LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091922\
Data File : BF130331.D
Acq On : 19 Sep 2022 20:57
Operator : CG\JU
Sample : N4613-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2-T-6-(10-18)

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_F\Methods\8270-BF091422.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130331.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.852	465	470	478	rVB	118623	146952	6.86%	0.816%
2	5.281	538	543	546	rBV	2157078	1909330	89.16%	10.597%
3	6.316	714	719	732	rBV	2127809	1913718	89.37%	10.621%
4	6.663	774	778	781	rBV	774302	612163	28.59%	3.397%
5	7.228	869	874	877	rBV	1483654	1241220	57.96%	6.889%
6	7.863	979	982	991	rBV2	25739	47784	2.23%	0.265%
7	7.945	991	996	999	rBV	852802	767384	35.84%	4.259%
8	9.022	1174	1179	1182	rBV	2456453	2141435	100.00%	11.885%
9	9.692	1289	1293	1296	rBV	874428	705061	32.92%	3.913%
10	9.910	1324	1330	1333	rBV3	29693	53239	2.49%	0.295%
11	10.481	1424	1427	1430	rBV	635252	456237	21.31%	2.532%
12	10.745	1469	1472	1475	rBV	43063	48066	2.24%	0.267%
13	10.845	1475	1489	1499	rVB3	127403	488919	22.83%	2.713%
14	11.169	1541	1544	1546	rBV	678307	546055	25.50%	3.031%
15	11.192	1546	1548	1552	rVB	191482	140206	6.55%	0.778%
16	11.245	1552	1557	1559	rBV	50623	51734	2.42%	0.287%
17	11.628	1619	1622	1626	rBV	35864	41100	1.92%	0.228%
18	11.669	1626	1629	1631	rBV	44241	39374	1.84%	0.219%
19	11.716	1631	1637	1640	rBV2	244361	349817	16.34%	1.941%
20	11.780	1645	1648	1650	rVV	72896	77857	3.64%	0.432%
21	11.804	1650	1652	1655	rVB	37870	31975	1.49%	0.177%
22	11.969	1677	1680	1681	rBV	38564	34039	1.59%	0.189%
23	11.998	1681	1685	1690	rVB	100306	122149	5.70%	0.678%
24	12.216	1720	1722	1725	rBV	45428	42891	2.00%	0.238%
25	12.375	1746	1749	1752	rBV	363394	374347	17.48%	2.078%
26	12.427	1752	1758	1766	rVV2	578437	1157899	54.07%	6.426%
27	12.498	1767	1770	1779	rVV4	171751	283835	13.25%	1.575%
28	12.604	1783	1788	1791	rVB	389068	373361	17.44%	2.072%
29	12.757	1810	1814	1817	rVB	1885696	1521071	71.03%	8.442%
30	12.933	1842	1844	1847	rVB	65132	55553	2.59%	0.308%
31	12.998	1853	1855	1858	rVB	44083	38027	1.78%	0.211%
32	13.033	1858	1861	1864	rBV2	59396	65049	3.04%	0.361%
33	13.157	1880	1882	1892	rVB3	39859	74106	3.46%	0.411%
34	13.798	1986	1991	1994	rBV2	780021	863553	40.33%	4.793%
35	13.822	1994	1995	2003	rVB	251215	188205	8.79%	1.045%
36	14.557	2118	2120	2124	rVB2	103950	88429	4.13%	0.491%

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091922\
Data File : BF130331.D
Acq On : 19 Sep 2022 20:57
Operator : CG\JU
Sample : N4613-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2-T-6-(10-18)

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_F\Methods\8270-BF091422.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.798	2158	2161	2164	rBV	183380	234915	10.97%	1.304%
38	15.127	2215	2217	2222	rVB	132870	134316	6.27%	0.745%
39	15.192	2224	2228	2231	rBV	480705	557002	26.01%	3.091%

