LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111722\
Data File : BG055681.D
Acq On : 18 Nov 2022 1:29
Operator : CG/JU
Sample : N5660-01 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : CL-02-11622

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-BG111622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055681.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.309	337	344	354	rVB	51656	84918	6.43%	0.715%
2	5.785	418	425	435	rBV	354950	584774	44.27%	4.925%
3	7.401	692	700	714	rVB	345978	618633	46.83%	5.210%
4	8.253	838	845	852	rBV	192725	330517	25.02%	2.784%
5	9.422	1037	1044	1052	rBV	212532	374487	28.35%	3.154%
6	11.085	1319	1327	1333	rBV	262010	470300	35.60%	3.961%
7	13.500	1731	1738	1746	rVB	516624	799666	60.53%	6.735%
8	14.604	1920	1926	1938	rBV	14775	31342	2.37%	0.264%
9	14.874	1965	1972	1979	rBV	408232	635982	48.14%	5.356%
10	14.939	1979	1983	1988	rVB2	13528	21442	1.62%	0.181%
11	15.268	2028	2039	2046	rVB4	12510	29963	2.27%	0.252%
12	15.914	2143	2149	2156	rBV2	18801	30770	2.33%	0.259%
13	16.214	2194	2200	2204	rVB2	12803	21640	1.64%	0.182%
14	16.355	2218	2224	2233	rVB	442830	683327	51.73%	5.755%
15	16.578	2258	2262	2269	rVB8	10622	22454	1.70%	0.189%
16	16.884	2310	2314	2317	rBV2	14975	23901	1.81%	0.201%
17	17.060	2340	2344	2350	rVB7	8068	15546	1.18%	0.131%
18	17.142	2350	2358	2360	rBV8	9756	23064	1.75%	0.194%
19	17.266	2375	2379	2386	rVB4	10730	20768	1.57%	0.175%
20	17.336	2388	2391	2396	rVV6	12121	16864	1.28%	0.142%
21	17.436	2404	2408	2414	rVB	12680	20420	1.55%	0.172%
22	17.618	2432	2439	2443	rBV	480416	770426	58.32%	6.489%
23	17.659	2443	2446	2453	rVV	199741	274816	20.80%	2.315%
24	17.747	2457	2461	2465	rVV	42337	64875	4.91%	0.546%
25	17.783	2465	2467	2475	rVB7	12027	28504	2.16%	0.240%
26	18.012	2502	2506	2514	rBV3	12804	30470	2.31%	0.257%
27	18.129	2522	2526	2530	rBV	14852	20214	1.53%	0.170%
28	18.200	2534	2538	2543	rVB2	19043	28895	2.19%	0.243%
29	18.335	2559	2561	2570	rVB5	13070	22886	1.73%	0.193%
30	18.406	2570	2573	2576	rBV5	8909	14901	1.13%	0.126%
31	18.476	2580	2585	2591	rVV2	130526	259831	19.67%	2.188%
32	18.535	2591	2595	2601	rVB	75578	114834	8.69%	0.967%
33	18.611	2605	2608	2614	rVB	22641	31382	2.38%	0.264%
34	18.682	2614	2620	2624	rBV2	84578	182629	13.82%	1.538%
35	18.717	2624	2626	2630	rVB	46027	55167	4.18%	0.465%
36	18.975	2666	2670	2674	rBV	42831	63456	4.80%	0.534%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111722\
Data File : BG055681.D
Acq On : 18 Nov 2022 1:29
Operator : CG/JU
Sample : N5660-01 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CL-02-11622

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-BG111622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	19.022	2674	2678	2687	rVB3	32083	62987	4.77%	0.530%
38	19.269	2717	2720	2724	rBV	24091	32565	2.47%	0.274%
39	19.393	2736	2741	2745	rBV	65109	109337	8.28%	0.921%
40	19.534	2760	2765	2770	rBV2	54172	116024	8.78%	0.977%
41	19.657	2780	2786	2791	rVB	586776	817830	61.91%	6.888%
42	19.739	2797	2800	2805	rVB4	49288	74510	5.64%	0.628%
43	19.986	2838	2842	2843	rBV2	67548	87845	6.65%	0.740%
44	20.015	2843	2847	2855	rVB	624148	899759	68.11%	7.578%
45	20.086	2855	2859	2864	rVB2	41943	67110	5.08%	0.565%
46	20.203	2874	2879	2884	rVB	714905	920789	69.70%	7.755%
47	21.520	3100	3103	3108	rVB	104798	137929	10.44%	1.162%
48	21.913	3162	3170	3175	rBV3	517853	1321050	100.00%	11.126%
49	21.966	3176	3179	3187	rVB	247927	401503	30.39%	3.382%

