LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111120\
Data File : BG047309.D
Acq On : 12 Nov 2020 10:16
Operator : CG/JU
Sample : L4622-05
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PAV-B12-10-17

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-BG110420.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG047309.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.571	371	380	388	rBV	771154	1257627	1.21%	0.736%
2	7.175	643	653	668	rBV	812130	1421769	1.37%	0.832%
3	13.268	1682	1690	1699	rBV	1323784	1970052	1.90%	1.153%
4	16.135	2170	2178	2185	rBV	940550	1486378	1.43%	0.870%
5	18.063	2498	2506	2510	rBV	10882971	14679760	14.13%	8.595%
6	19.202	2692	2700	2703	rBV	15176387	28539406	27.47%	16.709%
7	19.267	2703	2711	2717	rVB	46012139	103900060	100.00%	60.831%
8	19.361	2722	2727	2731	rVB	6327843	7463694	7.18%	4.370%
9	19.443	2737	2741	2753	rVB2	1176861	1848145	1.78%	1.082%
10	20.007	2832	2837	2843	rVB	1940339	2527073	2.43%	1.480%
11	20.330	2888	2892	2896	rVB	1446483	1680072	1.62%	0.984%
12	20.442	2907	2911	2914	rBV	939129	1086311	1.05%	0.636%
13	20.483	2914	2918	2923	rVV	689986	1223957	1.18%	0.717%
14	20.748	2959	2963	2968	rVB2	1241041	1715564	1.65%	1.004%

