LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112423\
Data File : BG059878.D
Acq On : 25 Nov 2023 4:29
Operator : MA/JU
Sample : 05420-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
72-12018

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-BG111623.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG059878.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.344	331	333	338	rVB4	9017	16473	1.25%	0.173%
2	5.602	374	377	383	rVB3	10222	17344	1.31%	0.182%
3	5.808	406	412	420	rBV2	402398	631720	47.79%	6.621%
4	6.930	596	603	610	rVB3	80855	139945	10.59%	1.467%
5	7.441	682	690	699	rBV2	397445	675158	51.07%	7.076%
6	7.712	730	736	744	rVB3	32242	59134	4.47%	0.620%
7	8.164	807	813	817	rBV4	8097	16607	1.26%	0.174%
8	8.317	833	839	846	rVB	103963	174877	13.23%	1.833%
9	9.515	1037	1043	1051	rVB2	239180	435232	32.92%	4.562%
10	11.166	1315	1324	1335	rBV	152590	275341	20.83%	2.886%
11	13.569	1726	1733	1742	rVB	657766	1016178	76.87%	10.650%
12	13.769	1761	1767	1772	rBV5	16748	25509	1.93%	0.267%
13	14.233	1842	1846	1849	rBV4	13854	18267	1.38%	0.191%
14	14.557	1895	1901	1905	rBV3	8846	17630	1.33%	0.185%
15	14.862	1949	1953	1958	rBV2	8654	14484	1.10%	0.152%
16	14.950	1960	1968	1975	rVB	237345	381121	28.83%	3.994%
17	15.144	1996	2001	2006	rBV3	12106	21014	1.59%	0.220%
18	16.431	2212	2220	2229	rBV	603023	911471	68.95%	9.553%
19	17.700	2430	2436	2440	rBV	303077	470188	35.57%	4.928%
20	17.741	2440	2443	2448	rVB2	58062	79342	6.00%	0.832%
21	17.835	2455	2459	2462	rVB4	15057	23550	1.78%	0.247%
22	18.105	2499	2505	2507	rBV4	7252	15365	1.16%	0.161%
23	18.287	2530	2536	2538	rBV5	8018	13669	1.03%	0.143%
24	18.511	2570	2574	2579	rBV3	76282	104768	7.92%	1.098%
25	18.564	2580	2583	2586	rVV3	13286	15907	1.20%	0.167%
26	18.599	2586	2589	2596	rVB7	14882	29406	2.22%	0.308%
27	19.110	2671	2676	2681	rBV9	13302	27310	2.07%	0.286%
28	19.163	2681	2685	2689	rVV4	22092	28040	2.12%	0.294%
29	19.357	2713	2718	2725	rBV	304885	352711	26.68%	3.697%
30	19.733	2777	2782	2786	rBV2	100257	138515	10.48%	1.452%
31	19.774	2786	2789	2794	rVB7	29909	37906	2.87%	0.397%
32	19.968	2821	2822	2829	rVB7	15087	29483	2.23%	0.309%
33	20.056	2829	2837	2840	rBV8	36009	74231	5.62%	0.778%
34	20.097	2840	2844	2850	rVB2	75822	108737	8.23%	1.140%
35	20.273	2868	2874	2880	rBV	1032504	1321998	100.00%	13.855%
36	20.485	2906	2910	2911	rBV4	21280	20519	1.55%	0.215%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112423\
Data File : BG059878.D
Acq On : 25 Nov 2023 4:29
Operator : MA/JU
Sample : 05420-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
72-12018

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-BG111623.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	20.978	2991	2994	2996	rVB3	22323	22886	1.73%	0.240%
38	21.014	2996	3000	3004	rBV6	42068	53216	4.03%	0.558%
39	21.155	3019	3024	3025	rBV5	15226	20680	1.56%	0.217%
40	21.255	3038	3041	3044	rVB5	12347	14303	1.08%	0.150%
41	21.554	3088	3092	3098	rBV8	35040	68357	5.17%	0.716%
42	21.719	3116	3120	3121	rBV4	11817	15670	1.19%	0.164%
43	21.825	3133	3138	3142	rBV	268575	364279	27.56%	3.818%
44	22.018	3164	3171	3177	rVV3	230540	472700	35.76%	4.954%
45	22.065	3177	3179	3185	rVB2	34572	57764	4.37%	0.605%
46	22.318	3219	3222	3224	rBV4	12274	16452	1.24%	0.172%
47	22.371	3227	3231	3234	rVB6	26352	38001	2.87%	0.398%
48	23.199	3368	3372	3376	rBV7	12450	17578	1.33%	0.184%
49	24.145	3531	3533	3535	rBV3	14579	16775	1.27%	0.176%
50	24.421	3578	3580	3588	rVB6	33729	70594	5.34%	0.740%
51	25.238	3715	3719	3729	rVB6	20632	60802	4.60%	0.637%
52	25.409	3743	3748	3750	rBV5	21445	30426	2.30%	0.319%
53	25.579	3769	3777	3789	rVB	119228	365233	27.63%	3.828%
54	25.661	3789	3791	3796	rBV5	11780	17872	1.35%	0.187%
55	27.095	4032	4035	4037	rBV4	10406	13707	1.04%	0.144%
56	28.352	4247	4249	4254	rVB6	12273	14104	1.07%	0.148%
57	29.645	4465	4469	4472	rBV6	8314	13679	1.03%	0.143%
58	32.424	4938	4942	4944	rBV5	8599	13623	1.03%	0.143%
59	32.600	4967	4972	4977	rBV9	10567	23546	1.78%	0.247%

