Cooperative Thiourea-Brønsted Acid Organocatalysis: Direct Enantioselective Cyanosilylation of Aldehydes with TMSCN

Zhiguo Zhang, Katharina M. Lippert, Heike Hausmann, Mike Kotke, and Peter R. Schreiner*

Institute of Organic Chemistry, Justus-Liebig University, Heinrich-Buff-Ring 58, 35392 Giessen, Germany; prs@org.chemie.uni-giessen.de, fax: +49-641-9934309

Supporting Information

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General Information

Materials. Unless otherwise noted, all materials were obtained from commercial suppliers and were used without further purification. Solvents for chromatography were of technical grade and were distilled prior to use. Solvents used in the reactions were reagent grade and were distilled from the indicated drying agents: toluene (P_2O_5), CH_2Cl_2 (P_2O_5), benzene (Na), diethyl ether (Na), MeCN (P_2O_5), 1,4-dioxane (Na), DMF (CaH_2), $CHCl_3$ (P_2O_5), THF (Na). For thin-layer chromatography (TLC), silica gel plates coated aluminum plates were used and chromatograms were visualized by irradiation with UV light at 254 nm. Column chromatography was performed using silica gel (70–230 mesh), or for flash chromatography using silica gel (particle size 230–400 mesh). Solvent mixtures are understood as volume/volume.

Instrumentation. All one-dimensional and two-dimensional NMR experiments were performed on a 400 MHz or 600 MHz NMR spectrometer equipped with a 5 mm probe at 295 K. The two-dimensional experiments were performed using apparatus standard pulse sequences and parameters. Proton and ^{13}C chemical shifts were referred to the solvent signal ($CDCl_3$) at 7.26 and 77 ppm, respectively. Data are presented as follows: chemical shift, integration, multiplicity (br = broad, s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, cm = complex multiplet) and coupling constant in Hertz (Hz). Infrared (IR) spectra were reported in terms of frequency of absorption (cm^{-1}), intensity of absorption (s = strong, m = medium, w = weak). Chiral gas chromatography (GC) analyses were performed with a Hydrodex-β-6-TBDM column or Chiraldex-γ-TA. Chiral high performance liquid chromatography (HPLC) analyses were performed on a Chirapak IA column. Optical rotations were measured using a 5 mL cell with a 1 dm path length on a digital polarimeter.

General Procedures. Unless otherwise noted, all reactions were performed in oven-dried Schlenk vials under an argon atmosphere. Plastic syringes with steel cannulae were used to transfer air- and moisture-sensitive liquids.

Computational Studies of the Binary Thiourea Catalyst/Benzoic Acid and Ternary Thiourea Catalyst/Benzoic Acid/Benzaldehyde Complexes

We computed various conformers of catalyst **4a** in combination with and without benzoic acid and in combination with benzoic acid and benzaldehyde to investigate the active catalysts system in solution. All computations were done with the Gaussian09 program suite. The M06 density functional theory method was used in conjunction with a 6–31G(d,p) basis set in the gas phase.[1] The computations were also performed with a self-consistent reaction field (SCRF) model to determine the solvent effects in benzene.[2] The bulk solvent was described with the United Atom topological model (UAHF) applied on radii optimized for the HF/6–31G(d) level of theory.[3] All given energies (ΔH_0) include ZPVE corrections.

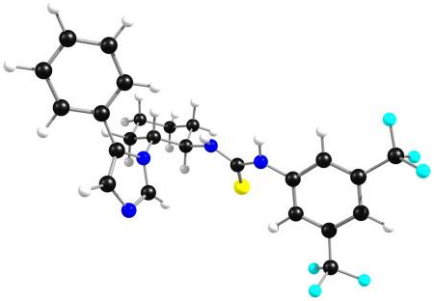
Table S1. Conformers of bifunctional catalyst **4a** in gas phase at M06/6–31G(d,p); the lowest lying conformer is highlighted in yellow. NIMAG = number of imaginary frequencies.

conformers	Energy (Hartree)	ZPVE (Hartree)	E+ZPVE (Hartree)	ΔH_0 (kcal/mol)	NIMAG	ΔG (Hartree)	ΔG_{298} (kcal/mol)
4a_1	–2143.1103560	0.4353720	–2142.6749840	2.4	0	–2142.742039	–1.5
4a_2	–2143.1099012	0.4372708	–2142.6726304	3.8	0	–2142.736698	1.8
4a_3	–2143.1162189	0.4374805	–2142.6787384	0	0	–2142.739638	0
4a_4	–2143.1150328	0.4368274	–2142.6782054	0.3	0	–2142.740890	–0.8
4a_5	–2143.1074719	0.4377691	–2142.6697028	5.7	0	–2142.730060	6.0
4a_6	–2143.1125895	0.4368873	–2142.6757022	1.9	0	–2142.738917	0.5

Table S2. Conformers of bifunctional catalyst **4a** in benzene at M06/6–31G(d,p)//PCM model//UAHF; the lowest lying conformers are highlighted in yellow. NIMAG = number of imaginary frequencies.

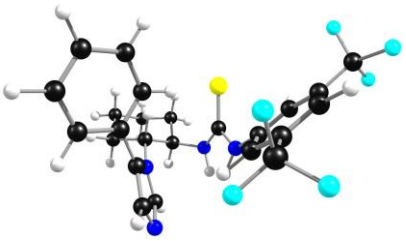
conformers	Energy (Hartree)	ZPVE (Hartree)	E+ZPVE (Hartree)	ΔH_0 (kcal/mol)	NIMAG	ΔG (Hartree)	ΔG_{298} (kcal/mol)
4a_1	–2143.1352057	0.4310907	–2142.7041150	0.7	0	–2142.771336	–3.5
4a_2	–2143.1327641	0.4326724	–2142.7000917	3.3	0	–2142.764774	0.7
4a_3	–2143.1392820	0.4339862	–2142.7052958	0	0	–2142.765834	0
4a_4	–2143.1379341	0.4318988	–2142.7060353	–0.5	0	–2142.769269	–2.2
4a_5	–2143.1317866	0.4324953	–2142.6992913	3.8	0	–2142.761239	2.9
4a_6	–2143.1343057	0.4328015	–2142.7015042	2.4	0	–2142.764561	0.8

4a_1



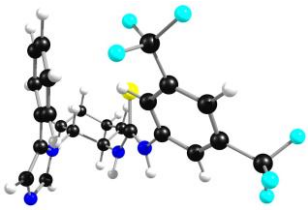
ΔH_0 = 2.4 (0.7), ΔG_{298} = –1.5 (–3.5)

4a_2



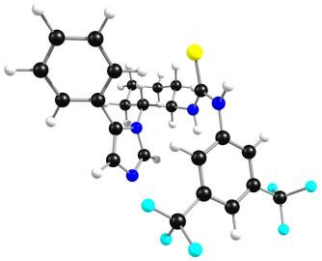
ΔH_0 = 3.8 (3.3), ΔG_{298} = 1.8 (0.7)
NH2···$N_{imidazole}$ d = 3.072 Å (3.462 Å)
H_{ortho}···$N_{imidazole}$ d = 3.582 Å (4.269 Å)

4a_3



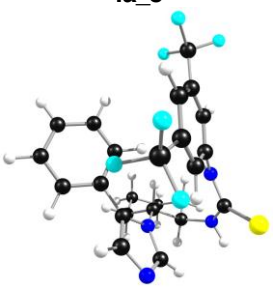
ΔH_0 = 0.0 (0.0), ΔG_{298} = 0.0 (0.0)

4a_4



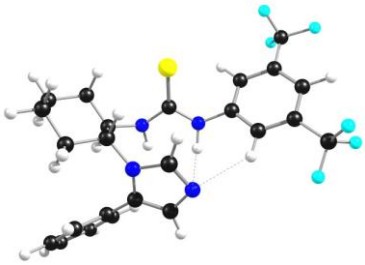
ΔH_0 = 0.3 (–0.5), ΔG_{298} = –0.8 (–2.2)
H_{ortho}···$N_{imidazole}$ d = 3.136 Å (3.251 Å)

4a_5



ΔH_0 = 5.7 (3.8), ΔG_{298} = 6.0 (2.9)
H_{ortho}···$N_{imidazole}$ d = 3.179 Å (3.411 Å)

4a_6



ΔH_0 = 1.9 (2.4), ΔG_{298} = 0.5 (0.8)
NH2···$N_{imidazole}$ d = 2.608 Å (2.851 Å)
H_{ortho}···$N_{imidazole}$ d = 2.627 Å (2.720 Å)

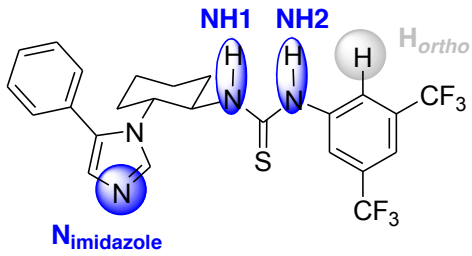


Figure S1. The conformers of catalyst **4a** at M06/6–31G(d,p)+SCRF(benzene).

Table S3. Bifunctional thiourea catalyst **4a** with benzoic acid (**9**) in gas phase at M06/6–31G(d,p); the lowest lying complex is highlighted in yellow.[a]

conformers	Energy (Hartree)	ZPVE (Hartree)	E+ZPVE (Hartree)	ΔH_0 (kcal/mol)	D_0 (kcal/mol)	ΔG (Hartree)	ΔG_{298} (kcal/mol)	D_{298} (kcal/mol)
4a·9_1	–2563.6963703	0.5542084	–2563.1421619	0	9.4	–2563.218377	0	–2.1
4a·9_2	–2563.7005042	0.5547423	–2563.1457619	–2.3	11.7	–2563.221154	–1.7	–0.4
4a·9_3	–2563.6999485	0.5546277	–2563.1453208	–2.0	11.4	–2563.214813	2.2	–4.4
4a·9_4[b]	–2563.6609162	0.5515961	–2563.1093201	20.6	–11.2	–2563.187621	19.3	–21.4
4a·9_5	–2563.6772312	0.5567864	–2563.1204448	13.6	–4.2	–2563.189400	18.2	–20.3
4a·9_6	–2563.7119245	0.5548971	–2563.1570274	–9.3	18.8	–2563.232039	–8.6	6.5
4a·9_7	–2563.7171927	0.5546508	–2563.1625419	–12.8	22.2	–2563.235463	–10.7	8.6
4a·9_8	–2563.7227274	0.5569867	–2563.1657407	–14.8	24.2	–2563.233249	–9.3	7.2

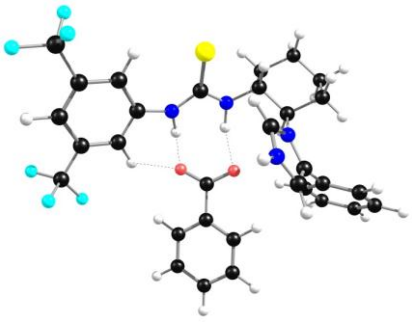
[a] If nothing is otherwise noted, all NIMAG (Number of imaginary frequencies) were zero. [b] The computation of complex **4a·9_4** contains a NIMAG = 1 at –9.97 cm^{-1} which is well within the expected numerical accuracy of the method.

Table S4. Bifunctional thiourea catalyst **4a** with benzoic acid (**9**) in benzene at M06/6–31G(d,p); the lowest lying complex is highlighted in yellow.[a]

conformers	Energy (Hartree)	ZPVE (Hartree)	E+ZPVE (Hartree)	ΔH_0 (kcal/mol)	D_0 (kcal/mol)	ΔG (Hartree)	ΔG_{298} (kcal/mol)	D_{298} (kcal/mol)
4a·9_1	–2563.7279290	0.5492317	–2563.1786973	0	8.3	–2563.254747	0	–3.7
4a·9_2	–2563.7252104	0.5493880	–2563.1758224	1.8	6.5	–2563.253471	0.8	–4.5
4a·9_3	–2563.7285536	0.5521300	–2563.1764236	1.4	6.9	–2563.245115	6.0	–9.8
4a·9_4	–2563.6609162	0.5515961	–2563.1451680	21.0	–12.7	–2563.219893	21.9	–25.6
4a·9_5	–2563.7097564	0.5519794	–2563.1577770	13.1	–4.8	–2563.227123	17.3	–21.1
4a·9_6	–2563.7327513	0.5494762	–2563.1832751	–2.9	11.2	–2563.257847	–1.9	–1.8
4a·9_7	–2563.7365711	0.5507977	–2563.1857734	–4.4	12.7	–2563.258193	–2.2	–1.6
4a·9_8	–2563.7456112	0.5520553	–2563.1935559	–9.3	17.6	–2563.261705	–4.4	0.6

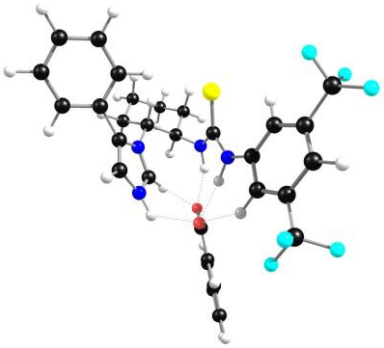
[a] If nothing is otherwise noted, all NIMAG (Number of imaginary frequencies) were zero.

4a·9_1



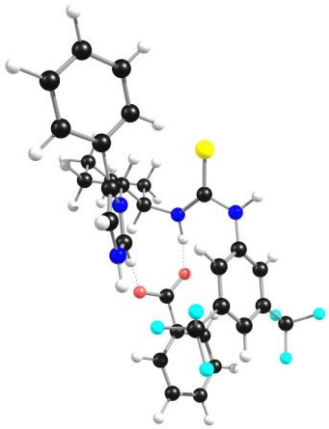
ΔH_0 = 0 (0), ΔG_{298} = 0 (0)
D_0 = 9.4 (8.3), D_{298} = –2.1 (–3.7)
NH1···O1 d = 1.812 Å (1.746 Å)
NH2···O2 d = 1.721 Å (1.751 Å)
H_{ortho}···O2 d = 2.264 Å (2.451 Å)

4a·9_2



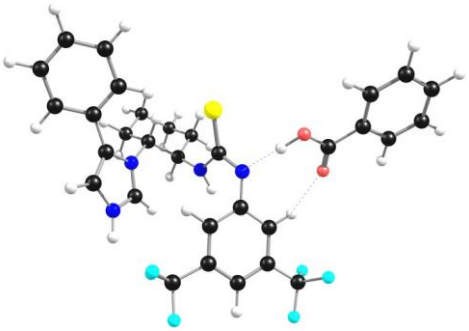
ΔH_0 = –2.3 (1.8), ΔG_{298} = –1.7 (0.8)
D_0 = 11.7 (6.5), D_{298} = –0.4 (–4.5)
NH1···O1 d = 1.875 Å (2.078 Å)
NH2···O2 d = 1.880 Å (1.794 Å)
H_{ortho}···O2 d = 2.348 Å (2.366 Å)
$NH_{imidazole}$···O2 d = 2.083 Å (2.807 Å)
$CH_{imidazole}$···O1 d = 1.964 Å (1.929 Å)

4a·9_3



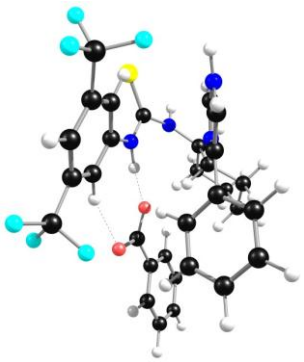
ΔH_0 = –2.0 (1.4), ΔG_{298} = 2.2 (6.0)
D_0 = 11.4 (6.9), D_{298} = –4.4 (–9.8)
NH1···O1 d = 1.625 Å (1.675 Å)
$CH_{imidazole}$···O2 d = 1.686 Å (1.795 Å)

4a·9_4

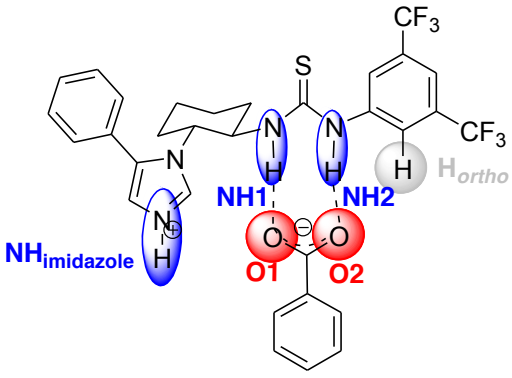


ΔH_0 = 20.6 (21.0), ΔG_{298} = 19.3 (21.9)
D_0 = –11.2 (–12.7), D_{298} = –21.4 (–25.6)
NH1···O1 d = 1.006 Å (1.017 Å)
H_{ortho}···O2 d = 2.136 Å (2.195 Å)
N···H2 d = 1.741 Å (1.685 Å)

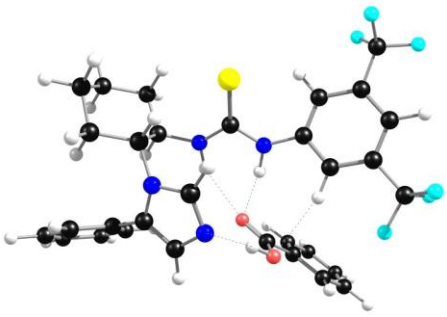
4a·9_5



ΔH_0 = 13.6 (13.1), ΔG_{298} = 18.2 (17.3)
D_0 = –4.2 (–4.8), D_{298} = –20.3 (–21.1)
NH2···O2 d = 1.721 Å (1.746 Å)
H_{ortho}···O1 d = 2.072 Å (2.112 Å)

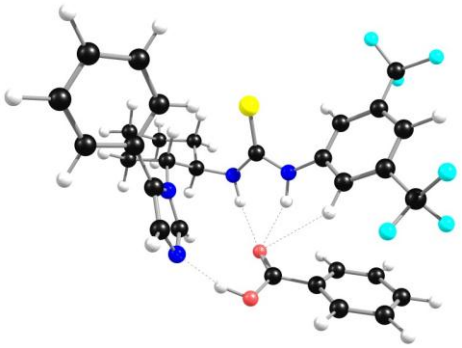


4a·9_6



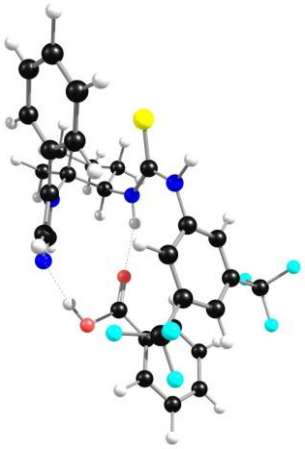
$\Delta H_0 = -9.3$ (–2.9), $\Delta G_{298} = -8.6$ (–1.9)
$D_0 = 18.8$ (11.2), $D_{298} = 6.5$ (–1.8)
NH1···O1 d = 2.324 Å (2.600 Å)
NH2···O1 d = 1.911 Å (1.897 Å)
H_{ortho}···O2 d = 2.411 Å (2.477 Å)
$N_{imidazole}$···OH2 d = 1.709 Å (1.721 Å)

4a·9_7



$\Delta H_0 = -12.8$ (–4.4), $\Delta G_{298} = -10.7$ (–2.2)
$D_0 = 22.2$ (12.7), $D_{298} = 8.6$ (–1.6)
NH1···O1 d = 2.111 Å (2.368 Å)
NH2···O1 d = 2.000 Å (2.052 Å)
H_{ortho}···O1 d = 3.379 Å (3.459 Å)
H_{ortho}···O2 d = 3.676 Å (3.481 Å)
$N_{imidazole}$···OH2 d = 1.725 Å (1.744 Å)

4a·9_8



$\Delta H_0 = -14.8$ (–9.3), $\Delta G_{298} = -9.3$ (–4.4)
$D_0 = 24.2$ (17.6), $D_{298} = 7.2$ (0.6)
NH1···O1 d = 2.021 Å (2.220 Å)
$N_{imidazole}$···OH2 d = 1.712 Å (1.746 Å)

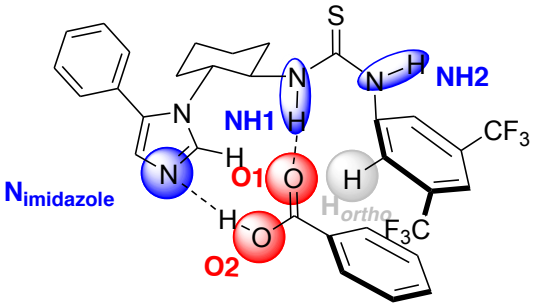


Figure S2. Complex of catalyst **4a** and benzoic acid (**9**) at M06/6–31G(d,p)+SCRF(benzene).

Table S5. Bifunctional thiourea catalyst **4a** with benzoic acid (**9**) and benzaldehyde (**7a**) in gas phase at M06/6–31G(d,p); the most stable complexes are highlighted in yellow.[a]

conformers	Energy (Hartree)	ZPVE (Hartree)	E+ZPVE (Hartree)	ΔH_0 (kcal/mol)	D_0 (kcal/mol)	ΔG (Hartree)	ΔG_{298} (kcal/mol)	D_{298} (kcal/mol)
4a·9·7a_1	–2909.0670070	0.6673356	–2908.3996714	5.4	29.8	–2908.480720	5.0	2.1
4a·9·7a_2	–2909.0722349	0.6696050	–2908.4026299	3.6	31.7	–2908.480270	5.3	1.9
4a·9·7a_3	–2909.0656882	0.6677342	–2908.3979540	6.5	28.7	–2908.477142	7.3	–0.1
4a·9·7a_4	–2909.0601554	0.6667860	–2908.3933694	9.4	25.8	–2908.475882	8.1	–0.9
4a·9·7a_5	–2909.0679273	0.6698420	–2908.3980853	6.4	28.8	–2908.474521	8.9	–1.7
4a·9·7a_6	–2909.0698862	0.6687103	–2908.4011759	4.5	30.7	–2908.478951	6.1	1.0
4a·9·7a_7	–2909.0757388	0.6674144	–2908.4083244	0.0	35.2	–2908.488721	0.0	7.2
4a·9·7a_8	–2909.0784090	0.6701793	–2908.4082297	0.1	35.2	–2908.485444	2.1	5.1
4a·9·7a_9	–2909.0817702	0.6701566	–2908.4116136	–2.1	37.3	–2908.485534	2.0	5.2
4a·9·7a_10	–2909.0487842	0.6671358	–2908.3816484	16.7	18.5	–2908.464606	15.1	–8.0

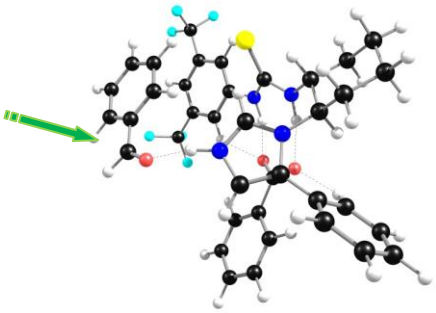
[a] If nothing is otherwise noted, all NIMAG (Number of imaginary frequencies) were zero.

Table S6. Bifunctional thiourea catalyst **4a** with benzoic acid (**9**) and benzaldehyde (**7a**) in benzene at M06/6–31G(d,p); the most stable complexes are highlighted in yellow.[a]

conformers	Energy (Hartree)	ZPVE (Hartree)	E+ZPVE (Hartree)	ΔH_0 (kcal/mol)	D_0 (kcal/mol)	ΔG (Hartree)	ΔG_{298} (kcal/mol)	D_{298} (kcal/mol)
4a·9·7a_1	–2909.0914623	0.6624849	–2908.4289774	4.4	20.6	–2908.510870	0.9	–6.9
4a·9·7a_2	–2909.0967911	0.6639125	–2908.4328786	1.9	23.0	–2908.512020	0.2	–6.2
4a·9·7a_3	–2909.0904675	0.6638616	–2908.4266059	5.9	19.1	–2908.506336	3.8	–9.7
4a·9·7a_4	–2909.0849569	0.6636903	–2908.4212666	9.2	15.7	–2908.501166	7.0	–13.0
4a·9·7a_5	–2909.0916770	0.6655064	–2908.4261706	6.2	18.8	–2908.503636	5.5	–11.4
4a·9·7a_6	–2909.0920081	0.6638249	–2908.4281832	4.9	20.1	–2908.507007	3.3	–9.3
4a·9·7a_7	–2909.1007157	0.6647361	–2908.4359796	0.0	25.0	–2908.512329	0.0	–6.0
4a·9·7a_8	–2909.1010144	0.6660475	–2908.4349669	0.6	24.3	–2908.509484	1.8	–7.8
4a·9·7a_9	–2909.0908253	0.6634723	–2908.4273530	5.4	19.5	–2908.502796	6.0	–12.0
4a·9·7a_10	–2909.0785386	0.6625289	–2908.4160097	12.5	12.4	–2908.498931	8.4	–14.4

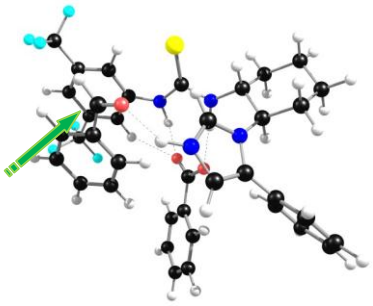
[a] If nothing is otherwise noted, all NIMAG (Number of imaginary frequencies) were zero.

