LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062223\
Data File : BG057823.D
Acq On : 23 Jun 2023 1:08
Operator : CG/JU
Sample : 03308-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SP-RIGHT

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-BG061923.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057823.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.030	323	330	340	rVB	298266	453156	24.93%	3.573%
2	5.489	402	408	418	rBV	462243	719944	39.61%	5.677%
3	6.105	507	513	521	rBV2	11787	18348	1.01%	0.145%
4	7.081	671	679	690	rBV	493023	834836	45.94%	6.583%
5	7.921	815	822	829	rBV	131475	218769	12.04%	1.725%
6	9.078	1012	1019	1028	rBV	279301	483160	26.59%	3.810%
7	10.724	1291	1299	1306	rBV	203534	360220	19.82%	2.840%
8	13.180	1710	1717	1724	rBV	780720	1172637	64.52%	9.247%
9	14.554	1944	1951	1958	rBV2	343076	540627	29.75%	4.263%
10	15.906	2175	2181	2187	rVB	211065	297632	16.38%	2.347%
11	16.041	2197	2204	2216	rBV	670884	1028028	56.57%	8.106%
12	16.470	2272	2277	2284	rVB	48347	69465	3.82%	0.548%
13	16.611	2296	2301	2308	rBV	9941	18637	1.03%	0.147%
14	17.298	2411	2418	2422	rBV	456200	691004	38.02%	5.449%
15	17.339	2422	2425	2430	rVB	106968	142631	7.85%	1.125%
16	17.433	2435	2441	2445	rVB	15203	23404	1.29%	0.185%
17	17.698	2477	2486	2491	rBV3	9852	20661	1.14%	0.163%
18	18.185	2562	2569	2579	rBV2	139406	257024	14.14%	2.027%
19	18.368	2595	2600	2603	rBV2	17929	27092	1.49%	0.214%
20	18.708	2655	2658	2665	rVB3	13343	19637	1.08%	0.155%
21	19.349	2759	2767	2772	rBV	191756	277960	15.29%	2.192%
22	19.460	2782	2786	2794	rBV3	45546	77046	4.24%	0.608%
23	19.707	2819	2828	2837	rBV	155042	273917	15.07%	2.160%
24	19.913	2857	2863	2869	rBV	1393736	1817353	100.00%	14.331%
25	20.712	2997	2999	3003	rVB	24070	24769	1.36%	0.195%
26	21.205	3079	3083	3091	rVB3	144831	251419	13.83%	1.983%
27	21.282	3092	3096	3105	rVB	80847	126326	6.95%	0.996%
28	21.446	3121	3124	3129	rVB	24542	28176	1.55%	0.222%
29	21.546	3134	3141	3146	rVV3	453073	854847	47.04%	6.741%
30	21.593	3146	3149	3161	rVB	77321	122604	6.75%	0.967%
31	21.746	3171	3175	3183	rBV2	53083	80888	4.45%	0.638%
32	22.345	3273	3277	3284	rVB4	55297	87646	4.82%	0.691%
33	23.021	3389	3392	3397	rVB	41024	62310	3.43%	0.491%
34	23.691	3501	3506	3513	rBV	51953	138991	7.65%	1.096%
35	23.808	3523	3526	3532	rVB4	35190	63506	3.49%	0.501%
36	24.543	3646	3651	3660	rVB	36856	80785	4.45%	0.637%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062223\
Data File : BG057823.D
Acq On : 23 Jun 2023 1:08
Operator : CG/JU
Sample : 03308-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SP-RIGHT

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-BG061923.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	24.695	3668	3677	3701	rVB	285596	916134	50.41%	7.224%

