LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121218\
Data File : BF111324.D
Acq On : 12 Dec 2018 16:31
Operator : JU/SJ
Sample : J6186-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DW-9

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-BF121218.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	5.004	487	496	505	rBV2	277036	460441	5.61%	0.654%
2	5.416	560	566	569	rBV	6589436	7157968	87.19%	10.160%
3	6.428	732	738	754	rBV	6814310	8209881	100.00%	11.653%
4	6.563	756	761	764	rBV	7621526	7485262	91.17%	10.625%
5	6.792	796	800	803	rBV	1990716	1759405	21.43%	2.497%
6	6.951	822	827	830	rBV	5929899	5440242	66.26%	7.722%
7	7.351	889	895	898	rBV	5025583	5007411	60.99%	7.108%
8	8.075	1013	1018	1021	rBV	2499136	2387253	29.08%	3.388%
9	9.151	1195	1201	1204	rBV	7849747	7243275	88.23%	10.281%
10	9.539	1260	1267	1270	rBV	914630	733739	8.94%	1.041%
11	9.827	1310	1316	1320	rBV	3232455	2787771	33.96%	3.957%
12	10.233	1382	1385	1389	rBV3	55891	82265	1.00%	0.117%
13	10.616	1445	1450	1453	rBV	4415365	4208107	51.26%	5.973%
14	11.310	1564	1568	1571	rBV	3228021	2722118	33.16%	3.864%
15	11.839	1653	1658	1663	rBV	895204	1346648	16.40%	1.911%
16	12.627	1786	1792	1806	rVB3	1676010	2943067	35.85%	4.177%
17	12.898	1833	1838	1841	rBV	6330213	5844401	71.19%	8.296%
18	13.815	1990	1994	2006	rBV	496588	863909	10.52%	1.226%
19	13.945	2012	2016	2024	rBV	1902803	1727116	21.04%	2.451%
20	14.745	2148	2152	2156	rBV	81298	90401	1.10%	0.128%
21	15.074	2204	2208	2211	rVB	130199	149427	1.82%	0.212%
22	15.392	2257	2262	2267	rVB	1170294	1423384	17.34%	2.020%
23	15.445	2267	2271	2277	rVB	150995	201084	2.45%	0.285%
24	15.868	2339	2343	2351	rVB	124902	177493	2.16%	0.252%

Sum of corrected areas: 70452068

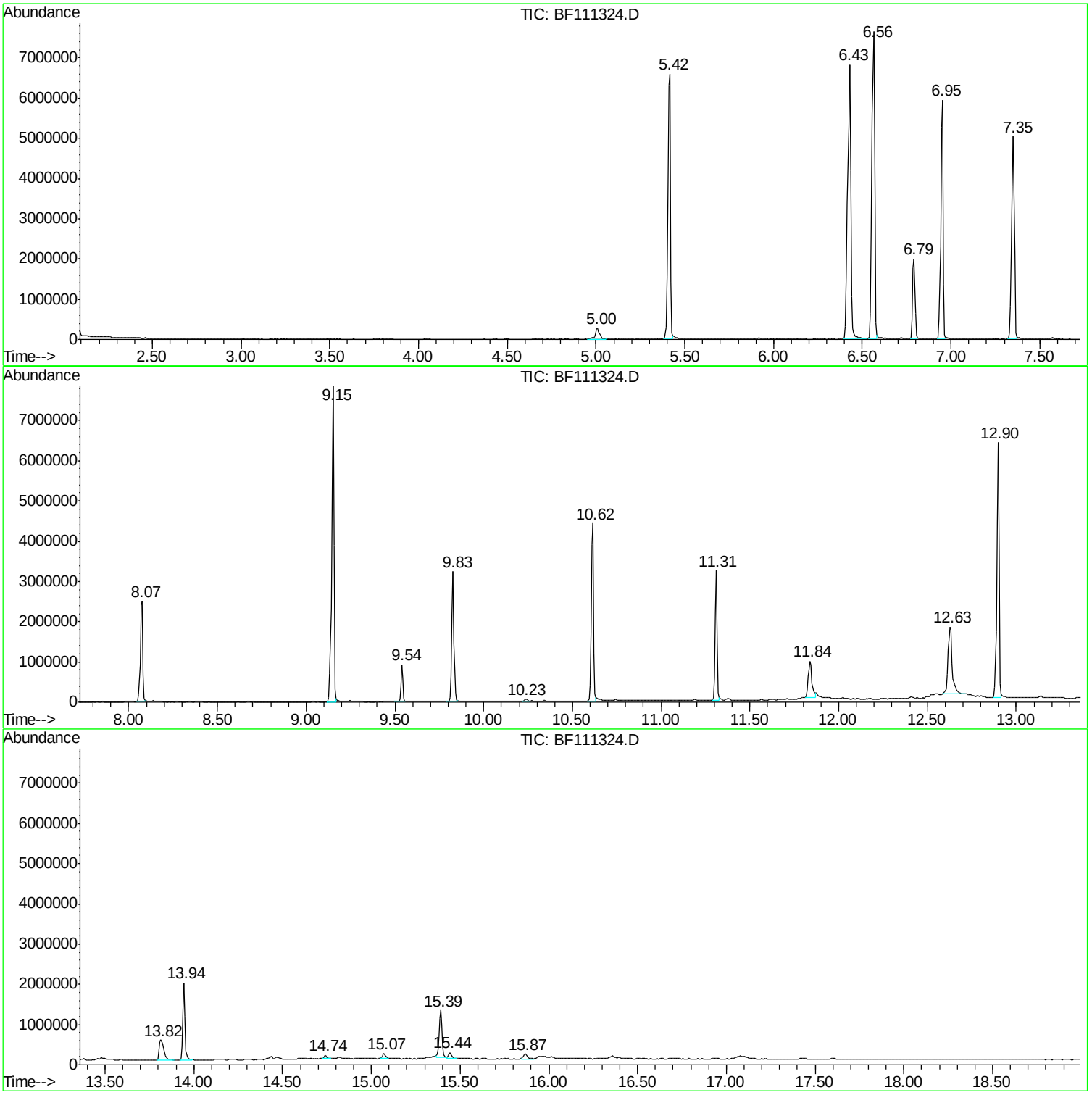
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121218\
Data File : BF111324.D
Acq On : 12 Dec 2018 16:31
Operator : JU/SJ
Sample : J6186-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DW-9

