LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100722\
Data File : BG055106.D
Acq On : 7 Oct 2022 19:46
Operator : CG/JU
Sample : N5018-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SASP2-T-3-(14-16)

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-BG100322.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055106.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.376	10	15	32	rVB	222035	371795	24.28%	4.226%
2	5.379	350	356	364	rVB	122070	189198	12.35%	2.151%
3	5.855	429	437	446	rVB	367920	602877	39.36%	6.853%
4	7.459	703	710	720	rBV	386164	670340	43.77%	7.620%
5	8.335	852	859	866	rBV	121512	209634	13.69%	2.383%
6	9.504	1048	1058	1067	rBV	255601	448498	29.28%	5.098%
7	11.167	1330	1341	1349	rVB	165582	304477	19.88%	3.461%
8	13.570	1742	1750	1758	rVB	702115	1091316	71.25%	12.405%
9	14.281	1865	1871	1878	rBV	297792	437048	28.54%	4.968%
10	14.939	1976	1983	1990	rVB	269932	422359	27.58%	4.801%
11	15.732	2113	2118	2126	rBV3	38238	67581	4.41%	0.768%
12	16.413	2228	2234	2240	rBV	536064	785711	51.30%	8.931%
13	16.637	2265	2272	2277	rBV	48197	92828	6.06%	1.055%
14	17.459	2408	2412	2415	rVB	69578	90723	5.92%	1.031%
15	17.671	2443	2448	2453	rBV	291061	452306	29.53%	5.141%
16	18.534	2591	2595	2600	rBV	317032	431403	28.17%	4.904%
17	20.191	2875	2877	2879	rBV	502216	597920	39.04%	6.796%
18	20.250	2884	2887	2892	rVB	1062441	1531579	100.00%	17.409%