Sum of corrected areas: 18018373

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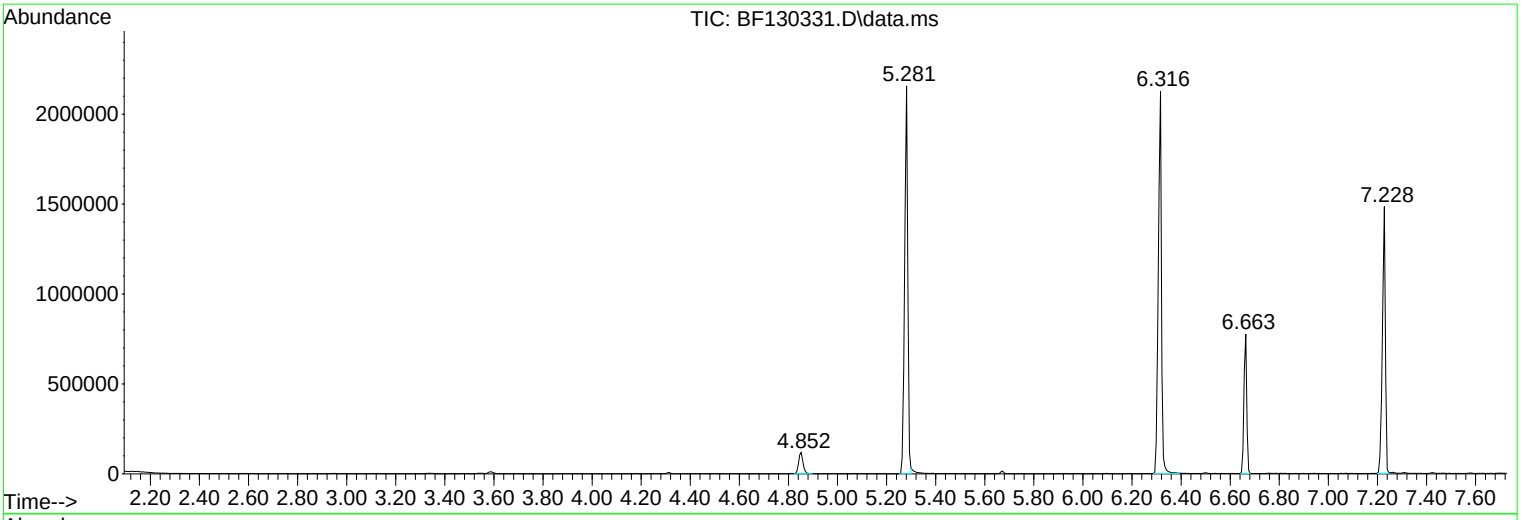
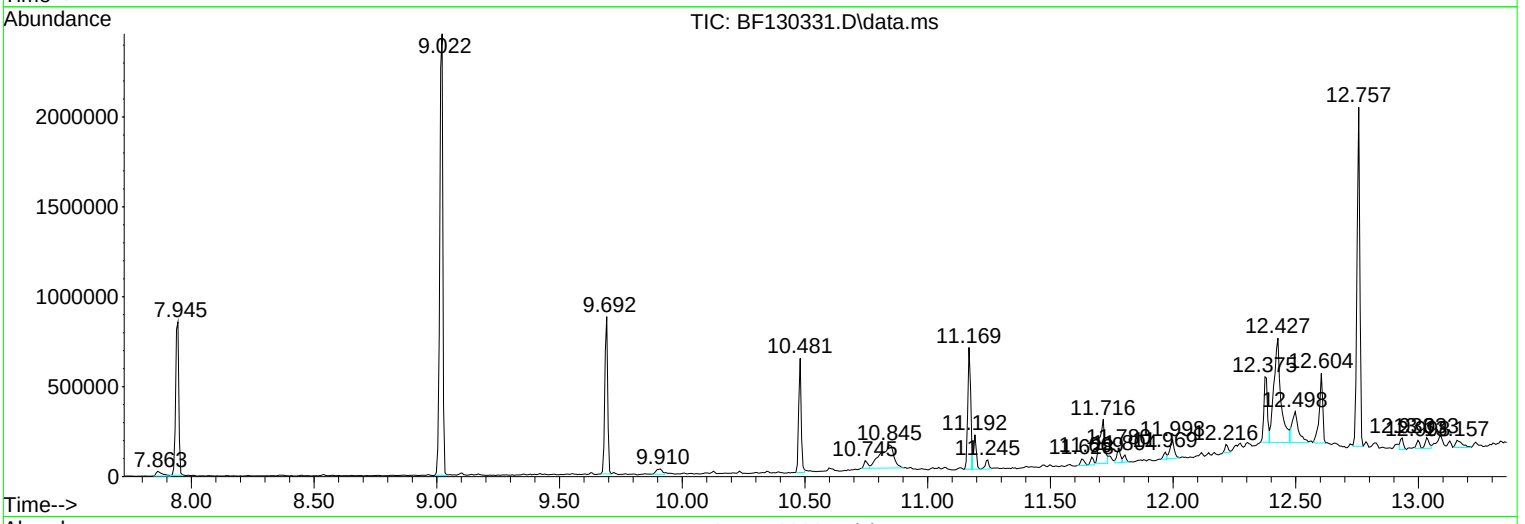
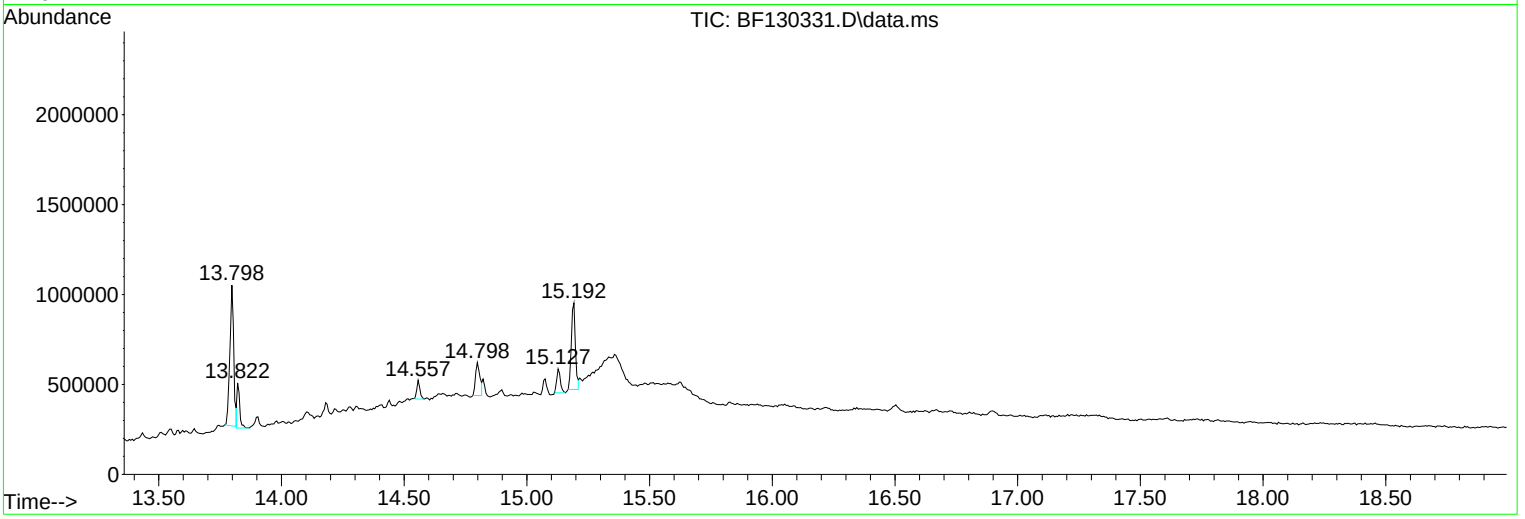
ClientSampleId :
SASP2-T-6-(10-18)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.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_F\Data\BF091922\
Data File : BF130331.D
Acq On : 19 Sep 2022 20:57
Operator : CG\JU
Sample : N4613-01
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Instrument :
BNA_F
ClientSampleId :
SASP2-T-6-(10-18)

