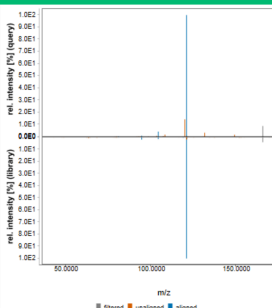


4,5,6,7-Tetrahydro-1H-benzo[d]imidazole-7-carboxylic acid

Matched signals: 9/36
Expl. intensity: 0.942

0.871



Compound information

Name: 4,5,6,7-Tetrahydro-1H-benzo[d]imidazole-7-carboxylic acid
Formula: C₈H₈N₂O₂
Exact mass: 166.074228
Ion type: [M+H]⁺
Precursor m/z: 167.081504
Charge: 1
RT: 0.715568
Polarity: +
InChI: InChI=1S/C₈H₈N₂O₂/c(11-8)(12)5-2-1-3-6-7(5)
InChI key: UGIMXCAKUNAE-UHFFFAOYSA-N
SMILES: NCC1C(=O)OCCCC1
Num peaks: 13

Instrument information

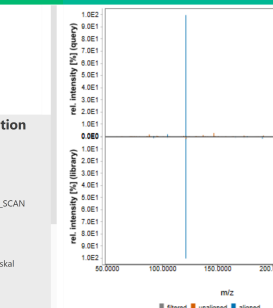
Instrument type: Orbitrap
Instrument: Orbitrap ID-X
Ion source: ESI
Ms level: 2.0
Collision energy: 30.0
Merged spec type: SINGLE_BEST_SCAN
Acquisition: Commercial
Software: mzmine3

Other information

Principal investigator: Tomas Pluskal
Data collector: Corinna Brungs

Database links

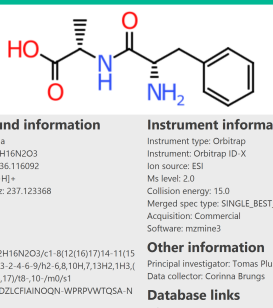
160



Phe-ala

Matched signals: 14/16
Expl. intensity: 0.981

0.985



Compound information

Name: Phe-ala
Formula: C₁₂H₁₆N₂O₃
Exact mass: 236.116092
Ion type: [M+H]⁺
Precursor m/z: 237.123368
Charge: 1
RT: 1.008481
Polarity: +
InChI: InChI=1S/C₁₂H₁₆N₂O₃/c(1-8)(12)(16)7(14-11)(15)(13)7-9-5-3-2-4-6-10(2)-8-11(12),13(14),15(16),17(18)-10-/m/s1
InChI key: MIDZLCFAIHOQNV-VRPWFQTSQ-A-N
SMILES: NCC1C(=O)OCCCC1

Instrument information

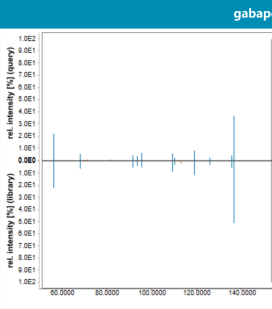
Instrument type: Orbitrap
Instrument: Orbitrap ID-X
Ion source: ESI
Ms level: 2.0
Collision energy: 15.0
Merged spec type: SINGLE_BEST_SCAN
Acquisition: Commercial
Software: mzmine3

Other information

Principal investigator: Tomas Pluskal
Data collector: Corinna Brungs

Database links

160



Compound information

Name: gabapentin
Formula: C₉H₁₇N₂O₂
Exact mass: 171.125929
Ion type: [M+H]⁺
Precursor m/z: 154.122645
Charge: 1
RT: 1.3277866
Polarity: +
InChI: InChI=1S/C₉H₁₇N₂O₂/c(10-7-9)(6-8)(11)2(4-2-1-3)-5-9(11)-7,10(12),11(12)
InChI key: UGIMXCAKUNAE-UHFFFAOYSA-N
SMILES: NCC1C(=O)OCCCC1
Num peaks: 13

