LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100623\
Data File : BF135634.D
Acq On : 06 Oct 2023 17:53
Operator : CG\JU
Sample : 04735-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT2662

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-BF091123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135634.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.116	3	5	12	rVB	40362	45852	1.24%	0.131%
2	2.799	116	121	127	rBV	24764	41087	1.11%	0.117%
3	4.340	380	383	395	rBV	178078	244704	6.63%	0.696%
4	4.981	485	492	516	rBV	2420173	3689964	100.00%	10.502%
5	5.381	557	560	580	rBV	3266503	3343226	90.60%	9.516%
6	5.763	621	625	634	rBV	101195	101259	2.74%	0.288%
7	6.392	728	732	756	rBV	3236413	3490510	94.59%	9.935%
8	6.739	787	791	802	rVB	953050	842252	22.83%	2.397%
9	7.304	883	887	900	rBV	2243587	2270941	61.54%	6.464%
10	8.016	1004	1008	1026	rVB	1304649	1170866	31.73%	3.333%
11	9.098	1186	1192	1195	rBV	3786503	3511210	95.16%	9.994%
12	9.216	1208	1212	1221	rVB	83588	88059	2.39%	0.251%
13	9.775	1303	1307	1311	rBV	1461327	1271333	34.45%	3.618%
14	10.569	1438	1442	1457	rBV	2099001	2120130	57.46%	6.034%
15	10.680	1458	1461	1465	rBV3	53741	66358	1.80%	0.189%
16	10.880	1491	1495	1498	rBV3	27579	37022	1.00%	0.105%
17	11.127	1533	1537	1540	rBV2	37846	50778	1.38%	0.145%
18	11.163	1540	1543	1548	rVB2	38730	48986	1.33%	0.139%
19	11.269	1557	1561	1563	rBV	1559751	1283929	34.80%	3.654%
20	11.292	1563	1565	1569	rVV	462304	385239	10.44%	1.096%
21	11.351	1572	1575	1577	rVB	54095	51754	1.40%	0.147%
22	11.516	1598	1603	1608	rBV4	54143	82593	2.24%	0.235%
23	11.774	1644	1647	1649	rBV	75569	64457	1.75%	0.183%
24	11.804	1649	1652	1659	rVV	441428	466726	12.65%	1.328%
25	11.886	1663	1666	1668	rVV	135131	132711	3.60%	0.378%
26	11.910	1668	1670	1674	rVB	57215	47614	1.29%	0.136%
27	12.074	1695	1698	1702	rBV	47580	44114	1.20%	0.126%
28	12.110	1702	1704	1708	rBV2	74564	76503	2.07%	0.218%
29	12.327	1738	1741	1743	rBV	56195	52286	1.42%	0.149%
30	12.363	1743	1747	1753	rBV6	56817	109235	2.96%	0.311%
31	12.421	1755	1757	1762	rVB2	60366	60711	1.65%	0.173%
32	12.486	1765	1768	1772	rBV	935539	896077	24.28%	2.550%
33	12.592	1783	1786	1790	rBV3	90307	108512	2.94%	0.309%
34	12.639	1792	1794	1798	rVV	69990	75352	2.04%	0.214%
35	12.721	1802	1808	1813	rVV	762627	857780	23.25%	2.441%
36	12.774	1813	1817	1821	rVB4	45607	69879	1.89%	0.199%

LSC Area Percent Report

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Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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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-BF091123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	12.863	1826	1832	1836	rBV	2913240	2906933	78.78%	8.274%
38	12.945	1842	1846	1850	rBV3	56410	89717	2.43%	0.255%
39	13.027	1857	1860	1863	rBV4	60589	94226	2.55%	0.268%
40	13.051	1863	1864	1868	rVB	87681	75887	2.06%	0.216%
41	13.121	1873	1876	1878	rVV	75630	77302	2.09%	0.220%
42	13.157	1879	1882	1889	rVB3	84658	111373	3.02%	0.317%
43	13.251	1895	1898	1900	rVB2	56562	46253	1.25%	0.132%
44	13.286	1901	1904	1907	rBV3	36846	48598	1.32%	0.138%
45	13.574	1950	1953	1957	rVB	85722	93590	2.54%	0.266%
46	13.680	1968	1971	1973	rBV2	82134	79724	2.16%	0.227%
47	13.704	1973	1975	1977	rVB	61948	46383	1.26%	0.132%
48	13.727	1977	1979	1981	rBV	48783	48351	1.31%	0.138%
49	13.786	1987	1989	1994	rVB2	93933	100287	2.72%	0.285%
50	13.927	2006	2013	2016	rBV2	945079	1203695	32.62%	3.426%
51	13.957	2016	2018	2023	rVB	334774	281278	7.62%	0.801%
52	14.557	2117	2120	2124	rBV2	82409	112606	3.05%	0.321%
53	14.651	2134	2136	2138	rBV2	43904	37641	1.02%	0.107%
54	14.974	2187	2191	2194	rBV	309957	470161	12.74%	1.338%
55	15.080	2207	2209	2213	rVB	56874	56080	1.52%	0.160%
56	15.274	2238	2242	2248	rVB	187799	245750	6.66%	0.699%
57	15.339	2249	2253	2258	rVB	205022	238517	6.46%	0.679%
58	15.398	2258	2263	2267	rBV	635047	797500	21.61%	2.270%
59	15.839	2336	2338	2345	rVB3	53870	78758	2.13%	0.224%
60	16.886	2512	2516	2523	rBV	84593	169256	4.59%	0.482%
61	17.339	2588	2593	2603	rVB2	74672	162570	4.41%	0.463%
62	17.956	2693	2698	2708	rVB9	62068	161861	4.39%	0.461%