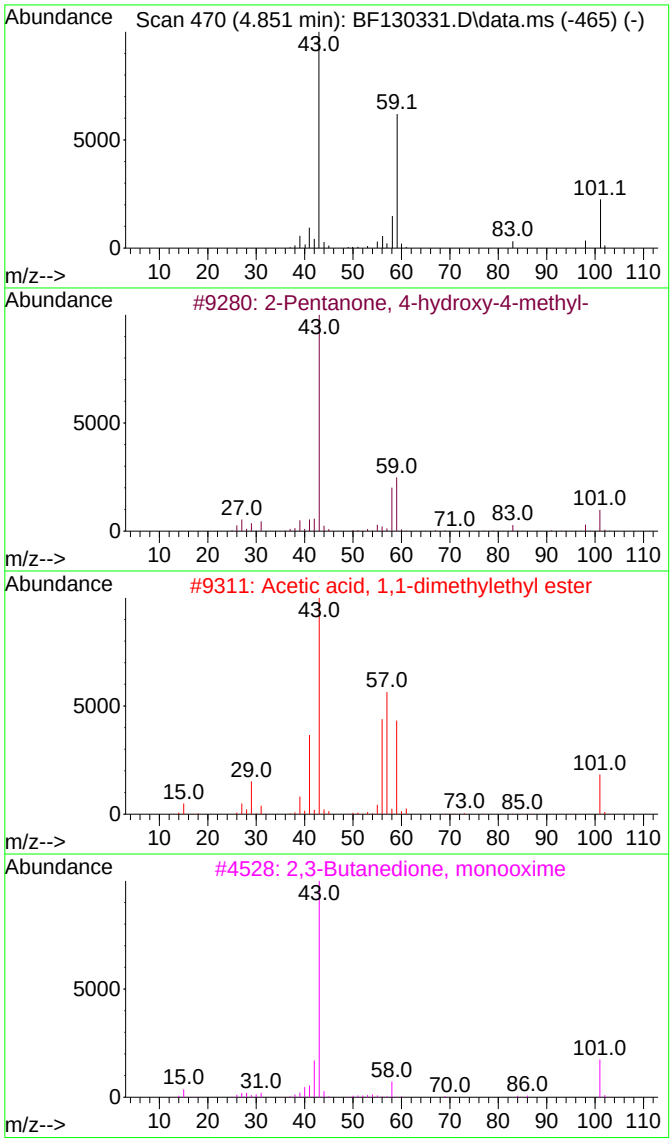
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

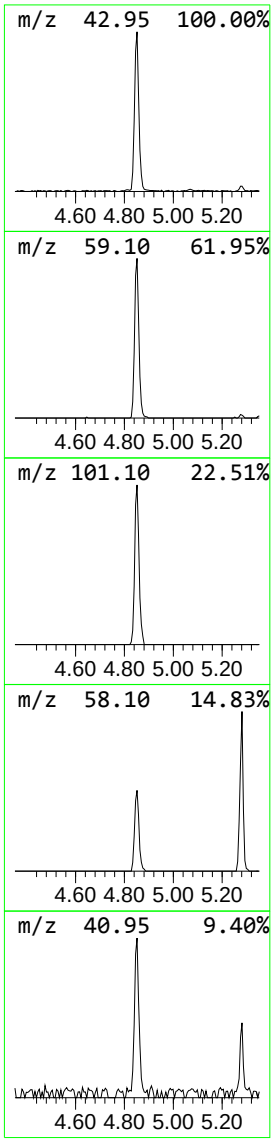
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.851	4.80 ng	146952	1,4-Dichlorobenzene-d4	6.663