Sum of corrected areas: 170799868

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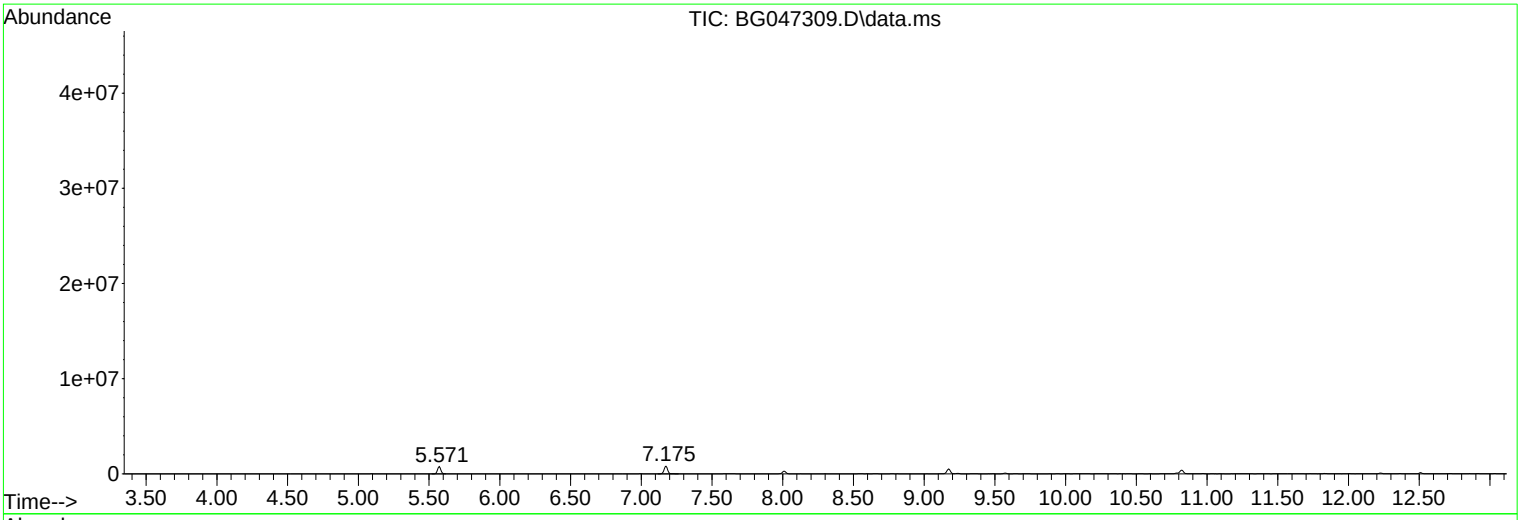
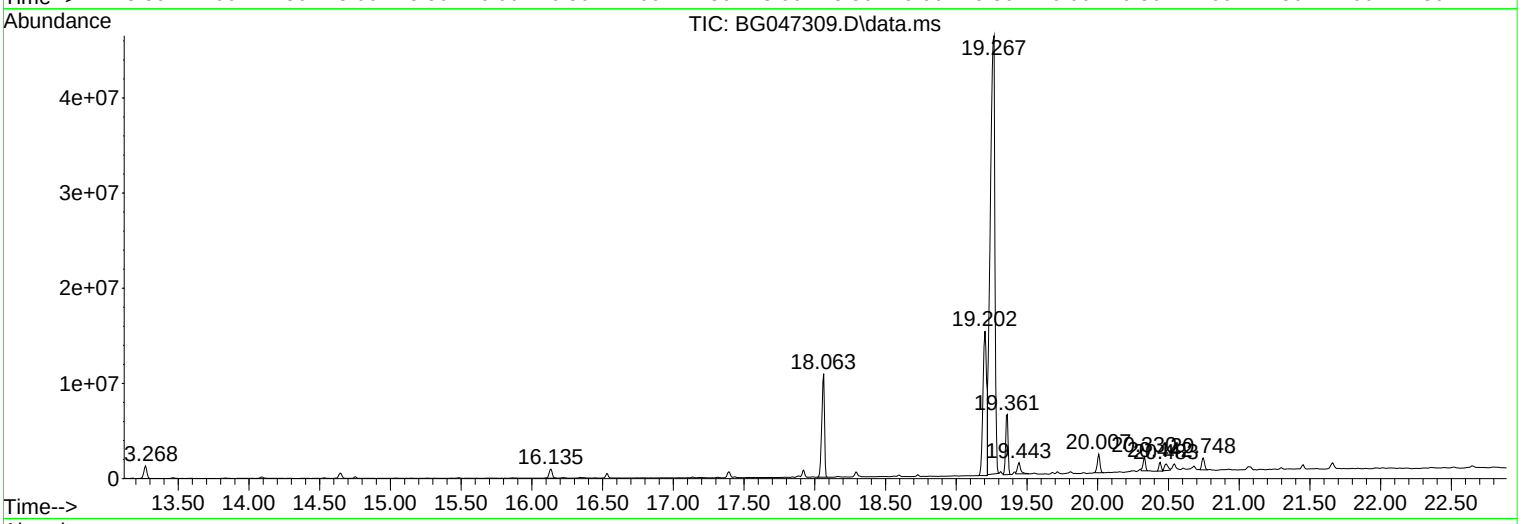
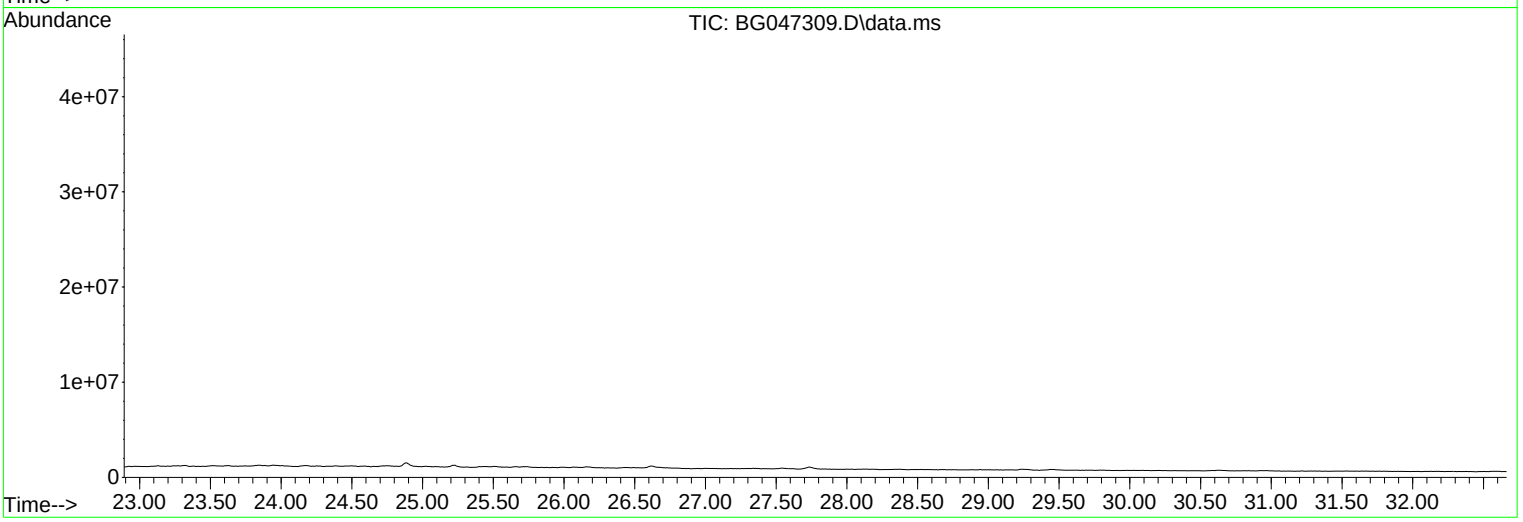
BNA_G
ClientSampleId :
PAV-B12-10-17

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG110420.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\BG111120\
Data File : BG047309.D
Acq On : 12 Nov 2020 10:16
Operator : CG/JU
Sample : L4622-05
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ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PAV-B12-10-17