4a·9·7a_1



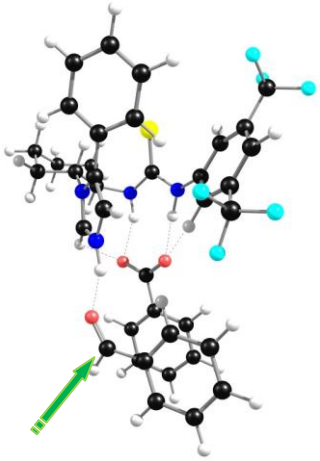
ΔH_0 = 5.4 (4.4), ΔG_{298} = 5.0 (0.9)
D_0 = 29.8 (20.6), D_{298} = 2.1 (–6.9)
NH1···O1 d = 1.871 Å (1.934 Å)
NH2···O2 d = 1.669 Å (1.700 Å)
H_{ortho}···O2 d = 2.246 Å (2.281 Å)
$NH_{imidazole}$···O3=C d = 1.736 Å (1.767 Å)
CH_{phenyl}···O1 d = 2.223 Å (2.375 Å)

4a·9·7a_2



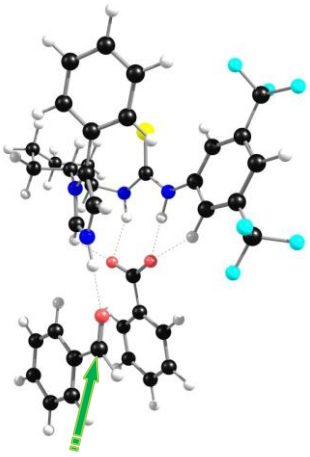
ΔH_0 = 3.6 (1.9), ΔG_{298} = 5.3 (0.2)
D_0 = 31.7 (23.0), D_{298} = 1.9 (–6.2)
NH1···O1 d = 1.776 Å (1.904 Å)
NH2···O2 d = 1.756 Å (1.775 Å)
H_{ortho}···O2 d = 2.322 Å (2.289 Å)
$NH_{imidazole}$···O3=C d = 1.824 Å (1.977 Å)

4a·9·7a_3



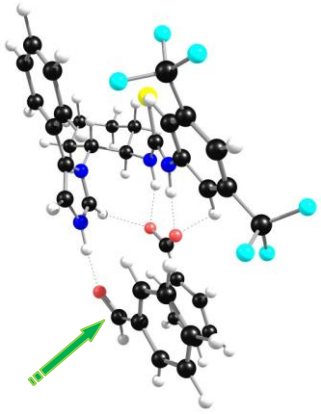
ΔH_0 = 6.5 (5.9), ΔG_{298} = 7.3 (3.8)
D_0 = 28.7 (19.1), D_{298} = –0.1 (–9.7)
NH1···O1 d = 1.870 Å (1.943 Å)
NH2···O2 d = 1.768 Å (1.776 Å)
H_{ortho}···O2 d = 2.323 Å (2.292 Å)
$NH_{imidazole}$···O3=C d = 1.767 Å (1.781 Å)
$CH_{imidazole}$···O1 d = 2.177 Å (2.239 Å)

4a·9·7a_4



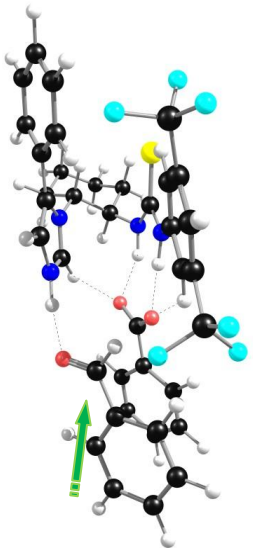
ΔH_0 = 9.4 (9.2), ΔG_{298} = 8.1 (7.0)
D_0 = 25.8 (15.7), D_{298} = –0.9 (–13.0)
NH1···O1 d = 1.950 Å (1.996 Å)
NH2···O2 d = 1.747 Å (1.769 Å)
H_{ortho}···O2 d = 2.272 Å (2.369 Å)
$NH_{imidazole}$···O3=C d = 1.758 Å (1.762 Å)
$CH_{imidazole}$···O2 d = 2.094 Å (2.155 Å)

4a·9·7a_5



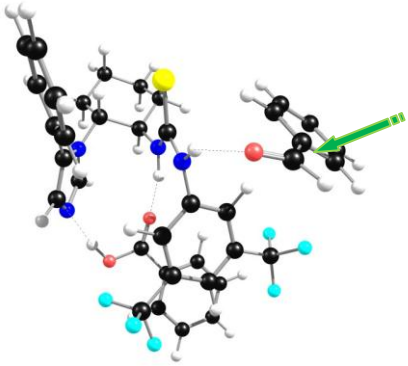
ΔH_0 = 6.4 (6.2), ΔG_{298} = 8.9 (5.5)
D_0 = 28.8 (18.8), D_{298} = –1.7 (–11.4)
NH1···O1 d = 1.893 Å (2.002 Å)
NH2···O2 d = 1.695 Å (1.726 Å)
H_{ortho}···O1 d = 2.474 Å (2.480 Å)
$NH_{imidazole}$···O3=C d = 1.710 Å (1.732 Å)
$CH_{imidazole}$···O1 d = 2.061 Å (2.131 Å)

4a·9·7a_6



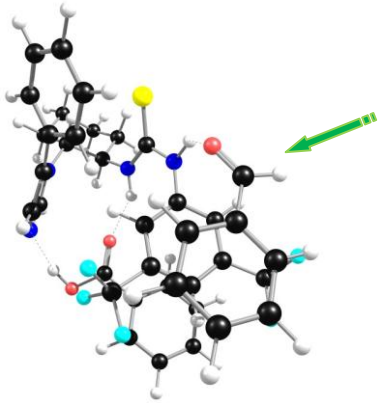
ΔH_0 = 4.5 (4.9), ΔG_{298} = 6.1 (3.3)
D_0 = 30.7 (20.1), D_{298} = 1.0 (–9.3)
NH1···O1 d = 1.866 Å (1.935 Å)
$CH_{imidazole}$···O1 d = 1.972 Å (2.041 Å)
NH2···O2 d = 1.777 Å (1.803 Å)
H_{ortho}···O2 d = 2.366 Å (2.330 Å)
$NH_{imidazole}$···O3=C d = 1.674 Å (1.713 Å)
N-$H_{imidazole}$ d = 1.046 Å (1.042 Å)

4a·9·7a_7



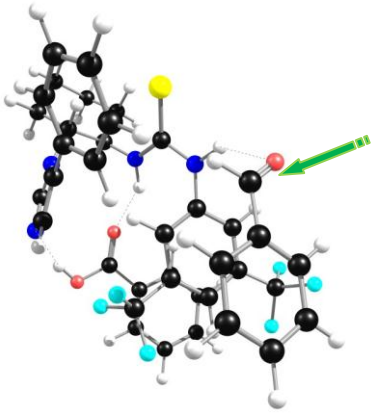
ΔH_0 = 0 (0), ΔG_{298} = 0 (0)
D_0 = 35.2 (25.0), D_{298} = 7.2 (–6.0)
NH1···O1 d = 2.044 Å (2.420 Å)
NH2···O3=C d = 2.080 Å (2.167 Å)
$N_{imidazole}$···HO2 d = 1.708 Å (1.743 Å)
H_{ortho}···Phenyl-Ring = 2.626 Å (2.585 Å)

4a·9·7a_8



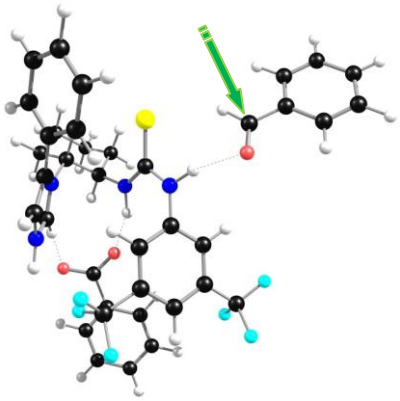
ΔH_0 = 0.1 (0.6), ΔG_{298} = 2.1 (1.8)
D_0 = 35.2 (24.3), D_{298} = 5.1 (–7.8)
NH1···O1 d = 1.953 Å (2.104 Å)
NH2···O3=C d = 2.315 Å (2.396 Å)
$N_{imidazole}$···HO2 d = 1.794 Å (1.812 Å)

4a·9·7a_9



$\Delta H_0 = -2.1$ (5.4), $\Delta G_{298} = 2.0$ (6.0)
$D_0 = 37.3$ (19.5), $D_{298} = 5.2$ (–12.0)
NH1···O1 d = 1.954 Å (2.067 Å)
NH2···O3=C d = 2.128 Å (2.172 Å)
N-$H_{imidazole}$ d = 1.812 Å (1.071 Å)
$NH_{imidazole}$···O2 d = 0.997 Å (1.591 Å)

4a·9·7a_10



$\Delta H_0 = 16.7$ (12.5), $\Delta G_{298} = 15.1$ (8.4)
$D_0 = 18.5$ (12.4), $D_{298} = -8.0$ (–14.4)
NH1···O1 d = 1.749 Å (1.795 Å)
NH2···O3=C d = 1.902 Å (1.899 Å)
$CH_{imidazole}$···O2 d = 1.723 Å (1.784 Å)

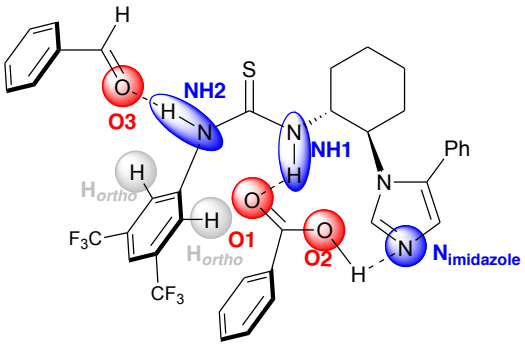


Figure S3. Complex of catalyst **4a**, benzoic acid **9**, and benzaldehyde **7a** at M06/6–31G(d,p)+SCRF(benzene)

NMR Studies of the Binary Bifunctional Thiourea Catalyst/Benzoic Acid Complex

In the phase-sensitive ^{1}H NOESY spectrum in [d_6]-benzene (Figure S4) all cross signals have the same sign as the diagonal signals, negative NOEs are observed indicating slowly tumbling molecules. Since the NOE effect changes its sign depending on the molecular correlation time we used 2D NMR ROESY experiments to identify possible intermolecular NOE's between **4a** and **11** because ROESY cross peaks have opposite phase to the diagonal signals regardless of molecular tumbling rates. As a result, the ROESY spectrum turned out to be complicated by overlapping of the solvent signal and its cross-peaks with relevant cross-peaks of the complex.

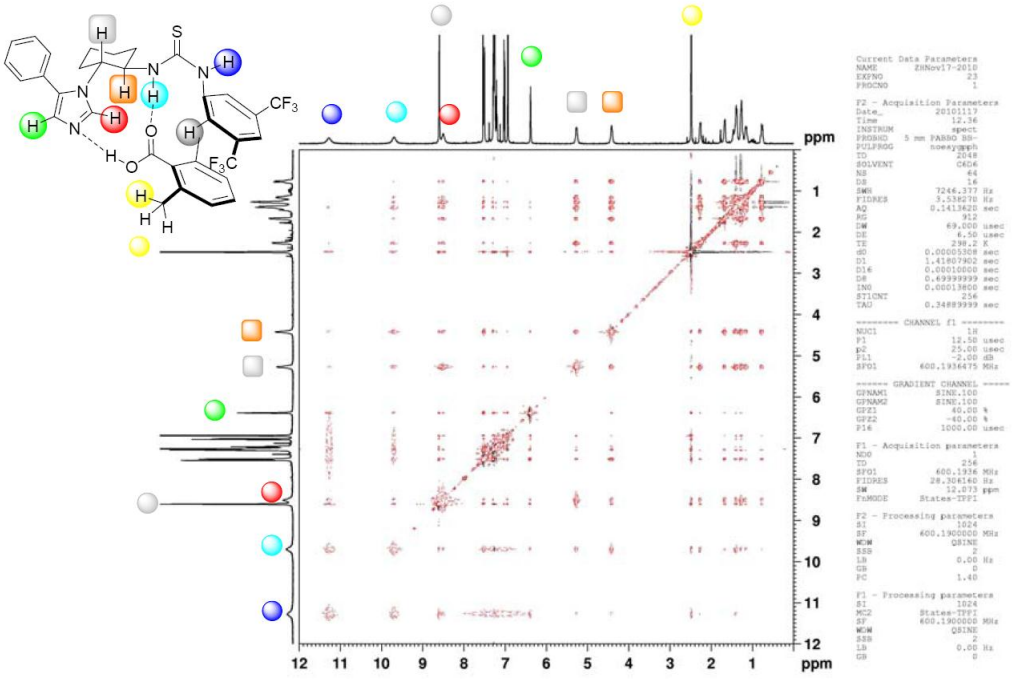


Figure S4. NOESY (600 MHz, 298.2 K) spectrum of a 1:1 mixture of **4a** (0.01 mmol) and **11** (0.01 mmol) in [d_6]-benzene.

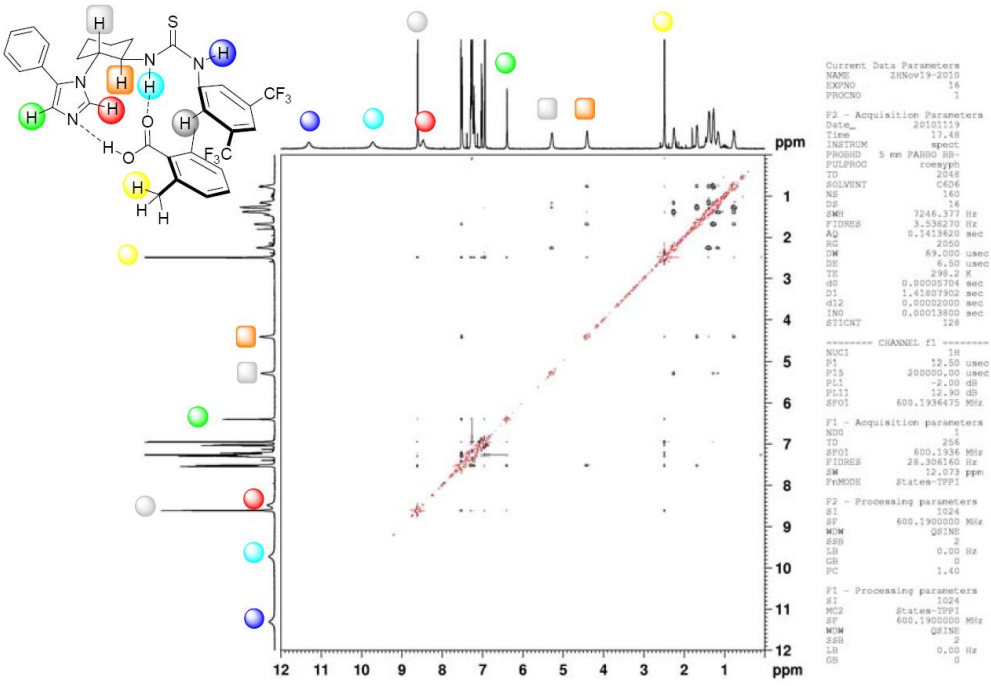


Figure S5. ^{1}H 2D ROESY spectrum of **4a** and **11** (1:1 mixture of **4a** (0.01 mmol) and **11** (0.01 mmol) in [d_6]-benzene).

The ^{1}H NMR concentration study in benzene at 25 °C supported the formation of the hydrogen-bonded complex **4a·11** (Figure S6 and relevant chemical shifts see Table S7).

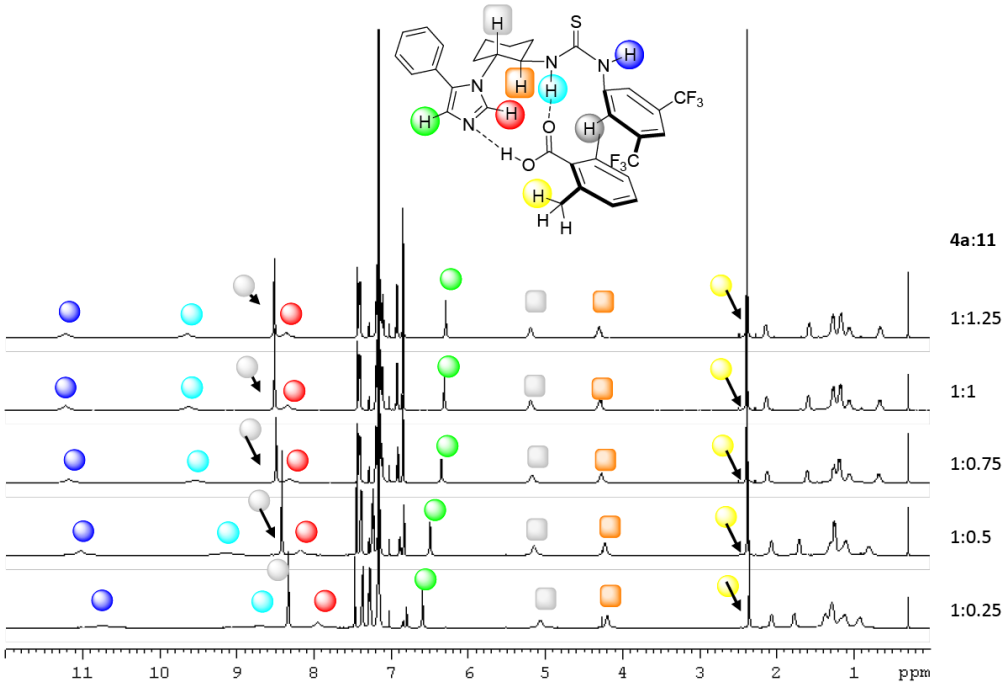


Figure S6. ^{1}H NMR spectra (600 MHz, 298.2 K) of **4a** with increasing concentration of **11**.

Table S7. Chemical shifts of ^{1}H NMR spectra of increasing concentration of **11**.

Stoichiometry **4a**:**11**	Proton species and shift (ppm)				
	NH2	NH1	*ortho*-H	$CH_{imidazole}$	$CH_{imidazole}$
4a:**11** 1:1.25	11.230	9.650	8.517	8.370	6.294
4a:**11** 1:1	11.227	9.627	8.514	8.347	6.343
4a:**11** 1:0.75	11.181	9.534	8.493	8.321	6.350
4a:**11** 1:0.5	11.029	9.140	8.419	8.177	6.497
4a:**11** 1:0.25	10.745	8.708	8.335	7.956	6.595

Parallel to the experimental NOE investigations we analyzed theoretically the lowest lying conformer (Figure S7) in gas phase (Table S8) and in benzene (Table S9).

Table S8. Bifunctional thiourea catalyst **4a** with **11** in the gas phase at M06/6–31G(d,p); the most stable complexes are highlighted in yellow.[a]

conformers	Energy (Hartree)	ZPVE (Hartree)	E+ZPVE (Hartree)	ΔH_0 (kcal/mol)	D_0 (kcal/mol)	ΔG (Hartree)	ΔG_{298} (kcal/mol)	D_{298} (kcal/mol)
4a·11_1	–2642.2707702	0.6110836	–2641.6596866	12.2	12.2	–2641.735807	7.9	–0.5
4a·11_2	–2642.2825266	0.6109888	–2641.6715378	4.8	19.6	–2641.747729	0.4	7.0
4a·11_3	–2642.2883193	0.6114352	–2641.6768841	1.4	22.9	–2641.751893	–2.2	9.6
4a·11_4	–2642.2937263	0.6145376	–2641.6791887	0.0	24.4	–2641.748345	0	7.4

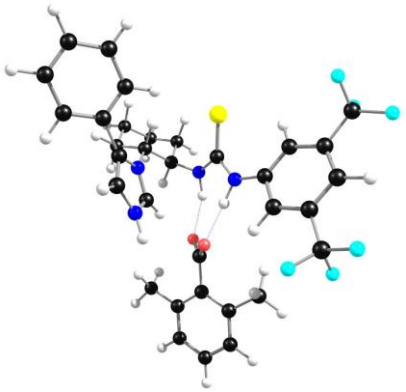
[a] If nothing is otherwise mentioned, all NIMAG (Number of imaginary frequencies) were zero.

Table S9. Bifunctional thiourea catalyst **4a** with **11** in benzene at M06/6–31G(d,p); the most stable complex is highlighted in yellow.[a]

conformers	Energy (Hartree)	ZPVE (Hartree)	E+ZPVE (Hartree)	ΔH_0 (kcal/mol)	D_0 (kcal/mol)	ΔG (Hartree)	ΔG_{298} (kcal/mol)	D_{298} (kcal/mol)
4a·11_1	–2642.2957912	0.6059360	–2641.6898552	8.2	7.3	–2641.767810	3.4	–5.8
4a·11_2	–2642.3036112	0.6064387	–2641.6971725	3.6	11.9	–2641.771897	0.9	–3.3
4a·11_3	–2642.3060009	0.6061204	–2641.6998805	1.9	13.6	–2641.774851	–1.0	–1.4
4a·11_4	–2642.3132987	0.6104022	–2641.7028965	0.0	15.5	–2641.773306	0.0	–2.4

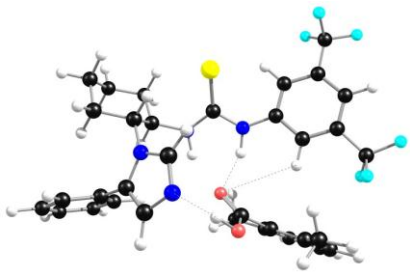
[a] If nothing is otherwise mentioned, all NIMAG (Number of imaginary frequencies) were zero.

4a·11_1



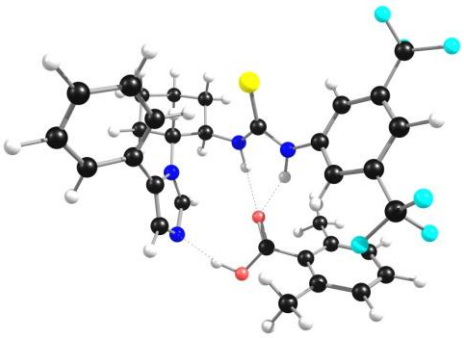
ΔH_0 = 12.2 (8.2), ΔG_{298} = 7.9 (3.4)
D_0 = 12.2 (7.3), D_{298} = –0.5 (–5.8)
NH1···O1 d = 1.877 Å (1.952 Å)
NH2···O2 d = 1.863 Å (1.826 Å)
H_{ortho}···O2 d = 2.299 Å (2.315 Å)
$NH_{imidazole}$···O2 d = 2.076 Å (2.536 Å)
$CH_{imidazole}$···O1 d = 1.993 Å (2.044 Å)

4a·11_2



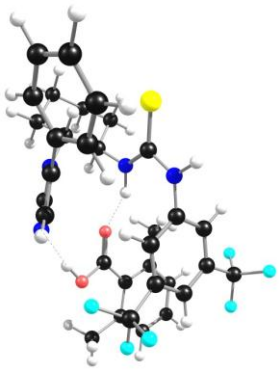
ΔH_0 = 4.8 (3.6), ΔG_{298} = 0.4 (0.9)
D_0 = 19.6 (11.9), D_{298} = 7.0 (–3.3)
NH1···O1 d = 2.170 Å (2.557 Å)
NH2···O1 d = 1.946 Å (1.956 Å)
H_{ortho}···O1 d = 3.141 Å (2.780 Å)
$N_{imidazole}$···HO2 d = 1.733 Å (1.713 Å)
H_{ortho}···CH_3 d = 2.910 Å (3.048 Å)

4a·11_3



ΔH_0 = 1.4 (1.9), ΔG_{298} = –2.2 (–1.0)
D_0 = 22.9 (13.6), D_{298} = 9.6 (–1.4)
NH1···O1 d = 2.019 Å (2.554 Å)
NH2···O1 d = 1.976 Å (1.862 Å)
$N_{imidazole}$···HO2 d = 1.762 Å (1.774 Å)

4a·11_4



ΔH_0 = 0 (0), ΔG_{298} = 0 (0)
D_0 = 24.4 (15.5), D_{298} = 7.4 (–2.4)
NH1···O1 d = 1.989 Å (2.084 Å)
$N_{imidazole}$···HO2 d = 1.818 Å (1.784 Å)

Figure S7. Complex of catalyst **4a** and **11** at M06/6–31G(d,p)+SCRF(benzene).

In a comparable experiment to our hydrogen-bonded complex the ^{1}H NMR spectrum of **11** and *N*-methylimidazole (1:1 mixture, Figure S8) in [d_6]-benzene confirms the hydrogen-bonded complex of **4a** and **11** with protonated **11** due integration of the signals; the existence of the benzoic acid proton in solution implies no deprotonation of **11**.

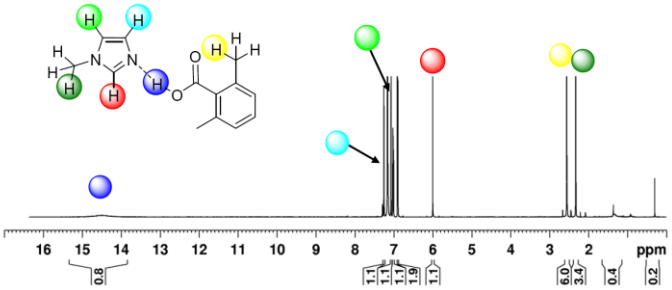


Figure S8. ^{1}H NMR spectrum (600 MHz, 298.2 K) of a 1:1 mixture of **11** (0.02 mmol) and *N*-methylimidazole (0.02 mmol) in [d_6]-benzene.

The cross-peaks of the NOESY spectrum in CD_2Cl_2 have the same sign as the cross-peaks of the diagonal (Figure S9). Due the sensibility of the NOESY measurement here only the NOE-effects for the benzoic acid proton are detected (Figure S10). No NOE-effect was detected for the benzoic acid proton due the ROESY measurement. The section of the NOESY spectrum in Figure S10 shows the NOE-effect of the acid proton with both NH-signals (dark and light blue), both methin-proton-signals (red and light green) of the imidazole-ring, phenyl-protons of the **11**, to a methin-proton (orange) of the cyclohexane-ring, and the methyl-group of the benzoic acid (yellow). The NOE-effects for the 2,6-dimethylbenzoic acid proton are summarized in Figure S10.

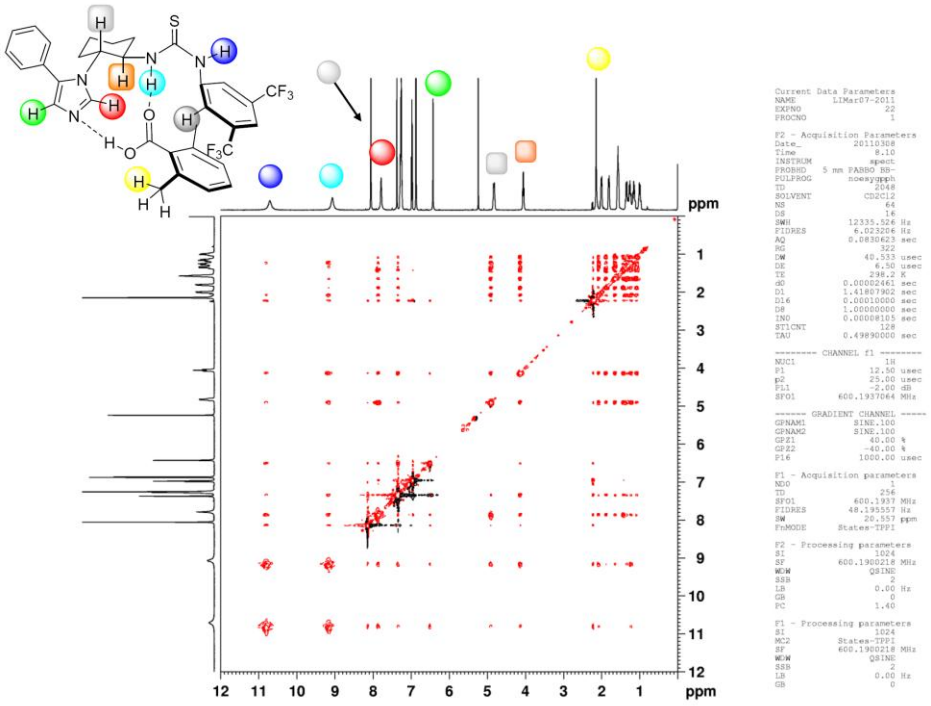


Figure S9. NOESY (600 MHz, 298.2 K) spectrum of a 1:1 mixture of **4a** (0.01 mmol) and **11** (0.01 mmol) in CD_2Cl_2.

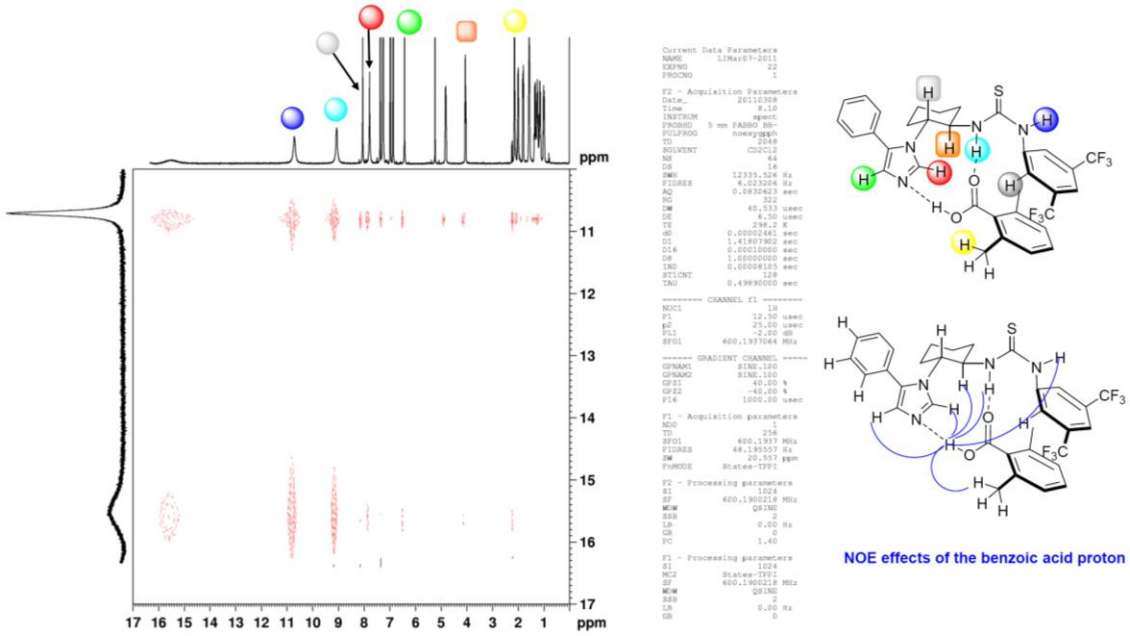


Figure S10. Section of NOESY (600 MHz, 298.2 K) spectrum of a 1:1 mixture of **4a** (0.01 mmol) and **11** (0.01 mmol) in CD_2Cl_2.