Sum of corrected areas: 8797593

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100722\
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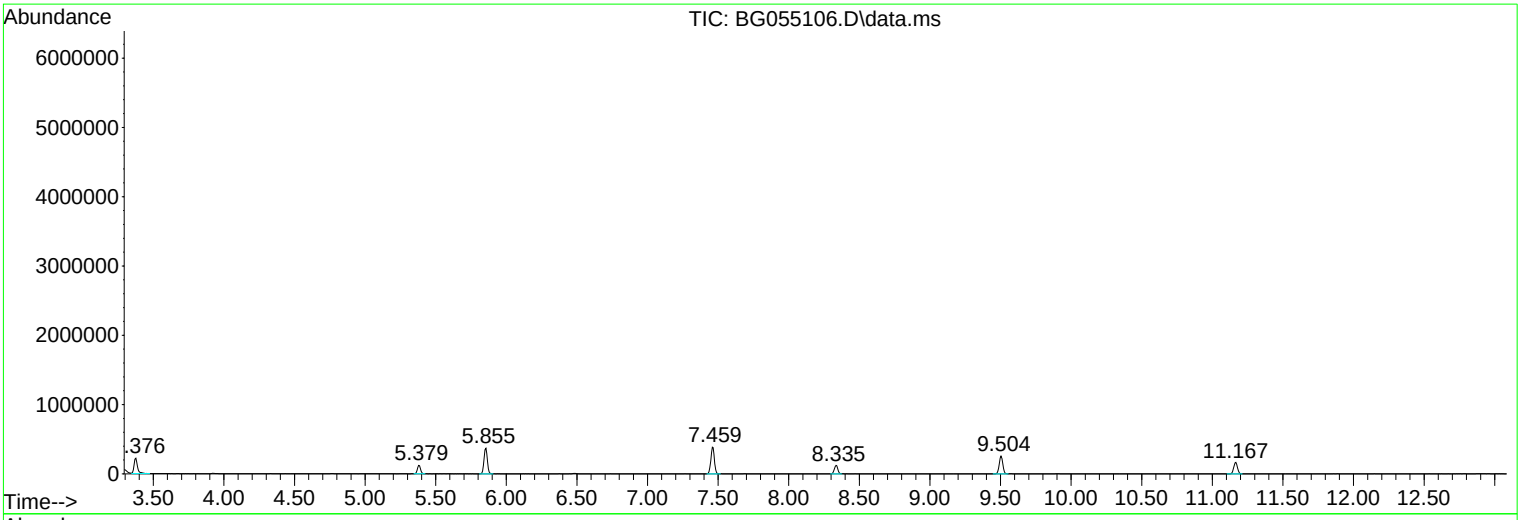
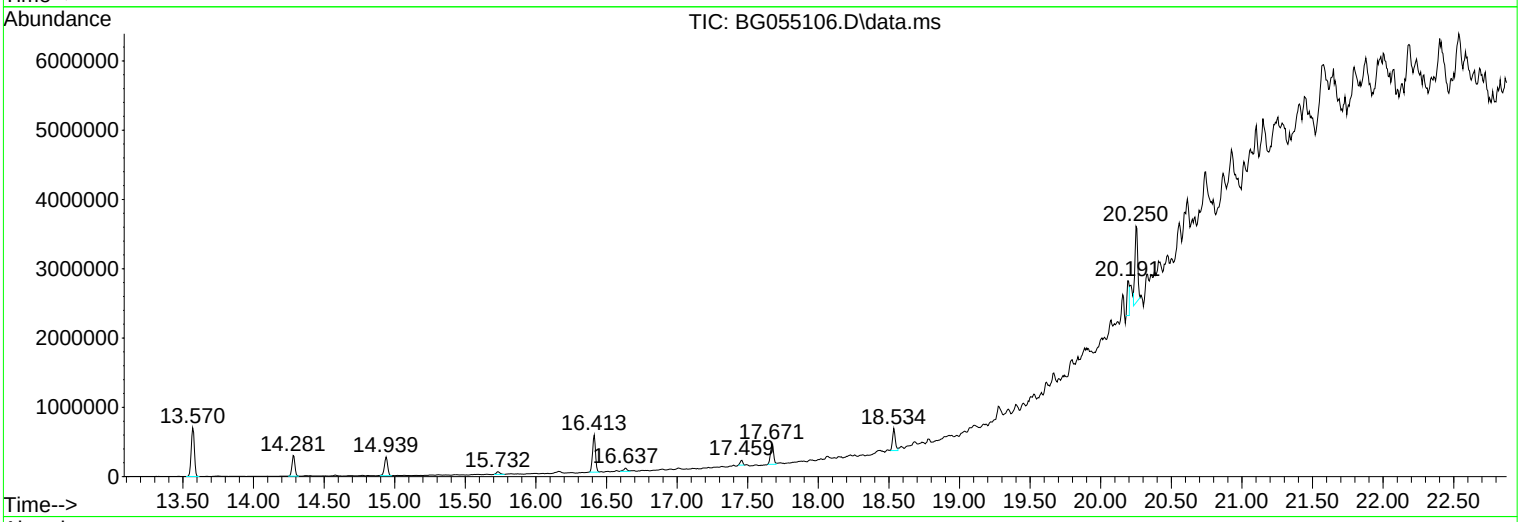
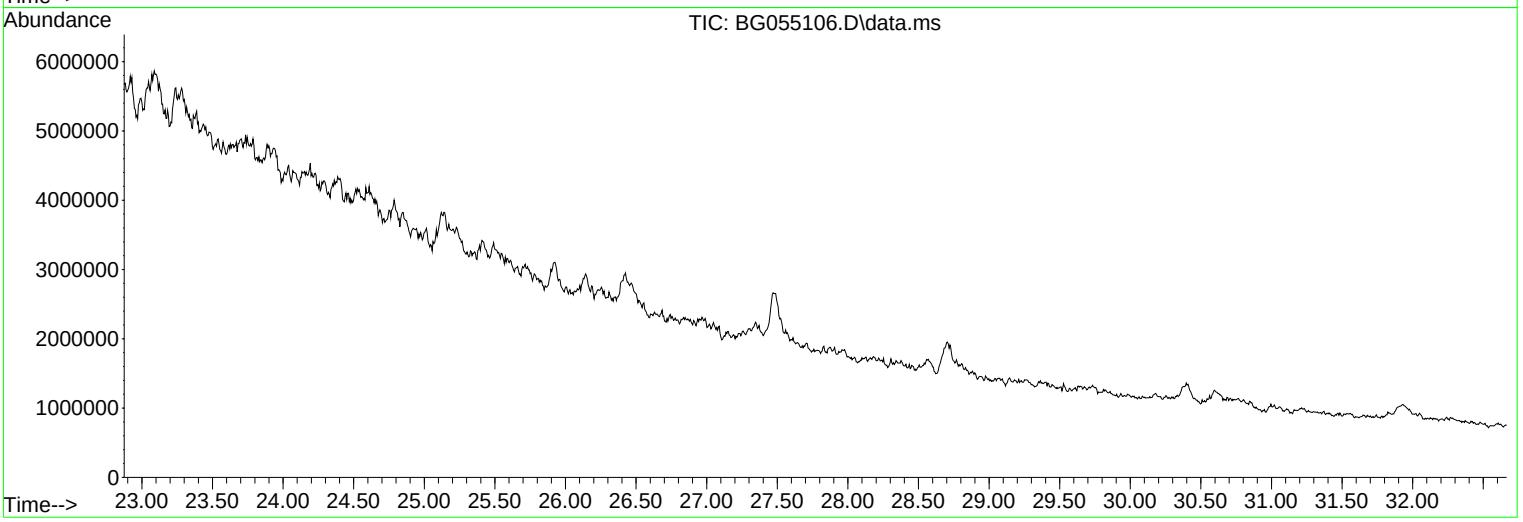
Instrument :
BNA_G
ClientSampleId :
SASP2-T-3-(14-16)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100322.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_G\Data\BG100722\
Data File : BG055106.D
Acq On : 7 Oct 2022 19:46
Operator : CG/JU
Sample : N5018-04
Misc :
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

