

Carltonine-Derived Compounds for Targeted Butyrylcholinesterase Inhibition

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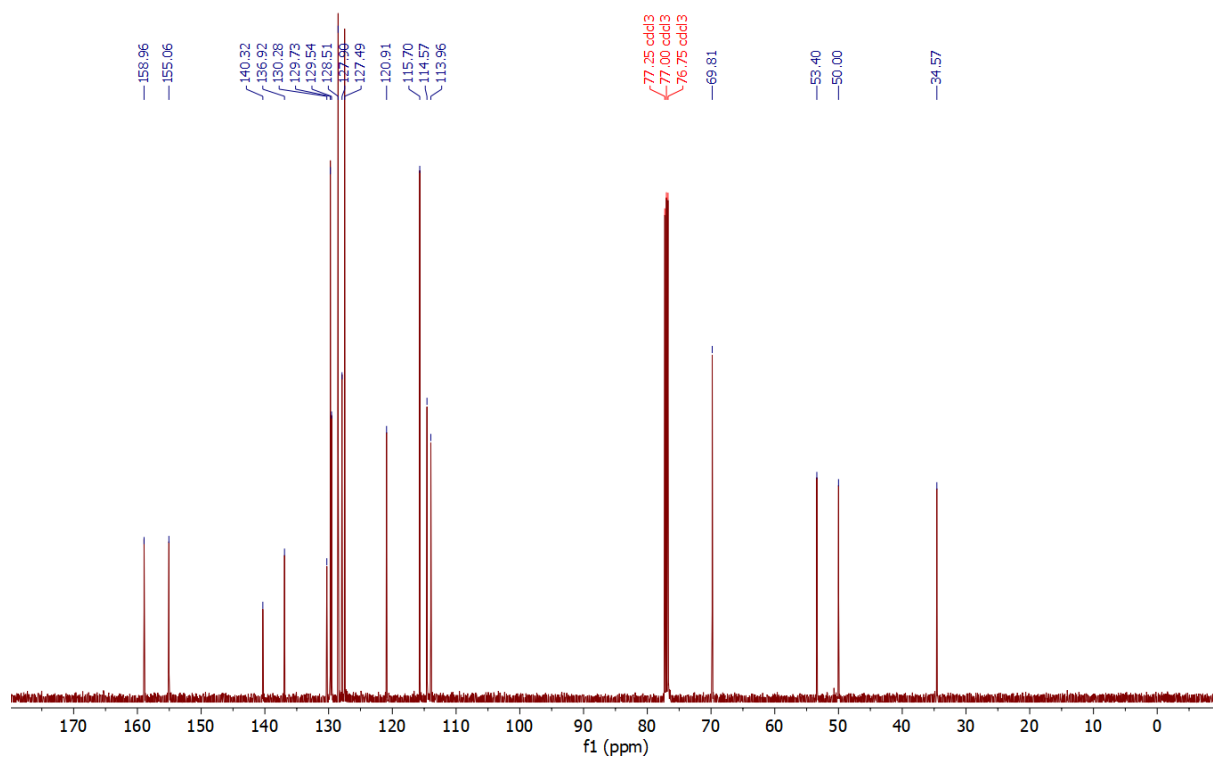
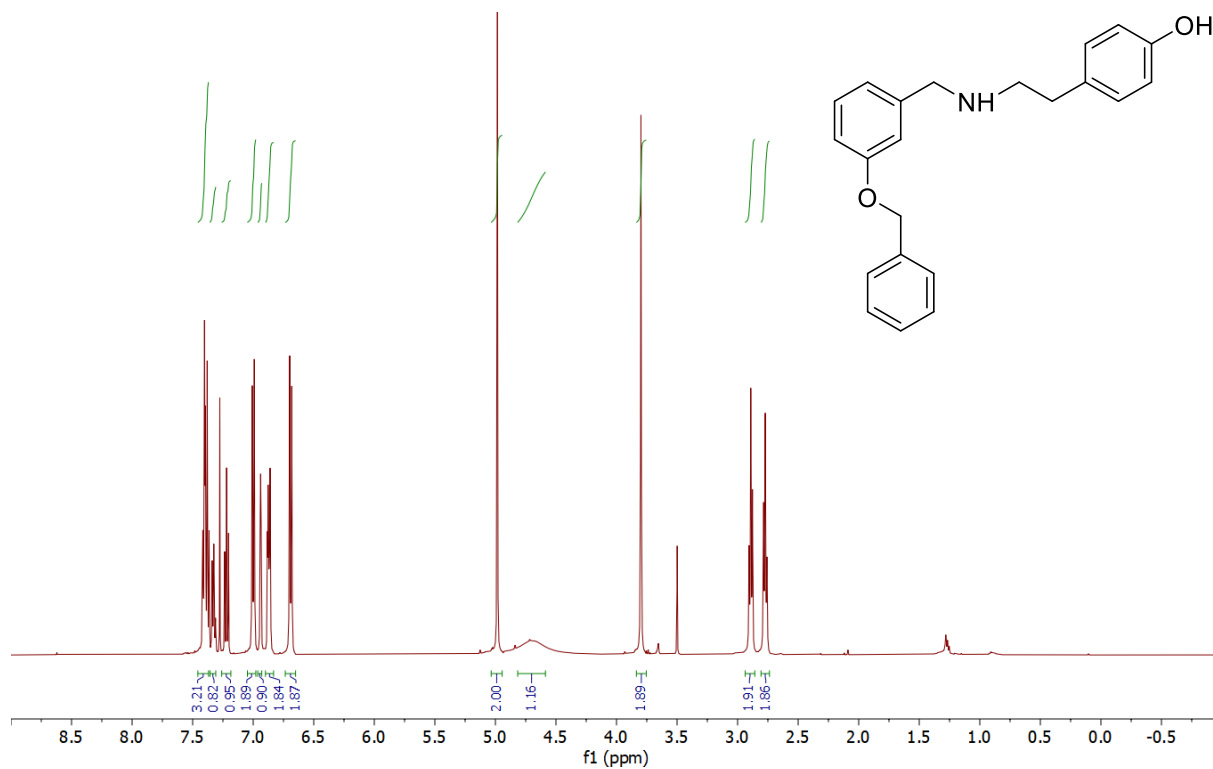
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jan.korabecny@fnhk.cz;

Lucie Cahlikova, ORCID ID: 0000-0002-1555-8870, e-mail: cahlikova@faf.cuni.cz

¹H NMR, ¹³C NMR, ESI-HRMS spectra and PDA chromatogram for final compounds

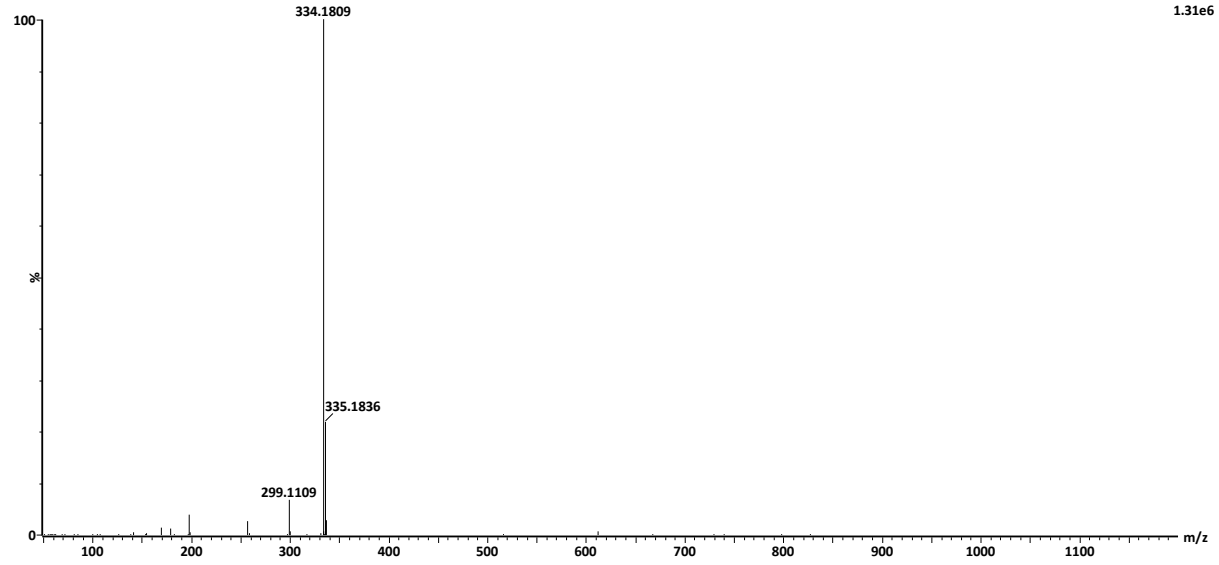
4-[2-({[3-(Benzyloxy)phenyl]methyl}amino)ethyl]phenol (4):



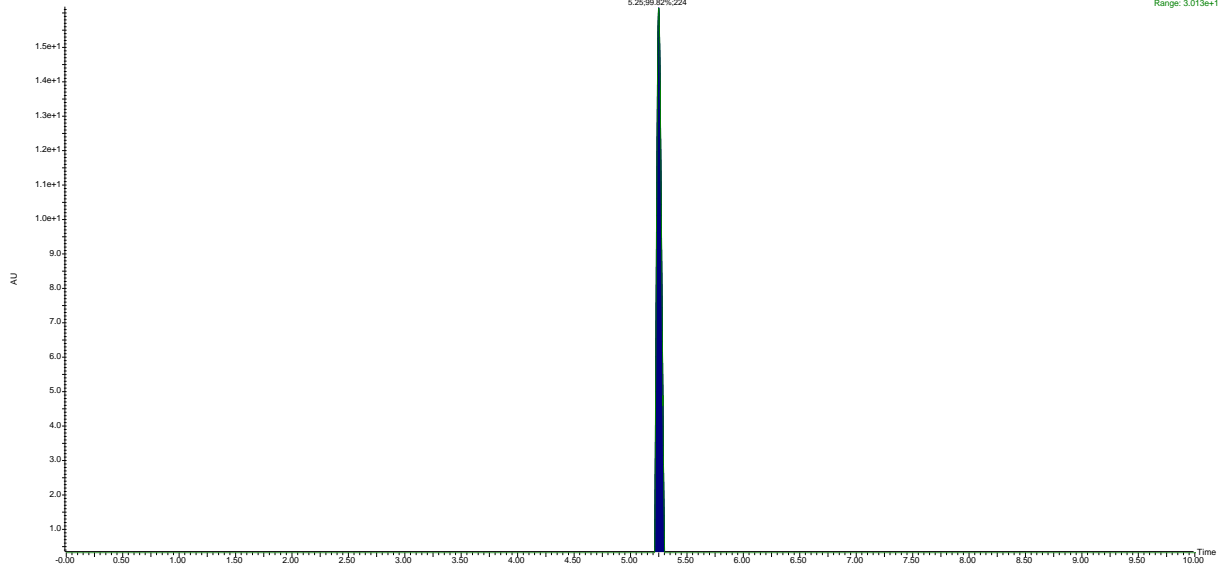
334.1802

2021 05 02 FC 012 A 1345 (2.323) Cm (1329:1366-(1194:1284+1458:1564))

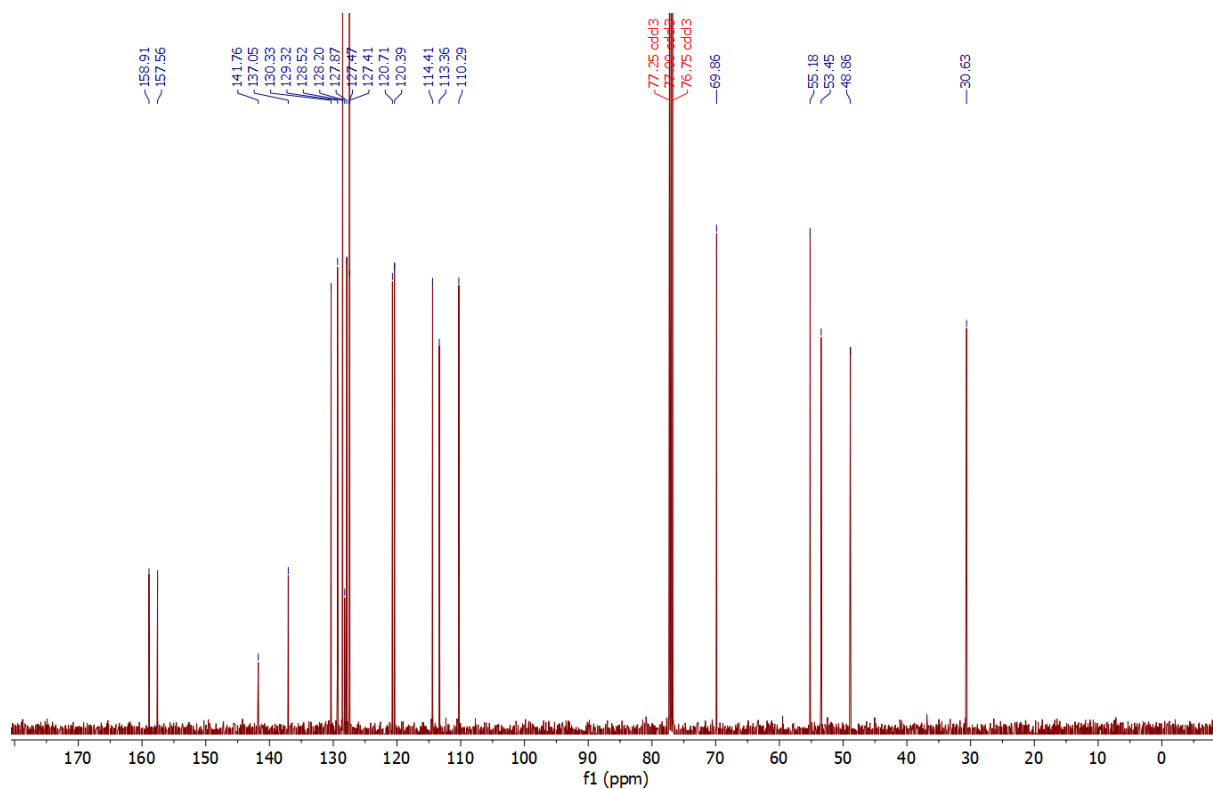
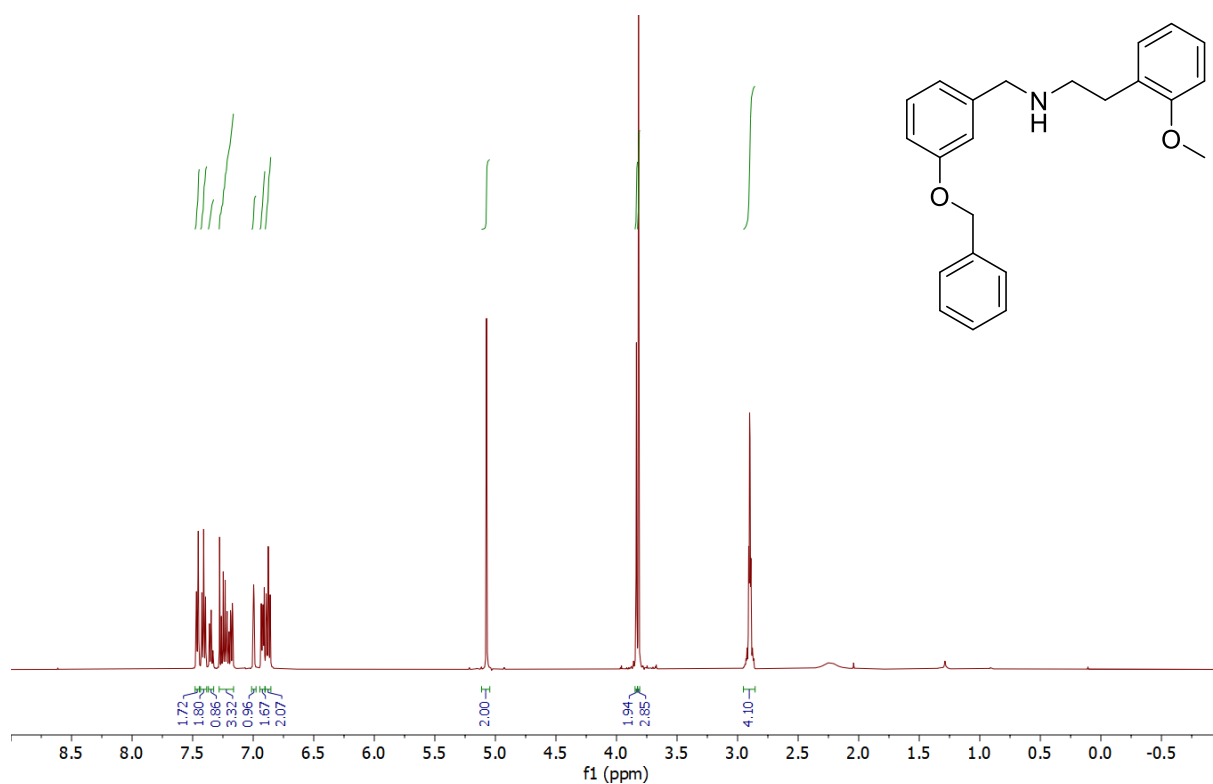
1: TOF MS ES+
1.31e6



FC012



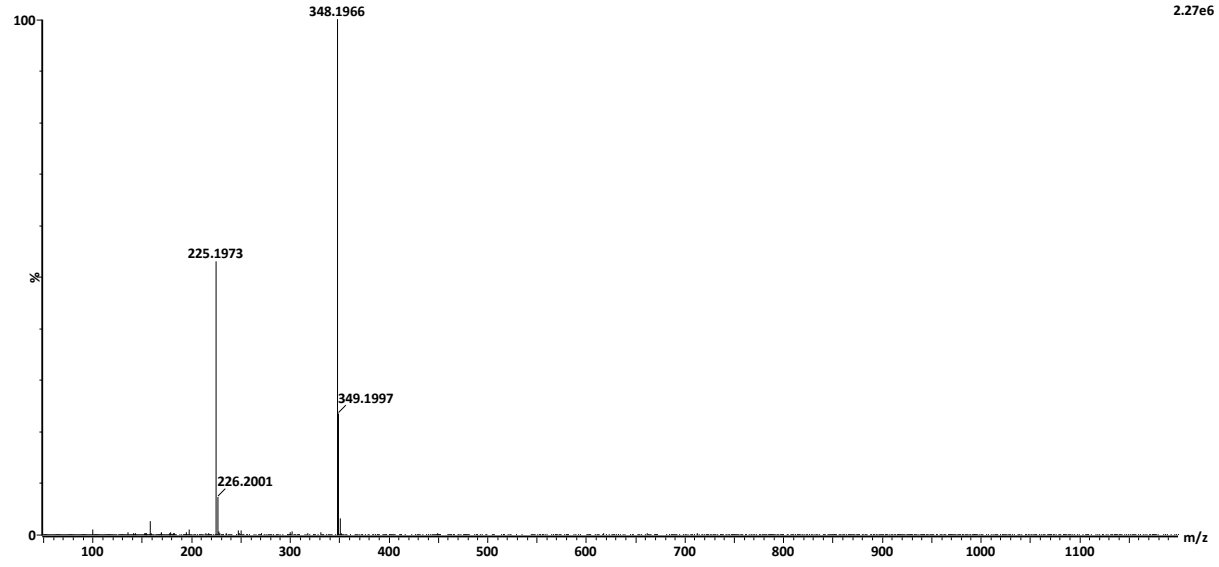
{[3-(Benzyloxy)phenyl]methyl}[2-(2-methoxyphenyl)ethyl]amine (5):



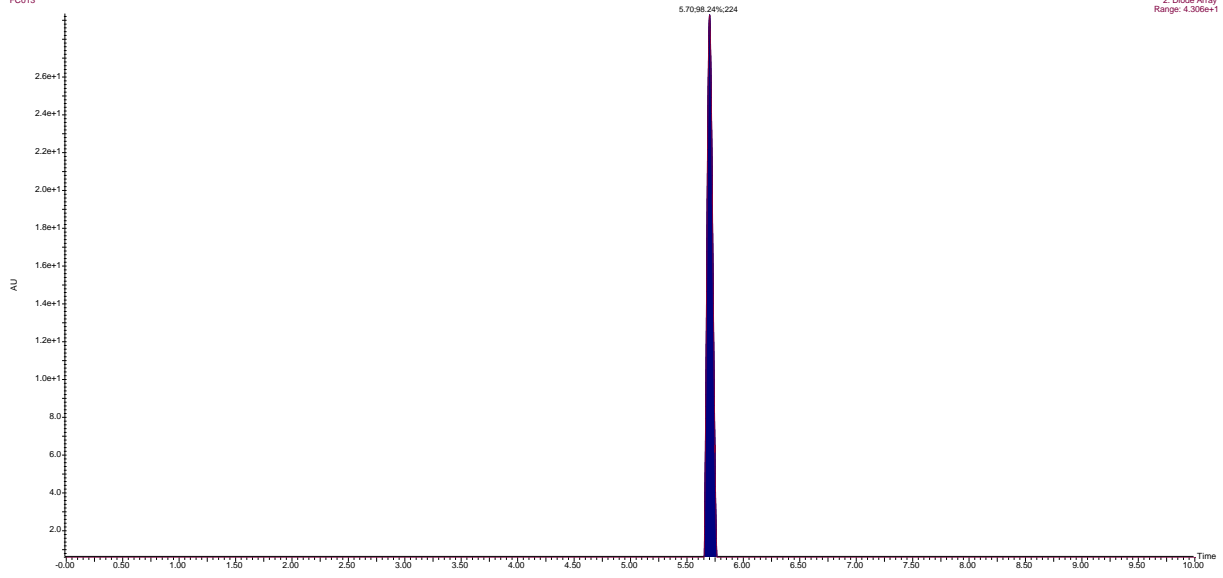
348,1958

2021 05 02 FC 013 A 1618 (2.788) Cm (1583:1619-(1502:1535+1663:1705))

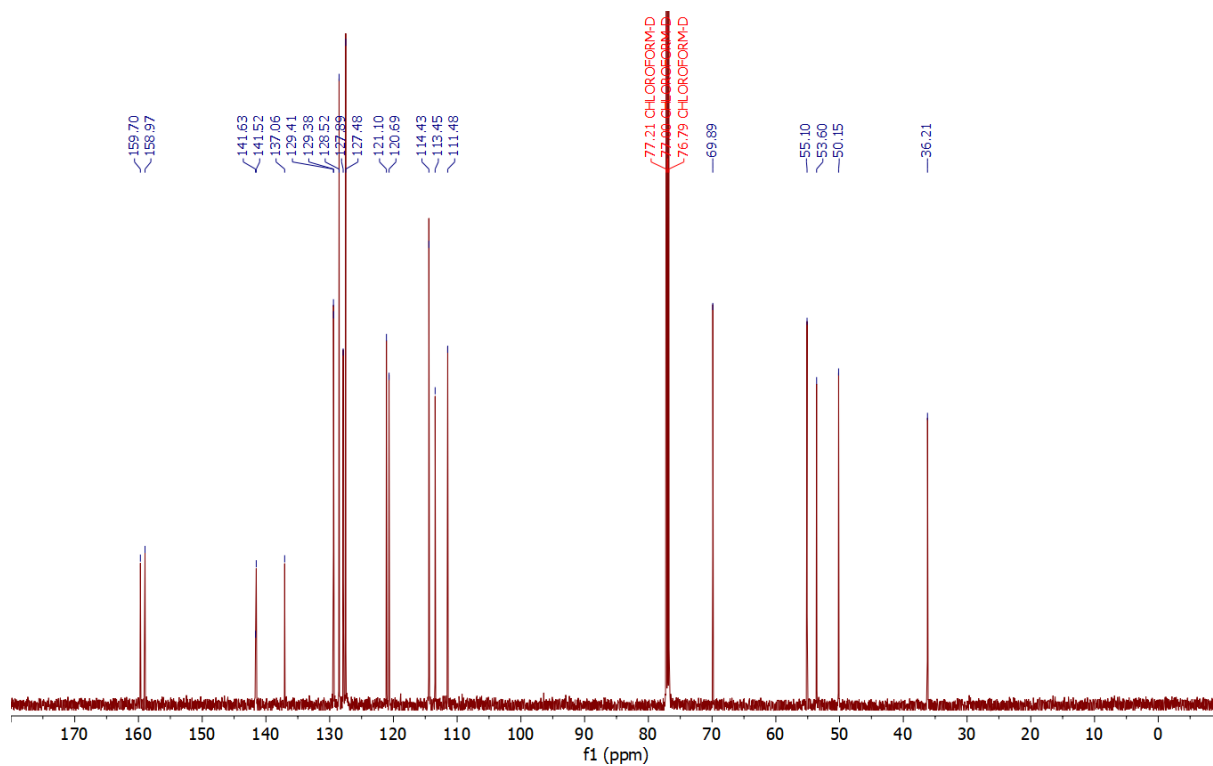
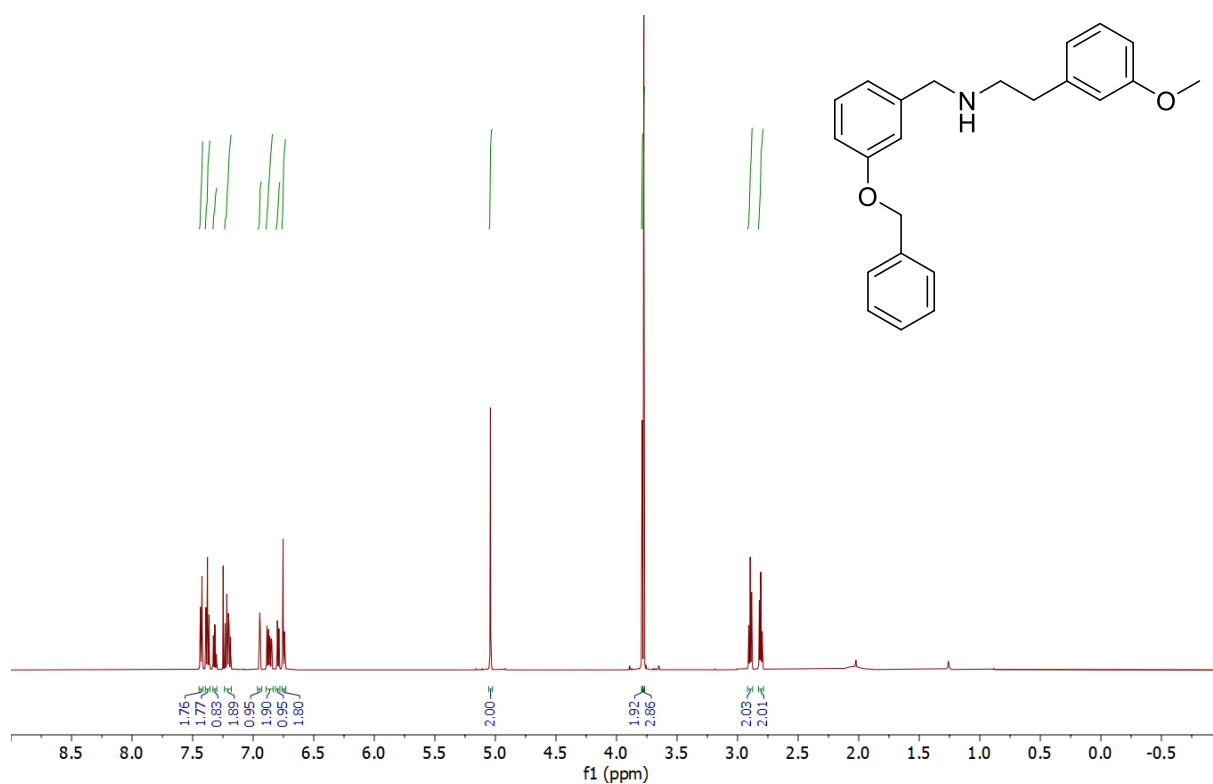
1: TOF MS ES+
2.27e6



FC013



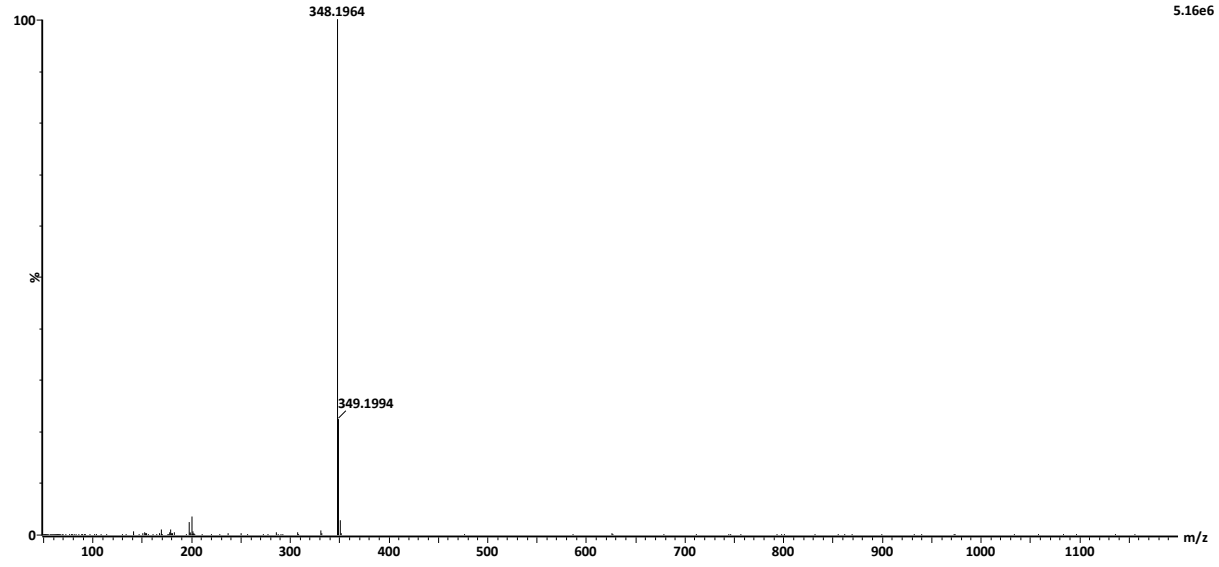
{[3-(Benzyloxy)phenyl]methyl}[2-(3-methoxyphenyl)ethyl]amine (6):



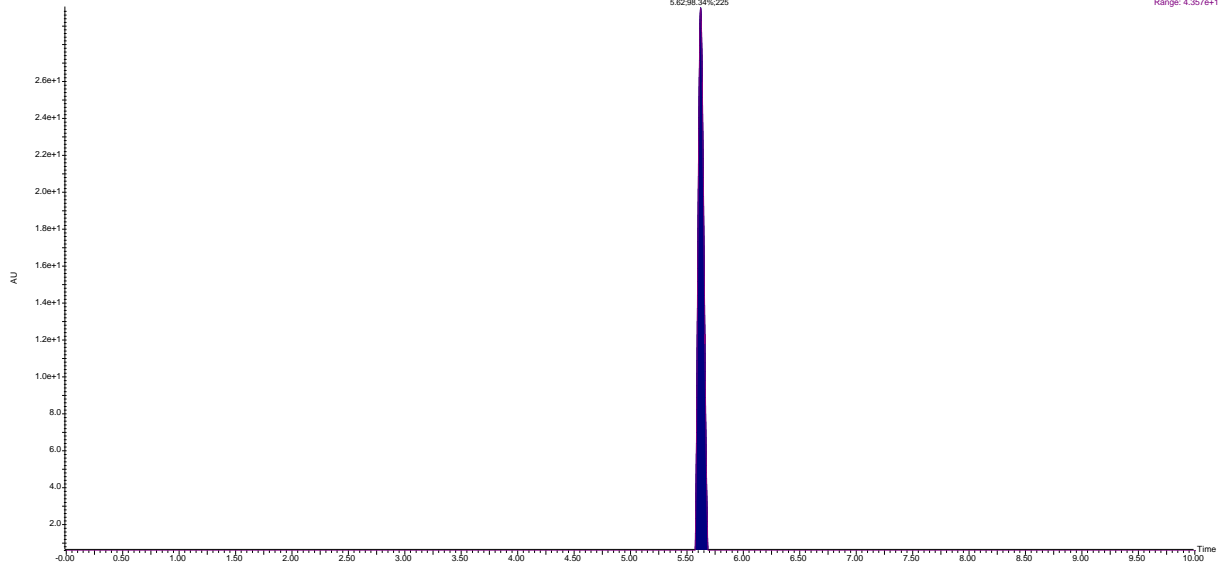
348.1958

2021 05 02 FC 018 A 1554 (2.677) Cm (1537:1579-(1349:1438+1658:1748))

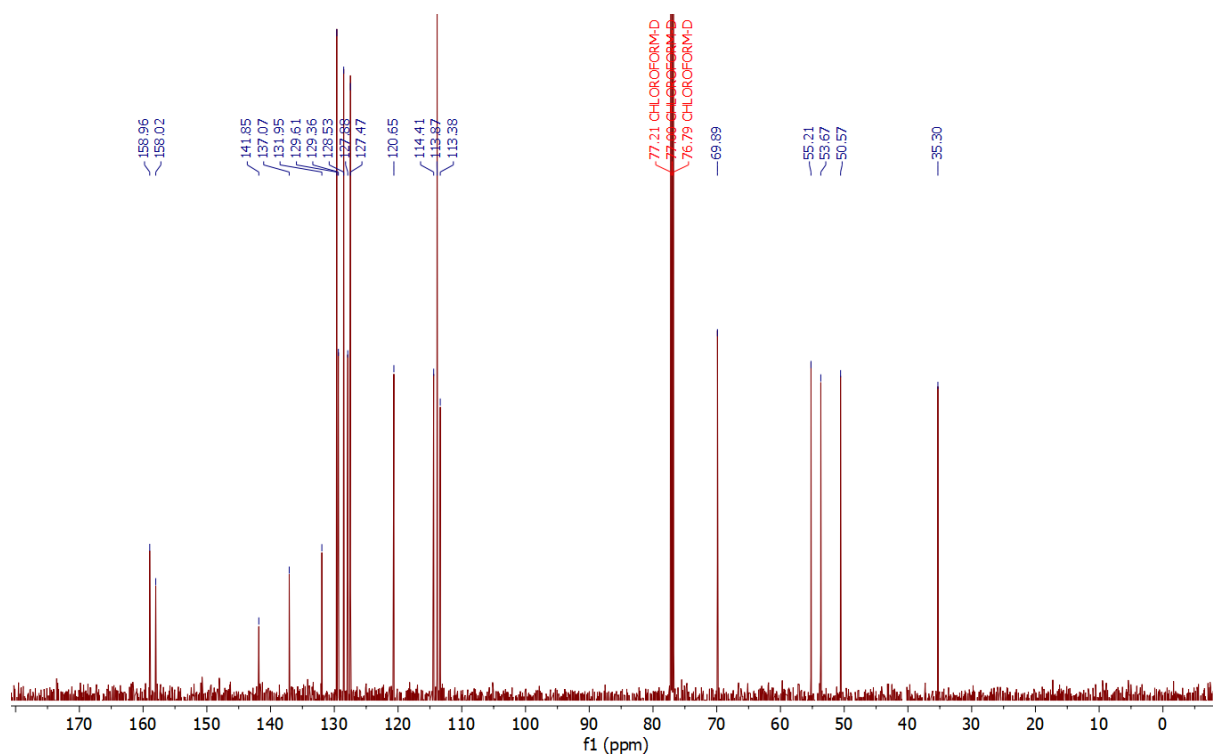
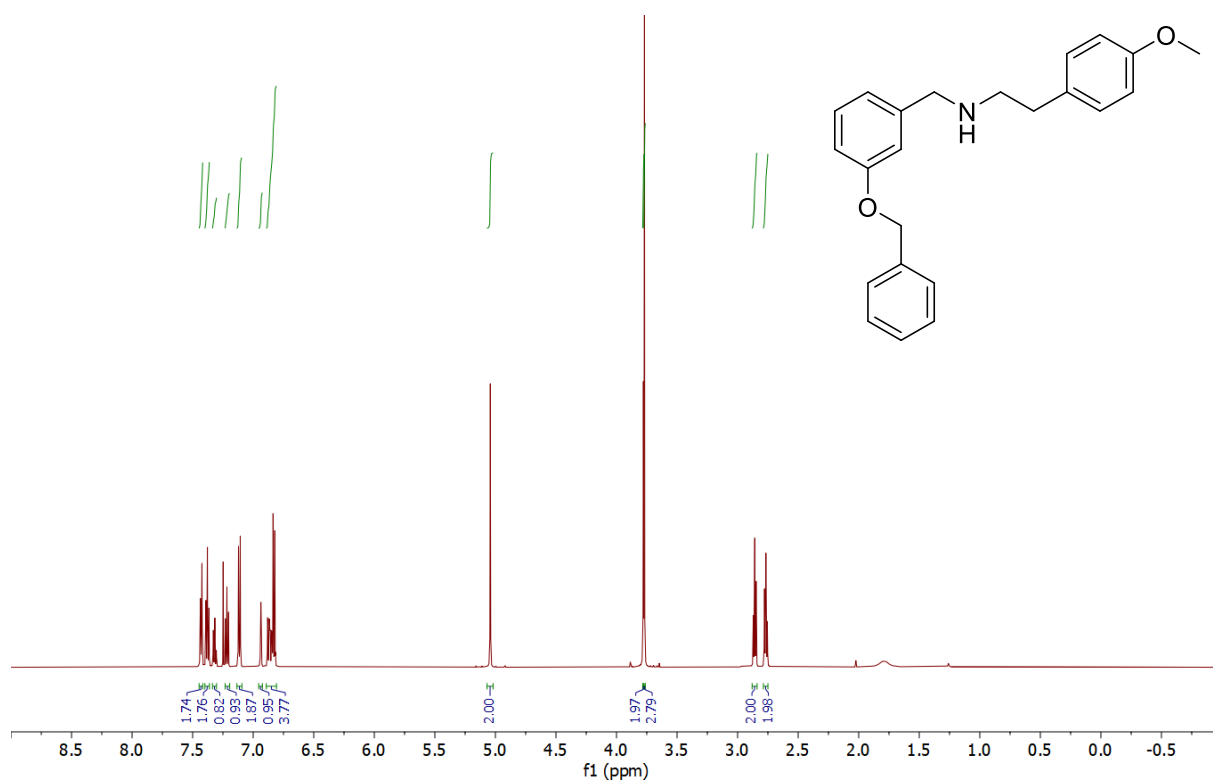
1: TOF MS ES+
5.16e6



FC018



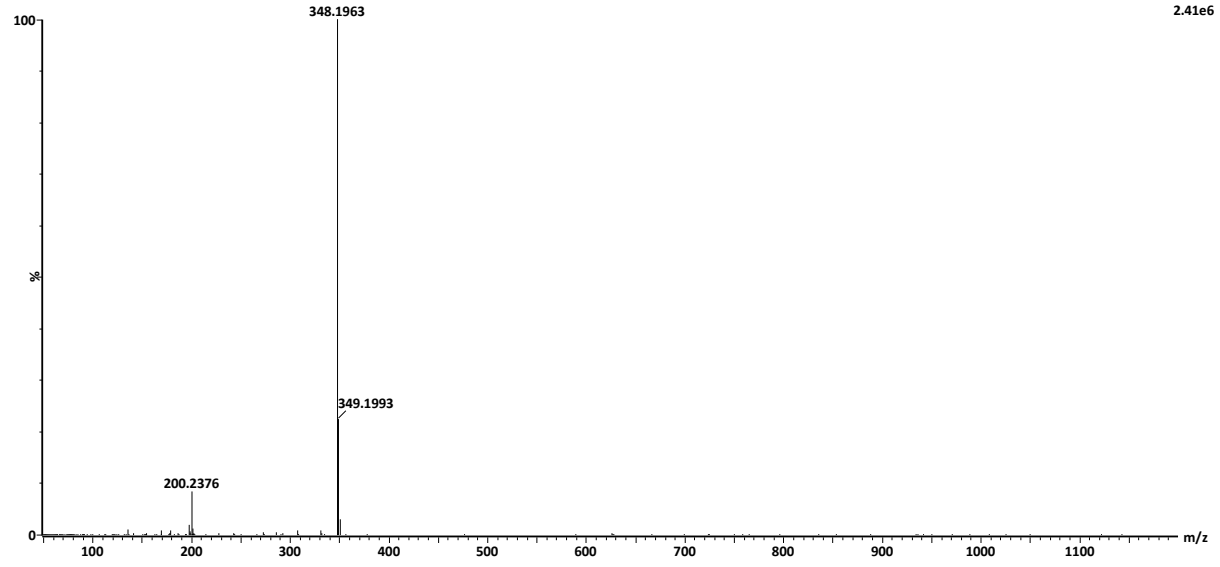
{[3-(Benzyloxy)phenyl]methyl}[2-(4-methoxyphenyl)ethyl]amine (7):



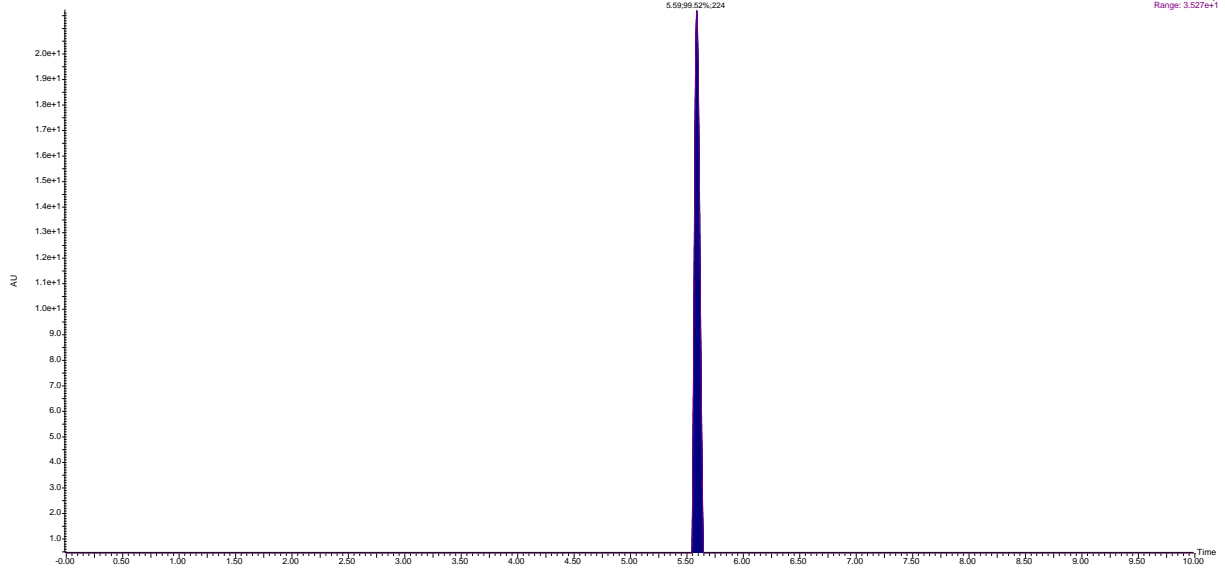
348.1958

2021 05 02 FC 017 B 1538 (2.652) Cm (1525:1563-(1401:1487+1621:1691))

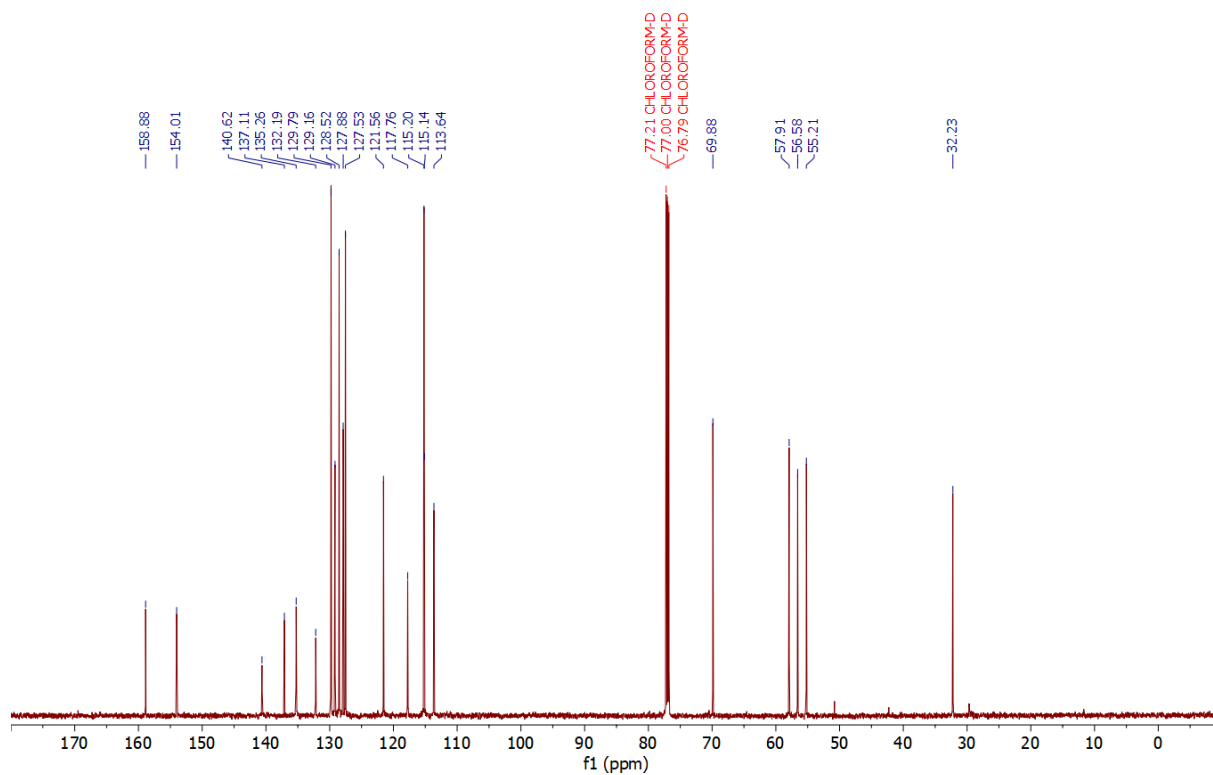
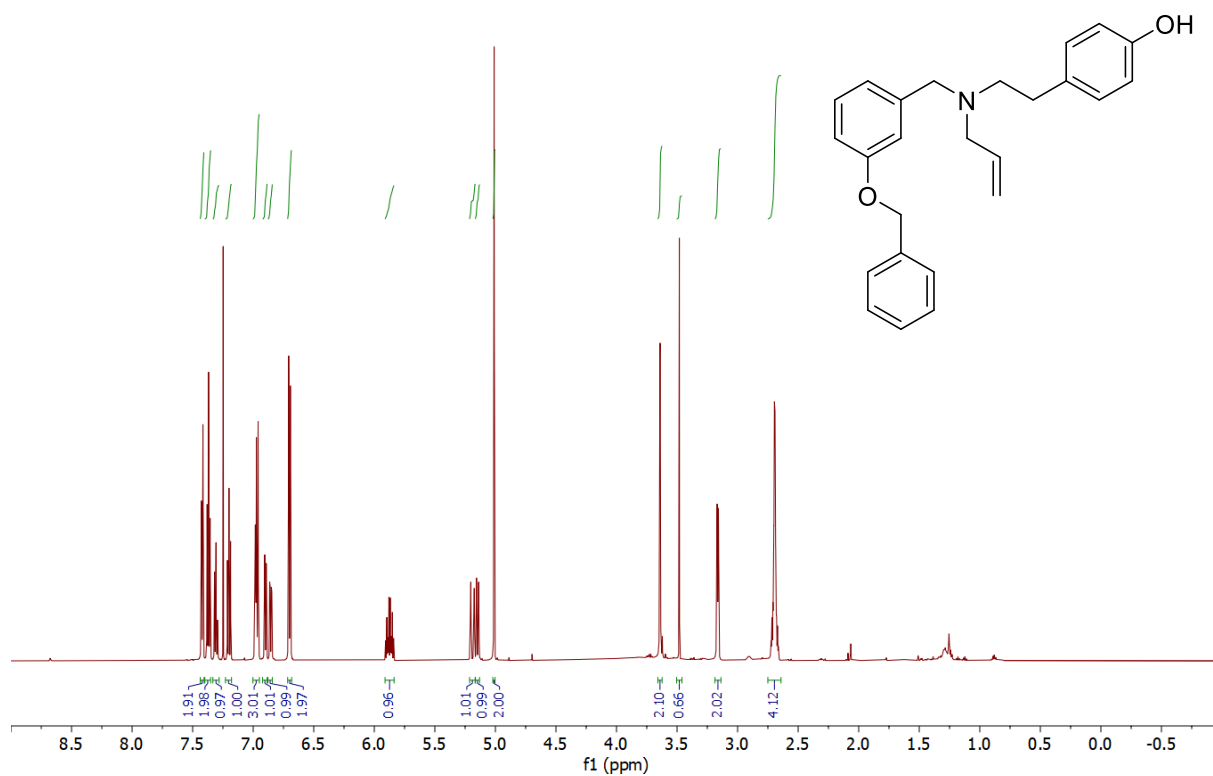
1: TOF MS ES+
2.41e6



FC017



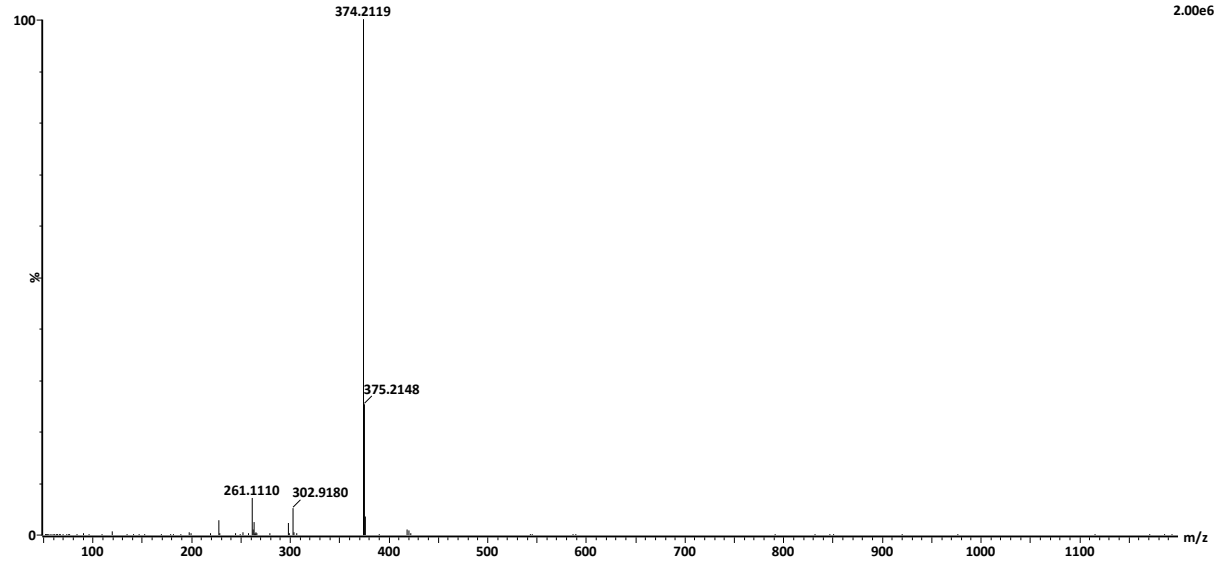
4-[2-({[3-(Benzyloxy)phenyl]methyl}(prop-2-en-1-yl)amino)ethyl]phenol (8):



374,2115

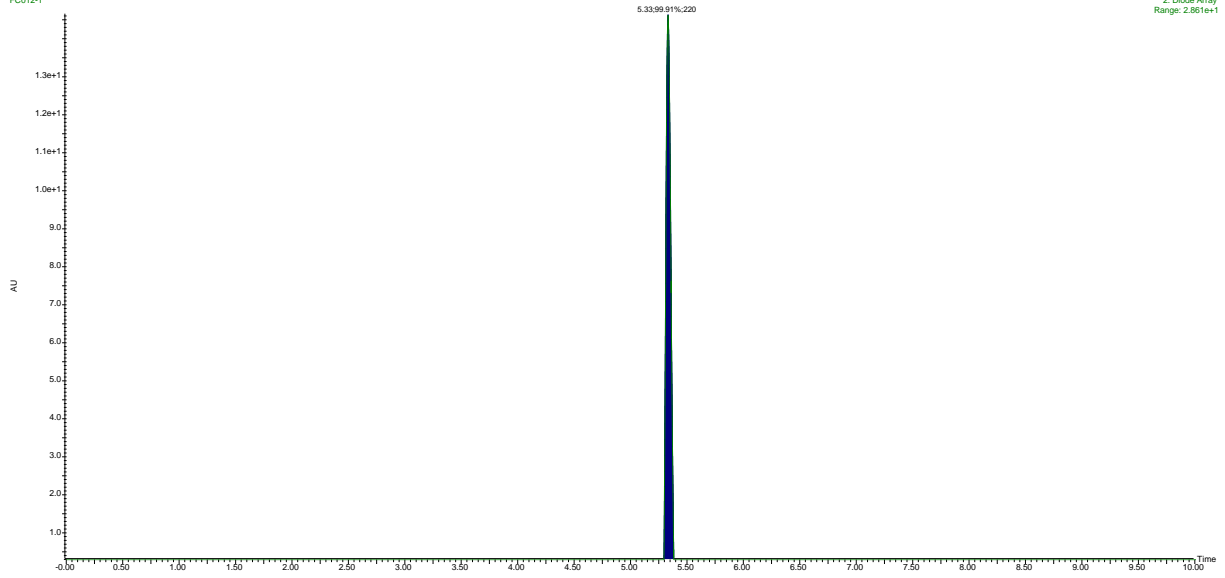
2021 05 02 FC 012-1 A 1468 (2.531) Cm (1453:1491-(1311:1403+1561:1667))

1: TOF MS ES+
2.00e6

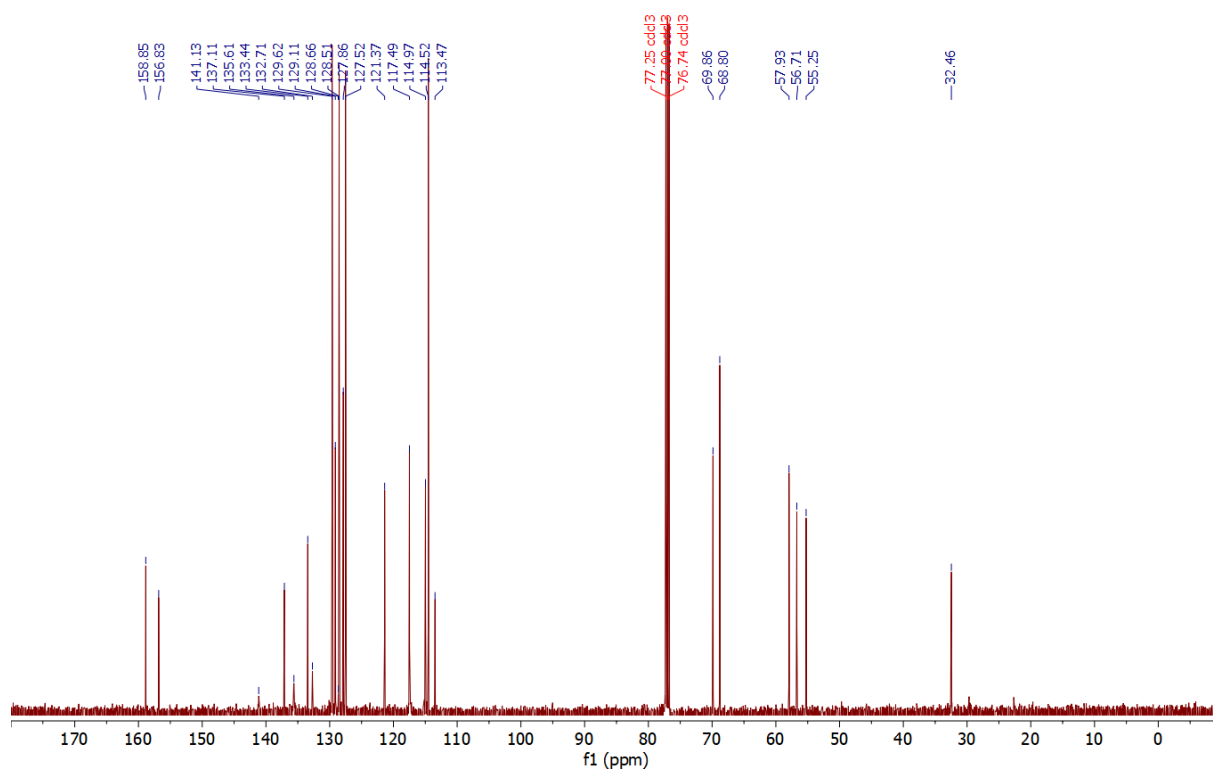
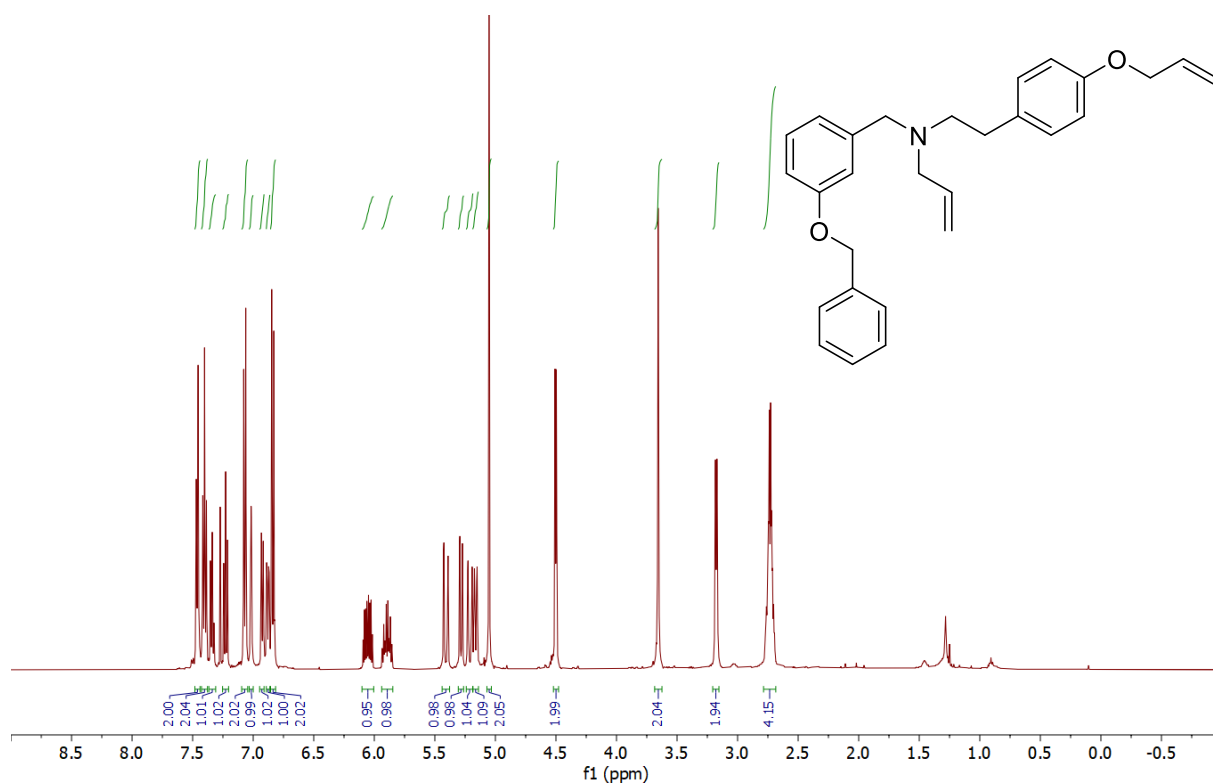


