LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061721\
Data File : BG049010.D
Acq On : 17 Jun 2021 11:38
Operator : CG/JU
Sample : M2678-12
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SPLP-AMND-COMP-F(CL-05)

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_G\METHODS\8270-BG061121.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG049010.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.157	15	20	29	rBV	165961	318195	9.20%	2.470%
2	3.233	29	33	41	rVB	73069	110810	3.20%	0.860%
3	5.666	439	447	461	rBV	317930	521859	15.09%	4.051%
4	7.270	709	720	729	rBV	191432	342610	9.90%	2.660%
5	8.116	857	864	870	rBV	123480	216682	6.26%	1.682%
6	9.285	1055	1063	1071	rBV	505293	904756	26.16%	7.024%
7	10.942	1337	1345	1352	rBV	158499	292972	8.47%	2.274%
8	13.380	1753	1760	1768	rBV	1189599	1909766	55.21%	14.826%
9	13.668	1802	1809	1816	rBV3	32209	60127	1.74%	0.467%
10	14.761	1988	1995	2001	rBV	265156	430280	12.44%	3.340%
11	15.160	2056	2063	2068	rBV2	36915	62318	1.80%	0.484%
12	16.247	2240	2248	2257	rVB	1207091	1848069	53.43%	14.347%
13	16.888	2352	2357	2367	rVB2	45684	63317	1.83%	0.492%
14	17.505	2457	2462	2468	rBV	376650	573998	16.59%	4.456%
15	18.269	2587	2592	2599	rBV3	46733	85183	2.46%	0.661%
16	18.386	2607	2612	2619	rBV2	68758	100130	2.89%	0.777%
17	19.655	2823	2828	2836	rBV5	38387	62350	1.80%	0.484%
18	20.061	2883	2897	2900	rBV7	34495	123823	3.58%	0.961%
19	20.113	2900	2906	2917	rVB	2497954	3459019	100.00%	26.853%
20	21.794	3185	3192	3200	rBV2	371425	642508	18.57%	4.988%
21	22.152	3245	3253	3257	rBV7	33549	93752	2.71%	0.728%
22	25.125	3749	3759	3770	rBV2	217814	658949	19.05%	5.115%

