LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111222\
Data File : BG055594.D
Acq On : 12 Nov 2022 18:01
Operator : CG/JU
Sample : N5431-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DISSOLVED-20221170-COMP-05-MODIFIED-ELUTRIATE

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-BG110922.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055594.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.325	3	6	22	rVB	468996	702116	36.61%	5.118%
2	4.706	236	241	245	rBV2	13624	19924	1.04%	0.145%
3	5.323	340	346	356	rVB	33150	52780	2.75%	0.385%
4	5.793	419	426	436	rVB	194396	320943	16.73%	2.340%
5	7.397	692	699	709	rBV	157736	270321	14.10%	1.971%
6	8.266	839	847	860	rBV	197729	338736	17.66%	2.469%
7	9.436	1039	1046	1054	rVB	253323	452051	23.57%	3.295%
8	11.092	1321	1328	1336	rBV	275281	496828	25.91%	3.622%
9	11.739	1433	1438	1446	rVB2	12809	20976	1.09%	0.153%
10	13.513	1731	1740	1748	rVB	738287	1125720	58.70%	8.206%
11	13.760	1777	1782	1790	rBV	18444	28028	1.46%	0.204%
12	14.324	1873	1878	1885	rBV2	19226	28634	1.49%	0.209%
13	14.888	1966	1974	1980	rVB	491366	770377	40.17%	5.616%
14	15.258	2032	2037	2043	rBV2	12928	20558	1.07%	0.150%
15	16.363	2218	2225	2232	rBV	679463	1058927	55.21%	7.719%
16	16.991	2324	2332	2340	rBV4	19035	33887	1.77%	0.247%
17	17.626	2434	2440	2446	rBV	702051	1054299	54.97%	7.686%
18	17.984	2496	2501	2511	rBV6	17659	45907	2.39%	0.335%
19	18.266	2545	2549	2554	rVB	68793	89135	4.65%	0.650%
20	18.360	2560	2565	2574	rVB4	21266	32912	1.72%	0.240%
21	18.490	2581	2587	2595	rBV	262498	407116	21.23%	2.968%
22	18.907	2654	2658	2662	rVB2	16894	20028	1.04%	0.146%
23	19.348	2727	2733	2738	rBV4	26787	56297	2.94%	0.410%
24	19.424	2742	2746	2750	rVB	200242	239932	12.51%	1.749%
25	19.553	2764	2768	2773	rVB	64989	77198	4.03%	0.563%
26	19.606	2773	2777	2779	rBV	49075	68292	3.56%	0.498%
27	19.747	2796	2801	2814	rBV	113751	178189	9.29%	1.299%
28	20.011	2842	2846	2855	rVB3	39103	58736	3.06%	0.428%
29	20.211	2874	2880	2887	rBV	1493753	1917832	100.00%	13.981%
30	20.505	2926	2930	2933	rVB	40256	42996	2.24%	0.313%
31	20.863	2988	2991	2997	rBV7	16056	29899	1.56%	0.218%
32	21.004	3011	3015	3019	rBV2	67263	84870	4.43%	0.619%
33	21.533	3100	3105	3119	rBV	196858	388452	20.25%	2.832%
34	21.792	3145	3149	3154	rVB2	24840	35560	1.85%	0.259%
35	21.927	3165	3172	3179	rBV	685029	1184210	61.75%	8.633%
36	22.109	3199	3203	3210	rBV	64528	96652	5.04%	0.705%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111222\
Data File : BG055594.D
Acq On : 12 Nov 2022 18:01
Operator : CG/JU
Sample : N5431-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DISSOLVED-20221170-COMP-05-MODIFIED-ELUTRIATE

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-BG110922.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	22.755	3309	3313	3320	rVB	53480	83166	4.34%	0.606%
38	23.496	3434	3439	3448	rVB2	48169	101339	5.28%	0.739%
39	23.701	3468	3474	3481	rVB	138824	283631	14.79%	2.068%
40	24.359	3583	3586	3593	rVB3	37851	76358	3.98%	0.557%
41	25.346	3744	3754	3769	rVB2	417471	1323994	69.04%	9.652%

