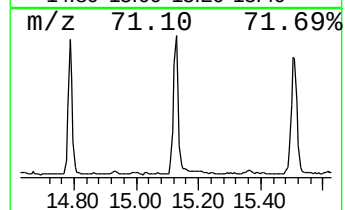
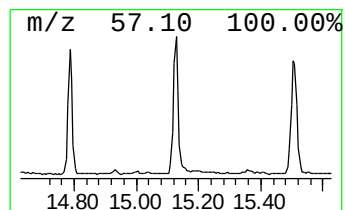
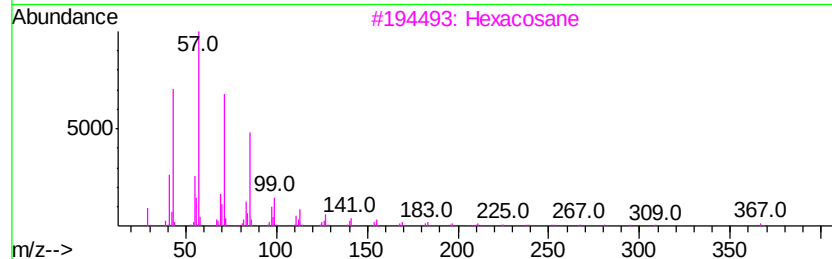
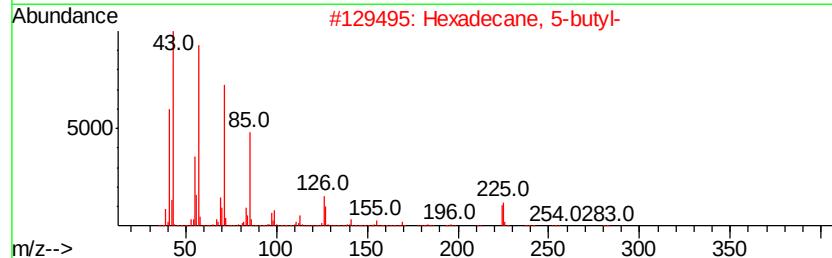
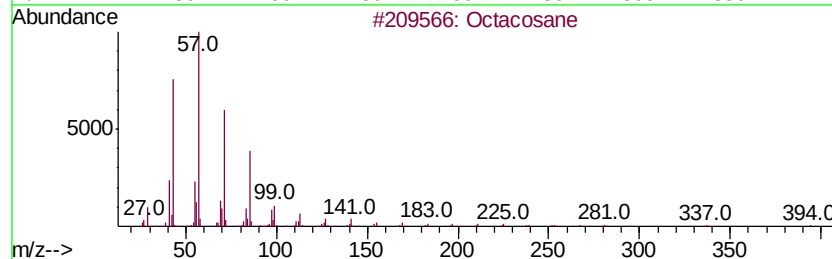
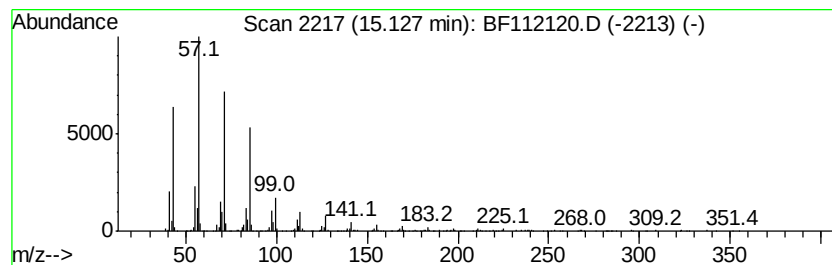
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 10 Octacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.13	5.72 ng	720436	Perylene-d12	15.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	91
2		Hexadecane, 5-butyl-	282	C20H42	006912-07-8	91
3		Hexacosane	366	C26H54	000630-01-3	91
4		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5		Heneicosane	296	C21H44	000629-94-7	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF011819\
Data File : BF112120.D
Acq On : 18 Jan 2019 11:58
Operator : JU/SJ
Sample : K1157-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

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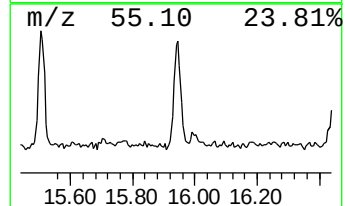
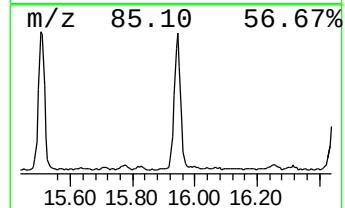