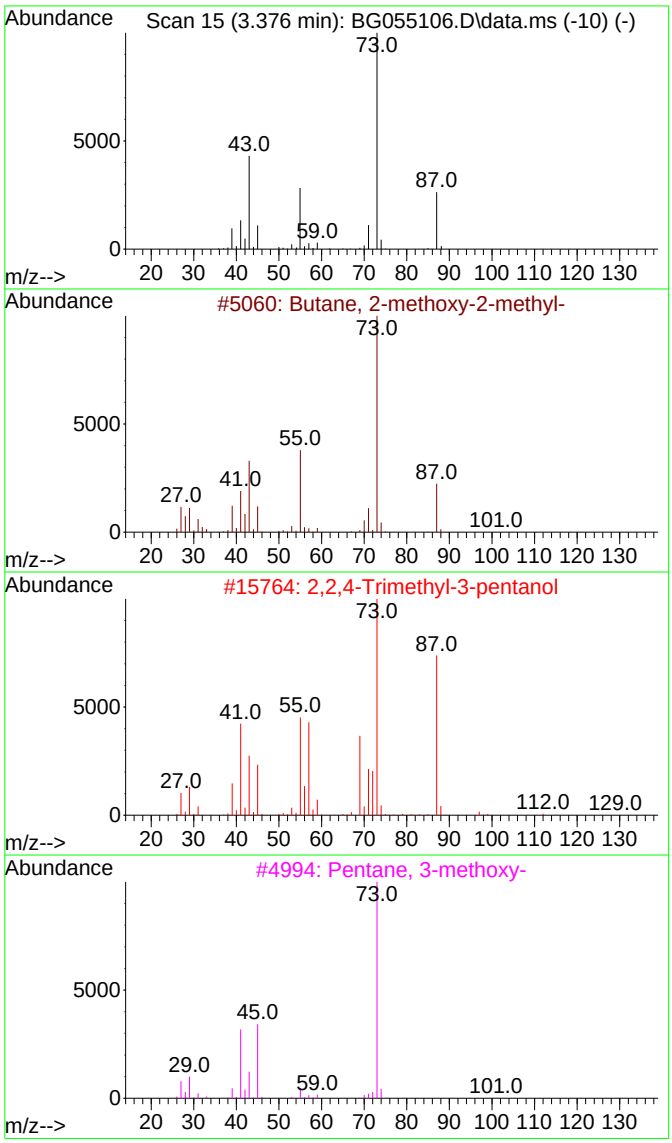
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

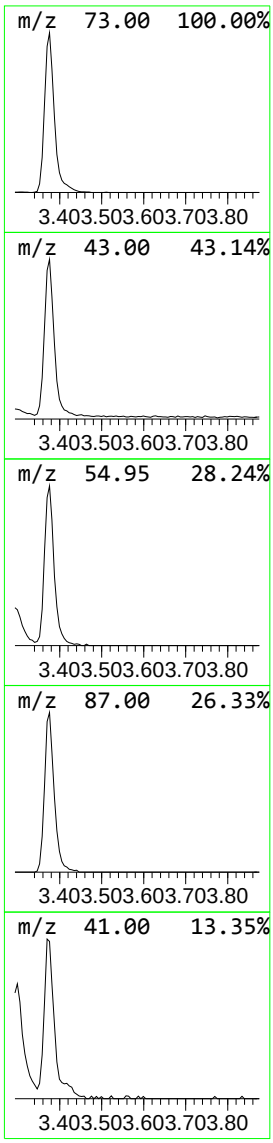
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.376	35.47 ng	371795	1,4-Dichlorobenzene-d4	8.340

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





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Acq On : 7 Oct 2022 19:46
Operator : CG/JU
Sample : N5018-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SASP2-T-3-(14-16)

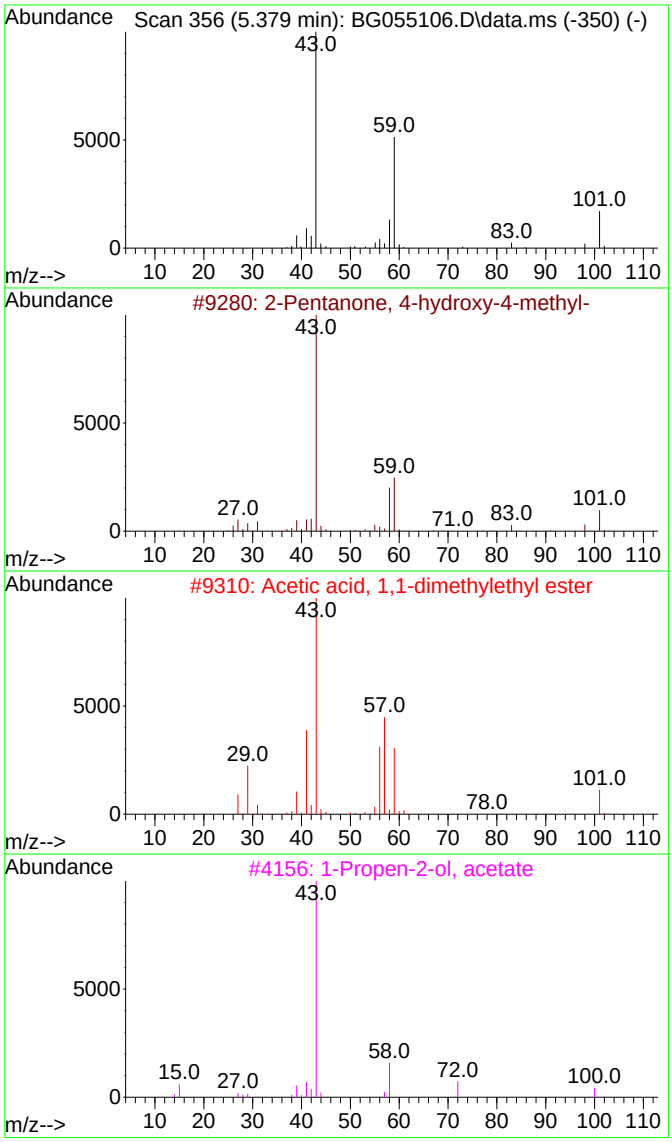
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