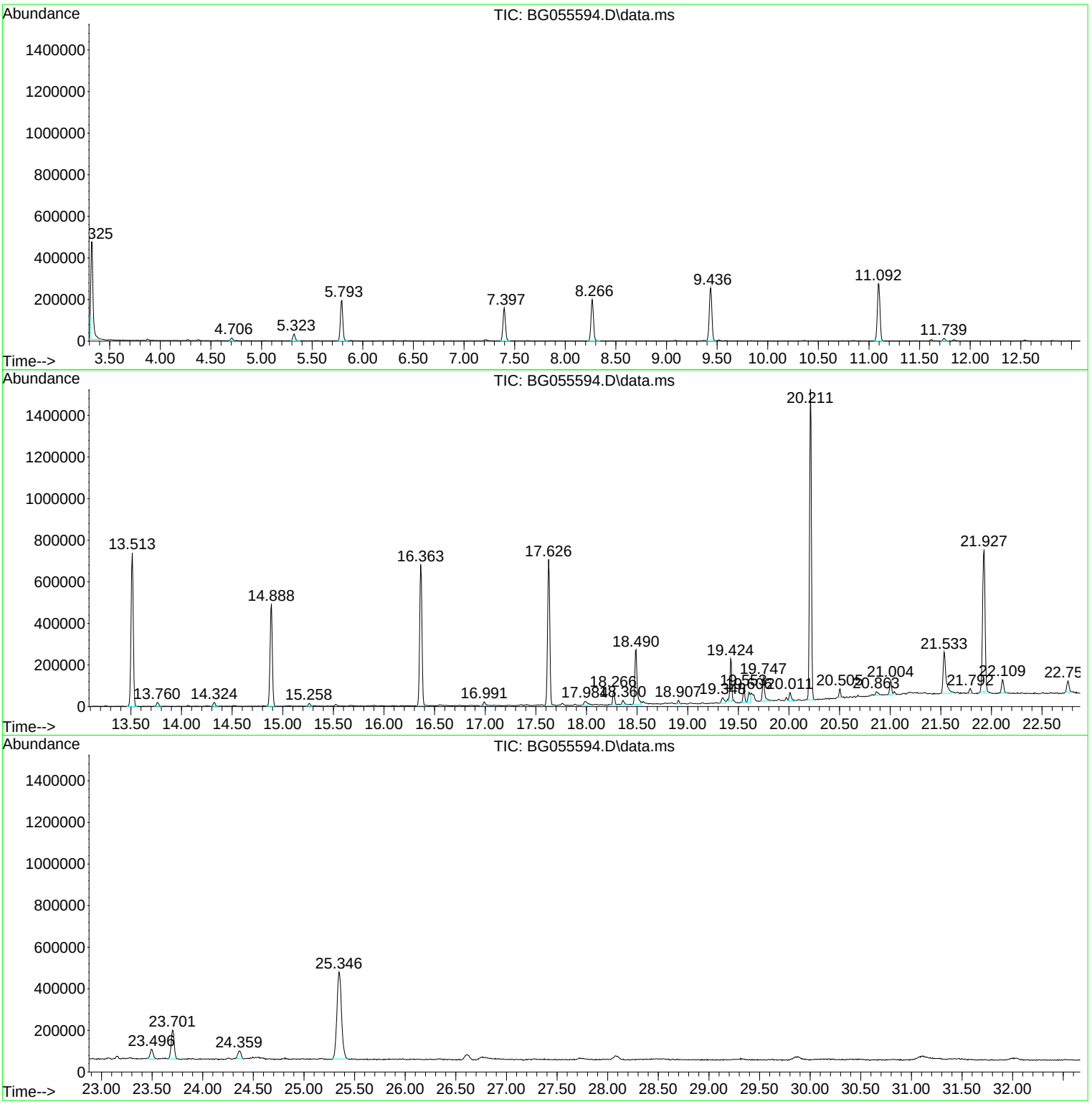
Sum of corrected areas: 13717806

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111222\
Data File : BG055594.D
Acq On : 12 Nov 2022 18:01
Operator : CG/JU
Sample : N5431-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DISSOLVED-20221170-COMP-05-MODIFIED-ELUTRIATE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111222\
Data File : BG055594.D
Acq On : 12 Nov 2022 18:01
Operator : CG/JU
Sample : N5431-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DISSOLVED-20221170-COMP-05-MODIFIED-ELUTRIATE

