Enantioselective Synthesis and Photoreactivity of a Diazirinyl-substituted (*R*)-*β*-Phenylalanine

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Supporting Information

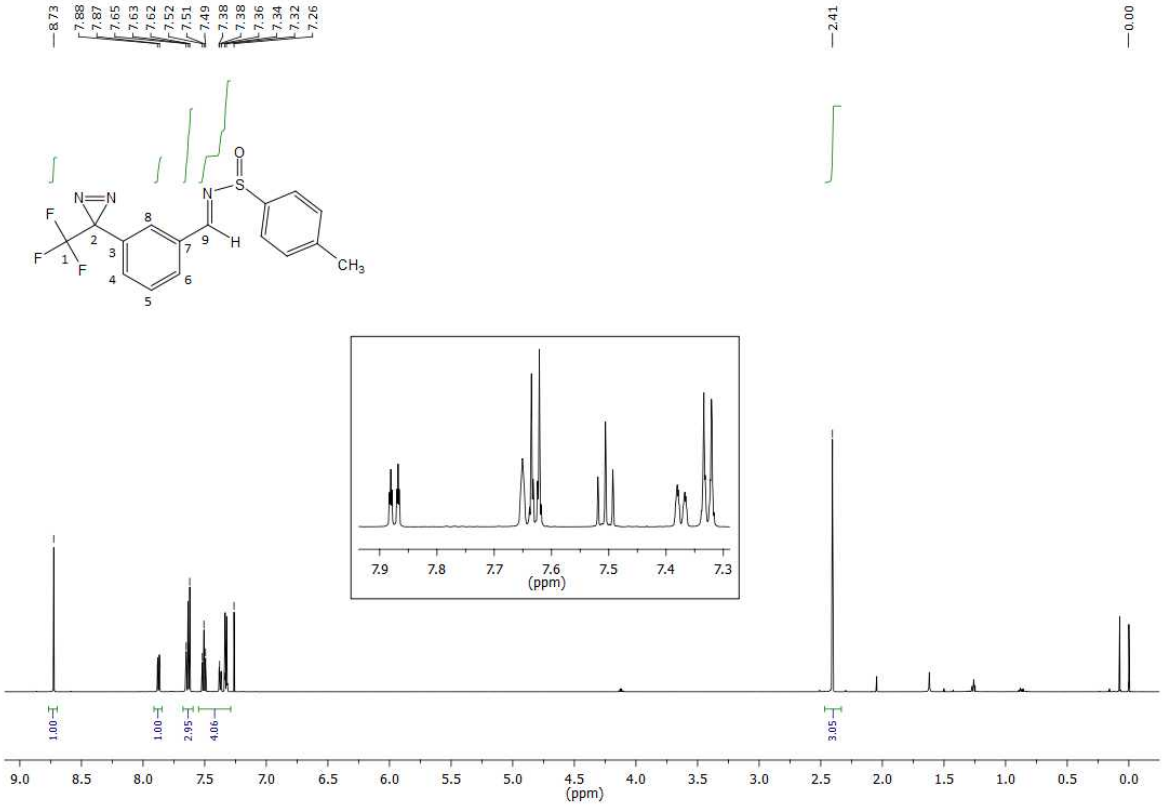
Mosher amides 10, 11

Methyl ester **9** (20 mg, 0.07 mmol) was dissolved in DCM (1 mL) and (*R*)-MTPA-Cl (26 mg, 0.104 mmol), HOBt (19 mg, 0.140 mmol), and EDC (20 mg, 0.104 mmol) were added. The resulting solution was stirred for 18 h at room temperature. Afterwards the reaction mixture was diluted with DCM (25 mL) and washed with 0.5 M HCl (2 x 15 mL), aqueous $NaHCO_3$ (5 %, 2 x 15 mL) and brine (15 mL). The combined organic layers were dried ($MgSO_4$) and concentrated in a vacuum. The crude product was purified by column chromatography (petroleum ether-EtOAc, 9 : 1 to 4 : 1) and Mosher amide **10** (15 mg, 0.030 mmol, 43%) was obtained as colorless oil. (*R*)-Mosher amide **11** was obtained in an analogous manner. **10**: – ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.94-7.92 (d, J = 8.3 Hz, 1H, N*H*), 7.55-7.52 (m, 2H, CH_{MTPA}), 7.45-7.41 (m, 3H, CH_{MTPA}), 7.39-7.32 (m, 2H, CH_{phenyl}), 7.14-7.10 (m, 2H, CH_{phenyl}), 5.42 (ddd, J = 6.0, 6.0, 8.4 Hz, 1H, C*H*CH_2), 3.59 (s, 3H, OCH_3), 3.42-3.41 (m, 3H, OCH_3, MTPA), 2.86 (m, 2H, CH_2) ppm. – ^{13}C NMR (100 MHz, $CDCl_3$): δ = 170.9 (1C, *C*$OOCH_3$), 165.9 (1C, *C*O), 141.2 (1C, $C_{q,\ phenyl}$), 132.2 (1C, $C_{q,\ MTPA}$), 129.8 (1C, $C_{q,\ phenyl}$), 129.6 (1C, *C*H_{MTPA}), 129.4 (1C, *C*H_{phenyl}), 128.6 (2C, *C*H_{MTPA}), 127.7 (2C, *C*H_{MTPA}), 127.6 (1C, *C*H_{phenyl}), 126.0 (1C, *C*H_{phenyl}), 124.0 (1C, *C*H_{phenyl}), 123.7 (1C, *C*F_3, MTPA), 122.1 (1C, *C*F_3), 84.1 (1C, $C_q$$CF_3$, MTPA), 55.0 (1C, O*C*$H_3$, MTPA), 52.0 (1C, O*C*$H_3$), 49.5 (1C,

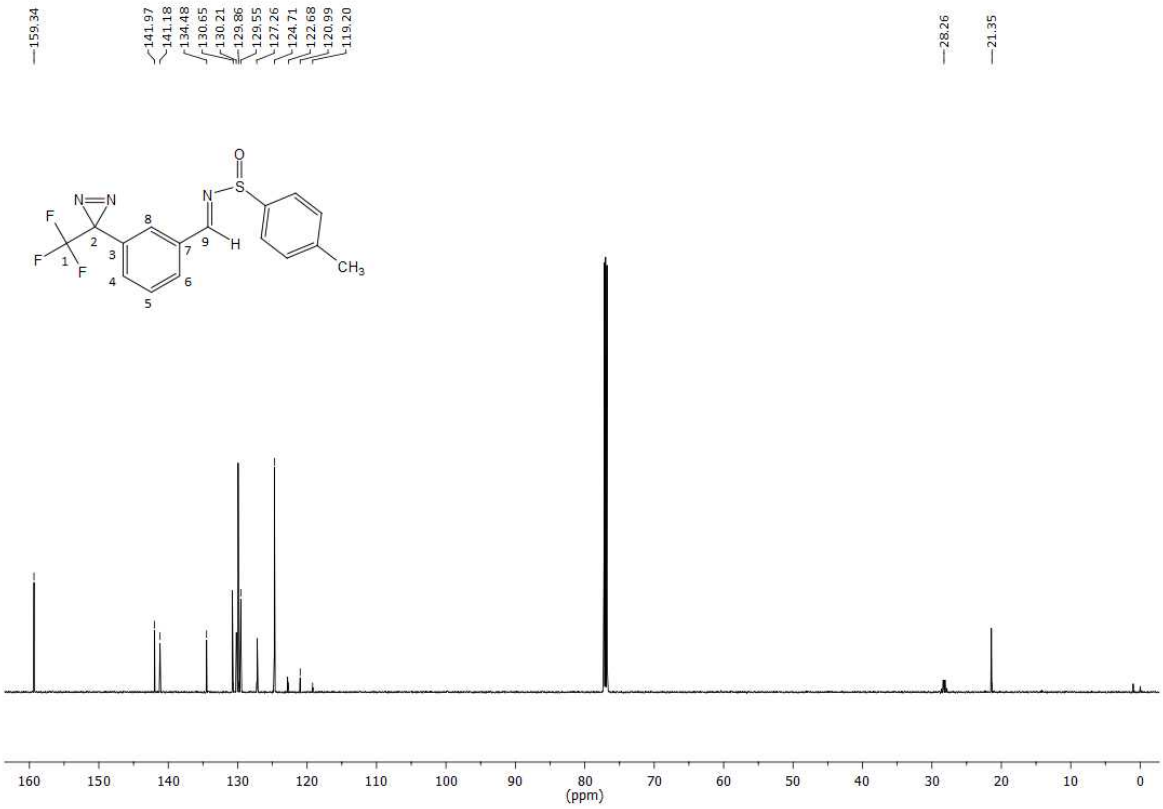
*C*HCH$_2$), 39.6 (1C, *C*H$_2$), 28.4 (1C, *C*$_q$CF$_3$) ppm. – ^{19}F NMR (376 MHz, CDCl$_3$): δ = –65.5833 (s, 3F, C*F*$_3$), –69.27 (s, 3F, C*F*$_3$, MTPA) ppm. – **11**: ^{1}H NMR (400 MHz, CDCl$_3$): δ = 7.89 (d, *J* = 8.2 Hz, 1H, N*H*), 7.46-7.43 (m, 2H, C*H*$_{MTPA}$), 7.41-7.38 (m, 3H, CH$_{MTPA}$), 7.34 (dd, *J* = 8.0, 8.0 Hz, 1H, C*H*$_{phenyl}$), 7.27-7.25 (m, 1H, C*H*$_{phenyl}$), 7.14 (d, *J* = 7.8 Hz, 1H, C*H*$_{phenyl}$), 6.98 (s, 1H, C*H*$_{phenyl}$), 5.43 (ddd, *J* = 5.9, 5.9, 8.4 Hz, 1H, C*H*CH$_2$), 3.65 (s, 3H, OC*H*$_3$), 3.47-3.46 (m, 3H, OCH$_3$, MTPA), 2.88 (m, 2H, C*H*$_2$) ppm. – ^{13}C NMR (100 MHz, CDCl$_3$): δ = 171.0 (1C, *C*$_q$OOCH$_3$), 165.9 (1C, *C*$_q$O), 141.2 (1C, *C*$_{q,\ phenyl}$), 132.3 (1C, *C*$_{qMTPA}$), 129.7 (1C, *C*$_{q,\ phenyl}$), 129.6 (1C, *C*H$_{MTPA}$), 192.3 (1C, *C*H$_{phenyl}$), 128.6 (2C, *C*H$_{MTPA}$), 127.7 (1C, *C*H$_{MTPA}$), 127.5 (2C, *C*H$_{MTPA}$), 126.0 (1C, *C*H$_{phenyl}$), 124.0 (1C, *C*H$_{phenyl}$), 123.7 (1C, q, $J_{C\text{-}F}$ = 290.0 Hz, *C*F$_{3,MTPA}$), 122.0 (1C, q, $J_{C\text{-}F}$ = 274.8 Hz, *C*F$_3$), 84.0 (1C, q, $J_{C\text{-}F}$ = 26.4 Hz, *C*$_q$CF$_3$, MTPA), 55.2 (1C, O*C*H$_3$, MTPA), 52.1 (1C, O*C*H$_3$), 39.6 (1C, *C*H$_2$), 28.4 (1C, q, $J_{C\text{-}F}$ = 40.4 Hz, *C*$_q$CF$_3$) ppm. – ^{19}F NMR (376 MHz, CDCl$_3$): δ = –65.5796 (s, 3F, C*F*$_3$), –69.30 (s, 3F, C*F*$_3$, MTPA) ppm.

NMR spectra

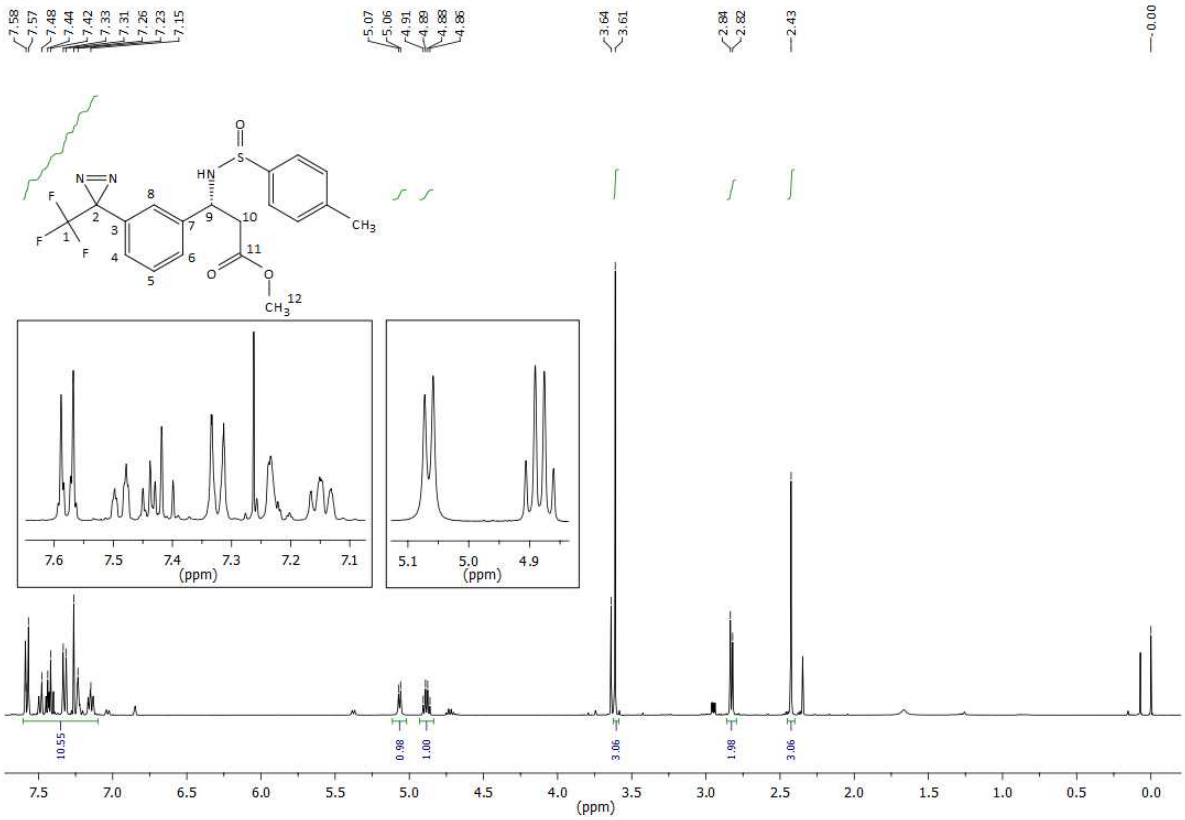
^{1}H NMR spectrum of **6** ($CDCl_3$, 400 MHz):



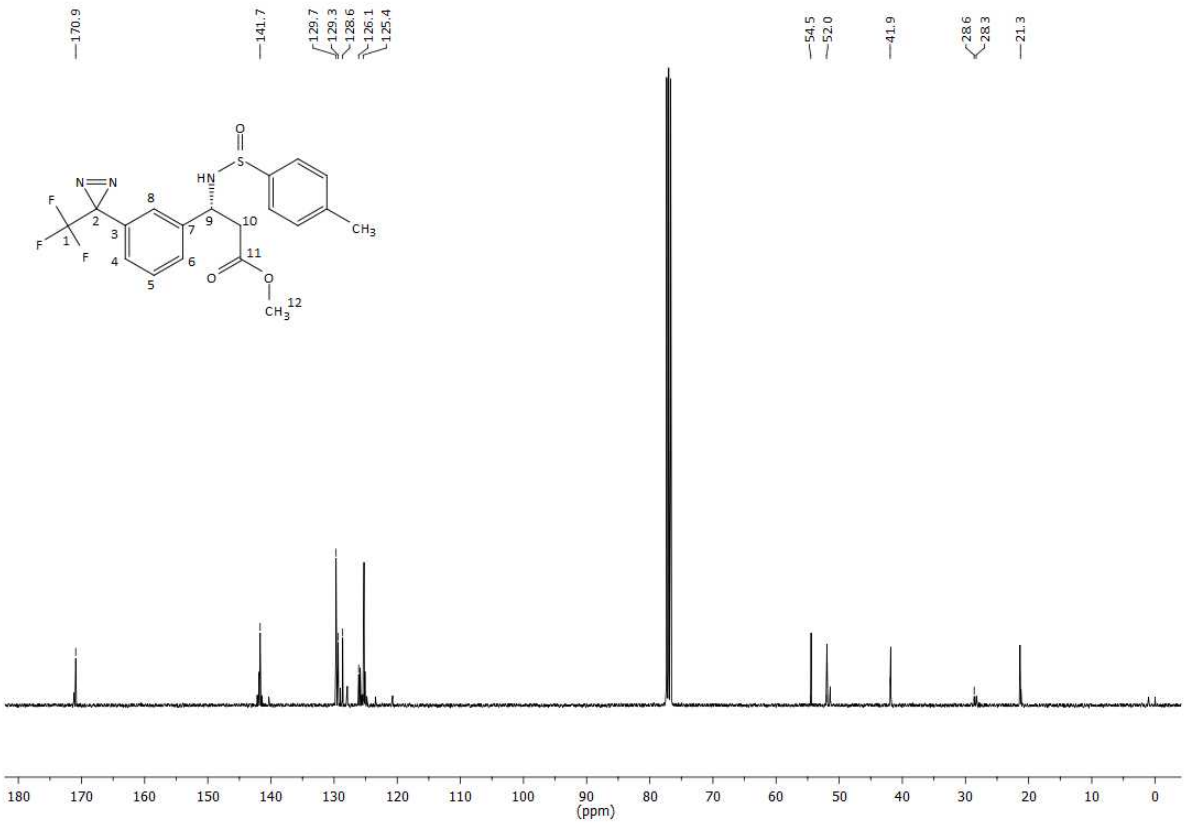
^{13}C NMR spectrum of **6** ($CDCl_3$, 100 MHz):