Sum of corrected areas: 9541397

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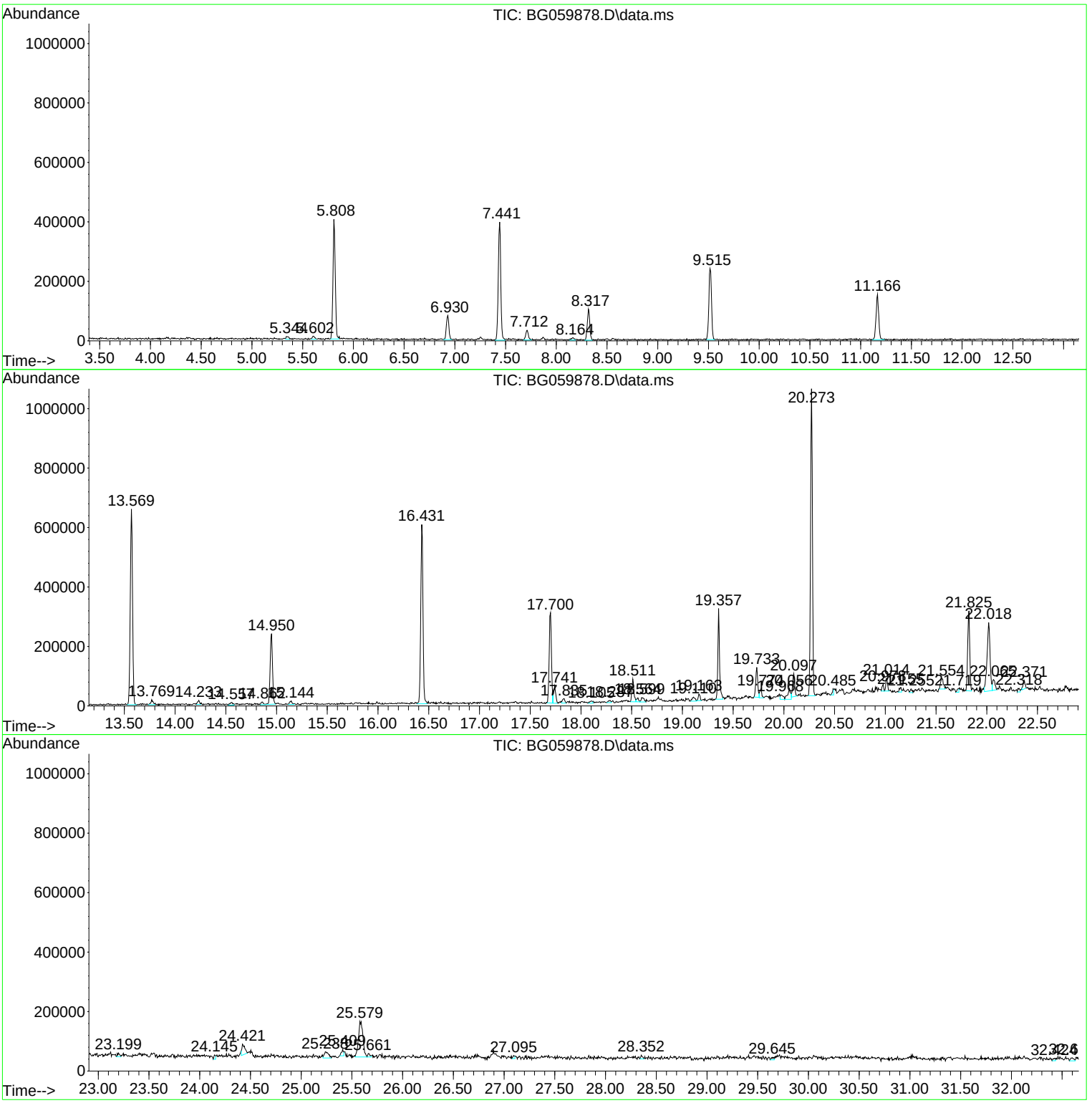
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
72-12018

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.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\BG112423\
Data File : BG059878.D
Acq On : 25 Nov 2023 4:29
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Sample : 05420-01
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