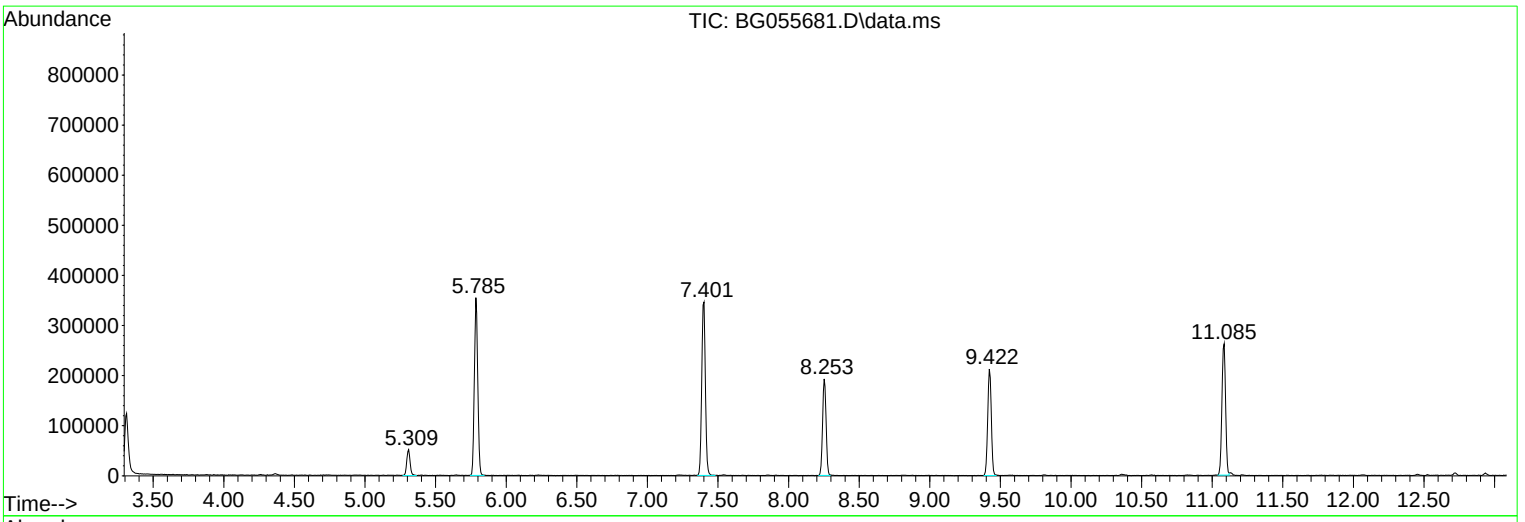
Sum of corrected areas: 11873302

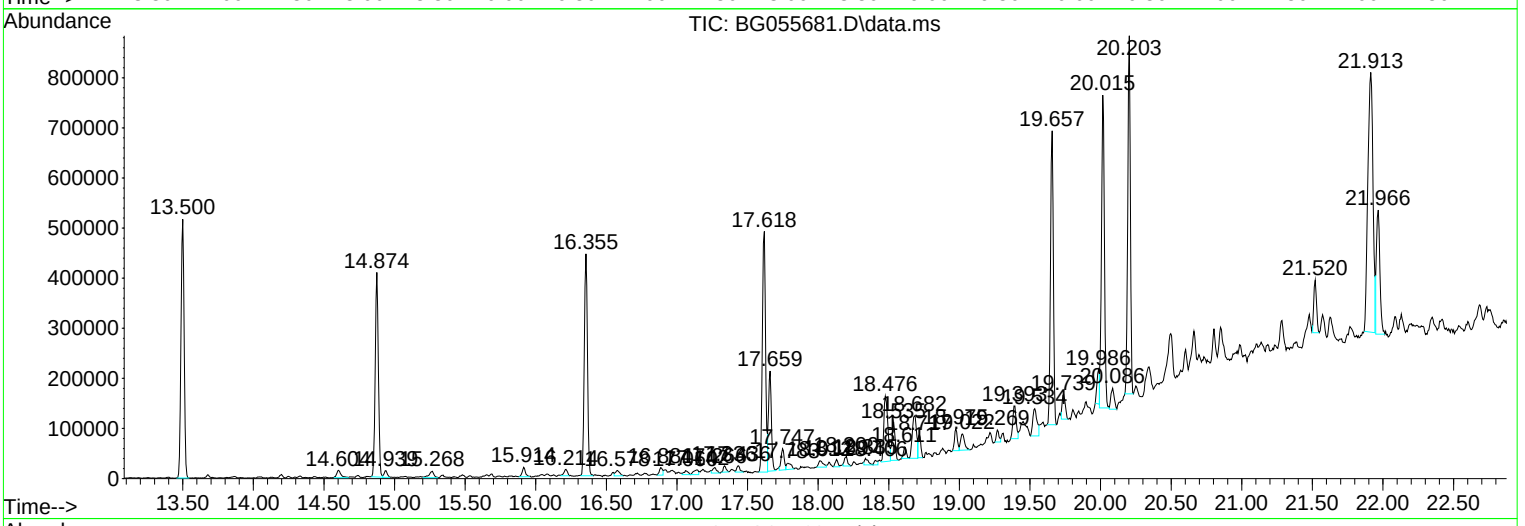
Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111722\
Data File : BG055681.D
Acq On : 18 Nov 2022 1:29
Operator : CG/JU
Sample : N5660-01 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