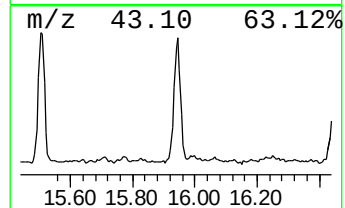
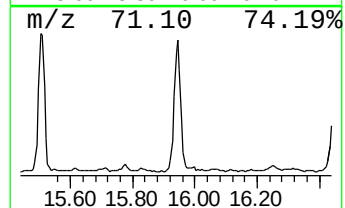
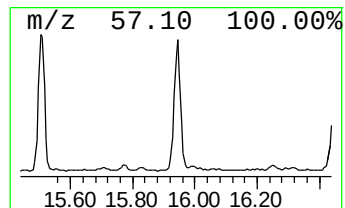
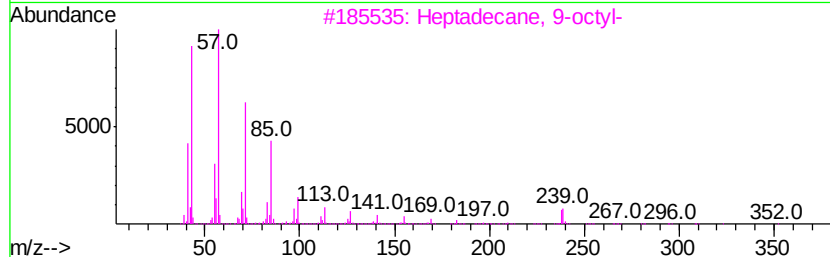
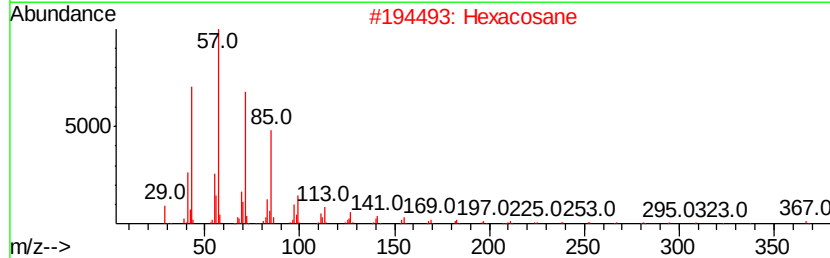
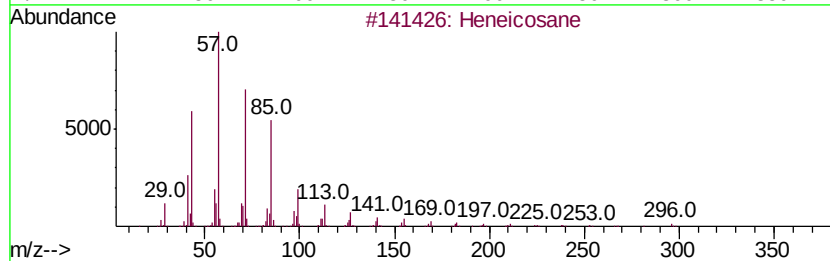
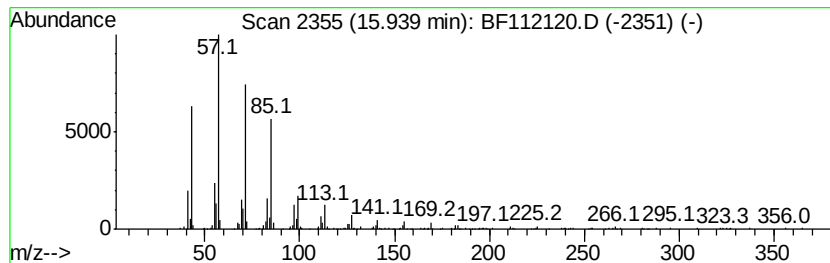
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.94	5.54 ng	697787	Perylene-d12	15.49

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	96
2			Hexacosane	366	C26H54	000630-01-3	94
3			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4			2-methyloctacosane	408	C29H60	1000376-72-8	91
5			Tetracosane	338	C24H50	000646-31-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF011819\
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Acq On : 18 Jan 2019 11:58
Operator : JU/SJ
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Misc :
ALS Vial : 8 Sample Multiplier: 1

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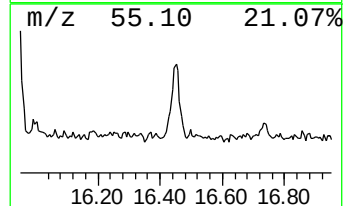
