

Supporting Information
for
Mechanistic studies on the CAN-mediated intramolecular
cyclization of δ -aryl- β -dicarbonyl compounds

Brian M. Casey, Dhandapani V. Sadasivam and Robert A. Flowers II*

Address: Department of Chemistry, Lehigh University, Bethlehem, PA 18015, USA

Email: Robert A. Flowers II - rof2@lehigh.edu

* Corresponding author

Characterization data for all compounds, copies of ^1H and ^{13}C NMR spectra of final products, computational details, absolute energies, and Cartesian coordinates of all optimized structures

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Characterization of starting materials and products

6-Phenyl-2,4-hexanedione (1a). Clear, colorless oil. ^1H NMR (CDCl_3 , 500 MHz) – (enol tautomer) δ 15.46 (br. s, 1H), 7.32-7.27 (m, 2H), 7.24-7.17 (m, 3H), 5.49 (s, 1H), 2.94 (t, 2H, J = 8.1 Hz), 2.60 (t, 2H, J = 8.2 Hz), 2.05 (s, 3H). ^{13}C NMR (CDCl_3 , 125 MHz) – δ 193.2, 191.0, 140.6, 128.8, 128.5, 128.5, 128.4, 128.3, 128.2, 126.4, 126.2, 100.0, 58.0, 45.2, 40.0, 38.1, 31.4, 29.4, 24.8. MS [m/z (rel int)] 190 (M^+ , 72), 172 (11), 129 (10), 104 (67), 91 (86), 85 (100), 77 (31).

Methyl 3-oxo-5-phenyl-pentanoate (1b). Clear, colorless oil. ^1H NMR (CDCl_3 , 500 MHz) – (keto tautomer) δ 7.31-7.27 (m, 2H), 7.22-7.17 (m, 3H), 3.72 (s, 3H), 3.44 (s, 2H), 2.95-2.86 (m, 4H). ^{13}C NMR (CDCl_3 , 125 MHz) – δ 201.7, 167.5, 140.4, 128.5, 128.4, 128.3, 126.2, 52.4, 49.2, 44.5, 29.4. MS [m/z (rel int)] 206 (M^+ , 28), 188 (41), 174 (25), 133 (50), 128 (34), 104 (100), 91 (100), 77 (47).

6-Methyl-6-phenyl-2,4-hexanedione (1c). Clear, light yellow oil. ^1H NMR (CDCl_3 , 500 MHz) – (enol tautomer) δ 15.52 (br. s, 1H), 7.34-7.29 (m, 2H), 7.26-7.20 (m, 3H), 5.43 (s, 1H), 3.29 (apparent sext, 1H, J = 7.1 Hz), 2.61 (dd, 1H, J = 14.7, 6.8 Hz), 2.49 (dd, 1H, J = 14.3, 8.2 Hz), 2.02 (s, 3H), 1.32 (d, 3H, J = 7.0 Hz). ^{13}C NMR (CDCl_3 , 125 MHz) – δ 202.9, 201.8, 191.9, 191.6, 145.8, 145.6, 128.4, 128.3, 126.6, 126.2, 100.6, 58.3, 51.6, 46.6, 46.5, 36.7, 36.6, 35.1, 35.1, 24.9, 24.8, 21.6, 21.5. MS [m/z (rel int)] 204 (M^+ , 36), 186 (9), 143 (18), 118 (41), 105 (100), 91 (23), 85 (54), 77 (32).

6-(3,5-Dimethoxyphenyl)-2,4-hexanedione (1d) Clear oil. ^1H NMR (CDCl_3 , 500 MHz) – (enol tautomer) δ 15.44 (br. s, 1H), 6.37-6.26 (m, 3H), 5.46 (s, 1H), 3.75 (s, 6H), 2.85 (t, 2H, J = 7.9 Hz), 2.56 (t, 2H, J = 7.9 Hz), 2.02 (s, 3H). ^{13}C NMR (CDCl_3 , 125 MHz) – δ 193.3, 190.9, 160.8, 143.1, 106.3, 100.0, 98.1, 55.2, 39.8, 31.7, 24.7. MS [m/z (rel int)] 250 (M^+ , 21), 232 (9), 165 (100), 151 (14), 91 (12), 85 (16), 77 (13).

6-(2-Methoxyphenyl)-2,4-hexanedione (1e). Clear, light yellow oil. ^1H NMR (CDCl_3 , 500 MHz) – (enol tautomer) δ 15.47 (br. s, 1H), 7.23-7.18 (m, 1H), 7.15-7.12 (m, 1H), 6.91-6.83 (m, 2H), 5.49 (s, 1H), 3.83 (s, 3H), 2.92 (t, 2H, J = 7.7 Hz), 2.58 (t, 2H, J = 7.7 Hz), 2.05 (s, 3H). ^{13}C NMR (CDCl_3 , 125 MHz) – δ 193.9, 191.0, 157.4, 129.8, 129.0, 127.5, 120.4, 110.2, 99.8, 55.18, 38.3, 26.6, 24.9. MS [m/z (rel int)] 220 (M^+ , 27), 146 (13), 134 (33), 121 (77), 91 (100), 85 (46), 77 (33).

6-(4-Methoxyphenyl)-2,4-hexanedione (1f). Clear, light yellow oil. ^1H NMR (CDCl_3 , 500 MHz) – (enol tautomer) δ 15.46 (br. s, 1H), 7.13-7.09 (m, 2H), 6.85-6.81 (m, 2H), 5.47 (s, 1H), 3.79 (s, 3H), 2.88 (t, 2H, J = 7.6 Hz), 2.56 (t, 2H, J = 7.6 Hz), 2.04 (s, 3H). ^{13}C NMR (CDCl_3 , 125 MHz) – δ 193.2, 191.1, 158.0, 132.7, 129.2, 129.2, 113.9, 113.8, 100.0, 55.2, 40.2, 30.6, 24.9. MS [m/z (rel int)] 220 (M^+ , 39), 163 (7), 134 (36), 121 (100), 91 (21), 85 (16), 77 (20).

6-(3-Methoxyphenyl)-2,4-hexanedione (1g). Clear, colorless oil. ^1H NMR (CDCl_3 , 500 MHz) – (enol tautomer) δ 15.46 (br. s, 1H), 7.23-7.19 (m, 1H), 6.81-6.72 (m, 3H), 5.49 (s, 1H), 3.80 (s, 3H), 2.92 (t, 2H, J = 7.9 Hz), 2.60 (t, 2H, J = 7.9 Hz), 2.05 (s, 3H). ^{13}C NMR (CDCl_3 , 125 MHz) – δ 193.3, 191.0, 159.7, 142.3, 129.5, 120.6, 114.0, 111.5, 100.0, 55.1, 39.9, 31.5, 24.8. MS [m/z

(rel int)] 220 (M^+ , 38), 202 (11), 162 (11), 135 (100), 121 (71), 105 (27), 91 (73), 85 (91), 77 (40).

6-(3-Chlorophenyl)-2,4-hexanedione (1h). 1H NMR ($CDCl_3$, 500 MHz) – (enol tautomer) δ 15.41 (br. s, 1H), 7.22-7.17 (m, 3H), 7.09-7.06 (m, 1H), 5.47 (s, 1H), 2.92 (t, 2H, J = 8.1 Hz), 2.59 (t, 2H, J = 8.1 Hz), 2.05 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz) – δ 192.9, 190.8, 142.7, 134.2, 129.8, 129.7, 128.5, 128.4, 126.5, 126.4, 100.0, 58.0, 44.8, 39.7, 31.0, 28.9, 24.7. MS [m/z (rel int)] 224 (M^+ , 38), 138 (33), 125 (42), 103 (35), 85 (100), 77 (28). IR (KBr) ν (cm^{-1}) 3644, 3167, 3064, 2939, 2670, 2365, 1843, 1592, 1438, 1330, 1262, 1142, 1038, 893, 785, 688. LC-HRMS calcd. for $C_{12}H_{14}ClO_2$ [$M+H$] 225.0677, found 225.0665.

6-(4-Chlorophenyl)-2,4-hexanedione (1i). White solid (mp 34–36 °C). 1H NMR ($CDCl_3$, 500 MHz) – (enol tautomer) δ 15.42 (br. s, 1H), 7.26-7.23 (m, 2H), 7.14-7.10 (m, 2H), 5.46 (s, 1H), 2.91 (t, 2H, J = 7.9 Hz), 2.57 (t, 2H, J = 7.9 Hz), 2.04 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz) – δ 192.9, 190.9, 139.1, 132.0, 129.6, 128.6, 100.1, 39.8, 30.7, 24.8. MS [m/z (rel int)] 224 (M^+ , 65), 138 (59), 125 (76), 103 (29), 85 (100), 77 (24). IR (KBr) ν (cm^{-1}) 3491, 2884, 2396, 2283, 1894, 1808, 1608, 1498, 1427, 1251, 1097, 1006, 940, 807. LC-HRMS calcd. for $C_{12}H_{13}ClNaO_2$ [$M+Na$] 247.0496, found 247.0487.

6-(2-Naphthyl)-2,4-hexanedione (1j). White solid (mp 57–58 °C). 1H NMR ($CDCl_3$, 500 MHz) – (enol tautomer) δ 15.51 (br. s, 1H), 7.84-7.75 (m, 3H), 7.67-7.62 (s, 1H), 7.51-7.42 (m, 2H), 7.37-7.32 (m, 1H), 5.50 (s, 1H), 3.12 (t, 2H, J = 8.0 Hz), 2.70 (t, 2H, J = 8.0 Hz), 2.05 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz) – δ 193.1, 191.0, 138.2, 133.5, 132.1, 128.1, 127.6, 127.4, 126.9, 126.4, 126.0, 125.3, 100.0, 39.9, 31.6, 24.8. MS [m/z (rel int)] 240 (M^+ , 55), 182 (12), 154 (65), 141 (100), 128 (35), 115 (62), 85 (40).

1-Acetyl-3,4-dihydro-2(2H)-naphthalenone (2a). Clear, light yellow oil. 1H NMR ($CDCl_3$, 500 MHz) – (enol tautomer – enol:keto >95:5) δ 16.53 (br. s, 1H), 7.25-7.18 (m, 3H), 7.15-7.10 (m, 1H), 2.86 (t, 2H, J = 6.9 Hz), 2.56 (t, 2H, J = 6.9 Hz), 2.39 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz) – δ 200.0, 183.8, 135.4, 132.8, 127.4, 126.5, 126.4, 125.4, 110.9, 35.3, 27.8, 23.3. MS [m/z (rel int)] 188 (M^+ , 26), 173 (23), 146 (21), 141 (21), 128 (24), 115 (100), 102 (10), 91 (24), 77 (16).

Methyl 3,4-dihydro-2(2H)-naphthalenone-1-carboxylate (2b). Clear, colorless oil. 1H NMR ($CDCl_3$, 500 MHz) – (enol tautomer – enol:keto >90:10) δ 13.32 (br. s, 1H), 7.72-7.67 (m, 1H), 7.22-7.18 (m, 1H), 7.15-7.12 (m, 1H), 7.10-7.06 (m, 1H), 3.93 (s, 3H), 2.83 (t, 2H, J = 7.4 Hz), 2.55 (t, 2H, J = 7.4 Hz). ^{13}C NMR ($CDCl_3$, 125 MHz) – δ 178.4, 172.4, 133.2, 131.3, 127.2, 126.4, 125.8, 125.0, 99.9, 51.7, 29.5, 27.7. MS [m/z (rel int)] 204 (not observed), 189 (2), 146 (56), 117 (44), 104 (100), 91 (23), 78 (33).

1-Acetyl-3,4-dihydro-4-methyl-2(2H)-naphthalenone (2c). Clear, light yellow oil. 1H NMR ($CDCl_3$, 500 MHz) – (enol tautomer – enol:keto >90:10) δ 16.56 (br. s, 1H), 7.26-7.15 (m, 4H), 3.07-3.00 (m, 1H), 2.66 (dd, 1H, J = 16.2, 5.1 Hz), 2.40 (s, 3H), 2.39 (dd, 1H, J = 7.6 Hz), 1.31 (d, 3H, J = 7.0 Hz). ^{13}C NMR ($CDCl_3$, 125 MHz) – δ 199.1, 183.6, 139.8, 132.1, 126.7, 126.2, 125.7, 110.8, 42.7, 32.4, 23.4, 18.9. MS [m/z (rel int)] 202 (M^+ , 62), 187 (25), 141 (44), 128 (38),

115 (100), 105 (25), 91 (31). IR (KBr) ν (cm⁻¹) 3089, 2958, 2549, 2411, 1595, 1408, 1271, 984, 759. LC-HRMS calcd. for C₁₃H₁₅O₂ [M+H] 203.1067, found 203.1060.

1-Acetyl-6,8-dimethoxy-3,4-dihydro-2(2H)-naphthalenone (2d) Clear, light yellow oil. ¹H NMR (CDCl₃, 500 MHz) – (enol tautomer – enol:keto 60:40) δ 15.56 (br. s, 1H), 6.41-6.32 (m, 2H), 3.80 (s, 3H), 3.77 (s, 3H), 3.19-2.37 (m, 4H), 2.00 (s, 3H). ¹³C NMR (CDCl₃, 125 MHz) – δ 206.4, 203.3, 198.2, 183.8, 160.2, 158.9, 157.4, 155.7, 138.8, 138.7, 114.6, 114.0, 107.4, 104.4, 104.2, 96.9, 96.8, 62.6, 55.4, 55.3, 55.0, 37.7, 35.2, 29.6, 29.0, 28.5, 23.1. MS [m/z (rel int)] 248 (M⁺, 32), 233 (6), 215 (21), 206 (100), 191 (30), 177 (34), 161 (13), 147 (11), 131 (11), 115 (11), 103 (11), 91 (15), 77 (13).

1-Acetyl-8-methoxy-3,4-dihydro-2(2H)-naphthalenone (2g) Single isomer existing in keto, *cis*-enol and *trans*-enol tautomers. Clear, light yellow oil. ¹H NMR (CDCl₃, 500 MHz) – (enol tautomers – enol:keto 70:30) δ 16.32 (br. s, 1H), 15.75 (br. s, 1H), 7.26-7.09 (m, 2H), 6.88-6.76 (m, 4H), 3.82 (s, 6H), 3.24-2.42 (m, 8H), 2.06 (s, 6H). ¹³C NMR (CDCl₃, 125 MHz) – δ 206.2, 202.9, 197.7, 185.5, 182.0, 157.4, 156.4, 154.6, 138.1, 137.8, 137.0, 128.6, 127.5, 126.8, 125.3, 121.8, 121.7, 120.5, 119.6, 113.2, 111.4, 110.5, 109.6, 108.5, 107.6, 63.0, 55.4, 55.3, 55.0, 37.7, 35.5, 34.9, 29.9, 28.5, 28.2, 28.1, 23.4, 23.0. MS [m/z (rel int)] 218 (M⁺, 31), 203 (14), 185 (17), 176 (100), 161 (48), 131 (31), 115 (43), 103 (28), 91 (20), 77 (20). IR (KBr) ν (cm⁻¹) 3635, 2948, 2823, 1712, 1597, 1461, 1425, 1260, 1167, 1086, 969. LC-HRMS calcd. for C₁₃H₁₅O₃ [M+H] 219.1016, found 219.1006.

4-Acetyl-1,2-dihydro-3(2H)-phenanthrenone (2j). Clear, light yellow oil. ¹H NMR (CDCl₃, 500 MHz) – (enol tautomer – enol:keto >90:10) δ 15.51 (br. s, 1H), 7.91-7.81 (m, 1H), 7.71 (d, 1H, J = 8.3 Hz), 7.64 (d, 1H, J = 8.2 Hz), 7.50-7.42 (m, 2H), 7.39 (d, 1H, J = 8.2 Hz), 3.18 (td, 1H, J = 15.0, 4.3 Hz), 2.93-2.85 (m, 1H), 2.71-2.62 (m, 1H), 2.51 (td, 1H, J = 15.6, 5.4 Hz), 1.91 (s, 3H). ¹³C NMR (CDCl₃, 125 MHz) – δ 206.4, 202.8, 201.7, 179.7, 135.4, 134.6, 133.1, 133.0, 131.3, 130.0, 129.4, 129.2, 128.6, 127.3, 126.9, 126.5, 125.8, 125.7, 125.7, 125.4, 125.0, 122.2, 110.1, 65.8, 37.3, 36.2, 29.2, 28.8, 28.7, 23.1. MS [m/z (rel int)] 238 (M⁺, 23), 196 (63), 178 (32), 165 (100), 152 (47), 139 (25), 115 (15). IR (KBr) ν (cm⁻¹) 3420, 3048, 2953, 2254, 1712, 1601, 1402, 1248, 1026, 915, 818, 739. LC-HRMS calcd. for C₁₆H₁₅O₂ [M+H] 239.1067, found 239.1062.

Computational results

Table S1: Absolute energies (Hartree), zero-point vibrational energies (ZPVE, kcal/mol) and dipole moments (Debye) for structures related to the anti-isomer of **1x'** as calculated at the UB3LYP/6-31G(d) level of theory.

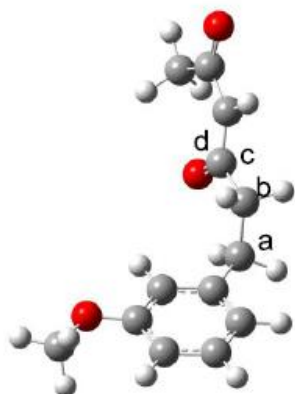
	E, Hartrees	ZPVE kcal/mol	Dipole, Debye
1a'	-615.50932	137.8	2.21
TS1a'	-615.50561	137.9	2.03
2a'	-615.50894	138.1	2.11
TS2a'	-615.48538	138.6	3.97
3a'	-615.49706	138.9	3.97
1g'	-730.03219	158.4	3.55
TS1g'	-730.02834	158.5	3.14
2g'	-730.03148	158.6	2.53
TS2g'	-730.01461	159.4	4.11
3g'	-730.02556	160.0	4.24
1g''	-730.03219	158.4	3.55
TS1g''	-730.02849	158.5	2.99
2g''	-730.03170	158.7	2.38
TS2g''	-730.01137	159.3	4.81
3g''	-730.02062	159.6	4.29
1f'	-730.03168	158.4	3.12
TS1f'	-730.02792	158.5	3.38
2f'	-730.03133	158.7	3.13
TS2f'	-730.00653	159.0	5.04
3f'	-730.01725	159.4	5.14
1h'	-1075.105489	131.8	1.98
TS1h'	-1075.10184	131.9	3.11
2h'	-1075.10524	132.1	3.55
TS2h'	-1075.07966	132.5	4.79
3h'	-1075.09142	133.2	4.97
1j'	-769.1534616	167.3	2.22
TS1j'	-769.1496332	167.3	2.07
2j'	-769.1531454	167.5	2.11
TS2j'	-769.1346359	168.0	4.05
3j'	-769.1495992	168.8	3.83

1j''	-769.1534616	167.3	2.22
TS1j''	-769.1499887	167.4	1.96
2j''	-769.1529335	167.6	2.02
TS2j''	-769.132151	168.0	4.11
3j''	-769.1455974	168.5	3.94

Table S2: Absolute energies (Hartree), relative energies (R.E. kcal/mol), zero-point vibrational energies (ZPVE, kcal/mol), low frequencies, and dipole moments (Debye) for structures related to the syn isomer (**1a**) as calculated at the UB3LYP/6-31G(d) level of theory.