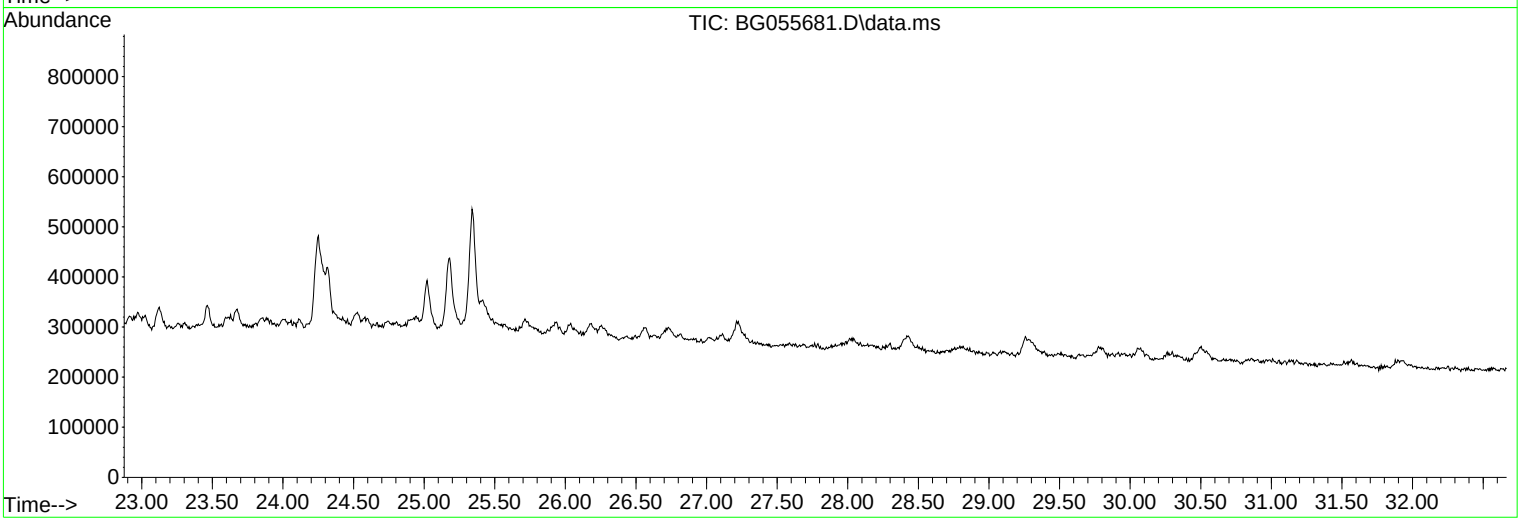
Instrument :
BNA_G
ClientSampleId :
CL-02-11622

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.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\BG111722\
Data File : BG055681.D
Acq On : 18 Nov 2022 1:29
Operator : CG/JU
Sample : N5660-01 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CL-02-11622

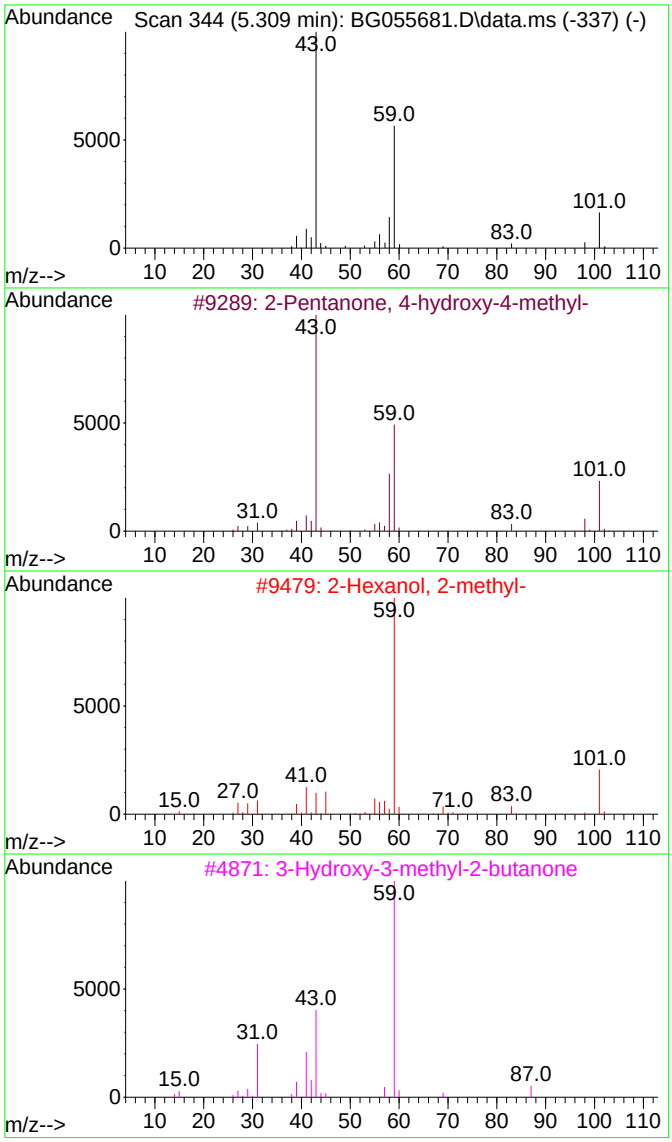
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

