LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120324\
Data File : BF140713.D
Acq On : 03 Dec 2024 16:16
Operator : RC/JU
Sample : P5052-19
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-640-COMP-63

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-BF112124.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF140713.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.152	3	10	23	rVB	740295	1218183	49.71%	7.054%
2	2.263	23	29	45	rVB	33856	56081	2.29%	0.325%
3	5.099	499	511	524	rBV	96392	153550	6.27%	0.889%
4	5.504	574	580	602	rBV	1235416	1645714	67.15%	9.530%
5	6.510	745	751	772	rBV	1277258	1741524	71.06%	10.085%
6	6.869	807	812	819	rBV	366428	448849	18.32%	2.599%
7	7.434	902	908	917	rBV	846972	1146312	46.78%	6.638%
8	7.687	946	951	966	rBV	26205	50357	2.05%	0.292%
9	8.151	1024	1030	1047	rBV	445665	607476	24.79%	3.518%
10	9.222	1206	1212	1222	rBV	1929530	2450659	100.00%	14.192%
11	9.904	1323	1328	1342	rBV	608536	778818	31.78%	4.510%
12	10.622	1444	1450	1458	rBV	318490	418203	17.06%	2.422%
13	10.698	1458	1463	1478	rBV	1214213	1599357	65.26%	9.262%
14	11.398	1577	1582	1590	rBV	641879	856918	34.97%	4.962%
15	11.916	1665	1670	1685	rBV	175831	312596	12.76%	1.810%
16	12.704	1799	1804	1817	rBV4	25043	58645	2.39%	0.340%
17	12.980	1845	1851	1857	rBV	1717754	2243435	91.54%	12.992%
18	13.880	1999	2004	2015	rBV	89719	156128	6.37%	0.904%
19	14.057	2029	2034	2047	rVB	361840	524318	21.39%	3.036%
20	14.210	2057	2060	2068	rVB6	12646	25550	1.04%	0.148%
21	14.845	2163	2168	2173	rBV2	43713	71356	2.91%	0.413%
22	15.586	2288	2294	2304	rVB	303540	511306	20.86%	2.961%
23	16.910	2514	2519	2526	rBV7	16678	36001	1.47%	0.208%
24	17.633	2635	2642	2658	rVB6	51789	157026	6.41%	0.909%

Sum of corrected areas: 17268362

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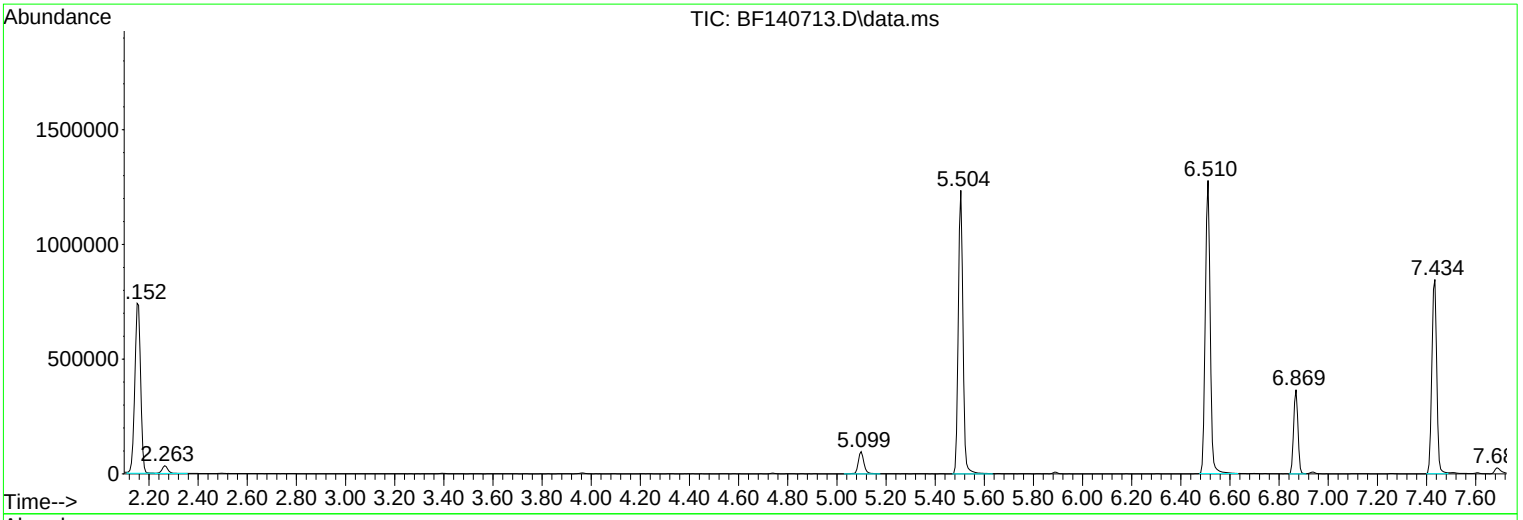
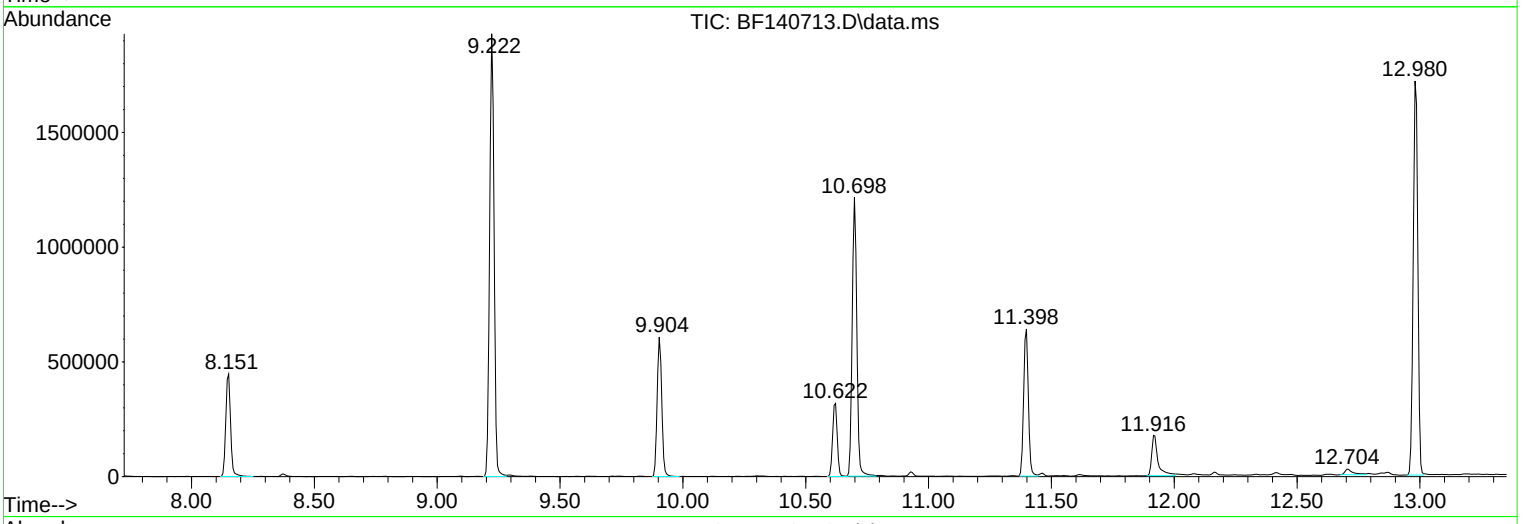
Misc :
ALS Vial : 13 Sample Multiplier: 1