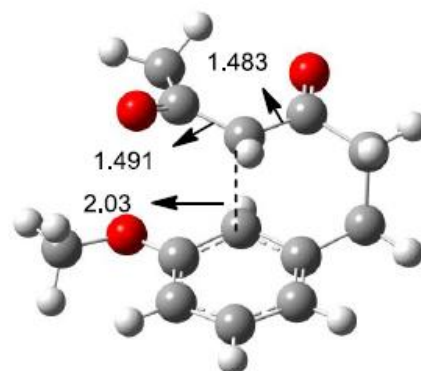
Syn	E, Hartrees	ZPVE (kcal/mol)	R.E.	R. E. + ZPVE (kcal/mol)	low freq. cm ⁻¹	Dipole, D
1a	-615.50152	137.43	0.00	0.0	22.4	4.80
Ts1a	-615.49791	137.47	2.26	2.3	49.7i	4.77
2a	-615.50123	137.66	0.18	0.4	15.2	4.61
TS2a	-615.48188	138.18	12.32	13.1	485.3i	5.47
3a	-615.50043	138.91	0.68	2.2	47.1	3.62

Calculated transition structures

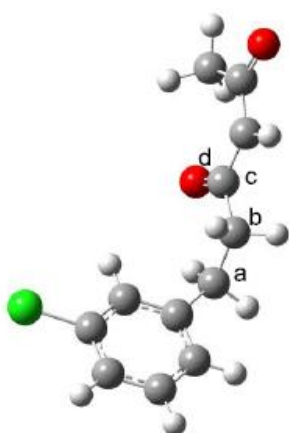


dihedral angle abcd = 4.2 deg

TS1g'

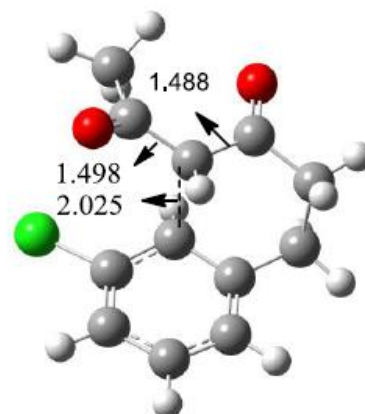


TS2g'

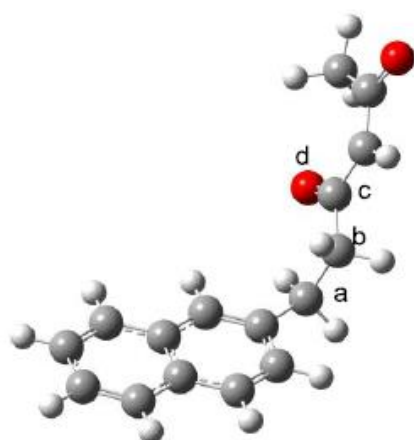


dihedral angle abcd = 6.3 deg

TS1h'

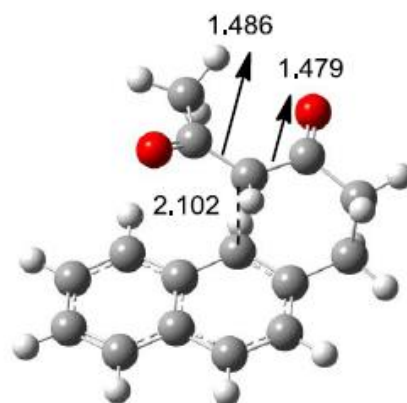


TS2h'

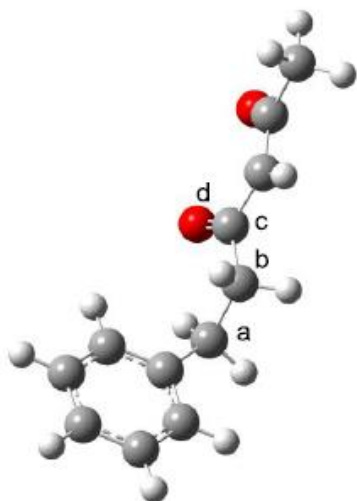


dihedral angle abcd = 1.1 deg

TS1j'

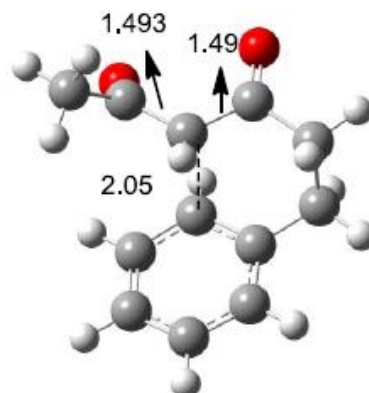


TS2j'

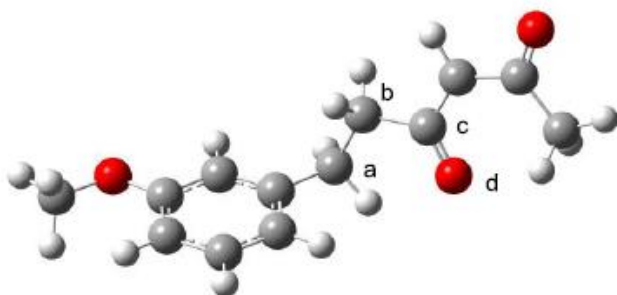


dihedral angle abcd = 6.4 deg

TS1a

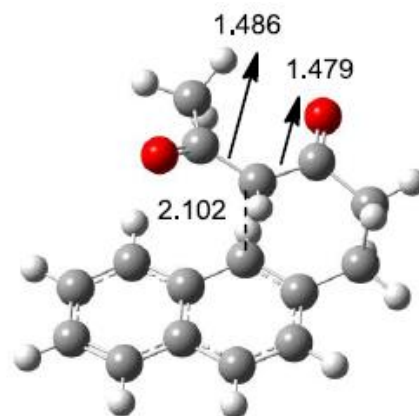


TS2a

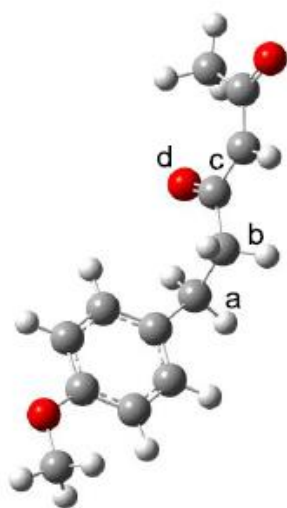


dihedral angle abcd = 1.1 deg

TS1g''

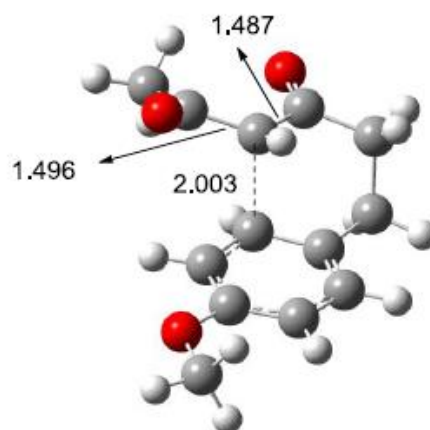


TS2g''

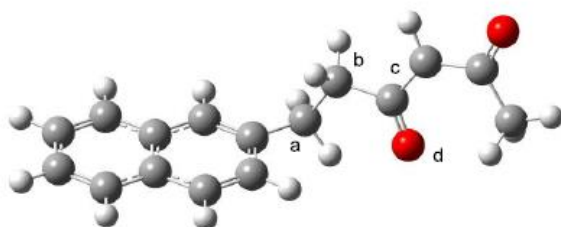


dihedral angle abcd = 4.4 deg

TS1f'

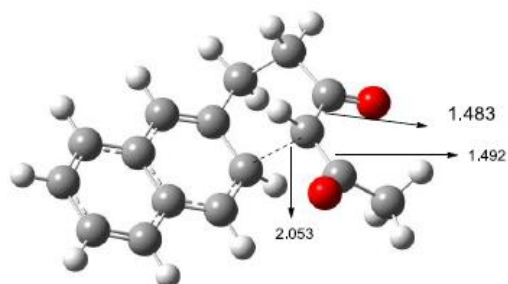


TS2f'



dihedral angle abcd = -9.3 deg

TS1j''



TS2j''

Cartesian coordinates

1a'

C	-2.712128	-0.760050	-0.000371
C	2.890457	0.154494	-1.203099
C	2.220285	0.413574	0.000221
C	0.796160	0.927563	0.000411
C	-0.232856	-0.213092	-0.001006
H	-2.404520	-1.803462	-0.000509
H	0.618851	1.561599	0.876219
H	0.619225	1.563408	-0.874161
H	-0.084516	-0.865142	-0.874447
H	-0.084396	-0.867581	0.870588
H	2.390507	0.360236	-2.147620
C	4.189859	-0.354207	-1.206130
C	4.843952	-0.611754	-0.000046
H	5.857274	-1.004263	-0.000139
C	4.190031	-0.354378	1.206163
H	4.693601	-0.544213	2.150580
C	2.890605	0.154275	1.203398
H	2.390771	0.359824	2.148019
C	-4.784399	0.810419	-0.000086
H	-4.458905	1.383905	-0.873760
H	-5.871003	0.702924	-0.000411
H	-4.459474	1.383686	0.873951
C	-1.677982	0.272816	-0.000310
C	-4.166451	-0.569922	0.000056
O	-4.865805	-1.587741	0.000615
O	-1.957433	1.474560	0.000275
H	4.693288	-0.543898	-2.150651

TS1a'

C	-2.681741	-0.568315	-0.548577
C	2.277297	1.082810	0.077486
C	2.155792	-0.265774	0.443895
C	0.872852	-0.775948	1.067156
C	-0.257152	-1.029415	0.040071
H	-2.547621	-1.310332	-1.332518
H	1.075301	-1.700467	1.618273
H	0.502548	-0.047405	1.796108
H	0.065523	-0.743817	-0.971393
H	-0.503942	-2.097199	-0.032859
H	1.451627	1.763787	0.274118
C	3.442179	1.559686	-0.523320
C	4.510914	0.693944	-0.766971
H	5.420466	1.064867	-1.231829
C	4.404587	-0.648914	-0.403368
H	5.232505	-1.329911	-0.583547
C	3.235735	-1.122141	0.196576
H	3.162634	-2.169884	0.481032
C	-4.405390	1.064238	0.513132

H	-3.759898	1.944129	0.427657
H	-5.448690	1.342922	0.351667
H	-4.266148	0.686192	1.530892
C	-1.549772	-0.263005	0.325033
C	-4.026169	0.016420	-0.509206
O	-4.836889	-0.384957	-1.349898
O	-1.635298	0.575740	1.224459
H	3.518402	2.609340	-0.795528

2a'

C	-2.376189	0.535465	0.605187
C	1.947333	-0.692954	-0.923375
C	1.954285	0.584081	-0.345758
C	1.038909	1.683109	-0.850410
C	-0.274191	1.802577	-0.054944
H	-2.398368	1.177360	1.482819
H	1.559495	2.646096	-0.788459
H	0.793794	1.515554	-1.903734
H	-0.074954	1.832566	1.023956
H	-0.769019	2.757340	-0.293732
H	1.276726	-0.894804	-1.753430
C	2.782607	-1.700429	-0.437253
C	3.638692	-1.448490	0.635869
H	4.290611	-2.232405	1.012173
C	3.655852	-0.180097	1.219329
H	4.323681	0.029158	2.051126
C	2.821173	0.824859	0.729734
H	2.848412	1.814172	1.183196
C	-3.624502	-1.404265	-0.596729
H	-2.743015	-2.051220	-0.649040
H	-4.523652	-2.001372	-0.431695
H	-3.680219	-0.891731	-1.562249
C	-1.287883	0.700859	-0.353942
C	-3.496076	-0.409735	0.535047
O	-4.332054	-0.356580	1.442238
O	-1.211562	0.008209	-1.373087
H	2.765377	-2.683623	-0.900670

TS2a'

C	0.897635	-0.055638	-0.567763
C	-0.578507	-0.232383	0.799414
C	-1.462791	0.834936	0.363976
C	-0.933657	2.242519	0.400446
C	0.253666	2.401704	-0.599774
H	0.272956	-0.196487	-1.447116
H	-1.721289	2.961118	0.150359
H	-0.570092	2.493805	1.405779
H	-0.125969	2.289836	-1.622548
H	0.710054	3.389599	-0.495651
H	0.089955	-0.001200	1.629580
C	-1.077313	-1.583831	0.742588

C	-2.284024	-1.865492	0.134951
H	-2.626674	-2.893772	0.061859
C	-3.086215	-0.823955	-0.363988
H	-4.039228	-1.048256	-0.834111
C	-2.666878	0.511797	-0.238253
H	-3.303208	1.309565	-0.615241
C	2.922340	-1.165463	0.653386
H	2.560962	-0.812027	1.626541
H	3.359151	-2.161603	0.753221
H	3.681219	-0.442850	0.339660
C	1.309889	1.346306	-0.299354
C	1.802223	-1.228019	-0.364745
O	1.582559	-2.251847	-1.001822
O	2.367795	1.652228	0.243570
H	-0.468887	-2.385646	1.148380

3a'

C	0.790780	-0.083526	-0.427461
C	-0.474907	-0.305652	0.515793
C	-1.480089	0.798984	0.281623
C	-0.957146	2.199181	0.435471
C	0.275914	2.437392	-0.475545
H	0.433148	-0.187664	-1.459339
H	-1.736288	2.934591	0.207429
H	-0.649377	2.375143	1.478453
H	-0.047114	2.413428	-1.525213
H	0.744483	3.405874	-0.279608
H	-0.084328	-0.204997	1.546973
C	-1.051392	-1.683931	0.345224
C	-2.350272	-1.892890	-0.022161
H	-2.714579	-2.910272	-0.142630
C	-3.235265	-0.809115	-0.248542
H	-4.263666	-0.992920	-0.542077
C	-2.768452	0.518141	-0.090500
H	-3.456205	1.343614	-0.265993
C	2.577614	-1.269475	1.089625
H	1.866994	-1.321691	1.923426
H	3.209520	-2.159887	1.088858
H	3.190568	-0.374661	1.239639
C	1.314624	1.348721	-0.263295
C	1.872342	-1.157798	-0.246592
O	2.133057	-1.902425	-1.172615
O	2.468589	1.603512	0.029808
H	-0.388810	-2.529432	0.510694

1g'

C	-3.453958	-0.401950	0.700954
C	2.212266	-0.384636	-0.576932
C	1.379138	0.709503	-0.346692
C	-0.052838	0.700018	-0.839026
C	-1.022801	0.141733	0.213005

H	-3.101797	-0.753497	1.668253
H	-0.369005	1.713862	-1.108536
H	-0.138546	0.101695	-1.752572
H	-0.735862	-0.881580	0.496483
H	-0.958482	0.723486	1.144512
H	1.861533	-1.244604	-1.141449
C	3.529293	-0.404351	-0.095607
C	4.024200	0.686511	0.627484
H	5.039881	0.695828	1.005709
C	3.187954	1.783792	0.855647
H	3.573397	2.634840	1.411336
C	1.881142	1.802921	0.378135
H	1.247707	2.668327	0.557665
O	4.243928	-1.531178	-0.388842
C	5.587350	-1.609535	0.058951
H	5.652670	-1.562191	1.154234
H	5.960743	-2.576940	-0.282125
H	6.204896	-0.810503	-0.372518
C	-5.578079	-0.092878	-0.766542
H	-5.170568	-0.634803	-1.625853
H	-6.649768	-0.280477	-0.673822
H	-5.393670	0.967700	-0.964814
C	-2.475912	0.127819	-0.247428
C	-4.903259	-0.527679	0.515250
O	-5.550508	-1.004738	1.452679
O	-2.807182	0.542322	-1.361298

TS1g'

C	-3.318897	-0.239366	-0.706410
C	1.762334	0.206695	0.444906
C	1.406220	-1.141587	0.384956
C	0.022556	-1.578691	0.821118
C	-1.071036	-1.318279	-0.242468
H	-3.251136	-0.711882	-1.683815
H	0.039224	-2.644673	1.071432
H	-0.263426	-1.043431	1.732535
H	-0.643997	-0.824685	-1.126825
H	-1.497535	-2.257586	-0.620376
H	1.069308	0.948748	0.832546
C	3.025562	0.638682	0.018428
C	3.951668	-0.288602	-0.474384
H	4.935481	0.021973	-0.806676
C	3.593882	-1.638352	-0.530126
H	4.313259	-2.360413	-0.908149
C	2.338231	-2.067597	-0.108256
H	2.078994	-3.122363	-0.155052
O	3.255693	1.981123	0.128204
C	4.522025	2.479980	-0.269385
H	4.714182	2.295269	-1.334888
H	4.489134	3.556543	-0.091556
H	5.334964	2.039870	0.323476

C	-4.815859	1.277392	0.784115
H	-4.026821	2.006087	0.995678
H	-5.781656	1.779693	0.699342
H	-4.820723	0.584212	1.631171
C	-2.226341	-0.442309	0.244075
C	-4.541536	0.546318	-0.511025
O	-5.339973	0.584803	-1.452542
O	-2.238483	0.074940	1.362825

2g'

C	2.965310	-0.362875	0.544165
C	-1.530002	-0.081929	-0.748644
C	-1.216682	-1.386576	-0.368904
C	-0.090451	-2.145208	-1.044755
C	1.249680	-2.045136	-0.292548
H	3.159270	-1.068251	1.348778
H	-0.360749	-3.205262	-1.116967
H	0.054957	-1.776917	-2.064708
H	1.116532	-2.270086	0.773058
H	1.948303	-2.805821	-0.675485
H	-0.978683	0.410784	-1.542798
C	-2.557782	0.626004	-0.107683
C	-3.281779	0.026075	0.928224
H	-4.081241	0.554177	1.434850
C	-2.965085	-1.282423	1.306864
H	-3.531119	-1.752730	2.106984
C	-1.948023	-1.986502	0.670609
H	-1.723180	-3.007390	0.970870
O	-2.772688	1.893610	-0.570821
C	-3.804320	2.660488	0.026958
H	-3.618674	2.826153	1.096779
H	-3.801994	3.621387	-0.491155
H	-4.786515	2.184792	-0.097164
C	3.657761	1.952236	-0.418167
H	2.637446	2.348722	-0.421843
H	4.370896	2.741416	-0.171234
H	3.839221	1.578916	-1.430946
C	1.948985	-0.696572	-0.448940
C	3.800874	0.842287	0.598567
O	4.628571	0.909659	1.512421
O	1.692194	0.059344	-1.390787

TS2g'

C	-0.750311	-0.760763	0.654704
C	-0.002041	0.566637	-0.686337
C	-0.815448	1.722230	-0.376942
C	-2.292799	1.600776	-0.631454
C	-2.916685	0.504433	0.291788
H	-0.600450	-0.138937	1.534554
H	-2.799065	2.555801	-0.455674
H	-2.483027	1.316407	-1.674802

H	-2.881455	0.855745	1.330072
H	-3.958354	0.324157	0.013201
H	-0.279066	-0.031877	-1.553154
C	1.417688	0.649501	-0.438327
C	1.946304	1.704818	0.292784
H	3.000879	1.738340	0.540647
C	1.106624	2.760052	0.678791
H	1.525168	3.590772	1.239417
C	-0.257097	2.768779	0.335823
H	-0.880130	3.608095	0.634905
O	2.116474	-0.391801	-0.943436
C	3.464789	-0.579054	-0.516321
H	3.507522	-0.691373	0.571864
H	3.799701	-1.500195	-0.994484
H	4.102607	0.252454	-0.839917
C	-0.001521	-3.059179	-0.320367
H	0.034163	-2.669231	-1.344516
H	0.803001	-3.783203	-0.173071
H	-0.979594	-3.535241	-0.209463
C	-2.142018	-0.801211	0.142900
C	0.164560	-1.937877	0.681405
O	1.073249	-1.949113	1.508562
O	-2.620245	-1.749908	-0.473908

3g'