Since the NOE effect changes its sign depending on the molecular correlation time we used the 2D NMR ROESY experiment to identify possible intermolecular NOE's between the **4a** and **11** because ROESY crosspeaks have opposite phase to the diagonal signals regardless of molecular tumbling rates (Figure S11).

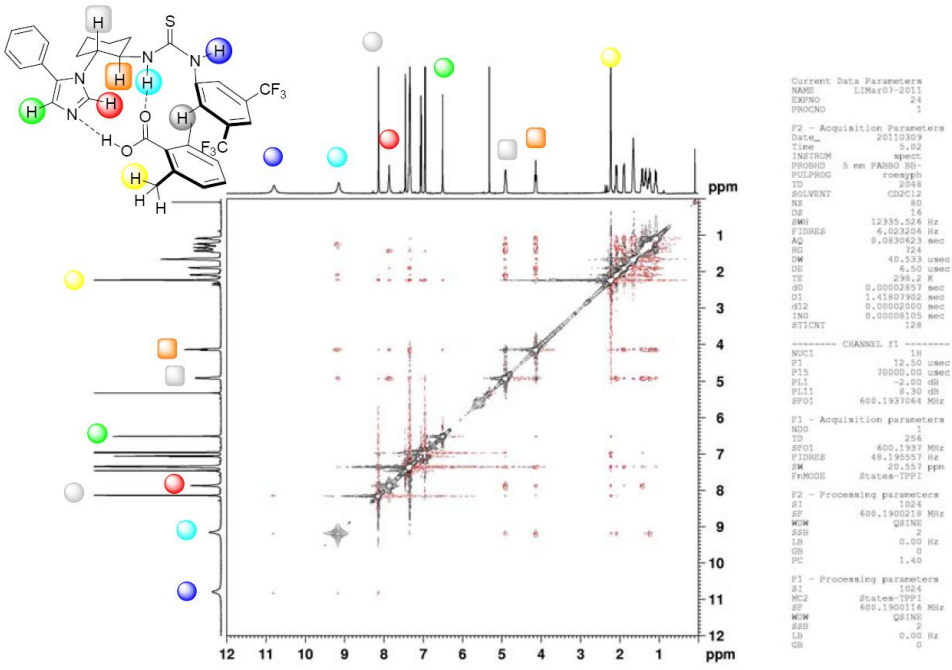


Figure S11. ^{1}H 2D ROESY spectrum of **4a** and **11** (1:1 mixture of **4a** (0.01 mmol) and **11** (0.01 mmol) in CD_2Cl_2).

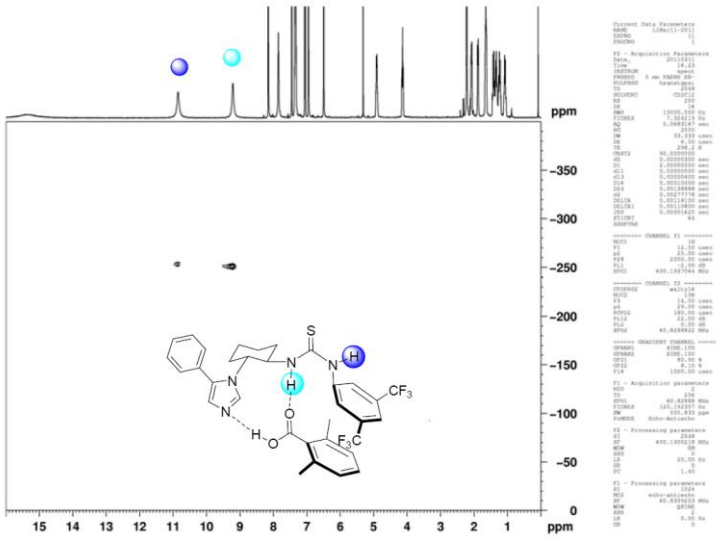


Figure S12. ^{1}H, ^{15}N-HSQC spectrum of **4a** and **11** (1:1 mixture of **4a** (0.01 mmol) and **11** (0.01 mmol) in CD_2Cl_2) showing the NH-signals, especially the one arising from the interaction **11**.

Further support for the confirmation of a hydrogen-bonded complex of **4a** and **11** through hydrogen-bonding of the NH-proton to the C=O-group and a hydrogen-bond of protonated **11** to the nitrogen of the imidazole ring we also measured a ^{1}H NMR spectrum of an excess of **11** with *N*-methylimidazole (10:1 mixture) in CD_2Cl_2 (Figure S13). The integration of the signals implies that **11** is not deprotonated.

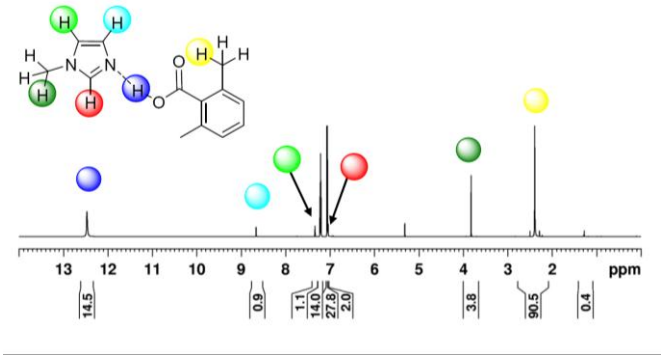


Figure S13. ^{1}H NMR spectrum (600 MHz, 298.2 K) of a 10:1 mixture **11** (0.2 mmol) and *N*-methylimidazole (0.02 mmol) in CD_2Cl_2.

A NOESY spectrum (Figure S14) was measured to underline our results that the proton of **11** shows NOE-effects to two of the methin-protons (light blue and light green) and to the methyl-protons (dark green) of *N*-methylimidazole. The red methin proton is overlapped by the phenyl protons of **11**. Additionally the methyl-group (yellow) of **11** shows crosspeaks to two methin protons (light blue and light green) of the imidazole-ring. A ^{1}H, ^{15}N HSQC measurement showed no signals for NH-

protons. Even after addition of ten equivalents of **11** no protonation of the imidazole-ring is visible.

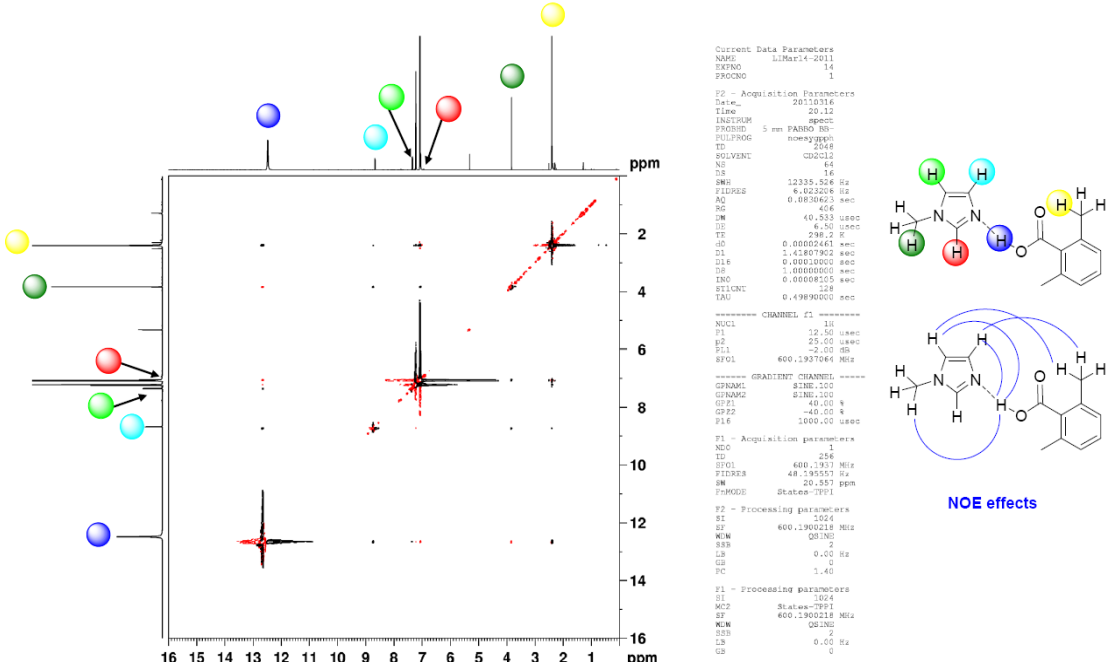


Figure S14. NOESY spectrum (600 MHz, 298.2 K) of a 10:1 mixture **11** (0.2 mmol) and *N*-methylimidazole (0.02 mmol) in CD_2Cl_2.

NMR Data Collection and Processing

The NMR spectra were recorded on a 600 MHz spectrometer equipped with a 5 mm broadband Z-gradient probe (maximum gradient strength 53.5 G/cm).

The phase-sensitive ^{1}H NOESY spectra were recorded using a mixing time of 1 s; the ROESY had a spin-lock pulse of 70 ms. The ^{1}H, ^{15}N HSQC spectra were acquired with pulsed field gradients. The delay was adjusted to a coupling constant of $^{1}J(^{1}H,^{15}N) = 90$ Hz.

All diffusion experiments were performed with a convection-suppressing double STE pulse sequence (dstegp3s)*[4] in pseudo-2D mode. The temperature was set and controlled at 298 K with an air flow of 535 l h^{-1}. For each experiment, 16 acquisition scans and 24 scans were used, with a relaxation delay of 2 s and a diffusion delay of 100 ms. The shape of the gradients were sinusoidal, with a length of 1 ms, and the strength was varied in 32 increments (2–95%) in a linear ramp.

ESI/MS Studies of the Binary Bifunctional Thiourea Catalyst/Benzoic Acid Complex

The proposed complex of thiourea **4a** and benzoic acid **9** was further confirmed by means of mass spectrometry (MS). Mass spectrometric analysis was performed using a quadrupole-time-of-flight mass spectrometer (Q-TOF) with orthogonal acceleration that allows acquisition in the positive and negative ion modes with highly accurate masses. Nano-electrospray ionization (nano-ESI)[5] was used as the ionization method using gold coated glass nano-emitters of 5 µm internal diameter. The instrument parameters were set to: ion spray (IS) voltage –950 V, declustering potential (DP) –100 V, focusing potential (FP) –60 V, curtain gas of 10 (arbitrary units) for the negative ion mode. From the 1:1 mixture of catalyst and benzoic acid in toluene an aliquot of 10 µL was filled into the nano-emitter using a 10 µL pipette with microloader tips. The ESI-MS spectrum (Figure S16) in negative mode shows the presence of [**4a**+PhCOO]$^-$, *m*/*z* 633.18, which is consistent with its isotopic pattern.

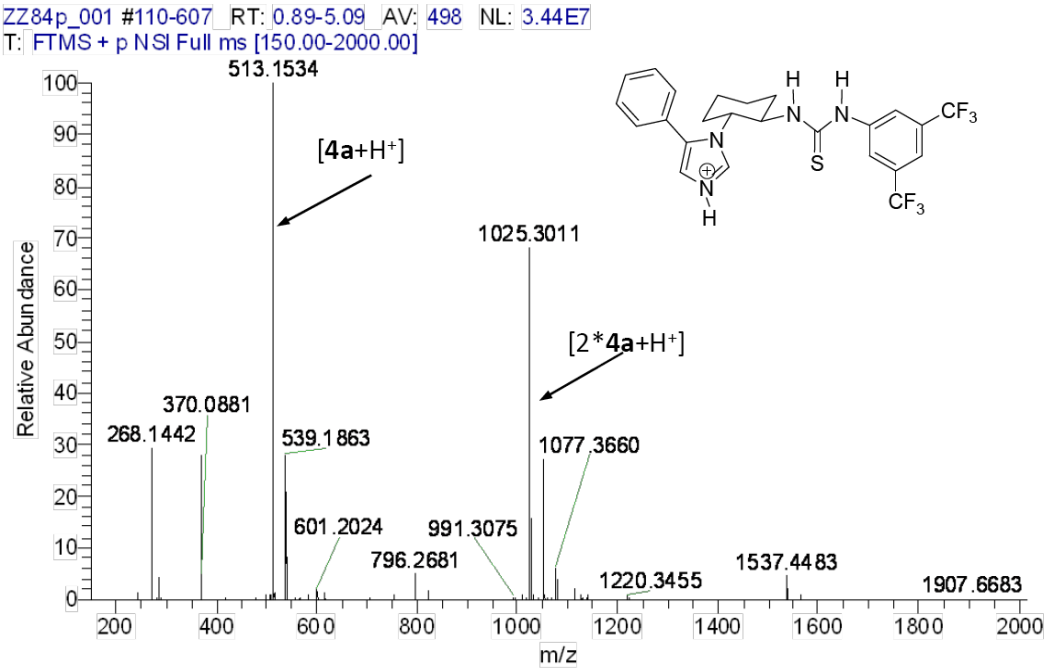


Figure S15. ESI/MS, positive mode; catalyst **4a** in toluene.

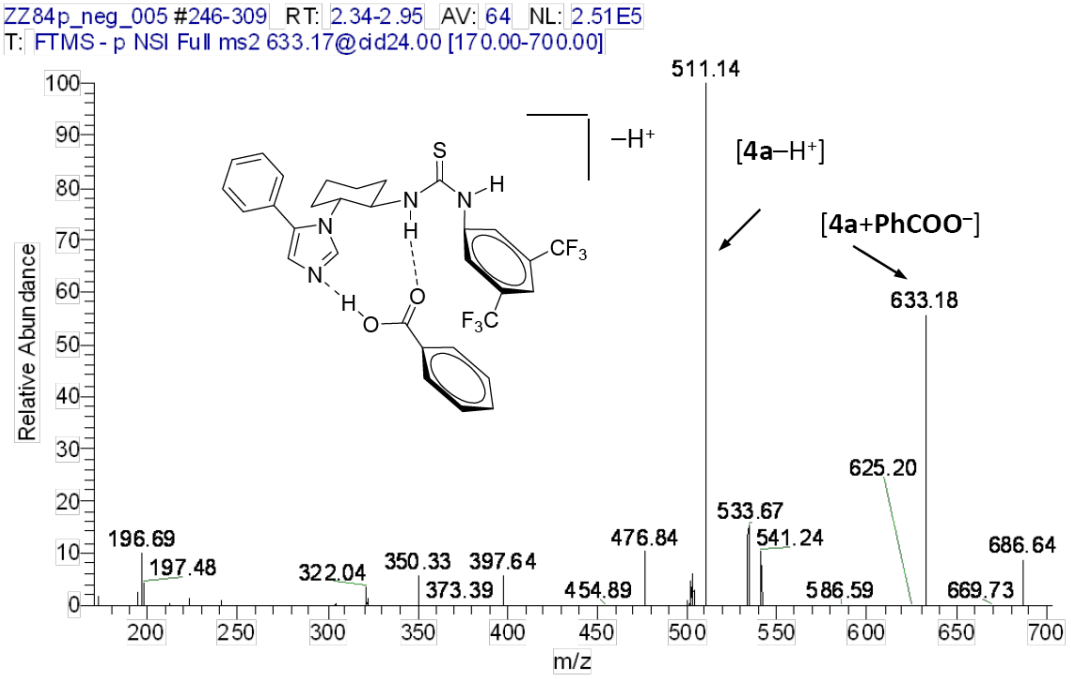


Figure S16. ESI/MS, negative mode; catalyst **4a** and **9** in toluene.

Full reference for Gaussian09

Gaussian 09, Revision B.01, 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.; P., H. H.; 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. T., J.; Cossi, M. R., 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. G., Inc., Wallingford CT, **2009**.

X,Y,Z-Coordinates in Å of the gas phase computations

Conformers of 4a

4a_1

6	4.754513000	-1.816556000	2.551583000	6	5.497185000	-1.144234000	1.020905000
6	4.575801000	-1.733871000	1.040966000	6	4.885081000	-0.096614000	0.097943000
6	3.448328000	-0.774026000	0.670655000	6	3.431404000	-0.437220000	-0.206835000
6	2.144939000	-1.194861000	1.340238000	6	3.320419000	-1.844724000	-0.817782000
6	2.330119000	-1.235094000	2.854355000	6	3.905405000	-2.881534000	0.133437000
6	3.447635000	-2.196230000	3.237844000	6	5.363066000	-2.545456000	0.432937000
7	1.071066000	-0.293134000	0.946903000	7	1.967854000	-2.127012000	-1.312169000
6	-0.233040000	-0.679425000	0.863817000	6	0.830652000	-1.899661000	-0.577536000
7	-1.037293000	0.348980000	0.418617000	7	-0.109275000	-1.202329000	-1.303280000
6	-2.423645000	0.326918000	0.185774000	6	-1.386343000	-0.804821000	-0.856033000
6	-3.170057000	1.438455000	0.582623000	6	-1.734517000	0.539187000	-0.989261000
6	-4.531858000	1.487451000	0.332113000	6	-2.996976000	0.964850000	-0.607432000
6	-5.175421000	0.430366000	-0.303899000	6	-3.920038000	0.066512000	-0.080199000
6	-4.425372000	-0.665868000	-0.700456000	6	-3.561255000	-1.267124000	0.049127000
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6	3.814620000	-0.359915000	-2.890276000	6	1.691413000	2.274519000	-1.872616000
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6	6.320054000	1.180990000	-1.716178000	6	2.108726000	3.409046000	1.044261000
6	4.625880000	2.179638000	-0.329471000	6	1.164824000	1.270391000	1.632666000
6	5.510528000	3.189650000	0.025458000	6	0.904079000	1.744440000	2.912538000
6	6.800895000	3.202846000	-0.494906000	6	1.237662000	3.049223000	3.260556000
6	7.199557000	2.199357000	-1.371888000	6	1.834227000	3.883086000	2.320564000
16	-0.774600000	-2.199485000	1.281046000	16	0.612821000	-2.403804000	0.995406000
6	-5.059373000	-1.809646000	-1.436789000	6	-4.511660000	-2.271518000	0.630042000
9	-6.388883000	-1.695933000	-1.494954000	9	-5.740514000	-1.772268000	0.783645000
9	-4.774105000	-2.978395000	-0.857033000	9	-4.093604000	-2.694792000	1.827164000
9	-4.604202000	-1.876313000	-2.693746000	9	-4.607464000	-3.353392000	-0.152192000
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1	7.491655000	3.996233000	-0.220881000	1	1.027032000	3.418024000	4.261480000
1	8.205777000	2.204375000	-1.783930000	1	2.092666000	4.906133000	2.583241000

4a_3

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6	-3.918013000	-0.462354000	-0.141587000	6	2.376912000	-1.114393000	-0.983523000

4a_4

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6	4.245517000	-0.008378000	-0.166435000	6	-3.738638000	0.789211000	-0.122277000
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6	1.856419000	0.374751000	-0.301210000	6	-2.835056000	-1.126362000	1.027250000
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6	-2.812557000	0.601941000	3.128032000	6	1.122386000	2.266739000	-1.309353000
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6	-2.071671000	1.835236000	1.007799000	6	3.119778000	1.684200000	0.200566000
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6	-0.015525000	3.079108000	0.690506000	6	4.268557000	1.360963000	2.305645000
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9	5.904237000	-2.389044000	-0.651629000	9	-2.640270000	2.969415000	-1.710405000
1	-5.066513000	-0.304708000	-2.667659000	1	4.712842000	-2.631206000	-0.990263000
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1	-5.788222000	0.556768000	-0.423849000	1	4.080571000	-0.512953000	-2.143528000
1	-3.366550000	0.255474000	-0.761408000	1	2.915058000	-1.027005000	-0.029688000
1	-3.790806000	-2.540045000	0.330680000	1	0.877265000	-2.386371000	-1.831358000
1	-3.088281000	-3.394706000	-1.828205000	1	1.408686000	-4.417685000	-0.585923000
1	-2.971057000	-1.765329000	-2.490349000	1	2.676974000	-3.576338000	0.299762000
1	-5.151474000	-2.763789000	-3.116506000	1	3.654220000	-4.785009000	-1.651347000
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1	-1.777479000	-2.107610000	1.058331000	1	-0.493864000	-1.611971000	-0.339092000
1	0.301355000	-2.293730000	0.833149000	1	-0.501012000	-0.905973000	2.956950000
1	2.524434000	-2.839343000	0.575418000	1	-0.546582000	1.387149000	0.910898000
1	5.264737000	0.357853000	-0.256293000	1	-4.556923000	1.277234000	-0.644800000
1	1.027739000	1.051743000	-0.478915000	1	-2.940793000	-2.141153000	1.406072000
1	-2.249511000	1.145235000	3.878480000	1	1.058526000	3.337369000	-1.154505000
1	-4.954037000	-1.553454000	2.207125000	1	0.139727000	-0.472868000	-2.578411000
1	-3.697680000	2.410576000	-0.287642000	1	3.987069000	3.143357000	-1.116004000
1	-0.281819000	1.523754000	2.157443000	1	2.473041000	0.324245000	1.748721000
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1	-0.004330000	4.512351000	-0.914279000	1	6.027002000	2.563158000	2.624213000
1	-2.371299000	4.073015000	-1.539250000	1	5.835871000	3.721857000	0.437211000

4a_5

6	3.851337000	-0.459012000	2.814064000	6	4.368020000	2.597829000	-2.032622000
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6	3.552973000	-1.124055000	-0.043989000	6	2.678155000	1.539549000	0.114608000
6	3.879418000	-2.197561000	0.997148000	6	2.897721000	3.041224000	-0.040703000
6	4.627367000	-1.611298000	2.188980000	6	4.249548000	3.313722000	-0.690627000
7	3.042570000	-1.698146000	-1.297552000	7	1.453776000	1.157598000	0.817915000
6	1.763192000	-1.751842000	-1.773226000	6	0.182059000	1.222865000	0.329592000
7	0.814843000	-1.914796000	-0.788009000	7	-0.609928000	0.219276000	0.860442000
6	-0.506988000	-1.446445000	-0.788531000	6	-1.976243000	0.032899000	0.564213000
6	-1.442843000	-2.091714000	0.013233000	6	-2.389360000	-1.203771000	0.067763000
6	-2.711765000	-1.543826000	0.181185000	6	-3.739906000	-1.431508000	-0.157269000
6	-3.067586000	-0.363565000	-0.451376000	6	-4.681540000	-0.433991000	0.076450000
6	-2.128139000	0.263430000	-1.267485000	6	-4.254331000	0.795518000	0.555534000
6	-0.860720000	-0.264608000	-1.446646000	6	-2.908862000	1.033072000	0.814557000
7	2.226950000	0.993440000	-0.303554000	7	2.453829000	-0.600939000	-1.089857000
6	1.213402000	1.918904000	-0.053385000	6	2.913562000	-1.512728000	-0.141421000
6	1.233937000	2.759099000	-1.142540000	6	1.923484000	-2.460465000	-0.042822000
7	2.209591000	2.408597000	-2.031732000	7	0.871232000	-2.174094000	-0.875236000
6	2.790398000	1.366359000	-1.495807000	6	1.221000000	-1.060530000	-1.470580000
6	0.363781000	2.010855000	1.137817000	6	4.204217000	-1.481403000	0.557885000
6	0.090911000	3.288801000	1.646422000	6	5.420968000	-1.502522000	-0.133751000
6	-0.255237000	0.914948000	1.751880000	6	4.226314000	-1.512030000	1.956305000
6	-1.117908000	1.087580000	2.826776000	6	5.431940000	-1.535939000	2.648087000
6	-1.380986000	2.362364000	3.315952000	6	6.634058000	-1.530163000	1.949833000
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6	-2.430497000	1.620015000	-1.837554000	6	-5.226071000	1.903176000	0.832431000
9	-3.736592000	1.774732000	-2.079888000	9	-6.483262000	1.560270000	0.539184000
9	-1.771447000	1.846561000	-2.973433000	9	-4.926390000	2.995850000	0.123200000
9	-2.074110000	2.582323000	-0.972420000	9	-5.196306000	2.260007000	2.123686000
6	-3.648535000	-2.233172000	1.124182000	6	-4.222928000	-2.738576000	-0.709092000
9	-3.734839000	-3.541523000	0.857964000	9	-3.287944000	-3.689216000	-0.660763000
9	-4.879703000	-1.725115000	1.085208000	9	-4.606579000	-2.611399000	-1.985325000
9	-3.209090000	-2.129022000	2.390031000	9	-5.289123000	-3.182687000	-0.030098000
1	2.921267000	-0.841780000	3.264456000	1	3.609197000	2.992867000	-2.725809000
1	4.423730000	-0.003457000	3.630223000	1	5.344272000	2.794130000	-2.491675000
1	4.403149000	1.059526000	1.360126000	1	4.962472000	0.705940000	-1.206453000
1	2.893466000	1.394647000	2.211851000	1	4.250818000	0.564730000	-2.819095000
1	1.815936000	-0.506314000	1.052331000	1	2.038258000	1.231146000	-1.910444000
1	4.509450000	-0.654426000	-0.328817000	1	3.487660000	1.156182000	0.756618000
1	4.461290000	-2.990716000	0.512776000	1	2.825308000	3.511631000	0.947535000
1	2.942623000	-2.667362000	1.342715000	1	2.089918000	3.461768000	-0.651486000
1	4.829401000	-2.393851000	2.929700000	1	4.389454000	4.393669000	-0.817435000
1	5.608361000	-1.245173000	1.847869000	1	5.059324000	2.969508000	-0.026918000
1	3.707427000	-1.710516000	-2.060845000	1	1.599485000	0.441003000	1.520657000
1	1.110865000	-2.408000000	0.045401000	1	-0.116524000	-0.658704000	1.003332000
1	-1.181998000	-3.017884000	0.523472000	1	-1.646784000	-1.969906000	-0.155832000
1	-4.053082000	0.067288000	-0.307322000	1	-5.735190000	-0.620759000	-0.109103000
1	-0.134153000	0.260699000	-2.059352000	1	-2.584086000	1.991726000	1.209754000
1	0.549226000	3.578233000	-1.333919000	1	1.950887000	-3.362577000	0.558586000
1	3.611558000	0.817287000	-1.940443000	1	0.605339000	-0.492463000	-2.161602000
1	0.574745000	4.148341000	1.187347000	1	5.411259000	-1.530189000	-1.221610000
1	-0.106088000	-0.086432000	1.357961000	1	3.281461000	-1.518758000	2.499097000
1	-1.605117000	0.217937000	3.262598000	1	5.431200000	-1.556012000	3.734970000
1	-2.060670000	2.498656000	4.153302000	1	7.578106000	-1.544212000	2.488628000
1	-0.970239000	4.464136000	3.092734000	1	7.562394000	-1.535253000	0.007109000

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Complex of catalyst 4a and benzoic acid 9

