

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040221\
 Data File : BG048574.D
 Acq On : 2 Apr 2021 18:37
 Operator : CG/JU
 Sample : M1836-07
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 B3-19-21

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_G\METHODS\8270-BG033021.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG048574.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.165	306	311	318	rVB2	30559	45163	3.76%	0.737%
2	5.641	383	392	400	rBV	290228	478810	39.88%	7.809%
3	7.245	656	665	674	rBV	312437	535282	44.59%	8.730%
4	8.097	803	810	817	rBV2	85644	147563	12.29%	2.407%
5	9.260	1001	1008	1016	rBV	190039	343938	28.65%	5.609%
6	10.923	1282	1291	1298	rBV	110930	195931	16.32%	3.195%
7	13.367	1699	1707	1717	rBV	505700	768958	64.05%	12.541%
8	14.184	1841	1846	1851	rBV	21533	31143	2.59%	0.508%
9	14.748	1936	1942	1951	rVB	176585	276589	23.04%	4.511%
10	16.234	2186	2195	2208	rBV	471476	698249	58.16%	11.388%
11	17.497	2404	2410	2417	rVB	250858	369938	30.81%	6.033%
12	18.379	2555	2560	2566	rBV3	45007	66526	5.54%	1.085%
13	19.648	2772	2776	2780	rBV3	13861	14812	1.23%	0.242%
14	20.106	2849	2854	2861	rVB	938738	1200547	100.00%	19.579%
15	21.422	3073	3078	3085	rBV6	43210	80614	6.71%	1.315%
16	21.798	3135	3142	3149	rVB2	241572	415228	34.59%	6.772%
17	21.992	3171	3175	3179	rVB5	7246	12221	1.02%	0.199%
18	23.537	3435	3438	3447	rVB5	15925	32306	2.69%	0.527%
19	25.136	3702	3710	3725	rVB2	137055	417895	34.81%	6.815%