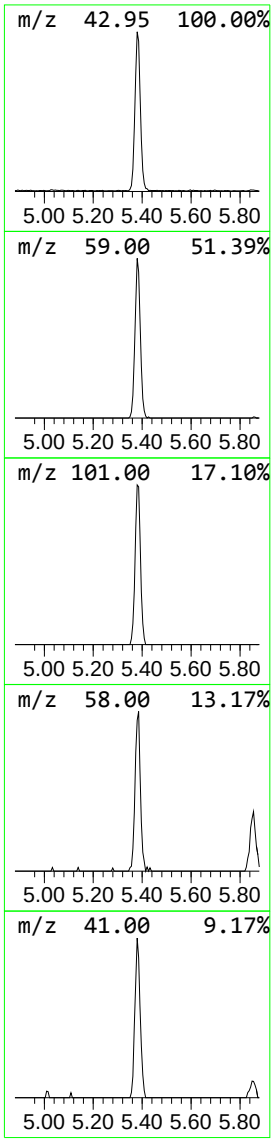
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.379	18.05 ng	189198	1,4-Dichlorobenzene-d4	8.340

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4	2-Pentanone	86	C5H10O	000107-87-9	10
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100722\
Data File : BG055106.D
Acq On : 7 Oct 2022 19:46
Operator : CG/JU
Sample : N5018-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SASP2-T-3-(14-16)

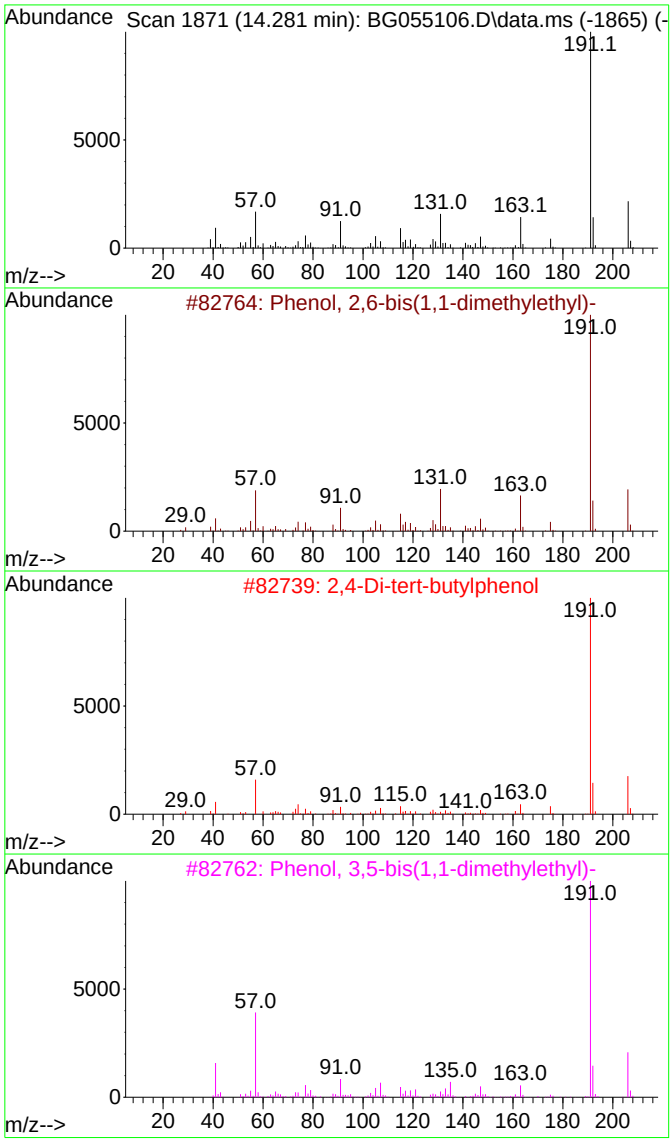
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

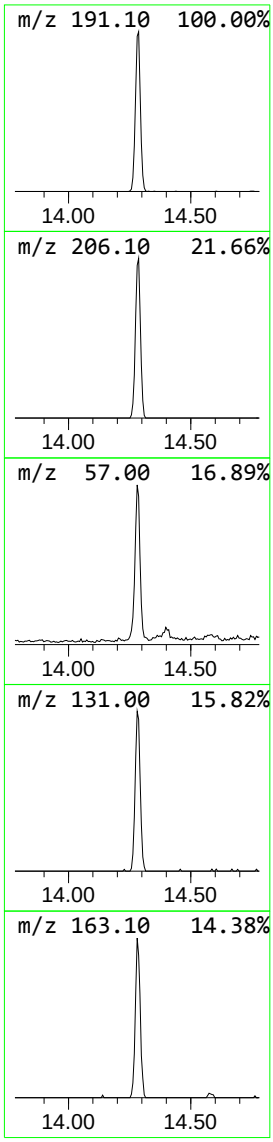
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Phenol, 2,6-bis(1,1-dimethy... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.281	20.70 ng	437048	Acenaphthene-d10	14.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,6-bis(1,1-dimethylethyl)-	206	C14H22O	000128-39-2	96
2	2,4-Di-tert-butylphenol	206	C14H22O	000096-76-4	87
3	Phenol, 3,5-bis(1,1-dimethylethyl)-	206	C14H22O	001138-52-9	81
4	2H-Indeno[1,2-b]furan-2-one, 3,3...	206	C13H18O2	1000196-74-3	80
5	3-(4-tert-Butylphenyl)propanoic ...	206	C13H18O2	001208-64-6	74





