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LC-HRMS Profile of Chemical Compounds in *Penicillium citrinum* XT6 Extract

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Abstract

Endophytes are a rich source of natural chemicals with diverse biological activities. Endophytic fungus *Penicillium citrinum* XT6 was isolated from the marine sponge *Xestospongia testudinaria.* It has the potential antibacterial, cytotoxic, antioxidant, and anti-diabetes. Using liquid chromatography-high resolution mass spectrometry (LC-HRMS), this study determines the chemical compound in *P.citrinum* XT6 extract. Based on the results of this study, we can determine that *P.citrinum* XT6 extract has several compounds with potential activity.

Keywords*:* LC-HRMS, compound, extract, *Penicillium citrinum*

1. Introduction

Endophytic fungi are a valuable source of new, potentially active, and active metabolites. Endophytes are a rich source of natural compounds with a wide range of biological activities such as anticancer, antibacterial, antiviral, immunomodulatory, antidiabetic, antioxidant, anti-arthritic, and anti-inflammatory (1). According to previous studies, *Penicillium citrinum* XT6 is an endophytic fungus isolated from the marine sponge *Xestospongia testudinaria* (2). This fungus exhibits antimicrobial, cytotoxic, antioxidant, and α-glucosidase and urease inhibitory action. It can also decrease blood glucose levels and stimulate adipocyte differentiation in 3T3-L1 preadipocytes (2–9). The bioactivity is due to the role of the compound content contained in the fungus.

This study determines the chemical compound in *P.citrinum* XT6 extract by using liquid chromatography-high resolution mass spectrometry (LC-HRMS). LC-HRMS provides more detailed information on the metabolic composition of samples through some chromatographic parameters such as retention time and peak shape of the analytes, allows comparison with standards, improves confidence level in structural annotations, distinguishing isobaric and isomeric metabolites that are not resolved through the fragmentation pattern, and accurate molecular mass (10).

2. Material and Methods

2.1 Extraction

P.citrinum XT6 was cultivated on rice medium for 4-8 weeks at 25°C. It was subsequently macerated (1:1) with ethyl acetate. The ethyl acetate was evaporated using a rotary evaporator (Heidolph) to yield the ethyl acetate extract.

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2.2 LC-HRMS analysis

The chemical constituents of a *P.citrinum* ethyl acetate extract were analyzed using liquid chromatography-high-resolution mass spectrometry (LC-HRMS) and an HPLC system (Thermo Scientific Dionex Ultimate 3000 RSLCnano with microflow meter) and a high-resolution mass spectrometer (Thermo Scientific Q Exactive). The HPLC apparatus used 0.1% formic acid in water (phase A) and 0.1% formic acid in acetonitrile (phase B). Hypersil GOLD aQ 50 x 1 mm x 1.9 m was used as the analytical column. The analytical flow rate was 40 L/min, the run time was 30 minutes, and the column oven's temperature was 30°C. HRMS was set up with full scan settings of 70,000 and an orbitrap resolution of 17,500. The data was processed using Compound Discoverer and the mzCLoud MS/MS library.

3. Results and Discussion

The chromatogram of the LC-HRMS analysis of *P.citrinum* extract is shown in Figure 1. Based on analysis and comparison to MS/MS library, it was estimated that the chemical compounds mentioned in Table 1.

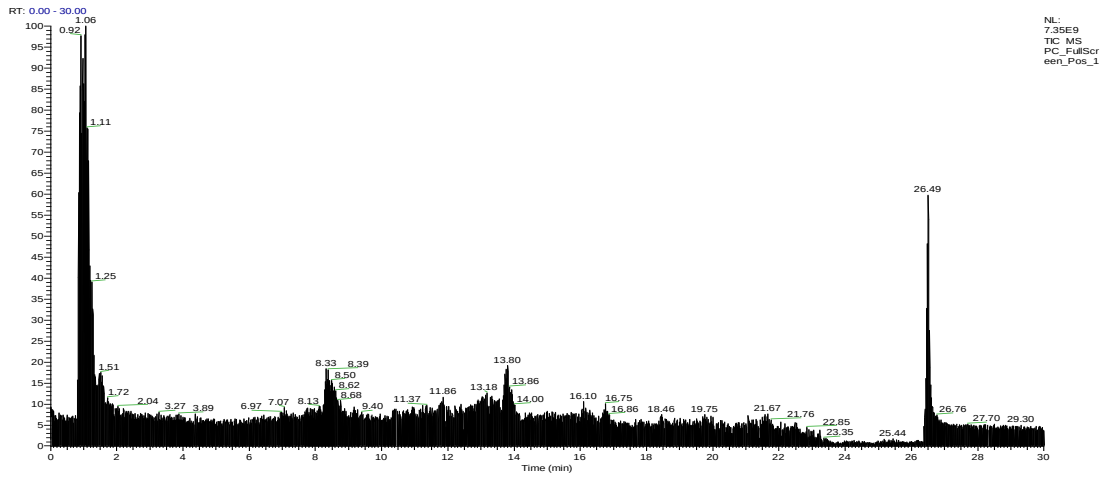

Figure 1: LC-HRMS chromatogram of *P.citrinum* extract

Based on the data in Table 1, several chemical compounds in *P.citrinum* XT6 extract have potential activities. (2S)-2-[(2R)-7-(2-Methoxyethoxy)-5,8-dimethyl-1,2,3,4-tetrahydro-2-naphthalenyl]-1-(1-piperidinyl)-1-propanone is contained in wine from Hungary's Tokaj Region and the wine has antiviral, anti-inflammatory and anticancer activities (11). 1-Linoleoyl glycerol in East Java red rice bran has antidiabetic potential (12). 4-Tert butyl-cyclohexyl acetate, benzaldehyde, phthalic acid, and violacerol II are the potential as antioxidants (13–16). The antidiabetic activity was shown by several compounds, like biochanin A, bis(2-ethylhexyl) phthalate, bis(4-ethyl benzylidene) sorbitol, esculetin, L-pyroglutamic acid, phthalic acid, tertiary butyl hydroquinone (TBHQ), tetralin, trans-3-indole acrylic acid, and xanthine (17–26). Quinine which has antimalarial activity found in the extract (27). Antibacterial activity was shown by sparfloxacin (28). Tecadenoson was found in the extract can be an adenosine receptor agonist (29). Thymol sulfate has antimicrobial, anticancer, antidiabetic, anti-neurodegenerative, and antirheumatic, and can prevent obesity (30,31). Tofisopam effect as anxiolytic and α-methyl-DL-histidine can inhibit histamine receptors (32).