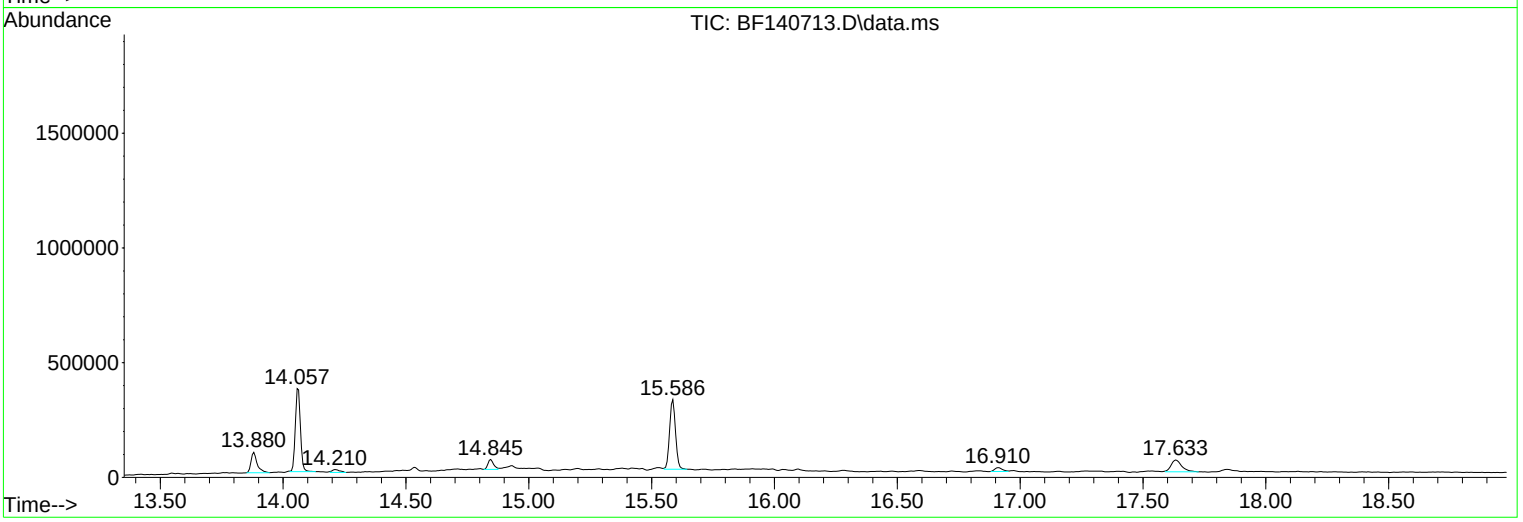
Instrument :
BNA_F
ClientSampleId :
OR-640-COMP-63