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

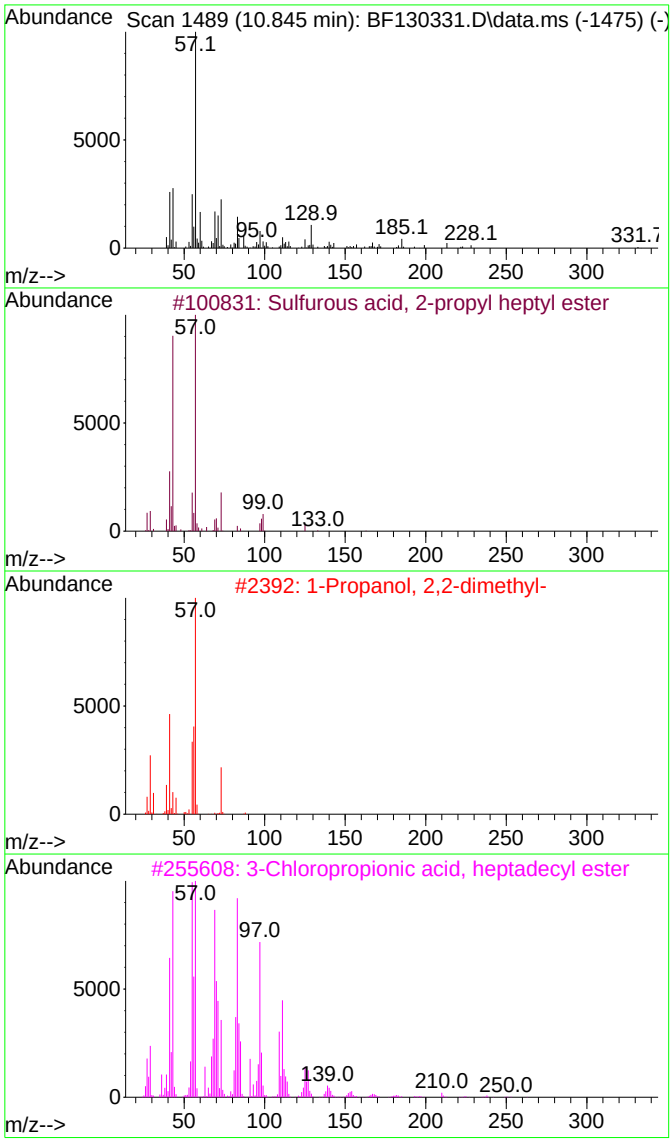
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

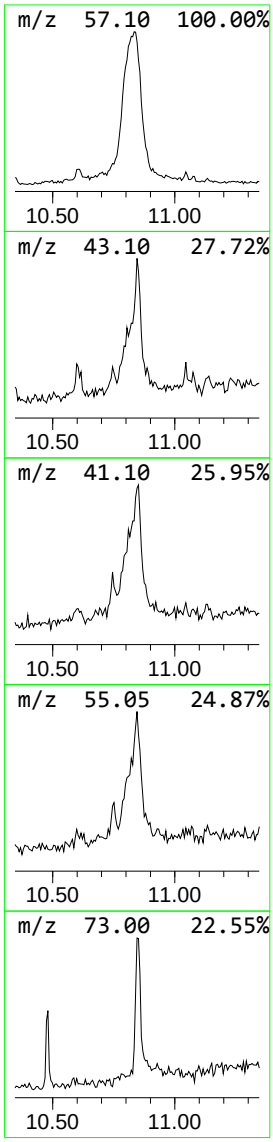
****

Peak Number 2 unknown10.845 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.845	17.91 ng	488919	Phenanthrene-d10	11.169

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, 2-propyl heptyl ...	222	C10H22O3S	1000309-11-8	38
2	1-Propanol, 2,2-dimethyl-	88	C5H12O	000075-84-3	35
3	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	22
4	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	14
5	Eicosyl nonyl ether	424	C29H60O	1000406-37-8	14





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Data File : BF130331.D
Acq On : 19 Sep 2022 20:57
Operator : CG\JU
Sample : N4613-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2-T-6-(10-18)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