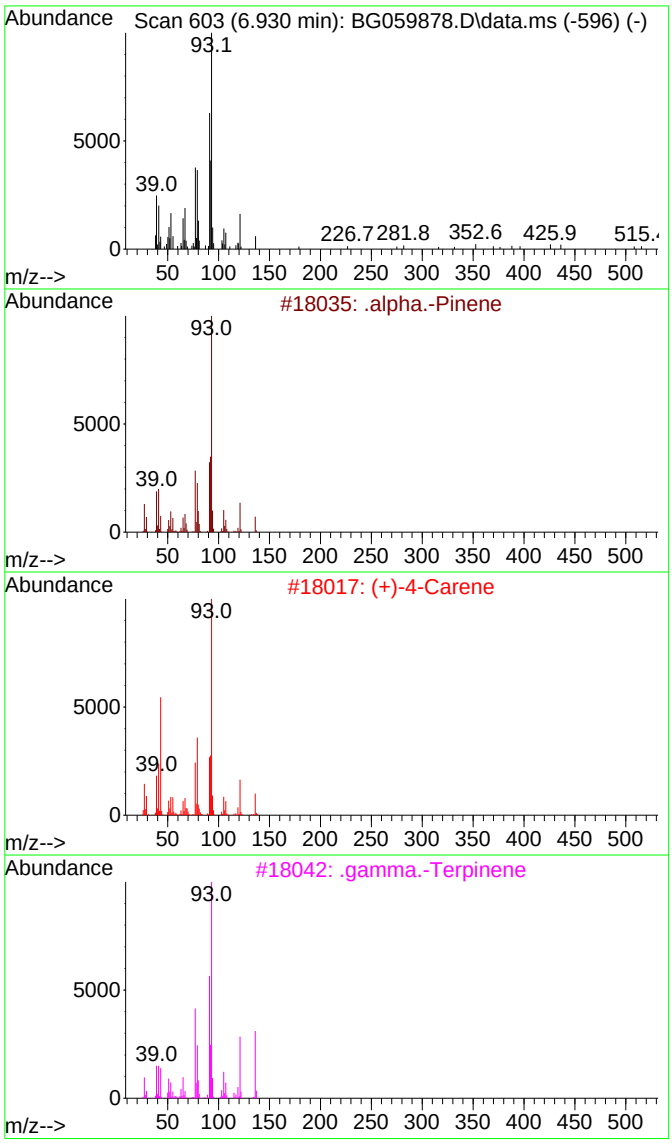
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

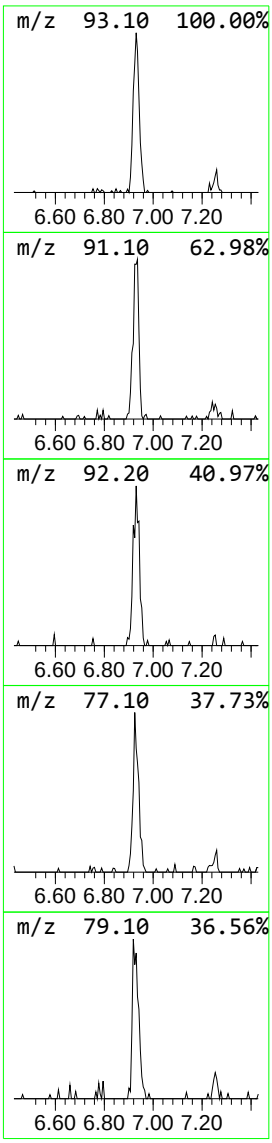
****

Peak Number 1 .alpha.-Pinene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.930	16.00 ng	139945	1,4-Dichlorobenzene-d4	8.317

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.alpha.-Pinene	136	C10H16	000080-56-8	90
2	(+)-4-Carene	136	C10H16	029050-33-7	87
3	.gamma.-Terpinene	136	C10H16	000099-85-4	81
4	(1S)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-26-4	72
5	Bicyclo[3.1.0]hex-2-ene, 2-methy...	136	C10H16	002867-05-2	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112423\
Data File : BG059878.D
Acq On : 25 Nov 2023 4:29
Operator : MA/JU
Sample : 05420-01
Misc :
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Instrument :
BNA_G
ClientSampleId :
72-12018

