LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071621\
Data File : BF124600.D
Acq On : 16 Jul 2021 17:14
Operator : JU/CG
Sample : M3061-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB-2021-WW-000-08

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-BF070721.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124600.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.228	20	24	28	rBB	22911	27002	8.99%	2.154%
2	3.081	165	169	173	rBB	2299	3047	1.01%	0.243%
3	4.681	435	441	444	rBB	263414	300282	100.00%	23.957%
4	5.528	582	585	588	rBB	54389	45979	15.31%	3.668%
5	6.528	752	755	759	rBB	33580	28958	9.64%	2.310%
6	6.922	819	822	825	rBB	42226	32101	10.69%	2.561%
7	7.481	913	917	920	rBB	82270	83903	27.94%	6.694%
8	8.104	1019	1023	1031	rBB	54824	54268	18.07%	4.330%
9	8.204	1036	1040	1043	rBB	55399	45966	15.31%	3.667%
10	8.480	1085	1087	1090	rBB	6626	4355	1.45%	0.347%
11	9.280	1219	1223	1226	rBV	190039	170680	56.84%	13.617%
12	9.375	1237	1239	1241	rBV	7689	5449	1.81%	0.435%
13	9.769	1303	1306	1313	rBB2	7793	12090	4.03%	0.965%
14	9.963	1336	1339	1342	rBB	73766	54523	18.16%	4.350%
15	10.163	1369	1373	1375	rBB	6735	5633	1.88%	0.449%
16	10.751	1469	1473	1476	rBB	121135	97786	32.56%	7.802%
17	11.451	1589	1592	1595	rBV	73870	58336	19.43%	4.654%
18	11.839	1656	1658	1660	rBB	5766	3837	1.28%	0.306%
19	11.968	1676	1680	1683	rBB	13713	9950	3.31%	0.794%
20	12.551	1776	1779	1781	rBB	9224	7228	2.41%	0.577%
21	12.757	1810	1814	1817	rBB	9766	7794	2.60%	0.622%
22	13.039	1858	1862	1865	rBV	164840	140544	46.80%	11.213%
23	14.092	2038	2041	2044	rBB	42285	31189	10.39%	2.488%
24	15.592	2291	2296	2299	rBB2	18303	22523	7.50%	1.797%

