LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110322\
Data File : BF130958.D
Acq On : 03 Nov 2022 12:20
Operator : CG\JU
Sample : N5395-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-11-103122

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-BF102722.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130958.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.240	17	26	32	rVB	474603	604173	32.61%	4.476%
2	2.352	40	45	50	rBV	37071	47872	2.58%	0.355%
3	4.040	327	332	338	rVB	199131	246282	13.29%	1.824%
4	5.151	516	521	532	rVB	389204	490427	26.47%	3.633%
5	5.545	581	588	591	rBV	1928469	1836117	99.11%	13.601%
6	6.545	752	758	761	rBV	1787167	1852658	100.00%	13.724%
7	6.922	818	822	825	rBV	514049	397501	21.46%	2.945%
8	7.316	883	889	899	rBV	116771	123196	6.65%	0.913%
9	7.487	913	918	921	rBV	1247570	1161615	62.70%	8.605%
10	7.916	987	991	999	rBV4	12963	25135	1.36%	0.186%
11	8.122	1021	1026	1033	rBV2	33161	84581	4.57%	0.627%
12	8.204	1037	1040	1043	rBV	505715	489398	26.42%	3.625%
13	9.286	1219	1224	1227	rBV	1787854	1623463	87.63%	12.026%
14	9.969	1335	1340	1343	rBV	559849	481044	25.97%	3.563%
15	10.157	1368	1372	1378	rBV4	23303	31018	1.67%	0.230%
16	10.610	1443	1449	1454	rBV3	19446	25734	1.39%	0.191%
17	10.757	1470	1474	1477	rBV	1149317	959189	51.77%	7.105%
18	10.804	1480	1482	1490	rVV	22943	32388	1.75%	0.240%
19	10.875	1490	1494	1502	rVB3	22424	35333	1.91%	0.262%
20	11.345	1571	1574	1579	rVB3	15798	20266	1.09%	0.150%
21	11.404	1579	1584	1588	rBV6	14624	19361	1.05%	0.143%
22	11.457	1590	1593	1596	rVV	472781	415705	22.44%	3.079%
23	11.480	1596	1597	1600	rVV	72972	46962	2.53%	0.348%
24	11.527	1602	1605	1609	rVB2	17543	23208	1.25%	0.172%
25	11.974	1676	1681	1686	rBV4	39630	57394	3.10%	0.425%
26	12.257	1724	1729	1732	rBV2	25294	29842	1.61%	0.221%
27	12.674	1797	1800	1804	rVB	113809	89968	4.86%	0.666%
28	12.904	1834	1839	1843	rBV	90362	93642	5.05%	0.694%
29	13.045	1859	1863	1867	rBV	1027548	955511	51.58%	7.078%
30	13.180	1884	1886	1889	rVB	24412	22156	1.20%	0.164%
31	14.033	2025	2031	2032	rBV5	29197	51289	2.77%	0.380%
32	14.110	2039	2044	2046	rBV2	337026	348277	18.80%	2.580%
33	14.133	2046	2048	2054	rVB	59867	51640	2.79%	0.383%
34	14.204	2057	2060	2064	rBV2	24709	32362	1.75%	0.240%
35	14.568	2119	2122	2124	rBV2	21679	21883	1.18%	0.162%
36	15.168	2221	2224	2228	rBV	49892	81630	4.41%	0.605%

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110322\
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Acq On : 03 Nov 2022 12:20
Operator : CG\JU
Sample : N5395-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-11-103122

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-BF102722.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.245	2234	2237	2240	rVB3	26380	26080	1.41%	0.193%
38	15.486	2276	2278	2284	rVB	32695	41948	2.26%	0.311%
39	15.551	2286	2289	2296	rVV	47803	65378	3.53%	0.484%
40	15.621	2296	2301	2311	rVB	284761	414703	22.38%	3.072%
41	17.151	2556	2561	2566	rBV2	21193	43231	2.33%	0.320%