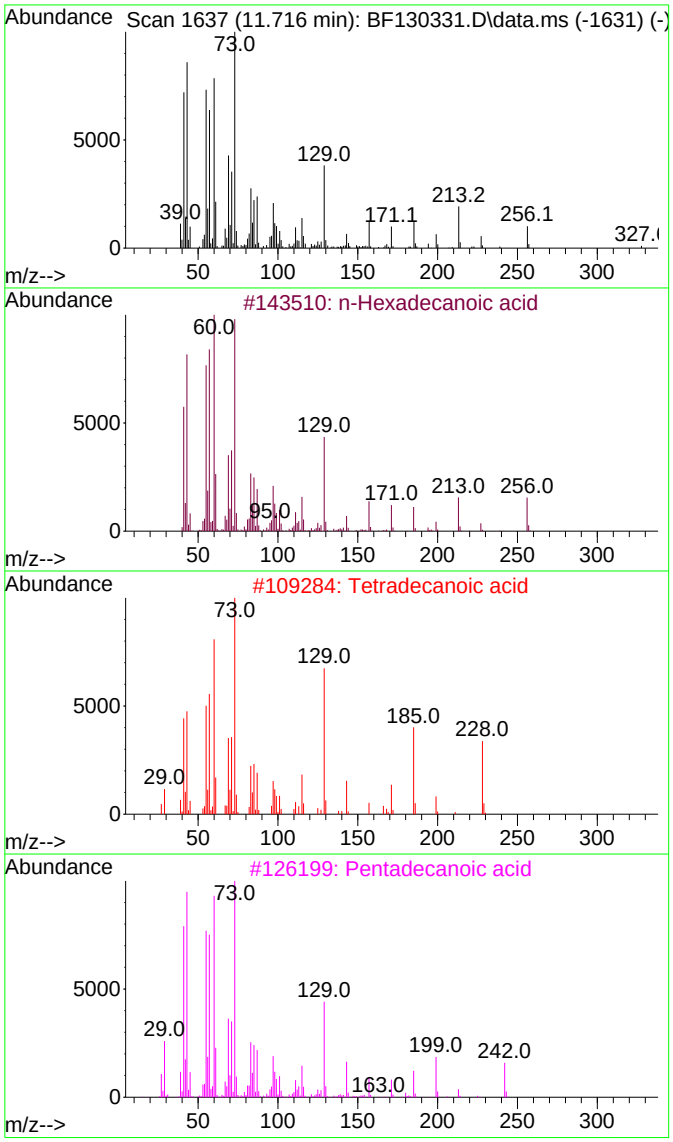
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

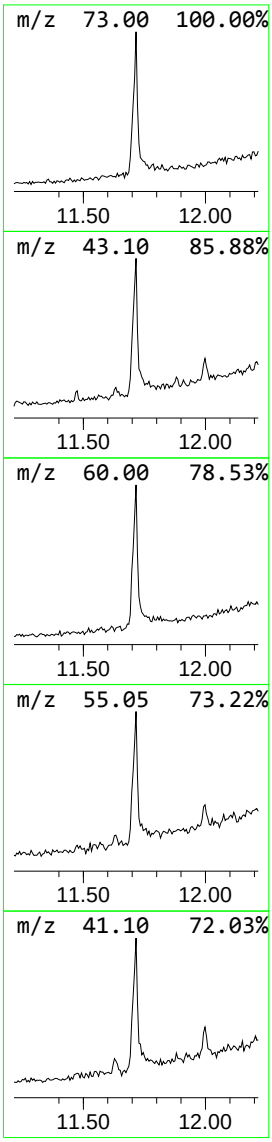
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.716	12.81 ng	349817	Phenanthrene-d10	11.169

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	Octadecanoic acid	284	C18H36O2	000057-11-4	87
5	Tridecanoic acid	214	C13H26O2	000638-53-9	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091922\
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Sample : N4613-01
Misc :
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Instrument :
BNA_F
ClientSampleId :
SASP2-T-6-(10-18)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

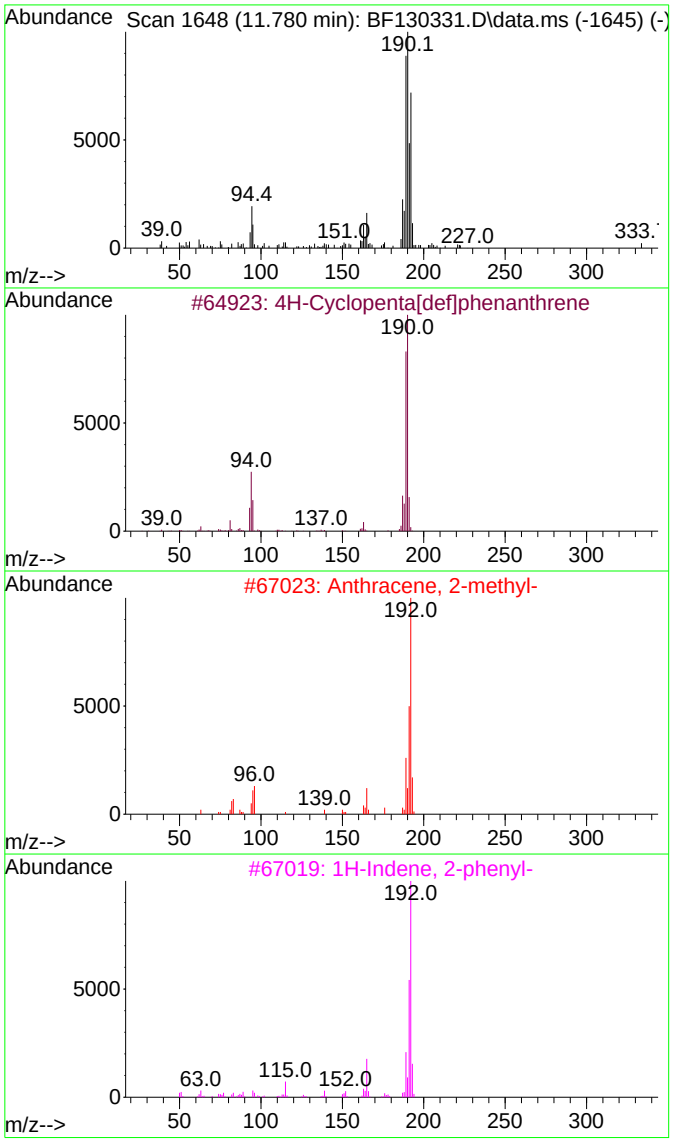
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