4. Conclusion

Based on the findings of this study, we can conclude that there are several chemical constituents with potential activities in *P.citrinum* Xt6 extract.

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Table 1. The chemical compounds in *P.citrinum* extract

Name	Formula	Molecular Weight	RT [min]	Area (Max.)	mzCloud Best Sim. Match
(+/-)-Cannabichromeorcin		178.05176	1.137	1,672,197.62	77.1
(1E,4S,5E,7R,9E,11aR,14S,14aR,15S,15aR,16aS)-7-Hydroxy-14-(1H-indol-3-ylmethyl)-4,6,15,15a-tetramethyl-4,7,14,14a,15,15a,16a,16b-octahydro-3H-cyclotrideca[d]oxireno[f]isoindole-8,11,12(13H)-trione	C14 H19 N7 O3	333.1563	9.834	185,845.71	75.9
(1R,9R)-5-(2-Naphthyl)-11-(propylsulfonyl)-7,11-diazatricyclo[7.3.1.02,7]trideca-2,4-dien-6-one	C12 H17 N2 O2 P	252.10265	10.359	5,326,074.71	73.1
(1S,5R,6S)-5-Acetoxy-3-(hydroxymethyl)-6-isopropyl-4-oxo-2-cyclohexen-1-yl (2E)-2-methyl-2-butenoate		205.55593	16.742	589,653.34	79.5
(2E,2'E)-N,N'-1,4-Butanediylbis[3-(4-hydroxyphenyl)acrylamide	C22 H24 N2 O4	380.17409	13.764	187,713,319.00	82.8
(2R)-4-(3-Fluorobenzoyl)-1-(4-methoxybenzoyl)-N-[(3S)-2-oxo-3-piperidinyl]-2-piperazine carboxamide	C23 H29 N4 O7 P	504.17778	7.758	574,530.74	77.6
(2S)-2-[(2R)-7-(2-Methoxyethoxy)-5,8-dimethyl-1,2,3,4-tetrahydro-2-naphthalenyl]-1-(1-piperidinyl)-1-propanone	C11 H25 N4 P	244.1819	1.069	2,990,859.76	90.4

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Name	Formula	Molecular Weight	RT [min]	Area (Max.)	mzCloud Best Sim. Match
(2S)-2-[(2R)-7-(2-Methoxyethoxy)-5,8-dimethyl-1,2,3,4-tetrahydro-2-naphthalenyl]-1-(1-piperidinyl)-1-propanone	C2 H6 N5 P	131.03656	1.171	922,048.37	64.5
(2S)-2-[(2R)-7-(2-Methoxyethoxy)-5,8-dimethyl-1,2,3,4-tetrahydro-2-naphthalenyl]-1-(1-piperidinyl)-1-propanone		131.05472	1.167	807,814.93	64.5
(2S)-2-[(2R)-7-(2-Methoxyethoxy)-5,8-dimethyl-1,2,3,4-tetrahydro-2-naphthalenyl]-1-(1-piperidinyl)-1-propanone	C6 H12 N8 O4	260.09693	1.128	348,603.65	64.5
(3R,4R)-3-({4-[(3,5-Dimethyl-1,2-oxazole-4-yl)methoxy]benzoyl}amino)-N-(4-fluorophenyl)-4-hydroxy-1-azepanecarboxamide	C24 H28 N6 O6	496.20854	16.37	415,038.09	76.8
(4aS,9aR)-2-Benzoyl-7-[2-(2-oxo-1-imidazolidinyl)ethyl]decahydro-6H-pyrido[3,4-d]azepin-6-one	C22 H31 O5 P	406.19197	13.133	4,623,830.53	78
(4aS,9aR)-7-Benzyl-2-[(4-methoxyphenyl)acetyl]decahydro-6H-pyrido[3,4-d]azepin-6-one	C7 H21 N3 O P2	225.11669	13.962	297,517.77	80.2
(5S)-3-Acetyl-4-hydroxy-5-{[4-(3-methyl-2-buten-1-yl)-1H-indol-3-yl]methyl}-1,5-dihydro-2H-pyrrole-2-one	C20 H22 N2 O3	338.1617	16.966	1,396,646.61	79.1
{3-[(E)-2-(1,3-Benzodioxol-5-yl)vinyl]-2-oxiranyl}(1-piperidinyl)methanone	C2 H2 N4 O S	129.9944	1.157	696,188.43	64.3