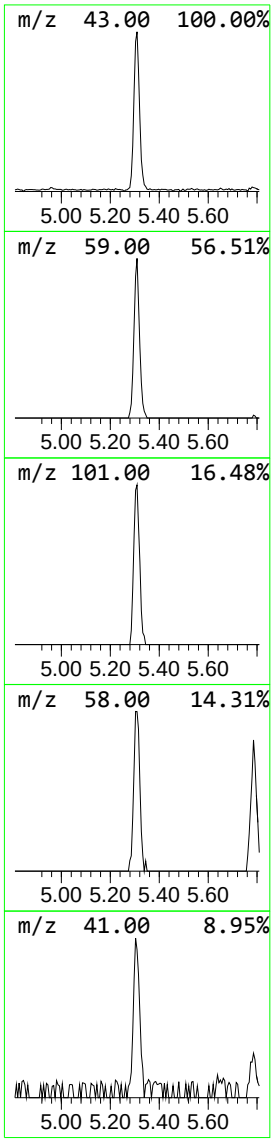
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.309	5.14 ng	84918	1,4-Dichlorobenzene-d4	8.253

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
3	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	23
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111722\
Data File : BG055681.D
Acq On : 18 Nov 2022 1:29
Operator : CG/JU
Sample : N5660-01 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CL-02-11622

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

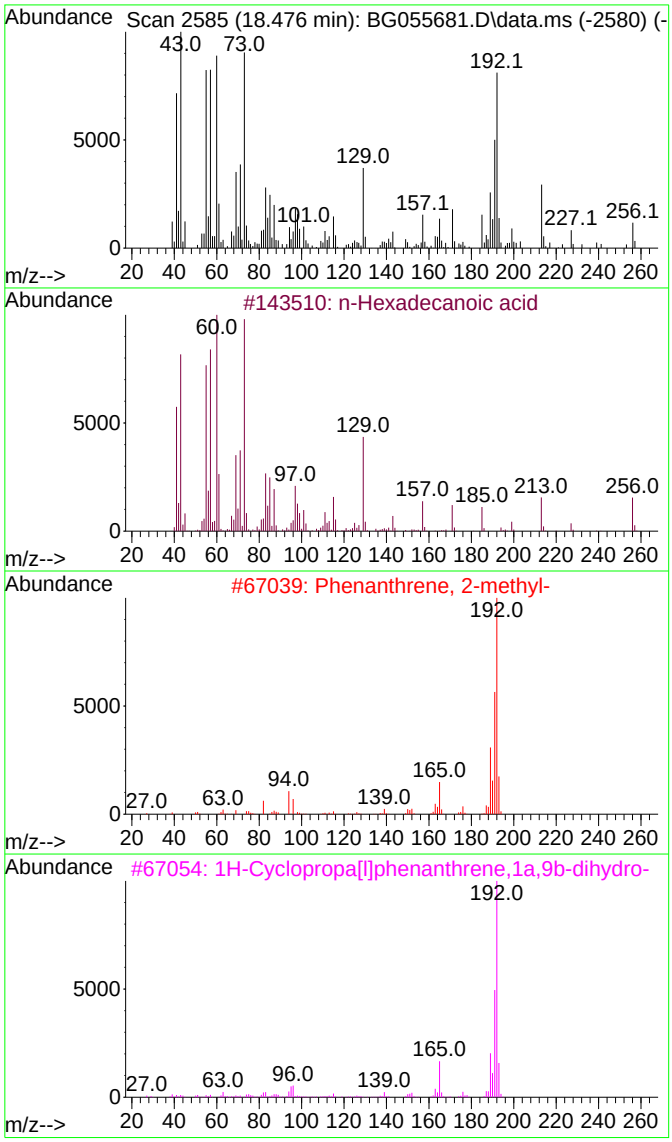
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

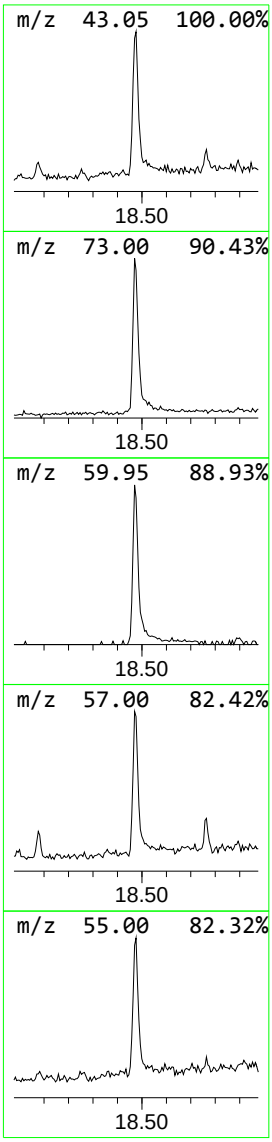
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.476	6.75 ng	259831	Phenanthrene-d10	17.618

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	68
3	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	64
4	Tridecanoic acid	214	C13H26O2	000638-53-9	64
5	Anthracene, 1-methyl-	192	C15H12	000610-48-0	62





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111722\
Data File : BG055681.D
Acq On : 18 Nov 2022 1:29
Operator : CG/JU
Sample : N5660-01 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CL-02-11622

