LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021521\
Data File : BF123209.D
Acq On : 15 Feb 2021 17:28
Operator : JU/CG
Sample : M1402-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-N9994

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-BF021221.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123209.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.140	3	9	15	rVB	420775	535305	12.56%	1.609%
2	5.487	573	578	581	rBV	3586095	3364551	78.93%	10.111%
3	6.492	744	749	765	rVB	3214131	3595407	84.34%	10.805%
4	6.869	809	813	816	rBV	1104536	859107	20.15%	2.582%
5	7.428	903	908	911	rBV	2281721	2243900	52.64%	6.743%
6	8.151	1027	1031	1035	rBV	1388579	1157757	27.16%	3.479%
7	9.228	1209	1214	1218	rBV	4165519	4011764	94.11%	12.056%
8	9.345	1230	1234	1246	rVB	684882	658228	15.44%	1.978%
9	9.622	1277	1281	1285	rBV	271168	212536	4.99%	0.639%
10	9.910	1323	1330	1333	rBV	1563483	1293084	30.33%	3.886%
11	10.492	1426	1429	1440	rBV	208513	315740	7.41%	0.949%
12	10.698	1459	1464	1468	rBV	2677008	2708726	63.54%	8.140%
13	11.398	1579	1583	1586	rBV	1473311	1371386	32.17%	4.121%
14	11.422	1586	1587	1590	rVV	206119	139838	3.28%	0.420%
15	11.474	1590	1596	1598	rVB2	44377	54927	1.29%	0.165%
16	11.892	1664	1667	1670	rBV3	35576	52873	1.24%	0.159%
17	11.927	1670	1673	1684	rVB2	606106	623704	14.63%	1.874%
18	12.016	1684	1688	1691	rBV	52477	60485	1.42%	0.182%
19	12.539	1774	1777	1782	rVB	52648	52453	1.23%	0.158%
20	12.616	1787	1790	1793	rVV	667538	528873	12.41%	1.589%
21	12.651	1793	1796	1799	rVB	122091	106999	2.51%	0.322%
22	12.716	1804	1807	1812	rBV2	213280	237030	5.56%	0.712%
23	12.845	1823	1829	1832	rBV	530858	486891	11.42%	1.463%
24	12.992	1848	1854	1860	rVB	4431328	4262935	100.00%	12.811%
25	13.174	1883	1885	1888	rVB	52118	44986	1.06%	0.135%
26	13.280	1898	1903	1905	rVB4	46991	51540	1.21%	0.155%
27	13.533	1942	1946	1948	rBV	42010	45169	1.06%	0.136%
28	13.568	1950	1952	1960	rVB6	30786	52230	1.23%	0.157%
29	13.680	1969	1971	1976	rVB	58715	56856	1.33%	0.171%
30	13.792	1985	1990	1993	rBV3	42219	68381	1.60%	0.205%
31	13.904	2004	2009	2026	rBV6	195569	621805	14.59%	1.869%
32	14.051	2026	2034	2036	rVV	1271224	1391796	32.65%	4.183%
33	14.074	2036	2038	2044	rVB	184783	170115	3.99%	0.511%
34	14.174	2052	2055	2059	rVB	273049	223823	5.25%	0.673%
35	14.521	2109	2114	2117	rBV3	58330	79850	1.87%	0.240%
36	14.563	2117	2121	2123	rBV4	36849	46379	1.09%	0.139%

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021521\
Data File : BF123209.D
Acq On : 15 Feb 2021 17:28
Operator : JU/CG
Sample : M1402-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RO-N9994

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-BF021221.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.827	2164	2166	2171	rVB2	37269	43130	1.01%	0.130%
38	14.910	2177	2180	2186	rVB3	33935	47574	1.12%	0.143%
39	15.092	2207	2211	2219	rVB	117531	235771	5.53%	0.709%
40	15.174	2221	2225	2228	rVB	62098	67727	1.59%	0.204%
41	15.398	2260	2263	2266	rVB	52856	57437	1.35%	0.173%
42	15.457	2270	2273	2279	rBV	49077	65264	1.53%	0.196%
43	15.527	2280	2285	2289	rBV	724110	891943	20.92%	2.680%
44	15.998	2361	2365	2370	rVB	58048	80061	1.88%	0.241%