Sum of corrected areas: 13499560

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110322\
Data File : BF130958.D
Acq On : 03 Nov 2022 12:20
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Instrument :
BNA_F
ClientSampleId :
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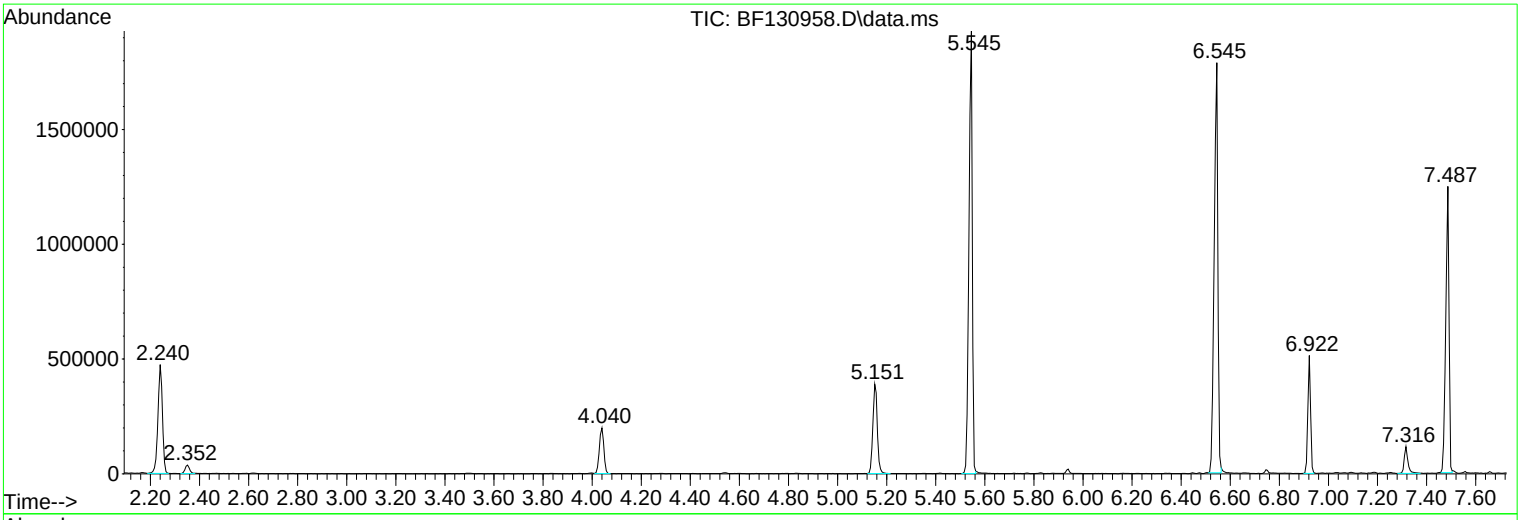
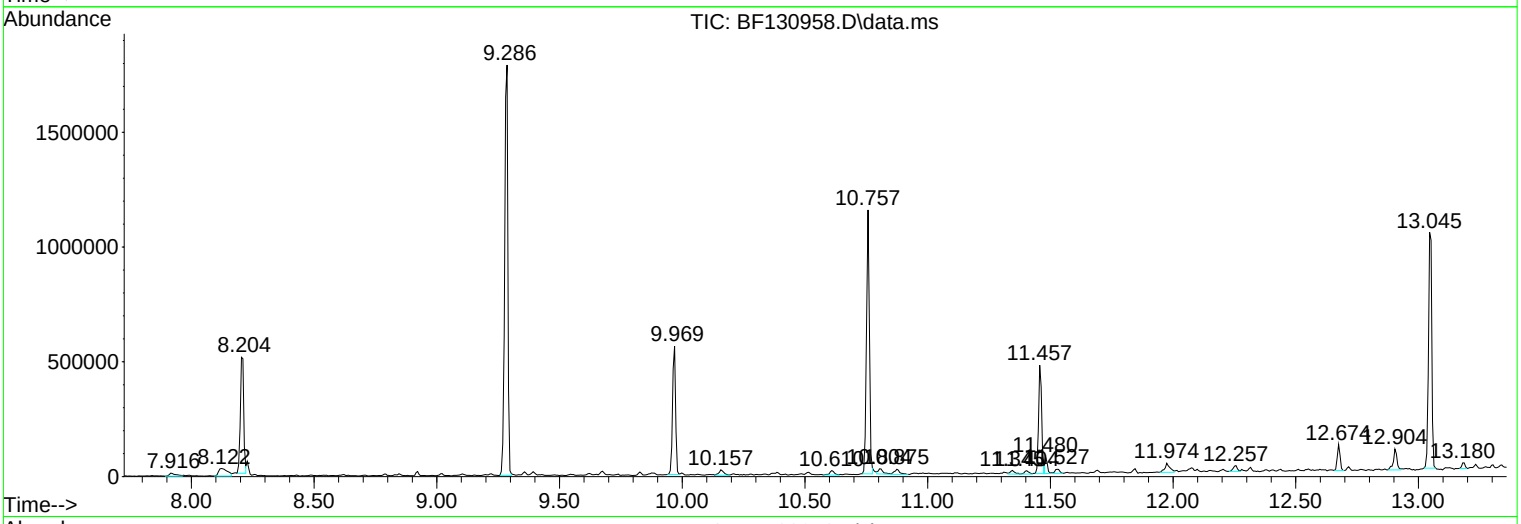
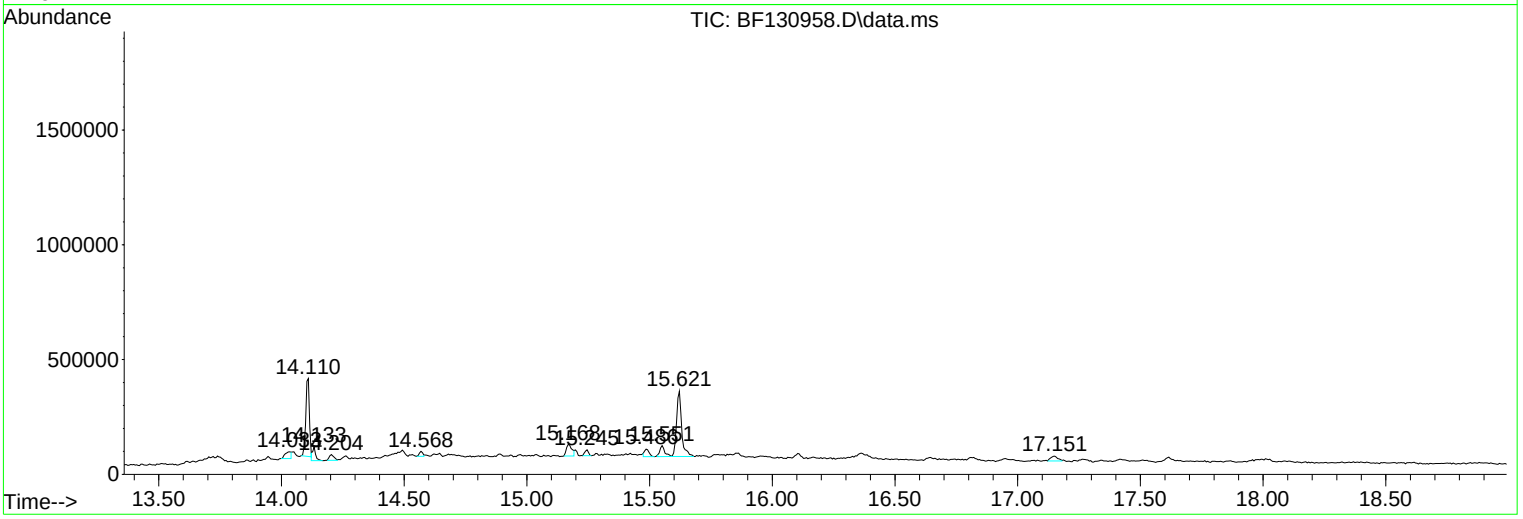
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110322\
Data File : BF130958.D
Acq On : 03 Nov 2022 12:20
Operator : CG\JU
Sample : N5395-03
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Instrument :
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ClientSampleId :
S-11-103122