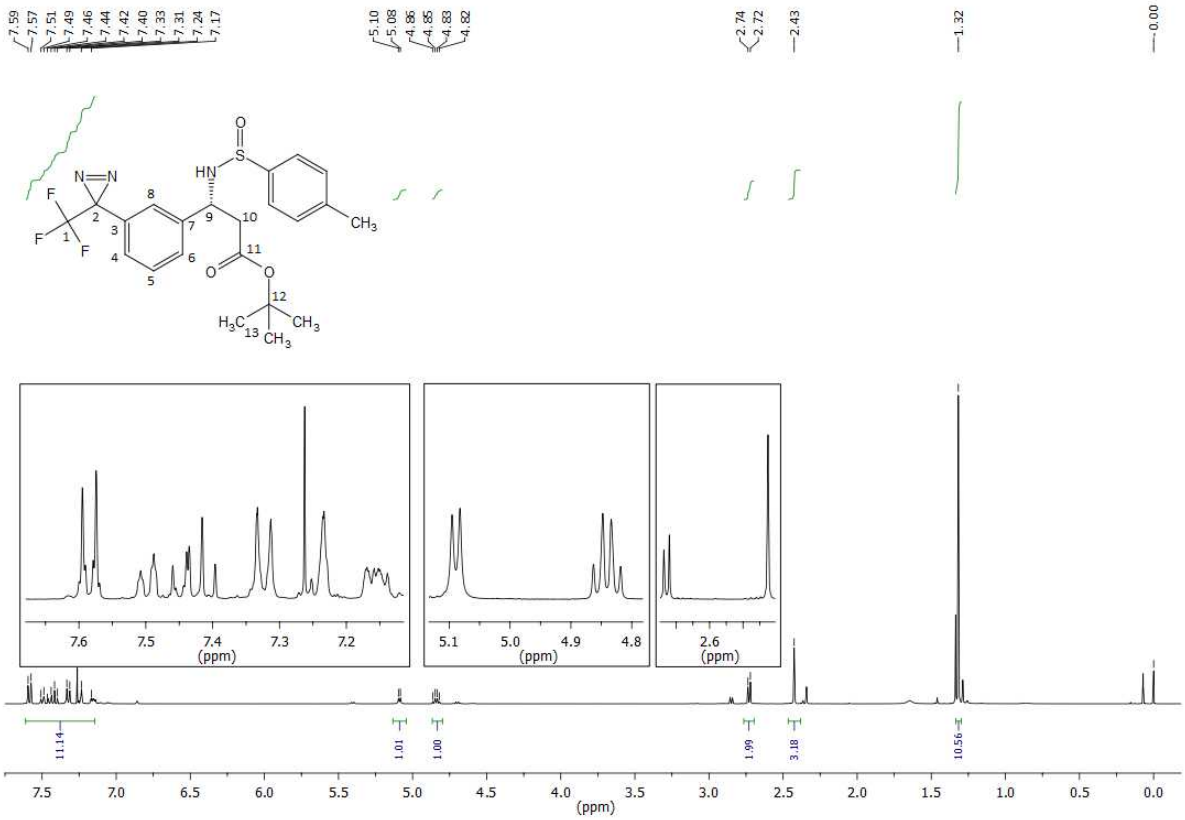
^{1}H NMR spectrum of **7** ($CDCl_3$, 400 MHz):



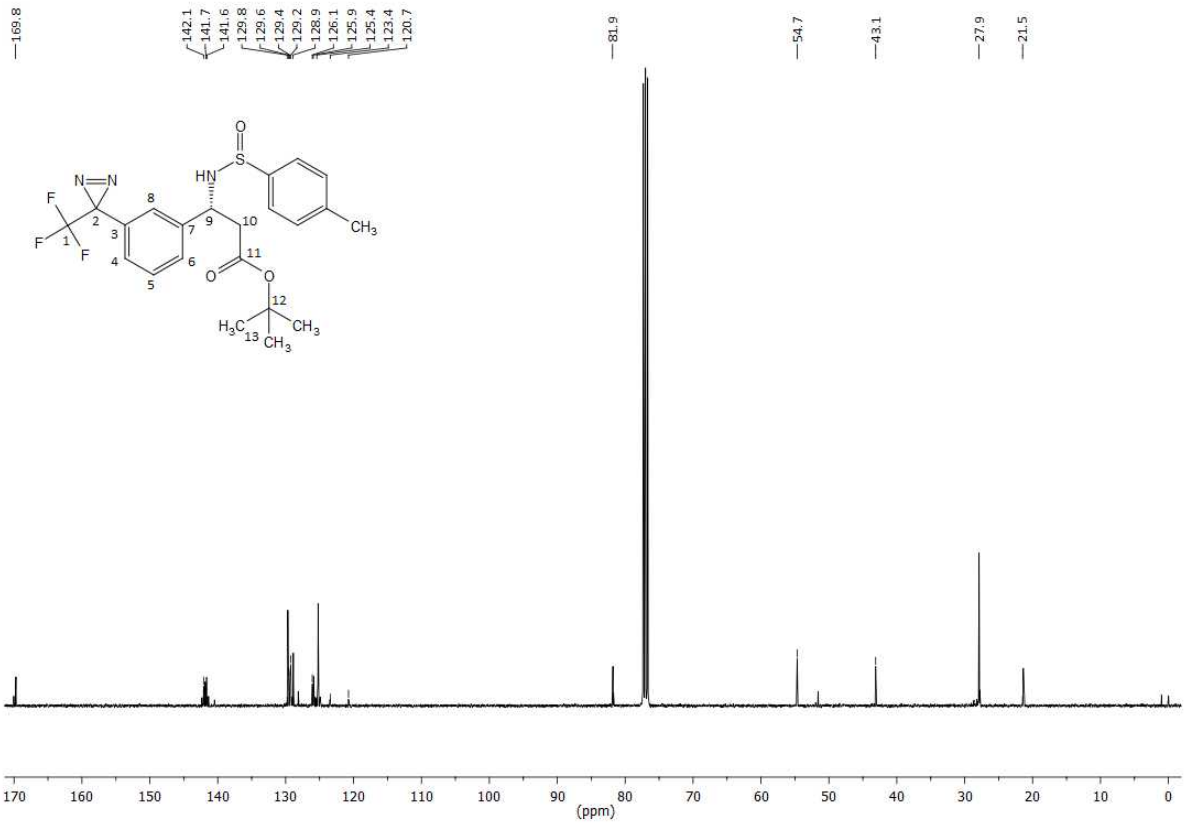
^{13}C NMR spectrum of **7** ($CDCl_3$, 100 MHz):



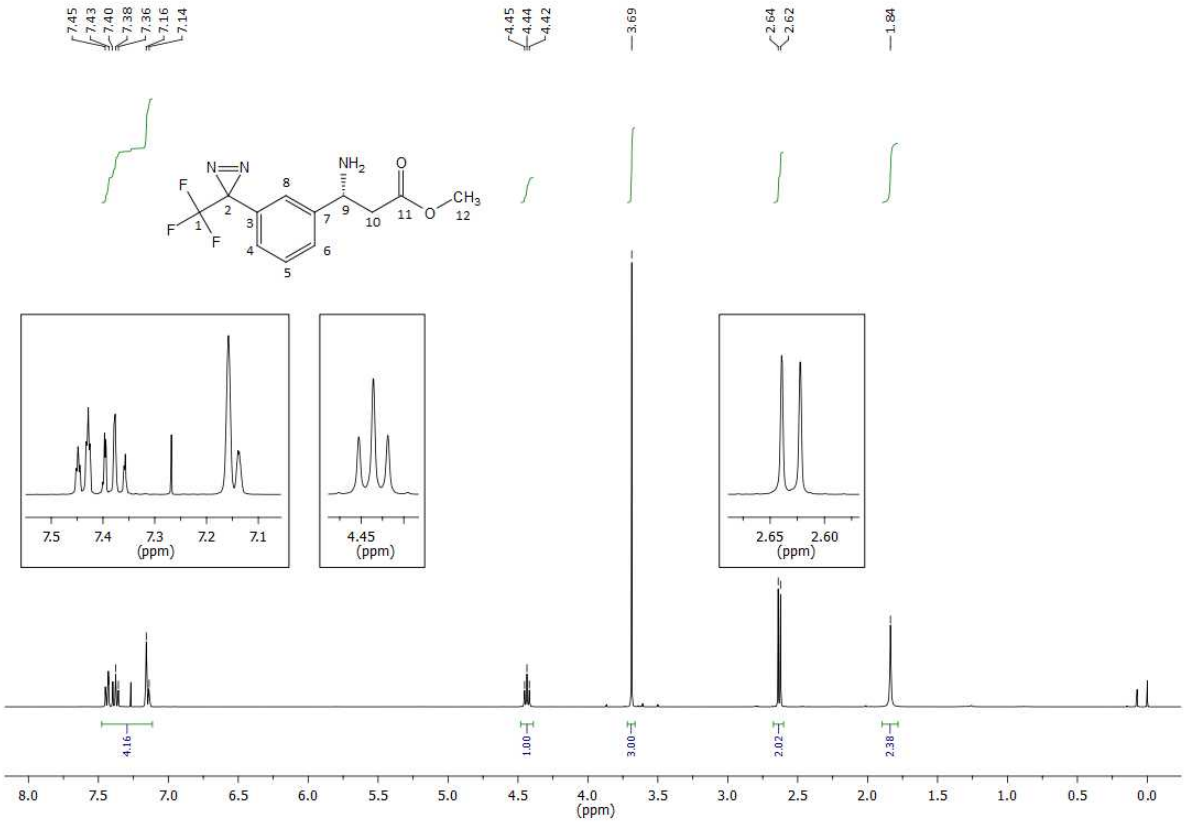
^{1}H NMR spectrum of **8** ($CDCl_3$, 400 MHz):



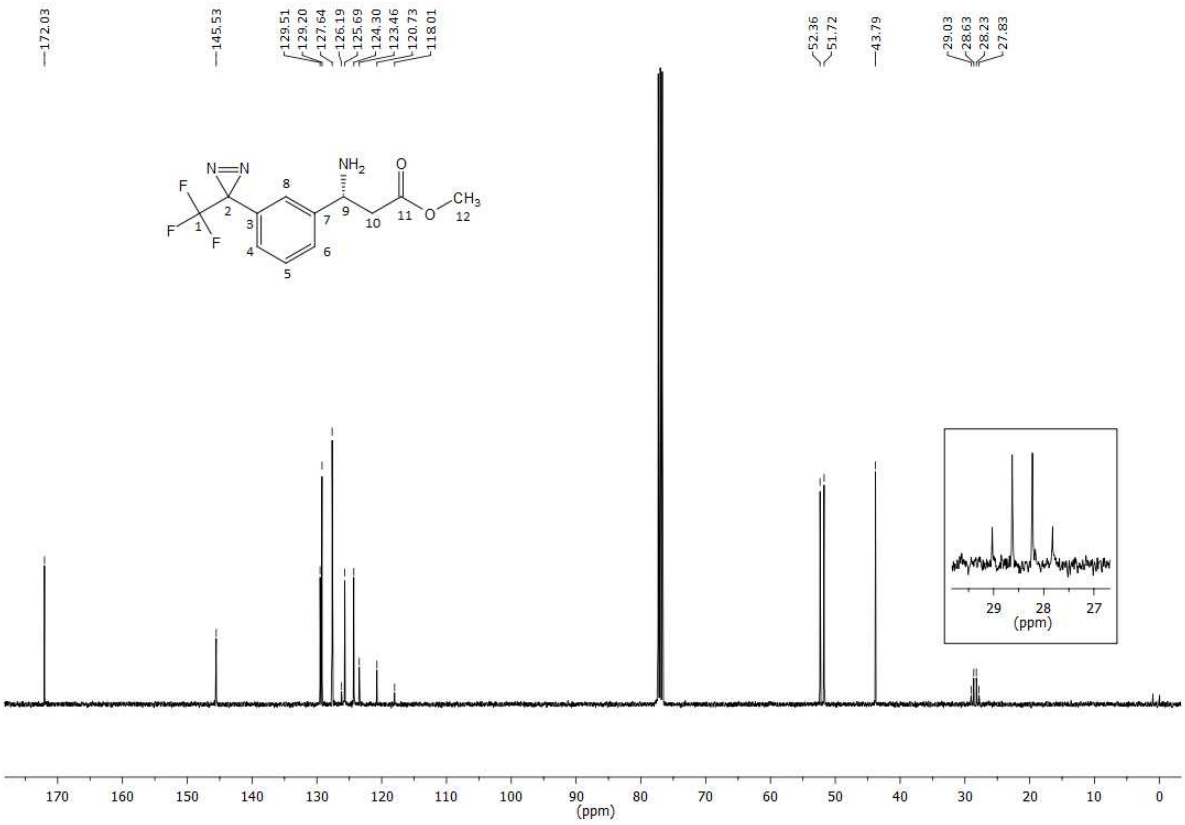
^{13}C NMR spectrum of **8** ($CDCl_3$, 100 MHz):



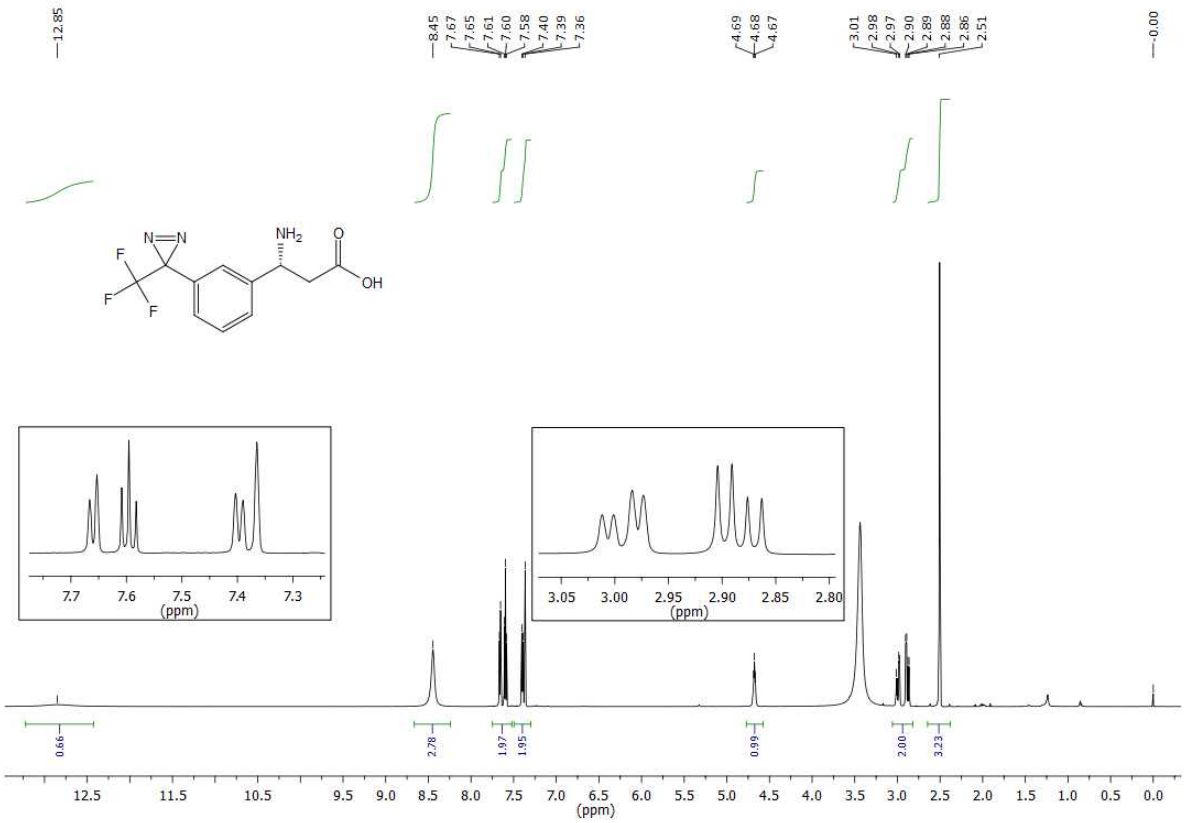
^{1}H NMR spectrum of **9** ($CDCl_3$, 400 MHz):



