LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101018\
Data File : BF109779.D
Acq On : 11 Oct 2018 9:02
Operator : JU/SJ
Sample : J5299-08
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 100518-SIDI-F-U-B

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

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

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-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	4.875	471	474	492	rBV	61017	86642	2.83%	0.505%
2	5.310	546	548	573	rBV	365029	610992	19.95%	3.558%
3	6.345	720	724	741	rBV	200896	429612	14.03%	2.502%
4	6.463	741	744	766	rVV	1191335	1404432	45.86%	8.179%
5	6.692	780	783	806	rVB	366662	520304	16.99%	3.030%
6	6.851	806	810	830	rBV	1962491	1981938	64.72%	11.542%
7	7.263	875	880	910	rBV	1178277	1729937	56.49%	10.075%
8	7.975	997	1001	1023	rBV	529323	659611	21.54%	3.841%
9	9.051	1180	1184	1212	rBV	2937192	3062124	100.00%	17.833%
10	9.445	1248	1251	1262	rBV	44823	48211	1.57%	0.281%
11	9.722	1294	1298	1313	rBV	745306	738307	24.11%	4.300%
12	10.510	1428	1432	1450	rBV	790173	1049223	34.26%	6.110%
13	11.198	1546	1549	1566	rBV	502754	662754	21.64%	3.860%
14	12.610	1785	1789	1795	rBV	77691	68404	2.23%	0.398%
15	12.780	1814	1818	1832	rBV	2320967	2421356	79.07%	14.101%
16	13.310	1905	1908	1912	rBV	52987	44183	1.44%	0.257%
17	13.686	1968	1972	1986	rBV2	29838	67503	2.20%	0.393%
18	13.827	1992	1996	2010	rBV	487291	553904	18.09%	3.226%
19	13.998	2021	2025	2030	rBV	40019	36402	1.19%	0.212%
20	14.298	2072	2076	2081	rBV	52800	54285	1.77%	0.316%
21	14.592	2121	2126	2131	rBV	88424	87905	2.87%	0.512%
22	14.904	2175	2179	2184	rBV	88900	95094	3.11%	0.554%
23	15.227	2229	2234	2245	rBV	336622	614972	20.08%	3.581%
24	15.645	2300	2305	2311	rBV	62128	87384	2.85%	0.509%
25	16.098	2378	2382	2390	rVB	36674	55958	1.83%	0.326%

Sum of corrected areas: 17171437

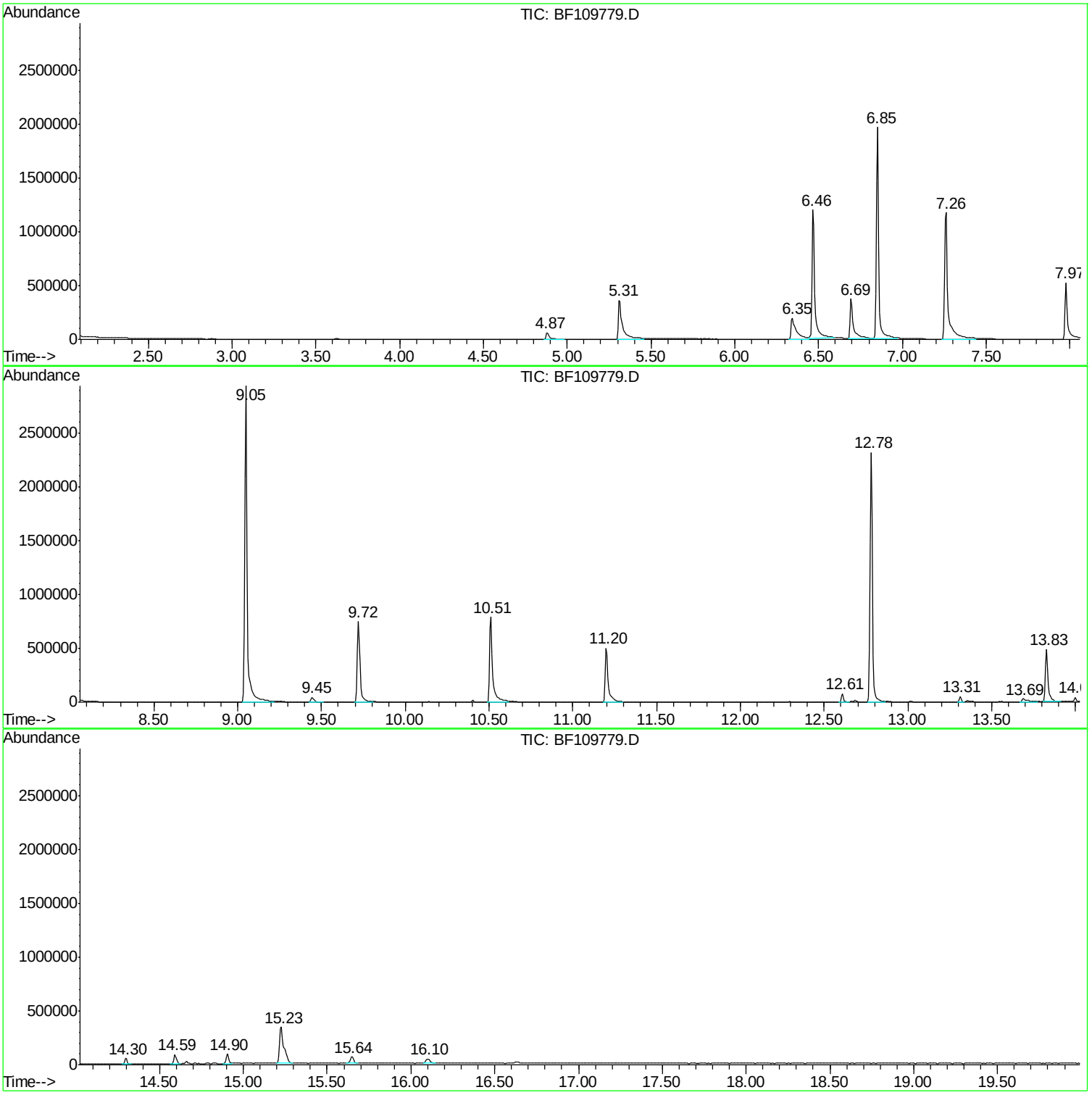
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101018\
Data File : BF109779.D
Acq On : 11 Oct 2018 9:02
Operator : JU/SJ
Sample : J5299-08
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
100518-SIDI-F-U-B

