LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041923\
Data File : BF132923.D
Acq On : 19 Apr 2023 21:12
Operator : CG\JU
Sample : 02366-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20230348-COMP-26

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-BF041723.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132923.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.957	479	488	496	rBV	121607	166646	2.23%	0.294%
2	5.363	552	557	560	rBV	5721509	5863657	78.40%	10.332%
3	6.104	679	683	697	rVB2	48279	103407	1.38%	0.182%
4	6.387	726	731	734	rBV	5510693	6129787	81.96%	10.801%
5	6.763	791	795	798	rBV	1999475	1586977	21.22%	2.796%
6	6.945	822	826	830	rVB	124188	106260	1.42%	0.187%
7	7.322	885	890	893	rBV	4071988	3889317	52.00%	6.853%
8	8.045	1009	1013	1015	rBV	2907982	2258193	30.19%	3.979%
9	8.069	1015	1017	1020	rVV	937952	720759	9.64%	1.270%
10	9.122	1192	1196	1200	rBV	7291726	6599231	88.23%	11.628%
11	9.798	1307	1311	1314	rVB	3401118	2570001	34.36%	4.529%
12	9.827	1314	1316	1319	rVB	203756	158252	2.12%	0.279%
13	10.086	1355	1360	1365	rBV	70633	83170	1.11%	0.147%
14	10.345	1401	1404	1410	rVB	95947	88725	1.19%	0.156%
15	10.516	1429	1433	1436	rVB	2306352	1963835	26.26%	3.460%
16	10.586	1441	1445	1448	rBV	5542854	4850683	64.85%	8.547%
17	10.816	1479	1484	1490	rBV2	456838	458151	6.13%	0.807%
18	10.910	1495	1500	1504	rVV3	57733	90796	1.21%	0.160%
19	11.157	1536	1542	1546	rBV7	44907	95220	1.27%	0.168%
20	11.280	1559	1563	1565	rBV	3593948	2813209	37.61%	4.957%
21	11.304	1565	1567	1570	rVV	336961	259854	3.47%	0.458%
22	11.351	1572	1575	1578	rVB	108410	95789	1.28%	0.169%
23	11.821	1650	1655	1659	rBV	924304	879562	11.76%	1.550%
24	12.074	1695	1698	1704	rVB2	369344	304712	4.07%	0.537%
25	12.486	1766	1768	1773	rBV	302310	265909	3.56%	0.469%
26	12.604	1784	1788	1793	rBV	252479	293961	3.93%	0.518%
27	12.716	1802	1807	1810	rBV	242426	243439	3.25%	0.429%
28	12.868	1829	1833	1837	rBV	7651546	7479381	100.00%	13.179%
29	13.110	1872	1874	1877	rVB	118927	106399	1.42%	0.187%
30	13.145	1877	1880	1888	rVB6	64763	87887	1.18%	0.155%
31	13.457	1930	1933	1938	rVB	107389	107875	1.44%	0.190%
32	13.774	1983	1987	1995	rBV2	493193	713264	9.54%	1.257%
33	13.915	2006	2011	2014	rBV	2768950	2580777	34.51%	4.547%
34	14.051	2032	2034	2039	rVB	101946	89613	1.20%	0.158%
35	14.098	2039	2042	2044	rVV	129401	110603	1.48%	0.195%
36	14.127	2044	2047	2053	rVB	244534	216528	2.89%	0.382%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041923\
Data File : BF132923.D
Acq On : 19 Apr 2023 21:12
Operator : CG\JU
Sample : 02366-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20230348-COMP-26

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-BF041723.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.404	2091	2094	2098	rBV	124304	135650	1.81%	0.239%
38	14.704	2142	2145	2152	rVB	94715	114793	1.53%	0.202%
39	15.033	2198	2201	2206	rVB2	95450	94064	1.26%	0.166%
40	15.345	2249	2254	2260	rBV	1520272	1800688	24.08%	3.173%
41	15.398	2260	2263	2269	rVB	56847	81574	1.09%	0.144%
42	15.868	2338	2343	2348	rBV6	50211	93023	1.24%	0.164%