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121218\
Data File : BF111324.D
Acq On : 12 Dec 2018 16:31
Operator : JU/SJ
Sample : J6186-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DW-9

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

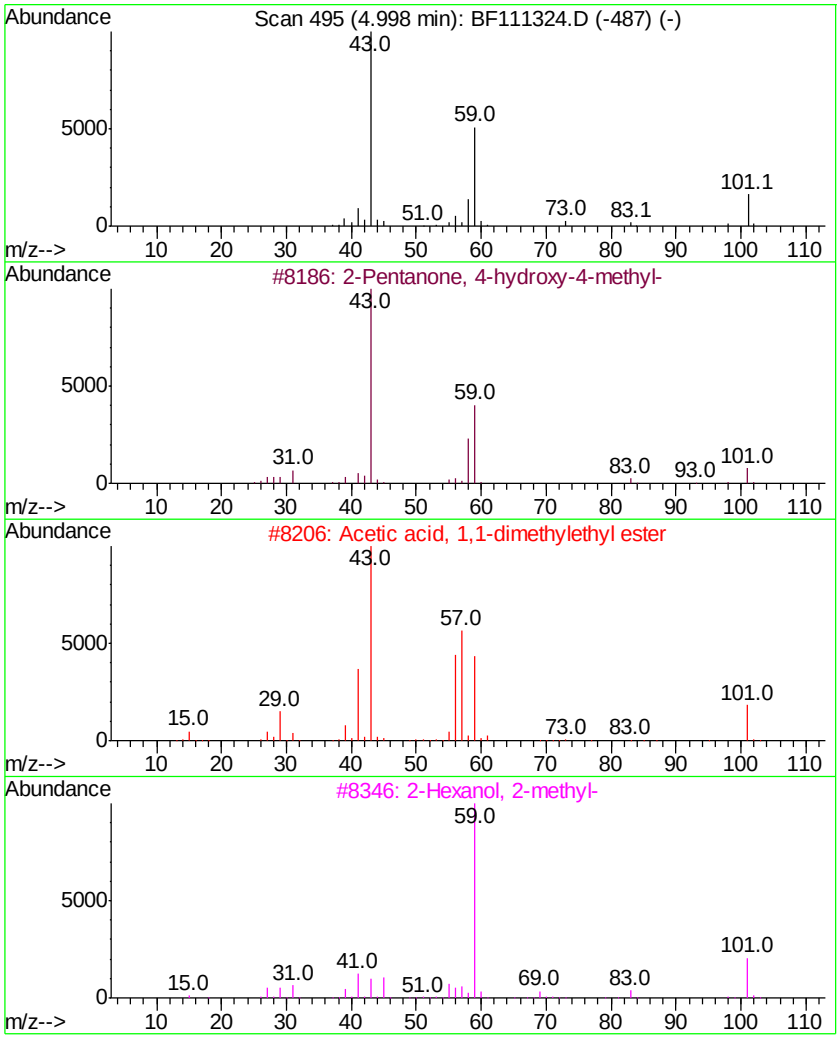
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