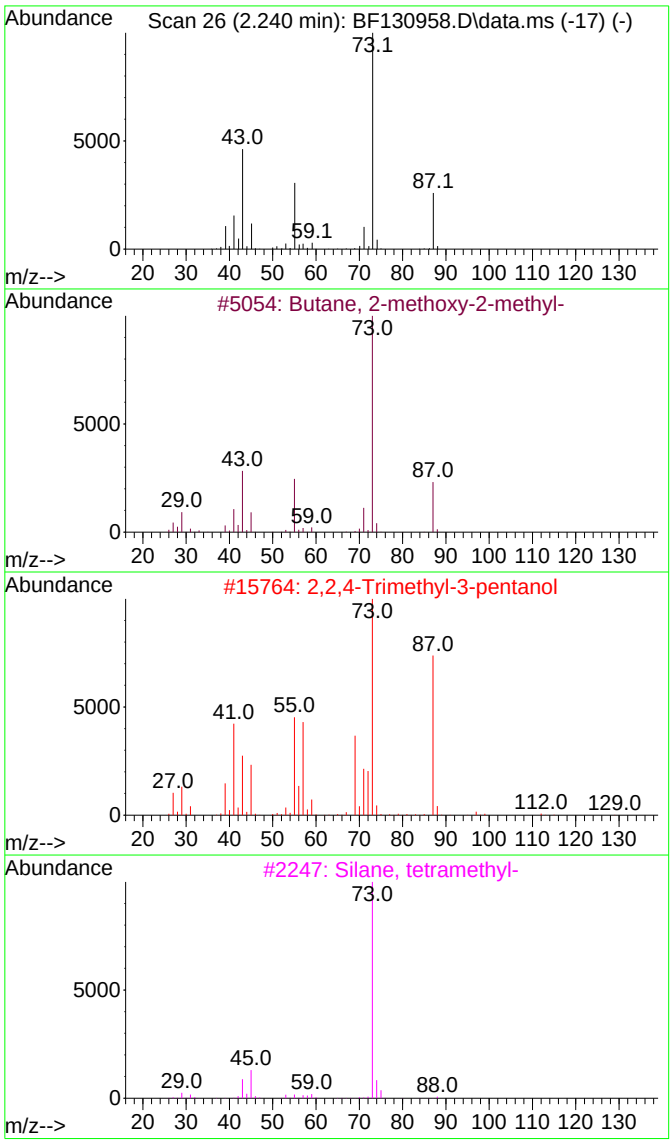
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