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Name	Formula	Molecular Weight	RT [min]	Area (Max.)	mzCloud Best Sim. Match
{5-Chloro-3-[(1E,3E)-3,5-dimethylhepta-1,3-dienyl]-8a-hydroxy-1-methoxy-7-methyl-6,8-dioxo-1H-isochromen-7-yl} acetate	C13 H23 N2 O7 P	350.12288	13.769	521,669.37	73
1-(4-Methoxyphenyl)-3-(1,4-thiazinan-4-yl)pyrrolidine-2,5-dione	C14 H18 N2 O2 S	278.1097	1.123	3,857,019.60	68.7
1,4:3,6-Dianhydro-2-[(4-carboxybutanoyl)amino]-2,5-dideoxy-5-{[4-(3-fluorophenyl)-2-pyrimidinyl]amino}-L-iditol	C13 H22 N2 O2 S	270.14104	0.931	129,691,186.32	69
1,4:3,6-Dianhydro-2-[(4-carboxybutanoyl)amino]-2,5-dideoxy-5-{[4-(3-fluorophenyl)-2-pyrimidinyl]amino}-L-iditol	C13 H22 N2 O2 S	270.14104	8.545	105,432,387.11	69.4
1,4:3,6-Dianhydro-2-[(4-carboxybutanoyl)amino]-2,5-dideoxy-5-{[4-(3-fluorophenyl)-2-pyrimidinyl]amino}-L-iditol	C13 H22 N2 O2 S	270.14104	1.046	44,045,133.33	69
1,4:3,6-Dianhydro-2-[(4-carboxybutanoyl)amino]-2,5-dideoxy-5-{[4-(3-fluorophenyl)-2-pyrimidinyl]amino}-L-iditol	C13 H12 N4 O4	288.08721	1.096	2,998,955.18	69
1,4:3,6-Dianhydro-2-[(4-carboxybutanoyl)amino]-2,5-dideoxy-5-{[4-(3-fluorophenyl)-2-pyrimidinyl]amino}-L-iditol	C6 H10 N10 O S	270.07588	6.079	287,155.76	71.7

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Name	Formula	Molecular Weight	RT [min]	Area (Max.)	mzCloud Best Sim. Match
1,4:3,6-Dianhydro-2-[(cyclohexylcarbonyl)amino]-2,5-dideoxy-5-{[4-(3-fluorophenyl)-2-pyrimidinyl]amino}-L-iditol		156.03992	1.109	2,473,559.86	60.6
1,4:3,6-Dianhydro-2-[(cyclohexyl carbonyl)amino]-2,5-dideoxy-5-{[4-(3-fluorophenyl)-2-pyrimidinyl]amino}-L-iditol	C4 H8 N6 O	156.07628	1.107	1,948,698.57	60.6
1,4:3,6-Dianhydro-2-[(cyclohexyl carbonyl)amino]-2,5-dideoxy-5-{[4-(3-fluorophenyl)-2-pyrimidinyl]amino}-L-iditol	C13 H20 N4 O5	312.1442	1.166	450,394.43	60.6
1,4:3,6-Dianhydro-2-[(cyclohexylcarbonyl)amino]-2,5-dideoxy-5-{[4-(3-fluorophenyl)-2-pyrimidinyl]amino}-L-iditol		114.01687	1.127	347,376.39	61.1
1,4:3,6-Dianhydro-2-deoxy-2-(2-furoylamino)-5-O-[(4-methoxyphenyl)carbamoyl]-D-glucitol	C6 H12 N6 P2	230.05991	0.904	170,202.26	66.7
1,4:3,6-Dianhydro-2-deoxy-2-[4-(methoxycarbonyl)-1H-1,2,3-triazol-1-yl]-D-glucitol	C9 H15 N2 O3 P	230.08129	6.084	1,308,339.34	61.7
1,4:3,6-Dianhydro-2-deoxy-5-O-[(4-isopropylphenyl)carbamoyl]-2-[(2-thienylsulfonyl)amino]-D-glucitol		127.05229	1.164	2,607,309.51	67.1
1,4:3,6-Dianhydro-2-deoxy-5-O-[(4-isopropyl phenyl)carbamoyl]-2-[(2-thienyl sulfonyl)amino]-D-glucitol	C3 H4 N4 S	128.01515	1.179	1,185,306.79	70.1
1,4:3,6-Dianhydro-2-deoxy-5-O-[(4-isopropylphenyl)carbamoyl]-2-[(2-thienylsulfonyl)amino]-D-glucitol		110.03204	0.039	354,239.91	62.5

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Name	Formula	Molecular Weight	RT [min]	Area (Max.)	mzCloud Best Sim. Match
1,4:3,6-Dianhydro-2-deoxy-5-O-[(4-isopropylphenyl)carbamoyl]-2-[(2-thienylsulfonyl)amino]-D-glucitol		127.55751	1.15	288,853.49	67.1
1,5-Anhydro-2-O-(6-O-benzoyl-α-L-galactopyranosyl)-D-glucitol	C9 H16 P2	186.07356	1.13	271,353.68	73.1
1-[2-(2-Chlorophenyl)-5-(3-pyridyl)-2,3-dihydro-1,3,4-oxadiazol-3-yl]ethan-1-one		123.05739	1.152	744,722.57	75.1
1-[2-(2-Chlorophenyl)-5-(3-pyridyl)-2,3-dihydro-1,3,4-oxadiazol-3-yl]ethan-1-one		123.04788	1.134	492,645.83	96.8
1-[3-Hydroxy-2-(2-hydroxy-2-propanyl)-2,3-dihydro-1-benzofuran-5-yl]ethanone	C13 H16 O4	236.10703	11.758	9,414,490.34	73.5
15-Acetyldeoxynivalenol	C5 H12 N2 O P2	178.04221	0.82	170,562.72	71.1
15-deoxy-Δ12,14-Prostaglandin J2-biotin	C20 H28 N4 O3 S	404.18764	9.913	250,707.84	75.3
1640340	C10 H17 N O3	199.12087	4.741	572,326.90	68.2
1733342	C8 H14	110.10967	19.396	978,900.66	81.3
1778635	C8 H12 O5	188.06844	0.909	13,462,460.48	83.6
1778635	C8 H12 O5	188.06844	1.052	1,372,266.67	83.6
1778635	C8 H12 O5	188.06844	2.075	1,255,745.82	66
1-Ethyl-6,7-dimethoxy isoquinoline-3-ol		188.06178	1.136	744,341.82	83.6
1-Ethyl-6,7-dimethoxyisoquinolin-3-ol	C5 H8 N4 S2	188.0199	1.091	554,104.96	83.6
1-Ethyl-6,7-dimethoxyisoquinolin-3-ol		187.08956	1.117	303,955.58	83.6
1-Linoleoyl glycerol	C20 H38 N2 O3	354.28636	20.311	1,210,666.92	68.7