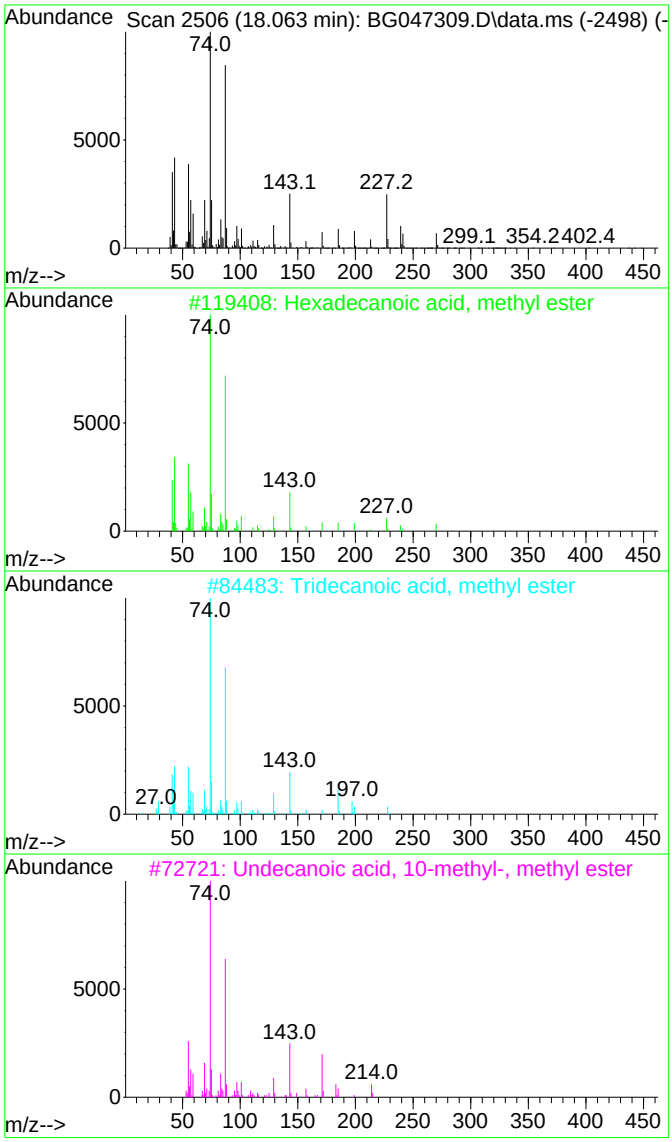
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG110420.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

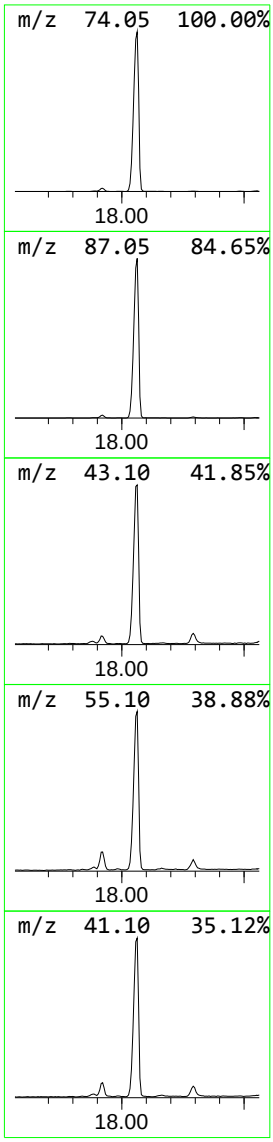
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Hexadecanoic acid, methyl e... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.063	20.00 ng	14679800	Phenanthrene-d10	17.393

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	95
2	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	91
3	Undecanoic acid, 10-methyl-, met...	214	C13H26O2	005129-56-6	80
4	Methyl 9-methyltetradecanoate	256	C16H32O2	213617-69-7	80
5	Methyl tetradecanoate	242	C15H30O2	000124-10-7	80





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Data File : BG047309.D
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Operator : CG/JU
Sample : L4622-05
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PAV-B12-10-17

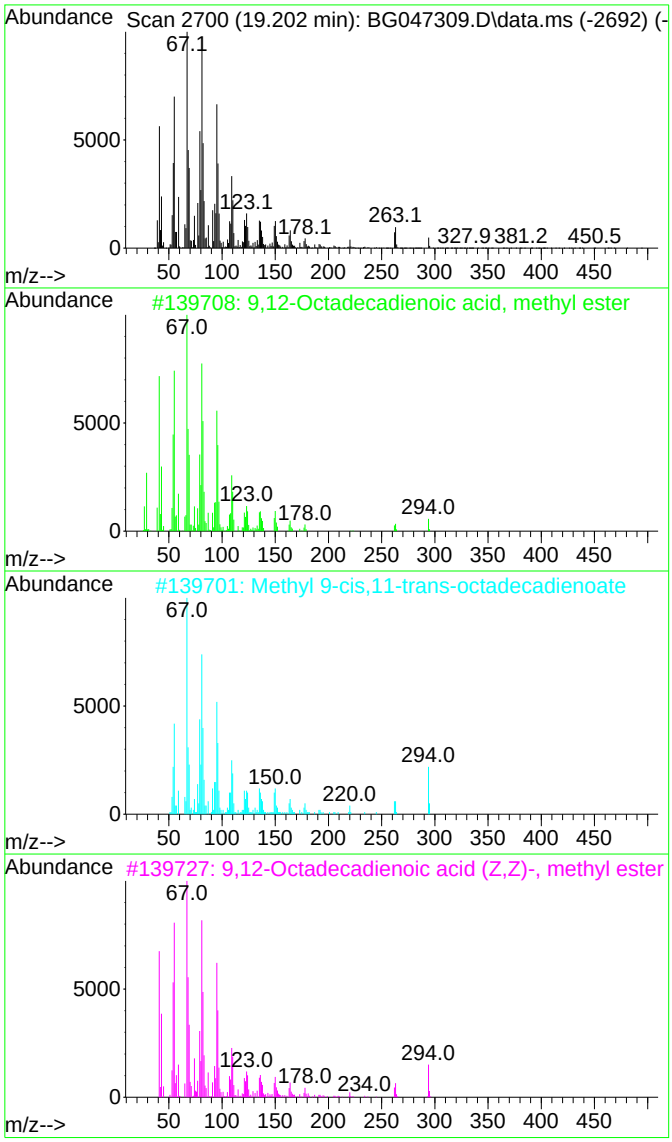
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG110420.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