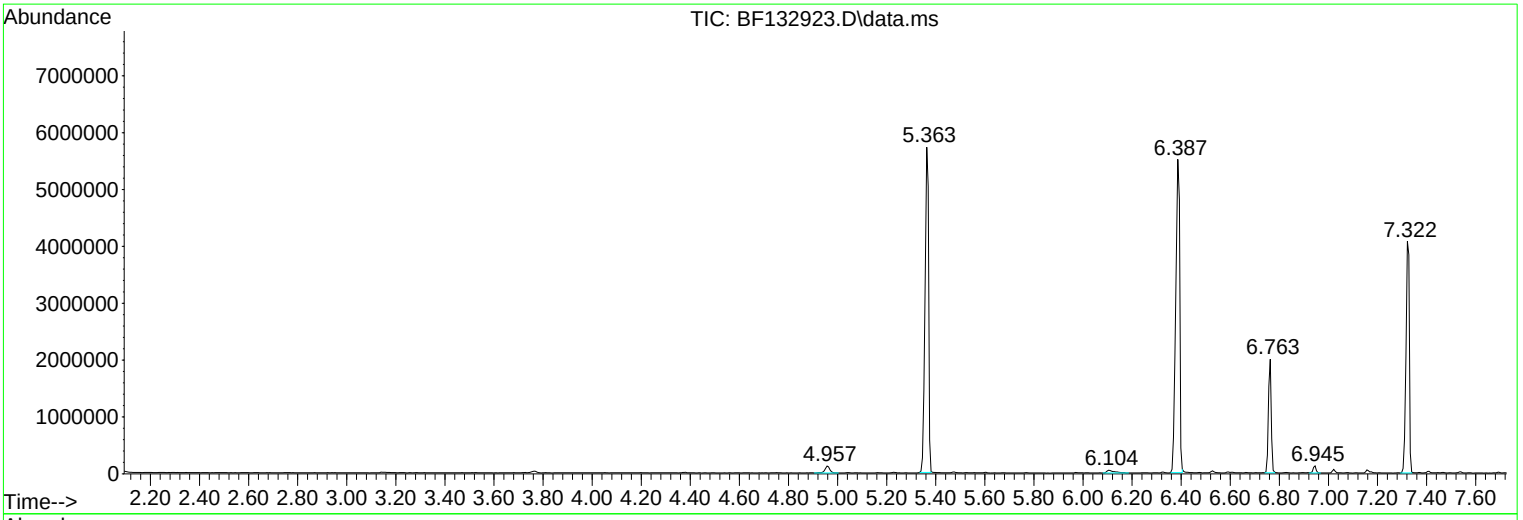
Sum of corrected areas: 56751621

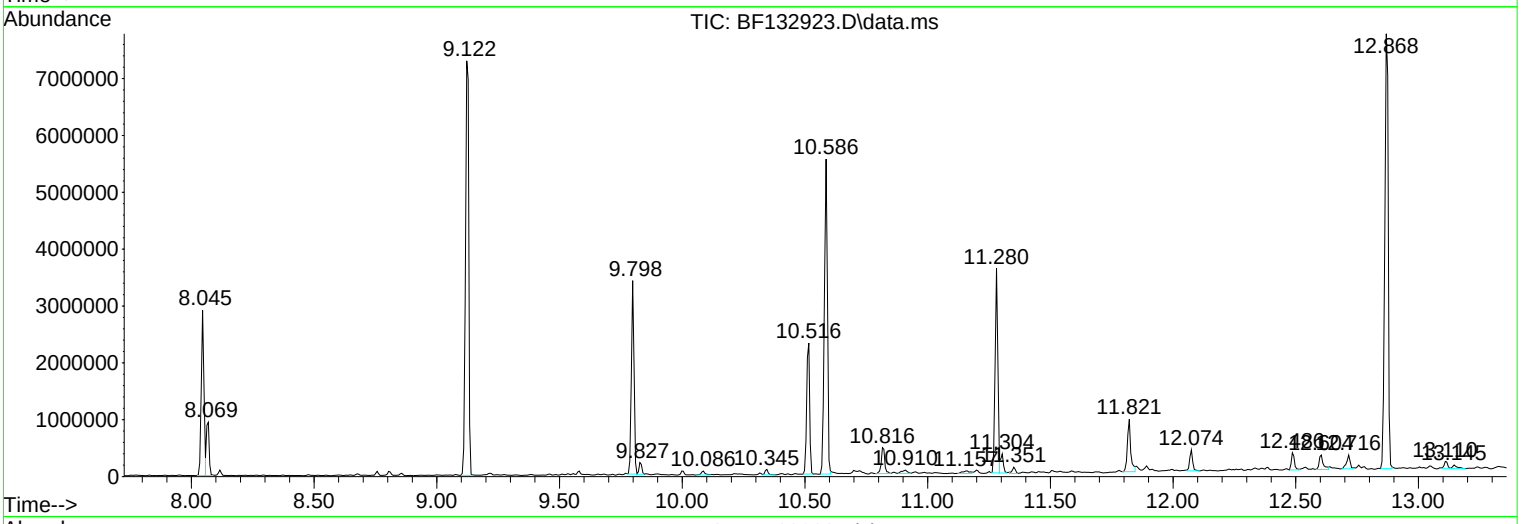
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041923\
Data File : BF132923.D
Acq On : 19 Apr 2023 21:12
Operator : CG\JU
Sample : 02366-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