C	-0.770005	-0.500961	0.454827
C	0.106370	0.442258	-0.491982
C	-0.356157	1.871418	-0.324295
C	-1.809240	2.110819	-0.614857
C	-2.698793	1.210192	0.282312
H	-0.563178	-0.181065	1.483895
H	-2.070729	3.163103	-0.459566
H	-2.035126	1.877177	-1.667103
H	-2.595733	1.539378	1.325223
H	-3.754815	1.269348	0.003530
H	-0.100830	0.104792	-1.522926
C	1.580197	0.274028	-0.232569
C	2.369847	1.276861	0.265950
H	3.419586	1.099125	0.472642
C	1.830835	2.568604	0.487783
H	2.466553	3.354328	0.882163
C	0.480154	2.837344	0.172687
H	0.092615	3.843374	0.322026
O	1.995224	-0.980479	-0.544790
C	3.330020	-1.358237	-0.226192
H	3.519002	-1.255295	0.848757
H	3.421952	-2.405519	-0.516353
H	4.054200	-0.754224	-0.786855
C	-0.588623	-2.754288	-0.892800
H	-0.158705	-2.212609	-1.741110
H	-0.111672	-3.732562	-0.801082

H	-1.659638	-2.882948	-1.080796
C	-2.261441	-0.242276	0.189824
C	-0.415055	-1.996922	0.406565
O	-0.038520	-2.544575	1.425931
O	-3.045721	-1.132376	-0.084385

TS1g''

C	3.444993	-0.755744	-0.467324
C	-2.437266	-0.630472	0.624077
C	-1.281400	0.147618	0.625855
C	-0.017341	-0.340922	1.303023
C	1.035834	-0.895730	0.314052
H	3.209291	-1.620238	-1.083953
H	0.445723	0.483504	1.855517
H	-0.269475	-1.113486	2.036693
H	1.203488	-1.970664	0.466177
H	0.680141	-0.808845	-0.722467
H	-2.464831	-1.591678	1.130143
C	-3.601112	-0.194559	-0.027484
C	-3.610826	1.037867	-0.688387
H	-4.498496	1.396847	-1.196298
C	-2.449650	1.818415	-0.683277
H	-2.458235	2.780177	-1.189962
C	-1.296101	1.387440	-0.036878
H	-0.405176	2.010569	-0.032945
O	-4.666779	-1.047164	0.043243
C	-5.872690	-0.666769	-0.598353
H	-5.732684	-0.540097	-1.680278
H	-6.577223	-1.481279	-0.419618
H	-6.279794	0.262526	-0.177864
C	5.346566	0.895685	0.180286
H	5.241177	0.728948	1.256995
H	6.396232	1.049061	-0.078427
H	4.764871	1.795496	-0.043482
C	2.392901	-0.193981	0.378817
C	4.828836	-0.289925	-0.603007
O	5.555069	-0.909534	-1.386599
O	2.592777	0.794901	1.087276

2g''

C	-2.949122	-0.216579	-0.928813
C	2.140011	0.729496	-0.617416
C	1.089178	1.127625	0.210245
C	0.071550	2.134286	-0.292041
C	-1.075125	1.494946	-1.097428
H	-2.803725	-0.373878	-1.994970
H	-0.359241	2.685231	0.549649
H	0.571408	2.865592	-0.937588
H	-1.630181	2.278174	-1.637745
H	-0.680350	0.821835	-1.868737
H	2.259118	1.151051	-1.612353

C	3.080056	-0.217454	-0.188213
C	2.972336	-0.775637	1.090439
H	3.689586	-1.505962	1.446919
C	1.920268	-0.373300	1.918613
H	1.838305	-0.803418	2.913633
C	0.984689	0.565573	1.493208
H	0.168393	0.863281	2.143400
O	4.061728	-0.522241	-1.089756
C	5.046812	-1.469696	-0.712491
H	4.603212	-2.450906	-0.496528
H	5.719449	-1.559520	-1.567652
H	5.617908	-1.133428	0.163273
C	-4.357162	-0.975754	1.122864
H	-4.639078	0.038706	1.421857
H	-5.176847	-1.670262	1.318087
H	-3.484660	-1.237455	1.729986
C	-2.098486	0.751155	-0.242761
C	-4.024421	-1.030906	-0.351322
O	-4.648484	-1.764857	-1.123698
O	-2.225344	0.983152	0.963388

TS2g''

C	1.462826	-0.268510	0.576156
C	-1.730129	1.310607	-0.074531
C	-0.431476	1.290081	-0.526927
C	0.472557	2.487659	-0.414728
C	1.532486	2.262607	0.709278
H	0.723428	-0.249256	1.373978
H	1.007216	2.656659	-1.358975
H	-0.104342	3.393157	-0.199322
H	2.253914	3.083959	0.718816
H	1.019491	2.225692	1.677767
H	-2.178576	2.230456	0.291110
C	-2.528247	0.141719	-0.070415
C	-2.000746	-1.072439	-0.551721
H	-2.610669	-1.967815	-0.586065
C	-0.701122	-1.116514	-1.016431
H	-0.308157	-2.048538	-1.408782
C	0.171502	0.026697	-0.930789
H	0.956758	0.085341	-1.685132
O	-3.787991	0.303752	0.405472
C	-4.650152	-0.827262	0.460179
H	-4.232045	-1.617053	1.096206
H	-5.584038	-0.466884	0.893949
H	-4.845494	-1.229878	-0.541482
C	3.250120	-1.870335	-0.450028
H	4.123799	-1.409007	0.019541
H	3.400038	-2.946126	-0.566627
H	3.157756	-1.392230	-1.432552
C	2.279807	0.961825	0.440867
C	2.012006	-1.643447	0.393975

O	1.406204	-2.587791	0.891169
O	3.429830	0.978463	0.008142

3g''

C	-1.423139	-0.228779	-0.431832
C	1.825640	1.257683	0.116731
C	0.493228	1.213510	0.399026
C	-0.370120	2.442224	0.447828
C	-1.545321	2.335890	-0.560897
H	-0.959685	-0.262850	-1.425239
H	-0.797282	2.564798	1.455689
H	0.218018	3.342527	0.240108
H	-2.253429	3.161556	-0.447211
H	-1.140699	2.361380	-1.581727
H	2.319698	2.210210	-0.060532
C	2.626468	0.083068	0.049163
C	2.033422	-1.179968	0.278215
H	2.634588	-2.082441	0.237751
C	0.696448	-1.285444	0.561461
H	0.265305	-2.267561	0.733483
H	-0.224132	-0.099554	0.619072
H	-0.719709	-0.068615	1.608595
O	3.941708	0.293648	-0.239179
C	4.804382	-0.830588	-0.328306
H	4.487034	-1.519311	-1.121959
H	5.791211	-0.431727	-0.569472
H	4.856064	-1.374727	0.623789
C	-2.998875	-1.782268	0.982734
H	-3.857719	-1.103131	0.991368
H	-3.340591	-2.819232	1.000694
H	-2.410311	-1.569347	1.883395
C	-2.295804	1.028745	-0.365404
C	-2.201983	-1.541043	-0.283056
O	-2.149474	-2.370195	-1.172739
O	-3.493958	0.998750	-0.147725

1f'

C	-3.576997	0.823682	0.110021
C	1.901434	-0.614433	1.258571
C	1.271157	-0.671996	0.004614
C	-0.183175	-1.071865	-0.121688
C	-1.138241	0.117747	0.058205
H	-3.203897	1.825654	0.310435
H	-0.369025	-1.528349	-1.100307
H	-0.434034	-1.839412	0.619462
H	-0.979211	0.597016	1.035637
H	-0.918700	0.902540	-0.680970
H	1.344011	-0.892157	2.151034
C	3.227012	-0.220307	1.387004
C	3.969678	0.131410	0.250337
C	3.363660	0.079338	-1.009303

H	3.914339	0.338114	-1.906584
C	2.027968	-0.320520	-1.115719
H	1.572888	-0.363592	-2.103343
C	-5.742808	-0.575368	-0.223747
H	-5.481830	-1.320765	0.534111
H	-6.819960	-0.396431	-0.224712
H	-5.426957	-0.998260	-1.182668
C	-2.610422	-0.259582	-0.060944
C	-5.039531	0.736352	0.044904
O	-5.673454	1.781857	0.219089
O	-2.965933	-1.418760	-0.290110
O	5.265104	0.501496	0.478334
C	6.065278	0.858317	-0.636499
H	5.656306	1.729173	-1.166275
H	7.047023	1.111901	-0.232141
H	6.169366	0.024266	-1.343397
H	3.713877	-0.183082	2.356682

TS1f'

C	-3.519489	0.148183	0.819972
C	1.417895	-0.618104	-0.772701
C	1.211764	0.739625	-0.472376
C	-0.137449	1.385495	-0.708702
C	-1.190107	1.047634	0.374890
H	-3.340064	0.428055	1.855666
H	-0.016498	2.472495	-0.768733
H	-0.538895	1.060914	-1.674735
H	-0.772487	0.355174	1.119651
H	-1.478429	1.938989	0.948990
H	0.605531	-1.197486	-1.206712
C	2.639350	-1.234420	-0.536760
C	3.703812	-0.501824	0.010163
C	3.522856	0.851346	0.312025
H	4.328782	1.444439	0.729395
C	2.283170	1.452625	0.068407
H	2.158573	2.507256	0.305586
C	-5.265995	-0.914858	-0.786946
H	-4.574088	-1.663073	-1.186412
H	-6.272683	-1.331192	-0.712715
H	-5.251151	-0.081509	-1.496547
C	-2.468411	0.404511	-0.164103
C	-4.833583	-0.460160	0.589064
O	-5.573725	-0.586038	1.569787
O	-2.608127	0.104588	-1.351671
O	4.865175	-1.196258	0.202675
C	5.977396	-0.502228	0.741972
H	5.761703	-0.107782	1.744170
H	6.784166	-1.234514	0.809695
H	6.292807	0.324668	0.091465
H	2.798886	-2.281725	-0.774505

2f'

C	3.079926	0.013990	-0.826905
C	-1.128762	0.283748	1.240622
C	-1.006336	1.299270	0.277300
C	0.142689	2.287631	0.305298
C	1.350391	1.858554	-0.549134
H	3.085720	0.277410	-1.881976
H	-0.204180	3.259283	-0.066151
H	0.483656	2.440706	1.334067
H	1.029373	1.562059	-1.555826
H	2.029811	2.714196	-0.690877
H	-0.387468	0.210485	2.030910
C	-2.174730	-0.629730	1.196485
C	-3.136849	-0.554385	0.179254
C	-3.035030	0.449953	-0.789599
H	-3.767964	0.538899	-1.583461
C	-1.976337	1.360541	-0.727182
H	-1.916956	2.142315	-1.482405
C	4.137316	-1.581683	0.934487
H	3.175693	-1.961728	1.293787
H	4.887386	-2.375112	0.947849
H	4.420388	-0.779134	1.622828
C	2.186107	0.740764	0.069794
C	4.016129	-1.061312	-0.480105
O	4.703633	-1.522985	-1.396067
O	2.134650	0.486862	1.277209
O	-4.126932	-1.495328	0.225010
C	-5.129776	-1.460677	-0.776340
H	-4.705873	-1.604215	-1.779421
H	-5.807647	-2.286123	-0.550894
H	-5.690139	-0.516260	-0.755632
H	-2.271039	-1.411157	1.944133

TS2f'

C	-1.328061	0.429766	-0.561956
C	-0.069726	-0.266839	0.831983
C	0.057035	-1.646440	0.383724
C	-1.179320	-2.503543	0.369995
C	-2.222008	-1.946003	-0.646751
H	-0.714867	0.190849	-1.428340
H	-0.930909	-3.537727	0.108470
H	-1.646853	-2.524073	1.363642
H	-1.825171	-2.062324	-1.662621
H	-3.165448	-2.492935	-0.568923
H	-0.772058	-0.085251	1.646587
C	1.109396	0.553160	0.838349
C	2.287978	0.113181	0.251042
C	2.365775	-1.193899	-0.268995
H	3.279779	-1.560530	-0.720688
C	1.249303	-2.048270	-0.183824
H	1.338037	-3.058786	-0.576823

C	-2.366740	2.497142	0.649350
H	-2.268636	2.004708	1.624463
H	-2.163213	3.565827	0.746455
H	-3.400696	2.328928	0.334574
C	-2.485693	-0.477391	-0.341017
C	-1.407900	1.910651	-0.366332
O	-0.648809	2.626016	-1.008556
O	-3.544263	-0.118989	0.166785
O	3.325508	0.997213	0.257843
C	4.564082	0.596100	-0.306865
H	4.462966	0.355844	-1.373315
H	5.232410	1.451365	-0.194068
H	4.990174	-0.267769	0.220725
H	1.080276	1.552258	1.259066

3f'

C	1.266120	-0.351839	-0.422368
C	0.114779	0.144850	0.561990
C	-0.157892	1.607600	0.308902
C	1.029032	2.525570	0.393635
C	2.168156	2.054839	-0.548290
H	0.867255	-0.263732	-1.440370
H	0.744200	3.554345	0.147686
H	1.422411	2.542665	1.422216
H	1.845097	2.184209	-1.590154
H	3.085707	2.629865	-0.395572
H	0.546148	0.047238	1.577161
C	-1.103120	-0.722342	0.465882
C	-2.343673	-0.225891	0.134437
C	-2.525218	1.155001	-0.118089
H	-3.495652	1.555373	-0.382528
C	-1.413347	2.032324	-0.021628
H	-1.578114	3.090522	-0.216954
C	2.168466	-2.293943	1.099128
H	1.516828	-1.989528	1.927033
H	2.265644	-3.381425	1.090636
H	3.147608	-1.832536	1.265409
C	2.475812	0.584945	-0.315245
C	1.631541	-1.831989	-0.240456
O	1.481064	-2.601245	-1.170273
O	3.595985	0.192136	-0.044308
O	-3.358274	-1.143039	0.075481
C	-4.658815	-0.698489	-0.273344
H	-4.682244	-0.253838	-1.277224
H	-5.289673	-1.589320	-0.262718
H	-5.050226	0.027602	0.451863
H	-1.006234	-1.788072	0.648992

1h'

C	3.392136	-0.325544	-0.719566
C	-2.276893	-0.403591	0.458176

C	-1.450819	0.723178	0.354476
C	-0.022720	0.672664	0.854517
C	0.954628	0.186285	-0.226356
H	3.053396	-0.602562	-1.715432
H	0.293342	1.663507	1.198223
H	0.053695	0.011712	1.724712
H	0.668456	-0.813237	-0.585186
H	0.902514	0.833815	-1.113987
H	-1.910621	-1.311447	0.928340
C	-3.579002	-0.359868	-0.035705
C	-4.092250	0.788129	-0.636516
H	-5.110264	0.801703	-1.010367
C	-3.269567	1.910718	-0.736373
H	-3.655845	2.816364	-1.195919
C	-1.963875	1.880014	-0.246749
H	-1.337340	2.765354	-0.324938
C	5.495636	-0.135001	0.797631
H	5.074308	-0.739982	1.606774
H	6.568118	-0.318445	0.706552
H	5.310842	0.907984	1.073720
C	2.402421	0.134680	0.251290
C	4.839041	-0.467954	-0.523238
O	5.497992	-0.872043	-1.486077
O	2.715940	0.465889	1.397602
Cl	-4.599675	-1.787517	0.109751

TS1h'

C	-3.262147	-0.349118	-0.676616
C	1.842449	0.265189	0.362105
C	1.511818	-1.097308	0.392638
C	0.134834	-1.527235	0.854282
C	-0.967265	-1.327981	-0.213989
H	-3.205491	-0.876533	-1.626188
H	0.164386	-2.579430	1.155681
H	-0.152124	-0.951458	1.740531
H	-0.556669	-0.849131	-1.114300
H	-1.367940	-2.289285	-0.562203
H	1.125938	1.009286	0.697355
C	3.097117	0.665299	-0.090044
C	4.049450	-0.260750	-0.514622
H	5.022033	0.073409	-0.859281
C	3.720545	-1.615471	-0.478347
H	4.452017	-2.351334	-0.801107
C	2.465413	-2.030632	-0.030495
H	2.225098	-3.090686	-0.005389
C	-4.764626	1.212676	0.761793
H	-3.990136	1.972012	0.909711
H	-5.744979	1.684937	0.672397
H	-4.731470	0.571192	1.648122
C	-2.140921	-0.464106	0.253324
C	-4.502520	0.412676	-0.494201

O	-5.324795	0.370751	-1.414395
O	-2.138246	0.115495	1.341233
Cl	3.491693	2.381625	-0.119117

2h'

C	2.928974	-0.532887	0.474254
C	-1.596159	0.073910	-0.636414
C	-1.359891	-1.287457	-0.402000
C	-0.268503	-2.027586	-1.151613
C	1.083694	-2.039102	-0.414792
H	3.134666	-1.328860	1.186167
H	-0.580697	-3.066811	-1.305822
H	-0.122409	-1.582996	-2.140681
H	0.955386	-2.338224	0.633345
H	1.743054	-2.798420	-0.863595
H	-1.000943	0.610720	-1.366554
C	-2.590766	0.736156	0.080682
C	-3.366300	0.079919	1.034580
H	-4.136708	0.616649	1.577591
C	-3.129929	-1.275779	1.265062
H	-3.729563	-1.805350	2.000393
C	-2.139119	-1.952702	0.554535
H	-1.973658	-3.011937	0.738185
C	3.683930	1.839132	-0.283087
H	2.690775	2.285925	-0.171055
H	4.456037	2.559816	-0.006293
H	3.776327	1.569886	-1.339960
C	1.838700	-0.712721	-0.478599
C	3.829263	0.619775	0.598676
O	4.713851	0.546815	1.456779
O	1.560169	0.149496	-1.317291
Cl	-2.875752	2.446774	-0.229725

TS2h'

C	-1.015377	-0.254008	0.661870
C	0.403966	0.409799	-0.621091
C	0.301067	1.835934	-0.353456
C	-0.994122	2.511216	-0.712936
C	-2.161197	1.958715	0.162382
H	-0.605562	0.217606	1.552606
H	-0.915988	3.594767	-0.576616
H	-1.240709	2.331611	-1.767566
H	-2.008460	2.277209	1.200573
H	-3.119326	2.348507	-0.191051
H	-0.105651	0.033865	-1.506659
C	1.667129	-0.211046	-0.316072
C	2.635992	0.431872	0.431561
H	3.551008	-0.087511	0.695191
C	2.441414	1.771384	0.795745
H	3.203247	2.283765	1.375235
C	1.288505	2.463846	0.382213
H	1.175356	3.514236	0.639023

C	-1.599707	-2.638012	-0.239058
H	-1.339003	-2.341290	-1.260921
H	-1.289202	-3.669077	-0.057753
H	-2.687444	-2.546287	-0.163945
C	-2.192128	0.438436	0.070322
C	-0.932788	-1.744674	0.783921
O	-0.302678	-2.207678	1.726671
O	-3.077315	-0.138681	-0.553069
Cl	1.962656	-1.825135	-0.917608

3h'

C	-0.860451	0.069226	0.476576
C	0.430693	0.186588	-0.458390
C	0.958600	1.605166	-0.350707
C	-0.011149	2.678760	-0.751433
C	-1.274978	2.613369	0.140730
H	-0.510093	0.218777	1.505825
H	0.450147	3.668860	-0.673655
H	-0.315807	2.547473	-1.800770
H	-0.998318	2.890970	1.167326
H	-2.057083	3.297660	-0.200158
H	0.077737	0.010404	-1.488312
C	1.501013	-0.823125	-0.134679
C	2.712348	-0.497560	0.413310
H	3.417365	-1.286646	0.655212
C	3.062944	0.853671	0.619711
H	4.022309	1.101612	1.061169
C	2.180350	1.878903	0.200394
H	2.488184	2.916893	0.308341
C	-2.212725	-1.798114	-0.804413
H	-1.631322	-1.543407	-1.695744
H	-2.336546	-2.881131	-0.740058
H	-3.196517	-1.326676	-0.902166
C	-1.851363	1.208318	0.168251
C	-1.581101	-1.293154	0.477478
O	-1.673537	-1.906170	1.522316
O	-3.033941	0.999920	-0.028206
Cl	1.172040	-2.497475	-0.537109

