LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112021\
Data File : BG051163.D
Acq On : 21 Nov 2021 1:28
Operator : CG/JU
Sample : M4768-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-1

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-BG111921.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG051163.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.744	377	384	390	rBV	212540	353683	23.26%	4.186%
2	5.808	390	395	404	rVB2	13835	30868	2.03%	0.365%
3	7.359	649	659	670	rBV	143589	275938	18.15%	3.266%
4	8.205	796	803	815	rBV	99683	173922	11.44%	2.059%
5	8.575	860	866	873	rVB	28260	47830	3.15%	0.566%
6	9.310	984	991	996	rBV2	17436	31299	2.06%	0.370%
7	9.380	996	1003	1013	rVV	333164	621820	40.89%	7.360%
8	9.833	1073	1080	1088	rVB	13134	22080	1.45%	0.261%
9	10.415	1169	1179	1185	rBV4	10205	19055	1.25%	0.226%
10	10.785	1234	1242	1248	rBV3	10275	21070	1.39%	0.249%
11	11.031	1274	1284	1296	rVV	139701	291985	19.20%	3.456%
12	11.131	1296	1301	1309	rVB	10843	20628	1.36%	0.244%
13	11.490	1357	1362	1368	rVB3	13888	22822	1.50%	0.270%
14	11.601	1376	1381	1389	rBV2	12227	23360	1.54%	0.276%
15	11.930	1429	1437	1441	rVB2	14278	23367	1.54%	0.277%
16	12.124	1465	1470	1477	rVB5	10304	20820	1.37%	0.246%
17	12.395	1511	1516	1523	rBV3	13288	24178	1.59%	0.286%
18	12.894	1590	1601	1608	rBV2	48523	111945	7.36%	1.325%
19	13.458	1688	1697	1703	rVB	814285	1318042	86.68%	15.601%
20	13.623	1720	1725	1728	rBV3	13290	19916	1.31%	0.236%
21	13.769	1745	1750	1754	rBV5	10940	21152	1.39%	0.250%
22	14.163	1811	1817	1828	rVB10	21401	62257	4.09%	0.737%
23	14.463	1864	1868	1873	rVB6	10986	21644	1.42%	0.256%
24	14.557	1880	1884	1890	rVB3	16393	29703	1.95%	0.352%
25	14.833	1921	1931	1939	rBV	225538	407159	26.78%	4.819%
26	14.903	1939	1943	1948	rVV5	18355	30678	2.02%	0.363%
27	15.326	2007	2015	2020	rBV	37390	77481	5.10%	0.917%
28	15.450	2030	2036	2040	rVB8	17600	32079	2.11%	0.380%
29	16.002	2127	2130	2135	rBV2	14136	25596	1.68%	0.303%
30	16.196	2157	2163	2171	rBV2	83439	193662	12.74%	2.292%
31	16.325	2179	2185	2196	rVB	614079	962440	63.29%	11.392%
32	17.036	2303	2306	2310	rBV4	17773	24130	1.59%	0.286%
33	17.583	2394	2399	2406	rBV	257388	401203	26.38%	4.749%
34	18.446	2542	2546	2551	rBV	60977	91194	6.00%	1.079%
35	20.174	2835	2840	2847	rVB	1171472	1520631	100.00%	17.998%
36	21.883	3126	3131	3138	rVB2	251142	424412	27.91%	5.023%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112021\
Data File : BG051163.D
Acq On : 21 Nov 2021 1:28
Operator : CG/JU
Sample : M4768-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-1

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-BG111921.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	23.388	3382	3387	3395	rVB2	84008	177514	11.67%	2.101%
38	25.285	3702	3710	3723	rVB	154174	471108	30.98%	5.576%