Instrument information

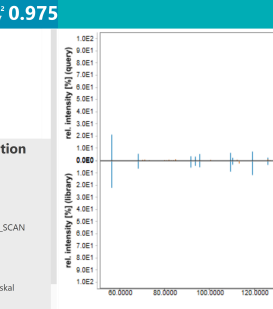
Instrument type: Orbitrap
Instrument: Orbitrap ID-X
Ion source: ESI
Ms level: 2.0
Collision energy: 20.0
Merged spec type: SINGLE_BEST_SCAN
Acquisition: Commercial
Software: mzmine3

Other information

Principal investigator: Tomas Pluskal
Data collector: Corinna Brungs

Database links

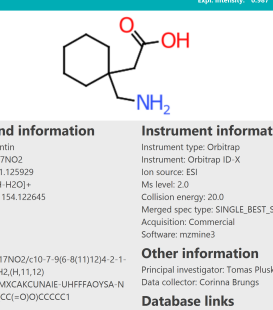
160



gabapentin

Matched signals: 11/12
Expl. intensity: 0.987

0.945



Compound information

Name: gabapentin
Formula: C₉H₁₇N₂O₂
Exact mass: 171.125929
Ion type: [M+H]⁺
Precursor m/z: 154.122645
Charge: 1
RT: 1.3277866
Polarity: +
InChI: InChI=1S/C₉H₁₇N₂O₂/c(10-7-9)(6-8)(11)2(4-2-1-3)-5-9(11)-7,10(12),11(12)
InChI key: UGIMXCAKUNAE-UHFFFAOYSA-N
SMILES: NCC1C(=O)OCCCC1
Num peaks: 13

Instrument information

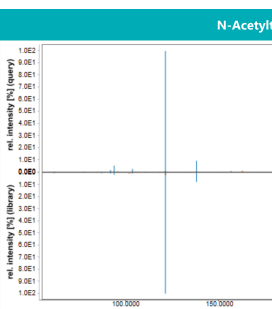
Instrument type: Orbitrap
Instrument: Orbitrap ID-X
Ion source: ESI
Ms level: 2.0
Collision energy: 20.0
Merged spec type: SINGLE_BEST_SCAN
Acquisition: Commercial
Software: mzmine3