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

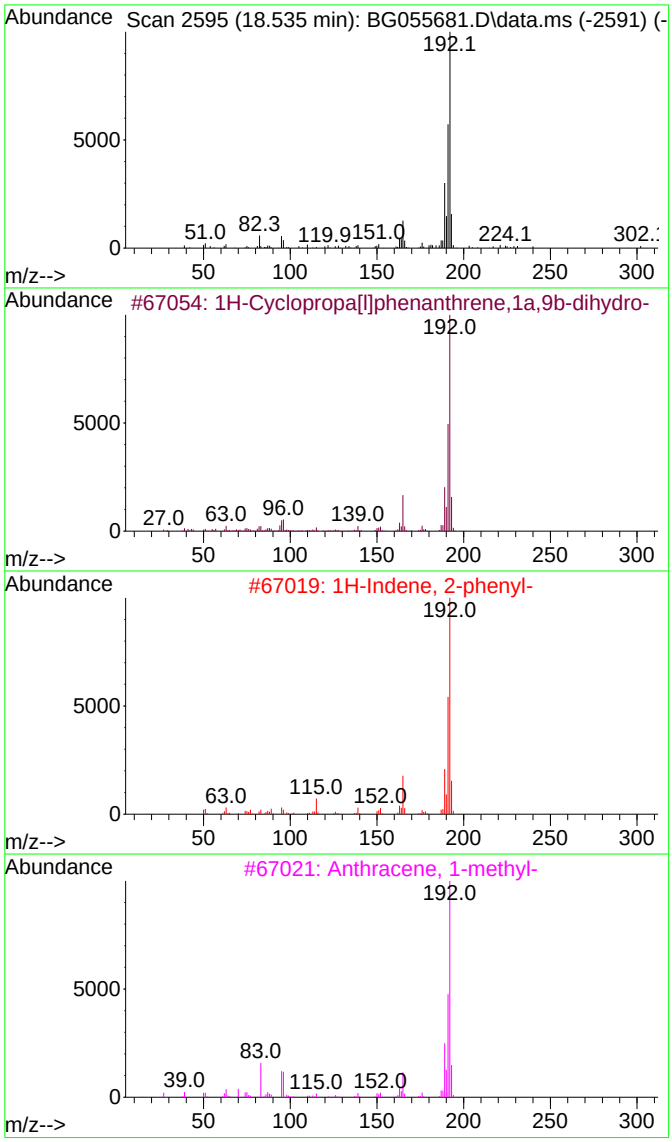
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

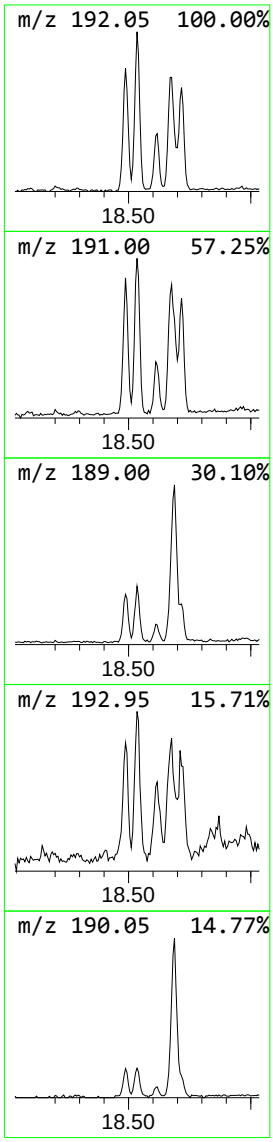
****

Peak Number 3 1H-Cyclopropa[l]phenanthren... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.535	2.98 ng	114834	Phenanthrene-d10	17.618

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	93
2	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	93
3	Anthracene, 1-methyl-	192	C15H12	000610-48-0	93
4	Naphtho[2,3-b]norbornadiene	192	C15H12	107426-38-0	91
5	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111722\
Data File : BG055681.D
Acq On : 18 Nov 2022 1:29
Operator : CG/JU
Sample : N5660-01 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CL-02-11622

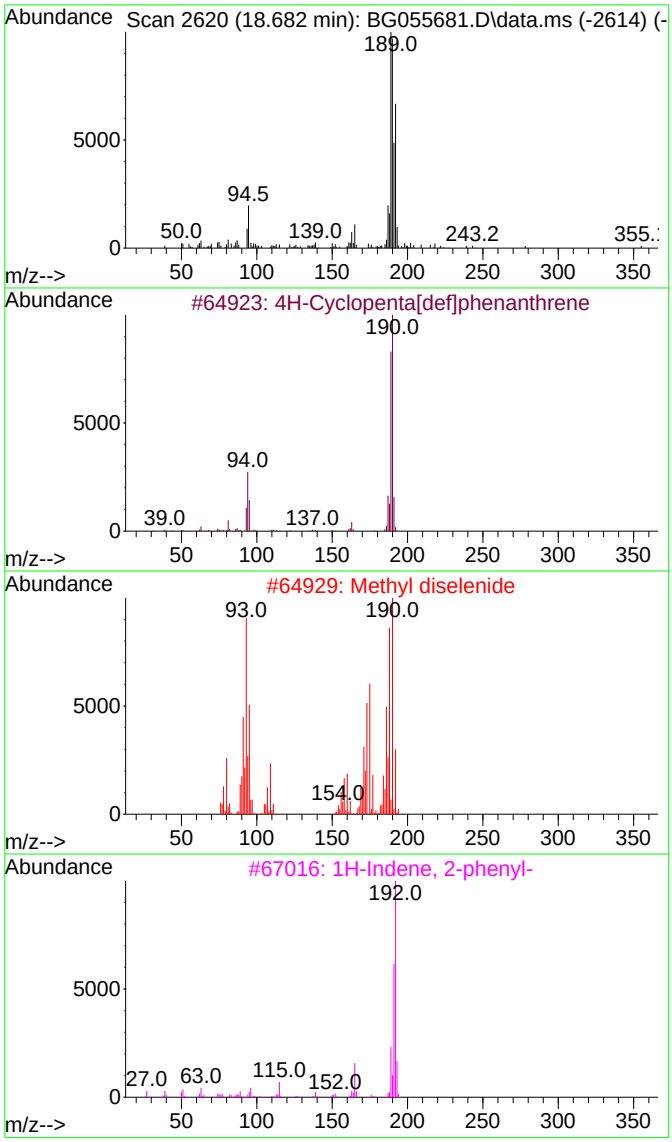
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