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Sample : N5018-04
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Instrument :
BNA_G
ClientSampleId :
SASP2-T-3-(14-16)

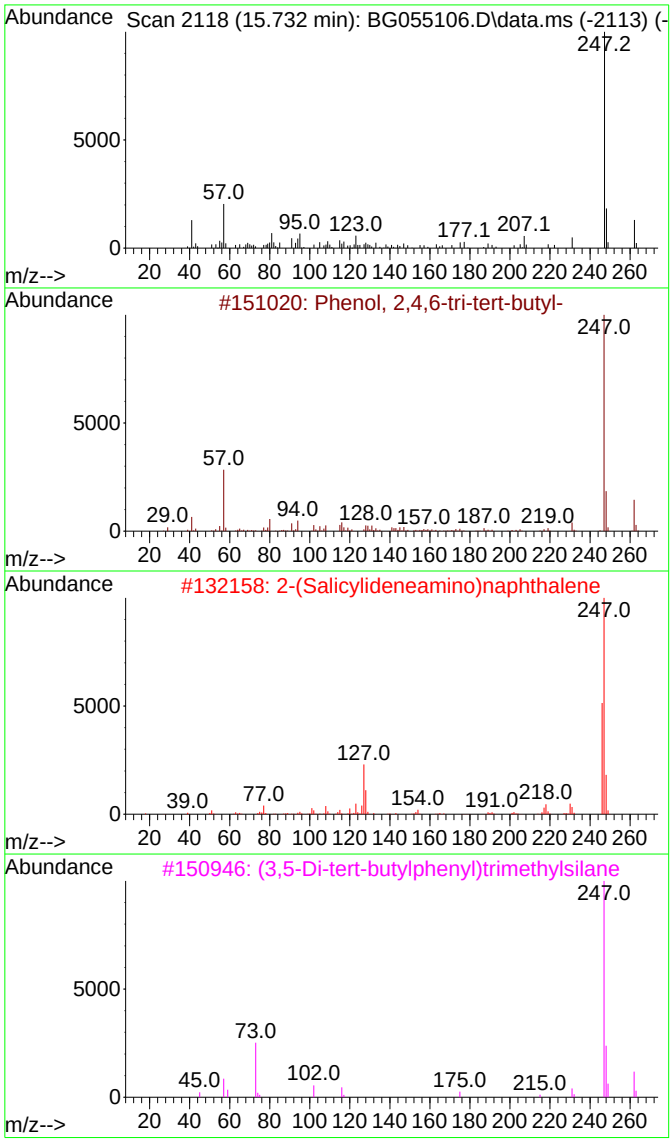
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

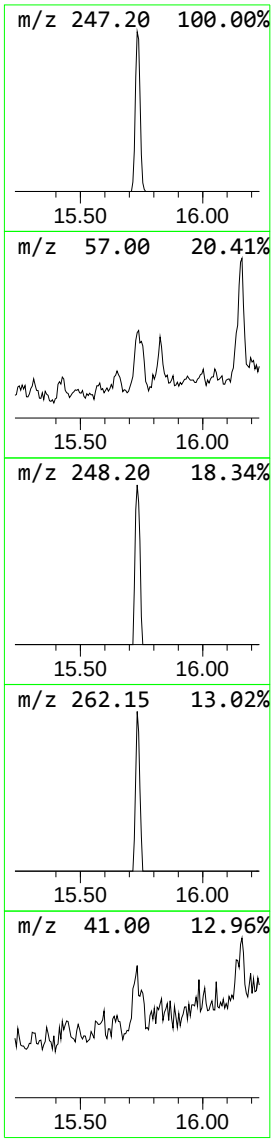
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Phenol, 2,4,6-tri-tert-butyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.732	3.20 ng	67581	Acenaphthene-d10	14.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,4,6-tri-tert-butyl-	262	C18H30O	000732-26-3	83
2	2-(Salicylideneamino)naphthalene	247	C17H13NO	001689-72-1	72
3	(3,5-Di-tert-butylphenyl)trimeth...	262	C17H30Si	1000423-71-8	72
4	Propanenitrile, 3-[1-(3-diethyla...	262	C16H26N2O	1000271-09-5	64
5	9H-Imidazo[1,2-a]benzimidazole, ...	247	C16H13N3	021431-82-3	59





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Sample : N5018-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

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BNA_G
ClientSampleId :
SASP2-T-3-(14-16)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