Other information

Principal investigator: Tomas Pluskal
Data collector: Corinna Brungs

Database links

160



Compound information

Name: N-Acetyltyramine
Formula: C₁₀H₁₃N₂O₂
Exact mass: 179.094629
Ion type: [M+H]⁺
Precursor m/z: 180.101905
Charge: 1
RT: 0.94919467
Polarity: +
InChI: InChI=1S/C₁₀H₁₃N₂O₂/c(1-8)(12)11-7-6-9-2-4-10(13)-3-9(12)-5,13(4)-7(12),13(14),15(15),16(16),17(17),18(18),19(19),20(20),21(21),22(22),23(23),24(24),25(25),26(26),27(27),28(28),29(29),30(30),31(31),32(32),33(33),34(34),35(35),36(36),37(37),38(38),39(39),40(40),41(41),42(42),43(43),44(44),45(45),46(46),47(47),48(48),49(49),50(50),51(51),52(52),53(53),54(54),55(55),56(56),57(57),58(58),59(59),60(60),61(61),62(62),63(63),64(64),65(65),66(66),67(67),68(68),69(69),70(70),71(71),72(72),73(73),74(74),75(75),76(76),77(77),78(78),79(79),80(80),81(81),82(82),83(83),84(84),85(85),86(86),87(87),88(88),89(89),90(90),91(91),92(92),93(93),94(94),95(95),96(96),97(97),98(98),99(99),100(100),101(101),102(102),103(103),104(104),105(105),106(106),107(107),108(108),109(109),110(110),111(111),112(112),113(113),114(114),115(115),116(116),117(117),118(118),119(119),120(120),121(121),122(122),123(123),124(124),125(125),126(126),127(127),128(128),129(129),130(130),131(131),132(132),133(133),134(134),135(135),136(136),137(137),138(138),139(139),140(140),141(141),142(142),143(143),144(144),145(145),146(146),147(147),148(148),149(149),150(150),151(151),152(152),153(153),154(154),155(155),156(156),157(157),158(158),159(159),160(160),161(161),162(162),163(163),164(164),165(165),166(166),167(167),168(168),169(169),170(170),171(171),172(172),173(173),174(174),175(175),176(176),177(177),178(178),179(179),180(180),181(181),182(182),183(183),184(184),185(185),186(186),187(187),188(188),189(189),190(190),191(191),192(192),193(193),194(194),195(195),196(196),197(197),198(198),199(199),200(200),201(201),202(202),203(203),204(204),205(205),206(206),207(207),208(208),209(209),210(210),211(211),212(212),213(213),214(214),215(215),216(216),217(217),218(218),219(219),220(220),221(221),222(222),223(223),224(224),225(225),226(226),227(227),228(228),229(229),230(230),231(231),232(232),233(233),234(234),235(235),236(236),237(237),238(238),239(239),240(240),241(241),242(242),243(243),244(244),245(245),246(246),247(247),248(248),249(249),250(250),251(251),252(252),253(253),254(254),255(255),256(256),257(257),258(258),259(259),260(260),261(261),262(262),263(263),264(264),265(265),266(266),267(267),268(268),269(269),270(270),271(271),272(272),273(273),274(274),275(275),276(276),277(277),278(278),279(279),280(280),281(281),282(282),283(283),284(284),285(285),286(286),287(287),288(288),289(289),290(290),291(291),292(292),293(293),294(294),295(295),296(296),297(297),298(298),299(299),300(300),301(301),302(302),303(303),304(304),305(305),306(306),307(307),308(308),309(309),310(310),311(311),312(312),313(313),314(314),315(315),316(316),317(317),318(318),319(319),320(320),321(321),322(322),323(323),324(324),325(325),326(326),327(327),328(328),329(329),330(330),331(331),332(332),333(333),334(334),335(335),336(336),337(337),338(338),339(339),340(340),341(341),342(342),343(343),344(344),345(345),346(346),347(347),348(348),349(349),350(350),351(351),352(352),353(353),354(354),355(355),356(356),357(357),358(358),359(359),360(360),361(361),362(362),363(363),364(364),365(365),366(366),367(367),368(368),369(369),370(370),371(371),372(372),373(373),374(374),375(375),376(376),377(377),378(378),379(379),380(380),381(381),382(382),383(383),384(384),385(385),386(386),387(387),388(388),389(389),390(390),391(391),392(392),393(393),394(394),395(395),396(396),397(397),398(398),399(399),400(400),401(401),402(402),403(403),404(404),405(405),406(406),407(407),408(408),409(409),410(410),411(411),412(412),413(413),414(414),415(415),416(416),417(417),418(418),419(419),420(420),421(421),422(422),423(423),424(424),425(425),426(426),427(427),428(428),429(429),430(430),431(431),432(432),433(433),434(434),435(435),436(436),437(437),438(438),439(439),440(440),441(441),442(442),443(443),444(444),445(445),446(446),447(447),448(448),449(449),450(450),451(451),452(452),453(453),454(454),455(455),456(456),457(457),458(458),459(459),460(460),461(461),462(462),463(463),464(464),465(465),466(466),467(467),468(468),469(469),470(470),471(471),472(472),473(473),474(474),475(475),476(476),477(477),478(478),479(479),480(480),481(481),482(482),483(483),484(484),485(485),486(486),487(487),488(488),489(489),490(490),491(491),492(492),493(493),494(494),495(495),496(496),497(497),498(498),499(499),500(500),501(501),502(502),503(503),504(504),505(505),506(506),507(507),508(508),509(509),510(510),511(511),512(512),513(513),514(514),515(515),516(516),517(517),518(518),519(519),520(520),521(521),522(522),523(523),524(524),525(525),526(526),527(527),528(528),529(529),530(530),531(531),532(532),533(533),534(534),535(535),536(536),537(537),538(538),539(539),540(540),541(541),542(542),543(543),544(544),545(545),546(546),547(547),548(548),549(549),550(550),551(551),552(552),553(553),554(554),555(555),556(556),557(557),558(558),559(559),560(560),561(561),562(562),563(563),564(564),565(565),566(566),567(567),568(568),569(569),570(570),571(571),572(572),573(573),574(574),575(575),576(576),577(577),578(578),579(579),580(58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