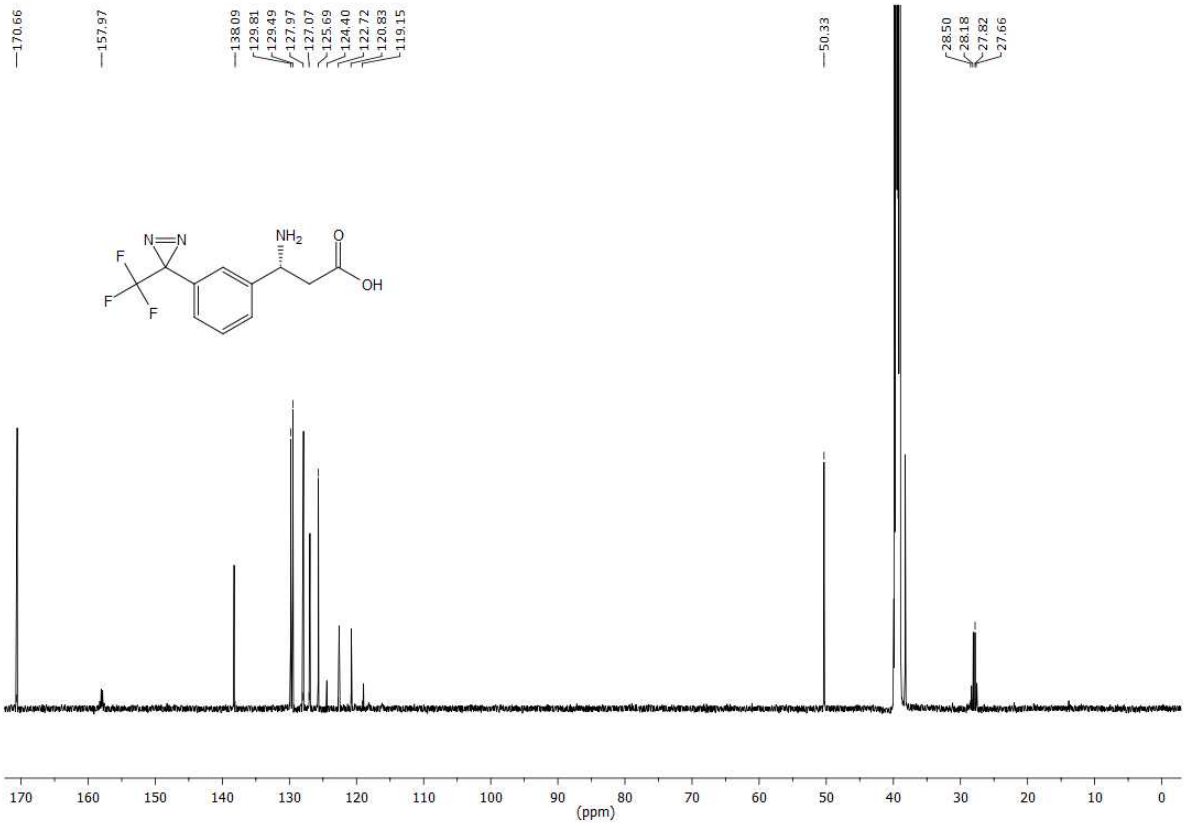
^{13}C NMR spectrum of **9** ($CDCl_3$, 100 MHz):



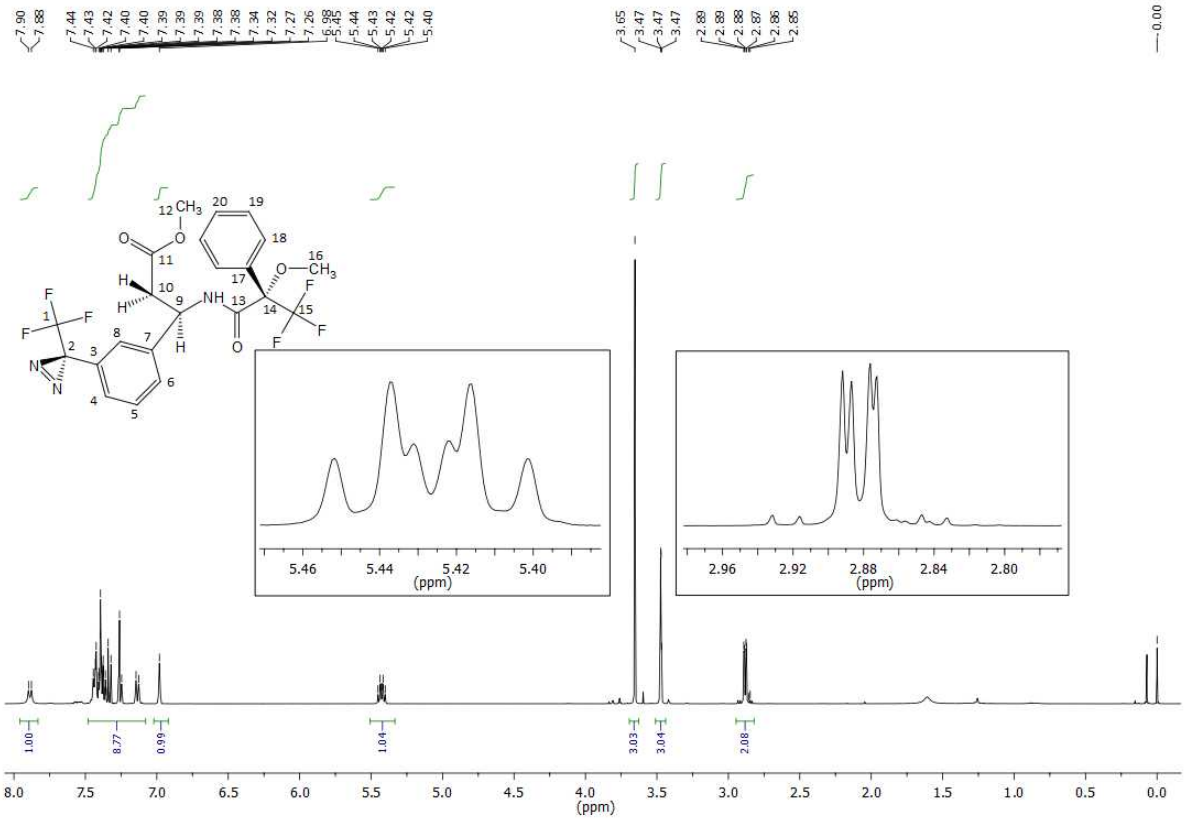
^{1}H NMR spectrum of **1** (DMSO-d_6, 600 MHz):



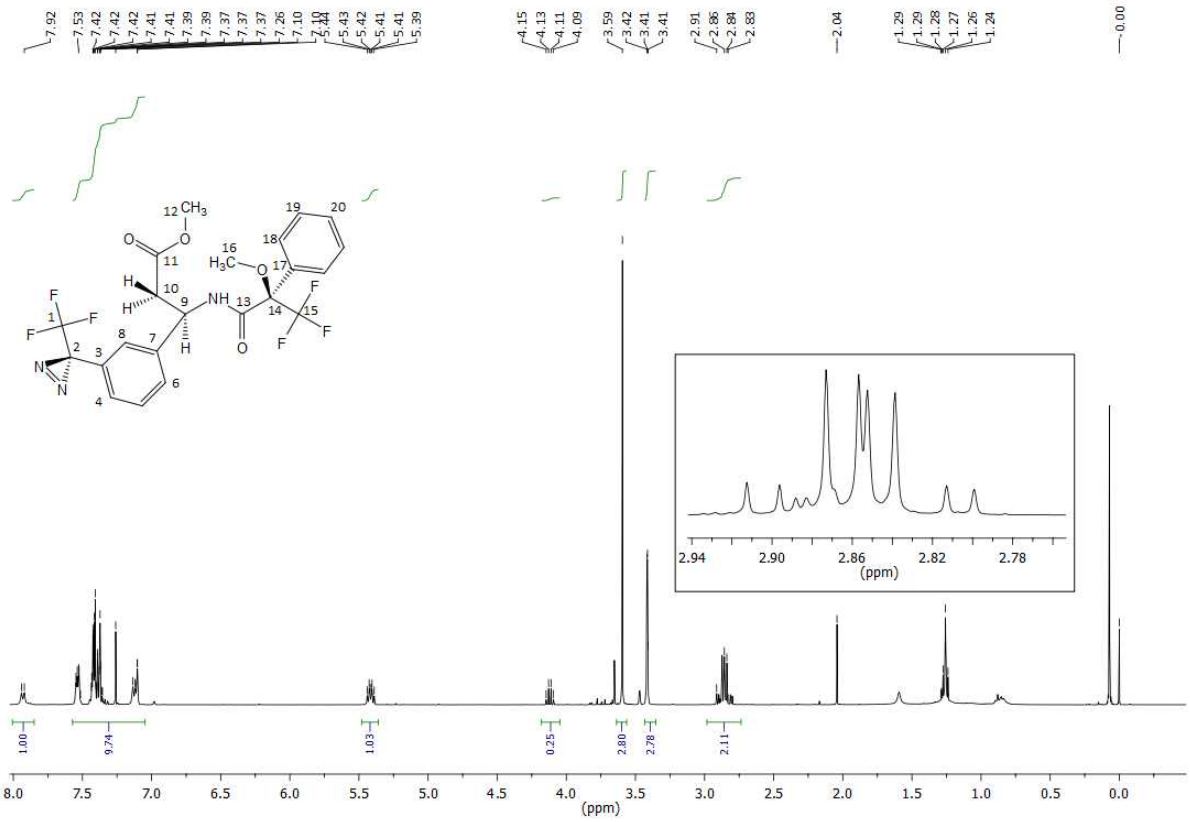
^{13}C NMR spectrum of **1** (DMSO-d_6, 150 MHz):



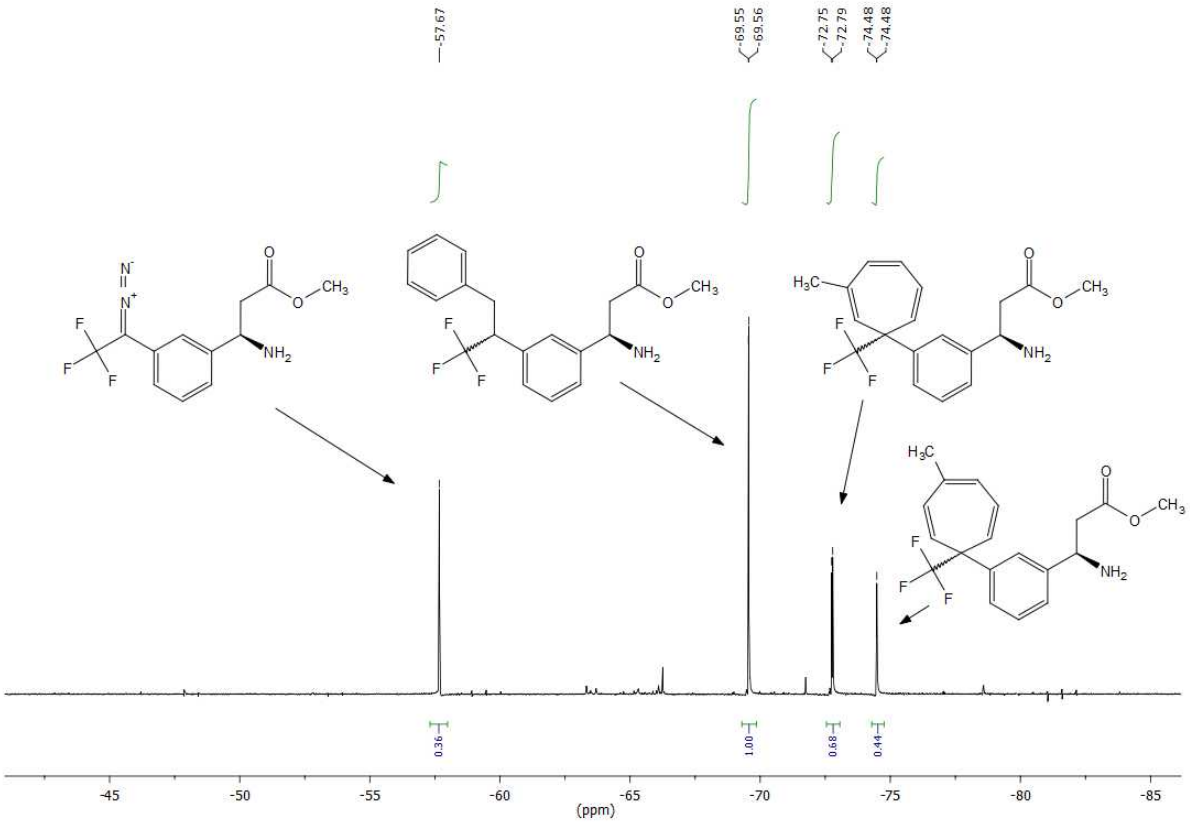
^{1}H NMR spectrum of (*S*)-**10** ($CDCl_3$, 400 MHz):



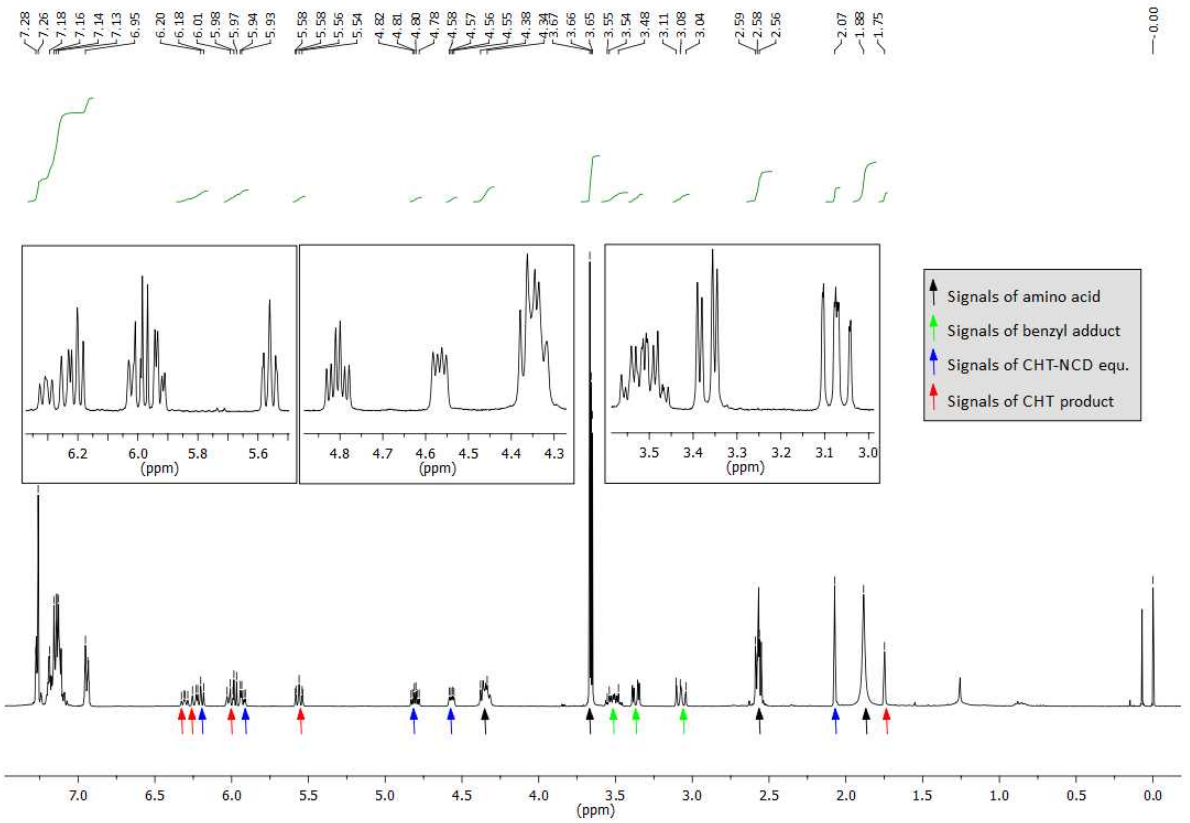
^{1}H NMR spectrum of (*R*)-**11** ($CDCl_3$, 400 MHz):