Sum of corrected areas: 8448671

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112021\
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Acq On : 21 Nov 2021 1:28
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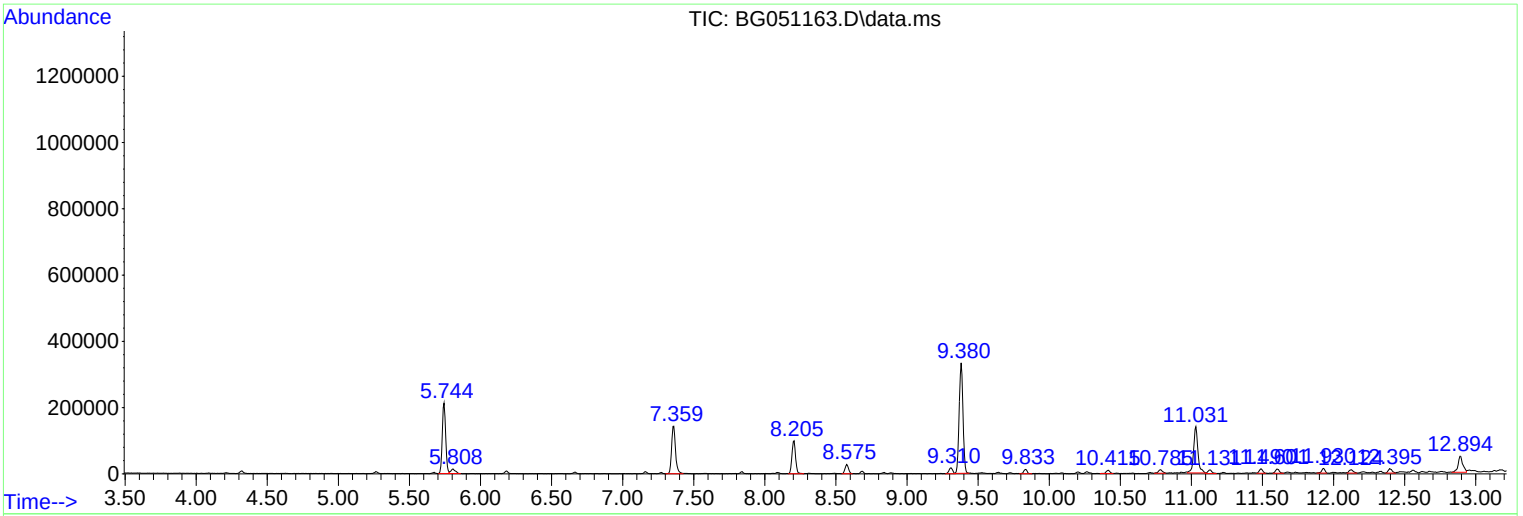
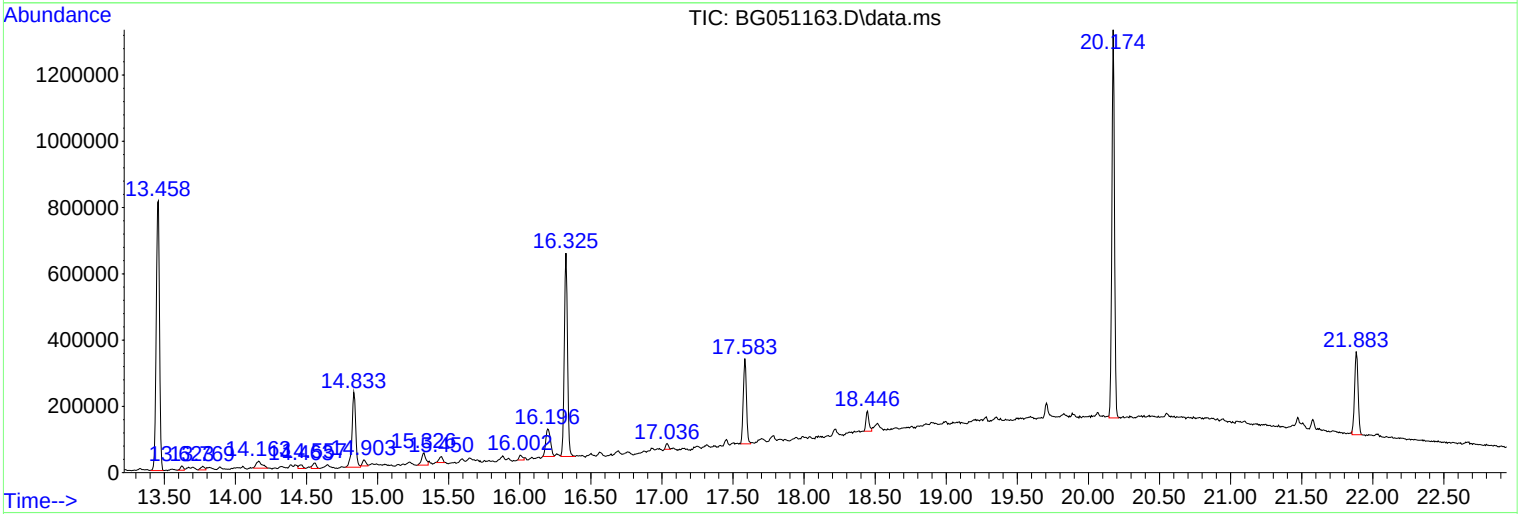
Misc :
ALS Vial : 18 Sample Multiplier: 1