Sum of corrected areas: 35134306

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Misc :
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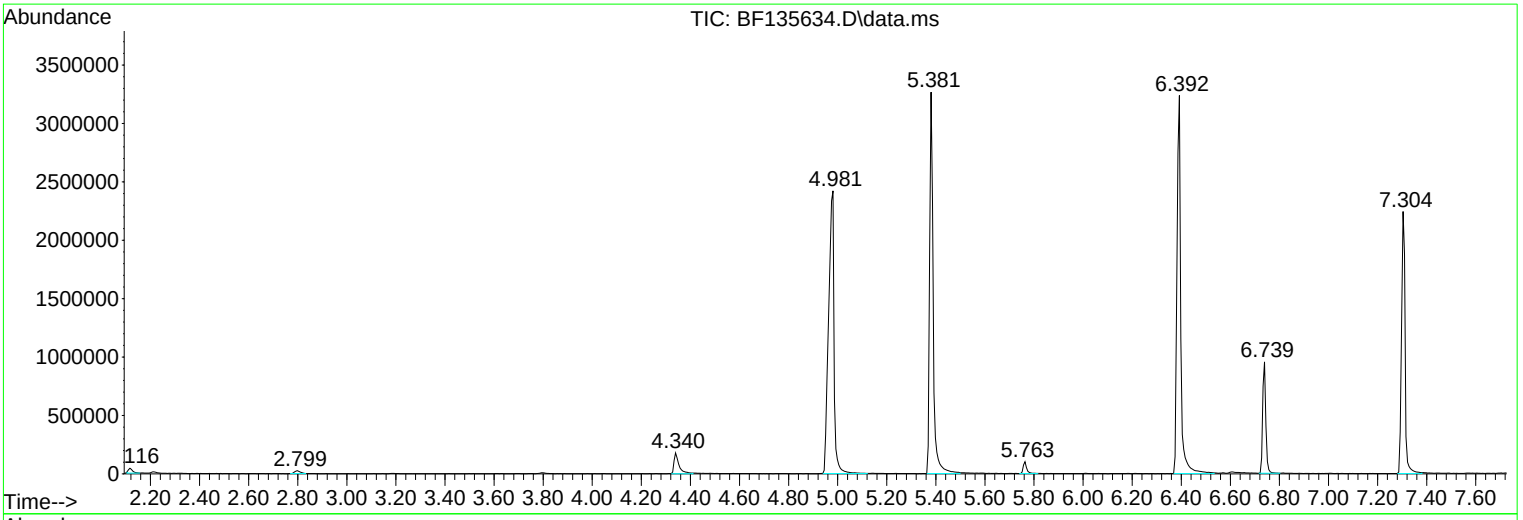
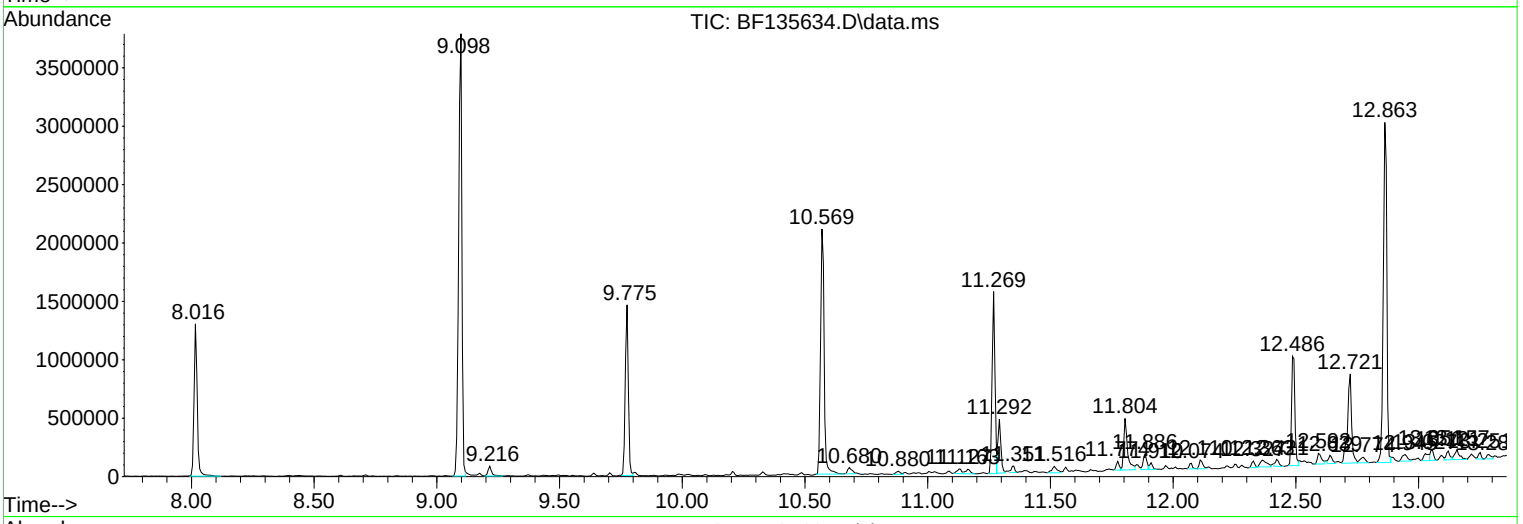
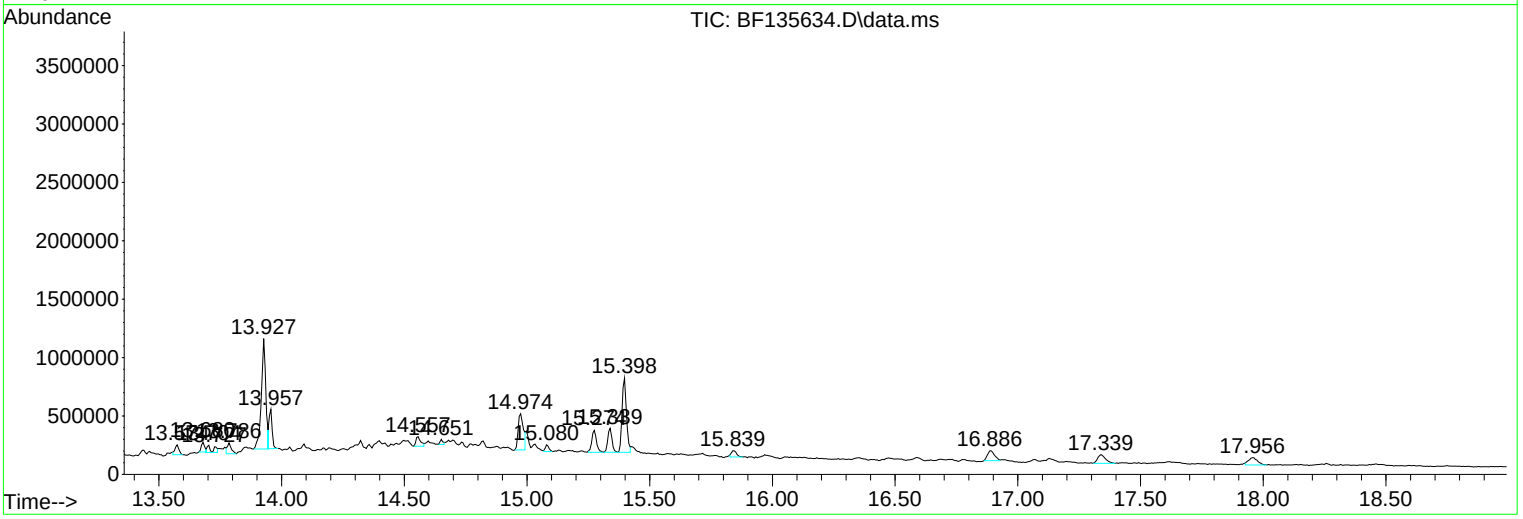
Instrument :
BNA_F
ClientSampleId :
RT2662