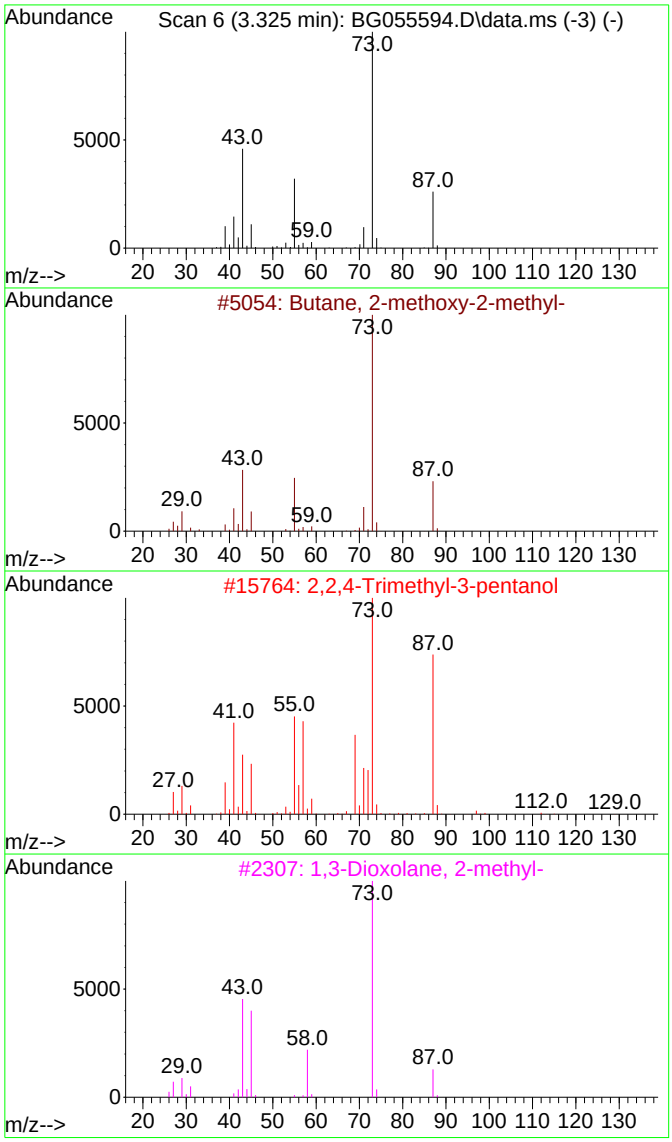
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

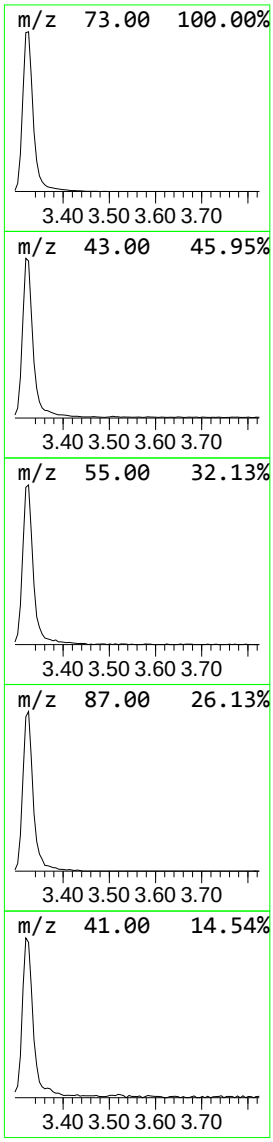
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.325	41.46 ng	702116	1,4-Dichlorobenzene-d4	8.266

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4	1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	17
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111222\
Data File : BG055594.D
Acq On : 12 Nov 2022 18:01
Operator : CG/JU
Sample : N5431-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DISSOLVED-20221170-COMP-05-MODIFIED-ELUTRIATE

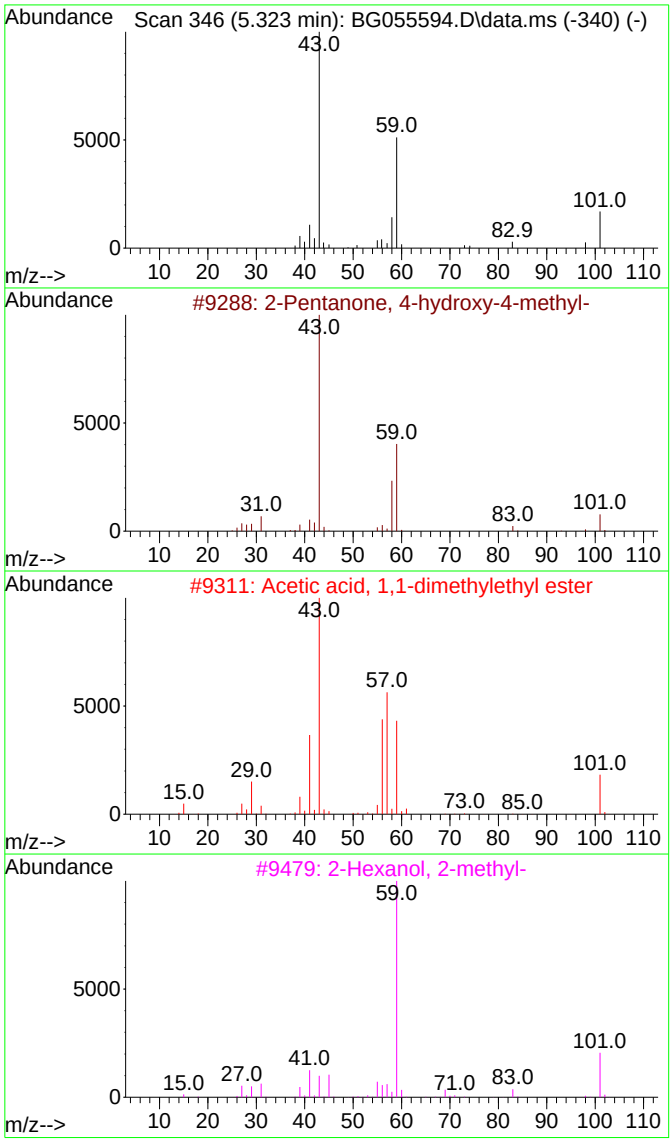
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