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.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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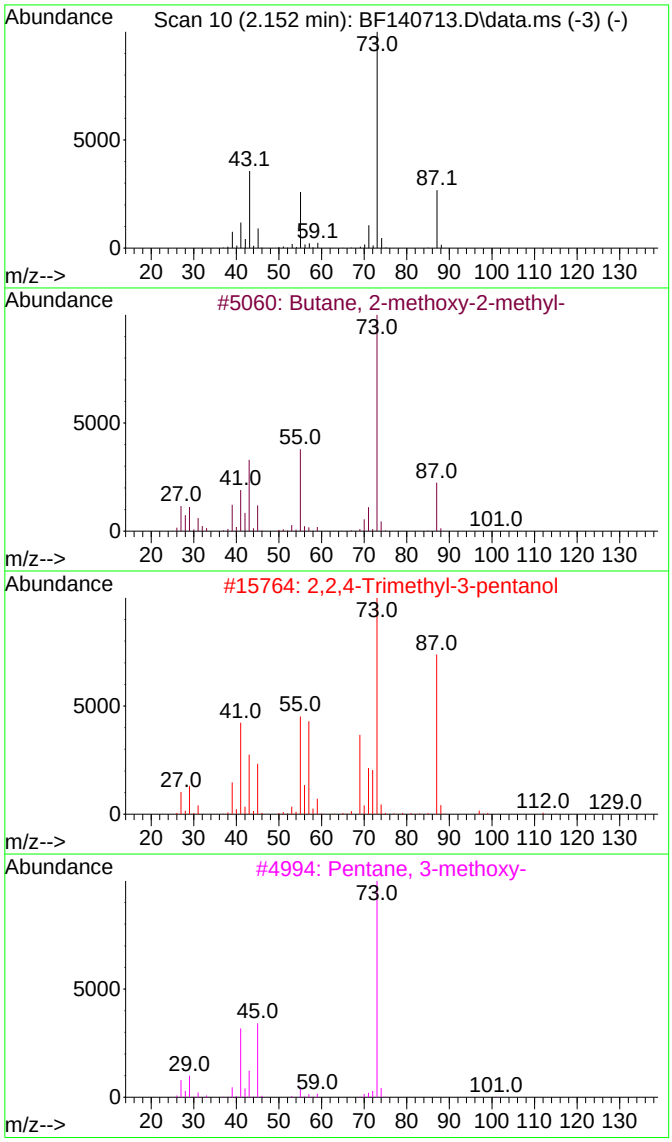
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

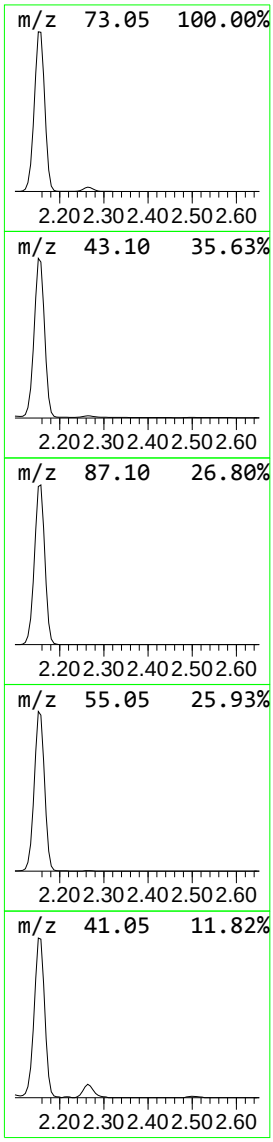
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.152	54.28 ng	1218180	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	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





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Acq On : 03 Dec 2024 16:16
Operator : RC/JU
Sample : P5052-19
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OR-640-COMP-63

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

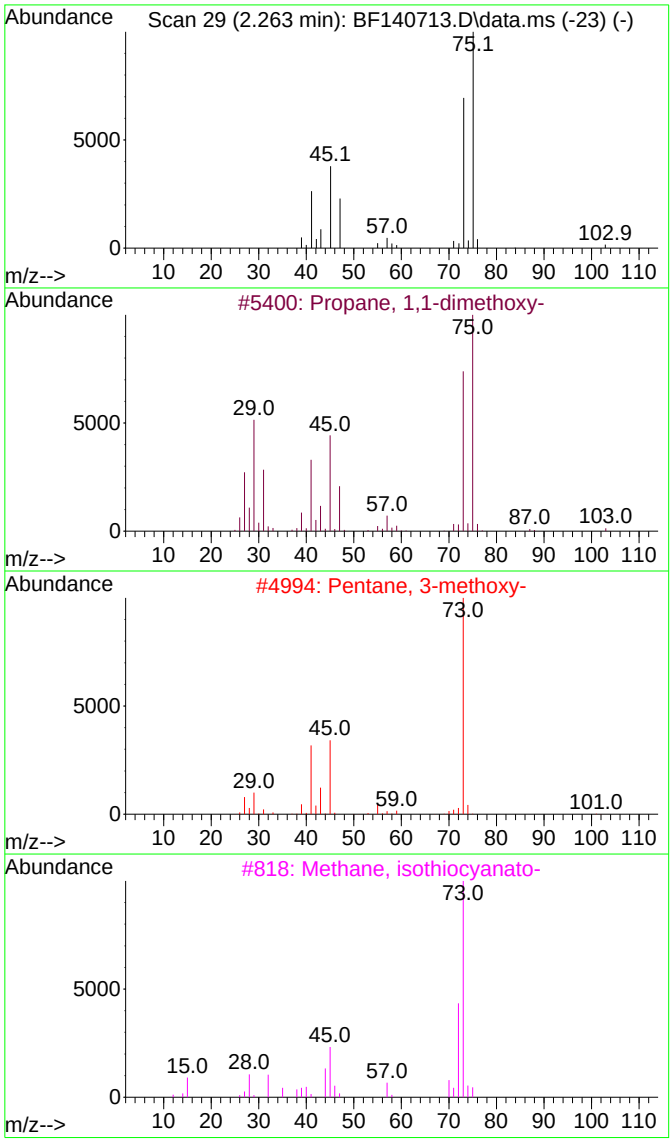
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

