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Molecular characterization of the ligninolytic Sundarban mangrove isolate *Stenotrophomonas maltophilia* GD1 and its promising applications in the dye and fiber industry

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Supplementary Material

Functional Group Analysis of 'GDI CR_I .asc'4:15:44PM 4/12/2023

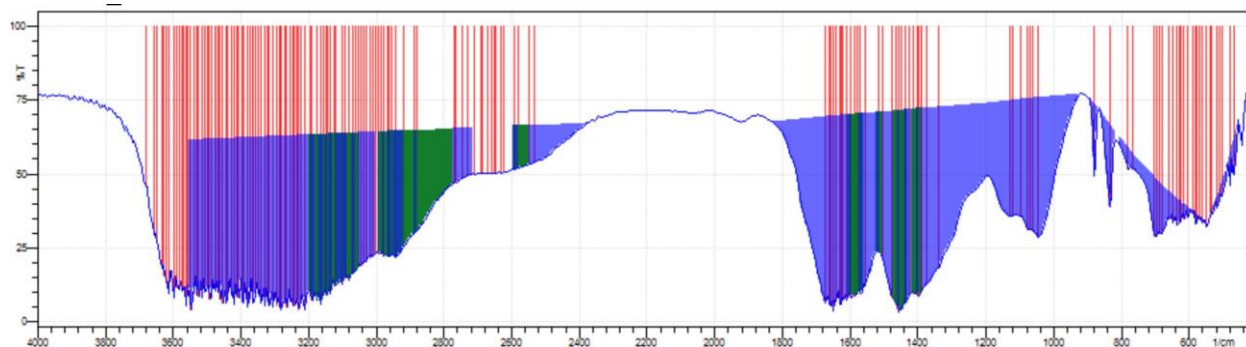
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GDICR I.asc



Matching Functional Groups

Quality	Functional Group	Chemical Sub Class	Chemical Class
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100	Aliphatic Alpha Amino Acid		Aliphatic Amino Acid
100	Aliphatic Amine, Primary, Branched		Aliphatic Amine
100	Aliphatic Amino Acid		Aliphatic Amino Acid
100	Aliphatic Nitrite		Aliphatic Nitro-oxy Compound
100	Aliphatic Sulphoxide	Aliphatic Sulfoxyc compound	Aliphatic Sulfur Compound
100	Aliphatic tert-Amino Acid		Aliphatic Amino Acid
100	Hydroxy, Possibly 1,2-Diol		Aliphatic Alcohol
100	N-MethylAmino Substituent	Substituent Group	Side Chain or Substituent
100	Primary Alcohol		Aliphatic Alcohol
100	Tertiary Alcohol		Aliphatic Alcohol
100	Unsaturated Hydrocarbon, Cis		Alkene
100	Unsaturated Hydrocarbon, Cyclic, > C5		
100	Unsaturated Hydrocarbon, Vinylidene		Alkene
98	Aliphatic Amine, Primary		Aliphatic Amine
97	Aliphatic Primary Amide, Linear		Aliphatic Amide
94	Unsaturated Hydrocarbon, Trisubstituted		Alkene
93	Carbonyl, Possibly Conjugated Aldehyde		Aliphatic Aldehyde
92	Aliphatic Alkoxy, Methoxy		Aliphatic Ether
92	Aliphatic Mercaptan, Branched, Methyl	Aliphatic Thiol	Aliphatic Thiocompound
91	Aliphatic Nitro Group		Aliphatic Nitro-oxy Compound

91	Aliphatic Primary Amide, Free NH2 Amino		Aliphatic Amide
88	3-Subst Pyridine	Pyridines	Other Aromatic Compounds

87	Aliphatic Primary Amide		Aliphatic Amide
87	Unsaturated Hydrocarbon, Trans Conjugated		Alkene
85	2-Subst Pyridine	Pyridines	Other Aromatic Compounds
81	Pyridines, General	Pyridines	Other Aromatic Compounds

Corresponding Chemical Classification Rules

Functional Group: 'Aliphatic Alpha Amino Acid', Chemical Class: 'Aliphatic Amino Acid'

Vibration	Start WN	End WN	Threshold	Priority
C-H Bend	1425	1390	Variable	Mandatory
C-H Bend, CH ₂ /CH ₃	1470	1430	Variable	Mandatory
N-H Bend	1530	1500	Variable	Mandatory
C=O Stretch	1600	1560	Strong	Mandatory
Bonded O-H	2600	2560	Variable	Mandatory
C-H Stretch, Alkyl	3000	2855	Variable	Mandatory
N-H Stretch, Bonded	3200	3050	Variable	Mandatory