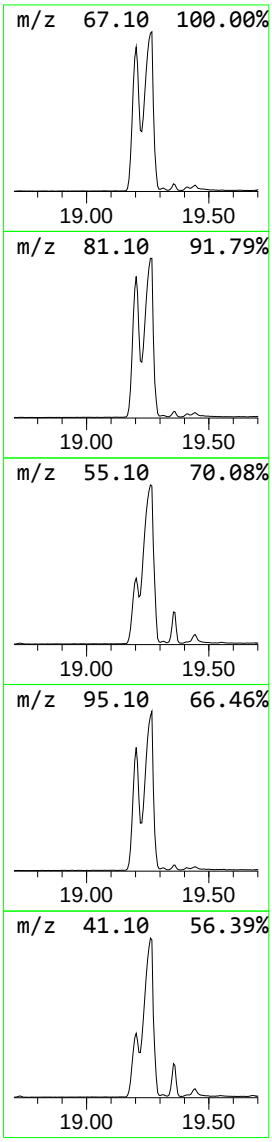
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 9,12-Octadecadienoic acid, ... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.202	38.88 ng	28539400	Phenanthrene-d10	17.393

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
2	Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	1000336-44-0	99
3	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
4	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	98
5	10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	98





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111120\
Data File : BG047309.D
Acq On : 12 Nov 2020 10:16
Operator : CG/JU
Sample : L4622-05
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PAV-B12-10-17

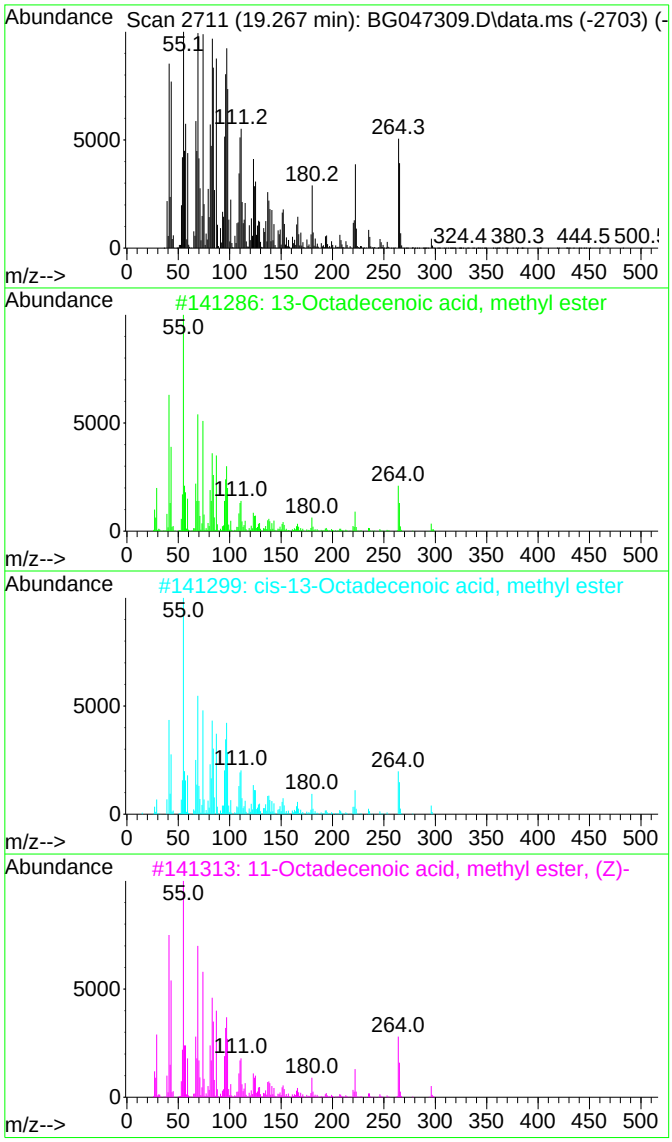
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG110420.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

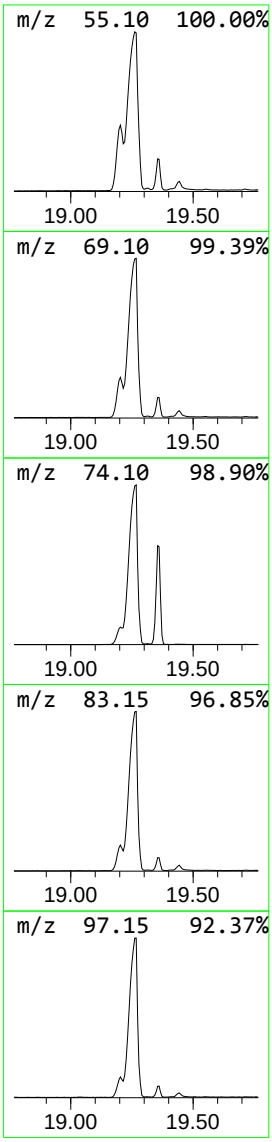
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 13-Octadecenoic acid, methy... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.267	141.56 ng	103900000	Phenanthrene-d10	17.393

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	99
2	cis-13-Octadecenoic acid, methyl...	296	C19H36O2	1000333-58-3	99
3	11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	99
4	8-Octadecenoic acid, methyl ester	296	C19H36O2	002345-29-1	99
5	9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	99





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111120\
Data File : BG047309.D
Acq On : 12 Nov 2020 10:16
Operator : CG/JU
Sample : L4622-05
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PAV-B12-10-17