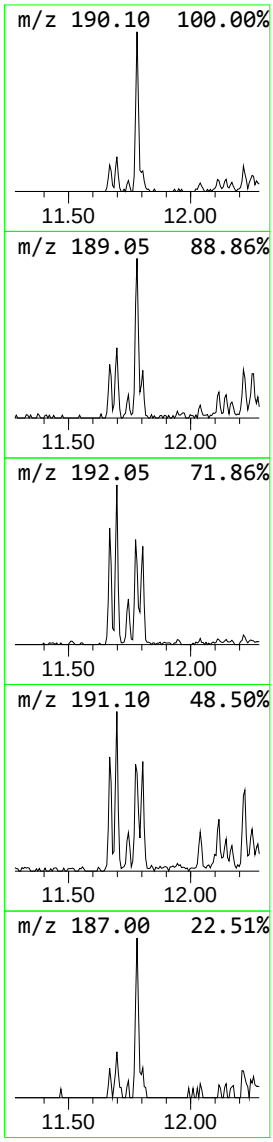
****

Peak Number 4 4H-Cyclopenta[def]phenanthrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.781	2.85 ng	77857	Phenanthrene-d10	11.169

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	70
2	Anthracene, 2-methyl-	192	C15H12	000613-12-7	38
3	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	38
4	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	38
5	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	35





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ALS Vial : 19 Sample Multiplier: 1

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SASP2-T-6-(10-18)

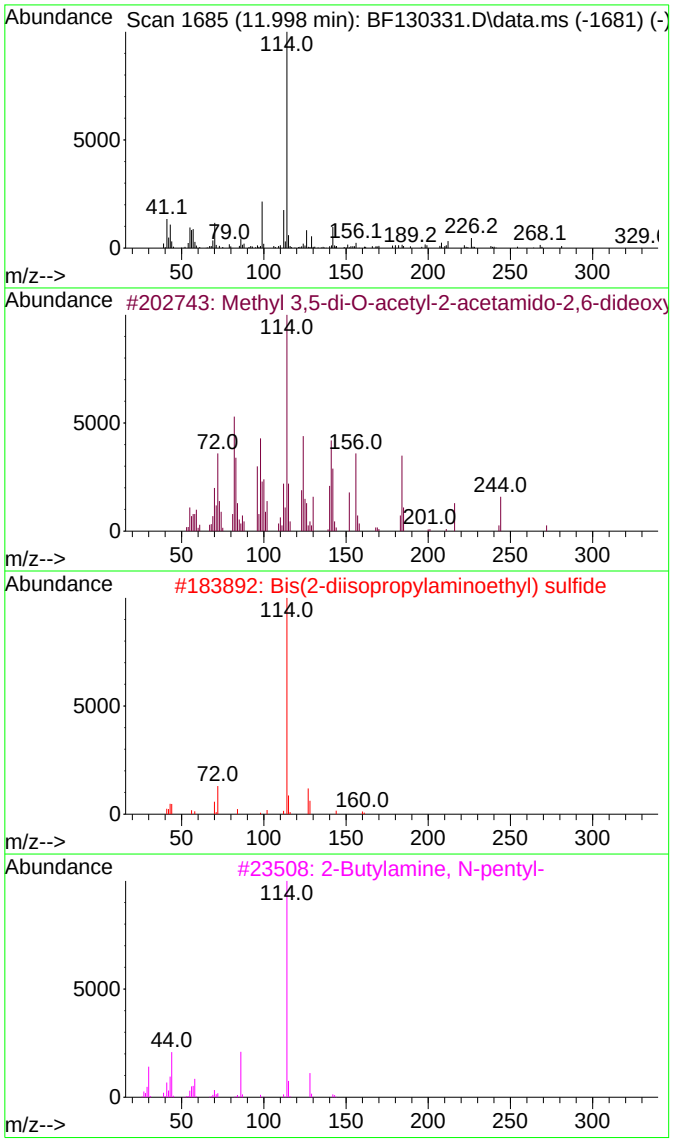
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