FC012-1

2: Diode Array
Range: 2.861e+1



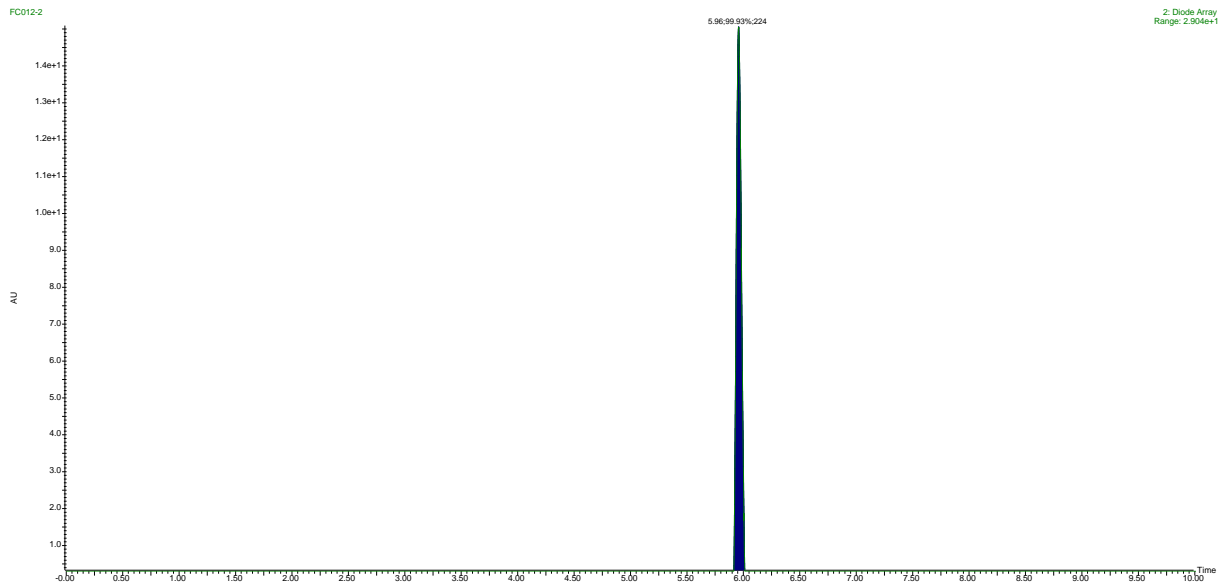
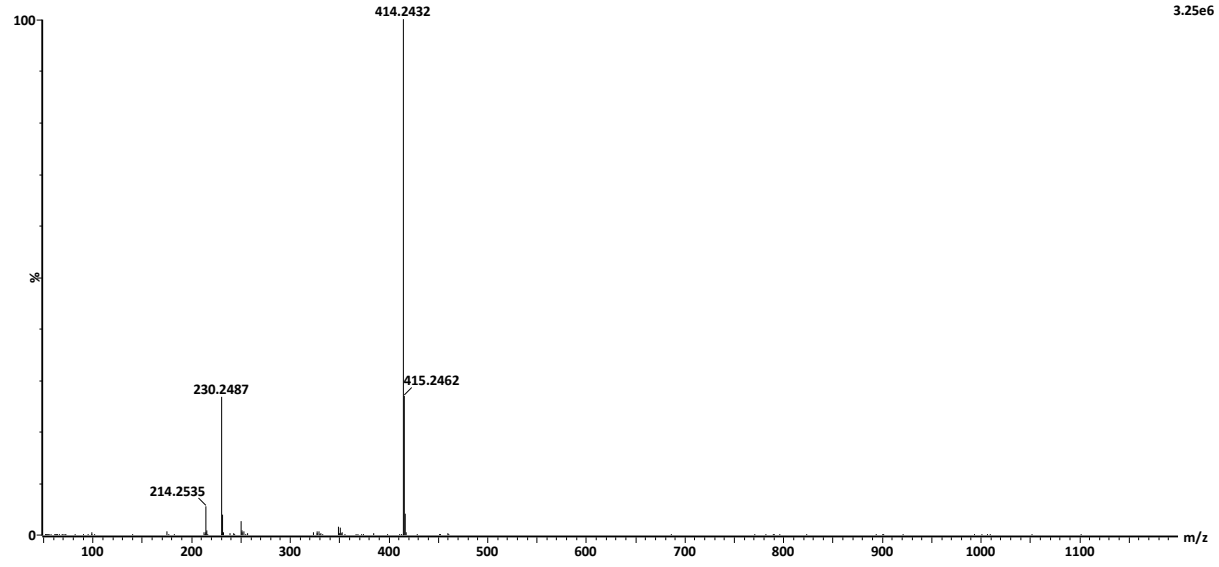
{[3-(Benzyloxy)phenyl]methyl}{prop-2-en-1-yl}{2-[4-(prop-2-en-1-yloxy)phenyl]ethyl}amine (9):



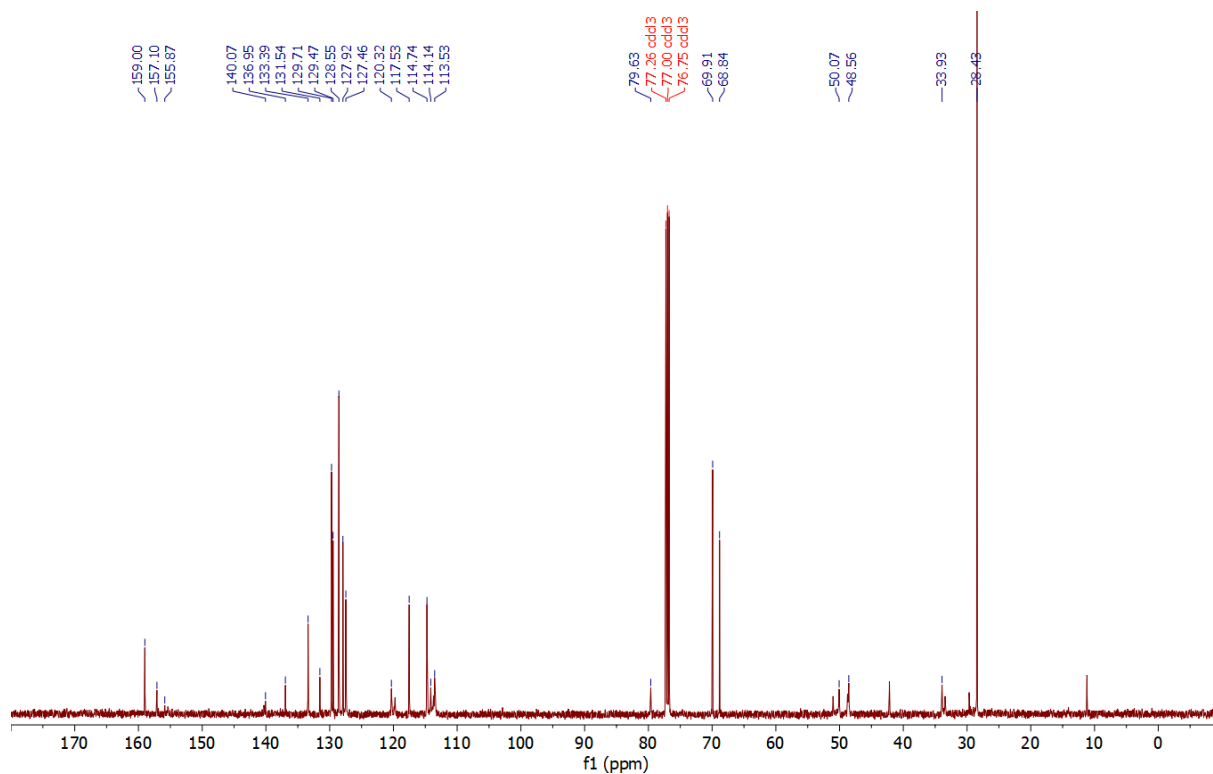
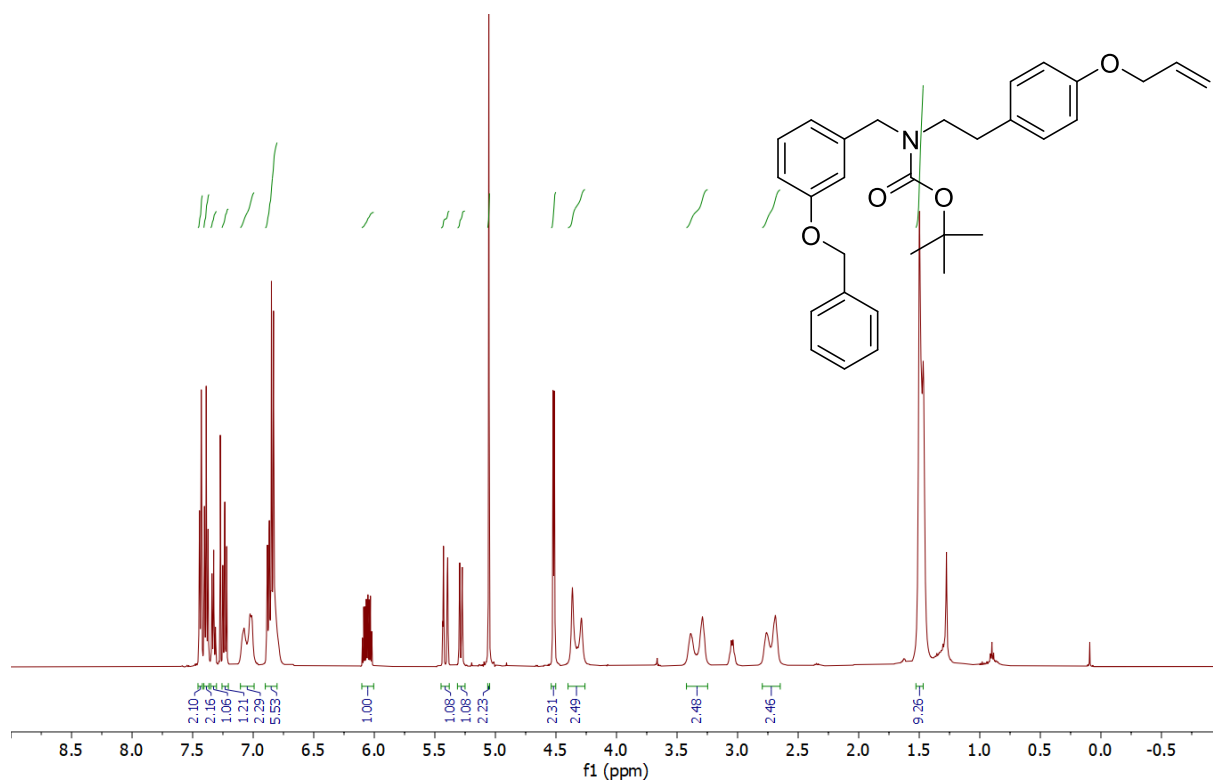
414,2428

2021 05 02 FC 012-2 B 1832 (3.155) Cm (1818:1854-(1700:1773+1943:2020))

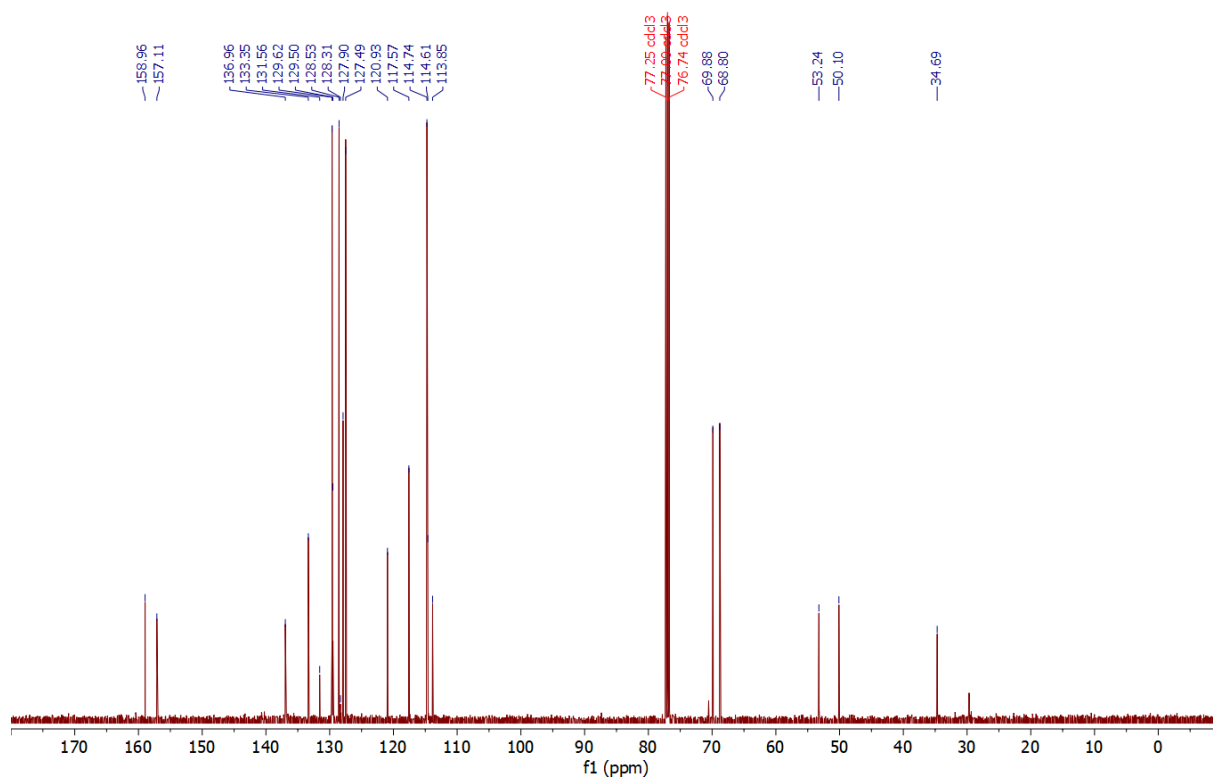
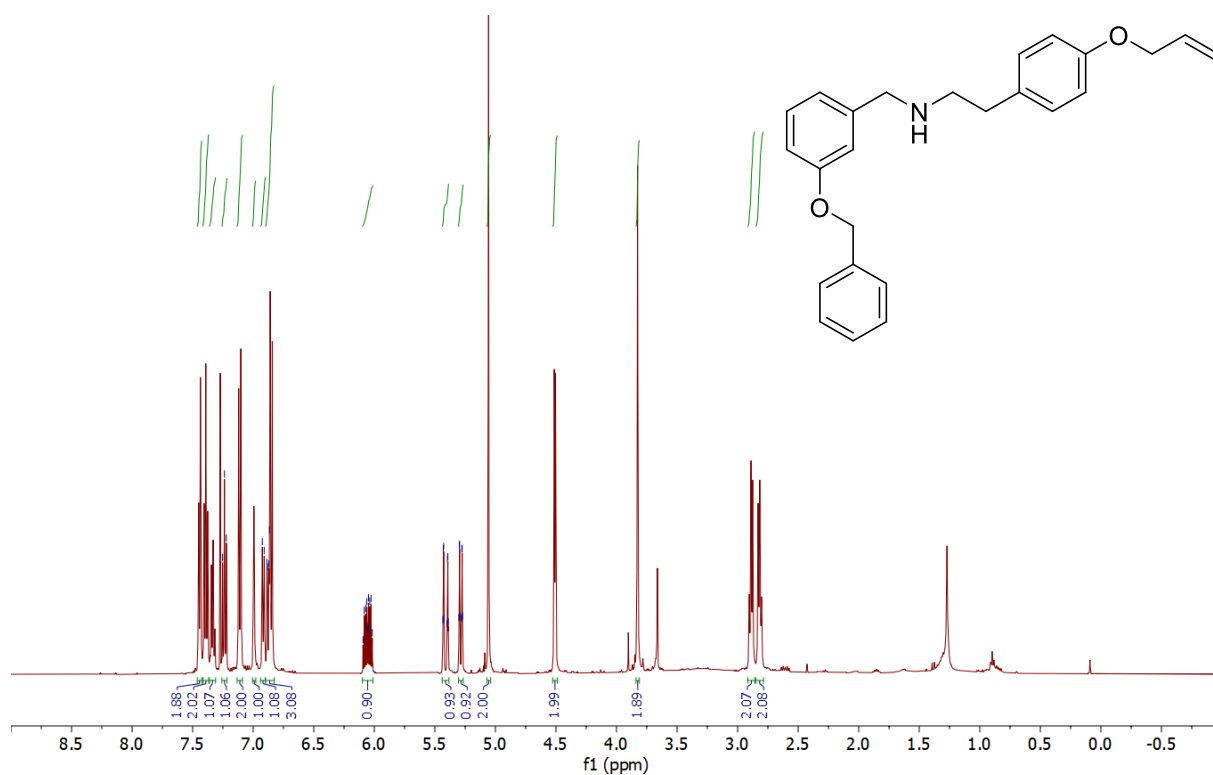
1: TOF MS ES+
3.25e6



Tert-butyl N-([3-(benzyloxy)phenyl]methyl)-N-{2-[4-(prop-2-en-1-yloxy)phenyl]ethyl}carbamate (11):



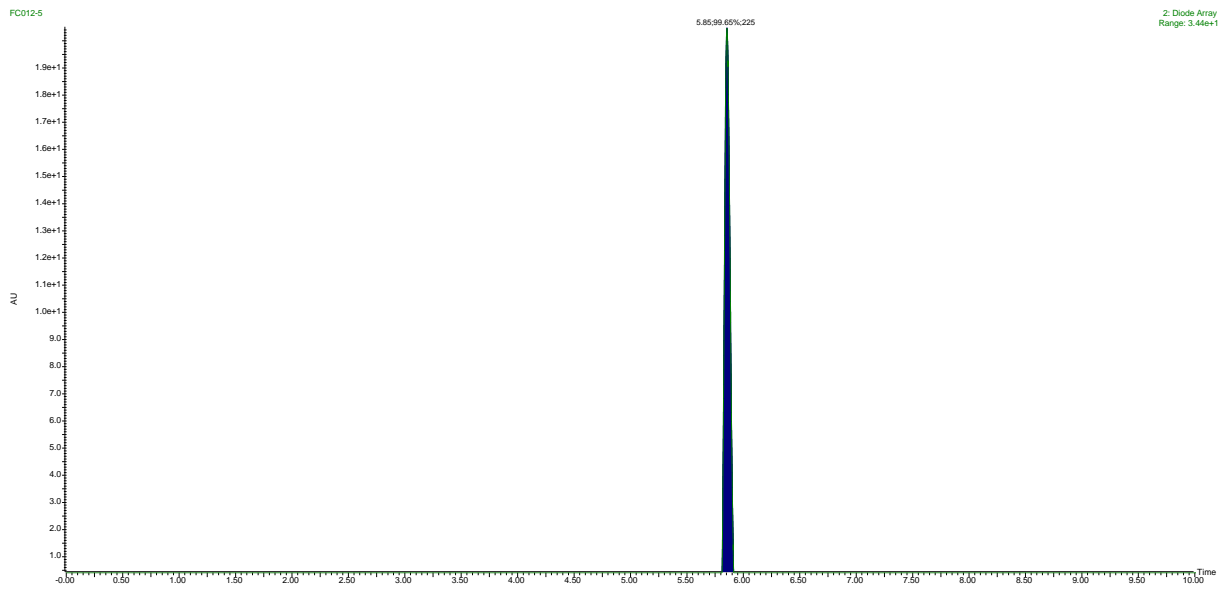
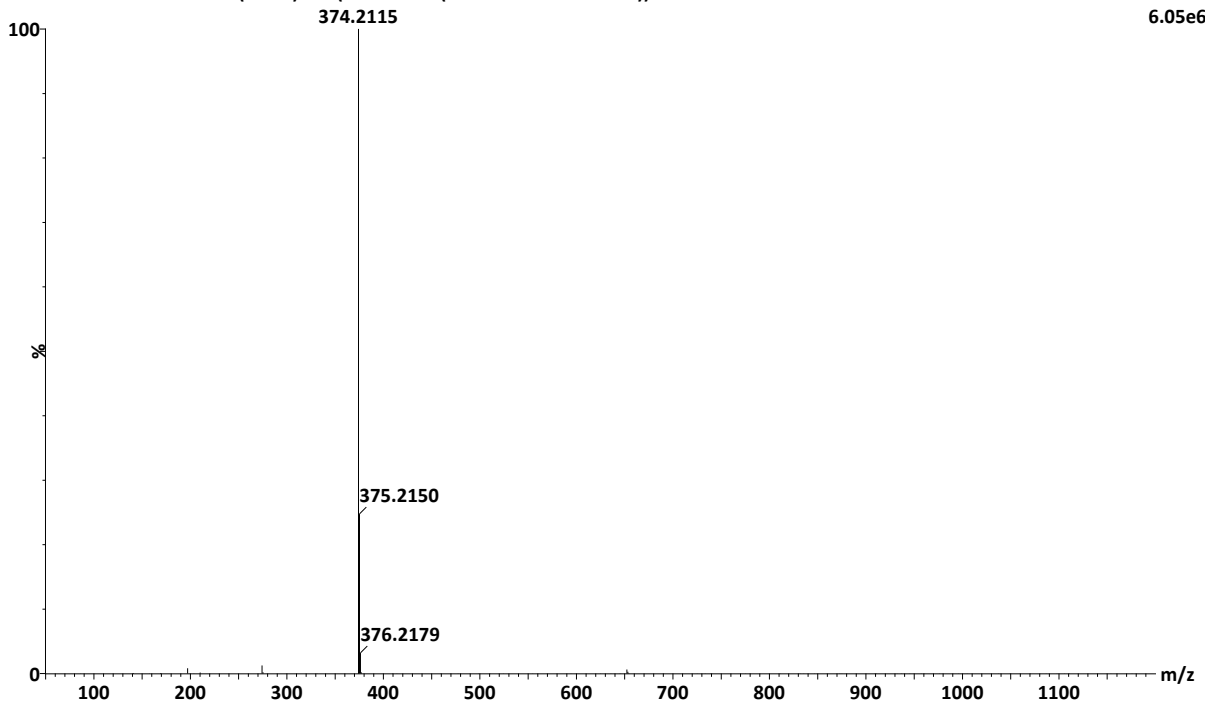
{[3-(Benzyloxy)phenyl]methyl}({2-[4-(prop-2-en-1-yloxy)phenyl]ethyl})amine (12):



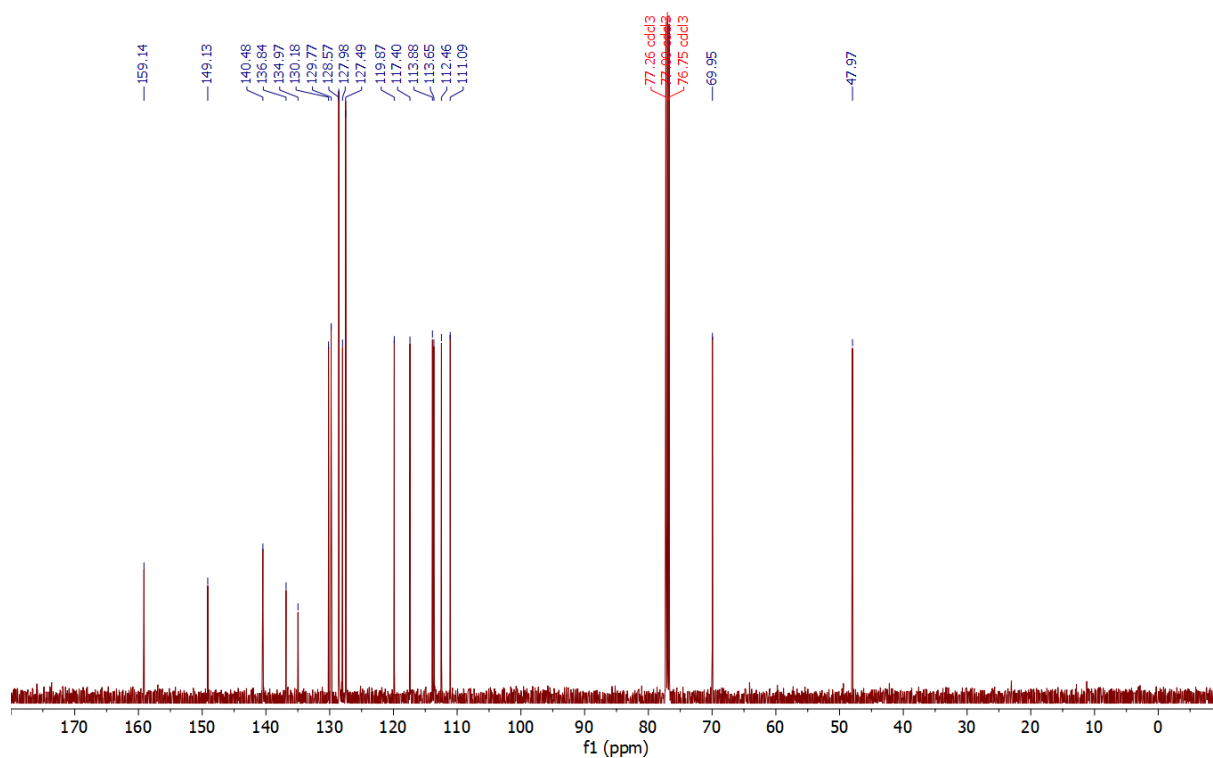
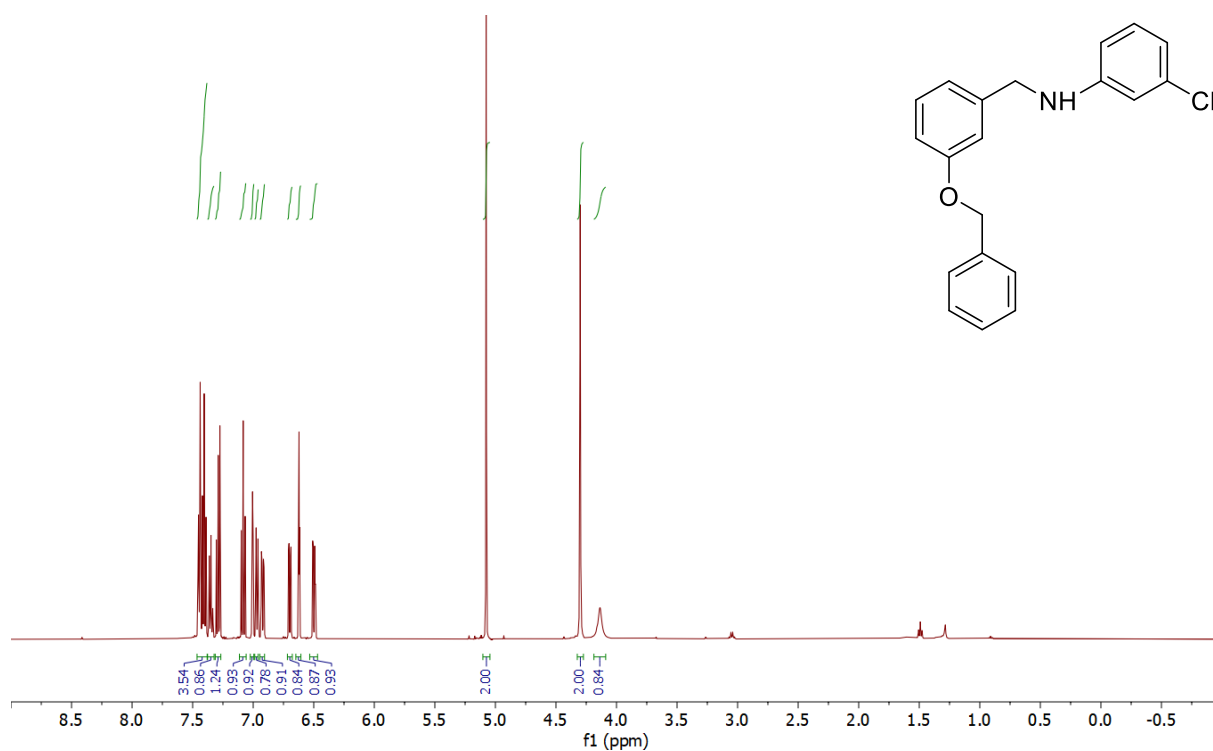
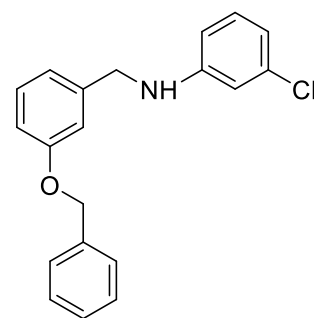
374.2115

2021 04 22 FC012-5B 1782 (3.104) Cm (1771:1802-(1576:1700+1886:1958))

1: TOF MS ES+
6.05e6



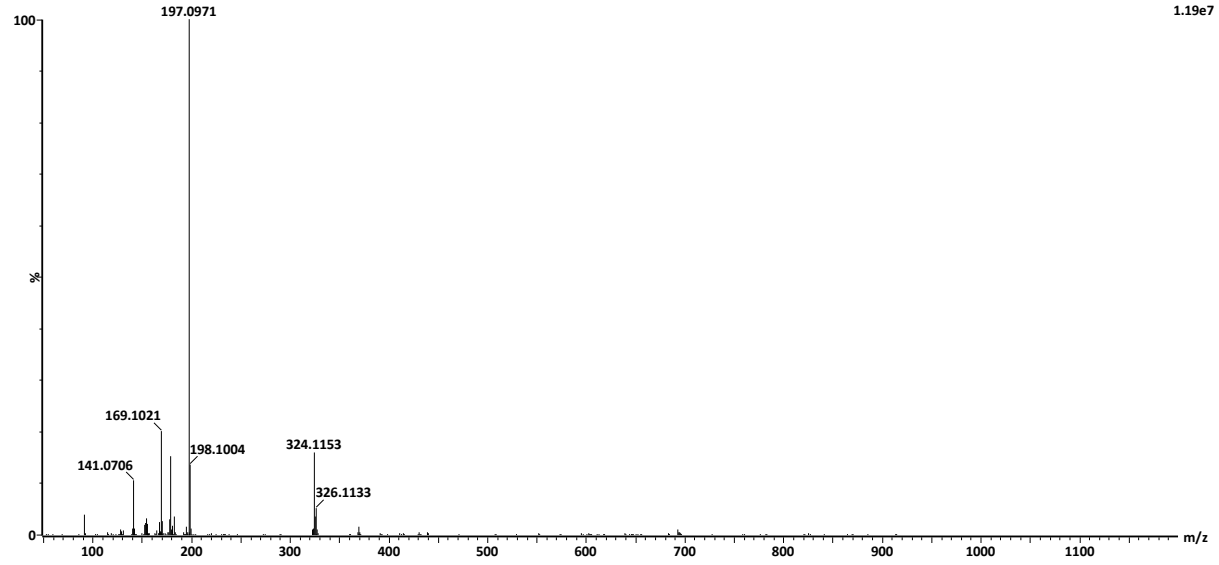
N-([3-(Benzyloxy)phenyl]methyl)-3-chloroaniline (13):



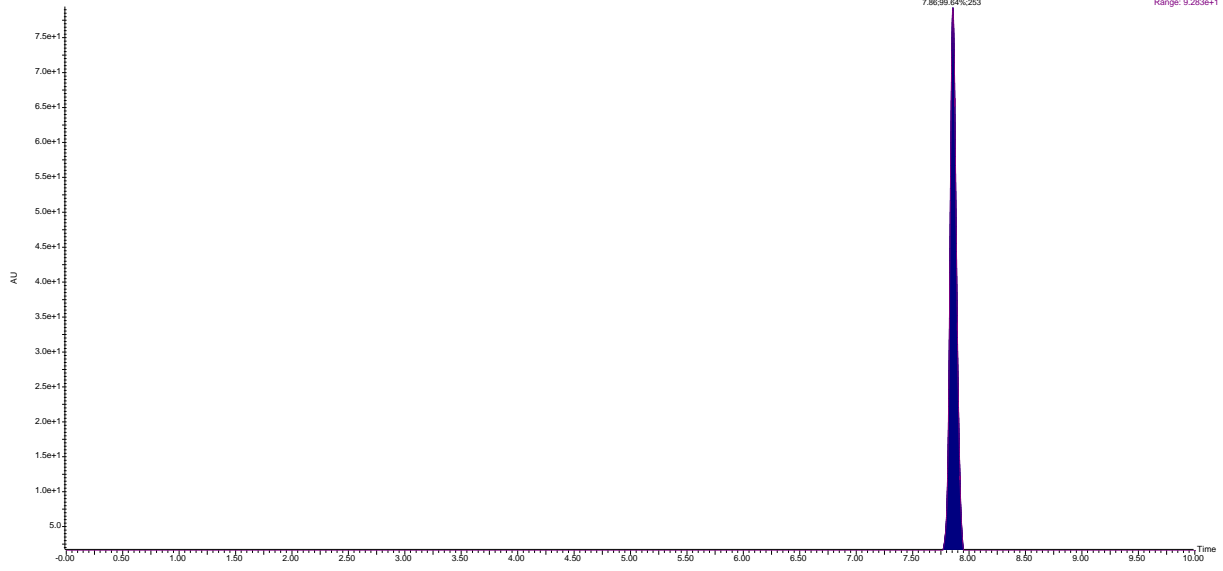
324.1150

2021 05 02 FC 022 B 2575 (4.424) Cm (2561:2597-(2448:2499+2678:2765))

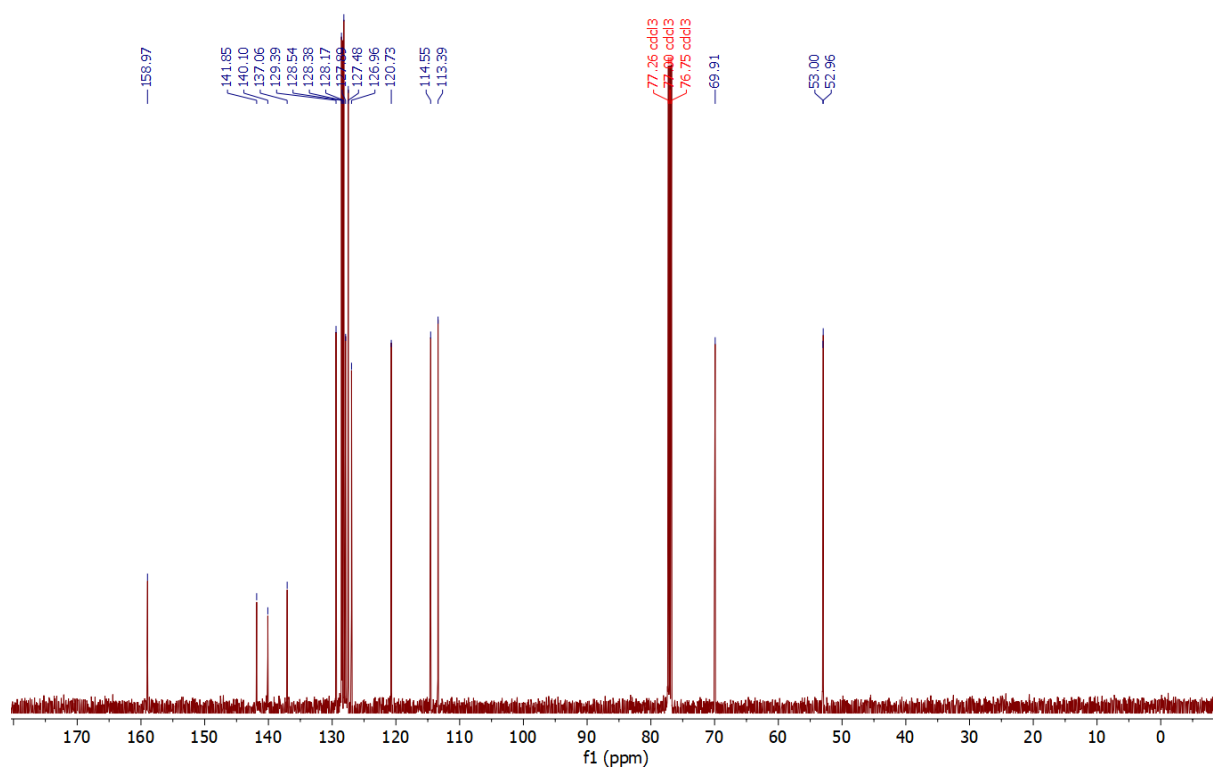
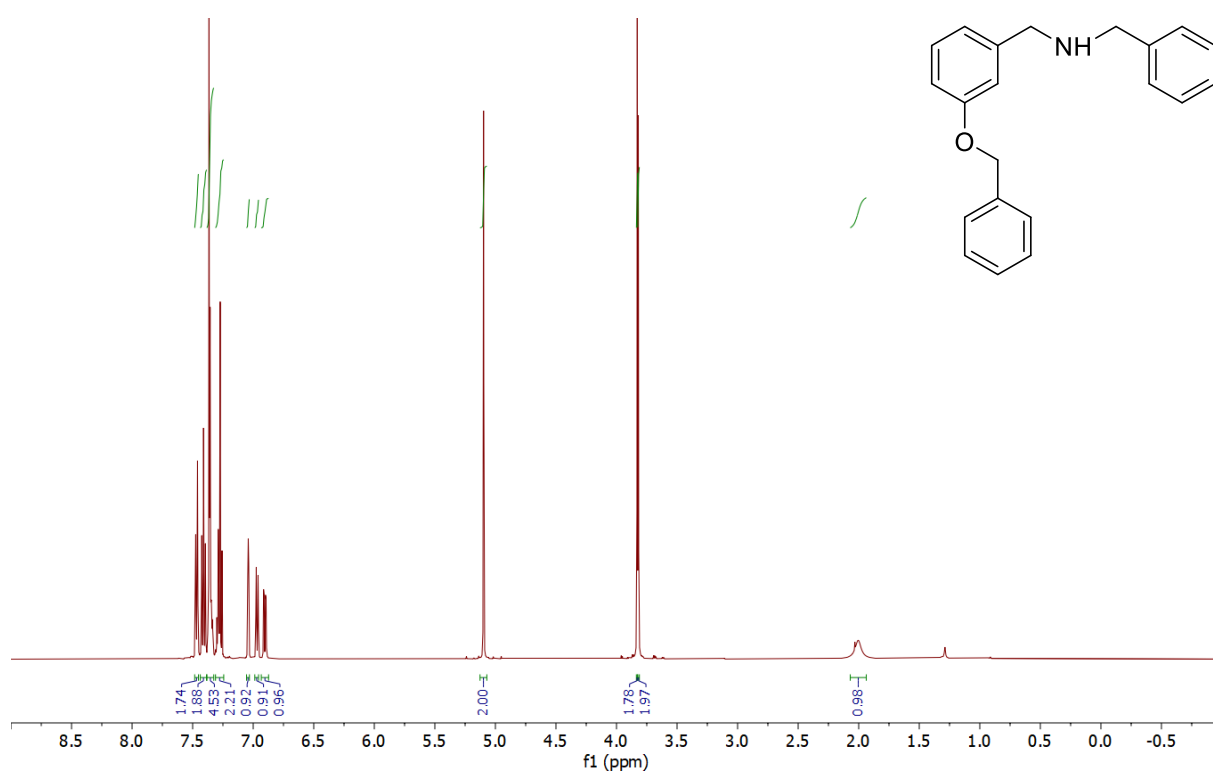
1: TOF MS ES+
1.19e7



FC022



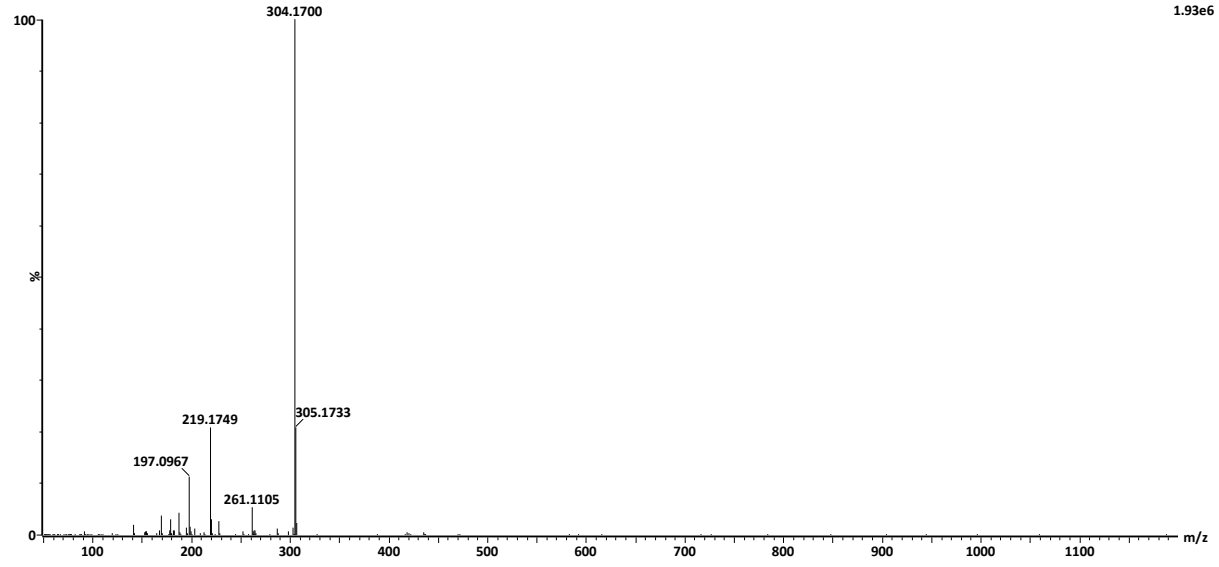
Benzyl({[3-(benzyloxy)phenyl]methyl})amine (14):



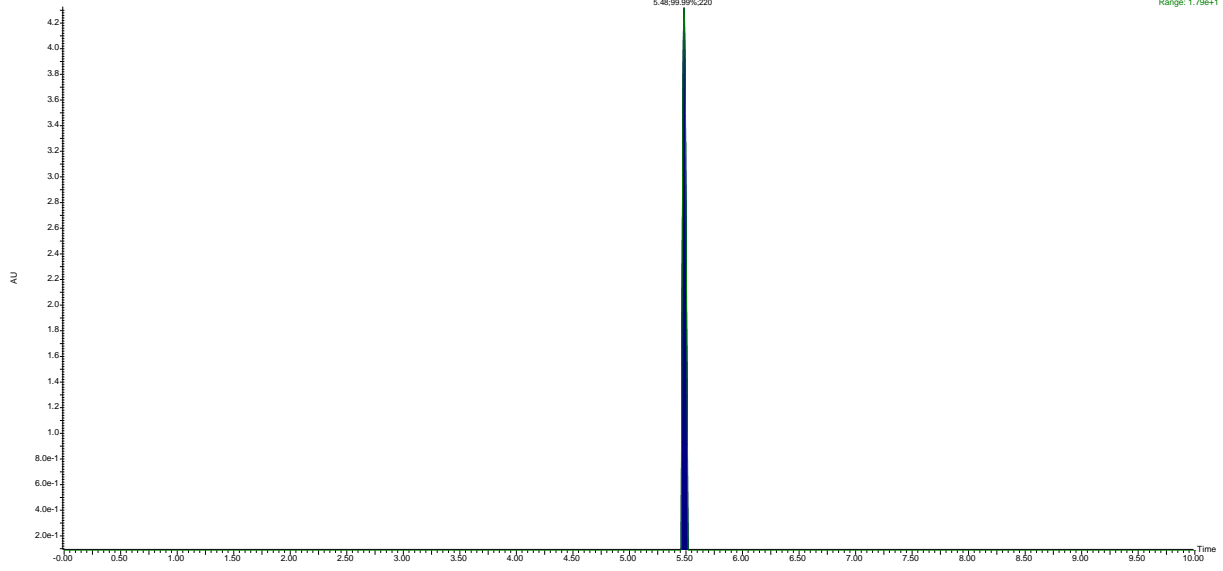
304.1696

2021 05 02 FC 019 A 1462 (2.520) Cm (1437:1477-(1241:1343+1526:1620))

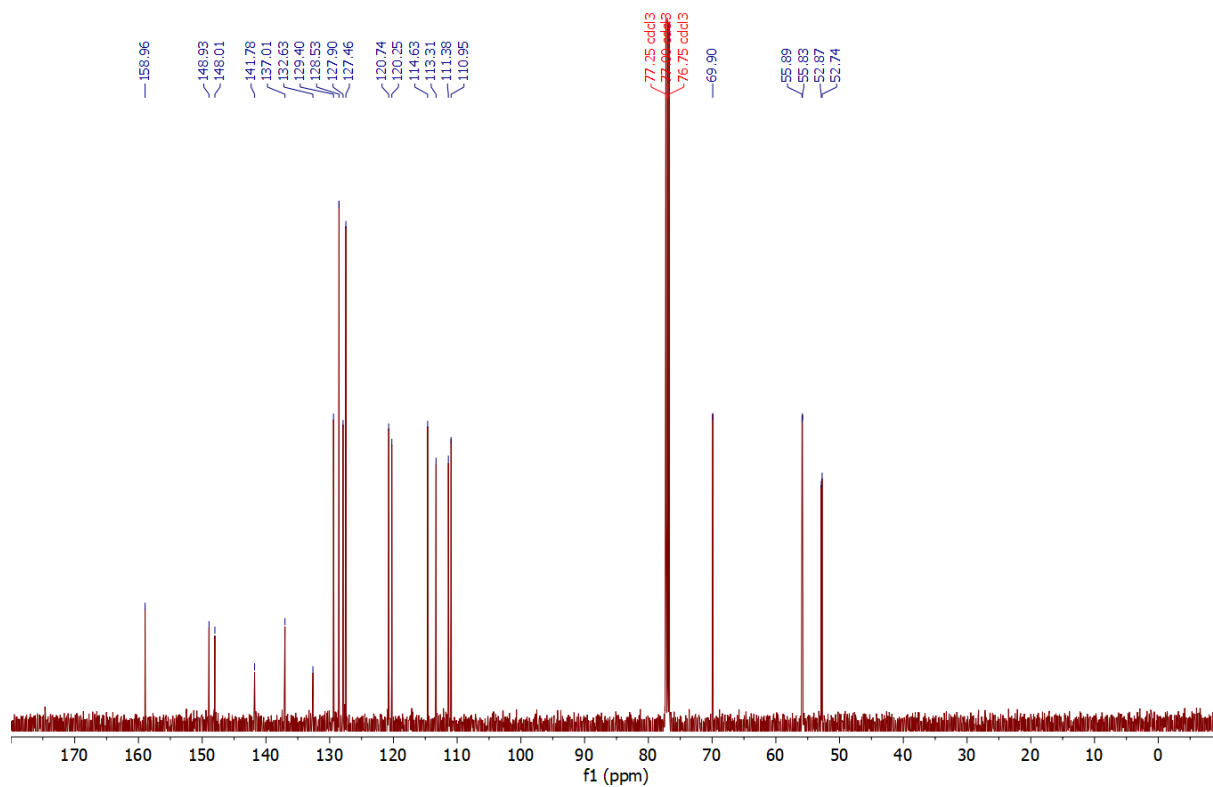
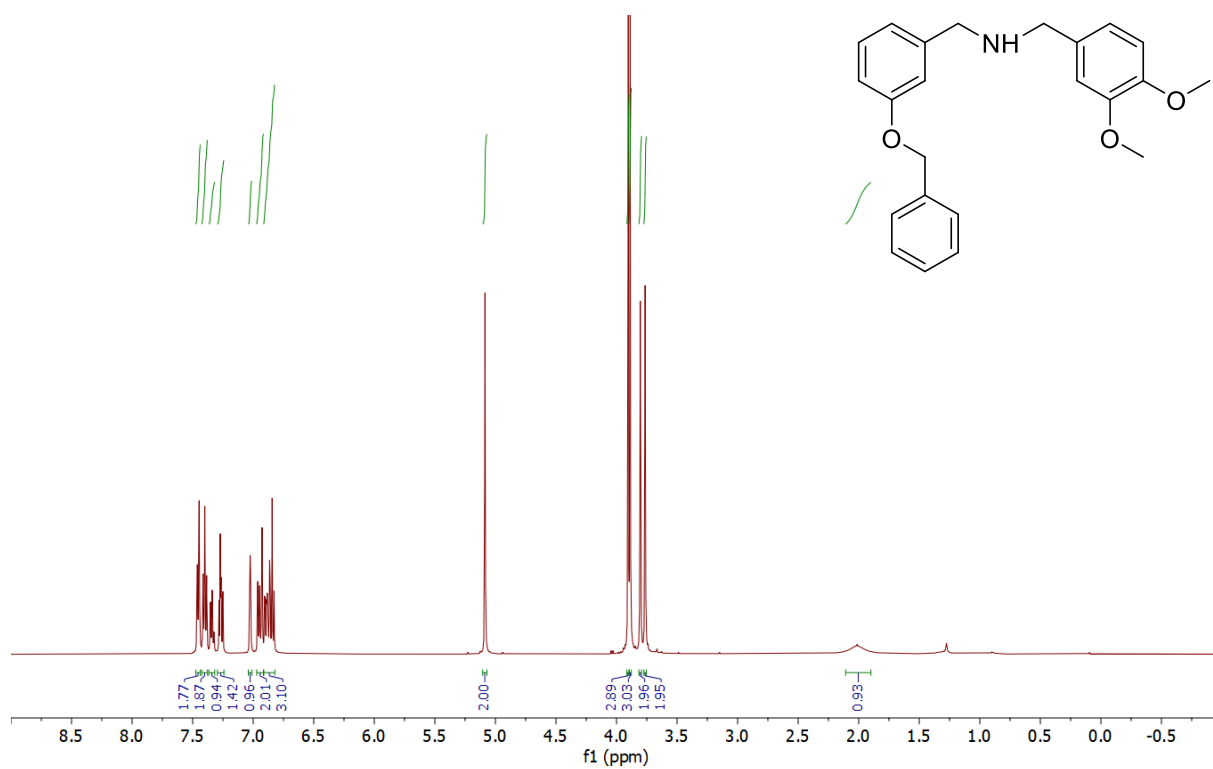
1: TOF MS ES+
1.93e6



FC019



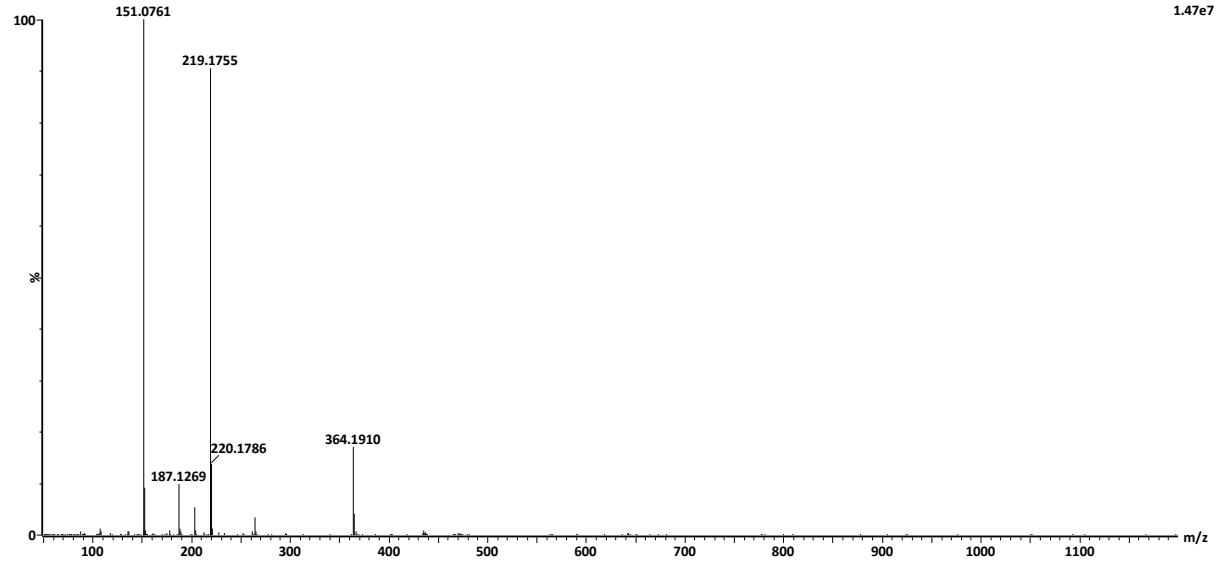
{{[3-(Benzyloxy)phenyl]methyl}[(3,4-dimethoxyphenyl)methyl]amine (15):



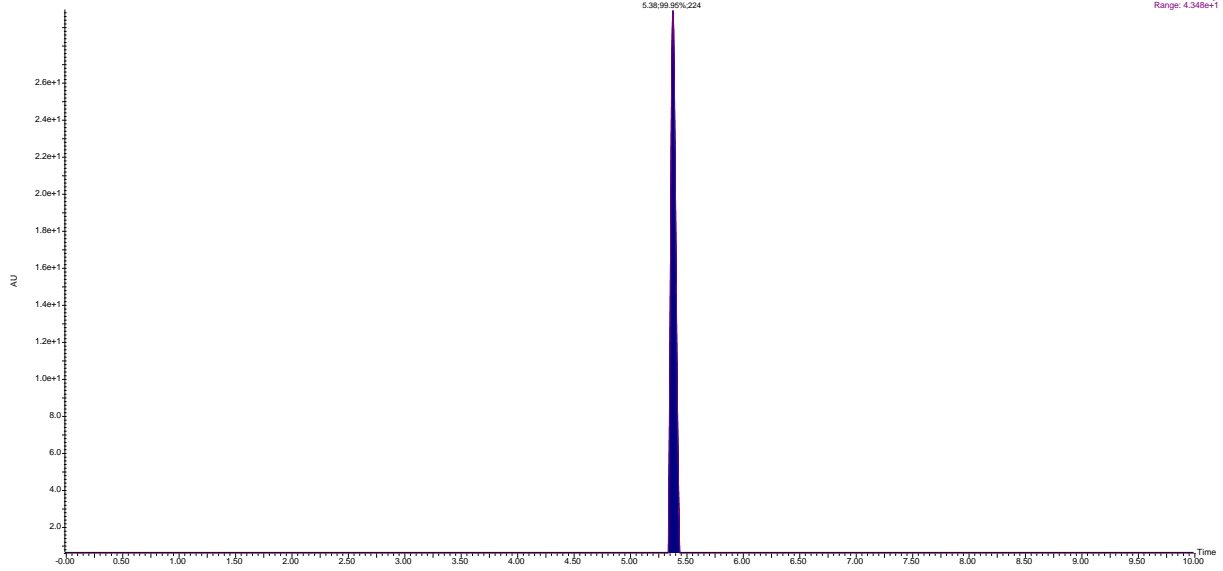
364.1907

2021 05 02 FC 021 A 1422 (2.450) Cm (1406:1452-(1182:1281+1527:1629))