1j'

C	-3.965970	0.037470	0.830593
C	1.351981	1.592155	-0.460020
C	0.866858	0.273254	-0.686822
C	-0.576957	0.055484	-1.083777
C	-1.533382	0.157231	0.113989
H	-3.599434	0.227437	1.836982
H	-0.880025	0.789906	-1.839534
H	-0.697628	-0.927196	-1.551833
H	-1.266477	-0.583686	0.881879
H	-1.430877	1.132566	0.612424
H	0.679503	2.434720	-0.608059
C	2.651151	1.817206	-0.070410

C	3.554702	0.736926	0.118482
C	3.082134	-0.595744	-0.110439
C	1.732823	-0.787201	-0.512273
H	1.384753	-1.803671	-0.688506
C	-6.116798	-0.384285	-0.568305
H	-7.190558	-0.457518	-0.384132
H	-5.908613	0.411072	-1.290957
H	-5.745323	-1.308322	-1.022555
C	-2.998039	-0.039339	-0.261689
C	-5.422589	-0.112985	0.747581
O	-6.058692	-0.008469	1.800908
O	-3.344878	-0.252071	-1.426432
H	3.006346	2.832187	0.093006
C	3.981090	-1.681120	0.071158
H	3.622050	-2.692752	-0.103974
C	4.903487	0.930210	0.519324
H	5.258147	1.943977	0.691078
C	5.283033	-1.461384	0.461819
H	5.959624	-2.300878	0.597481
C	5.749445	-0.143018	0.688309
H	6.779258	0.017321	0.995784

TS1j'

C	3.829870	-0.317977	0.685546
C	-1.592844	-2.036183	-0.046514
C	-0.841706	-1.010068	-0.686452
C	0.550993	-1.296677	-1.206705
C	1.633726	-1.314215	-0.100477
H	3.746679	-1.006169	1.523789
H	0.555411	-2.260346	-1.729564
H	0.834418	-0.537932	-1.942069
H	1.195638	-1.085864	0.881145
H	2.081283	-2.311350	0.013377
H	-1.163850	-3.032928	0.033392
C	-2.847096	-1.791083	0.460923
C	-3.435800	-0.501575	0.362252
C	-2.692985	0.539946	-0.282171
C	-1.400134	0.247688	-0.794133
H	-0.843035	1.044115	-1.284074
C	5.319541	1.543167	-0.353493
H	6.260757	2.042258	-0.114246
H	5.381235	1.067378	-1.337348
H	4.508455	2.274914	-0.422973
C	2.775735	-0.321167	-0.327798
C	5.032395	0.520937	0.723340
O	5.801668	0.355550	1.675162
O	2.810551	0.436231	-1.299394
H	-3.409034	-2.588277	0.942492
C	-3.276412	1.831329	-0.388372
H	-2.712193	2.621331	-0.878729
C	-4.728539	-0.210723	0.873563
H	-5.289235	-1.004828	1.361512

C	-4.531757	2.082474	0.118620
H	-4.965707	3.074927	0.030823
C	-5.265505	1.051795	0.756008
H	-6.255458	1.262515	1.151511

2j'

C	-3.397700	0.166171	0.638078
C	1.354753	2.115242	0.624875
C	0.644457	1.554810	-0.473963
C	-0.581014	2.264052	-1.014224
C	-1.850311	2.010346	-0.180578
H	-3.623043	0.826732	1.472073
H	-0.397339	3.345330	-1.033046
H	-0.772449	1.950554	-2.044606
H	-1.661094	2.184522	0.886425
H	-2.634100	2.729486	-0.466053
H	1.017753	3.061244	1.044386
C	2.459891	1.491378	1.154087
C	2.930193	0.262861	0.617223
C	2.225843	-0.311538	-0.489956
C	1.087443	0.361635	-1.009162
H	0.549906	-0.084680	-1.841784
C	-3.930370	-2.164842	-0.385310
H	-4.567751	-3.018207	-0.145066
H	-4.174181	-1.776378	-1.379148
H	-2.881467	-2.474533	-0.431287
C	-2.443512	0.615867	-0.370467
C	-4.132506	-1.103469	0.672569
O	-4.925026	-1.267323	1.605031
O	-2.155056	-0.081916	-1.347289
H	2.994142	1.937300	1.990071
C	2.691350	-1.539185	-1.034174
H	2.155121	-1.974461	-1.874244
C	4.069113	-0.410550	1.133617
H	4.601498	0.029915	1.973639
C	3.798317	-2.168727	-0.510581
H	4.143190	-3.107162	-0.936467
C	4.494597	-1.599116	0.583869
H	5.367202	-2.105365	0.987751

TS2j'

C	1.359148	0.540989	0.677862
C	-0.257636	-2.657297	0.275111
C	0.600180	-1.807513	-0.430241
C	2.039839	-2.167334	-0.673742
C	2.966804	-1.387061	0.310517
H	0.968299	-0.000493	1.535661
H	2.197926	-3.243731	-0.548439
H	2.336018	-1.910099	-1.698956
H	2.774743	-1.735311	1.332391
H	4.016803	-1.565688	0.064220
H	0.098844	-3.643124	0.565029

C	-1.551113	-2.274122	0.605471
C	-2.069418	-1.009579	0.203069
C	-1.223180	-0.112707	-0.516504
C	0.171581	-0.469655	-0.732155
H	0.665141	0.031994	-1.563115
C	1.506757	2.956564	-0.291495
H	0.925093	3.879962	-0.241412
H	2.553287	3.153716	-0.039667
H	1.519532	2.567170	-1.315767
C	2.683654	0.104406	0.183773
C	0.913283	1.958857	0.683955
O	0.032866	2.294306	1.470288
O	3.469014	0.841934	-0.408771
H	-2.199502	-2.956872	1.148515
C	-1.762857	1.095851	-0.994533
H	-1.127114	1.775654	-1.555733
C	-3.415400	-0.641716	0.446009
H	-4.053474	-1.325306	1.000823
C	-3.087766	1.427867	-0.757555
H	-3.485805	2.366088	-1.132992
C	-3.916183	0.557217	-0.024353
H	-4.950994	0.827511	0.166169

3j'

C	-1.180662	-0.416267	0.457631
C	0.370538	2.696957	0.136946
C	-0.539231	1.830800	-0.426496
C	-1.952415	2.228204	-0.733478
C	-2.924318	1.496459	0.227627
H	-0.878354	-0.091288	1.461417
H	-2.085391	3.311500	-0.641973
H	-2.214118	1.957909	-1.767691
H	-2.778708	1.891359	1.242794
H	-3.972425	1.644346	-0.048625
H	0.077331	3.732952	0.298168
C	1.662349	2.293406	0.503691
C	2.125260	0.967703	0.218121
C	1.242777	0.021326	-0.373461
C	-0.229129	0.359040	-0.568108
H	-0.534135	0.026997	-1.573330
C	-1.464158	-2.728411	-0.774162
H	-0.914590	-3.672055	-0.813766
H	-2.533491	-2.940892	-0.673400
H	-1.333102	-2.173364	-1.708873
C	-2.647252	0.002826	0.260005
C	-1.029142	-1.945346	0.451894
O	-0.586849	-2.507221	1.434513
O	-3.544123	-0.813678	0.148756
H	2.349850	3.003939	0.953269
C	1.754135	-1.216420	-0.768008
H	1.104980	-1.933586	-1.262244
C	3.470571	0.601817	0.448765

H	4.136601	1.327768	0.909310
C	3.089921	-1.557870	-0.547126
H	3.456948	-2.531127	-0.859914
C	3.947538	-0.647069	0.078910
H	4.985688	-0.910198	0.262212

TS1j''

C	-3.954342	-0.432707	0.752558
C	0.889512	1.018355	-0.520401
C	0.802581	-0.397353	-0.651385
C	-0.521574	-1.032568	-1.016923
C	-1.561160	-1.003883	0.129548
H	-3.765044	-0.991658	1.666269
H	-0.955993	-0.505076	-1.873603
H	-0.355502	-2.068005	-1.331711
H	-1.784502	-2.015198	0.493946
H	-1.160410	-0.470788	1.004019
H	0.003039	1.618896	-0.713023
H	2.070279	1.629253	-0.171241
H	3.245191	0.866363	0.069920
C	3.172860	-0.557941	-0.062496
C	1.933931	-1.153157	-0.424661
H	1.890096	-2.236391	-0.524643
C	-5.758474	0.938285	-0.524271
H	-6.794411	1.243478	-0.363385
H	-5.121799	1.817380	-0.666053
H	-5.673123	0.352705	-1.445065
C	-2.880457	-0.320992	-0.232946
C	-5.305537	0.132480	0.672571
O	-6.058590	-0.078779	1.628229
O	-3.029263	0.306976	-1.283610
H	2.121266	2.712108	-0.081743
C	4.343657	-1.327159	0.174172
H	4.288364	-2.408749	0.073215
C	4.482234	1.462565	0.431848
H	4.532504	2.544661	0.529866
C	5.528720	-0.719686	0.525088
H	6.416503	-1.320615	0.703223
C	5.599473	0.688969	0.655256
H	6.540468	1.156725	0.931912

2j''

C	3.439292	-0.151776	-0.905281
C	-0.611149	0.011099	1.439191
C	-0.628531	-1.160912	0.631382
C	0.511421	-2.159539	0.688562
C	1.654072	-1.855846	-0.299504
H	3.369014	-0.547435	-1.915827
H	0.928334	-2.199188	1.700173
H	0.125316	-3.159029	0.458411
H	2.294020	-2.745657	-0.409694

H	1.256107	-1.649841	-1.301312
H	0.228893	0.172193	2.107701
C	-1.633381	0.929647	1.376363
C	-2.738704	0.740746	0.504716
C	-2.770289	-0.436265	-0.311203
C	-1.698865	-1.363505	-0.218180
H	-1.737652	-2.259978	-0.835620
C	4.663977	1.605211	0.571005
H	5.441875	2.359923	0.438658
H	3.740187	2.070202	0.929581
H	4.958982	0.886569	1.342141
C	2.573706	-0.714549	0.127297
C	4.438726	0.911973	-0.753847
O	5.090196	1.215466	-1.757771
O	2.610531	-0.310731	1.293554
H	-1.607508	1.817966	2.003628
C	-3.875285	-0.636462	-1.182380
H	-3.898942	-1.531205	-1.800471
C	-3.810874	1.668585	0.415506
H	-3.783479	2.560641	1.037228
C	-4.898425	0.282383	-1.247158
H	-5.736929	0.117463	-1.918506
C	-4.866319	1.446746	-0.440236
H	-5.680265	2.164273	-0.499753

TS2j''

C	1.739158	0.341262	-0.610770
C	0.447474	-0.151278	0.906868
C	0.103780	-1.517669	0.509503
C	1.218590	-2.528483	0.456547
C	2.254698	-2.145333	-0.643275
H	1.032504	0.165892	-1.418352
H	1.742785	-2.575228	1.420690
H	0.823082	-3.529237	0.253132
H	3.113296	-2.821325	-0.609682
H	1.774919	-2.225295	-1.626190
H	1.229671	-0.045257	1.658315
C	-0.594402	0.820115	0.938067
C	-1.881869	0.541891	0.439852
C	-2.183685	-0.790418	-0.003097
C	-1.153497	-1.788232	0.056423
H	-1.398558	-2.794505	-0.279221
C	3.167904	2.261313	0.432232
H	3.113971	3.348163	0.527270
H	3.130636	1.791843	1.422317
H	4.127039	1.961071	0.000272
C	2.748212	-0.724503	-0.398679
C	2.023186	1.796219	-0.444810
O	1.278099	2.603008	-0.990915
O	3.866797	-0.519563	0.065401
H	-0.380430	1.815560	1.315507

C	-3.479562	-1.076903	-0.475739
H	-3.706480	-2.085700	-0.812609
C	-2.905964	1.528792	0.393768
H	-2.674180	2.537015	0.727139
C	-4.455544	-0.093730	-0.513365
H	-5.449956	-0.330986	-0.880949
C	-4.165181	1.216969	-0.074203
H	-4.937250	1.980357	-0.109452

3j''

C	1.672121	0.284441	-0.430214
C	0.512113	-0.047593	0.607708
C	0.041012	-1.470230	0.395837
C	1.114446	-2.522855	0.466811
C	2.256698	-2.220205	-0.535941
H	1.221799	0.235085	-1.429532
H	1.544421	-2.551392	1.479924
H	0.698863	-3.516831	0.270094
H	3.101084	-2.903291	-0.408527
H	1.871098	-2.331632	-1.558626
H	0.990319	0.008107	1.604123
C	-0.592061	0.961712	0.537771
C	-1.920558	0.633213	0.246817
C	-2.284944	-0.742280	0.028966
C	-1.248939	-1.752144	0.119414
H	-1.545080	-2.788006	-0.042321
C	2.918391	2.100767	1.001442
H	3.115044	3.174741	0.992801
H	2.322588	1.841454	1.884902
H	3.861341	1.548381	1.070209
C	2.759407	-0.796312	-0.362989
C	2.219648	1.711839	-0.285425
O	2.073706	2.501735	-1.198768
O	3.934914	-0.543156	-0.173771
H	-0.334011	2.005507	0.699554
C	-3.613728	-1.065450	-0.260810
H	-3.879552	-2.107613	-0.424238
C	-2.943767	1.622533	0.158041
H	-2.676581	2.664121	0.318508
C	-4.594202	-0.076382	-0.342424
H	-5.621456	-0.346660	-0.569034
C	-4.249712	1.271960	-0.130374
H	-5.014386	2.041316	-0.195299

Syn 1a

C	2.729449	0.584814	0.043985
C	-2.920640	0.215354	-1.179773
C	-2.241648	-0.390356	-0.113622
C	-0.840233	-0.933905	-0.293775
C	0.234226	0.130473	-0.025035

H	2.430044	1.626452	0.154243
H	-0.670492	-1.783357	0.376804
H	-0.706582	-1.320131	-1.310324
H	0.095371	0.993868	-0.692727
H	0.127457	0.535500	0.992296
H	-2.444777	0.262035	-2.157439
C	-4.198585	0.748752	-1.007328
C	-4.822063	0.683929	0.240079
H	-5.818927	1.094873	0.375628
C	-4.159060	0.080362	1.310106
H	-4.639196	0.017786	2.283352
C	-2.881133	-0.451270	1.131998
H	-2.374146	-0.927412	1.968998
C	5.096789	1.486226	0.196151
H	6.128808	1.137715	0.266410
H	4.980652	2.102964	-0.703774
H	4.870606	2.126177	1.058497
C	1.659992	-0.394092	-0.196018
C	4.162214	0.283926	0.156751
O	4.590280	-0.863461	0.231358
O	1.886595	-1.554177	-0.524375
H	-4.709661	1.209355	-1.848941

TS1a

C	2.670453	-0.240378	0.563453
C	-2.342640	1.023562	-0.339850
C	-2.184024	-0.370346	-0.351425
C	-0.896281	-0.988101	-0.855959
C	0.261844	-0.928486	0.168845
H	2.492170	-0.599895	1.576215
H	-1.076199	-2.029960	-1.141377
H	-0.565736	-0.463829	-1.758935
H	-0.053005	-0.399886	1.080081
H	0.551919	-1.932702	0.506991
H	-1.542798	1.652478	-0.725516
C	-3.512043	1.607244	0.147070
C	-4.548249	0.804851	0.630501
H	-5.461609	1.258205	1.006418
C	-4.404929	-0.583049	0.620588
H	-5.207691	-1.216838	0.988946
C	-3.231559	-1.162951	0.133688
H	-3.129427	-2.246260	0.125049
C	5.017047	0.253559	1.393708
H	5.989633	0.584189	1.024653
H	4.659126	0.954945	2.157673
H	5.127020	-0.724798	1.878597
C	1.517756	-0.215442	-0.348364
C	4.039546	0.171128	0.228534
O	4.389270	0.420450	-0.920790
O	1.549827	0.360253	-1.429941
H	-3.617701	2.689174	0.142309

2a

C	-2.332144	0.207078	0.616264
C	1.994999	-0.438368	-1.050177
C	2.000415	0.643423	-0.158354
C	1.067354	1.823963	-0.345155
C	-0.265632	1.678754	0.413777
H	-2.231978	0.364827	1.689043
H	1.561114	2.736588	0.008886
H	0.845547	1.966161	-1.407286
H	-0.088873	1.384401	1.456374
H	-0.774624	2.654470	0.458887
H	1.313491	-0.423695	-1.895492
C	2.845480	-1.527858	-0.854221
C	3.715953	-1.555121	0.236724
H	4.380353	-2.402176	0.386232
C	3.731593	-0.483422	1.131377
H	4.410784	-0.490675	1.980224
C	2.881234	0.604611	0.931988
H	2.907332	1.441432	1.627886
C	-4.397649	-1.135007	1.228486
H	-5.255266	-1.623449	0.762208
H	-3.818861	-1.875708	1.794261
H	-4.753332	-0.385231	1.946591
C	-1.248683	0.704535	-0.239685
C	-3.541395	-0.485203	0.149694
O	-3.860216	-0.525807	-1.034097
O	-1.144020	0.373863	-1.417599
H	2.829039	-2.355693	-1.558563

TS2a

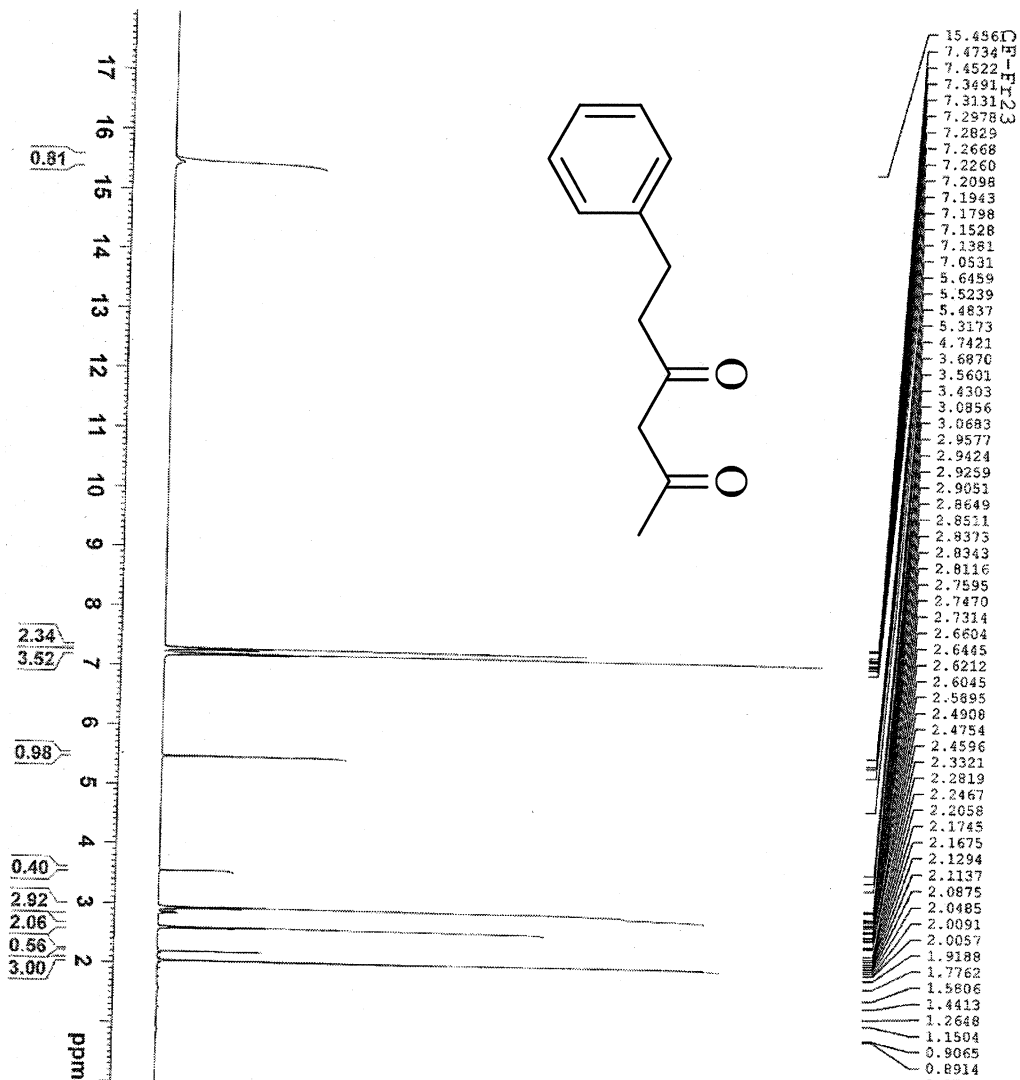
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H	-0.449468	-0.202876	1.426298
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H	0.772480	2.487469	-1.352289
H	0.170112	2.257292	1.646029
H	-0.539837	3.430935	0.509941
H	-0.051777	0.028561	-1.626410
C	1.033862	-1.612850	-0.758427
C	2.191654	-1.975692	-0.096929
H	2.481662	-3.021601	-0.040737
C	3.018439	-0.990037	0.470503
H	3.934107	-1.274670	0.980787
C	2.675362	0.366854	0.356278
H	3.331771	1.122215	0.783102
C	-2.353531	-2.064624	1.084672
H	-3.055706	-2.773701	0.641109
H	-1.470642	-2.602829	1.454187
H	-2.819407	-1.578696	1.950960