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6	-4.394964000	-3.649169000	-1.547973000	6	5.550683000	1.065384000	-1.886568000
6	-4.072607000	-3.025490000	-0.195157000	6	4.789657000	1.423897000	-0.614040000
6	-2.951060000	-2.003559000	-0.339692000	6	3.429912000	0.741245000	-0.628218000
6	-1.691686000	-2.647295000	-0.918928000	6	2.609670000	1.195212000	-1.849346000
6	-2.022129000	-3.271649000	-2.274105000	6	3.363832000	0.795543000	-3.116421000
6	-3.154676000	-4.283305000	-2.165542000	6	4.750885000	1.430878000	-3.132836000
7	-0.625015000	-1.680313000	-1.023060000	7	1.204720000	0.820042000	-1.814823000
6	0.643736000	-1.883911000	-0.576786000	6	0.684235000	-0.383350000	-1.452751000
7	1.433042000	-0.805534000	-0.799396000	7	-0.563268000	-0.233524000	-0.912028000
6	2.754573000	-0.523504000	-0.432732000	6	-1.554857000	-1.171234000	-0.605344000
6	3.116177000	0.833255000	-0.496637000	6	-2.577578000	-0.717320000	0.242815000
6	4.404029000	1.225009000	-0.183799000	6	-3.626967000	-1.553423000	0.575906000
6	5.365837000	0.294671000	0.207248000	6	-3.692780000	-2.855784000	0.084634000
6	5.004076000	-1.040015000	0.258195000	6	-2.685877000	-3.289795000	-0.760722000
6	3.714968000	-1.463691000	-0.062588000	6	-1.620049000	-2.465655000	-1.116228000
7	-2.675368000	-1.353399000	0.960092000	7	2.686427000	0.951064000	0.630132000
6	-3.476805000	-0.385730000	1.562015000	6	2.793881000	0.186897000	1.799040000
6	-2.847379000	-0.029674000	2.714931000	6	1.788244000	0.603580000	2.618673000
7	-1.686145000	-0.769565000	2.782678000	7	1.103991000	1.597314000	1.954758000
6	-1.596789000	-1.557596000	1.710814000	6	1.662059000	1.790559000	0.764994000
6	-4.756182000	0.095811000	1.022796000	6	3.842979000	-0.811656000	2.052251000
6	-5.915651000	-0.080238000	1.783848000	6	4.738292000	-0.595033000	3.103948000
6	-4.823028000	0.748469000	-0.213892000	6	3.939199000	-1.980794000	1.290797000
6	-6.051705000	1.199361000	-0.681244000	6	4.933458000	-2.908811000	1.574293000
6	-7.206730000	1.012518000	0.072434000	6	5.827325000	-2.685336000	2.616960000
6	-7.137842000	0.378344000	1.308710000	6	5.726399000	-1.530396000	3.385346000
16	1.095775000	-3.311125000	0.227994000	16	1.514797000	-1.840933000	-1.618494000
6	5.983729000	-2.085376000	0.697283000	6	-2.691064000	-4.685721000	-1.306476000
9	7.229227000	-1.607864000	0.790404000	9	-3.818828000	-5.340660000	-1.013001000
9	6.011148000	-3.120316000	-0.150244000	9	-1.672717000	-5.400185000	-0.811239000
9	5.656832000	-2.580526000	1.899323000	9	-2.555470000	-4.691372000	-2.637850000
6	4.796324000	2.670160000	-0.212947000	6	-4.708817000	-1.093537000	1.504241000
9	3.854103000	3.449874000	-0.745897000	9	-4.619563000	0.207381000	1.795224000
9	5.921249000	2.853598000	-0.917874000	9	-4.665331000	-1.766875000	2.663639000
9	5.043345000	3.126509000	1.024299000	9	-5.922300000	-1.309849000	0.982615000
1	-4.781713000	-2.866061000	-2.218798000	1	5.751583000	-0.017103000	-1.884564000
1	-5.197767000	-4.386824000	-1.433936000	1	6.526773000	1.564296000	-1.890841000
1	-3.744896000	-3.803324000	0.513060000	1	4.644991000	2.514190000	-0.544968000
1	-4.960486000	-2.546145000	0.237369000	1	5.348411000	1.114355000	0.279344000
1	-3.265690000	-1.187277000	-1.004752000	1	3.565977000	-0.343263000	-0.703988000
1	-1.354412000	-3.458088000	-0.252738000	1	2.583110000	2.299115000	-1.830814000
1	-1.104512000	-3.734978000	-2.656400000	1	2.772506000	1.113280000	-3.982824000
1	-2.290147000	-2.467953000	-2.978026000	1	3.430402000	-0.299733000	-3.160493000
1	-3.386310000	-4.701737000	-3.151948000	1	5.293676000	1.127693000	-4.035738000
1	-2.827860000	-5.126988000	-1.537913000	1	4.647787000	2.526621000	-3.185725000
1	-0.934912000	-0.697724000	-1.160795000	1	0.575057000	1.633262000	-1.741541000
1	0.946048000	0.020969000	-1.211773000	1	-0.775252000	0.704799000	-0.534499000
1	2.368779000	1.565666000	-0.798442000	1	-2.539951000	0.302681000	0.622505000
1	6.374898000	0.610829000	0.454946000	1	-4.516969000	-3.510436000	0.351903000
1	3.462836000	-2.517582000	-0.025055000	1	-0.846126000	-2.832919000	-1.781701000
1	-3.118076000	0.706299000	3.456075000	1	1.507265000	0.249916000	3.598830000
1	-0.772234000	-2.244862000	1.498830000	1	1.263148000	2.483006000	0.021116000
1	-5.852468000	-0.588717000	2.744622000	1	4.656533000	0.316326000	3.693478000
1	-3.896863000	0.934174000	-0.761496000	1	3.215649000	-2.171383000	0.497726000
1	-6.103288000	1.714558000	-1.636986000	1	4.999916000	-3.818489000	0.983279000
1	-8.162926000	1.370441000	-0.301315000	1	6.601246000	-3.417176000	2.834608000
1	-8.037110000	0.237101000	1.902663000	1	6.420082000	-1.355197000	4.203596000
1	-0.974380000	-0.705362000	3.496427000	6	-2.679614000	6.553601000	-0.799380000
6	-2.668031000	4.793720000	0.478556000	6	-3.726637000	6.494149000	0.116381000
6	-1.841443000	5.827167000	0.047411000	6	-3.901228000	5.359393000	0.903851000
6	-0.705147000	5.538260000	-0.702994000	6	-3.026496000	4.287777000	0.778530000
6	-0.397608000	4.221426000	-1.021467000	6	-1.973607000	4.343467000	-0.135112000
6	-1.226292000	3.180454000	-0.601442000	6	-1.806507000	5.481085000	-0.925581000
6	-2.360087000	3.477973000	0.154535000	6	-1.021709000	3.191919000	-0.265408000
6	-0.879159000	1.754699000	-0.947763000	8	-1.169593000	2.207038000	0.524184000
8	0.221427000	1.552347000	-1.516908000	8	-0.114331000	3.268631000	-1.137610000
8	-1.712521000	0.853467000	-0.637786000	1	-2.546588000	7.439355000	-1.416521000
1	-3.555108000	5.016661000	1.068256000	1	-4.411544000	7.333708000	0.214064000
1	-2.081666000	6.858320000	0.298100000	1	-4.723113000	5.310682000	1.614544000
1	-0.055331000	6.343616000	-1.038294000	1	0.161713000	1.963324000	2.108175000
1	0.488107000	3.971591000	-1.600105000	1	-0.982569000	5.499047000	-1.634378000
1	-2.993602000	2.658502000	0.487237000	1	-3.145824000	3.388916000	1.378600000

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6	-4.268951000	-2.150837000	2.710800000	6	-4.075738000	-2.079485000	3.286498000
6	-3.854745000	-0.740106000	2.308829000	6	-4.341719000	-0.966424000	2.279668000
6	-3.030587000	-0.778058000	1.027318000	6	-3.130695000	-0.784696000	1.374378000
6	-1.787682000	-1.652096000	1.210969000	6	-1.873896000	-0.453398000	2.183286000
6	-2.205964000	-3.067592000	1.609321000	6	-1.616805000	-1.574352000	3.194572000
6	-3.049453000	-3.050312000	2.877033000	6	-2.821626000	-1.788246000	4.101975000
7	-0.854695000	-1.610446000	0.099855000	7	-0.743750000	-0.089044000	1.353036000
6	-1.079457000	-1.915933000	-1.181323000	6	-0.097332000	-0.855071000	0.371448000
7	0.015658000	-1.757479000	-2.003054000	7	0.963400000	-0.315821000	-0.197526000
6	1.120880000	-0.911591000	-1.744989000	6	1.191179000	1.044431000	-0.183822000
6	0.915240000	0.420406000	-1.390715000	6	0.211861000	1.950661000	-0.631841000
6	1.999787000	1.240411000	-1.105923000	6	0.450974000	3.317848000	-0.651312000
6	3.300406000	0.757101000	-1.198980000	6	1.680985000	3.840166000	-0.261962000
6	3.497777000	-0.555112000	-1.606599000	6	2.668245000	2.943982000	0.134574000
6	2.419439000	-1.393197000	-1.865921000	6	2.441428000	1.573397000	0.183056000
7	-2.663569000	0.594873000	0.615887000	7	-3.406443000	0.252575000	0.351643000
6	-3.482783000	1.497567000	-0.067611000	6	-4.184021000	0.082105000	-0.794549000
6	-2.776867000	2.660057000	-0.153294000	6	-4.214777000	1.293493000	-1.421368000
7	-1.570601000	2.444959000	0.474497000	7	-3.468843000	2.164703000	-0.661251000
6	-1.513884000	1.194325000	0.937286000	6	-2.985931000	1.513697000	0.396410000
6	-4.845152000	1.232598000	-0.544252000	6	-4.844664000	-1.166653000	-1.189789000
6	-5.866231000	2.111292000	-0.166598000	6	-6.222499000	-1.148178000	-1.429028000
6	-5.133320000	0.167301000	-1.403419000	6	-4.116877000	-2.346252000	-1.379766000
6	-6.431529000	-0.016668000	-1.861863000	6	-4.778293000	-3.497964000	-1.787477000
6	-7.444773000	0.857474000	-1.480701000	6	-6.150428000	-3.479614000	-2.017622000
6	-7.160004000	1.925202000	-0.635914000	6	-6.872616000	-2.303153000	-1.843453000
16	-2.521544000	-2.470989000	-1.874579000	16	-0.650493000	-2.420267000	-0.043680000
6	4.880297000	-1.111635000	-1.778189000	6	4.022677000	3.438688000	0.549209000
9	5.827498000	-0.229760000	-1.456604000	9	4.127459000	4.771314000	0.452914000
9	5.084109000	-1.479452000	-3.051509000	9	4.987823000	2.906519000	-0.205258000
9	5.071733000	-2.205690000	-1.030696000	9	4.292899000	3.110501000	1.818458000
6	1.740034000	2.650228000	-0.681302000	6	-0.668988000	4.218253000	-1.034528000
9	0.809799000	3.236255000	-1.460793000	9	-1.630056000	4.257306000	-0.054323000

9	2.827078000	3.410829000	-0.706702000	9	-1.335732000	3.788304000	-2.124411000
9	1.238600000	2.717409000	0.574718000	9	-0.306560000	5.474237000	-1.250709000
1	-4.927069000	-2.565745000	1.931583000	1	-3.947681000	-3.028118000	2.743595000
1	-4.859454000	-2.115381000	3.634025000	1	-4.948224000	-2.204483000	3.938516000
1	-3.246440000	-0.281127000	3.105363000	1	-4.541981000	-0.017903000	2.806744000
1	-4.733694000	-0.098026000	2.161812000	1	-5.228080000	-1.191405000	1.671533000
1	-3.626763000	-1.196831000	0.208899000	1	-2.908943000	-1.703169000	0.816697000
1	-1.201483000	-1.234422000	2.050094000	1	-2.103312000	0.454613000	2.775568000
1	-1.291616000	-3.656079000	1.751027000	1	-0.725533000	-1.308434000	3.776328000
1	-2.760803000	-3.523033000	0.777238000	1	-1.371855000	-2.487969000	2.636778000
1	-3.357459000	-4.069263000	3.139643000	1	-2.623422000	-2.604939000	4.805732000
1	-2.439806000	-2.681187000	3.716911000	1	-2.991951000	-0.886378000	4.713336000
1	0.140846000	-1.553228000	0.450535000	1	-0.136563000	0.605391000	1.772646000
1	-0.127544000	-2.103491000	-2.943111000	1	2.190368000	-1.446710000	-0.693785000
1	-0.102759000	0.804813000	-1.341852000	1	-0.731969000	1.550359000	-0.999294000
1	4.148002000	1.385357000	-0.942647000	1	1.868076000	4.908134000	-0.278950000
1	2.582699000	-2.433400000	-2.139073000	1	3.219252000	0.877694000	0.504397000
1	-3.034422000	3.592930000	-0.631334000	1	-4.678532000	1.580290000	-2.352691000
1	-0.631910000	0.758276000	1.472033000	1	-2.322695000	1.940265000	1.132340000
1	-5.637479000	2.934723000	0.507787000	1	-6.779823000	-0.225564000	-1.274976000
1	-4.337240000	-0.502859000	-1.731099000	1	-3.034551000	-2.354169000	-1.228482000
1	-6.648007000	-0.845178000	-2.531166000	1	-4.211016000	-4.412759000	-1.936560000
1	-8.457681000	0.708754000	-1.846590000	1	-6.659205000	-4.385232000	-2.338614000
1	-7.947782000	2.611408000	-0.335706000	1	-7.944028000	-2.285833000	-2.025279000
6	4.766554000	1.758912000	2.613067000	6	7.300638000	-3.685703000	-0.038522000
6	5.806166000	0.929714000	2.199978000	6	7.128877000	-4.718926000	-0.955928000
6	5.525624000	-0.347610000	1.720622000	6	5.921620000	-4.856232000	-1.634791000
6	4.209106000	-0.784242000	1.642534000	6	4.885098000	-3.960743000	-1.401868000
6	3.161340000	0.046029000	2.041464000	6	5.055420000	-2.924149000	-0.483519000
6	3.450142000	1.316478000	2.538399000	6	6.265584000	-2.791795000	0.196995000
6	1.731465000	-0.393480000	1.832726000	6	3.976843000	-1.934983000	-0.200662000
8	1.563565000	-1.487217000	1.232000000	8	2.906284000	-2.105147000	-0.950850000
8	0.824976000	0.384657000	2.233136000	8	4.104320000	-1.061805000	0.642185000
1	4.984761000	2.754422000	2.994695000	1	8.244374000	-3.578241000	0.491317000
1	6.835449000	1.278415000	2.253229000	1	7.938782000	-5.421272000	-1.141719000
1	6.332796000	-0.997870000	1.388761000	1	5.788436000	-5.664584000	-2.350181000
1	3.961172000	-1.766850000	1.249296000	1	3.936225000	-4.054764000	-1.922339000
1	2.623735000	1.947315000	2.854659000	1	6.367490000	-1.975116000	0.906979000
1	-0.777818000	3.074434000	0.524617000	1	-3.200788000	3.115459000	-0.894365000

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6	-3.454619000	-2.197202000	1.439098000	6	-4.936091000	-3.596821000	-0.205353000
6	-2.019200000	-2.266345000	1.940878000	6	-4.789755000	-2.266437000	-0.935347000
6	-1.053406000	-2.086956000	0.770821000	6	-3.372048000	-1.739622000	-0.778855000
6	-1.253330000	-3.215300000	-0.235802000	6	-2.970532000	-1.619243000	0.704398000
6	-2.703369000	-3.209210000	-0.726666000	6	-3.211273000	-2.911742000	1.481370000
6	-3.709000000	-3.292604000	0.413658000	6	-4.633627000	-3.418230000	1.278042000
7	-0.334766000	-3.256446000	-1.384724000	7	-1.621523000	-1.077093000	0.860720000
6	0.723375000	-2.467030000	-1.762080000	6	-0.455133000	-1.628799000	0.422523000
7	0.553330000	-1.132917000	-1.586345000	7	0.585485000	-0.743624000	0.509777000
6	1.543275000	-0.158011000	-1.376313000	6	1.942061000	-0.956500000	0.212458000
6	1.136768000	1.181097000	-1.429236000	6	2.626296000	0.064668000	-0.451380000
6	2.013761000	2.187160000	-1.046715000	6	3.986163000	-0.052172000	-0.693507000
6	3.302284000	1.900607000	-0.608791000	6	4.684665000	-1.189100000	-0.300023000
6	3.702203000	0.572122000	-0.586178000	6	3.996173000	-2.200964000	0.352590000
6	2.848937000	-0.451799000	-0.980288000	6	2.634791000	-2.093437000	0.619878000
7	0.340337000	-1.989830000	1.283531000	7	-3.112539000	-0.451466000	-1.439967000
6	0.839311000	-0.917920000	2.035398000	6	-3.654659000	0.799698000	-1.143042000
6	2.148517000	-1.204238000	2.285210000	6	-2.749585000	1.706650000	-1.618885000
7	2.419425000	-2.418770000	1.700030000	7	-1.664384000	1.075829000	-2.172219000
6	1.318618000	-2.873084000	1.097732000	6	-1.911578000	-0.206411000	-2.033680000
6	0.065950000	0.248708000	2.473659000	6	-4.909127000	1.091305000	-0.433516000
6	0.070096000	0.584235000	3.832508000	6	-6.164727000	0.793047000	-0.972725000
6	-0.639024000	1.044145000	1.566995000	6	-4.839368000	1.774346000	0.784827000
6	-1.350802000	2.148564000	2.014985000	6	-5.999779000	2.130912000	1.462820000
6	-1.352177000	2.473208000	3.367613000	6	-7.242733000	1.812281000	0.927563000
6	-0.636655000	1.695171000	4.274259000	6	-7.322934000	1.145942000	-0.292599000
16	2.085008000	-3.235695000	-2.396723000	16	-0.289917000	-3.179961000	-0.203480000
6	5.048853000	0.171917000	-0.076296000	6	4.697042000	-3.455639000	0.780926000
9	5.802995000	1.211709000	0.274197000	9	6.026505000	-3.342028000	0.699674000
9	5.732297000	-0.556762000	-0.959957000	9	4.334993000	-4.496805000	0.024367000
9	4.928315000	-0.611273000	1.031245000	9	4.394227000	-3.771198000	2.046301000
6	1.507397000	3.600371000	-1.007600000	6	4.734266000	1.027731000	-1.413455000
9	0.724251000	3.879961000	-2.045803000	9	3.968214000	2.091802000	-1.674179000
9	2.516391000	4.485017000	-1.007010000	9	5.218968000	0.584421000	-2.579789000
9	0.796546000	3.821152000	0.106098000	9	5.784070000	1.450413000	-0.697269000
1	-3.624530000	-1.210252000	0.980017000	1	-4.241658000	-4.336247000	-0.634099000
1	-4.148213000	-2.280523000	2.283539000	1	-5.948510000	-3.991519000	-0.351980000
1	-1.823265000	-3.237399000	2.426038000	1	-5.507439000	-1.553641000	-0.508118000
1	-1.834123000	-1.487012000	2.689026000	1	-5.024690000	-2.359981000	-2.003770000
1	-1.273041000	-1.137331000	0.267835000	1	-2.682941000	-2.453570000	-1.251155000
1	-1.085694000	-4.163173000	0.315421000	1	-3.627907000	-0.847930000	1.138929000
1	-2.825815000	-4.049565000	-1.421985000	1	-3.001702000	-2.720673000	2.541174000
1	-2.833735000	-2.279542000	-1.295758000	1	-2.495578000	-3.670498000	1.145123000
1	-4.727999000	-3.218342000	0.014420000	1	-4.769623000	-4.363005000	1.817547000
1	-3.636485000	-4.276084000	0.906862000	1	-5.355061000	-2.704395000	1.708222000
1	-0.216501000	-4.192652000	-1.753958000	1	-1.590557000	-0.075937000	1.041394000
1	-0.430150000	-0.760189000	-1.600424000	1	0.334919000	0.226614000	0.702980000
1	0.105418000	1.436847000	-1.692812000	1	2.089817000	0.945092000	-0.798573000
1	3.975744000	2.692978000	-0.299575000	1	5.749852000	-1.279545000	-0.493966000
1	3.197410000	-1.479306000	-0.973936000	1	2.116573000	-2.887459000	1.147992000
1	2.910734000	-0.613141000	2.769288000	1	-2.830868000	2.787141000	-1.587912000
1	1.266217000	-3.776020000	0.506765000	1	-1.244760000	-1.017561000	-2.308476000
1	0.615967000	-0.039700000	4.538477000	1	-6.223818000	0.290534000	-1.936770000
1	-0.627667000	0.847927000	0.498234000	1	-3.856902000	2.020299000	1.188794000
1	-1.880987000	2.743169000	1.274504000	1	-5.931919000	2.658397000	2.411121000
1	-1.907475000	3.339605000	3.718361000	1	-8.151134000	2.088722000	1.457130000
1	-0.633518000	1.950754000	5.330877000	1	-8.293880000	0.910769000	-0.721732000
6	-6.235191000	0.154051000	-1.131509000	6	2.046520000	4.594929000	2.697415000
6	-6.760243000	1.385359000	-0.750106000	6	2.964824000	5.327500000	1.949320000
6	-5.909286000	2.468369000	-0.547028000	6	3.006494000	5.197018000	0.564180000
6	-4.539180000	2.317614000	-0.719637000	6	2.128545000	4.335513000	-0.079202000
6	-4.001655000	1.083556000	-1.087534000	6	1.207472000	3.598749000	0.669299000
6	-4.862891000	0.006382000	-1.299651000	6	1.170426000	3.729952000	2.059027000
6	-2.502877000	0.944651000	-1.239288000	6	0.269420000	2.652295000	0.025616000
8	-1.812689000	1.973330000	-1.122374000	8	0.375136000	2.611996000	-1.288799000
8	-2.060865000	-0.236313000	-1.434185000	8	-0.503053000	1.944299000	0.669432000
1	-6.899161000	-0.690610000	-1.305317000	1	2.017812000	4.698304000	3.779037000
1	-7.833821000	1.502808000	-0.617981000	1	3.654356000	6.003226000	2.449826000
1	-6.318322000	3.434221000	-0.257768000	1	3.727382000	5.767314000	-0.015648000
1	3.336305000	-2.836907000	1.612647000	1	0.445447000	3.143269000	2.617223000
1	-3.853268000	3.150827000	-0.585637000	1	2.149843000	4.221659000	-1.158735000
1	-4.439776000	-0.944440000	-1.616076000	1	-0.290400000	1.970164000	-1.689161000

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6	-5.790435000	0.928645000	-2.090899000	6	4.592259000	-3.511813000	-1.235011000
6	-5.285792000	-0.196744000	-1.197345000	6	4.102950000	-2.252484000	-1.940276000
6	-3.789847000	-0.055215000	-0.936264000	6	3.335956000	-1.357710000	-0.976915000
6	-3.013014000	-0.026278000	-2.262129000	6	2.182800000	-2.120657000	-0.298899000
6	-3.514539000	1.117295000	-3.141954000	6	2.669602000	-3.401305000	0.372648000
6	-5.010382000	0.975442000	-3.399974000	6	3.423353000	-4.274514000	-0.622458000
7	-1.562670000	-0.084203000	-2.109074000	7	1.386185000	-1.250666000	0.558667000
6	-0.759168000	0.768748000	-1.422209000	6	1.804563000	-0.595111000	1.661357000
7	0.495066000	0.236768000	-1.240525000	7	0.900082000	0.302427000	2.172034000
6	1.589530000	0.824315000	-0.584535000	6	-0.450612000	0.471157000	1.762922000
6	2.323725000	0.034074000	0.302701000	6	-1.448187000	-0.359311000	2.268382000
6	3.435483000	0.557014000	0.947234000	6	-2.775778000	-0.143578000	1.915210000
6	3.836219000	1.869654000	0.719279000	6	-3.119913000	0.890576000	1.052656000
6	3.107856000	2.644496000	-0.171606000	6	-2.117761000	1.701647000	0.535188000
6	1.994121000	2.133872000	-0.830360000	6	-0.786783000	1.490932000	0.879150000
7	-3.307245000	-1.121028000	-0.055673000	7	2.797774000	-0.168079000	-1.652943000
6	-3.346944000	-1.145879000	1.334617000	6	2.838988000	1.150129000	-1.208321000
6	-2.821521000	-2.362626000	1.685592000	6	1.835251000	1.792763000	-1.892045000
7	-2.464535000	-3.077277000	0.570235000	7	1.190366000	0.922107000	-2.733640000
6	-2.790279000	-2.309571000	-0.446617000	6	1.788798000	-0.232822000	-2.557039000
6	-3.879329000	-0.076568000	2.186468000	6	3.823275000	1.673776000	-0.265390000
6	-4.870917000	-0.390104000	3.122243000	6	5.161929000	1.269157000	-0.306961000
6	-3.387974000	1.232859000	2.128473000	6	3.435024000	2.620682000	0.687760000
6	-3.896132000	2.206941000	2.979058000	6	4.357639000	3.139084000	1.584722000
6	-4.885861000	1.887523000	3.903483000	6	5.680636000	2.710824000	1.551774000
6	-5.368255000	0.585024000	3.977873000	6	6.079921000	1.776877000	0.601683000
16	-1.223958000	2.281518000	-0.861784000	16	3.289828000	-0.756298000	2.436578000
6	3.503870000	4.059687000	-0.471168000	6	-2.433411000	2.854446000	-0.370586000
9	4.585830000	4.438184000	0.215604000	9	-3.713723000	2.868914000	-0.745503000
9	2.518497000	4.913818000	-0.178202000	9	-1.680376000	2.821461000	-1.475127000
9	3.777144000	4.216855000	-1.773353000	9	-2.176328000	4.020796000	0.236115000
6	4.243272000	-0.298271000	1.875521000	6	-3.816564000	-1.050565000	2.503830000
9	3.538349000	-1.328438000	2.355285000	9	-3.787733000	-1.007217000	3.841036000
9	4.695683000	0.402387000	2.921515000	9	-3.597294000	-2.327366000	2.157825000
9	5.319303000	-0.807616000	1.258064000	9	-5.051938000	-0.732398000	2.115578000
1	-5.671439000	1.887545000	-1.563502000	1	5.298743000	-3.230441000	-0.438657000
1	-6.863449000	0.805959000	-2.280144000	1	5.146085000	-4.143997000	-1.939343000
1	-5.468901000	-1.174677000	-1.673191000	1	3.446103000	-2.538244000	-2.778184000
1	-5.813215000	-0.208832000	-0.234401000	1	4.935623000	-1.685935000	-2.377786000
1	-3.601897000	0.894593000	-0.421325000	1	4.007242000	-1.000786000	-0.185133000
1	-3.259256000	-0.955315000	-2.803454000	1	1.476662000	-2.418838000	-1.090432000
1	-2.945888000	1.107272000	-4.079762000	1	1.800392000	-3.926551000	0.787540000
1	-3.299433000	2.073445000	-2.649239000	1	3.321511000	-3.143454000	1.215160000
1	-5.360020000	1.803472000	-4.027846000	1	3.776253000	-5.186490000	-0.126515000
1	-5.202702000	0.050665000	-3.968263000	1	2.743824000	-4.599677000	-1.427430000
1	-1.155402000	-0.995960000	-2.297777000	1	0.504573000	-0.963759000	0.132645000
1	0.570960000	-0.769964000	-1.392140000	1	1.218507000	0.753619000	3.020306000
1	2.012934000	-0.990374000	0.500423000	1	-1.177905000	-1.164027000	2.949569000
1	4.699588000	2.281646000	1.231849000	1	-4.157575000	1.058778000	0.780398000
1	1.440154000	2.750383000	-1.531202000	1	-0.000469000	2.118875000	0.465486000
1	-2.658067000	-2.739272000	2.687603000	1	1.576695000	2.844744000	-1.855991000
1	-2.625313000	-2.572553000	-1.482323000	1	1.488981000	-1.162653000	-3.026007000
1	-5.251088000	-1.409196000	3.164853000	1	5.486892000	0.564031000	-1.070612000
1	-2.584787000	1.482059000	1.434106000	1	2.394616000	2.938652000	0.728400000
1	-3.503922000	3.219635000	2.926551000	1	4.039508000	3.870579000	2.323566000
1	-5.276603000	2.652332000	4.570400000	1	6.400269000	3.106696000	2.263943000
1	-6.138746000	0.328007000	4.700846000	1	7.115636000	1.448670000	0.561743000
6	4.100735000	-2.809698000	-1.943252000	6	-4.956617000	-1.973716000	-0.795579000
6	4.829553000	-3.280013000	-0.853716000	6	-5.896791000	-1.139548000	-1.396835000
6	4.174256000	-3.799012000	0.259009000	6	-5.484729000	-0.103152000	-2.229725000
6	2.787088000	-3.854911000	0.286116000	6	-4.130693000	0.103807000	-2.464800000
6	2.052920000	-3.375734000	-0.801384000	6	-3.187781000	-0.725780000	-1.855762000
6	2.714938000	-2.851292000	-1.914925000	6	-3.604077000	-1.764193000	-1.021800000
6	0.571642000	-3.339813000	-0.777558000	6	-1.731070000	-0.490175000	-2.018733000
8	0.027443000	-4.065800000	0.169776000	8	-1.452965000	0.377992000	-2.969862000
8	-0.069420000	-2.655545000	-1.575468000	8	-0.896365000	-1.052879000	-1.321019000
1	4.615379000	-2.404763000	-2.810638000	1	-5.279719000	-2.778893000	-0.140890000
1	5.915628000	-3.233281000	-0.868206000	1	-6.956958000	-1.298402000	-1.213267000
1	4.747455000	-4.149662000	1.113258000	1	-6.220894000	0.548020000	-2.694386000
1	2.123463000	-2.482747000	-2.749919000	1	-0.479599000	0.625674000	-2.965152000
1	2.261555000	-4.248663000	1.151430000	1	-2.844870000	-2.386721000	-0.554487000
1	-0.954356000	-3.854963000	0.270512000	1	-3.790110000	0.915633000	-3.101716000