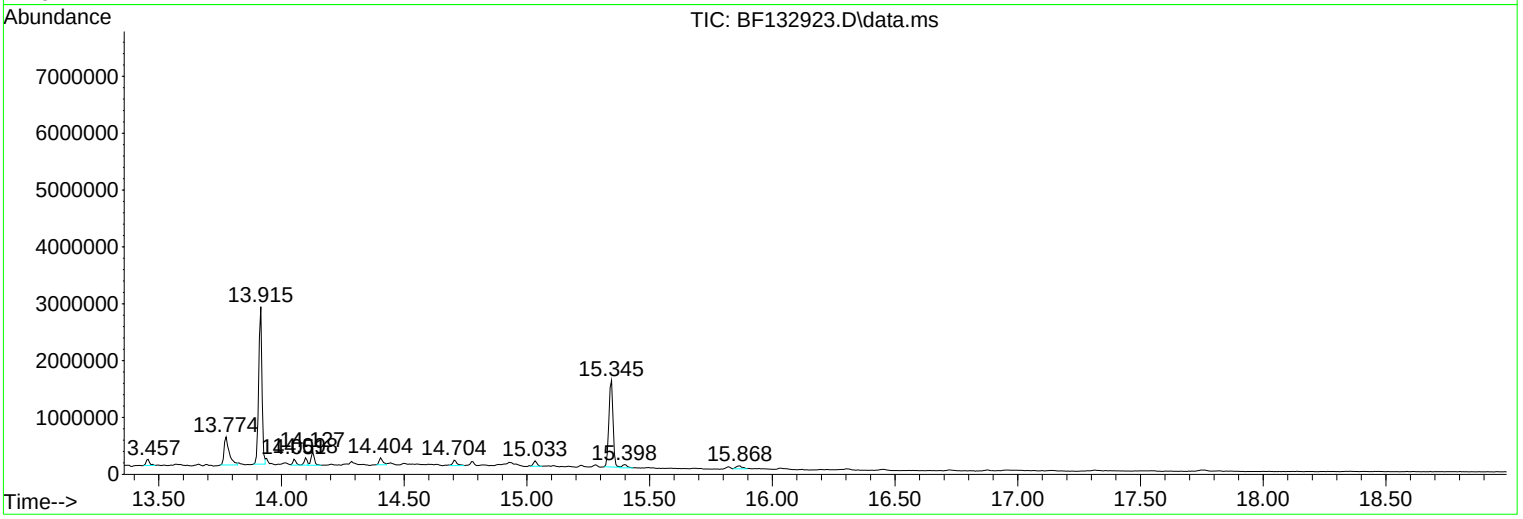
Instrument :
BNA_F
ClientSampleId :
20230348-COMP-26

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF041723.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\BF041923\
Data File : BF132923.D
Acq On : 19 Apr 2023 21:12
Operator : CG\JU
Sample : 02366-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20230348-COMP-26

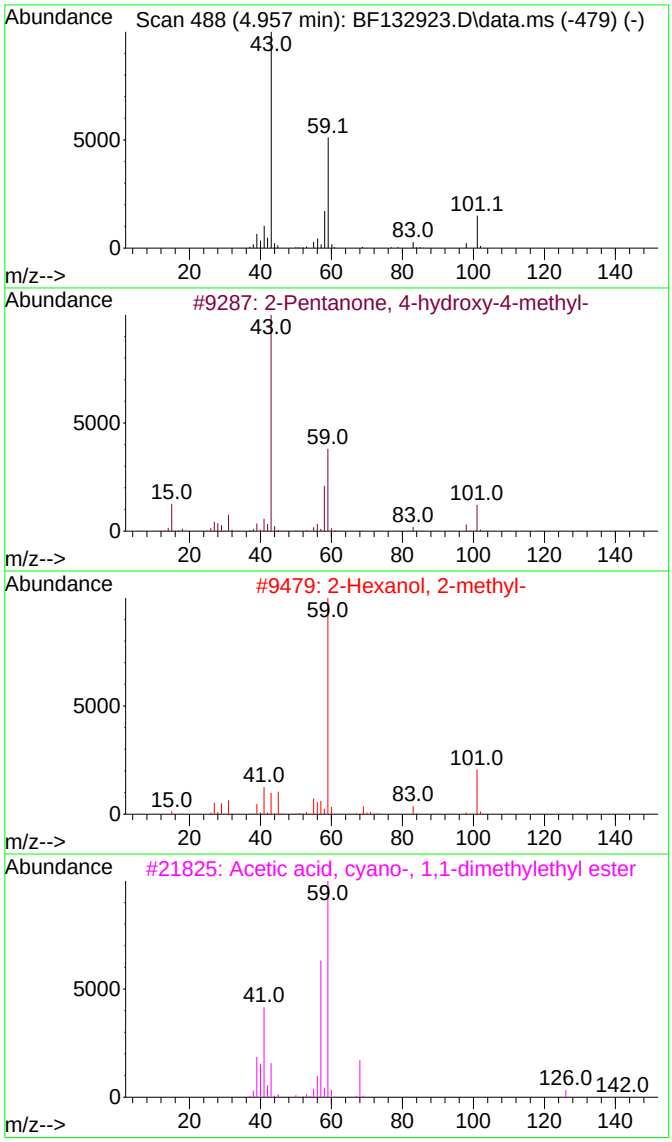
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF041723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