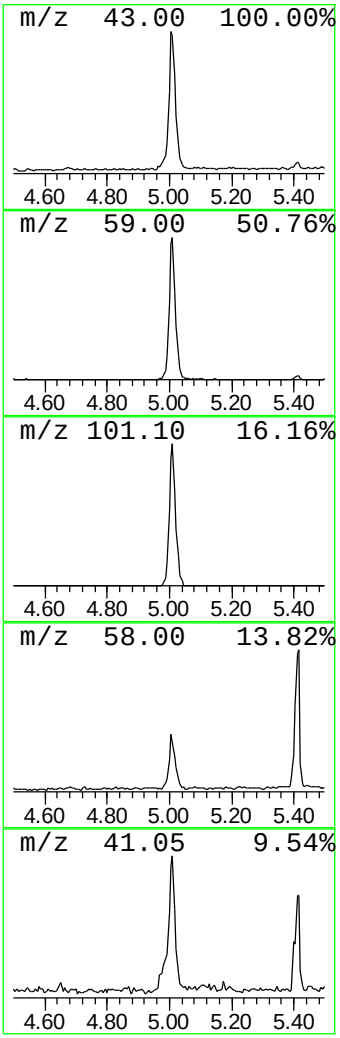
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	5.23 ng	460441	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121218\
Data File : BF111324.D
Acq On : 12 Dec 2018 16:31
Operator : JU/SJ
Sample : J6186-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DW-9

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

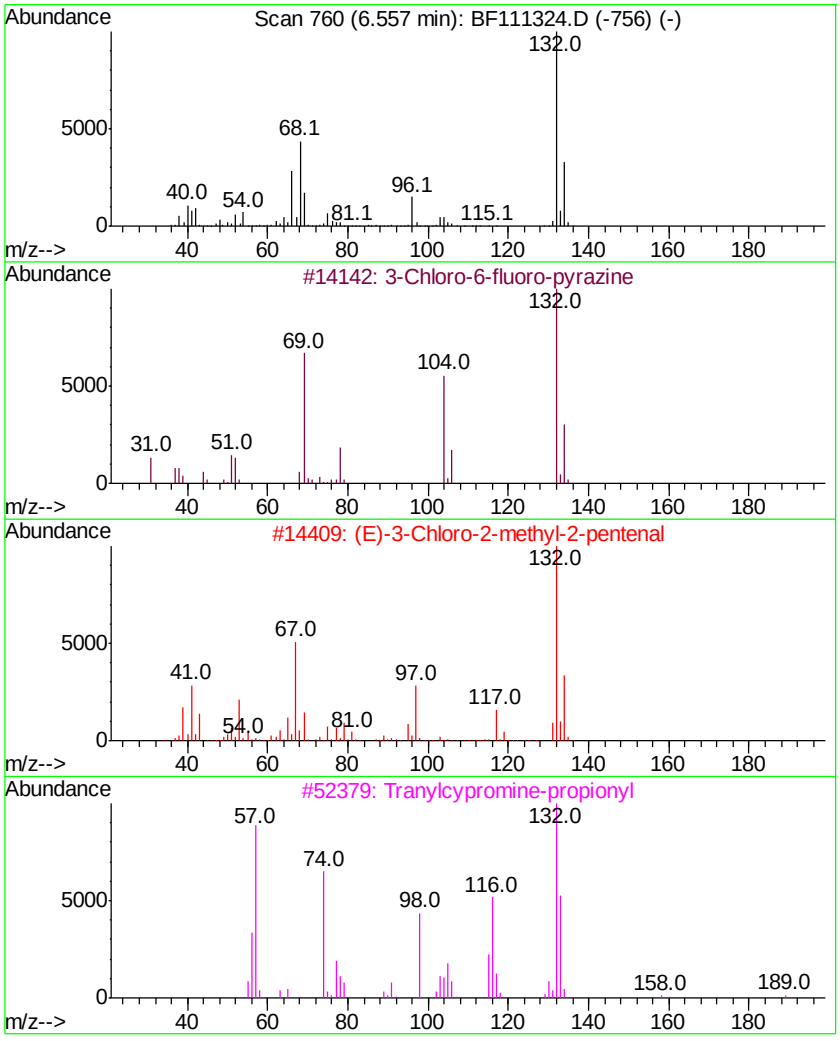
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

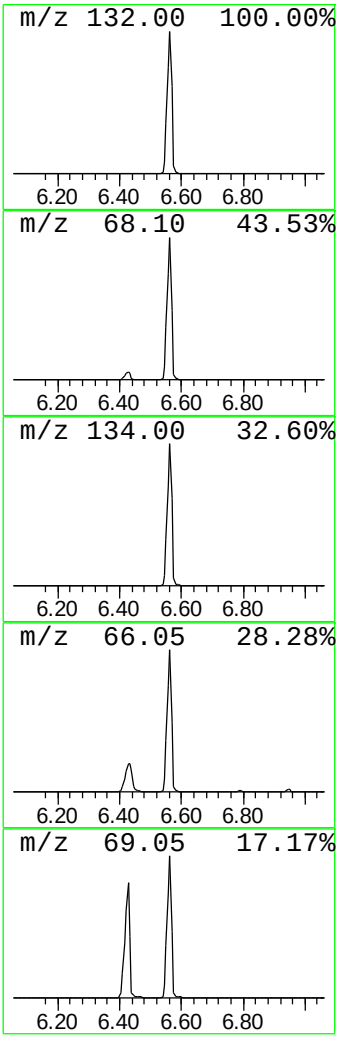
****

Peak Number 2 unknown6.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	85.09 ng	7485260	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121218\
Data File : BF111324.D
Acq On : 12 Dec 2018 16:31
Operator : JU/SJ
Sample : J6186-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DW-9