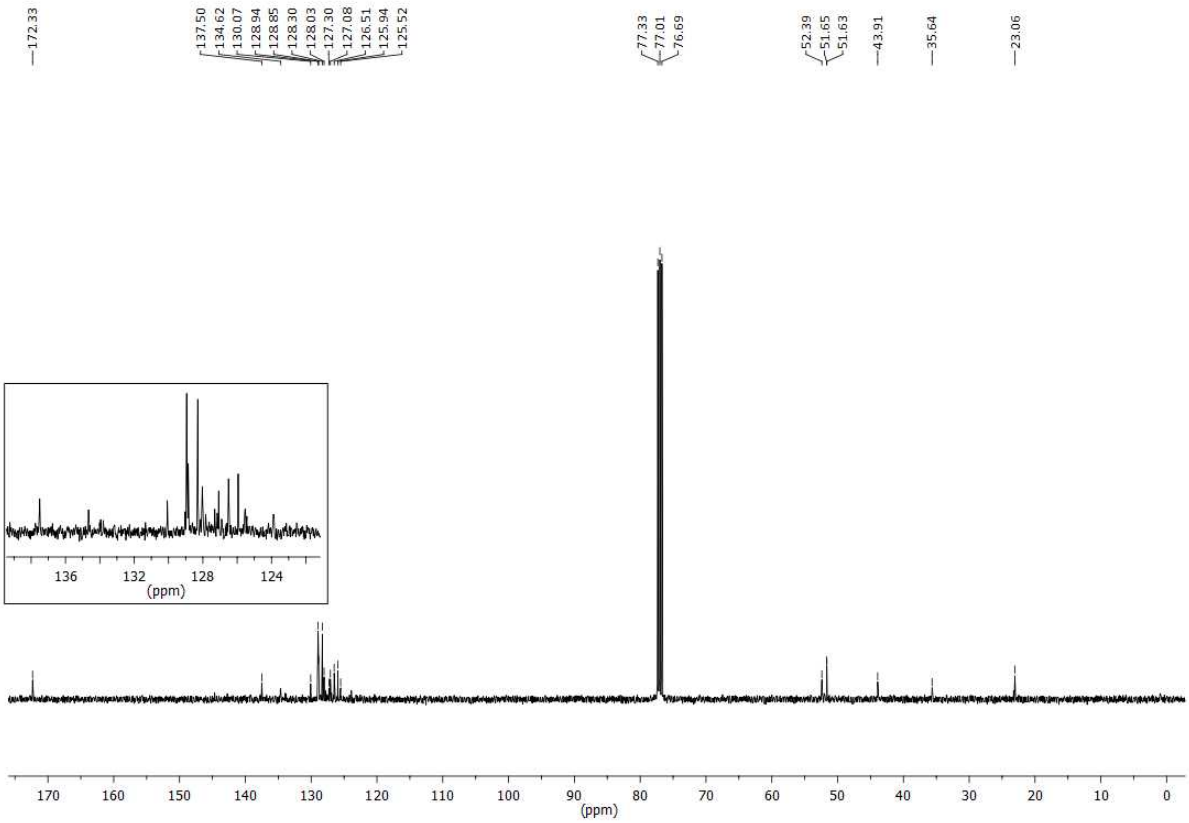
^{19}F NMR spectrum of crude irradiation mixture ($CDCl_3$, 188 MHz):



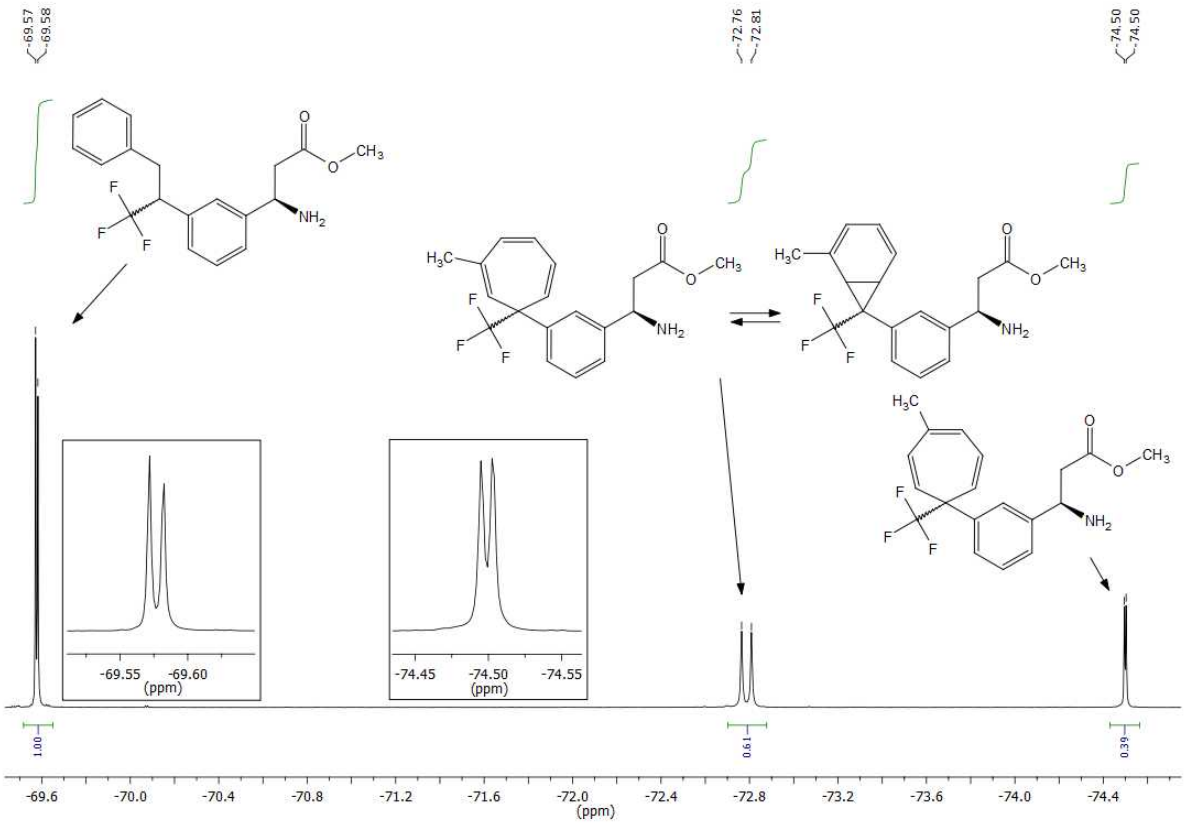
^{1}H NMR spectrum of irradiation products **12-16** ($CDCl_3$, 400 MHz):



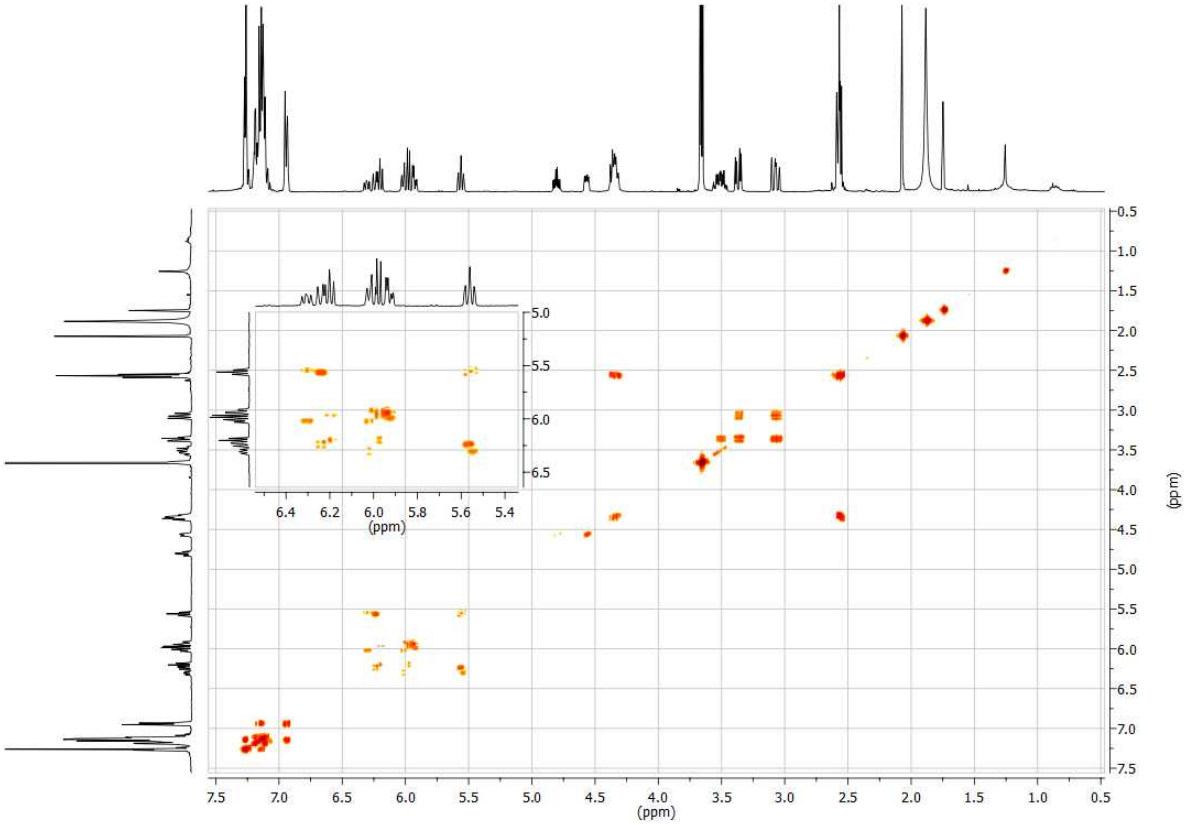
^{13}C NMR spectrum of irradiation products **12-16** ($CDCl_3$, 100 MHz):



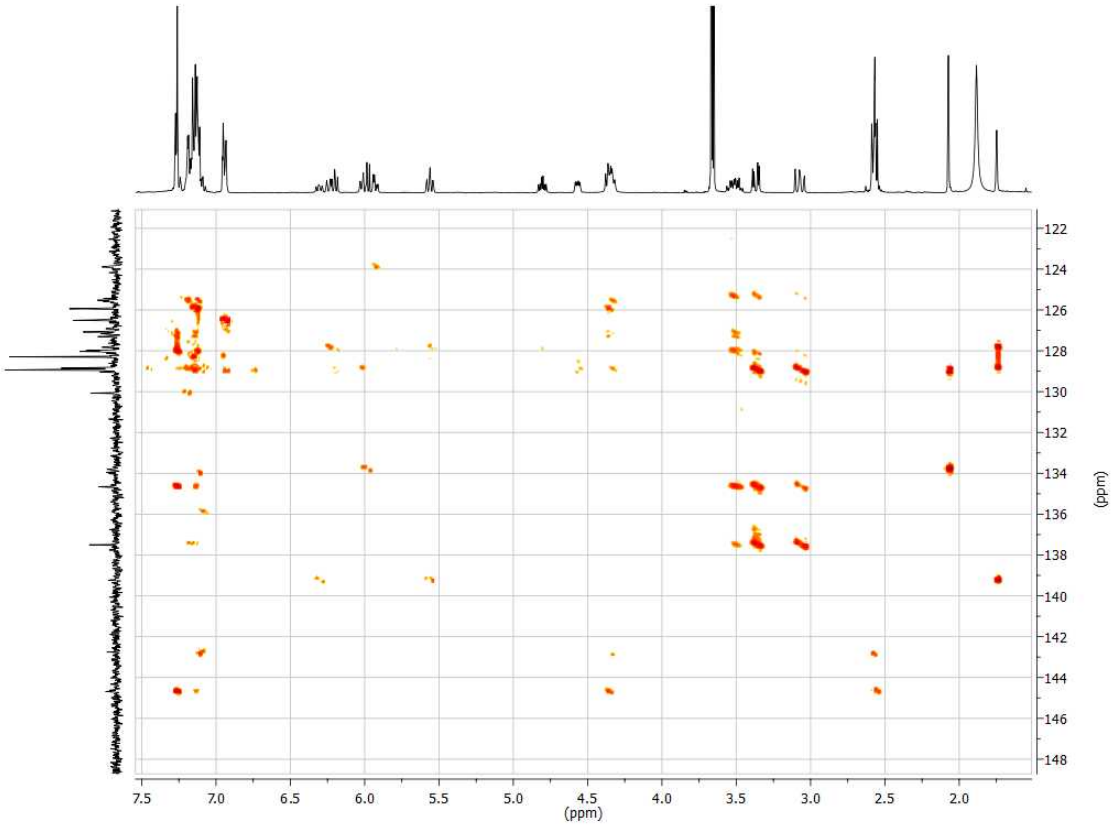
^{19}F NMR spectrum of irradiation products **12-16** ($CDCl_3$, 376 MHz):



COSY-spectrum of irradiation products **12-16** ($CDCl_3$, 400 MHz):

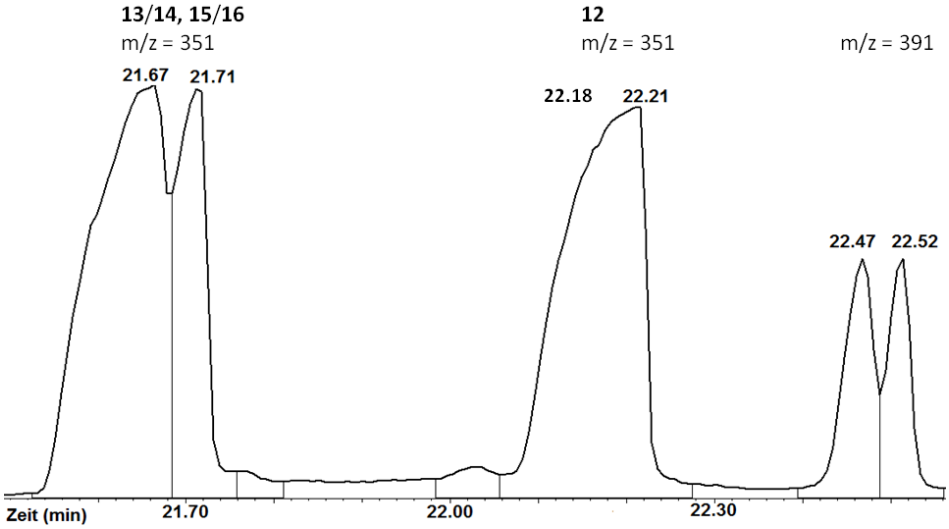


Section of HMBC spectrum of irradiation products **12-16** ($CDCl_3$, 400 MHz):