Sum of corrected areas: 1253423

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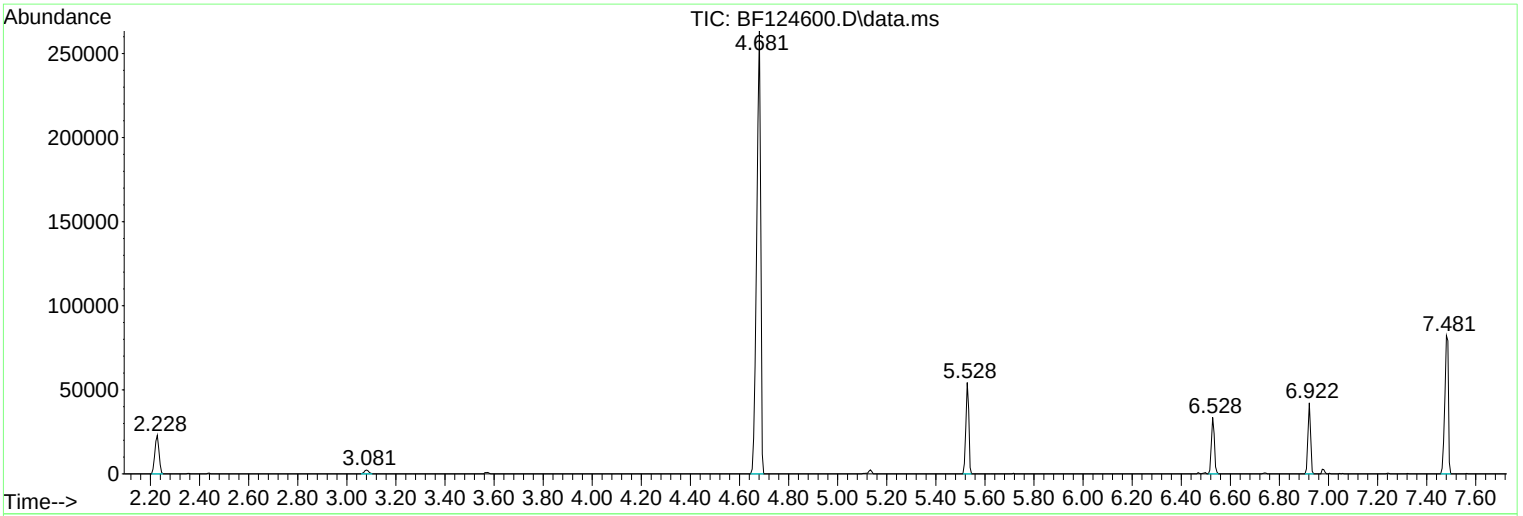
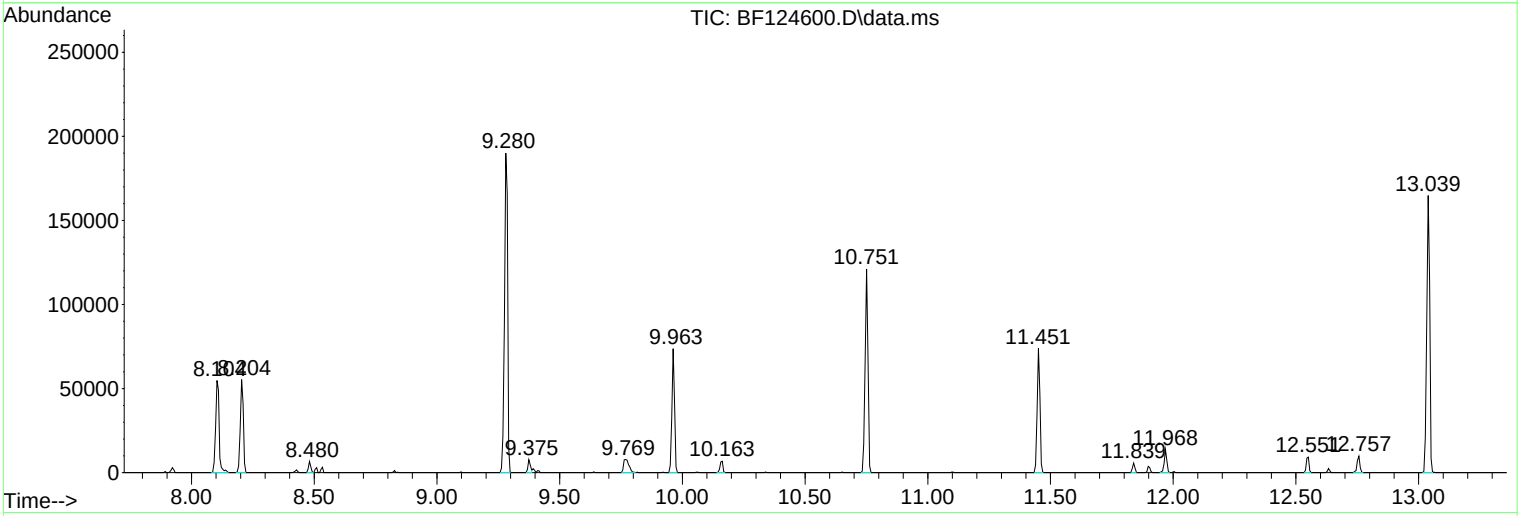
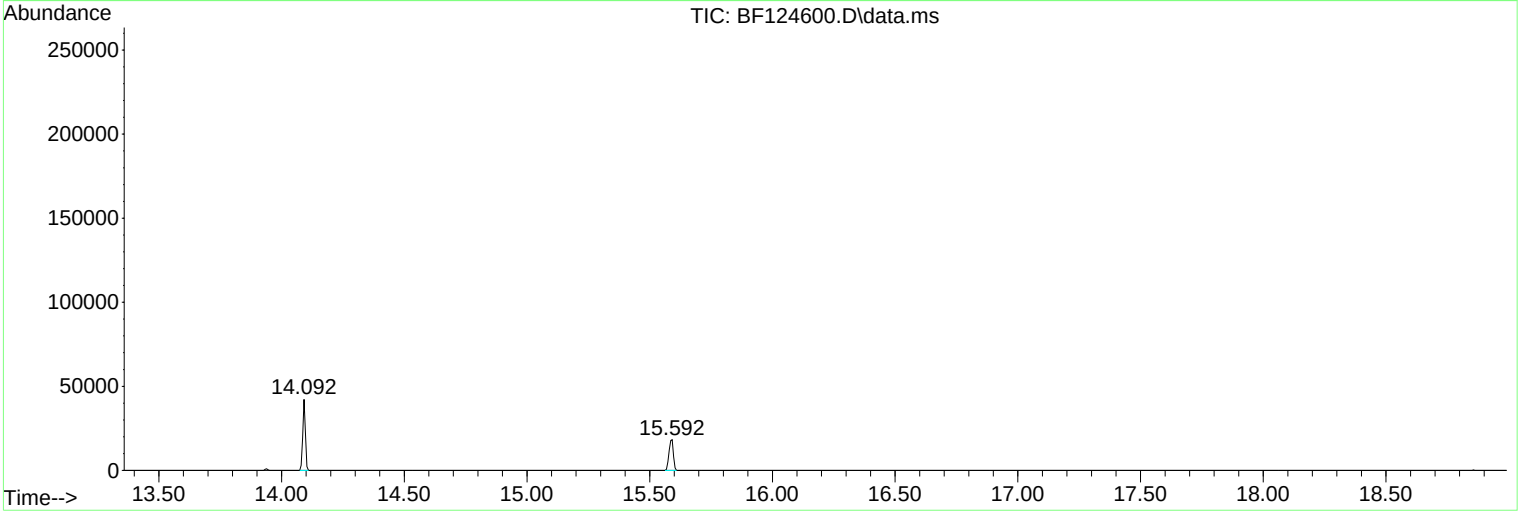
Instrument :
BNA_F
ClientSampleId :
PB-2021-WW-000-08