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121218.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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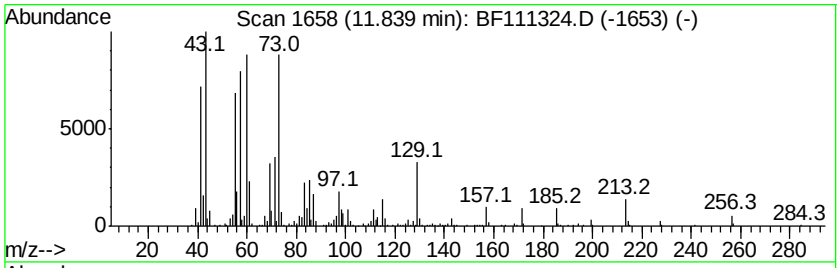
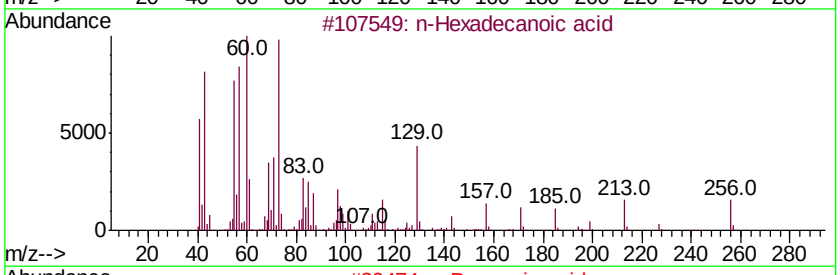
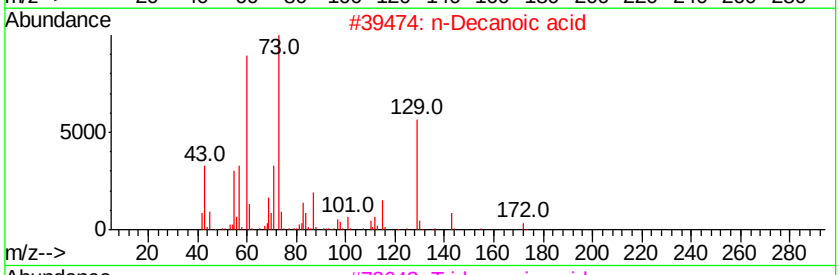
Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

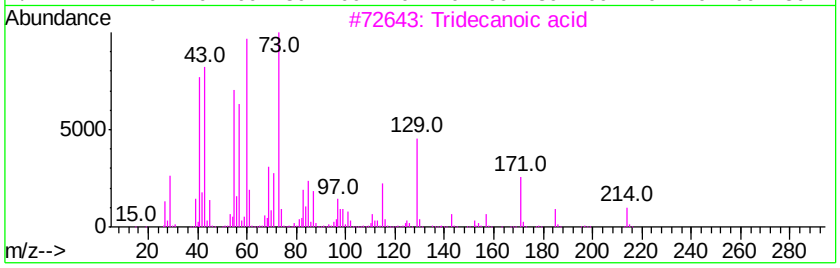
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.84	9.89 ng	1346650	Phenanthrene-d10	11.31

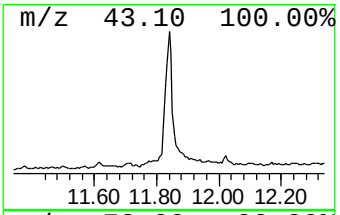
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	n-Decanoic acid	172	C10H20O2	000334-48-5	91
3	Tridecanoic acid	214	C13H26O2	000638-53-9	90
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	87

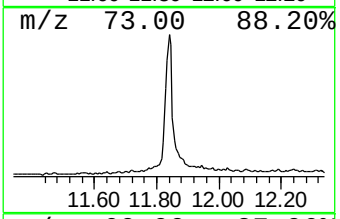


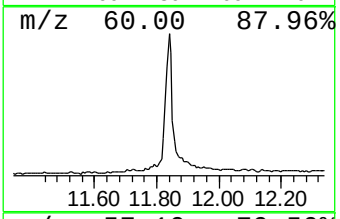


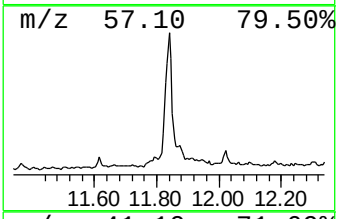


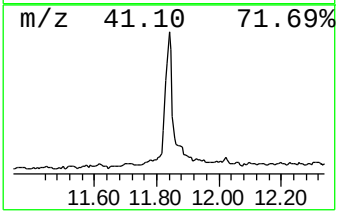












Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121218\
Data File : BF111324.D
Acq On : 12 Dec 2018 16:31
Operator : JU/SJ
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Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DW-9