C	-1.266799	1.438903	0.244814
C	-1.943127	-1.033302	0.045849
O	-2.360398	-1.072389	-1.100641
O	-2.300358	1.820279	-0.286663
H	0.407725	-2.362002	-1.234195

3a

C	0.785161	-0.115861	-0.308699
C	-0.540362	-0.346422	0.520203
C	-1.521403	0.773334	0.261734
C	-1.001842	2.160558	0.506523
C	0.263683	2.425732	-0.346896
H	0.541959	-0.250872	-1.373087
H	-1.765494	2.912772	0.280529
H	-0.733716	2.284860	1.567224
H	-0.023756	2.444726	-1.407826
H	0.732679	3.383212	-0.102386
H	-0.205821	-0.306735	1.572695
C	-1.117455	-1.712512	0.261782
C	-2.385284	-1.893442	-0.213606
H	-2.751833	-2.902455	-0.388822
C	-3.242038	-0.792891	-0.469306
H	-4.246991	-0.954388	-0.845934
C	-2.780624	0.521774	-0.216657
H	-3.449573	1.360548	-0.402823
C	2.986255	-1.356241	-0.928881
H	3.691827	-2.092955	-0.539366
H	2.557268	-1.715468	-1.872924
H	3.509142	-0.416171	-1.136359
C	1.298280	1.330364	-0.159475
C	1.895997	-1.103365	0.089121
O	1.885461	-1.643722	1.178115
O	2.462546	1.577530	0.095612
H	-0.481956	-2.563711	0.484205

NMR spectra of starting materials and products



Current Data Parameters
NAME 6-Ph-2,4-Hexan-1-one-103009
EXPNO 1
PROCNO 1

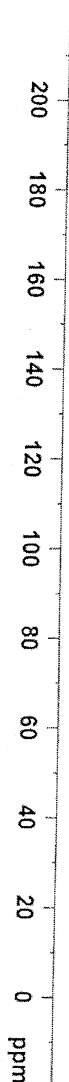
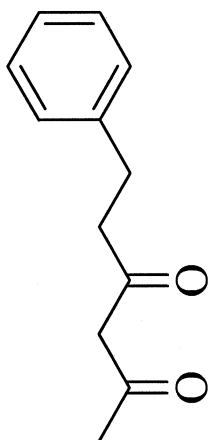
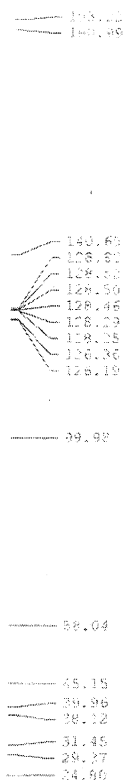
F2 - Acquisition Parameters
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Time 14.22
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT CDCl₃
NS 0
DS 0
SWH 8992.806 Hz
FIDRES 0.274439 Hz
AQ 1.8220063 sec
RG 322.5
INVM 55.600 usec
DE 28.100 usec
TE 298.2 K
D1 1.00000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.00 usec
PL1 0.00 dB
SFO1 500.136012 MHz

F2 - Processing parameters
SI 32768
SF 500.136012 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



1a
13C



Current Data Parameters
NAME 6-Ph-2,4-PentDione-090209
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters

Date_ 20090921
Time 15.14
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 29
DS 4
SWH 30010.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 2560.3
RG 16.680 usec
DE 1.0000000 usec
TE 297.2 K
D1 1.00000000 sec
d11 0.03000000 sec
ZPG 1

===== CHANNEL f1 =====

NUC1 13C
P1 8.46 usec
PL1 1.00 dB
SFO1 125.7703640 MHz

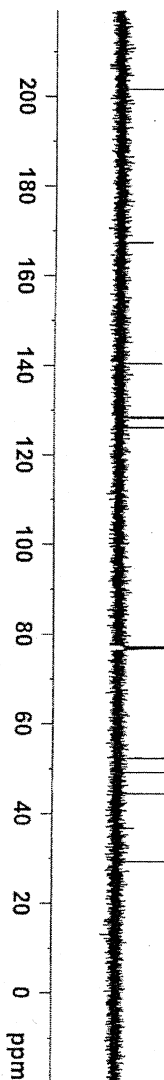
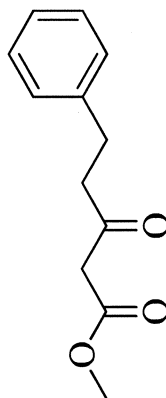
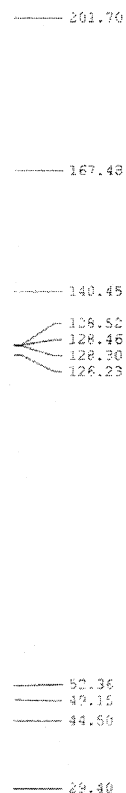
===== CHANNEL f2 =====

NUC2 13C
P2 100.00 usec
PL2 1.00 dB
SFO2 500.1322150 MHz

F2 - Processing parameters

SF 125.7577662 MHz
WDW EM
SSB 0
GB 1.00 Hz
PC 1.40

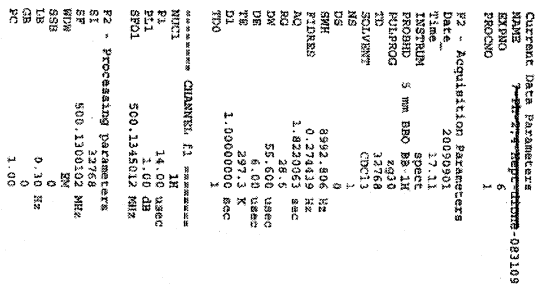
CF-Fr17
13C



Current Data Parameters
NAME Me-1-ph-3,5-Pent-on-ester-050209
PROCNO 1

F2 - Acquisition Parameters
Date_ 20011141
Time 17:41
INSTRUM spect
PROBHD 5 mm BBO BH-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 62
DS 4
SWH 30030.029 Hz
FIDRES 0.454222 Hz
RG 1.094096 sec
AQ 16.658 usec
DE 7.00 usec
TE 300.2 K
D1 1.00000000 sec
d11 0.01000000 sec
TDO 1

===== CHANNEL F1 =====
NUC1 13C
P1 9.00 usec
PL1 1.00 dB
FQ1 125.7702640 MHz
===== CHANNEL F2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 0.00 dB
PL12 17.50 dB
FQ2 500.1322180 MHz
F2 - Processing parameters
SI 32768
SF 500.1322180 MHz
GB 125.7577942 MHz
SB 1.00000000 MHz
LB 0
GB 0
LB 1.00 Hz
PC 1.40



CF-E133-35

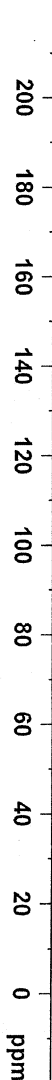
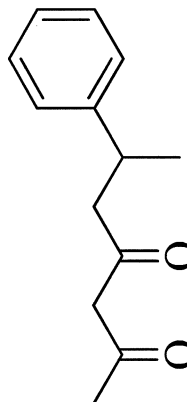
202.93
201.83
191.89-35
191.61

145.78
145.56

128.45
128.33
126.58
126.20

100.61

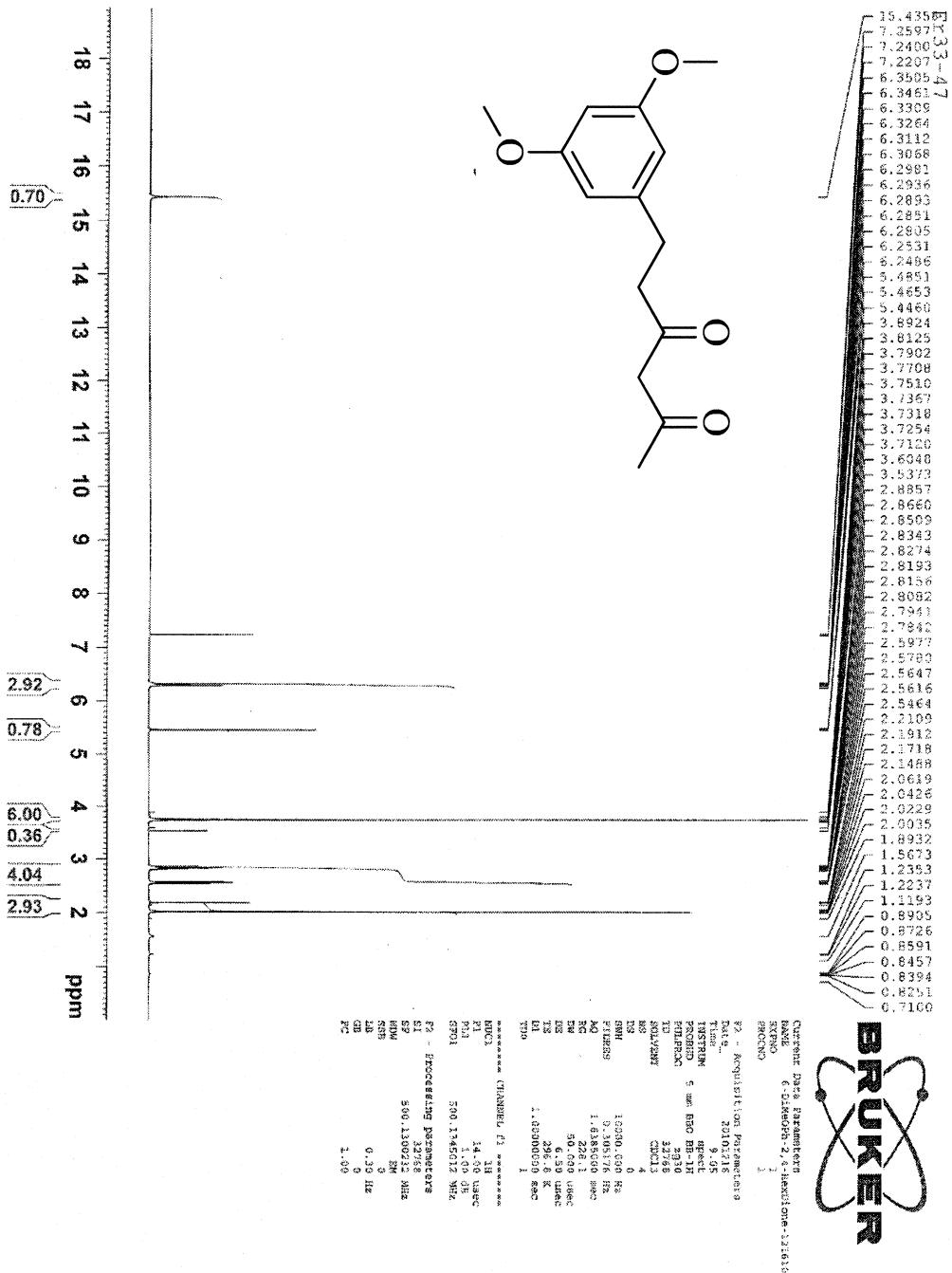
58.27
51.63
46.62
46.51
36.66
36.64
35.12
35.09
24.92
24.79
21.59
21.46



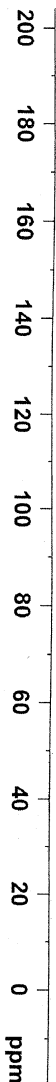
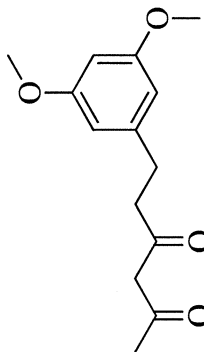
Current Data Parameters
NAME 7-Ph-2,4-Hept-dione-081109
EXPNO 7
PROCNO 1

PP - Acquisition Parameters
Date_ 20090901
Time 17.03
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 204
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 5160.8
DPR 1562.0 usec
DE 7.00 usec
TE 297.2 K
D1 1.0000000 sec
d11 0.0300000 sec
TD0 1

----- CHANNEL f1 -----
NUC1 13C
P1 5.00 usec
PL1 1.00 dB
SFO1 125.7703640 MHz
----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 24.00 dB
PL12 24.00 dB
SFO2 500.1322150 MHz
F2 - Processing parameters
SI 32768
SF 125.7578145 MHz
WDW EM
SSB 0
GB 0
PC 1.40



Fr33-47

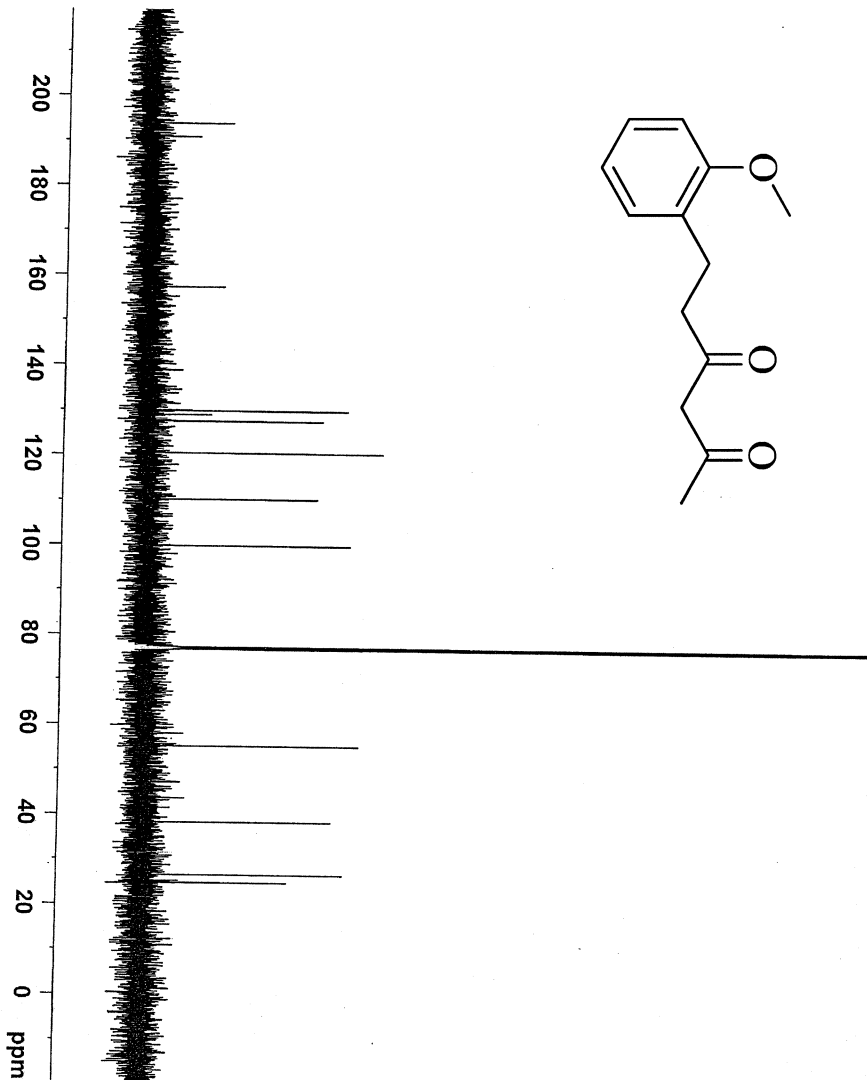
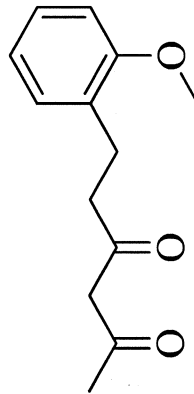


Current Data Parameters
NAME 6-Dimethyl-2,4-Hexadiene-1,2,3,4,5,6
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20101216
Time 12:12
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
SOLVENT CDCl3
NS 52
DS 4
SWH 30030.022 Hz
FIDRES 0.141242 Hz
AQ 1.0912410 sec
RG 7298.2
DM 16.550 usec
DE 2.750 usec
TE 300.2 K
D1 1.00000000 sec
d11 0.03000000 sec
TD0 1
===== CHANNEL f1 =====
NUC1 13C
P1 8.50 usec
PL1 1.00 dB
SFO1 125.7709540 MHz
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 1.00 dB
PL12 17.50 dB
SFO2 500.1322150 MHz
F2 - Processing parameters
SI 32768
SF 125.7577932 MHz
SDM 32
SOS 32
LB 1.00 Hz
GB 0
FC 1.40