Conformers of benzoic acid 9[6]

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6	1.893314000	1.184709000	-0.000001000	6	1.870043000	-1.187379000	0.133899000
6	2.557771000	-0.039178000	0.000001000	6	2.548757000	0.022944000	0.017721000
6	1.835847000	-1.229151000	0.000001000	6	1.838172000	1.209423000	-0.127944000
6	0.447676000	-1.200461000	0.000001000	6	0.449102000	1.188136000	-0.141406000
6	-0.219626000	0.026081000	-0.000001000	6	-0.237092000	-0.021325000	-0.011830000
6	0.506733000	1.217687000	-0.000001000	6	0.483511000	-1.210370000	0.109806000
6	-1.695942000	0.119368000	-0.000001000	6	-1.726355000	-0.120439000	-0.031081000
8	-2.298881000	-1.086638000	-0.000002000	8	-2.409350000	1.008238000	0.260251000
8	-2.326064000	1.152536000	0.000003000	8	-2.317172000	-1.137037000	-0.286905000
1	2.459876000	2.112405000	-0.000002000	1	2.425832000	-2.115487000	0.239967000
1	3.644900000	-0.066223000	0.000001000	1	3.635655000	0.040982000	0.032367000
1	2.357628000	-2.182892000	0.000003000	1	2.365774000	2.153067000	-0.240459000
1	-0.127536000	-2.121943000	0.000001000	1	-0.089526000	2.122288000	-0.298972000
1	-0.040298000	2.156923000	-0.000002000	1	-0.071214000	-2.141764000	0.186174000
1	-3.249649000	-0.899789000	0.000001000	1	-1.811164000	1.685357000	0.599163000

Conformer of 2,6-dimethylbenzoic acid 11

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6	1.999507000	1.092026000	-0.088254000
6	2.620967000	-0.146072000	-0.035593000
6	1.855983000	-1.299105000	0.051621000
6	0.462993000	-1.243852000	0.068773000
6	-0.159084000	0.022022000	0.012629000
6	0.610740000	1.203823000	-0.050085000
6	-1.637463000	0.162572000	0.046683000
8	-2.289666000	-0.826267000	-0.601487000
8	-2.248542000	1.068799000	0.568422000
1	2.597562000	1.998993000	-0.153404000
1	3.706211000	-0.213531000	-0.057178000
1	2.342457000	-2.271192000	0.109950000
6	-0.291676000	-2.538370000	0.180738000
6	0.008332000	2.577703000	-0.094948000
1	0.392042000	-3.349327000	0.449990000
1	-1.081177000	-2.494169000	0.937468000
1	-0.781943000	-2.801861000	-0.761812000
1	-0.473059000	2.832146000	0.854067000
1	-0.770678000	2.666730000	-0.859135000
1	0.783025000	3.321464000	-0.306091000
1	-3.230560000	-0.613992000	-0.498712000

Coordinates for complex 4a_2,6-dimethylbenzoic acid 11

4a·11_1

6	5.575122000	1.045146000	-2.041826000
6	4.825607000	1.442203000	-0.774188000
6	3.506152000	0.686560000	-0.701769000
6	2.634162000	1.004996000	-1.930368000
6	3.382044000	0.569247000	-3.189425000
6	4.725914000	1.283084000	-3.286305000
7	1.258542000	0.547020000	-1.833652000
6	0.818014000	-0.668239000	-1.409935000
7	-0.421424000	-0.560579000	-0.843807000
6	-1.379041000	-1.520815000	-0.508190000
6	-2.418950000	-1.064130000	0.311267000
6	-3.470815000	-1.898996000	0.645993000
6	-3.509657000	-3.214977000	0.197351000
6	-2.467657000	-3.663517000	-0.602579000
6	-1.407716000	-2.837588000	-0.967500000
7	2.780894000	0.953025000	0.557416000
6	2.951625000	0.279217000	1.773004000
6	1.947598000	0.706538000	2.588956000
7	1.200420000	1.618757000	1.877517000
6	1.718905000	1.749347000	0.660861000
6	4.042283000	-0.662753000	2.061976000
6	4.956417000	-0.350974000	3.072391000
6	4.151623000	-1.877940000	1.378272000
6	5.177556000	-2.758318000	1.697829000
6	6.089237000	-2.441647000	2.700358000
6	5.976189000	-1.239329000	3.390593000
16	1.720883000	-2.085877000	-1.532021000
6	-2.436381000	-5.080098000	-1.092326000
9	-3.560723000	-5.742214000	-0.801373000
9	-1.419924000	-5.758561000	-0.545293000
9	-2.267291000	-5.134532000	-2.418922000
6	-4.603877000	-1.316983000	1.434128000
9	-4.167418000	-0.486439000	2.391614000
9	-5.347184000	-2.257704000	2.022911000
9	-5.418774000	-0.597695000	0.648449000
1	5.837609000	-0.022045000	-1.977550000
1	6.520609000	1.596502000	-2.103178000
1	4.619996000	2.524923000	-0.771275000
1	5.423414000	1.224468000	0.120777000
1	3.700970000	-0.392226000	-0.696631000
1	2.539071000	2.104334000	-1.983373000
1	2.750747000	0.794043000	-4.056673000
1	3.514253000	-0.520609000	-3.165311000
1	5.263877000	0.953975000	-4.182909000
1	4.556447000	2.365346000	-3.405414000
1	0.576714000	1.319505000	-1.791012000
1	-0.671458000	0.381881000	-0.498320000
1	-2.392349000	-0.037389000	0.673764000
1	-4.329906000	-3.872942000	0.464549000
1	-0.612426000	-3.216363000	-1.601370000
1	1.706947000	0.410141000	3.598383000
1	1.263825000	2.356762000	-0.122277000
1	4.862641000	0.595895000	3.601158000
1	3.414696000	-2.140102000	0.617781000
1	5.255572000	-3.704147000	1.168156000
1	6.887561000	-3.136833000	2.947827000
1	6.683875000	-0.991179000	4.177385000
6	-2.530518000	6.336584000	0.011954000
6	-3.883638000	6.070101000	0.169903000
6	-4.332334000	4.757810000	0.159249000
6	-3.443666000	3.692559000	0.006648000
6	-2.077761000	3.975322000	-0.170496000
6	-1.614366000	5.302950000	-0.174084000
6	-1.096901000	2.849475000	-0.345811000
8	-1.152464000	1.889487000	0.484047000
8	-0.256071000	2.922684000	-1.281207000
1	-2.171834000	7.365039000	0.024426000
1	-4.590164000	6.886989000	0.299539000
1	-5.394037000	4.544144000	0.275234000
6	-0.161079000	5.638651000	-0.350850000
6	-3.989320000	2.293034000	0.016597000
1	0.011108000	6.706196000	-0.178101000
1	0.476677000	5.080714000	0.348458000
1	0.185209000	5.380274000	-1.356006000
1	-5.068227000	2.302826000	-0.170385000
1	-3.523130000	1.657909000	-0.745325000
1	-3.826743000	1.796550000	0.982021000
1	0.236781000	1.929705000	2.026420000

4a·11_2

6	4.900234000	3.611788000	-0.338501000
6	4.826430000	2.214005000	-0.937769000
6	3.411443000	1.657355000	-0.837643000
6	2.880672000	1.697725000	0.605490000
6	3.045429000	3.071792000	1.252627000
6	4.478040000	3.572152000	1.125488000
7	1.527442000	1.157280000	0.717626000
6	0.372523000	1.679867000	0.223789000
7	-0.700915000	0.855642000	0.478428000
6	-2.065019000	1.077925000	0.261274000
6	-2.872655000	-0.038642000	0.029212000
6	-4.244322000	0.108703000	-0.135052000
6	-4.842578000	1.359773000	-0.073555000
6	-4.036194000	2.462419000	0.176905000
6	-2.664573000	2.336491000	0.353131000
7	3.297463000	0.301183000	-1.385258000
6	4.045155000	-0.841270000	-1.111818000
6	3.451651000	-1.836397000	-1.838517000
7	2.365115000	-1.361901000	-2.527380000
6	2.304062000	-0.083516000	-2.224696000
6	5.190409000	-0.937467000	-0.188019000
6	6.502308000	-0.866681000	-0.663394000
6	4.974722000	-1.158581000	1.175141000
6	6.047715000	-1.268329000	2.052323000
6	7.349572000	-1.174689000	1.571224000
6	7.575679000	-0.981381000	0.211818000
16	0.262559000	3.125632000	-0.624562000
6	-4.619083000	3.842618000	0.252624000
9	-5.955549000	3.827094000	0.273622000
9	-4.242290000	4.585378000	-0.793711000
9	-4.205449000	4.483412000	1.353000000
6	-5.067339000	-1.125991000	-0.337409000
9	-4.555036000	-1.904280000	-1.303477000
9	-6.328448000	-0.847819000	-0.676691000
9	-5.106037000	-1.867524000	0.776730000
1	4.236089000	4.293151000	-0.892893000
1	5.917795000	4.006860000	-0.442313000
1	5.522890000	1.563902000	-0.390295000
1	5.140249000	2.202794000	-1.989832000
1	2.741890000	2.278050000	-1.450111000
1	3.502114000	0.998153000	1.185761000
1	2.740042000	2.993212000	2.303600000
1	2.362913000	3.783073000	0.774478000
1	4.565540000	4.564148000	1.584247000
1	5.162477000	2.907264000	1.678716000
1	1.485397000	0.174224000	0.971080000
1	-0.455805000	-0.122769000	0.636387000
1	-2.430854000	-1.036183000	-0.016726000
1	-5.913054000	1.469767000	-0.206486000
1	-2.062176000	3.213242000	0.562756000
1	3.746504000	-2.878126000	-1.880233000
1	1.553519000	0.621997000	-2.566207000
1	6.668696000	-0.706716000	-1.727263000
1	3.950953000	-1.261004000	1.536676000
1	5.867681000	-1.438357000	3.111005000
1	8.189777000	-1.261655000	2.255688000
1	8.592461000	-0.920273000	-0.168355000
6	-2.044530000	-3.965027000	2.299416000
6	-3.113158000	-4.503139000	1.599590000
6	-3.136483000	-4.433958000	0.215701000
6	-2.100208000	-3.835341000	-0.499224000
6	-1.019572000	-3.278632000	0.224153000
6	-0.992461000	-3.335808000	1.637111000
6	0.077900000	-2.558091000	-0.472827000
8	0.377318000	-3.015407000	-1.669523000
8	0.659056000	-1.597196000	0.028427000
1	-2.020722000	-4.023978000	3.385924000
1	-3.934068000	-4.974483000	2.134630000
1	-3.986817000	-4.833984000	-0.333043000
6	1.053737000	-2.412315000	-2.102288000
6	0.119025000	-2.770823000	2.478020000
1	1.108073000	-2.947433000	2.045926000
1	0.022843000	-1.683948000	2.598240000
1	0.091129000	-3.215462000	3.477956000
6	-2.232287000	-3.764202000	-1.993913000
1	-3.213810000	-4.138071000	-2.298395000
1	-2.140493000	-2.735414000	-2.361044000
1	-1.460390000	-4.348615000	-2.501183000

4a·11_3

6	-5.871147000	1.379191000	-1.890154000
6	-5.407116000	0.173454000	-1.084228000
6	-3.901669000	0.218375000	-0.842620000
6	-3.140633000	0.323136000	-2.175472000
6	-3.611032000	1.539354000	-2.970001000
6	-5.114270000	1.471647000	-3.210594000
7	-1.693069000	0.202616000	-2.035141000
6	-0.847070000	1.015233000	-1.350955000
7	0.383687000	0.425384000	-1.173762000
6	1.509750000	0.984992000	-0.547933000
6	2.216603000	0.203140000	0.367227000
6	3.355320000	0.705917000	0.982170000
6	3.810850000	1.987918000	0.694693000
6	3.110559000	2.753250000	-0.227350000
6	1.969814000	2.264295000	-0.853306000
7	-3.462824000	-0.952278000	-0.076424000
6	-3.368708000	-1.082169000	1.305430000
6	-2.976024000	-2.380009000	1.514693000
7	-2.834515000	-3.046043000	0.323939000
6	-3.152185000	-2.163864000	-0.597643000
6	-3.686476000	-0.040506000	2.287244000
6	-4.570830000	-0.347542000	3.327827000
6	-3.094217000	1.227039000	2.251880000
6	-3.399053000	2.168767000	3.226492000
6	-4.281847000	1.855981000	4.255302000
6	-4.862129000	0.592691000	4.307860000
16	-1.233248000	2.547376000	-0.782493000

4a·11_4

6	-4.689917000	3.631077000	-0.881249000
6	-4.170846000	2.450689000	-1.693615000
6	-3.427423000	1.469139000	-0.798740000
6	-2.288799000	2.171315000	-0.036809000
6	-2.809619000	3.363398000	0.761924000
6	-3.548731000	4.332429000	-0.153212000
7	-1.475210000	1.231580000	0.727928000
6	-1.878974000	0.478359000	1.771472000
7	-0.956310000	-0.425065000	2.236683000
6	0.342682000	-0.692421000	1.730517000
6	1.462305000	-0.203195000	2.395700000
6	2.737360000	-0.528327000	1.940646000
6	2.904003000	-1.353765000	0.838742000
6	1.780152000	-1.853616000	0.185299000
6	0.503024000	-1.510491000	0.610892000
7	-2.887049000	0.335409000	-1.559007000
6	-3.019608000	-1.015893000	-1.258373000
6	-2.015181000	-1.640191000	-1.956279000
7	-1.268348000	-0.726177000	-2.659328000
6	-1.823790000	0.434728000	-2.397536000
6	-4.065692000	-1.583765000	-0.411593000
6	-5.398149000	-1.169831000	-0.512517000
6	-3.737372000	-2.585522000	0.507186000
6	-4.715951000	-3.159383000	1.306104000
6	-6.035500000	-2.730304000	1.209523000
6	-6.372997000	-1.733790000	0.299464000
16	-3.371513000	0.546800000	2.547359000

6	3.541933000	4.153067000	-0.547817000	6	1.961900000	-2.891498000	-0.882521000
9	4.776840000	4.412647000	-0.106268000	9	3.117035000	-2.731732000	-1.537945000
9	2.721317000	5.051619000	0.006080000	9	0.973085000	-2.889675000	-1.776957000
9	3.529218000	4.376141000	-1.867467000	9	1.993071000	-4.114821000	-0.334844000
6	4.129100000	-0.137487000	1.949192000	6	3.915743000	-0.002158000	2.704623000
9	3.379886000	-1.113165000	2.478007000	9	3.975795000	-0.558631000	3.921632000
9	4.611134000	0.590949000	2.961857000	9	3.819635000	1.320704000	2.892959000
9	5.182198000	-0.722599000	1.360757000	9	5.072757000	-0.246485000	2.090606000
1	-5.693012000	2.295070000	-1.306112000	1	-5.420714000	3.267359000	-0.142227000
1	-6.952538000	1.321587000	-2.061919000	1	-5.224229000	4.330506000	-1.535345000
1	-5.647388000	-0.756974000	-1.625155000	1	-3.490155000	2.818949000	-2.478876000
1	-5.920934000	0.116537000	-0.115567000	1	-4.986665000	1.926585000	-2.208653000
1	-3.654460000	1.105420000	-0.246087000	1	-4.116228000	1.050130000	-0.052612000
1	-3.422849000	-0.556411000	-2.778040000	1	-1.588681000	2.572501000	-0.786179000
1	-3.054477000	1.570564000	-3.914724000	1	-1.958194000	3.849179000	1.255301000
1	-3.354611000	2.451862000	-2.419465000	1	-3.477893000	3.003533000	1.553952000
1	-5.439255000	2.349716000	-3.781106000	1	-3.928848000	5.179887000	0.429562000
1	-5.355688000	0.591416000	-3.828998000	1	-2.850363000	4.753192000	-0.895406000
1	-1.333321000	-0.731018000	-2.214887000	1	-0.574034000	1.031957000	0.291143000
1	0.404598000	-0.589985000	-1.288412000	1	-1.263048000	-0.909610000	3.070665000
1	1.864748000	-0.797008000	0.613751000	1	1.333639000	0.435909000	3.267049000
1	4.696533000	2.384510000	1.181463000	1	3.900581000	-1.600444000	0.483922000
1	1.441036000	2.873559000	-1.579312000	1	-0.382181000	-1.875591000	0.090831000
1	-2.768580000	-2.852907000	2.467008000	1	-1.830459000	-2.706013000	-2.020805000
1	-3.127464000	-2.354967000	-1.662680000	1	-1.453267000	1.388725000	-2.751666000
1	-5.033042000	-1.332719000	3.352904000	1	-5.672059000	-0.414660000	-1.248038000
1	-2.370309000	1.469535000	1.473930000	1	-2.696285000	-2.888862000	0.609704000
1	-2.930331000	3.148976000	3.185904000	1	-4.445242000	-3.932746000	2.020667000
1	-4.512886000	2.594894000	5.018820000	1	-6.800039000	-3.170290000	1.844895000
1	-5.550335000	0.340364000	5.111054000	1	-7.404351000	-1.400185000	0.214465000
6	3.758278000	-3.423619000	0.404836000	6	4.667227000	2.283895000	-0.026954000
6	4.476120000	-3.119235000	-0.742064000	6	5.717231000	1.677323000	-0.696806000
6	3.811094000	-2.896438000	-1.937749000	6	5.454647000	0.855967000	-1.780435000
6	2.420444000	-2.948977000	-2.006619000	6	4.149549000	0.581225000	-2.192712000
6	1.699975000	-3.267094000	-0.834659000	6	3.076945000	1.151042000	-1.459188000
6	2.367819000	-3.515297000	0.384690000	6	3.342179000	2.048059000	-0.390308000
6	0.216178000	-3.235467000	-0.889614000	6	1.660134000	0.789369000	-1.729836000
8	-0.389403000	-2.382248000	-1.536711000	8	1.497468000	-0.226944000	-2.563848000
8	-0.398719000	-4.166007000	-0.194973000	8	0.705897000	1.345356000	-1.198940000
1	4.282213000	-3.565066000	1.347789000	1	4.869031000	2.950145000	0.809232000
1	5.559833000	-3.042318000	-0.696474000	1	6.743100000	1.863651000	-0.387645000
1	4.374365000	-2.664579000	-2.839737000	1	6.279468000	0.413927000	-2.336132000
1	-1.371881000	-3.932065000	-0.101659000	1	0.527635000	-0.443595000	-2.659492000
6	1.650623000	-3.803495000	1.673328000	6	4.005142000	-0.273956000	-3.421844000
1	1.155620000	-4.778599000	1.650641000	1	4.978970000	-0.368824000	-3.912959000
1	2.354718000	-3.790534000	2.510013000	1	3.641662000	-1.277854000	-3.186320000
1	0.868038000	-3.063353000	1.882259000	1	3.297116000	0.149463000	-4.138648000
6	1.768270000	-2.679584000	-3.334158000	6	2.289357000	2.783912000	0.390588000
1	2.502717000	-2.786263000	-4.138553000	1	1.646329000	3.384659000	-0.259008000
1	0.935028000	-3.357286000	-3.541503000	1	1.615521000	2.107442000	0.928763000
1	1.362625000	-1.661992000	-3.388332000	1	2.766991000	3.447490000	1.118496000

Benzaldehyde 7a

7a

6	1.318599000	-1.327680000	0.000038000
6	2.205141000	-0.250599000	-0.000048000
6	1.728662000	1.056772000	-0.000041000
6	0.359042000	1.287999000	0.000085000
6	-0.530344000	0.213816000	0.000040000
6	-0.047689000	-1.097338000	0.000002000
6	-1.981872000	0.466875000	-0.000025000
8	-2.832064000	-0.394302000	-0.000040000
1	1.701535000	-2.345122000	0.000206000
1	3.277217000	-0.433625000	-0.000158000
1	2.424861000	1.891526000	-0.000202000
1	-0.033370000	2.304789000	0.000253000
1	-0.767348000	-1.912704000	-0.000027000
1	-2.255622000	1.550475000	-0.000067000

Ternary complex of catalyst 4a/benzoic acid 9/benzaldehyde 7a

4a·9·7a_1

6	-4.758245000	-4.179296000	-0.293650000
6	-4.378564000	-3.051258000	0.657996000
6	-3.357047000	-2.127681000	0.003190000
6	-2.105327000	-2.901281000	-0.402366000
6	-2.490747000	-4.030588000	-1.356497000
6	-3.526254000	-4.958540000	-0.736316000
7	-1.116290000	-2.022340000	-0.989303000
6	0.200525000	-2.050350000	-0.664024000
7	0.917562000	-1.102319000	-1.316276000
6	2.269214000	-0.773125000	-1.172326000
6	2.596843000	0.587723000	-1.267965000
6	3.915840000	0.990553000	-1.156339000
6	4.935626000	0.064251000	-0.944929000
6	4.603394000	-1.279200000	-0.877622000
6	3.284948000	-1.710253000	-1.003917000
7	-3.033862000	-0.991245000	0.885217000
6	-3.853431000	0.114911000	1.092138000
6	-3.143097000	0.973593000	1.875018000
7	-1.921793000	0.392111000	2.120704000
6	-1.874044000	-0.787803000	1.512045000
6	-5.216753000	0.248630000	0.557842000
6	-6.284892000	0.356417000	1.452687000
6	-5.457690000	0.289933000	-0.821057000
6	-6.760918000	0.418039000	-1.286065000
6	-7.823378000	0.513186000	-0.391844000
6	-7.584178000	0.489876000	0.977953000
16	0.821380000	-3.116011000	0.508824000
6	5.640141000	-2.318668000	-0.590218000
9	6.877922000	-1.814679000	-0.560901000
9	5.622622000	-3.307985000	-1.487254000
9	5.420687000	-2.887618000	0.611995000
6	4.284856000	2.440196000	-1.221146000
9	3.234851000	3.230576000	-1.453747000
9	5.187384000	2.671300000	-2.182910000
9	4.846019000	2.848418000	-0.069513000
1	-5.258556000	-3.748125000	-1.175253000
1	-5.489186000	-4.840180000	0.186627000
1	-3.937643000	-3.462918000	1.579812000
1	-5.264127000	-2.473102000	0.952924000
1	-3.792904000	-1.676384000	-0.898512000
1	-1.655787000	-3.361275000	0.492294000
1	-1.573327000	-4.571759000	-1.618111000
1	-2.879418000	-3.589742000	-2.288197000
1	-3.802107000	-5.748451000	-1.444628000
1	-3.082474000	-5.461988000	0.136651000
1	-1.489020000	-1.187206000	-1.482554000
1	0.360549000	-0.346599000	-1.783368000
1	1.797913000	1.309485000	-1.431981000
1	5.967323000	0.388449000	-0.836758000
1	3.048023000	-2.768100000	-0.948570000
1	-3.395721000	1.962845000	2.225548000
1	-1.028764000	-1.473304000	1.533143000
1	-6.088067000	0.325027000	2.522941000
1	-4.606106000	0.270874000	-1.503033000
1	-6.945666000	0.457379000	-2.356629000
1	-8.839843000	0.614190000	-0.764371000
1	-8.410398000	0.571962000	1.679617000
1	-1.133254000	0.835977000	2.620290000
6	-3.459260000	4.447388000	-0.665295000
6	-2.469379000	5.423981000	-0.723553000
6	-1.179256000	5.077660000	-1.114649000
6	-0.881094000	3.760903000	-1.443322000
6	-1.865994000	2.773585000	-1.382213000
6	-3.156992000	3.130533000	-0.992541000
6	-1.511427000	1.341185000	-1.707385000
8	-0.337470000	1.134716000	-2.106832000
8	-2.390684000	0.451296000	-1.537822000
1	-4.472003000	4.714809000	-0.369868000
1	-2.704266000	6.455270000	-0.468184000
1	-0.403367000	5.838513000	-1.166572000
1	0.120311000	3.472380000	-1.754612000
1	-3.923877000	2.360885000	-0.953307000
8	0.042710000	1.923325000	3.290622000
1	1.528326000	3.254090000	3.550140000
6	1.227353000	2.221324000	3.268276000
6	2.334448000	1.341873000	2.918955000
6	2.126957000	0.004295000	2.556340000
1	1.114803000	-0.393406000	2.498879000
6	3.207776000	-0.807954000	2.261945000
6	4.501912000	-0.287904000	2.328597000
6	4.717314000	1.042696000	2.676563000
6	3.634145000	1.857613000	2.968280000
1	3.784063000	2.903255000	3.234561000
1	5.726502000	1.444867000	2.705108000
1	5.345713000	-0.931111000	2.088981000
1	3.039204000	-1.837332000	1.951121000

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6	-4.919721000	-3.412514000	-2.015340000
6	-4.566805000	-2.927022000	-0.615209000
6	-3.383568000	-1.967311000	-0.662153000
6	-2.163583000	-2.616126000	-1.313743000
6	-2.530873000	-3.108731000	-2.713043000
6	-3.715015000	-4.065020000	-2.682194000
7	-1.063728000	-1.680633000	-1.351924000
6	0.222408000	-1.989844000	-1.041943000
7	1.038926000	-0.912463000	-1.202888000
6	2.397195000	-0.714396000	-0.958776000
6	2.867454000	0.581504000	-1.243706000
6	4.192467000	0.906133000	-1.031013000
6	5.093709000	-0.029412000	-0.523258000
6	4.622280000	-1.299166000	-0.239237000
6	3.292554000	-1.659628000	-0.456692000
7	-3.063671000	-1.485821000	0.695035000
6	-3.795940000	-0.552741000	1.424570000
6	-3.134834000	-0.387141000	2.605315000
7	-2.029764000	-1.202739000	2.569985000
6	-1.996255000	-1.844204000	1.407405000
6	-5.019699000	0.107685000	0.952581000
6	-6.203510000	-0.036111000	1.681376000
6	-4.996478000	0.919064000	-0.187357000
6	-6.157771000	1.563956000	-0.594265000
6	-7.337591000	1.412425000	0.128376000
6	-7.359010000	0.616760000	1.269336000
16	0.673359000	-3.525605000	-0.488575000
6	5.504702000	-2.302107000	0.435177000
9	6.794733000	-1.956640000	0.401279000
9	5.393463000	-3.519639000	-0.098524000
9	5.166316000	-2.421649000	1.737302000
6	4.695454000	2.289156000	-1.308132000
9	3.730526000	3.120736000	-1.702991000
9	5.644380000	2.286092000	-2.252507000
9	5.257963000	2.828851000	-0.209291000
1	-5.254492000	-2.554697000	-2.619302000
1	-5.766109000	-4.107304000	-1.964150000
1	-4.293266000	-3.781902000	0.023747000
1	-5.423494000	-2.430556000	-0.140637000
1	-3.650764000	-1.068967000	-1.237758000
1	-1.855677000	-3.494682000	-0.722381000
1	-1.639919000	-3.583941000	-3.141088000
1	-2.760014000	-2.234930000	-3.343145000
1	-3.965847000	-4.392359000	-3.697896000
1	-3.436324000	-4.970950000	-2.121578000
1	-1.322900000	-0.675804000	-1.291184000
1	0.563481000	-0.051802000	-1.546983000
1	2.164675000	1.329258000	-1.607953000
1	6.131654000	0.236139000	-0.342953000
1	2.949869000	-2.665756000	-0.234971000
1	-3.356995000	0.265987000	3.435284000
1	-1.203888000	-2.529969000	1.107095000
1	-6.211092000	-0.667938000	2.568058000
1	-4.048429000	1.067476000	-0.705794000
1	-6.135936000	2.202000000	-1.474050000
1	-8.241898000	1.922762000	-0.194033000
1	-8.277893000	0.501615000	1.838632000
1	-1.208617000	-1.256209000	3.185810000
6	-2.666834000	4.804552000	0.569312000
6	-2.010030000	5.834006000	-0.099292000
6	-1.061595000	5.536200000	-1.074142000
6	-0.771705000	4.212651000	-1.380744000
6	-1.435978000	3.175481000	-0.724763000
6	-2.380933000	3.480836000	0.256295000
6	-1.100264000	1.741415000	-1.051734000
8	-0.137524000	1.533170000	-1.827136000
8	-1.812890000	0.842628000	-0.512003000
1	-3.402916000	5.035977000	1.336367000
1	-2.234857000	6.870646000	0.142751000
1	-0.545124000	6.340361000	-1.593792000
1	-0.028849000	3.952025000	-2.130218000
1	-2.877392000	2.660164000	0.771360000
8	0.506471000	-1.870316000	3.090944000
1	2.491097000	-2.038390000	2.775646000
6	1.580988000	-1.400482000	2.746342000
6	1.819550000	-0.023470000	2.316186000
6	0.790740000	0.824409000	1.881304000
1	-0.229827000	0.457980000	1.769064000
6	1.087437000	2.130991000	1.525023000
6	2.397505000	2.601584000	1.617659000
6	3.423090000	1.761635000	2.040872000
6	3.136138000	0.445724000	2.371716000
1	3.931813000	-0.240242000	2.661816000
1	4.445821000	2.124480000	2.079375000
1	2.622049000	3.626902000	1.332152000
1	0.297026000	2.785846000	1.163944000