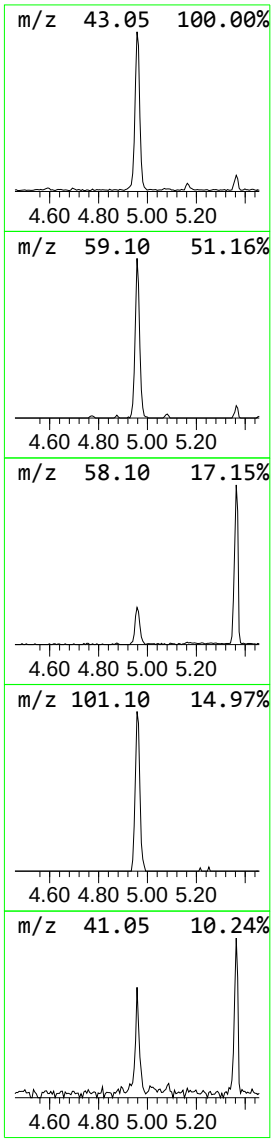
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.957	2.10 ng	166646	1,4-Dichlorobenzene-d4	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041923\
Data File : BF132923.D
Acq On : 19 Apr 2023 21:12
Operator : CG\JU
Sample : 02366-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20230348-COMP-26

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF041723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

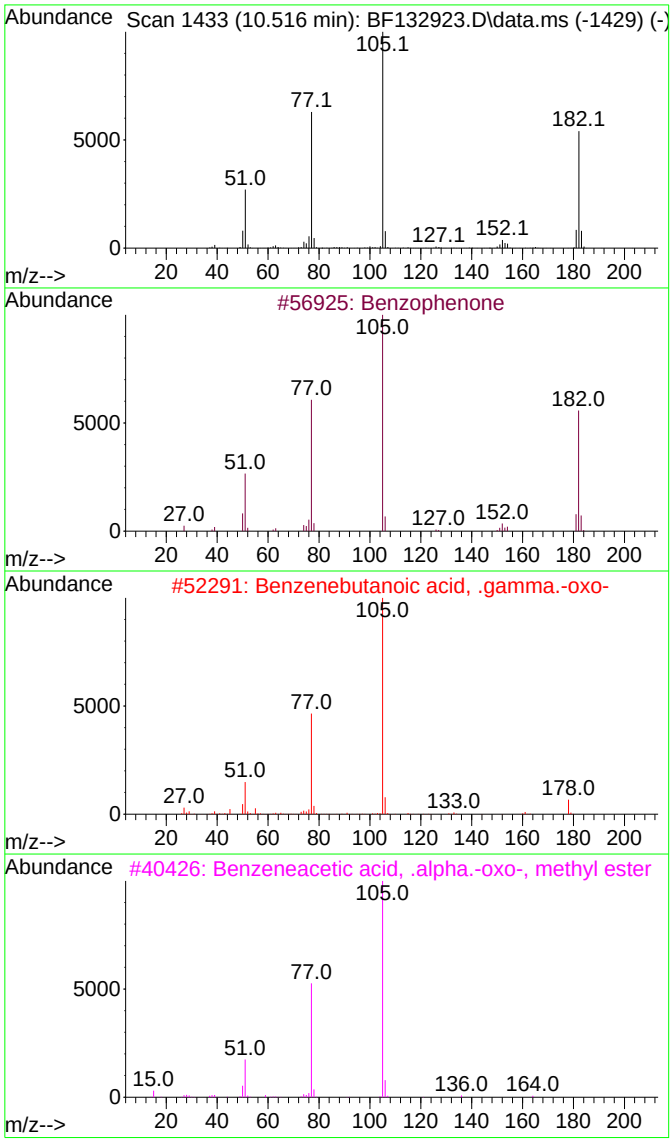
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

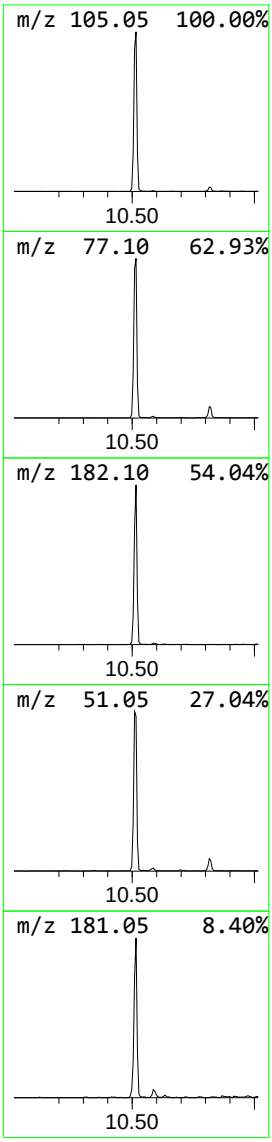
****

Peak Number 2 Benzophenone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.516	15.28 ng	1963840	Acenaphthene-d10	9.798

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	49
3	Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	49
4	N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47
5	Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041923\
Data File : BF132923.D
Acq On : 19 Apr 2023 21:12
Operator : CG\JU
Sample : 02366-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20230348-COMP-26