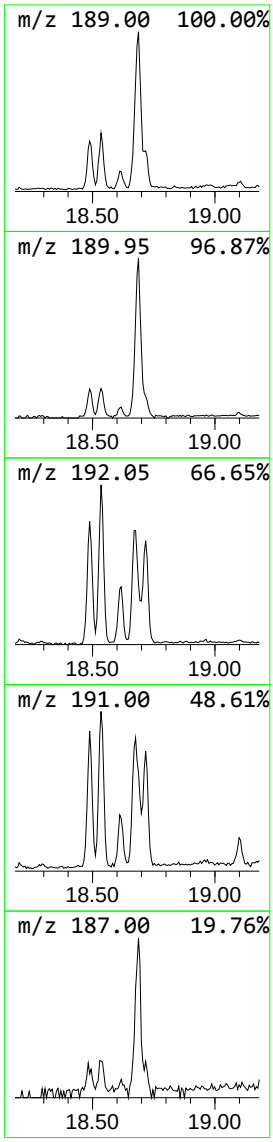
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 4H-Cyclopenta[def]phenanthrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.682	4.74 ng	182629	Phenanthrene-d10	17.618

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	70
2	Methyl diselenide	190	C2H6Se2	007101-31-7	45
3	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	38
4	5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	38
5	Anthracene, 9-methyl-	192	C15H12	000779-02-2	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111722\
Data File : BG055681.D
Acq On : 18 Nov 2022 1:29
Operator : CG/JU
Sample : N5660-01 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CL-02-11622

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

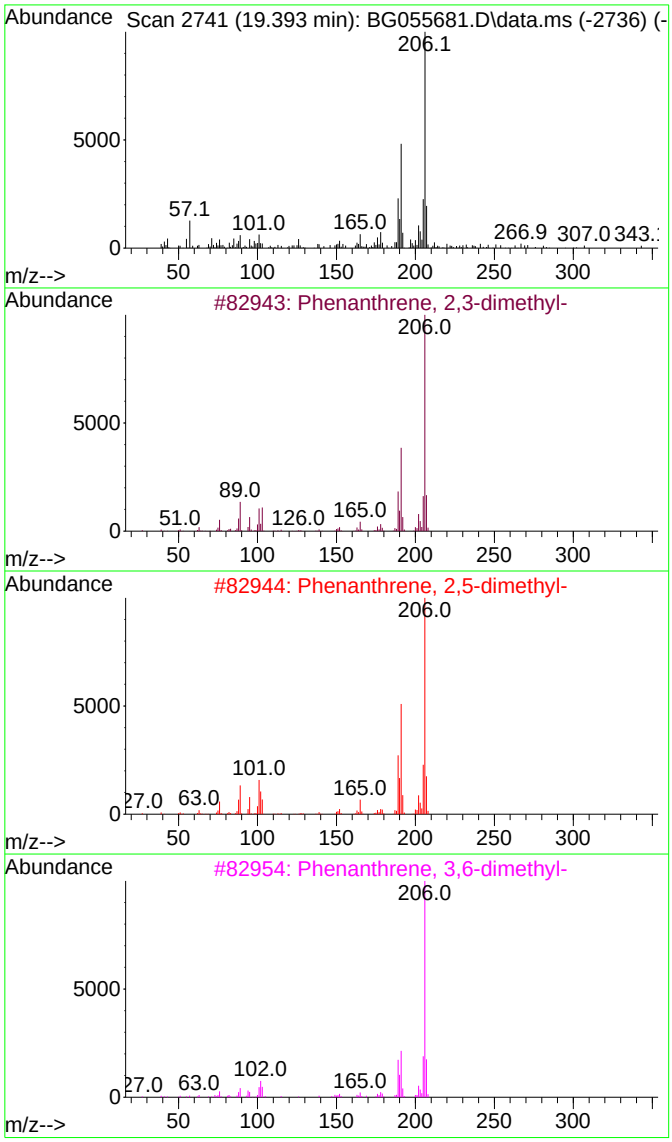
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