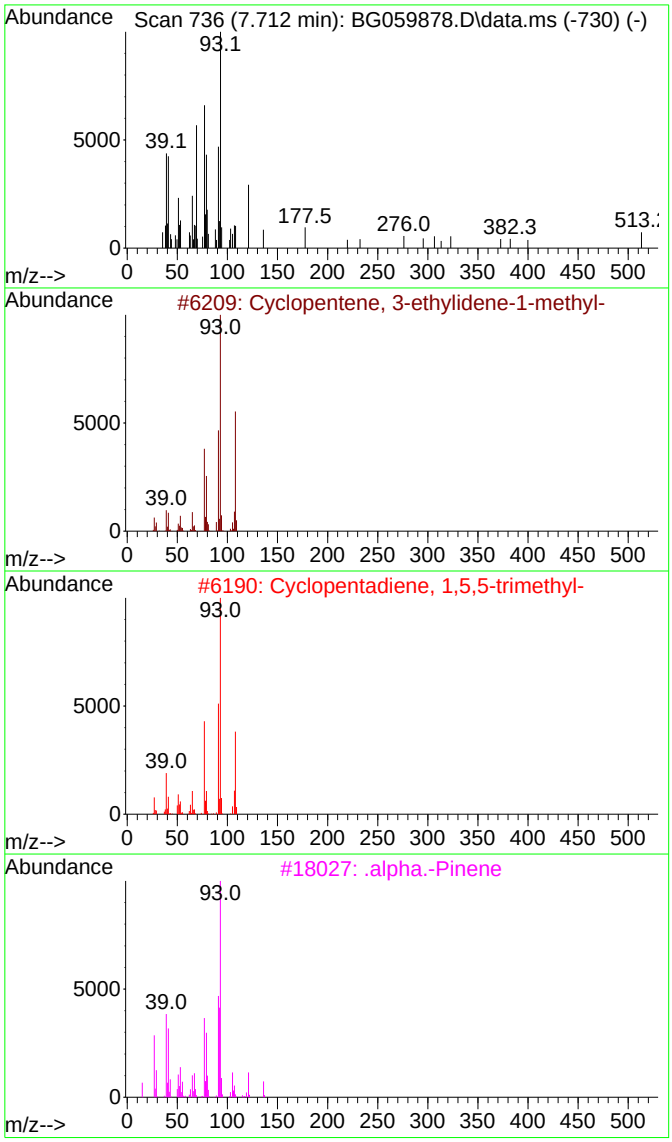
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

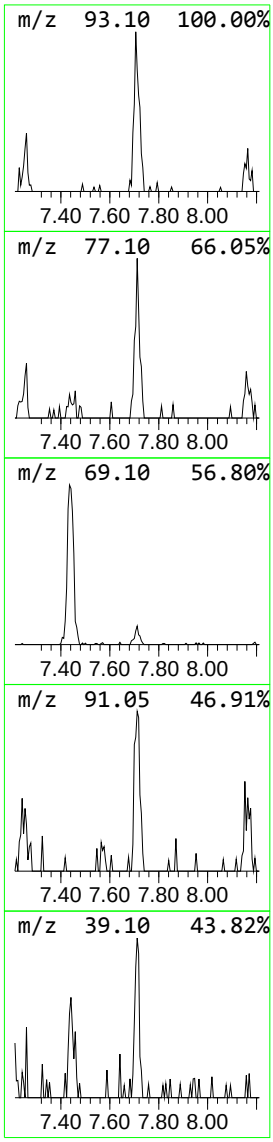
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Cyclopentene, 3-ethylidene-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.712	6.76 ng	59134	1,4-Dichlorobenzene-d4	8.317

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentene, 3-ethylidene-1-met...	108	C8H12	062338-00-5	72
2	Cyclopentadiene, 1,5,5-trimethyl-	108	C8H12	004249-09-6	64
3	.alpha.-Pinene	136	C10H16	000080-56-8	58
4	1,3,6-Octatriene, 3,7-dimethyl-,...	136	C10H16	003338-55-4	58
5	(+)-4-Carene	136	C10H16	029050-33-7	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112423\
Data File : BG059878.D
Acq On : 25 Nov 2023 4:29
Operator : MA/JU
Sample : 05420-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
72-12018

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

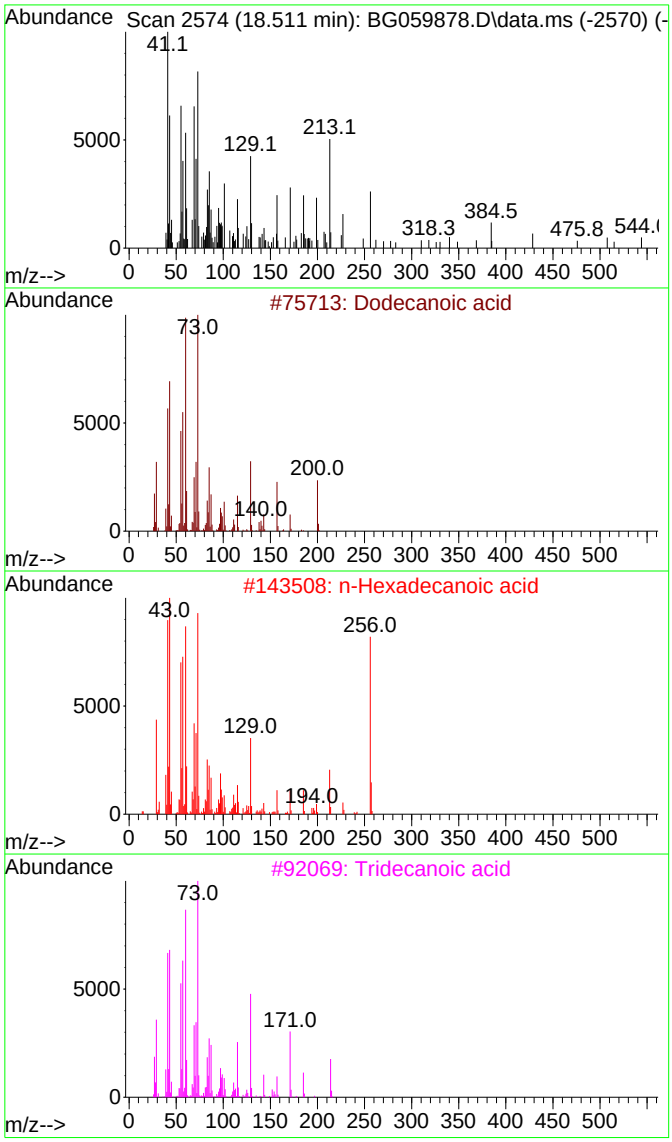
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