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101018\
Data File : BF109779.D
Acq On : 11 Oct 2018 9:02
Operator : JU/SJ
Sample : J5299-08
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 100518-SIDI-F-U-B

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

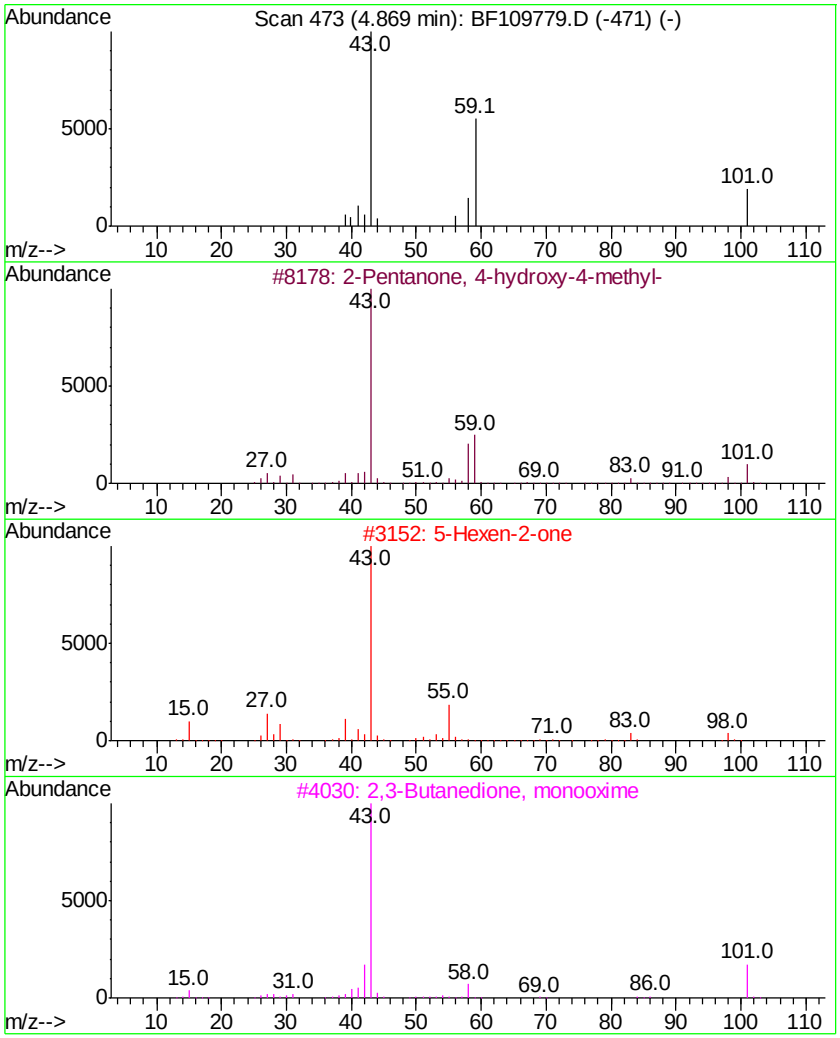
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