Sum of corrected areas: 12881473

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061721\
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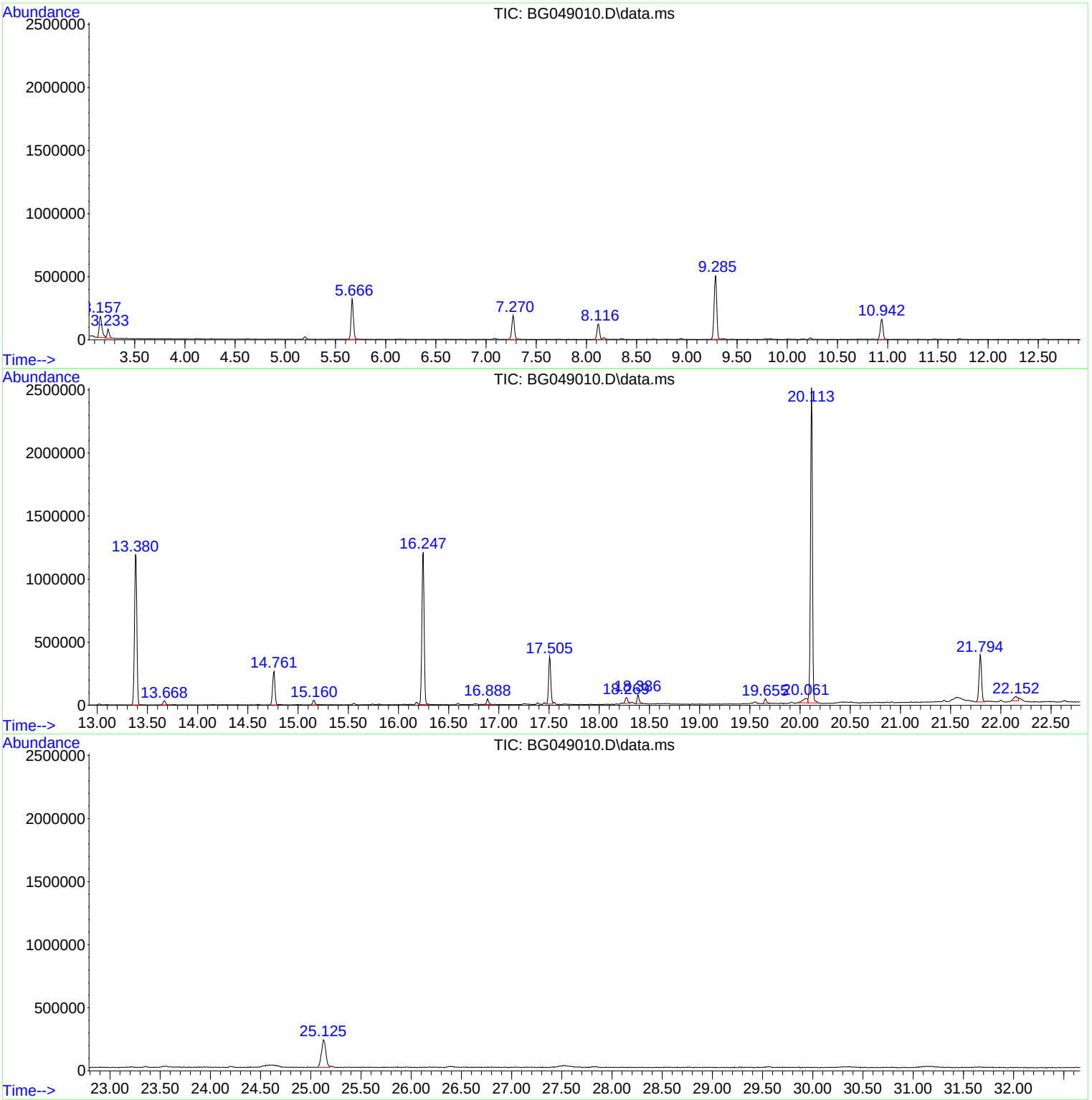
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SPLP-AMND-COMP-F(CL-05)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.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_G\Data\BG061721\
Data File : BG049010.D
Acq On : 17 Jun 2021 11:38
Operator : CG/JU
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ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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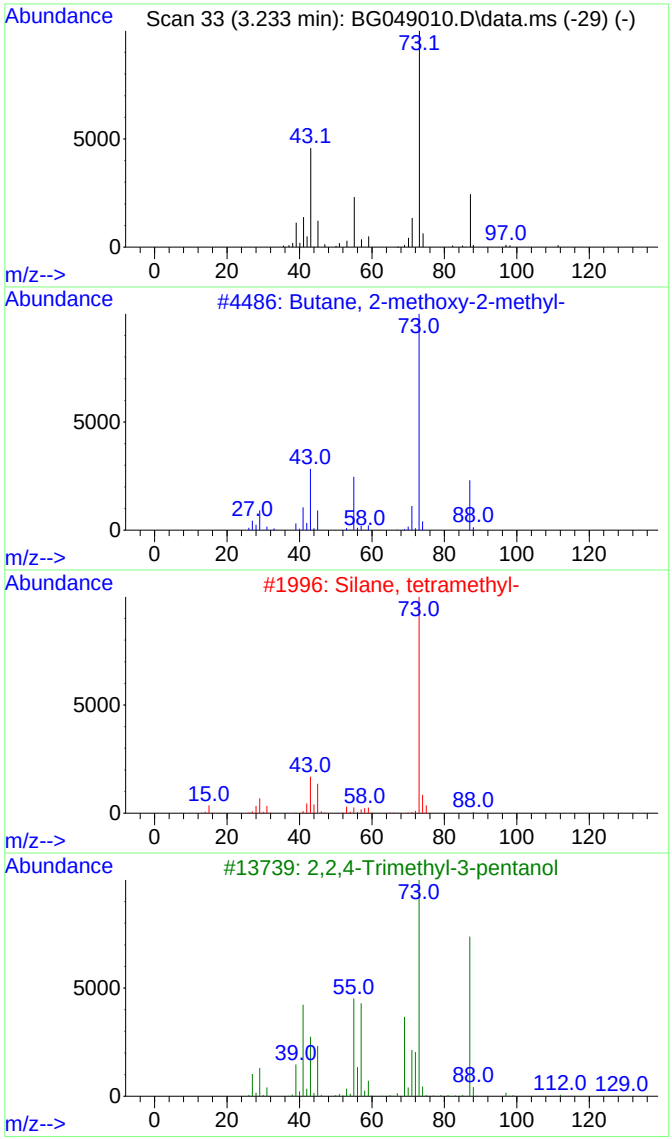
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

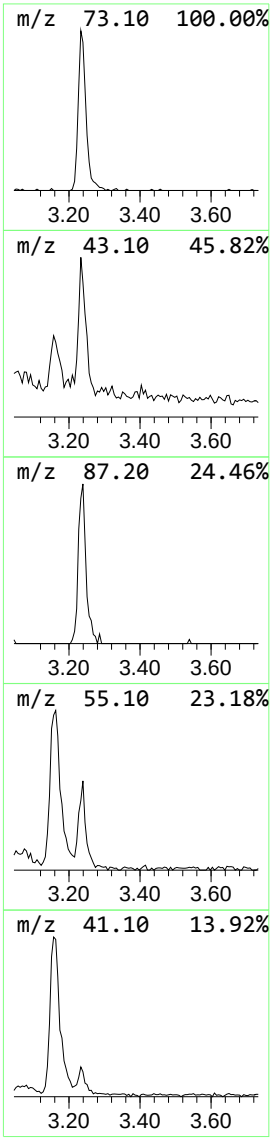
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.233	10.23 ng	110810	1,4-Dichlorobenzene-d4	8.116