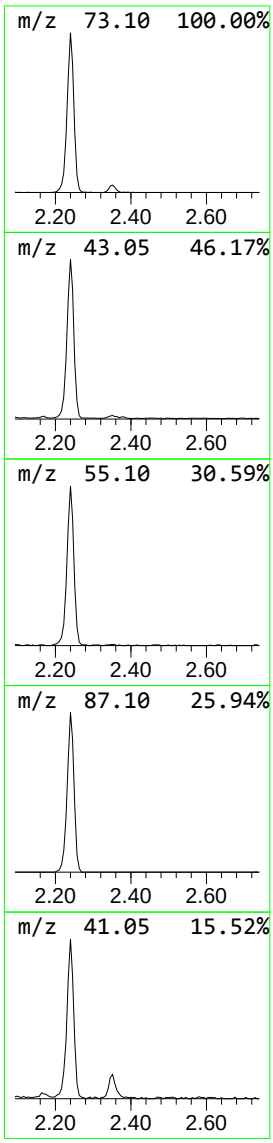
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.240	30.40 ng	604173	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	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5	1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23





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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

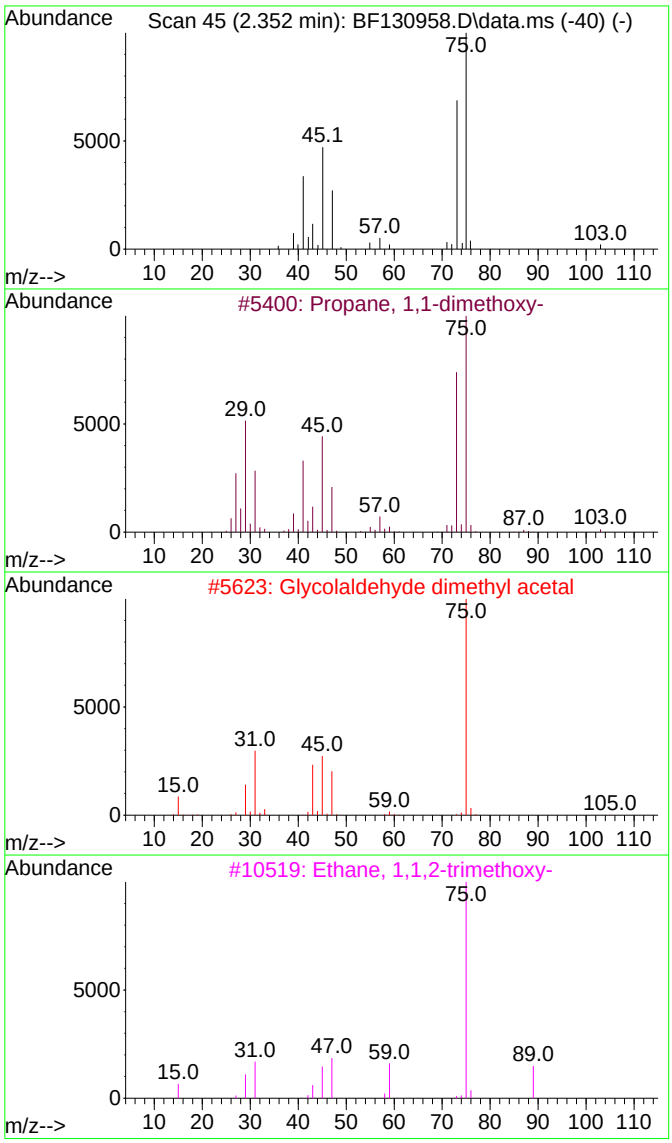
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

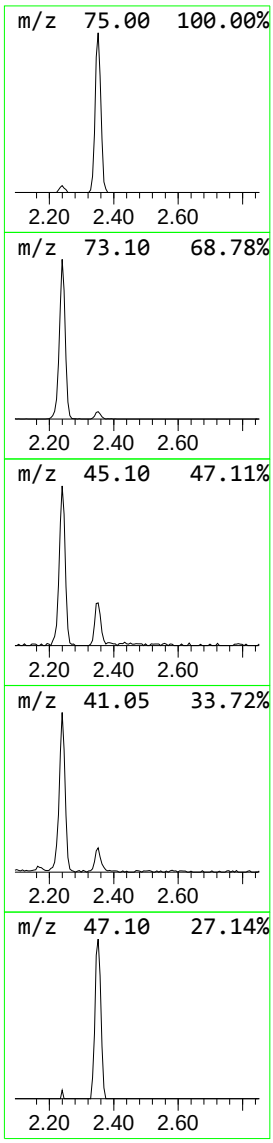
****

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.352	2.41 ng	47872	1,4-Dichlorobenzene-d4	6.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	64
2	Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	9
3	Ethane, 1,1,2-trimethoxy-	120	C5H12O3	024332-20-5	9
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
5	Aminoacetaldehyde dimethyl acetal	105	C4H11NO2	022483-09-6	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110322\
Data File : BF130958.D
Acq On : 03 Nov 2022 12:20
Operator : CG\JU
Sample : N5395-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-11-103122