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Name	Formula	Molecular Weight	RT [min]	Area (Max.)	mzCloud Best Sim. Match
1-Linoleoyl glycerol	C16 H34 N8 O	354.28688	17.807	437,070.21	69.3
1-Linoleoyl glycerol		262.23363	20.333	1,112,300.70	79.7
1-Linoleoyl glycerol		262.23363	19.765	767,660.63	78.2
1-Linoleoyl glycerol		262.23363	17.8	238,908.83	77.2
2-(2-Methyl-1,3-thiazol-4-yl)-5-[4-(trifluoromethyl)phenyl]-1,3,4-oxadiazole	C8 H12 N P S	185.04196	16.73	585,460.93	63.6
2-(4-Methyl-3-cyclohexen-1-yl)-2-propanyl 6-O-(6-deoxy-α-L-mannopyranosyl)-β-D-glucopyranoside	C26 H44 O8	484.30206	19.974	4,257,618.06	93.6
2-(4-Methyl-3-cyclohexen-1-yl)-2-propanyl 6-O-(6-deoxy-α-L-mannopyranosyl)-β-D-glucopyranoside	C26 H44 O8	484.30159	20.14	1,162,183.17	93.8
2,5-Dimethyl-3-[4-(trifluoromethyl)phenyl]-7-{[4-(trifluoromethyl)phenyl]methylene}-3,3a,4,5,6,7-hexahydro-2H-pyrazolo[4,3-c]pyridine	C17 H17 N4 O3 P	356.10462	11.755	568,486.38	90.1
2,6-Dimethoxyphenol	C8 H10 O3	154.063	6.358	2,780,084.00	90.7
2-[(2S,3R,4S,5R)-5-(Acetamidomethyl)-3,4-dihydroxytetrahydro-2-furanyl]-N-(4-fluorobenzyl)acetamide	C21 H25 P S	340.14089	11.469	282,559.37	78
2-[2-(3,4,5-Trimethoxybenzylidene)hydrazono]-1,3-thiazolan-4-one	C11 H26 O3 P2	268.13536	7.487	1,749,955.58	63.8
2-Amino-1-methyl-6-phenylimidazo(4,5-b)pyridine	C13 H12 N4	224.10625	10.505	429,331.91	62.6
2-Hydroxy-3,4,5-trimethoxybenzoic acid	C10 H12 O6	228.06331	1.001	4,304,705.87	79.3

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2-Methoxy-1-(3-methyl-2-buten-1-yl)-4-[(Z)-2-phenylvinyl]benzene	C20 H22 O	278.16825	1.047	777,909.73	68.7
2-Methoxy-3,5-dimethyl-6-(tetrahydro-4-(2-methyl-3-(4-nitrophenyl)-2-propenylidene)-2-furanyl)-4H-pyran-4-one	C11 H24 O5 S	268.13536	7.745	523,183.34	62.5
2-Methoxy-3,5-dimethyl-6-(tetrahydro-4-(2-methyl-3-(4-nitrophenyl)-2-propenylidene)-2-furanyl)-4H-pyran-4-one	C10 H22 O5 S	254.11859	6.764	446,660.21	70.4
2-Methoxy-3,5-dimethyl-6-(tetrahydro-4-(2-methyl-3-(4-nitrophenyl)-2-propenylidene)-2-furanyl)-4H-pyran-4-one	C10 H22 O5 S	254.11859	6.543	382,064.91	70.9
2-O-Ethyl Ascorbic Acid	C8 H12 O6	204.06404	1.451	626,837.02	80.1
3-(3,5-Dimethoxyphenyl)propanoic acid	C11 H14 O4	210.08982	6.979	2,201,664.90	66.8
3-(3,5-Dimethoxyphenyl)propanoic acid	C11 H14 O4	210.08953	11.238	602,908.33	67.7
3,4,5-Trimethoxyphenyl 6-O-pentopyranosyl-β-D-glucopyranoside	C6 H12 N6 O	184.10761	1.092	675,381.76	67.6
3,4,5-Trimethoxyphenyl 6-O-pentopyranosyl-β-D-glucopyranoside		183.56061	1.13	323,497.73	67.5
3,4-Dimethoxy-α-pyrrolidinohexanophenone	C11 H15 N2 O2 P	238.08615	6.948	1,259,700.65	73.6
3-{[(4-Methoxy-1-methyl-1H-indazol-3-yl)amino]carbonyl}-2-pyrazinecarboxylic acid	C10 H19 N O5 S	265.0992	7.909	1,109,804.92	65.9

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Name	Formula	Molecular Weight	RT [min]	Area (Max.)	mzCloud Best Sim. Match
3635	C5 H6 O3	114.03167	0.911	13,411,968.52	64.8
3635	C5 H6 O3	114.03168	1.262	6,903,129.39	64.8
3-Aminophenol	C7 H14 N4 O2 S	218.08357	1.171	9,359,672.49	76.2
3-Aminophenol	C6 H12 N4 O3 S	220.06298	1.179	469,472.26	76.2
4-[(2S,3S,4S)-4-[4-(β-D-Glucopyranosyloxy)-3-methoxybenzyl]-3-(hydroxymethyl)tetrahydro-2-furanyl]-2-methoxyphenyl-β-D-glucopyranoside	C6 H12 N2 O2 P2	206.03774	1.857	1,050,987.41	73.5
4-Aminobiphenyl	C2 H5 N O4 P2	168.9698	26.71	660,604.14	60.7
4-Aminophenol		109.53945	1.138	1,263,064.02	76.2
4-Aminophenol		110.05833	1.134	2,783,326.71	72.2
4-Guanidinobutyric acid		145.07033	1.154	816,484.45	63.4
4-Guanidinobutyric acid	C8 H7 N3	145.06445	1.133	134,627.21	63.4
4-Guanidinobutyric acid		147.04955	1.16	311,046.00	63.4
4-Guanidinobutyric acid		292.17365	1.137	4,791,036.96	63.4
4-Hydroxy-3-nitrosobenzamide	C7 H6 N2 O3	166.03786	0.897	2,329,035.16	66
4-Methoxy-5-methyl-6-[(2S,3S)-2-methyl-3-[(2Z,4E)-4-methyl-5-[(1S,2S,4R,5R)-1,2,4-trimethyl-3,6-dioxabicyclo[3.1.0]hexan-4-yl]penta-2,4-dien-2-yl]oxiran-2-yl]pyran-2-one	C12 H19 N2 O2 P	254.11859	9.579	268,094.52	66.3
4-Tert-Butylcyclohexyl acetate	C12 H22 O2	198.16171	19.398	1,642,532.93	66.9