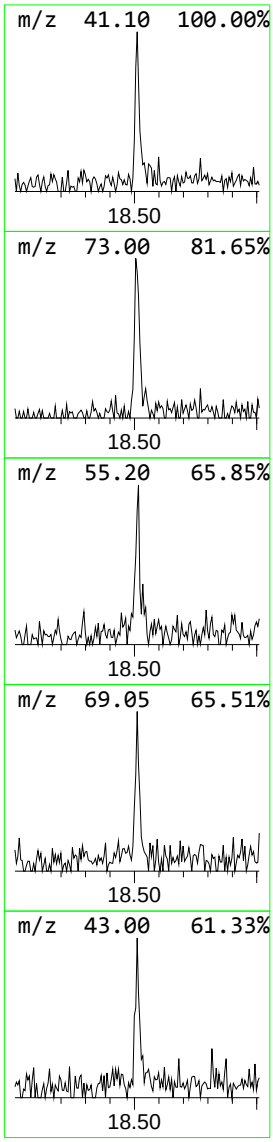
****

Peak Number 3 Dodecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.511	4.46 ng	104768	Phenanthrene-d10	17.694

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	86
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	60
3	Tridecanoic acid	214	C13H26O2	000638-53-9	52
4	Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	38
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112423\
Data File : BG059878.D
Acq On : 25 Nov 2023 4:29
Operator : MA/JU
Sample : 05420-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
72-12018

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

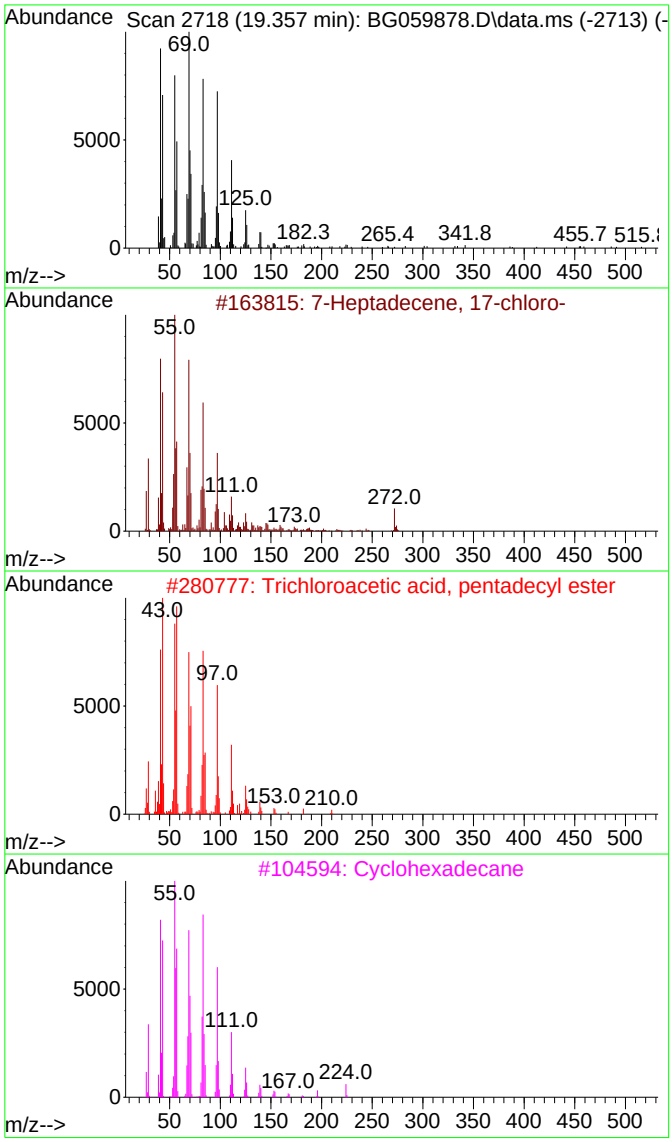
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