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.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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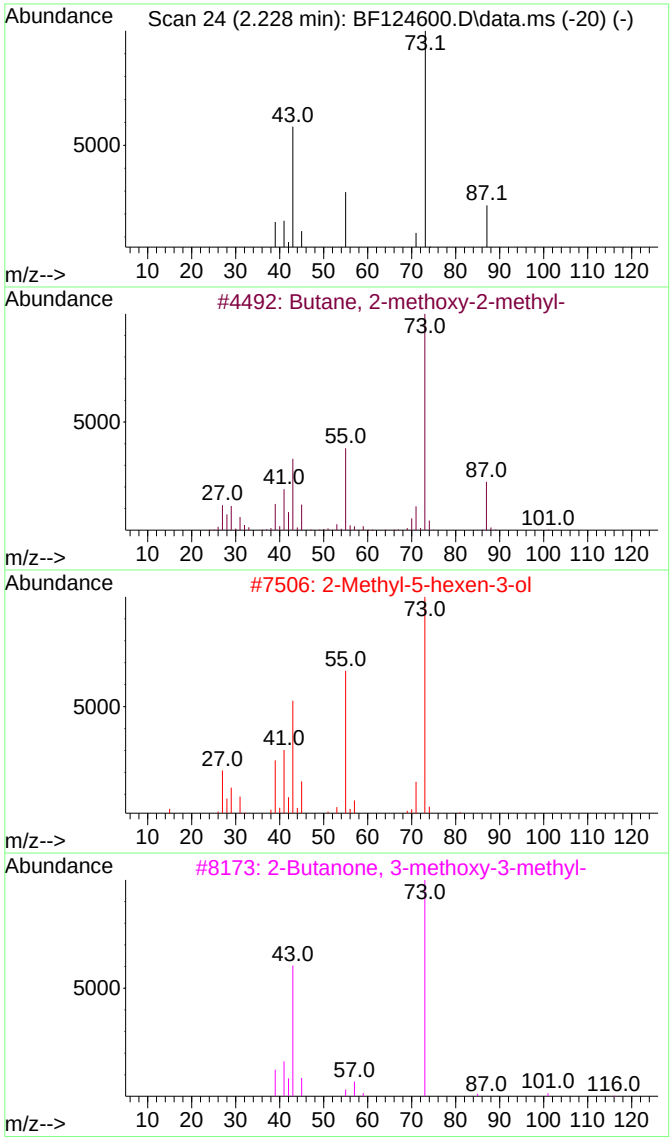
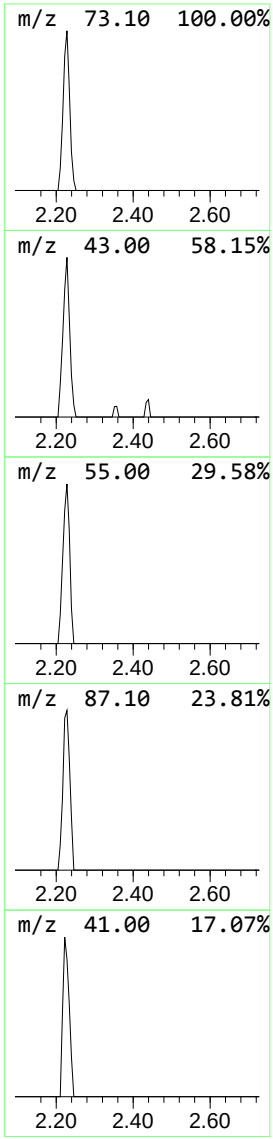
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.228	16.82 ng	27002	1,4-Dichlorobenzene-d4	6.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	33
3	2-Butanone, 3-methoxy-3-methyl-	116	C6H12O2	036687-98-6	9
4	Isobutylamine	73	C4H11N	000078-81-9	5
5	N-Ethylformamide	73	C3H7NO	000627-45-2	5





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Data File : BF124600.D
Acq On : 16 Jul 2021 17:14
Operator : JU/CG
Sample : M3061-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB-2021-WW-000-08

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

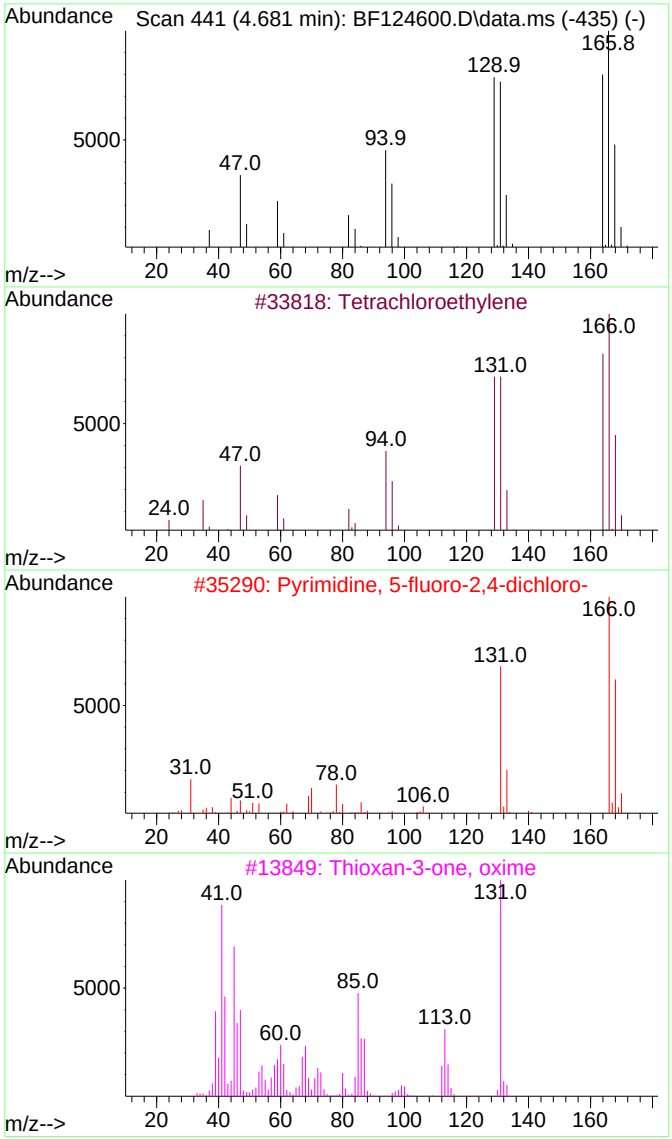
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