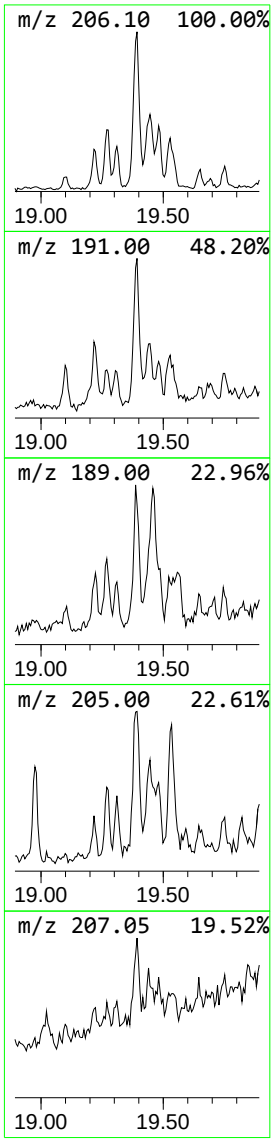
****

Peak Number 5 Phenanthrene, 2,3-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.393	2.84 ng	109337	Phenanthrene-d10	17.618

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2,3-dimethyl-	206	C16H14	003674-65-5	93
2	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	93
3	Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	91
4	Anthracene, 1,4-dimethyl-	206	C16H14	000781-92-0	91
5	Phenanthrene, 1,7-dimethyl-	206	C16H14	000483-87-4	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111722\
Data File : BG055681.D
Acq On : 18 Nov 2022 1:29
Operator : CG/JU
Sample : N5660-01 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CL-02-11622

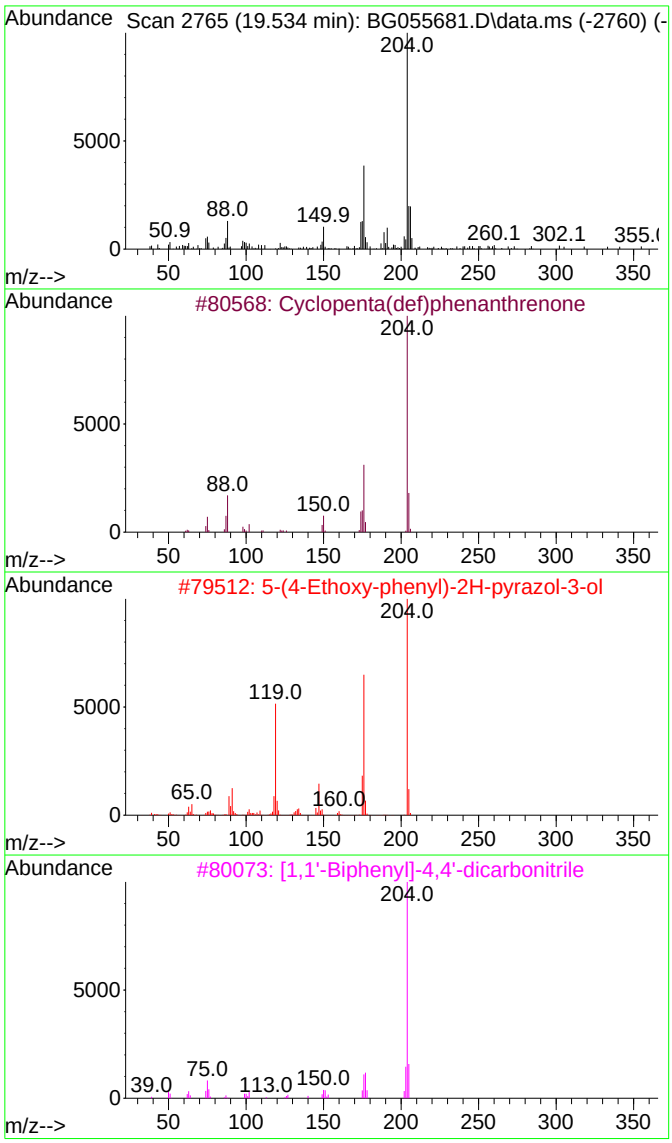
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

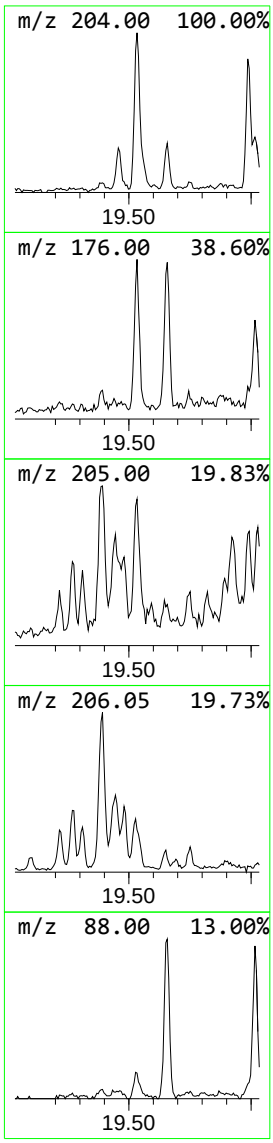
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Cyclopenta(def)phenanthrenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.534	3.01 ng	116024	Phenanthrene-d10	17.618

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopenta(def)phenanthrenone	204	C15H8O	005737-13-3	70
2	5-(4-Ethoxy-phenyl)-2H-pyrazol-3-ol	204	C11H12N2O2	1000278-26-8	50
3	[1,1'-Biphenyl]-4,4'-dicarbonitrile	204	C14H8N2	001591-30-6	47
4	5H-Dibenzo[a,d]cycloheptene, 5-m...	204	C16H12	002975-79-3	43
5	Quinoline, 8-methoxy-5-nitro-	204	C10H8N2O3	1000298-88-7	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111722\
Data File : BG055681.D
Acq On : 18 Nov 2022 1:29
Operator : CG/JU
Sample : N5660-01 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CL-02-11622