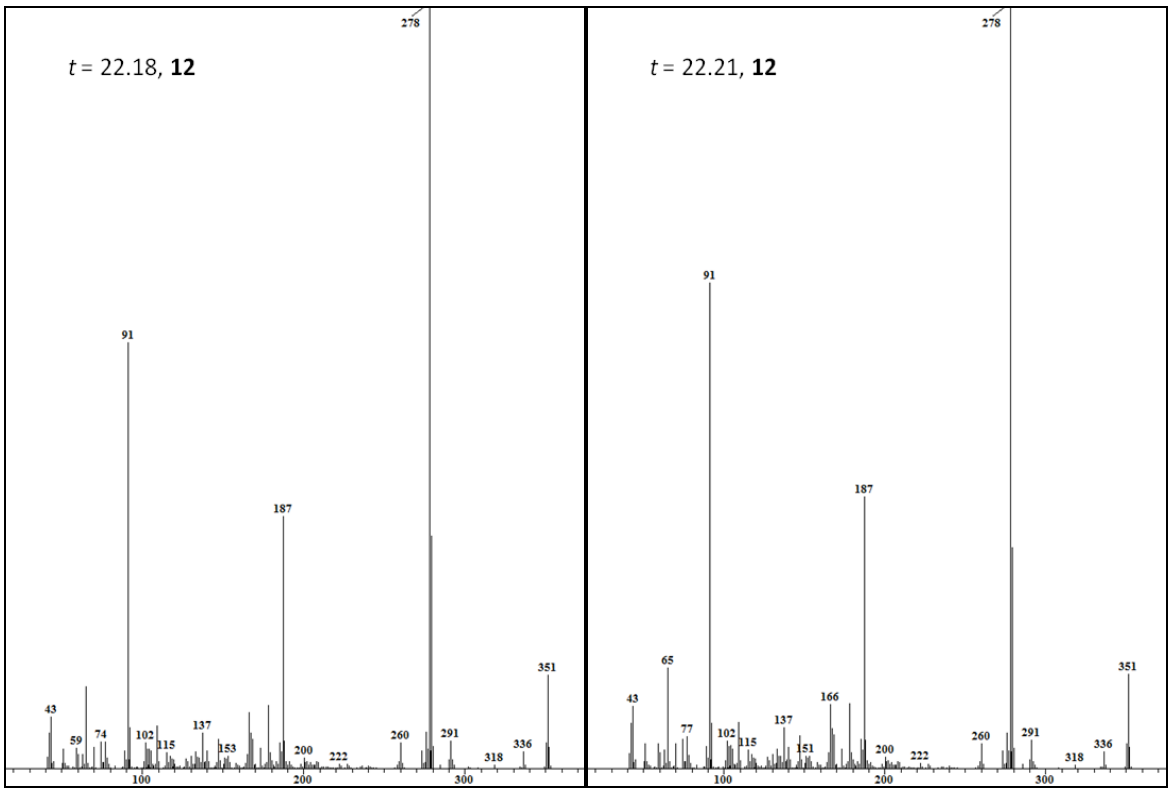
Irradiation products

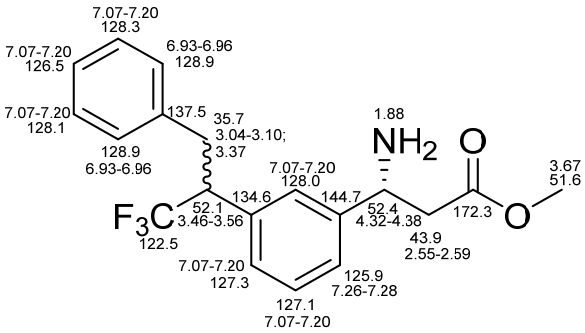
GC:

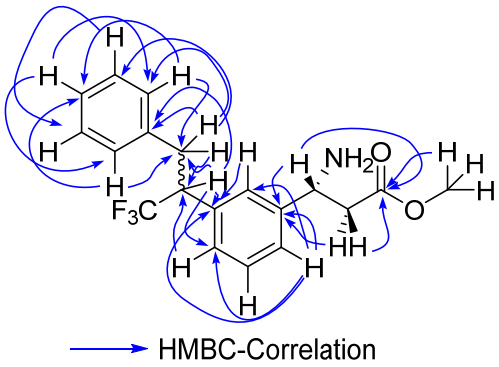


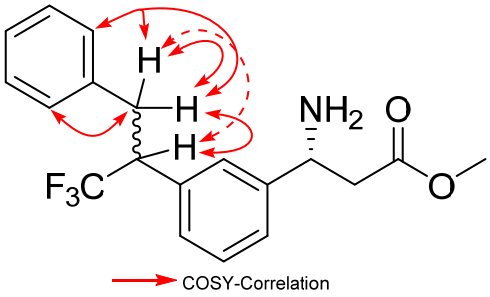
Benzyl adduct 12:

GC/MS (EI, 70 eV): *t* = 22.18 min (*m/z* (%) = 351.15 (12) [M^+], 278.15 (100), 187.06 (33), 91.06 (55)); 22.21 min (*m/z* (%) = 351.14 (10) [M^+], 278.12 (100), 187.06 (20), 91.06 (77)).



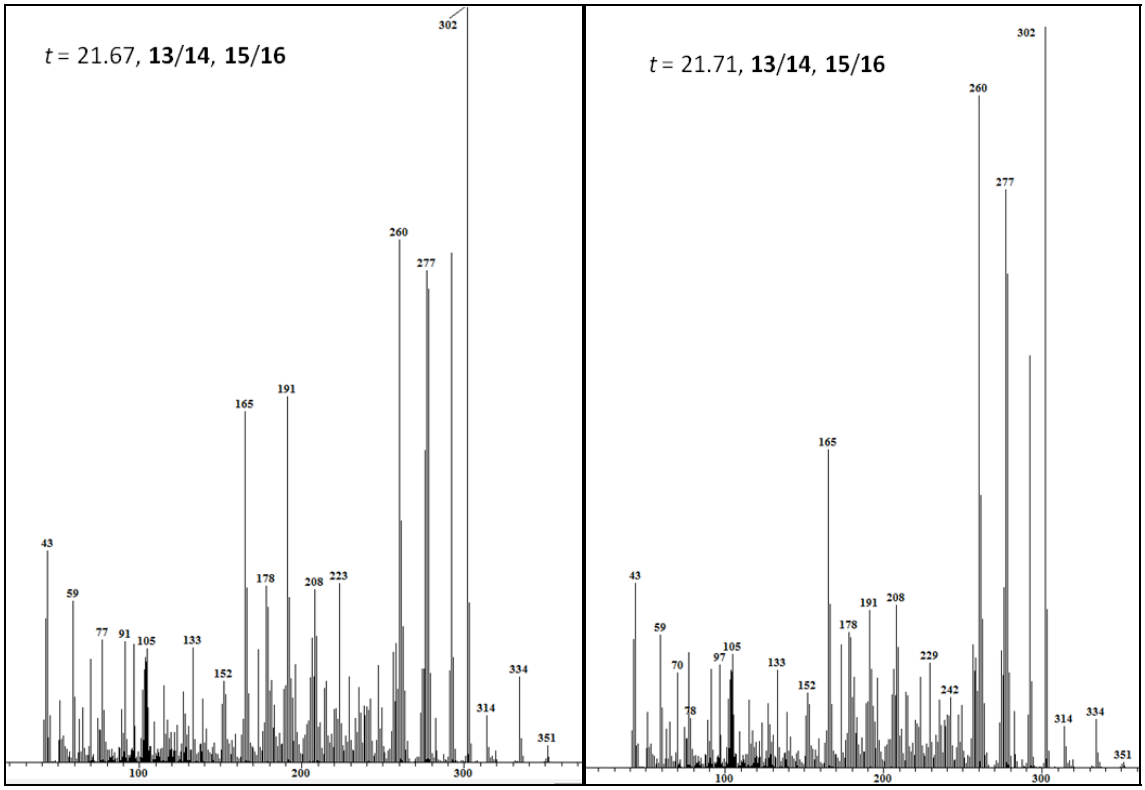

7.07-7.20
128.3
7.07-7.20
126.5
6.93-6.96
128.9
7.07-7.20
128.1
137.5
35.7
3.04-3.10;
3.37
128.9
6.93-6.96
1.88
NH2
O
3.67
51.6
7.07-7.20
128.0
134.6
144.7
F3C
52.1
3.46-3.56
52.4
4.32-4.38
172.3
O
122.5
43.9
2.55-2.59
7.07-7.20
127.3
125.9
7.26-7.28
127.1
7.07-7.20

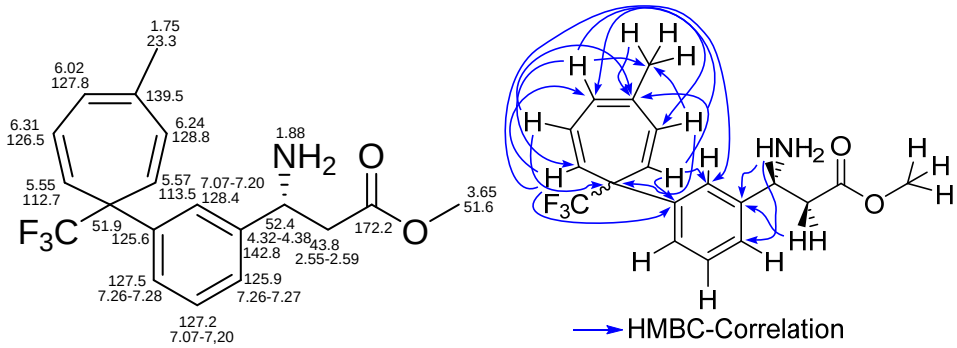

H
H
H
H
H
H
H
H
H
H
F3C
H
NH2
O
H
H
H
O
HH
H
H
H
HMBC-Correlation

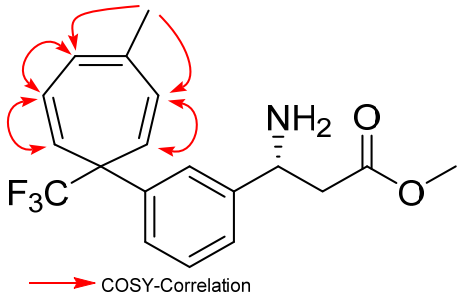

H
H
H
NH2
O
F3C
O
COSY-Correlation

Cycloheptatriene 13:

GC/MS (EI, 70 eV): *t* = 21.67 min (*m/z* (%) = 351.15 (3) [M$^+$], 334.12 (11), 302.10 (100), 277.11 (65), 260.08 (70), 165.07 (46)); 21.71 min (*m/z* (%) = 351.16 (1) [M$^+$], 334.12 (7), 302.10 (100), 277.11 (76), 260.08 (89), 165.07 (42)).

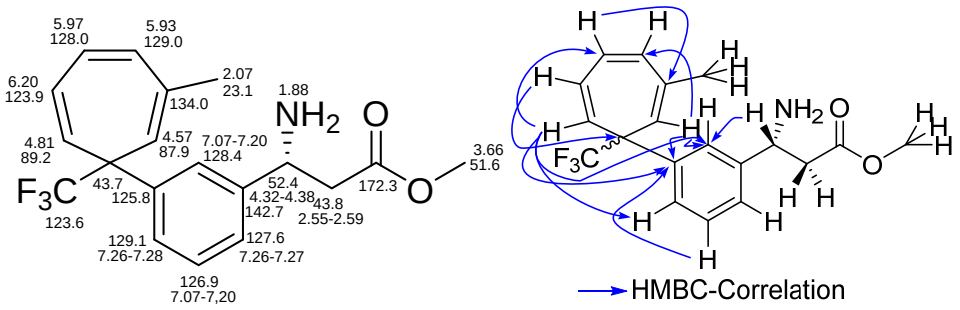


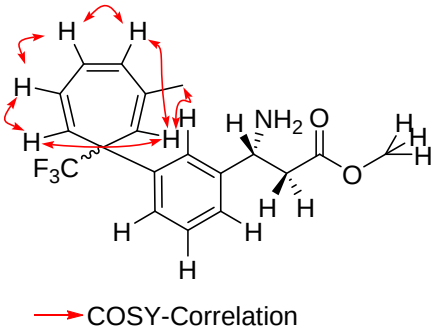




Cyclohexatriene/norcaradiene equilibrium (15, 16):

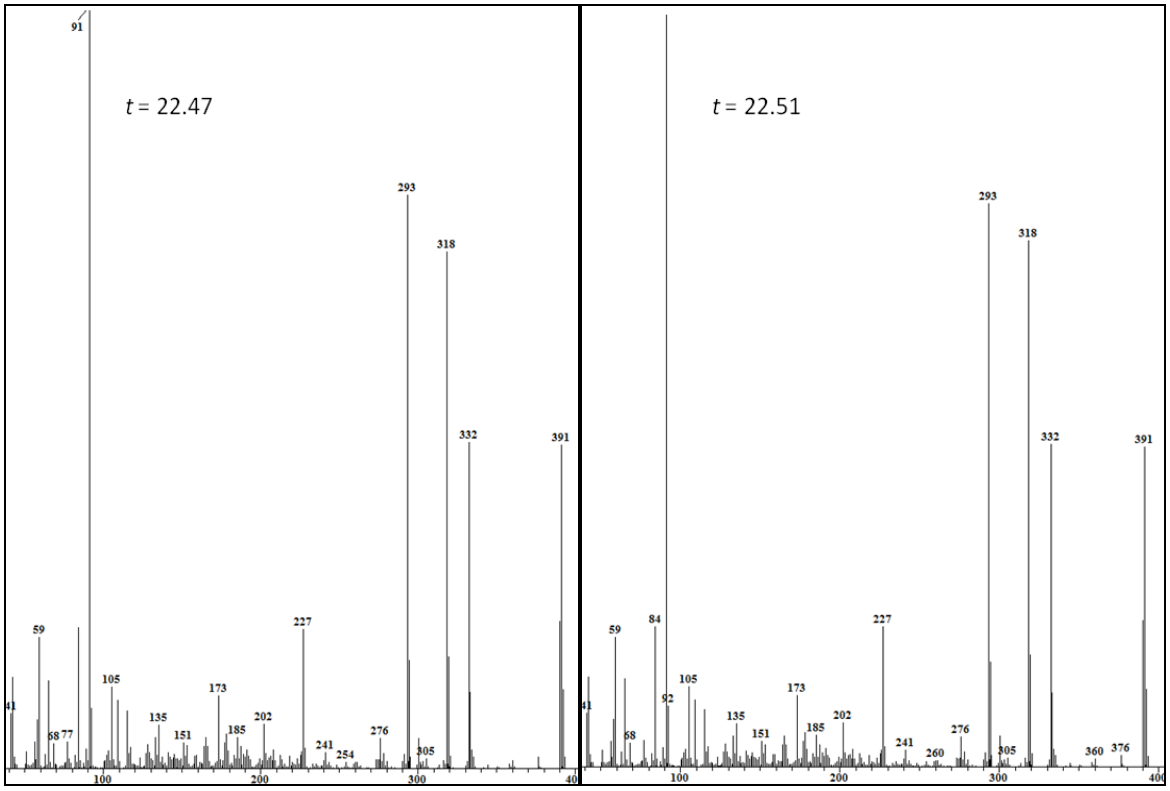
GC/MS (EI, 70 eV): t = 21.67 min (m/z (%) = 351.15 (3) [M^+], 334.12 (11), 302.10 (100), 277.11 (65), 260.08 (70), 165.07 (46)); 21.71 min (m/z (%) = 351.16 (1) [M^+], 334.12 (7), 302.10 (100), 277.11 (76), 260.08 (89), 165.07 (42)).



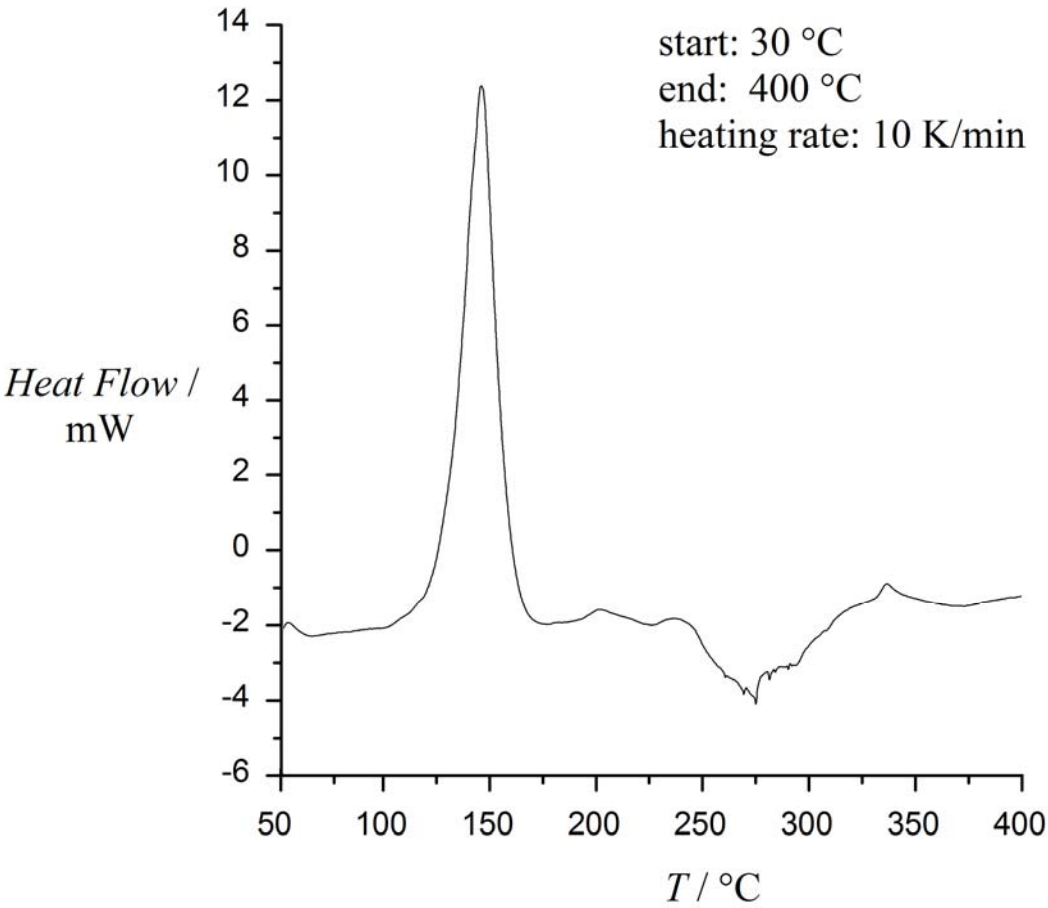


Unknown structure (not detectable in NMR):

GC/MS (EI, 70 eV): *t* = 22.47 min (*m*/*z* (%) = 391.19 (42), 332.16 (42), 318.15 (77), 293.12 (74), 91.06 (100)); 22.52 min (*m*/*z* (%) = 391.19 (42), 332.18 (43), 318.15 (70), 293.12 (74), 91.06 (100)).