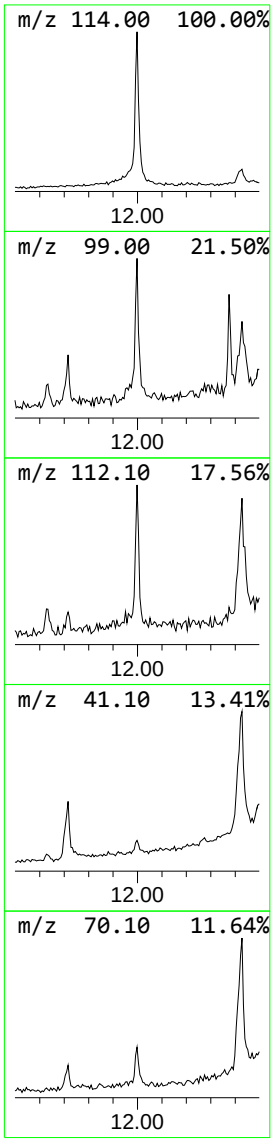
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Methyl 3,5-di-O-acetyl-2-ac... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.998	4.47 ng	122149	Phenanthrene-d10	11.169

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl 3,5-di-O-acetyl-2-acetami...	303	C13H21NO7	093250-08-9	64
2	Bis(2-diisopropylaminoethyl) sul...	288	C16H36N2S	110501-56-9	47
3	2-Butylamine, N-pentyl-	143	C9H21N	1000463-86-2	47
4	7-Tridecylamine	199	C13H29N	022513-16-2	47
5	Bis(2-N,N-dipropylaminoethyl)dis...	320	C16H36N2S2	106479-14-5	43





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Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
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SASP2-T-6-(10-18)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

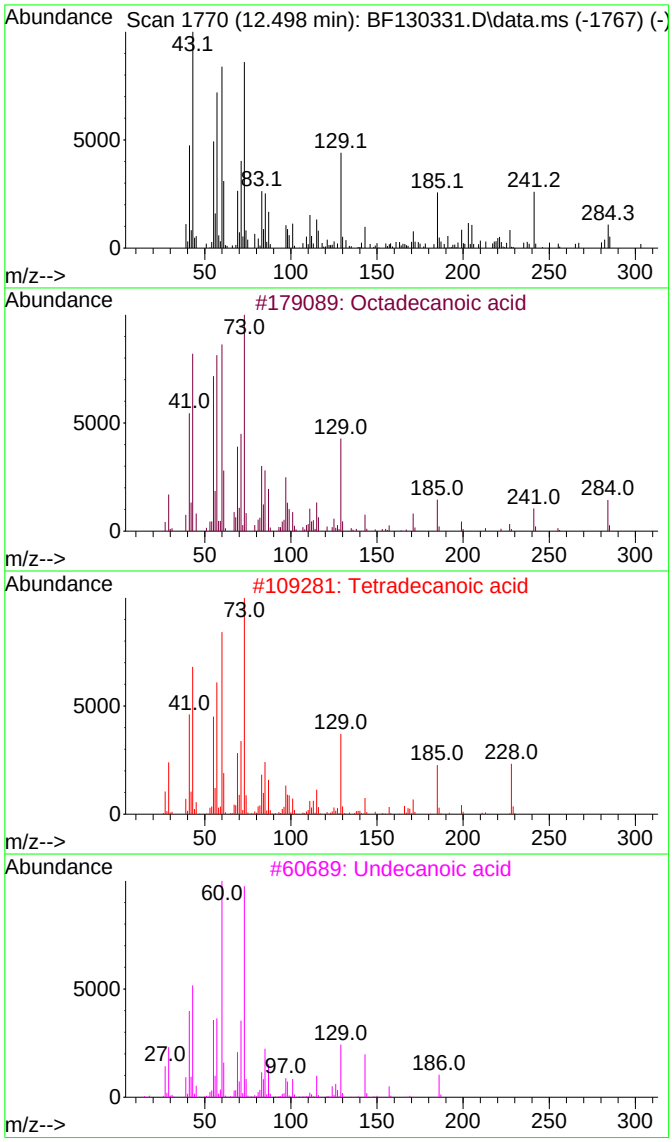
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

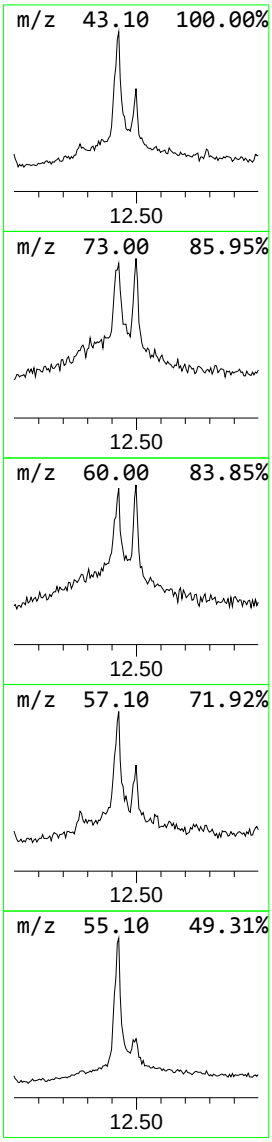
****

Peak Number 6 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.498	6.57 ng	283835	Chrysene-d12	13.798