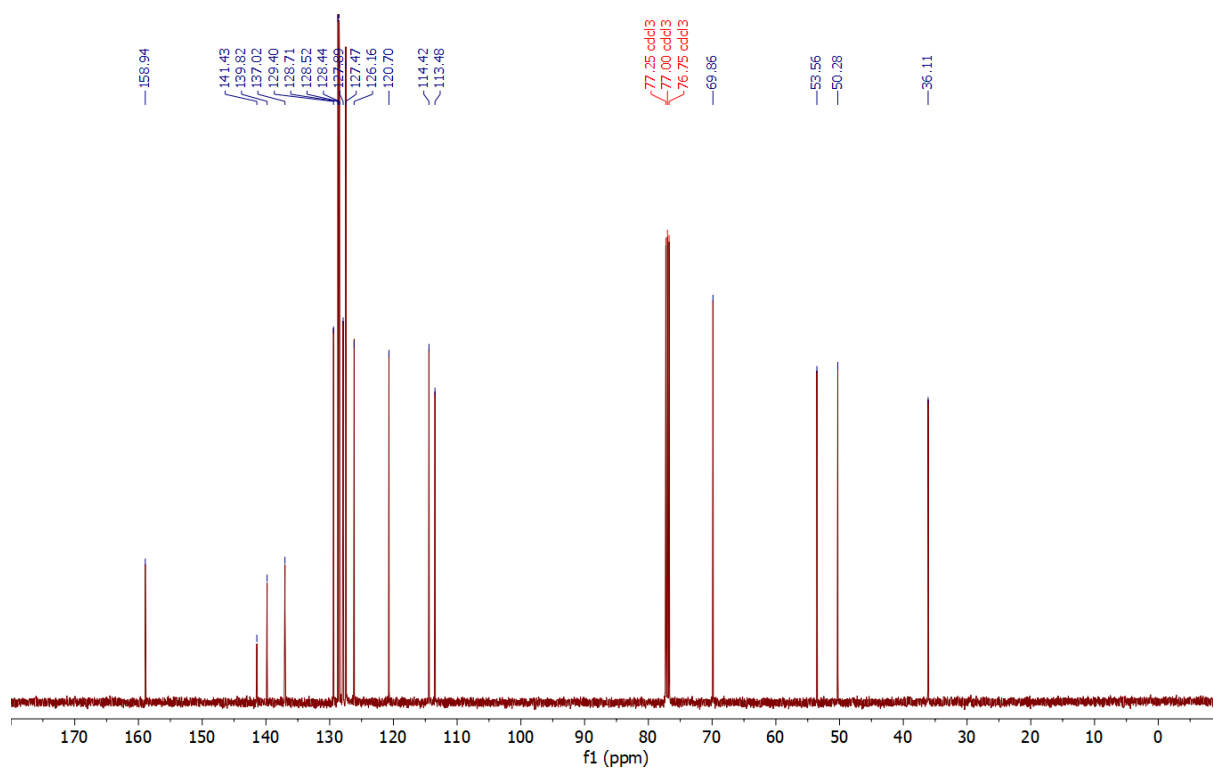
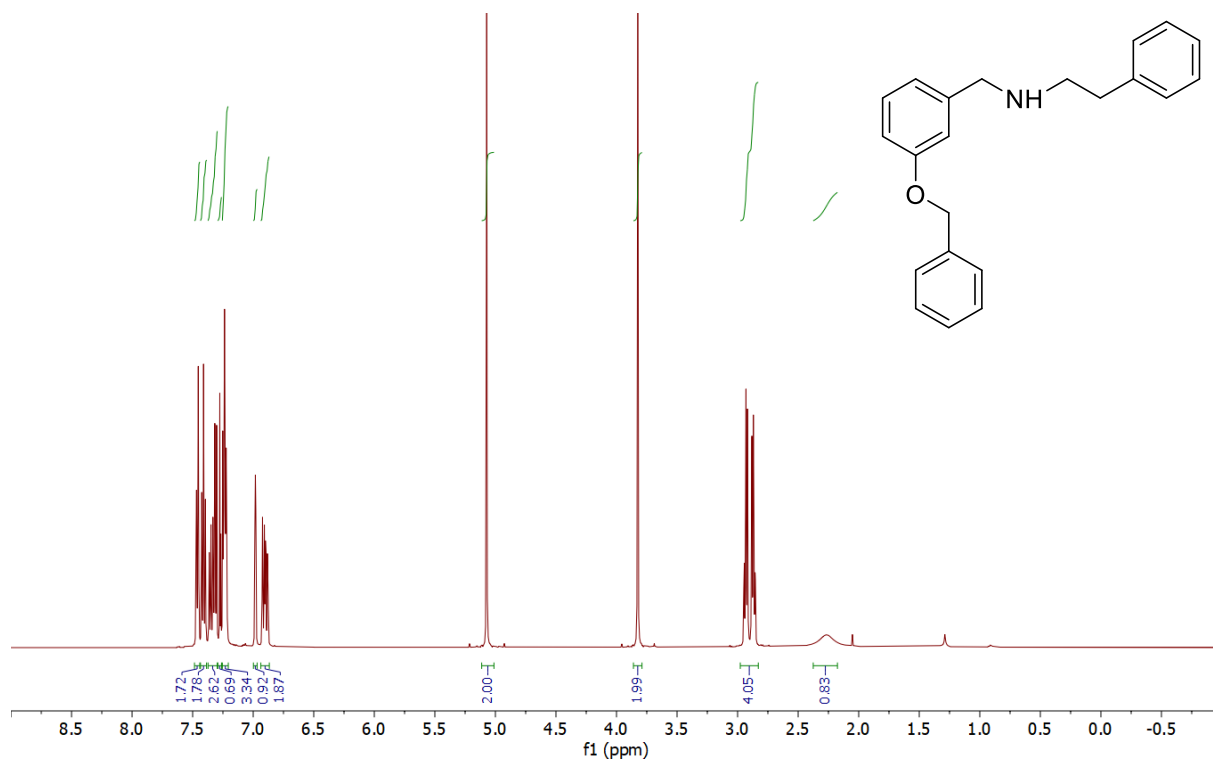
1: TOF MS ES+
1.47e7



FC021



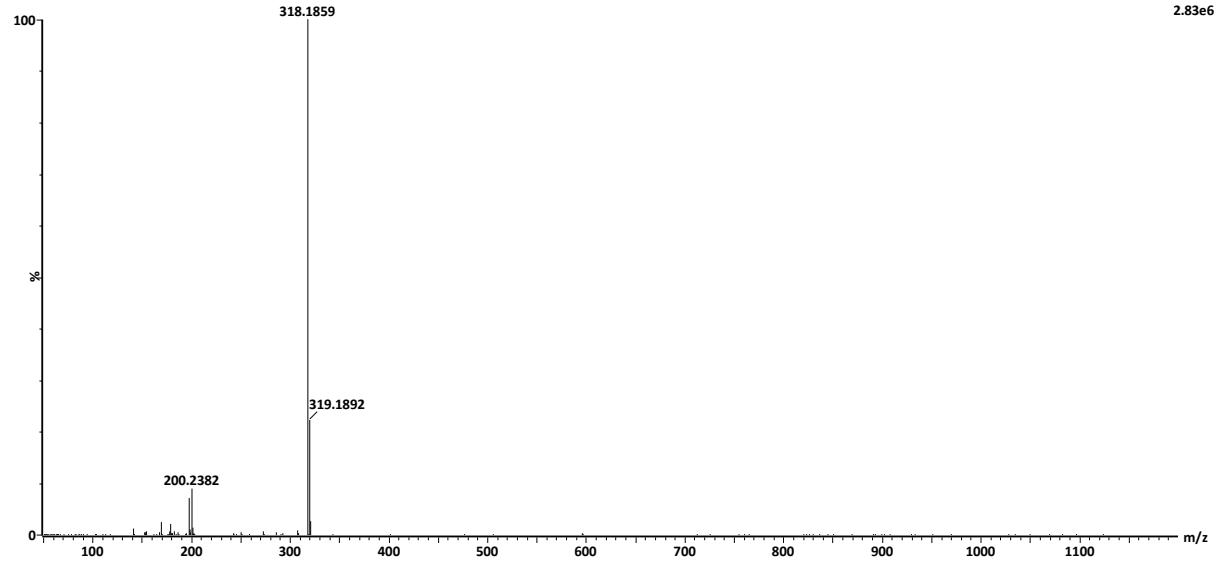
{[3-(Benzyloxy)phenyl]methyl}(2-phenylethyl)amine (16):



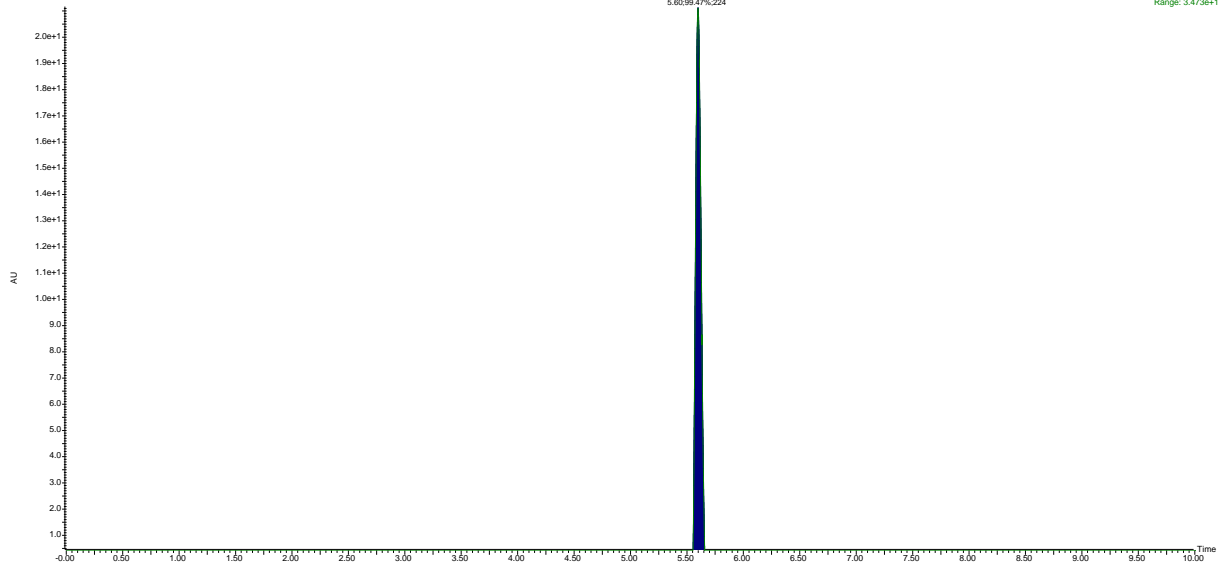
318,1852

2021 05 02 FC 015 A 1548 (2.668) Cm (1525:1567-(1383:1459+1635:1718))

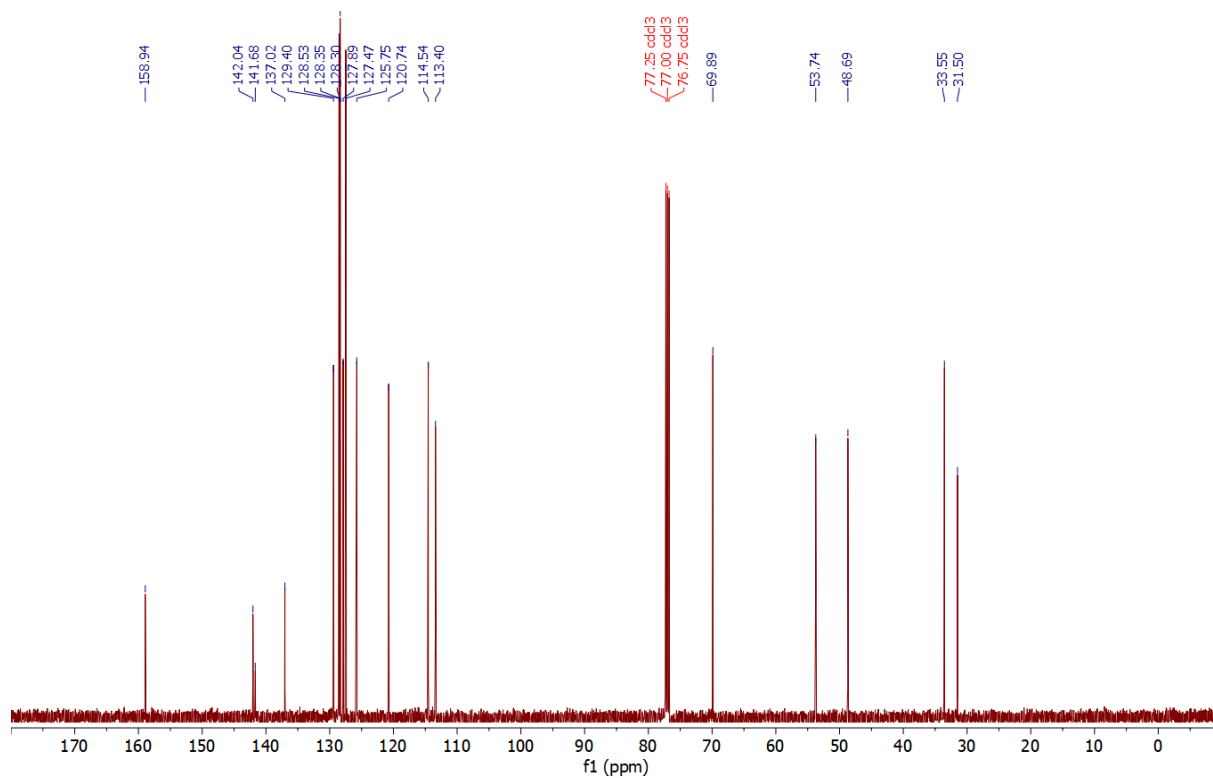
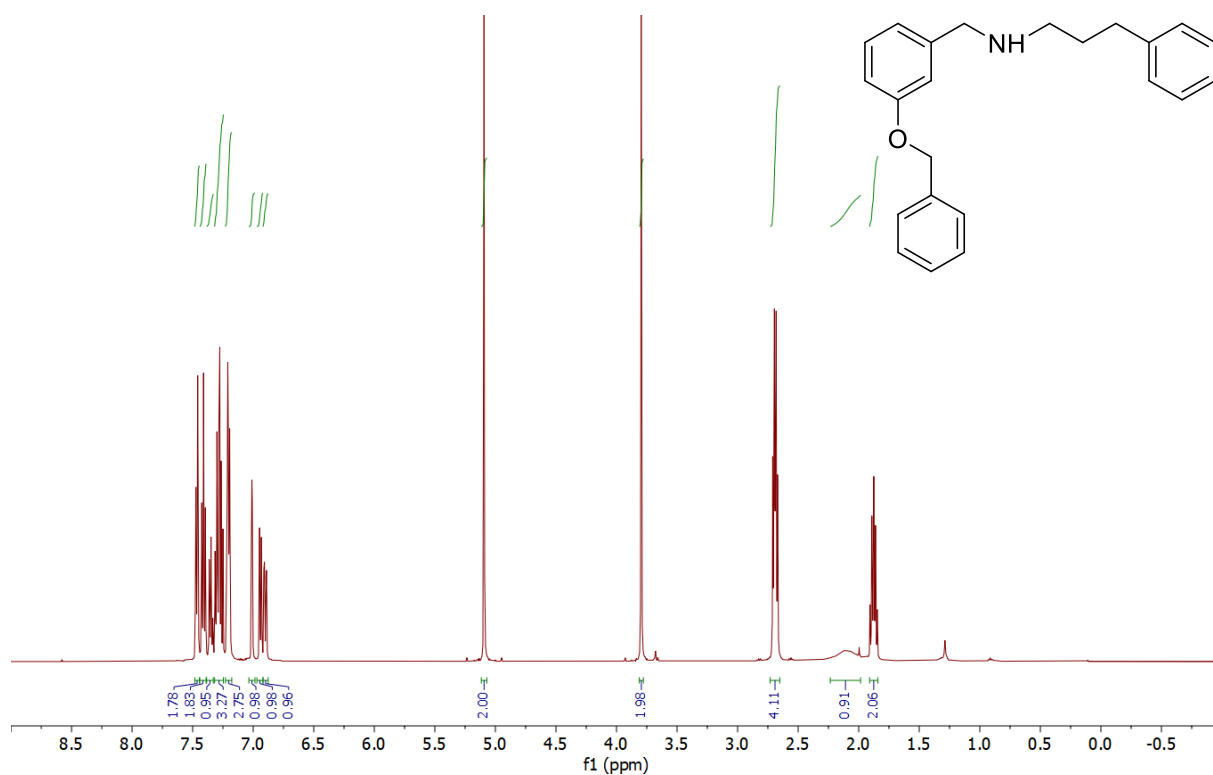
1: TOF MS ES+
2.83e6



FC015



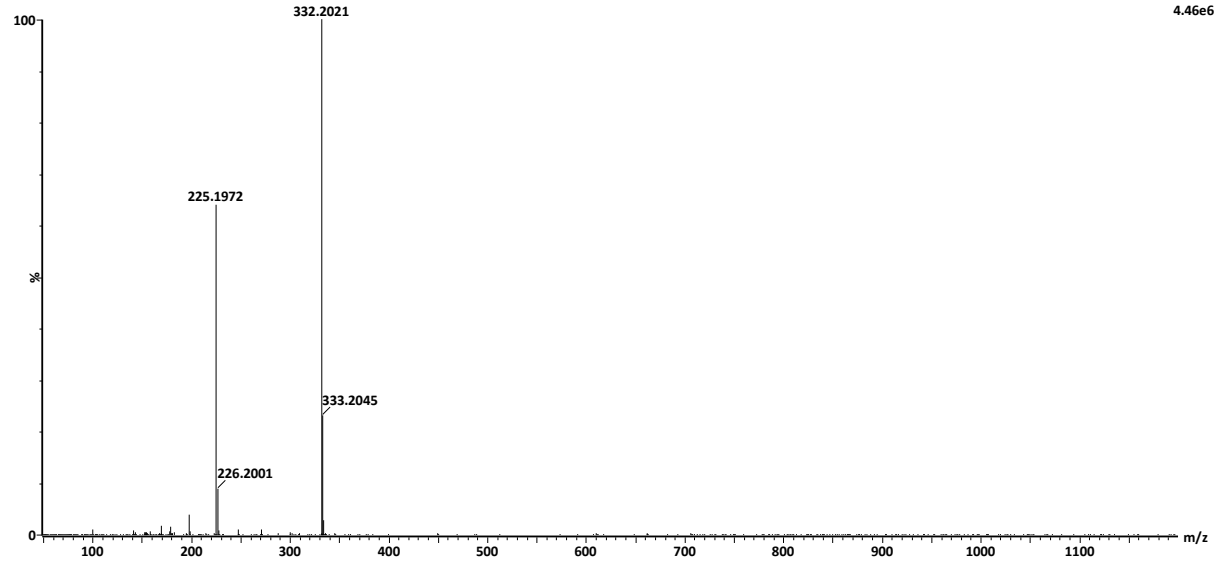
{[3-(Benzyloxy)phenyl]methyl}(3-phenylpropyl)amine (17):



332,2009

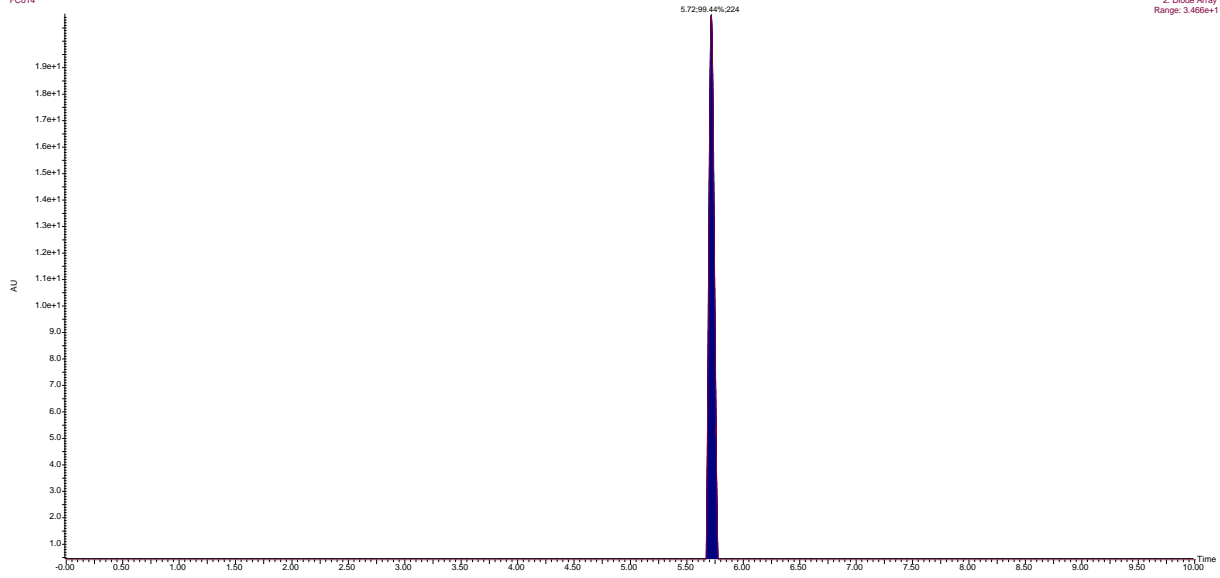
2021 05 02 FC 014 A 1619 (2.789) Cm (1603:1643-(1499:1542+1701:1770))

1: TOF MS ES+
4.46e6

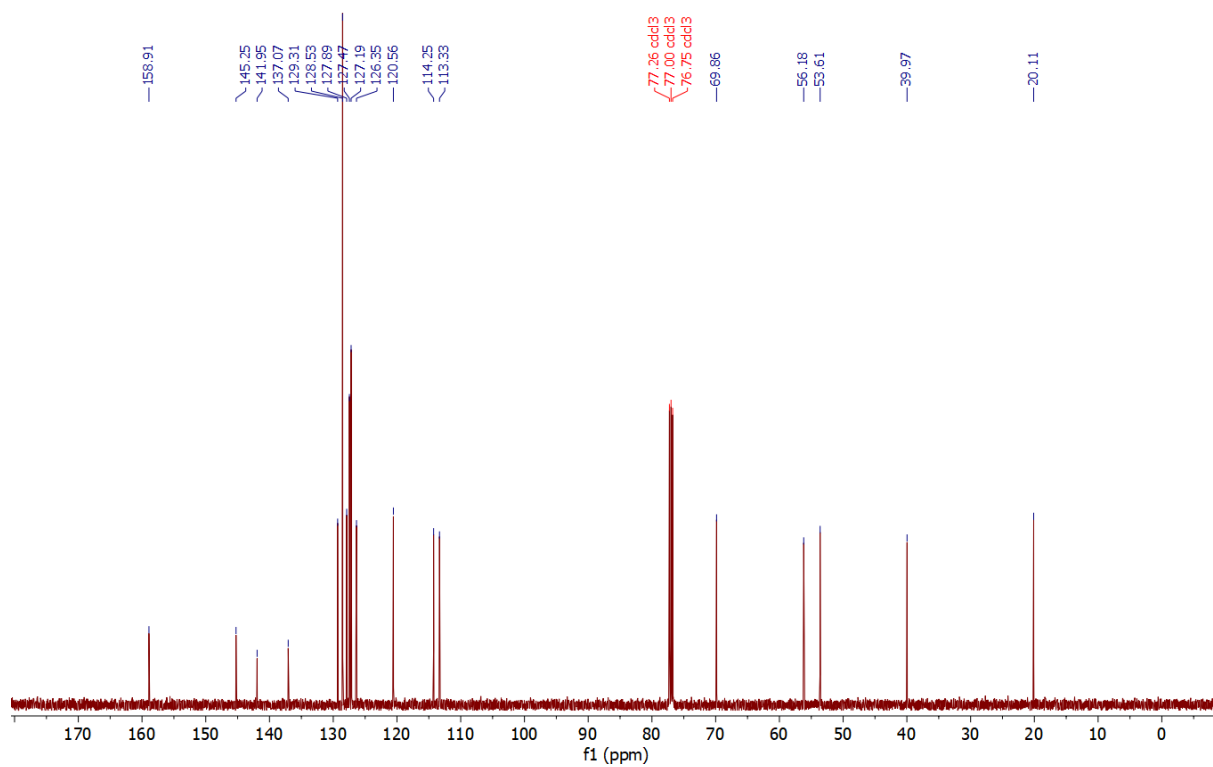
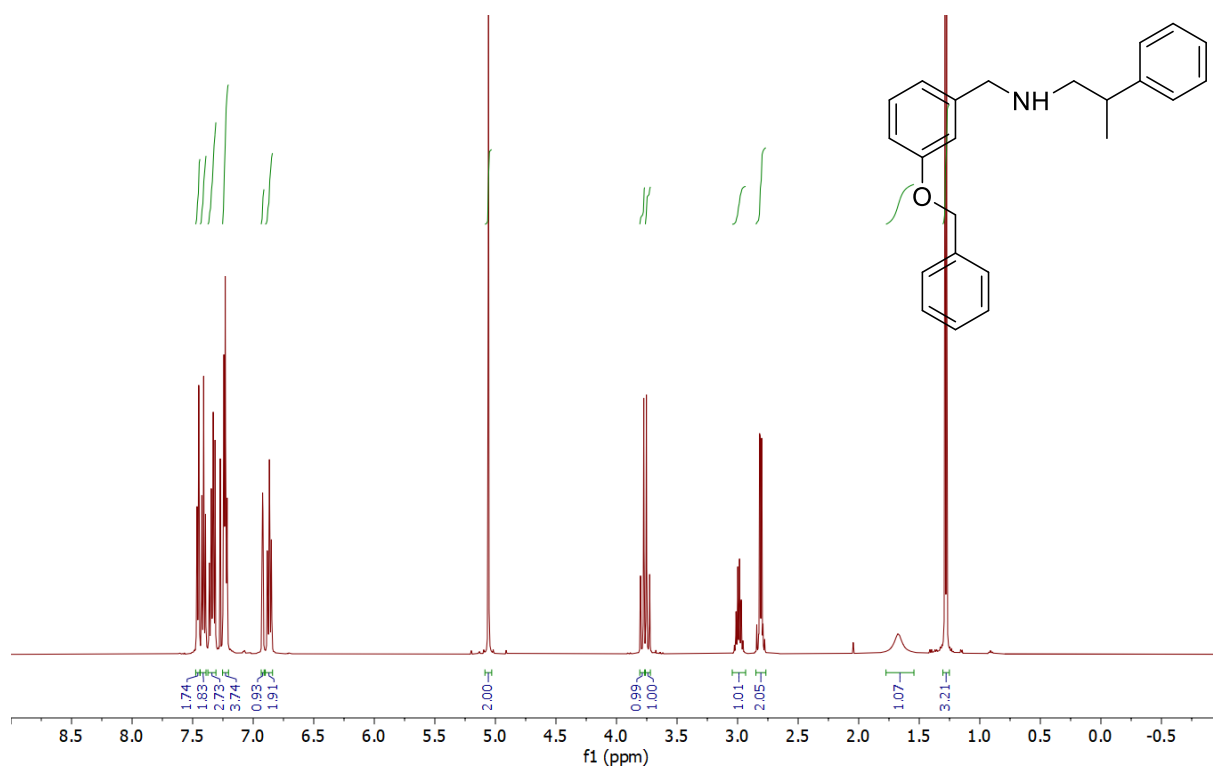


FC014

2: Diode Array
Range: 3.466e+1



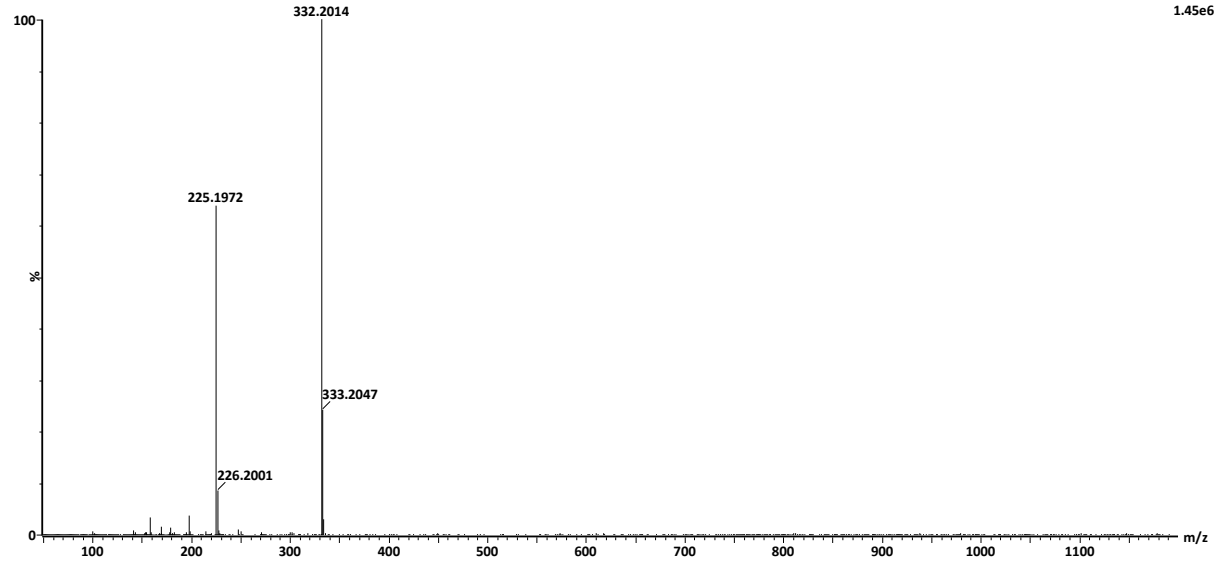
{[3-(Benzyloxy)phenyl]methyl}(2-phenylpropyl)amine (18):



332.2009

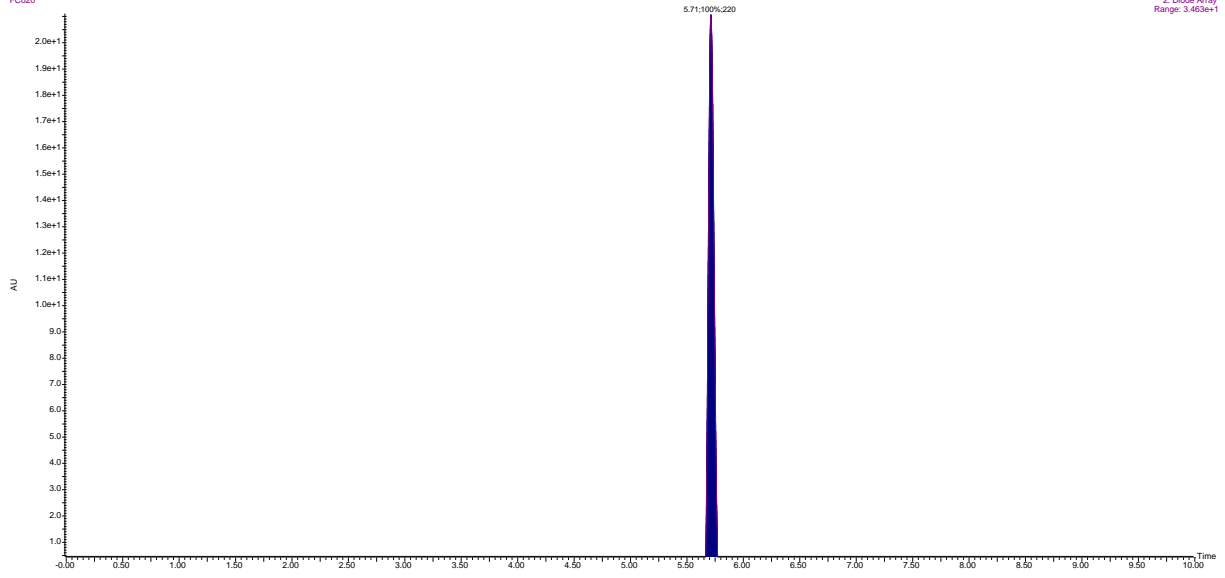
2021 05 02 FC 020 B 1618 (2.787) Cm (1583:1618-(1505:1540+1664:1710))

1: TOF MS ES+
1.45e6

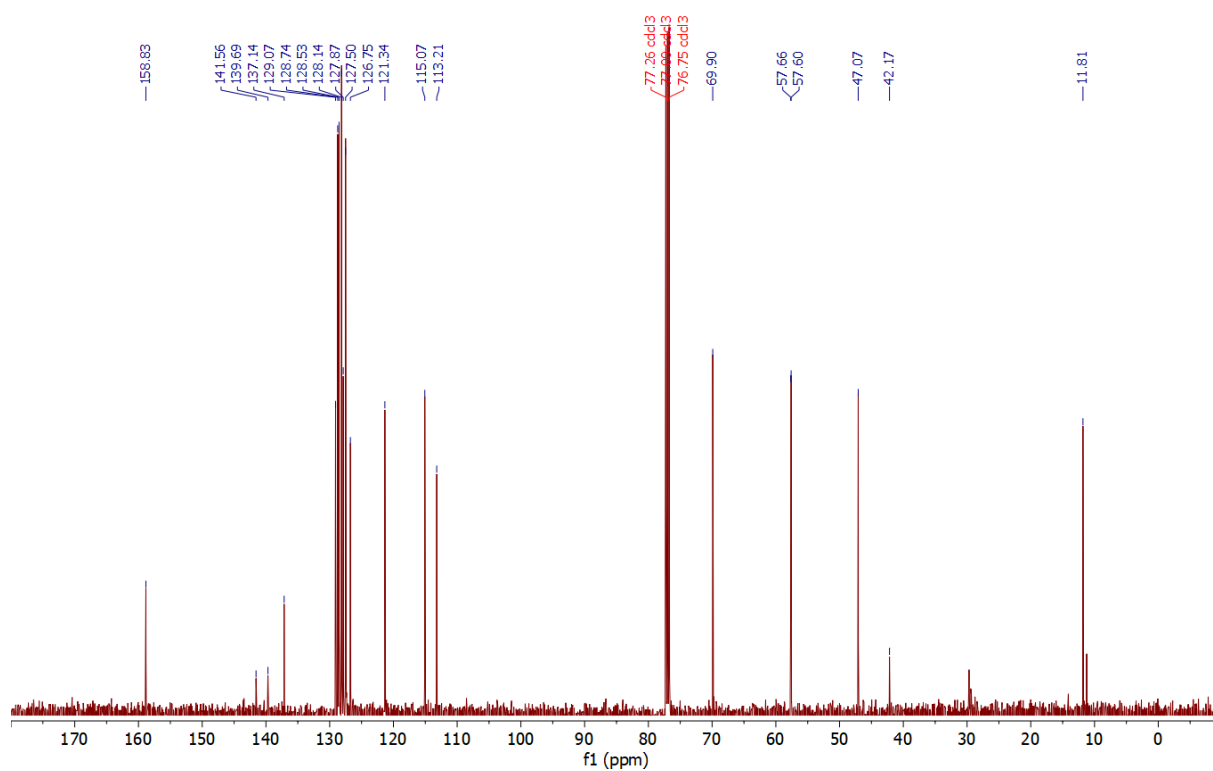
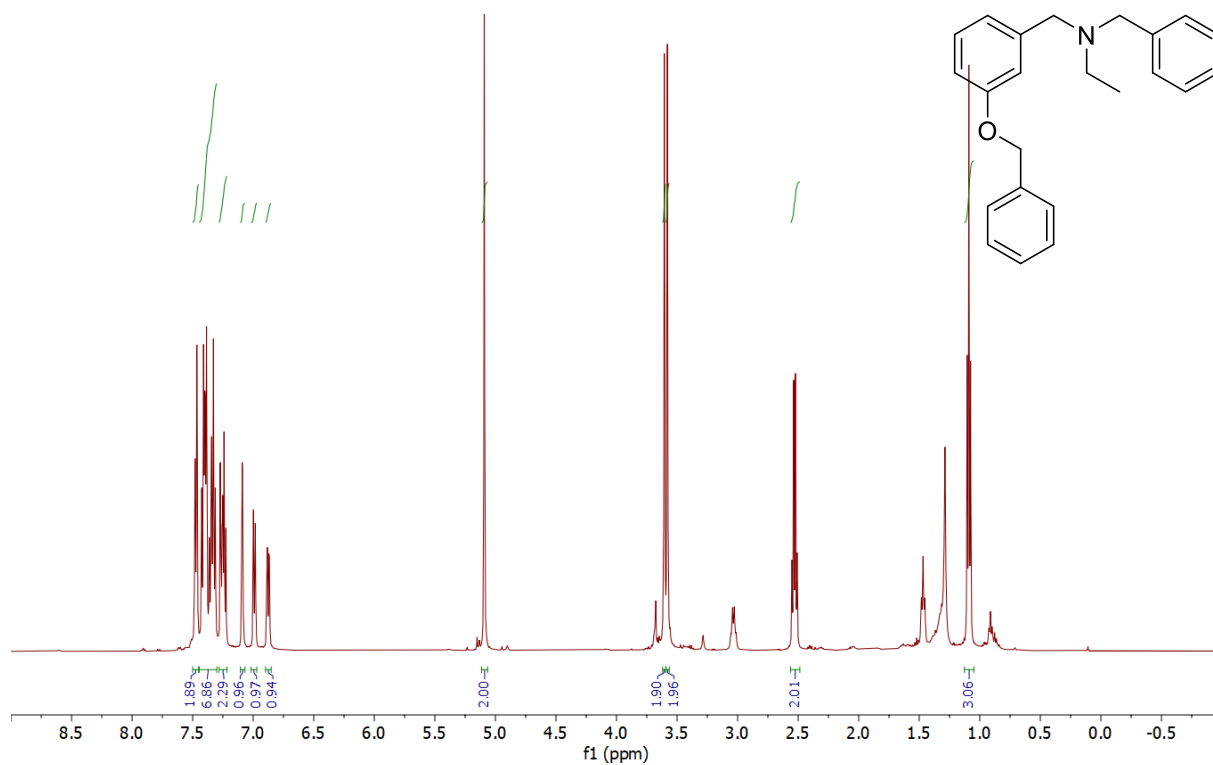


FC020

2: Diode Array
Range: 3.463e+1



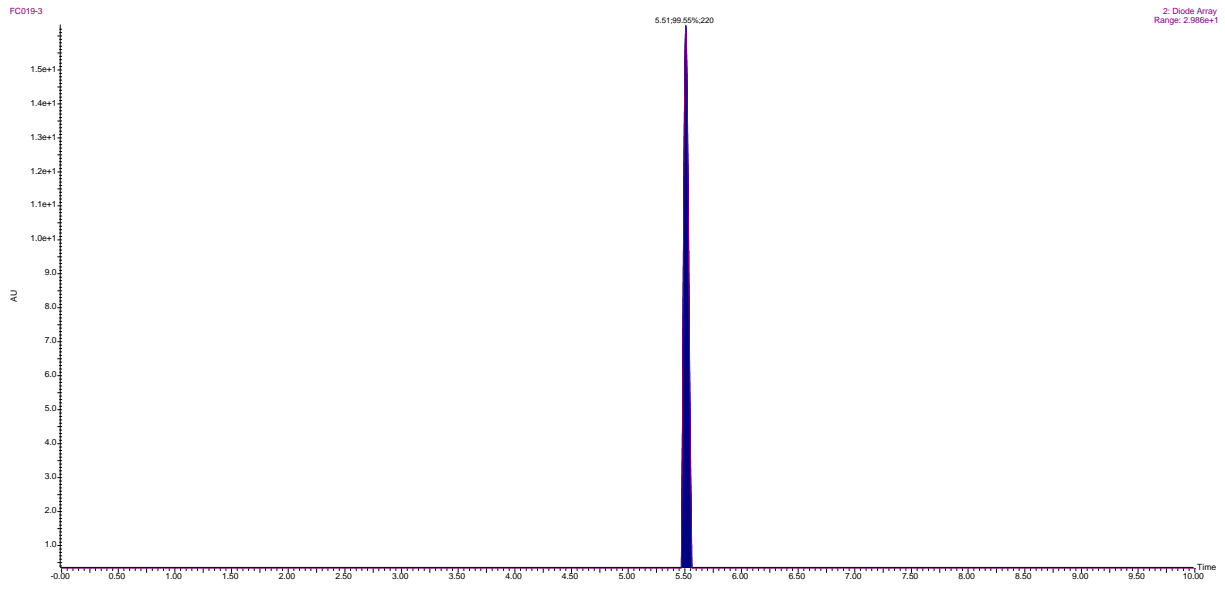
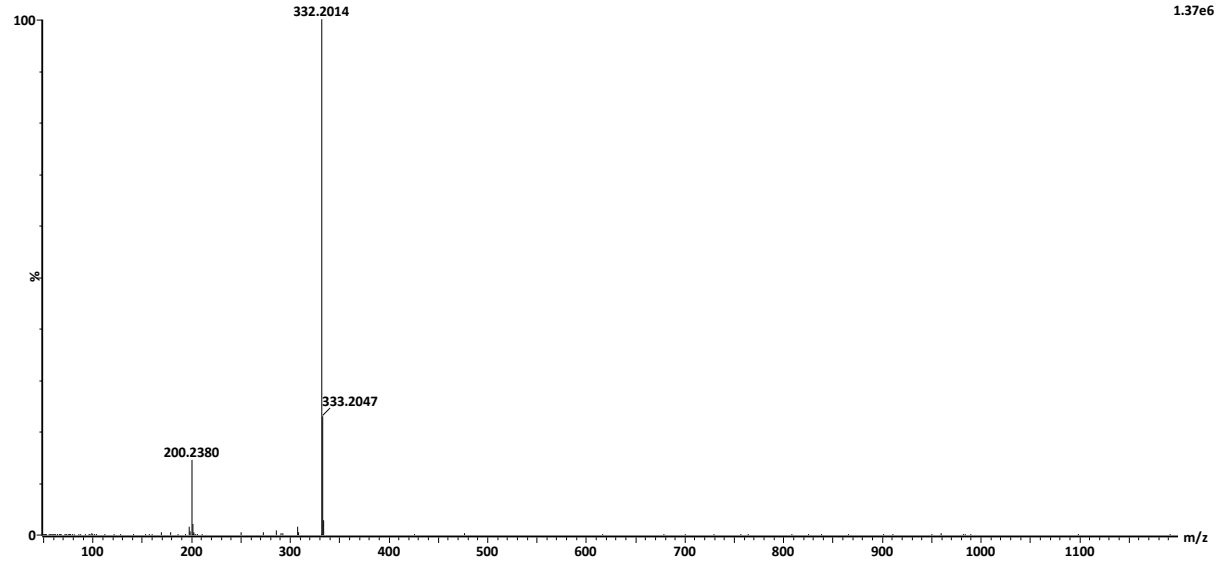
Benzyl([3-(benzyloxy)phenyl]methyl)ethylamine (19):



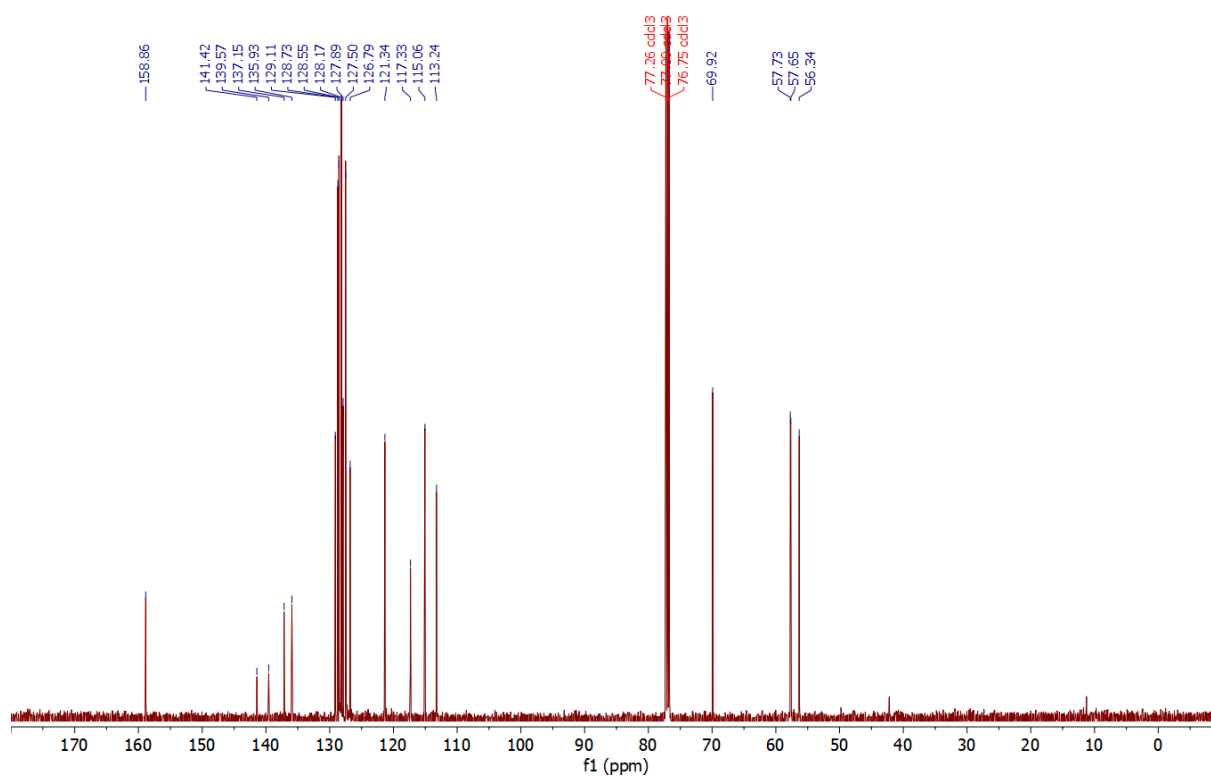
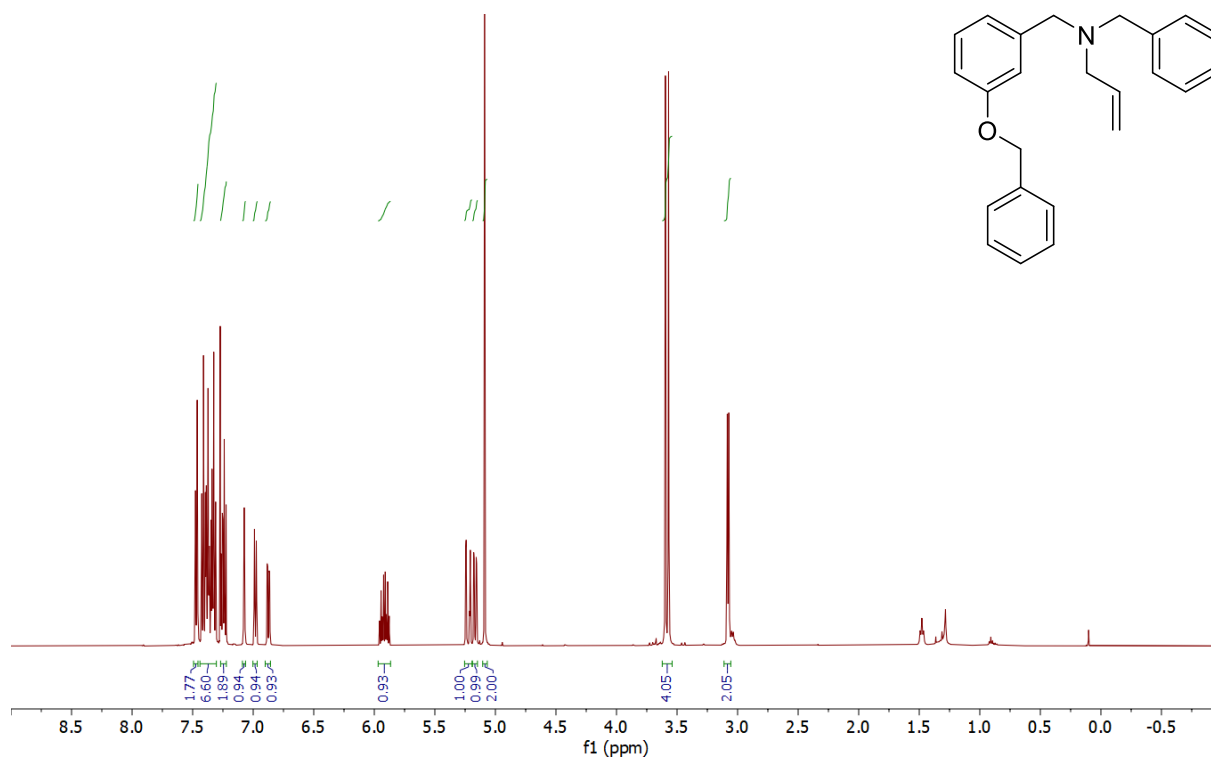
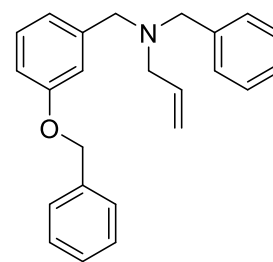
332.2009

2021 05 02 FC 019-3 B 1541 (2.656) Cm (1529:1569-(1369:1445+1639:1744))

1: TOF MS ES+
1.37e6



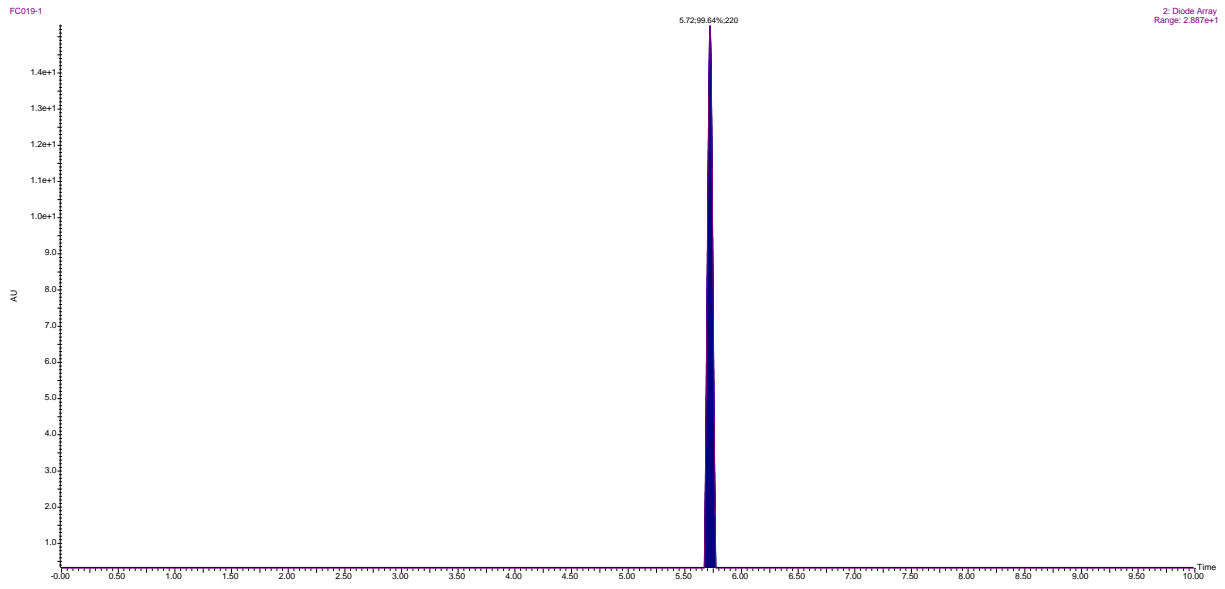
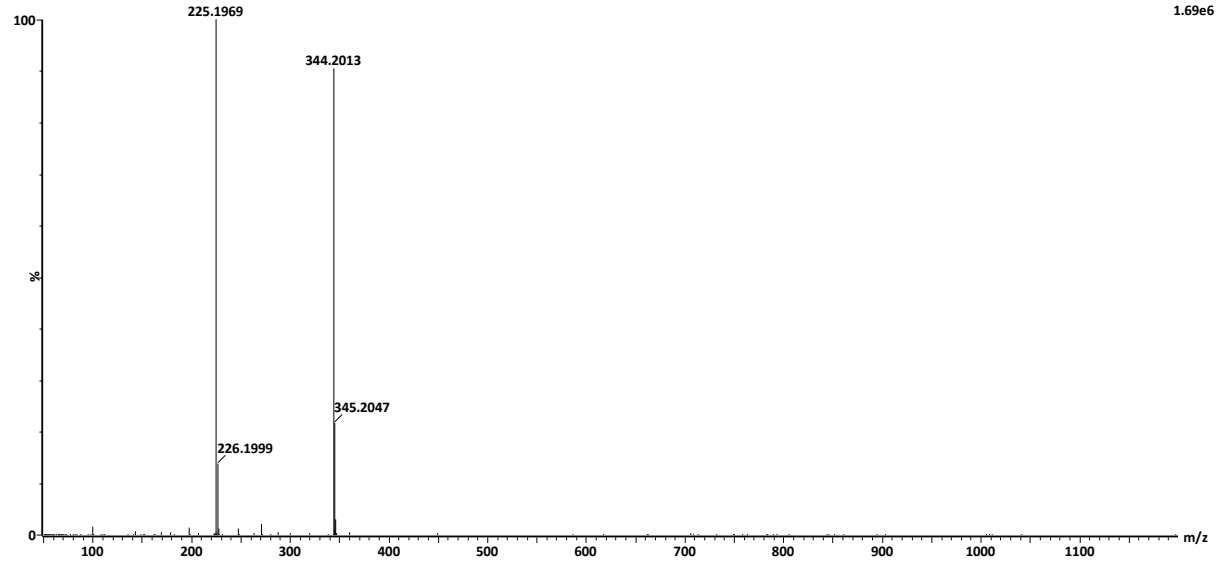
Benzyl({[3-(benzyloxy)phenyl]methyl})(prop-2-en-1-yl)amine (20):