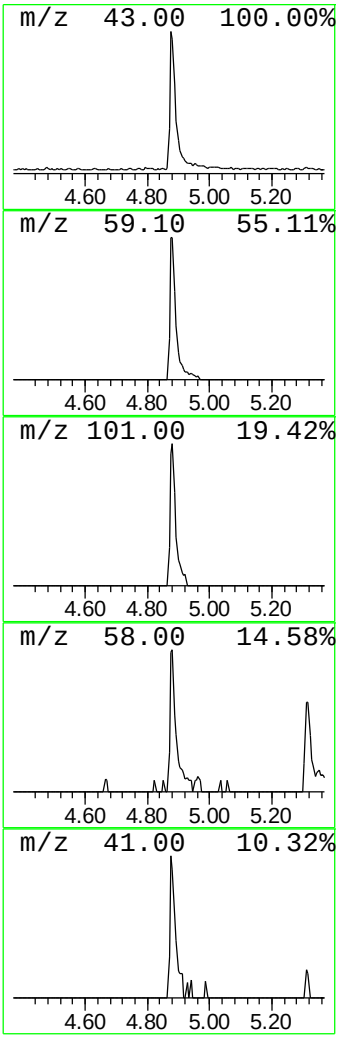
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.87	3.33 ng	86642	1,4-Dichlorobenzene-d4	6.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	5-Hexen-2-one	98	C6H10O	000109-49-9	9
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101018\
Data File : BF109779.D
Acq On : 11 Oct 2018 9:02
Operator : JU/SJ
Sample : J5299-08
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 100518-SIDI-F-U-B

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

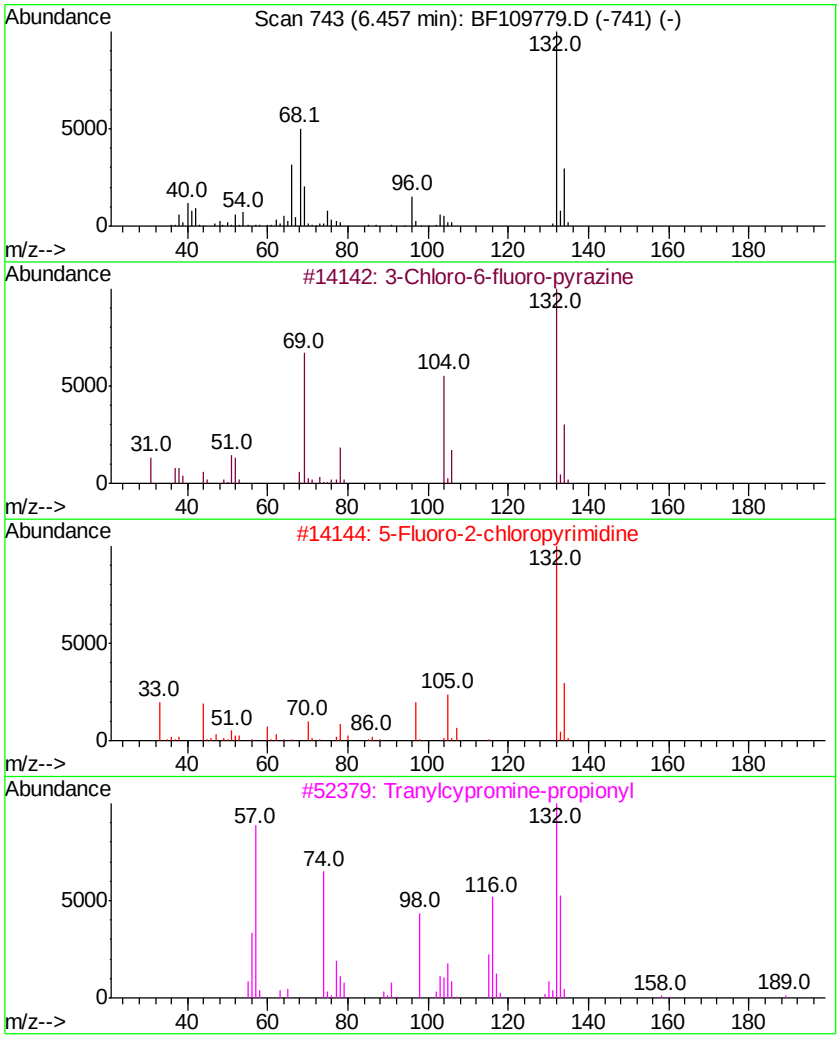
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