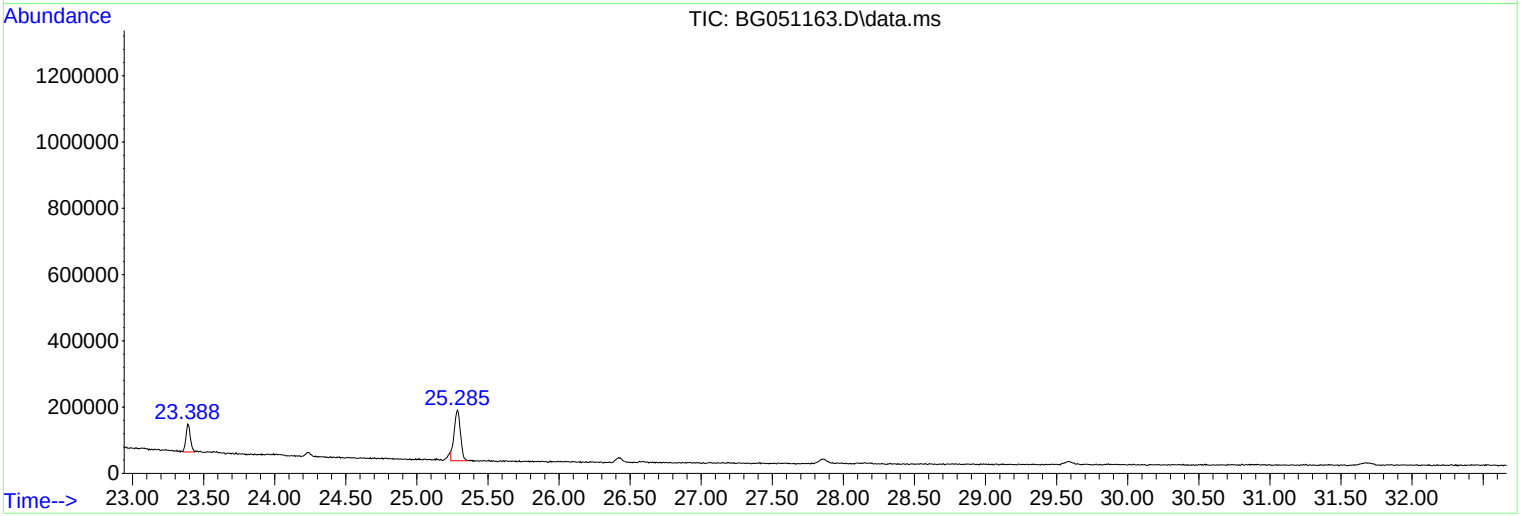
Instrument :
BNA_G
ClientSampleId :
MW-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111921.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\BG112021\
Data File : BG051163.D
Acq On : 21 Nov 2021 1:28
Operator : CG/JU
Sample : M4768-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

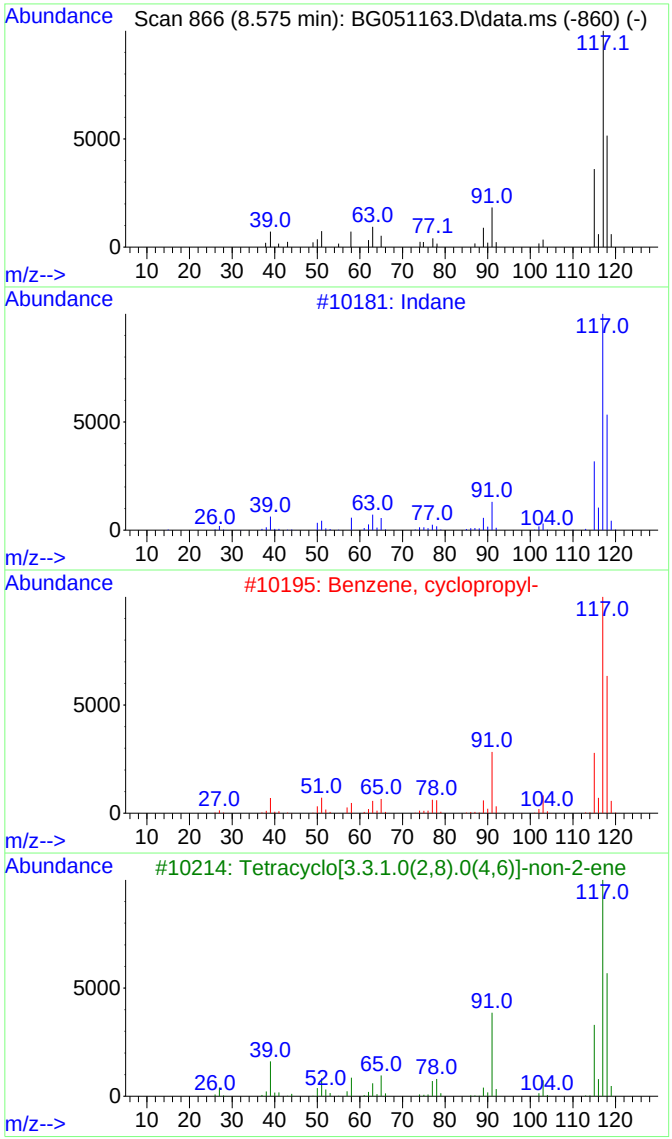
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

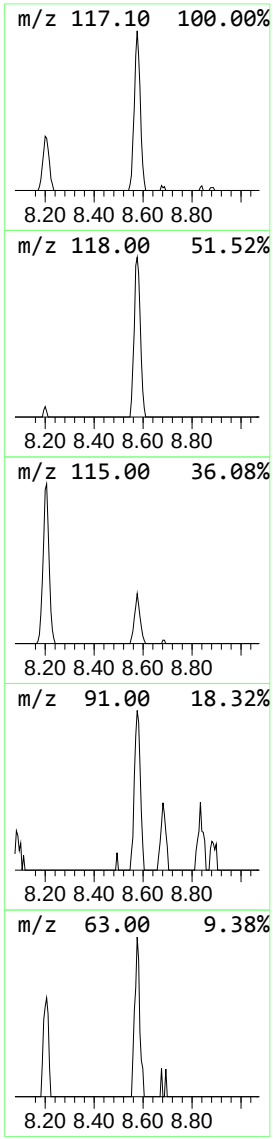
****

Peak Number 2 Indane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.575	5.50 ng	47830	1,4-Dichlorobenzene-d4	8.205