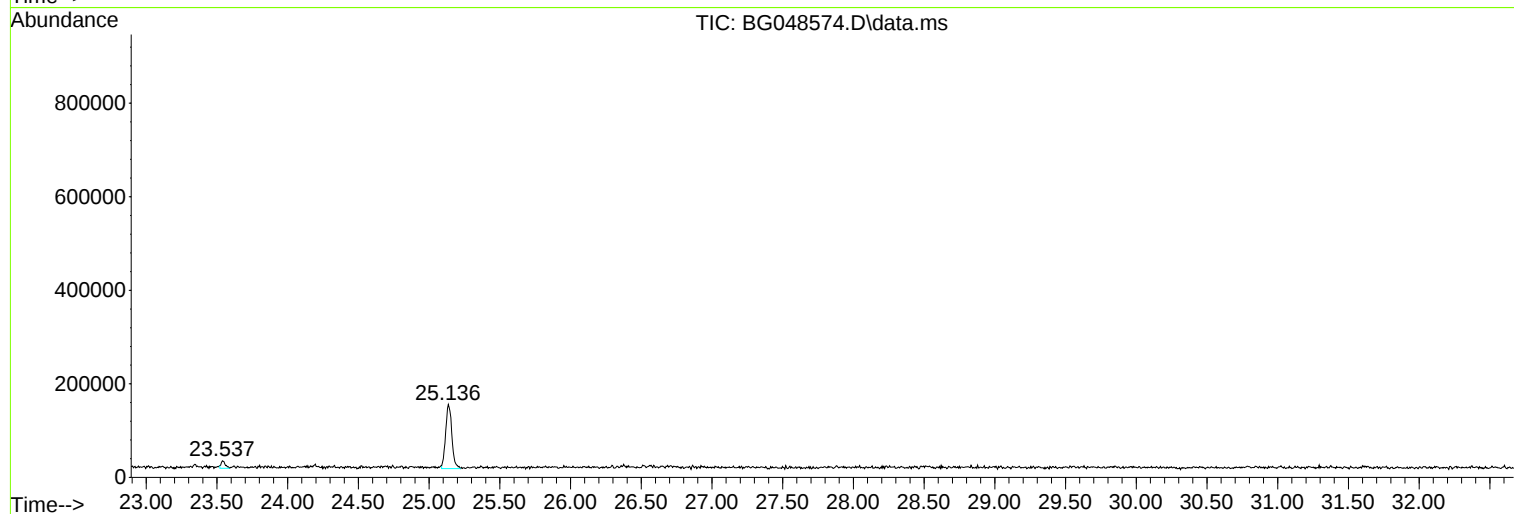
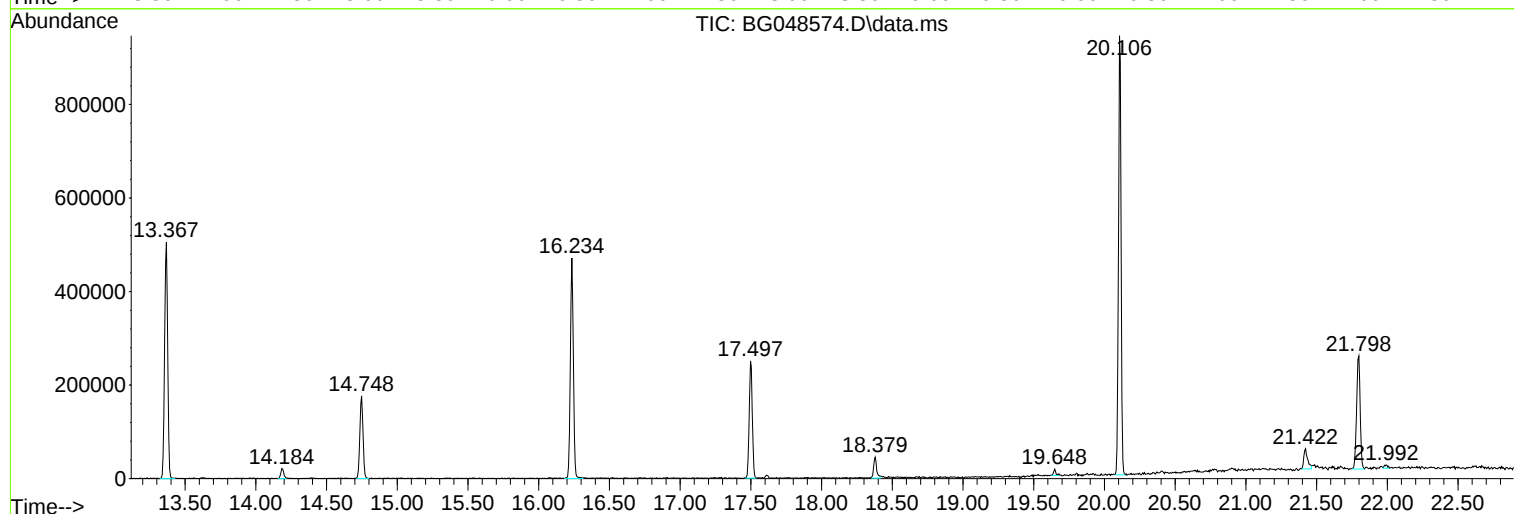
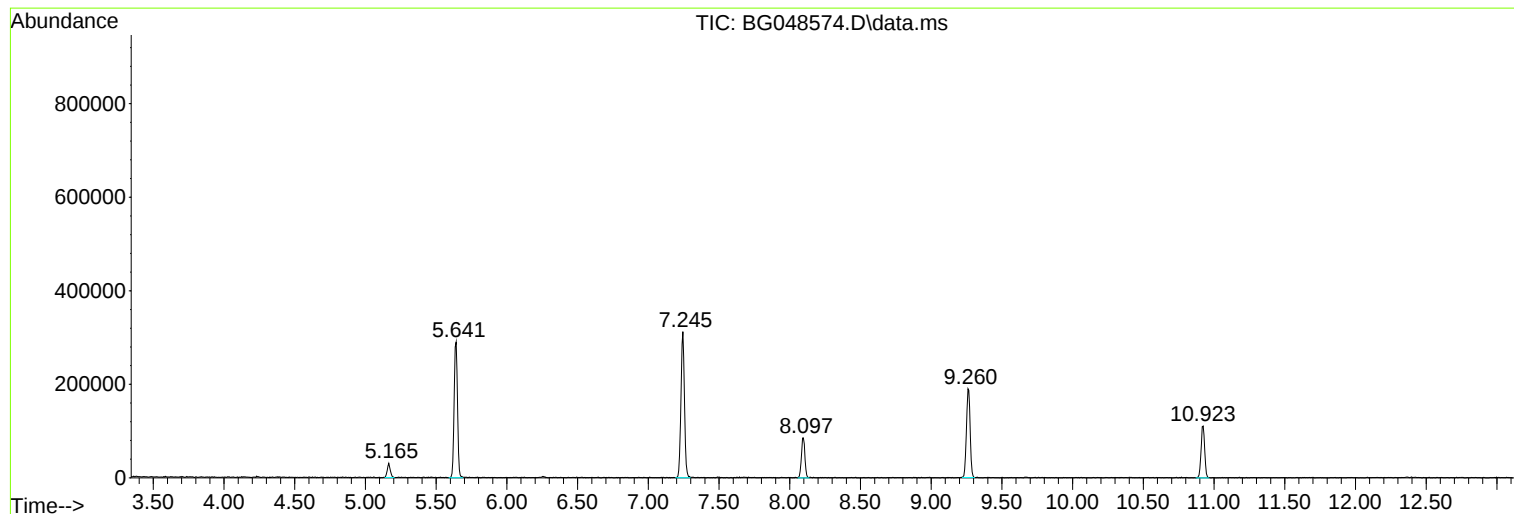
Sum of corrected areas: 6131713