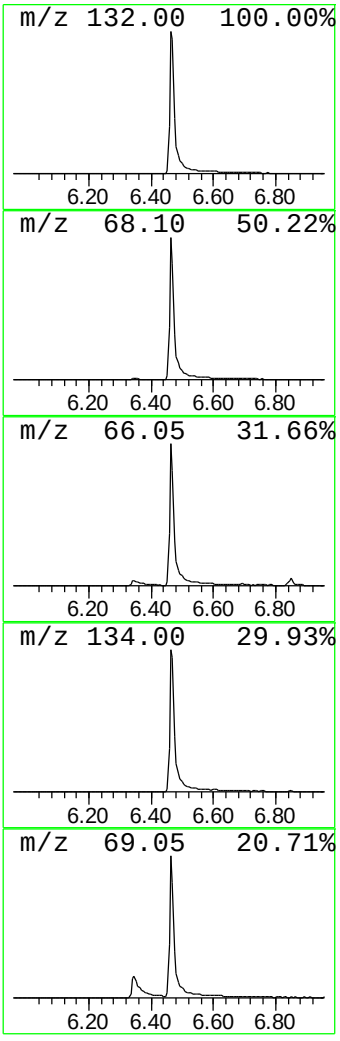
****

Peak Number 2 unknown6.46 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.46	53.99 ng	1404430	1,4-Dichlorobenzene-d4	6.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5	5-Aminoindole	132	C8H8N2	005192-03-0	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101018\
Data File : BF109779.D
Acq On : 11 Oct 2018 9:02
Operator : JU/SJ
Sample : J5299-08
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 100518-SIDI-F-U-B

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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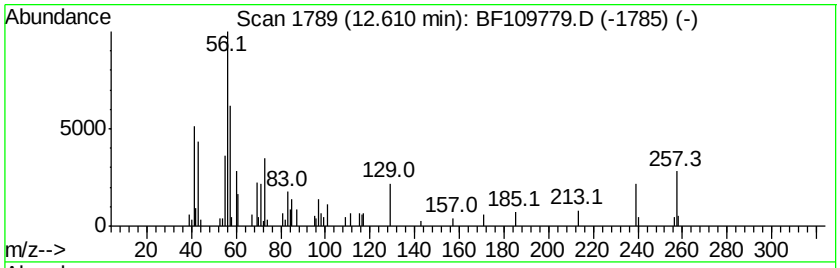
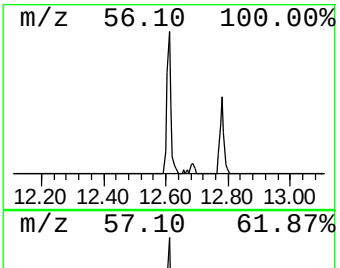
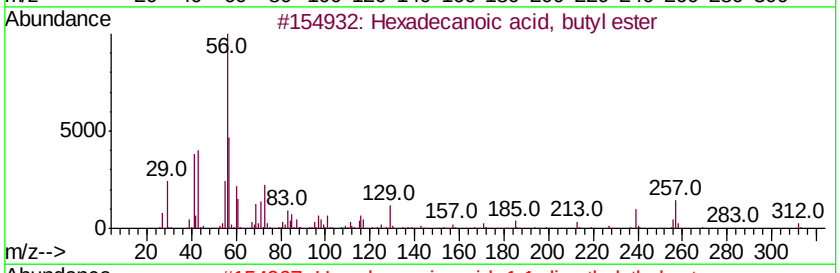
Peak Number 4 Hexadecanoic acid, butyl ester Concentration Rank 7

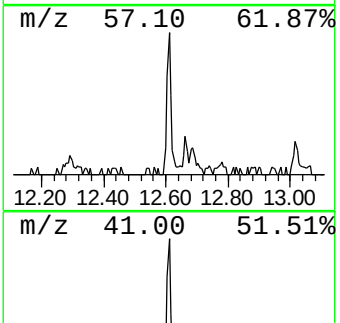
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.61	2.47 ng	68404	Chrysene-d12	13.83

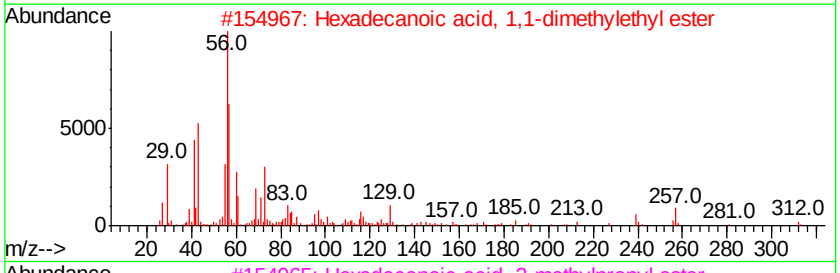
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	90
3	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	32
4	Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	27
5	1-Heptene, 2-methyl-	112	C8H16	015870-10-7	27