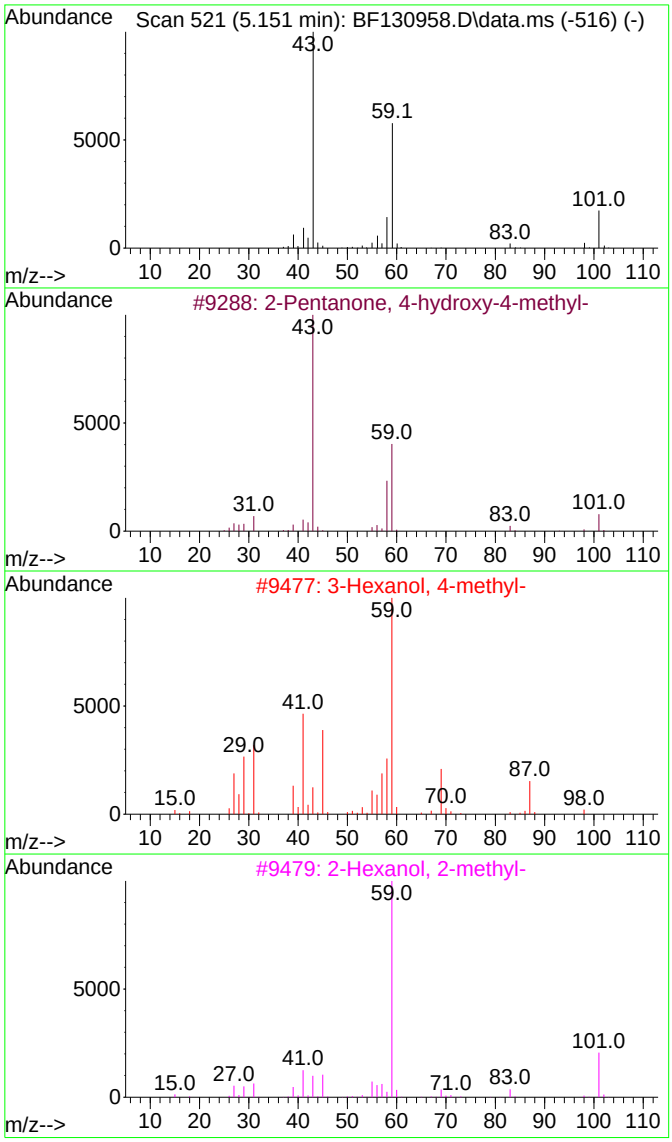
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

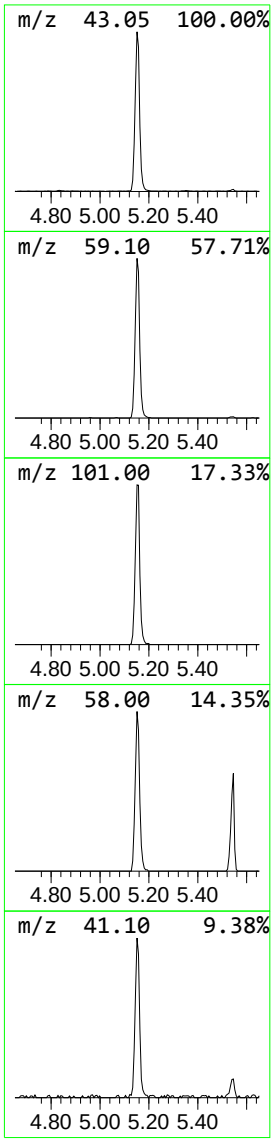
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.151	24.68 ng	490427	1,4-Dichlorobenzene-d4	6.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	25
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110322\
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Sample : N5395-03
Misc :
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Instrument :
BNA_F
ClientSampleId :
S-11-103122

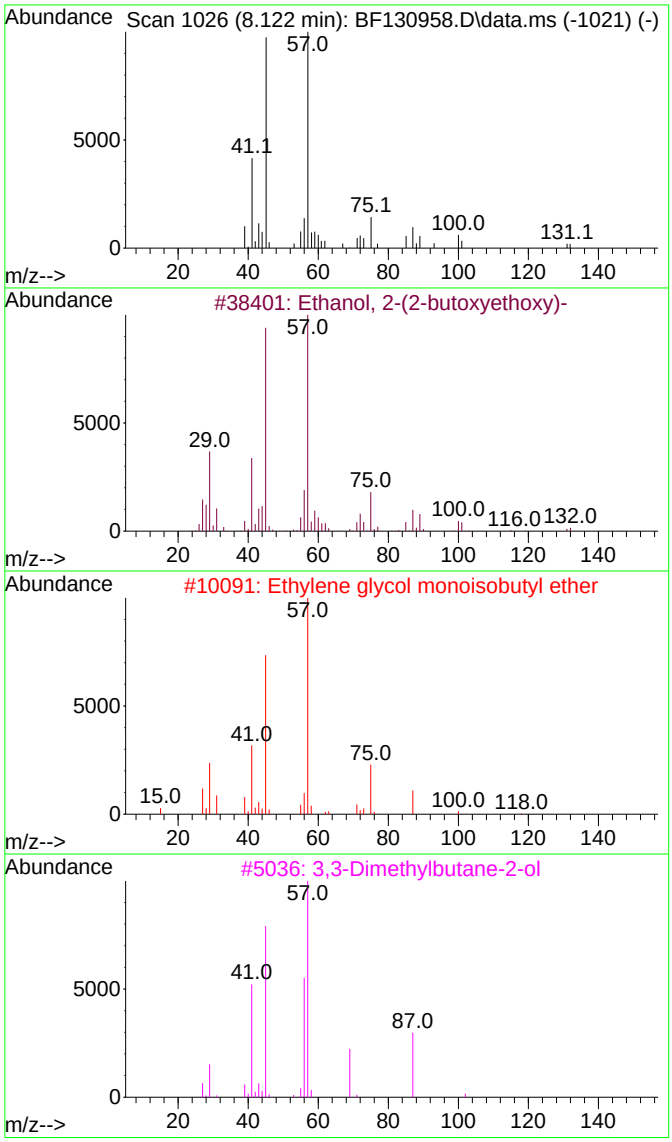
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