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG110420.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

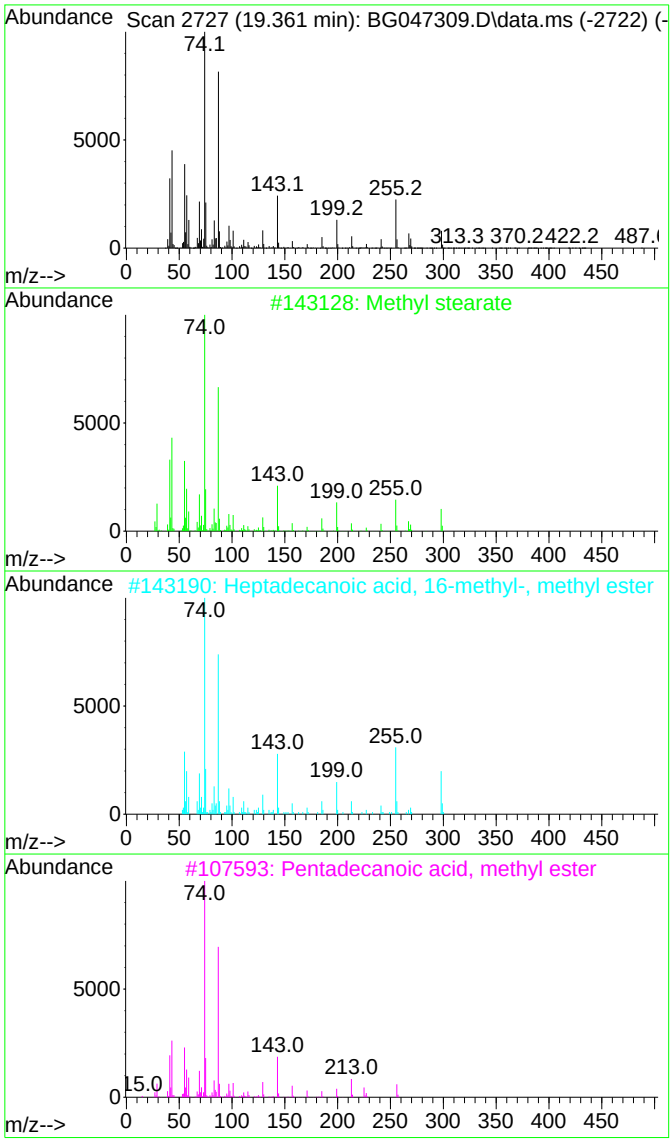
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

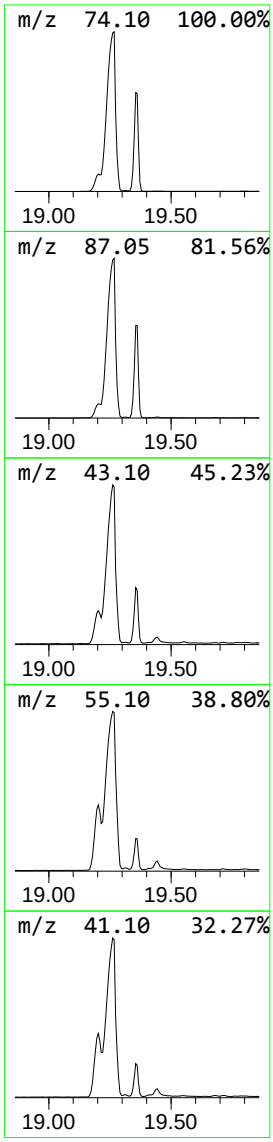
****

Peak Number 4 Methyl stearate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.361	10.17 ng	7463690	Phenanthrene-d10	17.393

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl stearate	298	C19H38O2	000112-61-8	98
2	Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	94
3	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	87
4	Methyl 9-methyltetradecanoate	256	C16H32O2	213617-69-7	83
5	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	80





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111120\
Data File : BG047309.D
Acq On : 12 Nov 2020 10:16
Operator : CG/JU
Sample : L4622-05
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PAV-B12-10-17

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG110420.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

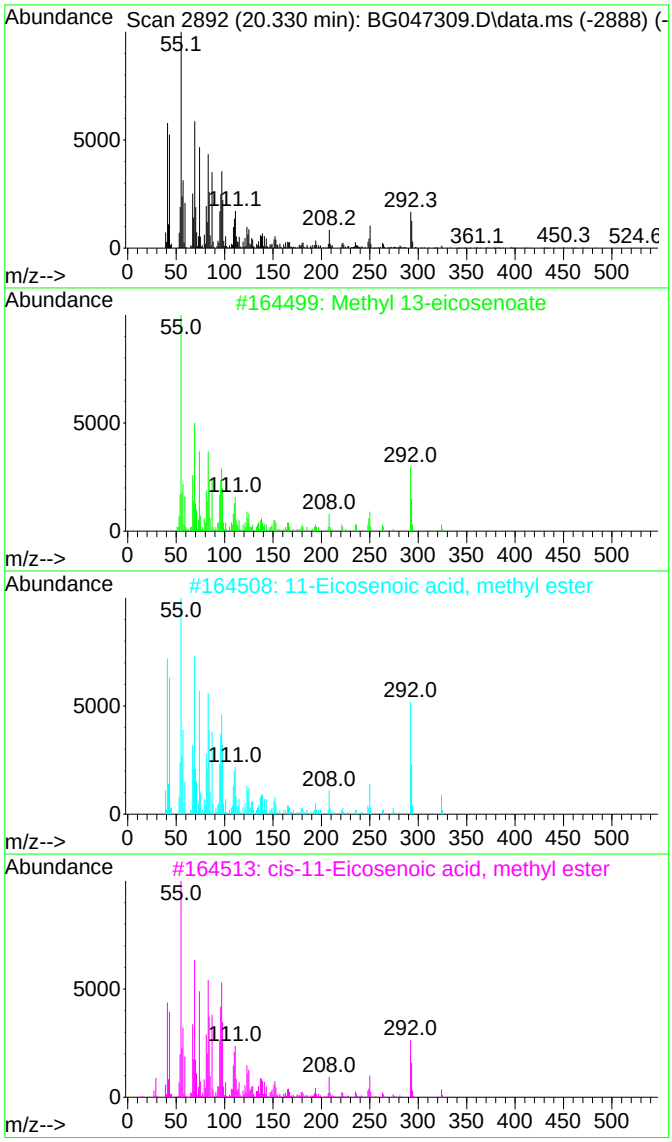
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