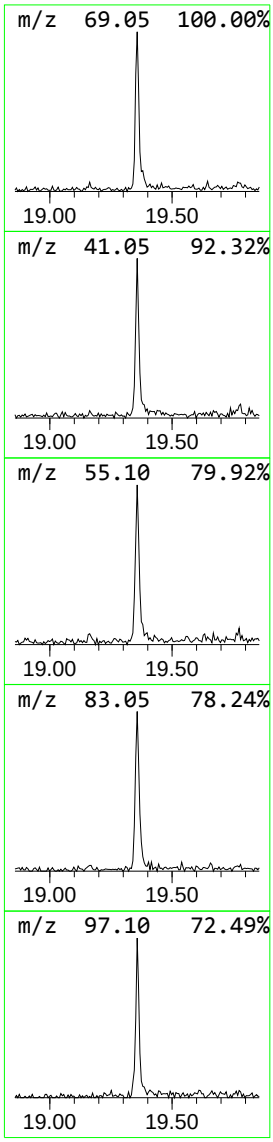
****

Peak Number 4 7-Heptadecene, 17-chloro- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.357	15.00 ng	352711	Phenanthrene-d10	17.694

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Heptadecene, 17-chloro-	272	C17H33Cl	056554-79-1	93
2	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	87
3	Cyclohexadecane	224	C16H32	000295-65-8	83
4	Bacteriochlorophyll-c-stearyl	841	C52H72MgN4O4	1010164-49-7	70
5	1-Nonadecene	266	C19H38	018435-45-5	68





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Instrument :
BNA_G
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

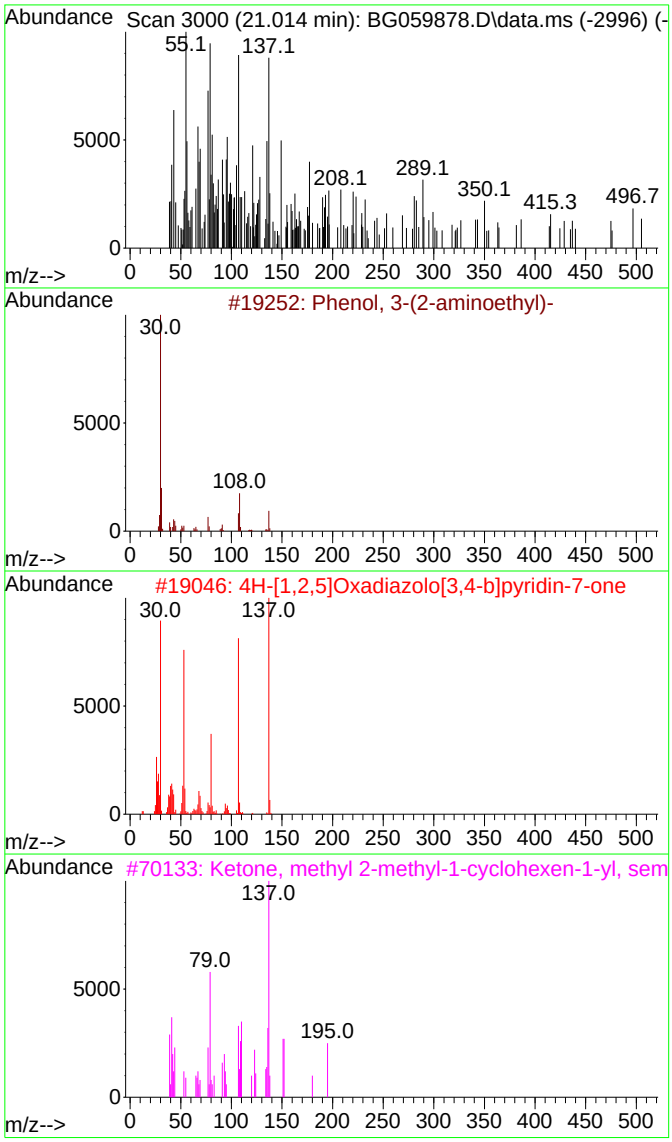
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

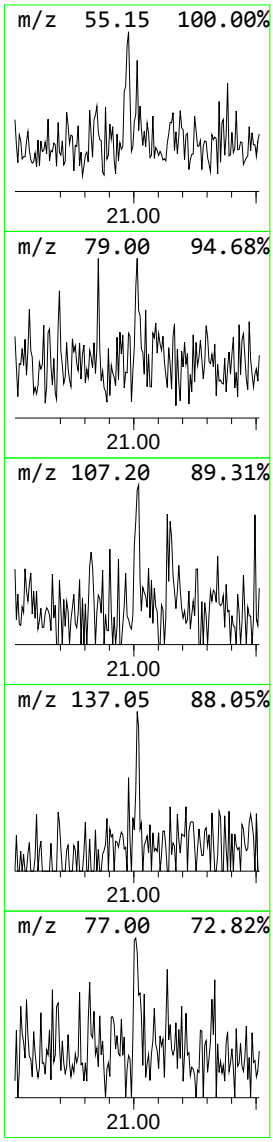
****

Peak Number 5 Phenol, 3-(2-aminoethyl)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.014	2.25 ng	53216	Chrysene-d12	22.018