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

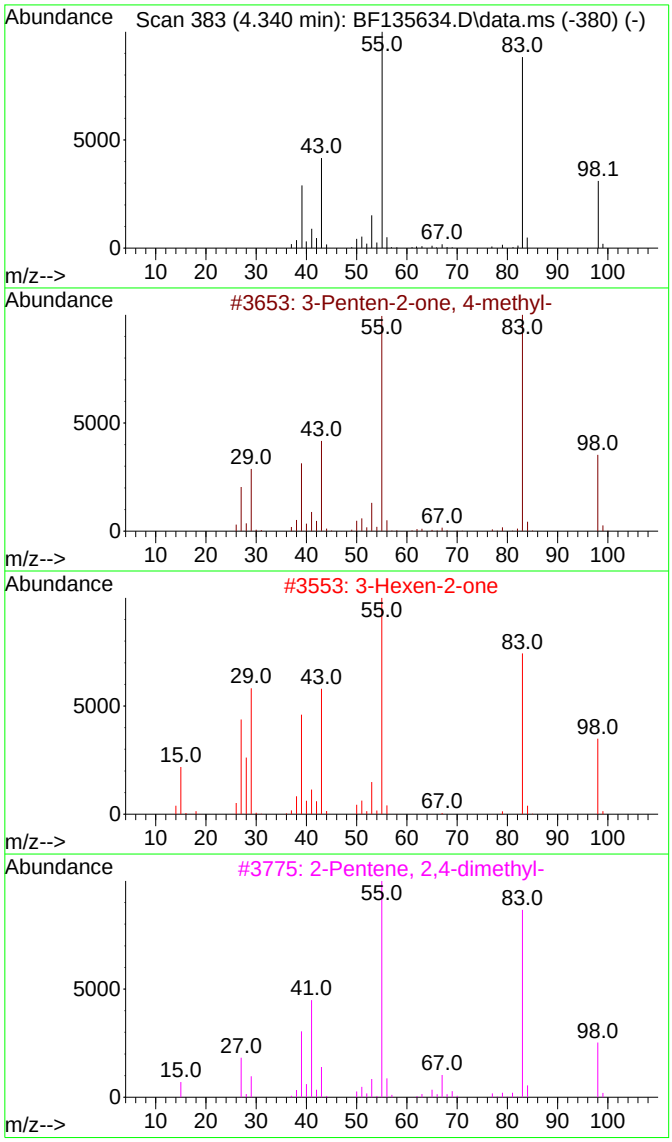
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