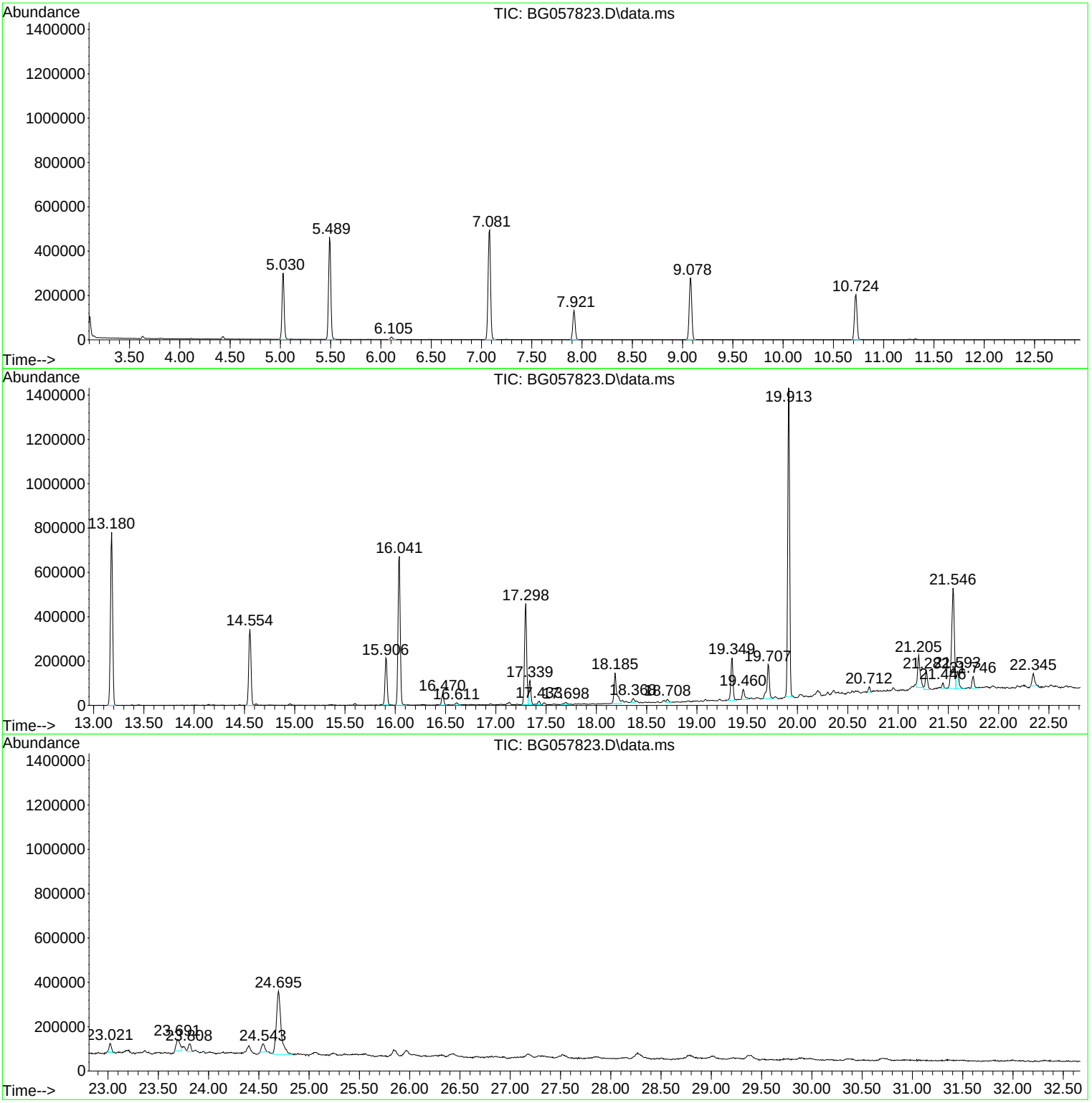
Sum of corrected areas: 12681589

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062223\
Data File : BG057823.D
Acq On : 23 Jun 2023 1:08
Operator : CG/JU
Sample : 03308-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SP-RIGHT

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.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\BG062223\
Data File : BG057823.D
Acq On : 23 Jun 2023 1:08
Operator : CG/JU
Sample : 03308-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SP-RIGHT

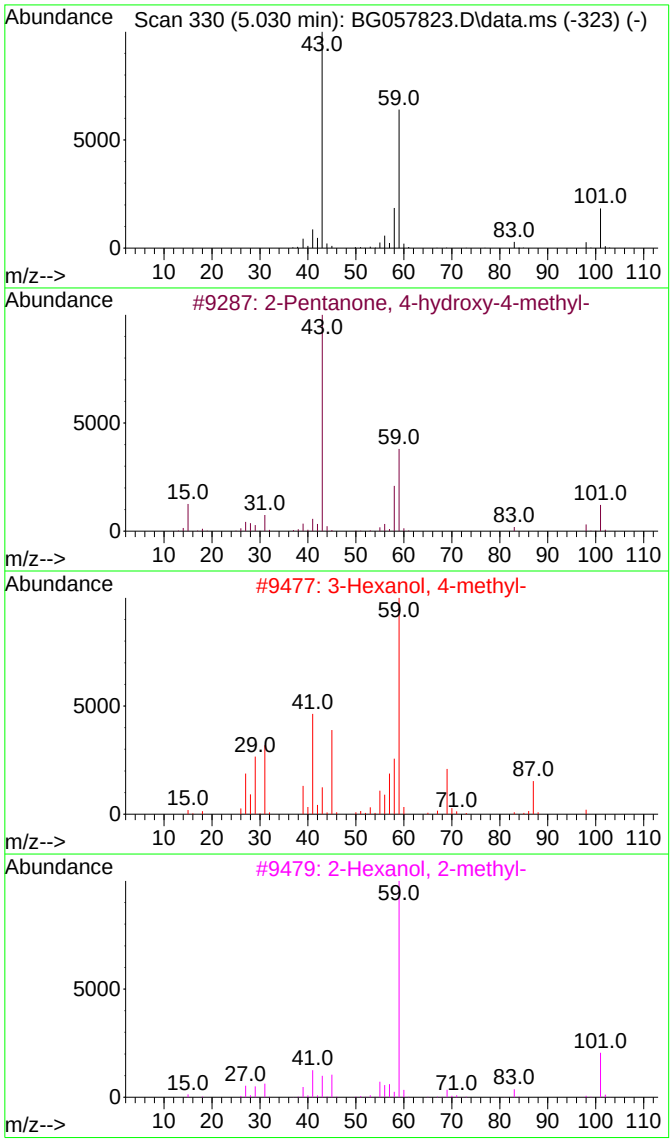
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