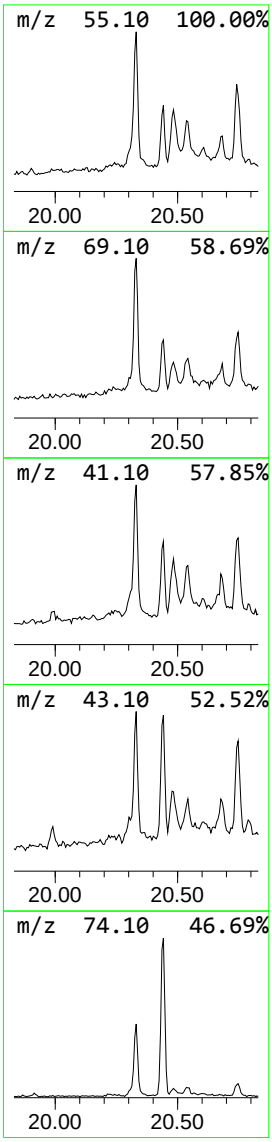
****

Peak Number 5 Methyl 13-eicosenoate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.331	19.59 ng	1680070	Chrysene-d12	21.658

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl 13-eicosenoate	324	C21H40O2	1000336-48-4	99
2	11-Eicosenoic acid, methyl ester	324	C21H40O2	003946-08-5	94
3	cis-11-Eicosenoic acid, methyl e...	324	C21H40O2	1000333-63-8	93
4	Methyl 9-eicosenoate	324	C21H40O2	1000336-50-5	91
5	Cyclopropaneoctanoic acid, 2-hex...	282	C18H34O2	010152-61-1	90





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Data File : BG047309.D
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Operator : CG/JU
Sample : L4622-05
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PAV-B12-10-17

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG110420.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

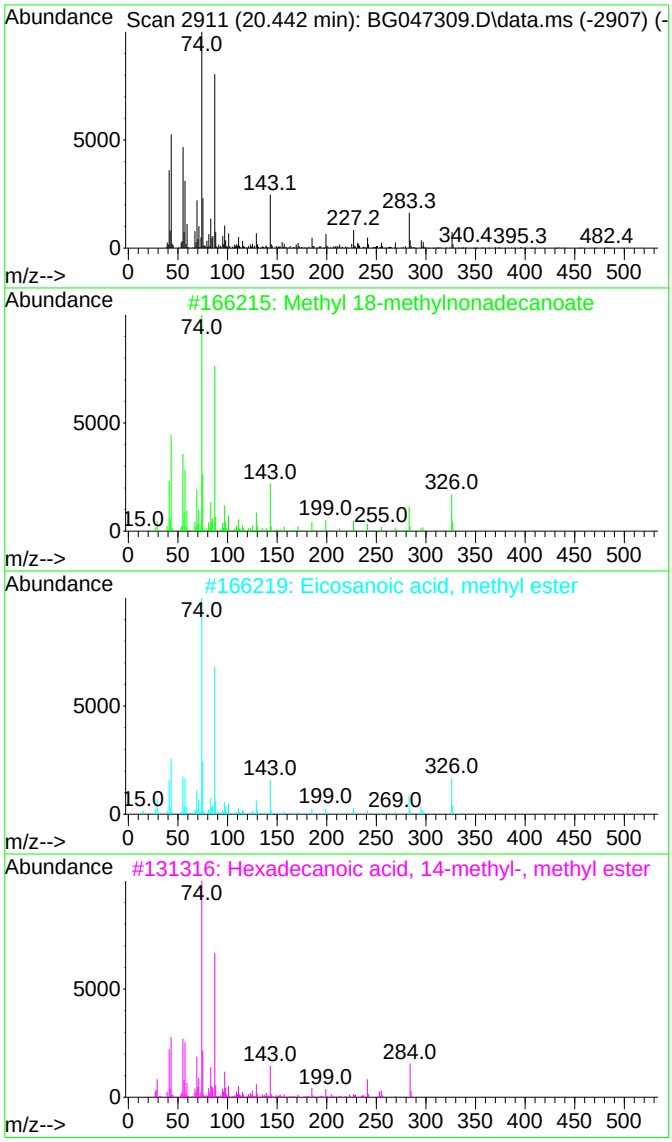
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