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6	2.300228000	5.778130000	0.613587000
6	1.449377000	4.736960000	1.333951000
6	1.463934000	3.435668000	0.546428000
6	0.908336000	3.659023000	-0.874403000
6	1.780576000	4.682765000	-1.597527000
6	1.815235000	5.992876000	-0.816887000
7	0.648964000	2.418343000	-1.581629000
6	1.508744000	1.366094000	-1.650085000
7	0.832338000	0.171959000	-1.735257000
6	1.347253000	-1.076813000	-1.371098000
6	0.580701000	-1.819562000	-0.467905000
6	1.054205000	-3.028052000	0.023862000
6	2.283217000	-3.530049000	-0.386700000
6	3.015999000	-2.808227000	-1.323712000
6	2.565281000	-1.592221000	-1.824032000
7	0.733413000	2.356637000	1.243797000
6	1.279334000	1.196423000	1.807440000
6	0.216426000	0.415087000	2.164810000
7	-0.925926000	1.093706000	1.825402000
6	-0.599226000	2.249765000	1.268120000
6	2.707032000	0.905031000	1.931649000
6	3.627312000	1.869337000	2.354397000
6	3.160073000	-0.380640000	1.615235000
6	4.511163000	-0.685567000	1.692147000
6	5.423489000	0.286609000	2.088533000
6	4.978615000	1.560637000	2.427081000
16	3.184024000	1.509891000	-1.605081000
6	4.346878000	-3.359903000	-1.734582000
9	4.253218000	-4.652437000	-2.073788000
9	5.224783000	-3.298001000	-0.716917000
9	4.882537000	-2.708106000	-2.764549000
6	0.330256000	-3.702672000	1.142817000
9	-0.958019000	-3.332150000	1.217887000
9	0.885658000	-3.380258000	2.327052000
9	0.364774000	-5.032616000	1.049217000
1	3.345027000	5.429484000	0.596473000
1	2.292457000	6.720729000	1.173640000
1	0.410615000	5.094974000	1.426471000
1	1.813849000	4.564964000	2.356022000
1	2.491849000	3.065775000	0.447247000
1	-0.092941000	4.110829000	-0.772417000
1	1.373042000	4.830436000	-2.604397000
1	2.791721000	4.272854000	-1.718507000
1	2.455223000	6.720776000	-1.329264000
1	0.804578000	6.431466000	-0.790215000
1	-0.362031000	2.209622000	-1.574015000
1	-0.183968000	0.237390000	-1.532149000
1	-0.377491000	-1.417695000	-0.142584000
1	2.664027000	-4.469736000	0.006940000
1	3.155227000	-1.035992000	-2.542087000
1	0.200460000	-0.557010000	2.636350000
1	-1.314741000	2.918473000	0.804926000
1	3.283408000	2.862383000	2.639572000
1	2.453063000	-1.134194000	1.269056000
1	4.851039000	-1.678088000	1.406824000
1	6.483941000	0.051927000	2.132388000
1	5.687369000	2.318054000	2.752011000
6	-6.316386000	1.764358000	-1.485421000
6	-6.748227000	0.521787000	-1.942346000
6	-5.825488000	-0.499763000	-2.156057000
6	-4.478512000	-0.284113000	-1.892990000
6	-4.037832000	0.959793000	-1.441215000
6	-4.963041000	1.986778000	-1.252360000
6	-2.574980000	1.188783000	-1.156100000
8	-1.861395000	0.162254000	-0.977713000
8	-2.169152000	2.380472000	-1.123531000
1	-7.035746000	2.565264000	-1.326533000
1	-7.804888000	0.350974000	-2.138416000
1	-6.160843000	-1.470059000	-2.516760000
1	-1.912577000	0.803674000	1.899316000
1	-4.594415000	2.953718000	-0.917051000
1	-3.741457000	-1.071783000	-2.028643000
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6	-4.096849000	-2.911558000	0.752444000
6	-5.409474000	-3.381514000	0.697410000
6	-6.480887000	-2.529043000	0.946387000
6	-6.237244000	-1.197802000	1.253742000
6	-4.710022000	0.681593000	1.654753000
8	-3.633265000	1.204641000	1.898008000
1	-5.635867000	1.295011000	1.696776000
1	-2.838011000	-1.189579000	1.057525000
1	-3.266806000	-3.579886000	0.541824000
1	-5.597033000	-4.424043000	0.450566000
1	-7.500288000	-2.901838000	0.893119000
1	-7.061556000	-0.507878000	1.431528000

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6	0.298673000	5.958065000	-0.210056000
6	-0.155657000	4.789127000	0.658989000
6	0.410602000	3.489026000	0.107403000
6	-0.066852000	3.272384000	-1.343091000
6	0.428648000	4.428018000	-2.209557000
6	-0.099299000	5.752599000	-1.668716000
7	0.190521000	1.932035000	-1.836268000
6	1.372617000	1.262594000	-1.679921000
7	1.158420000	-0.075757000	-1.499675000
6	2.026762000	-1.088969000	-1.089582000
6	1.407347000	-2.182867000	-0.457784000
6	2.166497000	-3.229866000	0.030144000
6	3.555760000	-3.228412000	-0.087964000
6	4.156144000	-2.160211000	-0.733428000
6	3.413638000	-1.095417000	-1.244927000
7	0.068169000	2.328383000	0.955752000
6	0.941918000	1.560155000	1.732320000
6	0.217509000	0.483940000	2.160458000
7	-1.049290000	0.606103000	1.650351000
6	-1.117339000	1.711005000	0.921175000
6	2.360131000	1.845656000	1.942166000
6	2.828091000	3.126211000	2.251296000
6	3.274192000	0.795209000	1.806574000
6	4.633809000	1.025361000	1.956539000
6	5.093143000	2.306455000	2.244335000
6	4.189885000	3.353585000	2.396208000
16	2.868511000	2.031302000	-1.686729000
6	5.646681000	-2.088895000	-0.866271000
9	6.244886000	-3.230654000	-0.512695000
9	6.156666000	-1.119409000	-0.085375000
9	6.020242000	-1.804937000	-2.116701000
6	1.518180000	-4.376847000	0.741658000
9	0.185262000	-4.326987000	0.691328000
9	1.869162000	-4.396486000	2.037903000
9	1.900074000	-5.551644000	0.225841000
1	1.394386000	6.045050000	-0.139429000
1	-0.115457000	6.895832000	0.179410000
1	-1.256633000	4.727737000	0.665870000
1	0.157738000	4.926352000	1.702831000
1	1.506920000	3.525177000	0.101754000
1	-1.168483000	3.336045000	-1.341604000
1	0.090812000	4.254924000	-3.237835000
1	1.525759000	4.422725000	-2.229346000
1	0.266465000	6.584722000	-2.281731000
1	-1.198522000	5.769239000	-1.746677000
1	-0.677334000	1.377665000	-1.836719000
1	0.164066000	-0.331124000	-1.343011000
1	0.323019000	-2.187567000	-0.355457000
1	4.147350000	-4.049648000	0.306062000
1	3.909332000	-0.268302000	-1.741715000
1	0.512705000	-0.343315000	2.788186000
1	-1.948500000	1.961569000	0.268188000
1	2.122531000	3.943878000	2.391000000
1	2.916106000	-0.196493000	1.531581000
1	5.334870000	0.207745000	1.815584000
1	6.159551000	2.490694000	2.346563000
1	4.547189000	4.352904000	2.631404000
6	-6.054936000	-1.236162000	-2.068758000
6	-6.043899000	-2.595420000	-1.765474000
6	-4.870608000	-3.198612000	-1.318816000
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6	-3.721594000	-1.076638000	-1.466226000
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6	-2.475236000	-0.250124000	-1.273547000
8	-1.439593000	-0.859424000	-0.894080000
8	-2.555871000	0.991513000	-1.485084000
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1	-6.950024000	-3.186580000	-1.882324000
1	-4.857087000	-4.262601000	-1.090609000
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1	-4.880931000	0.583246000	-2.141679000
1	-2.782182000	-2.884839000	-0.825896000
6	-5.331786000	-0.726314000	1.477229000
6	-5.103082000	0.623953000	1.197048000
6	-6.169080000	1.464249000	0.926136000
6	-7.469417000	0.958894000	0.935143000
6	-7.704528000	-0.385549000	1.205130000
6	-6.633645000	-1.229007000	1.470124000
6	-4.223831000	-1.631710000	1.788797000
8	-3.059226000	-1.306030000	1.937558000
1	-4.518271000	-2.695878000	1.921111000
1	-4.080032000	0.992156000	1.178003000
1	-5.993919000	2.512437000	0.698825000
1	-8.305943000	1.620592000	0.723125000
1	-8.719427000	-0.773950000	1.203715000
1	-6.797273000	-2.286720000	1.674077000

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6	-4.147324000	-4.961816000	-0.637178000
6	-3.191974000	-4.426692000	0.425316000
6	-2.665756000	-3.067685000	-0.009346000
6	-1.917483000	-3.185561000	-1.350020000
6	-2.886269000	-3.691933000	-2.416445000
6	-3.468805000	-5.039699000	-2.001944000
7	-1.153240000	-1.998089000	-1.675776000
6	-1.607714000	-0.715246000	-1.584843000
7	-0.588320000	0.141502000	-1.281992000
6	-0.560188000	1.525430000	-1.126247000
6	0.705294000	2.129682000	-1.228227000
6	0.840825000	3.496142000	-1.047120000
6	-0.257836000	4.296524000	-0.737697000
6	-1.497740000	3.689641000	-0.618624000
6	-1.665244000	2.321392000	-0.814836000
7	-1.803700000	-2.441371000	1.013616000
6	-2.096974000	-1.311660000	1.784714000
6	-0.931581000	-0.968442000	2.408655000
7	0.030845000	-1.862933000	2.010218000
6	-0.507530000	-2.732740000	1.168058000
6	-3.383031000	-0.618433000	1.817334000

4a·9·7a_6

6	-3.545633000	-5.342659000	-0.018559000
6	-2.721627000	-4.473655000	0.927497000
6	-2.421561000	-3.144343000	0.249614000
6	-1.603833000	-3.389138000	-1.034257000
6	-2.457442000	-4.209053000	-1.999419000
6	-2.836343000	-5.540055000	-1.355903000
7	-0.974051000	-2.195608000	-1.566741000
6	-1.569164000	-0.973104000	-1.663825000
7	-0.658103000	0.031930000	-1.468372000
6	-0.822476000	1.392226000	-1.225575000
6	0.356327000	2.121599000	-1.008676000
6	0.298584000	3.465908000	-0.667334000
6	-0.915980000	4.126106000	-0.529771000
6	-2.078266000	3.400068000	-0.758888000
6	-2.050303000	2.056802000	-1.109793000
7	-1.751126000	-2.183552000	1.147207000
6	-2.316401000	-1.037751000	1.717417000
6	-1.278501000	-0.346070000	2.275988000
7	-0.127499000	-1.052427000	2.033342000
6	-0.428623000	-2.149699000	1.352030000
6	-3.721040000	-0.640381000	1.641777000

6	-4.603185000	-1.297337000	1.876765000	6	-4.783423000	-1.542250000	1.751782000
6	-3.380673000	0.779408000	1.760265000	6	-3.999679000	0.716829000	1.446402000
6	-4.574173000	1.486610000	1.738340000	6	-5.307121000	1.164435000	1.338885000
6	-5.784499000	0.801144000	1.773946000	6	-6.357790000	0.256560000	1.428513000
6	-5.796438000	-0.587671000	1.850026000	6	-6.093279000	-1.092271000	1.640408000
16	-3.219722000	-0.289304000	-1.829348000	16	-3.209972000	-0.784419000	-1.987494000
6	-2.683162000	4.483329000	-0.163179000	6	-3.404771000	4.050837000	-0.509941000
9	-2.533213000	5.792901000	-0.375368000	9	-3.391813000	5.353001000	-0.806461000
9	-2.878075000	4.321803000	1.163441000	9	-3.740111000	3.956648000	0.796221000
9	-3.813518000	4.098946000	-0.759792000	9	-4.395129000	3.481989000	-1.198296000
6	2.175190000	4.165691000	-1.168055000	6	1.584195000	4.171888000	-0.374926000
9	3.153386000	3.325295000	-1.507067000	9	2.090978000	3.776124000	0.810639000
9	2.532370000	4.736567000	0.002822000	9	1.447048000	5.496197000	-0.318754000
9	2.149421000	5.150644000	-2.071643000	9	2.523832000	3.899225000	-1.292025000
1	-5.017981000	-4.289805000	-0.698730000	1	-4.517464000	-4.851951000	-0.188586000
1	-4.529735000	-5.944170000	-0.335570000	1	-3.761086000	-6.309323000	0.451988000
1	-2.344100000	-5.119126000	0.556433000	1	-1.773510000	-4.975318000	1.181166000
1	-3.688160000	-4.349818000	1.402611000	1	-3.251578000	-4.308626000	1.875894000
1	-3.496970000	-2.366784000	-0.154932000	1	-3.359017000	-2.654595000	-0.037744000
1	-1.146087000	-3.965848000	-1.233633000	1	-0.744218000	-4.024316000	-0.761027000
1	-2.344532000	-3.768385000	-3.366240000	1	-1.885838000	-4.364605000	-2.921451000
1	-3.681107000	-2.949349000	-2.561333000	1	-3.351753000	-3.632845000	-2.270417000
1	-4.179420000	-5.393050000	-2.758360000	1	-3.468373000	-6.123584000	-2.035630000
1	-2.663122000	-5.790284000	-1.958038000	1	-1.924371000	-6.136113000	-1.191673000
1	-0.144893000	-2.162190000	-1.531578000	1	0.037341000	-2.217112000	-1.367343000
1	0.347067000	-0.302760000	-1.143580000	1	0.315357000	-0.284074000	-1.280385000
1	1.572849000	1.508167000	-1.444653000	1	1.318051000	1.615100000	-1.103865000
1	-0.142849000	5.367349000	-0.593925000	1	-0.955776000	5.175714000	-0.257911000
1	-2.646519000	1.864747000	-0.728380000	1	-2.971073000	1.513005000	-1.290669000
1	-0.732977000	-0.173272000	3.111773000	1	-1.286931000	0.578997000	2.832490000
1	0.070445000	-3.460710000	0.607221000	1	0.316928000	-2.816164000	0.918584000
1	-4.619446000	-2.383108000	1.953520000	1	-4.589453000	-2.597045000	1.937824000
1	-2.432208000	1.308987000	1.679188000	1	-3.175657000	1.418625000	1.337524000
1	-4.552192000	2.570728000	1.662430000	1	-5.493894000	2.220322000	1.160651000
1	-6.721562000	1.350887000	1.740100000	1	-7.384550000	0.599976000	1.331774000
1	-6.741446000	-1.123314000	1.889858000	1	-6.912376000	-1.802066000	1.723159000
6	5.465676000	-4.058969000	-0.645870000	6	5.725017000	-3.556642000	-0.265522000
6	6.414328000	-3.043237000	-0.749032000	6	6.592141000	-2.633659000	-0.844272000
6	6.003218000	-1.721669000	-0.896233000	6	6.091398000	-1.449920000	-1.379075000
6	4.647367000	-1.415107000	-0.932884000	6	4.729527000	-1.182970000	-1.318926000
6	3.692415000	-2.427615000	-0.831848000	6	3.854439000	-2.107700000	-0.749519000
6	4.111597000	-3.751752000	-0.692716000	6	4.359884000	-3.300388000	-0.232495000
6	2.222405000	-2.094213000	-0.867333000	6	2.376705000	-1.835486000	-0.714995000
8	1.918860000	-0.870708000	-0.860274000	8	2.001401000	-0.635537000	-0.843851000
8	1.405190000	-3.052774000	-0.909780000	8	1.610215000	-2.826096000	-0.569584000
1	5.786131000	-5.092607000	-0.534391000	1	6.114928000	-4.484253000	0.148477000
1	7.474934000	-3.284509000	-0.720353000	1	7.659896000	-2.839984000	-0.882435000
1	6.741506000	-0.926296000	-0.981601000	1	6.767013000	-0.725544000	-1.829890000
1	1.045705000	-1.857399000	2.223927000	1	0.857607000	-0.776724000	2.250701000
1	3.349837000	-4.524112000	-0.622763000	1	3.659190000	-4.018192000	0.186388000
1	4.305409000	-0.386621000	-1.030820000	1	4.320296000	-0.255754000	-1.712993000
6	3.965976000	-0.205676000	1.962945000	6	4.318354000	0.695385000	1.330476000
6	2.881981000	0.641345000	1.708738000	6	5.291832000	-0.109292000	1.932352000
6	3.104701000	1.986348000	1.467769000	6	6.632355000	0.155491000	1.711045000
6	4.404794000	2.490612000	1.473743000	6	7.002370000	1.220719000	0.889571000
6	5.487942000	1.653322000	1.727752000	6	6.036559000	2.017704000	0.281624000
6	5.266811000	0.305988000	1.969521000	6	4.690963000	1.754654000	0.500474000
6	3.783598000	-1.636683000	2.187744000	6	2.903453000	0.429961000	1.570109000
8	2.715317000	-2.210969000	2.335968000	8	2.502095000	-0.466392000	2.305857000
1	4.726204000	-2.223525000	2.240320000	1	2.191269000	1.120884000	1.073606000
1	1.877007000	0.229729000	1.651084000	1	4.967787000	-0.942146000	2.551564000
1	2.269797000	2.650053000	1.257357000	1	7.394858000	-0.471974000	2.165163000
1	4.567104000	3.545207000	1.266710000	1	8.056530000	1.426334000	0.716744000
1	6.498938000	2.051816000	1.727180000	1	6.333456000	2.841629000	-0.361843000
1	6.101347000	-0.371938000	2.145686000	1	3.923377000	2.361440000	0.024964000

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6	4.633236000	-0.647832000	3.817433000
6	4.177309000	-1.717064000	2.831972000
6	3.410256000	-1.092734000	1.675021000
6	2.225019000	-0.249000000	2.184197000
6	2.687887000	0.807948000	3.184070000
6	3.444496000	0.154992000	4.334452000
7	1.399476000	0.256290000	1.094609000
6	1.782907000	1.093749000	0.105689000
7	0.888046000	1.225543000	-0.917433000
6	-0.428736000	0.688264000	-0.944450000
6	-1.474553000	1.365575000	-0.320207000
6	-2.773927000	0.882445000	-0.425025000
6	-3.042342000	-0.281993000	-1.134425000
6	-1.992467000	-0.967537000	-1.733144000
6	-0.686764000	-0.494050000	-1.632294000
7	2.920337000	-2.113819000	0.740023000
6	2.998696000	-2.103572000	-0.649892000
6	2.042708000	-2.996352000	-1.070120000
7	1.391161000	-3.547818000	0.003915000
6	1.939291000	-2.993166000	1.059752000
6	3.967241000	-1.326394000	-1.418709000
6	5.292094000	-1.181156000	-0.992416000
6	3.573418000	-0.718048000	-2.614591000
6	4.472963000	0.037875000	-3.352288000
6	5.778195000	0.204519000	-2.901608000
6	6.186937000	-0.412945000	-1.724789000
16	3.235571000	1.951622000	0.036598000
6	-2.239862000	-2.193533000	-2.562599000
9	-3.512658000	-2.593651000	-2.514281000
9	-1.477205000	-3.217330000	-2.168152000
9	-1.939103000	-1.960695000	-3.847238000
6	-3.873263000	1.667942000	0.224703000
9	-3.940426000	2.909353000	-0.279204000
9	-3.665966000	1.802405000	1.542103000
9	-5.072813000	1.109344000	0.057842000
1	5.337704000	0.031809000	3.313331000
1	5.181136000	-1.111926000	4.646357000
1	3.528899000	-2.440109000	3.353437000
1	5.027247000	-2.289494000	2.437453000
1	4.072660000	-0.429105000	1.104155000
1	1.547182000	-0.928448000	2.725424000
1	1.806766000	1.355787000	3.542584000
1	3.331379000	1.532698000	2.670594000
1	3.779536000	0.920379000	5.044809000
1	2.771114000	-0.515417000	4.893562000
1	0.539658000	-0.276595000	0.961245000

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6	6.419228000	-1.439589000	1.331680000
6	5.699226000	-1.350614000	-0.006552000
6	4.346055000	-0.665914000	0.138794000
6	3.479959000	-1.325564000	1.228992000
6	4.232749000	-1.501464000	2.547222000
6	5.566811000	-2.204186000	2.336525000
7	2.186441000	-0.662618000	1.381121000
6	1.957796000	0.578877000	1.856059000
7	0.636792000	0.954235000	1.923521000
6	-0.482534000	0.402556000	1.261011000
6	-1.657044000	0.215022000	1.987373000
6	-2.838105000	-0.127636000	1.335868000
6	-2.874172000	-0.273950000	-0.044550000
6	-1.695574000	-0.100368000	-0.762067000
6	-0.500959000	0.202410000	-0.119242000
7	3.619872000	-0.675978000	-1.138134000
6	2.909594000	0.367587000	-1.724410000
6	2.115552000	-0.230073000	-2.674344000
7	2.315144000	-1.589801000	-2.691420000
6	3.212263000	-1.810107000	-1.758506000
6	3.108150000	1.777299000	-1.379448000
6	4.399207000	2.303555000	-1.254154000
6	2.015124000	2.627078000	-1.180996000
6	2.206331000	3.961380000	-0.847499000
6	3.493492000	4.467304000	-0.706702000
6	4.589173000	3.636293000	-0.917135000
16	3.116331000	1.675408000	2.392105000
6	-1.683348000	-0.150992000	-2.261718000
9	-2.912131000	-0.212557000	-2.779446000
9	-0.994370000	-1.198101000	-2.725292000
9	-1.086063000	0.941214000	-2.772185000
6	-4.074739000	-0.276684000	2.167473000
9	-4.323343000	0.847962000	2.864231000
9	-3.946569000	-1.251660000	3.075809000
9	-5.157379000	-0.541251000	1.435164000
1	6.610127000	-0.424920000	1.714367000
1	7.396962000	-1.918422000	1.198915000
1	5.559528000	-2.369705000	-0.402494000
1	6.294146000	-0.808008000	-0.753353000
1	4.495179000	0.384597000	0.419631000
1	3.216949000	-2.331091000	0.864728000
1	3.589250000	-2.065411000	3.234380000
1	4.399716000	-0.516855000	2.999707000
1	6.090343000	-2.302192000	3.295062000
1	5.402749000	-3.228860000	1.963397000
1	1.402173000	-1.218163000	1.041077000

1	1.120894000	1.926530000	-1.622124000	1	0.511120000	1.913742000	2.240292000
1	-1.259467000	2.276141000	0.237383000	1	-1.642660000	0.371813000	3.064632000
1	-4.060008000	-0.653782000	-1.207350000	1	-3.807810000	-0.495835000	-0.552094000
1	0.141462000	-1.037537000	-2.086806000	1	0.411541000	0.324412000	-0.701149000
1	1.832589000	-3.306653000	-2.086844000	1	1.440232000	0.257616000	-3.366730000
1	1.621215000	-3.160910000	2.081876000	1	3.561323000	-2.790649000	-1.456539000
1	5.624550000	-1.686899000	-0.086955000	1	5.258473000	1.661177000	-1.442148000
1	2.544933000	-0.826709000	-2.953855000	1	1.004120000	2.237630000	-1.286578000
1	4.147520000	0.516300000	-4.272533000	1	1.343602000	4.599067000	-0.670701000
1	6.477620000	0.811789000	-3.470651000	1	3.643610000	5.508504000	-0.432641000
1	7.210971000	-0.300853000	-1.376964000	1	5.598139000	4.030017000	-0.821095000
6	-4.887252000	-1.184847000	2.188312000	6	-2.913504000	-3.722681000	1.265450000
6	-5.776901000	-2.065912000	1.577316000	6	-3.886654000	-4.084686000	0.337155000
6	-5.298789000	-3.152952000	0.851030000	6	-3.561971000	-4.194341000	-1.012364000
6	-3.930257000	-3.363030000	0.732215000	6	-2.264454000	-3.940198000	-1.438412000
6	-3.037758000	-2.479402000	1.341930000	6	-1.289163000	-3.567396000	-0.510283000
6	-3.520604000	-1.391003000	2.070028000	6	-1.619589000	-3.457172000	0.841052000
6	-1.569461000	-2.626338000	1.169952000	6	0.082221000	-3.194704000	-0.934581000
8	-1.228285000	-3.781747000	0.635644000	8	0.354590000	-3.479359000	-2.195156000
8	-0.781685000	-1.744344000	1.487699000	8	0.875084000	-2.650818000	-0.177186000
1	-5.259481000	-0.324274000	2.738898000	1	-3.169514000	-3.634065000	2.317327000
1	-6.848382000	-1.900726000	1.663612000	1	-4.903767000	-4.281178000	0.668533000
1	-5.995247000	-3.836005000	0.371115000	1	-4.323693000	-4.477050000	-1.734735000
1	-0.258795000	-3.790839000	0.370841000	1	1.123764000	-2.916994000	-2.496824000
1	-2.805187000	-0.705988000	2.519180000	1	-0.850859000	-3.145900000	1.544534000
1	-3.539105000	-4.195448000	0.153501000	1	-1.996622000	-4.013433000	-2.488713000
6	-0.505928000	4.593712000	-0.937442000	6	-3.030820000	3.225668000	0.317971000
6	0.548003000	4.327246000	-0.056863000	6	-2.559791000	3.264457000	-0.997722000
6	0.382538000	4.557647000	1.299841000	6	-3.427192000	3.003827000	-2.047249000
6	-0.828417000	5.062112000	1.777044000	6	-4.761903000	2.694803000	-1.786412000
6	-1.870177000	5.353279000	0.899646000	6	-5.238741000	2.665213000	-0.478672000
6	-1.704492000	5.128169000	-0.460886000	6	-4.373566000	2.938078000	0.572695000
6	-0.403649000	4.219440000	-2.352602000	6	-2.107020000	3.390328000	1.450006000
8	0.449875000	3.489768000	-2.819115000	8	-0.902547000	3.518730000	1.353287000
1	-1.208250000	4.634449000	-3.003665000	1	-2.603242000	3.357556000	2.450194000
1	1.486407000	3.922117000	-0.435915000	1	-1.509788000	3.489663000	-1.173926000
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4a·9·7a_9