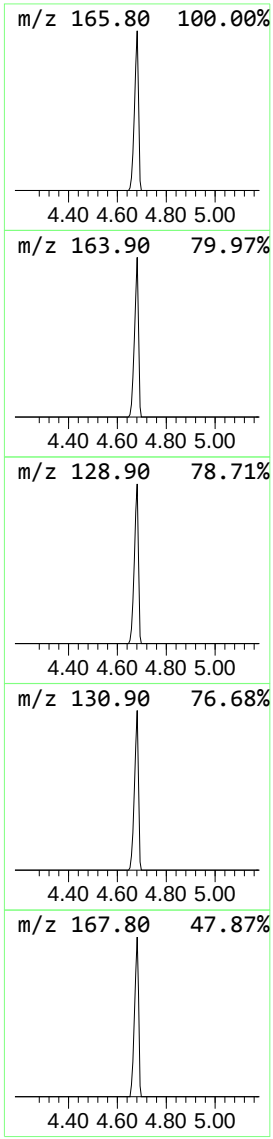
****

Peak Number 2 unknown4.681 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.681	187.09 ng	300282	1,4-Dichlorobenzene-d4	6.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetrachloroethylene	164	C2Cl4	000127-18-4	98
2	Pyrimidine, 5-fluoro-2,4-dichloro-	166	C4HCl2FN2	002927-71-1	35
3	Thioxan-3-one, oxime	131	C5H9NOS	058230-51-6	9
4	1,3-Dichloro-4-fluorobenzene	164	C6H3Cl2F	001435-48-9	9
5	2-Chloroquinoxaline	164	C8H5ClN2	001448-87-9	9





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Sample : M3061-02
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Instrument :
BNA_F
ClientSampleId :
PB-2021-WW-000-08

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.M
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TIC Library : C:\DATABASE\NIST11.L
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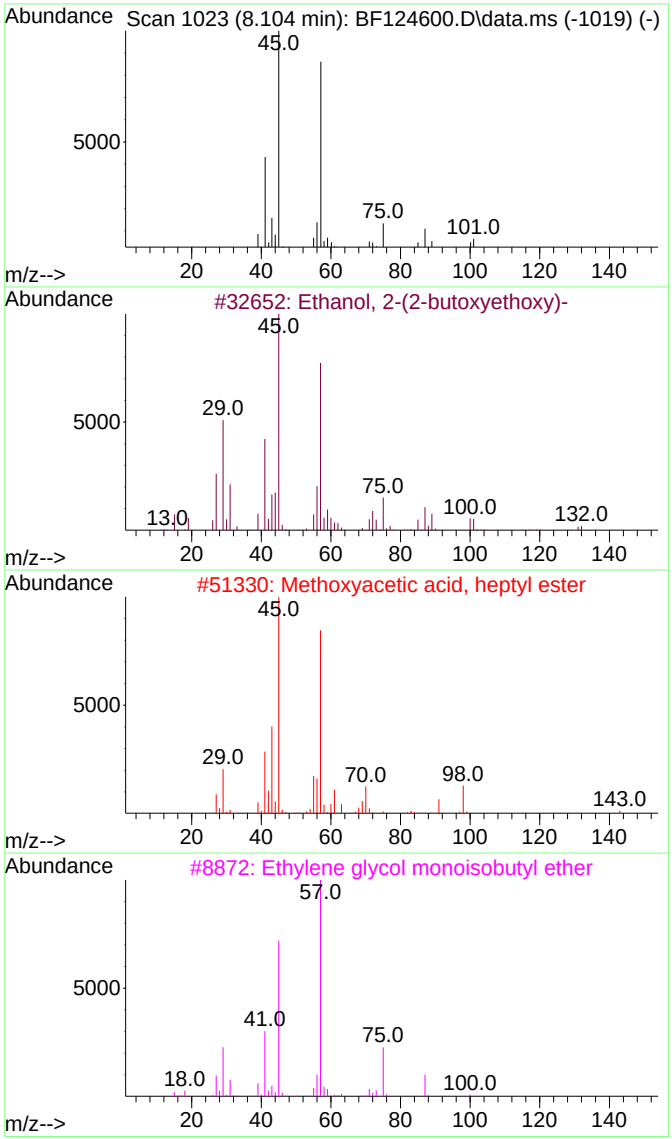
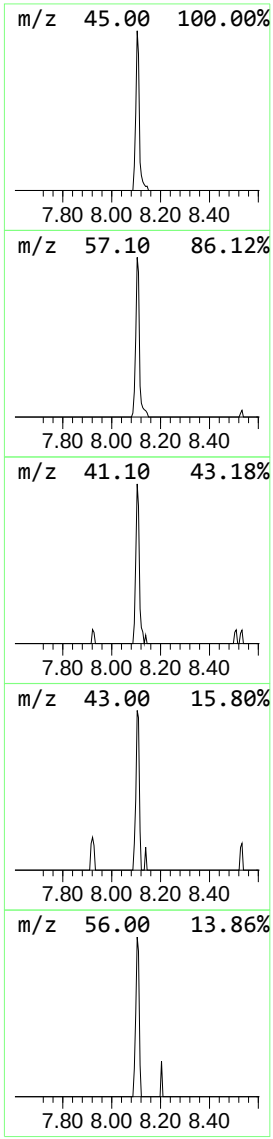
****
Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.104	23.61 ng	54268	Naphthalene-d8	8.204