Sum of corrected areas: 33276336

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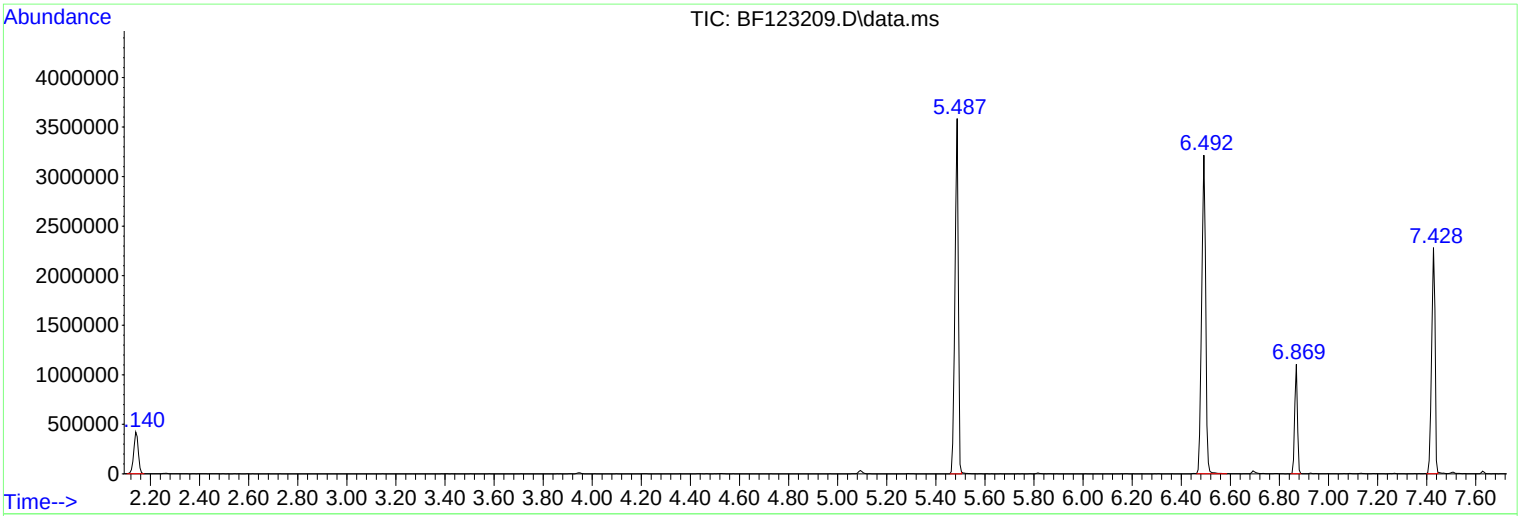
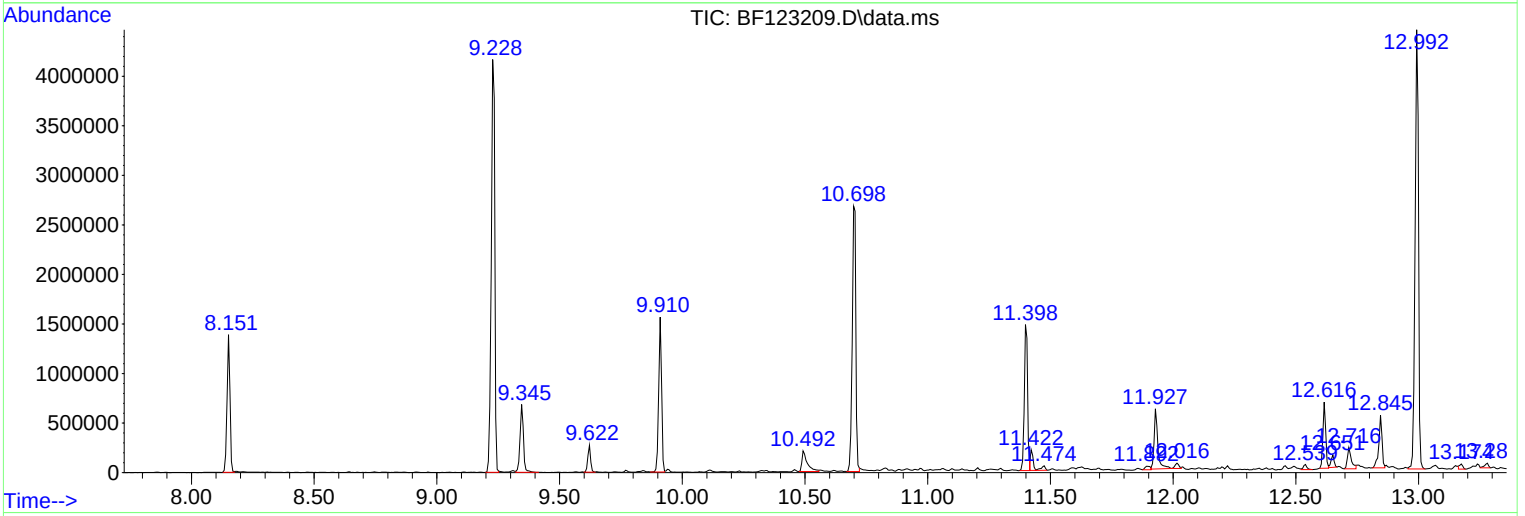
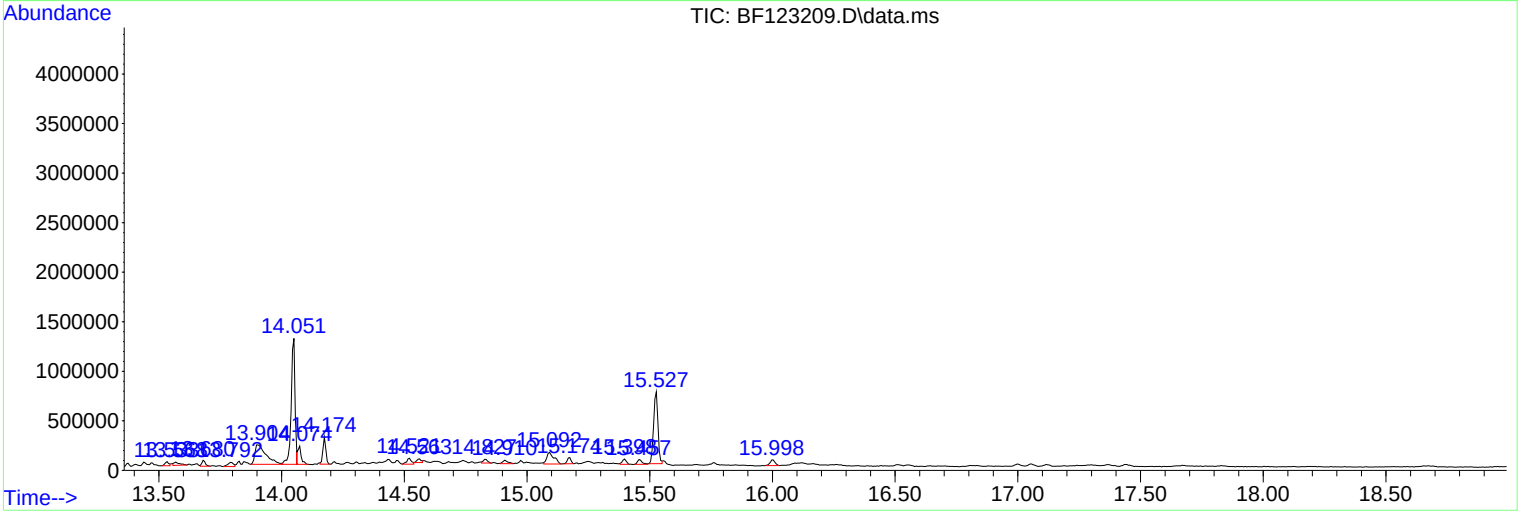
Instrument :
BNA_F
ClientSampleId :
RO-N9994