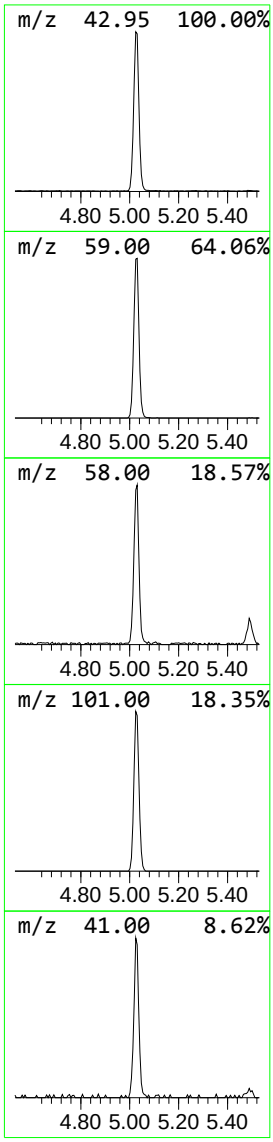
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.030	41.43 ng	453156	1,4-Dichlorobenzene-d4	7.921

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	Acetone	58	C3H6O	000067-64-1	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062223\
Data File : BG057823.D
Acq On : 23 Jun 2023 1:08
Operator : CG/JU
Sample : 03308-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SP-RIGHT

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

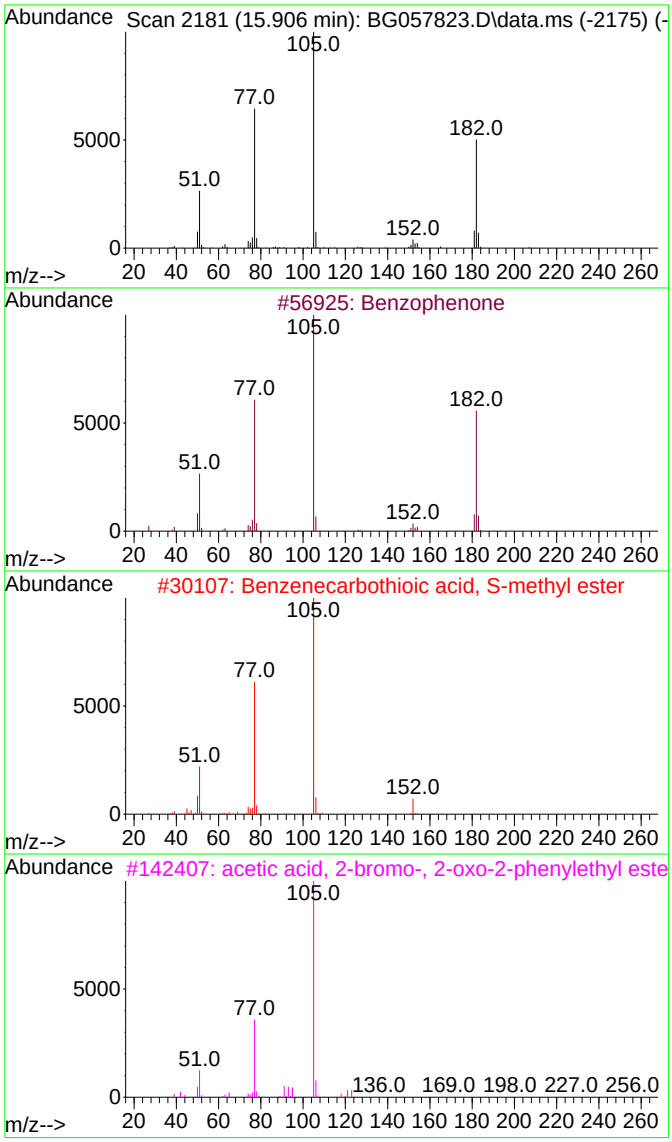
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