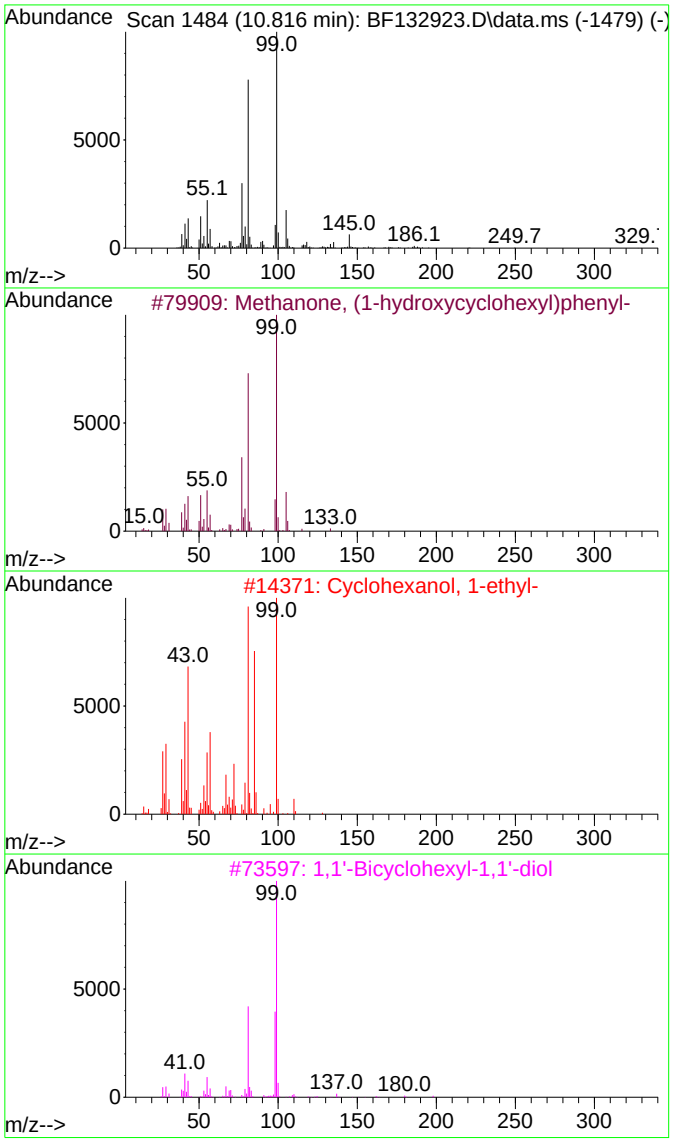
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF041723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

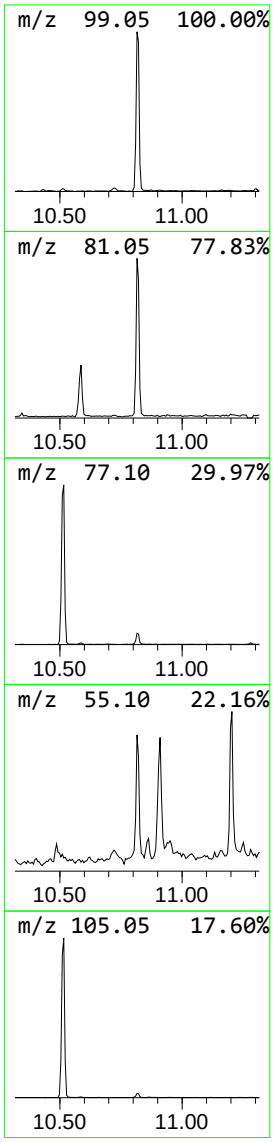
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Methanone, (1-hydroxycycloh... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.816	3.26 ng	458151	Phenanthrene-d10	11.280

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methanone, (1-hydroxycyclohexyl)...	204	C13H16O2	000947-19-3	91
2	Cyclohexanol, 1-ethyl-	128	C8H16O	001940-18-7	45
3	1,1'-Bicyclohexyl-1,1'-diol	198	C12H22O2	002888-11-1	45
4	Cyclohexanol, 1-(aminomethyl)-	129	C7H15NO	004000-72-0	45
5	1-(Prop-2-yn-1-yl)cyclohexyl car...	181	C10H15NO2	000358-52-1	45





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041923\
Data File : BF132923.D
Acq On : 19 Apr 2023 21:12
Operator : CG\JU
Sample : 02366-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20230348-COMP-26

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF041723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