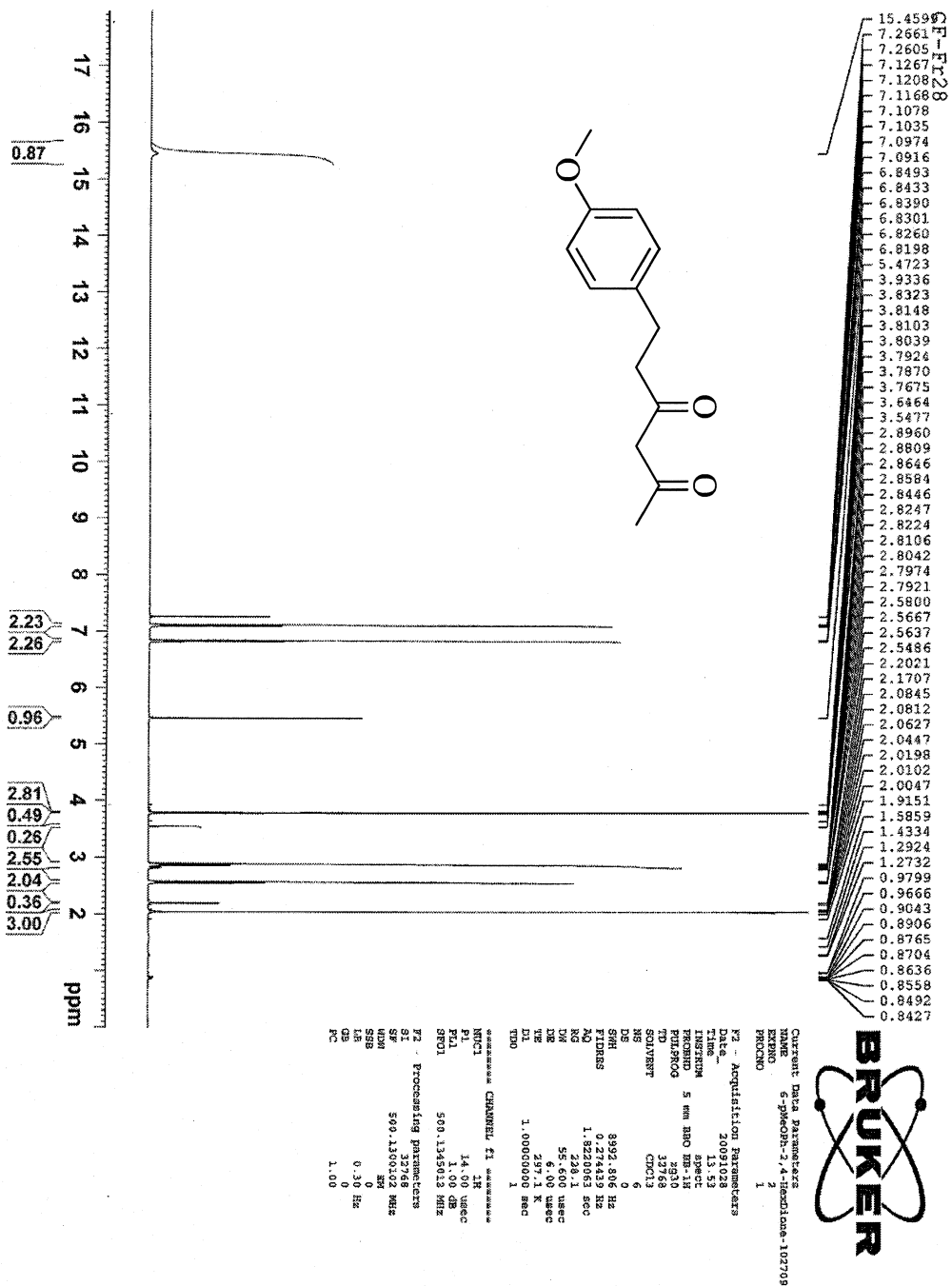


CF-Fr18
13C NMR

193.94
190.95
157.40
129.83
128.97
127.53
120.43
110.18
99.85
55.18
38.31
26.56
24.86

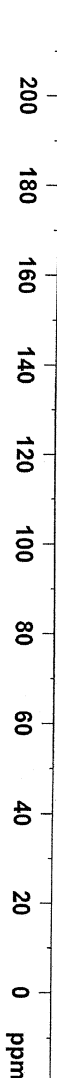
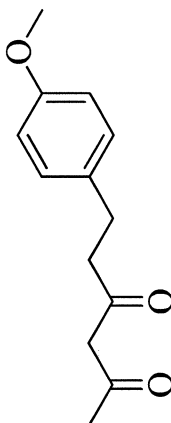


Current Data Parameters
NAME 6-methoxy-2,4-hexadione-102909
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20091029
Time 15:53
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
FOLPROG zgpg30
SOLVENT CDCl3
NS 231
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 2.80
RG 4096
DM 16.650 usec
DE 7.00 usec
TE 296.8 K
D1 1.0000000 sec
d11 0.0300000 sec
TD0 1
===== CHANNEL f1 =====
NUC1 13C
P1 8.40 usec
PL1 1.00 dB
SFO1 125.7703640 MHz
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
P2 1.00 dB
PL2 1.00 dB
SFO2 500.132150 MHz
F2 - Processing parameters
SI 32768
SF 125.757724 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

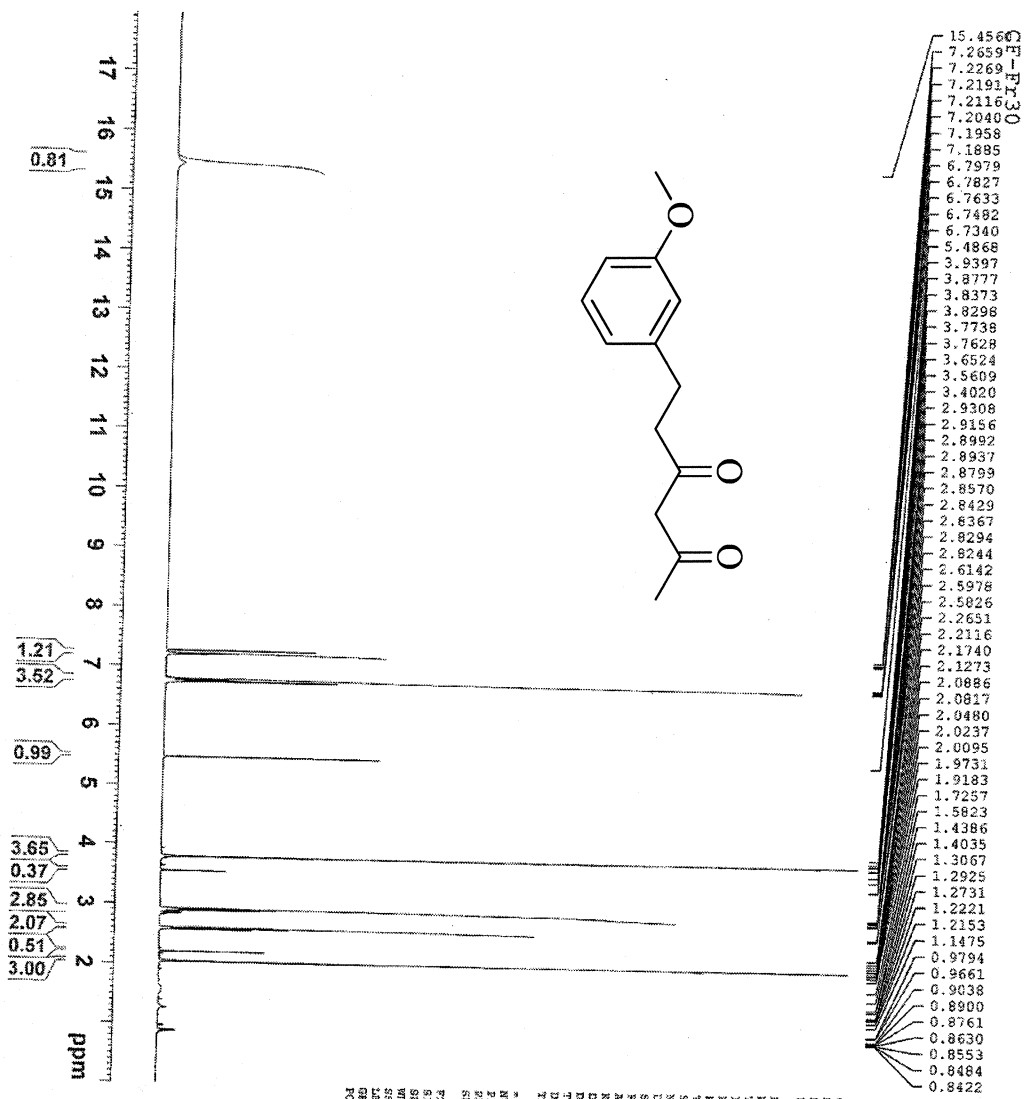


CF-Ft28
13C NMR

193.23
191.14
158.01
132.72
129.24
129.20
113.93
113.87
100.03
55.24
30.64
24.86



Current Data Parameters
NAME 6-JNMRP2.4-RedDione-102709
EXPNO 3
PROCNO 1
P2 - Acquisition Parameters
Date_ 20091024
Time 13.56
INSTRUM spect
PROBHD 5 mm BBO HS-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 48
DS 4
SWH 30330.023 Hz
FIDRES 0.445622 Hz
AQ 1.0912410 sec
RG 1448.2
DM 16.650 usec
DE 23.74 usec
TE 300.2 K
D1 1.00000000 sec
d11 0.03000000 sec
TD0 1
----- CHANNEL f1 -----
NUC1 13C
P1 8.60 usec
PL1 1.00 dB
SFO1 125.7703640 MHz
----- CHANNEL f2 -----
CYPDPRG2 waltz16
NUC2 1H
P2 160.10 usec
PL2 1.00 dB
PL12 17.50 dB
SFO2 500.1322150 MHz
P2 - Processing parameters
SI 32768
SF 125.757323 MHz
WDW EM
SSB 0
GB 0
PC 1.40

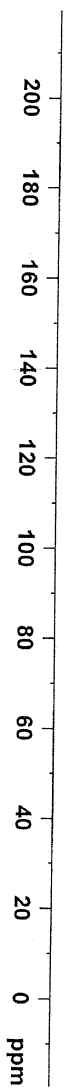
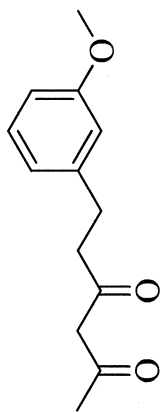


Current Data Parameters
 NAME 6-methoxy-2,4-heptanedione-111003
 EXPNO 3
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20091110
 Time 8.53
 INSTRUM spect
 PULPROG zgpg30
 TD 32768
 SFO 500.136012
 SOLVENT CDCl3
 NS 6
 DS 4
 SWH 8994.806 Hz
 FIDRES 0.274439 Hz
 AQ 1.820063 sec
 RG 487.4
 DQ 55.608 usec
 DE 277.3 X
 TE 300.2 K
 DI 1.0000000 sec
 TO 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 14.00 usec
 PL 0.00 dB
 SFO1 500.136012 MHz
 F2 - Processing parameters
 SI 32768
 SF 500.136012 MHz
 BRW 3K
 SSF 0.30 Hz
 LB 0
 GB 0
 PC 1.00

CF-Fr9-13
13C NMR

- 193.29
- 190.95
- 159.69
- 142.31
- 129.47
- 120.62
- 114.05
- 111.51
- 100.01
- 55.14
- 39.90
- 31.49
- 24.80



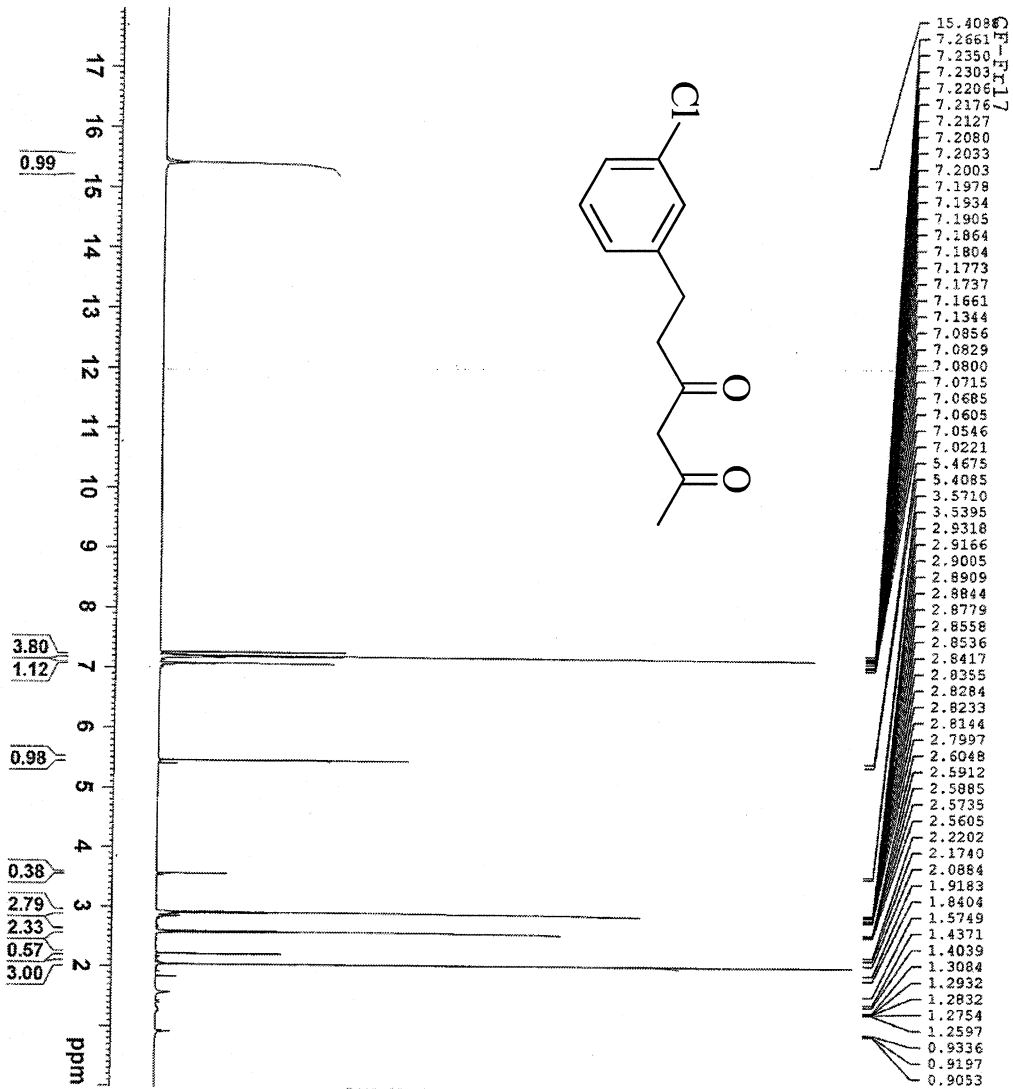
Current Data Parameters
NAME 6-methoxy-2,4-hexanedione-102109
EXFNO 4
PROCNO 1

P2 - Acquisition Parameters
Date_ 20091021
Time_ 14.49
INSTRUM spect
PROBHD 5 mm BBO BB-HF
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 105
DS 4
SWH 30280.029 Hz
FIDRES 14.6442248
AQ 1.0912410 sec
RG 2896.3
DW 16.650 usec
DE 297.873
DI1 1.00000000 sec
TD1 0.03000000 sec
TPO 1

===== CHANNEL f1 =====
NUC1 13C
P1 8.60 usec
PL1 1.00 dB
SFO1 125.7703640 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P2 100.00 usec
PL2 1.00 dB
PL12 17.50 dB
SFO2 500.132150 MHz

P3 - Processing parameters
SI 32768
SF 125.7577920 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Current Data Parameters
 NAME 6-methyl-2,4-heptadiene-100709
 EXNO 2
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20091007
 Time 16.11
 INSTRUM spect
 PROCD 5 mm BBO
 PULPROG zgpg30
 TD 65536
 SFO 127.60
 SOLVENT CDCl3
 NS 5
 DS 0
 SWH 9992.840 Hz
 FIDRES 0.217449 Hz
 AQ 1.6220663 sec
 RG 362
 DW 55.600 usec
 DE 2.500 V
 TE 300.2 K
 D1 1.00000000 sec
 TDO 1
 CHANNEL f1
 NUC1 13C
 P1 14.00 usec
 PL 1.00 dB
 SFO1 500.1345012 MHz
 F2 - Processing parameters
 SI 32768
 SF 500.1306102 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

CF-Ft17
13C

192.91
190.77

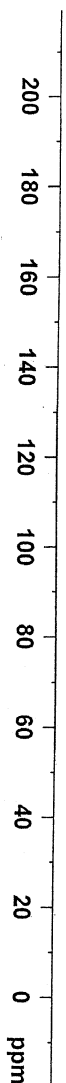
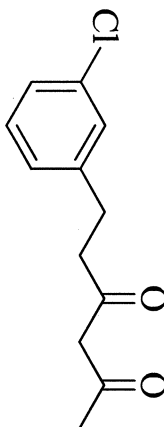
142.70
134.21
129.78
129.73
128.47
128.44
126.52
126.43

100.04

57.99

44.75
39.66

30.97
28.91
24.72



Current Data Parameters
NAME 6-AClPr-2,4-Hexadione-100709
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters

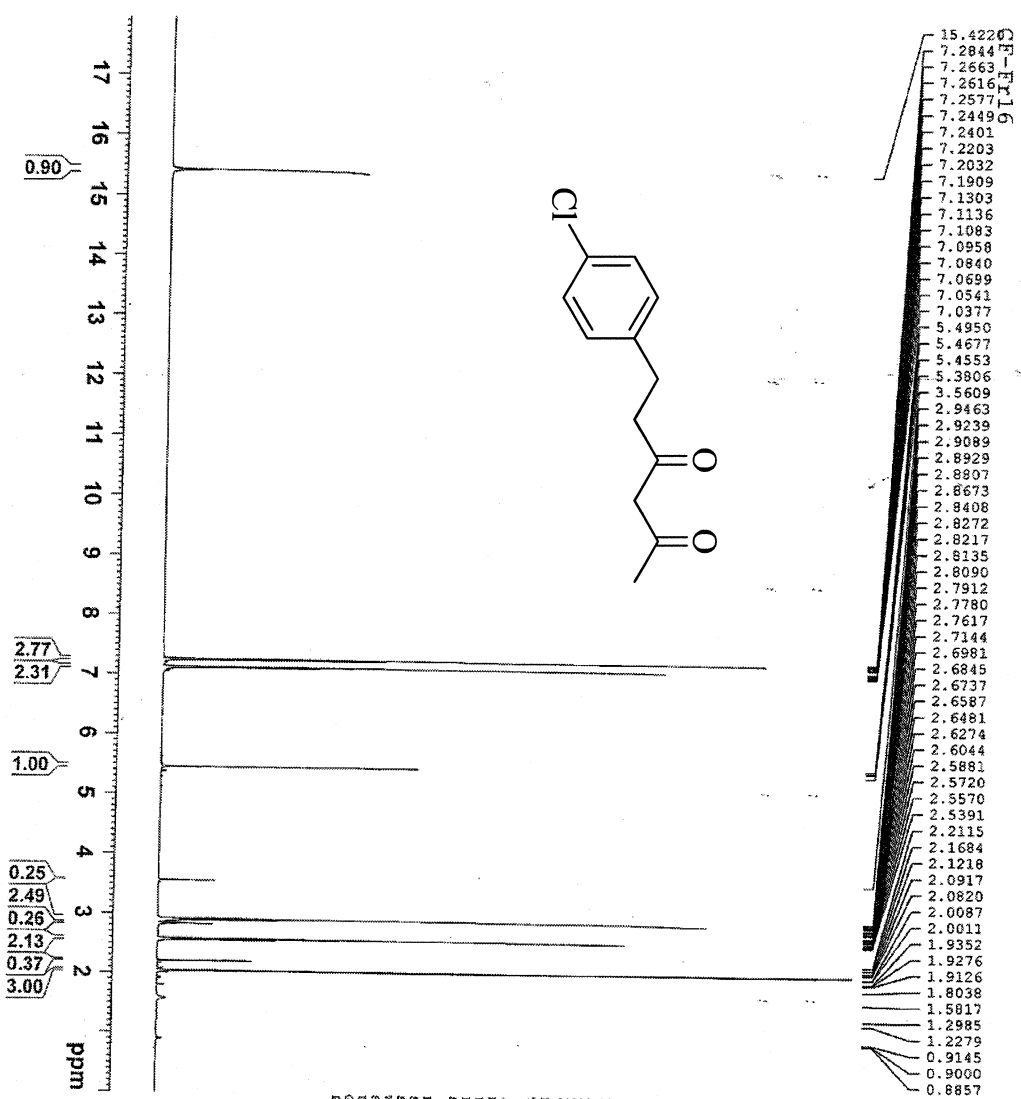
File 20091007
Date_ 11/11/07
Time 11:45
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SFO200.132150
AQ 177
DS 4
SWH 30030.029 Hz
FIDRES 0.456222 Hz
AQ 1.091240 sec
RG 327.5
DE 16.650 usec
TE 297.4 K
D1 1.0000000 sec
d11 0.0300000 sec
D10 1