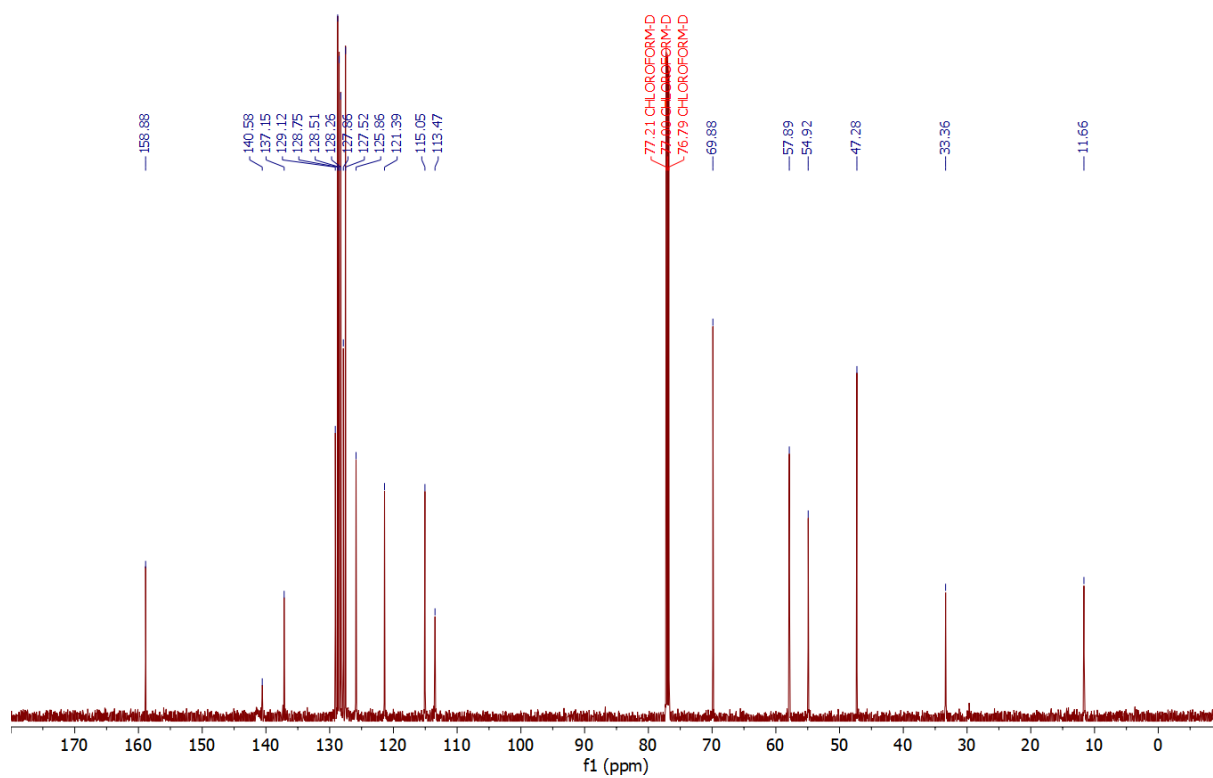
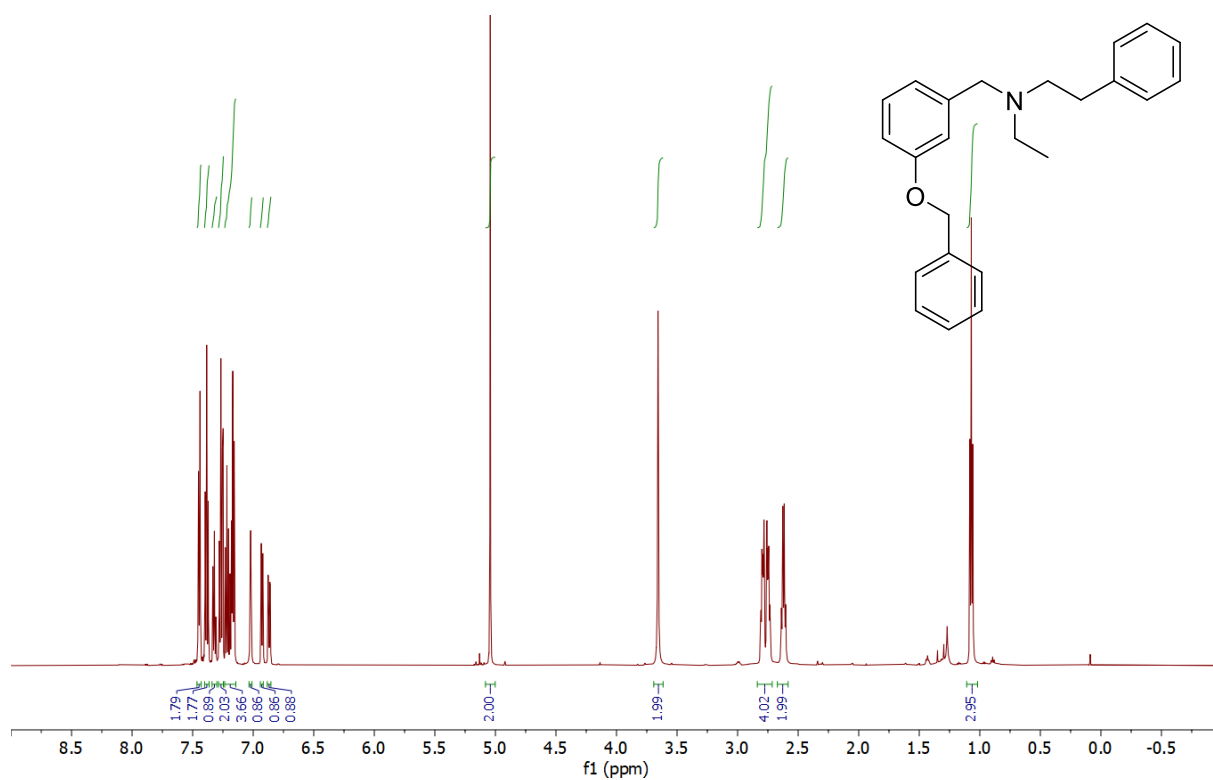
344,2009

2021 05 02 FC 019-1 B 1638 (2.821) Cm (1618:1659-(1470:1555+1732:1828))

1: TOF MS ES+
1.69e6



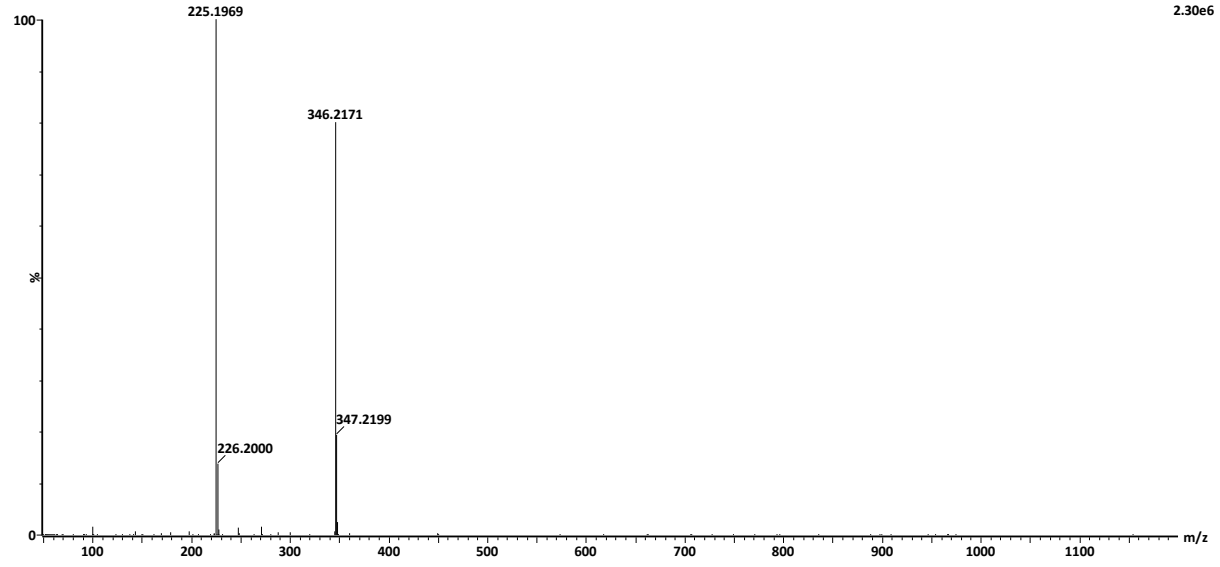
{[3-(Benzyloxy)phenyl]methyl}(ethyl)(2-phenylethyl)amine (21):



346.2165

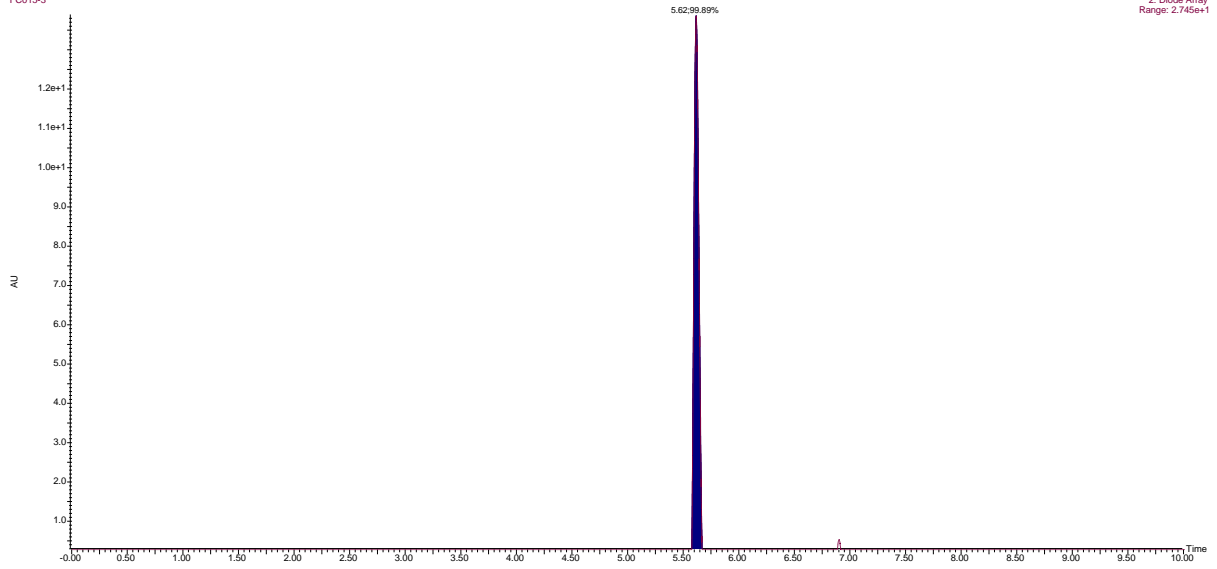
2021 05 02 FC 015-3 A 1627 (2.803) Cm (1610:1658-(1423:1508+1763:1897))

1: TOF MS ES+
2.30e6

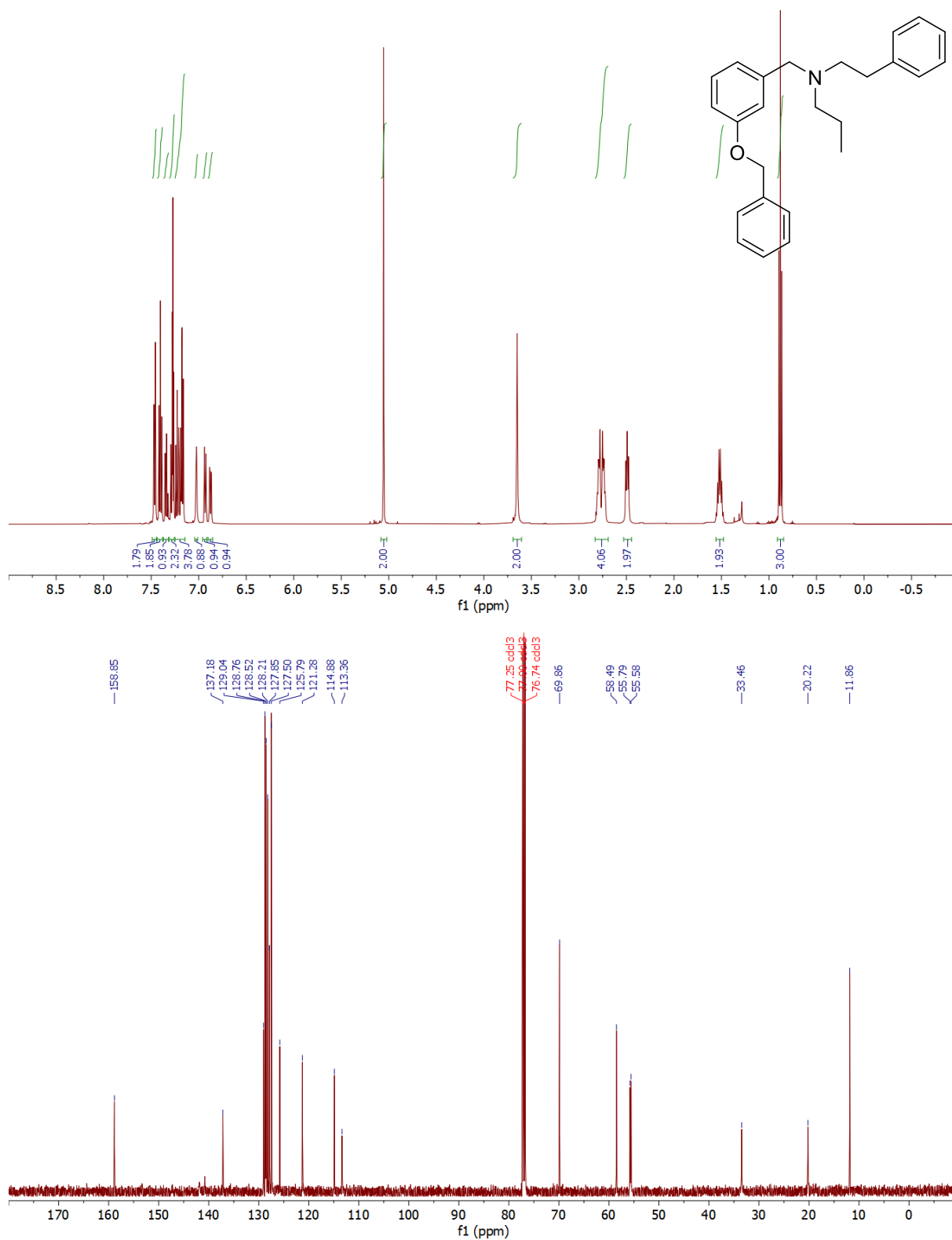


FC015-3

2: Diode Array
Range: 2.745e+1



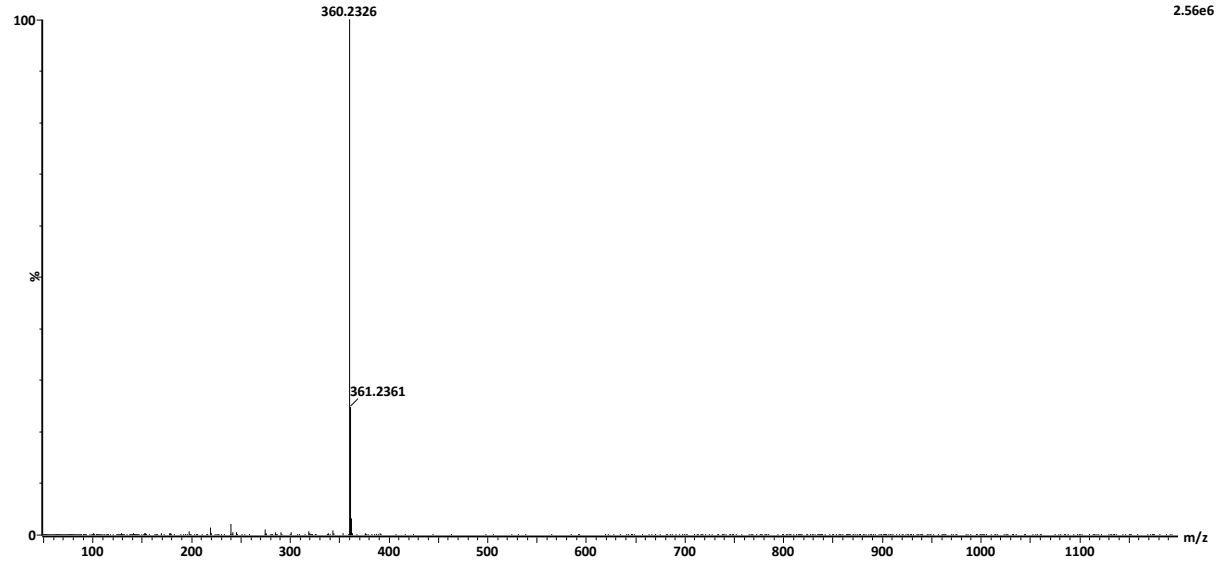
{[3-(Benzyloxy)phenyl]methyl}(2-phenylethyl)propylamine (22):



360.2322

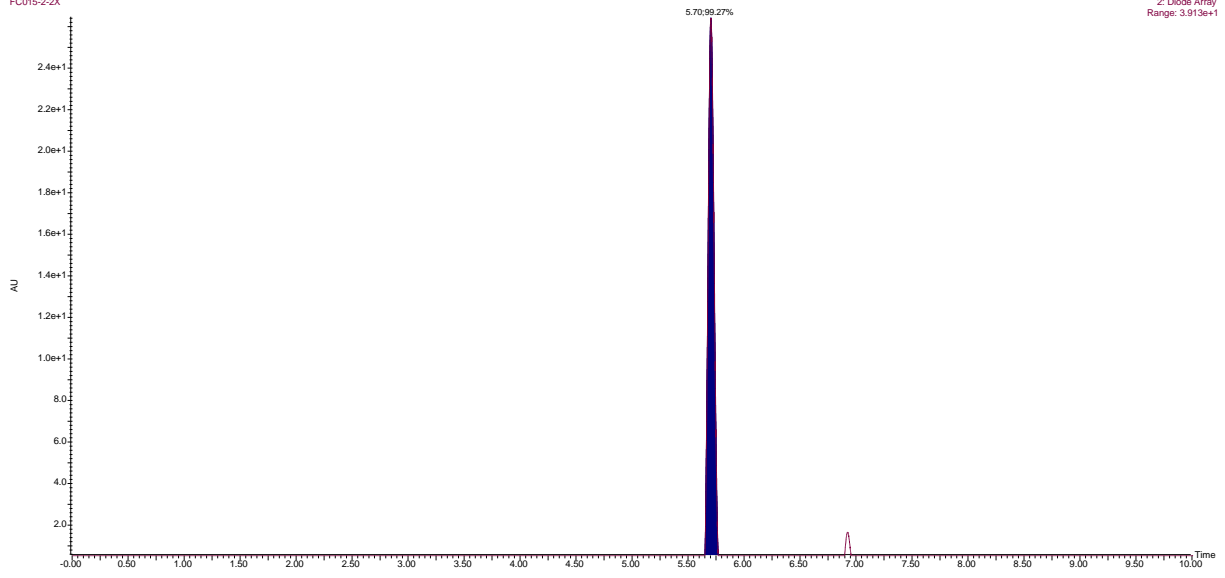
2021 05 02 FC 015-2 A 1716 (2.954) Cm (1699:1737-(1617:1660+1783:1840))

1: TOF MS ES+
2.56e6

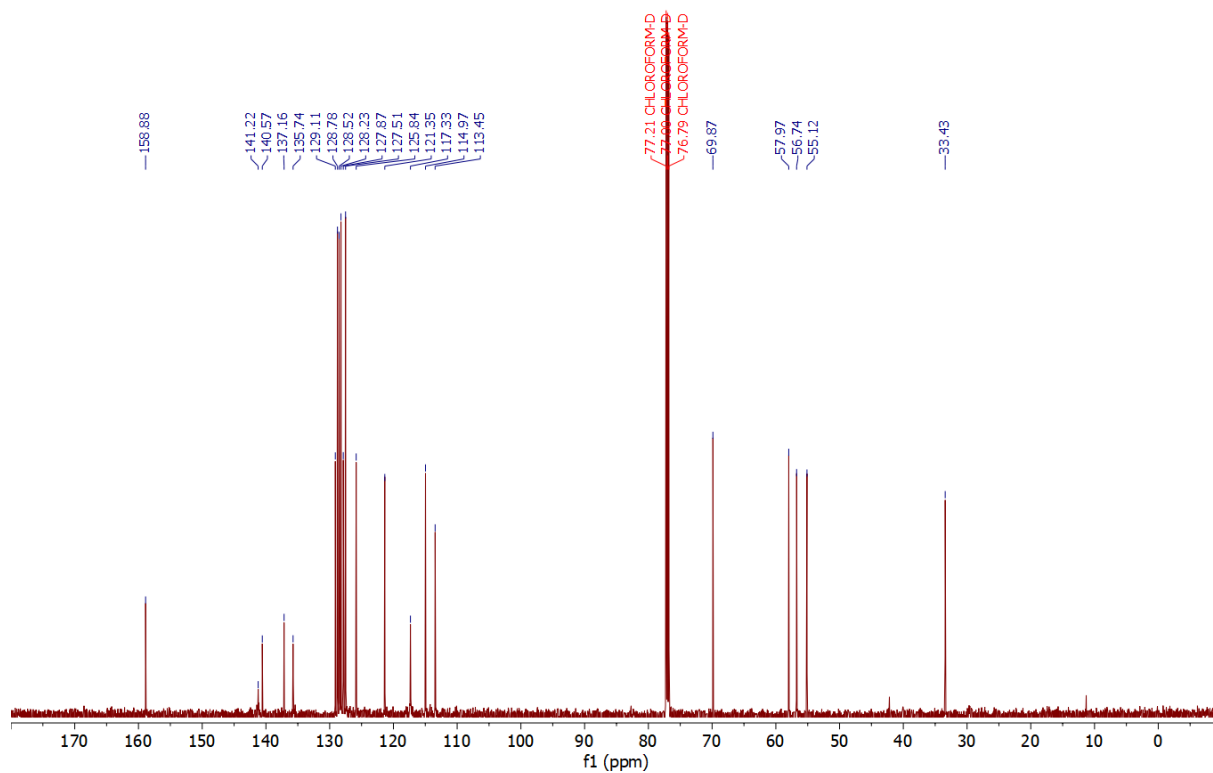
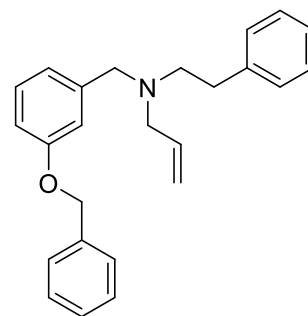
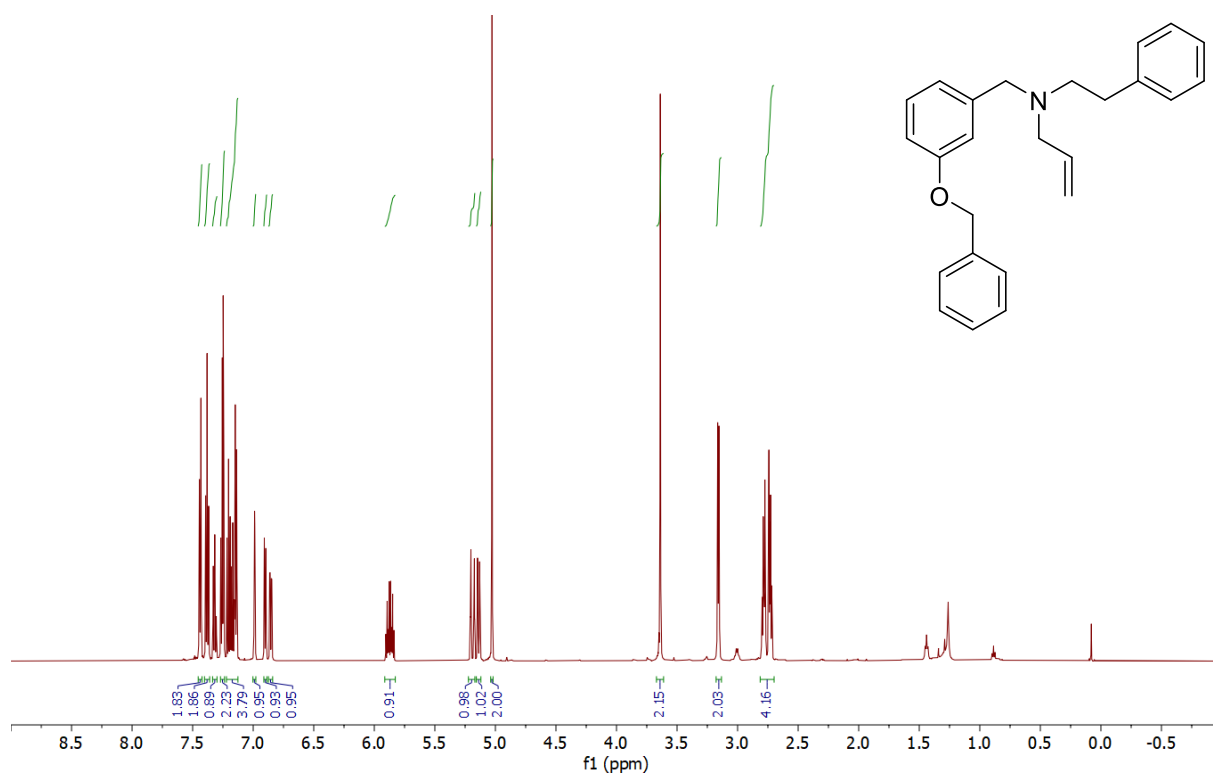


FC015-2-2X

2: Diode Array
Range: 3.913e+1



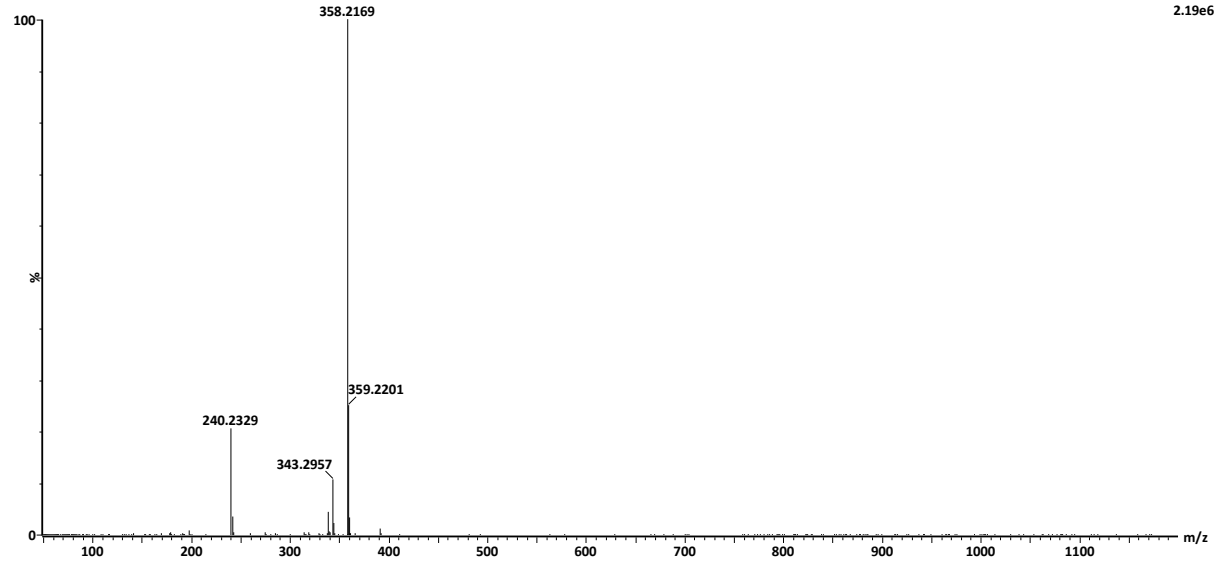
{[3-(Benzyloxy)phenyl]methyl}(2-phenylethyl)(prop-2-en-1-yl)amine (23):



358,2165

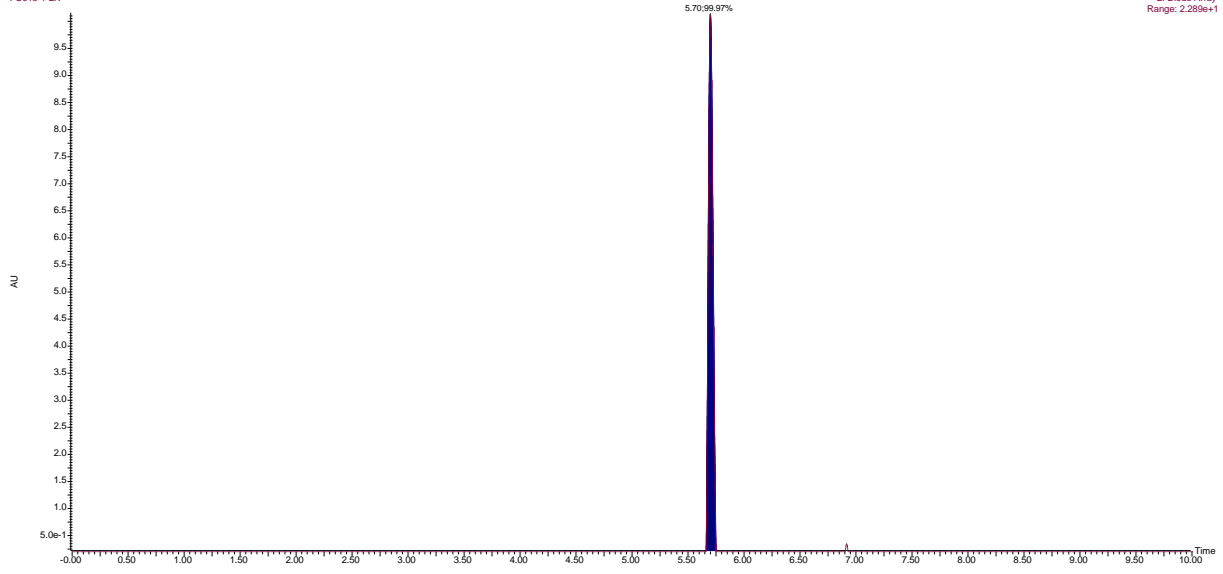
2021 05 02 FC 015-1 B 1689 (2.910) Cm (1673:1712-(1572:1618+1780:1862))

1: TOF MS ES+
2.19e6

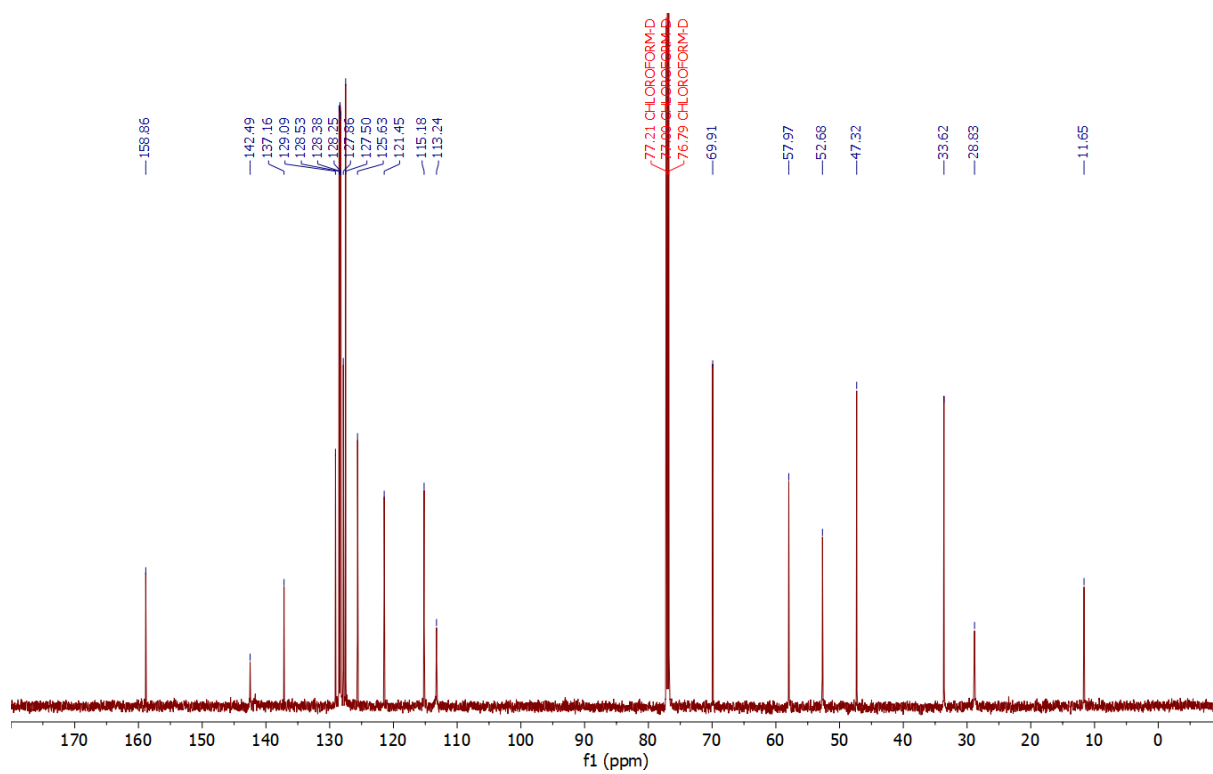
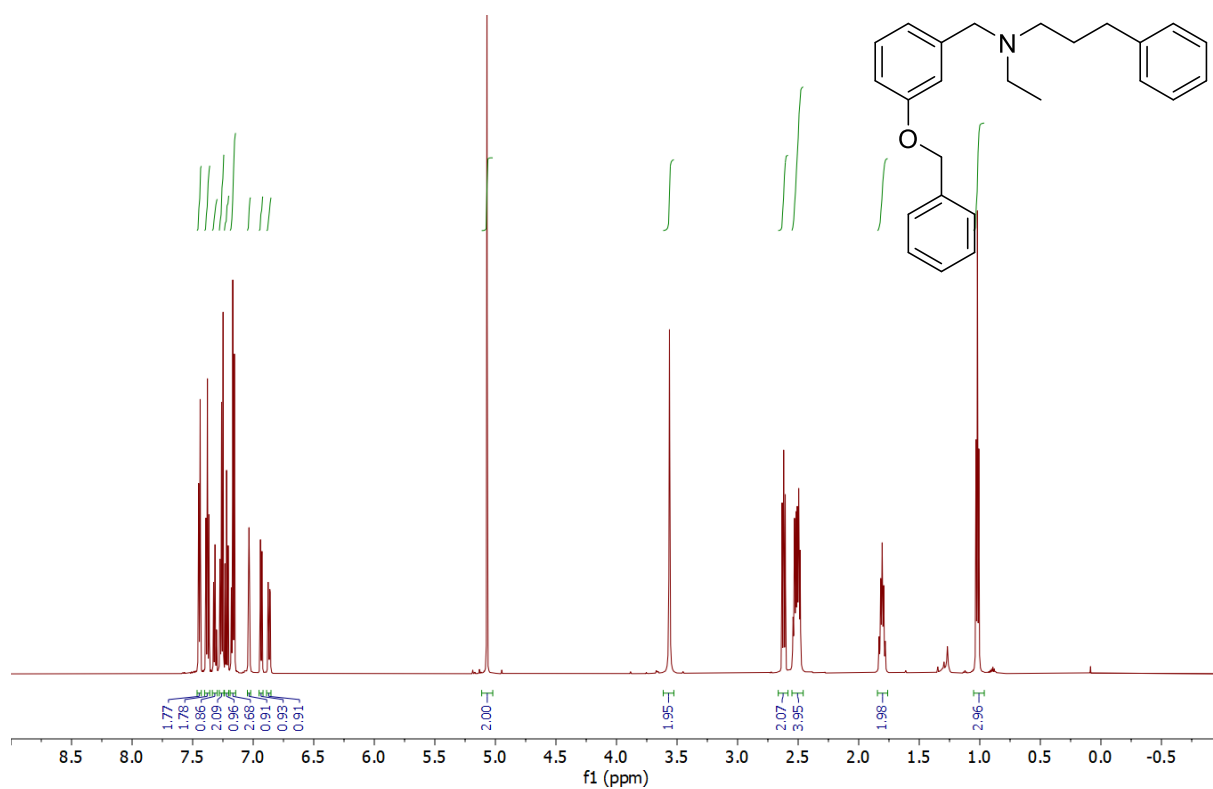


FC015-1-2X

2: Diode Array
Range: 2.289e+1



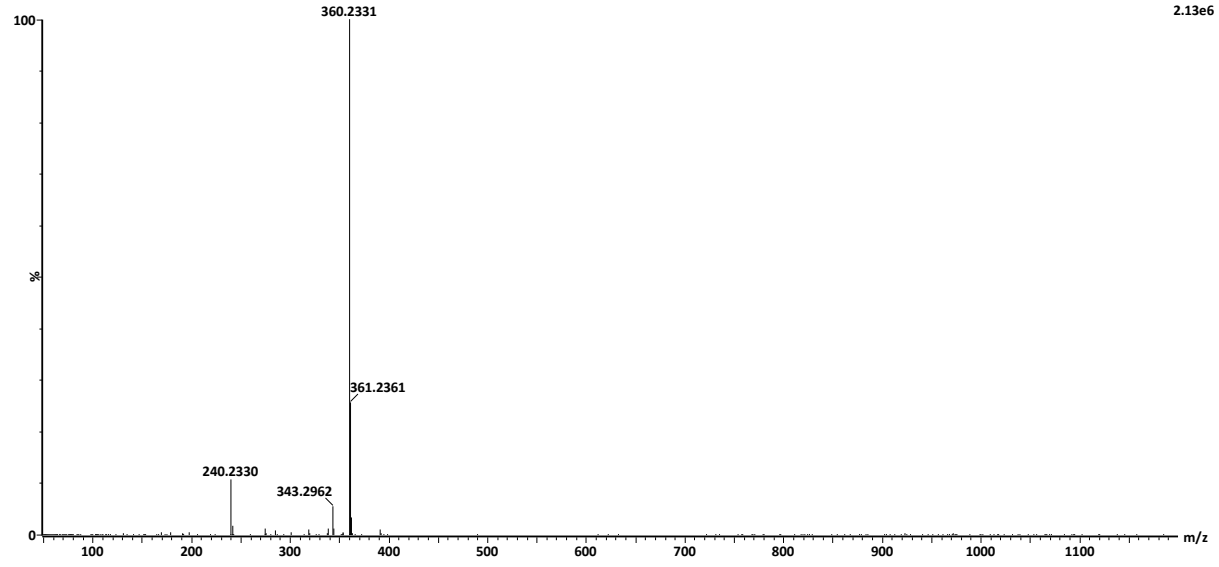
{[3-(Benzyloxy)phenyl]methyl}(ethyl)(3-phenylpropyl)amine (24):



360,2322

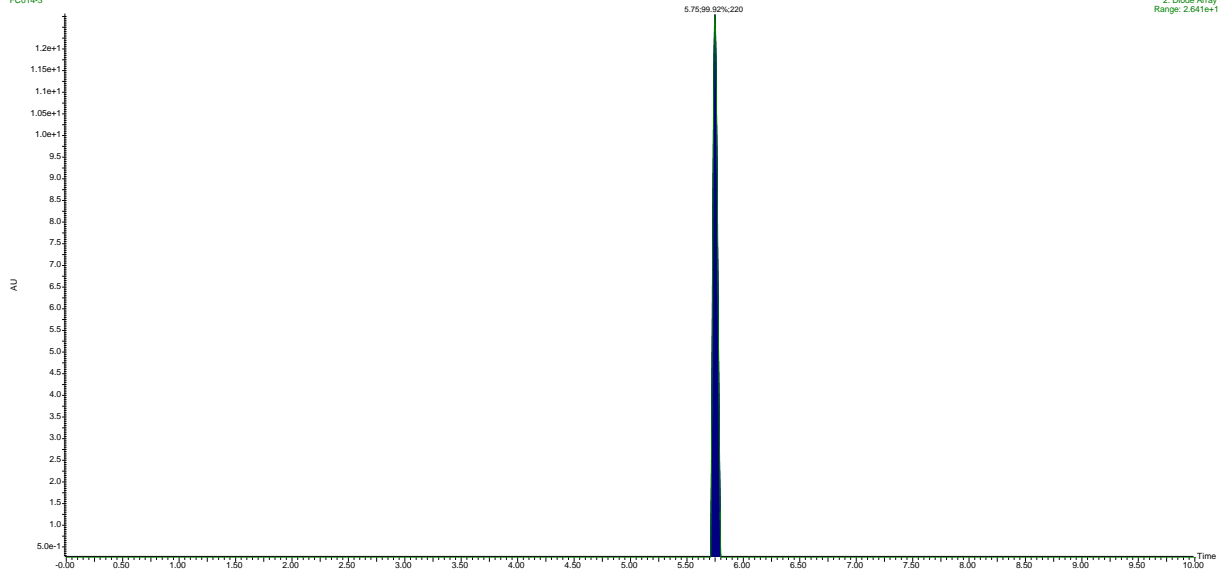
2021 05 02 FC 014-3 A 1702 (2.931) Cm (1689:1730-(1559:1620+1776:1850))

1: TOF MS ES+
2.13e6

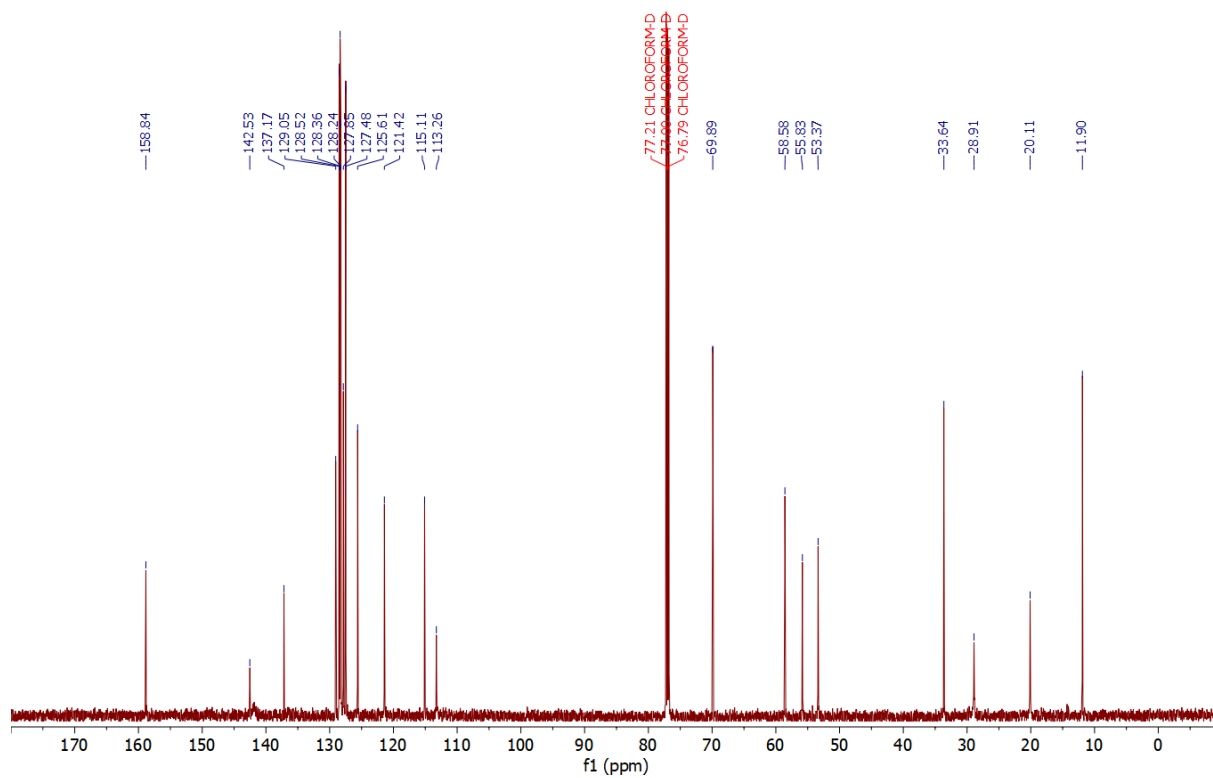
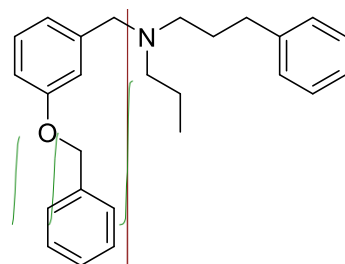
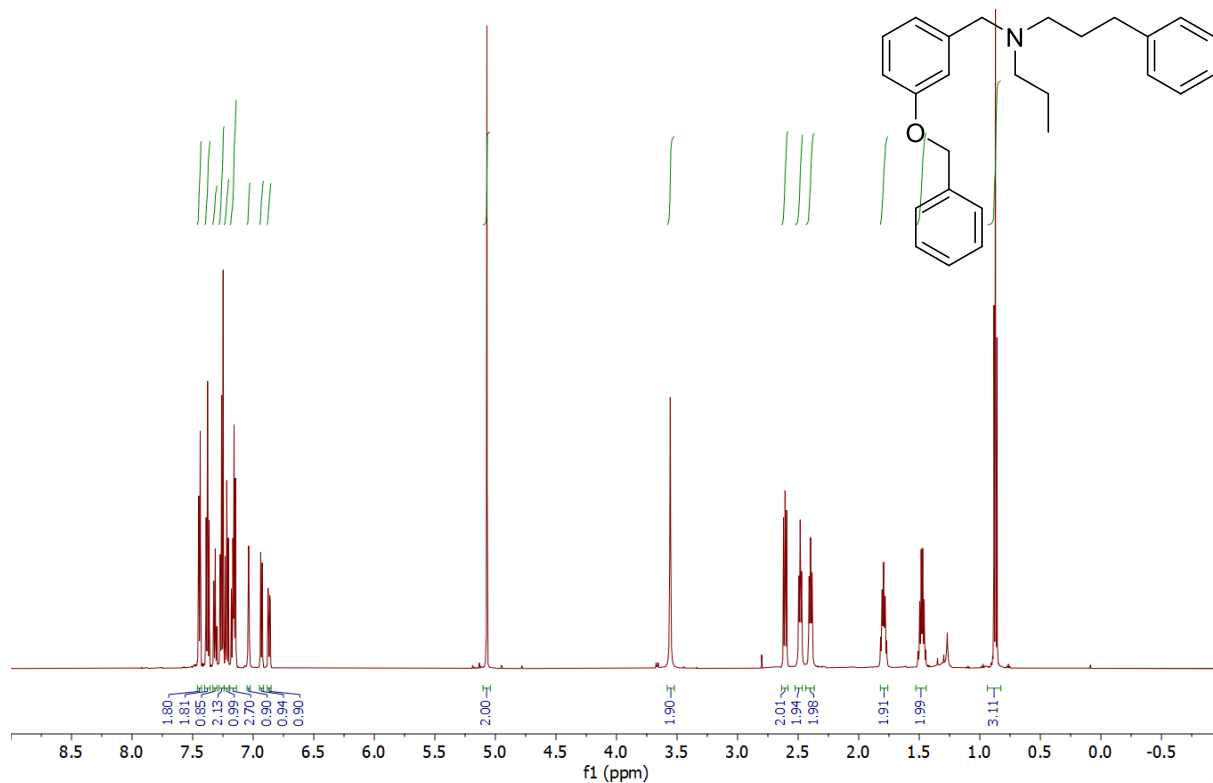


FC014-3

2: Diode Array
Range: 2.641e+1



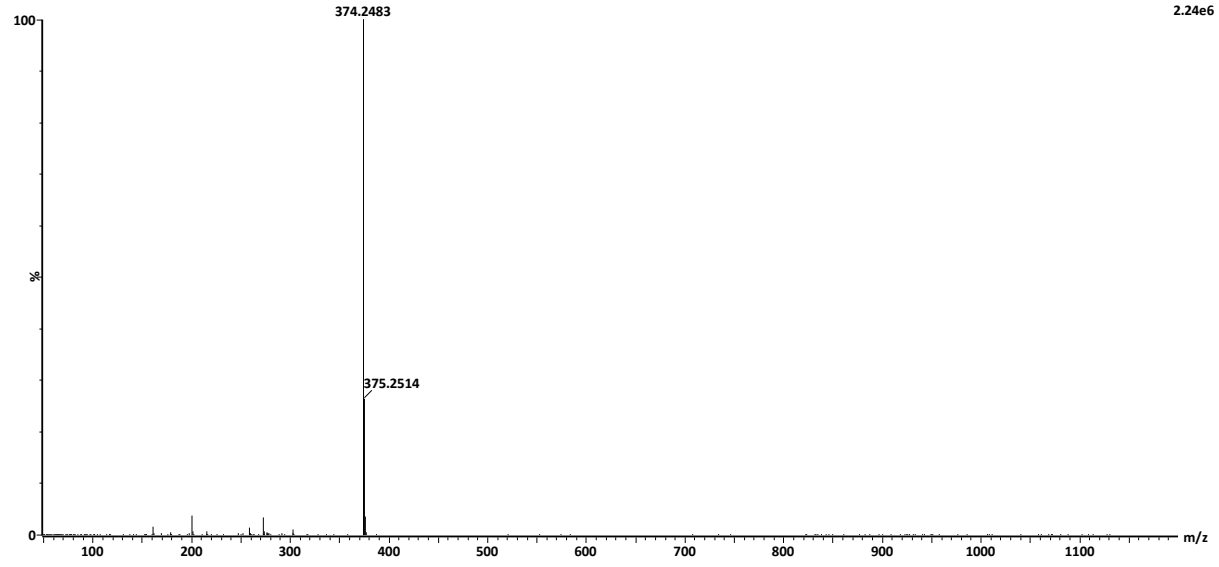
{[3-(Benzyloxy)phenyl]methyl}(3-phenylpropyl)propylamine (25):



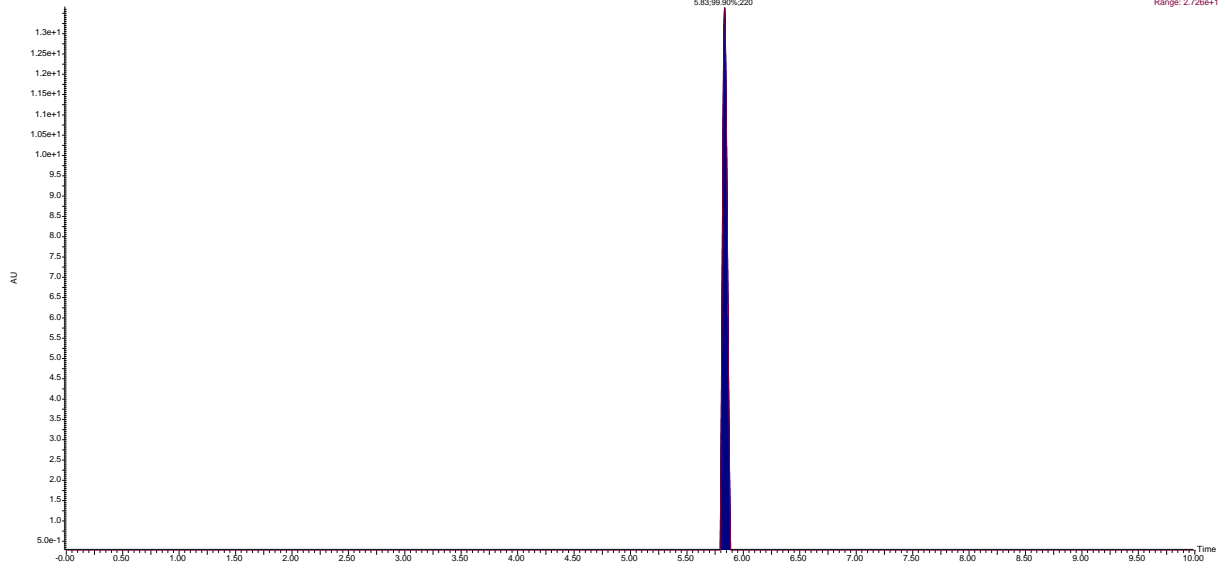
374,2478

2021 05 02 FC 014-2 A 1784 (3.072) Cm (1772:1807-(1649:1720+1899:1947))

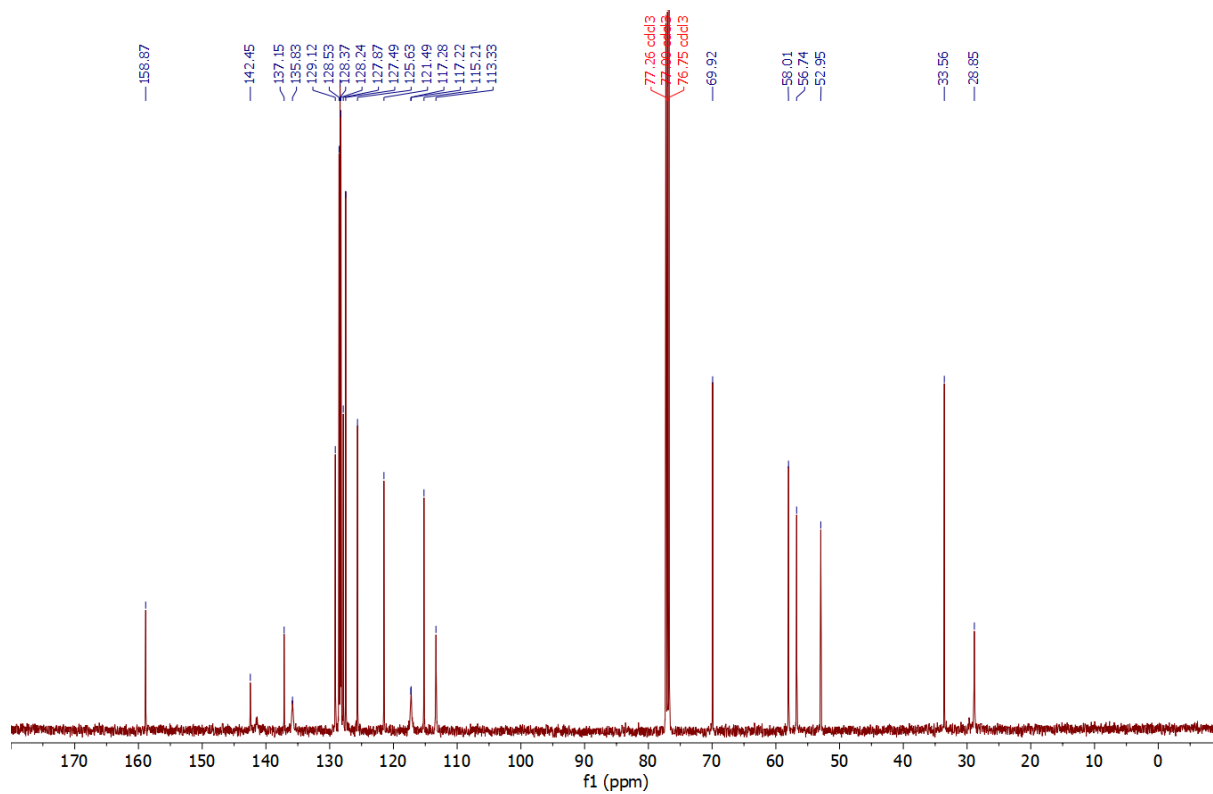
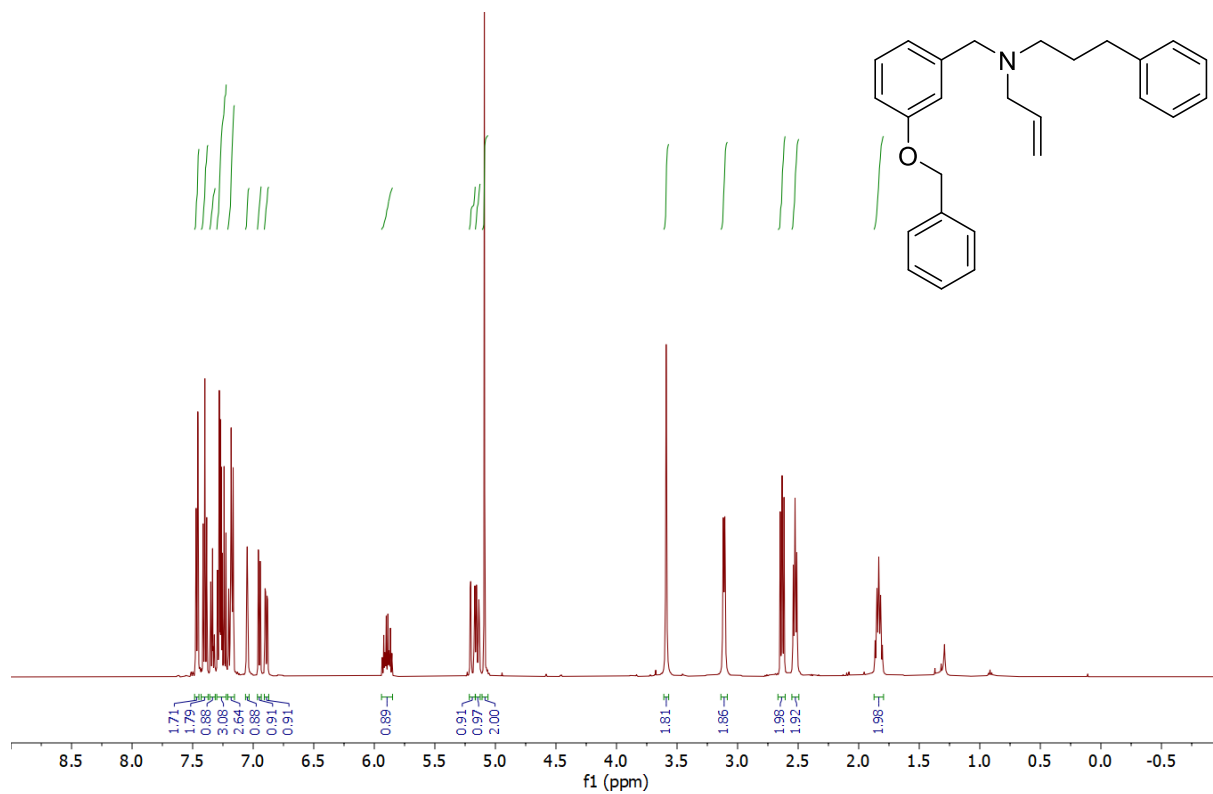
1: TOF MS ES+
2.24e6