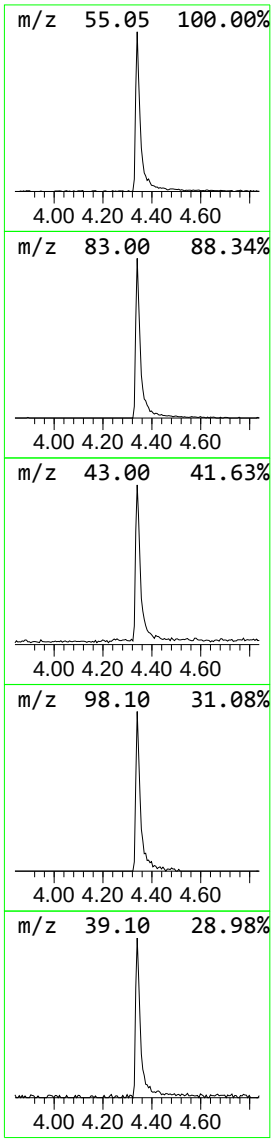
****

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.340	5.81 ng	244704	1,4-Dichlorobenzene-d4	6.739

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	94
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91
3	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
4	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	80
5	2,4-Azetidinedione, 3,3-diethyl-	141	C7H11NO2	042282-85-9	78





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Operator : CG\JU
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ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT2662

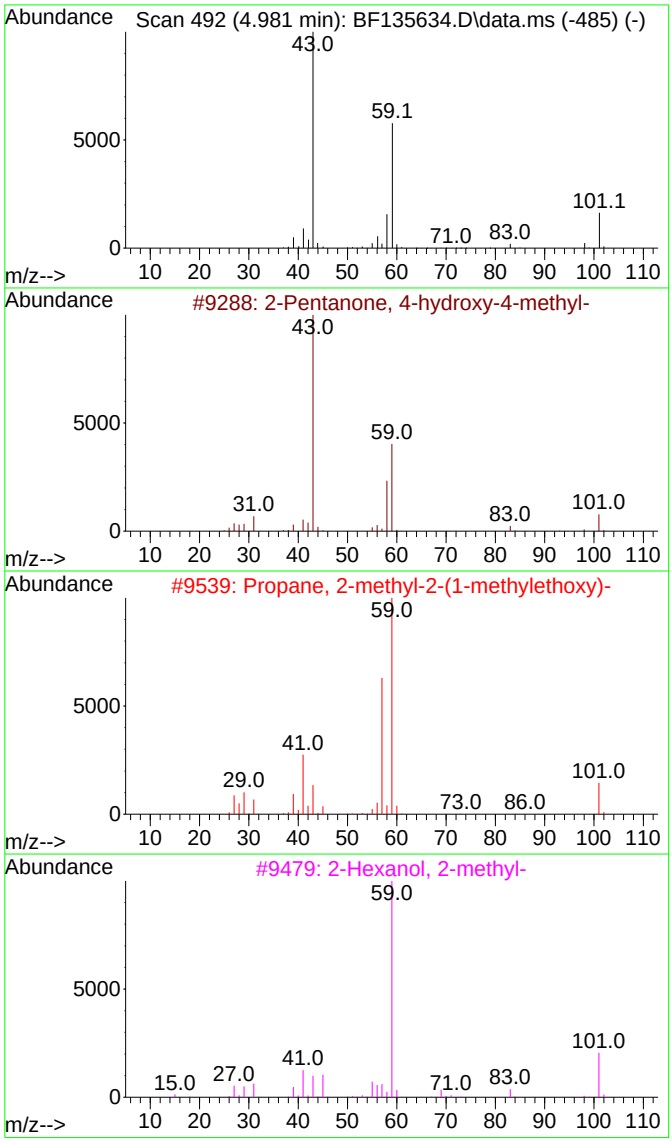
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

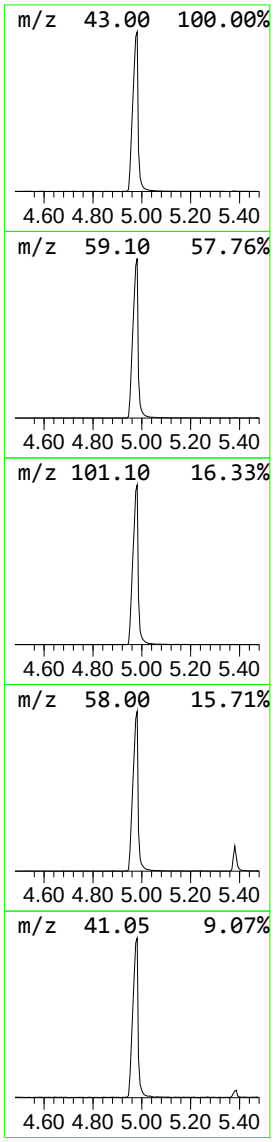
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.981	87.62 ng	3689960	1,4-Dichlorobenzene-d4	6.739