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2	Silane, tetramethyl-	88	C4H12Si	000075-76-3	25
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	25
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5	2-Methyl-1,5-pentanediamine	116	C6H16N2	015520-10-2	9





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Data File : BG049010.D
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Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SPLP-AMND-COMP-F(CL-05)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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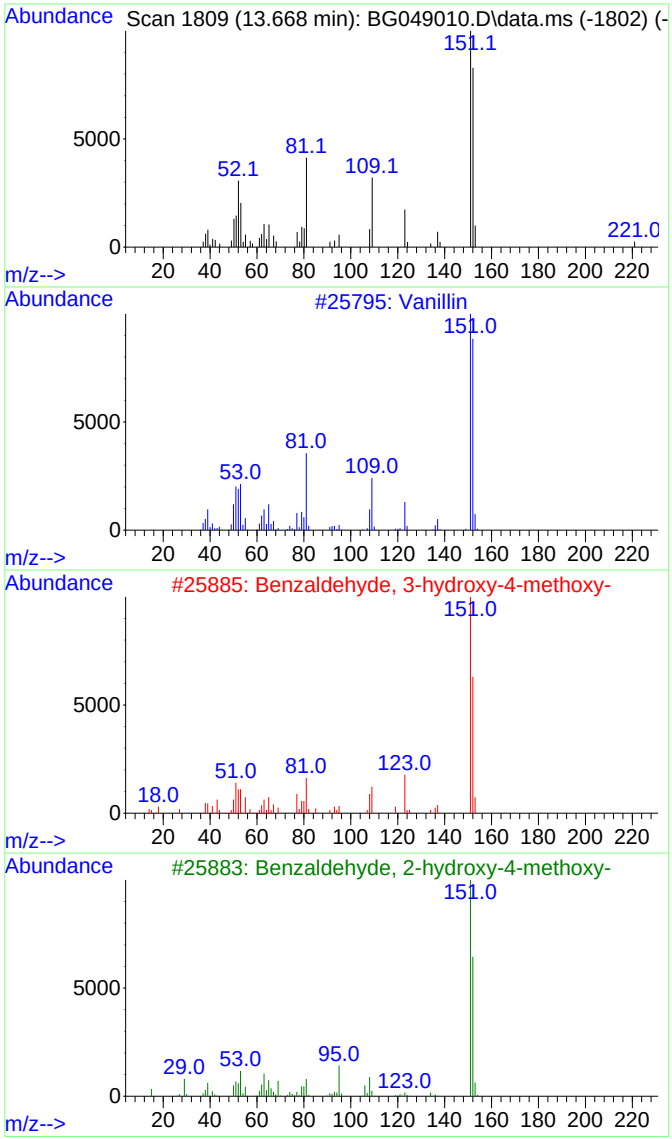
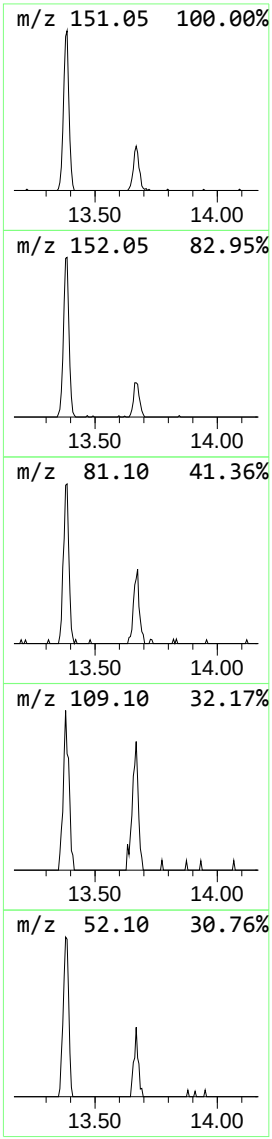
****

Peak Number 3 Vanillin Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.668	2.79 ng	60127	Acenaphthene-d10	14.761

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Vanillin	152	C8H8O3	000121-33-5	93
2	Benzaldehyde, 3-hydroxy-4-methoxy-	152	C8H8O3	000621-59-0	70
3	Benzaldehyde, 2-hydroxy-4-methoxy-	152	C8H8O3	000673-22-3	49
4	4-Hydroxy-2-methoxybenaldehyde	152	C8H8O3	018278-34-7	47
5	Benzaldehyde, 2,4-dihydroxy-6-me...	152	C8H8O3	000487-69-4	46





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Operator : CG/JU
Sample : M2678-12
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SPLP-AMND-COMP-F(CL-05)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