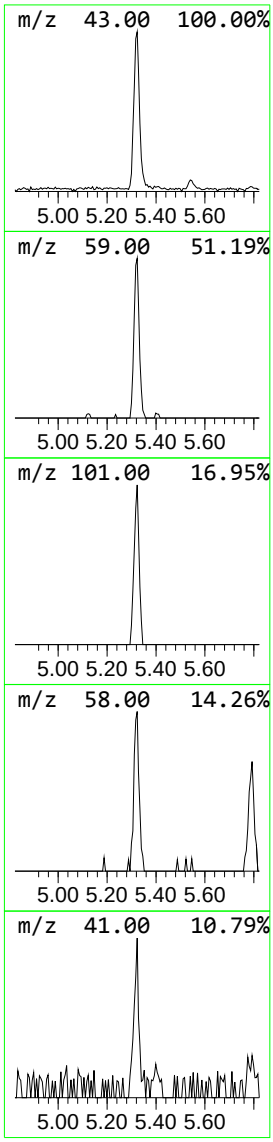
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.323	3.12 ng	52780	1,4-Dichlorobenzene-d4	8.266

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	50
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111222\
Data File : BG055594.D
Acq On : 12 Nov 2022 18:01
Operator : CG/JU
Sample : N5431-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DISSOLVED-20221170-COMP-05-MODIFIED-ELUTRIATE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

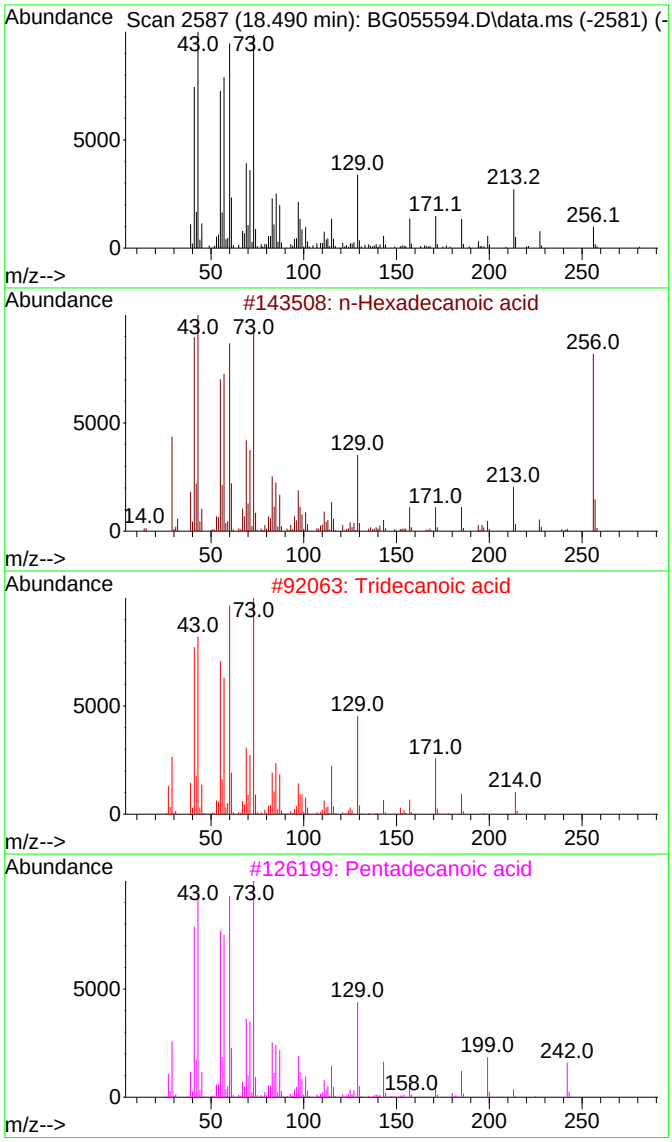
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