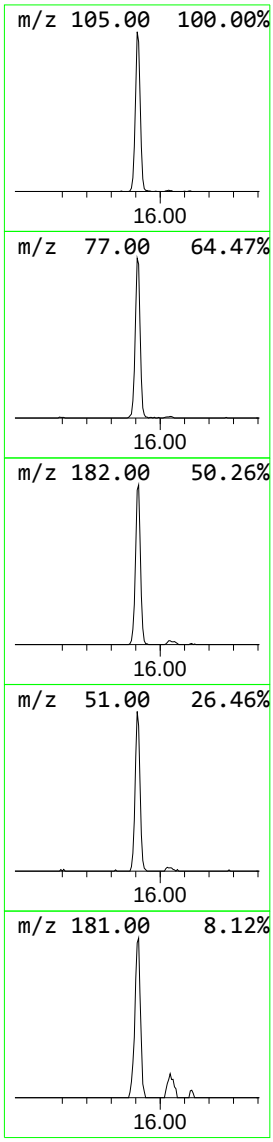
****

Peak Number 2 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.906	11.01 ng	297632	Acenaphthene-d10	14.554

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	52
3	acetic acid, 2-bromo-, 2-oxo-2-p...	256	C10H9BrO3	1000401-50-0	47
4	2-Benzoyl-4-bromo-5-methyl-1,2-o...	281	C11H8BrNO3	1000444-92-3	47
5	1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062223\
Data File : BG057823.D
Acq On : 23 Jun 2023 1:08
Operator : CG/JU
Sample : 03308-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SP-RIGHT

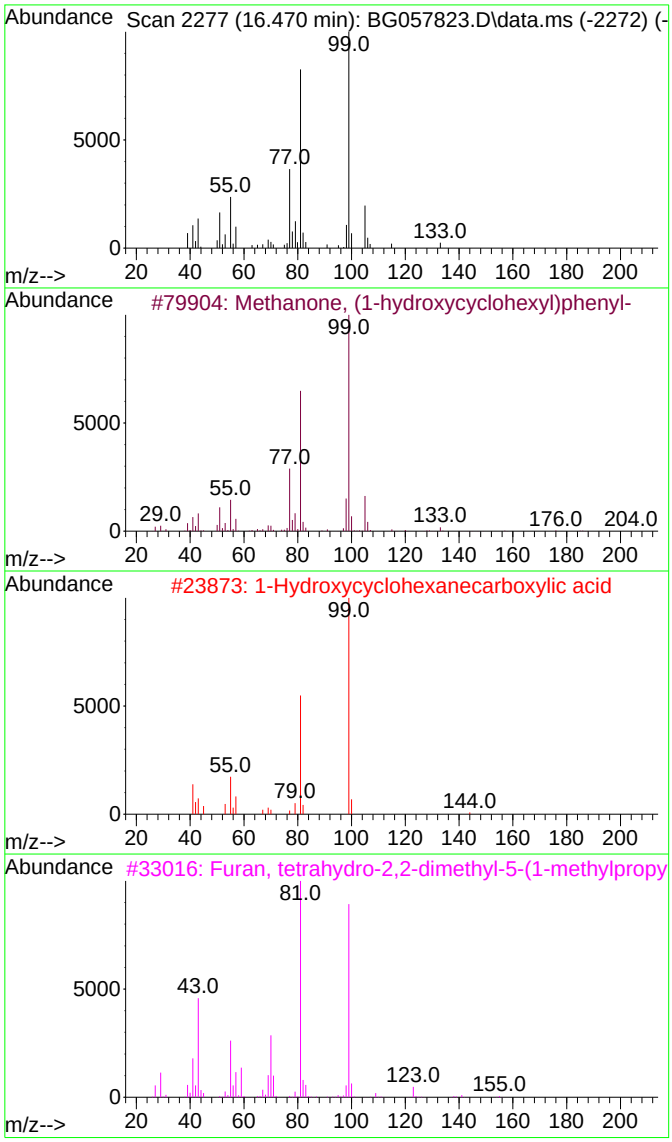
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