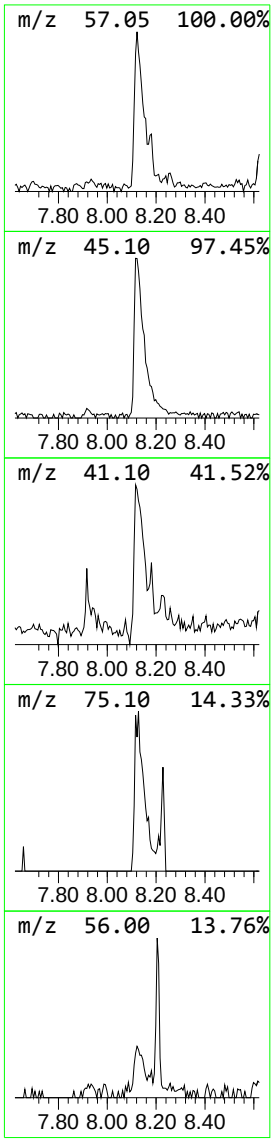
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.122	3.46 ng	84581	Naphthalene-d8	8.210

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
3	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53
4	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50
5	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	47





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

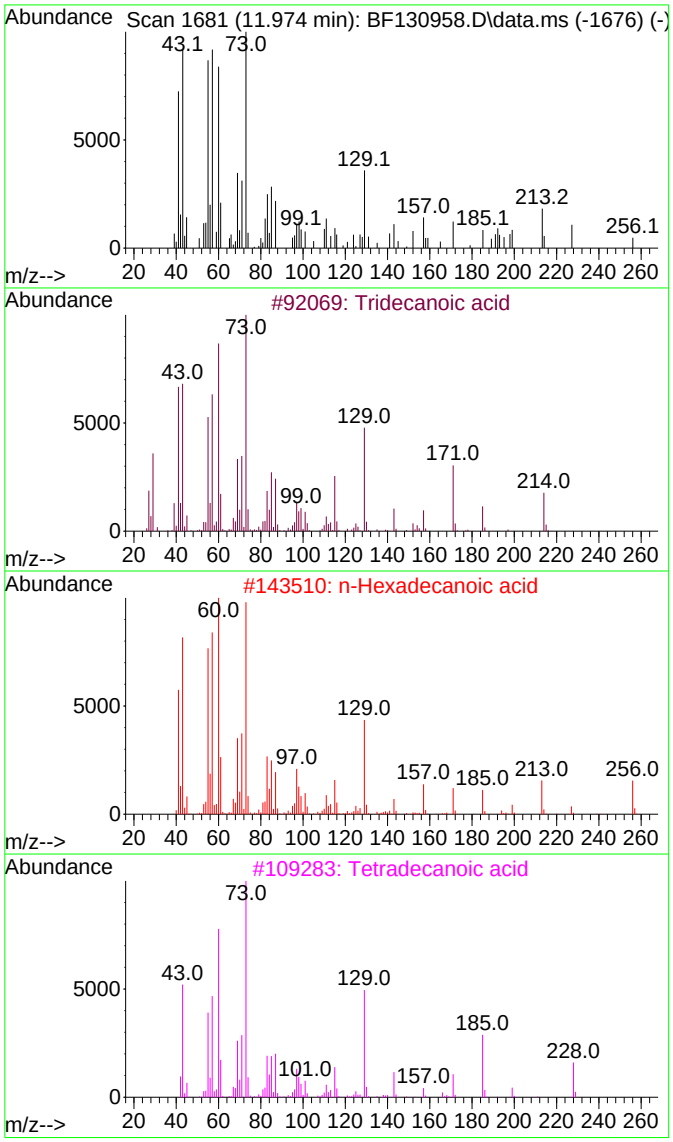
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