Missing Chemical Classification Rules

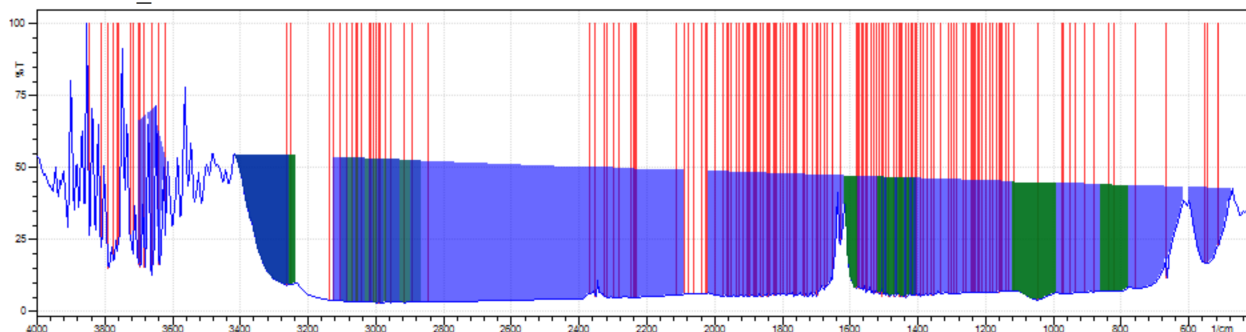
Functional Group: 'Aliphatic Alpha Amino Acid', Chemical Class: 'Aliphatic Amino Acid'

Vibration	Start WN	End WN	Threshold	Priority
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Matching Functional Groups

Quality	Functional Group	Chemical Sub Class	Chemical Class
100	1,4 Substituted Aryl Alcohol	Aromatic Alcohol	Aromatic Hydroxy Compound
100	Aliphatic Anhydride - Carbonyl Compound		Aliphatic Anhydride
100	Aliphatic Ether or Sulfonate Salt	Substituent Group	Side Chain or Substituent
100	Aliphatic Ether or Sulfoxide	Substituent Group	Side Chain or Substituent
100	Aliphatic Hydroxy, 2-Amino		Aliphatic Amine
100	Aliphatic Sulphoxide	Aliphatic Sulfoxy-compound	Aliphatic Sulfur Compound
100	Alkoxy Substituent	Substituent Group	Side Chain or Substituent
100	Alkyl-Aryl Phosphonate		Aromatic Phosphorus Compounds
100	Aromatic Sulfonate	Aromatic Sulfoxy Compound	Aromatic Sulfur Compound
100	Aromatic, Nonconjugated Ester, Acetate	Aryl Substituted Ester	Aromatic or Conjugated Ester
100	Cyclic Anhydride, Six Membered		Aliphatic Anhydride
100	Hydroxy Compound	Substituent Group	Side Chain or Substituent
100	Possibly Primary Hydroxy	Substituent Group	Side Chain or Substituent
99	Polysiloxanes	Siloxanes	Aliphatic Silicon Compound
95	1,2 Aryl Subs. Isocyanate	Aryl Isocyanate	Aromatic Nitrile or Multiple Bonded Nitrogen
95	1,4 Aryl Subs. Isocyanate	Aryl Isocyanate	Aromatic Nitrile or Multiple Bonded Nitrogen
95	Aliphatic Sulfonic Acid	Aliphatic Sulfoxy-compound	Aliphatic Sulfur Compound
95	Nitrile, 2-Aryl Substituted	Aryl Substituted Nitrile	Aromatic Nitrile or Multiple Bonded Nitrogen
95	Nitrile, 4-Aryl Substituted	Aryl Substituted Nitrile	Aromatic Nitrile or Multiple Bonded Nitrogen