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

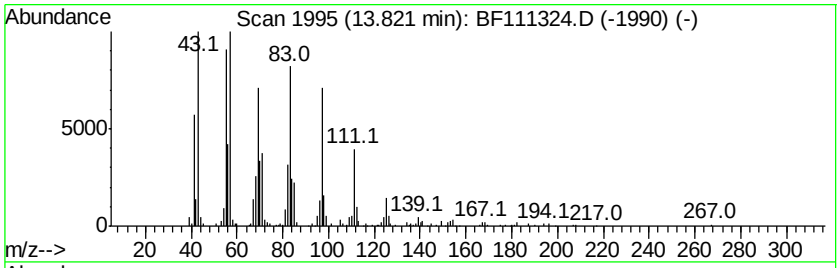
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

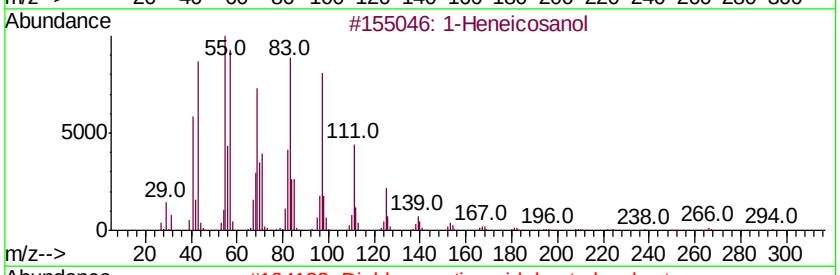
****

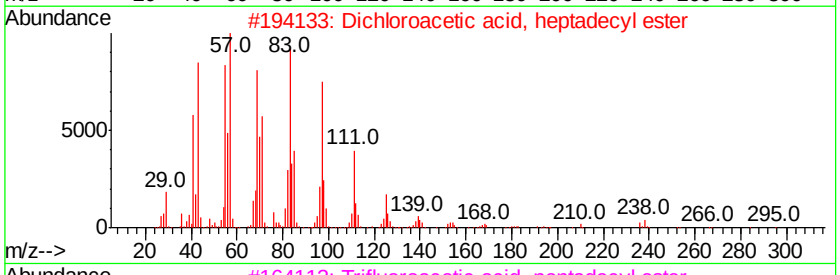
Peak Number 5 1-Heneicosanol Concentration Rank 3

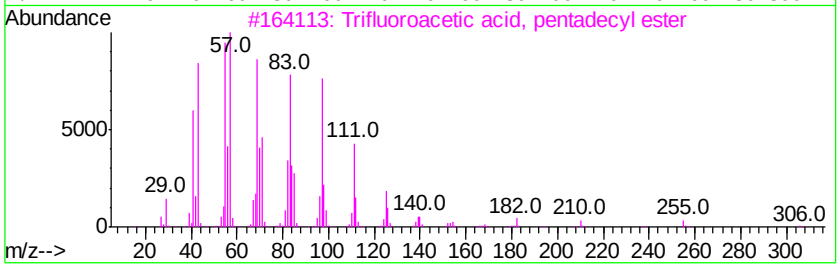
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	10.00 ng	863909	Chrysene-d12	13.94

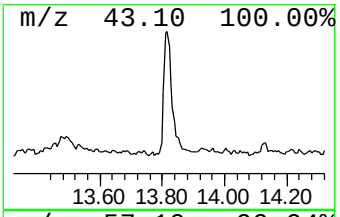
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
3	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
4	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
5	Behenic alcohol	326	C22H46O	000661-19-8	93

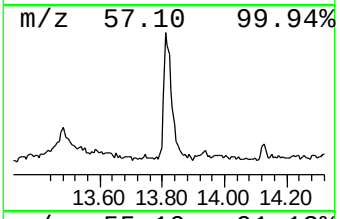


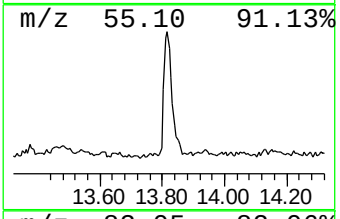


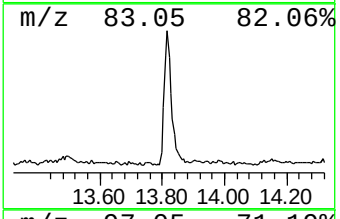


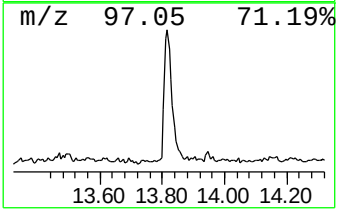












Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121218\
Data File : BF111324.D
Acq On : 12 Dec 2018 16:31
Operator : JU/SJ
Sample : J6186-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DW-9