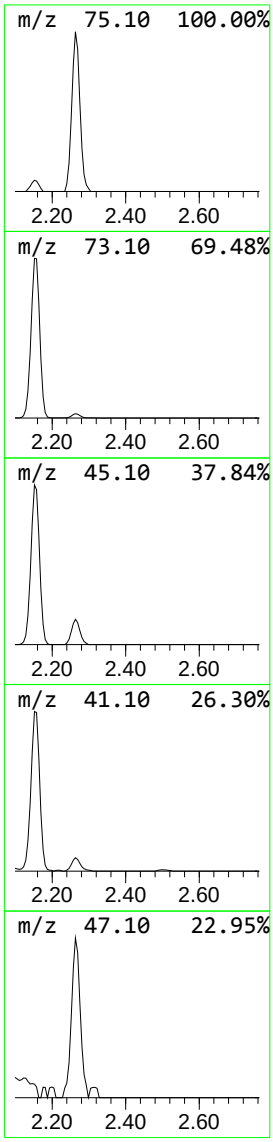
****

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.263	2.50 ng	56081	1,4-Dichlorobenzene-d4	6.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	64
2	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	10
3	Methane, isothiocyanato-	73	C2H3NS	000556-61-6	9
4	2-Propanol, 1,1-dimethoxy-	120	C5H12O3	042919-42-6	9
5	Ethane, 1,1,2-trimethoxy-	120	C5H12O3	024332-20-5	9





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Acq On : 03 Dec 2024 16:16
Operator : RC/JU
Sample : P5052-19
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OR-640-COMP-63

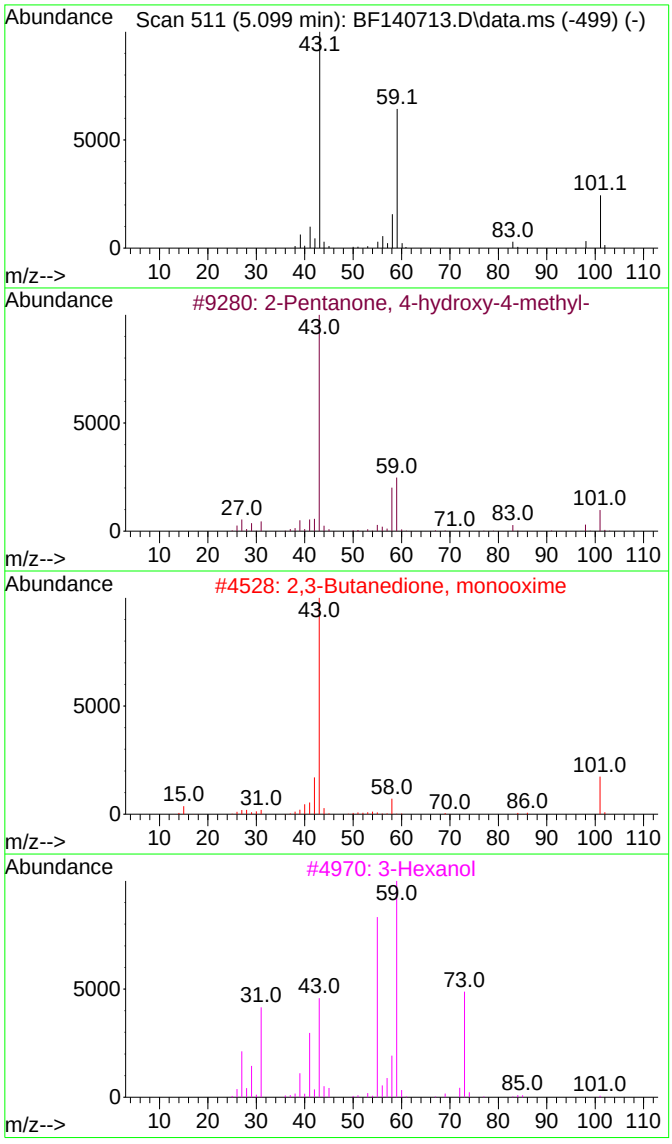
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