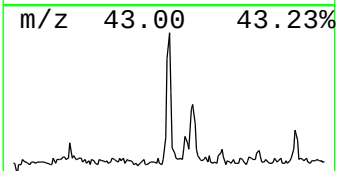


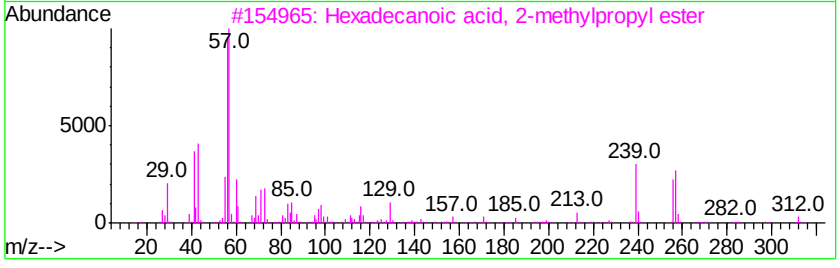


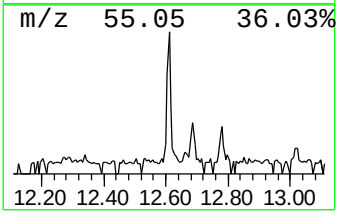












Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101018\
Data File : BF109779.D
Acq On : 11 Oct 2018 9:02
Operator : JU/SJ
Sample : J5299-08
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 100518-SIDI-F-U-B

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

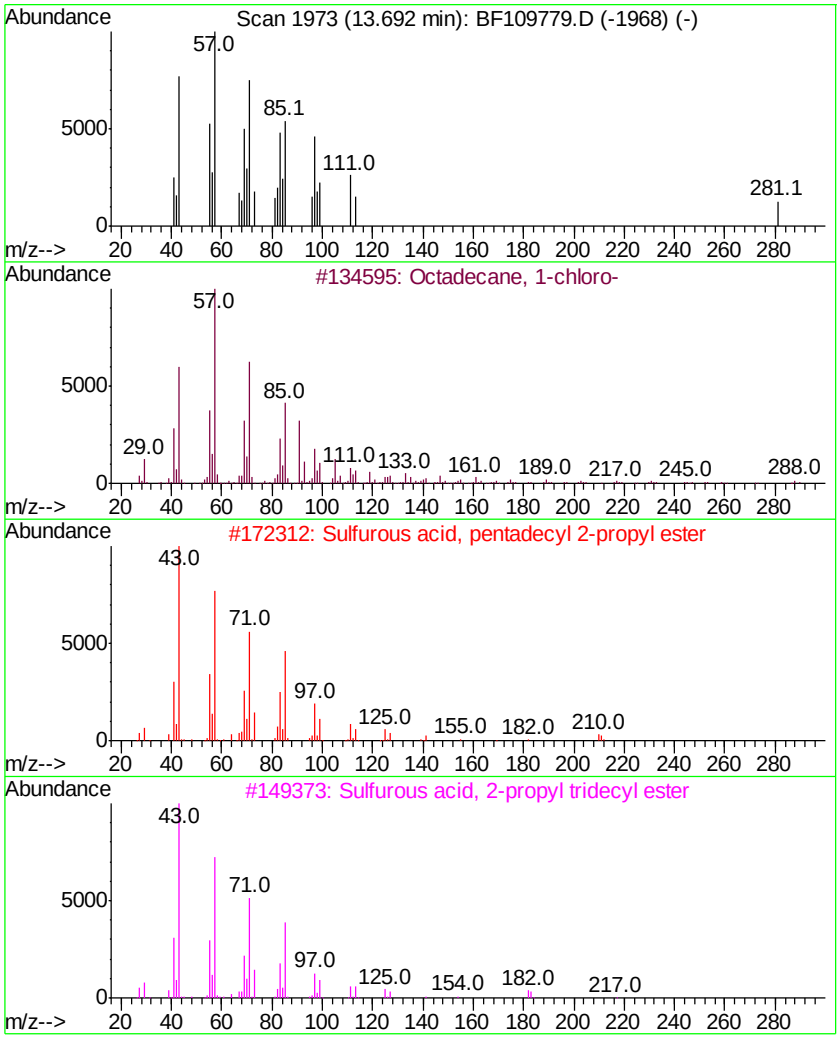
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

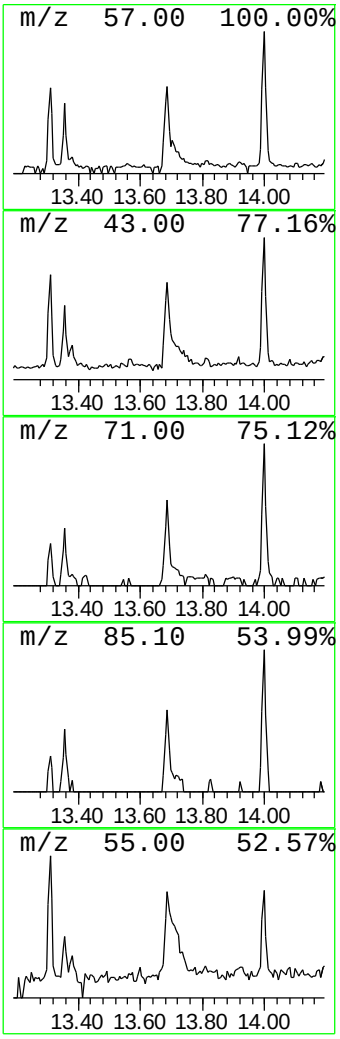
****

Peak Number 5 Octadecane, 1-chloro- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.69	2.44 ng	67503	Chrysene-d12	13.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	90
2	Sulfurous acid, pentadecyl 2-pro...	334	C18H38O3S	1000309-12-6	90
3	Sulfurous acid, 2-propyl tridecy...	306	C16H34O3S	1000309-12-4	90
4	1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	90
5	Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	90