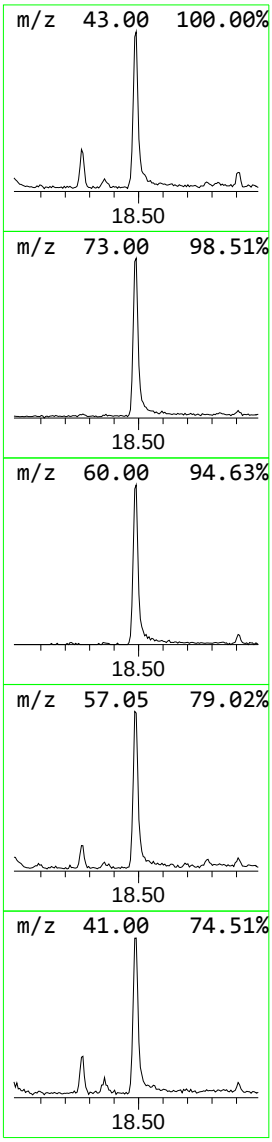
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.490	7.72 ng	407116	Phenanthrene-d10	17.626

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Undecanoic acid	186	C11H22O2	000112-37-8	76
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111222\
Data File : BG055594.D
Acq On : 12 Nov 2022 18:01
Operator : CG/JU
Sample : N5431-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DISSOLVED-20221170-COMP-05-MODIFIED-ELUTRIATE

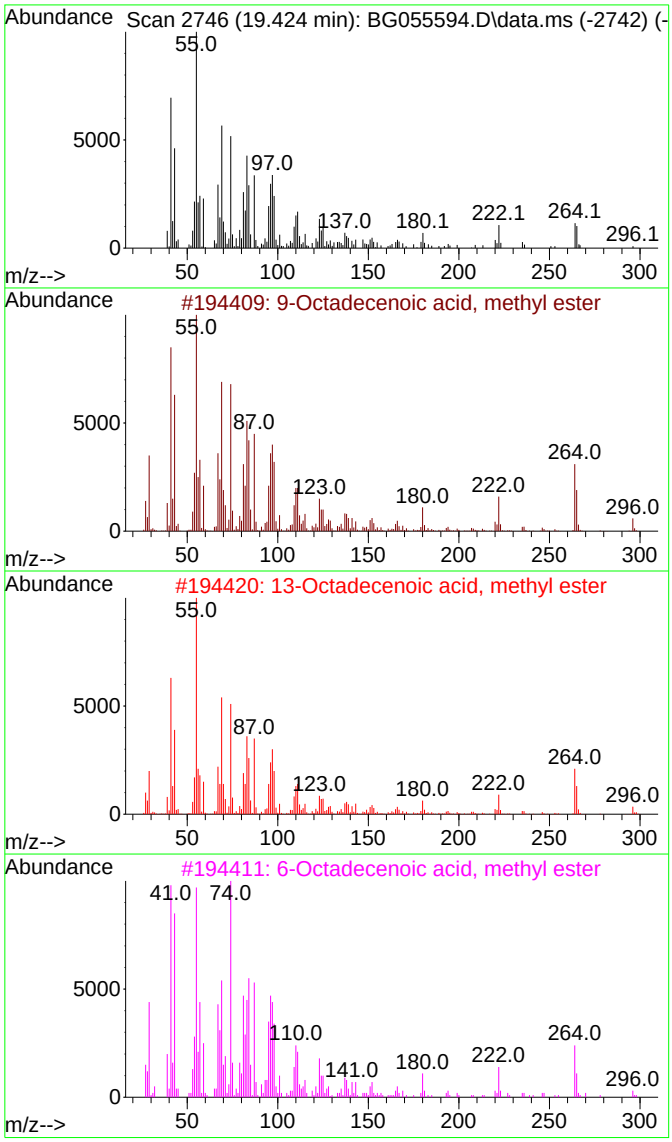
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