===== CHANNEL f1 =====

NUC1 13C
P1 8.60 usec
PL1 1.00 dB
SFO1 125.7705450 MHz

===== CHANNEL f2 =====

NAME 6-AClPr-2,4-Hexadione-100709
EXPNO 3
PROCNO 1
F2 - Processing parameters
SI 327.5
SF 125.777721 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Current Data Parameters
 NAME 5-PClP-2,4-Hexadione-091009
 EXNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20090930
 Time 14.54
 INSTRUM spect
 PROBD 5 mm BBO
 PULPROG zgpg30
 TD 32768
 SOLVENT CHCl3
 NS 6
 DS 4
 SWH 9972.400 Hz
 FIDRES 0.374419 Hz
 AQ 1.820063 sec
 RG 256
 DN 55.606 usec
 DE 3.00 usec
 TE 300.2 K
 D1 1.0000000 sec
 TDO 1

===== CHANNEL f1 =====
 NUCL1 1H
 P1 18 usec
 PL 14.00 dB
 SFO1 500.1345012 MHz

F2 - Processing parameters
 SI 32768
 SF 500.134505 MHz
 KW 50
 SSB 0
 GB 0
 CB 0.36 Hz
 PC 1.00

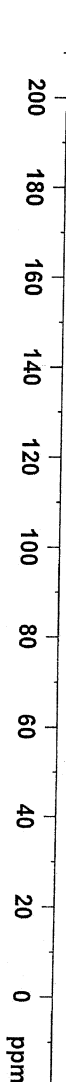
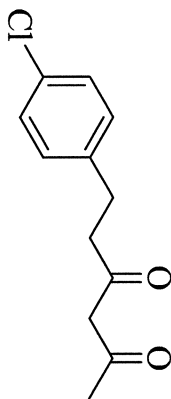
CF-Et16
13C NMR

192.91
190.87

139.10
131.95
129.65
128.57

100.07

39.79
30.69
24.75



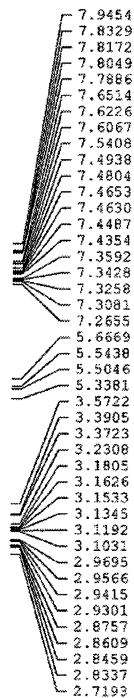
Current Data Parameters
NAME 6-PClPh-2,4-HexDione-093009
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090930
Time 15.19
INSTRUM spect
PROBHD 5 mm BBO 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 35
DS 4
SWH 30030.022 Hz
FIDRES 0.456222 Hz
AQ 1.0912410 sec
RG 4096
DW 16.650 usec
DE 2.00 usec
TE 300.7 K
D1 1.00000000 sec
d11 0.03000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 13C
P1 8.60 usec
PL1 1.00 dB
SFO1 125.7703640 MHz
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 1.00 dB
PL12 1.50 dB
SFO2 500.1322150 MHz
F2 - Processing parameters
SI 32768
SF 125.7577935 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Vialed-Cong

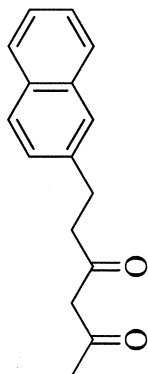
15.5135



Current Data Parameters
NAME 6-Sept-24-Hexadec-102309
EXPNO 8
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090326
Time 14:46
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CHCl3
NS 4
DS 0
SWH 8992.806 Hz
FIDRES 0.274439 Hz
AQ 1.822063 sec
RG 101.6
DB 55.682 dB
BPC 287.1
T2 1.00000000 sec
TPO 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.00 usec
PL1 1.00 dB
SFO1 500.1345012 MHz
F2 - Processing parameters
SI 32768
SF 500.1345012 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



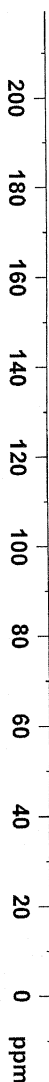
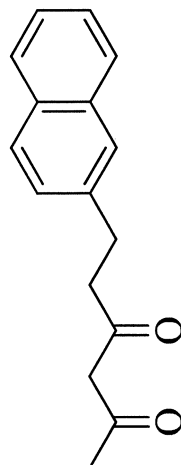
Viald-Conc
13C NMR

193.14
191.00

138.16
133.54
132.08
128.96
127.58
127.44
126.94
126.41
126.00
125.34

100.04

39.87
31.57
24.78



Current Data Parameters
NAME 6-Naph-2,4-Hexdione-102309
EXPNO 9
PROCNO 1

F2 - Acquisition Parameters
Date_ 20091026
Time 16.49

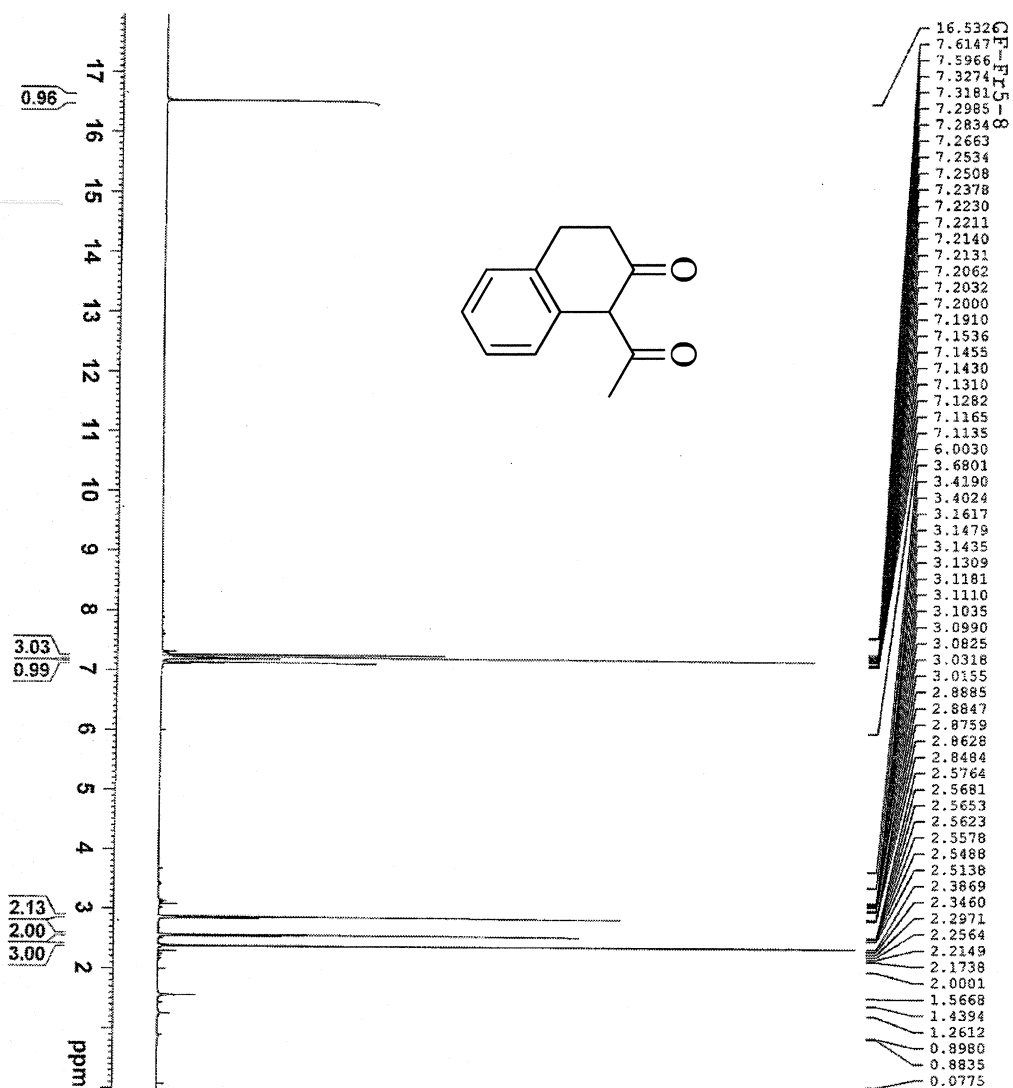
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 21
DS 4

SWH 30030.029 Hz
FIDRES 0.46822 Hz
AQ 1.0914096 sec
RG 320
DE 16.650 usec
TE 297.5 K
D1 1.0000000 sec
D11 0.0300001 sec
ID0 1

===== CHANNEL f1 =====
NUC1 13C
P1 8.60 usec
PL1 1.00 dB
SFO1 125.7703640 MHz

===== CHANNEL f2 =====
CPOPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 19.00 dB
PL12 17.50 dB
SFO2 500.1322150 MHz

F2 - Processing parameters
SI 32768
SF 125.757792 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

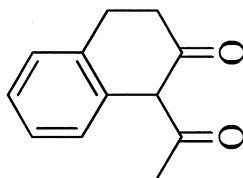


Output Data Parameters
NAME 4-PP-2-4-BROUCLON-CON-MECH-110109
EXPNO 6
PROCNO 1
F2 - Acquisition Parameters
Date_ 20091104
Time 22.41
INSTRUM spect
PROBHD 5 mm HNP 1H-13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 6
DS 0
SWH 8922.806 Hz
FIDRES 0.276439 Hz
AQ 1.8220491 sec
RG 327.5
EW 55.400 Hz
F2 500.1300102 MHz
F1 100.6261000 MHz
TMR 1
TE 300.2 K
===== CHANNEL f1 =====
NUC1 1H
P1 14.00 Hz
PC1 1.00
SFO1 500.1345012 MHz
F2 - Processing parameters
SI 32768
SF 500.1300102 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



CF-Et5-8
13C NMR

200.38
183.77
135.38
132.81
127.36
126.43
126.38
125.45
110.93

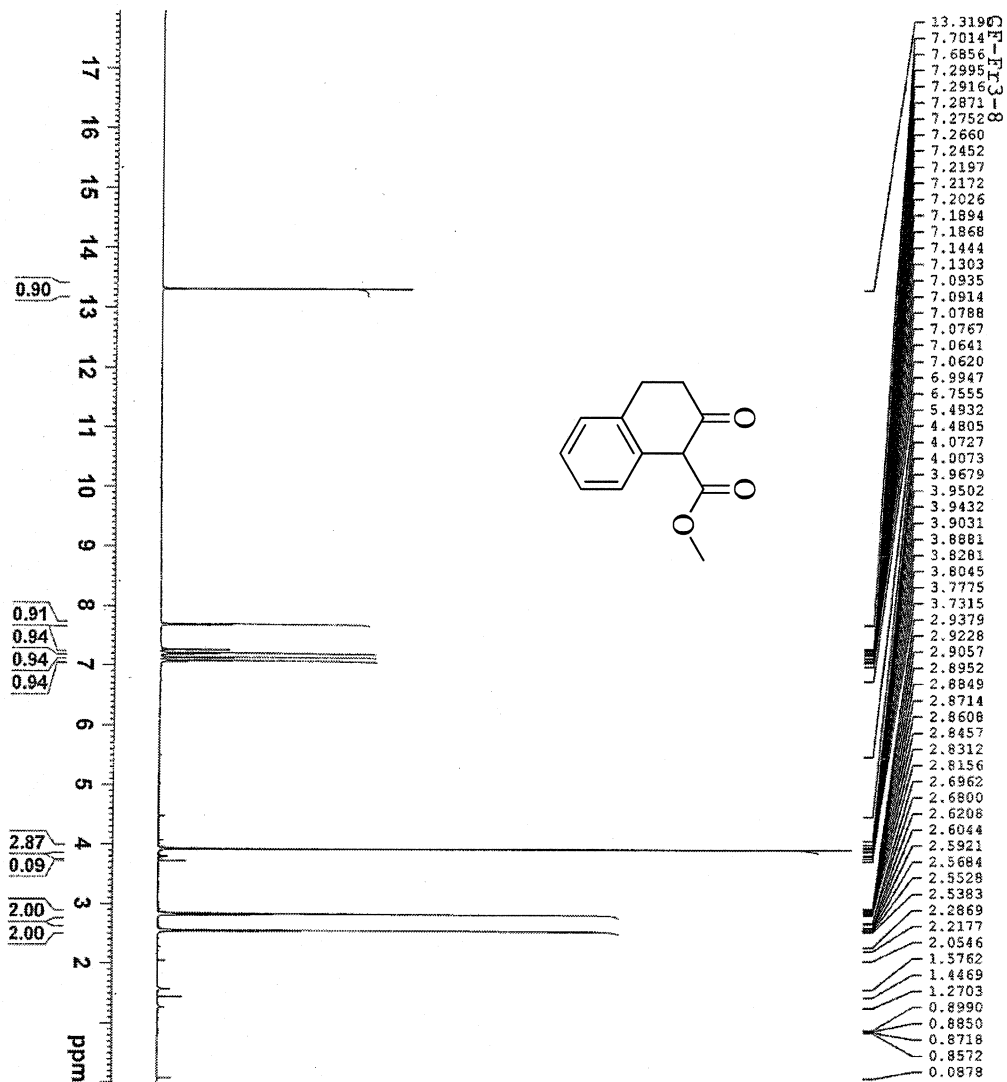


35.32
27.76
23.31

200
180
160
140
120
100
80
60
40
20
0
ppm



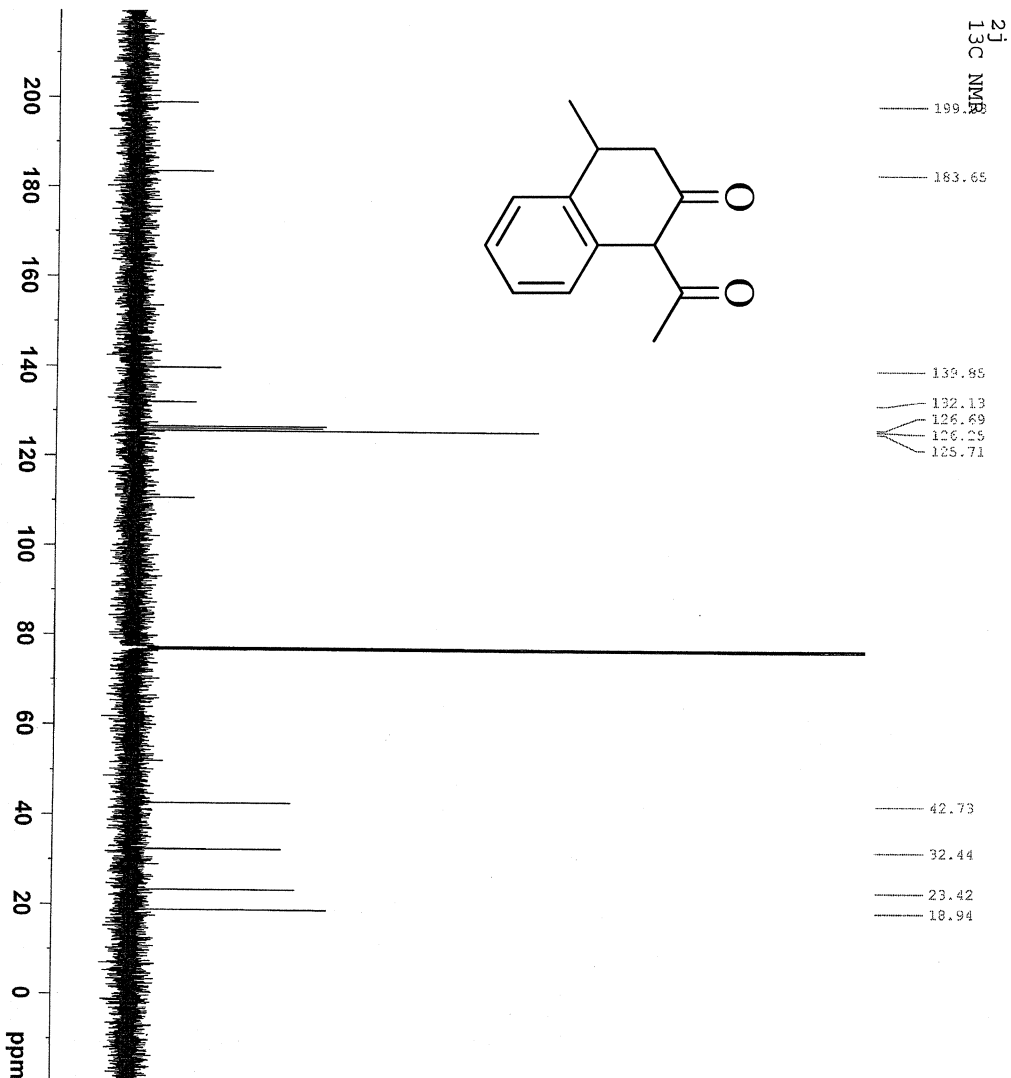
Current Data Parameters
NAME 670724-HS0001-CON-MACH-110109
EXPNO 7
PROCNO 1
F2 - Acquisition Parameters
Date_ 20091104
Time 11:11
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
AQ 0.45513
SOLVENT CDCl3
NS 125
DS 4
SWH 10030.428 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 320
GB 1
PC 1
DE 16.450 usec
TE 300.2 K
D1 1.0000000 sec
d11 0.0300000 sec
TDO 1
===== CHANNEL f1 =====
NUC1 13C
P1 1.00 usec
PL1 0.00 dB
SFO1 125.7703640 MHz
===== CHANNEL f2 =====
NUC2 1H
P2 1.00 usec
PL2 0.00 dB
SFO2 500.132450 MHz
F2 - Processing parameters
SI 32768
SF 125.7577221 MHz
WDW EM
SSB 0
GB 0
PC 1.40



Bruker Data Parameters
 Name: 1-methoxy-1,2,3,4-tetrahydronaphthalen-2-one
 Date: 20081111
 Time: 14:14:11
 Instrument: spect
 Processor: spectpro
 Acquisition: 32768
 Resolution: 0.390625
 F2: 299.613 MHz
 A1: 101.625 MHz
 SFO1: 500.135260 MHz
 PC: 32768
 REW: 500.135260 MHz
 ASB: 0.390625 MHz
 GB: 0.390625 MHz
 PC: 1.000000 MHz