95	Possibly Aromatic Nitrile	Substituent Group	Side Chain or Substituent
94	1,2 Substituted Aryl Alcohol	Aromatic Alcohol	Aromatic Hydroxy Compound
94	Aliphatic Alkoxy, Methoxy		Aliphatic Ether
94	Aliphatic Amino Acid - Carbonyl Compound		Aliphatic Amino Acid
94	Aliphatic Conjugated Ester		Aliphatic Ester
94	Aliphatic Cyanate	Aliphatic Cyanate	Aliphatic Nitrile or Multiple Bonded Nitrogen
94	Aliphatic Ester, Oxalate		Aliphatic Ester
94	Aliphatic Ether or Sulfone	Substituent Group	Side Chain or Substituent
94	Aliphatic Ketone or Carbonyl Compound		Aliphatic Ketone
94	Aliphatic Nitrile	Aliphatic Nitrile	Aliphatic Nitrile or Multiple Bonded Nitrogen
94	Aliphatic Nitrile, Conjugated	Aliphatic Nitrile	Aliphatic Nitrile or Multiple Bonded Nitrogen
94	Aliphatic Sulfonate or Sulfate	Aliphatic Sulfoxy-compound	Aliphatic Sulfur Compound
94	Aromatic Subst., Possibly Secondary Amide	Aromatic Substituted Amide	Aromatic or Conjugated Amide
94	Aromatic Substituted, Possibly Tertiary Amide	Aromatic Substituted Amide	Aromatic or Conjugated Amide
94	Aromatic, Nonconjugated Ketone	Aryl Substituted Ketone	Aromatic or Conjugated Ketone
94	Aromatic, Possibly Tertiary Amide or Ketone	Aromatic Substituted Amide	Aromatic or Conjugated Amide
94	Carbonyl, Possibly Conjugated Ketone		Aliphatic Ketone
94	CHF2	Fluorine compounds	Organic Halogen Compounds
94	Linear Bromo Compound	Aliphatic Brominated Compound	Aliphatic Halogen Compound
94	Pyridines, General	Pyridines	Other Aromatic Compounds
94	Tertiary Alcohol		Aliphatic Alcohol
94	Unsaturated Hydrocarbon, Cyclic, > C5		Alkene
94	Unsaturated Hydrocarbon, Generic, Isolated		Alkene
93	2-Substituted Phenol	Phenol	Aromatic Hydroxy Compound
93	2-Substituted Phenol, Hindered	Phenol	Aromatic Hydroxy Compound
93	Aliphatic Chloroformyl Ester	Aliphatic Chloroformate	Aliphatic Acid Halide
93	Aliphatic Thioether	Aliphatic Thioether	Aliphatic Thiocompound
93	Aromatic Ester	Aromatic Ester	Aromatic or Conjugated Ester
93	Aromatic Ester, Nitro Substituted	Aromatic Ester	Aromatic or Conjugated Ester
93	Aromatic, Alpha Methylene Ketone	Aryl Substituted Ketone	Aromatic or Conjugated Ketone

93	Aromatic, Ketone	Aromatic Ketone	Aromatic or Conjugated Ketone
93	Aromatic, Nonconjugated Methyl Ketone	Aryl Substituted Ketone	Aromatic or Conjugated Ketone
93	Aryl Aryl Ketone	Aromatic Ketone	Aromatic or Conjugated Ketone
93	Aryl Strained Ring or Activated Carbonyl	Substituent Group	Side Chain or Substituent
93	Carbonyl, Alpha Methylene	Substituent Group	Side Chain or Substituent
93	Metal Carbonyl, Terminal + Bridging		Metal Carbonyl
93	Metal Carbonyl, Terminal + Cyclopentadienyl		Metal Carbonyl
93	Metal Carbonyl, Terminal or Metal Cyano Complex		Metal Carbonyl
93	N-Methyl Amino, Tertiary, Aryl Subs.	Aryl Substituted Aliphatic Amine	Aromatic Amine
93	Terminal Allene		Alkene
92	4-Substituted Phenol	Phenol	Aromatic Hydroxy Compound
92	Aromatic, Possibly Sulfonamide, Secondary	Aromatic Sulfoxy Compound	Aromatic Sulfur Compound
92	Aromatic, Possibly Sulfonyl Fluoride	Aromatic Sulfoxy Compound	Aromatic Sulfur Compound
92	Aromatic, Possibly Sulfonyl Halide	Aromatic Sulfoxy Compound	Aromatic Sulfur Compound
92	Cyclic Anhydride, Five Membered		Aliphatic Anhydride
92	Generic Aromatic	Aryl Group	Aromatic Compound
92	Possibly Aromatic Nitro	Substituent Group	Side Chain or Substituent
92	Possibly Aromatic Tertiary Amine	Aryl Group	Aromatic Compound
92	Strained Ring or Activated Carbonyl	Substituent Group	Side Chain or Substituent
92	Substituted Allene		Alkene
92	t-Butoxy Substituent	Substituent Group	Side Chain or Substituent
91	Aliphatic Amido, Possibly Subs. Urea		Aliphatic Amide
91	Aliphatic Linear Acyl Anhydride		Aliphatic Anhydride
91	Aryl Halo Phosphate		Aromatic Phosphorus Compounds
91	CF3 group	Fluorine compounds	Organic Halogen Compounds
91	Epoxy Substituent	Substituent Group	Side Chain or Substituent
91	Tetramethyl Ammonium Salt		Aliphatic Amine
91	Triaryl Phosphate		Aromatic Phosphorus Compounds
88	Primary Alcohol		Aliphatic Alcohol