Library Search Compound Report

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Instrument : BNA_F
ClientSampleId : 100518-SIDI-F-U-B

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
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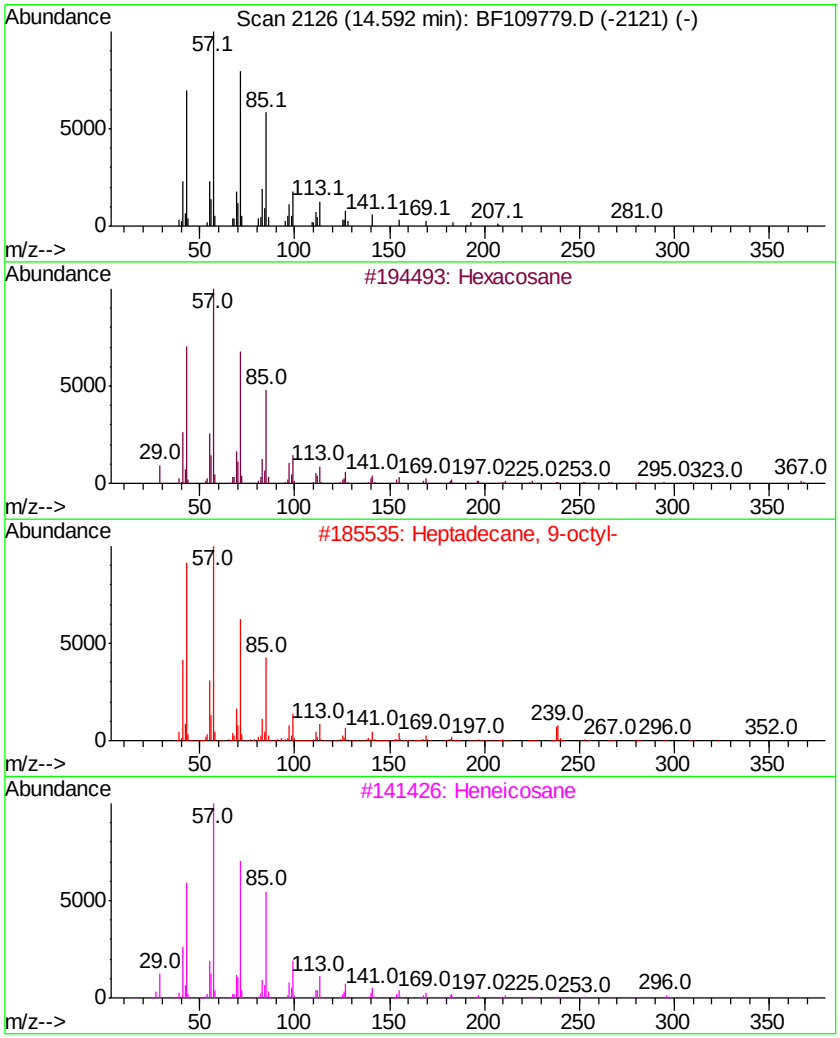
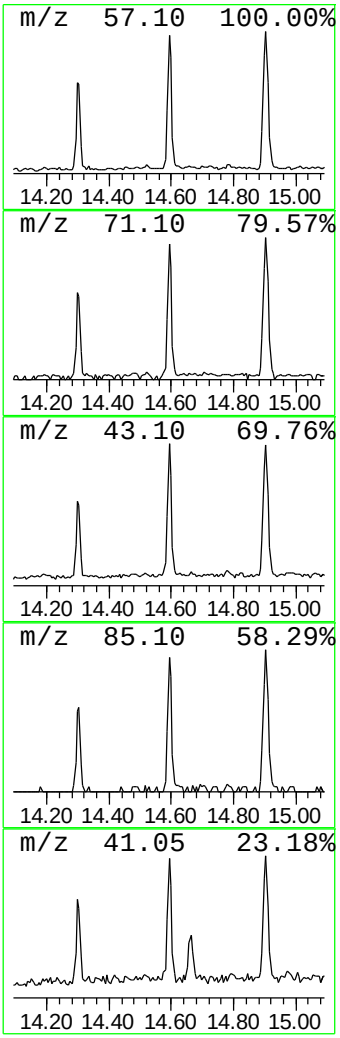
****

Peak Number 6 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.59	2.86 ng	87905	Perylene-d12	15.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
3	Heneicosane	296	C21H44	000629-94-7	90
4	Heptadecane	240	C17H36	000629-78-7	90
5	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	90





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Operator : JU/SJ
Sample : J5299-08
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 100518-SIDI-F-U-B