Differential scanning calorimetry of 1



Calculations

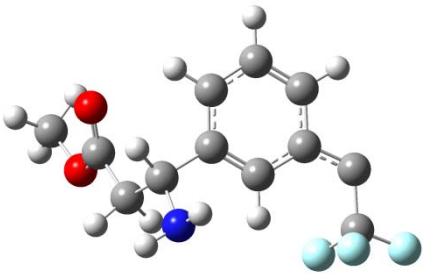
All structures were optimized at the B3LYP 6-311G (2s,2p) level of theory. Solvent effects were investigated with the polarized continuum model (PCM) as implemented in Gaussian 09.

Full reference to the GAUSSIAN 09 program:

GAUSSIAN 09, Revision A.1, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara,M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene,M.; Knox, J. E.; Cross, J.B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT (USA), **2009**.

For each optimized structure the output summary is given. The summary contains information about the level of theory, the atom coordinates and the energy.

Carbene 17



Singlet in the gas phase

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0.8599482495,0.5887828738\C,3.678873228,0.2921732618,0.7685334522\F,3.6888919223,
-0.9782387091,1.2644857565\F,4.3530658383,0.2843860481,-0.414726008\F,4.4267521415,
1.0150294363,1.6213601127\\Version=EM64L-G09RevA.02\State=1-A\HF=-930.1004324\RMSD=
8.560e-09\RMSF=5.521e-06\Dipole=-1.3765947,-1.4732096,-1.5307132\Quadrupole=-2.9069813,
2.998874,-0.0918927,-4.9321159,-5.5958764,-4.3601814\PG=C01 [X(C11H10F3N1O2)]\\@

Triplet in the gas phase

1\1\GINC-LINDEL22\FOpt\UB3LYP\6-311G(2d,2p)\C11H10F3N1O2(3)\ALEX\26-Jun-2013\0\\#
opt freq=noraman ub3lyp/6-311g(2d,2p)
geom=connectivity\\JNS1Conf1antiTgas\\0,3\H,0.7357661005,
-0.9209438079,0.499476052\C,0.4276851291,0.1097119634,0.4066549165\C,-0.3622053262,
2.7767469313,0.2099298094\C,-0.8693909905,0.4631922967,0.7429497376\C,1.360417643,
1.0877287402,-0.0403783195\C,0.9303977818,2.4381882802,-0.1309765788\C,-1.2629343749,
1.8036053977,0.6461064631\H,1.629747868,3.1906531776,-0.4663162489\H,-2.2766204529,
2.0780622481,0.9006666261\H,-0.6816221751,3.8077902882,0.1414795244\C,-1.8623969147,
-0.5992485174,1.1972574226\H,-2.6544759606,-0.09029806,1.7547365785\C,-2.5248465192,
-1.3049640807,0.0016053583\H,-1.7755720795,-1.666289616,-0.7009238267\H,-3.0649844736,
-2.1894820398,0.3543380426\C,-3.5382929076,-0.4569013052,-0.7280960232\O,-3.7935015251,

-0.9429069579,-1.9635538864\H,-4.4721137634,-0.369081111,-2.3475497782\O,-4.0983911956,
0.5157751996,-0.2895507356\N,-1.1668851317,-1.6256124995,1.9874470543\H,-0.730118384,
-1.19880441,2.7964213525\H,-1.8327350839,-2.303362668,2.3398519782\C,2.6608755059,
0.7327641958,-0.3795824193\C,3.4370343966,-0.5101266332,-0.416282229\F,3.5886559496,
-1.0621130869,0.8140702987\F,2.8482206116,-1.4619325404,-1.1850862738\F,4.6695062722,
-0.303325385,-0.9131308957\\Version=EM64L-G09RevA.02\State=3-A\HF=-930.1067727\S2=
2.035537\S2-1=0.\S2A=2.000602\RMSD=7.998e-09\RMSF=3.432e-06\Dipole=-
1.2673203,0.2171077,
0.3100732\Quadrupole=-5.1831067,2.1366915,3.0464152,6.4518007,1.5190432,-3.0106304\PG=
C01 [X(C11H10F3N1O2)]\\@

Singlet in cyclohexane

1\1\GINC-LINDEL22\FOpt\UB3LYP\6-311G(2d,2p)\C11H10F3N1O2\ALEX\26-Jun-2 013\0\\# opt
freq=noraman ub3lyp/6-311g(2d,2p) scrf=(solvent=cyclohexane) geom=connectivity
\\JNS1Conf1antiScyc\\0,1\H,0.7745085626,-0.897629 475,0.4570716258\C,0.4650077103,
0.1323047015,0.3797596915\C,-0.3485796 889,2.8064577491,0.2413929441\C,-0.8286033035,
0.4627626898,0.740211515 4\C,1.3880107848,1.1226414193,-0.0679766229\C,0.9378460364,
2.469597199 2,-0.1279807091\C,-1.2210851924,1.8084373339,0.6713856949\H,1.64346606
5,3.2132476601,-0.4680606134\H,-2.232339247,2.0688317403,0.9522847535\H,-0.6835077001,
3.8331715244,0.2008320255\C,-1.8118997637,-0.607803459 3,1.1980234257\H,-2.6067530181,
-0.106858181,1.7590606767\C,-2.46874492 18,-1.3238785411,0.0066015878\H,-1.714372599,
-1.7116218863,-0.67736929 71\H,-3.0266181886,-2.193649422,0.3665267604\C,-3.4523040494,
-0.475232 4017,-0.7605879334\O,-3.7811243877,-1.0443221142,-1.9380051017\H,-4.43 24761054,
-0.4649665957,-2.3600844392\O,-3.9284239725,0.5700727613,-0.3 901245406\N,-1.0988858231,
-1.6219230148,1.9862640727\H,-0.6998217544,- 1.196462407,2.8153731065\H,-1.7480816291,
-2.3298620104,2.3092222266\C, 2.7288195691,0.9171042692,-0.4758102721\C,3.2312950125,
-0.4935451453,- 0.4079052097\F,3.1592146976,-1.0304586722,0.8426382839\F,2.5487395005,
-1.3132720647,-1.2546543739\F,4.5279334059,-0.5943176573,-0.7665252779 \\Version=EM64L
-G09RevA.02\State=1-A\HF=-930.1066159\S2=0.\S2-1=0.\S2A =0.\RMSD=5.151e-
09\RMSF=4.616e
-06\Dipole=-2.7502019,0.1224904,0.789821 9\Quadrupole=-9.9442103,4.3907206,5.5534897,
3.5863616,3.2568135,-1.614 0527\PG=C01 [X(C11H10F3N1O2)]\\@

Triplet in cyclohexane

1\1\GINC-LINDEL22\FOpt\UB3LYP\6-311G(2d,2p)\C11H10F3N1O2(3)\ALEX\28-Jun-2013\0\\#
opt freq=noraman ub3lyp/6-311g(2d,2p) scrf=(solvent=cyclohexane) geom=connectivity\\
JNS1Conf1antiTcyc\\0,3\H,0.7253850005,-0.9209681106,0.4957890906\C,0.4200854885,
0.1107164058,0.4065266396\C,-0.3618514643,2.7814453069,0.2247078667\C,-0.8739607352,
0.4662990671,0.7521584387\C,1.3528161338,1.0874660136,-0.0430273354\C,0.9274088366,
2.4402438134,-0.1262253947\C,-1.2625253005,1.8086283623,0.6629724523\H,1.6268250528,
3.1918018098,-0.4632759491\H,-2.27250287,2.0868543257,0.9279514622\H,-0.6784768549,
3.8136753517,0.1630201303\C,-1.8670365515,-0.5949815104,1.2090586482\H,-2.6625041023,
-0.083810323,1.7591852719\C,-2.5215706441,-1.3113932332,0.0154626985\H,-1.7673782783,
-1.691717571,-0.6714353768\H,-3.0765367685,-2.1829543718,0.3770042916\C,-3.5171551549,
-0.4662375697,-0.7410062435\O,-3.7300842648,-0.9451174348,-1.9851842823\H,-4.4025231264,
-0.3789758832,-2.391845248\O,-4.0977588378,0.5004149291,-0.3122984482\N,-1.1744224756,

-1.613560793,2.012434609\H,-0.7605659341,-1.179009917,2.8296102342\H,-1.8432702779,
-2.2931458624,2.3563849946\C,2.6499667685,0.7296945808,-0.3917909448\C,3.4221658681,
-0.5130010424,-0.4451999688\F,3.5679570079,-1.0894661482,0.7759419176\F,2.8390734526,
-1.4528517682,-1.2341517716\F,4.6596600319,-0.301222427,-0.9312037827\\Version=EM64L-
G09RevA.02\State=3-A\HF=-930.1108838\S2=2.035296\S2-1=0.\S2A=2.000594\RMSD=4.443e
-09\RMSF=7.535e-06\Dipole=-1.378803,0.2393834,0.3480795\Quadrupole=-5.8756247,2.4425315,
3.4330932,7.0287864,1.5425146,-3.0245951\PG=C01 [X(C11H10F3N1O2)]\\@

Singlet in toluene

1\1\GINC-LINDEL22\FOpt\RB3LYP\6-311G(2d,2p)\C11H10F3N1O2\ALEX\09-Jul-2013\0\\# opt
freq
=noraman rb3lyp/6-311g(2d,2p) scrf=(solvent=toluene) geom=connectivity\\JNS1Conf1antiStoluol\\
0,1\H,0.7721993755,-0.8972830119,0.4560545302\C,0.4634672144,0.1329435973,0.3798696473\C,
-0.3481363594,2.8080784461,0.2452787866\C,-0.8293973249,0.46372407,0.7419450703\C,
1.3870755315,1.1232828391,-0.0674793905\C,0.9377343806,2.4710247104,-0.1251205926\C,
-1.2208387036,1.8098520765,0.6748571687\H,1.6431772305,3.2152245206,-0.4642917083\H,
-2.2313878595,2.0709081179,0.9575850942\H,-0.6825009603,3.8349926351,0.2064258434\C,
-1.8127359806,-0.6067022465,1.199876974\H,-2.6086625182,-0.1054702153,1.7589532989\C,
-2.4670528389,-1.3252119381,0.008601043\H,-1.7113295388,-1.7161364184,-0.6720543636\H,
-3.0273965255,-2.1928368569,0.3697697522\C,-3.4470329525,-0.4776326957,-0.7641834907\O,
-3.7703903314,-1.0479758892,-1.9421547901\H,-4.4201982121,-0.4700074382,-2.3686713216\O,
-3.9247496396,0.5683282326,-0.3969405171\N,-1.1002862691,-1.6187697516,1.9915057678\H,
-0.7077238928,-1.1913773338,2.8227976431\H,-1.7499160287,-2.327540353,2.3119740936\C,
2.7266283691,0.9165955063,-0.4762457152\C,3.2268430492,-0.4950081949,-0.4141165549\F,
3.1599831325,-1.0344333669,0.8354851885\F,2.5412364415,-1.3133372151,-1.2596417511\F,
4.5226112109,-0.5964058264,-0.7785157061\\Version=EM64L-G09RevA.02\State=1-A\HF=
-930.1078047\RMSD=7.175e-09\RMSF=4.770e-06\Dipole=-2.8115668,0.12797,0.8123459\
Quadrupole=-10.1612123,4.497482,5.6637303,3.6096917,3.258212,-1.5770052\PG=C01
[X(C11H10F3N1O2)]\\@

Triplet in toluene

1\1\GINC-LINDEL22\FOpt\UB3LYP\6-311G(2d,2p)\C11H10F3N1O2(3)\ALEX\09-Jul-2013\0\\#
opt freq=noraman ub3lyp/6-311g(2d,2p) scrf=(solvent=toluene) geom=connectivity\\
JNS1Conf1antiTtoluol\\0,3\H,0.7234331055,-0.9210456385,0.494280404\C,0.4186991739,
0.1108807034,0.4061182313\C,-0.3616004471,2.7823659185,0.2277045193\C,-0.8747297393,
0.4668420655,0.7536254534\C,1.3515144242,1.0874564982,-0.0436373049\C,0.9270285834,
2.4406933885,-0.1251591684\C,-1.2623070936,1.8095723162,0.6661635221\H,1.6264848999,
3.1921456225,-0.4623227828\H,-2.2715560203,2.0884753715,0.9332005035\H,-0.6776242638,
3.8148485275,0.1675066366\C,-1.8678522328,-0.5942282226,1.2108699858\H,-2.6639641046,
-0.0827112495,1.7596254959\C,-2.5208679498,-1.3125956396,0.0176226732\H,-1.7657902558,
-1.6960020468,-0.6665666471\H,-3.0782242966,-2.1820028419,0.3805939629\C,-3.5133992436,
-0.4680983008,-0.7434415339\O,-3.7192188622,-0.9458904711,-1.9888568345\H,-4.3906276487,
-0.3811885021,-2.3994004617\O,-4.0973829168,0.4976530929,-0.316602512\N,-1.1759103931,
-1.6113796642,2.0168142534\H,-0.7662332058,-1.1752043547,2.835296495\H,-1.8456093159,
-2.2908263334,2.359568401\C,2.6480400222,0.7291540476,-0.3941729826\C,3.4194990887,
-0.51352559,-0.4501418692\F,3.5657834983,-1.0929720628,0.7697613098\F,2.8363859267,

-1.4521143187,-1.2408719773\F,4.6572492671,-0.3014763158,-0.9360137726\\Version=EM64L-G09RevA.02\State=3-A\HF=-930.1116636\S2=2.035251\S2-1=0.\S2A=2.000593\RMSD=4.099e-09\RMSF=7.324e-06\Dipole=-1.3995504,0.2449968,0.3555516\Quadrupole=-5.9897037,2.4910813,3.4986224,7.1396668,1.535407,-3.0216401\PG=C01 [X(C11H10F3N1O2)]\\@