87	Possibly Methyl Siloxane or Silane	Substituent Group	Side Chain or Substituent
86	Aliphatic Amido, Cyclic, Lactam		Aliphatic Amide
85	Alkyl Aryl Ketone	Aromatic Ketone	Aromatic or Conjugated Ketone
82	N-Methyl Amino, Tertiary, Aliphatic		Aliphatic Amine
82	Unsaturated Hydrocarbon, Trans Conjugated		Alkene
82	Unsaturated Hydrocarbon, Vinylidene		Alkene
80	Alkene Conjugated Ketone	Conjugated Ketone	Aromatic or Conjugated Ketone
78	4-Subst Pyridine	Pyridines	Other Aromatic Compounds
78	Isothiocyanate	Aliphatic Thiocyanate	Aliphatic Nitrile or Multiple Bonded Nitrogen
78	Unsaturated Hydrocarbon, Trans Alkene		Alkene
77	2-Subst Pyridine	Pyridines	Other Aromatic Compounds
77	Methoxy Substituent	Substituent Group	Side Chain or Substituent
76	Aliphatic Acid Halide, Linear		Aliphatic Acid Halide
76	Aliphatic Acid Halide, Long Chain Linear		Aliphatic Acid Halide
76	Carbonyl, Possibly Methyl Ketone		Aliphatic Ketone
73	Carbonyl, Possibly Alpha Methylene Ketone		Aliphatic Ketone
70	Aliphatic Ester, Acetate		Aliphatic Ester
68	Metal Carbonyl, Terminal + Aryl		Metal Carbonyl
68	Silanol	Silanol	Aliphatic Silicon Compound
67	Unsaturated Hydrocarbon, Ether Conjugated		Alkene
66	Unsaturated Hydrocarbon, Trisubstituted		Alkene
60	Linear Chloro Compound	Aliphatic Chlorinated Compound	Aliphatic Halogen Compound
57	Aliphatic Tertiary		Aliphatic Amide

Corresponding Chemical Classification Rules

Functional Group: '1,4 Substituted Aryl Alcohol', Chemical Class: 'Aromatic Hydroxy Compound',
Chemical Sub Class: 'Aromatic Alcohol'

Vibration	Start WN	End WN	Threshold	Priority
C-H Bend, OOP, 1,4 Subs	840	790	Strong	Mandatory
C-O Stretch	1125	1000	Strong	Mandatory
C-H Bend, CH ₂ /CH ₃	1480	1410	Variable	Mandatory

C-C Stretch, Ring	1520	1485	Variable	Mandatory
C-C Stretch, Ring	1615	1580	Variable	Mandatory
C-H Stretch, Alkyl	3000	2855	Variable	Medium
C-H Stretch, Aryl	3100	3000	Variable	Medium
O-H Stretch	3450	3225	Variable	Mandatory