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

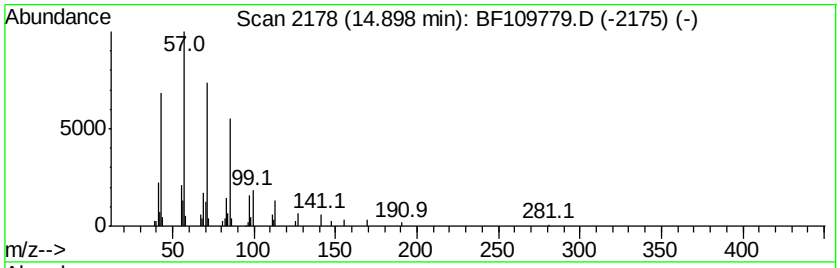
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

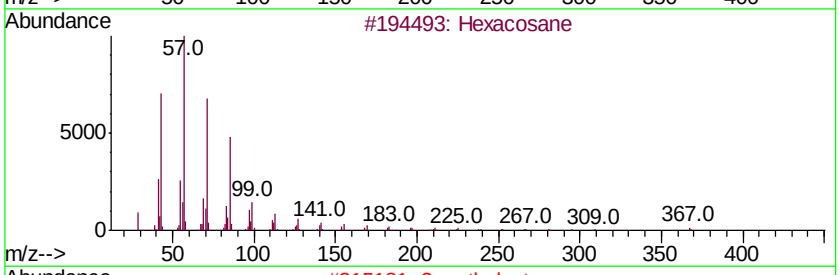
****

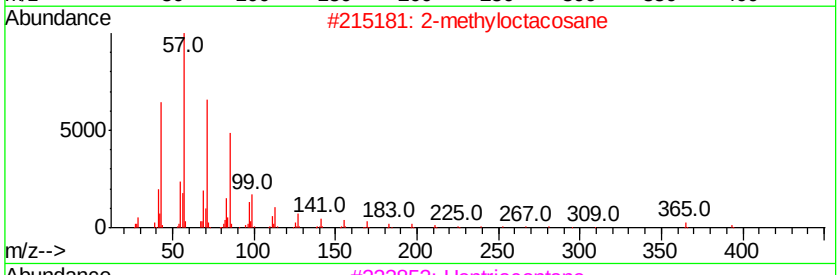
Peak Number 7 2-methyloctacosane Concentration Rank 4

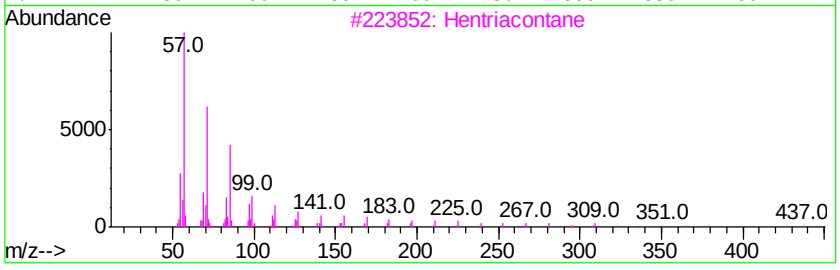
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.90	3.09 ng	95094	Perylene-d12	15.23

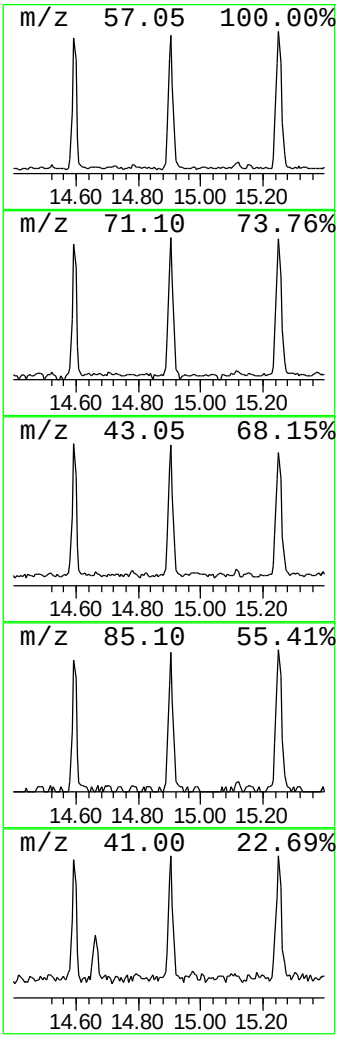
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	2-methyloctacosane	408	C29H60	1000376-72-8	91
3	Hentriacontane	437	C31H64	000630-04-6	91
4	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	90
5	Heneicosane	296	C21H44	000629-94-7	87