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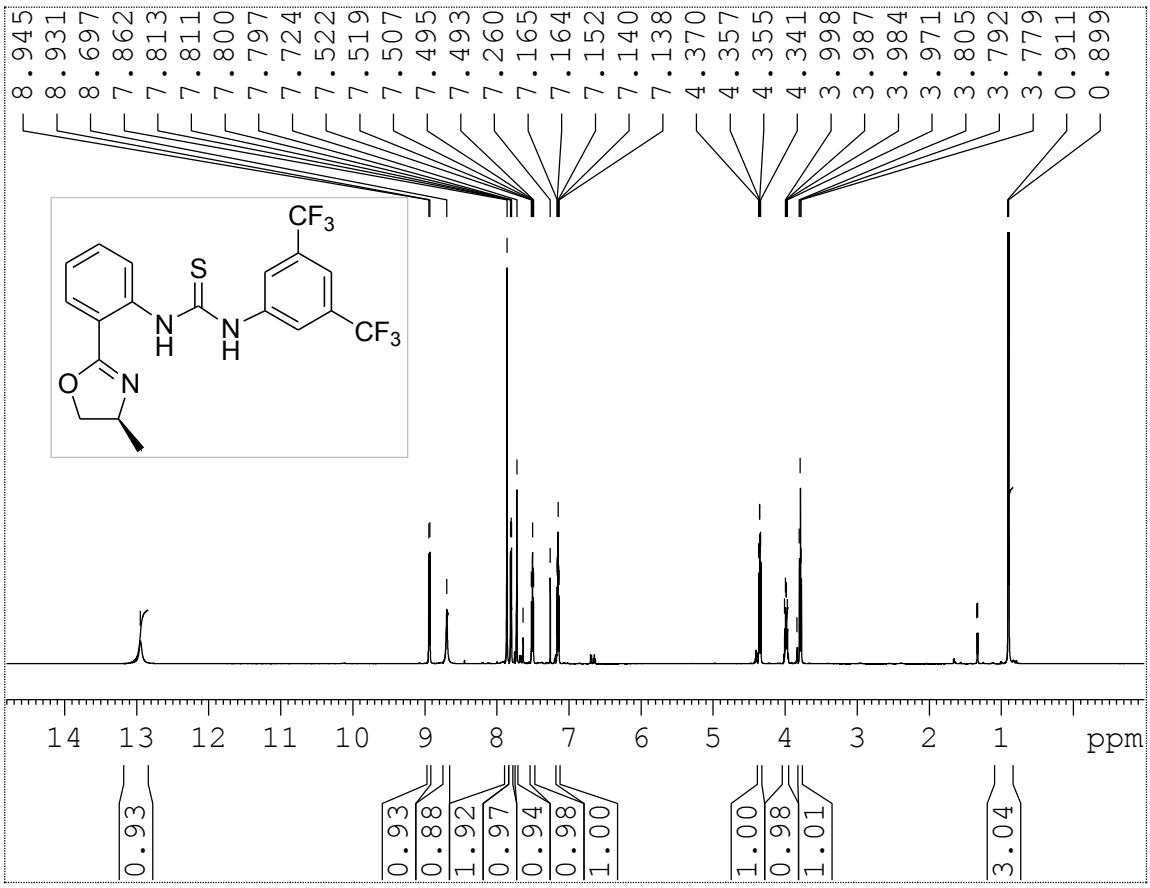
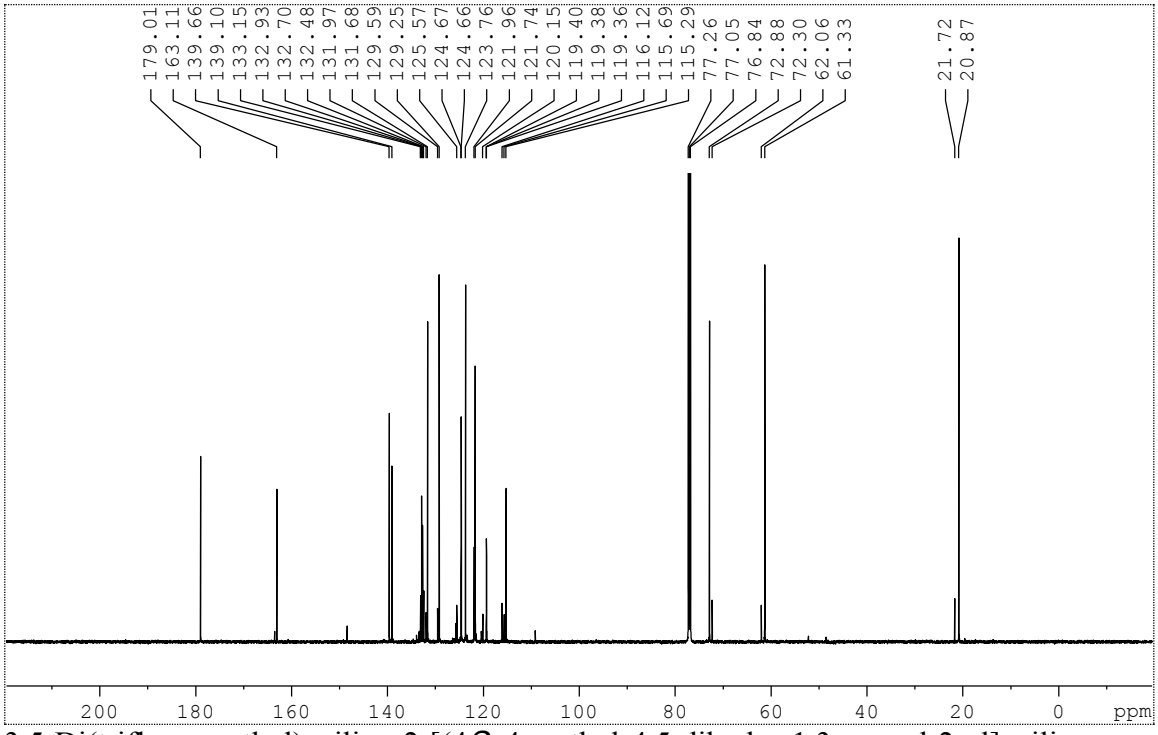
1	-0.962120000	3.745864000	-1.509441000	1	-6.713761000	-0.864947000	1.598348000

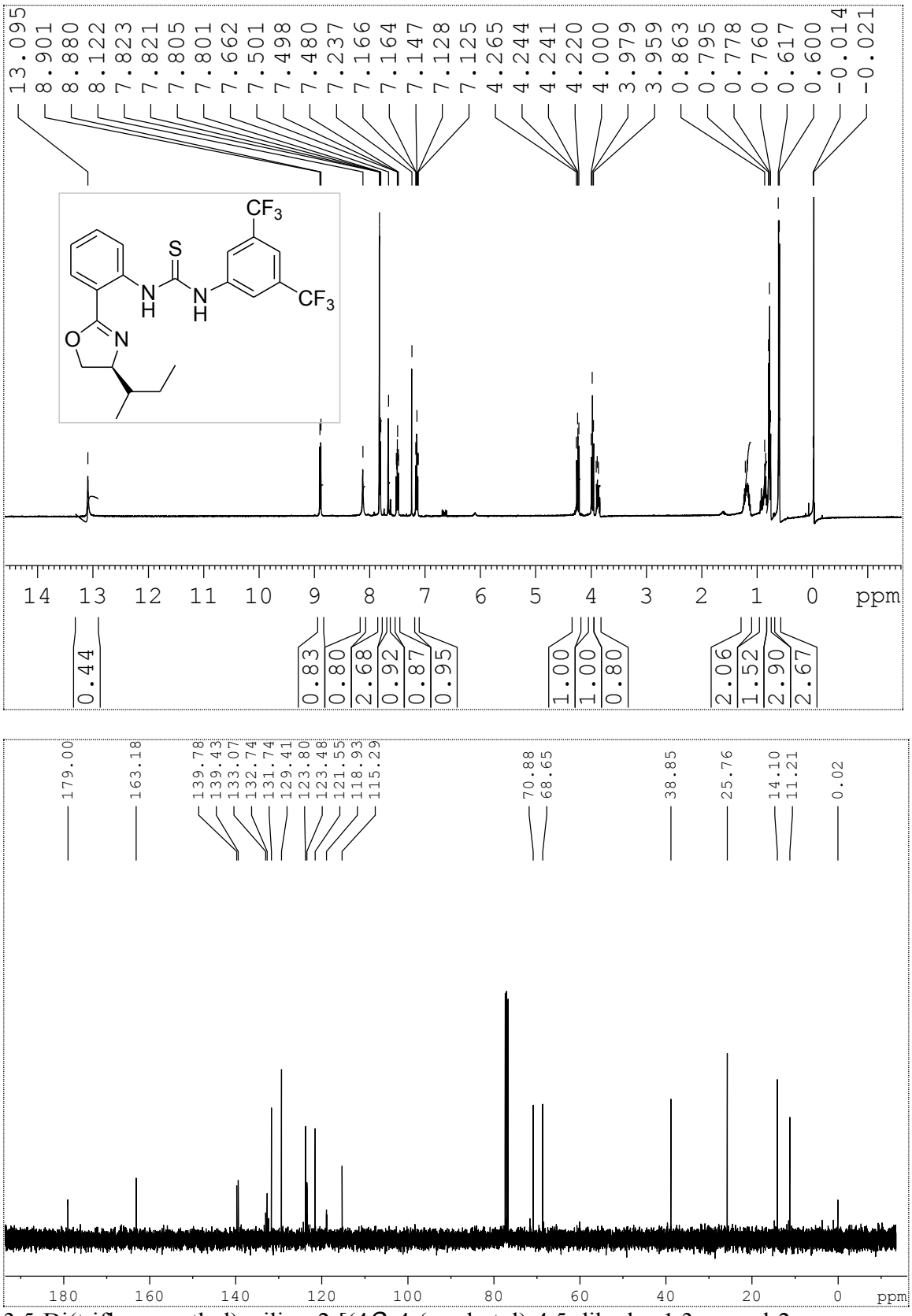
Copies of NMR spectra of 2a–g, 3a, 4a–b, and 7l–m



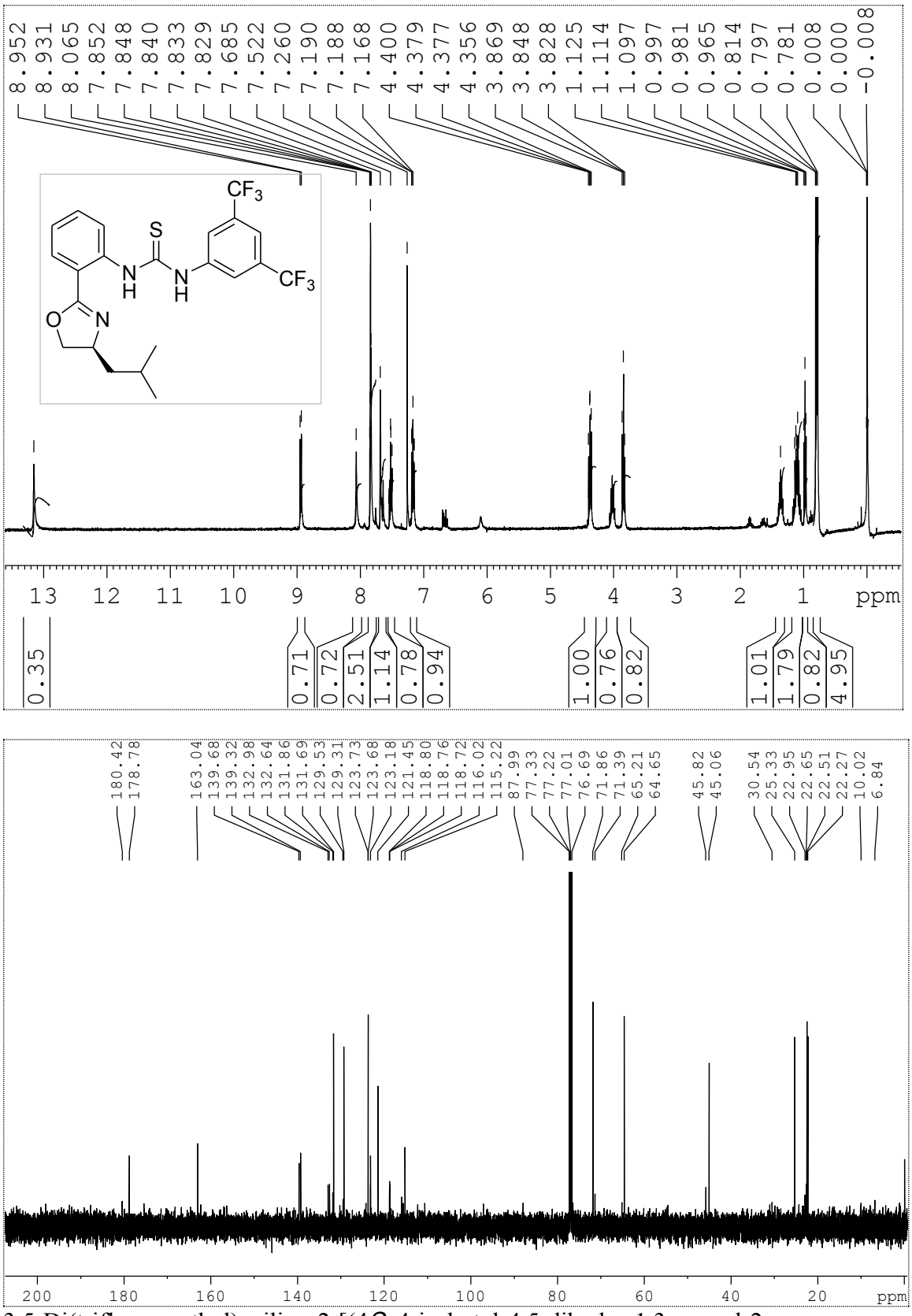


3,5-Di(trifluoromethyl)anilino-2-[(4*S*)-4-methyl-4,5-dihydro-1,3-oxazol-2-yl]aniline-methanethione (**2a**)

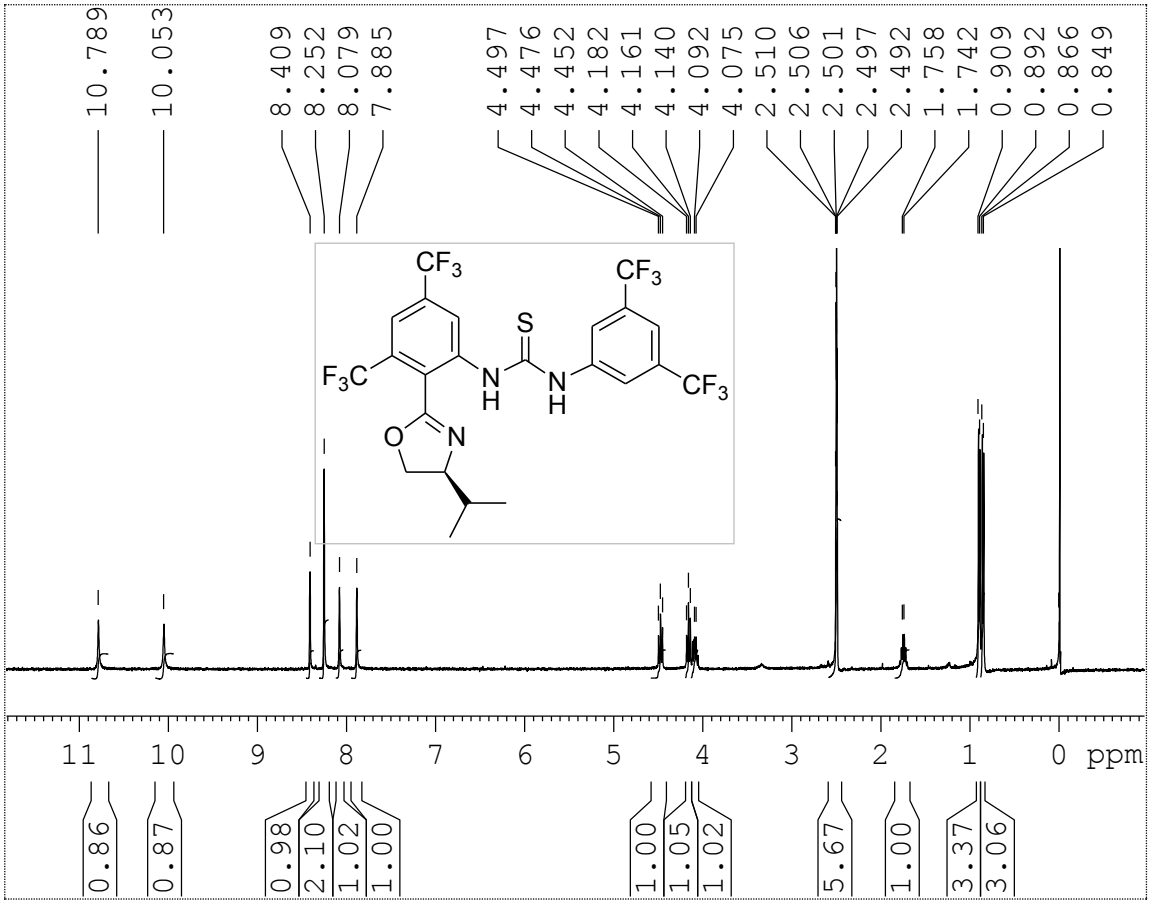
2-[(4*S*)-4-Benzyl-4,5-dihydro-1,3-oxazol-2-yl]anilino-3,5-di(trifluoromethyl)anilino-methanethione (**2b**)

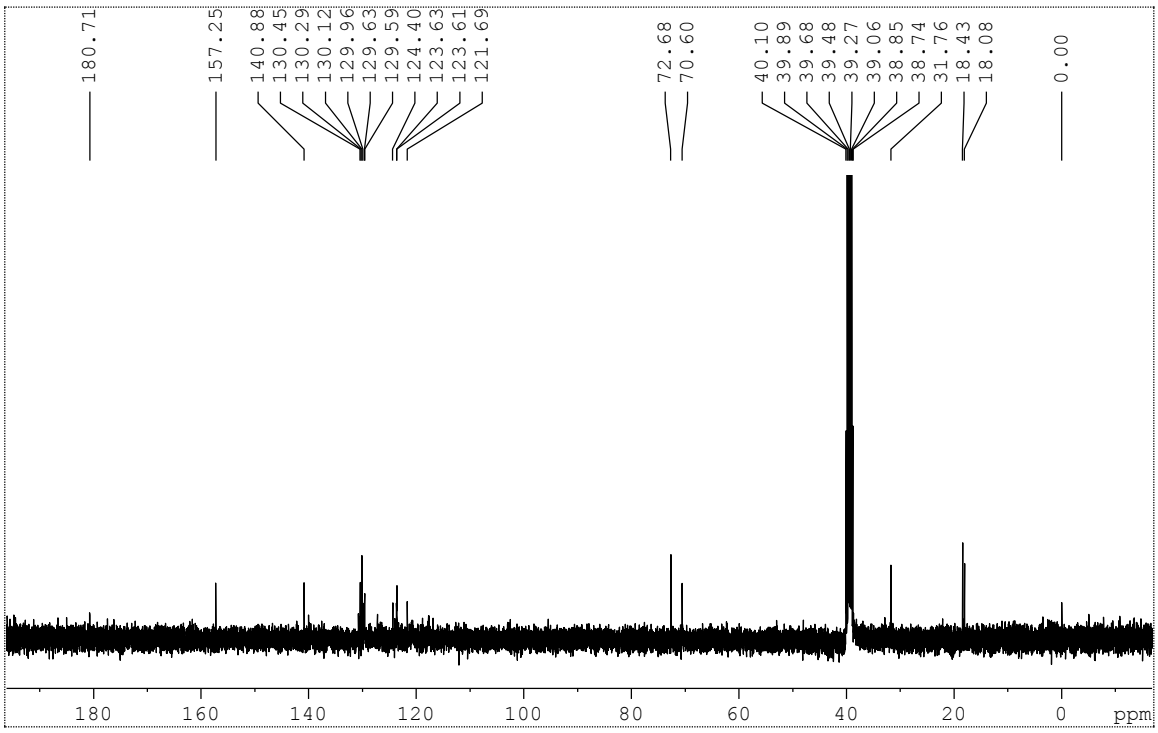


3,5-Di(trifluoromethyl)anilino-2-[(4*S*)-4-(*sec*-butyl)-4,5-dihydro-1,3-oxazol-2-yl]aniline methanethione (**2c**)

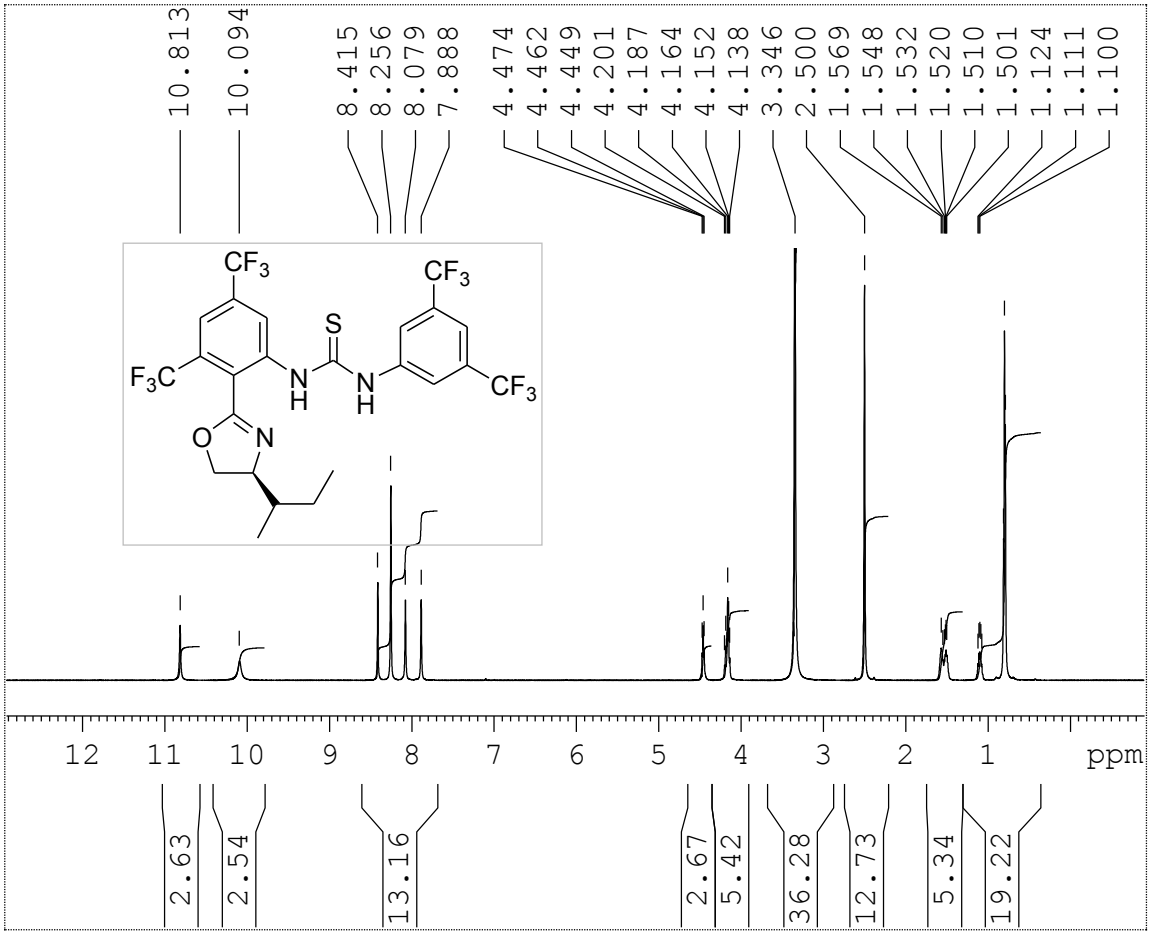


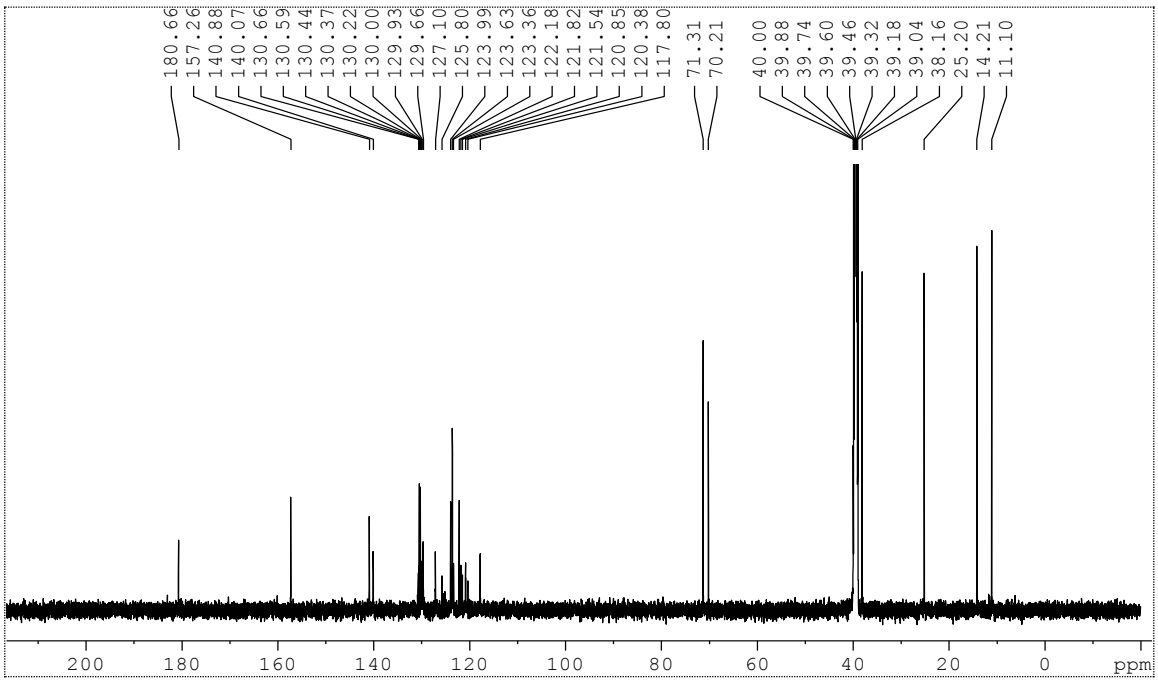
3,5-Di(trifluoromethyl)anilino-2-[(4*S*)-4-isobutyl-4,5-dihydro-1,3-oxazol-2-yl]aniline-methanethione (**2d**)





3,5-Di(trifluoromethyl)anilino-2-[(4*S*)-4-isopropyl-4,5-dihydro-1,3-oxazol-2-yl]-3,5-di(trifluoromethyl)anilinomethanethione (**2e**)