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P







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Operator : JU/CG
Sample : M1402-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-N9994

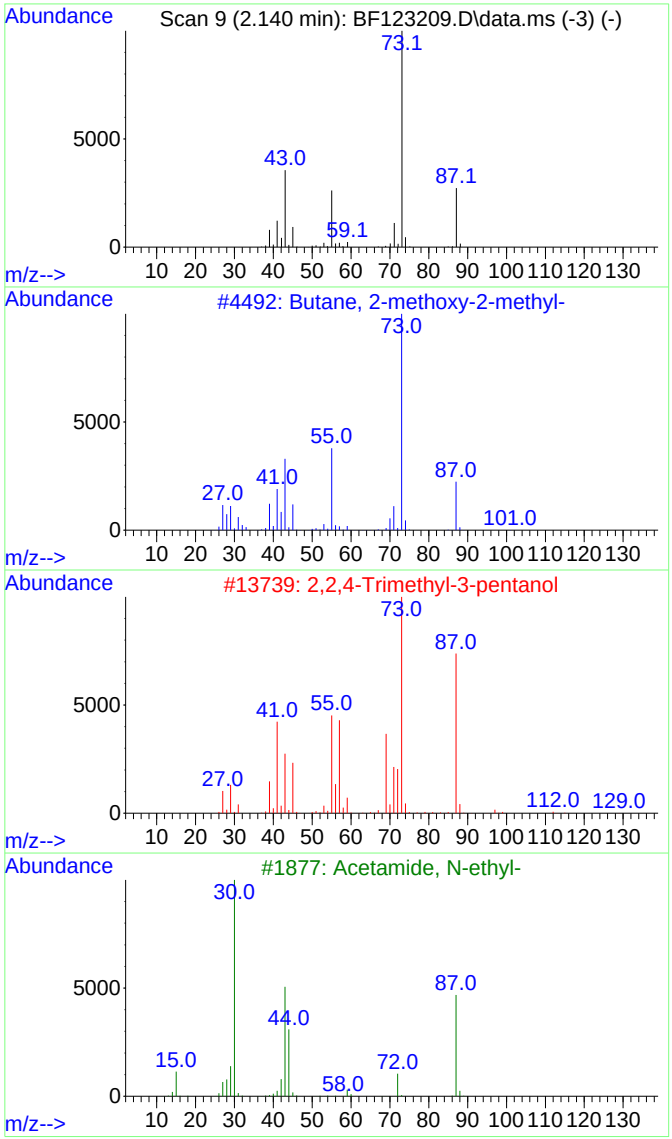
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