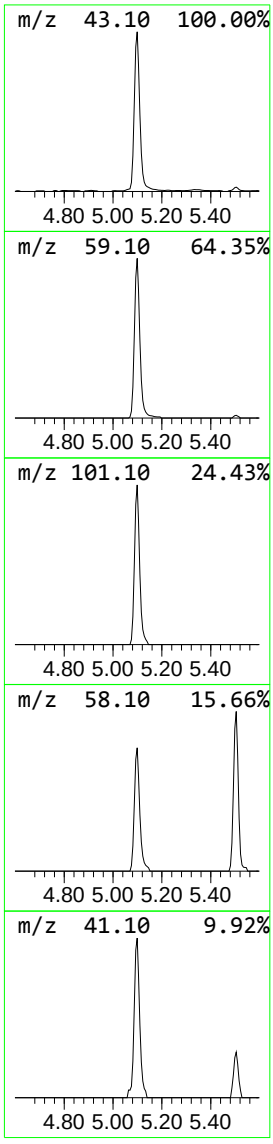
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.099	6.84 ng	153550	1,4-Dichlorobenzene-d4	6.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
3	3-Hexanol	102	C6H14O	000623-37-0	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10





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Sample : P5052-19
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OR-640-COMP-63

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

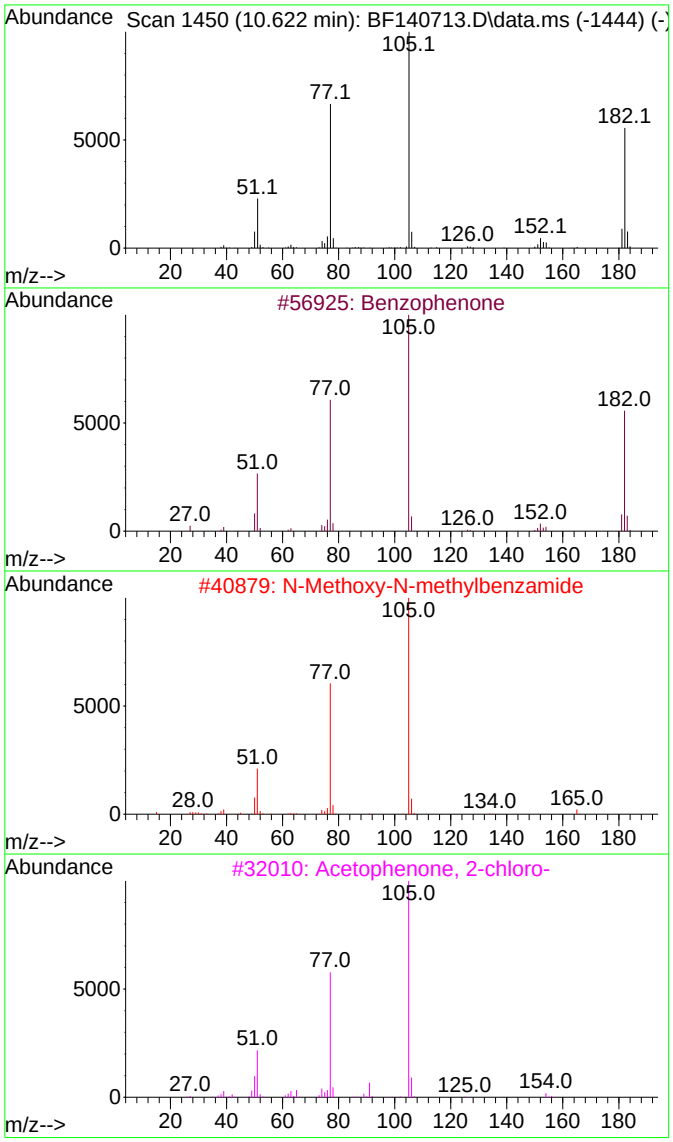
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

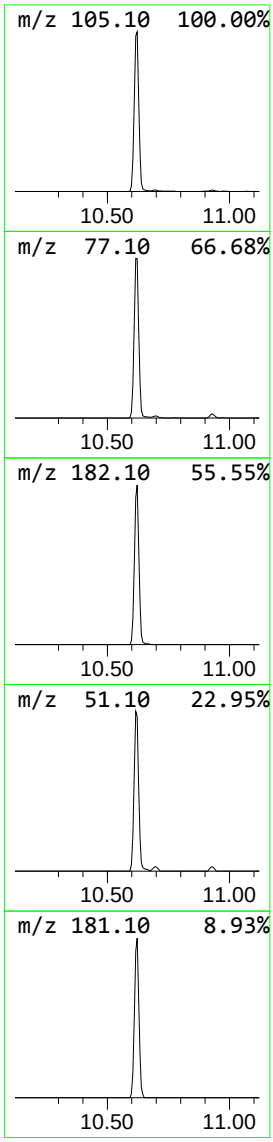
****

Peak Number 4 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.622	10.74 ng	418203	Acenaphthene-d10	9.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	49
3	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
4	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	47
5	1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47





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Operator : RC/JU
Sample : P5052-19
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OR-640-COMP-63