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

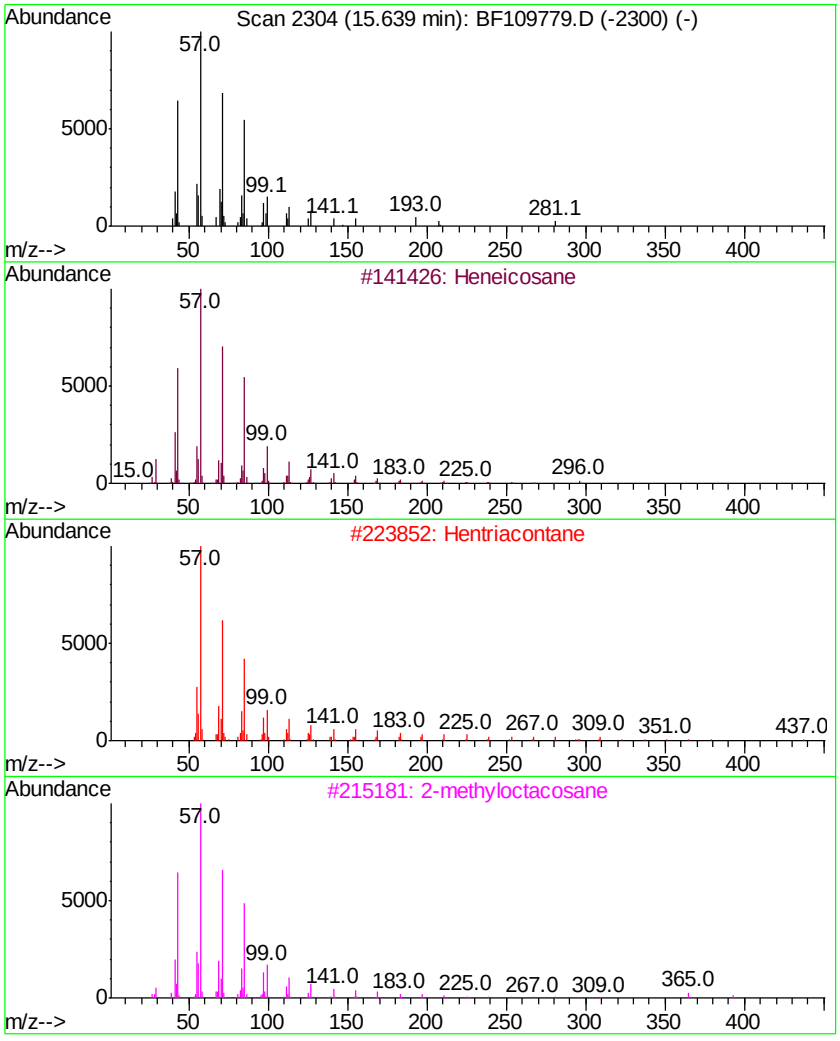
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

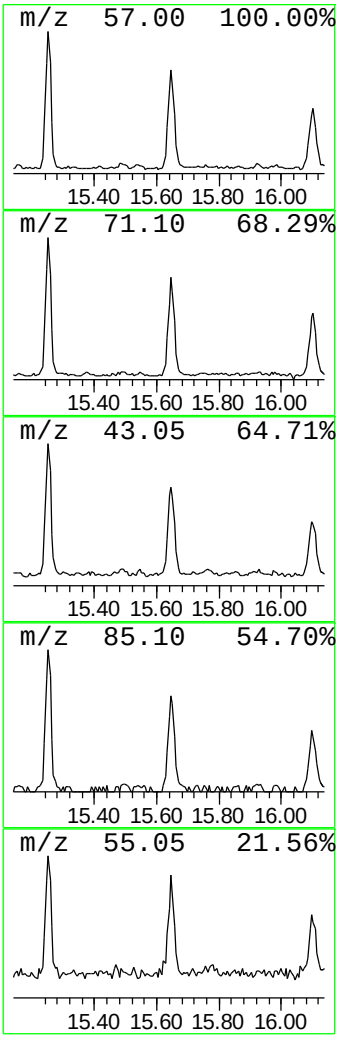
****

Peak Number 8 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.64	2.84 ng	87384	Perylene-d12	15.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Hentriacontane	437	C31H64	000630-04-6	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	91
4	Hexacosane	366	C26H54	000630-01-3	91
5	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF101018\
Data File : BF109779.D
Acq On : 11 Oct 2018 9:02
Operator : JU/SJ
Sample : J5299-08
Misc :
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Instrument : BNA_F
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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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.87	3.3	ng	86642	1	6.69	520304	20.0
unknown6.46	6.46	54.0	ng	1404430	1	6.69	520304	20.0
Hexadecanoic acid...	12.61	2.5	ng	68404	5	13.83	553904	20.0
Octadecane, 1-chl...	13.69	2.4	ng	67503	5	13.83	553904	20.0
Hexacosane	14.59	2.9	ng	87905	6	15.23	614972	20.0
2-methyloctacosane	14.90	3.1	ng	95094	6	15.23	614972	20.0
Heneicosane	15.64	2.8	ng	87384	6	15.23	614972	20.0