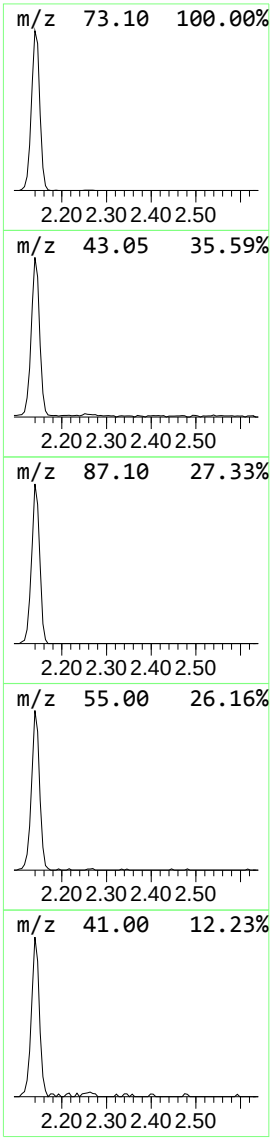
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.140	12.46 ng	535305	1,4-Dichlorobenzene-d4	6.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5	Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9





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Sample : M1402-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-N9994

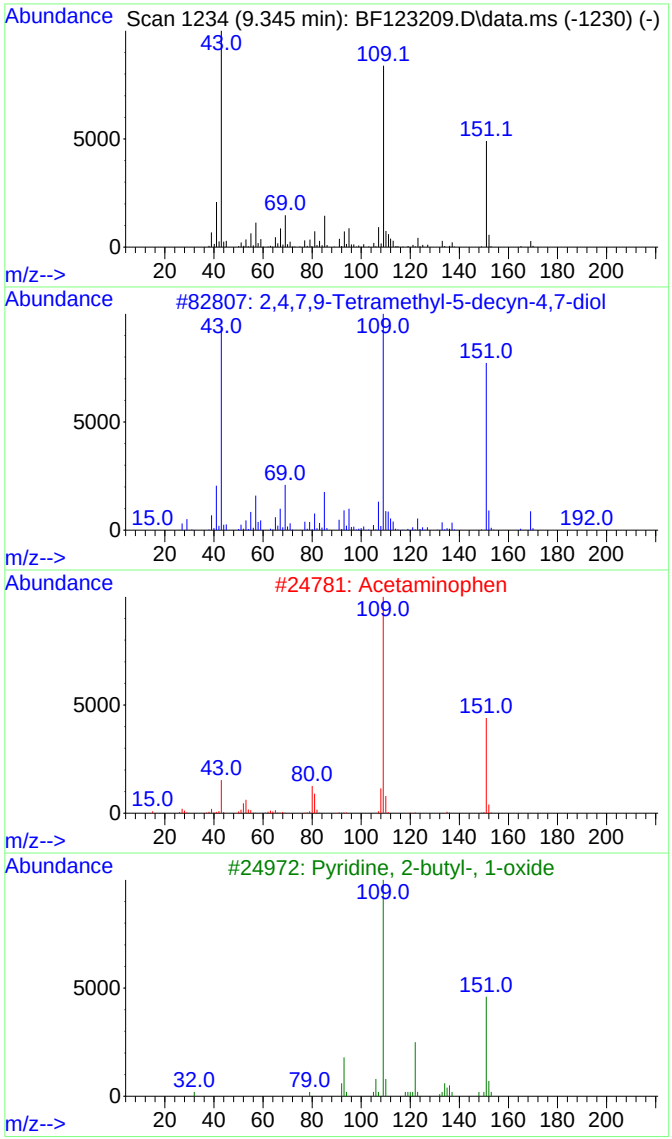
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

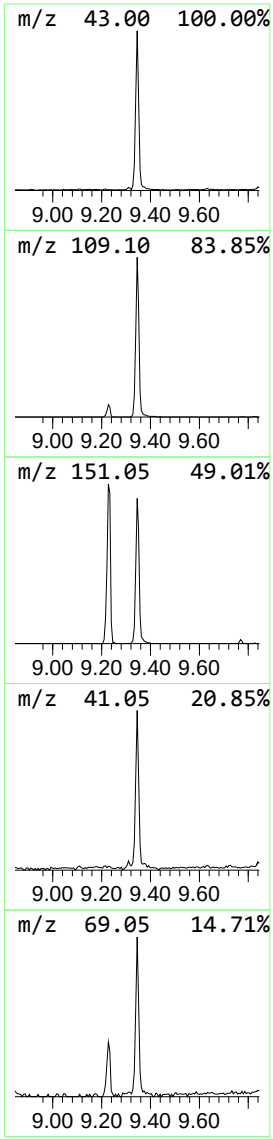
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.345	10.18 ng	658228	Acenaphthene-d10	9.910

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	91
2	Acetaminophen	151	C8H9NO2	000103-90-2	59
3	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	59
4	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	59
5	Metacetamol	151	C8H9NO2	000621-42-1	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021521\
Data File : BF123209.D
Acq On : 15 Feb 2021 17:28
Operator : JU/CG
Sample : M1402-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RO-N9994