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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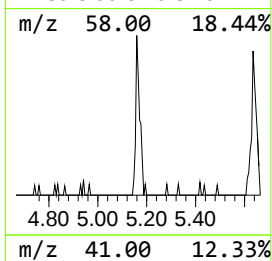
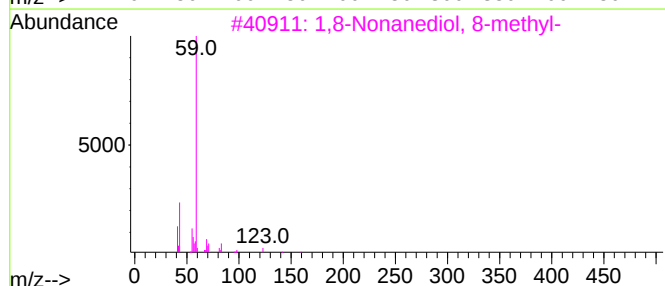
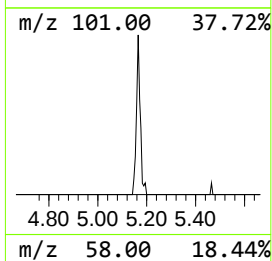
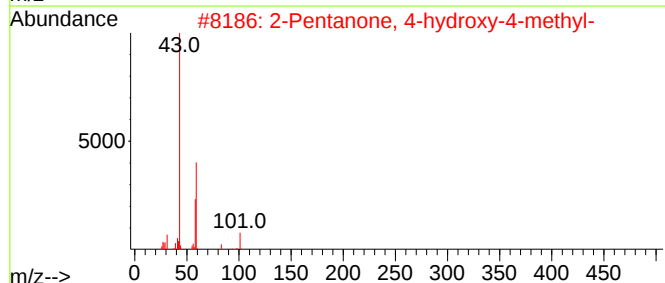
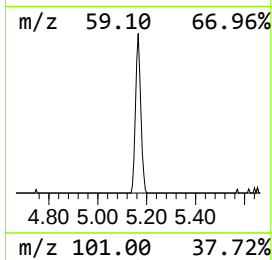
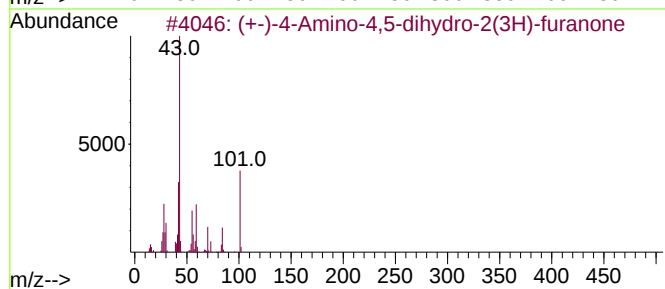
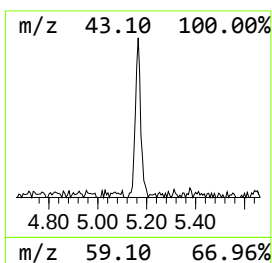
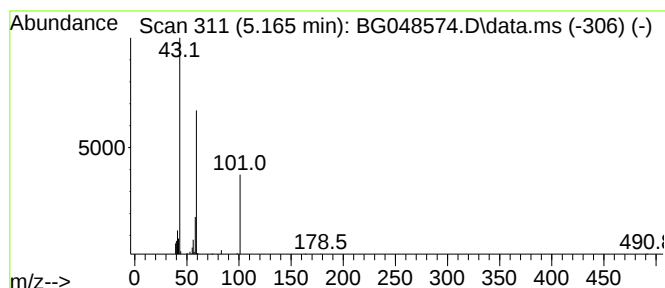
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Peak Number 1 unknown5.165 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.165	6.12 ng	45163	1,4-Dichlorobenzene-d4	8.097