FC014-2



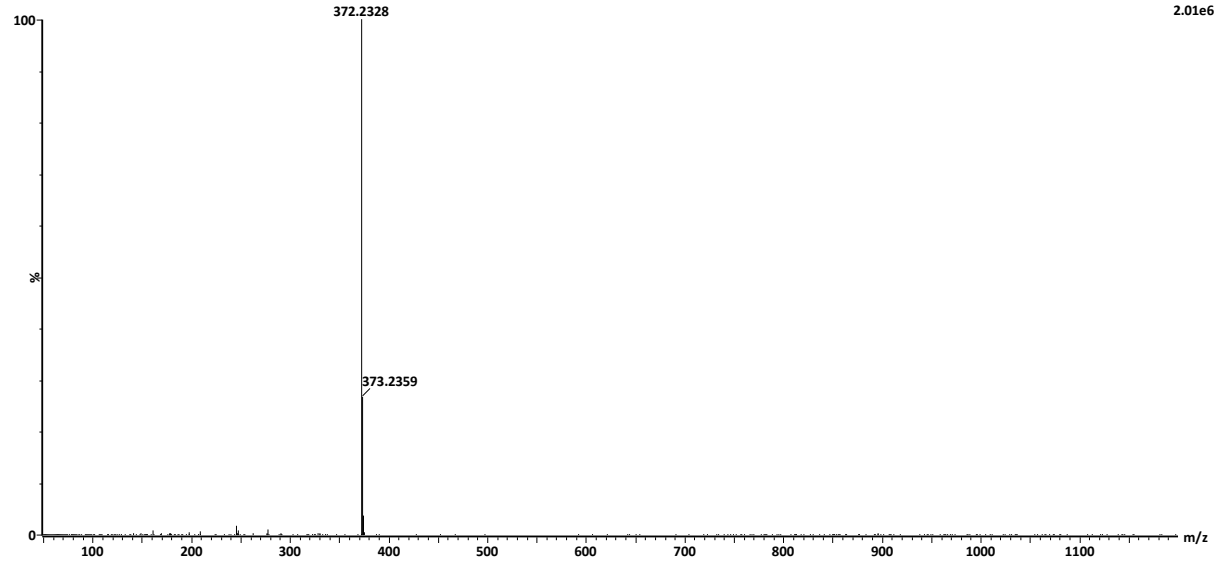
{[3-(Benzyloxy)phenyl]methyl}(3-phenylpropyl)(prop-2-en-1-yl)amine (26):



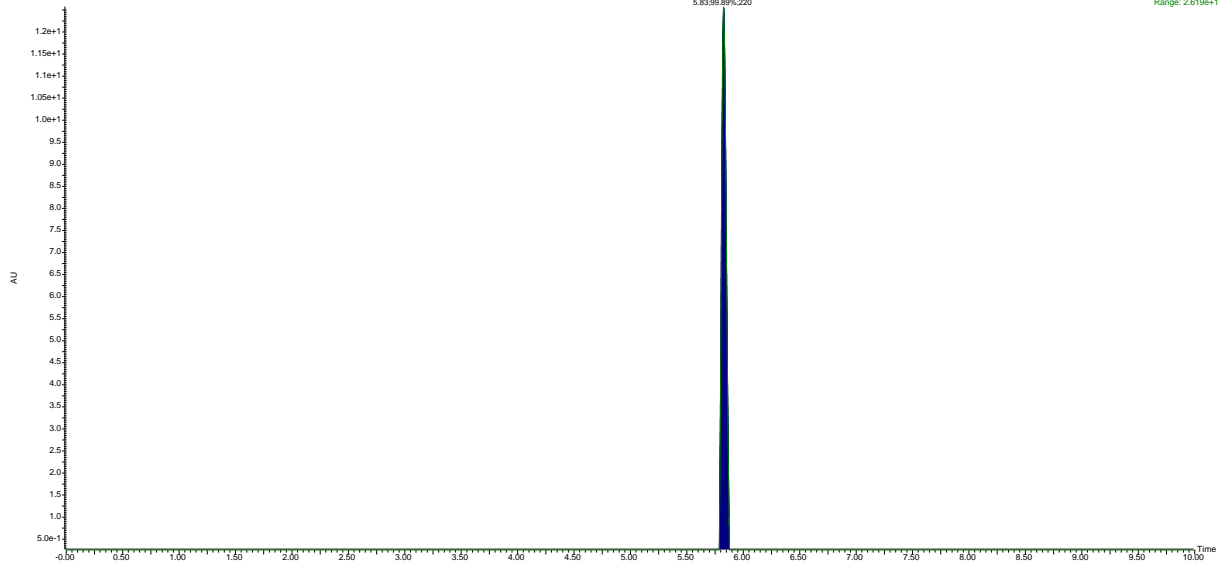
372.2322

2021 05 02 FC 014-1 B 1751 (3.017) Cm (1741:1776-(1655:1710+1824:1876))

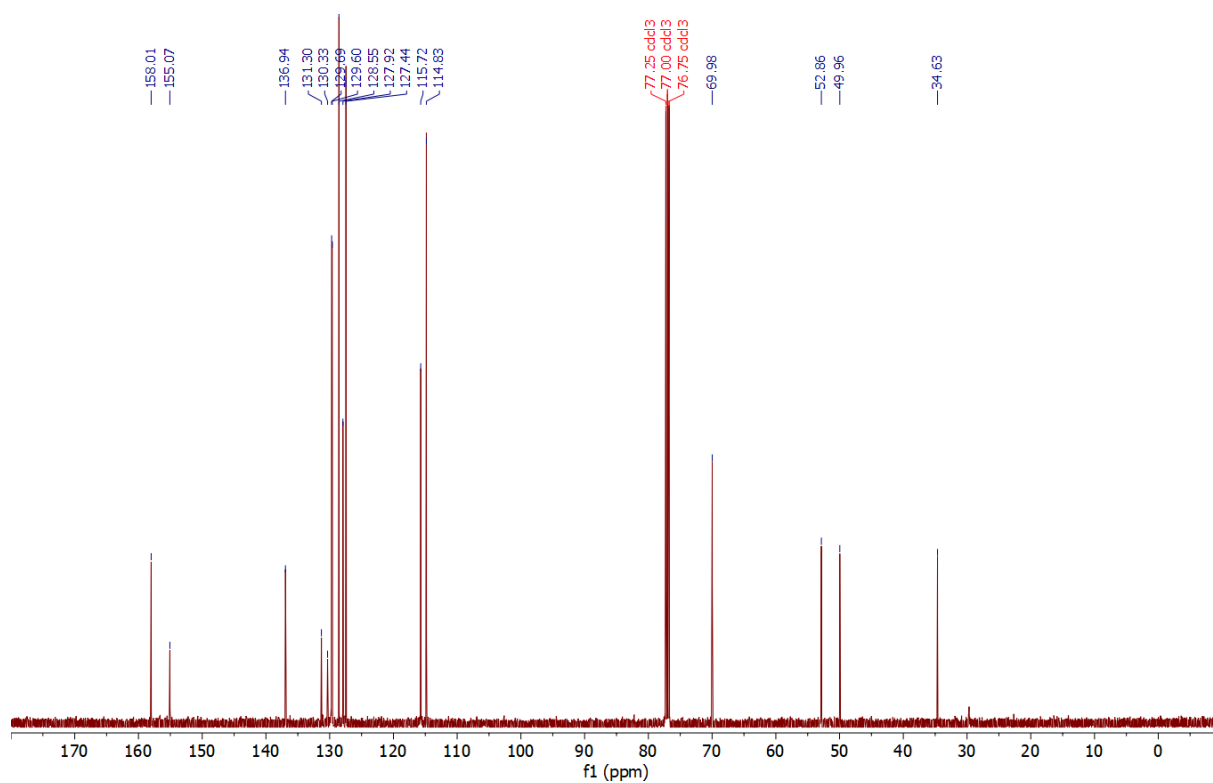
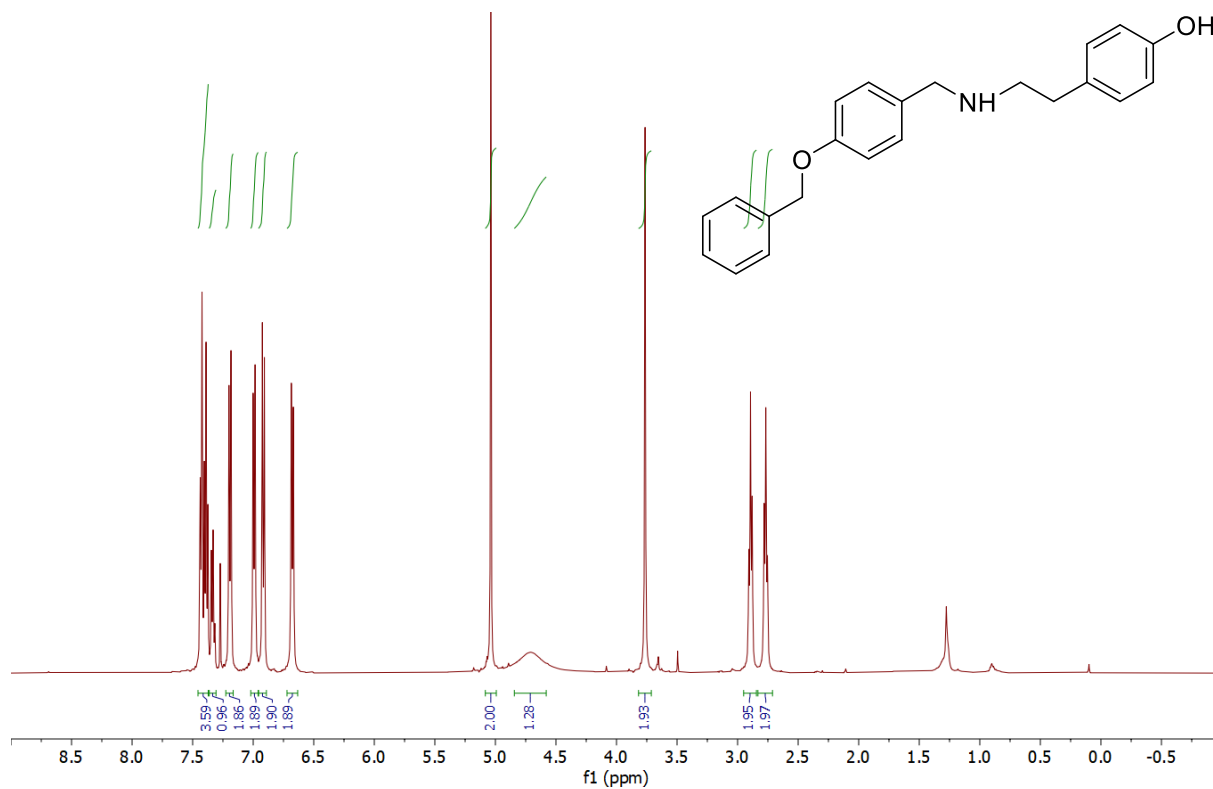
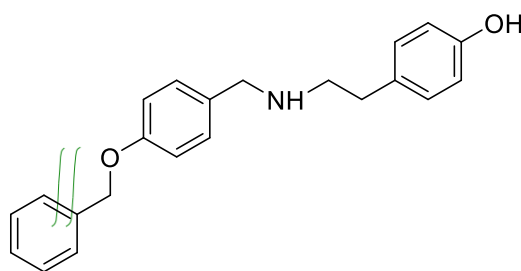
1: TOF MS ES+
2.01e6



FC014-1



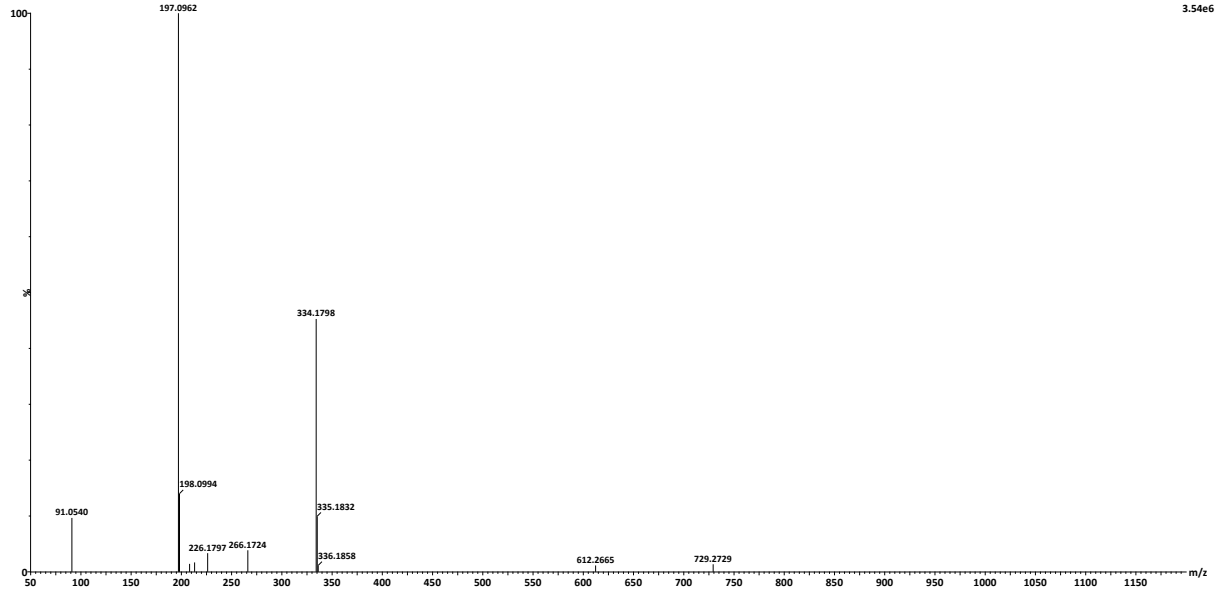
4-[2-({[4-(Benzyloxy)phenyl]methyl}amino)ethyl]phenol (28):



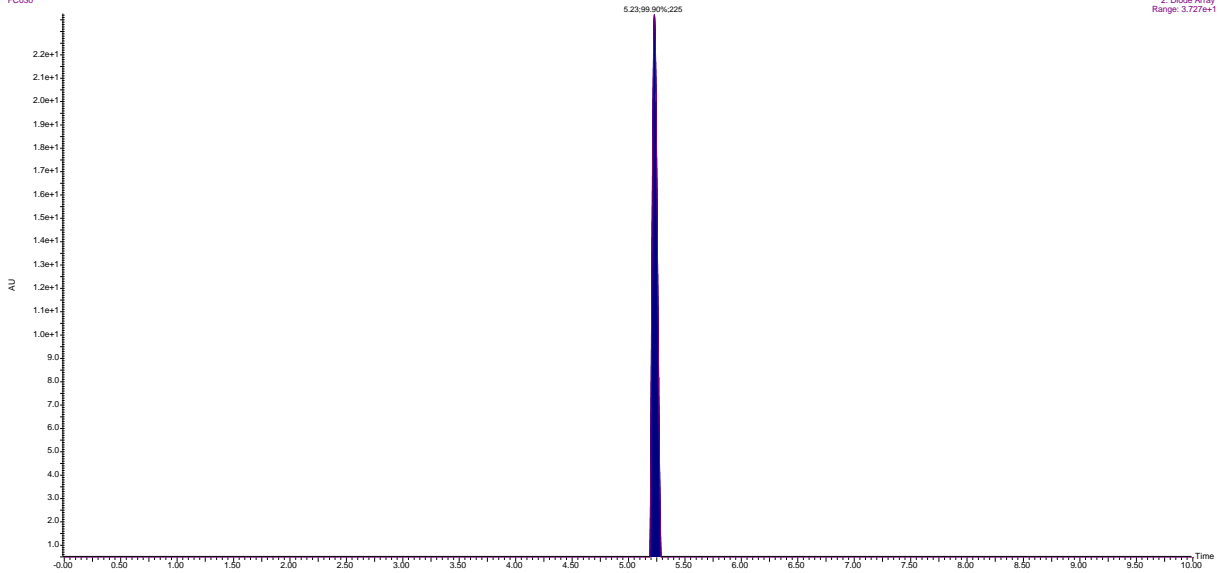
2041802

2022 08 03 FC030A 1393 (2.429) Cm (1379:1418-1126:1281+1500:1595)

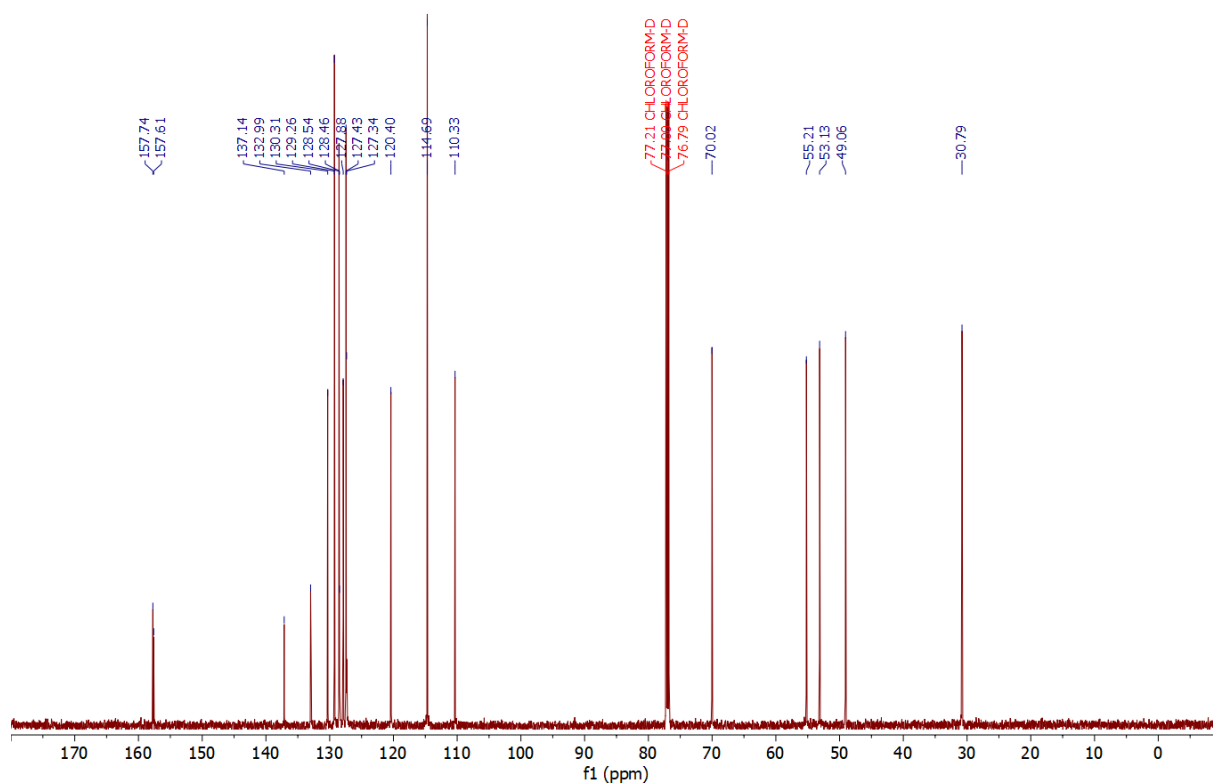
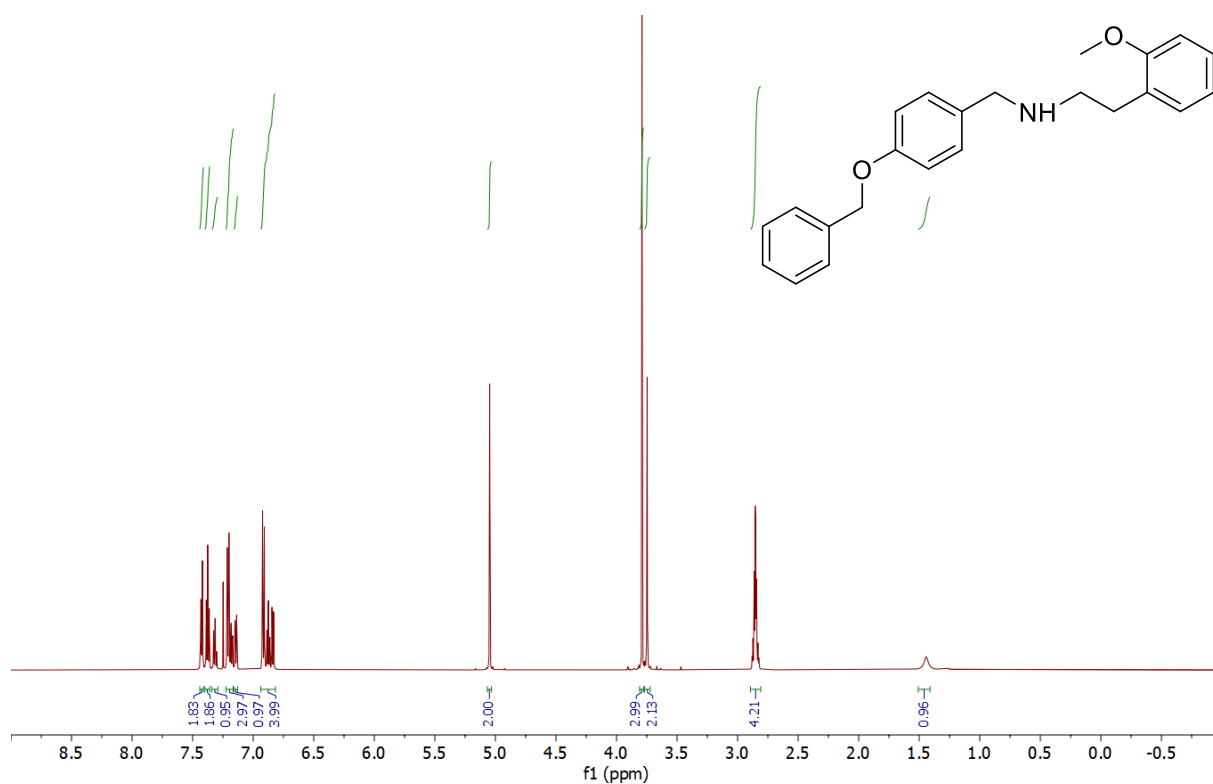
1: TOF MS ES+
3.54e6



FC030



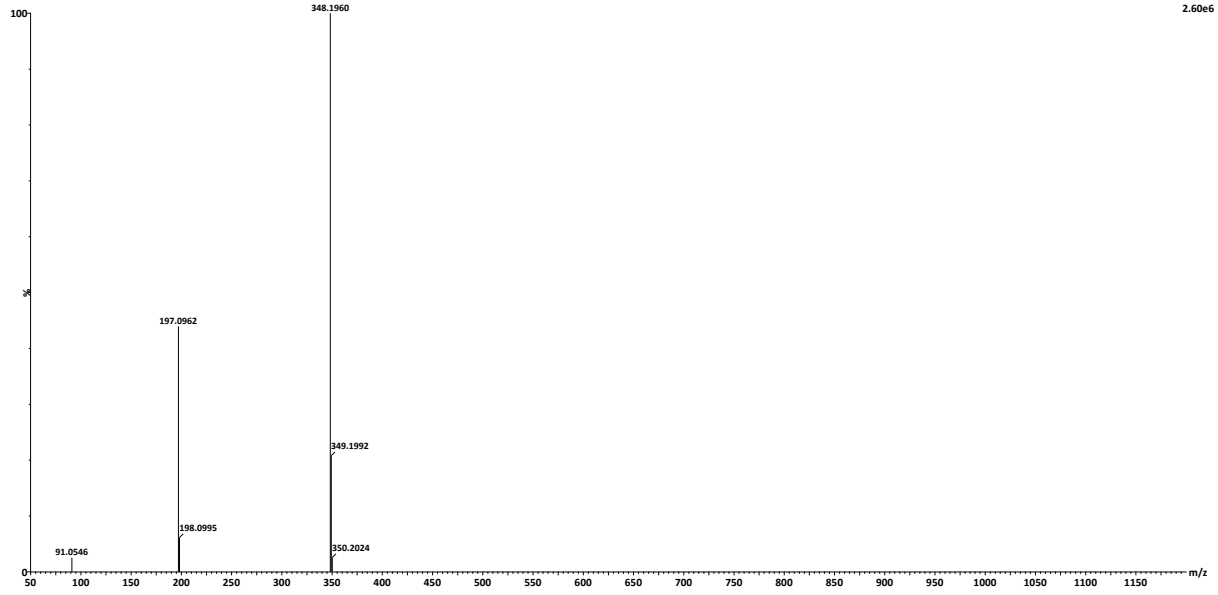
{{[4-(Benzyloxy)phenyl]methyl}[2-(2-methoxyphenyl)ethyl]amine (29):



348.1960

2022 08 03 FC044A 1656 (2.887) Cm (1647:1678-(1449:1545+1752:1890))

1: TOF MS ES+
2.60e6



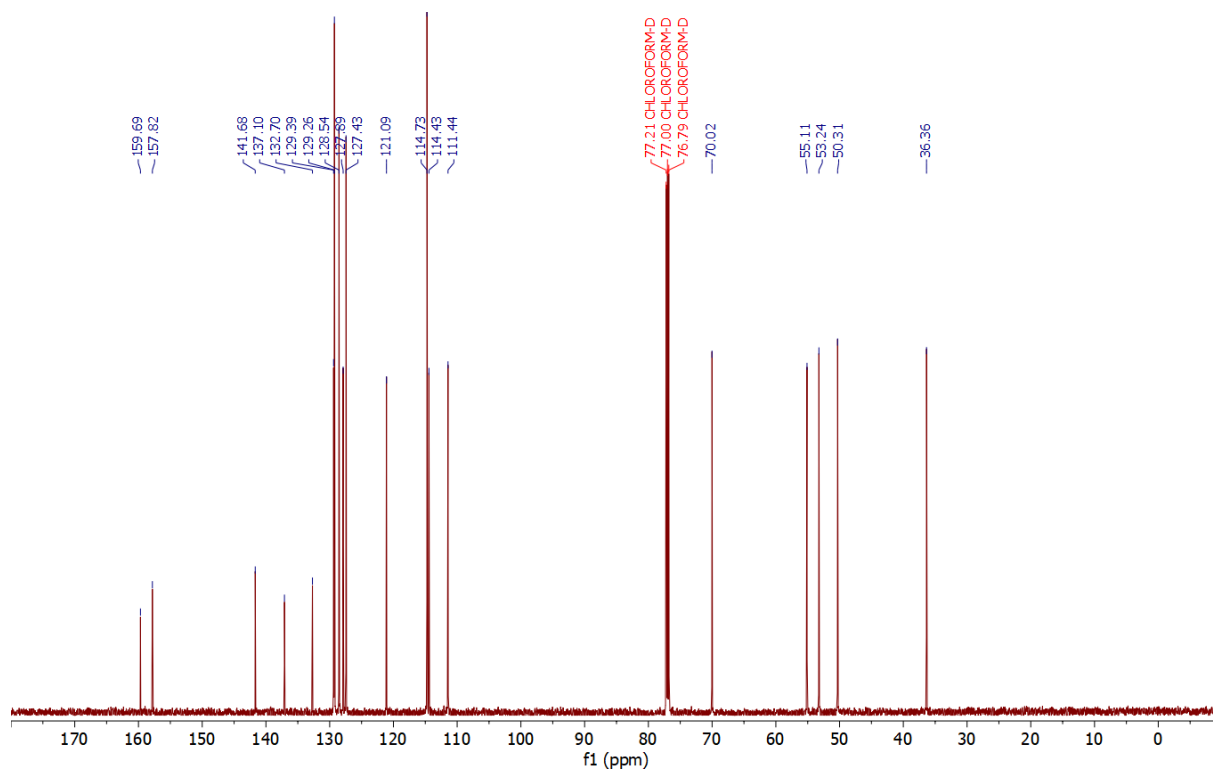
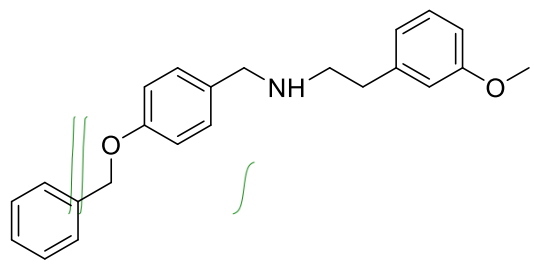
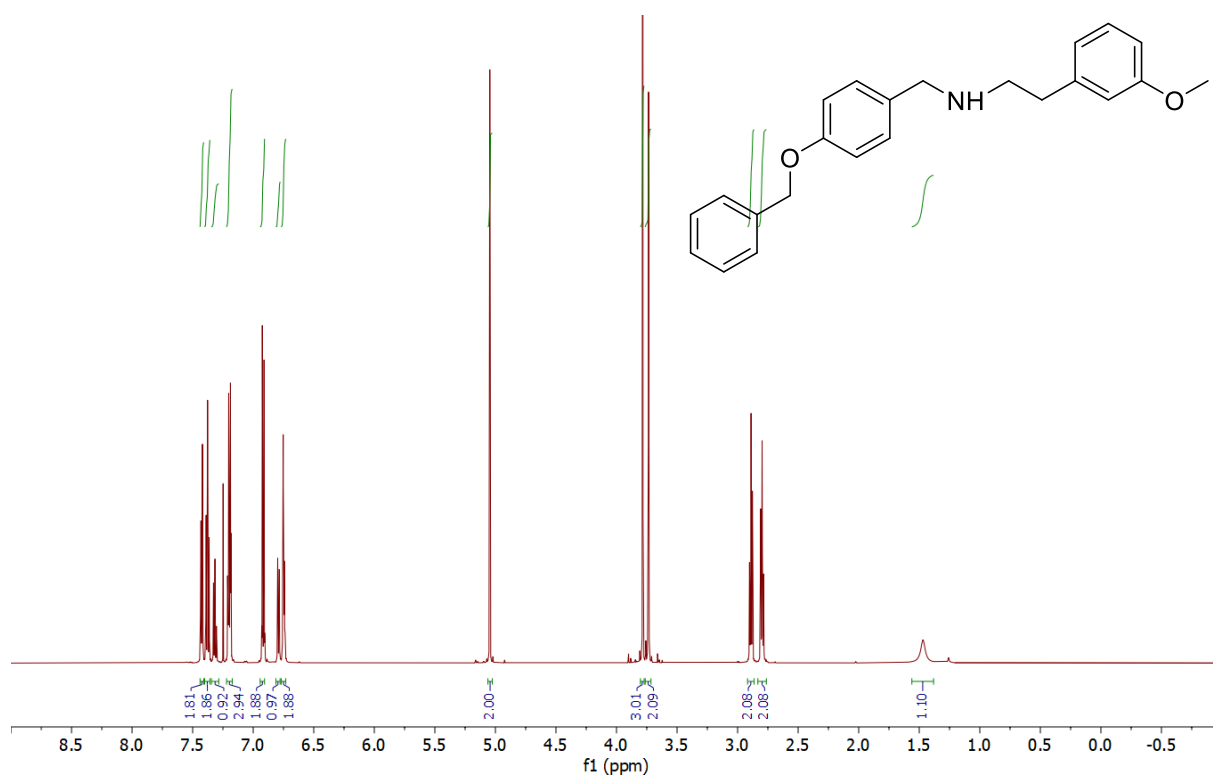
FC044

5.6739.87%:225

2: Diode Array
Range: 3.504e+1



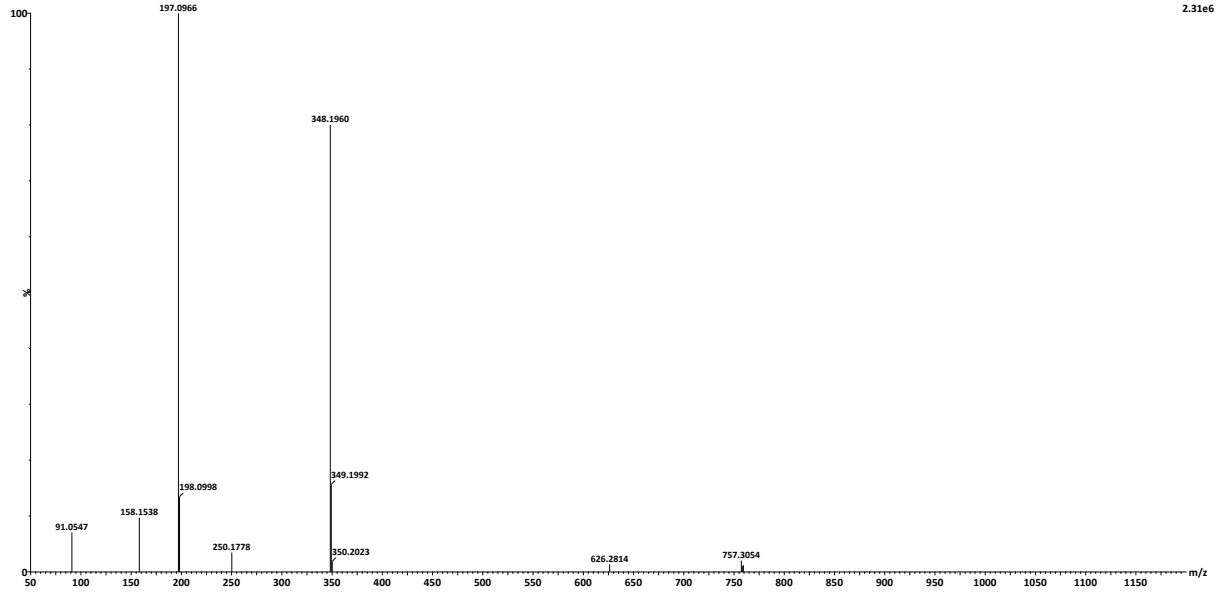
{{[4-(Benzyloxy)phenyl]methyl}[2-(3-methoxyphenyl)ethyl]amine (30):



348.1958

2022 08 03 FC045A 1613 (2.811) Cm (1597:1638-(1277:1426+1802:1958))

1: TOF MS ES+
2.31e6

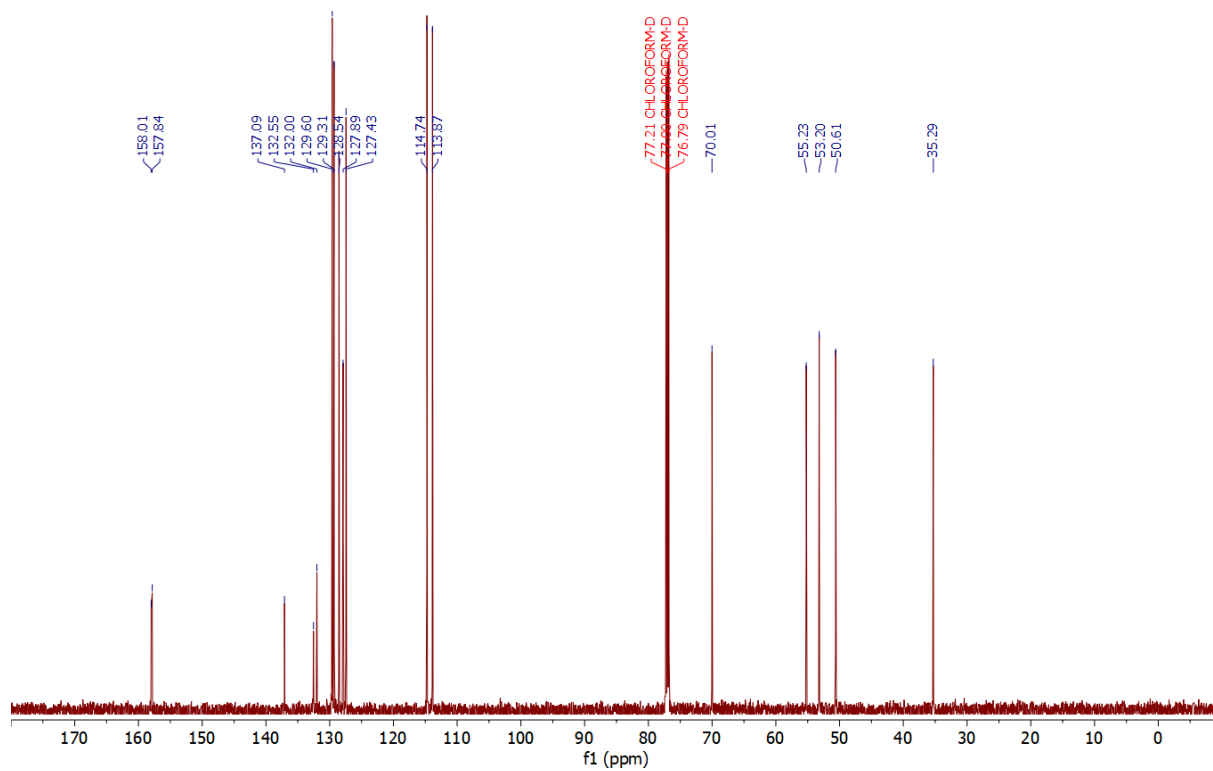
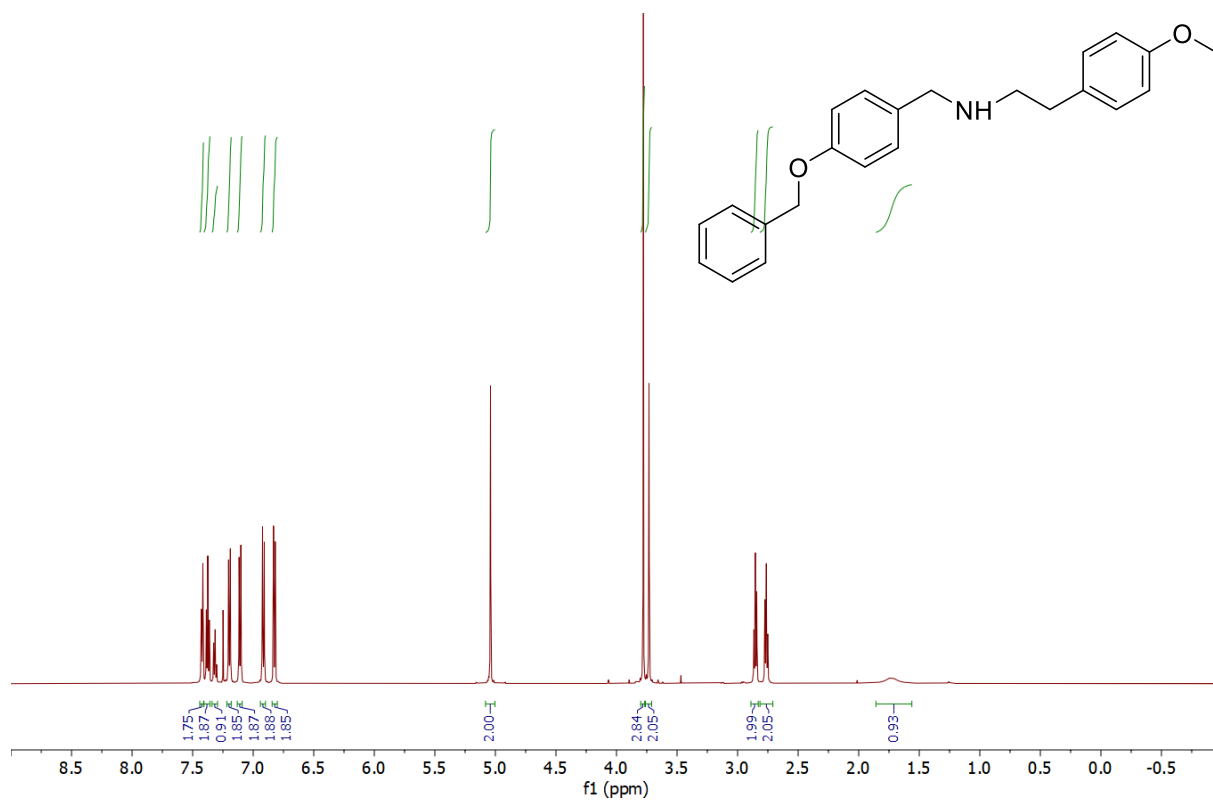


FC045



2: Diode Array
Range: 5.773e+1

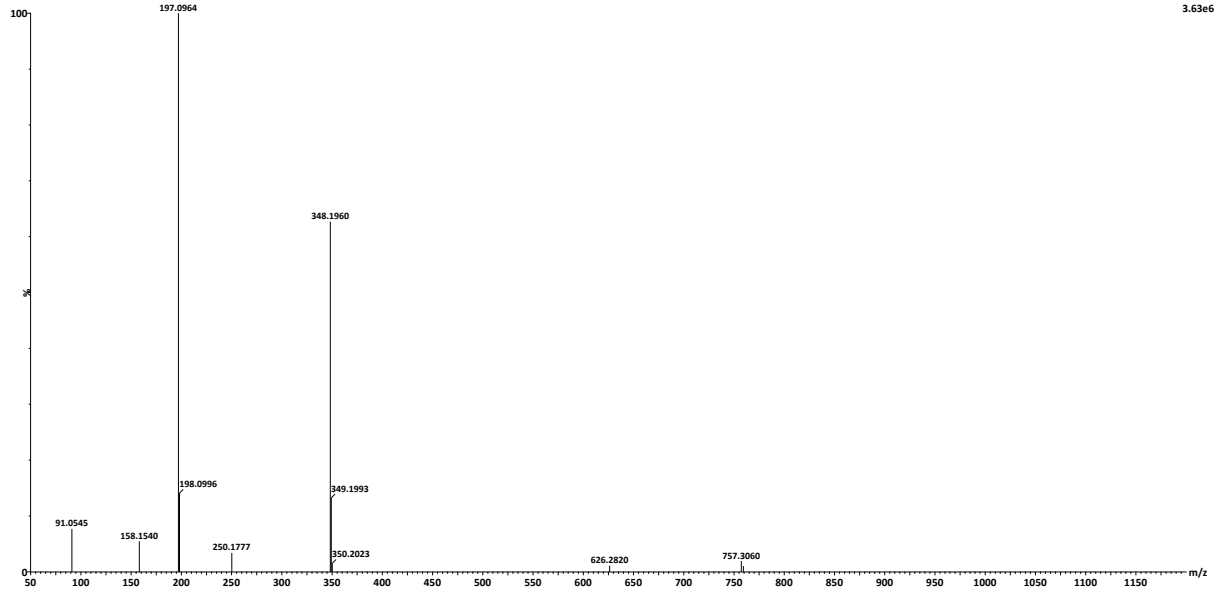
{{[4-(Benzyloxy)phenyl]methyl}[2-(4-methoxyphenyl)ethyl]amine (31):



348.1958

2022 08 03 FC042A 1602 (2.793) Cm (1590:1624-(1358:1429+1684:1799))

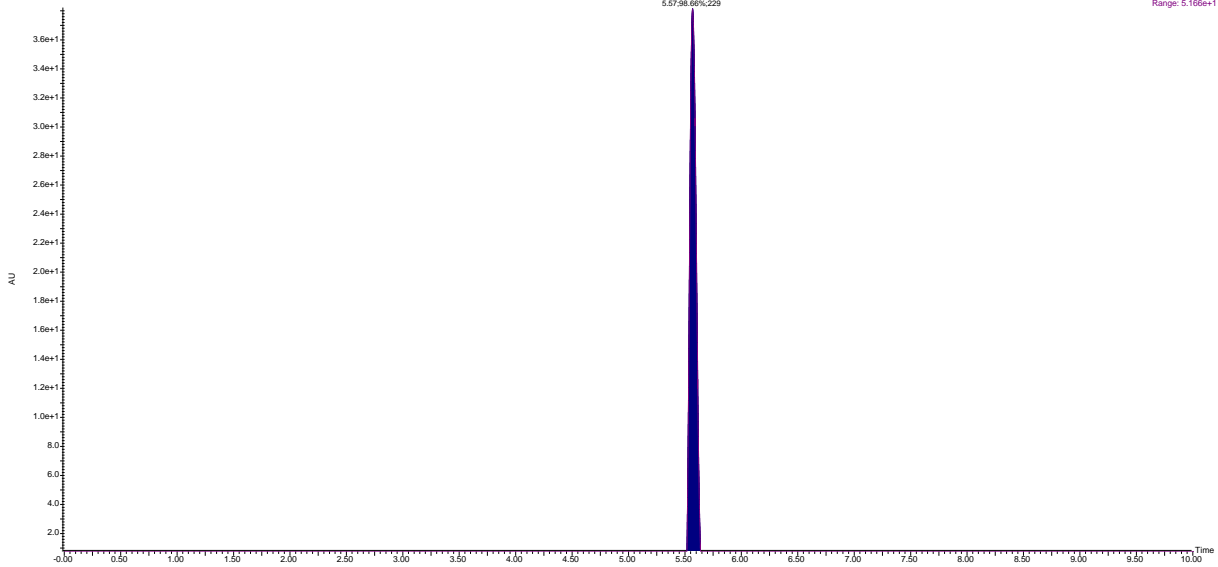
1: TOF MS ES+
3.63e6



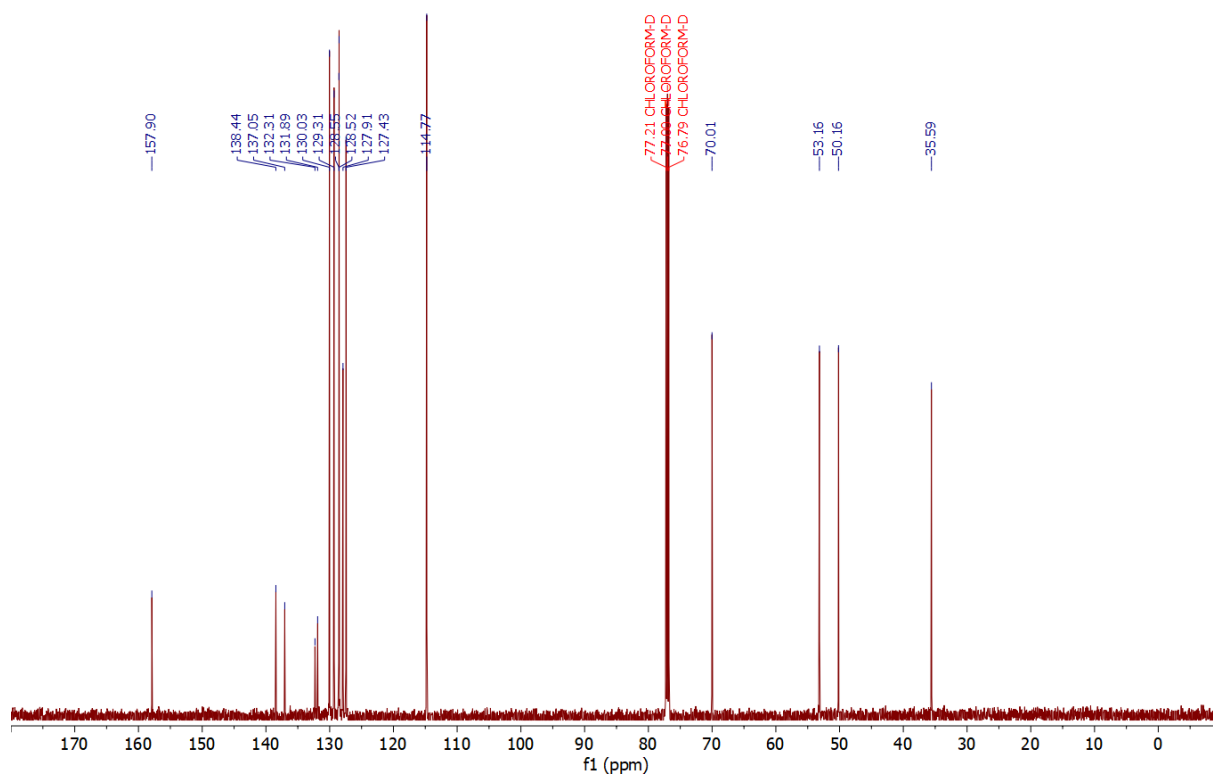
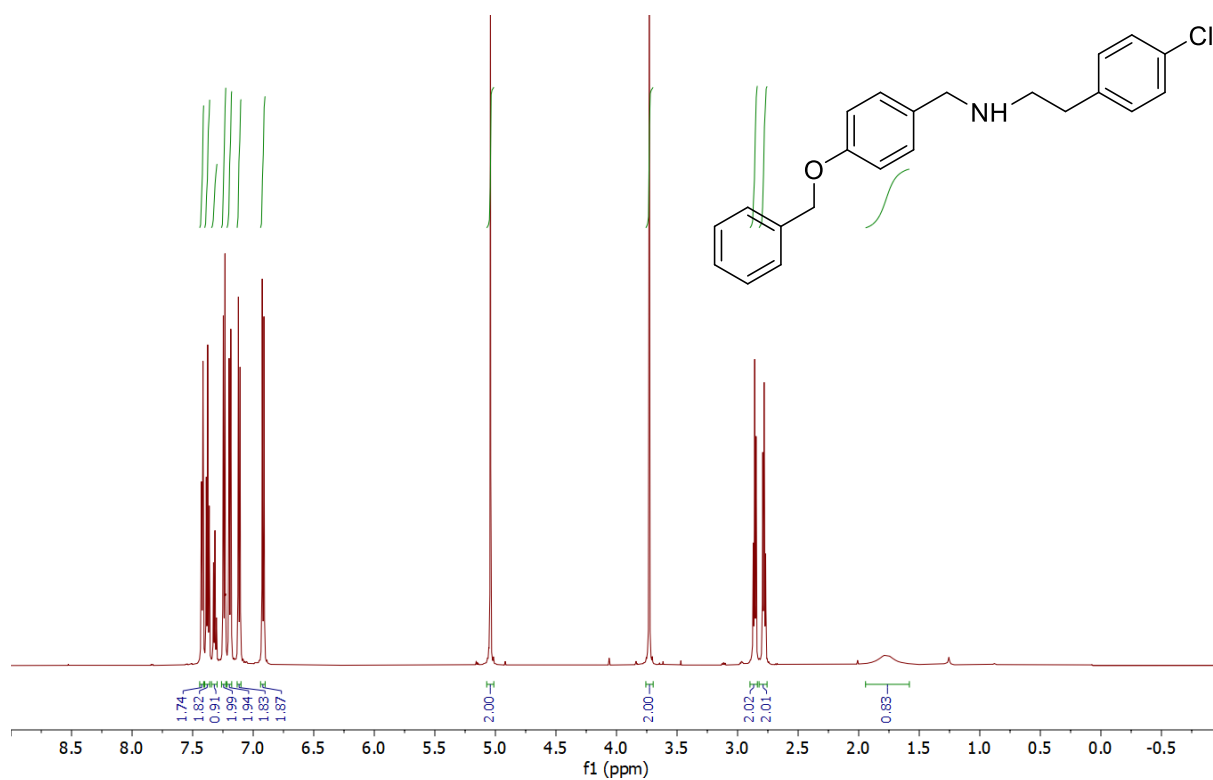
FC042

5.573868% (229)

2: Diode Array
Range: 5.168e+1



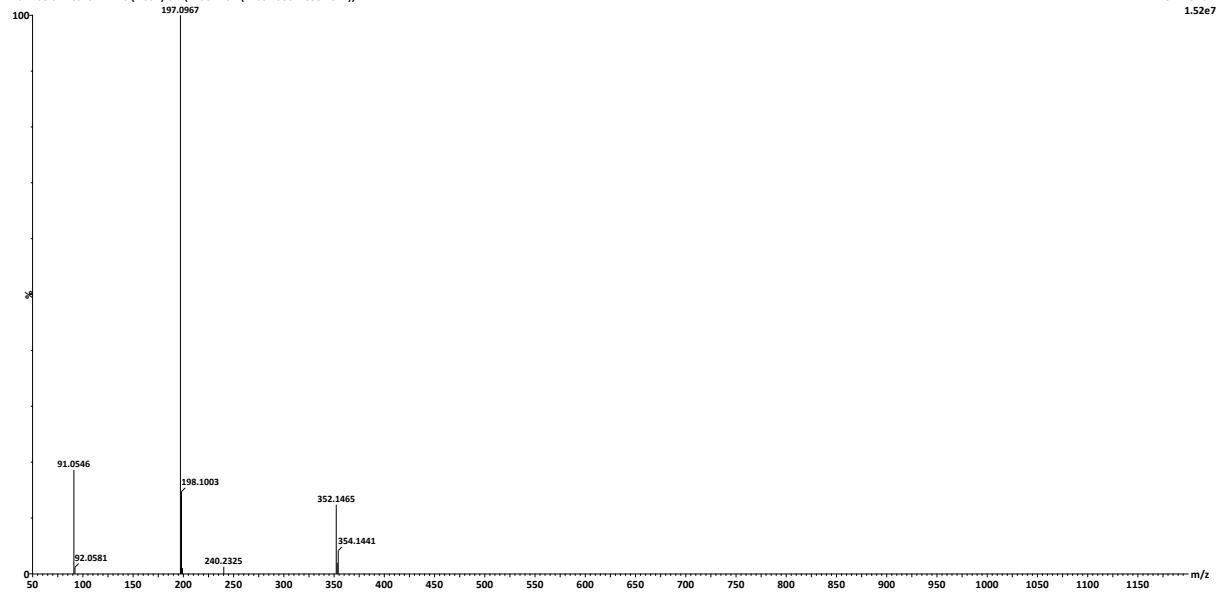
{[4-(Benzyloxy)phenyl]methyl}[2-(4-chlorophenyl)ethyl]amine (32):



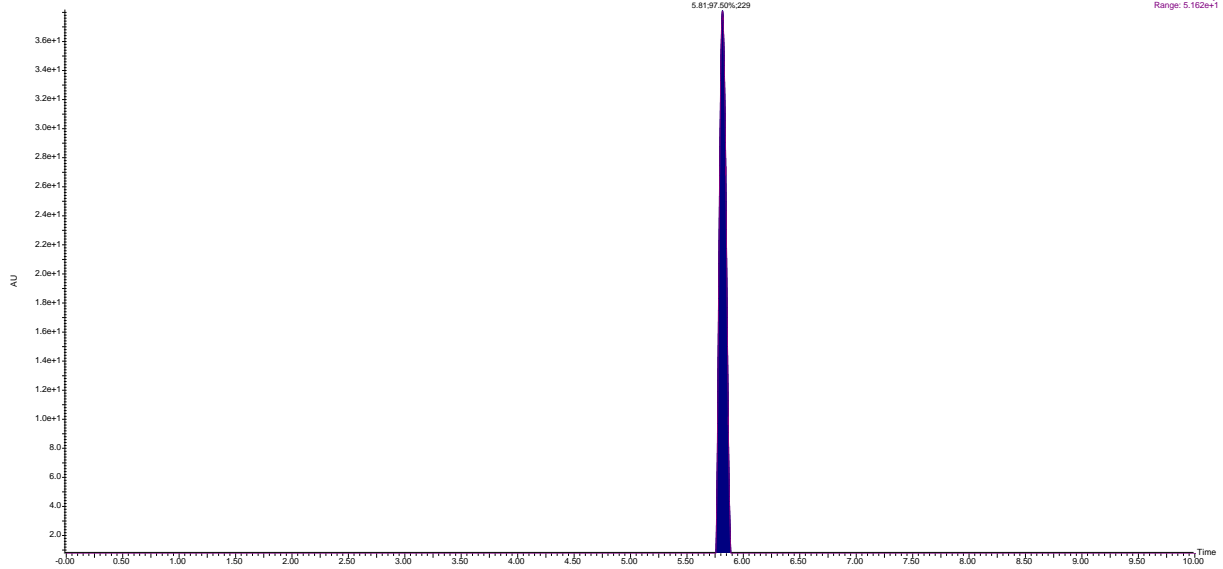
3021463

2022 08 04 FC043 A 1716 (2.991) Cm (1706:1734-(1460:1580+1855:1974))