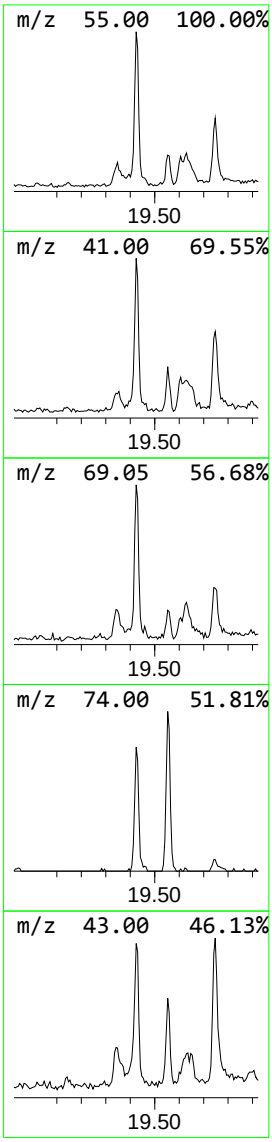
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 9-Octadecenoic acid, methyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.424	4.55 ng	239932	Phenanthrene-d10	17.626

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid, methyl ester	296	C19H36O2	002462-84-2	99
2	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	98
3	6-Octadecenoic acid, methyl ester	296	C19H36O2	052355-31-4	95
4	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	95
5	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	94





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111222\
Data File : BG055594.D
Acq On : 12 Nov 2022 18:01
Operator : CG/JU
Sample : N5431-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DISSOLVED-20221170-COMP-05-MODIFIED-ELUTRIATE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

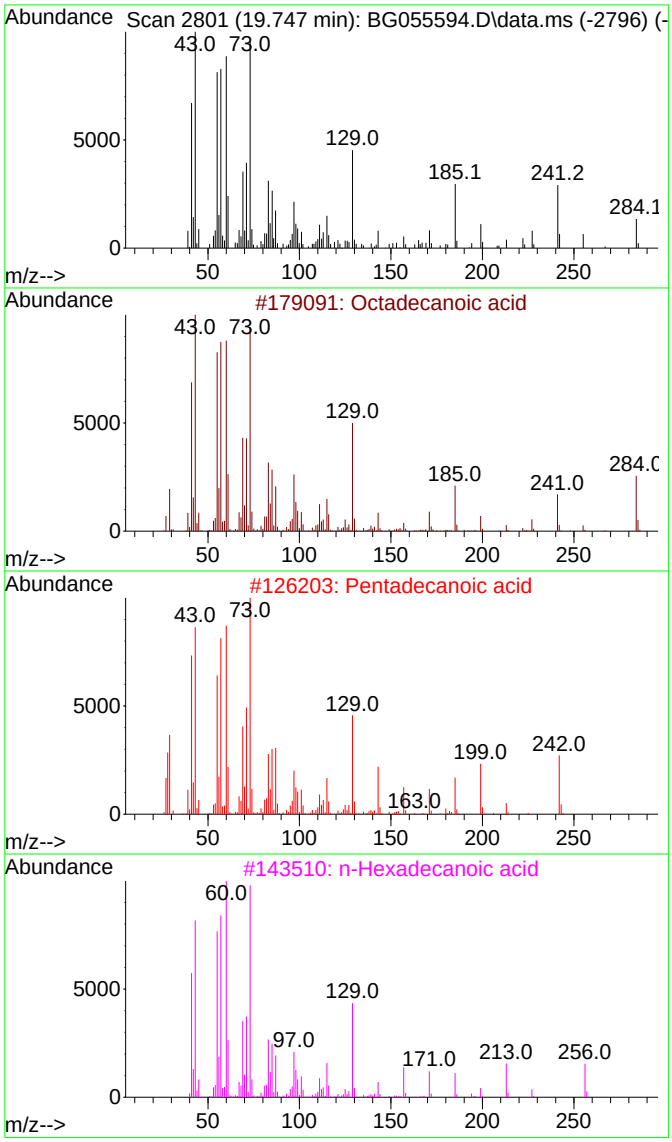
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

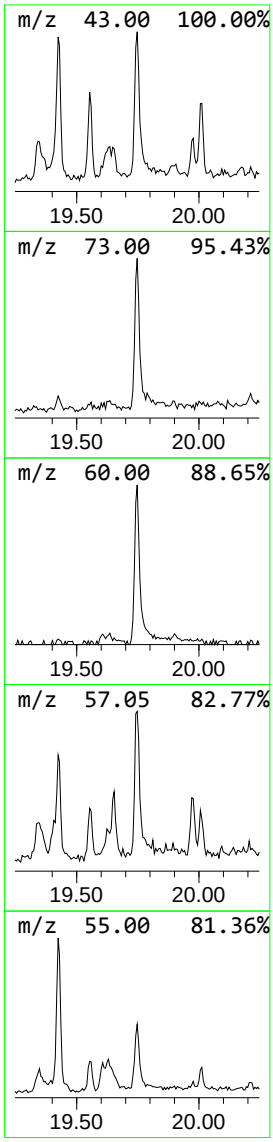
****

Peak Number 5 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.747	3.38 ng	178189	Phenanthrene-d10	17.626