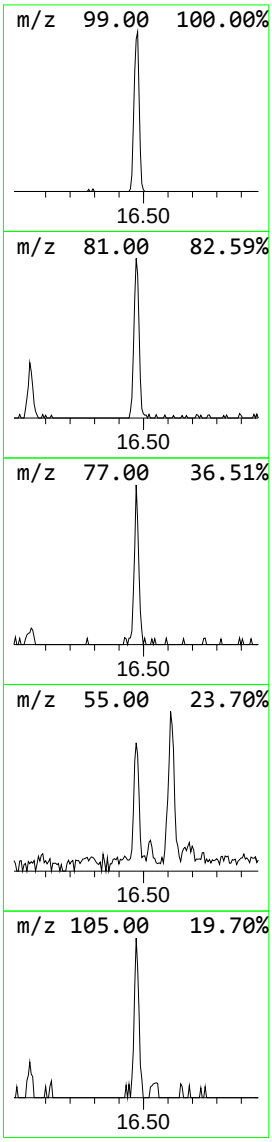
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Methanone, (1-hydroxycycloh... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.470	2.01 ng	69465	Phenanthrene-d10	17.298

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methanone, (1-hydroxycyclohexyl)...	204	C13H16O2	000947-19-3	90
2	1-Hydroxycyclohexanecarboxylic acid	144	C7H12O3	001123-28-0	59
3	Furan, tetrahydro-2,2-dimethyl-5...	156	C10H20O	033978-70-0	53
4	2-Methylcyclosarin	194	C8H16FO2P	085473-32-1	50
5	Cyclohexanol, 1-(aminomethyl)-	129	C7H15NO	004000-72-0	45





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062223\
Data File : BG057823.D
Acq On : 23 Jun 2023 1:08
Operator : CG/JU
Sample : 03308-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SP-RIGHT

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

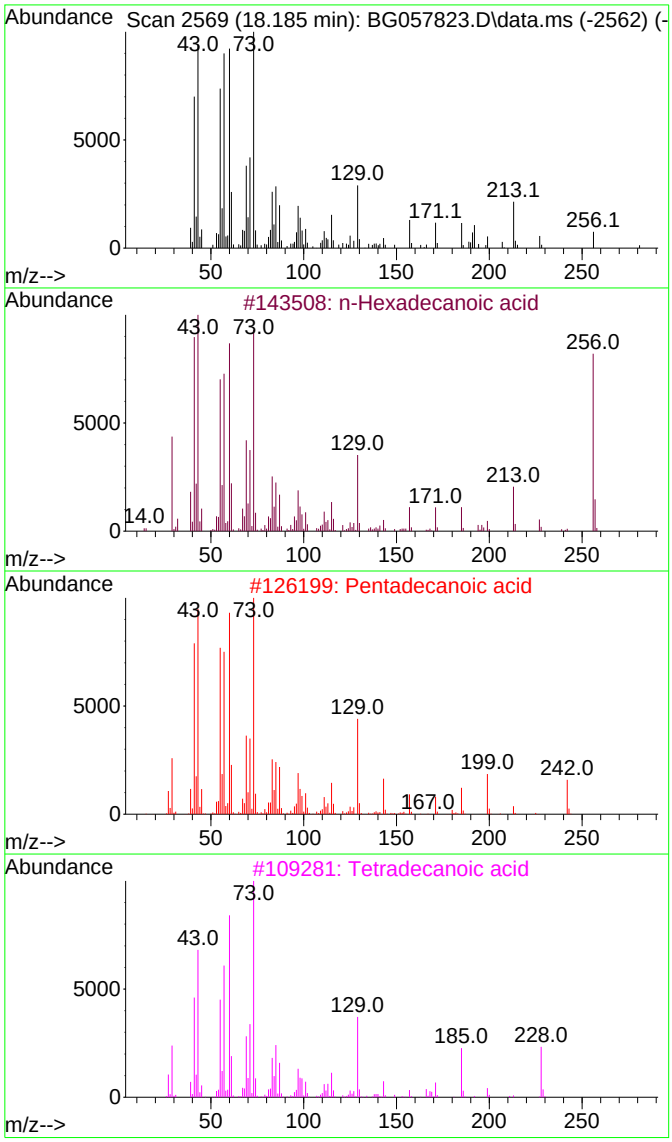
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