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23





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Instrument :
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ClientSampleId :
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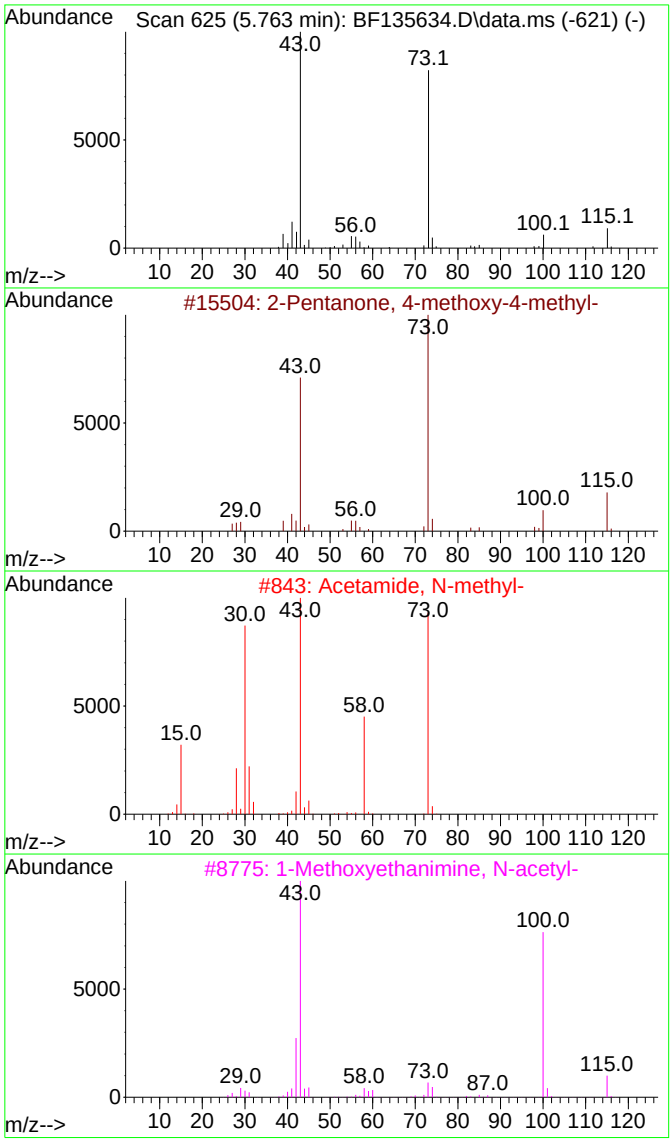
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

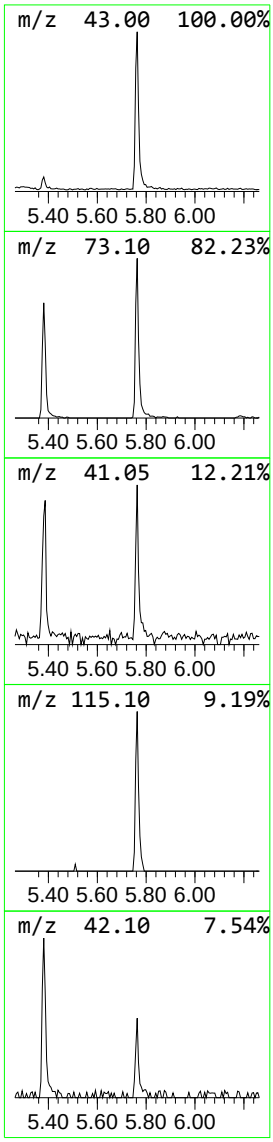
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.763	2.40 ng	101259	1,4-Dichlorobenzene-d4	6.739

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	38
3	1-Methoxyethanimine, N-acetyl-	115	C5H9NO2	099028-43-0	37
4	1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	35
5	N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	33