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 3-(2-aminoethyl)-	137	C8H11NO	000588-05-6	50
2	4H-[1,2,5]Oxadiazolo[3,4-b]pyrid...	137	C5H3N3O2	1000489-26-2	40
3	Ketone, methyl 2-methyl-1-cycloh...	195	C10H17N3O	016983-67-8	32
4	Isolongifolene, 9-hydroxy-	220	C15H24O	1000163-46-6	25
5	3-Cyclopropyl-2-fluoropyridine	137	C8H8FN	1227177-68-5	22





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Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

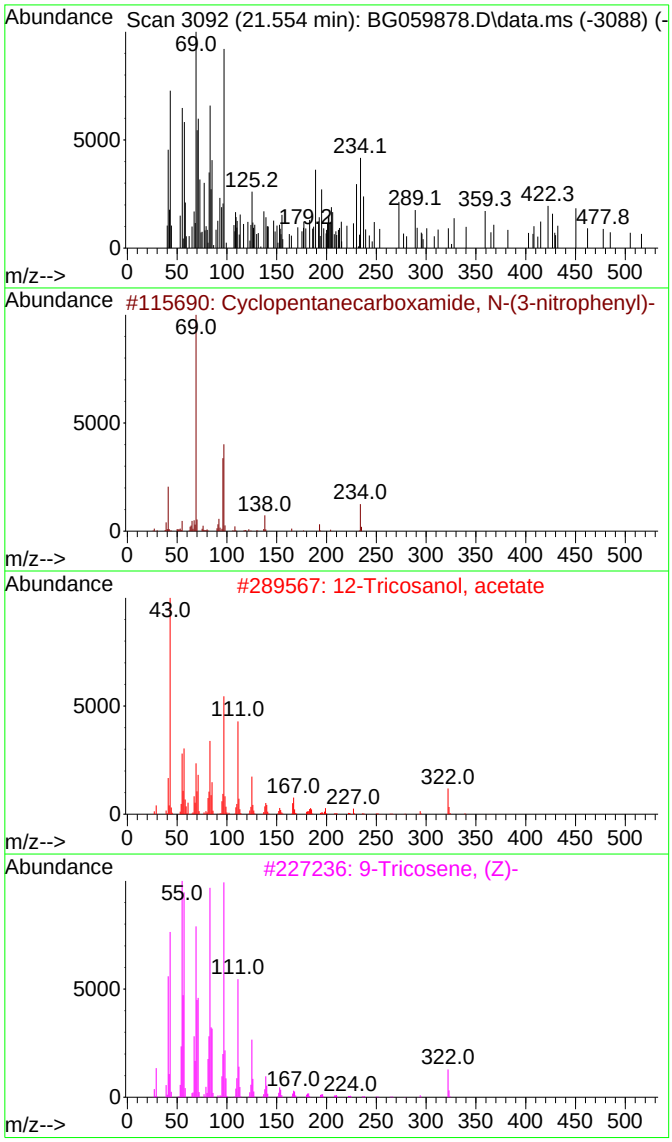
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

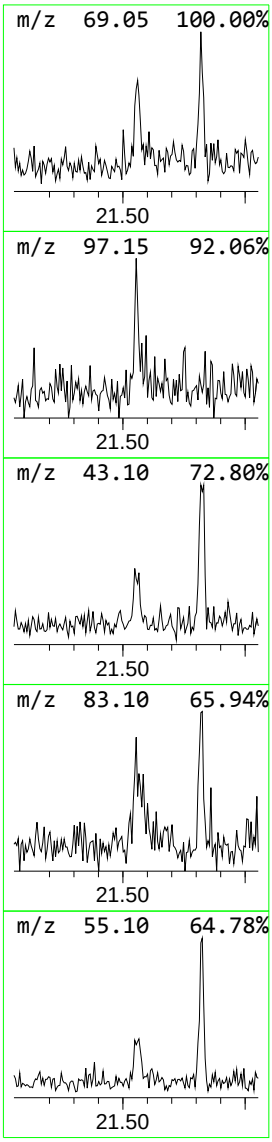
****

Peak Number 6 unknown21.554 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.554	2.89 ng	68357	Chrysene-d12	22.018

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentanecarboxamide, N-(3-ni...	234	C12H14N2O3	1000307-03-0	47
2	12-Tricosanol, acetate	382	C25H50O2	1000506-70-0	16
3	9-Tricosene, (Z)-	322	C23H46	027519-02-4	16
4	Phosphorothioic acid, O-(1,6-dih...	340	C14H17N2O4PS	000119-12-0	12
5	myo-Inositol, hexakis(trifluoroa...	756	C18H6F18O12	1000380-31-6	12





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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