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

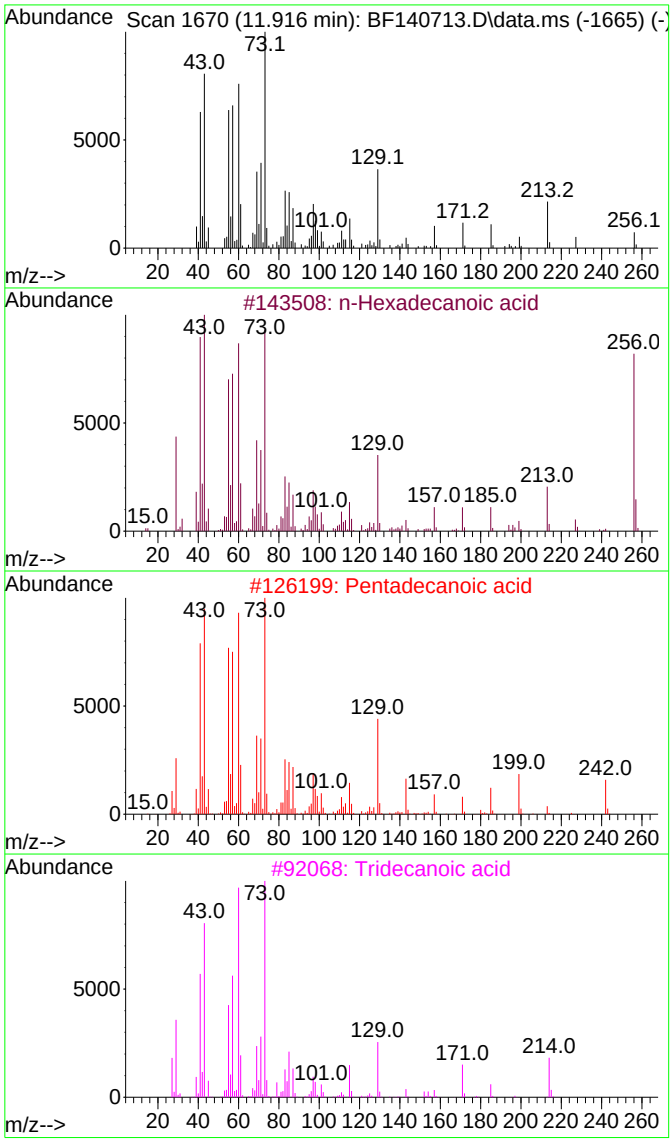
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

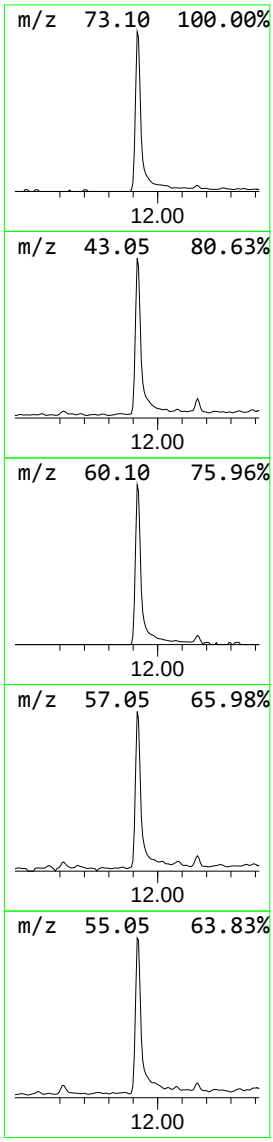
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	7.30 ng	312596	Phenanthrene-d10	11.398

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	87
3	Tridecanoic acid	214	C13H26O2	000638-53-9	74
4	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	55
5	Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	35





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Instrument :
BNA_F
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.M
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TIC Library : C:\Database\NIST20.L
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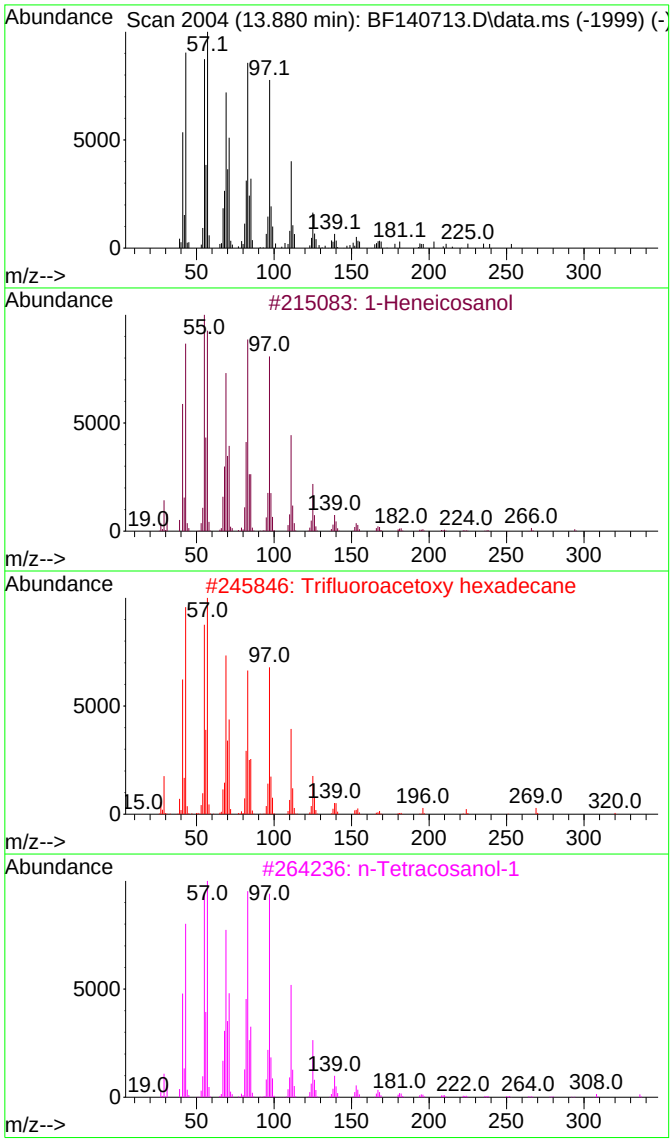
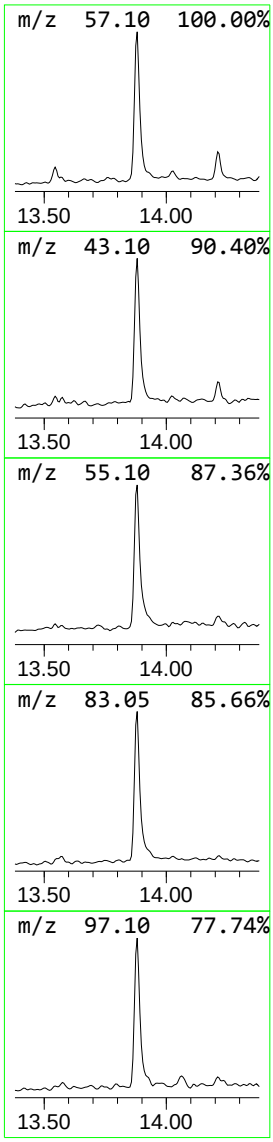
****