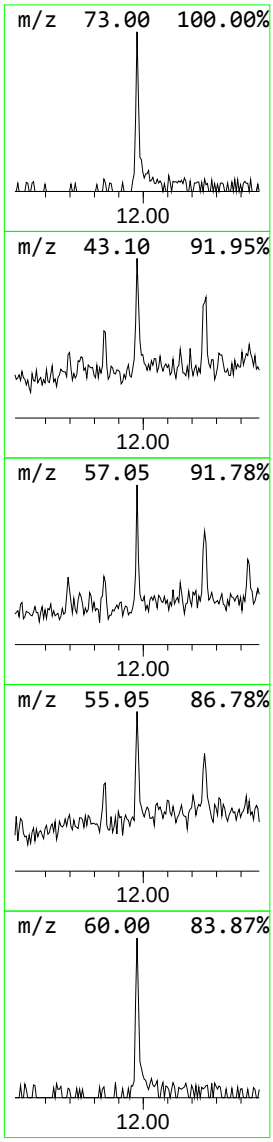
****

Peak Number 6 Tridecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.975	2.76 ng	57394	Phenanthrene-d10	11.457

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	93
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	78
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	59
4	Undecanoic acid	186	C11H22O2	000112-37-8	53
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	53





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Sample : N5395-03
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ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

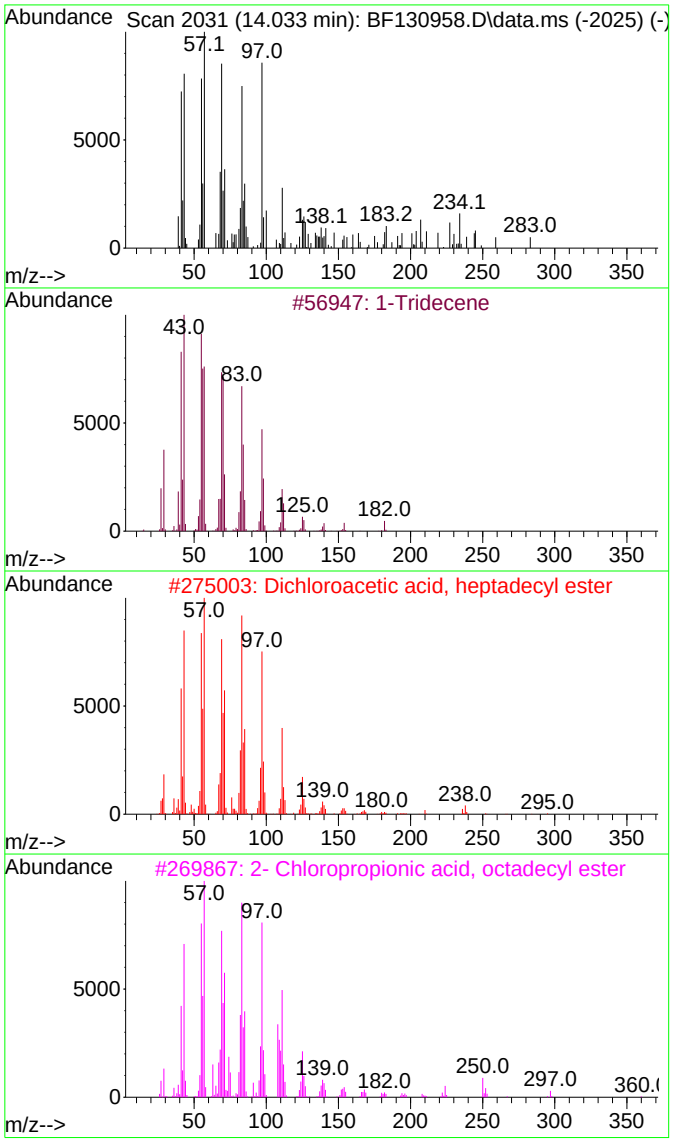
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

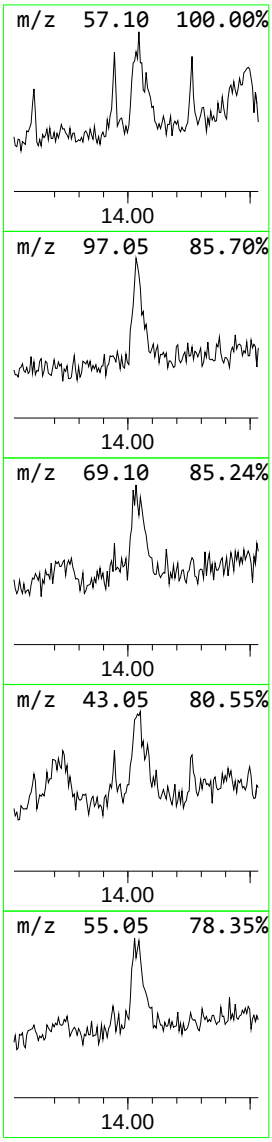
****

Peak Number 7 1-Tridecene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.033	2.95 ng	51289	Chrysene-d12	14.110