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

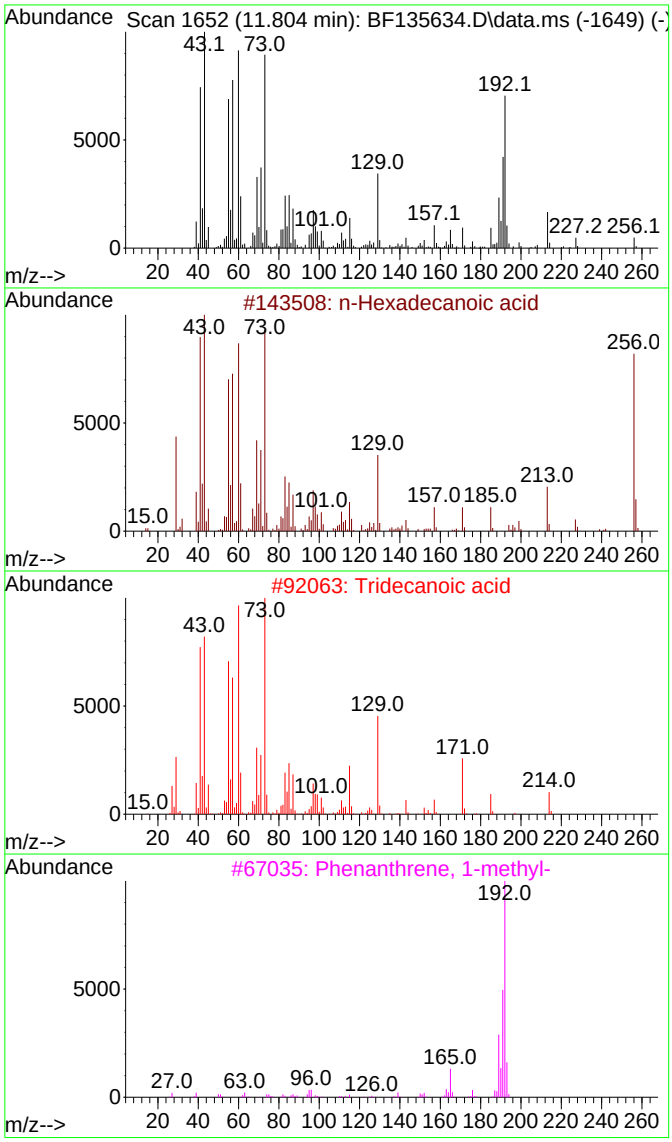
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

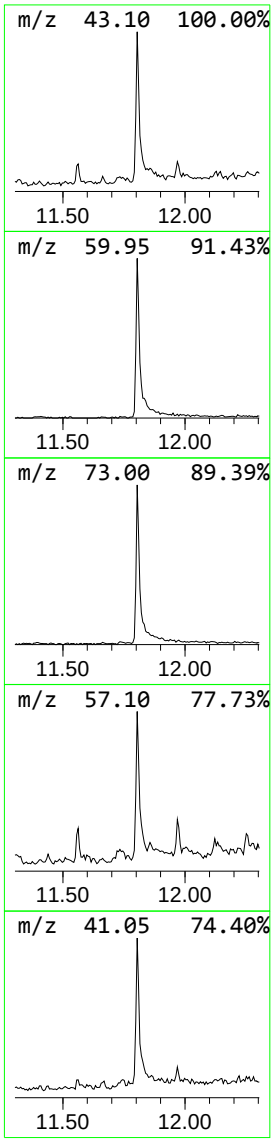
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.804	7.27 ng	466726	Phenanthrene-d10	11.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tridecanoic acid	214	C13H26O2	000638-53-9	70
3	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	64
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	55
5	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	53





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ALS Vial : 16 Sample Multiplier: 1

Instrument :
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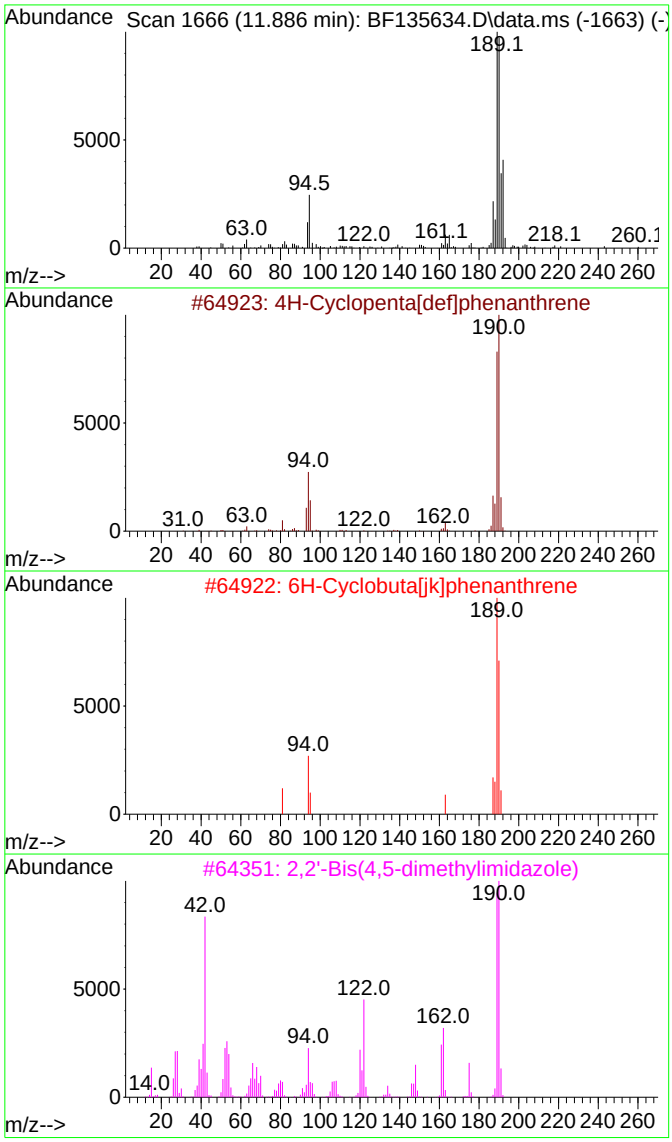
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