Peak Number 6 1-Heneicosanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.880	5.96 ng	156128	Chrysene-d12	14.057

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
5	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91





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Sample : P5052-19
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OR-640-COMP-63

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

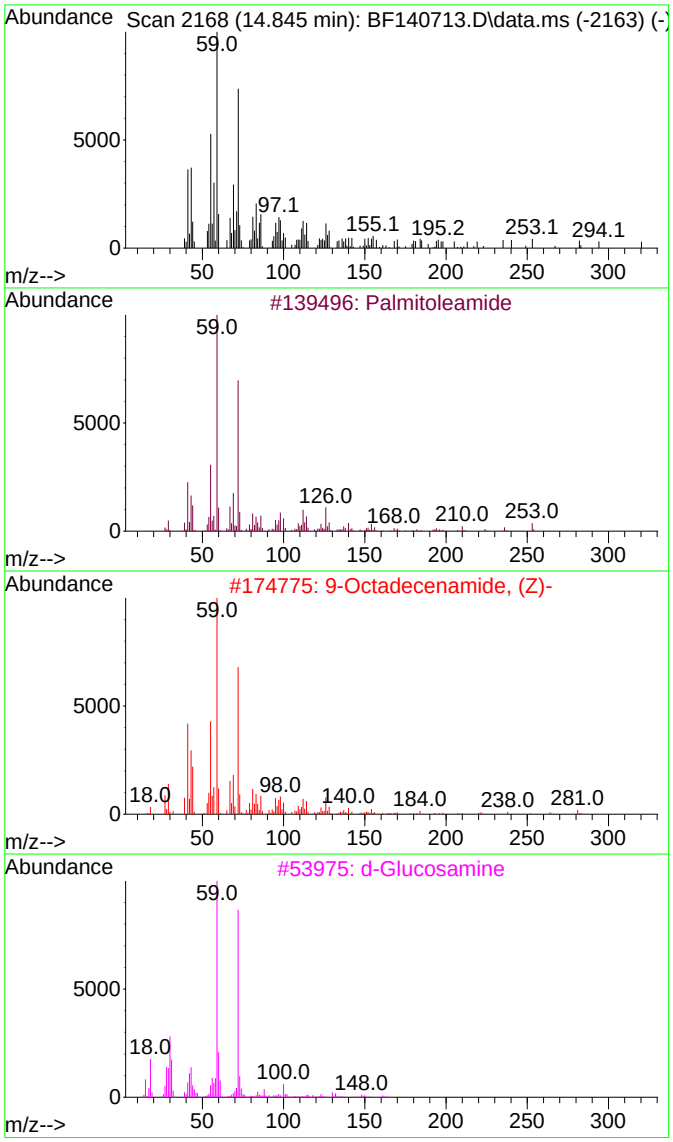
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

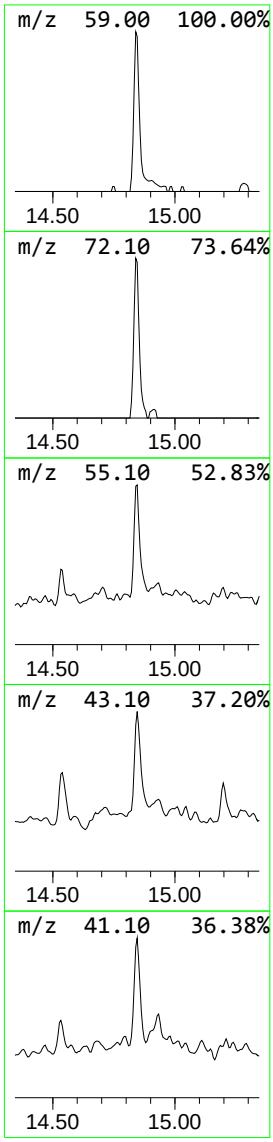
****

Peak Number 7 Palmitoleamide Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.845	2.79 ng	71356	Perylene-d12	15.586