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	87
2	Benzene, cyclopropyl-	118	C9H10	000873-49-4	72
3	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	72
4	(Z)-1-Phenylpropene	118	C9H10	000766-90-5	72
5	Deltacyclene	118	C9H10	007785-10-6	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112021\
Data File : BG051163.D
Acq On : 21 Nov 2021 1:28
Operator : CG/JU
Sample : M4768-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-1

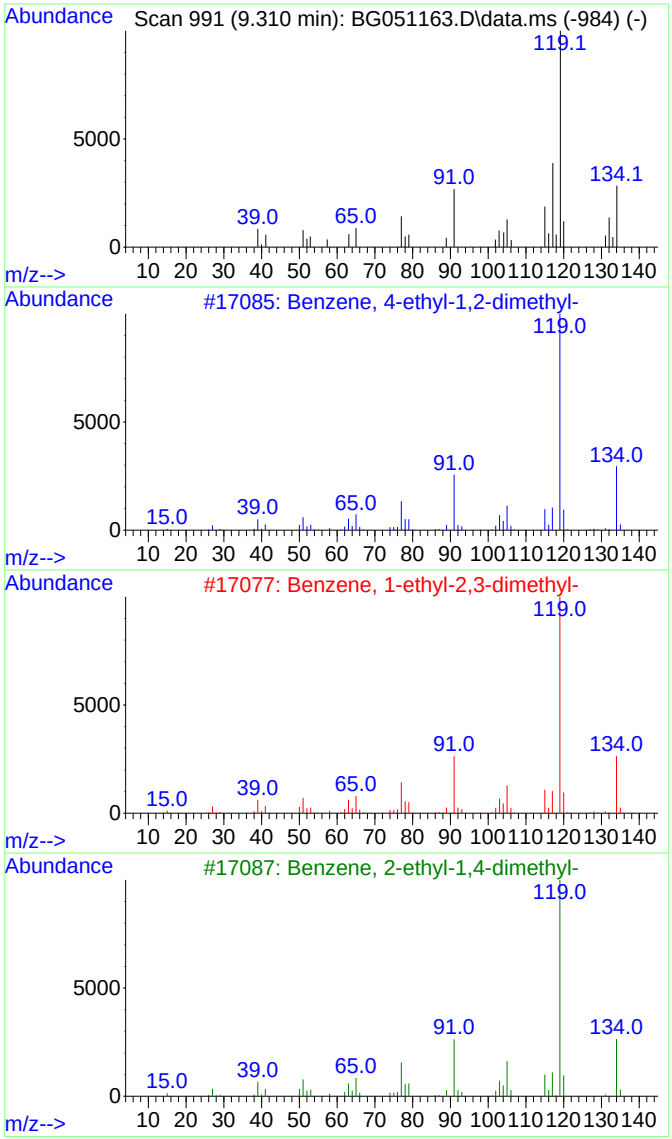
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

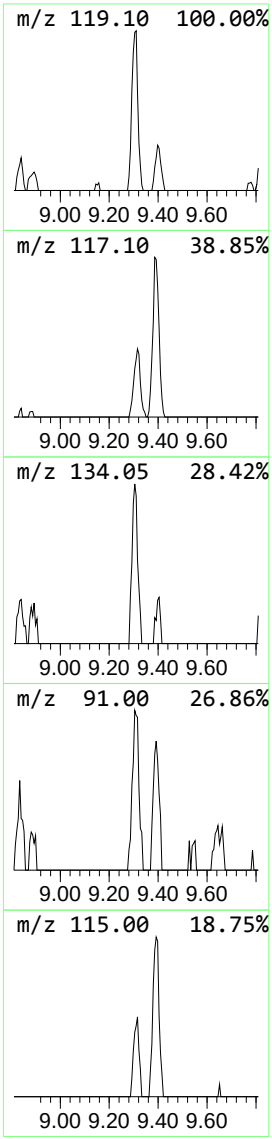
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Benzene, 4-ethyl-1,2-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.310	3.60 ng	31299	1,4-Dichlorobenzene-d4	8.205

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	70
2	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	70
3	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	64
4	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	62
5	7-Methoxymethyl-2,7-dimethylcycl...	164	C11H16O	073992-48-0	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112021\
Data File : BG051163.D
Acq On : 21 Nov 2021 1:28
Operator : CG/JU
Sample : M4768-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