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	72
2	Methoxyacetic acid, heptyl ester	188	C10H20O3	168920-36-3	53
3	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	45
4	2-Propanol, 1-butoxy-	132	C7H16O2	005131-66-8	45
5	Propanoic acid, 2-(methoxymethoxy)-	134	C5H10O4	081327-29-9	43





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Sample : M3061-02
Misc :
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Instrument :
BNA_F
ClientSampleId :
PB-2021-WW-000-08

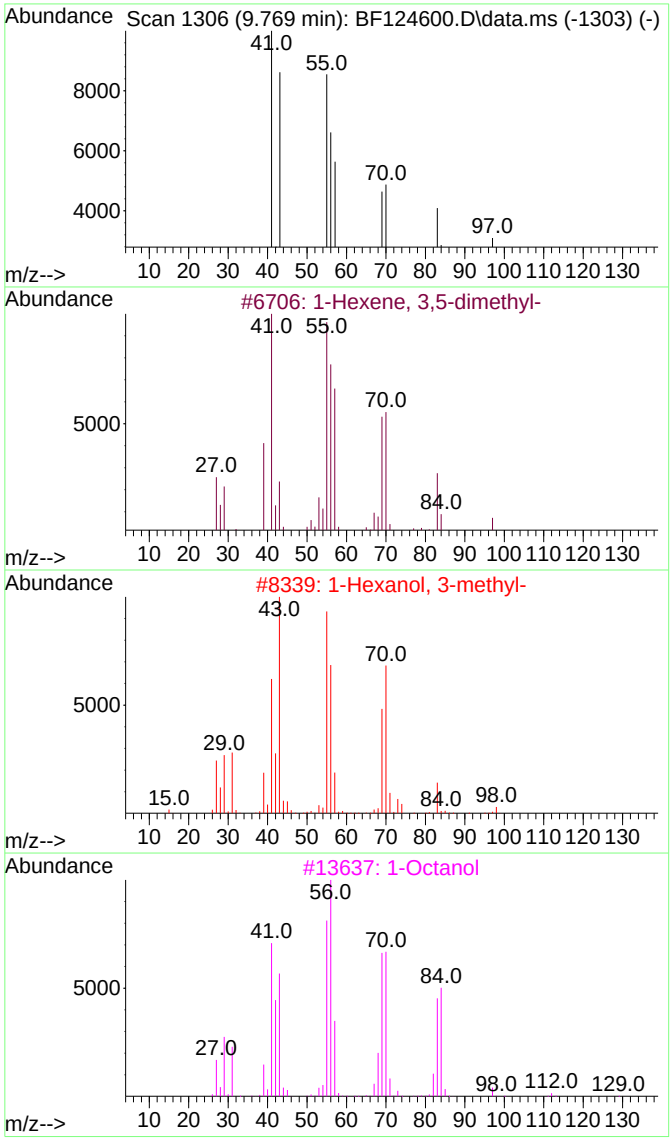
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

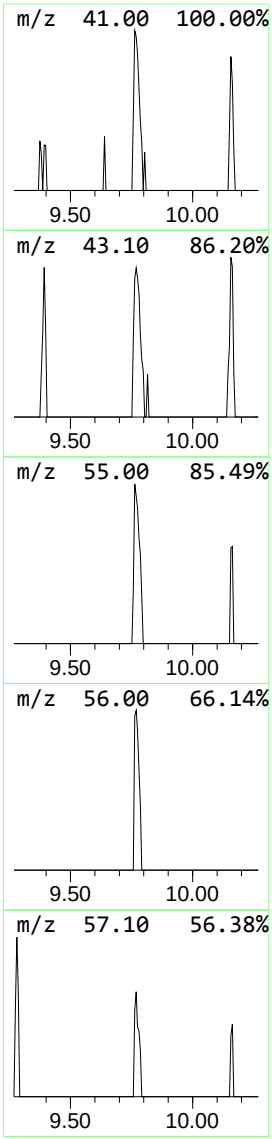
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1-Hexene, 3,5-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.769	4.43 ng	12090	Acenaphthene-d10	9.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexene, 3,5-dimethyl-	112	C8H16	007423-69-0	53
2	1-Hexanol, 3-methyl-	116	C7H16O	013231-81-7	50
3	1-Octanol	130	C8H18O	000111-87-5	45
4	1-Heptanol, 4-methyl-	130	C8H18O	000817-91-4	40
5	1-Heptanol, 6-methyl-	130	C8H18O	001653-40-3	38





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Sample : M3061-02
Misc :
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Instrument :
BNA_F
ClientSampleId :
PB-2021-WW-000-08