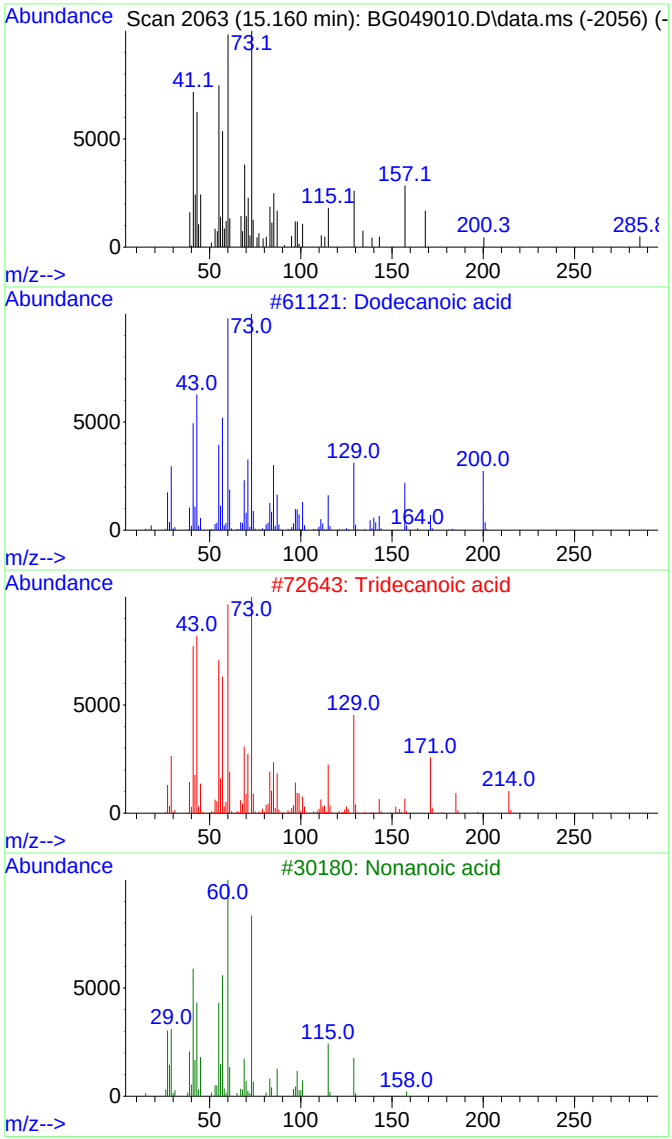
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

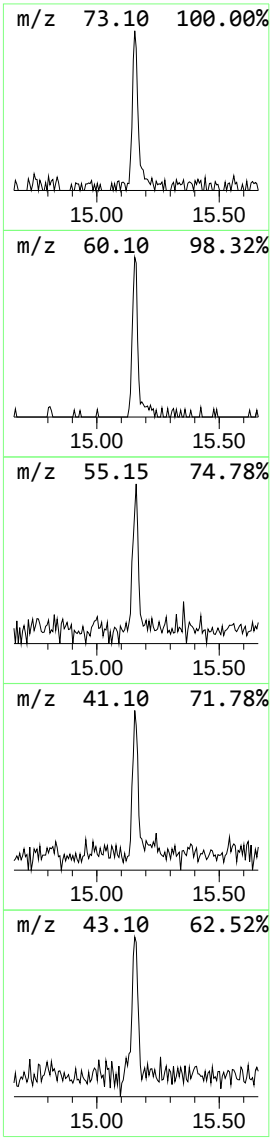
****

Peak Number 4 Dodecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.161	2.90 ng	62318	Acenaphthene-d10	14.761

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	80
2	Tridecanoic acid	214	C13H26O2	000638-53-9	59
3	Nonanoic acid	158	C9H18O2	000112-05-0	50
4	n-Decanoic acid	172	C10H20O2	000334-48-5	50
5	12-Bromododecanoic acid	278	C12H23BrO2	073367-80-3	47





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Data File : BG049010.D
Acq On : 17 Jun 2021 11:38
Operator : CG/JU
Sample : M2678-12
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SPLP-AMND-COMP-F(CL-05)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