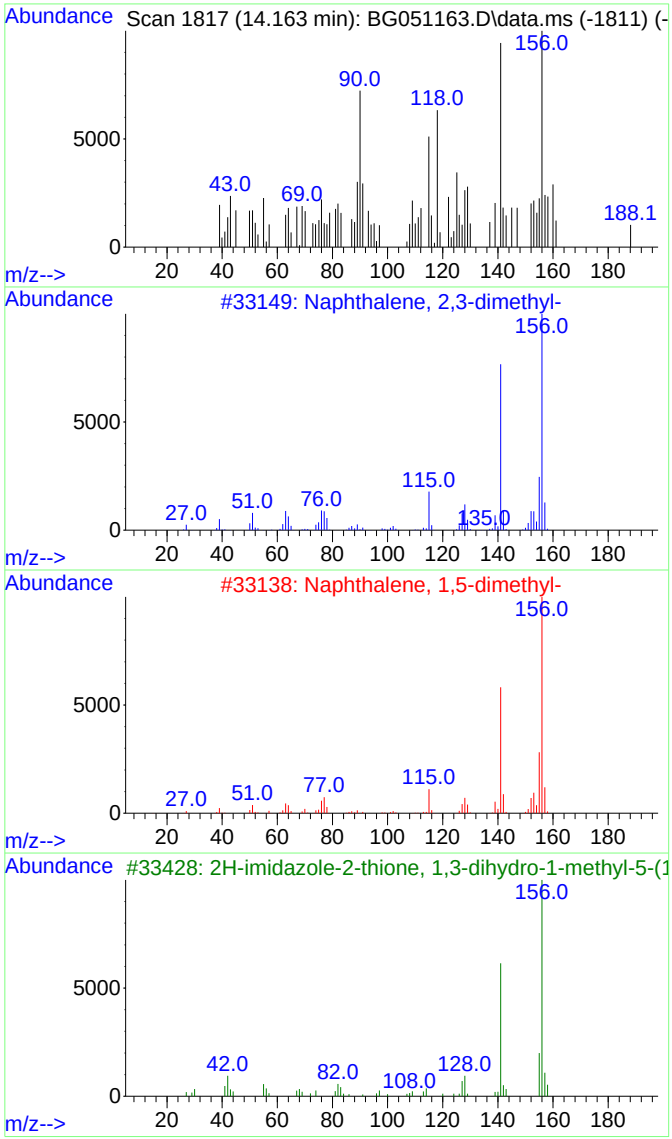
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

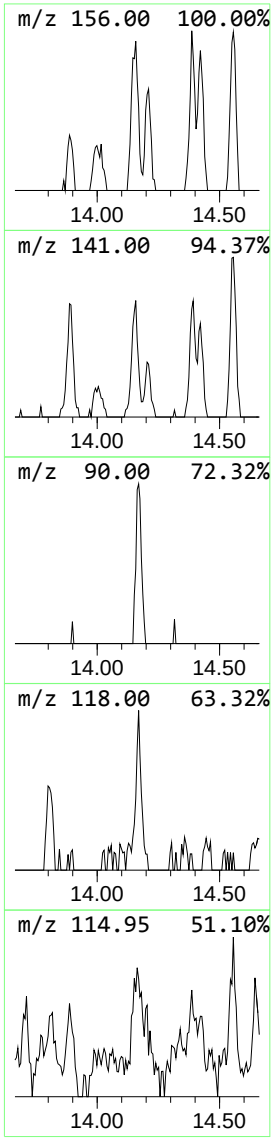
****

Peak Number 4 unknown14.163 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.163	3.06 ng	62257	Acenaphthene-d10	14.833

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	46
2	Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	46
3	2H-imidazole-2-thione, 1,3-dihyd...	156	C7H12N2S	1000404-33-5	43
4	Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	43
5	Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112021\
Data File : BG051163.D
Acq On : 21 Nov 2021 1:28
Operator : CG/JU
Sample : M4768-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

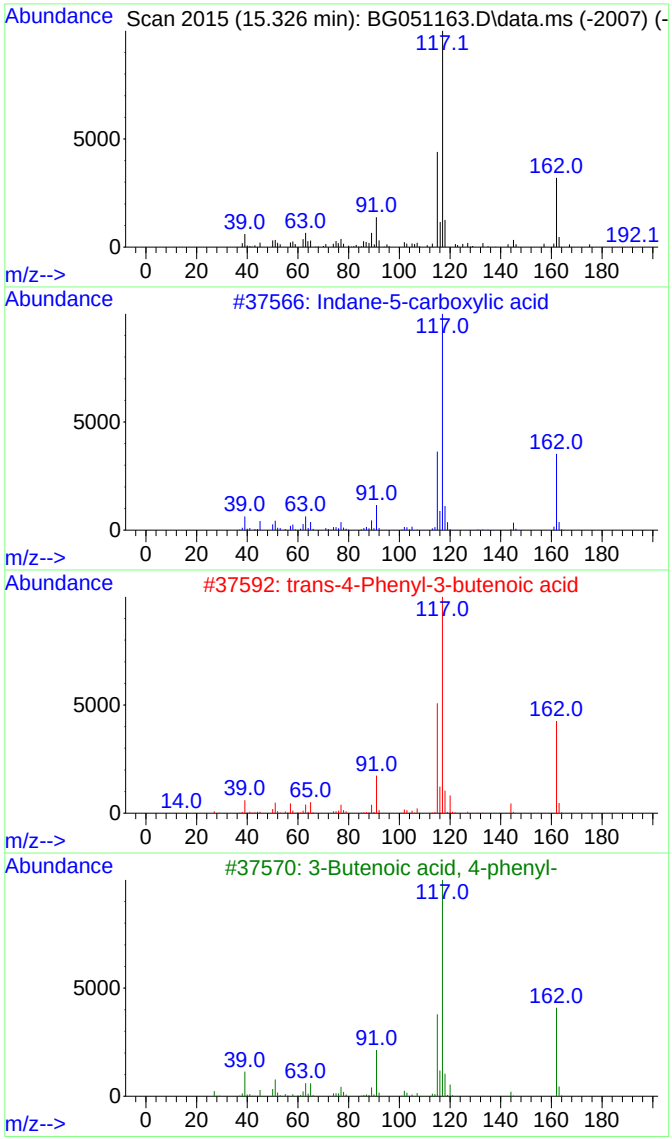
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