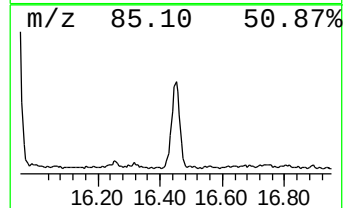
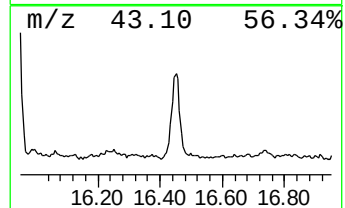
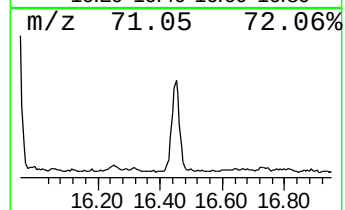
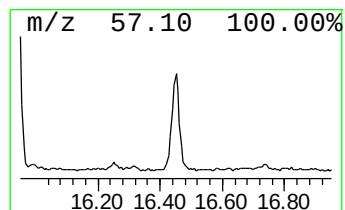
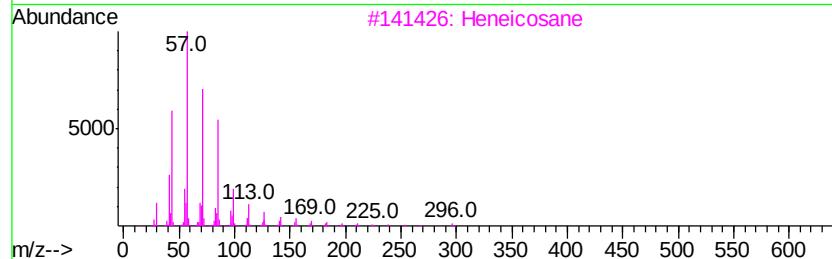
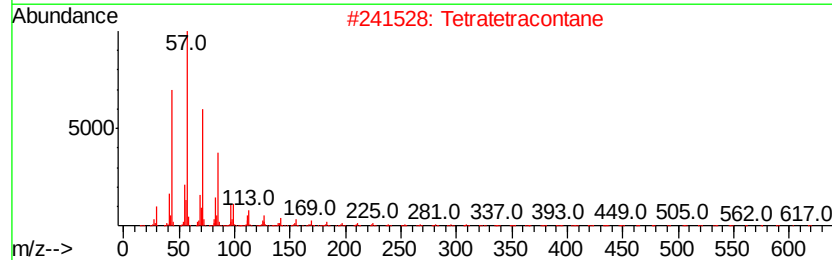
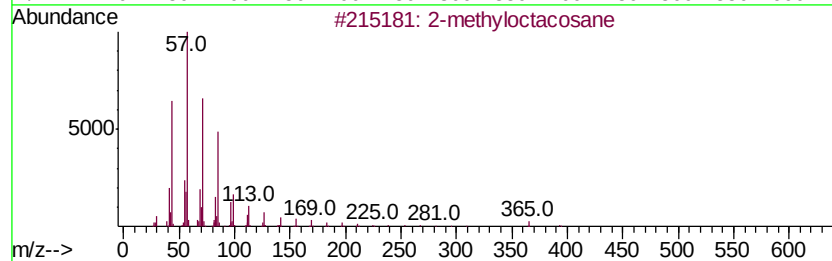
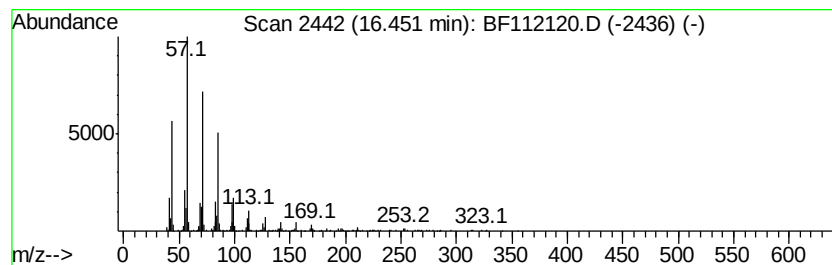
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 2-methyloctacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.45	3.69 ng	464783	Perylene-d12	15.49

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-methyloctacosane	408	C29H60	1000376-72-8	91
2			Tetratetracontane	619	C44H90	007098-22-8	91
3			Heneicosane	296	C21H44	000629-94-7	90
4			Octadecane	254	C18H38	000593-45-3	87
5			Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF011819\
Data File : BF112120.D
Acq On : 18 Jan 2019 11:58
Operator : JU/SJ
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Misc :
ALS Vial : 8 Sample Multiplier: 1