Singlet in diethylether

1\1\GINC-LINDEL22\FOpt\UB3LYP\6-311G(2d,2p)\C11H10F3N1O2\ALEX\10-Jul-2013\0\\# opt freq=noraman ub3lyp/6-311g(2d,2p) scrf=(solvent=diethylether) geom=connectivity \\JNS1Conf1antiSet2o\\0,1\H,0.7642399543,-0.8752226058,0.5019985517\C,0.4587598149,0.152491243,0.3886783539\C,-0.3446455949,2.8240886757,0.1588939447\C,-0.8341956784,0.4981326639,0.7338690871\C,1.3875753885,1.1248459965,-0.0891151717\C,0.9411653657,2.4718509765,-0.1950217643\C,-1.2211197571,1.8425666522,0.6195099568\H,1.6480974166,3.2039058501,-0.5566159926\H,-2.2310660996,2.116655688,0.8915393764\H,-0.6765056552,3.8496866738,0.0842359963\C,-1.8216662969,-0.5534896835,1.2248422607\H,-2.6232162701,-0.0309353014,1.7550824324\C,-2.4625232727,-1.3214779715,0.0575930861\H,-1.6992675835,-1.7448710483,-0.5947224906\H,-3.0312861002,-2.1697496335,0.4498633833\C,-3.4280499712,-0.5067587761,-0.7664961393\O,-3.7354081873,-1.1274112447,-1.9221780619\H,-4.3779665246,-0.5697076796,-2.3855227419\O,-3.9076746774,0.5562756373,-0.4527012841\N,-1.1170020963,-1.5308688722,2.0664779259\H,-0.7460147934,-1.0679231928,2.8888525138\H,-1.7714453442,-2.2278572281,2.4034156504\C,2.7258773014,0.8990383026,-0.4836273038\C,3.2225670969,-0.5103751181,-0.371344551\F,3.1496103347,-1.011805028,0.8934005346\F,2.5445330468,-1.3561528941,-1.1951298208\F,4.5228071829,-0.623978082,-0.7240957322\\Version=EM64L-G09RevA.02\State=1-A\HF=-930.1112148\S2=0.\S2-1=0.\S2A=0.\RMSD=9.275e-09\RMSF=2.346e-05\Dipole=-3.0001106,0.1798994,0.8566335\Quadrupole=-10.7665596,4.6704797,6.0960799,3.7991598,2.9947697,-1.3567158\PG=C01 [X(C11H10F3N1O2)]\\@

Triplet in diethylether

1\1\GINC-LINDEL22\FOpt\UB3LYP\6-311G(2d,2p)\C11H10F3N1O2(3)\ALEX\17-Jul-2013\0\\# opt freq=noraman ub3lyp/6-311g(2d,2p) scrf=(solvent=diethylether) geom=connectivity\\ JNS1Conf1antiTet2o\\0,3\H,0.7241899027,-0.9221541526,0.5030046543\C,0.4181955584,0.1085051685,0.4058870824\C,-0.3624823023,2.7793770643,0.2148618976\C,-0.8744712718,0.4659920662,0.7544948168\C,1.3500510517,1.082941128,-0.0510441915\C,0.9251762135,2.4358751008,-0.1399233291\C,-1.2616090909,1.8086266062,0.6613128028\H,1.6236039446,3.1856429258,-0.482795525\H,-2.2691425773,2.0897890094,0.9323183719\H,-0.6785010718,3.8115548933,0.150553669\C,-1.8674132257,-0.5919332223,1.2196080736\H,-2.660102401,-0.0773108387,1.7700885951\C,-2.5265411653,-1.3133449932,0.0315087654\H,-1.7749413724,-1.7043001603,-0.652175047\H,-3.0877556935,-2.1770501641,0.4017633587\C,-3.5172263967,-0.4696265611,-0.7325092372\O,-3.712890781,-0.9416275792,-1.9806911583\H,-4.3856885175,-0.3809168429,-2.3949789245\O,-4.1081097825,0.4921233888,-0.3041389559\N,-1.1755788727,-1.6076446658,2.0278901022\H,-0.7724305769,-1.168929814,2.8484581588\H,-1.8476294051,-2.2853374425,2.3700237896\C,2.6474741242,0.7260616758,-0.3990942427\C,3.4251215422,-0.5109720392,-0.4644419222\F,3.4268390853,-1.1893645129,0.7138497295\F,2.9510140679,-1.381373205,-1.3934003346\F,4.7120690139,-0.2657768333,-0.7788669997\\Version=EM64L-G09RevA.02\State=3-A\HF=-930.1138826\S2=2.035194\S2-1=0.\S2A=2.000591\RMSD=9.129e-09\RMSF=6.089e-06\Dipole=-1.4652729,0.2607538,0.3811508\Quadrupole=-6.2694641,2.6152862,3.6541778,7.4313087,1.6078827,-3.1253751\PG=C01 [X(C11H10F3N1O2)]\\@

Singlet in tetrahydrofuran

1\1\GINC-LINDEL22\FOpt\UB3LYP\6-311G(2d,2p)\C11H10F3N1O2\ALEX\09-Jul-2013\0\\# opt freq=noraman ub3lyp/6-311g(2d,2p) scrf=(solvent=thf) geom=connectivity\\JNS1Conf1antiSthf\\ 0,1\H,0.7572210277,-0.8565305548,0.5389678009\C,0.454048227,0.1680607112,0.3957026919\C, -0.3438411082,2.8339728679,0.0879778187\C,-0.8393480993,0.5248590305,0.7259286085\C, 1.3864359795,1.1255277093,-0.1059248895\C,0.9421678101,2.4702295574,-0.2518019367\C, -1.2231956994,1.8665151397,0.5729699461\H,1.6505176733,3.1916937784,-0.6313710836\H, -2.2329993289,2.1502496896,0.835223461\H,-0.6738428173,3.8575365635,-0.0158449455\C, -1.8302910557,-0.510885272,1.2425989992\H,-2.6358264706,0.0279044325,1.7496050503\C, -2.461075969,-1.3168236242,0.0957384826\H,-1.6924392294,-1.7649705521,-0.5333389962\H, -3.0370041402,-2.1487315412,0.5116389656\C,-3.4148241417,-0.5290885142,-0.7671573334\O, -3.709009462,-1.1876320854,-1.90471286\H,-4.3458073941,-0.64665556,-2.3953357695\O, -3.8959571626,0.5451069435,-0.4952015555\N,-1.1325063599,-1.4596641685,2.1221996346\H, -0.775602961,-0.9689588195,2.9347291515\H,-1.7911623426,-2.145728747,2.4733101071\C, 2.7244518066,0.8854656119,-0.4881997707\C,3.2189148598,-0.5203474225,-0.3318811074\F, 3.1361138735,-0.9897297332,0.9443415166\F,2.5491888235,-1.3878513266,-1.139149593\F, 4.5235636609,-0.6432791138,-0.6699783935\\Version=EM64L-G09RevA.02\State=1-A\HF= -930.1134326\S2=0.\S2-1=0.\S2A=0.\RMSD=8.166e-09\RMSF=1.095e-05\Dipole=-3.1251063, 0.2231729,0.8815591\Quadrupole=-11.1450126,4.7724466,6.3725661,3.9112208,2.7503317, -1.1726284\PG=C01[X(C11H10F3N1O2)]\\@

Triplet in tetrahydrofuran

1\1\GINC-LINDEL22\FOpt\UB3LYP\6-311G(2d,2p)\C11H10F3N1O2(3)\ALEX\11-Jul-2013\0\\# opt freq=noraman ub3lyp/6-311g(2d,2p) scrf=(solvent=thf) geom=connectivity\\JNS1Conf1antiTthf \\0,3\H,0.6868475688,-0.8894865475,0.5624878367\C,0.3734900508,0.1346176207,0.4271878946 \C,-0.4268370135,2.7909401321,0.1385279438\C,-0.9291762053,0.4899866399,0.7387627909\C, 1.3056915665,1.1034695775,-0.0408185442\C,0.8708084921,2.4491303507,-0.1798504051\C, -1.3259879089,1.825477348,0.5966149419\H,1.5691678623,3.1948222922,-0.5315377455\H, -2.3408760121,2.1056584083,0.839777416\H,-0.7506343024,3.8176204321,0.0365192284\C, -1.9214250728,-0.5626154362,1.2169186118\H,-2.7340698122,-0.0384517512,1.7275381452\C, -2.5403638719,-1.3362337064,0.0401655475\H,-1.7663831034,-1.7454648822,-0.6069428926\H, -3.1035659503,-2.1905411563,0.4285637932\C,-3.5169294133,-0.5335457486,-0.7836063274\O, -3.6705401099,-1.0535285811,-2.0179202176\H,-4.3375632453,-0.5184366713,-2.4736896814\O, -4.1302912589,0.4369263221,-0.4086627074\N,-1.2395646131,-1.5385102479,2.0814047541\H, -0.8679460651,-1.0630412063,2.8965092734\H,-1.9145984314,-2.2098628698,2.4305676702\C, 2.613136777,0.7487143193,-0.3515986339\C,3.4035269086,-0.4812395385,-0.3654172792\F, 3.3791098487,-1.1322977278,0.8283939635\F,2.9650006708,-1.3790982011,-1.2861693035\F, 4.6968996442,-0.2310341707,-0.6495780732\\Version=EM64L-G09RevA.02\State=3-A\HF= -930.1153124\S2=2.035114\S2-1=0.\S2A=2.000589\RMSD=7.706e-09\RMSF=2.527e-06\Dipole= -1.5164617,0.2708451,0.3576423\Quadrupole=-6.6297779,2.6200197,4.0097583,7.6594202, 1.0844726,-2.8510691\PG=C01 [X(C11H10F3N1O2)]\\@

Singlet in dichloromethane

1\1\GINC-LINDEL22\FOpt\UB3LYP\6-311G(2d,2p)\C11H10F3N1O2\ALEX\27-Jun-2013\0\\# opt freq=noraman ub3lyp/6-311g(2d,2p) scrf=(solvent=dichloromethane) geom=connectivity

\\JNS1Conf1antiSdcm\\0,1\H,0.760997502,-0.8966710844,0.4442180088\C,0.4561489574,
0.1351557896,0.3762763028\C,-0.344877715,2.8155295154,0.264579932\C,-0.8321583648,
0.4674463732,0.7488041418\C,1.3819755956,1.1255711497,-0.0710468543\C,0.93616229,
2.4770531625,-0.1171108185\C,-1.2176065488,1.816247583,0.694042777\H,1.6392261649,
3.2237774608,-0.4554115359\H,-2.2233523391,2.0807391036,0.9898246569\H,-0.6760295582,
3.8435649489,0.2363433292\C,-1.8158384929,-0.602046613,1.2071738741\H,-2.6150400387,
-0.0998414601,1.7595895818\C,-2.4607582269,-1.3302180643,0.0170302038\H,-1.699985971,
-1.7354835327,-0.6495841255\H,-3.0321459317,-2.1879004313,0.3839169846\C,-3.4243245296,
-0.4873186574,-0.7802722791\O,-3.73157269,-1.0684372708,-1.9557751498\H,-4.3743159732,
-0.4968048216,-2.401920444\O,-3.9022680724,0.5659977155,-0.4314772779\N,-1.1062721462,
-1.6067344122,2.0124317578\H,-0.7407545405,-1.1707633412,2.8519562697\H,-1.7605584898,
-2.3154171938,2.3248735599\C,2.7141761376,0.9129521182,-0.4870166334\C,3.2090713144,
-0.5004687807,-0.4376697509\F,3.1487928574,-1.0556479987,0.8048366999\F,2.5249032786,
-1.3116588229,-1.2901047678\F,4.5076255311,-0.5997964352,-0.8069444428\\Version=EM64L
-G09RevA.02\State=1-A\HF=-930.1139735\S2=0.\S2-1=0.\S2A=0.\RMSD=5.740e-09\RMSF=3.928e
-06\Dipole=-3.1427125,0.1635642,0.9498757\Quadrupole=-11.1621523,4.9847063,6.177446,
3.6781089,3.2272538,-1.2905606\PG=C01 [X(C11H10F3N1O2)]\\@

Triplet in dichloromethane

1\1\GINC-LINDEL22\FOpt\UB3LYP\6-311G(2d,2p)\C11H10F3N1O2(3)\ALEX\28-Jun-2013\0\\#
opt freq=noraman ub3lyp/6-311g(2d,2p) scrf=(solvent=dichloromethane) geom=connectivity\\
JNS1Conf1antiTdcm\\0,3\H,0.7177067302,-0.922378127,0.4972253932\C,0.4140147679,
0.109365032,0.4046006164\C,-0.3596482181,2.7832601943,0.2265159877\C,-0.8766640182,
0.468766304,0.7586860188\C,1.3471479688,1.0829717702,-0.0514398468\C,0.9260051432,
2.4377014624,-0.1336894361\C,-1.2599549657,1.8128866812,0.6719260499\H,1.6252829167,
3.1870334667,-0.4756234464\H,-2.2653320275,2.0963310933,0.9485188272\H,-0.6728858794,
3.8165727014,0.1676813303\C,-1.8704939789,-0.5882576179,1.2234825746\H,-2.6662217703,
-0.0725150697,1.7680908251\C,-2.5224826128,-1.3167221832,0.0358384812\H,-1.7668057087,
-1.7130571607,-0.6403124853\H,-3.0871425795,-2.177091351,0.4083815389\C,-3.5065542269,
-0.4774423978,-0.7411080514\O,-3.6918311831,-0.9558062618,-1.9877151031\H,-4.3620312085,
-0.3994254075,-2.4123308045\O,-4.1004075706,0.4874466287,-0.3225748276\N,-1.1817537603,
-1.5988069527,2.0416044514\H,-0.7883173879,-1.153444039,2.8634785576\H,-1.8575799699,
-2.2729979524,2.3838216606\C,2.6426348888,0.724269006,-0.4047713313\C,3.417461058,
-0.5131318258,-0.4805434621\F,3.4104839202,-1.2076360124,0.6888957236\F,2.9490243277,
-1.3716353543,-1.4239327833\F,4.7075653448,-0.2674306269,-0.7831424585\\Version=EM64L-
G09RevA.02\State=3-A\HF=-930.1156598\S2=2.035097\S2-1=0.\S2A=2.000589\RMSD=9.009e
-09\RMSF=8.382e-06\Dipole=-1.5142716,0.2794389,0.4067298\Quadrupole=-6.4217612,2.6476097,
3.7741515,7.7070243,1.5194118,-3.0598802\PG=C01 [X(C11H10F3N1O2)]\\@

Singlet in acetone

1\1\GINC-LINDEL22\FOpt\UB3LYP\6-311G(2d,2p)\C11H10F3N1O2\ALEX\09-Jul-2 013\0\\# opt
freq=noraman ub3lyp/6-311g(2d,2p) scrf=(solvent=acetone) geom=connectivity
\\JNS1Conf1antiSaceton\\0,1\H,0.7569801129,-0.8966836 849,0.4382084533\C,0.4535661125,
0.1357736779,0.3741883155\C,-0.3432635 644,2.8180263171,0.272174989\C,-0.8330141268,
0.4687163281,0.7508760945 \C,1.3800830655,1.126148329,-0.0730768546\C,0.9357137584,
2.4788119472, -0.1146896472\C,-1.2160950742,1.8185017247,0.7015066263\H,1.6380583952,

3.226118421,-0.4531721109\H,-2.2200071023,2.0841123092,1.0023238838\H,-0.6729608215,
3.846569644,0.2483002154\C,-1.8170101726,-0.6003742194, 1.2090299669\H,-2.6174893407,-
0.0977625595,1.7588723634\C,-2.458496145 8,-1.3318789162,0.0192348874\H,-1.6958955993,-
1.7413158582,-0.64281383 97\H,-3.0330864224,-2.1866934129,0.3875844678\C,-3.4167609569,-
0.49070 31983,-0.7860050674\O,-3.722436505,-1.0778866919,-1.9586025974\H,-4.36 2557092,-
0.5079679883,-2.4108473828\O,-3.8918686934,0.5667569889,-0.44 51757756\N,-1.1087834873,-
1.6025972741,2.0191911469\H,-0.7497962682,-1 .163148001,2.8598509587\H,-1.7651376783,-
2.3097667904,2.3312231038\C,2 .7098062995,0.9116394289,-0.4924358485\C,3.2037509393,-
0.5020499956,-0.4449298842\F,3.1402329023,-1.0641104739,0.7942623027\F,2.5231106898,-
1.309311773,-1.3035081413\F,4.5045767757,-0.6000982785,-0.8100066257\\ Version=EM64L-
G09RevA.02\State=1-A\HF=-930.1155799\S2=0.\S2-1=0.\S2A=0 .\RMSD=4.258e-
09\RMSF=3.505e-06\Dipole=-3.2325041,0.1761578,0.995463\Q uadrupole=-
11.3778023,5.0754683,6.302334,
3.6853112,3.1853021,-1.163507 9\PG=C01 [X(C11H10F3N1O2)]\\@