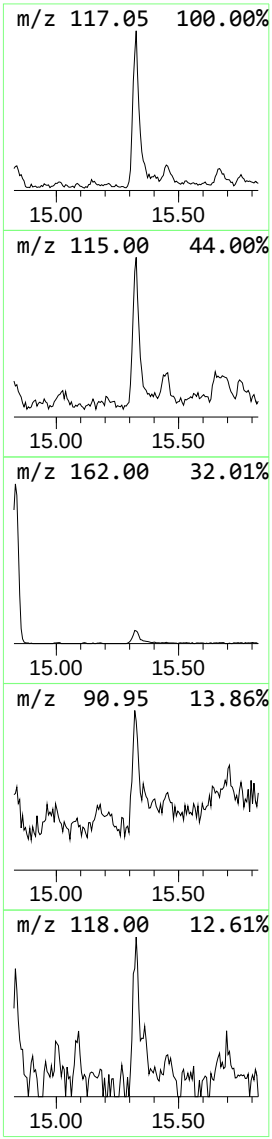
****

Peak Number 5 Indane-5-carboxylic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.326	3.81 ng	77481	Acenaphthene-d10	14.833

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane-5-carboxylic acid	162	C10H10O2	065898-38-6	95
2	trans-4-Phenyl-3-butenoic acid	162	C10H10O2	001914-58-5	91
3	3-Butenoic acid, 4-phenyl-	162	C10H10O2	002243-53-0	91
4	Benzene, 1-(chloromethyl)-3-ethe...	152	C9H9Cl	039833-65-3	72
5	3-Phenylbut-1-ene	132	C10H12	000934-10-1	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112021\
Data File : BG051163.D
Acq On : 21 Nov 2021 1:28
Operator : CG/JU
Sample : M4768-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-1

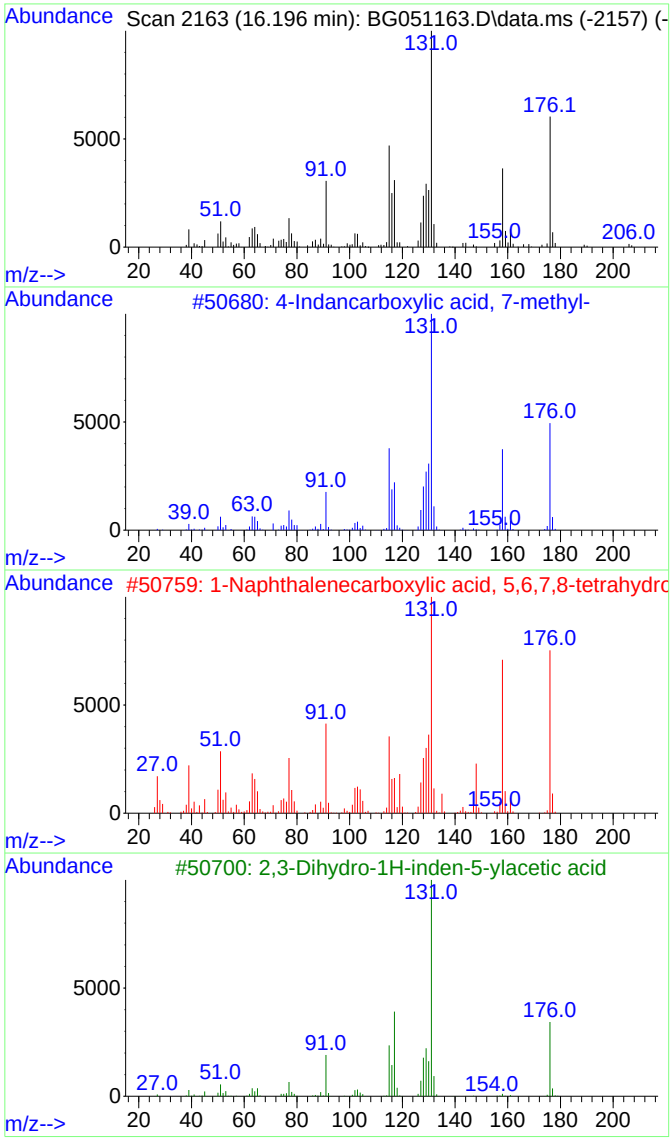
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