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Name	Formula	Molecular Weight	RT [min]	Area (Max.)	mzCloud Best Sim. Match
5-(4-Chlorophenyl)-3-{[(4-chlorophenyl)thio]methyl}-1H-1,2,4-triazole		264.093	1.165	15,686,133.31	63.9
5-(4-Chlorophenyl)-3-{[(4-chlorophenyl)thio]methyl}-1H-1,2,4-triazole	C5 H12 Cl N9 O2	265.08064	1.234	227,764.93	63.9
5,5-Dimethyl-4-(3-oxobutyl)dihydro-2(3H)-furanone	C10 H16 O3	184.11001	0.913	1,366,090.55	66.1
5-Amino-3-(4-methoxyphenyl)-5-oxopentanoic acid	C9 H19 N O4 S	237.10246	6.002	303,885.85	69
5-Chloro-2-methyl-4-isothiazolin-3-one	C4 H4 Cl N O S	148.97017	4.825	1,999,923.70	65.5
5-Methoxy-3-indoleaceate	C11 H11 N O3	205.07462	8.827	520,406.41	74.2
5-O-[(4-Acetylphenyl)carbamoyl]-1,4:3,6-dianhydro-2-deoxy-2-[(ethylcarbamoyl)amino]-D-glucitol	C3 H4 N4 S	128.01515	1.514	332,266.33	85.8
5-O-[(4-Acetylphenyl)carbamoyl]-1,4:3,6-dianhydro-2-deoxy-2-[(ethylcarbamoyl)amino]-D-glucitol	C2 H4 N6 O	128.04505	1.108	141,427.43	60.3
6-(1,3-Dithiolan-2-yl)-2,2-dimethylchromane	C5 H10 N6 O5	234.07071	6.409	849,723.98	67.7
6-(1-Hydroxyethyl)-3-(hydroxymethyl)-2,7-dioxabicyclo[4.1.0]hept-3-en-5-one	C8 H10 O5	186.05293	1.365	550,852.83	73.1
6,12-Dihydrobenzo[b]chromeno[4,3-e][1,4]thiazin-6-one	C13 H9 N S	211.04605	17.693	714,252.29	94.9
6',7',10,11-Tetramethoxy-1',2'-didehydroemetan	C16 H21 N5 O4 S	379.13047	11.232	280,724.37	76.2

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Name	Formula	Molecular Weight	RT [min]	Area (Max.)	mzCloud Best Sim. Match
6-Methoxy-2-Oxo-3-[(2-Oxo-2H-Chromen-7-Yl)Oxy]-2H-Chromen-7-Yl 6-O-(4-Carboxy-3-Hydroxy-3-Methylbutanoyl)Hexopyranoside	C9 H15 N2 O4 P	246.07712	1.587	648,647.77	63.6
6-Methyl-2-nitro-3-pyridyl 3-chlorobenzo[b]thiophene-2-carboxylate	C2 H4 N4 O P2 S	193.95851	26.653	392,039.33	64.2
Acetyl Proline	C7 H11 N O3	157.07397	1.02	1,622,679.44	75.4
ACPC	C4 H7 N O2	101.04816	0.913	1,526,662.26	72.2
Adenine	C5 H5 N5	135.05451	7.298	223,333.15	88.3
Adipic acid	C6 H10 O4	146.05786	1.456	2,195,058.17	71.4
AF4878000	C11 H12 O3	192.07865	0.89	459,315.11	68
AF4878000	C11 H12 O3	192.07865	10.773	334,935.45	77.6
Aminolevulinic acid	C5 H9 N O3	131.05839	1.481	611,430.72	65.3
Arecoline	C8 H13 N O2	155.09466	1.054	2,384,005.39	60.6
Arecoline	C8 H13 N O2	155.09462	0.926	650,548.59	60.6
Avermectin B1a	C H2 N6 O	114.02951	1.108	117,452.72	64.8
Basic Red 9		287.67342	8.654	345,785.51	63.7
Benzaldehyde	C7 H6 O	106.04209	10.435	1,936,518.63	96.9
Biacetyl	C4 H6 O2	86.0368	1.038	722,182.58	78.8
Biochanin A	C16 H12 O5	284.07393	16.249	613,103.43	93.4
Bis(2-ethylhexyl) phthalate	C23 H38 N2 O3	390.28868	22.999	20,698,943.61	94.3
Bis(2-ethylhexyl) phthalate	C21 H43 O4 P	390.28868	22.516	18,779,635.93	94.3