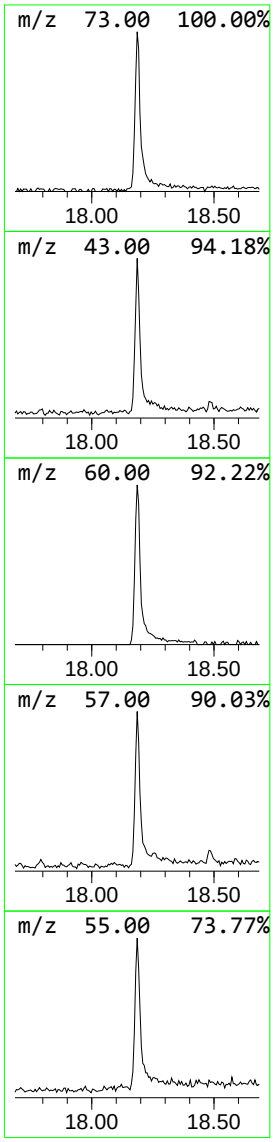
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.185	7.44 ng	257024	Phenanthrene-d10	17.298

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	Tridecanoic acid	214	C13H26O2	000638-53-9	70
5	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	49





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062223\
Data File : BG057823.D
Acq On : 23 Jun 2023 1:08
Operator : CG/JU
Sample : 03308-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SP-RIGHT

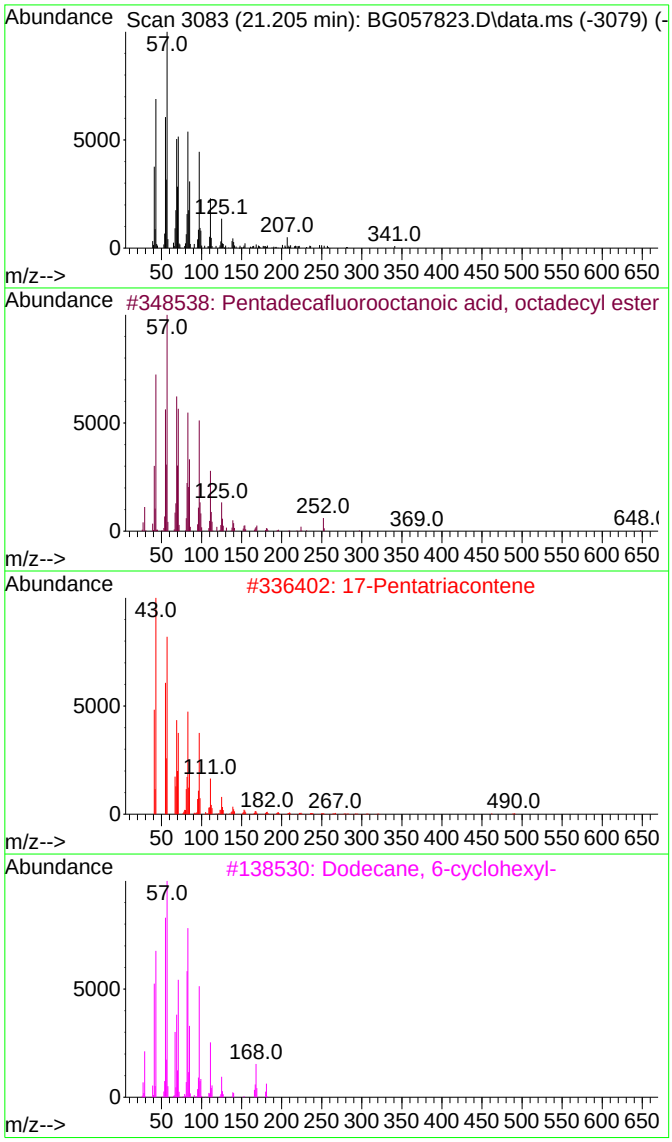
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

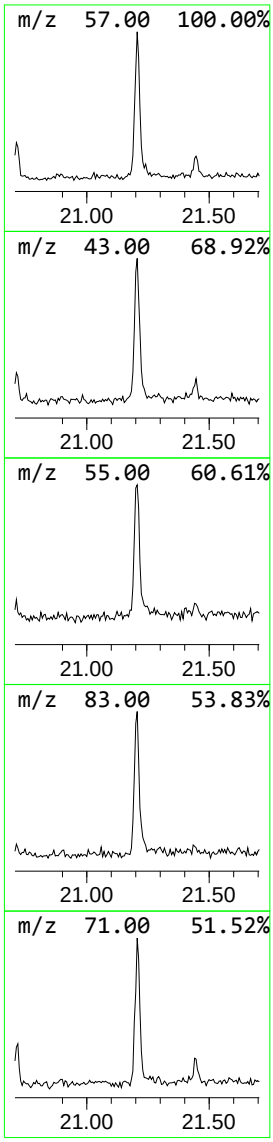
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Pentadecafluorooctanoic aci... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.205	5.88 ng	251419	Chrysene-d12	21.546