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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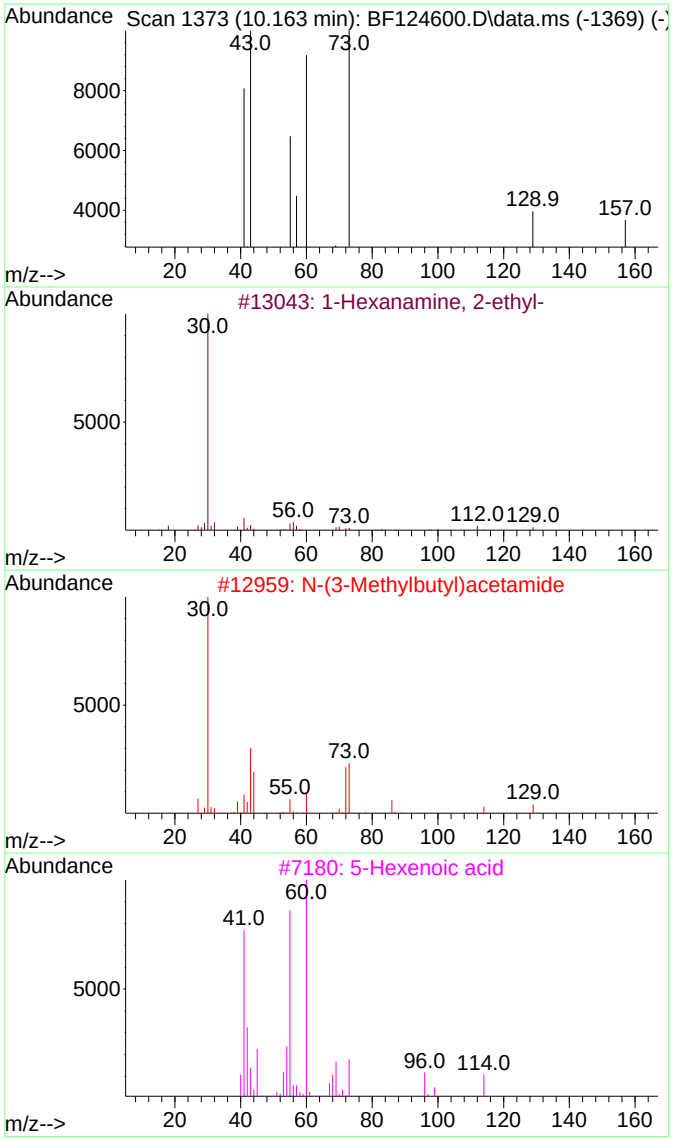
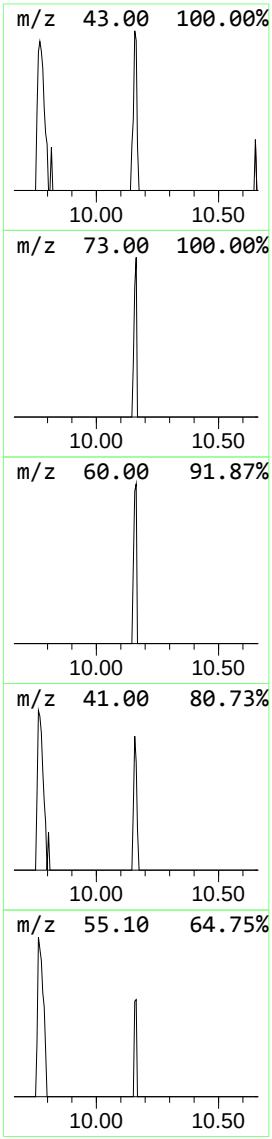
****

Peak Number 5 unknown10.163 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.163	2.07 ng	5633	Acenaphthene-d10	9.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanamine, 2-ethyl-	129	C8H19N	000104-75-6	9
2	N-(3-Methylbutyl)acetamide	129	C7H15NO	013434-12-3	9
3	5-Hexenoic acid	114	C6H10O2	001577-22-6	9
4	Guanidine, methyl-	73	C2H7N3	000471-29-4	7
5	Acetic acid	60	C2H4O2	000064-19-7	7





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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.M
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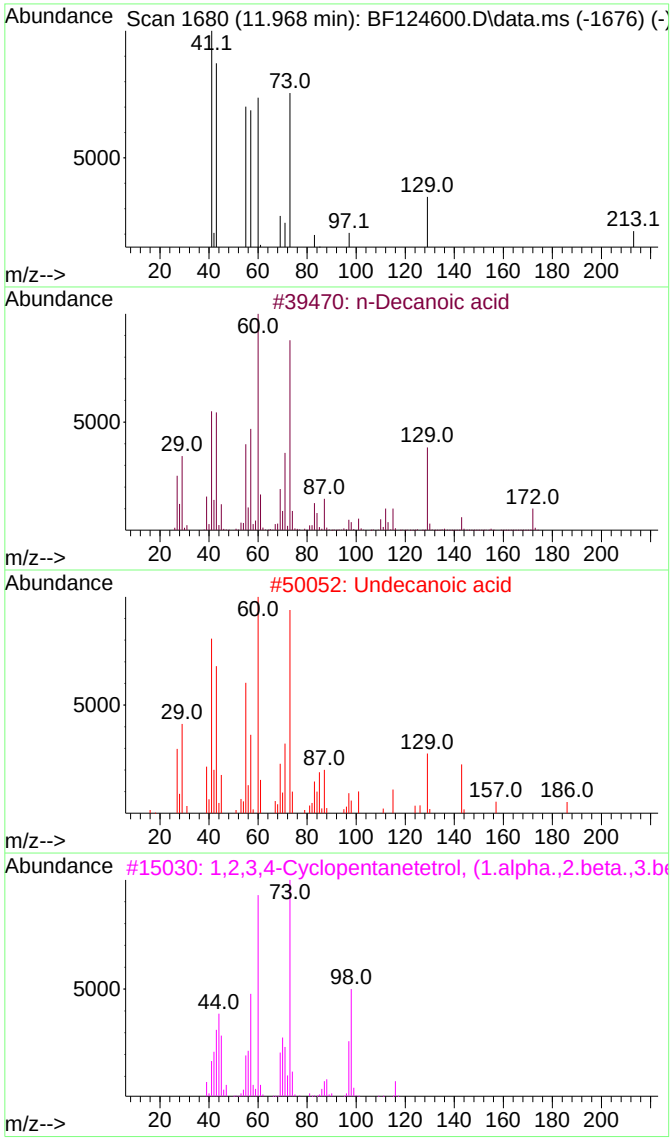
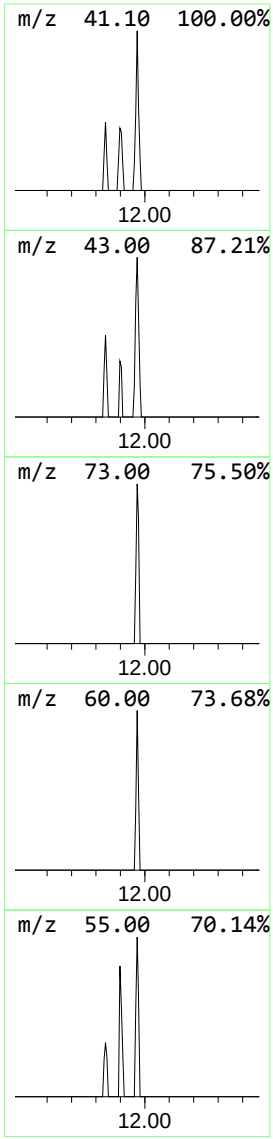
****