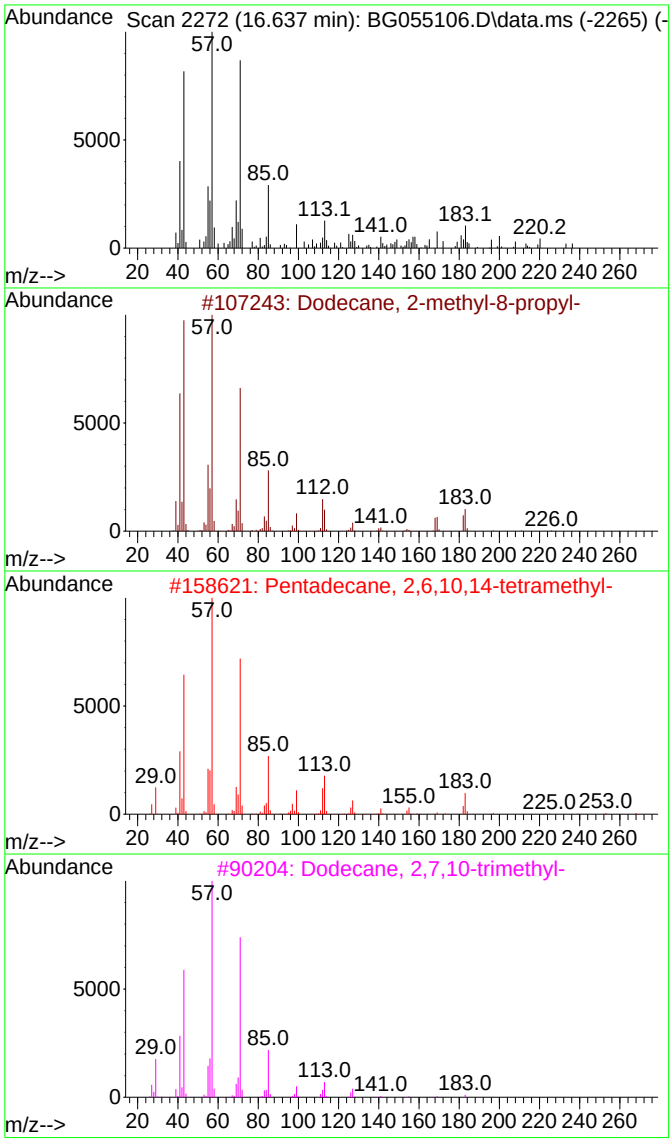
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

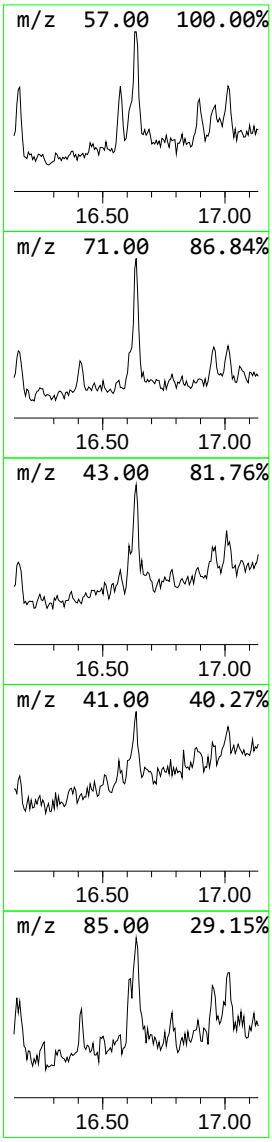
****

Peak Number 5 Dodecane, 2-methyl-8-propyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.637	4.10 ng	92828	Phenanthrene-d10	17.671

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2-methyl-8-propyl-	226	C16H34	055045-07-3	86
2	Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	80
3	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	80
4	Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	72
5	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	64





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BNA_G
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SASP2-T-3-(14-16)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

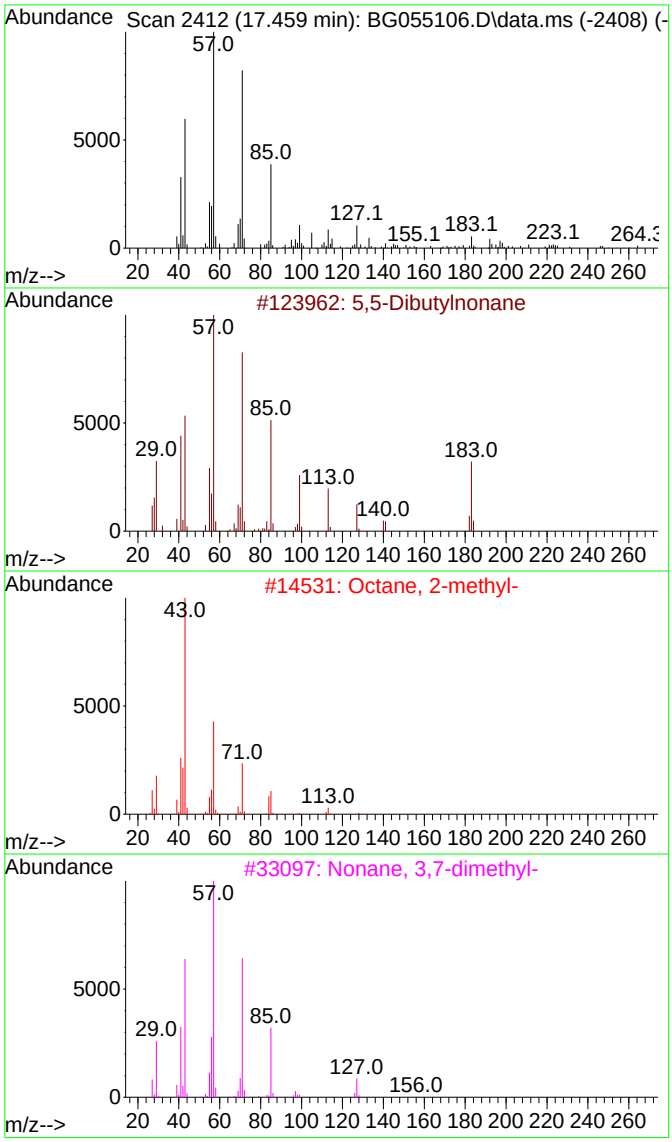
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