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
2	17-Pentatriacontene	491	C35H70	006971-40-0	91
3	Dodecane, 6-cyclohexyl-	252	C18H36	013151-86-5	86
4	Butyl hexadecyl ether	298	C20H42O	1010406-40-5	80
5	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	74





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Data File : BG057823.D
Acq On : 23 Jun 2023 1:08
Operator : CG/JU
Sample : 03308-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SP-RIGHT

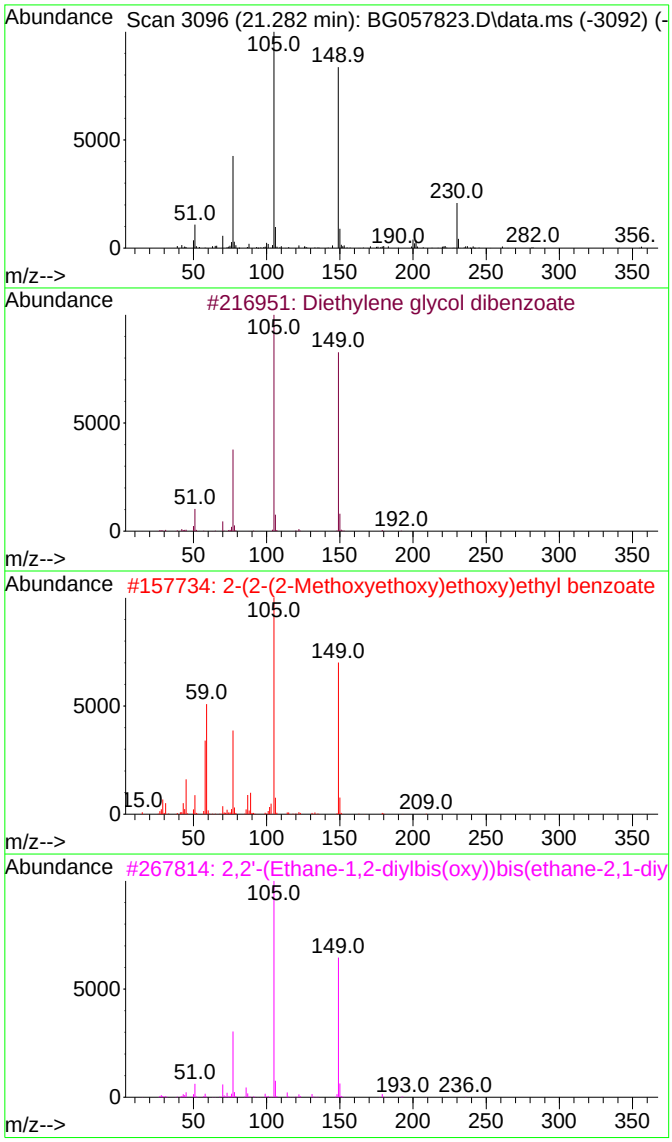
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

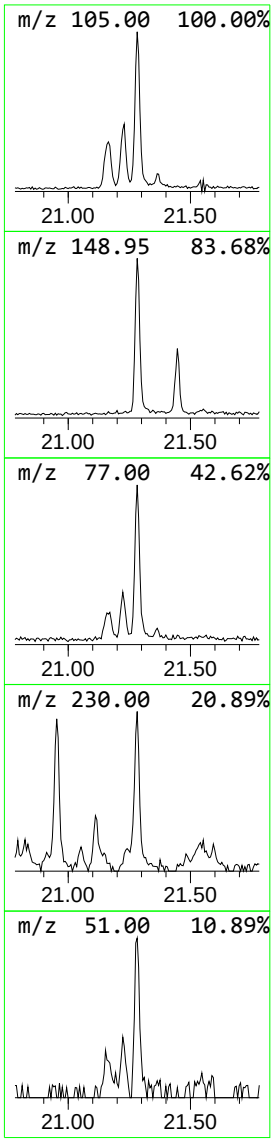
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Diethylene glycol dibenzoate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.282	2.96 ng	126326	Chrysene-d12	21.546

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	72
2	2-(2-(2-Methoxyethoxy)ethoxy)eth...	268	C14H20O5	1000366-99-1	64
3	2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	53
4	Benzamide, N-(5-acetyl-1,2,3-tri...	230	C11H10N4O2	129959-33-7	43
5	Cycloheptanone, 2-(2-oxo-2-pheny...	230	C15H18O2	054669-79-3	43





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Acq On : 23 Jun 2023 1:08
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Sample : 03308-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SP-RIGHT