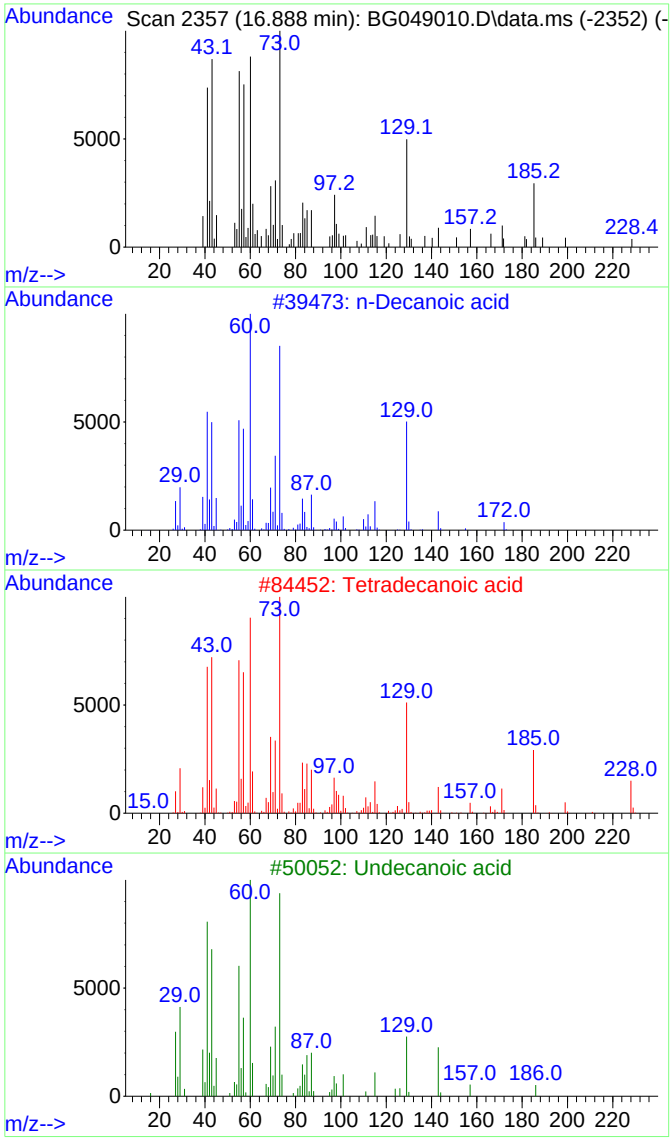
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

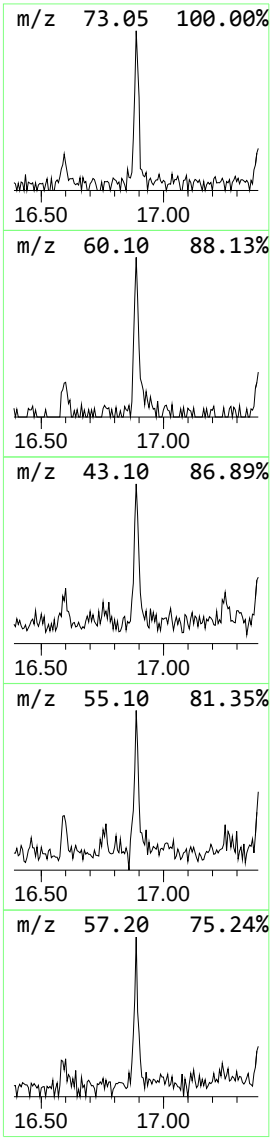
****

Peak Number 5 n-Decanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.888	2.21 ng	63317	Phenanthrene-d10	17.505

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Decanoic acid	172	C10H20O2	000334-48-5	92
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
3	Undecanoic acid	186	C11H22O2	000112-37-8	53
4	Tridecanoic acid	214	C13H26O2	000638-53-9	50
5	Dodecanoic acid	200	C12H24O2	000143-07-7	50





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Data File : BG049010.D
Acq On : 17 Jun 2021 11:38
Operator : CG/JU
Sample : M2678-12
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SPLP-AMND-COMP-F(CL-05)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

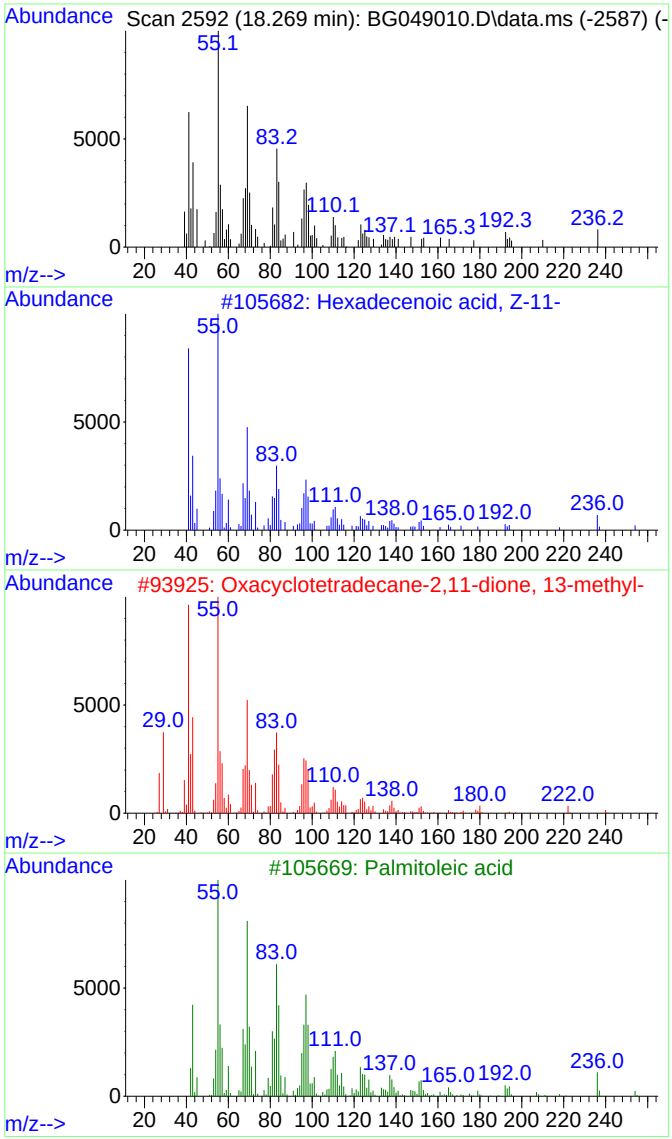
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