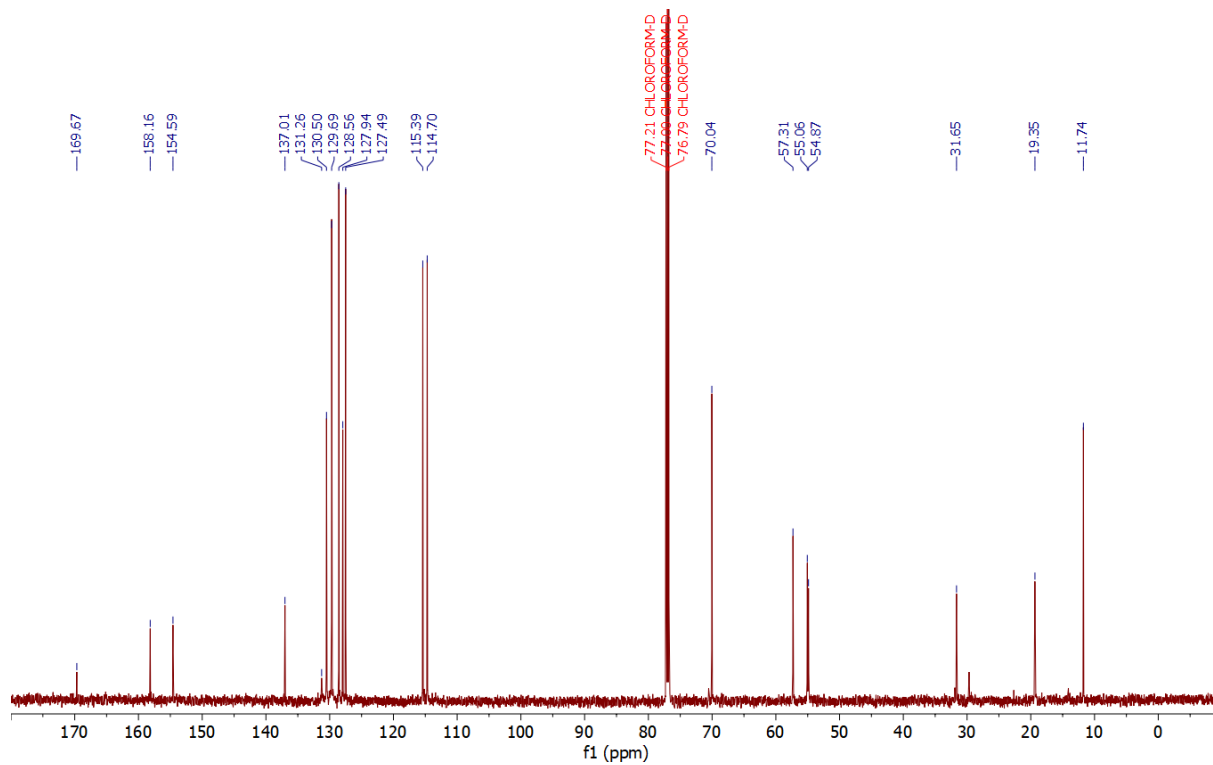
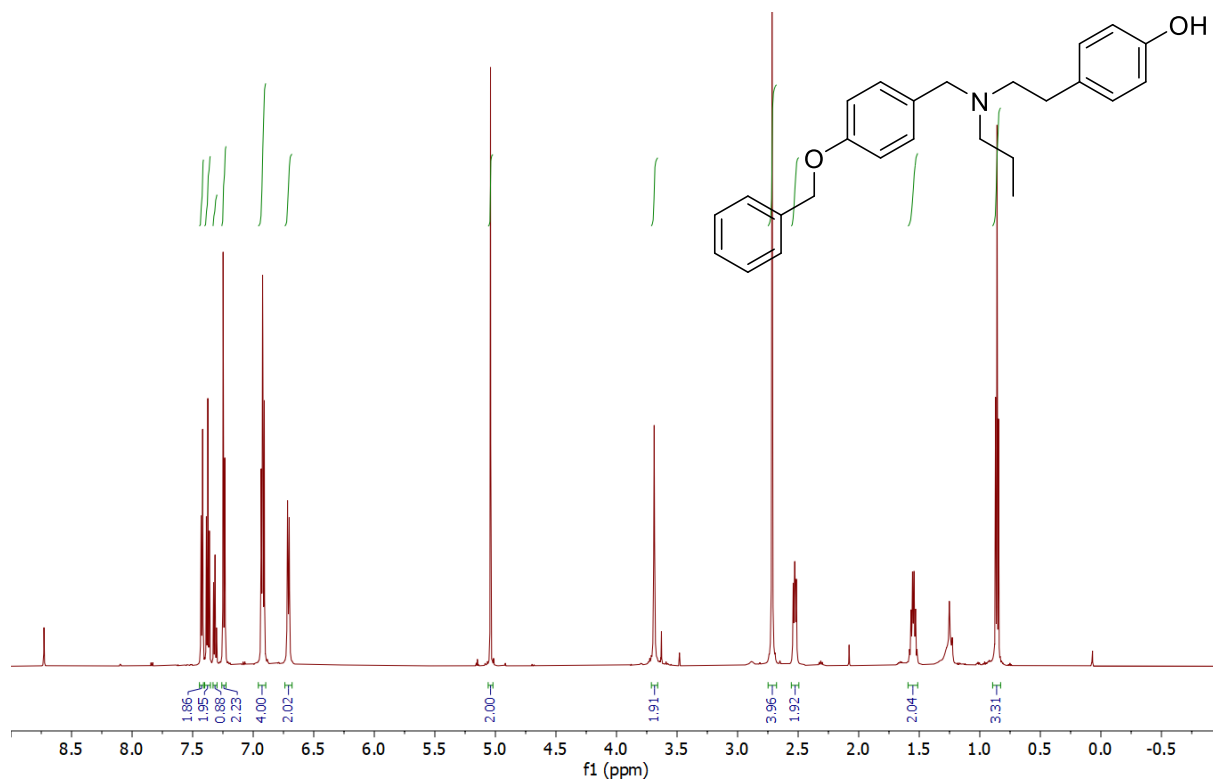
1: TOF MS ES+
1.52e7



FC043



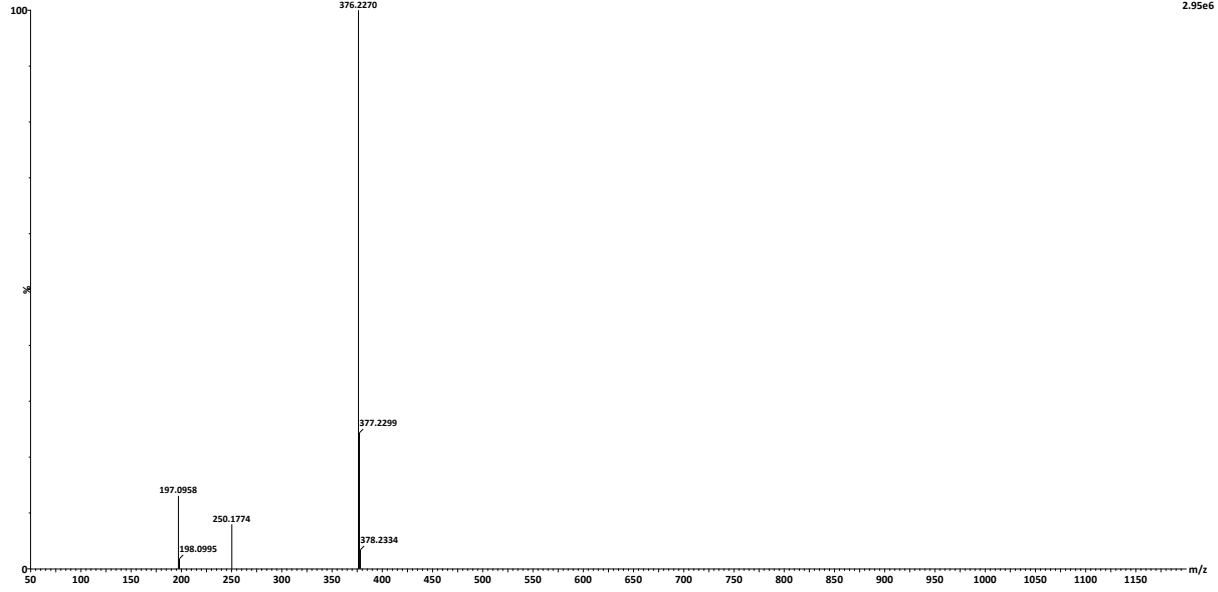
4-[2-({[4-(Benzyloxy)phenyl]methyl}(propyl)amino)ethyl]phenol (33):



376.2270

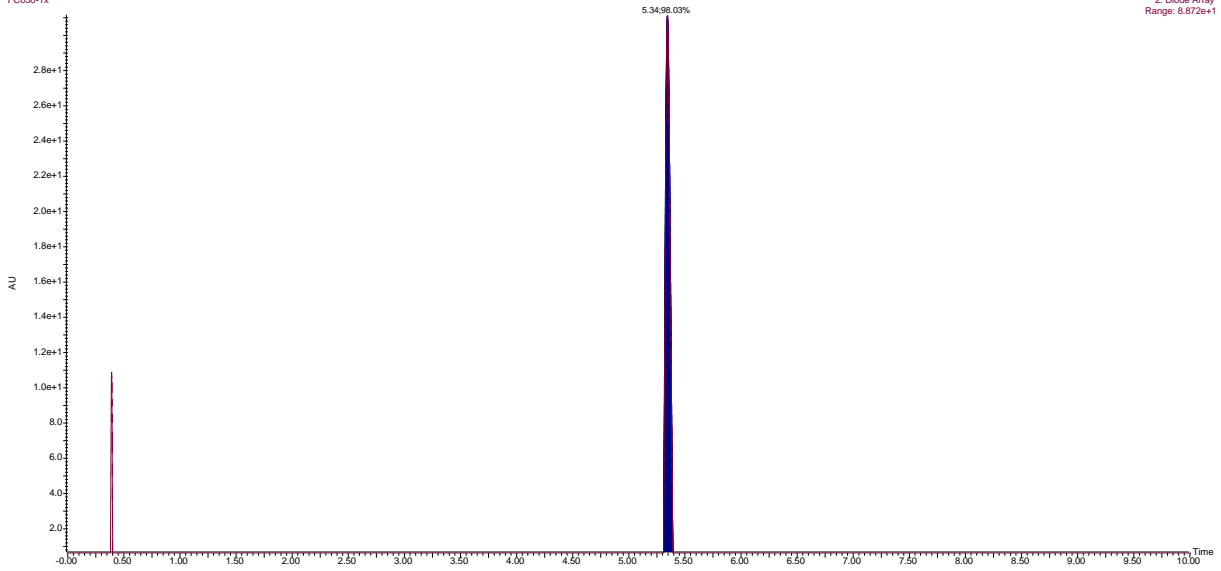
2022 08 03 FC030-1A 1566 (2.729) Cm (1553:1593-(1320:1415+1670:1743))

1: TOF MS ES+
2.95e6

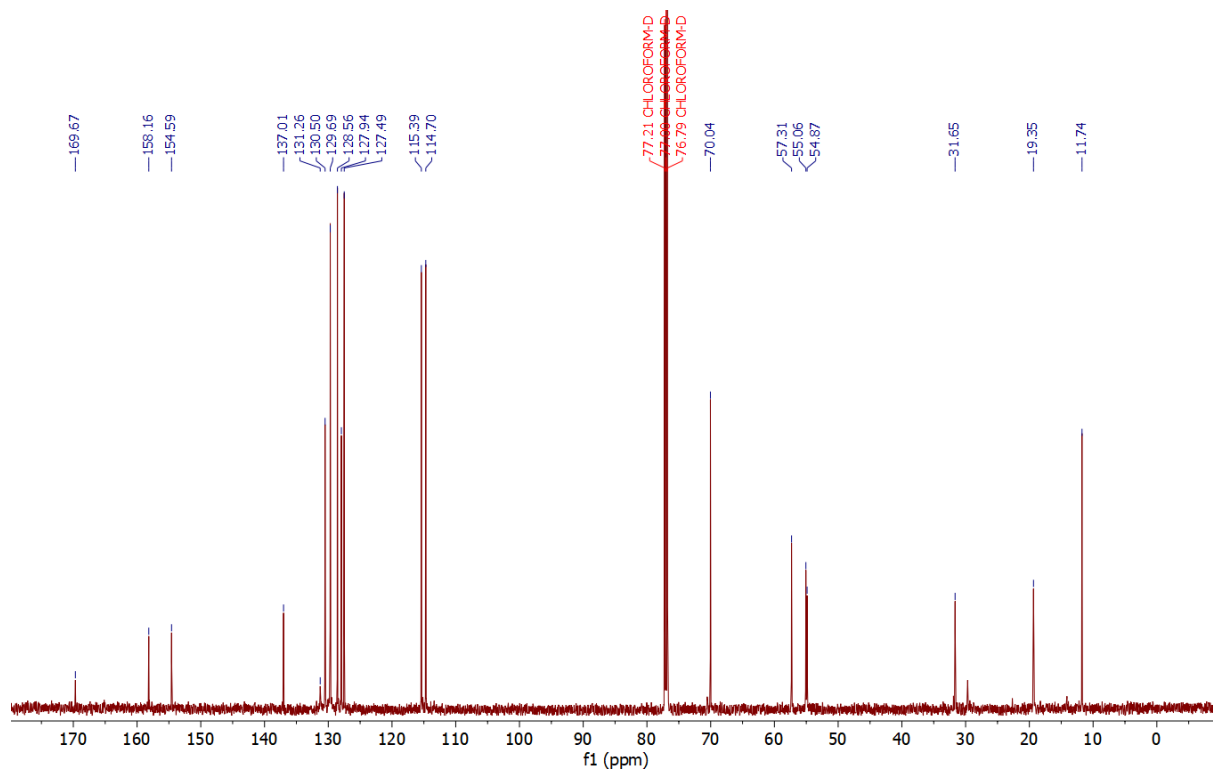
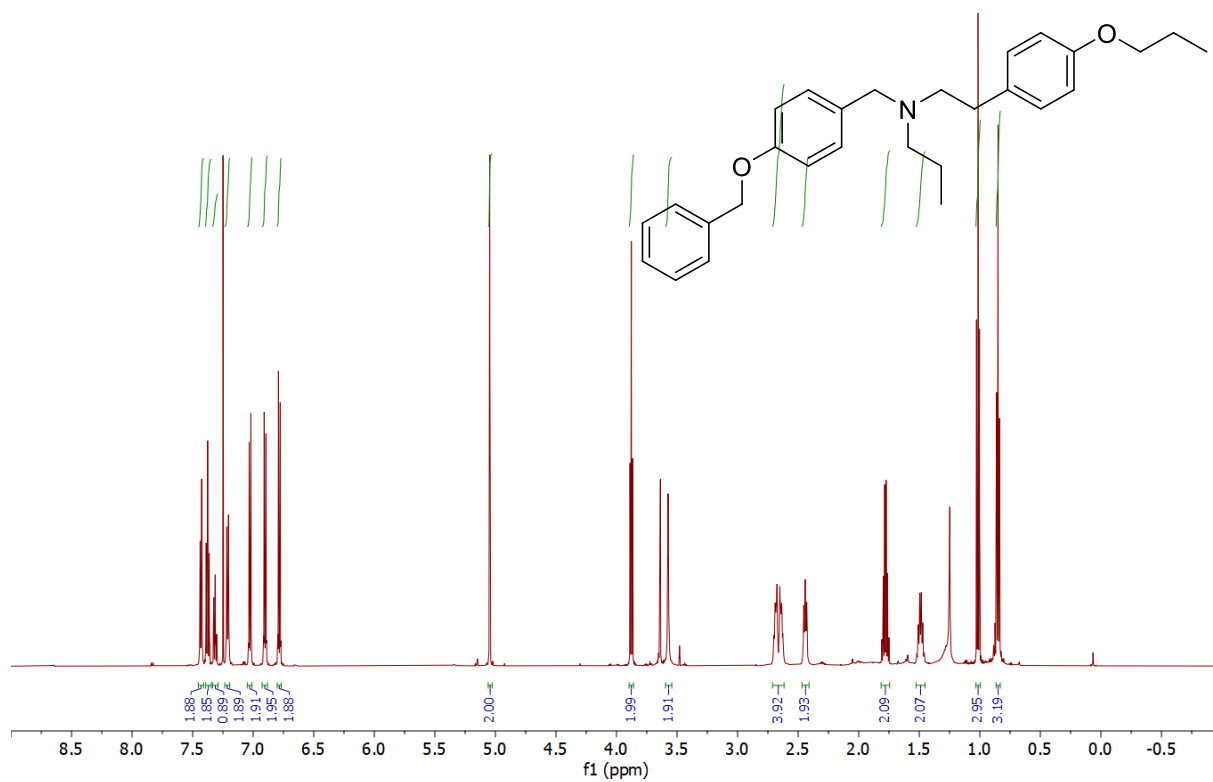


FC030-1x

2: Diode Array
Range: 8.872e+1



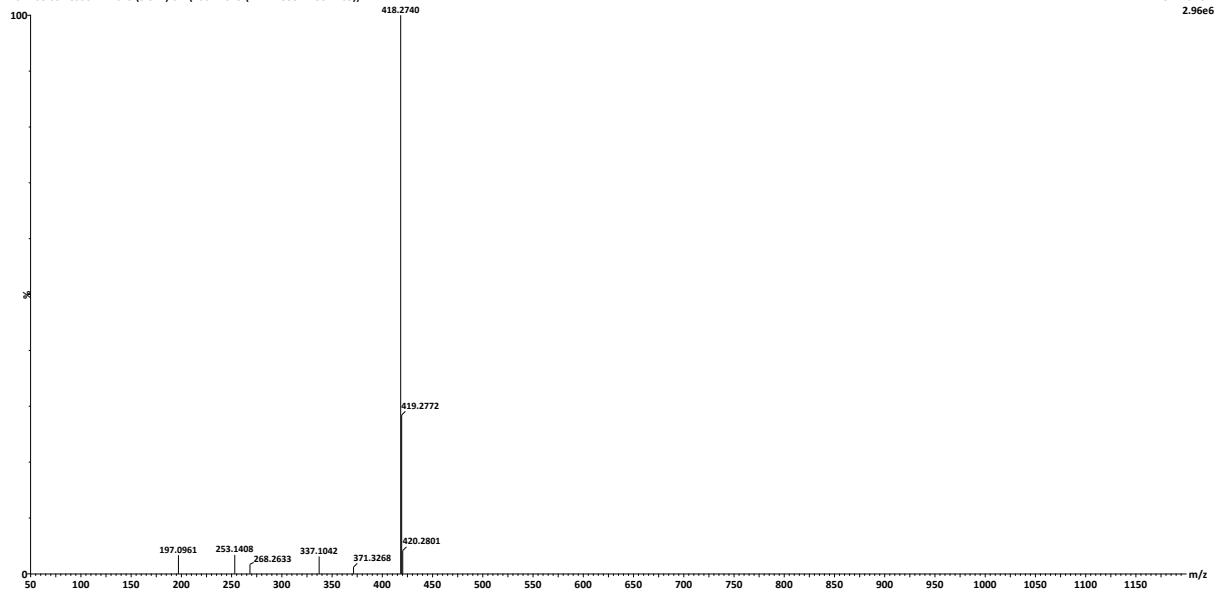
{[4-(Benzyloxy)phenyl]methyl}[2-(4-propoxyphenyl)ethyl]propylamine (34):



418.2741

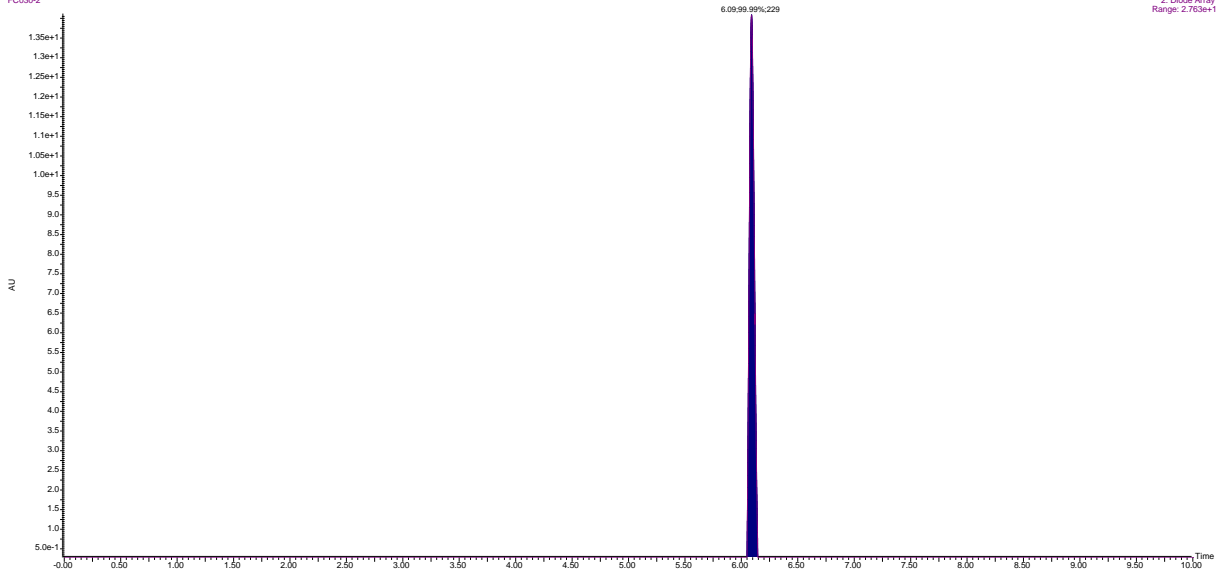
2022 08 03 FC030-2A 2019 (3.514) Cm (2007:2048-(1771:1888+2153:2265))

1: TOF MS ES+
2.96e6

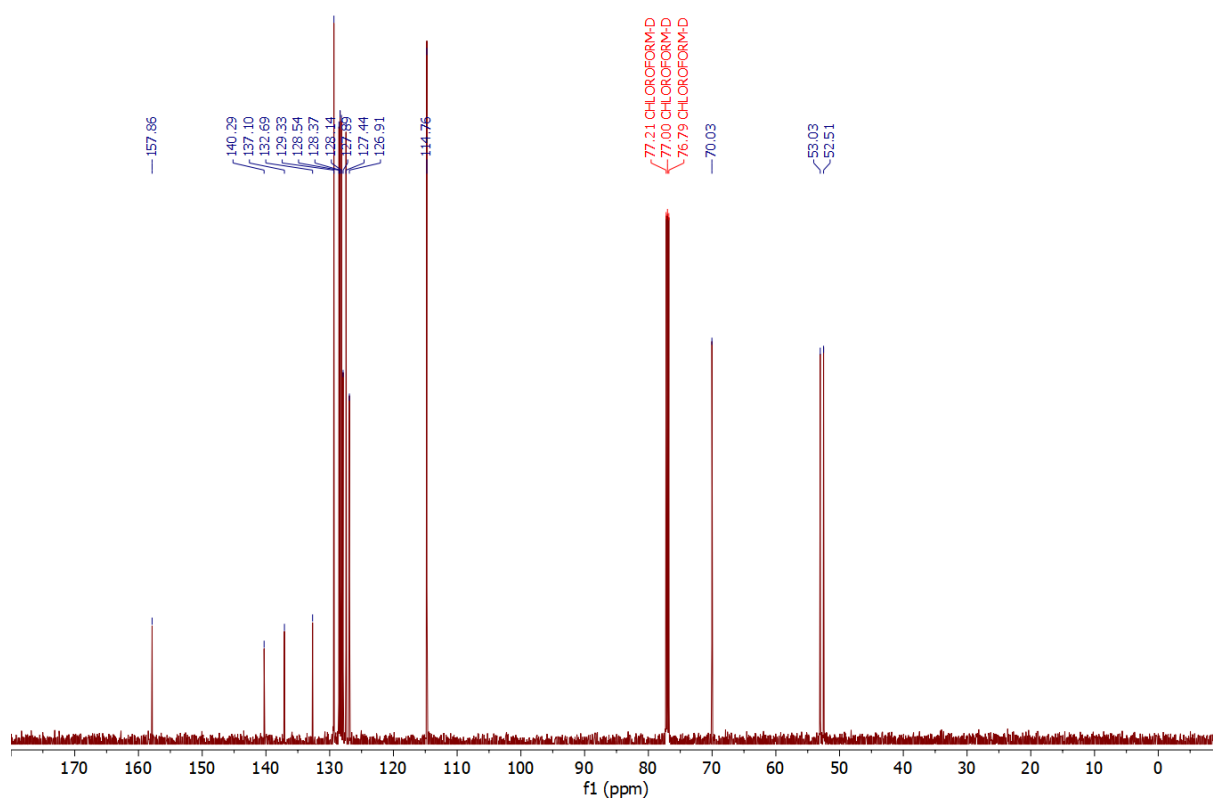
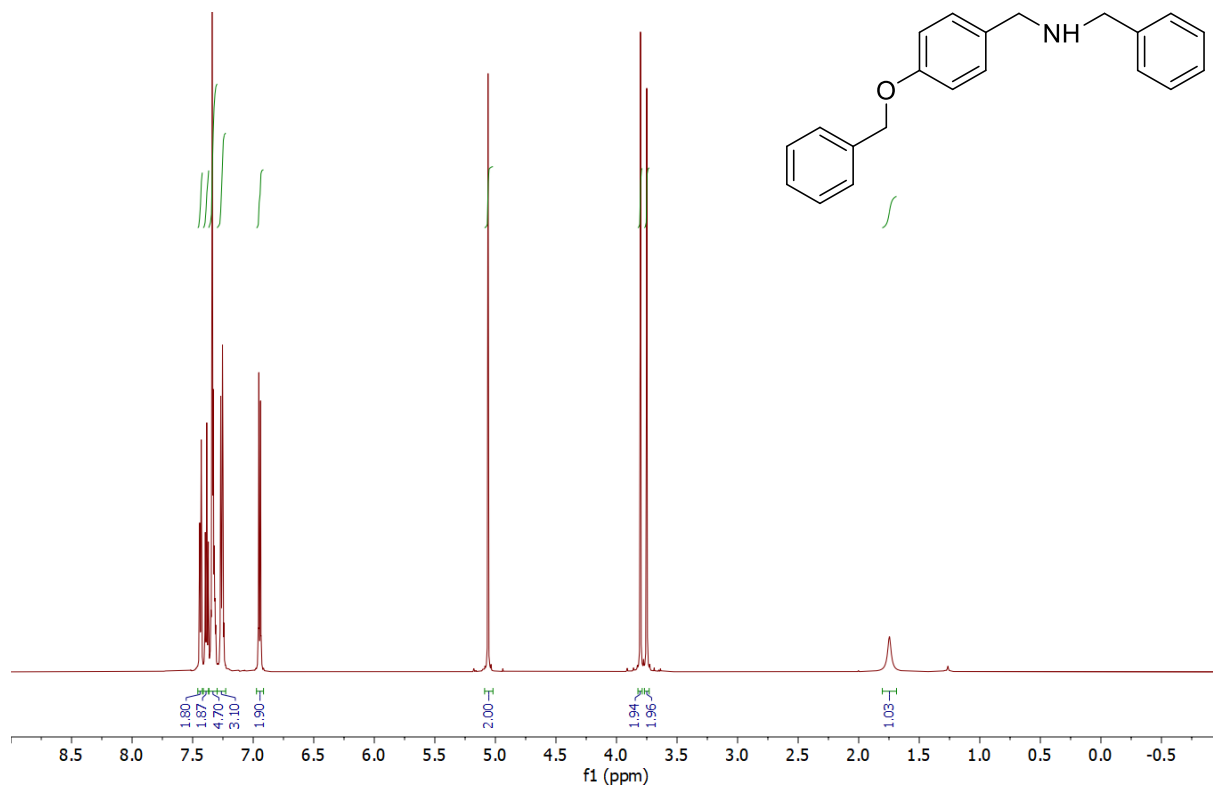
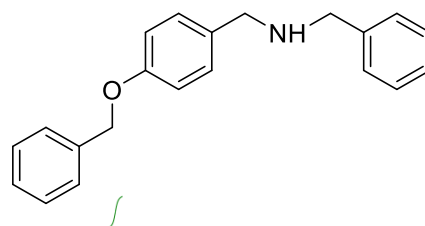


FC030-2

2: Diode Array
Range: 2.763e+1



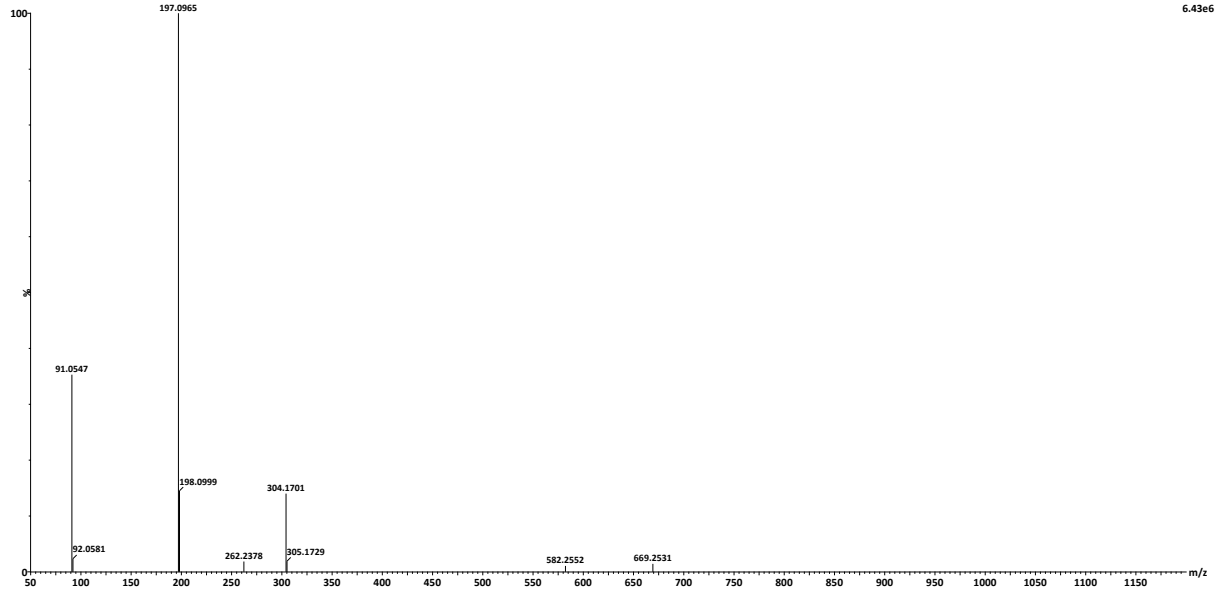
Benzyl([4-(benzyloxy)phenyl]methyl)amine (35):



2041696

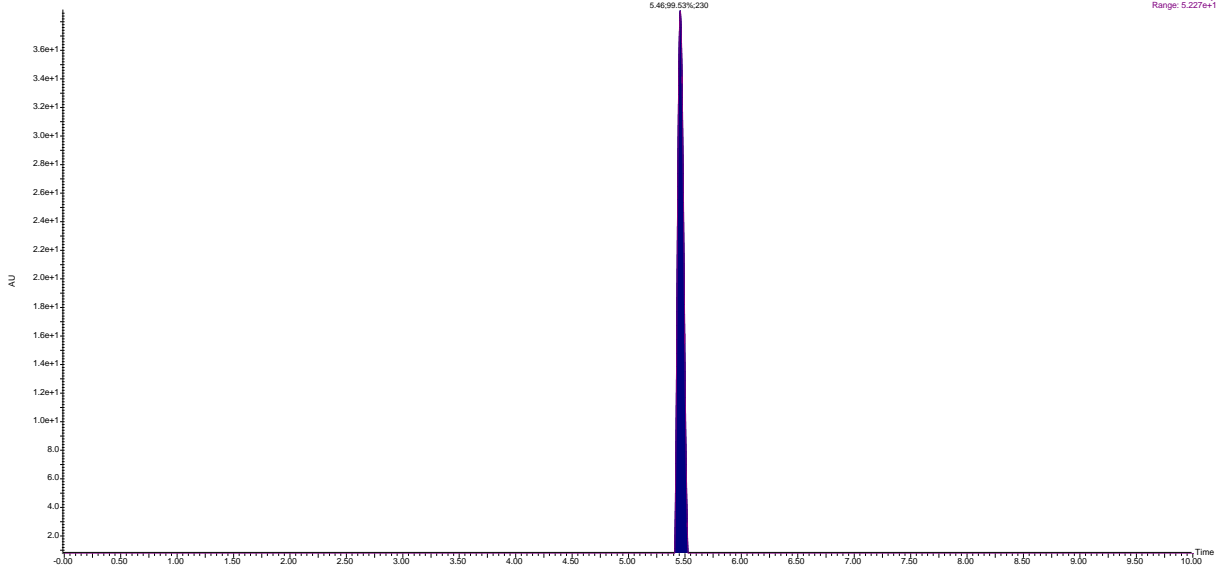
2022 08 04 FC046 B 1505 (2.623) Cm (1490:1525-(1087:1224+1660:1775))

1: TOF MS ES+
6.43e6

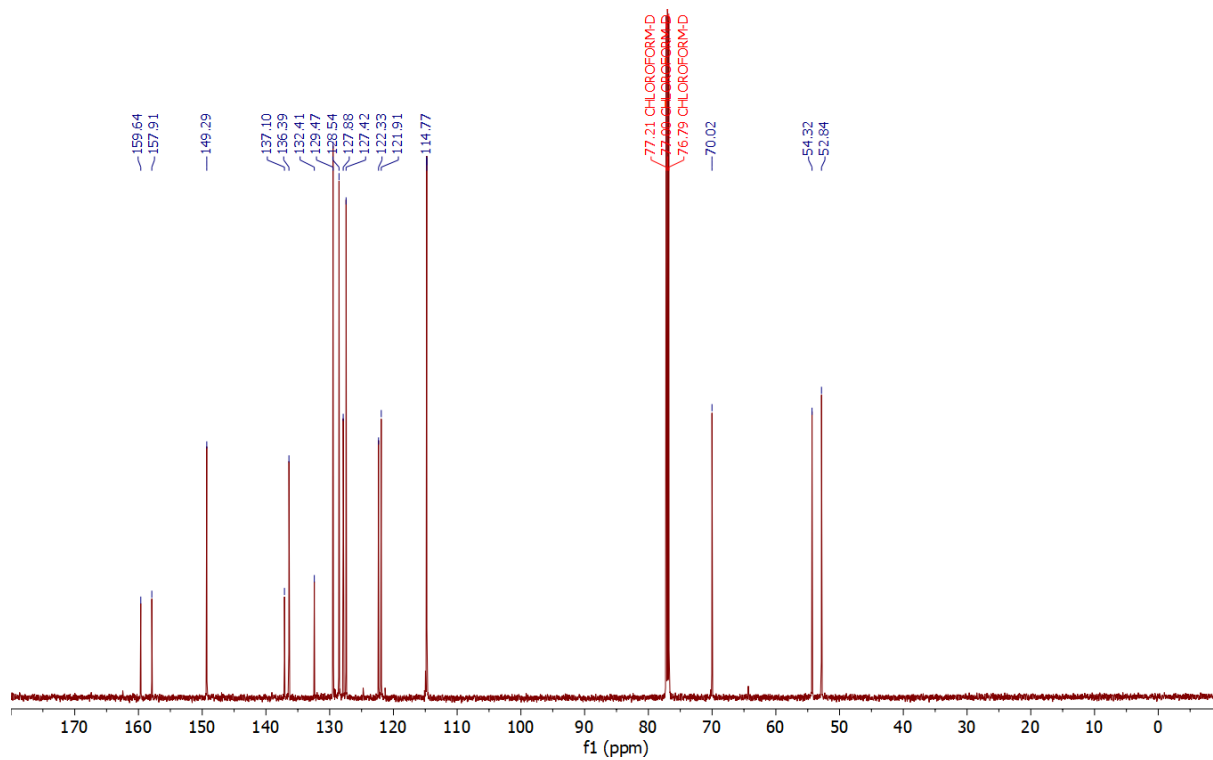
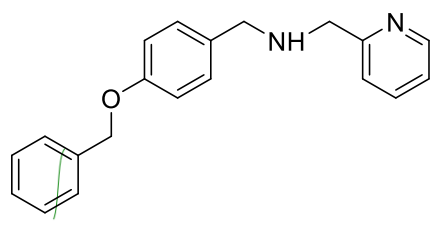
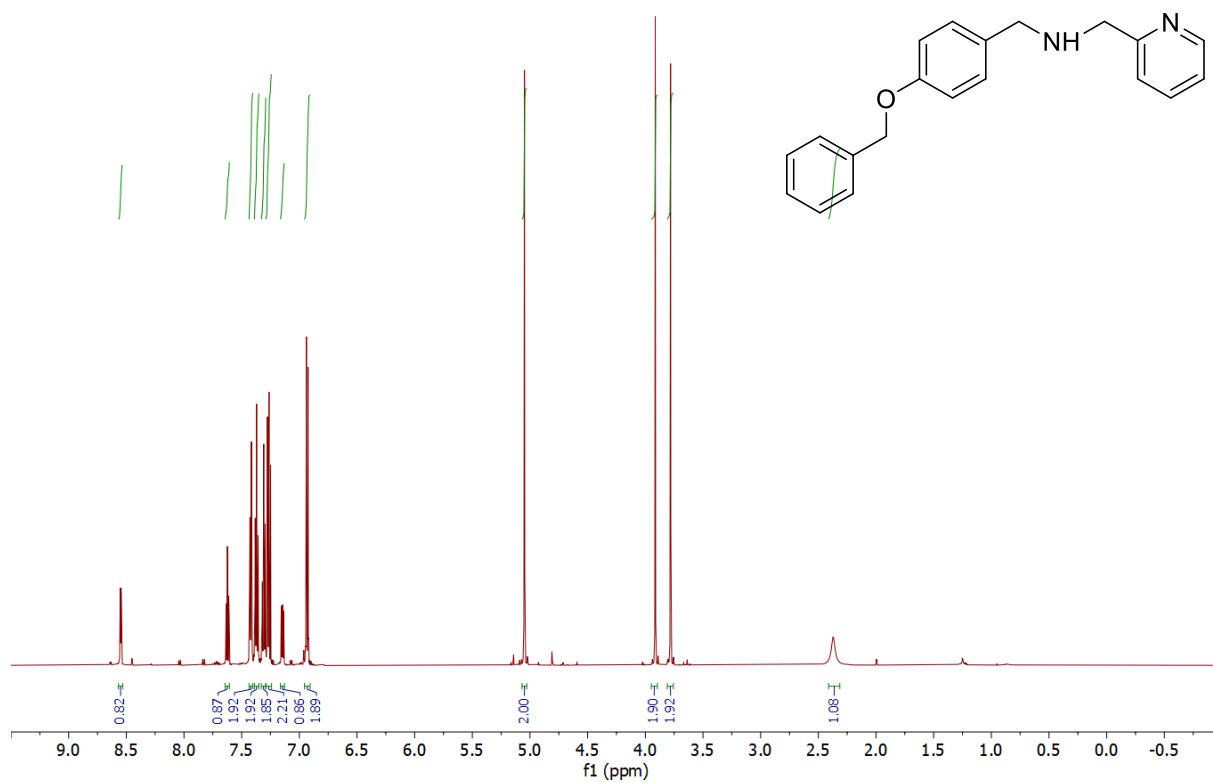


FC046

2: Diode Array
Range: 5.227e+1



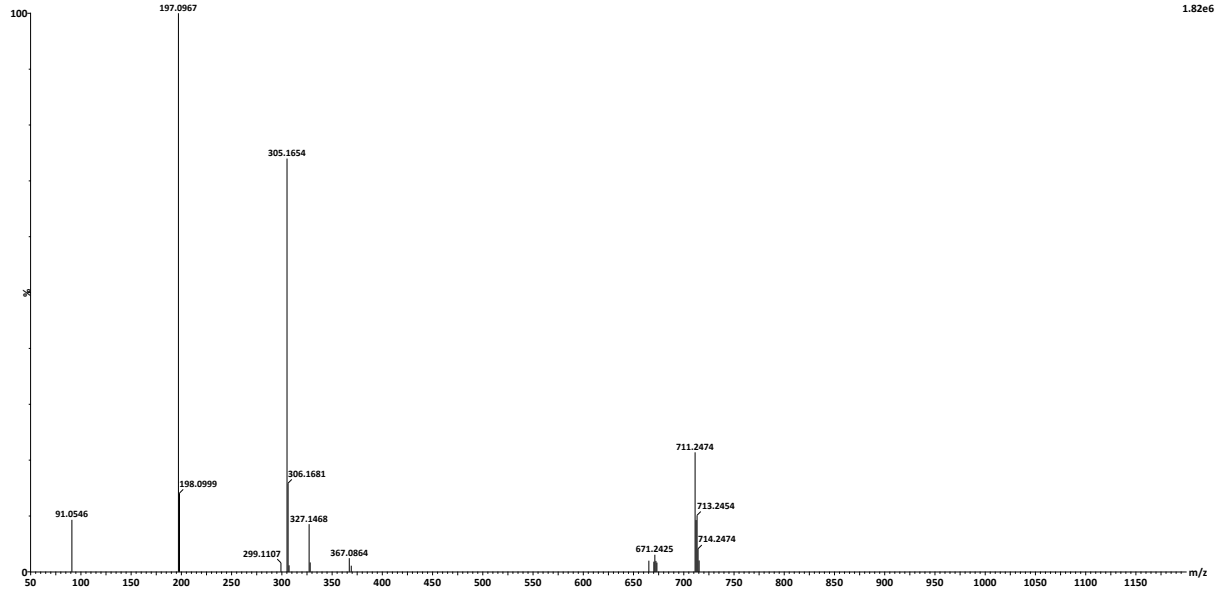
{[4-(Benzyloxy)phenyl]methyl}[(pyridin-2-yl)methyl]amine (36):



2022-08-03

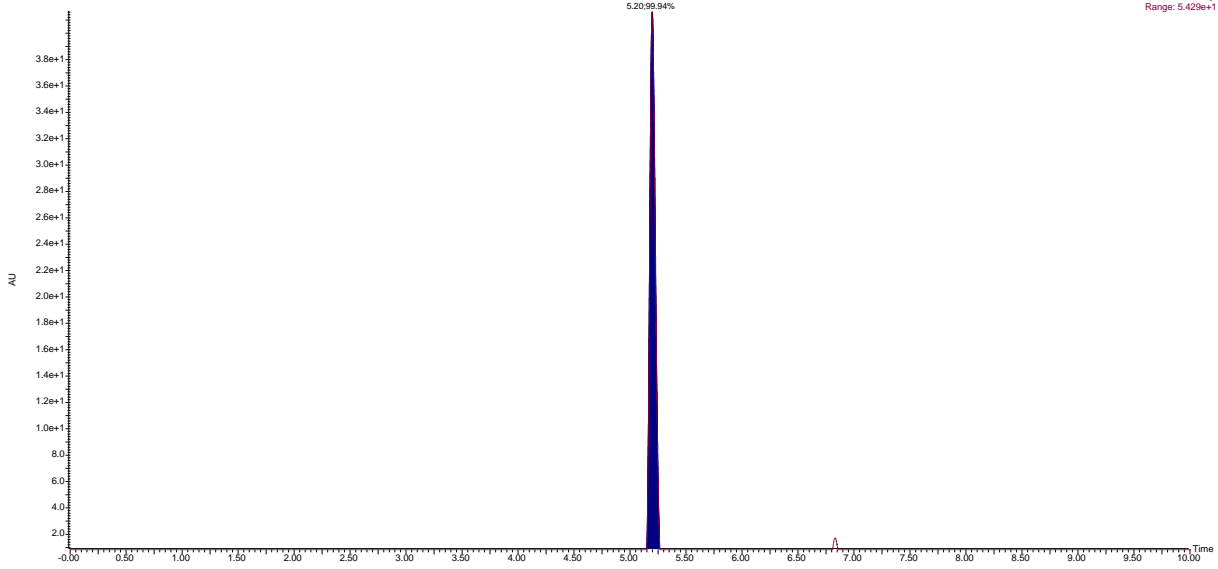
2022 08 03 F0409B 1365 (2.382) Cm (1349:1387-[117:1221+1444:1522])

1: TOF MS ES+
1.82e6

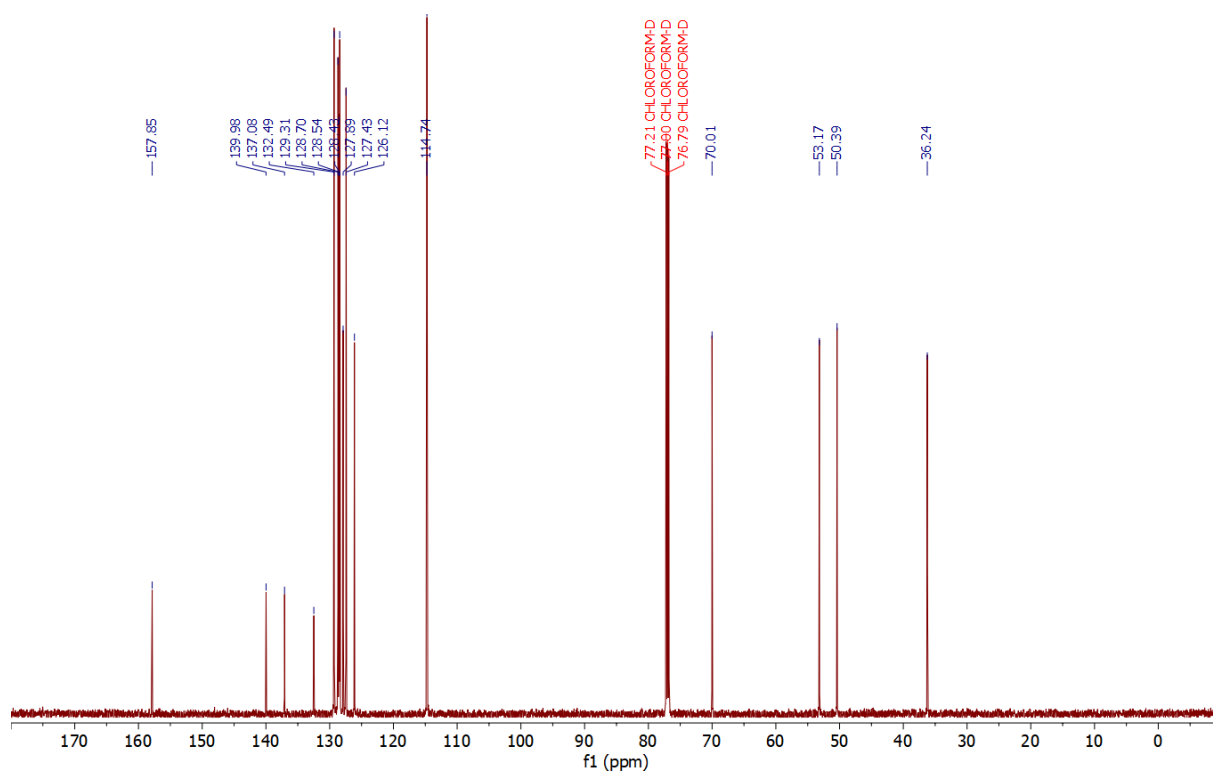
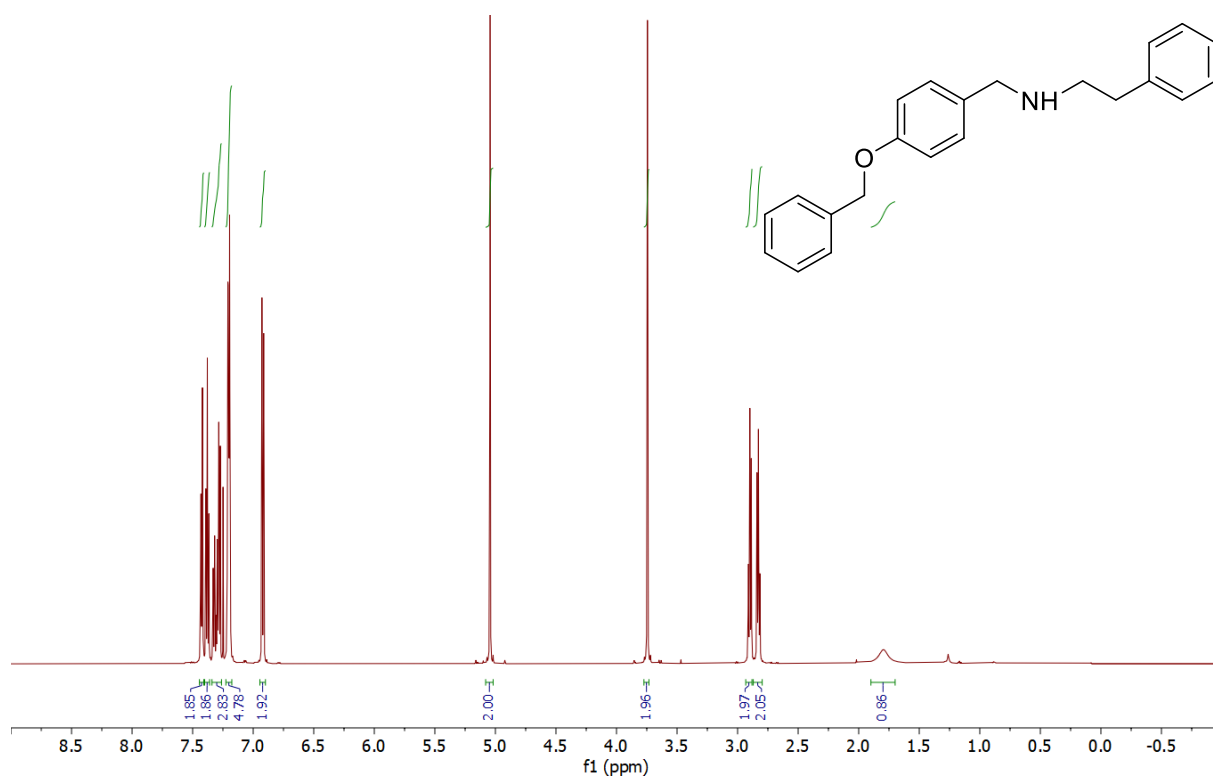


FC0409-2X

2: Diode Array
Range: 5.429e+1



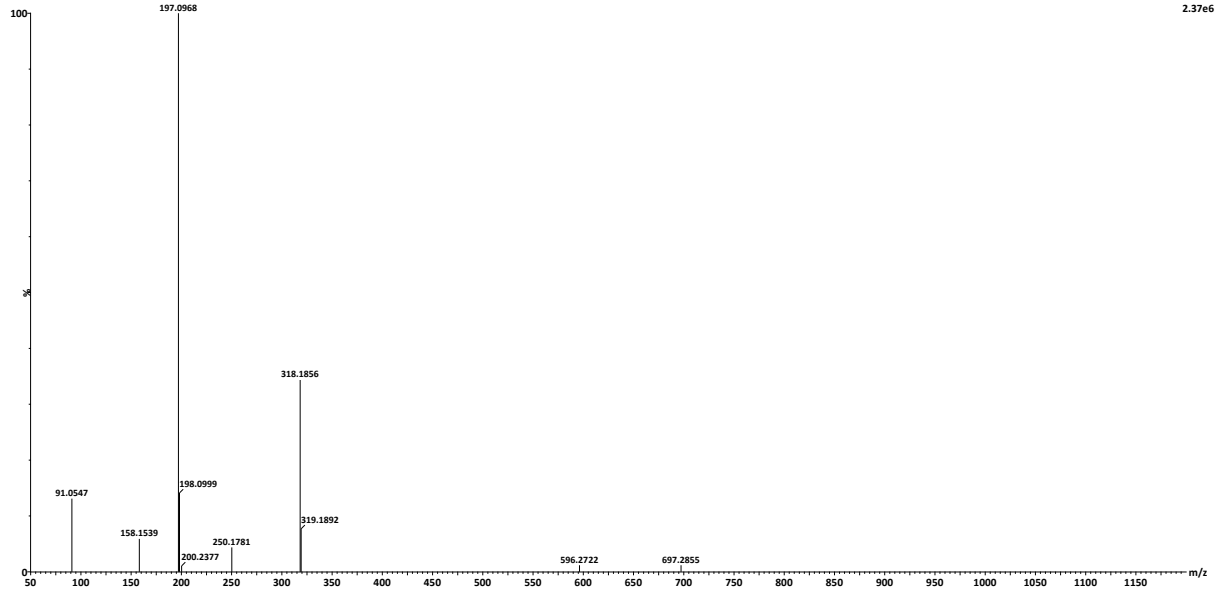
{[4-(Benzyloxy)phenyl]methyl}(2-phenylethyl)amine (37):



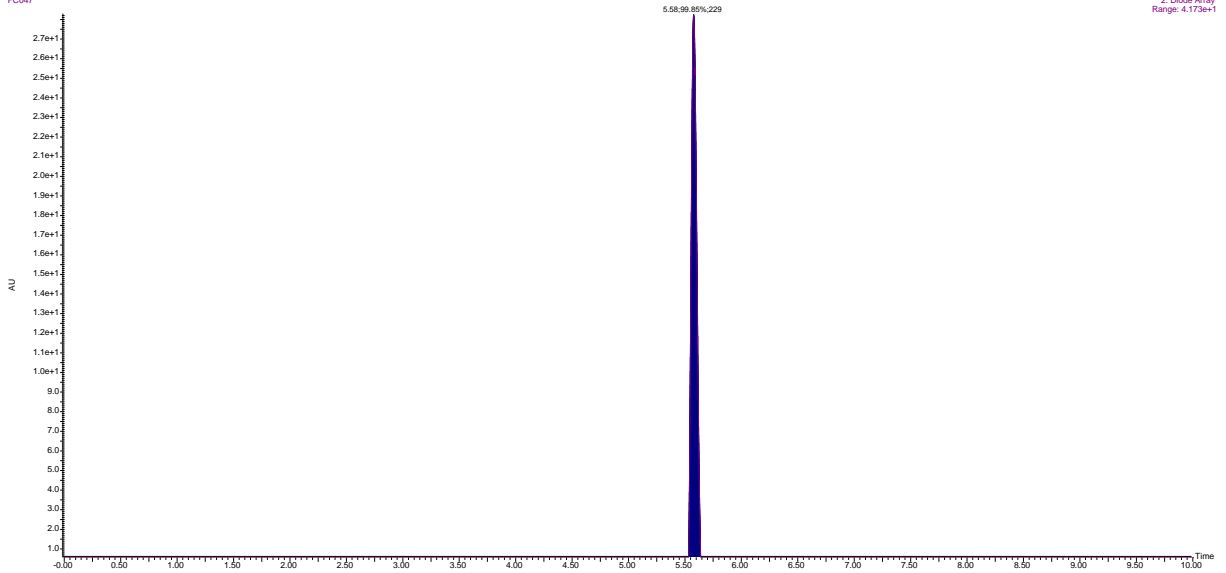
318.1802

2022 08 03 FC0478 1602 (2.793) Cm (1592:1623-(1401:1503+1700:1801))

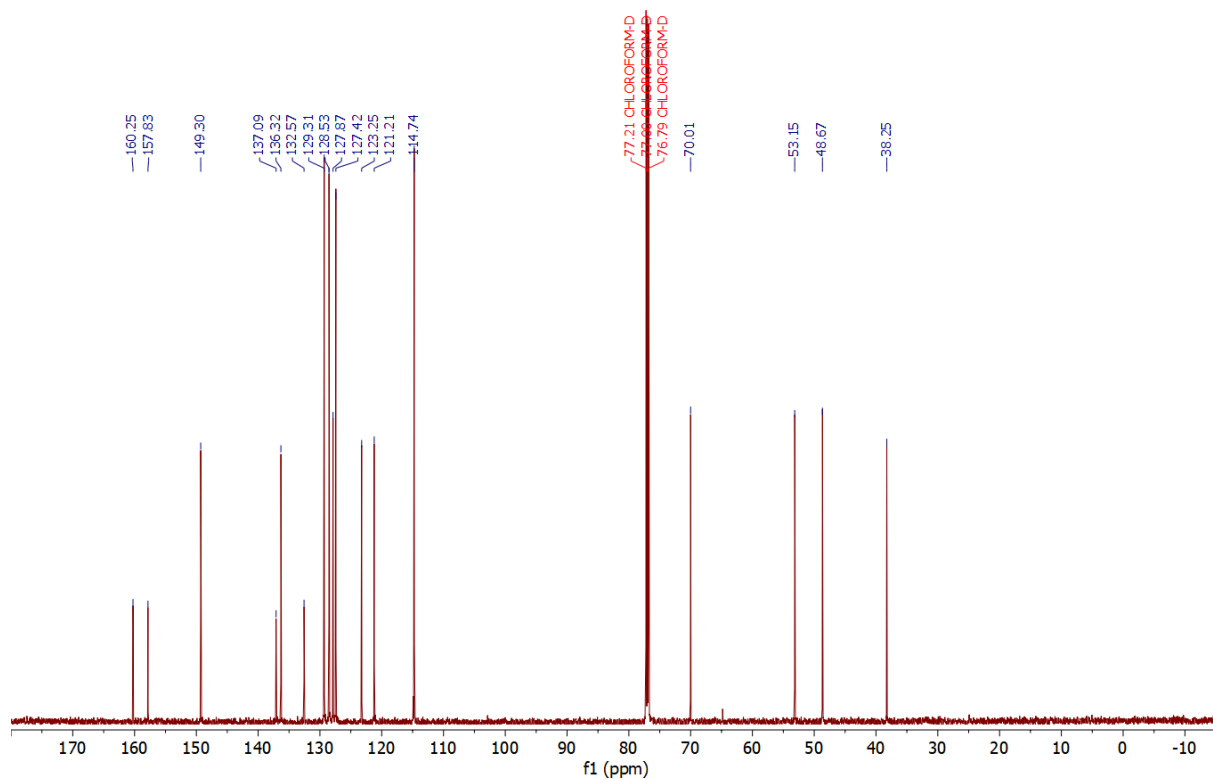
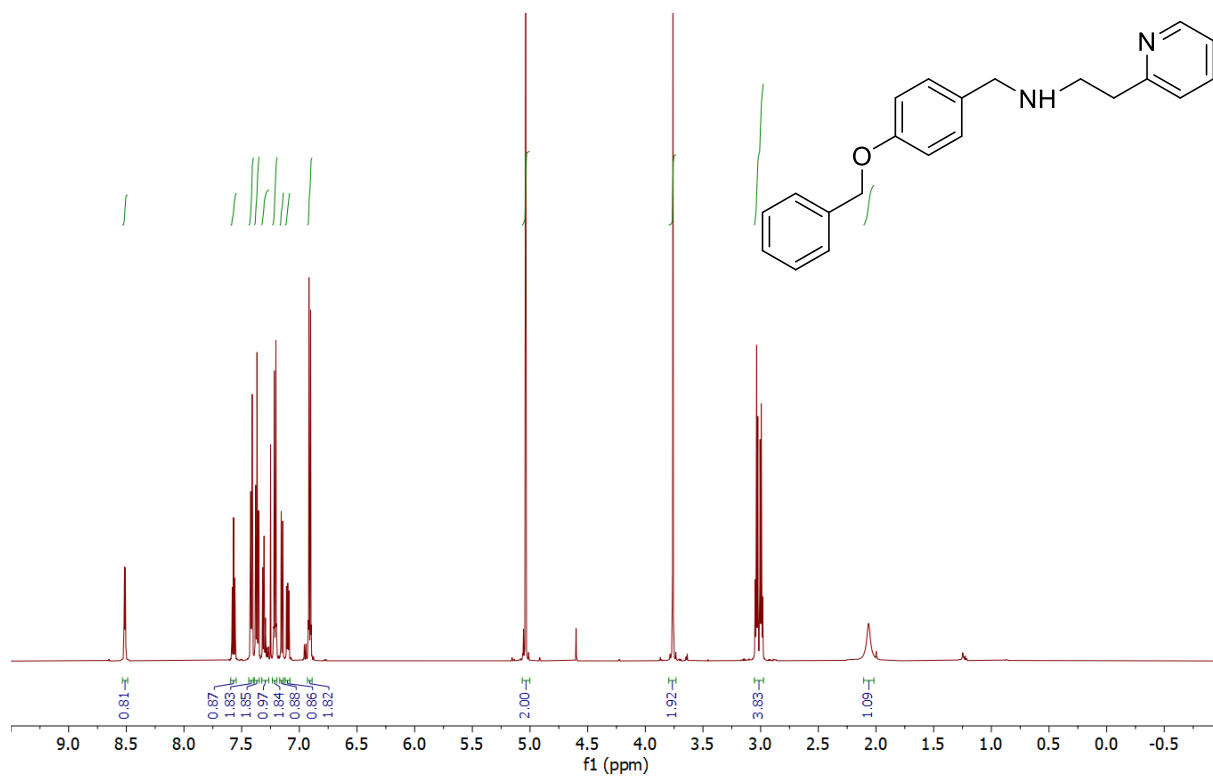
1: TOF MS ES+
2.37e6