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	n-Decanoic acid	172	C10H20O2	000334-48-5	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111222\
Data File : BG055594.D
Acq On : 12 Nov 2022 18:01
Operator : CG/JU
Sample : N5431-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DISSOLVED-20221170-COMP-05-MODIFIED-ELUTRIATE

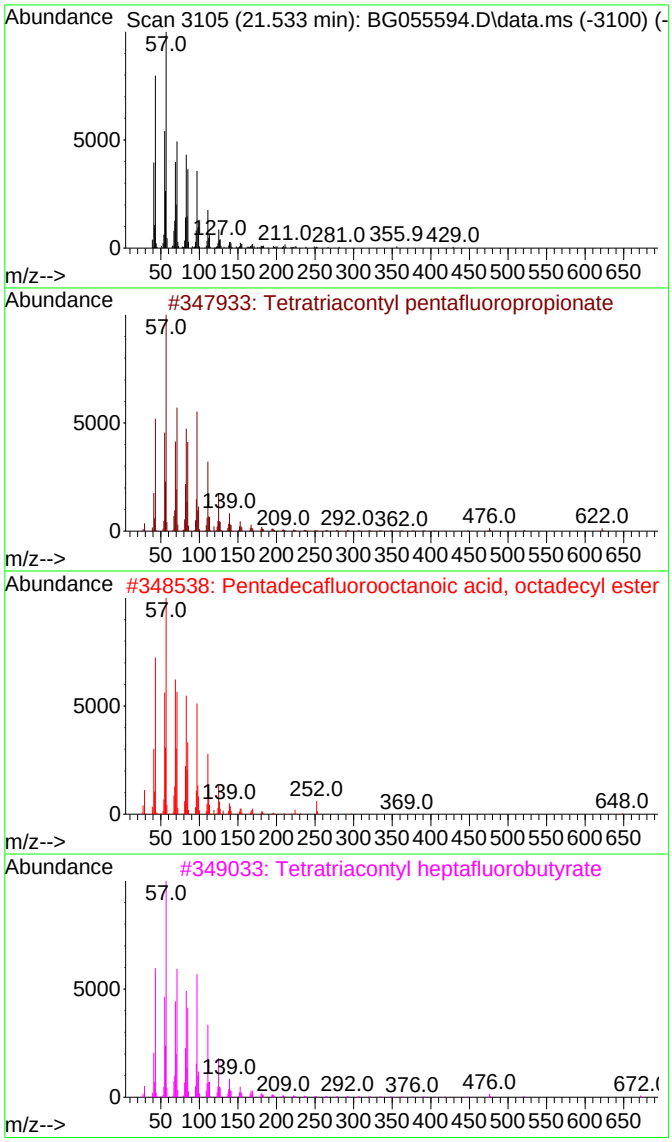
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

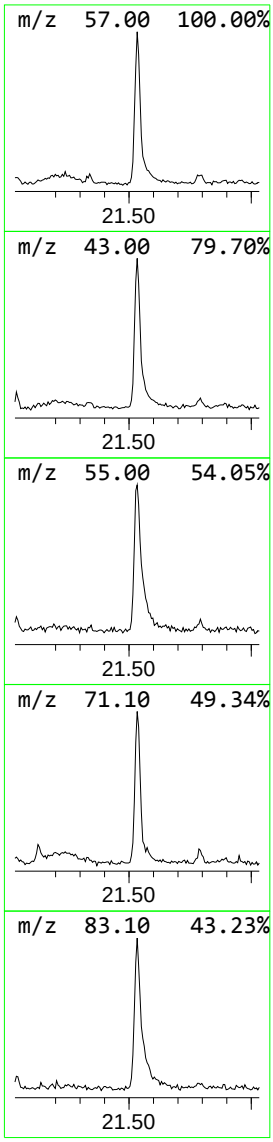
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Tetratriacontyl pentafluoro... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.533	6.56 ng	388452	Chrysene-d12	21.927

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratriacontyl pentafluoropropi...	641	C37H69F5O2	1000351-81-5	91
2	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	91
3	Tetratriacontyl heptafluorobutyrate	691	C38H69F7O2	1000351-84-1	91
4	Dotriacontyl pentafluoropropionate	612	C35H65F5O2	1010351-81-4	91
5	Oxalic acid, isobutyl octadecyl ...	398	C24H46O4	1000309-38-3	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111222\
Data File : BG055594.D
Acq On : 12 Nov 2022 18:01
Operator : CG/JU
Sample : N5431-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DISSOLVED-20221170-COMP-05-MODIFIED-ELUTRIATE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