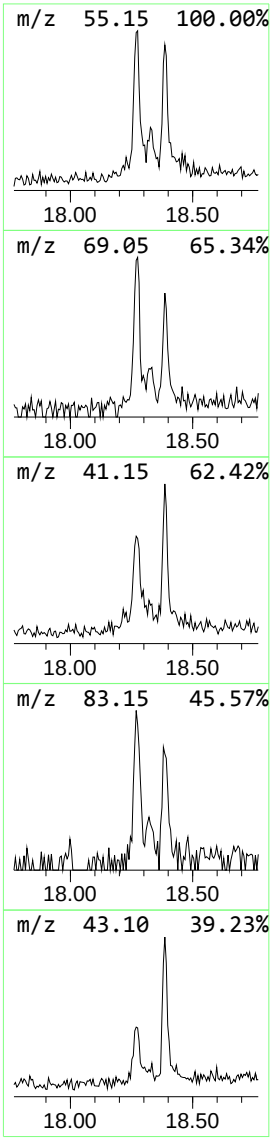
****

Peak Number 6 Hexadecenoic acid, Z-11- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.269	2.97 ng	85183	Phenanthrene-d10	17.505

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecenoic acid, Z-11-	254	C16H30O2	002416-20-8	78
2	Oxacyclotetradecane-2,11-dione, ...	240	C14H24O3	074685-36-2	64
3	Palmitoleic acid	254	C16H30O2	000373-49-9	47
4	Cyclopentadecane	210	C15H30	000295-48-7	43
5	1-Cyclohexyl-2-methyl-prop-2-en-...	152	C10H16O	025183-82-8	35





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Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SPLP-AMND-COMP-F(CL-05)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

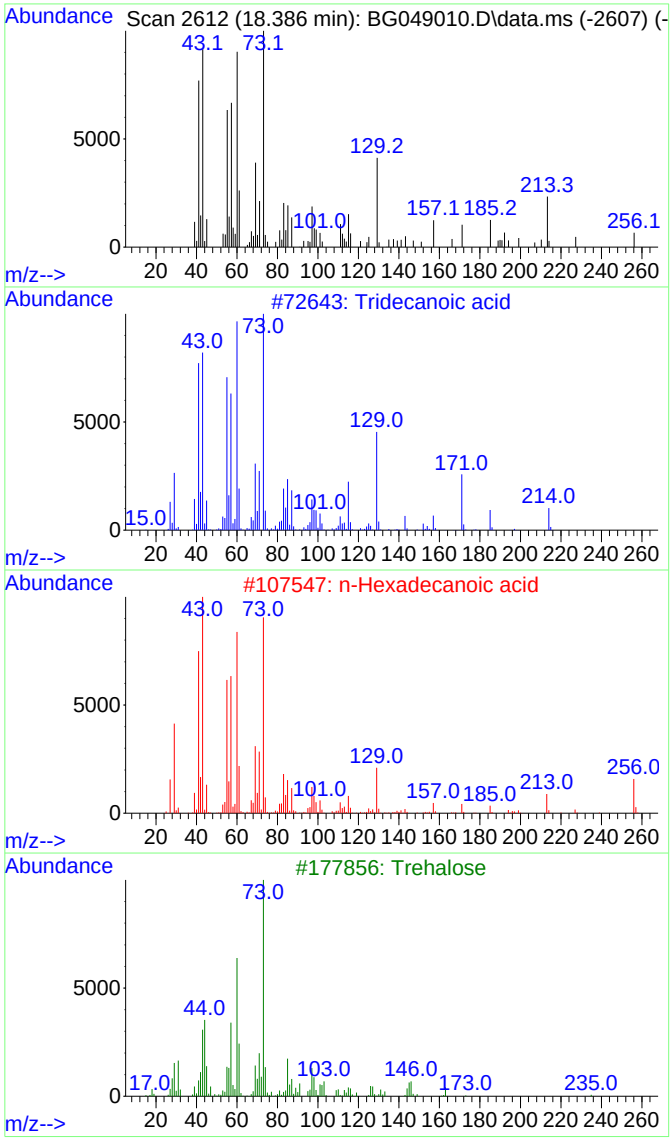
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