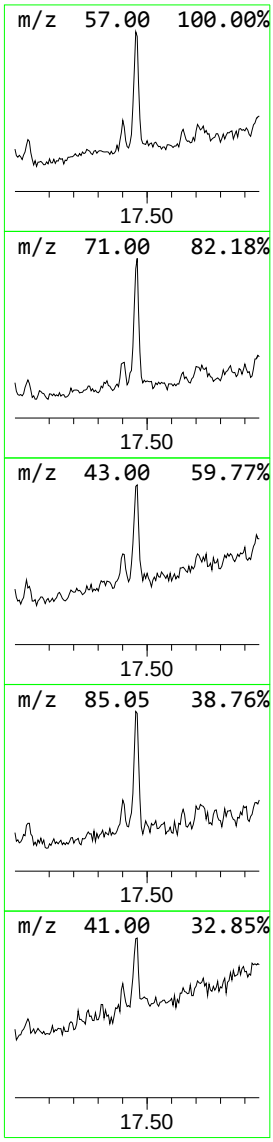
****

Peak Number 6 5,5-Dibutylnonane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.459	4.01 ng	90723	Phenanthrene-d10	17.671

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5,5-Dibutylnonane	240	C17H36	006008-17-9	72
2	Octane, 2-methyl-	128	C9H20	003221-61-2	72
3	Nonane, 3,7-dimethyl-	156	C11H24	017302-32-8	72
4	Undecane, 6-ethyl-	184	C13H28	017312-60-6	70
5	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	64





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

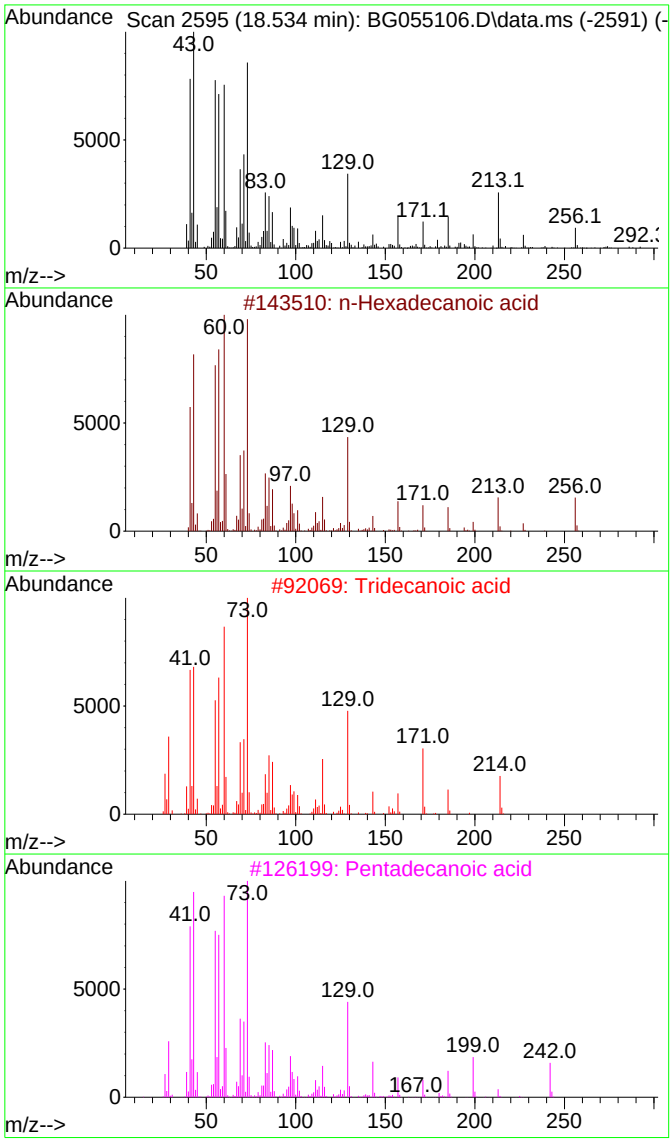
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

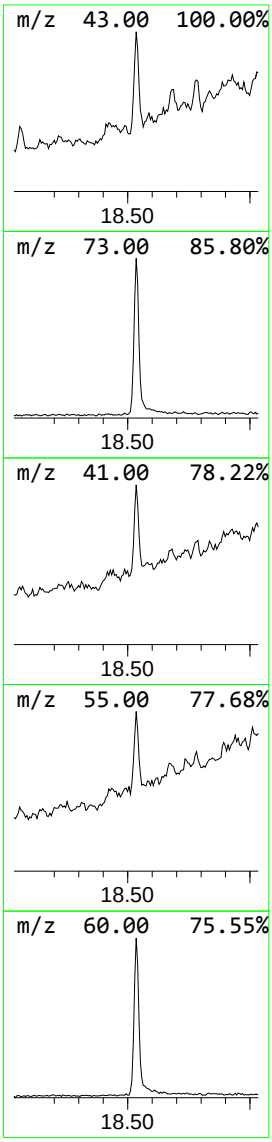
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.534	19.08 ng	431403	Phenanthrene-d10	17.671