Peak Number 6 unknown11.969 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.969	3.41 ng	9950	Phenanthrene-d10	11.451

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Decanoic acid	172	C10H20O2	000334-48-5	47
2	Undecanoic acid	186	C11H22O2	000112-37-8	45
3	1,2,3,4-Cyclopentanetetrol, (1.a...	134	C5H10O4	014003-71-5	40
4	1-(p-Toluidino)-1-deoxy-.beta.-d...	269	C13H19NO5	1000226-06-4	38
5	11-Bromoundecanoic acid	264	C11H21BrO2	002834-05-1	37





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ClientSampleId :
PB-2021-WW-000-08

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.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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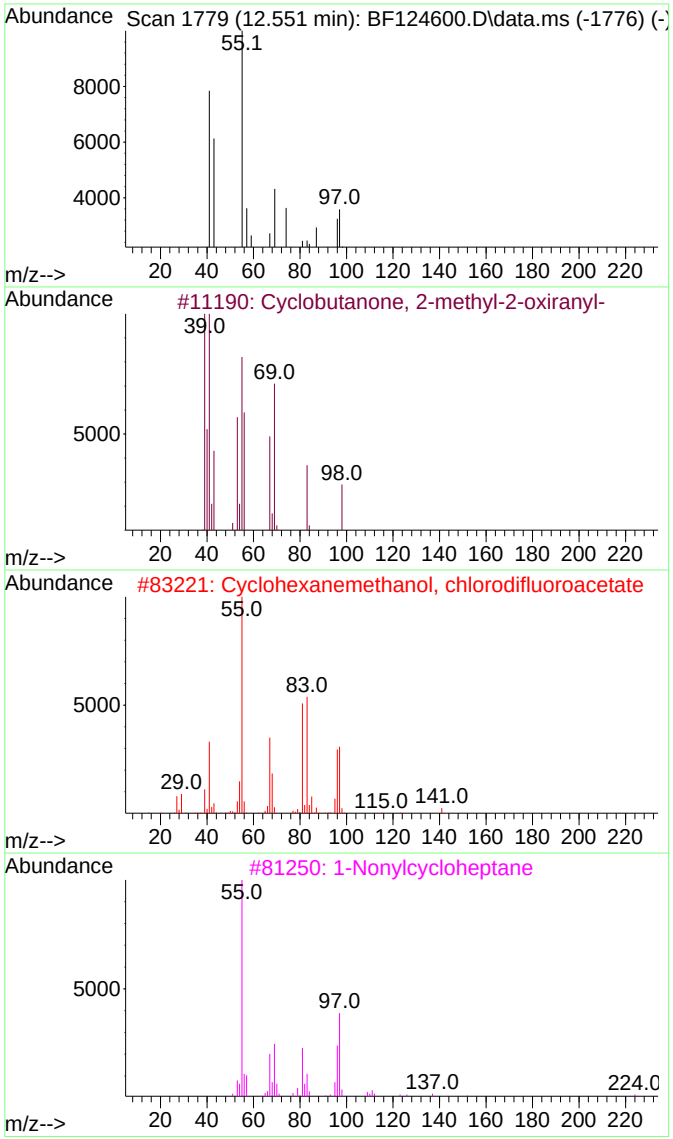
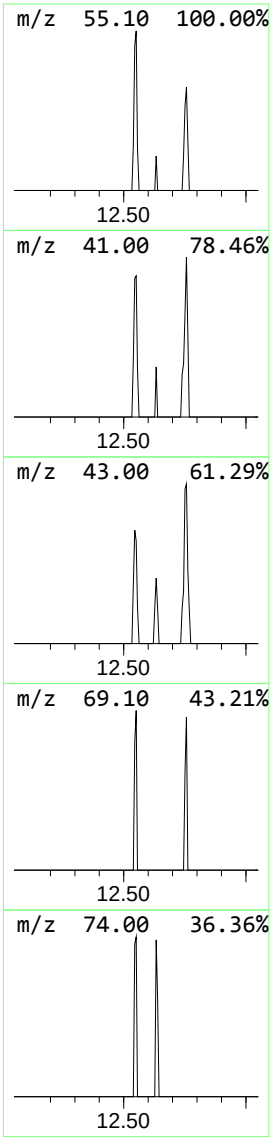
Peak Number 7 unknown12.551 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.551	2.48 ng	7228	Phenanthrene-d10	11.451