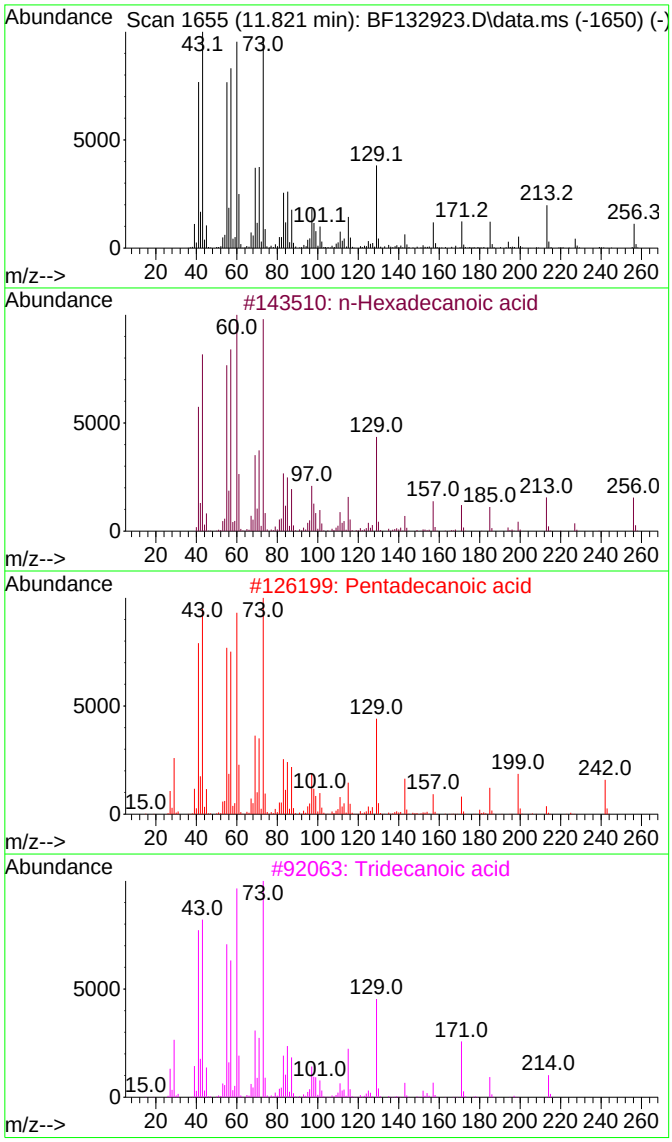
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

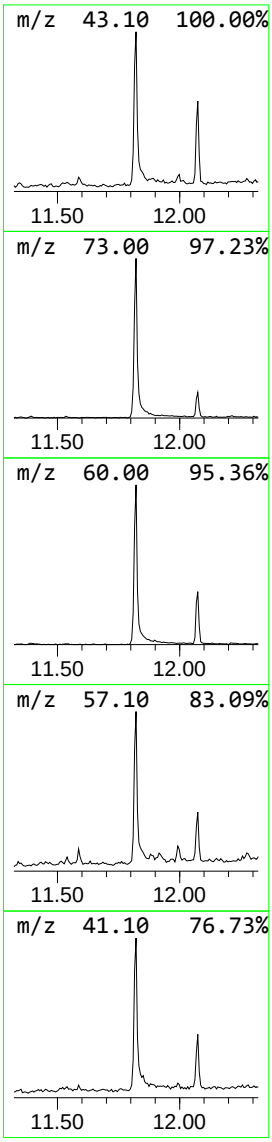
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.822	6.25 ng	879562	Phenanthrene-d10	11.280

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tridecanoic acid	214	C13H26O2	000638-53-9	89
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5	n-Decanoic acid	172	C10H20O2	000334-48-5	60





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041923\
Data File : BF132923.D
Acq On : 19 Apr 2023 21:12
Operator : CG\JU
Sample : 02366-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20230348-COMP-26

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF041723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

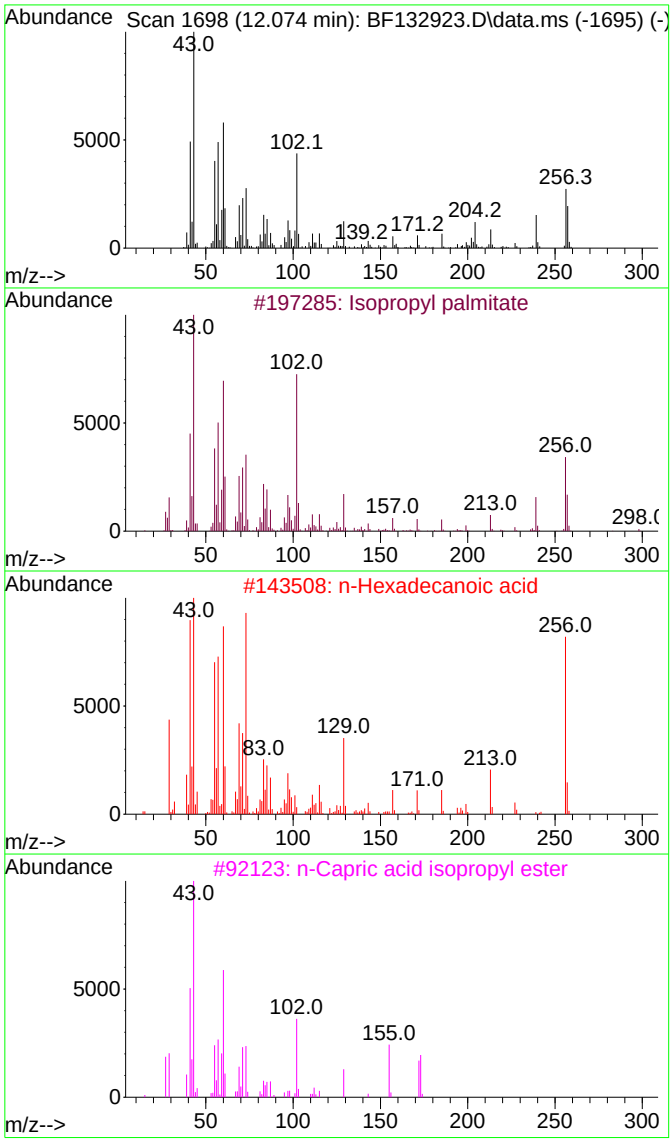
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