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Bis(2-ethylhexyl) phthalate	C21 H43 O4 P	390.28868	22.176	12,711,704.11	94.3
Bis(2-ethylhexyl) phthalate	C22 H49 N3 O3 S	435.35121	23.003	2,575,951.29	86.6
Bis(2-ethylhexyl) phthalate	C19 H45 N7 O4	435.35121	22.802	1,692,475.67	80.8
Bis(4-ethylbenzylidene)sorbitol	C28 H30 O3	414.21855	15.122	729,202.36	78.3
Butyl acrylate	C7 H12 O2	128.08377	0.907	652,107.41	69.1
Butyl acrylate	C7 H12 O2	128.0838	1.029	615,762.99	69.1
Butyl benzoate	C11 H14 O2	178.09924	10.639	537,441.02	64.6
Butyl palmitate		274.25588	19.957	525,174.30	68.4
Butyl palmitate	C14 H33 N2 P	260.23976	18.807	1,063,790.55	74
Butylparaben	C11 H14 O3	194.09429	6.097	503,207.64	69.5
Caffeine	C17 H17 N4 O5 P	388.09452	16.734	1,164,617.65	71.5
Camptothecin	C6 H10 N4 O6	234.06026	1.266	193,994.88	73.1
Camptothecin	C6 H10 N4 O4 S	234.04328	1.142	1,299,742.27	74.7
Camptothecin		233.12824	0.937	859,947.09	72.3
Camptothecin		233.08867	1.152	175,907.65	74.7
Camptothecin		233.05234	1.161	220,415.92	75
Camptothecin		232.14403	1.108	344,192.87	75
Camptothecin	C4 H8 N6 O	156.0753	1.099	533,030.50	75
Camptothecin	C10 H20 O5 S	252.10266	0.893	1,977,641.55	72.3
Cannabisativine	C21 H39 N3 O3	381.29973	19.112	2,048,406.84	74.2

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Caprolactam	C6 H11 N O	113.08429	1.05	520,468.89	64.8
Cardiopetalidine	C21 H33 N O4	363.24126	8.498	869,452.13	87.9
Choline		102.53171	1.17	2,154,771.85	89.2
Cis-2-Carboxycyclohexyl-acetic acid	C9 H14 O4	186.08965	1.05	331,930.72	73.1
Coenzyme Q1	C28 H36 N2 O3	448.27403	10.364	653,123.15	64.1
Coenzyme Q2		251.21272	8.334	352,959.61	63.3
Coenzyme Q2	C20 H39 N3 O4	385.29473	13.861	577,537.56	68.3
Colistin	C10 H19 N4 O P	242.12982	5.734	711,719.50	74.5
Coproporphyrin III tetramethyl ester	C29 H41 N8 O5 P	612.29296	21.553	723,621.90	60.6
Cyclo(leucylprolyl)	C11 H18 N2 O2	210.13741	6.444	609,828.07	61.4
Cymarin	C8 H19 N2 O3 P	222.11425	1.264	362,179.21	82.7
Cymarin		112.03758	1.133	1,747,696.71	86.8
Diazepam	C13 H10 N4 O	238.08599	9.364	2,839,465.87	61.9
Diethyl tartrate	C8 H14 O6	206.07904	1.785	12,756,191.87	73.5
Difenacoum	C12 H20 N2 O2 S	256.12435	0.927	4,751,707.60	74.4
Difenacoum	C12 H22 N3 O P	255.15026	6.973	309,507.31	73.5
DMPHEN	C14 H12 N2	208.09938	0.898	2,600,401.75	66.7
Docetaxel	C3 H11 N5 O2 S	181.06297	1.134	348,112.86	72.1
Epsilon-Caprolactone	C6 H10 O2	114.06824	0.993	8,391,889.41	64.8
Esculetin	C9 H6 O4	178.02654	10.796	820,634.34	64.6

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Ethionamide S-oxide	C8 H10 N2 O S	182.05229	1.164	404,675.48	71.9
Ethyl 1-[(2-phenoxy-3-pyridinyl)carbonyl]-4-piperidinecarboxylate	C22 H27 P S	354.15688	12.425	576,708.22	79.6
Flumethasone	C21 H31 O6 P	410.18736	10.988	7,440,882.00	73.4
Flumethasone	C21 H31 O6 P	410.18736	10.72	6,696,014.10	70.1
Flumethasone	C21 H31 O6 P	410.18736	11.632	5,834,967.09	71
FR140423		222.12699	0.896	2,201,494.42	65.8
Furaneol	C6 H8 O3	128.04744	0.896	2,453,076.00	69.1
Furaneol	C6 H8 O3	128.04744	1.034	1,411,192.83	69.1
g-Butyrobetaine	C7 H15 N O2	145.11025	0.997	1,812,344.98	72.8
Guaietolin	C11 H16 O4	212.10552	6.881	6,280,546.96	71.3
Guaietolin	C11 H16 O4	212.10552	0.914	5,826,571.75	67.6
Guaifenesin	C10 H14 O4	198.08914	5.612	1,625,580.50	68.2
Guvacine	C6 H9 N O2	127.06342	0.927	2,198,486.73	67.9
Guvacine	C6 H9 N O2	127.06342	1.596	668,550.71	85.8
Hexyl 2-furoate	C11 H16 O3	196.10981	7.091	17,757,937.52	65.6
Hydralazine pyruvic acid hydrazone	C11 H10 N4 O2	230.08129	1.309	576,906.49	62.8
Ibufenac	C12 H16 O2	192.11501	10.937	253,490.74	77.7
Ilomastat	C20 H28 N4 O4	388.21214	9.594	394,275.42	76.4
Jasmonic acid	C12 H18 O3	210.12568	7.283	5,787,857.34	65.5