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

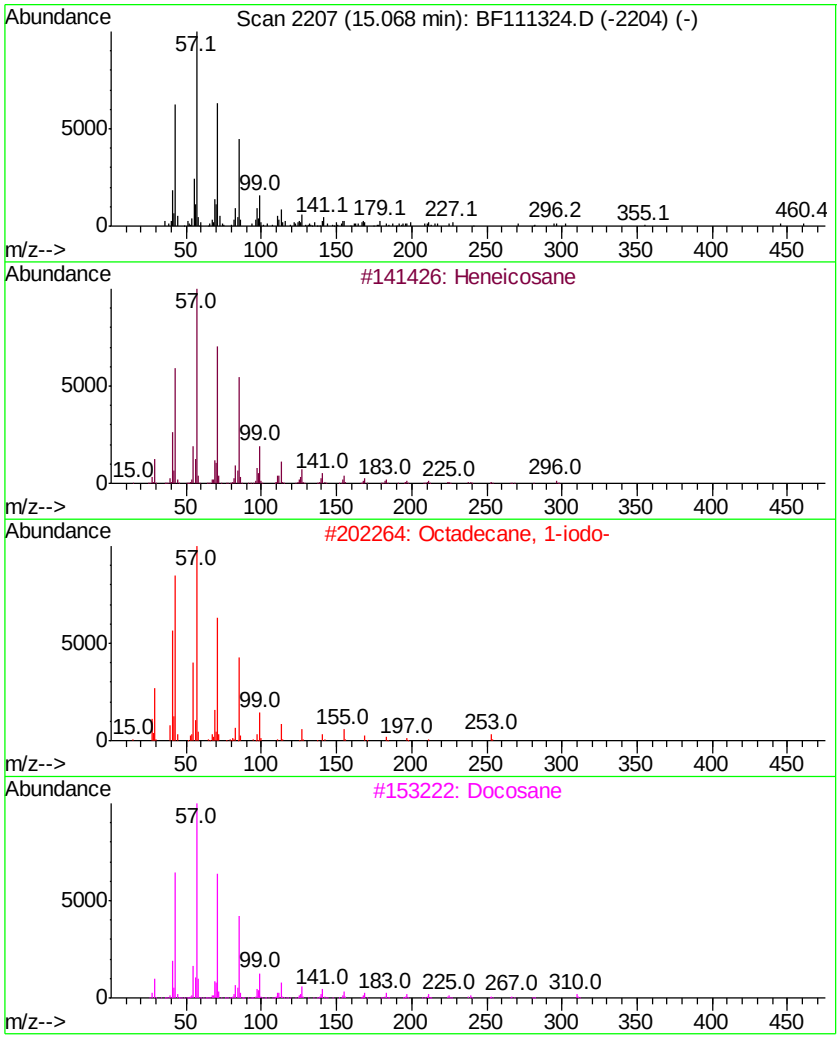
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

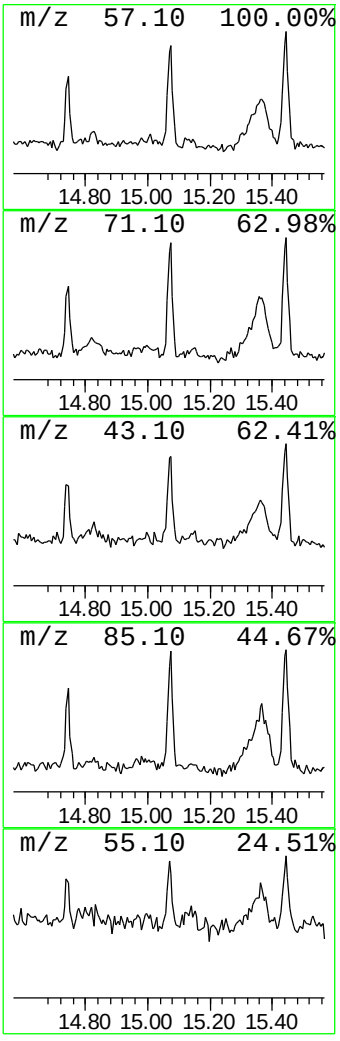
****

Peak Number 6 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.07	2.10 ng	149427	Perylene-d12	15.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	97
2	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	83
3	Docosane	310	C22H46	000629-97-0	83
4	Eicosane	282	C20H42	000112-95-8	80
5	Tetracosane	338	C24H50	000646-31-1	62