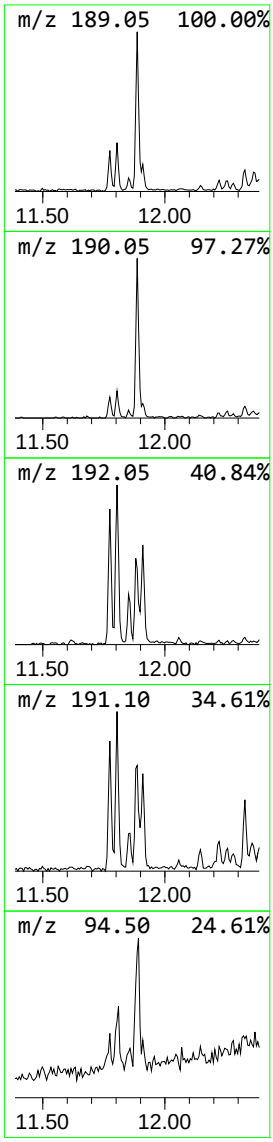
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.886	2.07 ng	132711	Phenanthrene-d10	11.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	93
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	45
3	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	42
4	2,4(1H,3H)-Pyrimidinedione, 5-br...	190	C4H3BrN2O2	000051-20-7	32
5	2-Amino-4,6-dichloropyrimidine-5...	191	C5H3Cl2N3O	005604-46-6	23





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BNA_F
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

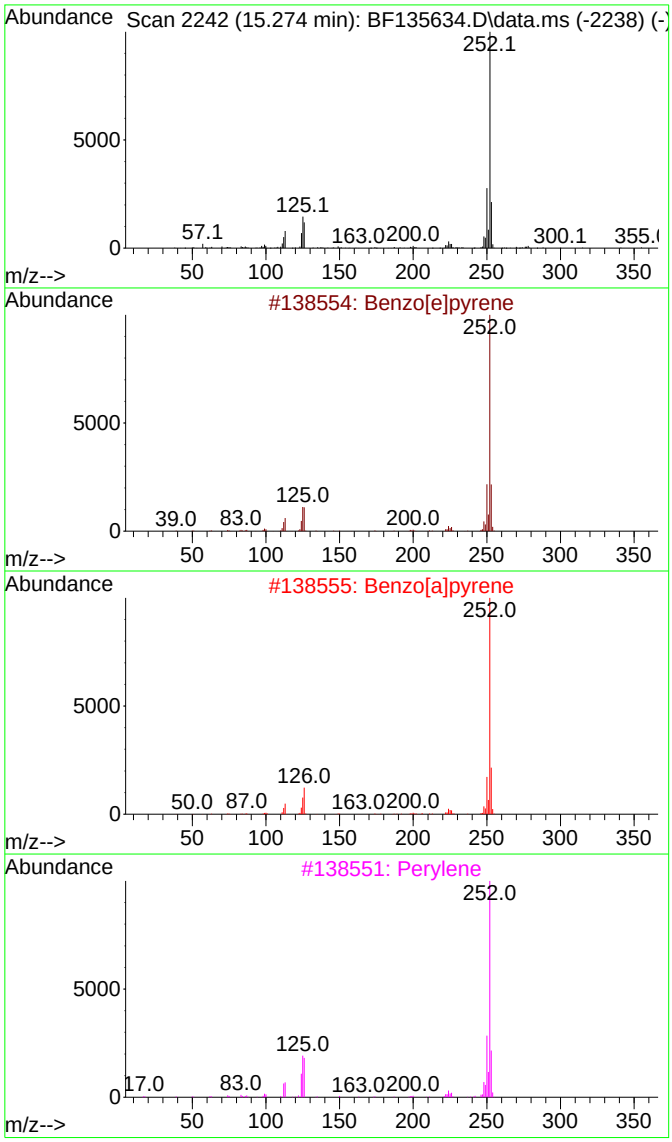
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

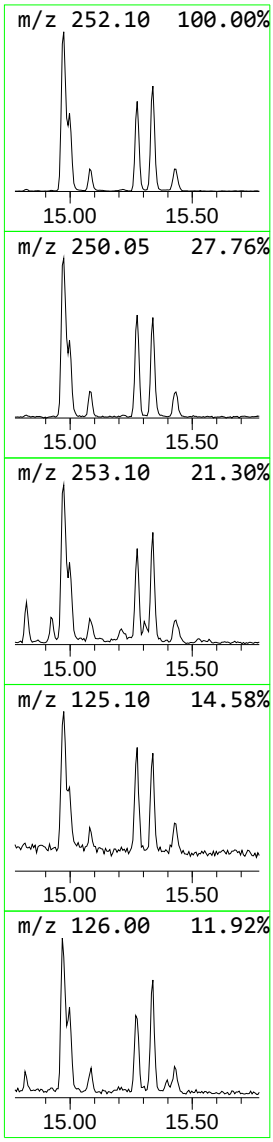
****

Peak Number 6 Benzo[e]pyrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.274	6.16 ng	245750	Perylene-d12	15.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benzo[a]pyrene	252	C20H12	000050-32-8	93
3	Perylene	252	C20H12	000198-55-0	90
4	Benzo[k]fluoranthene	252	C20H12	000207-08-9	90
5	Benzo[b]fluoranthene	252	C20H12	000205-99-2	90