FC047



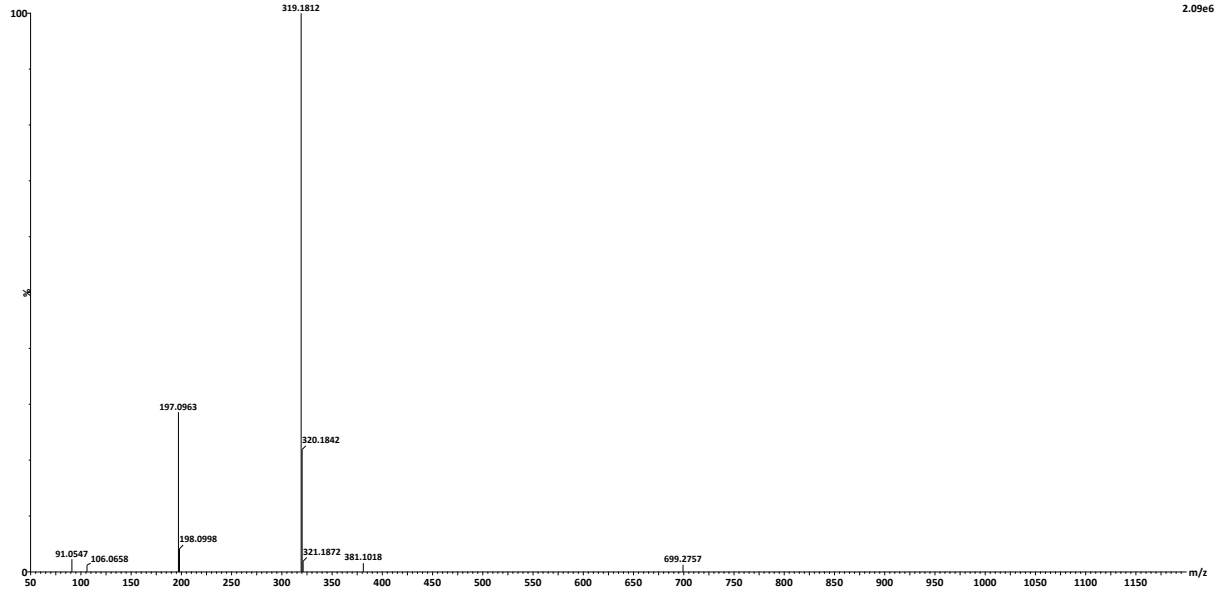
{[4-(Benzyloxy)phenyl]methyl}[2-(pyridin-2-yl)ethyl]amine (38):



310.1805

2022 08 03 FC050A 1299 (2.270) Cm (1285:1322-(1102:1183+1398:1480))

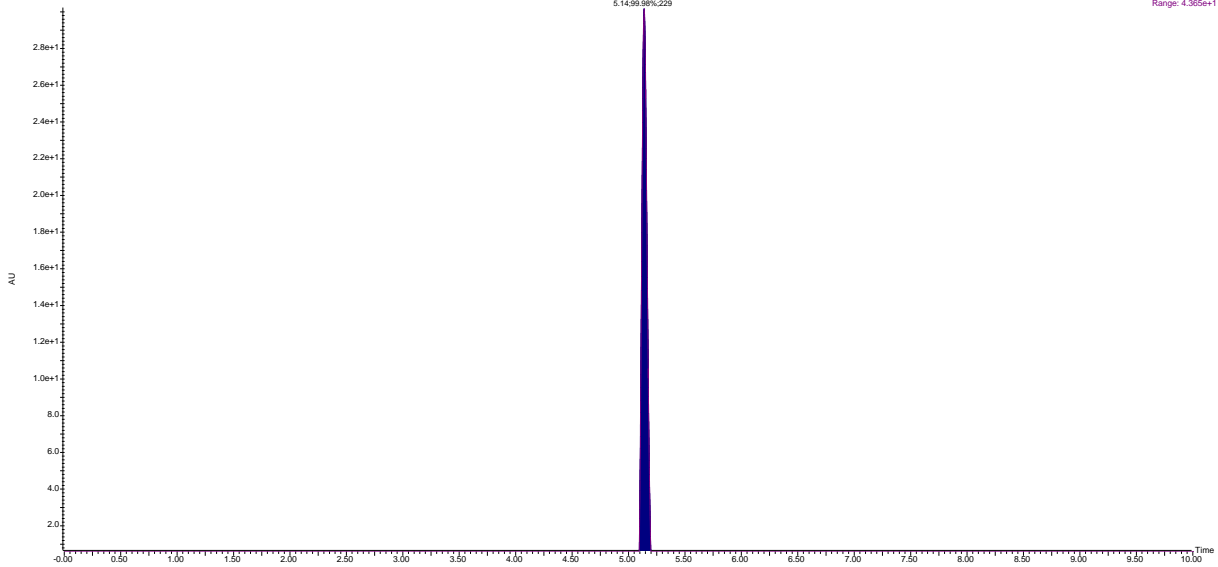
1: TOF MS ES+
2.09e6



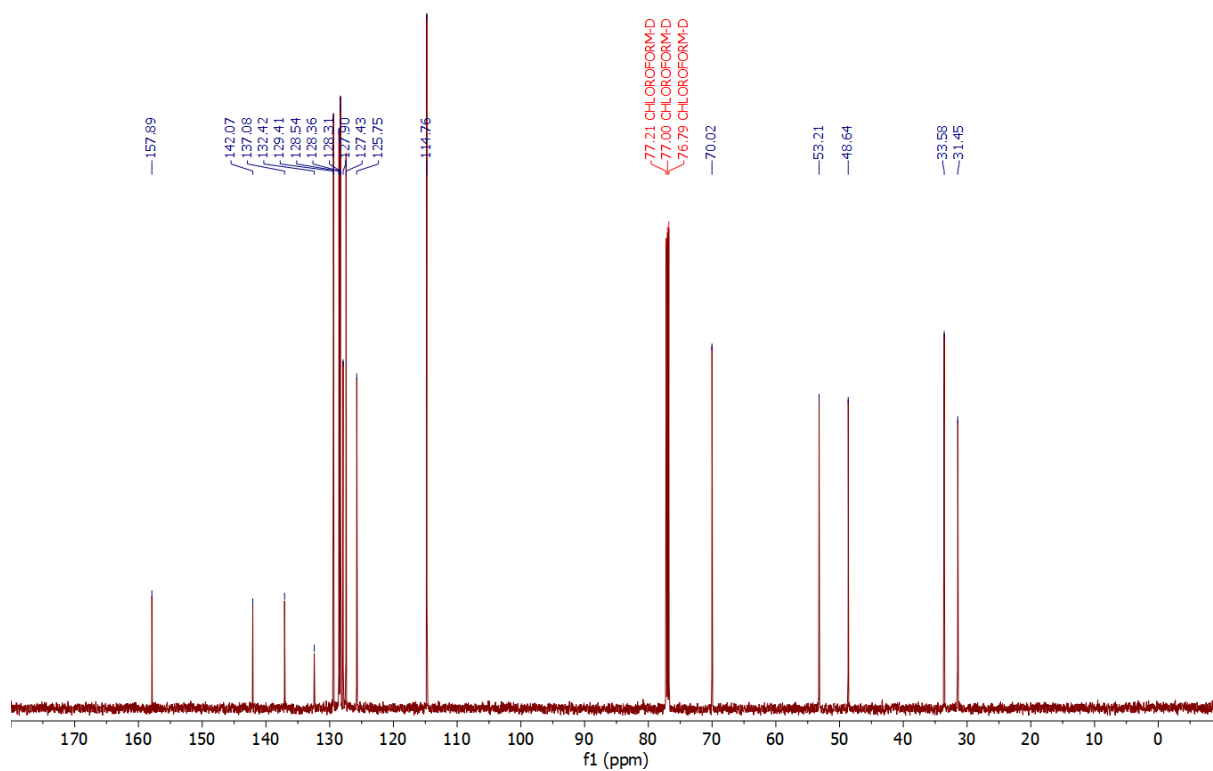
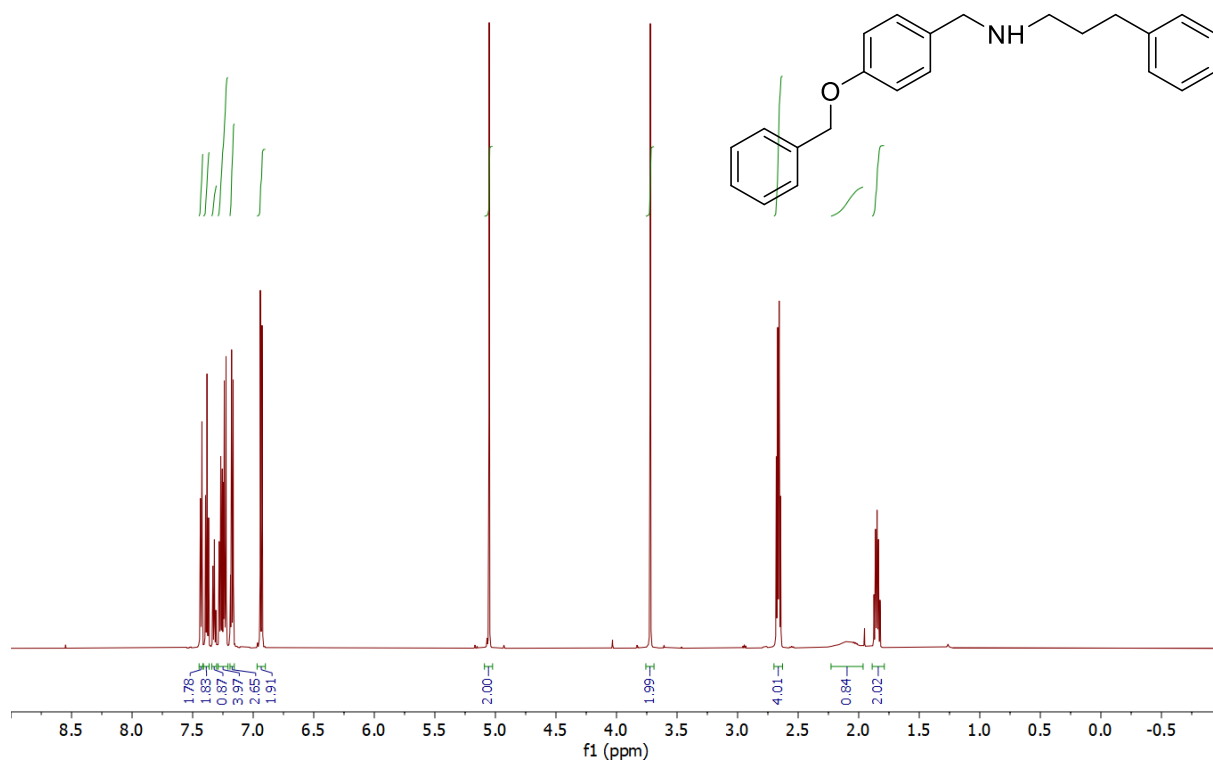
FC050

5.149998%229

2: Diode Array
Range: 4.365e+1



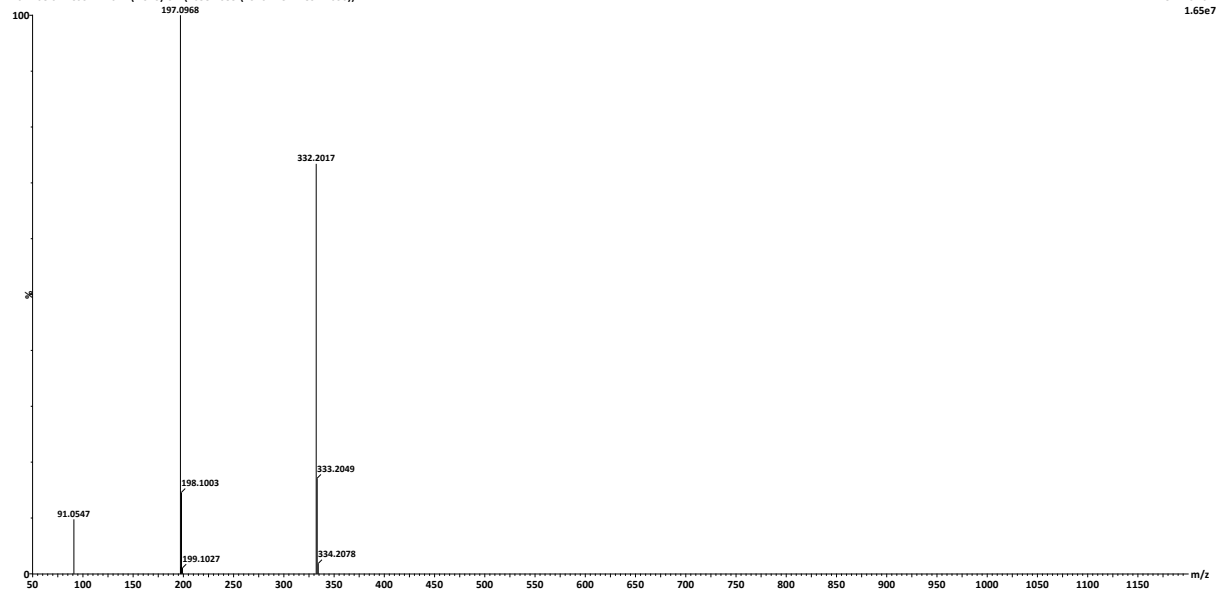
{[4-(Benzyloxy)phenyl]methyl}(3-phenylpropyl)amine (39):



201-1096

2022 08 04 FC032 B 1672 (2.913) Cm (1658:1685-(1320:1454+1897:2030))

1: TOF MS ES+
1.65e7

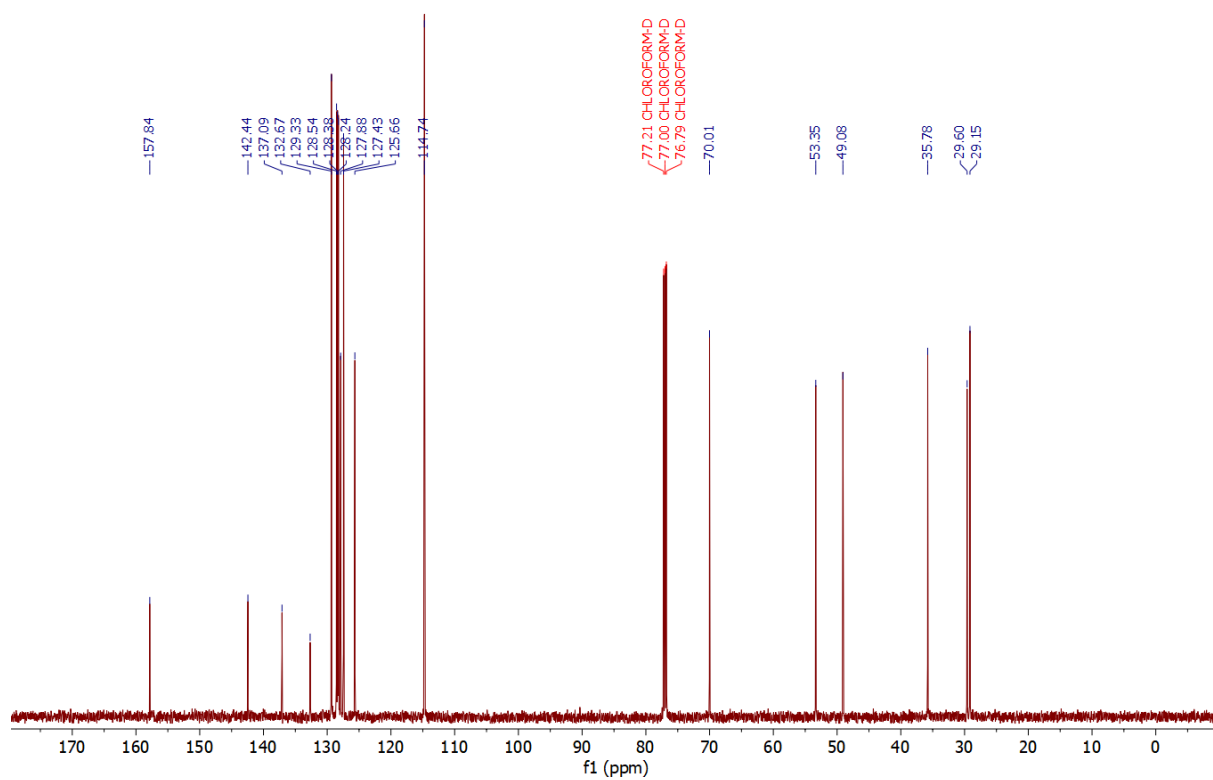
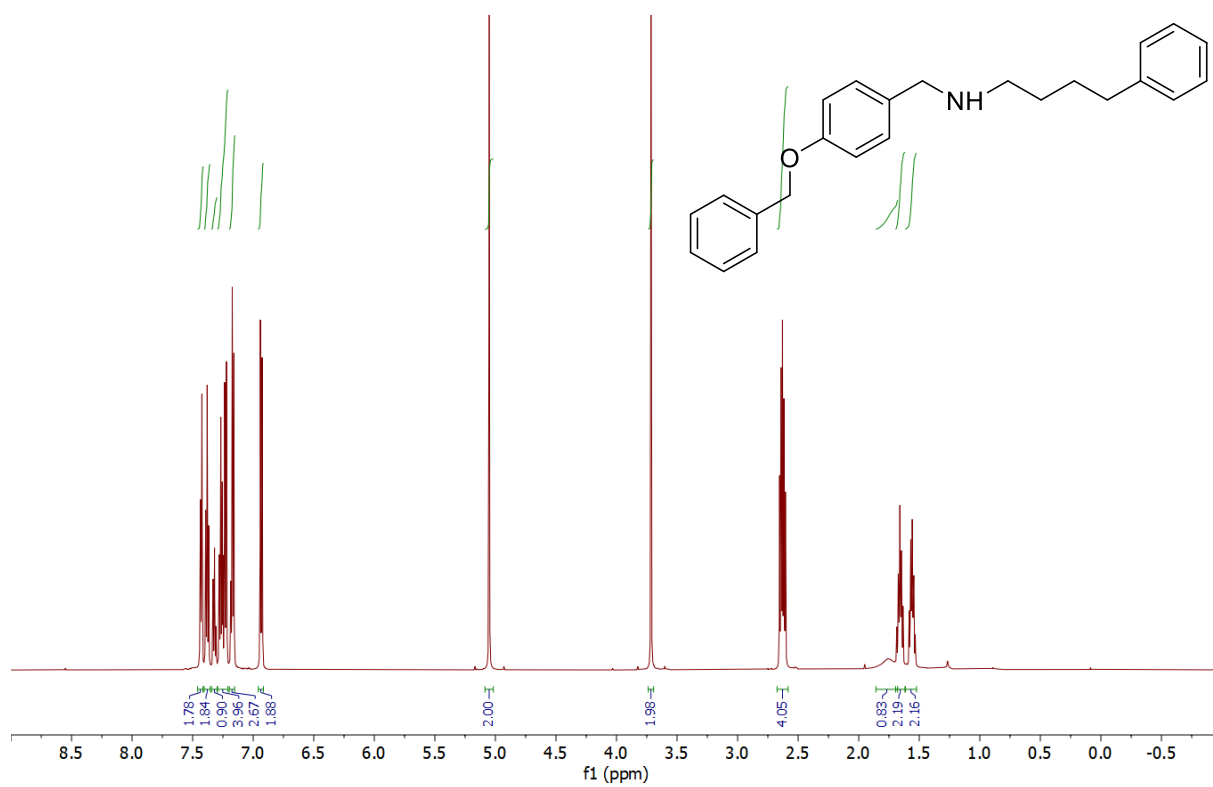


FC032

2: Diode Array
Range: 4.672e+1



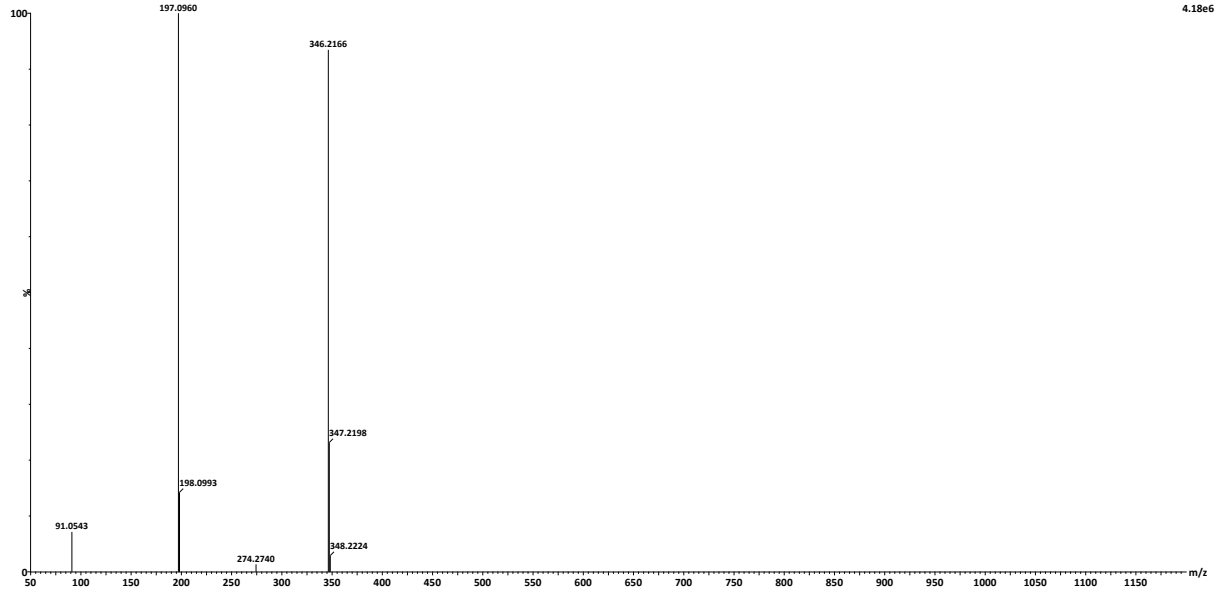
{[4-(Benzyloxy)phenyl]methyl}{4-phenylbutyl}amine (40):



346.2166

2022 08 03 FC034A 1767 (3.074) Cm (1754:1788-(1515:1615+1870:1953))

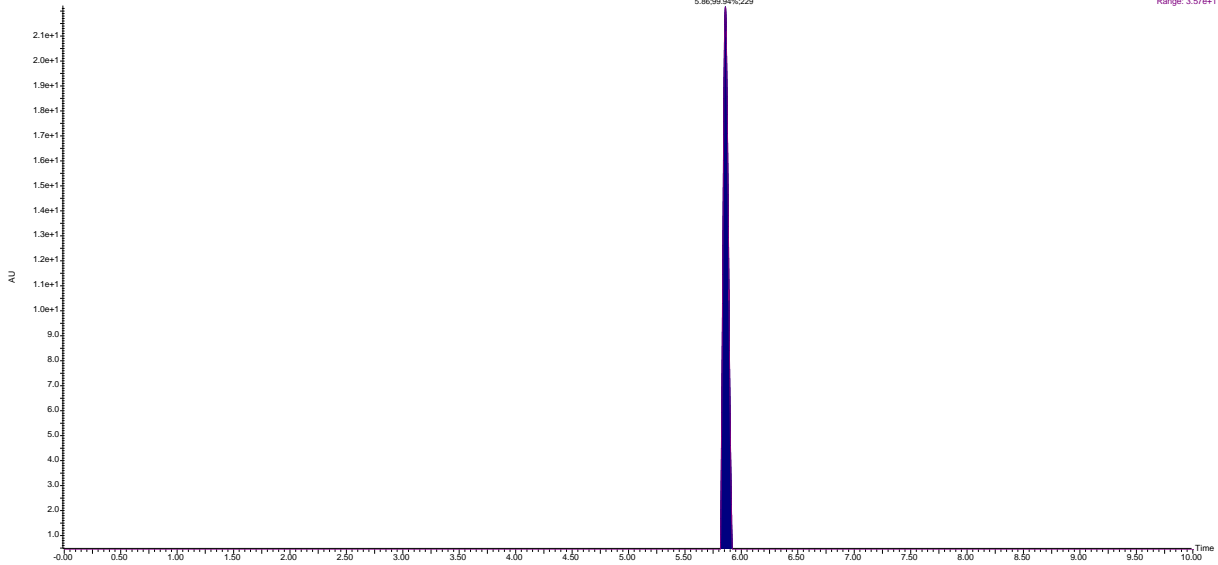
1: TOF MS ES+
4.18e6



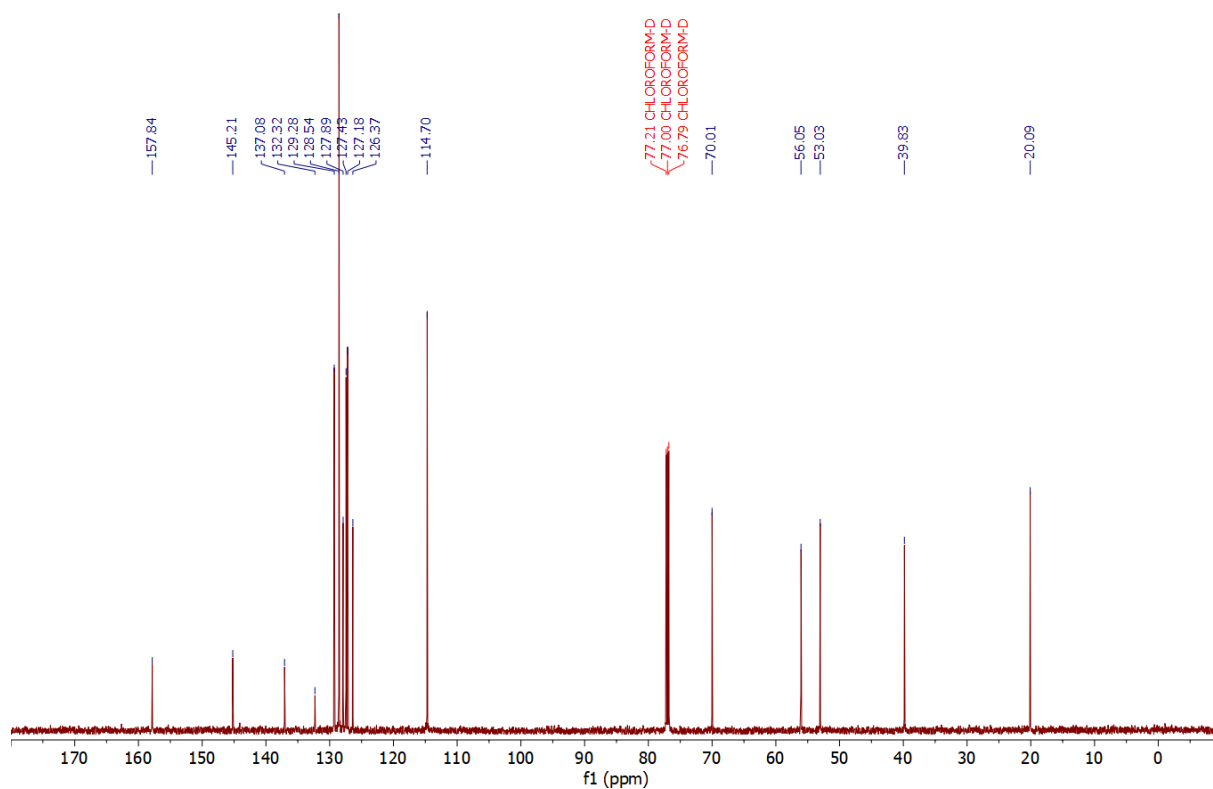
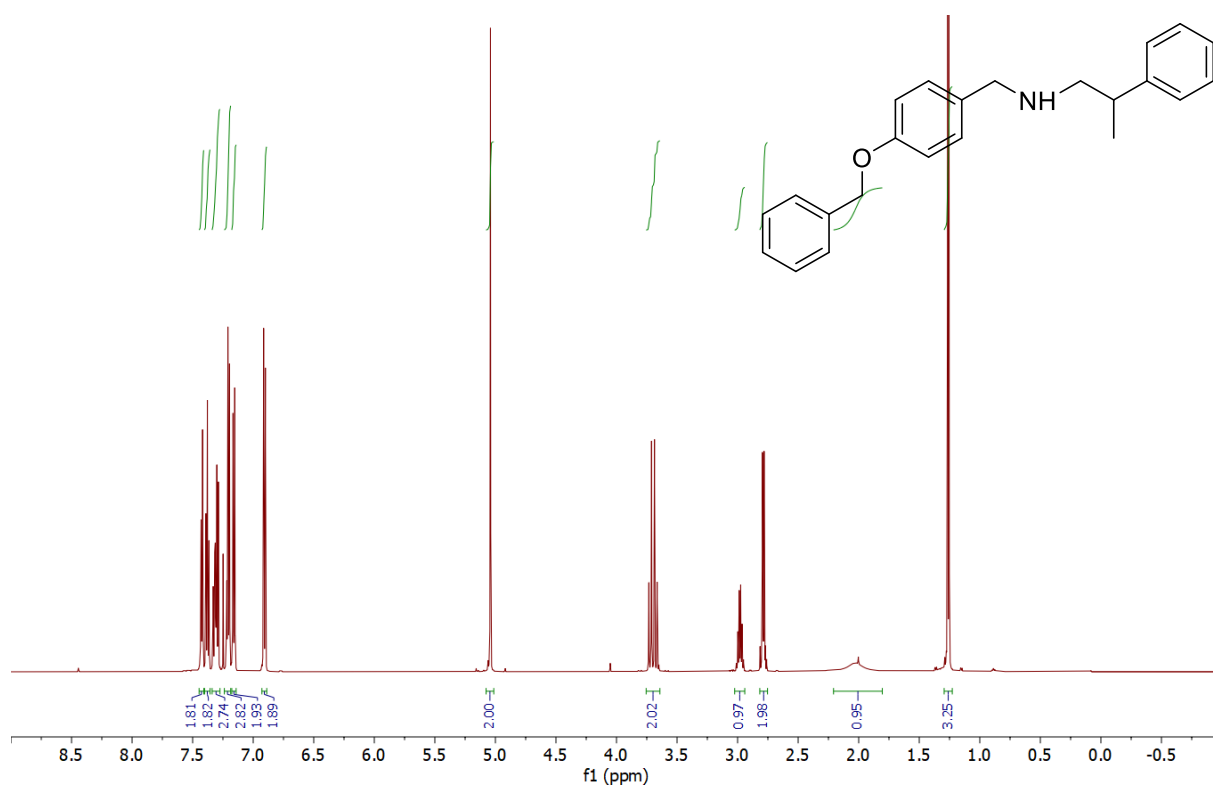
FC034

5.663934%(229)

2: Diode Array
Range: 3.57e+1



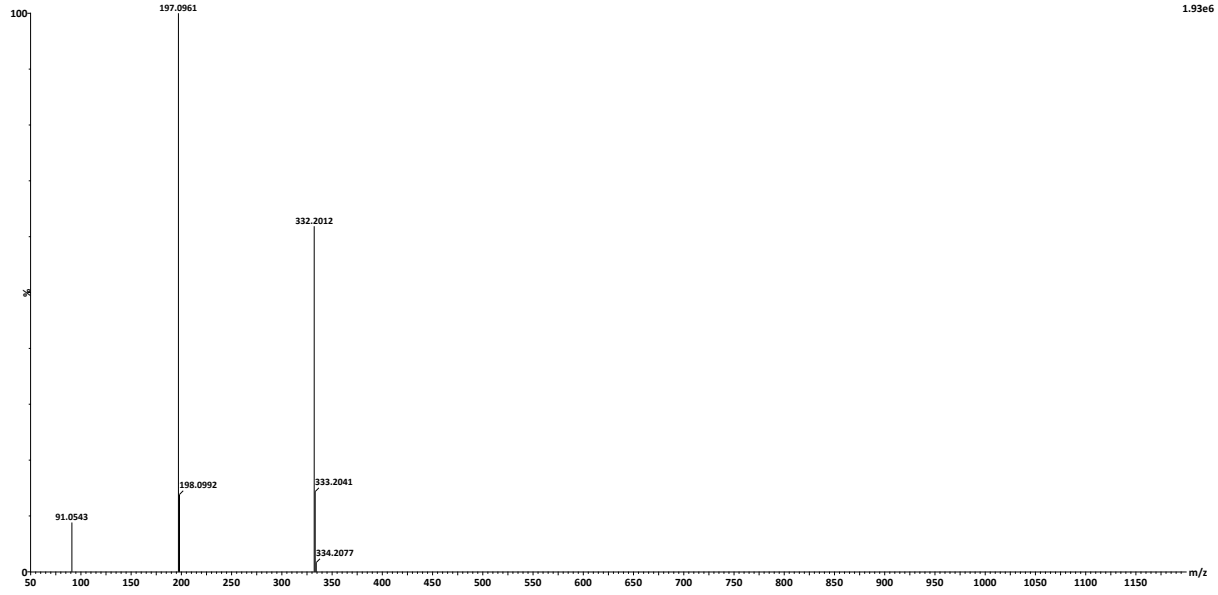
{[4-(Benzyloxy)phenyl]methyl}(2-phenylpropyl)amine (41):



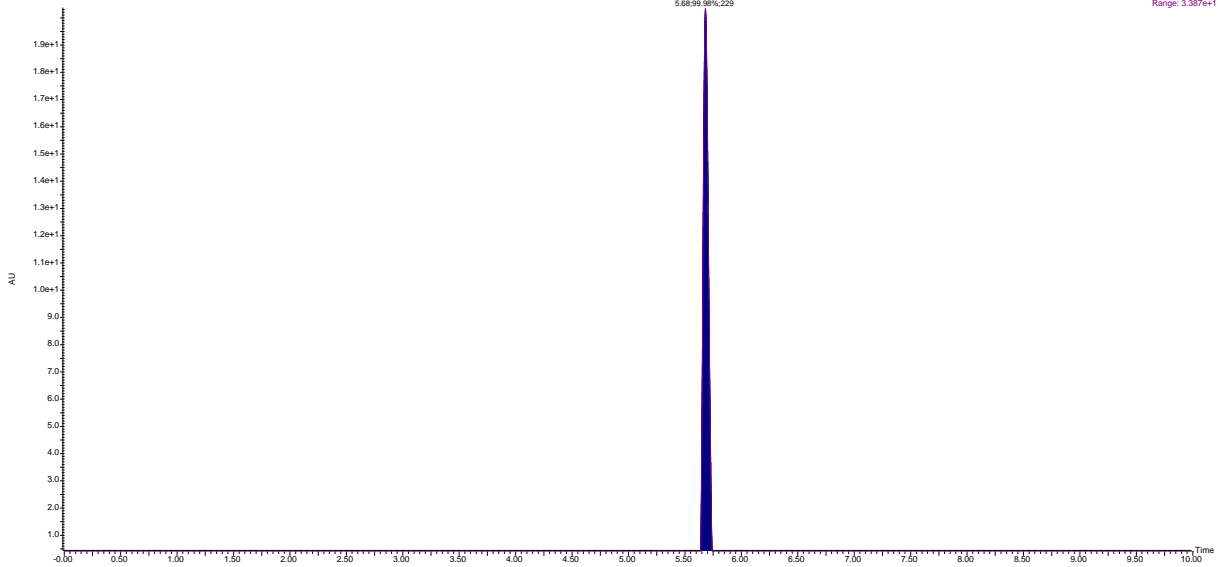
20220809

2022 08 03 FC031 B 1656 (2.886) Cm (1649:1679-(1450:1545+1758:1860))

1: TOF MS ES+
1.93e6

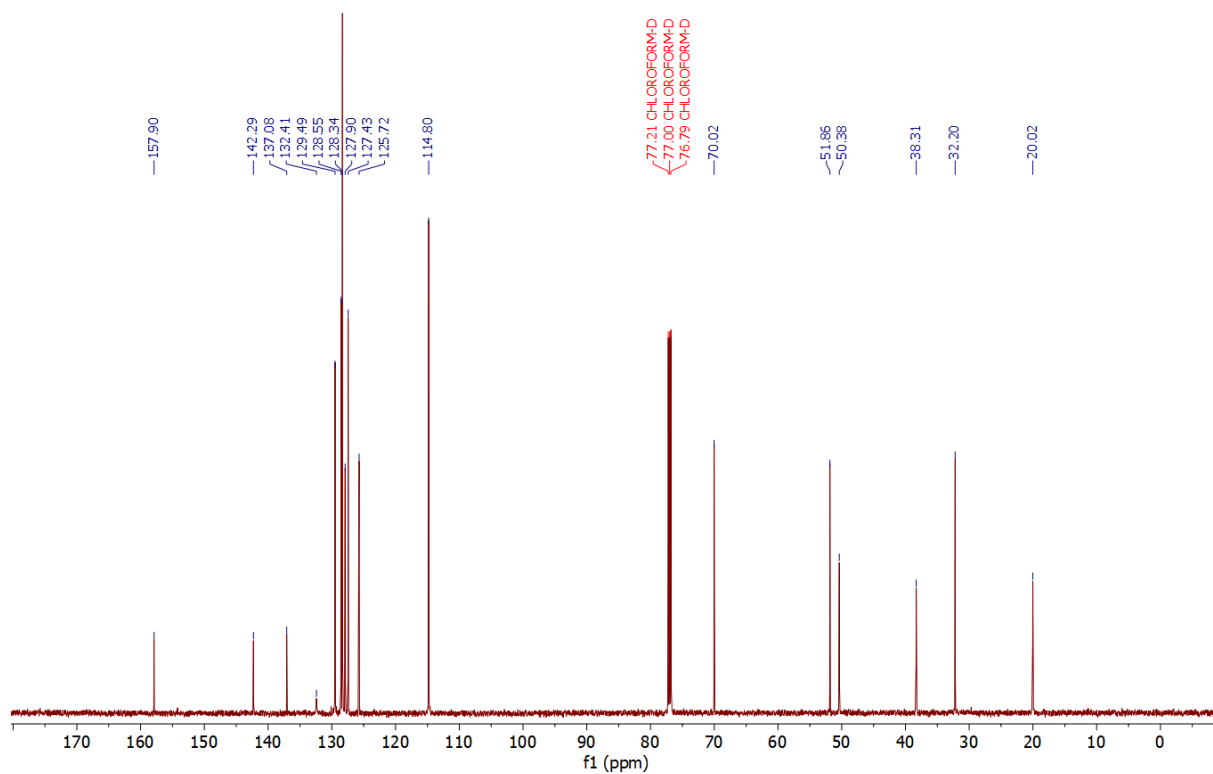
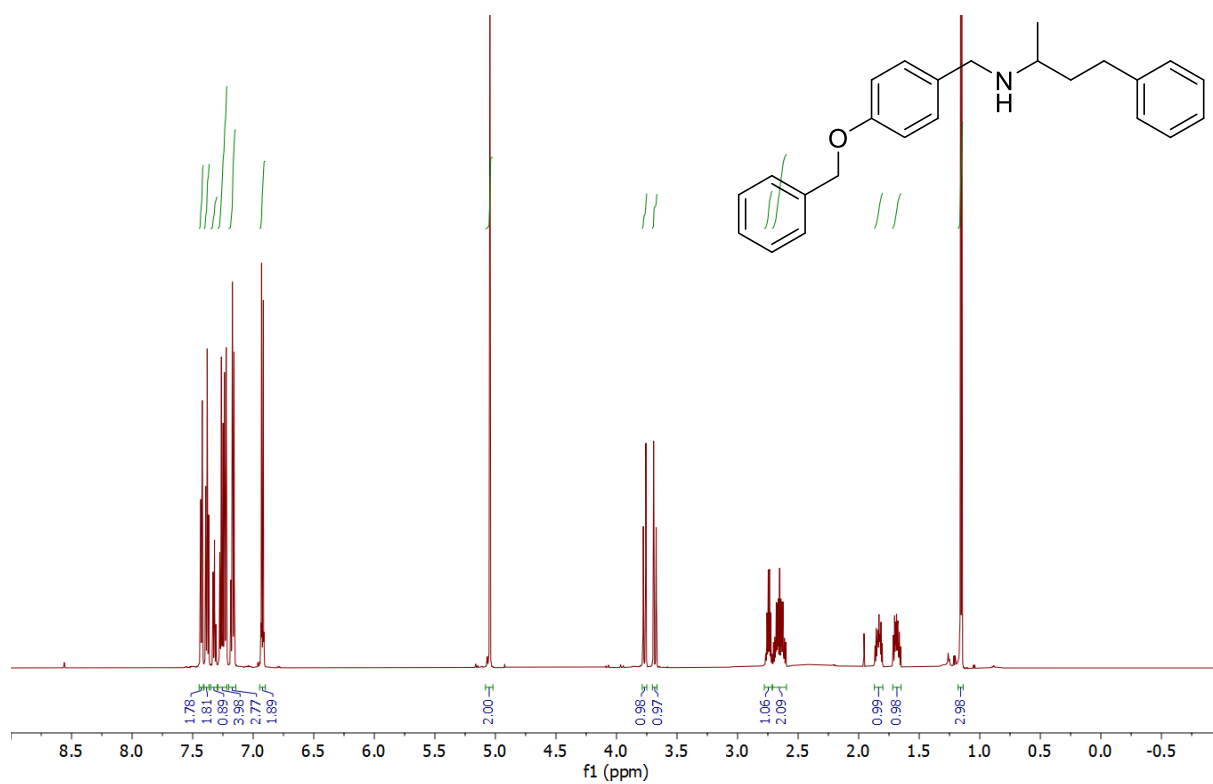


FC031



2: Diode Array
Range: 3.387e+1

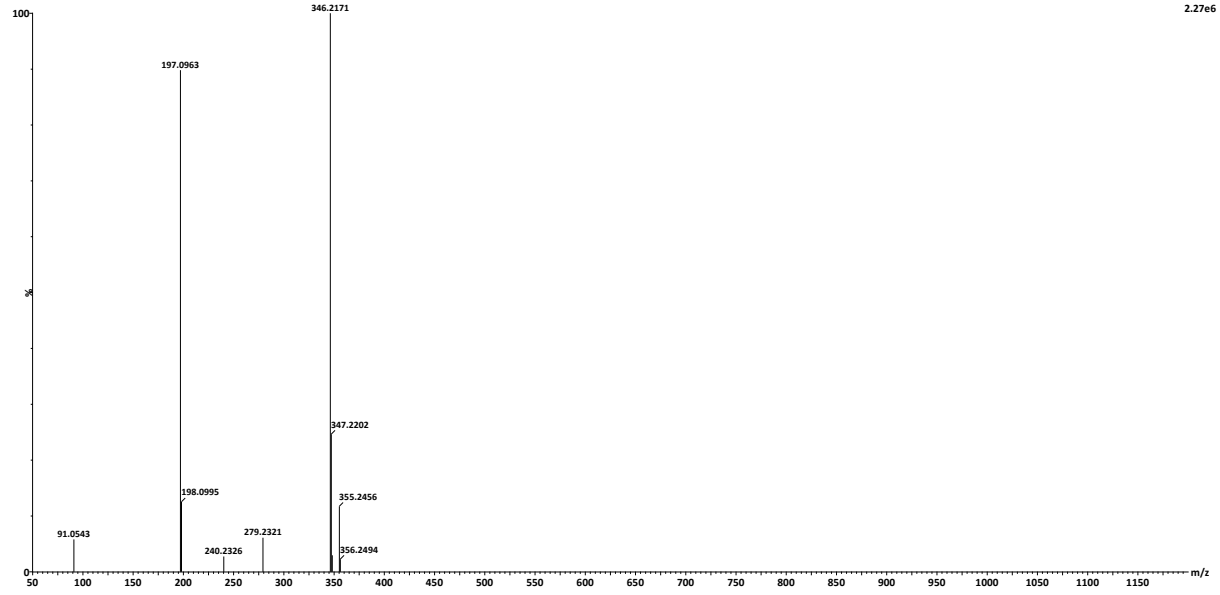
{[4-(Benzyloxy)phenyl]methyl}{4-phenylbutan-2-yl}amine (42):



346.2165

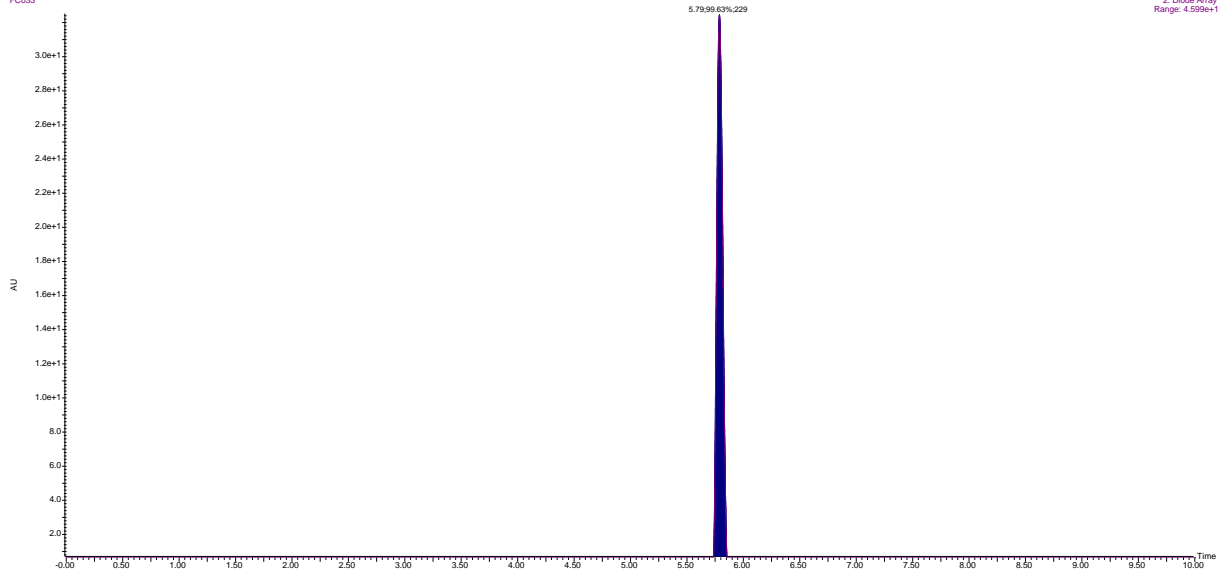
2022 08 03 FC033A 1726 (3.007) Cm (1712:1742-(1440:1558+1820:1932))

1: TOF MS ES+
2.27e6

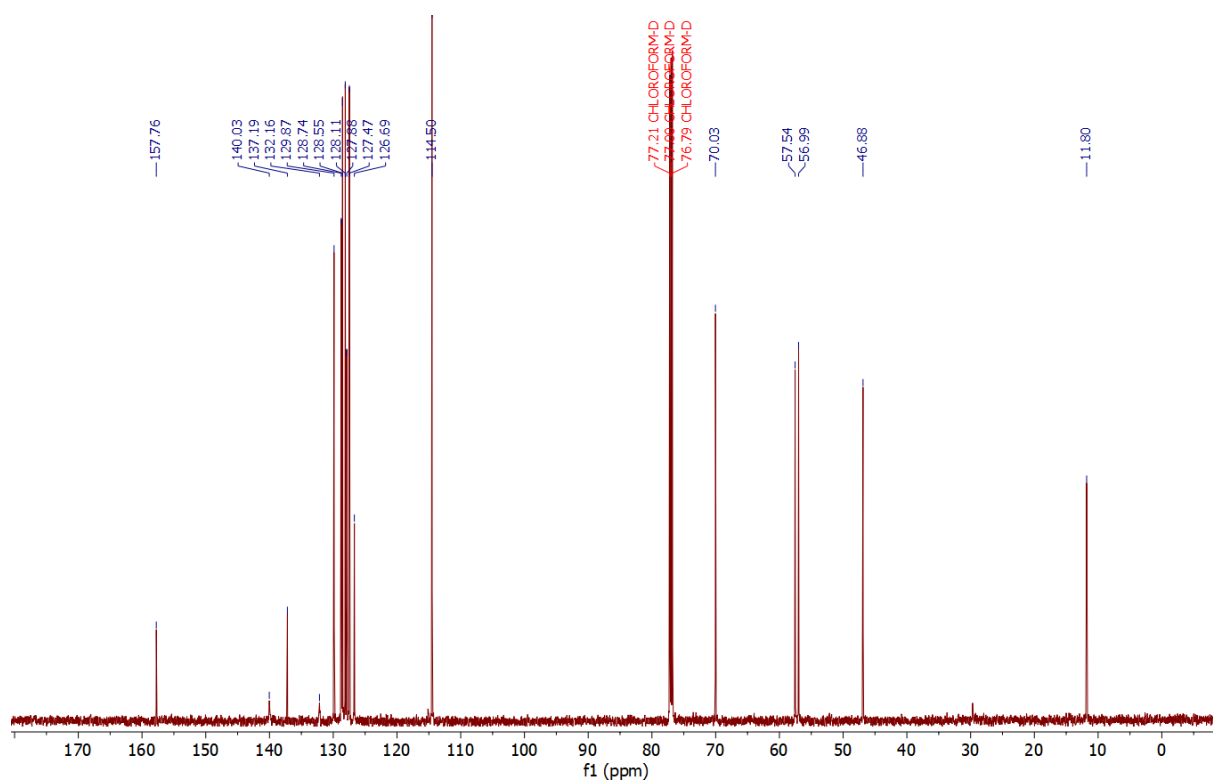
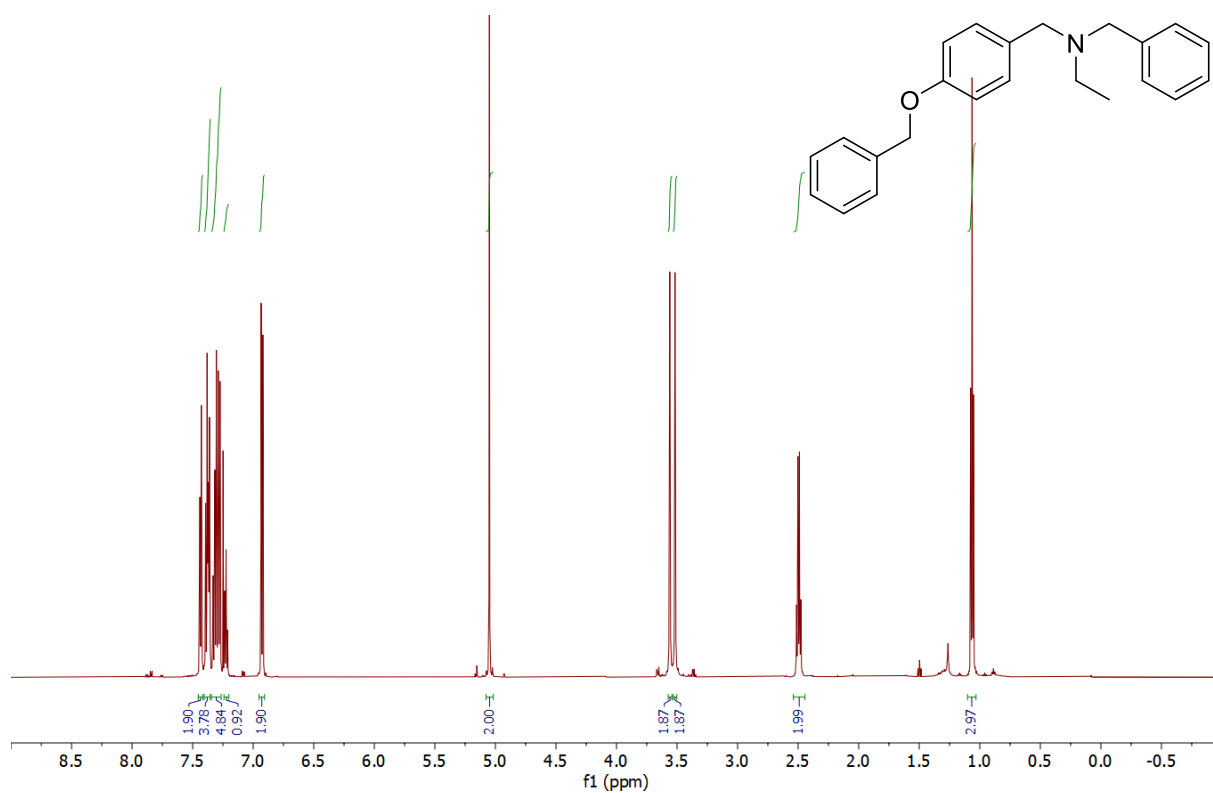


FC033

2: Diode Array
Range: 4.599e+1



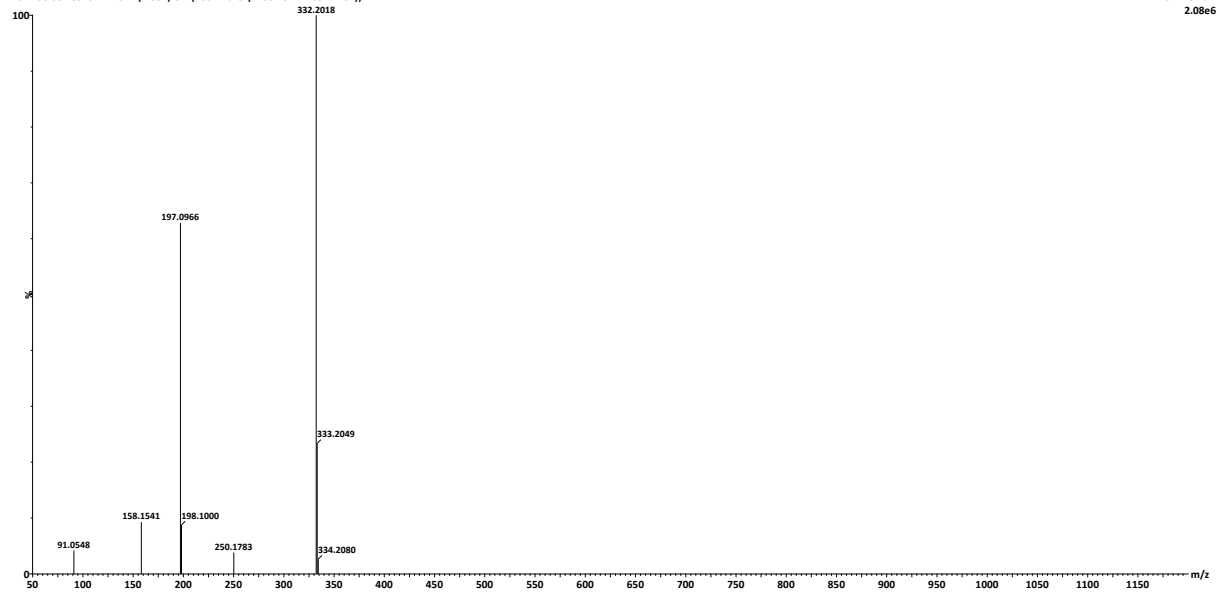
Benzyl([4-(benzyloxy)phenyl]methyl)ethylamine (43):