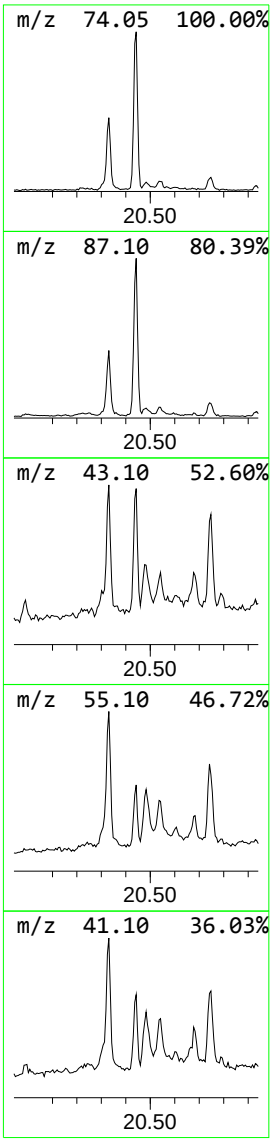
****

Peak Number 6 Methyl 18-methylnonadecanoate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.442	12.66 ng	1086310	Chrysene-d12	21.658

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl 18-methylnonadecanoate	326	C21H42O2	1000352-20-6	96
2	Eicosanoic acid, methyl ester	326	C21H42O2	001120-28-1	95
3	Hexadecanoic acid, 14-methyl-, m...	284	C18H36O2	002490-49-5	95
4	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	94
5	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	90





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Instrument : BNA_G
ClientSampleId : PAV-B12-10-17

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG110420.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

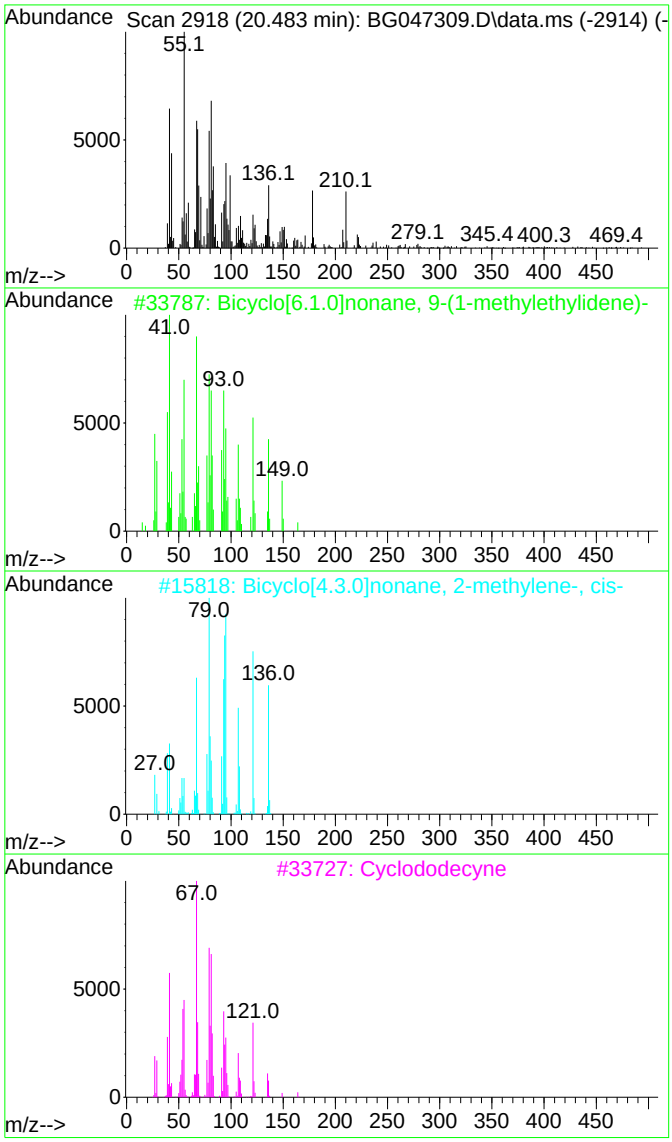
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

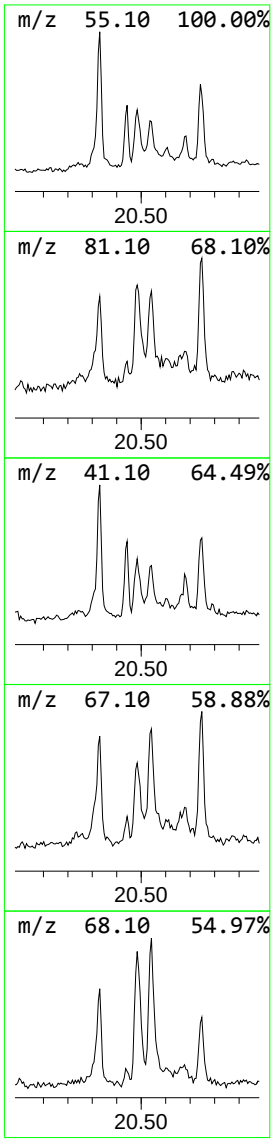
****

Peak Number 7 Bicyclo[6.1.0]nonane, 9-(1-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.483	14.27 ng	1223960	Chrysene-d12	21.658