Triplet in acetone

1\1\GINC-LINDEL22\FOpt\UB3LYP\6-311G(2d,2p)\C11H10F3N1O2(3)\ALEX\11-Jul-2013\0\\#
opt freq=noraman ub3lyp/6-311g(2d,2p) scrf=(solvent=acetone) geom=connectivity\\
JNS1Conf1antiTaceton\\0,3\H,0.7128971408,-0.9222932034,0.4922760725\C,0.4108871283,
0.1102900703,0.4035748257\C,-0.3575267569,2.7864107461,0.2361061577\C,-0.8782458969,
0.4710062635,0.7618928999\C,1.3450391589,1.0834544567,-0.0514484967\C,0.9265816291,
2.4394245624,-0.1284191459\C,-1.2586919431,1.8162556426,0.6804747701\H,1.6264678513,
3.1885346935,-0.4695514732\H,-2.2624826531,2.1011782537,0.9612682175\H,-0.6686970817,
3.8205548005,0.1815840949\C,-1.872788829,-0.5854409086,1.2263206429\H,-2.6707705051,
-0.0689579093,1.7666398806\C,-2.5194424454,-1.3190519674,0.0390389629\H,-1.7606517755,
-1.7200731041,-0.6309222055\H,-3.0874165033,-2.1765295588,0.4130518292\C,-3.4975397812,
-0.4828810831,-0.7485342514\O,-3.6780017117,-0.9694973966,-1.9922774617\H,-4.3453930111,
-0.4158625691,-2.4250564686\O,-4.0907788889,0.4868720678,-0.339709413\N,-1.1862418368,
-1.5922548728,2.0514267757\H,-0.7991463744,-1.1422470414,2.8738903882\H,-1.8643239971,
-2.2642746356,2.3938571711\C,2.6390236694,0.7233270194,-0.408950704\C,3.4112561637,
-0.5147547588,-0.4925112687\F,3.3982863611,-1.2202830626,0.6706192465\F,2.9454854254,
-1.3644722446,-1.4454912535\F,4.703435463,-0.2696082602,-0.7875857934\\Version=EM64L-
G09RevA.02\State=3-A\HF=-930.1166877\S2=2.035034\S2-1=0.\S2A=2.000587\RMSD=9.065e
-09\RMSF=2.248e-06\Dipole=-1.5439864,0.2905223,0.4264547\Quadrupole=-6.4719136,2.6322783,
3.8396353,7.8838785,1.4249063,-2.9957341\PG=C01 [X(C11H10F3N1O2)]\\@

Singlet in methanol

1\1\GINC-LINDEL22\FOpt\UB3LYP\6-311G(2d,2p)\C11H10F3N1O2\ALEX\26-Jun-2013\0\\# opt
freq=noraman ub3lyp/6-311g(2d,2p) scrf=(solvent=methanol) geom=connectivity\\
JNS1Conf1antiSmeoh\\0,1\H,0.7557057199,-0.8967660468,0.4360430008\C,0.4526886642,
0.1358731542,0.3733459594\C,-0.3428861935,2.8186771193,0.2744267212\C,-0.833295756,
0.4689903149,0.7515156646\C,1.3793454379,1.1262399361,-0.0740850091\C,0.9353547409,
2.4792364105,-0.1143544008\C,-1.2156505992,1.8190854776,0.7039233642\H,1.6373732898,
3.2267229921,-0.4531163972\H,-2.2189259124,2.0850304455,1.0065251627\H,-0.6721358883,
3.8473741087,0.2519493133\C,-1.8173489886,-0.5999567636,1.2096882785\H,-2.6181904771,
-0.0972254554,1.7587722175\C,-2.4578860523,-1.3324623858,0.0200339795\H,-1.6947911553,

-1.7433516616,-0.6405596366\H,-3.0336367483,-2.1862371524,0.3889200328\C,-3.4143960052,
-0.4916524253,-0.7876080756\O,-3.71894836,-1.0800655329,-1.9597801326\H,-4.3582798738,
-0.5105995465,-2.4137631427\O,-3.8890663044,0.5667329377,-0.448791261\N,-1.1095303713,
-1.6014556232,2.0213564382\H,-0.7522537184,-1.1608377495,2.8621836708\H,-1.7666261087,
-2.3079209146,2.3336065909\C,2.7082421277,0.9111513451,-0.4946448114\C,3.2022013561,
-0.5024772568,-0.4470689034\F,3.1367511762,-1.0668996498,0.7909580387\F,2.5233896526,
-1.3084618772,-1.3081928153\F,4.5040163476,-0.5999182004,-0.8097198474\\Version=EM64L-
G09RevA.02\State=1-A\HF=-930.1160711\S2=0.\S2-1=0.\S2A=0.\RMSD=7.215e-09\RMSF=6.595e
-06\Dipole=-3.2595322,0.1807666,1.0100799\Quadrupole=-11.4432946,5.1033981,6.3398966,
3.6859009,3.1741537,-1.1223627\PG=C01 [X(C11H10F3N1O2)]\\@

Triplet in methanol

1\1\GINC-LINDEL22\FOpt\UB3LYP\6-311G(2d,2p)\C11H10F3N1O2(3)\ALEX\29-Jun-2013\0\\#
opt freq=noraman ub3lyp/6-311g(2d,2p) scrf=(solvent=methanol) geom=connectivity\\
JNS1Conf1antiTmeoh\\0,3\H,0.7114589864,-0.9223311269,0.4907871329\C,0.4099200227,
0.110483711,0.4032065482\C,-0.3569754141,2.7872320296,0.2387717345\C,-0.8787323086,
0.4715887907,0.7628633943\C,1.3443243306,1.0834924297,-0.0516527964\C,0.9266427914,
2.4398225683,-0.1271189841\C,-1.2583447878,1.8171614657,0.6829913487\H,1.6266710741,
3.1888545247,-0.4681058429\H,-2.2616172196,2.1025399953,0.9651638171\H,-0.6675360401,
3.8216182151,0.1855122007\C,-1.8734671515,-0.5846648015,1.2272700219\H,-2.6719742086,
-0.0679758984,1.7665287602\C,-2.5188120984,-1.3196837792,0.0401819363\H,-1.7592499237,
-1.7225281223,-0.6278309737\H,-3.088198623,-2.1759509923,0.4147804976\C,-3.494766385,
-0.4841914454,-0.750695523\O,-3.6733400764,-0.9729218623,-1.9937729615\H,-4.3397409812,
-0.4200069094,-2.4290525735\O,-4.0878892172,0.4869375635,-0.3447391119\N,-1.1874740315,
-1.5904834873,2.0542200866\H,-0.8024172588,-1.139241619,2.8770000684\H,-1.8661231474,
-2.2620809067,2.396475052\C,2.63786421,0.7229733586,-0.4103754014\C,3.409454959,
-0.5152370548,-0.4959469944\F,3.3950125257,-1.2235962146,0.6655733126\F,2.9443890905,
-1.3627404338,-1.4513423727\F,4.7021408826,-0.2702439983,-0.7891283763\\Version=EM64L-
G09RevA.02\State=3-A\HF=-930.1170005\S2=2.035017\S2-1=0.\S2A=2.000586\RMSD=9.928e
-09\RMSF=2.261e-06\Dipole=-1.5531604,0.293878,0.4326029\Quadrupole=-6.4869288,2.6276201,
3.8593087,7.938773,1.3929262,-2.9778388\PG=C01 [X(C11H10F3N1O2)]\\@

Singlet in DMSO

1\1\GINC-LINDEL22\FOpt\UB3LYP\6-311G(2d,2p)\C11H10F3N1O2\ALEX\11-Jul-2013\0\\# opt
freq=noraman ub3lyp/6-311g(2d,2p) scrf=(solvent=dmso) geom=connectivity
\\JNS1Conf1antiSdmso\\0,1\H,0.7532163714,-0.8752956677,0.4872621532\C,0.4515247854,
0.1544477742,0.383930192\C,-0.3410006548,2.832214676,0.1796008675\C,-0.8368489391,
0.5020596393,0.7400632779\C,1.3824077915,1.1270614126,-0.0928449183\C,0.9399824932,
2.4780336265,-0.1861496601\C,-1.2177729839,1.8496436774,0.6392791994\H,1.6452086463,
3.2122440943,-0.5465892063\H,-2.2230204489,2.1272319269,0.9243326222\H,-0.6692740668,
3.8595257813,0.116533231\C,-1.8249053425,-0.5486143806,1.2307125745\H,-2.6300773046,
-0.0252814614,1.7535269972\C,-2.4556194995,-1.3264293715,0.0648656095\H,-1.6871280425,
-1.7624824918,-0.5729966826\H,-3.0347150389,-2.1653669885,0.4614484155\C,-3.4047788368,
-0.5174617605,-0.7829283658\O,-3.7021768004,-1.152477303,-1.9323862525\H,-4.3370867704,
-0.6008933704,-2.4138470379\O,-3.8796668737,0.5546785387,-0.4908016507\N,-1.1239951248,
-1.5179993115,2.0862582177\H,-0.7744401413,-1.0451239768,2.9126894212\H,-1.7840126822,

-2.2119398012,2.4197383688\C,2.7141888981,0.8956222504,-0.4948162416\C,3.2050744413,
-0.5163315426,-0.3942421834\F,3.1355904473,-1.0323261586,0.8644222189\F,2.527759579,
-1.3542640544,-1.2255155476\F,4.5077450974,-0.6295217568,-0.7498636197\\Version=EM64L-
G09RevA.02\State=1-A\HF=-930.1163288\S2=0.\S2-1=0.\S2A=0.\RMSD=5.744e-09\RMSF=7.864e
-06\Dipole=-3.2833742,0.2211391,0.9848092\Quadrupole=-11.5167391,5.0236354,6.4931037,
3.8077081,2.8697217,-1.0253944\PG=C01 [X(C11H10F3N1O2)]\\@

Triplet in DMSO

1\1\GINC-LINDEL22\FOpt\UB3LYP\6-311G(2d,2p)\C11H10F3N1O2(3)\ALEX\13-Jul-2013\0\\#
opt freq=noraman ub3lyp/6-311g(2d,2p) scrf=(solvent=dmso)
geom=connectivity\\JNS1Conf1antiTdmso
\\0,3\H,0.6783872092,-0.8898335248,0.5537071317\C,0.367838113,0.1360154512,0.4252990547
\C,-0.4236612158,2.797003612,0.1554562632\C,-0.9323329935,0.4940046715,0.7443177609\C,
1.3017717136,1.1041264316,-0.0408545465\C,0.8714506943,2.4524055775,-0.1704360979\C,
-1.3243358453,1.8318238867,0.6116201177\H,1.5708719759,3.1977607579,-0.5205905554\H,
-2.3365833707,2.1149457445,0.8622421876\H,-0.743953588,3.8254752351,0.0611626548\C,
-1.9258127054,-0.5576645033,1.2215920128\H,-2.7423052647,-0.0325758877,1.724529561\C,
-2.5351182792,-1.340241008,0.0459518867\H,-1.7557554648,-1.7572818324,-0.5897758052\H,
-3.1042835063,-2.1894222217,0.4366542594\C,-3.5006402655,-0.5435819101,-0.7961094586\O,
-3.6446695488,-1.0770211865,-2.025149621\H,-4.3064129409,-0.5472589304,-2.4949894849\O,
-4.113202512,0.4343991771,-0.4381945716\N,-1.248147187,-1.5265742376,2.0980878933\H,
-0.8881418261,-1.0429627018,2.9138066964\H,-1.9272643477,-2.194142991,2.4472857892\C,
2.6068166126,0.7467915249,-0.3587962044\C,3.3933143293,-0.4845896175,-0.3866496786\F,
3.3594804065,-1.1556128706,0.7964982852\F,2.9597939428,-1.3675984173,-1.3246343158\F,
4.6898228647,-0.2344152295,-0.6578832146\\Version=EM64L-G09RevA.02\State=3-A\HF=
-930.1171645\S2=2.035006\S2-1=0.\S2A=2.000586\RMSD=5.071e-09\RMSF=3.269e-06\Dipole=-
1.5709527,0.2915705,0.3909278\Quadrupole=-6.7250363,2.6135854,4.1114509,7.9662908,
0.9001025,-2.7281611\PG=C01 [X(C11H10F3N1O2)]\\@

Singlet in water

1\1\GINC-LINDEL22\FOpt\UB3LYP\6-311G(2d,2p)\C11H10F3N1O2\ALEX\26-Jun-2013\0\\# opt
freq=noraman ub3lyp/6-311g(2d,2p) scrf=(solvent=water) geom=connectivity\\JNS1Conf1antiSh2o
\\0,1\H,0.7543571352,-0.8967851545,0.4338825321\C,0.4518308155,0.1360620672,0.3725792456
\C,-0.3423297891,2.8194679004,0.2769391951\C,-0.8335586039,0.4693933277,0.7521937134\
C,1.3786828998,1.1263959469,-0.0749143436\C,0.9351632698,2.4797650526,-0.113739205\C,
-1.2151095255,1.8198118343,0.7064648745\H,1.636916392,3.2274190033,-0.4526793581\H,
-2.2177427199,2.086119051,1.010826449\H,-0.6710740181,3.848336218,0.255951643\C,
-1.8177213875,-0.5994293182,1.2102561097\H,-2.6189986751,-0.0965760119,1.7584740748\C,
-2.4570900764,-1.332993883,0.0206818055\H,-1.6933852628,-1.745084273,-0.638492512\H,
-3.0337926885,-2.1859279032,0.3899437606\C,-3.411947527,-0.492744358,-0.7894225437\O,
-3.7163635043,-1.0832508246,-1.9604955649\H,-4.3548423951,-0.5142804645,-2.4163490786\O,
-3.8854484273,0.5670857444,-0.4532619107\N,-1.1103793141,-1.6001283672,2.0235613821\H,
-0.7550894574,-1.1583126451,2.8646490334\H,-1.7682174092,-2.3059657112,2.3358449003\C,
2.7067316351,0.9106751452,-0.4967318827\C,3.2005516593,-0.5029728021,-0.4493246732\F,
3.1331374155,-1.0699681073,0.7874163923\F,2.5235540597,-1.3074552461,-1.3131403899\F,
4.5033854994,-0.5998302211,-0.8095496488\\Version=EM64L-G09RevA.02\State=1-A\HF=

-930.1165706\S2=0.\S2-1=0.\S2A=0.\RMSD=6.696e-09\RMSF=6.216e-06\Dipole=-3.2879026,
0.1852004,1.0255513\Quadrupole=-11.5040162,5.1275852,6.376431,3.6866095,3.1582474,
-1.0765093\PG=C01 [X(C11H10F3N1O2)]\\@

Triplet in water

1\1\GINC-LINDEL22\FOpt\UB3LYP\6-311G(2d,2p)\C11H10F3N1O2(3)\ALEX\29-Jun-2013\0\\#
opt freq=noraman ub3lyp/6-311g(2d,2p) scrf=(solvent=water)
geom=connectivity\\JNS1Conf1antiTh2o
\\0,3\H,0.7101784801,-0.9223337463,0.4893180396\C,0.4090296517,0.1106821149,0.4027723867
\C,-0.3565619694,2.7879725318,0.2411197652\C,-0.8791574152,0.4721031219,0.7637814045\C,
1.3435946953,1.0835661721,-0.0520553675\C,0.9265680787,2.4402008999,-0.126192798\C,
-1.2580336365,1.8179696337,0.6853569469\H,1.6266570503,3.189170711,-0.4671758527\H,
-2.2607807291,2.1037577345,0.9689704513\H,-0.66659578,3.8225666249,0.189003555\C,
-1.8740045081,-0.5839938064,1.2282884418\H,-2.6729017305,-0.067136747,1.7667170271\C,
-2.5183581505,-1.3203252708,0.041512475\H,-1.7582071893,-1.7250837308,-0.6246955044\H,
-3.0891933155,-2.1753056155,0.4168090392\C,-3.4922434662,-0.4854540176,-0.7524929935\O,
-3.6692776053,-0.9763913538,-1.9948127465\H,-4.3347761092,-0.4242180525,-2.4324601192\O,
-4.0850591153,0.4871396371,-0.3493675456\N,-1.1884054148,-1.588902603,2.056838214\H,
-0.8053775812,-1.1365353373,2.8799848572\H,-1.8675224867,-2.2602141583,2.3988440611\C,
2.6367287989,0.7227551329,-0.4119350015\C,3.4079216347,-0.5154235798,-0.4993752648\F,
3.3910139353,-1.227131841,0.6601827379\F,2.9446234469,-1.3603474761,-1.458011894\F,
4.701360431,-0.2702609787,-0.7893603147\\Version=EM64L-G09RevA.02\State=3-A\HF=
-930.1173177\S2=2.035\S2-1=0.\S2A=2.000586\RMSD=9.685e-09\RMSF=2.784e-06\Dipole=
-1.5628934,0.2969514,0.4390672\Quadrupole=-6.5002477,2.6226579,3.8775898,7.9947293,
1.3609964,-2.9620079\PG=C01 [X(C11H10F3N1O2)]\\@