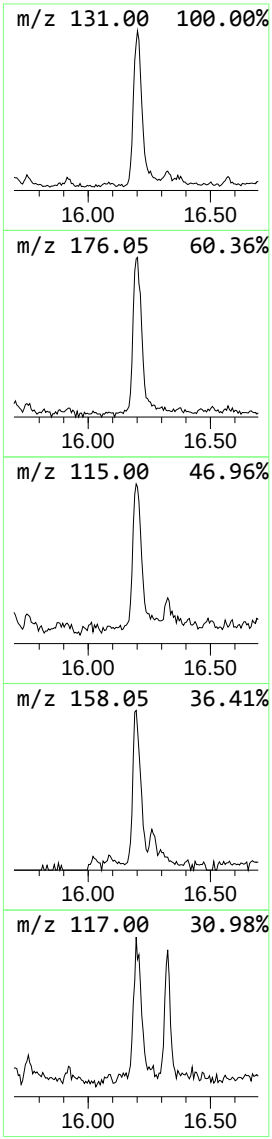
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 4-Indancarboxylic acid, 7-m... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.196	9.51 ng	193662	Acenaphthene-d10	14.833

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Indancarboxylic acid, 7-methyl-	176	C11H12O2	071042-74-5	98
2	1-Naphthalenecarboxylic acid, 5,...	176	C11H12O2	004242-18-6	93
3	2,3-Dihydro-1H-inden-5-ylacetic ...	176	C11H12O2	005453-98-5	68
4	3-Pentenoic acid, 4-phenyl-	176	C11H12O2	053774-19-9	47
5	Cinnamic acid, .alpha.,.beta.-di...	176	C11H12O2	1000151-56-4	43





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Acq On : 21 Nov 2021 1:28
Operator : CG/JU
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Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

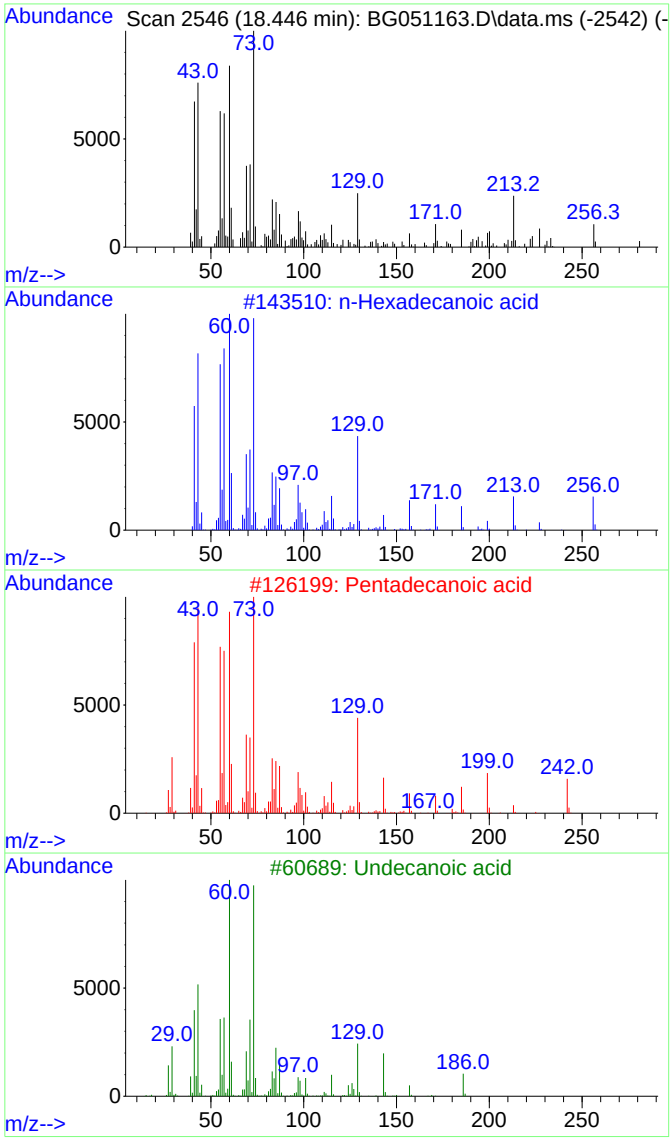
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

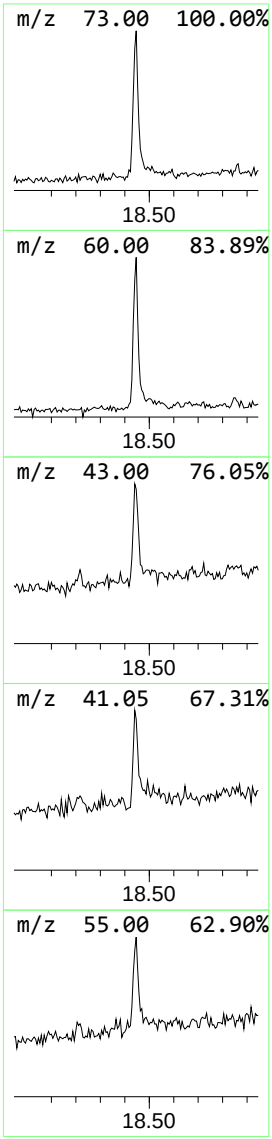
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.446	4.55 ng	91194	Phenanthrene-d10	17.583