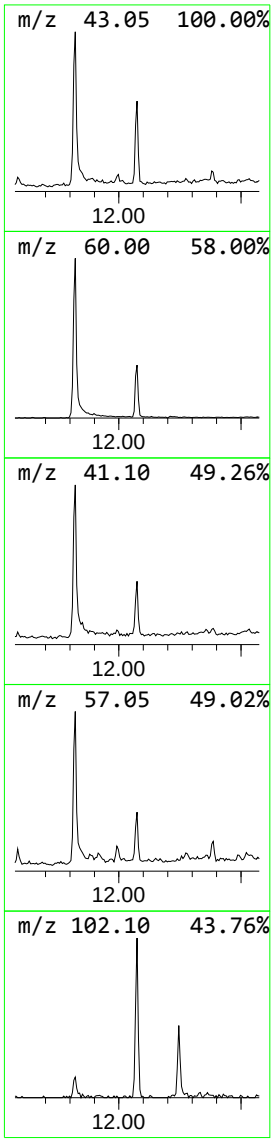
****

Peak Number 5 Isopropyl palmitate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.074	2.17 ng	304712	Phenanthrene-d10	11.280

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl palmitate	298	C19H38O2	000142-91-6	87
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	86
3	n-Capric acid isopropyl ester	214	C13H26O2	002311-59-3	47
4	Nonanoic acid, 1-methylethyl ester	200	C12H24O2	028267-32-5	35
5	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	22





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041923\
Data File : BF132923.D
Acq On : 19 Apr 2023 21:12
Operator : CG\JU
Sample : 02366-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20230348-COMP-26

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF041723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

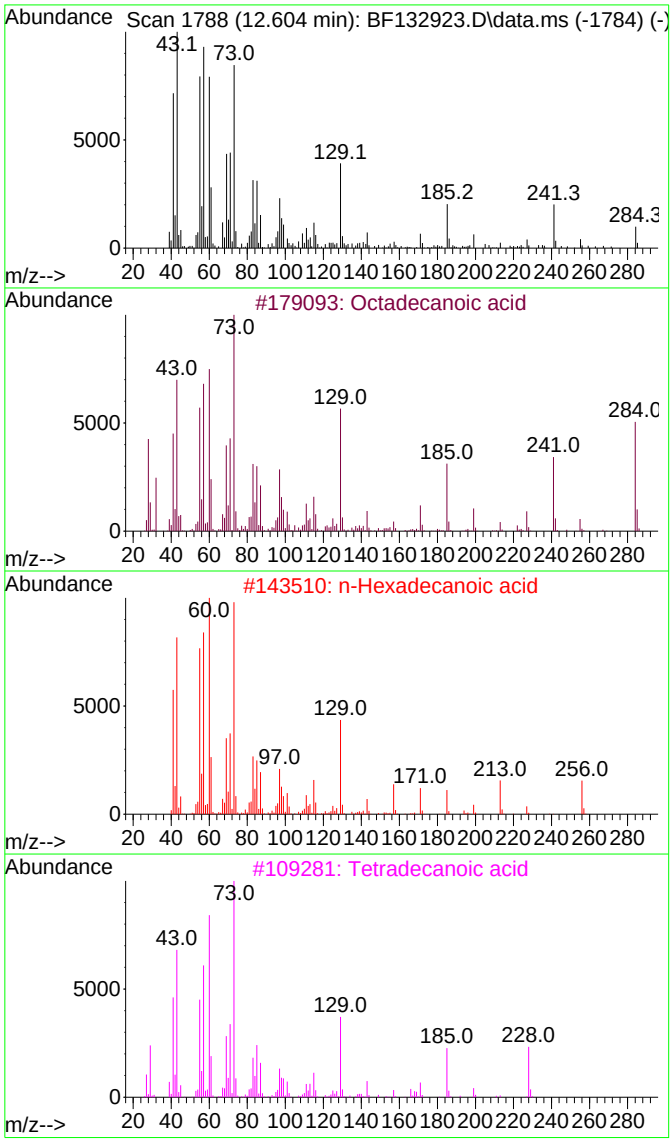
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

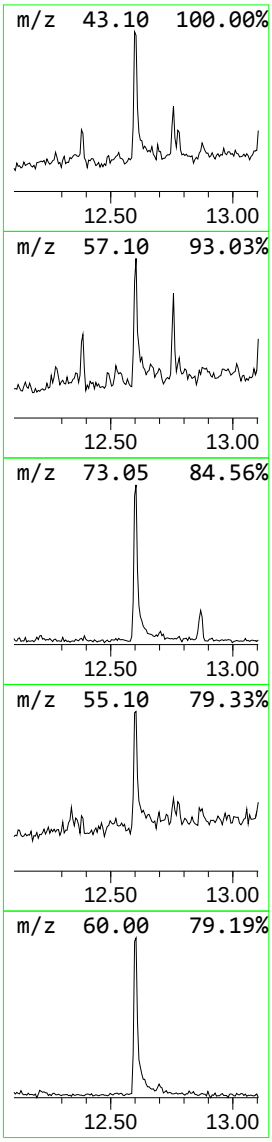
****

Peak Number 6 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.604	2.28 ng	293961	Chrysene-d12	13.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4	n-Decanoic acid	172	C10H20O2	000334-48-5	49
5	Oxalic acid, propyl tetradecyl e...	328	C19H36O4	1000309-26-7	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041923\
Data File : BF132923.D
Acq On : 19 Apr 2023 21:12
Operator : CG\JU
Sample : 02366-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20230348-COMP-26