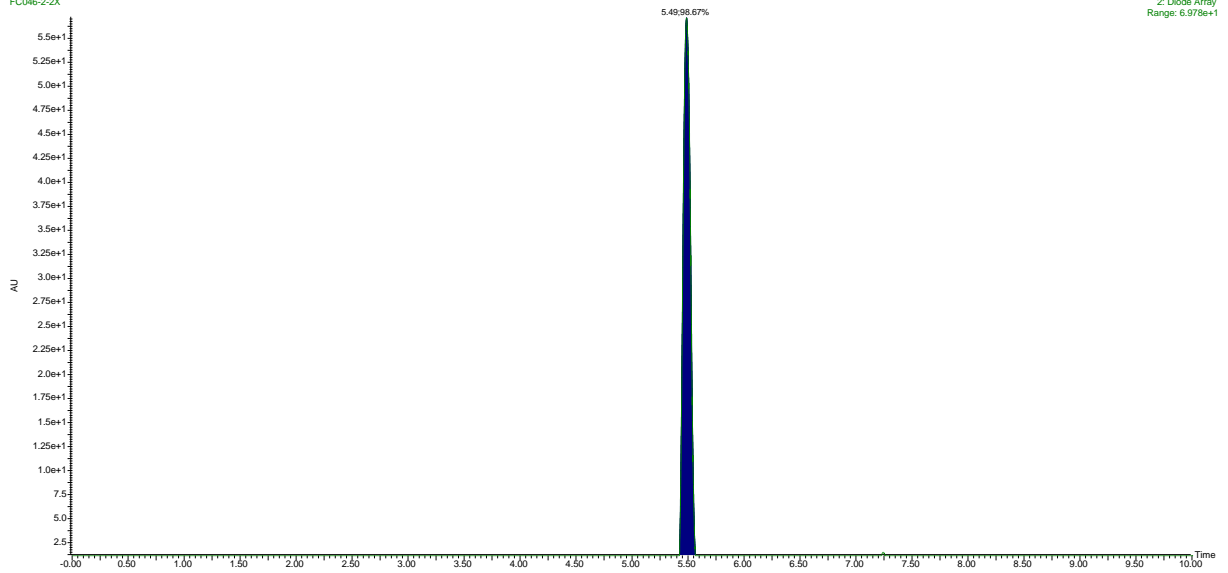
20220809

2022 08 03 FC046-2A 1611 (2.807) Cm (1601:1629-(1430:1514+1687:1781))

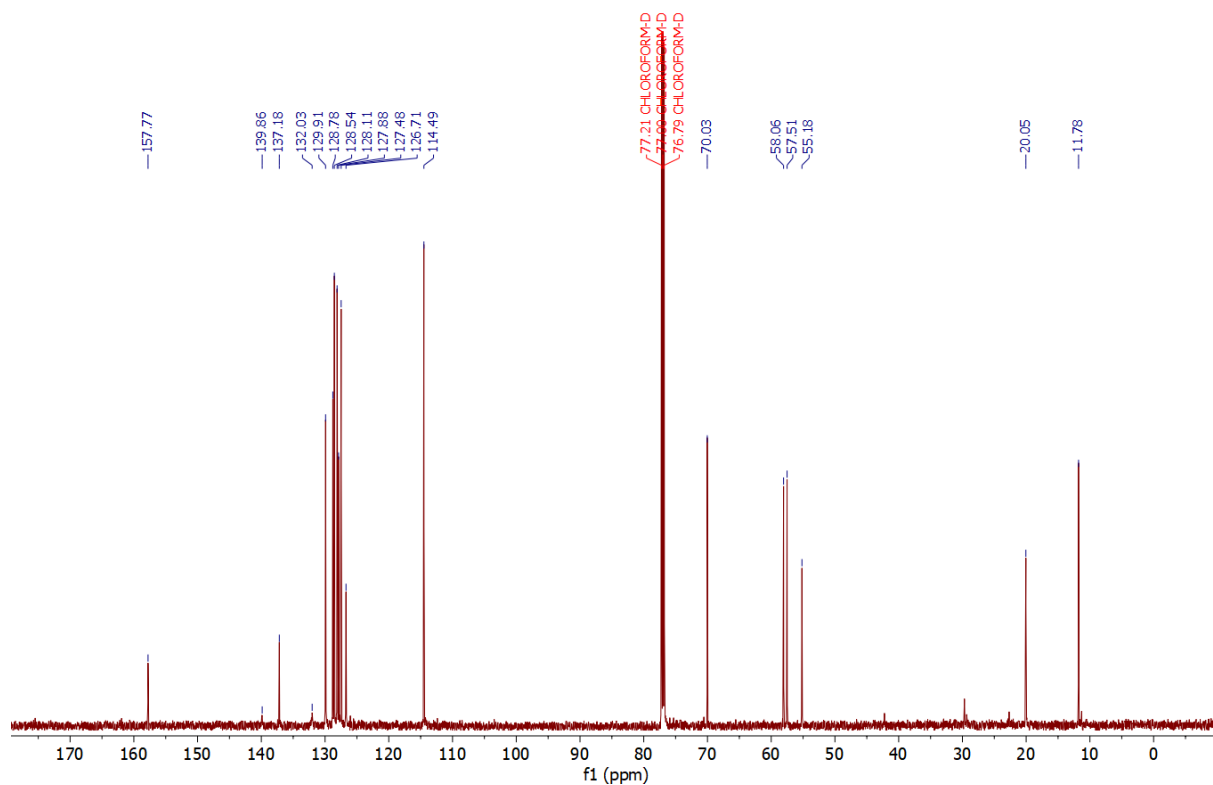
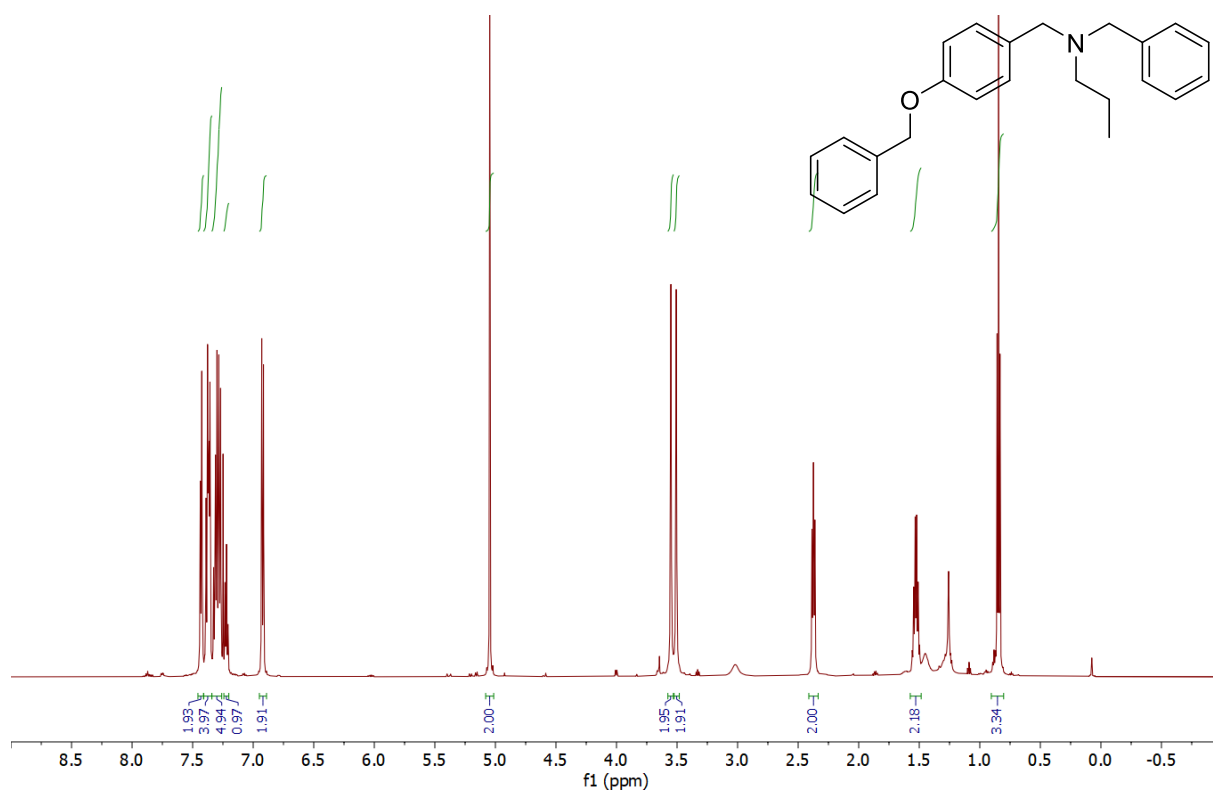
1: TOF MS ES+
2.08e6



FC046-2-2X



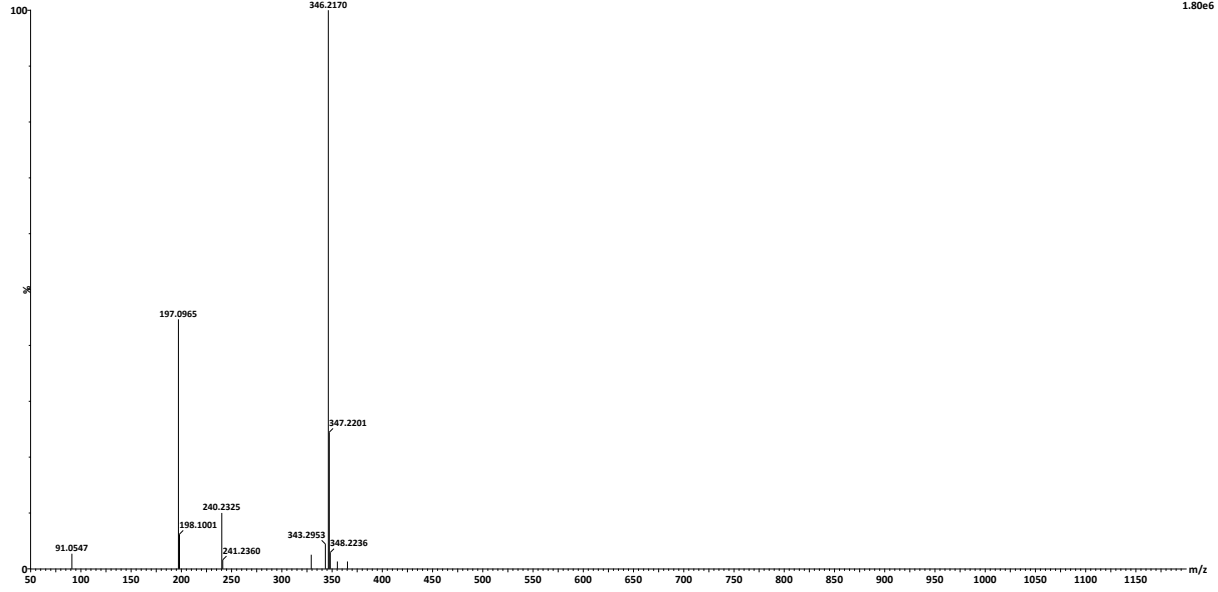
Benzyl({[4-(benzyloxy)phenyl]methyl})propylamine (44):



346.2165

2022 08 03 F0406-1A 1711 (2.978) Cm (1700:1726-(1521:1594+1788:1855))

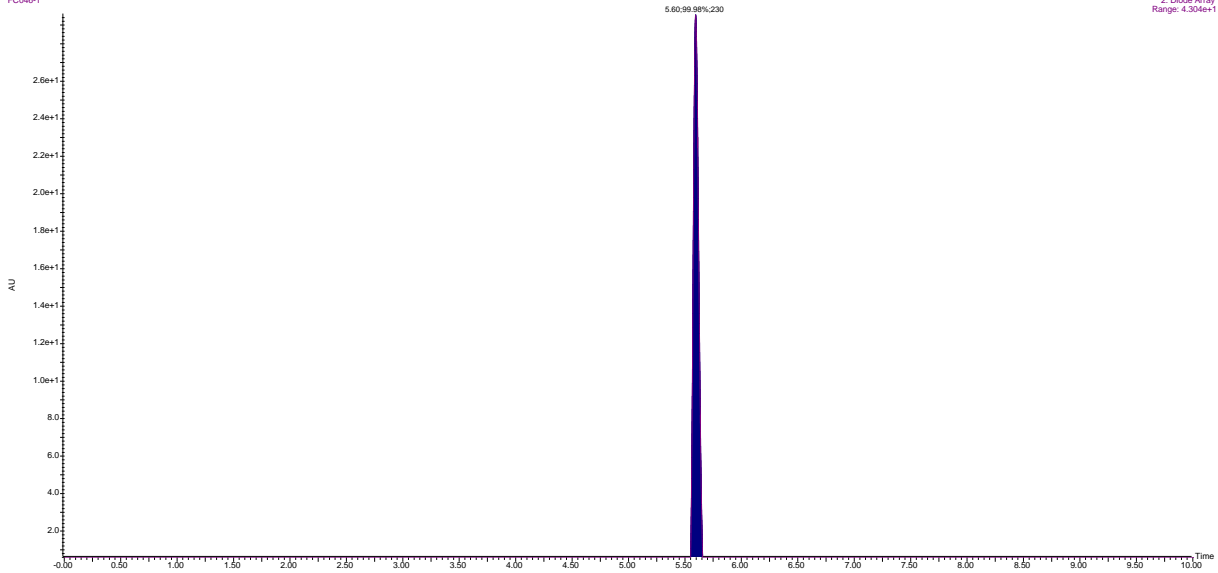
1: TOF MS ES+
1.80e6



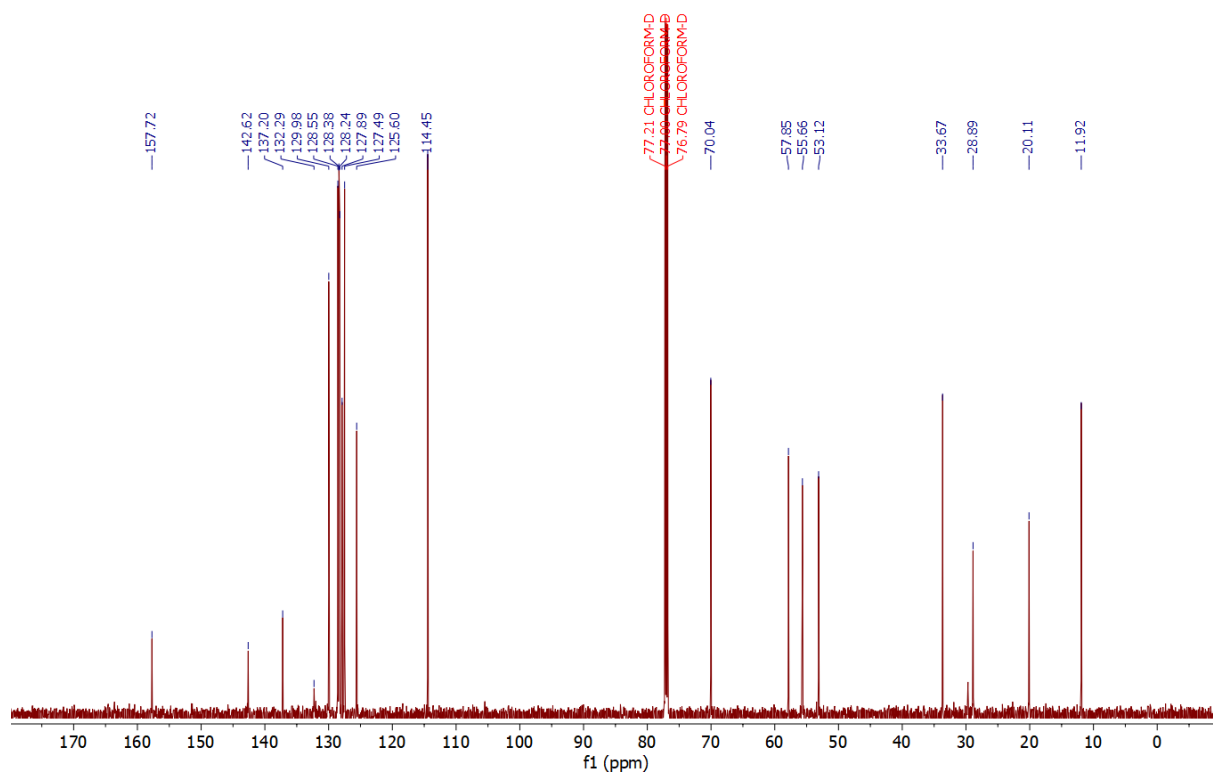
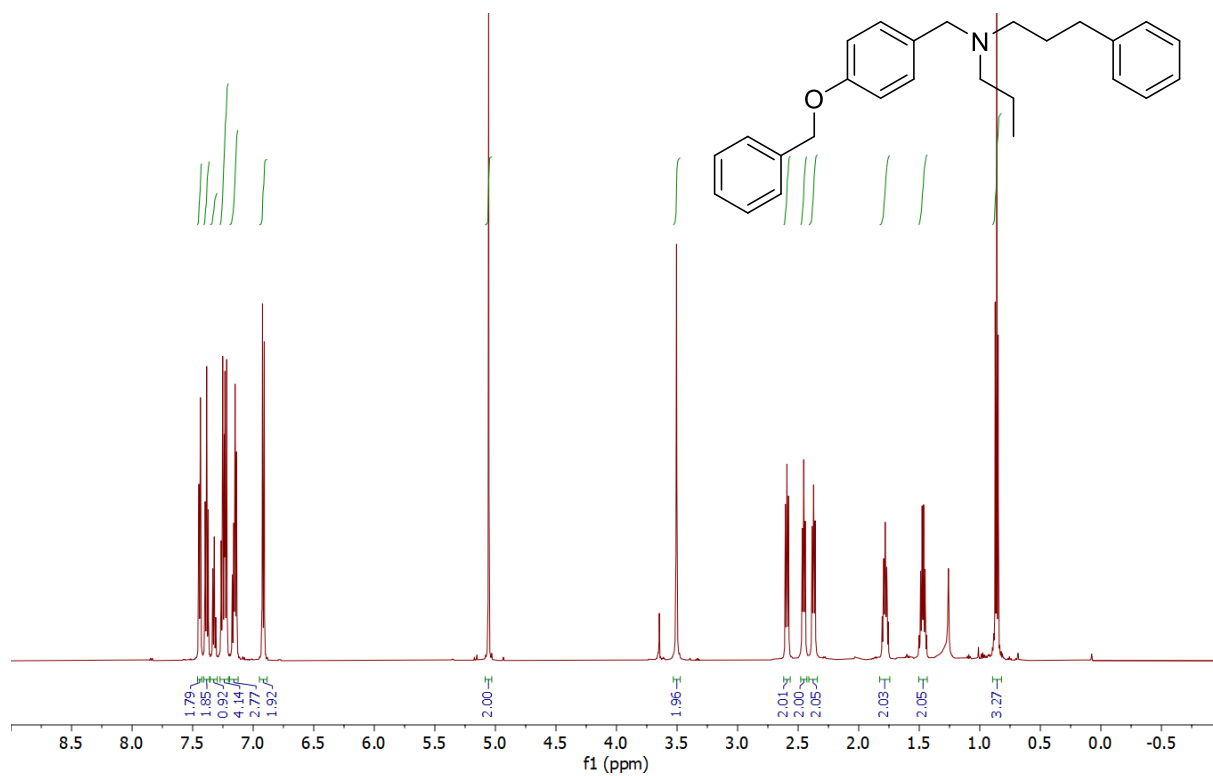
F0406-1

5.60:99.98%:230

2: Diode Array
Range: 4.304e+1



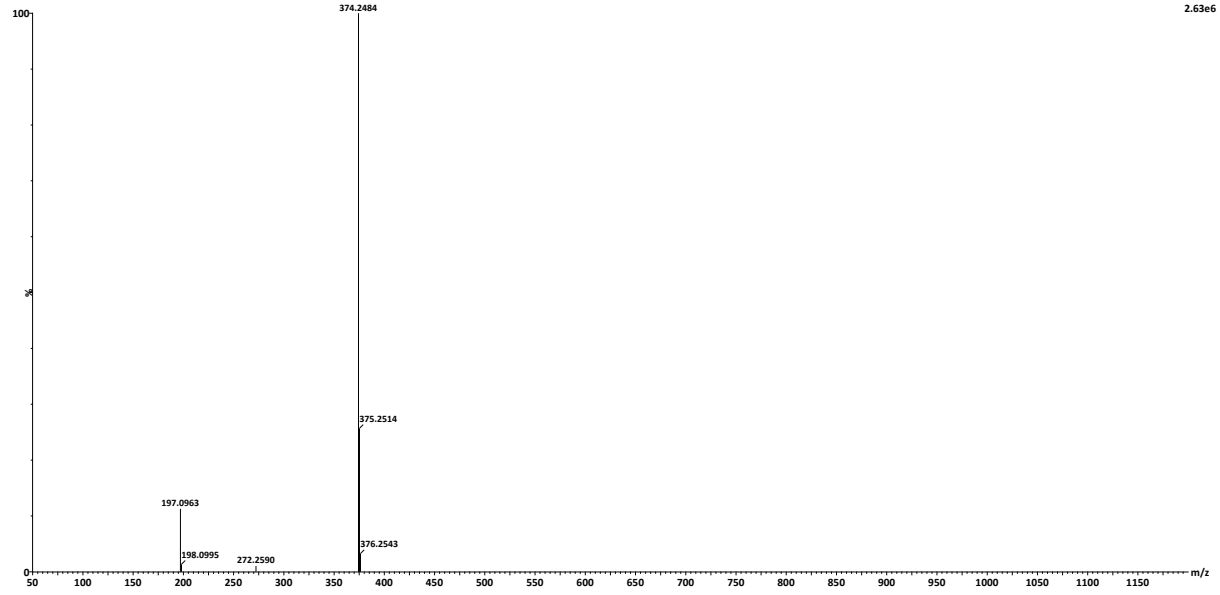
{[4-(Benzyloxy)phenyl]methyl}(3-phenylpropyl)propylamine (45):



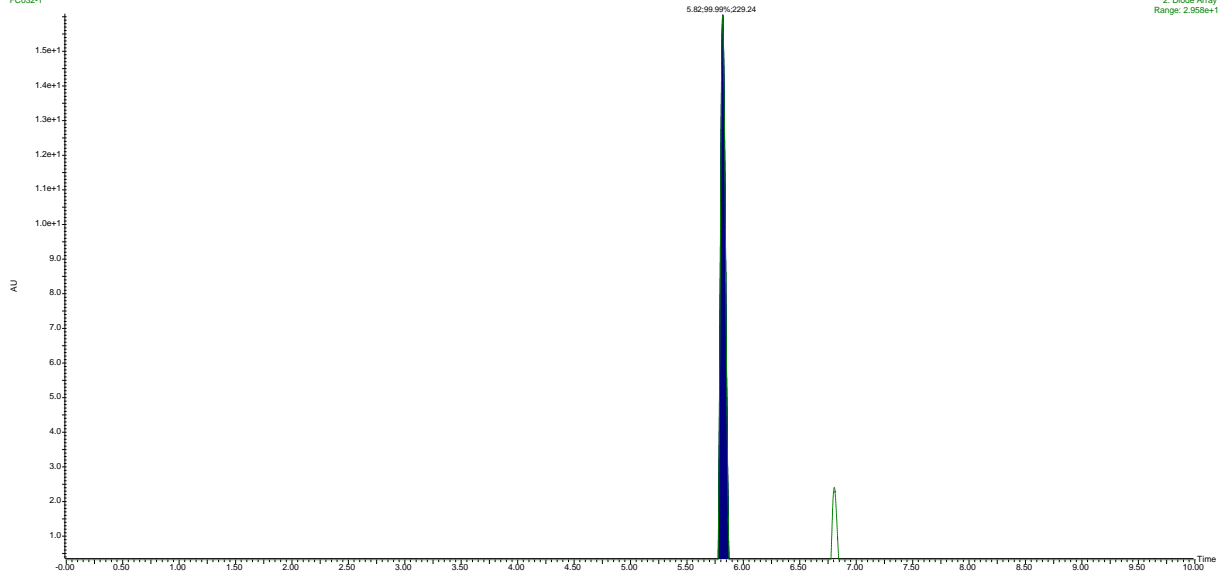
374.2478

2022 08 03 FC032-18 1858 (3.235) Cm (1845:1880-(1497:1642+2012-2136))

1: TOF MS ES+
2.63e6

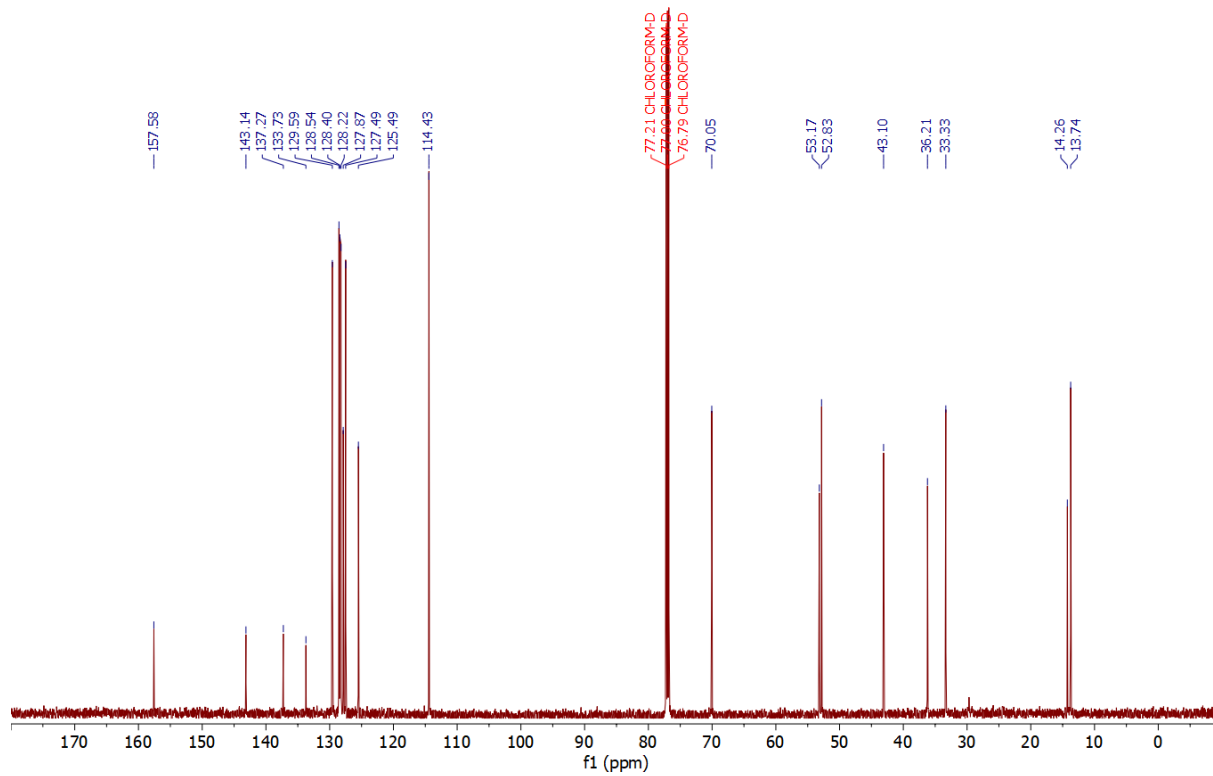
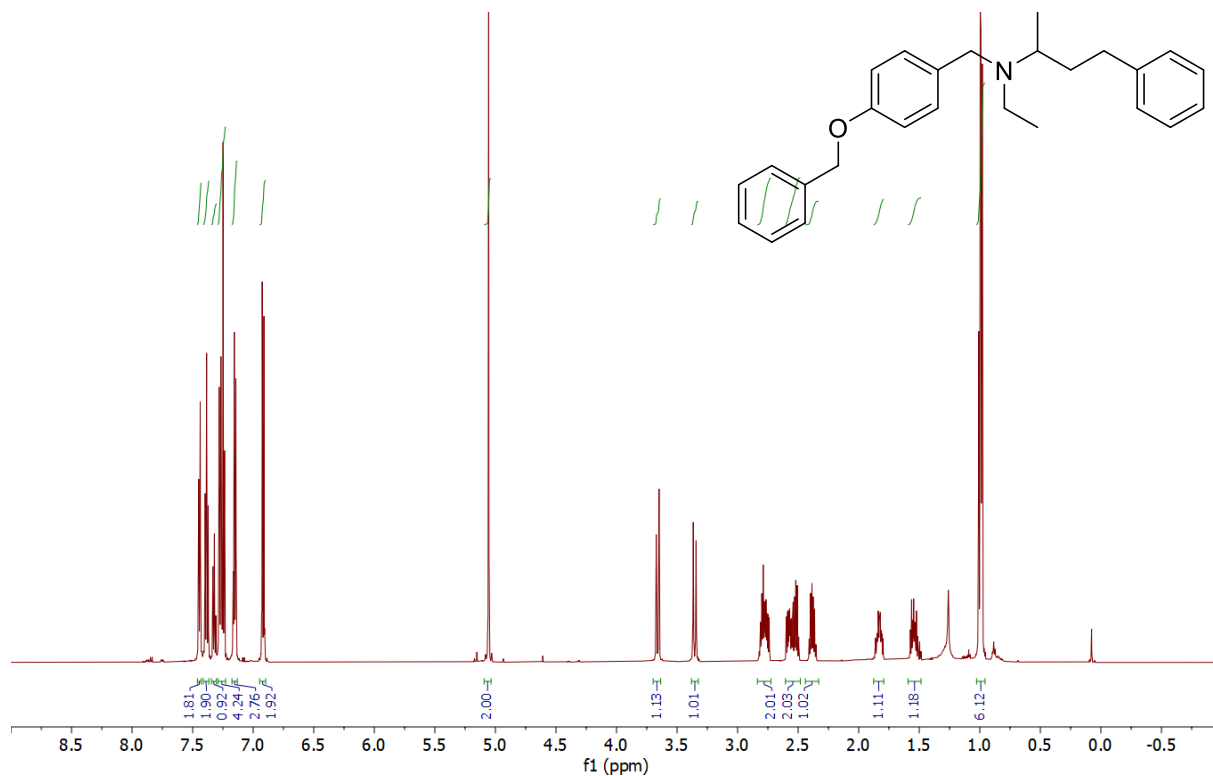


FC032-1



2: Diode Array
Range: 2.958e+1

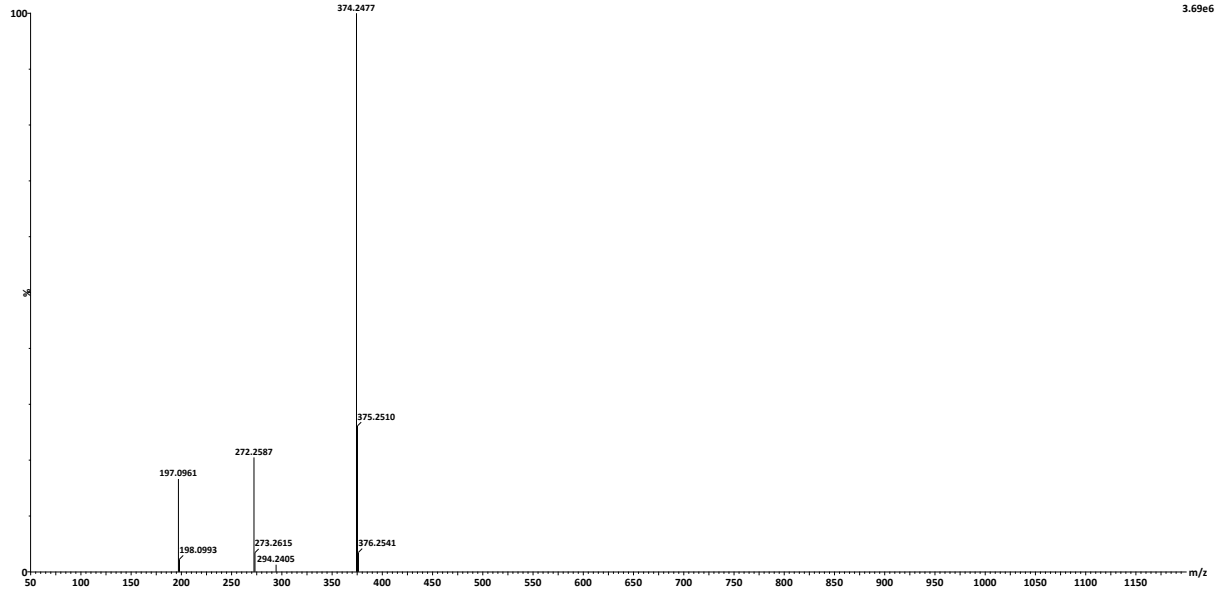
{[4-(Benzyloxy)phenyl]methyl}(ethyl)(4-phenylbutan-2-yl)amine (46):



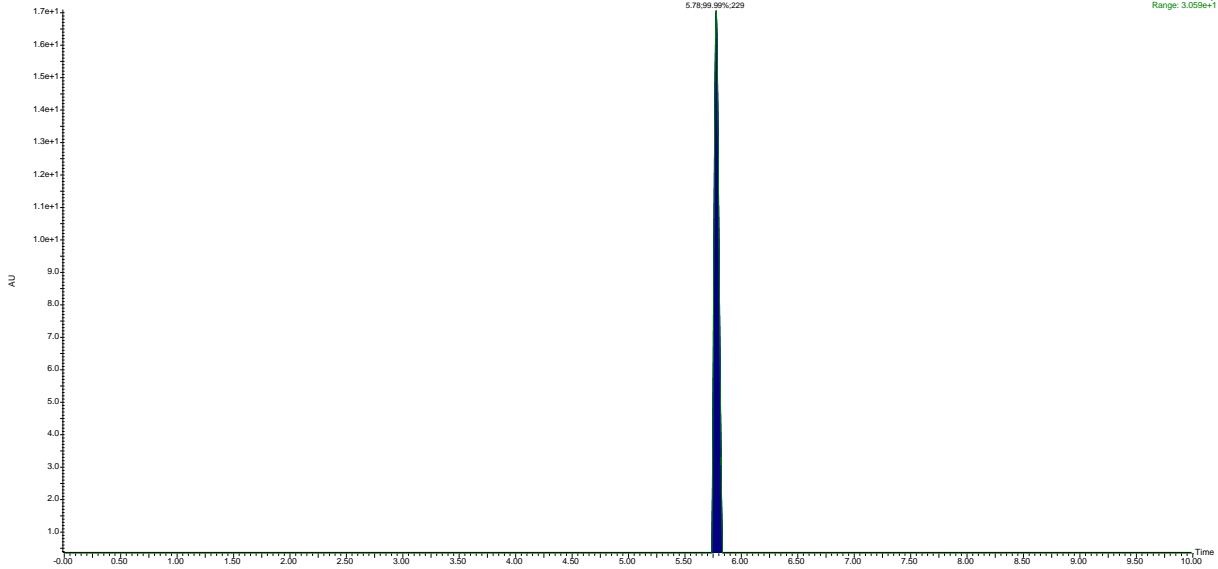
2142478

2022 08 03 FC033-28 1808 (3.146) Cm (1797:1829-(1656:1744+1913:2035))

1: TOF MS ES+
3.69e6

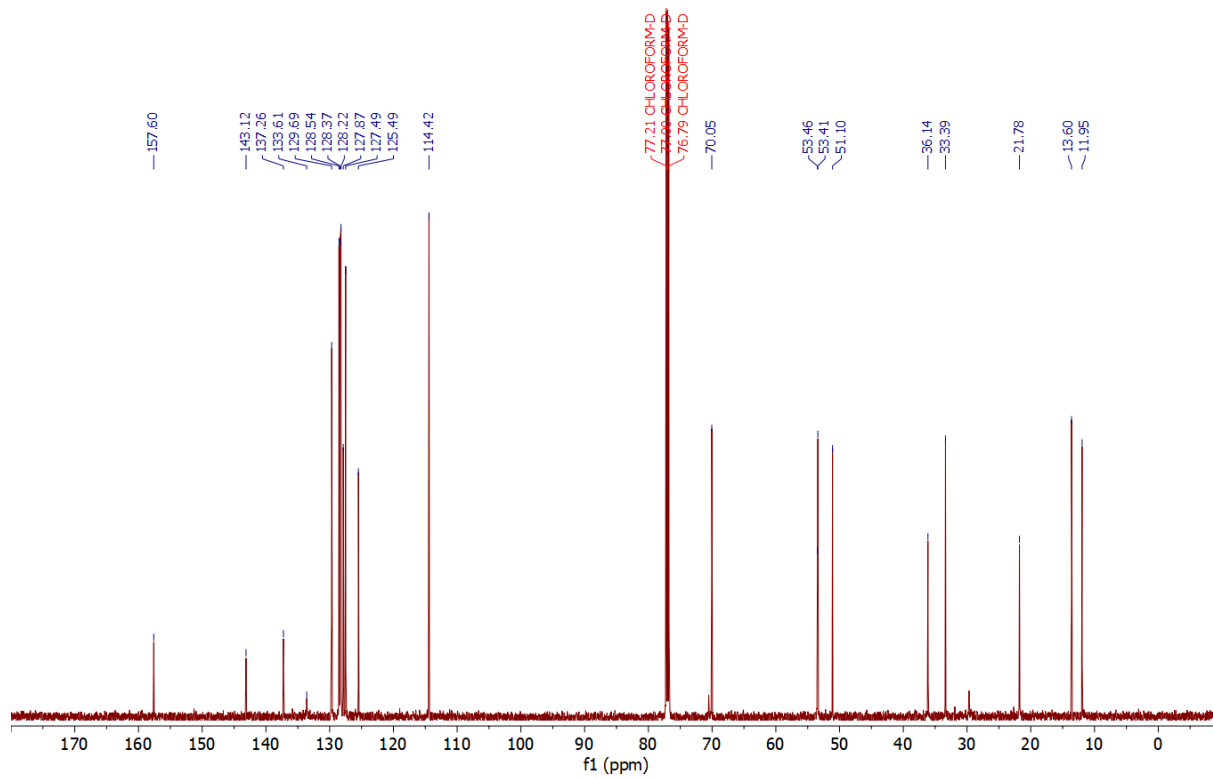
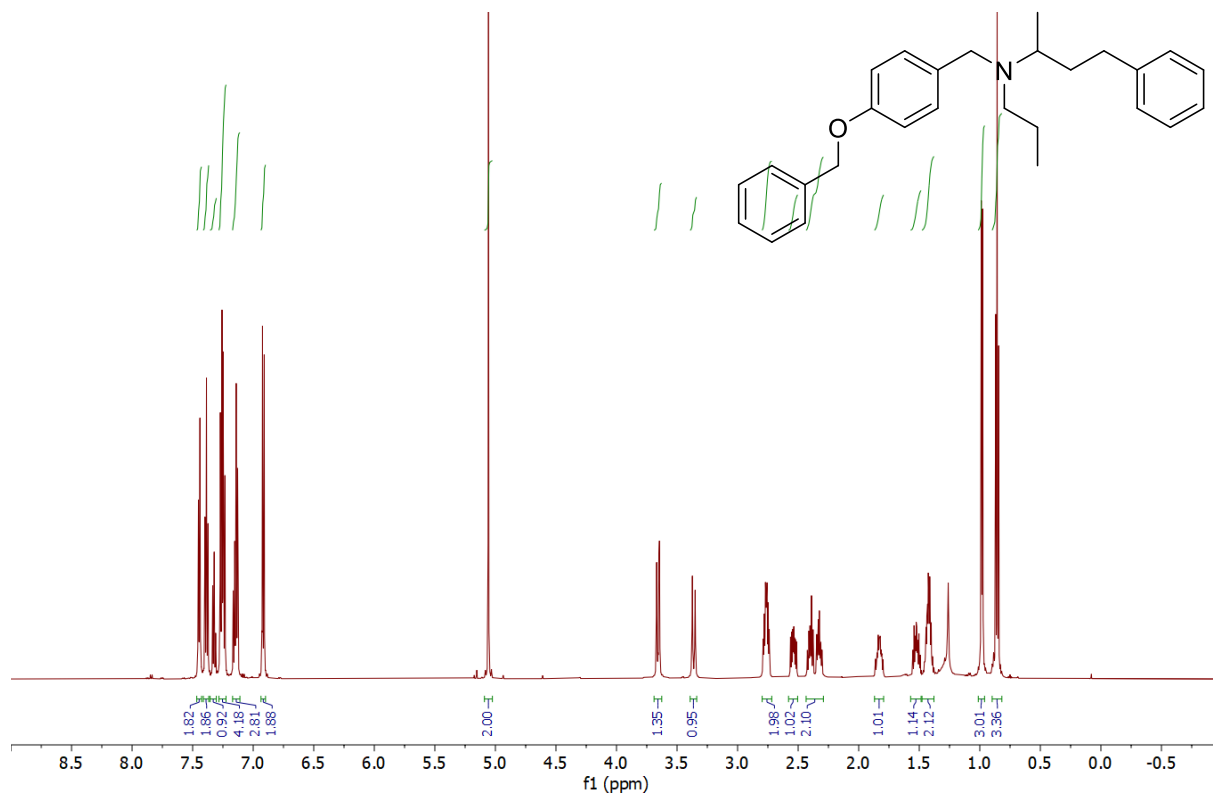


FC033-2



2: Diode Array
Range: 3.059e+1

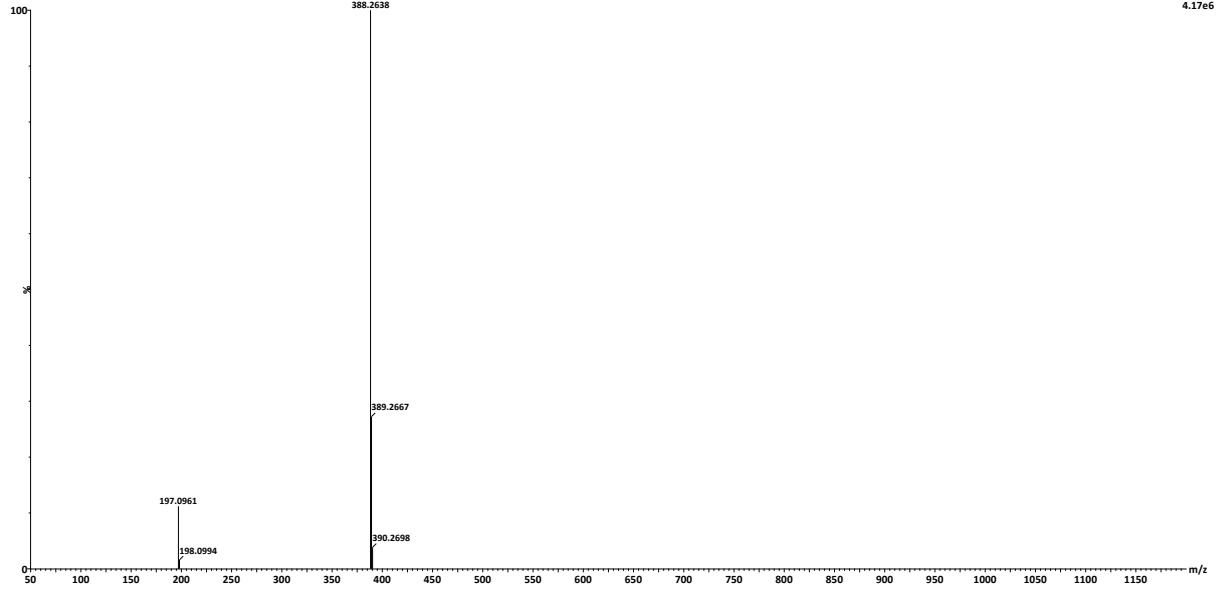
{[4-(Benzyloxy)phenyl]methyl}{4-phenylbutan-2-yl}propylamine (47):



388.2638

2022 08 03 FC033-18 1896 (3.302) Cm (1886:1910-(1755:1815+1956:2001))

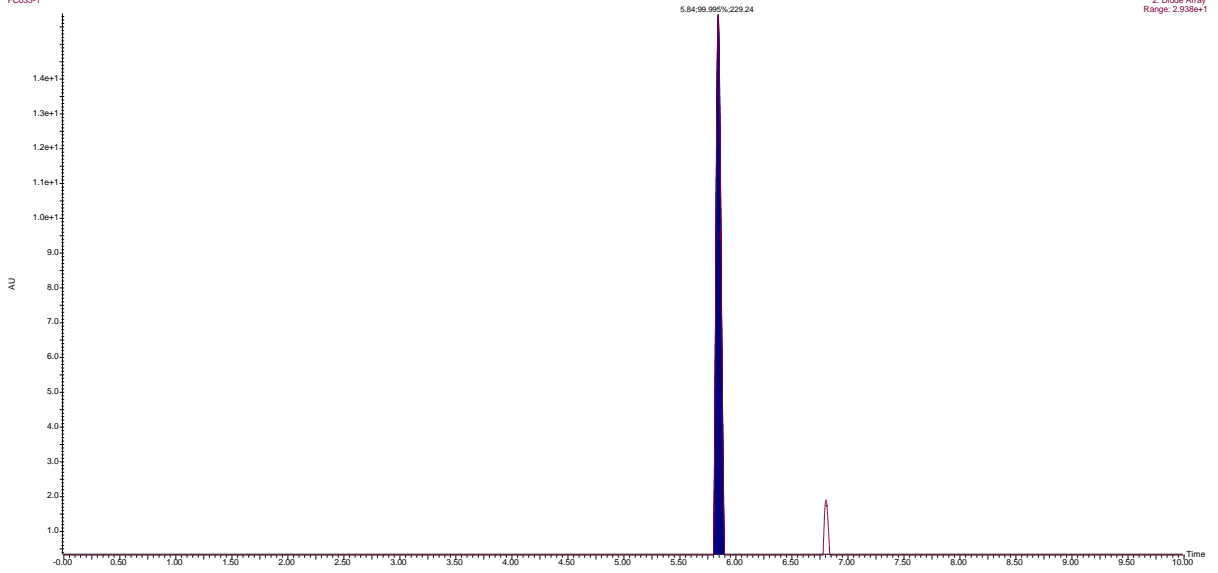
1: TOF MS ES+
4.17e6



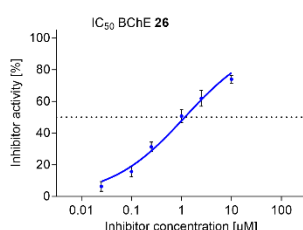
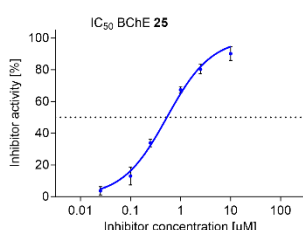
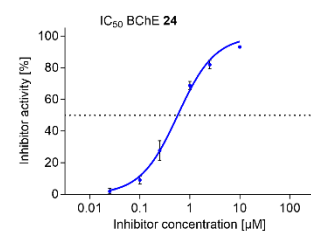
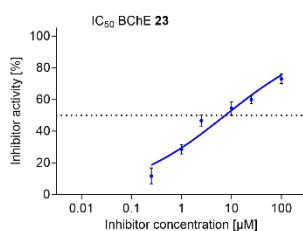
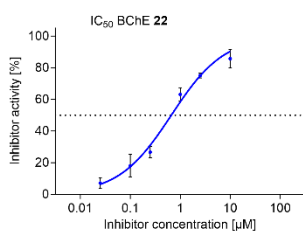
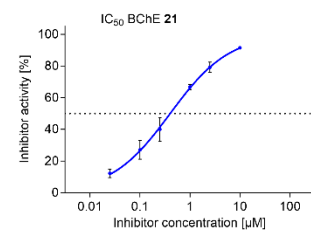
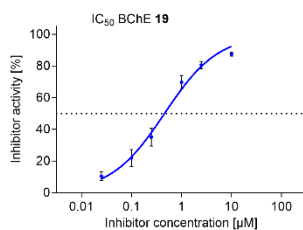
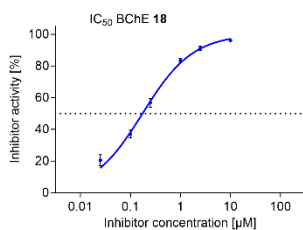
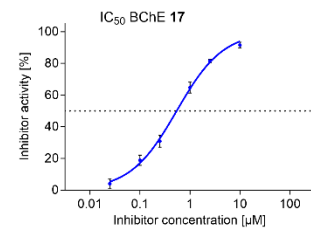
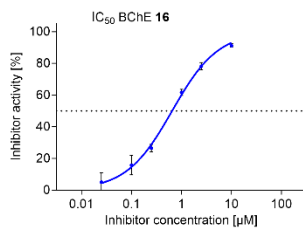
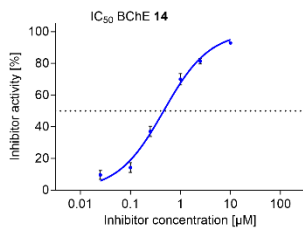
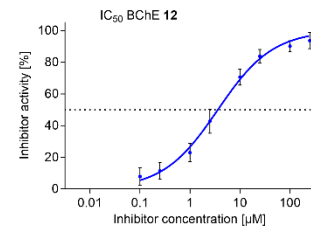
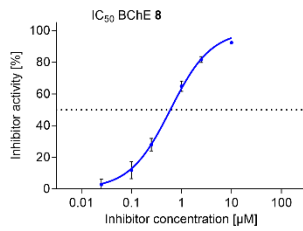
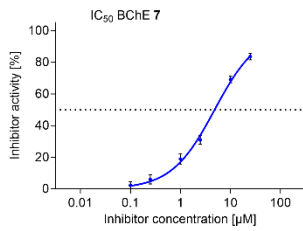
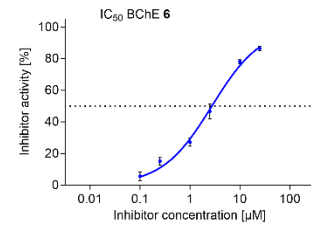
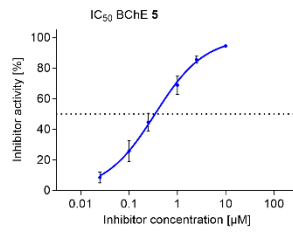
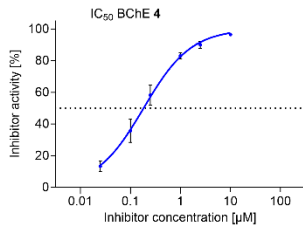
FC033-1

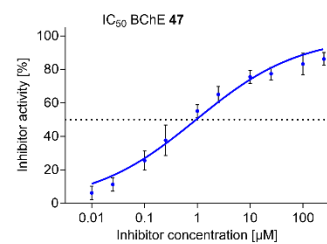
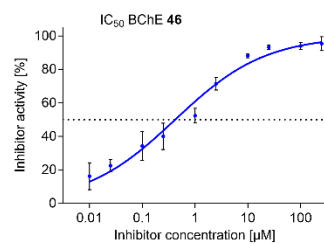
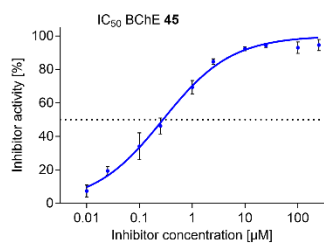
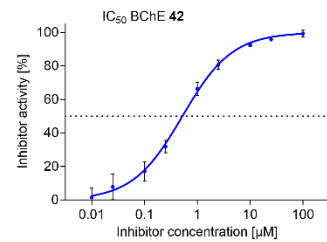
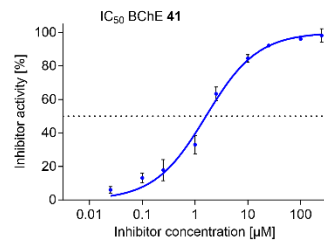
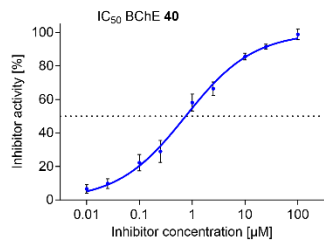
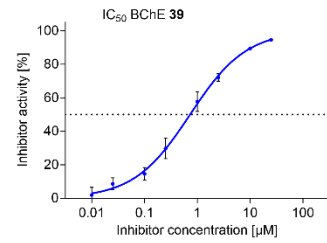
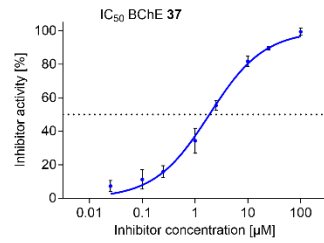
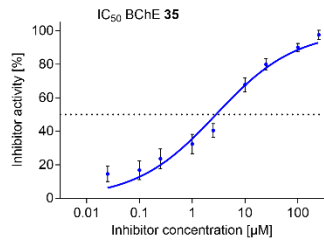
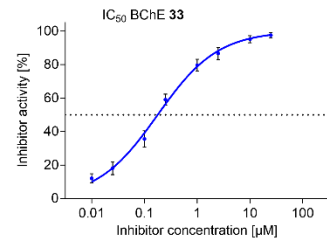
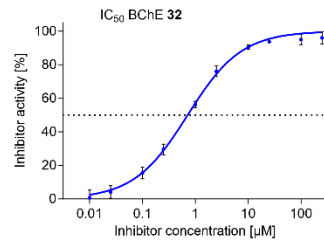
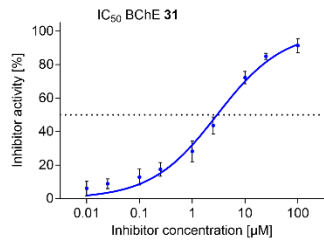
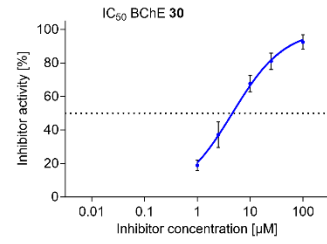
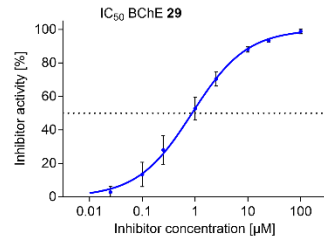
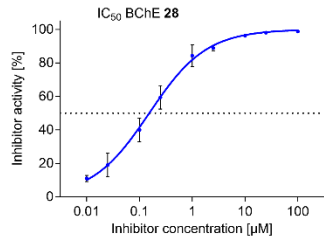
5.84-99.995%, 229.24

2: Diode Array
Range: 2.938e+1

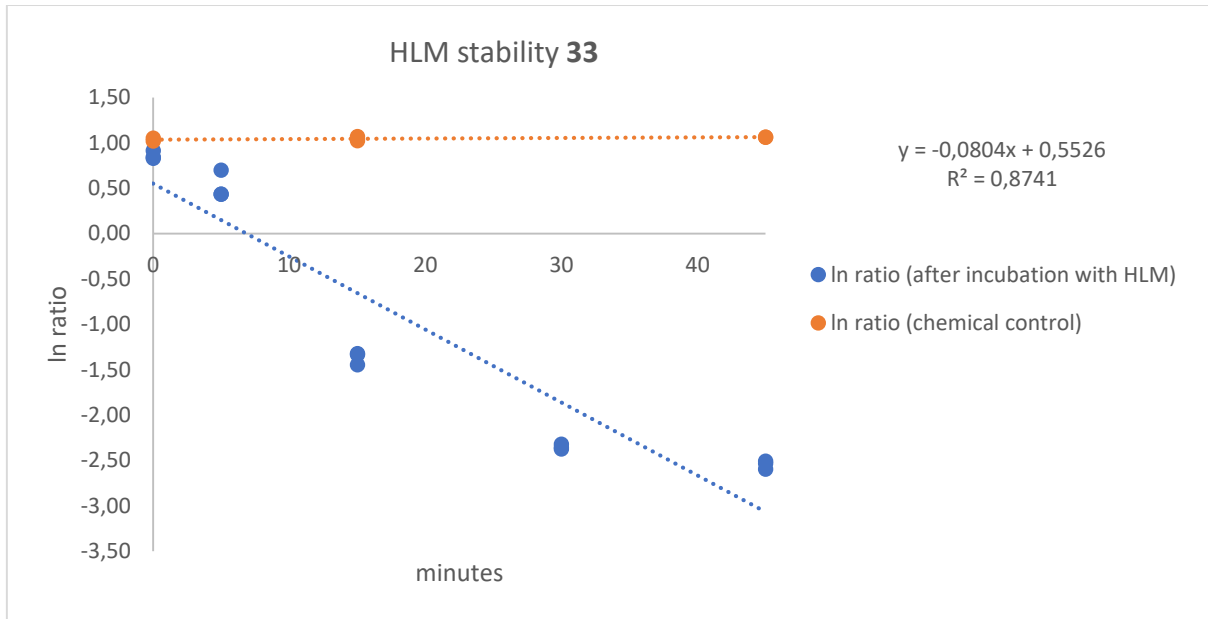


Dose-response curves for calculation IC₅₀ BChE values





HLM stability



Human plasma stability