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
3	Undecanoic acid	186	C11H22O2	000112-37-8	72
4	Dodecanoic acid	200	C12H24O2	000143-07-7	62
5	Tridecanoic acid	214	C13H26O2	000638-53-9	62





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Data File : BG051163.D
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Operator : CG/JU
Sample : M4768-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

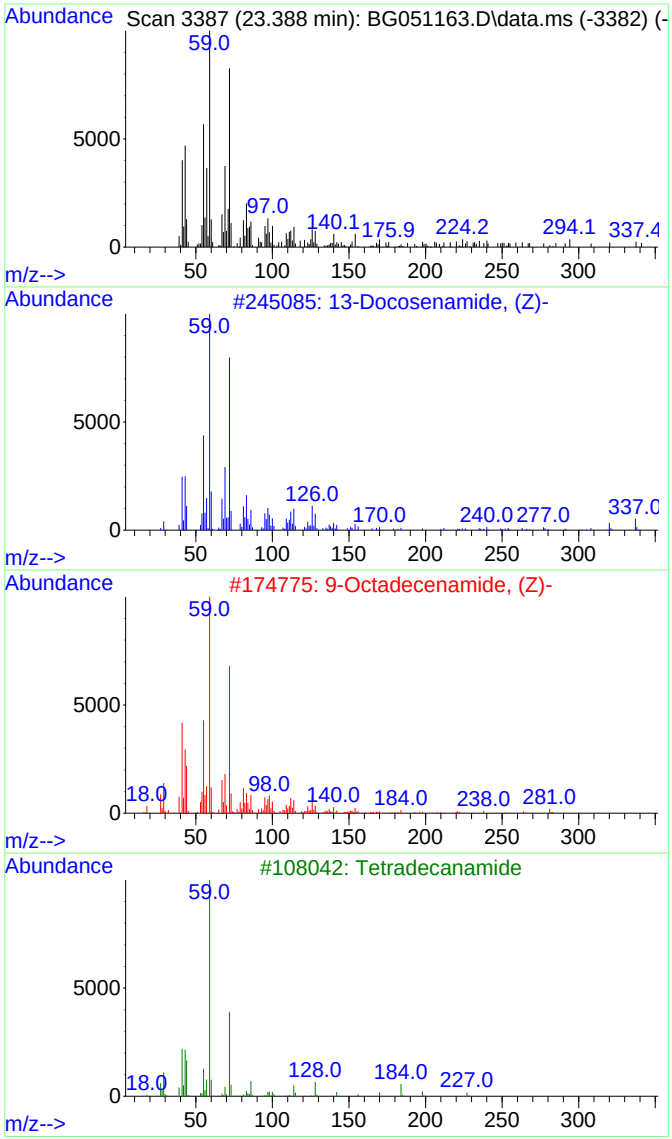
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

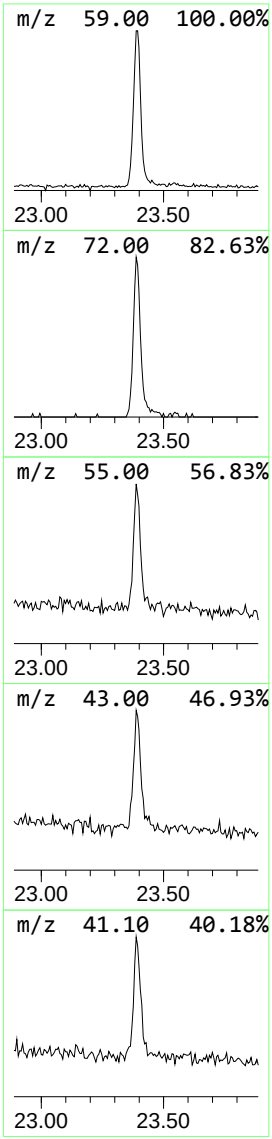
****

Peak Number 8 13-Docosenamide, (Z)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.387	8.37 ng	177514	Chrysene-d12	21.883

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	93
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	87
3	Tetradecanamide	227	C14H29NO	000638-58-4	58
4	9-Octadecenamide	281	C18H35NO	003322-62-1	47
5	Dodecanamide	199	C12H25NO	001120-16-7	46





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112021\
Data File : BG051163.D
Acq On : 21 Nov 2021 1:28
Operator : CG/JU
Sample : M4768-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111921.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
Indane	8.575	5.5	ng	47830	1	8.205	173922	20.0
Benzene, 4-ethy...	9.310	3.6	ng	31299	1	8.205	173922	20.0
unknown14.163	14.163	3.1	ng	62257	3	14.833	407159	20.0
Indane-5-carbox...	15.326	3.8	ng	77481	3	14.833	407159	20.0
4-Indancarboxyl...	16.196	9.5	ng	193662	3	14.833	407159	20.0
n-Hexadecanoic ...	18.446	4.5	ng	91194	4	17.583	401203	20.0
13-Docosenamide...	23.387	8.4	ng	177514	5	21.883	424412	20.0