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

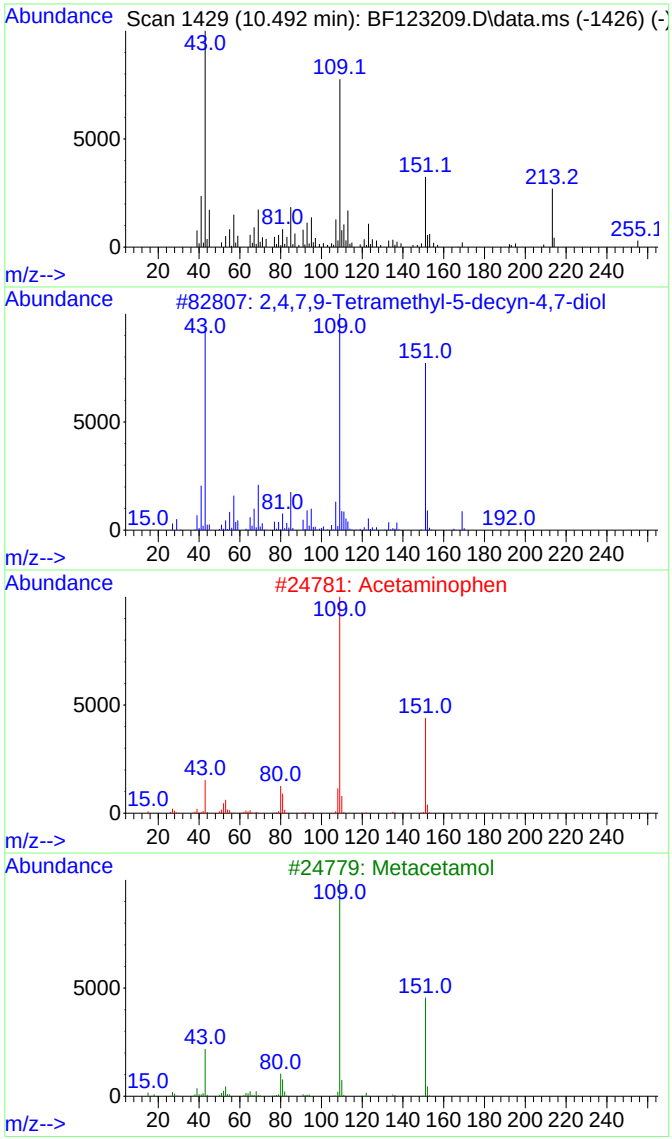
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

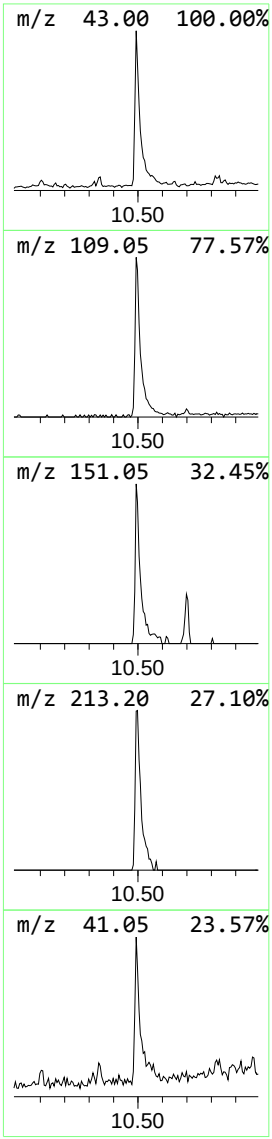
****

Peak Number 3 unknown10.492 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.492	4.88 ng	315740	Acenaphthene-d10	9.910

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	59
2	Acetaminophen	151	C8H9NO2	000103-90-2	46
3	Metacetamol	151	C8H9NO2	000621-42-1	46
4	4-Pyridinemethanol, acetate (ester)	151	C8H9NO2	001007-48-3	43
5	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021521\
Data File : BF123209.D
Acq On : 15 Feb 2021 17:28
Operator : JU/CG
Sample : M1402-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-N9994

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

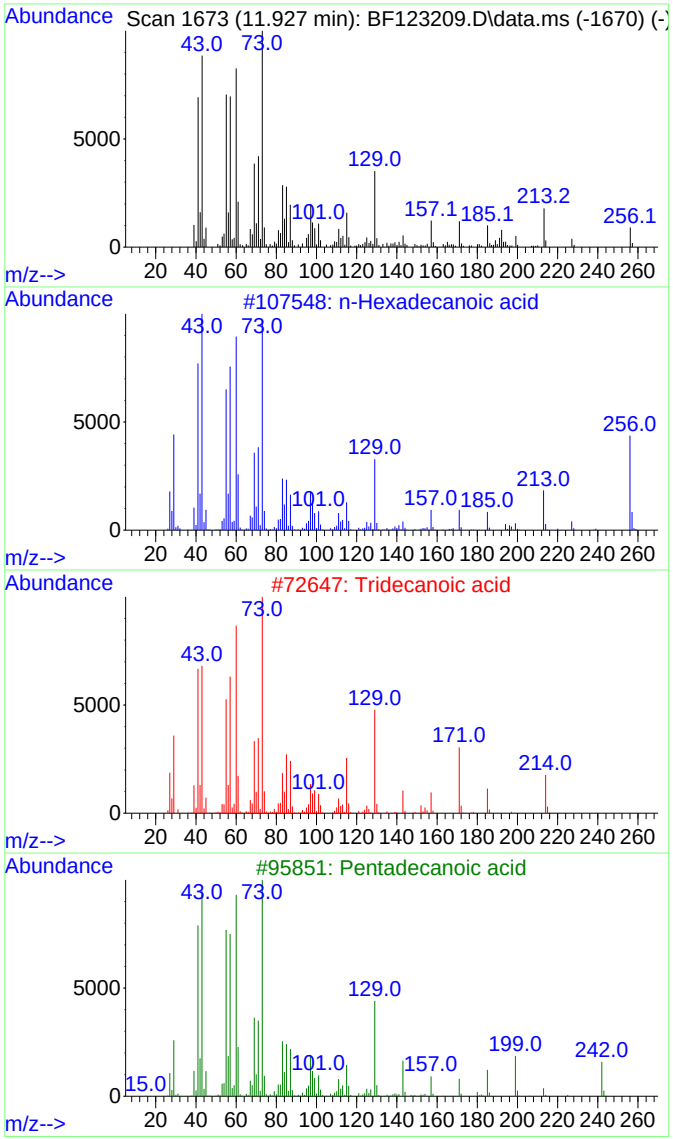
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