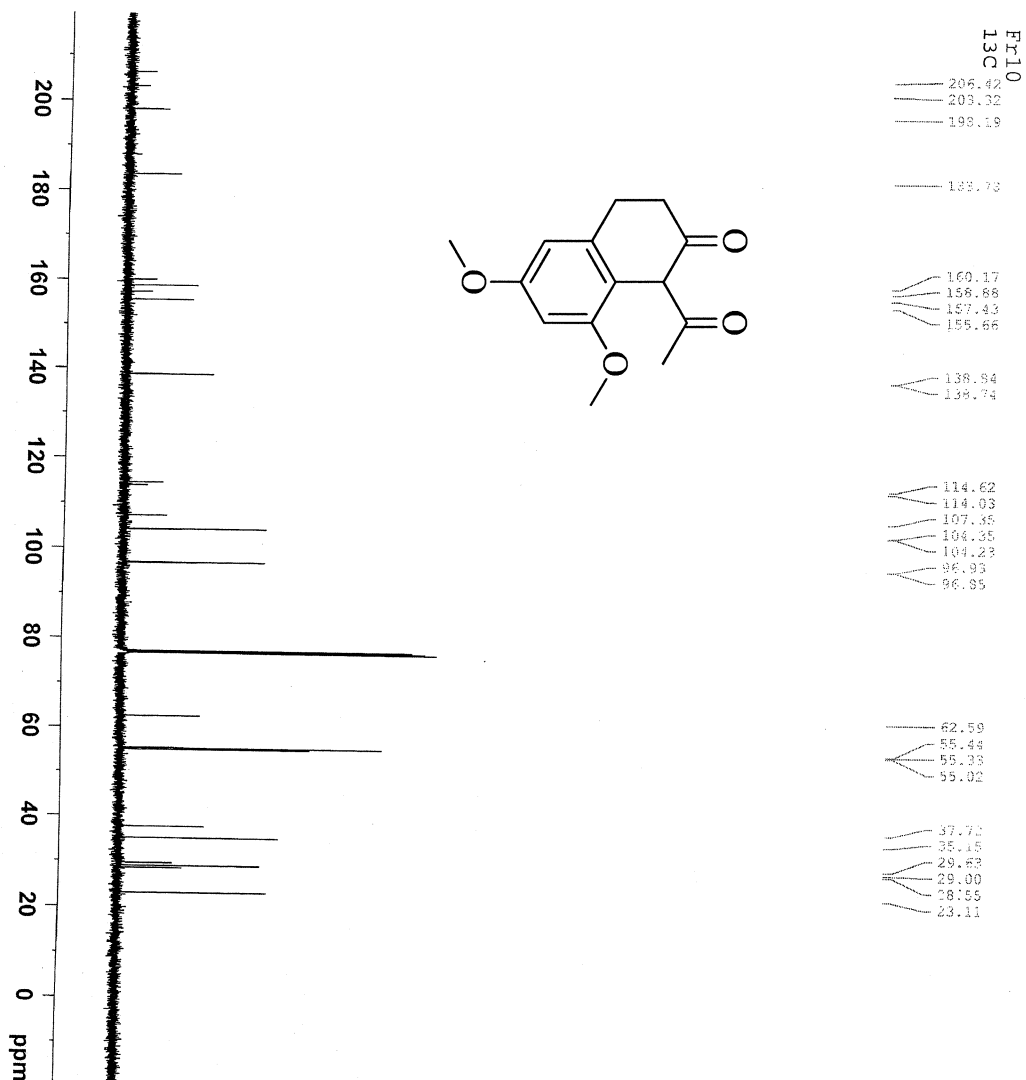






Current Data Parameters
 EXNO 4
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20091201
 Time 12:52:52
 INSTRUM spect
 PULPROG zgpg30
 TD 65536
 FIDRES 0.459222 Hz
 AQ 1.091440 sec
 SFO1 125.7703640 MHz
 D1 1.00000000 sec
 T2 1.00000000 sec
 T20 1.00000000 sec
 T200 1.00000000 sec
 ===== CHANNEL f1 =====
 NUC1 ¹³C
 P1 1.00 usec
 PL1 0.00 dB
 SFO1 125.7703640 MHz
 ===== CHANNEL f2 =====
 NUC2 ¹³C
 P2 1.00 usec
 PL2 0.00 dB
 SFO2 500.1321150 MHz
 F2 - Processing parameters
 SI 32768
 SF 500.132115 MHz
 WDM 1.00 Hz
 SSB 0
 GB 0
 PC 1.40





BRUKER

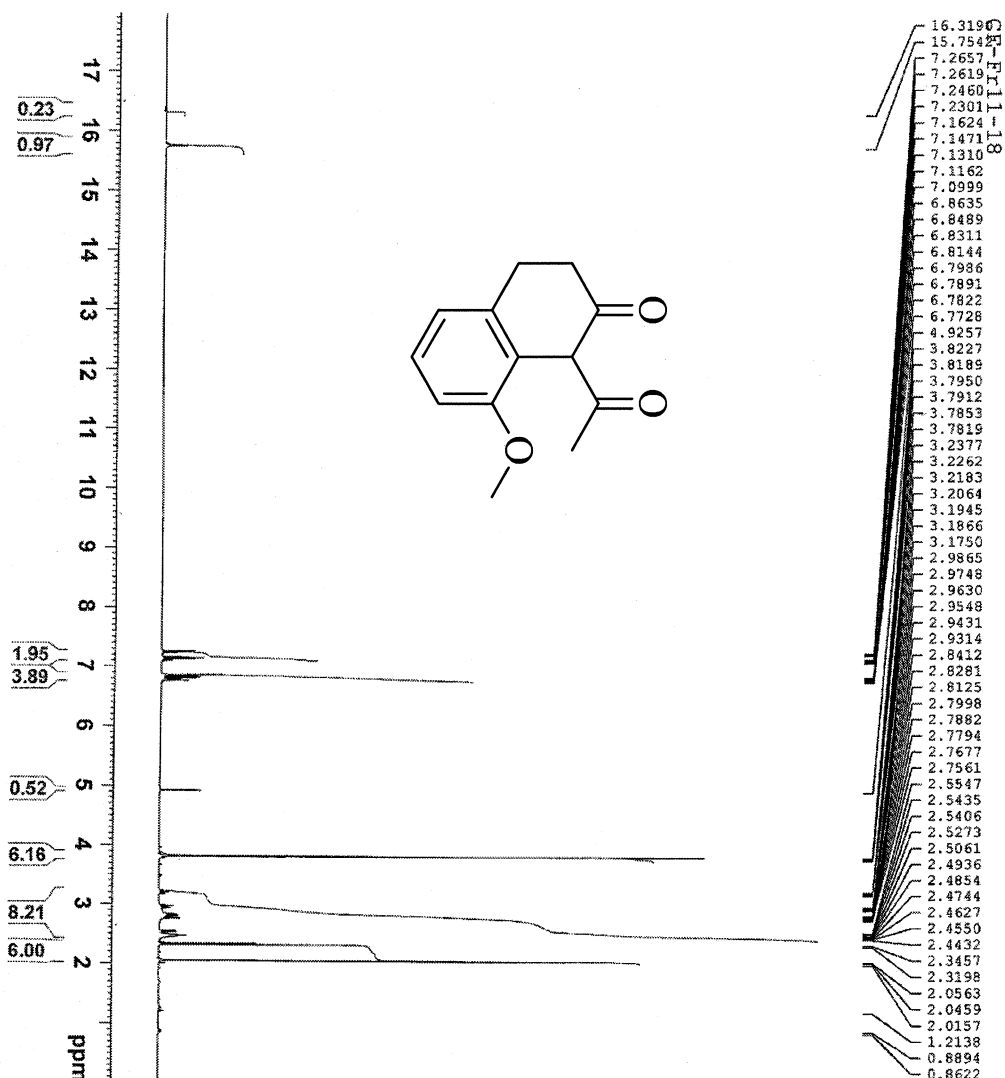
Current Data Parameters
NAME 6-DIMETHY-2,4-METHYLENE-CAN-MWOK-121710
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20101217
Time 18:20
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 4
DS 4
SWH 30063.422 MHz
FIDRES 0.045422 Hz
AQ 1.0912410 sec
RG 327.5
DWD 16.650 uSAC
DE 7.00 uSAC
TE 300.2 K
D1 1.00000000 sec
D11 0.01000000 sec
D12 1

===== CHANNEL F1 =====
NUC1 13C
P1 12.50
PL1 0.00
SFO1 125.761440 MHz

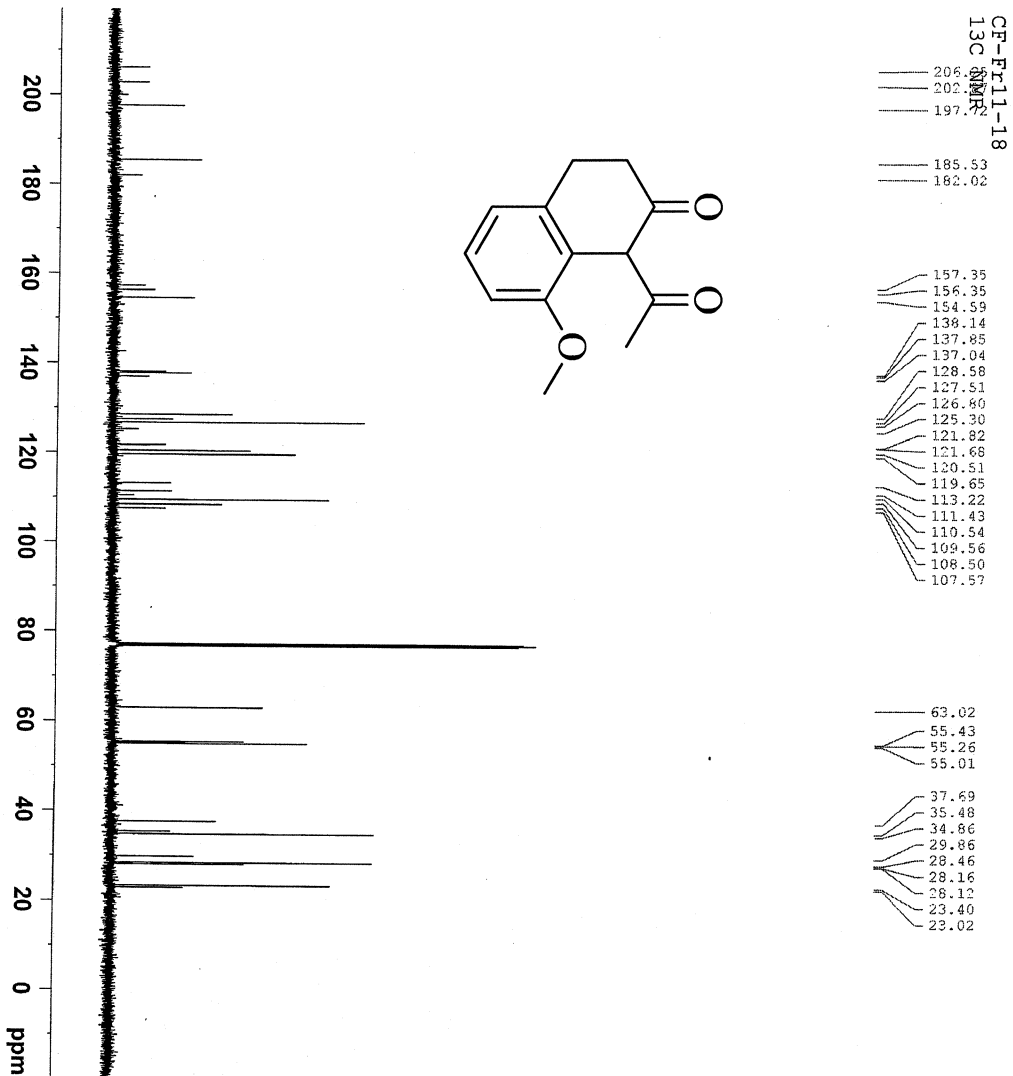
===== CHANNEL F2 =====
CPOBPR2 waltz16
NUC2 1H
PCPB2 100.00 uSAC
PULP2 zgpg30
RG 327.5
SFO2 500.132150 MHz

F1 - Processing parameters
SI 32768
WDW EM
SSB 0
GB 1.00 Hz
PC 1.40



Current Data Parameters
 Name: 1
 Date: 2013.12.14
 Time: 13.13.24
 Instrument: spect
 Processor: 5 mm BBO
 P1: 12.00
 P2: 12.00
 P3: 12.00
 P4: 12.00
 P5: 12.00
 P6: 12.00
 P7: 12.00
 P8: 12.00
 P9: 12.00
 P10: 12.00
 P11: 12.00
 P12: 12.00
 P13: 12.00
 P14: 12.00
 P15: 12.00
 P16: 12.00
 P17: 12.00
 P18: 12.00
 P19: 12.00
 P20: 12.00
 P21: 12.00
 P22: 12.00
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 P92: 12.00
 P93: 12.00
 P94: 12.00
 P95: 12.00
 P96: 12.00
 P97: 12.00
 P98: 12.00
 P99: 12.00
 P100: 12.00





Current Data Parameters
NAME 6-methoxy-2,4-hexadiene-ONE-MCHC-120109
EXPNO 1
PROCNO 1

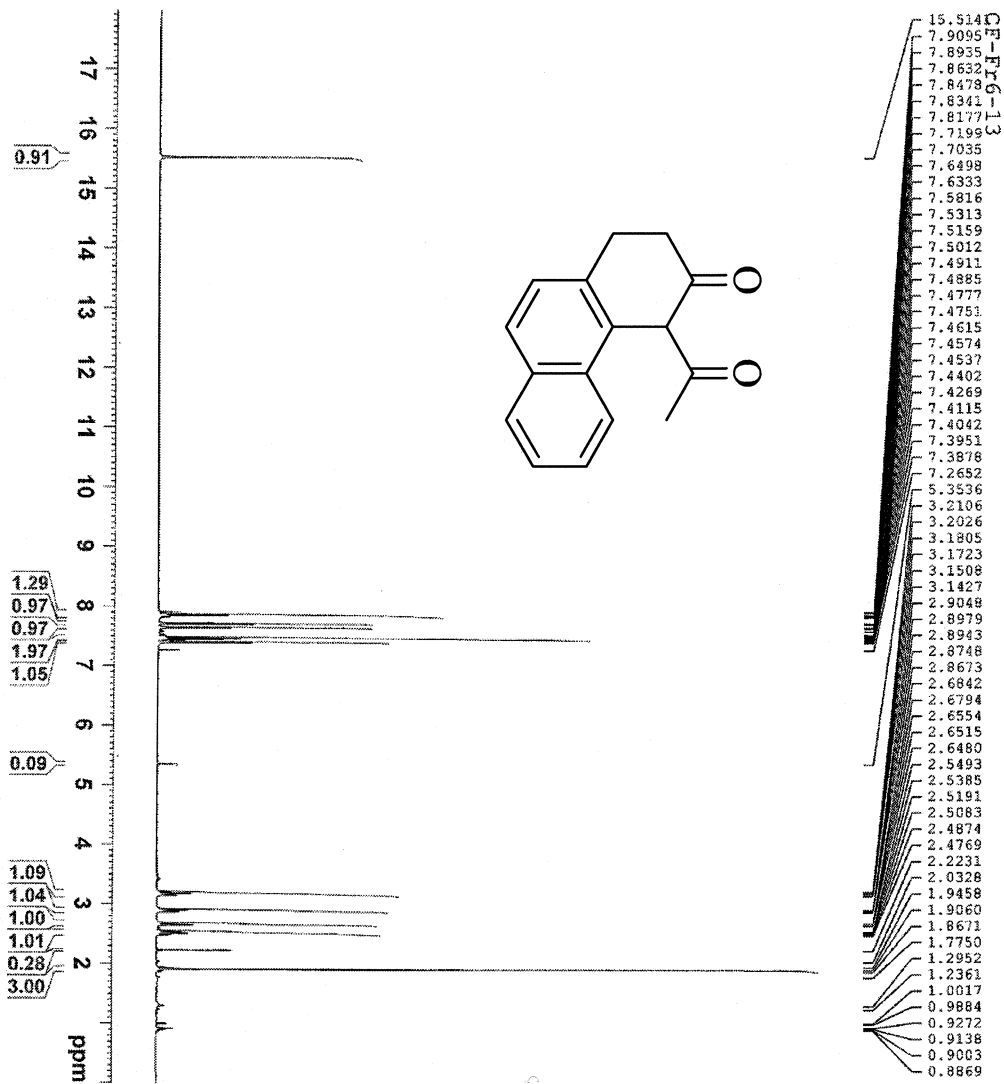
F2 - Acquisition Parameters
Date_ 20091203
Time_ 16:46
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 4
DS 4
SWH 30013.029 Hz
F2 300.13 MHz
AQ 1.0912410 sec
RG 16.496
DE 16.453 usec
TE 300.2 K
D1 1.0000000 sec
D11 0.0100000 sec
D10 1

===== CHANNEL f1 =====
NUC1 13C
P1 8.40 usec
PL1 1.00 dB
SFO1 125.770540 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 0.00 dB
PL12 17.50 dB
SFO2 500.132150 MHz

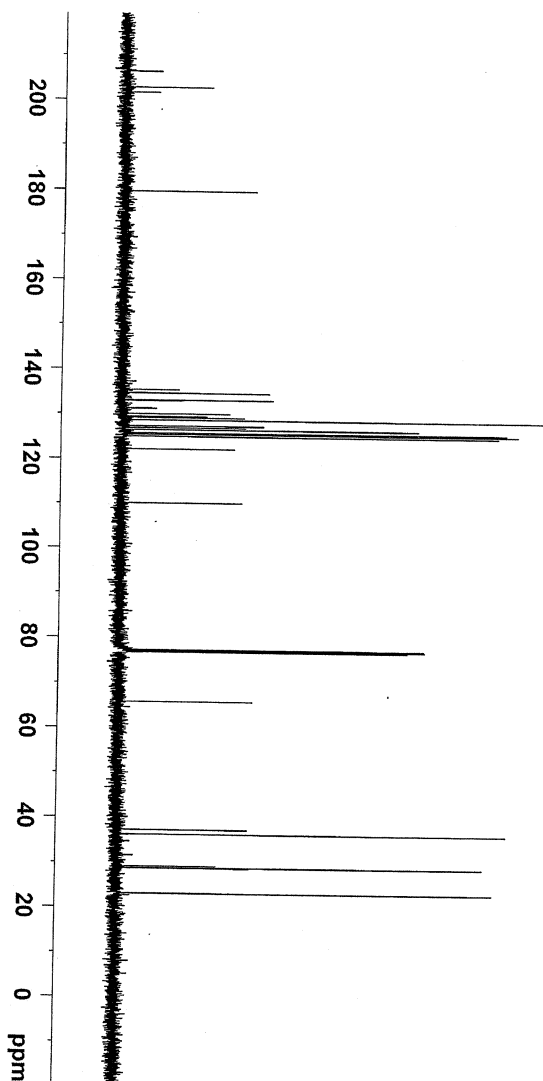
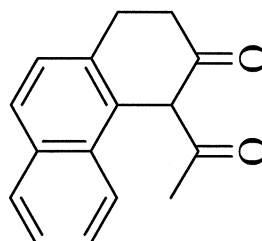
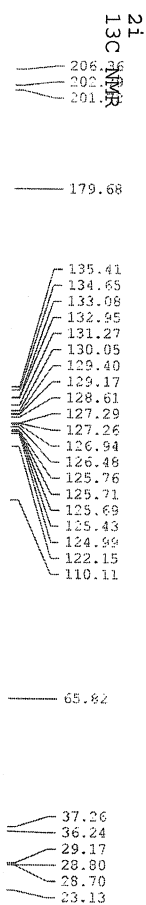
F2 - Processing parameters
SI 32768
SF 500.132150 MHz
SF2 125.757772 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.46





Current Data Parameters
 6-MHz 2,4-Hexanedione-CH2-NOCH3-11203
 F2 - Acquisition Parameters
 Date_ 20031120
 Time_ 15.43
 Instrument_ spect
 Processor_ 5 Hz CFI 1H/2
 P1/P2/PC 1/2/2
 F1/F2 499.9/124.999
 SOLVENT CDCl3
 NS 5
 DS 5
 SWH 892.806 Hz
 FIDRES 0.214419 Hz
 AQ 1.022813 sec
 NO 488.3
 DM 55.603 L/sec
 T2 286.7 K/sec
 T1 1.0000000 sec
 D1 1
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Current Data Parameters
NAME 6-Methyl-2,4-Heptanedione-CN-Mech-11209
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20091201
Time 9.09
INSTRUM spect
PROBHD 5 mm BBO BE-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 61
DS 4
SWH 30630.024 Hz
AQ 0.463222 sec
RG 1.0914440 sec
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00000000 sec
D1 0.01000000 sec
D11 100

===== CHANNEL f1 =====
NUC1 13C
P1 1.00
PL1 0.00 dB
SFO1 125.7703540 MHz

===== CHANNEL f2 =====
NAME2 1H
NUC2 1H
P2 100.00
PL2 0.00 dB
SFO2 500.1322150 MHz

F2 - Processing parameters
SI 32768
SF 500.1322150 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