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[6.1.0]nonane, 9-(1-methy...	164	C12H20	056666-90-1	64
2	Bicyclo[4.3.0]nonane, 2-methylen...	136	C10H16	040954-37-8	55
3	Cyclododecyne	164	C12H20	001129-90-4	49
4	9,12-Tetradecadien-1-ol, acetate...	252	C16H28O2	031654-77-0	46
5	9,12,15-Octadecatrienoic acid, (...	278	C18H30O2	000463-40-1	46





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Instrument : BNA_G
ClientSampleId : PAV-B12-10-17

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG110420.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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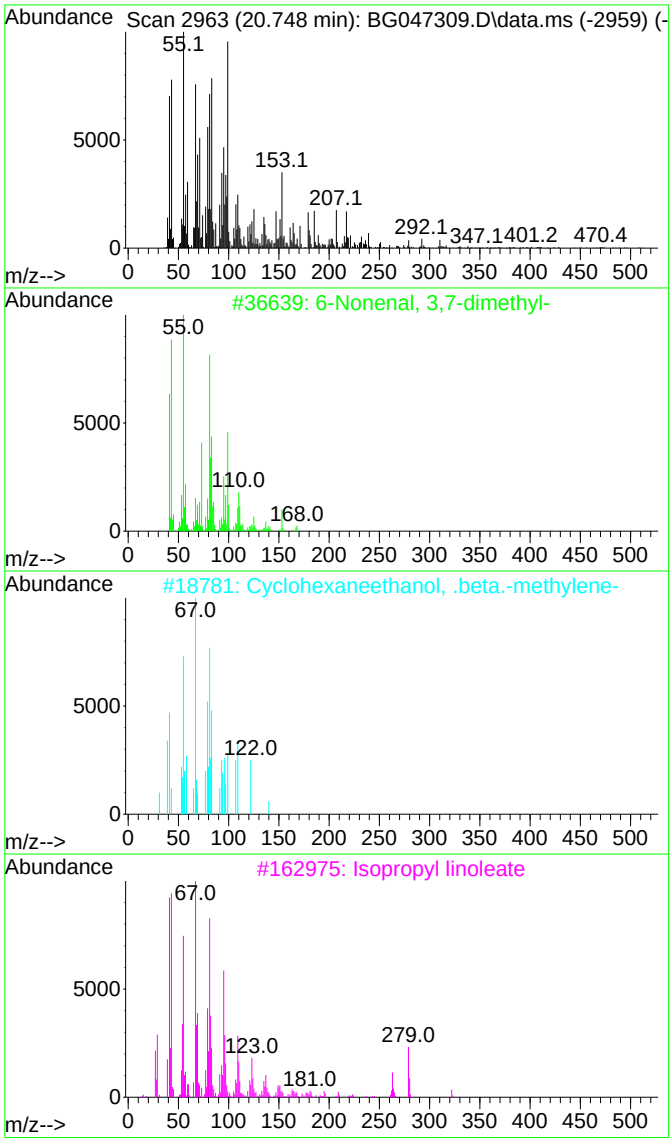
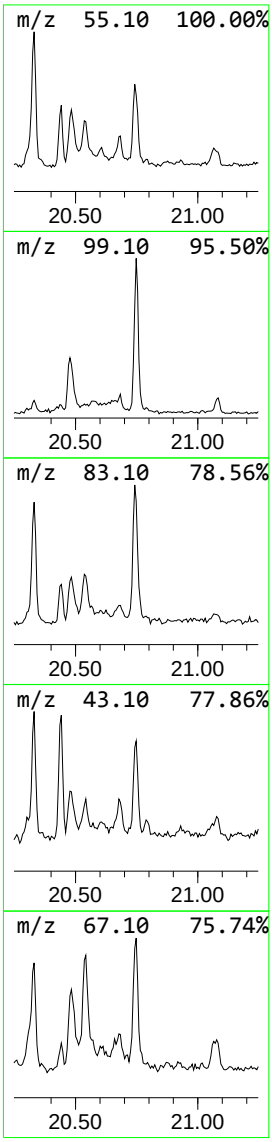
****

Peak Number 8 unknown20.74 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.748	20.00 ng	1715560	Chrysene-d12	21.658

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-Nonenal, 3,7-dimethyl-	168	C11H20O	1000132-43-9	49
2	Cyclohexaneethanol, .beta.-methy...	140	C9H16O	007697-55-4	42
3	Isopropyl linoleate	322	C21H38O2	022882-95-7	38
4	9-Methyl-10,12-hexadecadien-1-ol...	294	C19H34O2	1000130-87-7	25
5	2,3-Diazaspiro[4.5]deca-1,3-dien...	164	C10H16N2	105786-97-8	25





Tentatively Identified Compound (LSC) summary

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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
Hexadecanoic ac...	18.063	20.0	ng	14679800	4	17.393	14679800	20.0
9,12-Octadecadi...	19.202	38.9	ng	28539400	4	17.393	14679800	20.0
13-Octadecenoic...	19.267	141.6	ng	103900000	4	17.393	14679800	20.0
Methyl stearate	19.361	10.2	ng	7463690	4	17.393	14679800	20.0
Methyl 13-eicos...	20.331	19.6	ng	1680070	5	21.658	1715560	20.0
Methyl 18-methy...	20.442	12.7	ng	1086310	5	21.658	1715560	20.0
Bicyclo[6.1.0]n...	20.483	14.3	ng	1223960	5	21.658	1715560	20.0
unknown20.74	20.748	20.0	ng	1715560	5	21.658	1715560	20.0