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Lactide	C6 H8 O4	144.0424	0.878	960,437.65	64.4
L-Alanine methyl ester	C21 H39 N3 O2	365.30428	21.109	1,053,397.47	64.5
L-Pyroglutamic acid	C5 H7 N O3	129.04262	0.911	1,172,176.30	69.1
LQ1825000	C7 H13 N O	127.09979	0.926	1,521,975.62	69.1
MA4000000	C5 H7 N O2	113.0478	0.992	5,763,301.08	85.5
MA4000000	C5 H7 N O2	113.04775	1.291	1,353,453.27	82.7
Mabuterol	C14 H22 N4 O9	390.13681	8.621	4,704,888.01	72
Mabuterol	C20 H19 N6 O P	390.13681	9.077	2,417,292.79	74.8
Maraniol	C12 H12 O3	204.07944	18.439	2,046,723.44	91.8
Medazepam	C19 H30 N4 O4	378.22762	0.917	20,273,468.69	87.2
Medazepam	C10 H22 O4	206.15199	8.34	399,903.76	75.4
Mephenesin	C10 H14 O3	182.09432	6.373	1,030,255.99	79.4
Methyl 2-cyano-3-{1-[4-(trifluoromethyl)phenyl]-1H-pyrrol-2-yl}acrylate	C29 H31 N3 O4 P2 S	579.1525	16.739	256,433.27	62
Methyl-5-acetoxy-6,10-dihydroxy-2,4b,7,7,10a,12a-hexamethyl-12-methylene-1,4,8-trioxohexadecahydro-2H-naphtho[1,2-H]isochromene-2-carboxylate	C13 H19 N2 P	234.12776	15.443	1,244,984.32	63.8
Methylone	C6 H3 N6 P	190.01547	1.159	405,788.27	88.4
Methylone		189.09644	1.147	402,431.42	88.4
Metoxuron	C10 H21 N4 P	228.14964	1.051	955,951.12	79.3

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Metoxuron	C10 H14 O7	246.07395	1.103	18,426,782.56	79.3
Mevalonolactone	C3 H6 N4 O2	130.04842	1.255	1,306,037.23	65.3
MFCD00070502	C4 H8 O3	104.04736	0.916	5,630,676.56	89.2
MFCD00070502	C4 H8 O3	104.04768	1.268	602,558.31	89.2
MFCD27967839	C19 H20 O	264.15167	1.098	367,651.55	60.9
Microcystin LF	C8 H9 N	119.07363	9.571	393,561.67	65.5
Milbemycin A3 oxime	C17 H23 N3 O5	349.16283	5.566	317,478.53	66.1
Myriocin	C14 H33 N9	327.28533	21.106	1,291,753.31	67.8
N-{[(2R,3S,4S,5S)-5-(2-{[2-(Dimethylamino)ethyl]amino}-2-oxoethyl)-3,4-dihydroxytetrahydro-2-furanyl]methyl}-1,3-benzodioxole-5-carboxamide	C21 H43 O4 P	390.28868	21.616	10,607,276.41	94.1
N-{[(2R,3S,4S,5S)-5-(2-{[2-(Dimethylamino)ethyl]amino}-2-oxoethyl)-3,4-dihydroxytetrahydro-2-furanyl]methyl}-1,3-benzodioxole-5-carboxamide	C23 H38 N2 O3	390.28868	23.23	4,147,098.32	94.8
N'1-(2-Cyano-3-fluorophenyl)-N'1-methylethanimidohydrazide	C7 H16 N2 O P2	206.07431	6.416	536,524.67	74.3
N1-(4-Chlorophenyl)-2-{2-[(3-methoxypropyl)amino]-4-oxo-4,5-dihydro-1,3-thiazol-5-yl}acetamide	C11 H9 N4 P	228.05573	6.101	445,608.22	85.5
N'1-{[1-(4-Fluorophenyl)-4-oxo-1,4-dihydropyridazin-3-yl]carbonyl}-2-chlorobenzene-1-sulfonohydrazide	C11 H18 N2 O8	306.10616	1.143	2,753,637.76	63.5

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N2-{[(3R,4S)-3-{[5-(4-methoxyphenyl)-1,2-oxazol-3-yl]methyl}-4-piperidinyl]acetyl}-N2-methylglycinamide	C21 H32 N2 O3 P2	422.18724	18.327	1,632,200.34	68.2
N8-Acetylspermidine		172.05881	1.127	3,338,656.06	78.3
N8-Acetylspermidine	C7 H15 N2 O2 P	190.08691	1.007	1,089,611.38	84.6
N-Acetyl-L-leucine	C8 H15 N O3	173.10524	0.952	3,724,530.41	84.6
N-Acetyl-L-leucine	C8 H15 N O3	173.10524	4.713	769,478.43	67.8
N-Acetyl-L-phenylalanine	C11 H13 N O3	207.08946	1.026	11,426,559.47	74.8
N-Acetyl-L-phenylalanine	C11 H13 N O3	207.08951	0.907	4,623,561.68	76.8
N-Acetyl-L-phenylalanine	C11 H13 N O3	207.09041	6.852	1,254,056.22	74.6
N-Acetylputrescine		173.06319	1.539	612,423.76	85
N-Acetylvaline	C7 H13 N O3	159.0895	0.975	13,082,095.67	83.3
N-Arachidonoyl-L-serine	C20 H37 N3 O3	367.28371	18.618	2,607,481.53	66.2
n-Butyl lactate	C7 H14 O3	146.09419	0.891	675,078.02	65.4
N-Desmethylclomipramine	C31 H44 N6 O P2	578.3076	18.433	196,356.10	89.3
Nebivolol	C13 H26 O7	294.16896	1.501	807,870.95	67.5
Nebivolol	C4 H12 N2 P2	150.04721	1.496	2,346,445.52	64.3
N-Ethylbuphedrone	C16 H36 N4 P2	346.24073	17.299	1,065,048.65	86.3
N-ethylmaleimide	C6 H7 N O2	125.04787	0.98	227,934.15	75.4
Netilmicin	C18 H26 O2 S	306.16503	9.564	2,301,398.17	71.1