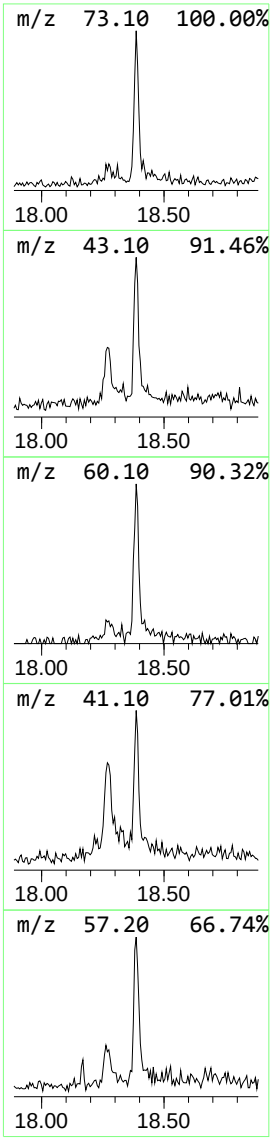
****

Peak Number 7 Tridecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.386	3.49 ng	100130	Phenanthrene-d10	17.505

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	64
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
3	Trehalose	342	C12H22O11	000099-20-7	49
4	d-Glucohexodialdose	178	C6H10O6	1000149-19-1	43
5	.alpha.-Methyl-D-mannopyranoside	194	C7H14O6	000617-04-9	38





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Sample : M2678-12
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Instrument :
BNA_G
ClientSampleId :
SPLP-AMND-COMP-F(CL-05)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

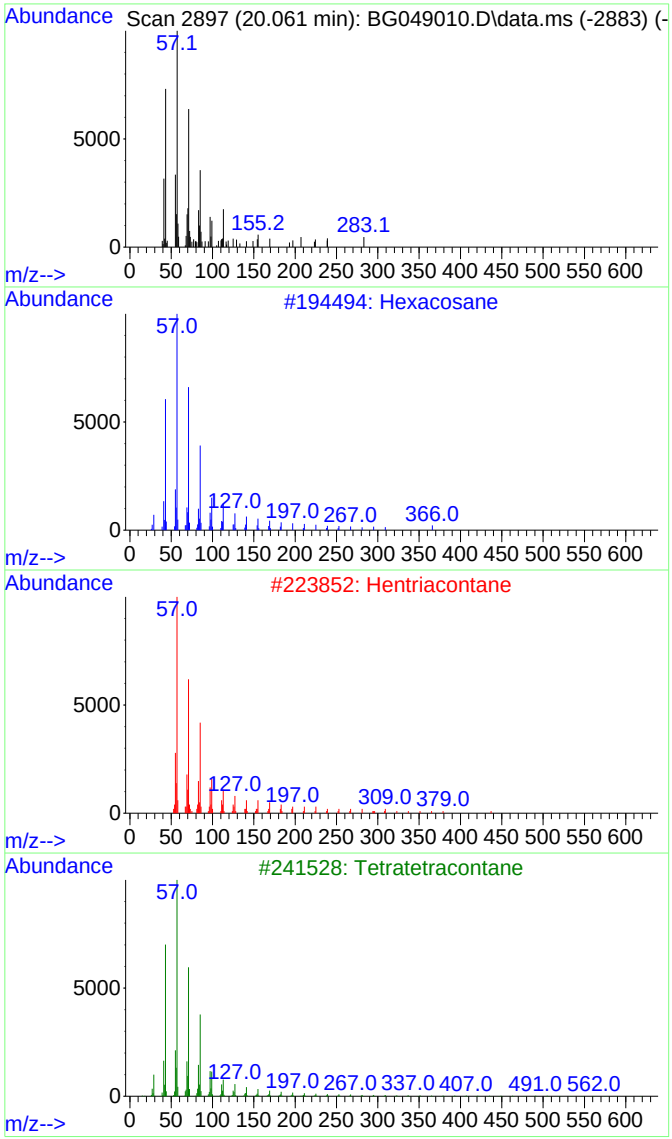
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

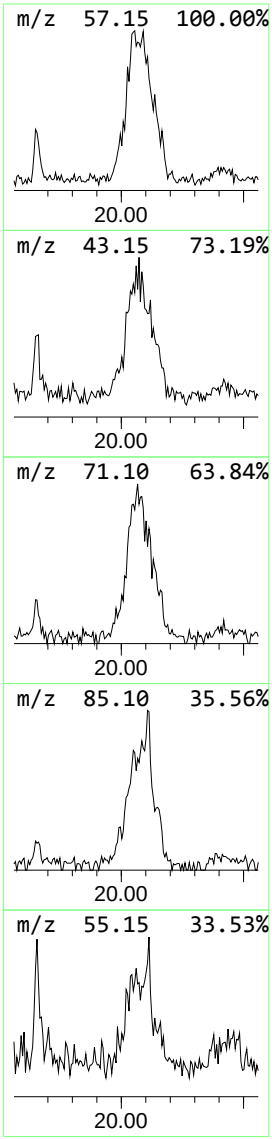
****

Peak Number 8 Hexacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.061	3.85 ng	123823	Chrysene-d12	21.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	80
2	Hentriacontane	437	C31H64	000630-04-6	80
3	Tetratetracontane	619	C44H90	007098-22-8	80
4	Octacosane	394	C28H58	000630-02-4	72
5	Octadecane	254	C18H38	000593-45-3	72