Missing Chemical Classification Rules

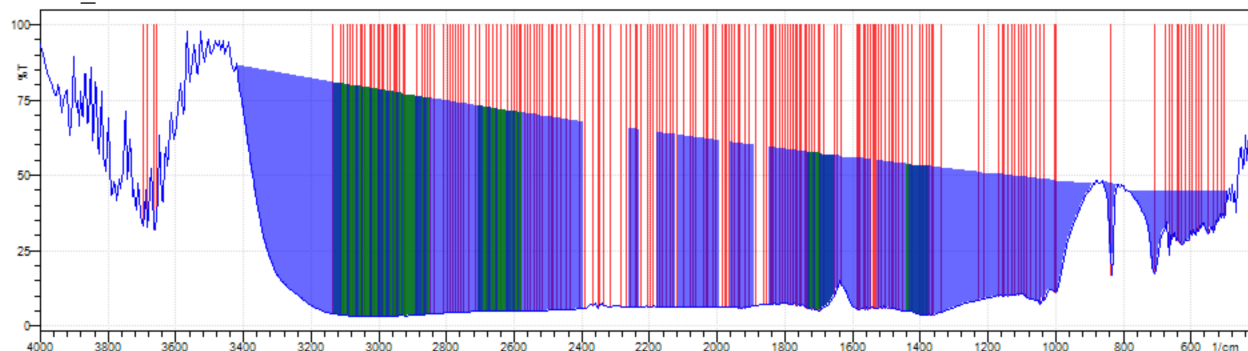
Functional Group: '1,4 Substituted Aryl Alcohol', Chemical Class: 'Aromatic Hydroxy Compound',
Chemical Sub Class: 'Aromatic Alcohol'

Vibration	Start WN	End WN	Threshold	Priority
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Matching Functional Groups

Quality	Functional Group	Chemical Sub Class	Chemical Class
100	Aliphatic Acid or Carbonyl Compound		Aliphatic Carboxylic Acid
100	Aliphatic Alpha Amino Acid		Aliphatic Amino Acid
100	Aliphatic Amino Acid		Aliphatic Amino Acid
100	Aliphatic Amino Acid - Carbonyl Compound		Aliphatic Amino Acid
100	Aliphatic Linear Acyl Anhydride		Aliphatic Anhydride
100	Aliphatic Sulfite	Aliphatic Sulfoxy-compound	Aliphatic Sulfur Compound
100	Aliphatic tert-Amino Acid		Aliphatic Amino Acid
100	Alkoxy Substituent	Substituent Group	Side Chain or Substituent
100	Aromatic Amino Acid, Bonded		Aromatic Amino Acid
100	Branched, Gem Dimethyl	Alkyl Group	Aliphatic Compound
100	Carbonyl, Alpha Alkyl Substituted	Substituent Group	Side Chain or Substituent
100	Carbonyl, Alpha Methylene	Substituent Group	Side Chain or Substituent
100	Carbonyl, Possibly Alpha Methyl Aldehyde		Aliphatic Aldehyde
100	CF3 group	Fluorine compounds	Organic Halogen Compounds
100	Linear Bromo Compound	Aliphatic Brominated Compound	Aliphatic Halogen Compound
100	Methoxy Substituent	Substituent Group	Side Chain or Substituent
100	N-MethylAmino Substituent	Substituent Group	Side Chain or Substituent
100	Unsaturated Hydrocarbon, Cis Alkene		Alkene
97	Methyl Mercapto	Aliphatic Thioether	Aliphatic Thiocompound
96	Aliphatic Aldehyde		Aliphatic Aldehyde
96	Aliphatic Amine Salt, Primary, Hydrochloride		Aliphatic Amine

96	Aliphatic Amine Salt, Secondary		Aliphatic Amine
96	Aliphatic Anhydride - Carbonyl Compound		Aliphatic Anhydride
96	Aliphatic Carboxylate, General		Aliphatic Carboxylate
96	Aliphatic Cyanate	Aliphatic Cyanate	Aliphatic Nitrile or Multiple Bonded Nitrogen
96	Aliphatic Ether or Sulfoxide	Substituent Group	Side Chain or Substituent
96	Aliphatic Isonitrile	Aliphatic Nitrile	Aliphatic Nitrile or Multiple Bonded Nitrogen
96	Aliphatic Mercapto Group	Substituent Group	Side Chain or Substituent
96	Aliphatic Nitrile	Aliphatic Nitrile	Aliphatic Nitrile or Multiple Bonded Nitrogen
96	Aliphatic Sulphoxide	Aliphatic Sulfoxy-compound	Aliphatic Sulfur Compound
96	Carbonyl, Possibly Alpha Methylene Aldehyde		Aliphatic Aldehyde
96	Isothiocyanate	Aliphatic Thiocyanate	Aliphatic Nitrile or Multiple Bonded Nitrogen
96	Unsaturated Hydrocarbon, Cyclic, > C5		Alkene
94	Aryl Ether, Aryloxy (possible 4-subst)	Phenoxy or Aryloxy Ether	Aromatic Ether
93	Metal Carbonyl, Terminal + Bridging		Metal Carbonyl
93	Metal Carbonyl, Terminal + Cyclopentadienyl		Metal Carbonyl
93	Metal Carbonyl, Terminal or Metal Cyano Complex		Metal Carbonyl
92	4-Subst Pyridine	Pyridines	Other Aromatic Compounds
92	Carbonyl, Possibly Conjugated Aldehyde		Aliphatic Aldehyde
91	Strained Ring or Activated Carbonyl	Substituent Group	Side Chain or Substituent
90	Aliphatic Nitro Group		Aliphatic Nitro-oxy Compound
89	Unsaturated Hydrocarbon, Trisubstituted		Alkene
88	Aliphatic Alkoxy, Methoxy		Aliphatic Ether
88	Aliphatic Ester, Acetate		Aliphatic Ester
88	Pyridines, General	Pyridines	Other Aromatic Compounds
87	Aliphatic Thiocyanate	Aliphatic Thiocyanate	Aliphatic Nitrile or Multiple Bonded Nitrogen
82	Unsaturated Hydrocarbon, Trans Conjugated		Alkene
80	2-Subst Pyridine	Pyridines	Other Aromatic Compounds
78	Aliphatic Tertiary		Aliphatic Amide
71	Aliphatic Acid Halide, Linear		Aliphatic Acid Halide