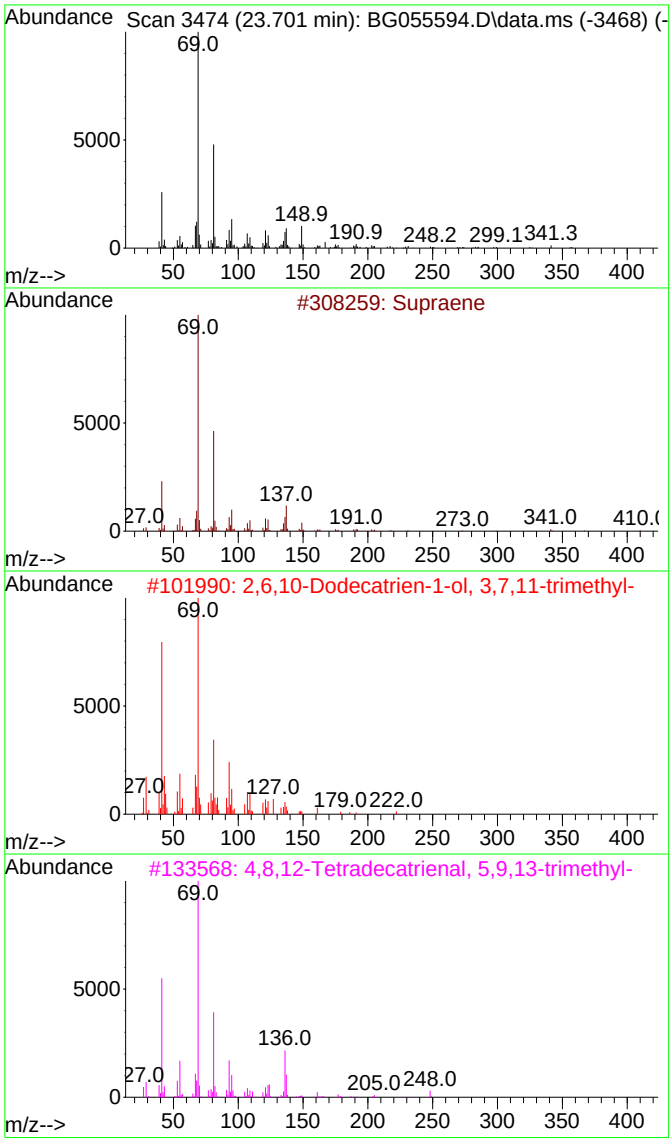
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

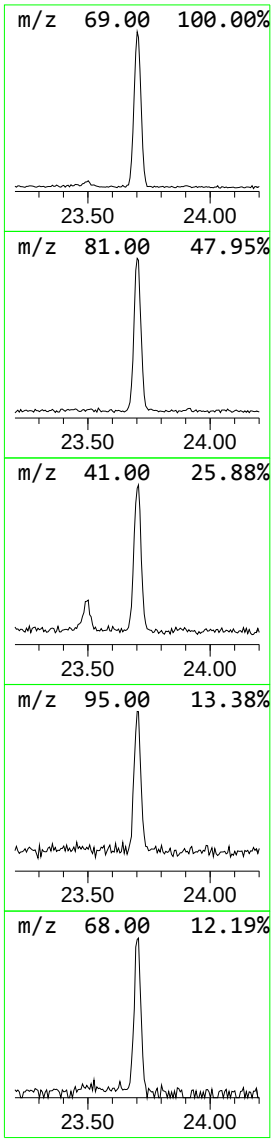
****

Peak Number 7 Supraene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.701	4.28 ng	283631	Perylene-d12	25.346

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	87
2	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	72
3	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72
4	2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	64
5	5-Bromo-1-pentanol	166	C5H11BrO	034626-51-2	59





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111222\
Data File : BG055594.D
Acq On : 12 Nov 2022 18:01
Operator : CG/JU
Sample : N5431-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DISSOLVED-20221170-COMP-05-MODIFIED-ELUTRIATE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	3.325	41.5	ng	702116	1	8.266	338736	20.0
2-Pentanone, 4-...	5.323	3.1	ng	52780	1	8.266	338736	20.0
n-Hexadecanoic ...	18.490	7.7	ng	407116	4	17.626	1054300	20.0
9-Octadecenoic ...	19.424	4.5	ng	239932	4	17.626	1054300	20.0
Octadecanoic acid	19.747	3.4	ng	178189	4	17.626	1054300	20.0
Tetratriacontyl...	21.533	6.6	ng	388452	5	21.927	1184210	20.0
Supraene	23.701	4.3	ng	283631	6	25.346	1323990	20.0