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

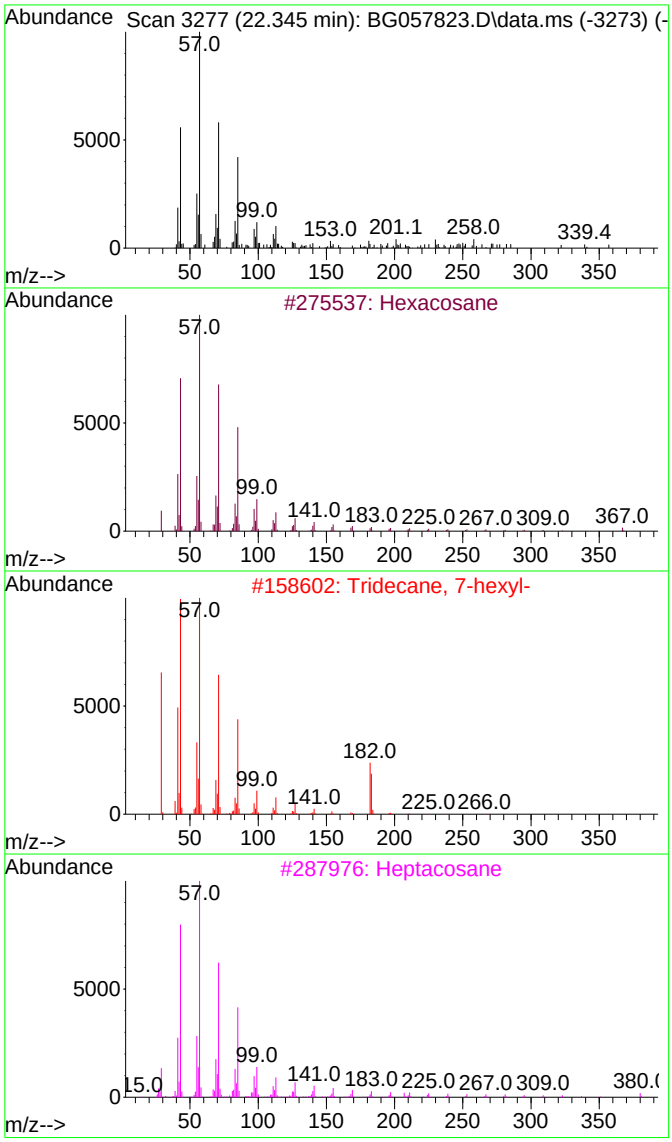
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

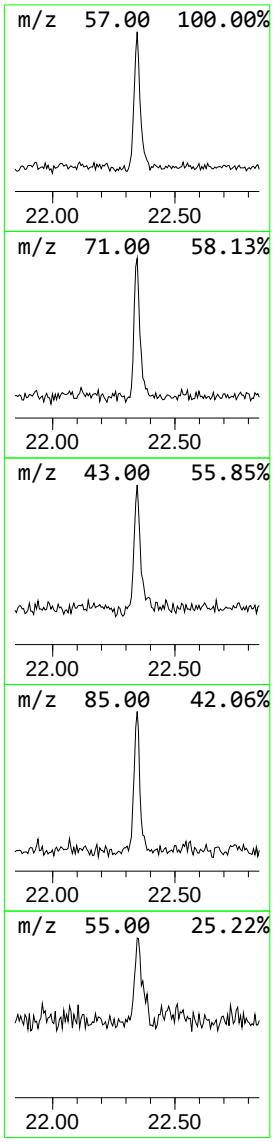
****

Peak Number 7 Hexacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.345	2.05 ng	87646	Chrysene-d12	21.546

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	87
2	Tridecane, 7-hexyl-	268	C19H40	007225-66-3	87
3	Heptacosane	380	C27H56	000593-49-7	83
4	10-Methylnonadecane	282	C20H42	056862-62-5	83
5	Docosane, 7-hexyl-	394	C28H58	055373-86-9	80





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062223\
Data File : BG057823.D
Acq On : 23 Jun 2023 1:08
Operator : CG/JU
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.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-...	5.030	41.4	ng	453156	1	7.921	218769	20.0
Benzophenone	15.906	11.0	ng	297632	3	14.554	540627	20.0
Methanone, (1-h...	16.470	2.0	ng	69465	4	17.298	691004	20.0
n-Hexadecanoic ...	18.185	7.4	ng	257024	4	17.298	691004	20.0
Pentadecafluoro...	21.205	5.9	ng	251419	5	21.546	854847	20.0
Diethylene glyc...	21.282	3.0	ng	126326	5	21.546	854847	20.0
Hexacosane	22.345	2.0	ng	87646	5	21.546	854847	20.0