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

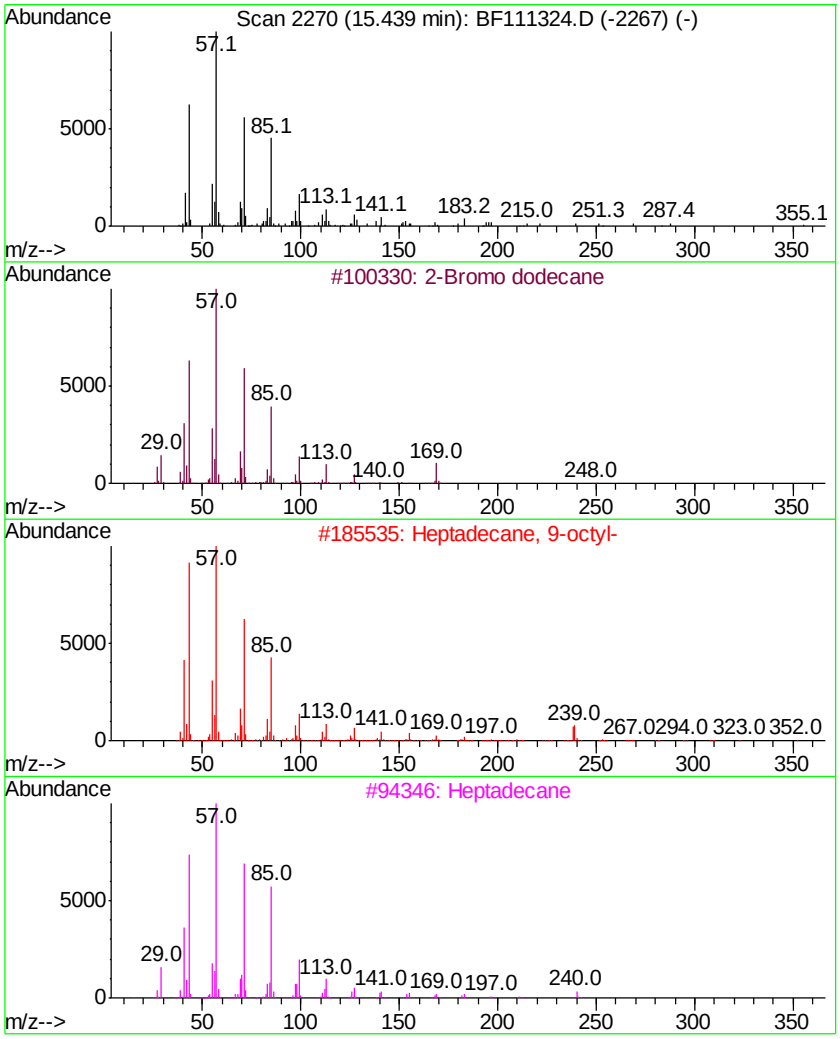
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

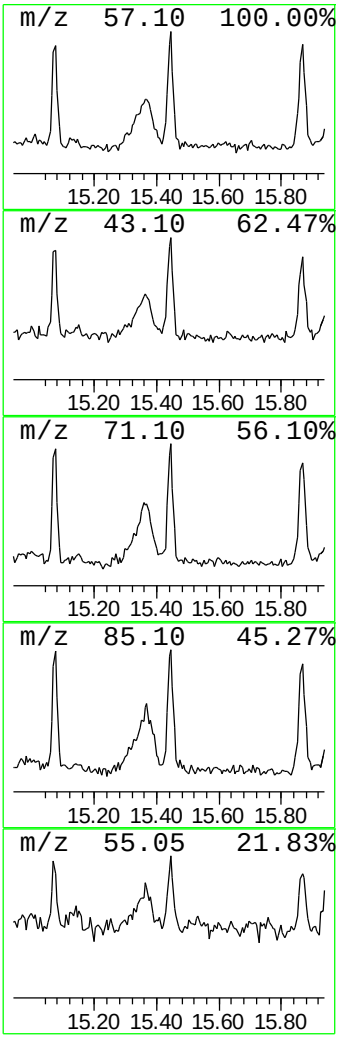
****

Peak Number 7 2-Bromo dodecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.44	2.83 ng	201084	Perylene-d12	15.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Bromo dodecane	248	C12H25Br	013187-99-0	90
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
3	Heptadecane	240	C17H36	000629-78-7	87
4	Octacosane	394	C28H58	000630-02-4	87
5	Hentriacontane	437	C31H64	000630-04-6	86





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Data File : BF111324.D
Acq On : 12 Dec 2018 16:31
Operator : JU/SJ
Sample : J6186-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DW-9