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	97
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	70
4	n-Decanoic acid	172	C10H20O2	000334-48-5	64
5	Octadecanoic acid	284	C18H36O2	000057-11-4	58





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TIC Library : C:\Database\NIST20.L
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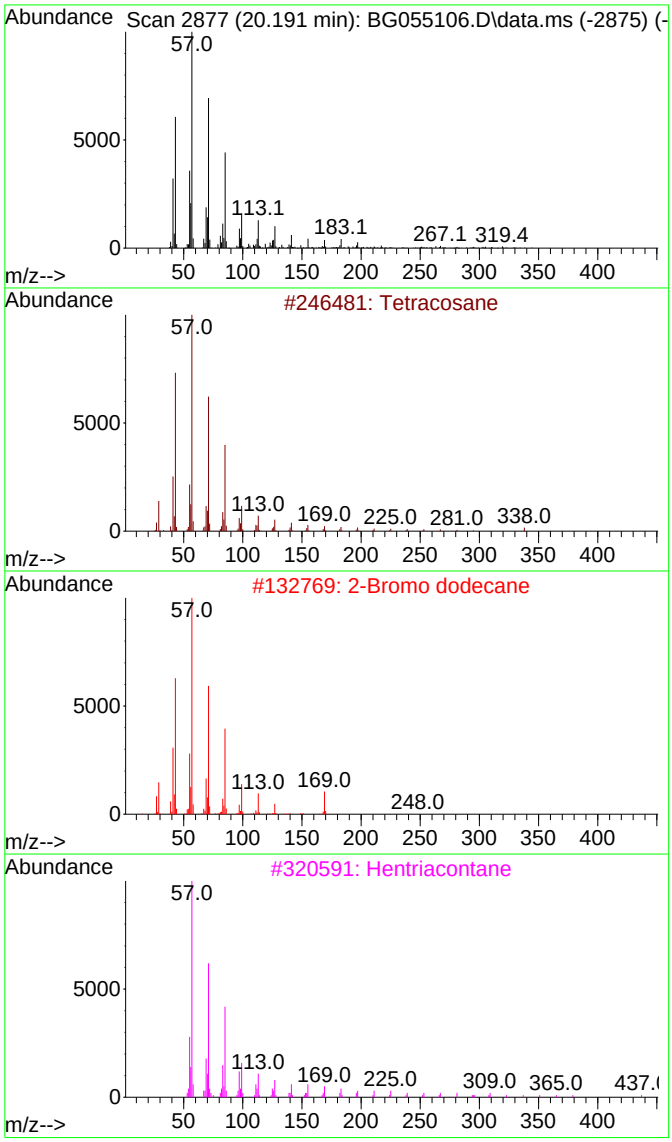
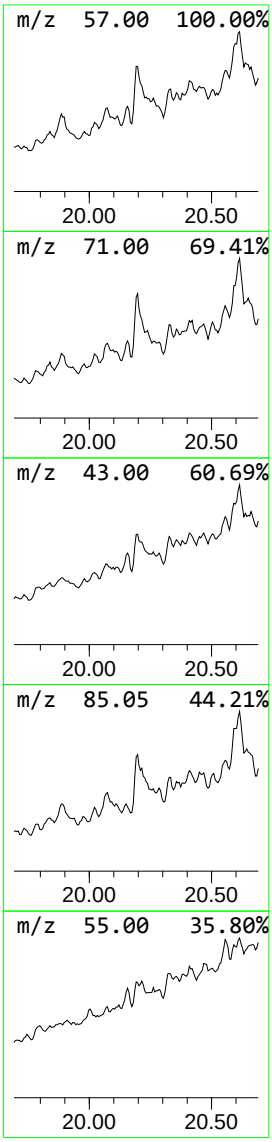
****

Peak Number 8 Tetracosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.191	7.81 ng	597920	Chrysene-d12	21.983

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	93
2	2-Bromo dodecane	248	C12H25Br	013187-99-0	93
3	Hentriacontane	437	C31H64	000630-04-6	91
4	Hexacosane	366	C26H54	000630-01-3	90
5	Heneicosane	296	C21H44	000629-94-7	90





Tentatively Identified Compound (LSC) summary

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100322.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...	3.376	35.5	ng	371795	1	8.340	209634	20.0
2-Pentanone, 4-...	5.379	18.1	ng	189198	1	8.340	209634	20.0
Phenol, 2,6-bis...	14.281	20.7	ng	437048	3	14.939	422359	20.0
Phenol, 2,4,6-t...	15.732	3.2	ng	67581	3	14.939	422359	20.0
Dodecane, 2-met...	16.637	4.1	ng	92828	4	17.671	452306	20.0
5,5-Dibutylnonane	17.459	4.0	ng	90723	4	17.671	452306	20.0
n-Hexadecanoic ...	18.534	19.1	ng	431403	4	17.671	452306	20.0
Tetracosane	20.191	7.8	ng	597920	5	21.983	1531580	20.0