62	Unsaturated Hydrocarbon, Ether Conjugated	Alkene
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Corresponding Chemical Classification Rules

Functional Group: 'Aliphatic Acid or Carbonyl Compound', Chemical Class: 'Aliphatic Carboxylic Acid'

Vibration	Start WN	End WN	Threshold	Priority
C-H Bend, CH ₂ /CH ₃	1450	1380	Variable	Mandatory
C=O Stretch	1730	1680	Strong	Mandatory
O-H Bonded, Acid	2710	2580	Variable	Mandatory
C-H Stretch, Alkyl	3120	2855	Variable	Mandatory

Missing Chemical Classification Rules

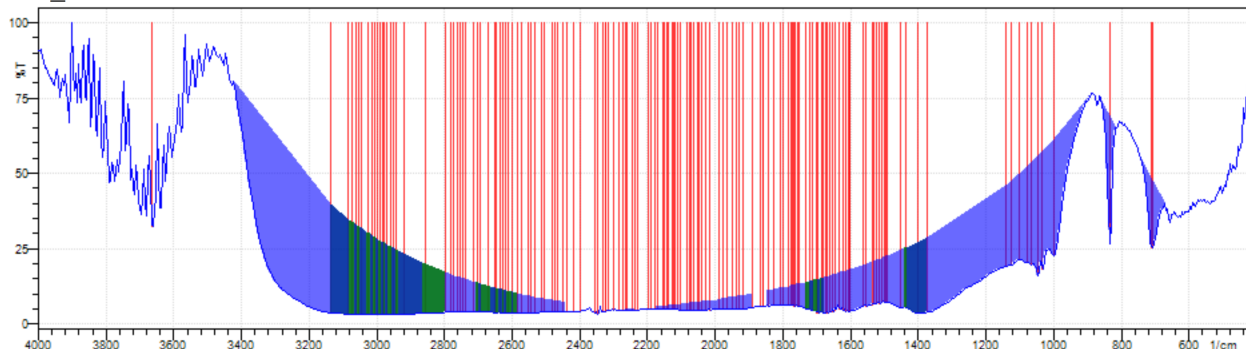
Functional Group: 'Aliphatic Acid or Carbonyl Compound', Chemical Class: 'Aliphatic Carboxylic Acid'

Vibration	Start WN	End WN	Threshold	Priority
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Matching Functional Groups