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Data File : BF135634.D
Acq On : 06 Oct 2023 17:53
Operator : CG\JU
Sample : 04735-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT2662

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

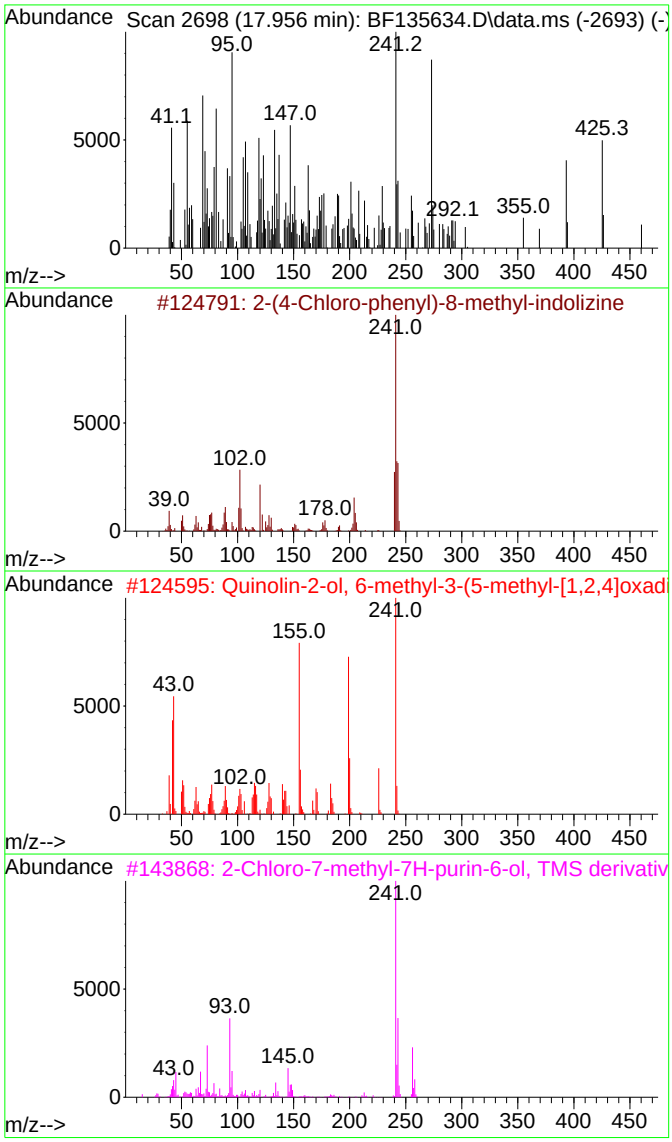
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

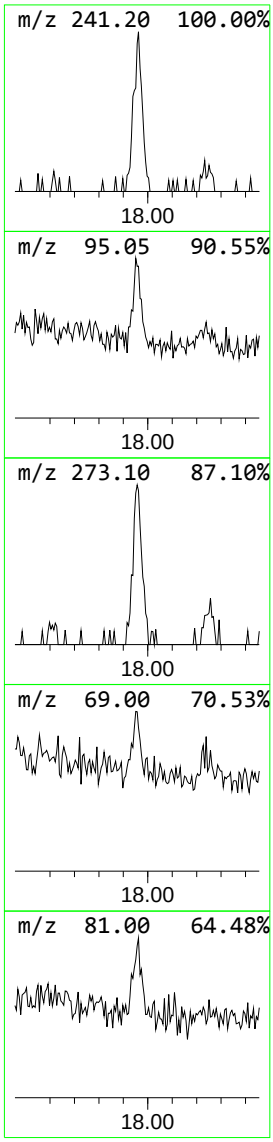
****

Peak Number 7 unknown17.956 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.956	4.06 ng	161861	Perylene-d12	15.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(4-Chloro-phenyl)-8-methyl-ind...	241	C15H12ClN	1000337-21-4	25
2	Quinolin-2-ol, 6-methyl-3-(5-met...	241	C13H11N3O2	1000317-00-2	25
3	2-Chloro-7-methyl-7H-purin-6-ol,...	256	C9H13ClN4OSi	1000471-30-2	25
4	8-Nitropyrimido[4,5-b][1,4]benzo...	273	C11H7N5O2S	089046-89-9	15
5	1,2,4-Oxadiazole, 3-chloromethyl...	256	C11H13ClN2OS	1000266-38-4	15





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100623\
Data File : BF135634.D
Acq On : 06 Oct 2023 17:53
Operator : CG\JU
Sample : 04735-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT2662

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.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
3-Penten-2-one,...	4.340	5.8	ng	244704	1	6.739	842252	20.0
2-Pentanone, 4-...	4.981	87.6	ng	3689960	1	6.739	842252	20.0
2-Pentanone, 4-...	5.763	2.4	ng	101259	1	6.739	842252	20.0
n-Hexadecanoic ...	11.804	7.3	ng	466726	4	11.269	1283930	20.0
4H-Cyclopenta[d...	11.886	2.1	ng	132711	4	11.269	1283930	20.0
Benzo[e]pyrene	15.274	6.2	ng	245750	6	15.398	797500	20.0
unknown17.956	17.956	4.1	ng	161861	6	15.398	797500	20.0