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N-Hydroxy-1-methyl-6-phenyl-1H-imidazo[4,5-b]pyridin-2-amine	C13 H12 N4 O	240.10208	7.769	7,803,067.45	75
N-Hydroxy-1-methyl-6-phenyl-1H-imidazo[4,5-b]pyridin-2-amine	C13 H12 N4 O	240.10208	0.88	6,000,985.40	75
Nicotinamide	C6 H6 N2 O	122.0481	1.453	394,271.71	88.6
Nicotinamide	C6 H6 N2 O	122.0481	0.887	336,194.23	90.4
N-Methyl-2-[(3R,4S)-3-{[5-(phenoxymethyl)-1,2-oxazol-3-yl]methyl}-4-piperidinyl]-N-(2-propyn-1-yl)acetamide	C27 H46 N5 O6 P	567.31638	12.846	619,091.41	61.3
Noradrenaline	C8 H11 N O3	169.07377	0.999	2,927,701.57	80
Nα-({1,3,4-trihydroxy-5-[(N-methylvalyl)amino] cyclohexyl}carbonyl)phenylalaninamide	C12 H26 N2 P2	260.15676	9.526	621,503.48	64.2
Nα-[(1,3,4-trihydroxy-5-{[2-methoxy-4-(methylsulfanyl)benzoyl] amino}cyclohexyl)carbonyl]tryptophanamide	C7 H13 N4 P S	216.05936	3.843	2,514,176.55	66.6
Octylamine	C8 H19 N	129.15187	1.026	400,438.73	65
Oleoyl ethanolamide		323.29054	19.55	1,102,631.45	63.9
Olodaterol	C21 H26 N2 O5	386.18517	14.81	5,757,373.92	62.9
Paraldehyde	C6 H12 O3	132.07872	1.2	5,736,319.46	63.6
Paraldehyde	C6 H12 O3	132.07873	1.042	1,020,625.90	63.6
PEG Monolaurate n3	C14 H34 N8 O	330.28455	21.64	22,470,219.06	61.9
PEG Monolaurate n7		274.25588	20.297	808,040.85	76.2
Phalloidin	C10 H22 N3 O P	231.14922	7.747	339,186.18	66.6
Phalloidin	C5 H12 N2 O P2	178.04212	1.561	1,276,503.43	63

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Phalloidin		159.05834	1.126	1,235,152.00	73.9
Phalloidin		158.55753	1.136	163,395.74	73.9
Phthalic acid	C8 H4 O3	148.0159	18.451	6,508,528.25	95.8
Phthalic acid	C8 H4 O3	148.0159	22.943	4,135,075.41	96.2
Phthalic acid	C8 H4 O3	148.0159	22.514	3,786,563.93	96.4
Pivagabine	C9 H17 N O3	187.12074	1.016	1,235,028.08	83.6
Pivagabine	C9 H17 N O3	187.12079	6.211	857,927.51	80
Pivagabine	C9 H17 N O3	187.12079	8.074	513,339.40	75.1
Proline	C12 H30 N3 O P S	295.1852	12.425	516,338.00	61.2
Prostaglandin E2-biotin		226.16951	8.986	755,855.85	68.4
Quinine	C10 H22 N2 O2 P2	264.11537	8.879	1,251,243.63	65.7
Ranitidine		156.06618	10.357	186,815.42	74.9
Sorbicillin		222.12693	9.569	8,482,067.01	62.9
Sparfloxacin	C19 H20 N O P	309.12819	7.996	726,665.29	61.6
Succinylacetone	C7 H10 O4	158.05792	1.228	4,088,532.24	75.4
Succinylacetone	C7 H10 O4	158.05783	0.891	1,624,534.54	72.2
TBHQ	C10 H14 O2	166.09935	9.707	380,559.15	73.8
TBHQ	C10 H14 O2	166.09935	1.046	231,523.02	61.5
Tecadenoson	C14 H19 N5 O5	337.14012	9.028	654,114.52	92.6
Tetralin	C10 H12	132.09349	19.973	186,449.65	83

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Threonine	C19 H39 N3 O4	373.29463	14.461	524,960.51	64.5
Thymol sulfate	C10 H14 O4 S	230.06114	0.889	1,253,370.31	76.7
Tofisopam	C22 H26 N2 O4	382.18996	18.164	524,791.00	61.2
Tolfamide	C8 H12 N3 O2 P	213.06676	8.534	743,521.62	78.1
Trans-3-Indoleacrylic acid	C19 H21 N3 O3	339.15669	13.148	245,852.78	77
Trans-Zeatin	C5 H12 P2	134.04178	1.18	1,199,491.08	99.4
Triazoxide	C5 H12 O4 P2	198.0219	26.636	1,332,320.41	70.2
Triazoxide	C6 H8 N4 P2	198.0219	26.784	1,158,167.79	70.2
Trifloxystrobin	C20 H19 F3 N2 O4	408.12809	1.285	1,532,153.07	80.1
Trimethadione	C6 H9 N O3	143.05827	0.929	5,656,429.65	64.4
Trimethadione	C6 H9 N O3	143.05826	1.62	1,977,212.10	63.1
Trimethoprim impurity C	C16 H10 N4	258.09062	1.102	298,724.29	81.5
Uracil	C4 H4 N2 O2	112.02757	1.273	747,177.28	82.7
Uracil	C4 H4 N2 O2	112.02757	1.469	539,073.32	79.3
Violacerol II	C25 H32 N6 P2	478.21865	14.891	561,019.43	65.7
Xanthine	C5 H4 N4 O2	152.03339	1.282	940,190.53	65.6
Zeatin-7-N-glucoside	C27 H40 N7 O7 P	605.27172	10.509	489,507.98	63.7
Zeatin-7-N-glucoside	C17 H21 N7 O2	355.17458	7.292	1,606,651.62	90.8
α-Methyl-DL-histidine	C6 H9 N3	123.07971	24.714	240,352.70	96.1
α-Methyl-DL-histidine	C6 H9 N3	123.07971	23.674	203,340.38	94.8

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