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tridecene	182	C13H26	002437-56-1	58
2	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	49
3	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	46
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	46
5	Cyclotridecane	182	C13H26	000295-02-3	44





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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

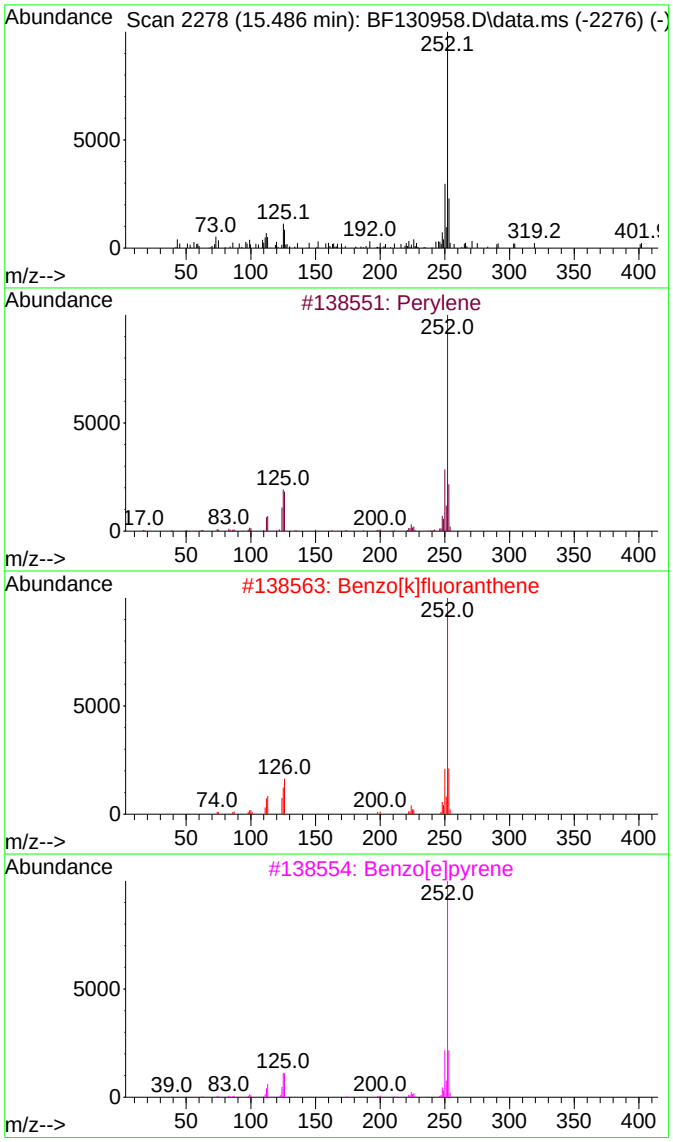
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

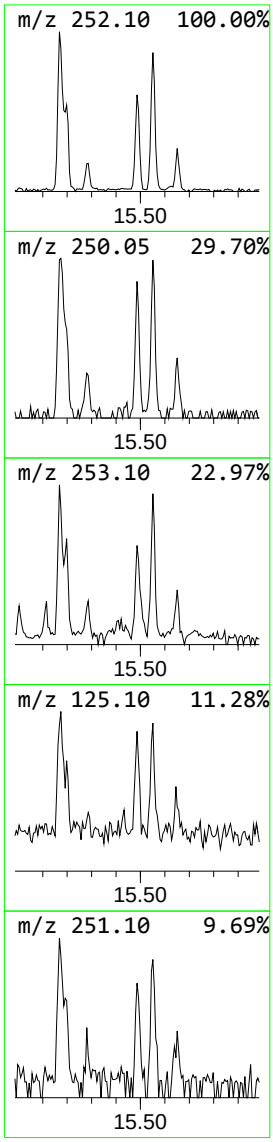
****

Peak Number 8 Perylene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.486	2.02 ng	41948	Perylene-d12	15.621

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Perylene	252	C20H12	000198-55-0	81
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	81
3	Benzo[e]pyrene	252	C20H12	000192-97-2	81
4	Benzo[b]fluoranthene	252	C20H12	000205-99-2	81
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	81





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110322\
Data File : BF130958.D
Acq On : 03 Nov 2022 12:20
Operator : CG\JU
Sample : N5395-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-11-103122

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.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
Butane, 2-metho...	2.240	30.4	ng	604173	1	6.922	397501	20.0
Propane, 1,1-di...	2.352	2.4	ng	47872	1	6.922	397501	20.0
2-Pentanone, 4-...	5.151	24.7	ng	490427	1	6.922	397501	20.0
Ethanol, 2-(2-b...	8.122	3.5	ng	84581	2	8.210	489398	20.0
Tridecanoic acid	11.975	2.8	ng	57394	4	11.457	415705	20.0
1-Tridecene	14.033	3.0	ng	51289	5	14.110	348277	20.0
Perylene	15.486	2.0	ng	41948	6	15.621	414703	20.0