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

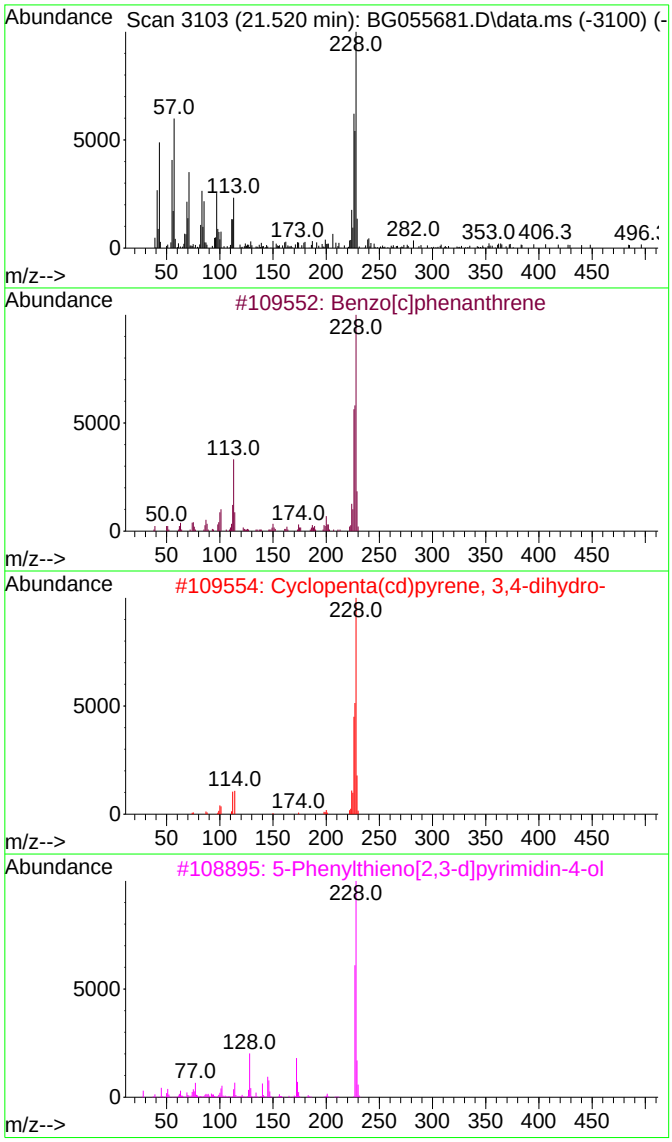
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

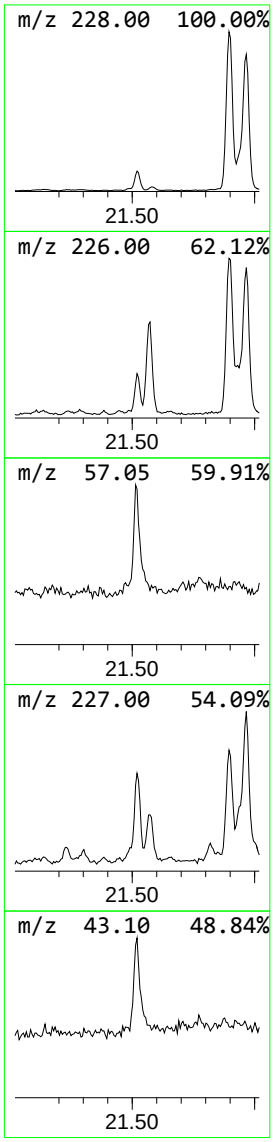
****

Peak Number 7 unknown21.520 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.520	2.09 ng	137929	Chrysene-d12	21.919

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[c]phenanthrene	228	C18H12	000195-19-7	49
2	Cyclopenta(cd)pyrene, 3,4-dihydro-	228	C18H12	025732-74-5	43
3	5-Phenylthieno[2,3-d]pyrimidin-4-ol	228	C12H8N2OS	035978-39-3	43
4	Naphthacene	228	C18H12	000092-24-0	25
5	2,5-Dimethyl-4-(3-nitrophenyl)py...	228	C13H12N2O2	068018-39-3	25





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111722\
Data File : BG055681.D
Acq On : 18 Nov 2022 1:29
Operator : CG/JU
Sample : N5660-01 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CL-02-11622

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.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
2-Pentanone, 4-...	5.309	5.1	ng	84918	1	8.253	330517	20.0
n-Hexadecanoic ...	18.476	6.8	ng	259831	4	17.618	770426	20.0
1H-Cyclopropa[l...	18.535	3.0	ng	114834	4	17.618	770426	20.0
4H-Cyclopenta[d...	18.682	4.7	ng	182629	4	17.618	770426	20.0
Phenanthrene, 2...	19.393	2.8	ng	109337	4	17.618	770426	20.0
Cyclopenta(def)...	19.534	3.0	ng	116024	4	17.618	770426	20.0
unknown21.520	21.520	2.1	ng	137929	5	21.919	1321050	20.0