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Palmitoleamide	253	C16H31NO	106010-22-4	93
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	87
3	d-Glucosamine	179	C6H13NO5	000090-77-7	59
4	Isobutyramide, N-propyl-N-hexyl-	213	C13H27NO	1000437-74-1	38
5	7-Nonenamide	155	C9H17NO	090949-53-4	35





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TIC Library : C:\Database\NIST20.L
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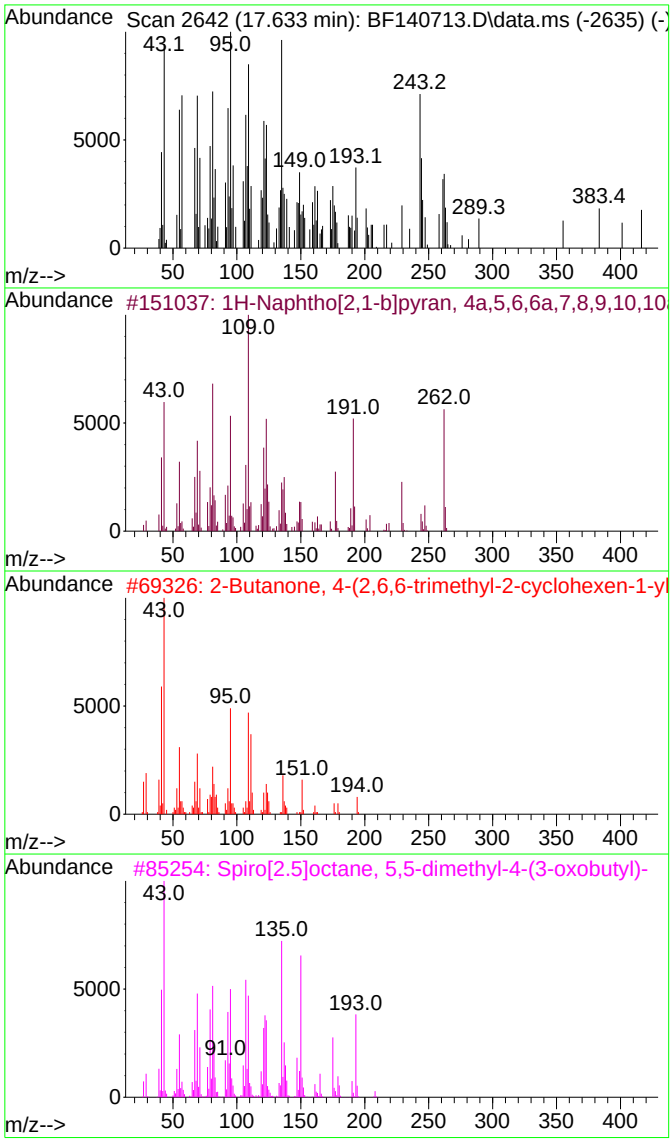
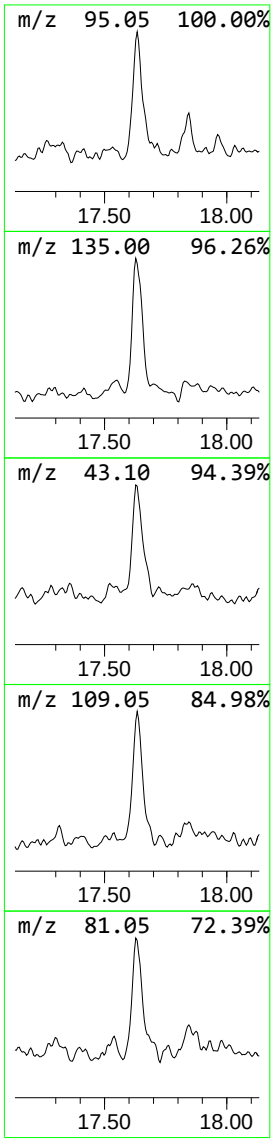
Peak Number 8 unknown17.633 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.633	6.14 ng	157026	Perylene-d12	15.586

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Naphtho[2,1-b]pyran, 4a,5,6,6...	262	C18H30O	005153-92-4	38
2	2-Butanone, 4-(2,6,6-trimethyl-2...	194	C13H22O	039721-65-8	30
3	Spiro[2.5]octane, 5,5-dimethyl-4...	208	C14H24O	077143-32-9	27
4	trans-Chrysanthenol	152	C10H16O	038043-83-3	15
5	5-Octen-2-one, 6-methyl-8-(2,6,6...	262	C18H30O	055638-41-0	15





Tentatively Identified Compound (LSC) summary

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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...	2.152	54.3	ng	1218180	1	6.869	448849	20.0
Propane, 1,1-di...	2.263	2.5	ng	56081	1	6.869	448849	20.0
2-Pentanone, 4-...	5.099	6.8	ng	153550	1	6.869	448849	20.0
Benzophenone	10.622	10.7	ng	418203	3	9.904	778818	20.0
n-Hexadecanoic ...	11.916	7.3	ng	312596	4	11.398	856918	20.0
1-Heneicosanol	13.880	6.0	ng	156128	5	14.057	524318	20.0
Palmitoleamide	14.845	2.8	ng	71356	6	15.586	511306	20.0
unknown17.633	17.633	6.1	ng	157026	6	15.586	511306	20.0