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	25		
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	23		
3	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	17		
4	Acetone	58	C3H6O	000067-64-1	9		
5	Butane	58	C4H10	000106-97-8	9		



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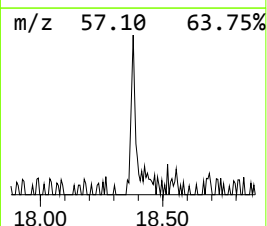
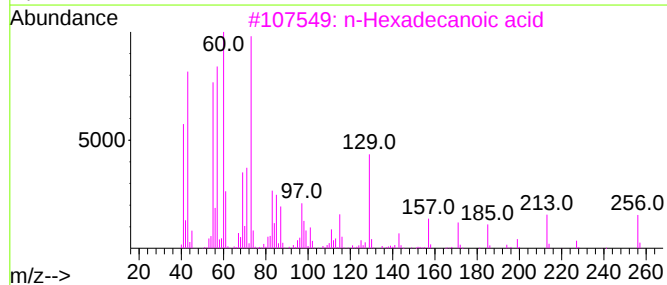
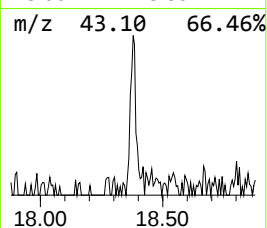
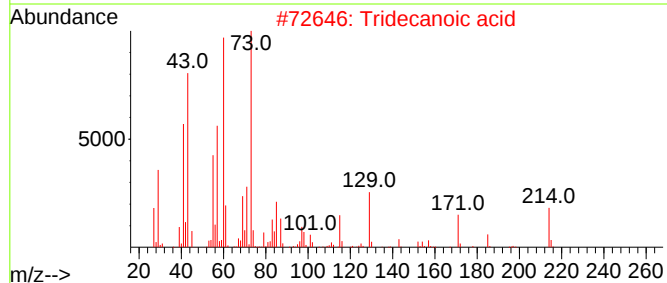
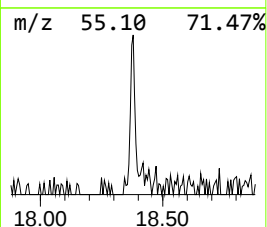
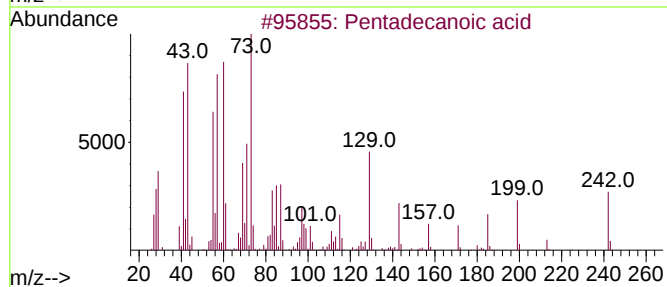
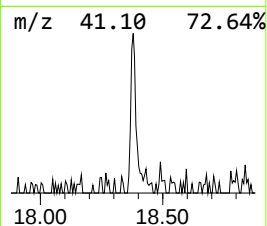
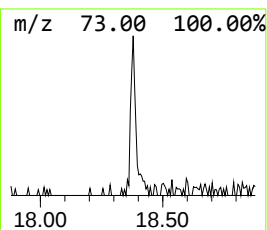
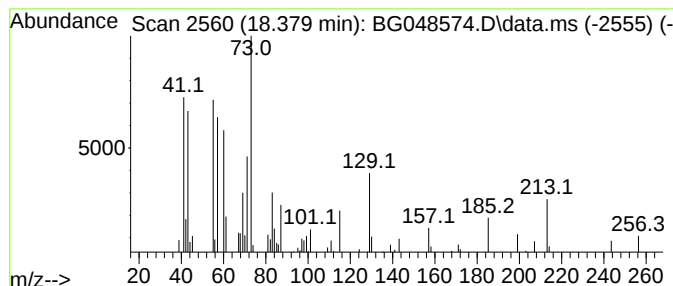
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Peak Number 2 Pentadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.379	3.60 ng	66526	Phenanthrene-d10	17.497

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecanoic acid	242	C15H30O2	001002-84-2	72
2			Tridecanoic acid	214	C13H26O2	000638-53-9	52
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	49
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	43
5			D-Glucopyranoside, 4-O-decyl-	320	C16H32O6	1000158-00-4	43