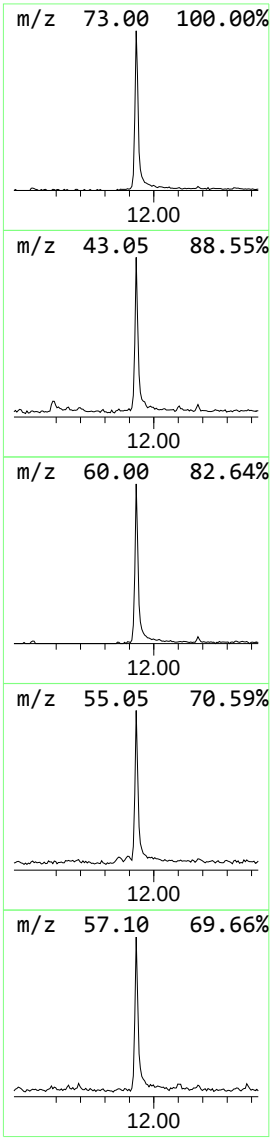
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.927	9.10 ng	623704	Phenanthrene-d10	11.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	Oxalic acid, dodecyl propyl ester	300	C17H32O4	1000309-26-5	25





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Data File : BF123209.D
Acq On : 15 Feb 2021 17:28
Operator : JU/CG
Sample : M1402-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-N9994

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

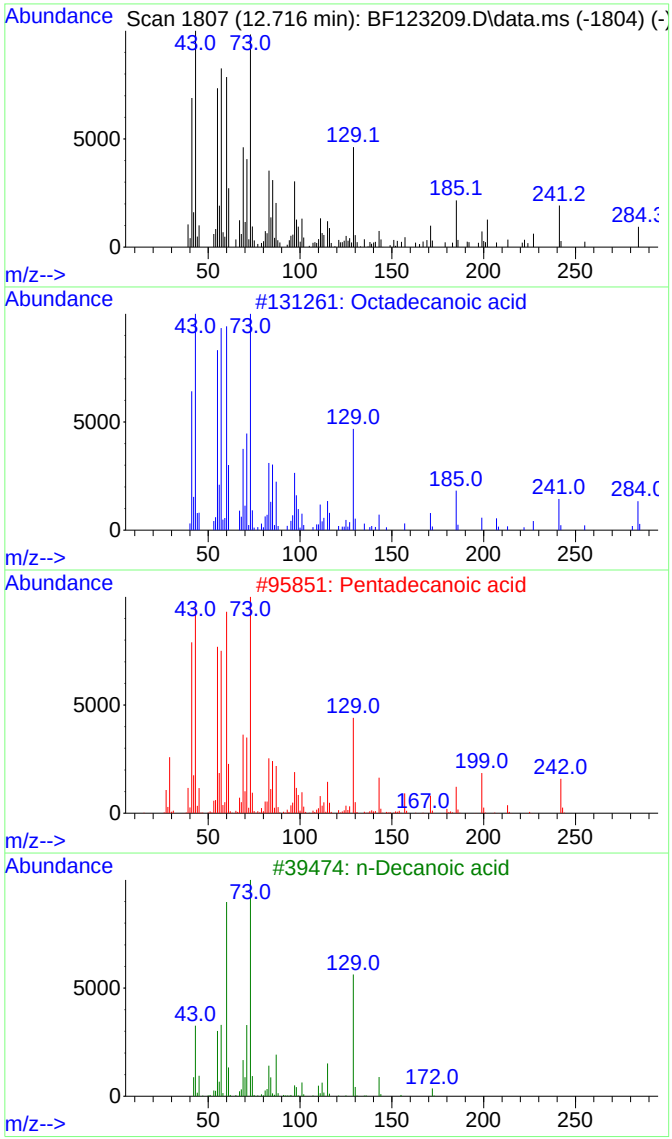
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