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF041723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

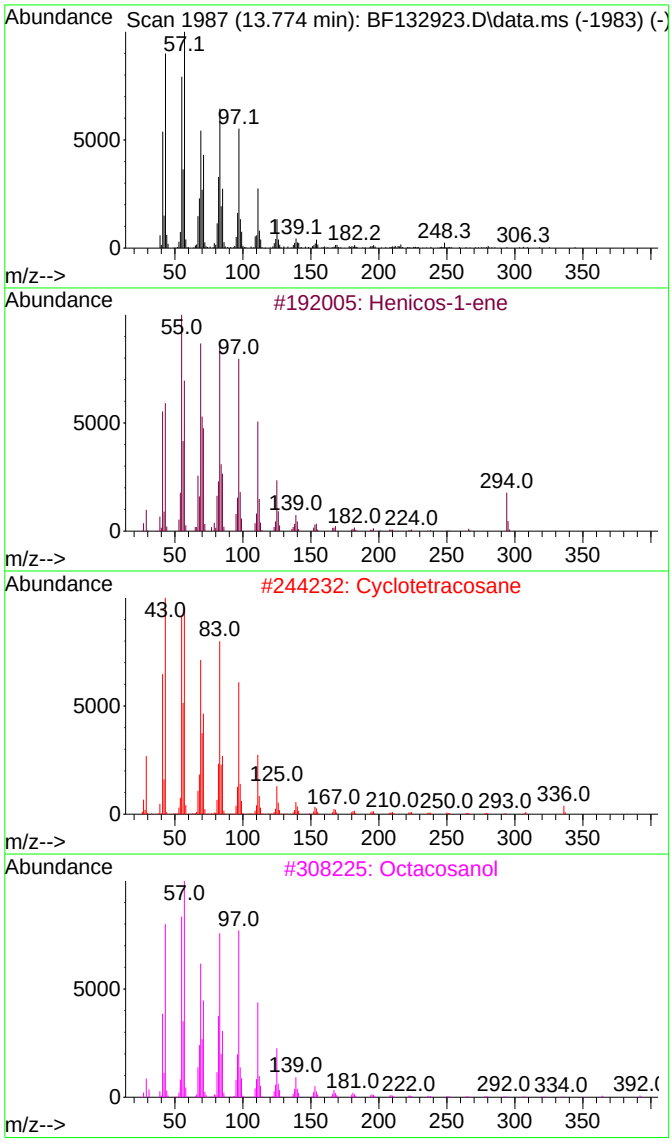
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

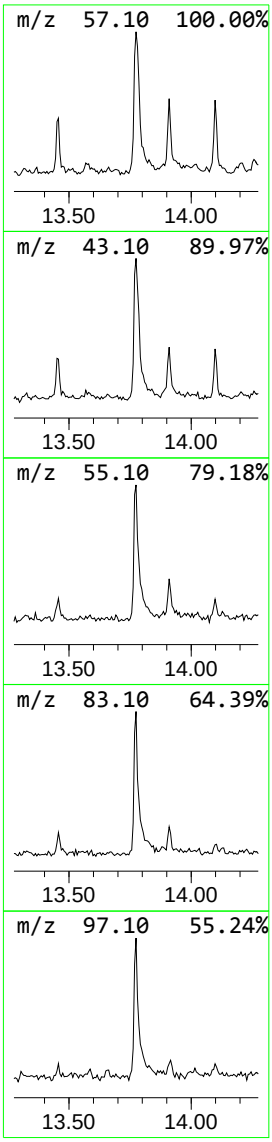
****

Peak Number 7 Henicos-1-ene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.774	5.53 ng	713264	Chrysene-d12	13.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Henicos-1-ene	294	C21H42	001599-68-4	95
2	Cyclotetracosane	336	C24H48	000297-03-0	95
3	Octacosanol	410	C28H58O	000557-61-9	94
4	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91
5	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041923\
Data File : BF132923.D
Acq On : 19 Apr 2023 21:12
Operator : CG\JU
Sample : 02366-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20230348-COMP-26

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF041723.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-...	4.957	2.1	ng	166646	1	6.763	1586980	20.0
Benzophenone	10.516	15.3	ng	1963840	3	9.798	2570000	20.0
Methanone, (1-h...	10.816	3.3	ng	458151	4	11.280	2813210	20.0
n-Hexadecanoic ...	11.822	6.3	ng	879562	4	11.280	2813210	20.0
Isopropyl palmi...	12.074	2.2	ng	304712	4	11.280	2813210	20.0
Octadecanoic acid	12.604	2.3	ng	293961	5	13.916	2580780	20.0
Henicos-1-ene	13.774	5.5	ng	713264	5	13.916	2580780	20.0