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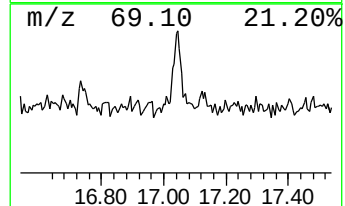
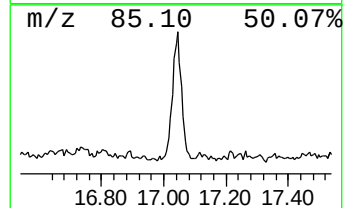
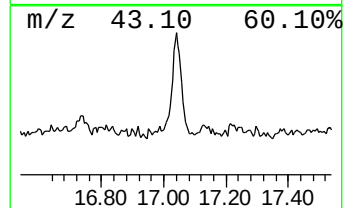
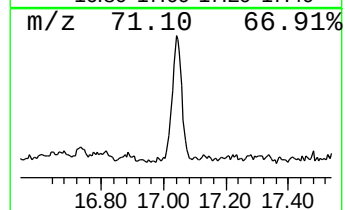
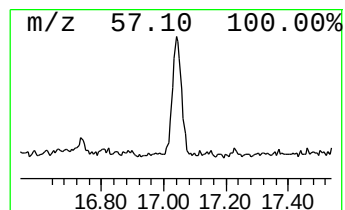
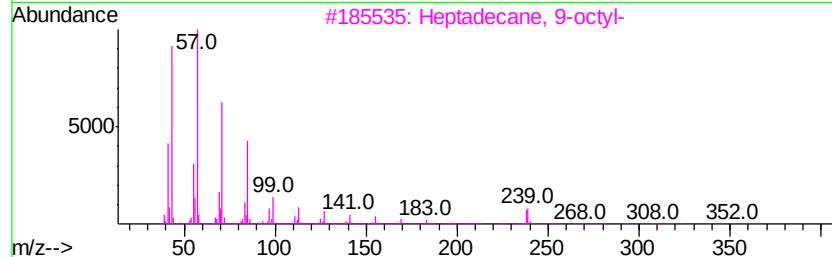
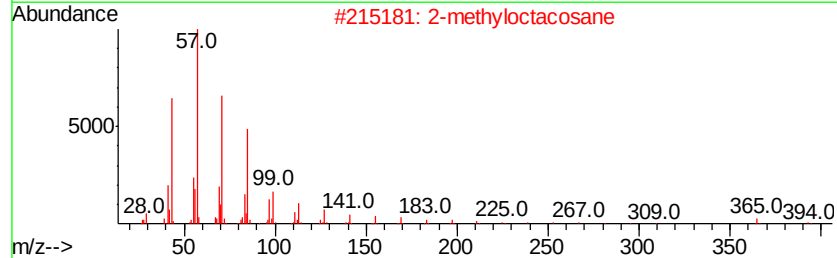
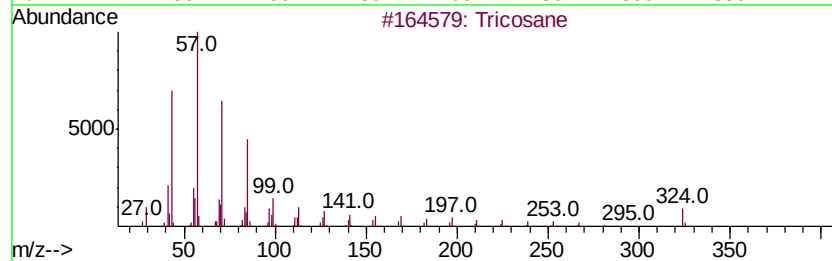
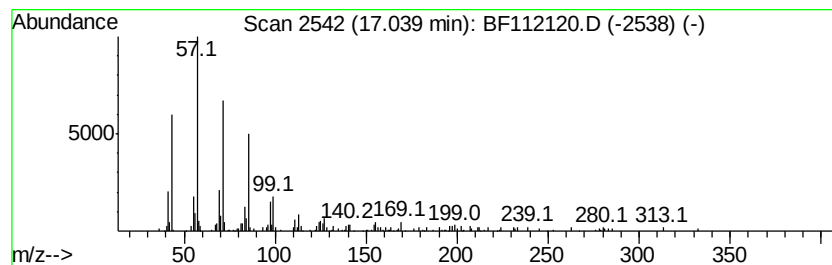
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Tricosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.04	2.08 ng	261445	Perylene-d12	15.49

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tricosane	324	C23H48	000638-67-5	87
2			2-methyloctacosane	408	C29H60	1000376-72-8	87
3			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	86
4			Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	86
5			Docosane	310	C22H46	000629-97-0	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF011819\
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 Acq On : 18 Jan 2019 11:58
 Operator : JU/SJ
 Sample : K1157-13
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 ALS Vial : 8 Sample Multiplier: 1

Instrument :
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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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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2-Pentanone, 4-hy...	5.07	3.6	ng	288855	1	6.86	1610630	20.0
unknown6.63	6.63	61.3	ng	4936810	1	6.86	1610630	20.0
1-Heneicosyl formate	13.85	4.7	ng	401030	5	14.02	1719060	20.0
Hexatriacontane	14.18	2.6	ng	221800	5	14.02	1719060	20.0
Octadecane	14.48	5.5	ng	475744	5	14.02	1719060	20.0
Eicosane	14.79	4.3	ng	535245	6	15.49	2517520	20.0
Octacosane	15.13	5.7	ng	720436	6	15.49	2517520	20.0
Heneicosane	15.94	5.5	ng	697787	6	15.49	2517520	20.0
2-methyloctacosane	16.45	3.7	ng	464783	6	15.49	2517520	20.0
Tricosane	17.04	2.1	ng	261445	6	15.49	2517520	20.0