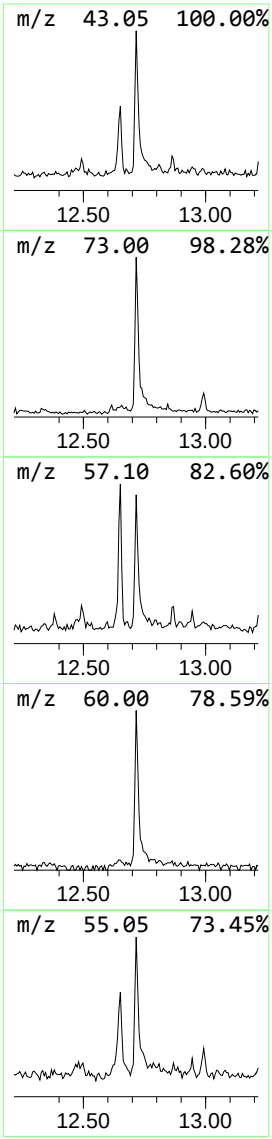
****

Peak Number 5 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.716	3.46 ng	237030	Phenanthrene-d10	11.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	n-Decanoic acid	172	C10H20O2	000334-48-5	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021521\
Data File : BF123209.D
Acq On : 15 Feb 2021 17:28
Operator : JU/CG
Sample : M1402-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-N9994

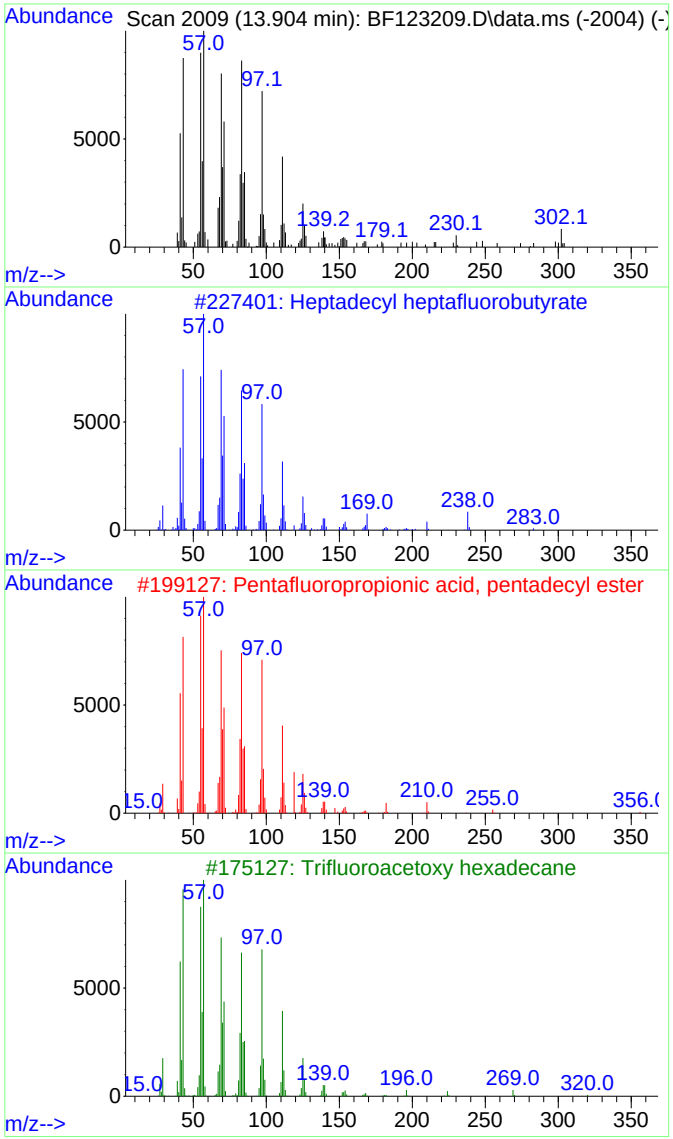
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

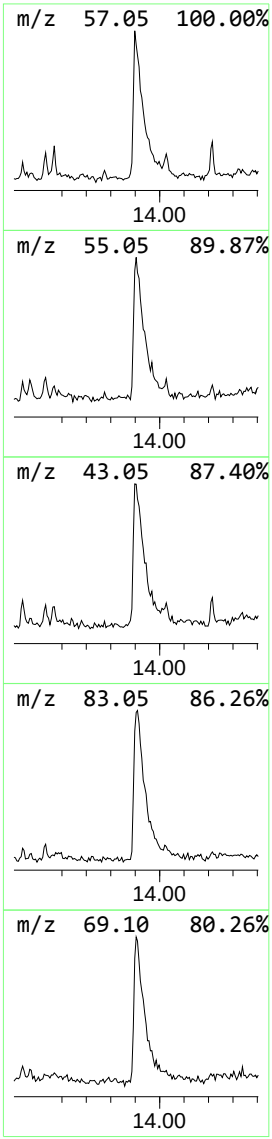
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Heptadecyl heptafluorobutyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.904	8.94 ng	621805	Chrysene-d12	14.051