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BNA_G
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
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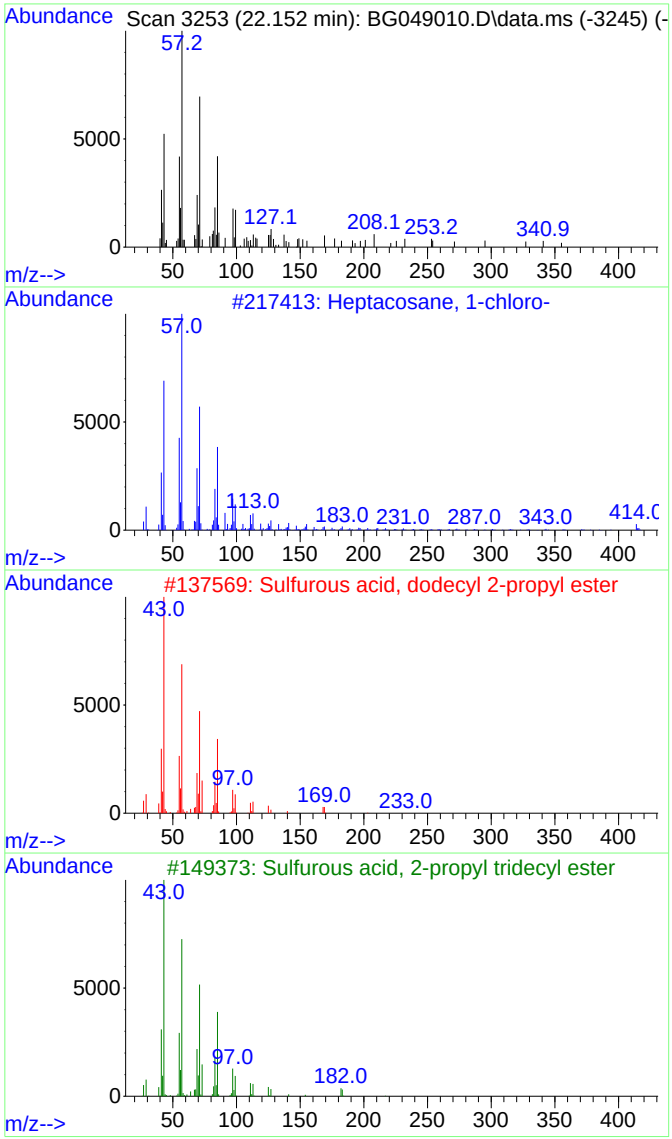
TIC Integration Parameters: LSCINT.P

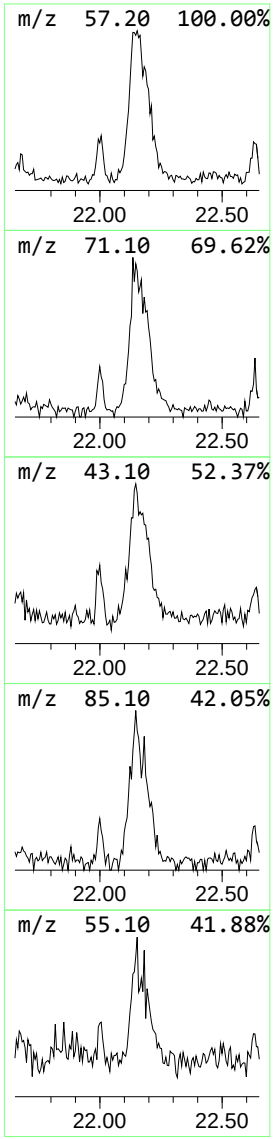
****

Peak Number 9 Heptacosane, 1-chloro- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.152	2.92 ng	93752	Chrysene-d12	21.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	80
2	Sulfurous acid, dodecyl 2-propyl...	292	C15H32O3S	1000309-12-3	80
3	Sulfurous acid, 2-propyl tridecy...	306	C16H34O3S	1000309-12-4	80
4	Octadecane	254	C18H38	000593-45-3	74
5	Tetracosane, 11-decyl-	479	C34H70	055429-84-0	72





Tentatively Identified Compound (LSC) summary

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	3.233	10.2	ng	110810	1	8.116	216682	20.0
Vanillin	13.668	2.8	ng	60127	3	14.761	430280	20.0
Dodecanoic acid	15.161	2.9	ng	62318	3	14.761	430280	20.0
n-Decanoic acid	16.888	2.2	ng	63317	4	17.505	573998	20.0
Hexadecenoic ac...	18.269	3.0	ng	85183	4	17.505	573998	20.0
Tridecanoic acid	18.386	3.5	ng	100130	4	17.505	573998	20.0
Hexacosane	20.061	3.9	ng	123823	5	21.794	642508	20.0
Heptacosane, 1-...	22.152	2.9	ng	93752	5	21.794	642508	20.0