Quality	Functional Group	Chemical Sub Class	Chemical Class
100	Aliphatic Acid or Carbonyl Compound		Aliphatic Carboxylic Acid
100	Aliphatic Alpha Amino Acid		Aliphatic Amino Acid
100	Aliphatic Amino Acid		Aliphatic Amino Acid
100	Aliphatic Amino Acid - Carbonyl Compound		Aliphatic Amino Acid
100	Aliphatic Carboxylate, General		Aliphatic Carboxylate
100	Aliphatic Linear Acyl Anhydride		Aliphatic Anhydride
100	Aliphatic tert-Amino Acid		Aliphatic Amino Acid
100	Aromatic Amino Acid, Bonded		Aromatic Amino Acid
100	Carbonyl, Alpha Methylene	Substituent Group	Side Chain or Substituent
99	Aliphatic Carboxylate, Possibly 2-Keto Substituted		Aliphatic Carboxylate
99	Carbonyl, Alpha Alkyl Substituted	Substituent Group	Side Chain or Substituent
98	Aliphatic Amine Salt, Primary, Hydrochloride		Aliphatic Amine
98	Long Chain Substituent	Alkyl Group	Aliphatic Compound
98	N-MethylAmino Substituent	Substituent Group	Side Chain or Substituent
97	Unsaturated Hydrocarbon, Cyclic, > C5		Alkene
96	Aliphatic Cyanate	Aliphatic Cyanate	Aliphatic Nitrile or Multiple Bonded Nitrogen
96	Metal Carbonyl, Terminal + Bridging		Metal Carbonyl
96	Metal Carbonyl, Terminal + Cyclopentadienyl		Metal Carbonyl
96	Metal Carbonyl, Terminal or Metal Cyano Complex		Metal Carbonyl

95	Aliphatic Aldehyde		Aliphatic Aldehyde
95	Aliphatic Carbodiimide	Aliphatic Carbodiimide	Aliphatic Nitrile or Multiple Bonded Nitrogen
95	Aliphatic Isonitrile	Aliphatic Nitrile	Aliphatic Nitrile or Multiple Bonded Nitrogen
94	Aliphatic Anhydride - Carbonyl Compound		Aliphatic Anhydride
93	Strained Ring or Activated Carbonyl	Substituent Group	Side Chain or Substituent
91	Unsaturated Hydrocarbon, Cis Alkene		Alkene
88	Aliphatic Sulphoxide	Aliphatic Sulfoxy-compound	Aliphatic Sulfur Compound
86	4-Subst Pyridine	Pyridines	Other Aromatic Compounds
86	Carbonyl, Possibly Alpha Methyl Aldehyde		Aliphatic Aldehyde
85	Carbonyl, Possibly Conjugated Aldehyde		Aliphatic Aldehyde
84	Unsaturated Hydrocarbon, Trans Conjugated		Alkene
82	2-Subst Pyridine	Pyridines	Other Aromatic Compounds
82	Aliphatic Tertiary		Aliphatic Amide
82	Pyridines, General	Pyridines	Other Aromatic Compounds
80	Aliphatic Alkoxy, Methoxy		Aliphatic Ether
80	Unsaturated Hydrocarbon, Trisubstituted		Alkene
78	Isothiocyanate	Aliphatic Thiocyanate	Aliphatic Nitrile or Multiple Bonded Nitrogen
66	Aliphatic Acid Halide, Linear		Aliphatic Acid Halide

Corresponding Chemical Classification Rules

Functional Group: 'Aliphatic Acid or Carbonyl Compound', Chemical Class: 'Aliphatic Carboxylic Acid'

Vibration	Start WN	End WN	Threshold	Priority
C-H Bend, CH ₂ /CH ₃	1450	1380	Variable	Mandatory
C=O Stretch	1730	1680	Strong	Mandatory
O-H Bonded, Acid	2710	2580	Variable	Mandatory
C-H Stretch, Alkyl	3120	2855	Variable	Mandatory

Missing Chemical Classification Rules

Functional Group: 'Aliphatic Acid or Carbonyl Compound', Chemical Class: 'Aliphatic Carboxylic Acid'

Vibration	Start WN	End WN	Threshold	Priority
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>GU972589.1 *Bacillus* sp. LS04 laccase (cotA) gene, complete cds

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>KC010297.2 *Bacillus pumilus* strain DSKK1 laccase (lacc1) gene, complete cds

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>AF184209.1 *Marinomonas mediterranea* polyphenol oxidase (ppoA) gene, complete cds

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>stenotrophomonas maltophilia GD1

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>JF821185.1 *Streptomyces* sp. C1 laccase gene, partial cds

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>HQ857207.1 *Streptomyces cyaneus* strain CECT 3335 laccase (sclA) gene, complete cds

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>MW344649.1 *Geobacillus stearothermophilus* laccase (lacsagzm) gene, complete cds

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>AB092576.1 *Streptomyces lavendulae* gene for laccase, complete cds

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>XM_001389488.2 *Aspergillus niger* CBS 513.88 laccase, mRNA

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