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	95
2	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
4	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	94
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94





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Sample : M1402-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-N9994

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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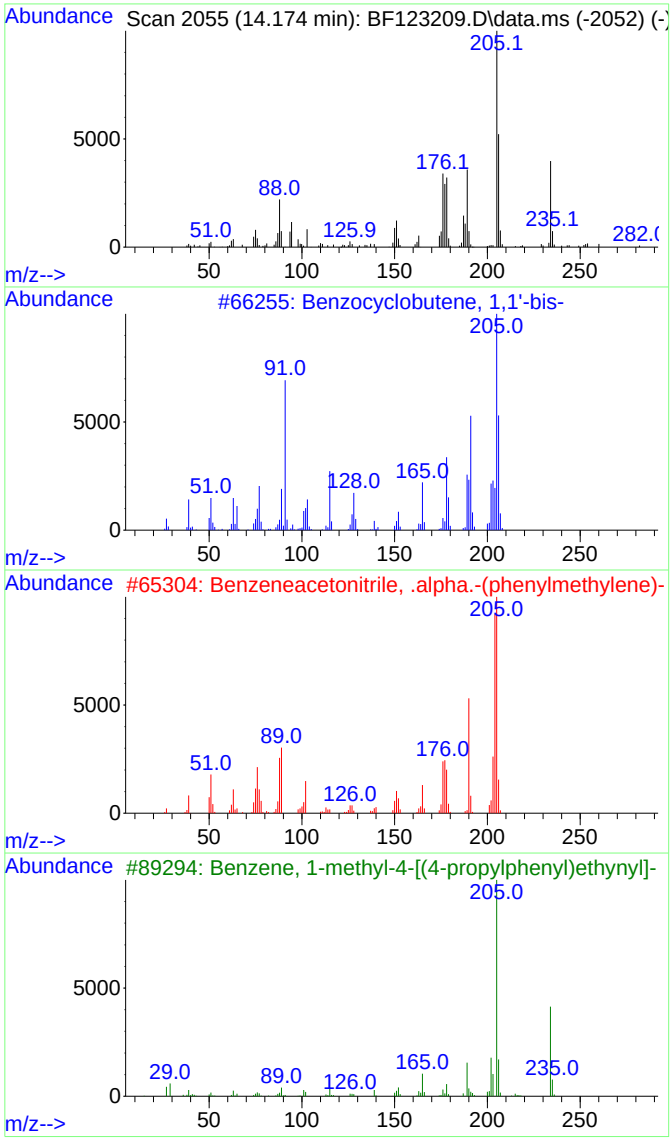
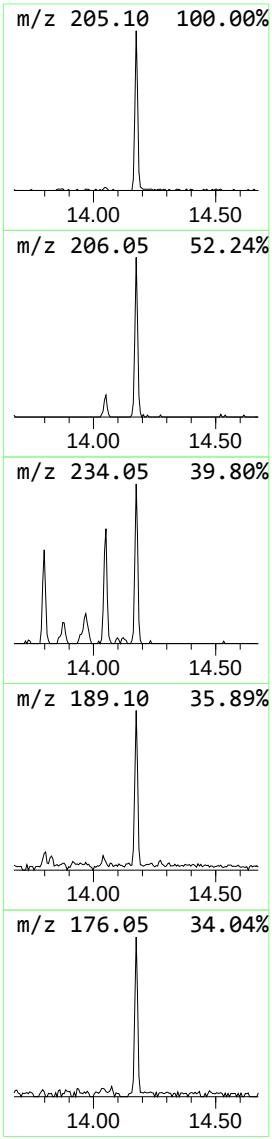
Peak Number 7 unknown14.174 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.174	3.22 ng	223823	Chrysene-d12	14.051

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzocyclobutene, 1,1'-bis-	206	C16H14	121754-51-6	47
2	Benzeneacetonitrile, .alpha.-(ph...	205	C15H11N	002510-95-4	43
3	Benzene, 1-methyl-4-[(4-propylph...	234	C18H18	184161-94-2	43
4	Phenanthrene-9-carboxaldehyde	206	C15H10O	004707-71-5	42
5	Phthalazine, 1-phenyl-	206	C14H10N2	007188-22-9	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021521\
Data File : BF123209.D
Acq On : 15 Feb 2021 17:28
Operator : JU/CG
Sample : M1402-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-N9994

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.140	12.5	ng	535305	1	6.869	859107	20.0
2,4,7,9-Tetrame...	9.345	10.2	ng	658228	3	9.910	1293080	20.0
unknown10.492	10.492	4.9	ng	315740	3	9.910	1293080	20.0
n-Hexadecanoic ...	11.927	9.1	ng	623704	4	11.398	1371390	20.0
Octadecanoic acid	12.716	3.5	ng	237030	4	11.398	1371390	20.0
Heptadecyl hept...	13.904	8.9	ng	621805	5	14.051	1391800	20.0
unknown14.174	14.174	3.2	ng	223823	5	14.051	1391800	20.0