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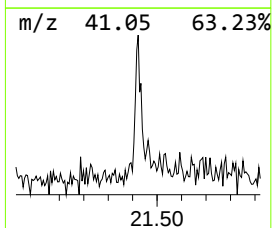
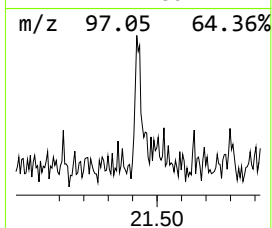
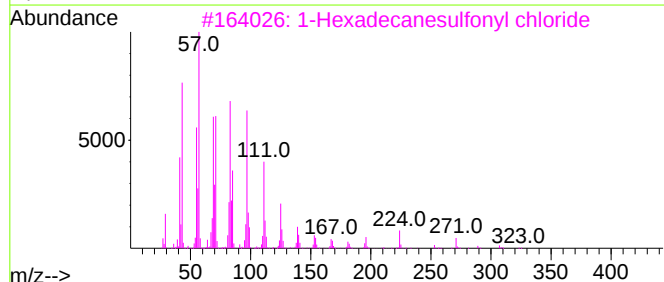
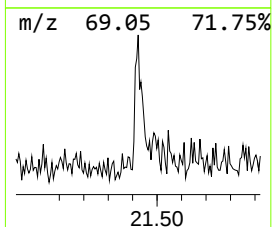
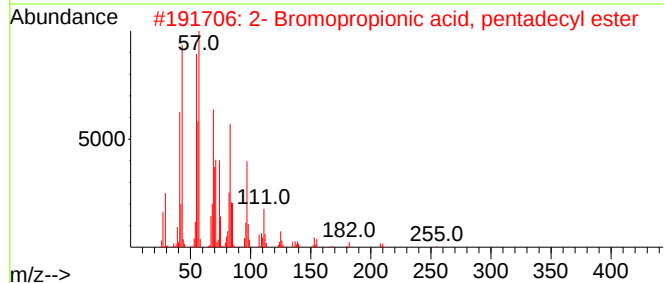
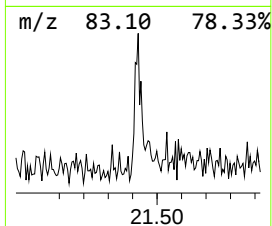
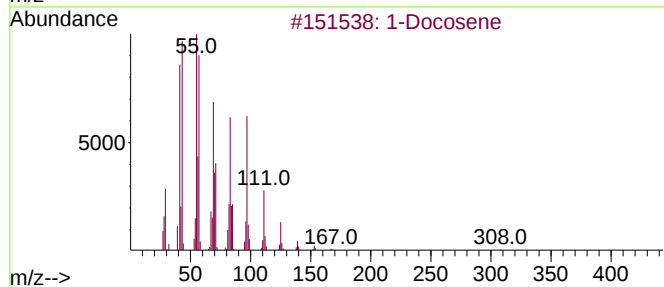
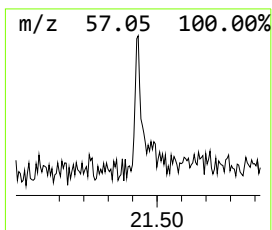
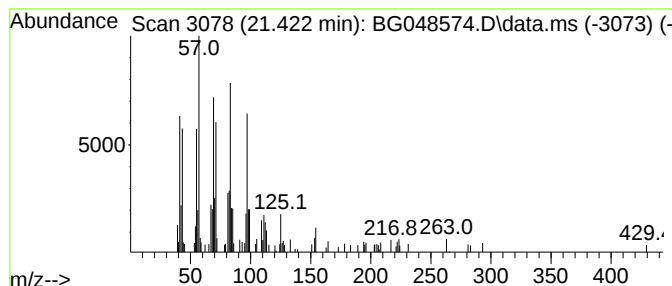
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Peak Number 3 1-Docosene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.422	3.88 ng	80614	Chrysene-d12	21.798

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene			308	C22H44	001599-67-3	83
2	2- Bromopropionic acid, pentadec...			362	C18H35BrO2	1000292-44-2	72
3	1-Hexadecanesulfonyl chloride			324	C16H33ClO2S	038775-38-1	72
4	n-Tetracosanol-1			354	C24H50O	000506-51-4	64
5	Docosyl pentafluoropropionate			472	C25H45F5O2	1000351-80-9	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown5.165	5.165	6.1	ng	45163	1	8.097	147563	20.0
Pentadecanoic acid	18.379	3.6	ng	66526	4	17.497	369938	20.0
1-Docosene	21.422	3.9	ng	80614	5	21.798	415228	20.0