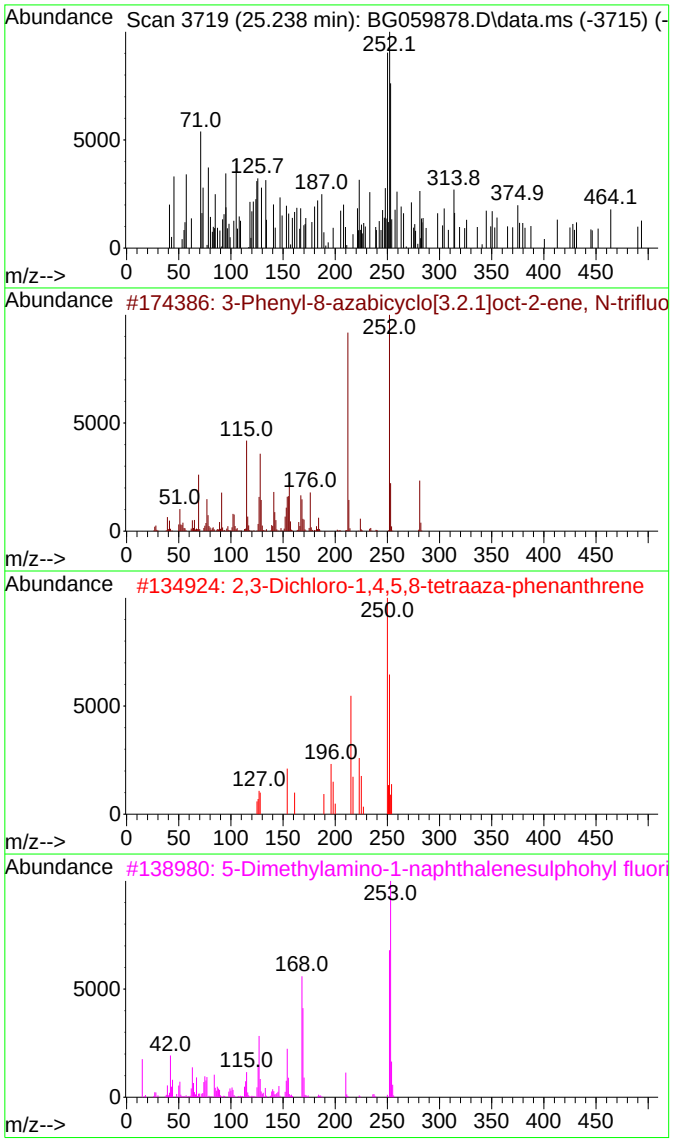
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

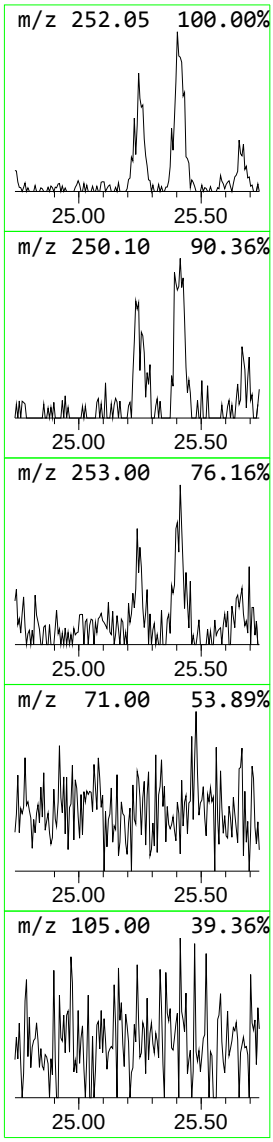
****

Peak Number 7 unknown25.238 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.238	3.33 ng	60802	Perylene-d12	25.591

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Phenyl-8-azabicyclo[3.2.1]oct-...	281	C15H14F3NO	1000507-85-8	35
2	2,3-Dichloro-1,4,5,8-tetraaza-ph...	250	C10H4Cl2N4	071222-45-2	25
3	5-Dimethylamino-1-naphthalenesul...	253	C12H12FNO2S	1000342-78-6	25
4	5-(4-Methoxycinnamoyl)-2-methyl-...	253	C16H15NO2	094298-96-1	18
5	Phenol, 2,4-dibromo-	250	C6H4Br2O	000615-58-7	18





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112423\
Data File : BG059878.D
Acq On : 25 Nov 2023 4:29
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Misc :
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Instrument :
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ClientSampleId :
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
.alpha.-Pinene	6.930	16.0	ng	139945	1	8.317	174877	20.0
Cyclopentene, 3...	7.712	6.8	ng	59134	1	8.317	174877	20.0
Dodecanoic acid	18.511	4.5	ng	104768	4	17.694	470188	20.0
7-Heptadecene, ...	19.357	15.0	ng	352711	4	17.694	470188	20.0
Phenol, 3-(2-am...	21.014	2.3	ng	53216	5	22.018	472700	20.0
unknown21.554	21.554	2.9	ng	68357	5	22.018	472700	20.0
unknown25.238	25.238	3.3	ng	60802	6	25.591	365233	20.0