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	89
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
3	Undecanoic acid	186	C11H22O2	000112-37-8	70
4	n-Decanoic acid	172	C10H20O2	000334-48-5	60
5	Dodecanoic acid	200	C12H24O2	000143-07-7	60





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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

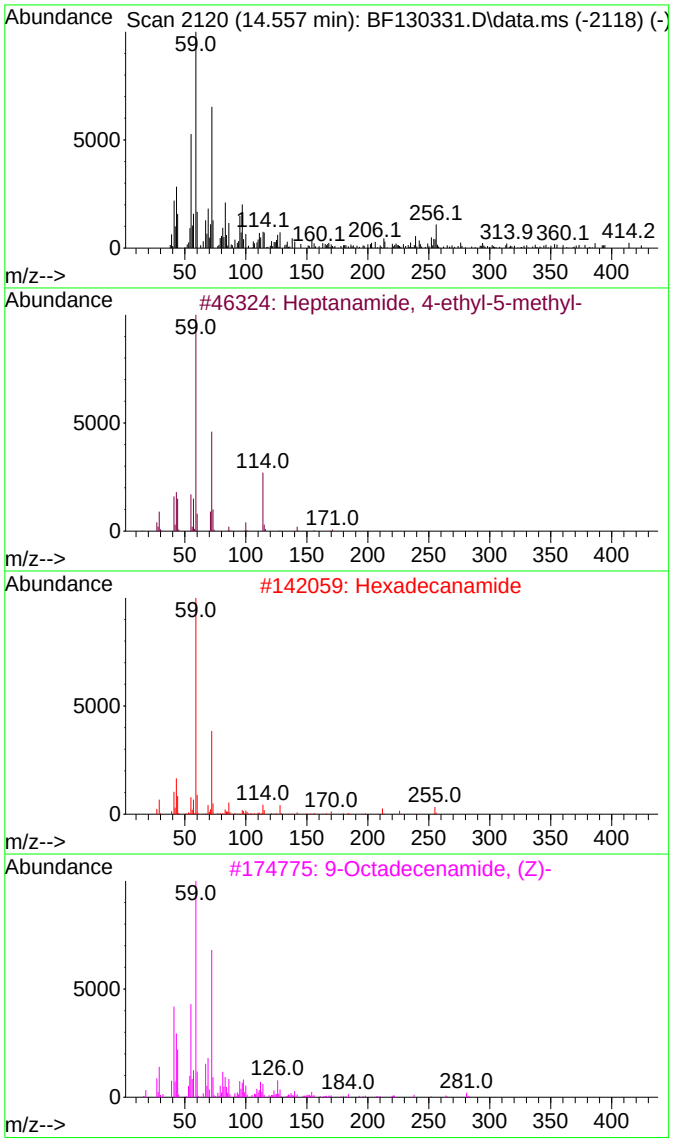
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

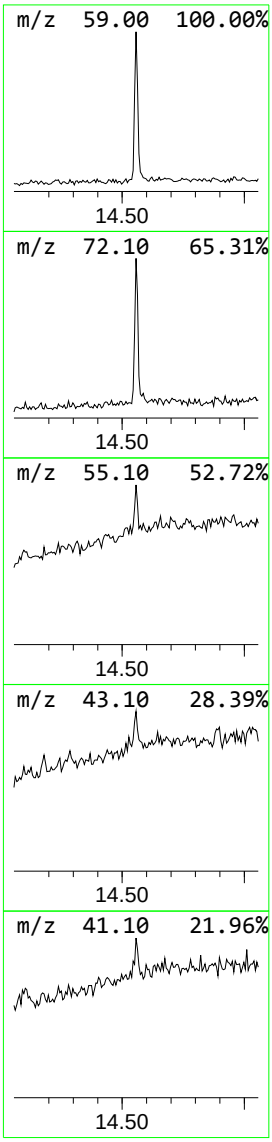
****

Peak Number 7 Heptanamide, 4-ethyl-5-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.557	3.18 ng	88429	Perylene-d12	15.192

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	62
2	Hexadecanamide	255	C16H33NO	000629-54-9	58
3	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	58
4	Tetradecanamide	227	C14H29NO	000638-58-4	53
5	d-Glucosamine	179	C6H13NO5	000090-77-7	53





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091922\
Data File : BF130331.D
Acq On : 19 Sep 2022 20:57
Operator : CG\JU
Sample : N4613-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2-T-6-(10-18)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.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-...	4.851	4.8	ng	146952	1	6.663	612163	20.0
unknown10.845	10.845	17.9	ng	488919	4	11.169	546055	20.0
n-Hexadecanoic ...	11.716	12.8	ng	349817	4	11.169	546055	20.0
4H-Cyclopenta[d...	11.781	2.9	ng	77857	4	11.169	546055	20.0
Methyl 3,5-di-O...	11.998	4.5	ng	122149	4	11.169	546055	20.0
Octadecanoic acid	12.498	6.6	ng	283835	5	13.798	863553	20.0
Heptanamide, 4-...	14.557	3.2	ng	88429	6	15.192	557002	20.0