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

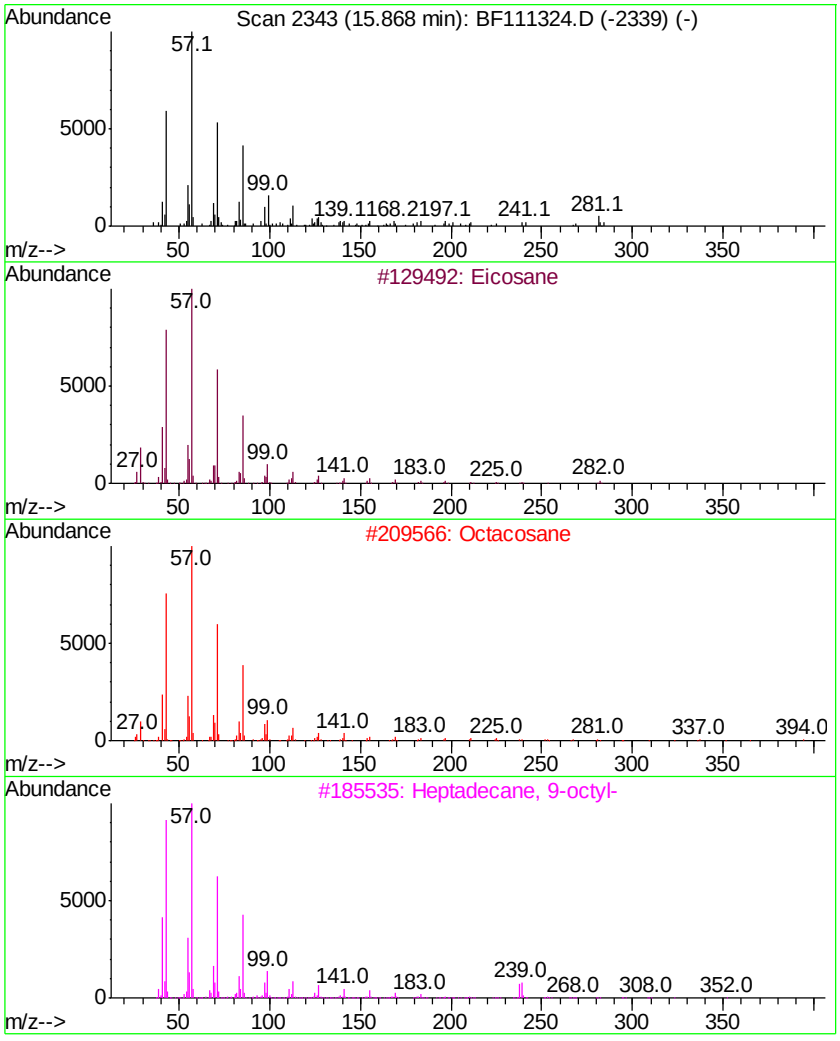
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

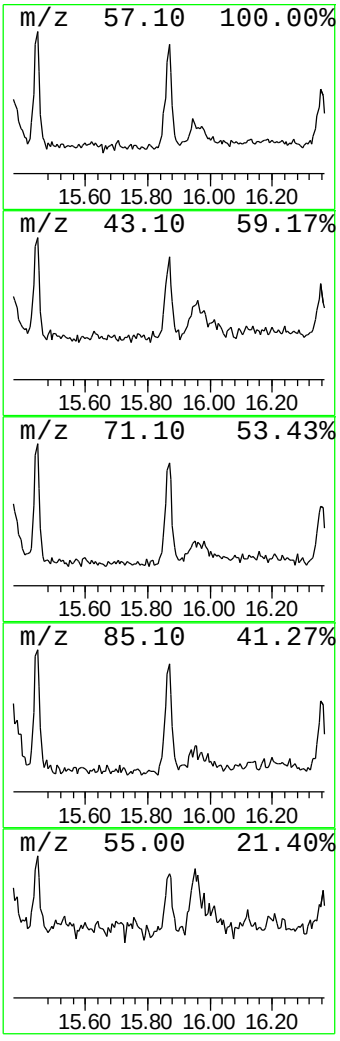
****

Peak Number 8 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.87	2.49 ng	177493	Perylene-d12	15.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Octacosane	394	C28H58	000630-02-4	86
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	83
4	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	83
5	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	80





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF121218\
Data File : BF111324.D
Acq On : 12 Dec 2018 16:31
Operator : JU/SJ
Sample : J6186-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DW-9

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121218.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...	5.00	5.2	ng	460441	1	6.79	1759410	20.0
unknown6.56	6.56	85.1	ng	7485260	1	6.79	1759410	20.0
n-Hexadecanoic acid	11.84	9.9	ng	1346650	4	11.31	2722120	20.0
1-Heneicosanol	13.82	10.0	ng	863909	5	13.94	1727120	20.0
Heneicosane	15.07	2.1	ng	149427	6	15.39	1423380	20.0
2-Bromo dodecane	15.44	2.8	ng	201084	6	15.39	1423380	20.0
Eicosane	15.87	2.5	ng	177493	6	15.39	1423380	20.0