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclobutanone, 2-methyl-2-oxiranyl-	126	C7H10O2	075314-19-1	10
2	Cyclohexanemethanol, chlorodiflu...	226	C9H13ClF2O2	1000376-25-9	9
3	1-Nonylcycloheptane	224	C16H32	1000371-47-7	9
4	1-Heptanol, 6-methyl-	130	C8H18O	001653-40-3	9
5	Cyclopropane, 1-ethyl-2-methyl-,...	84	C6H12	019781-68-1	9





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TIC Library : C:\DATABASE\NIST11.L
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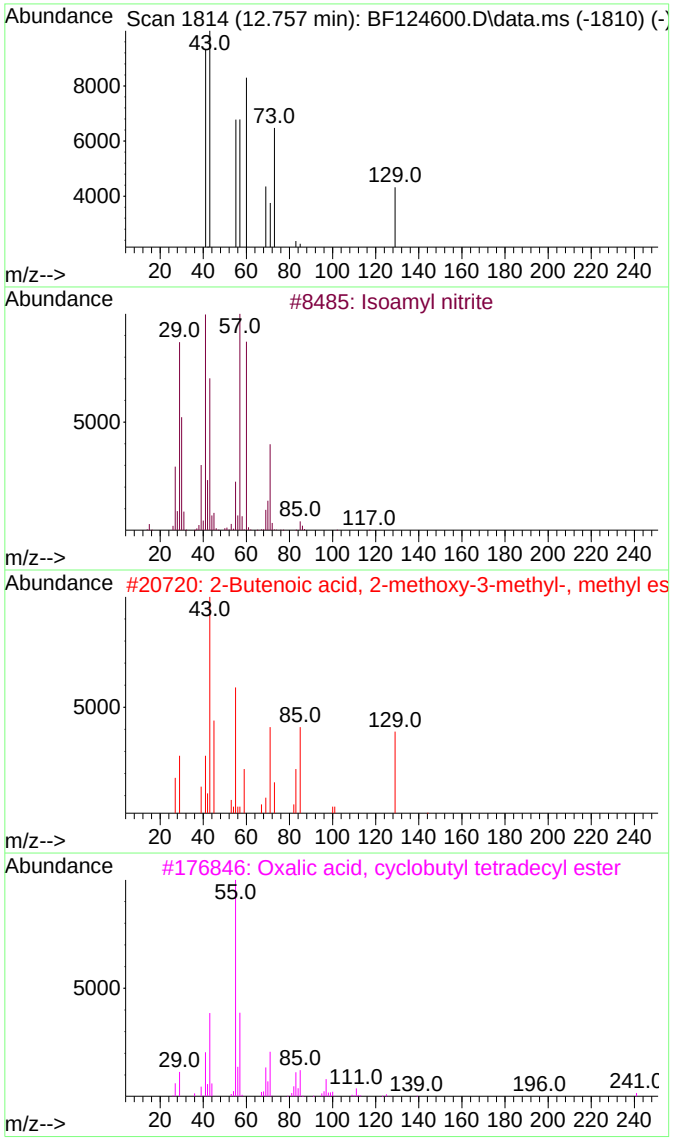
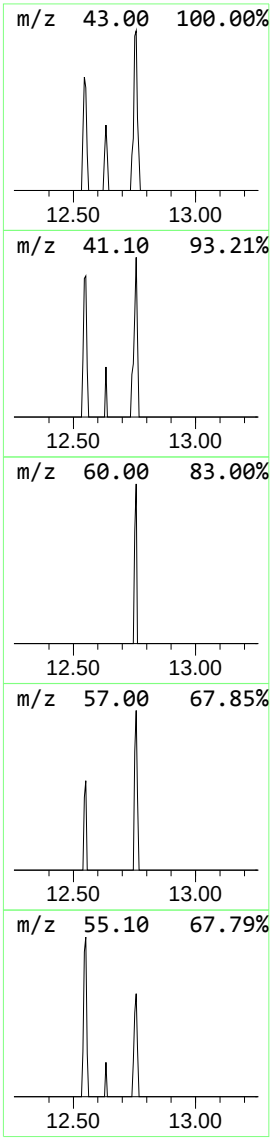
****

Peak Number 8 unknown12.757 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.757	2.67 ng	7794	Phenanthrene-d10	11.451

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isoamyl nitrite	117	C5H11NO2	000110-46-3	37
2	2-Butenoic acid, 2-methoxy-3-met...	144	C7H12O3	056009-32-6	12
3	Oxalic acid, cyclobutyl tetradec...	340	C20H36O4	1000309-70-9	10
4	N-(3-Methylbutyl)acetamide	129	C7H15NO	013434-12-3	9
5	2,4,6,8-Tetramethyl-1-undecene	210	C15H30	059920-26-2	9





Tentatively Identified Compound (LSC) summary

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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.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...	2.228	16.8	ng	27002	1	6.922	32101	20.0
unknown4.681	4.681	187.1	ng	300282	1	6.922	32101	20.0
Ethanol, 2-(2-b...	8.104	23.6	ng	54268	2	8.204	45966	20.0
1-Hexene, 3,5-d...	9.769	4.4	ng	12090	3	9.963	54523	20.0
unknown10.163	10.163	2.1	ng	5633	3	9.963	54523	20.0
unknown11.969	11.969	3.4	ng	9950	4	11.451	58336	20.0
unknown12.551	12.551	2.5	ng	7228	4	11.451	58336	20.0
unknown12.757	12.757	2.7	ng	7794	4	11.451	58336	20.0