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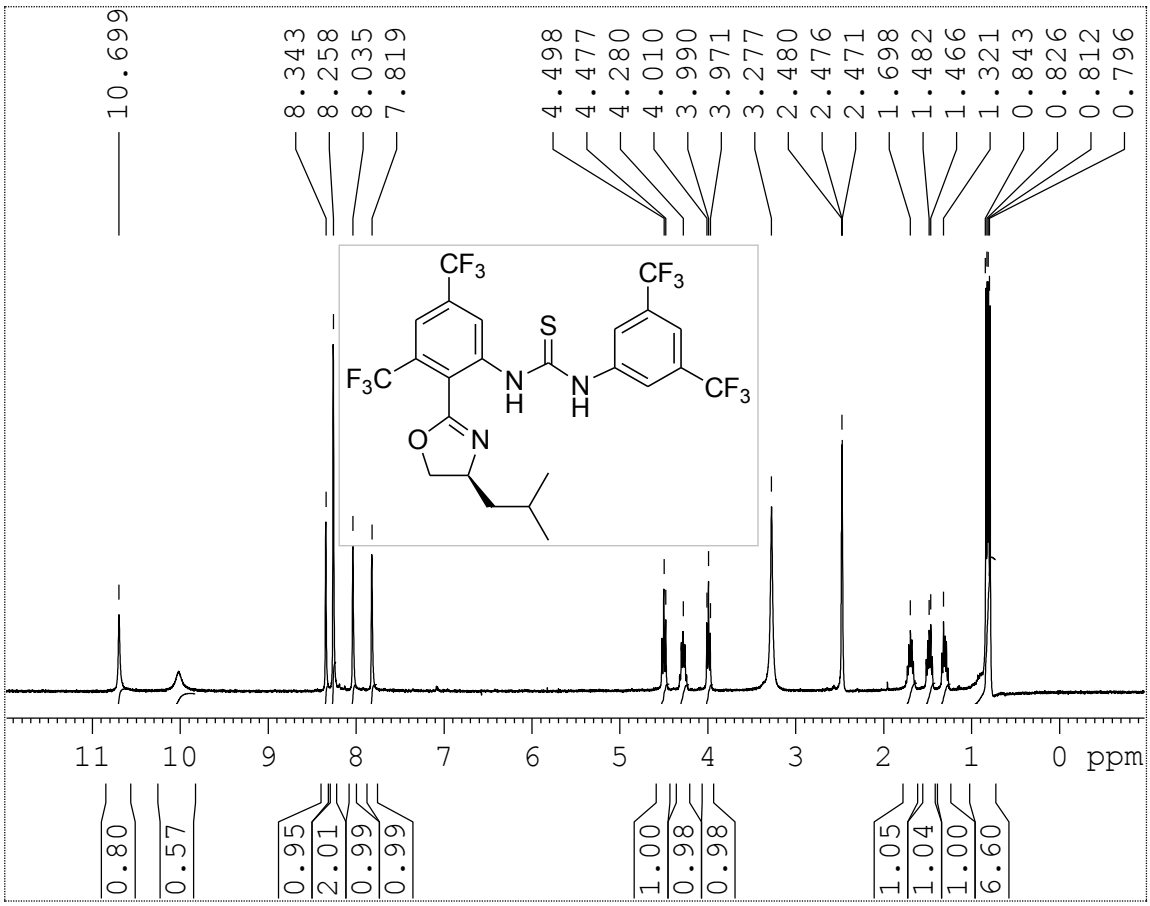
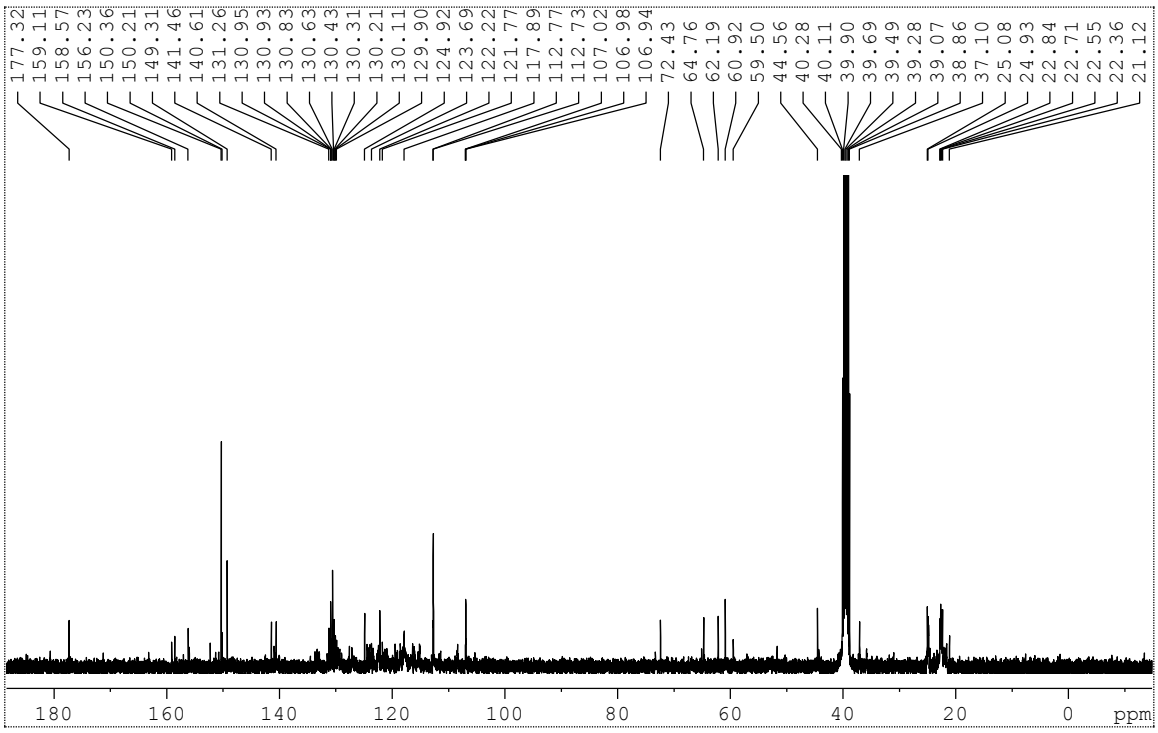
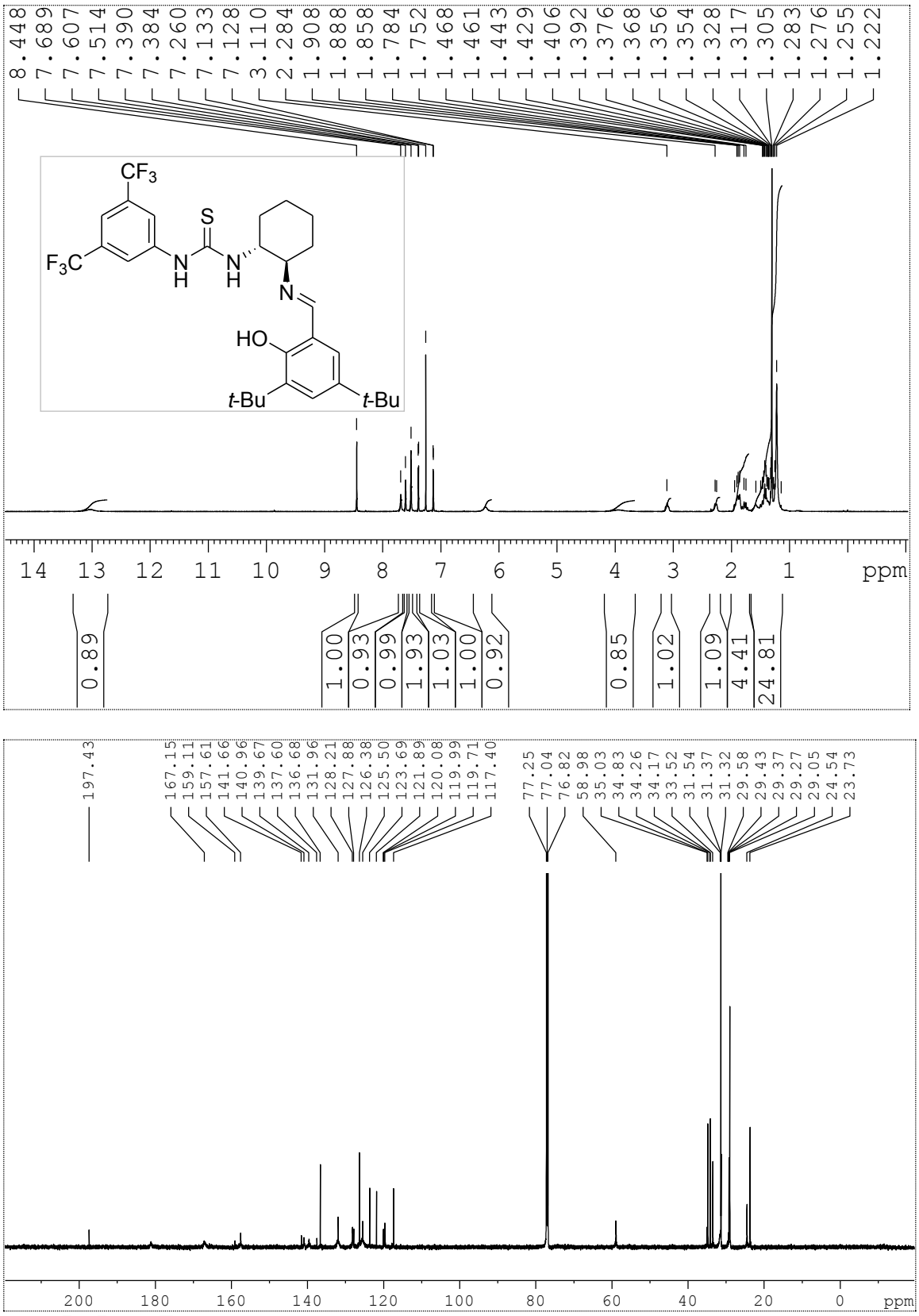
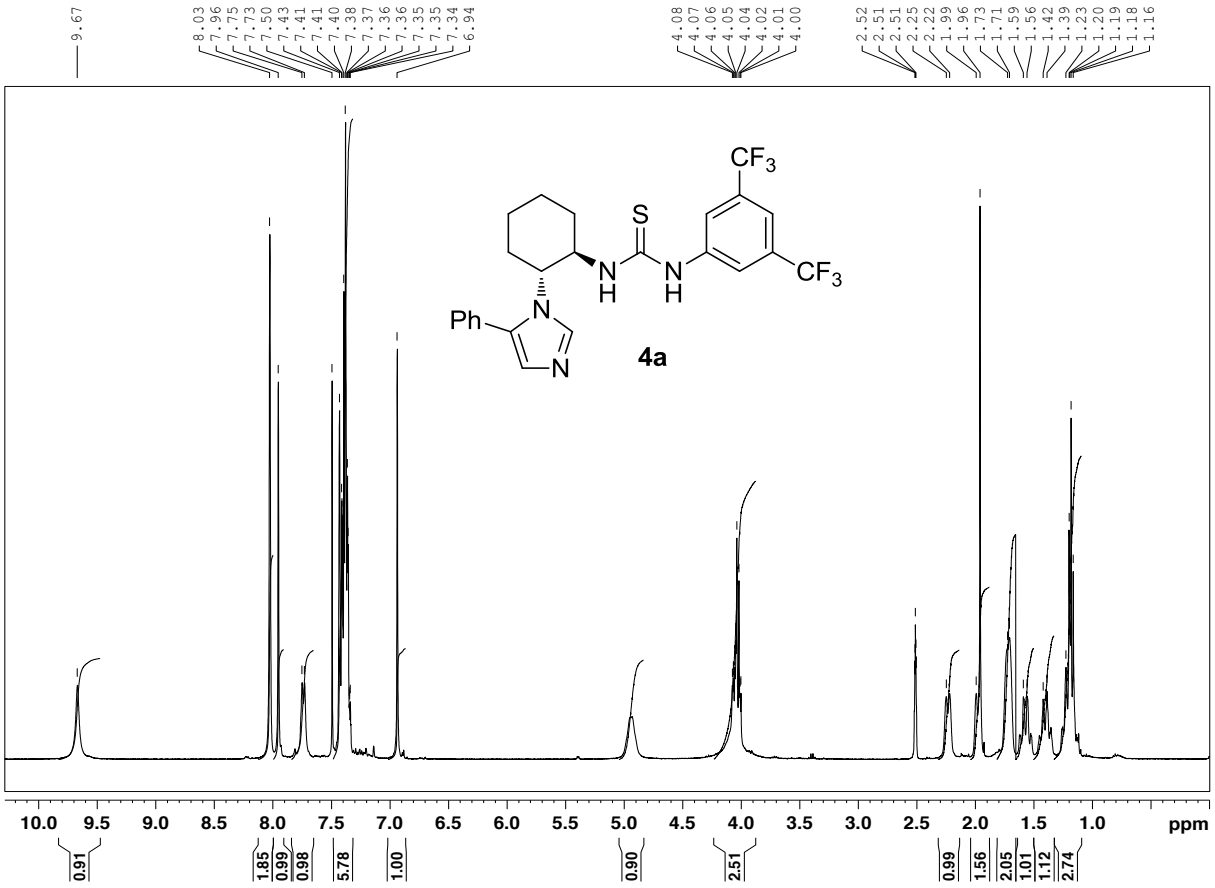




3,5-Di(trifluoromethyl)anilino-2-[(4*S*)-4-isobutyl-4,5-dihydro-1,3-oxazol-2-yl]-3,5-di(trifluoromethyl)anilinomethanethione (**2g**)



of (1*R*,2*R*)-2-(*E*)-1-[3,5-di(*tert*-butyl)-2-hydroxyphenyl] methylideneaminocyclohexylamino-3,5-di(trifluoromethyl)anilinomethanethione (**3b**)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H
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Ph
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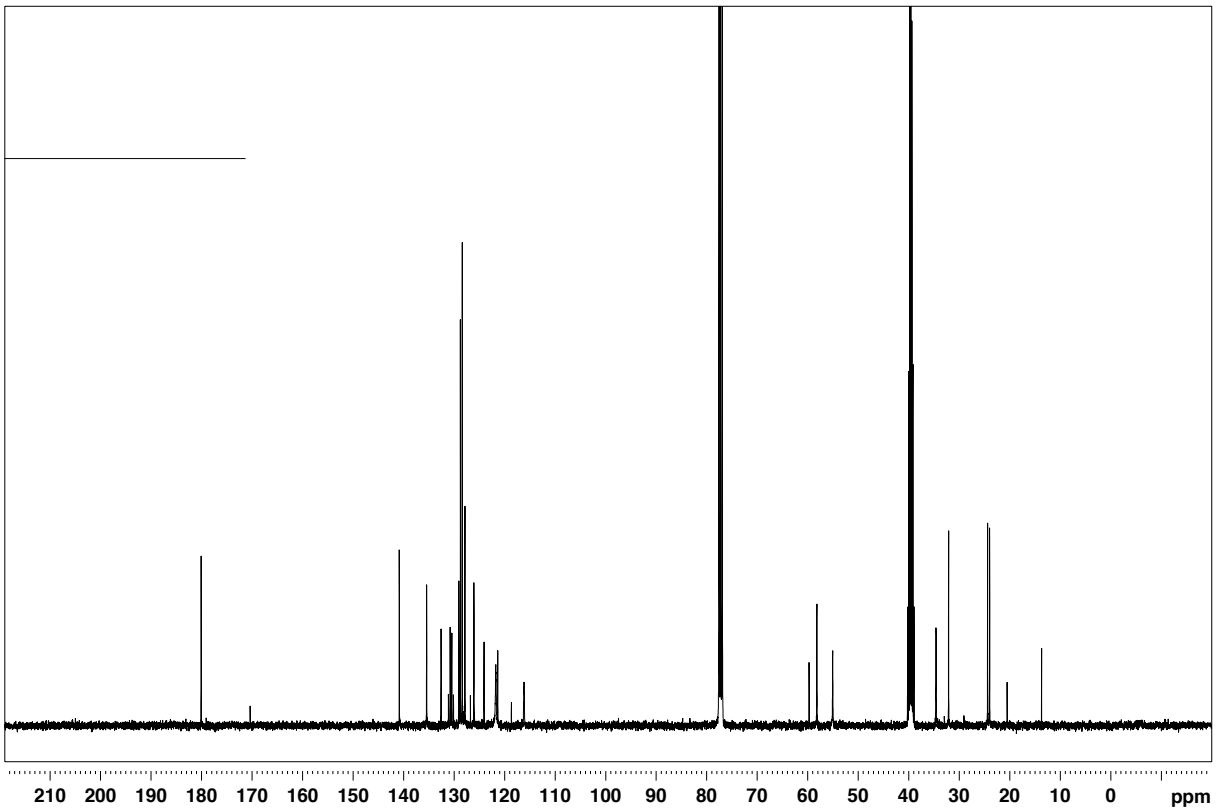
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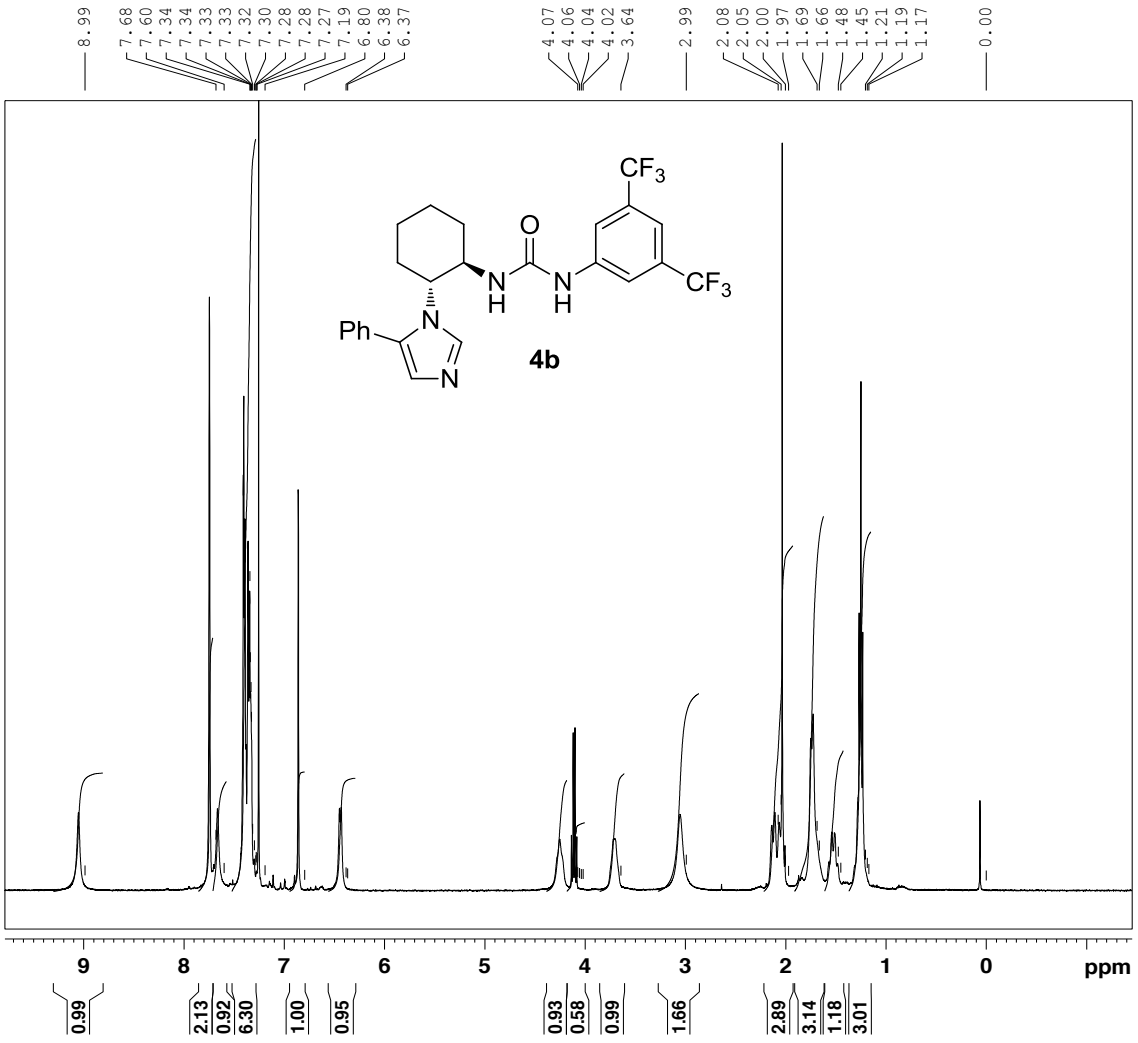
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N
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Ph
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N
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5
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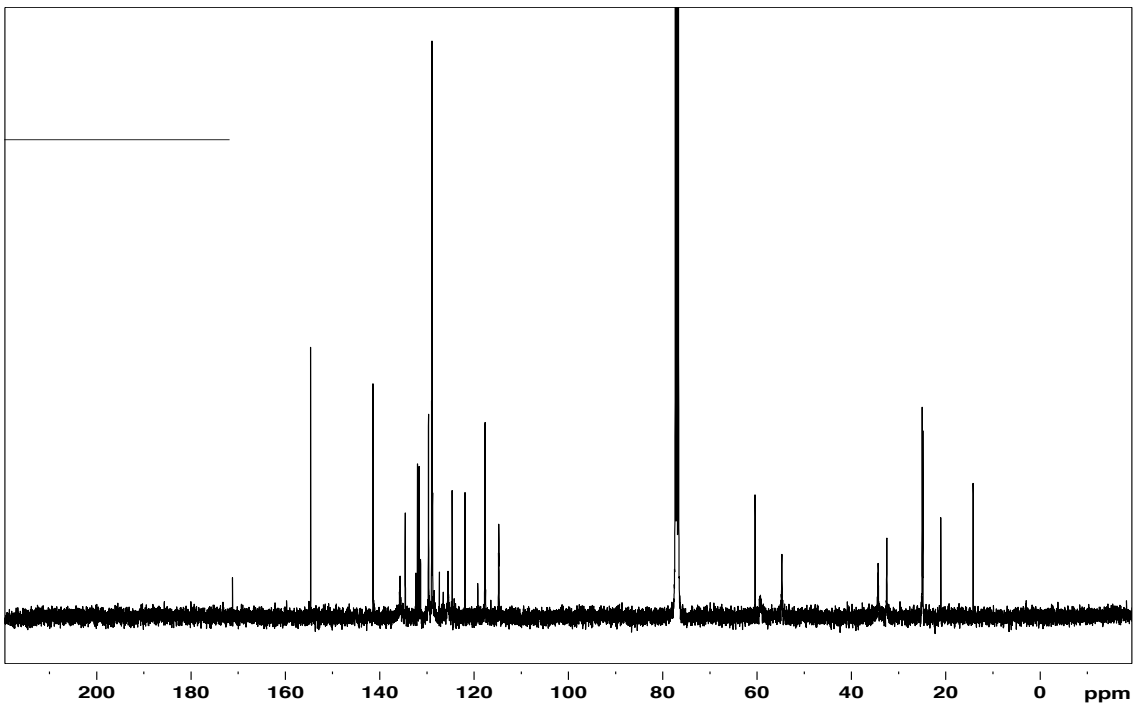
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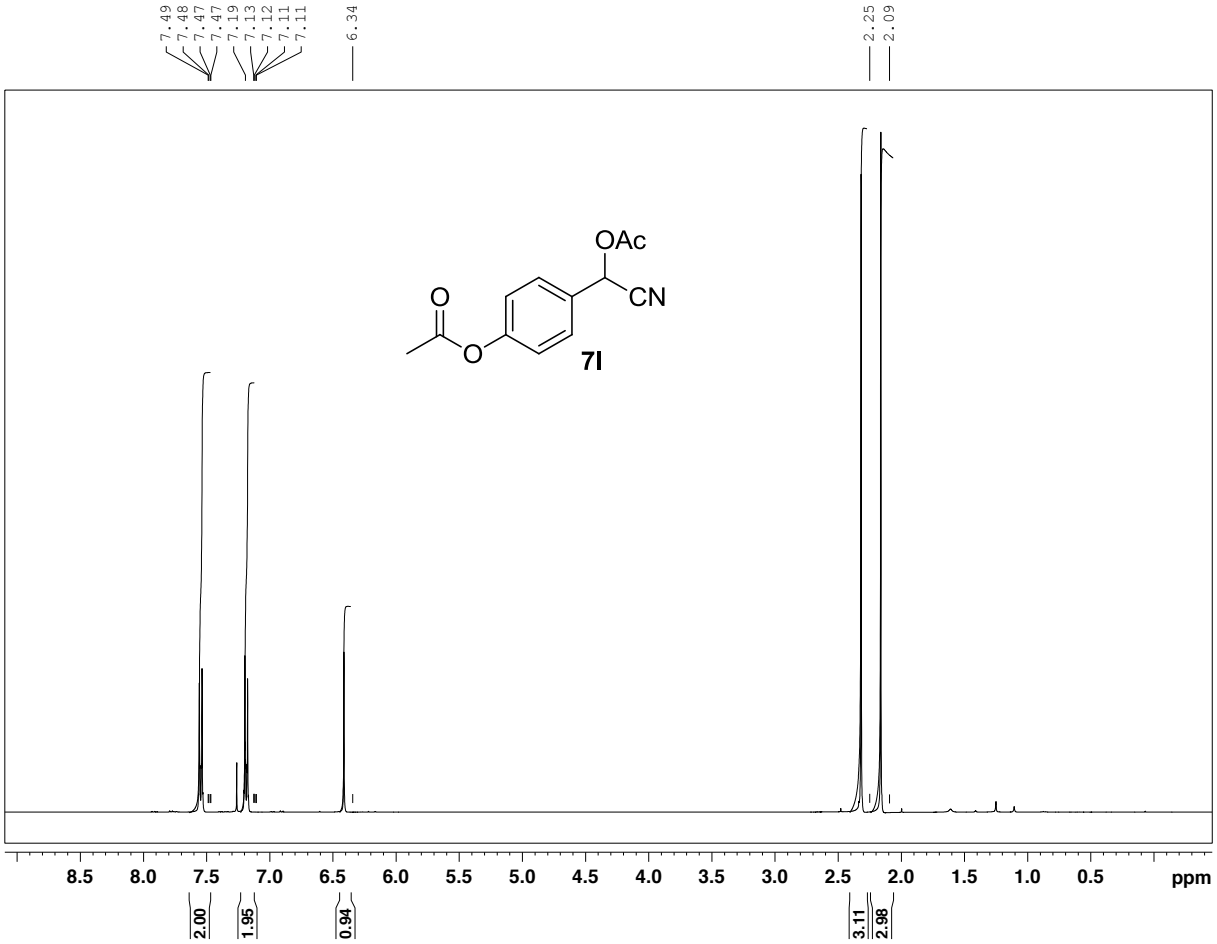
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CN
O
O
7l
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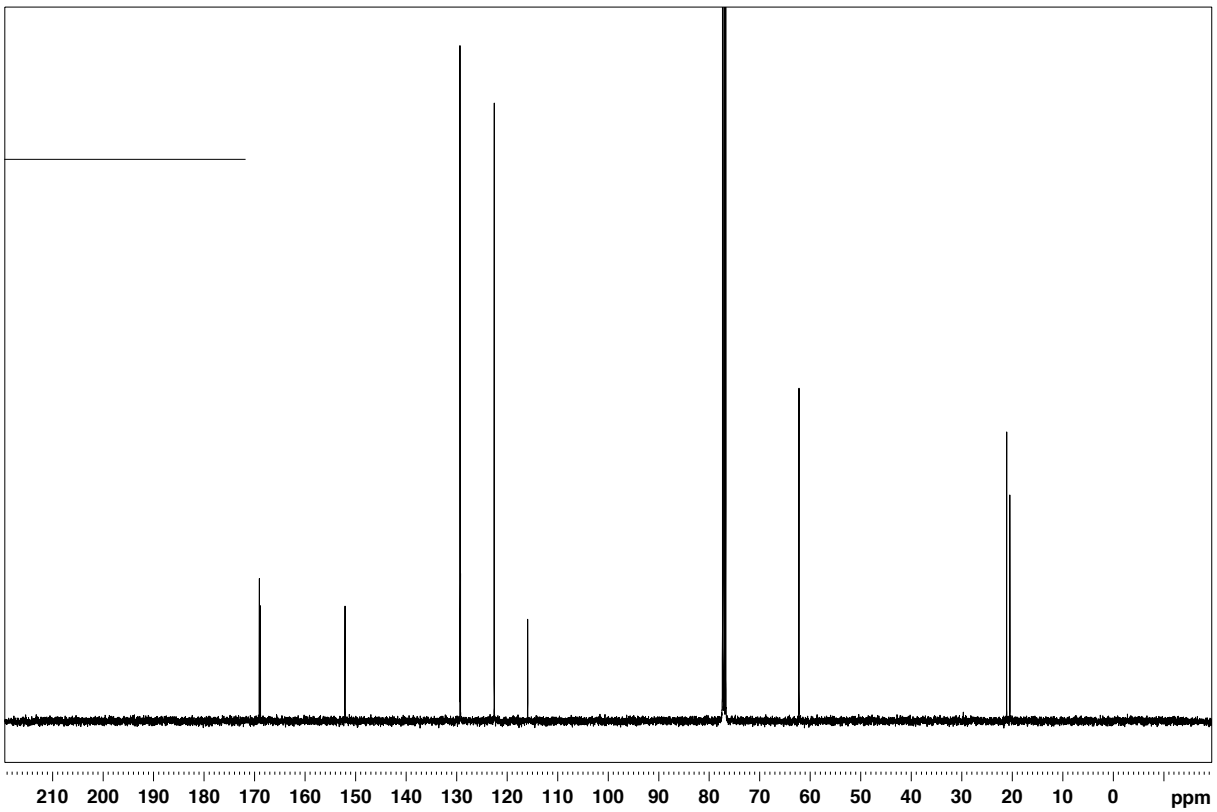
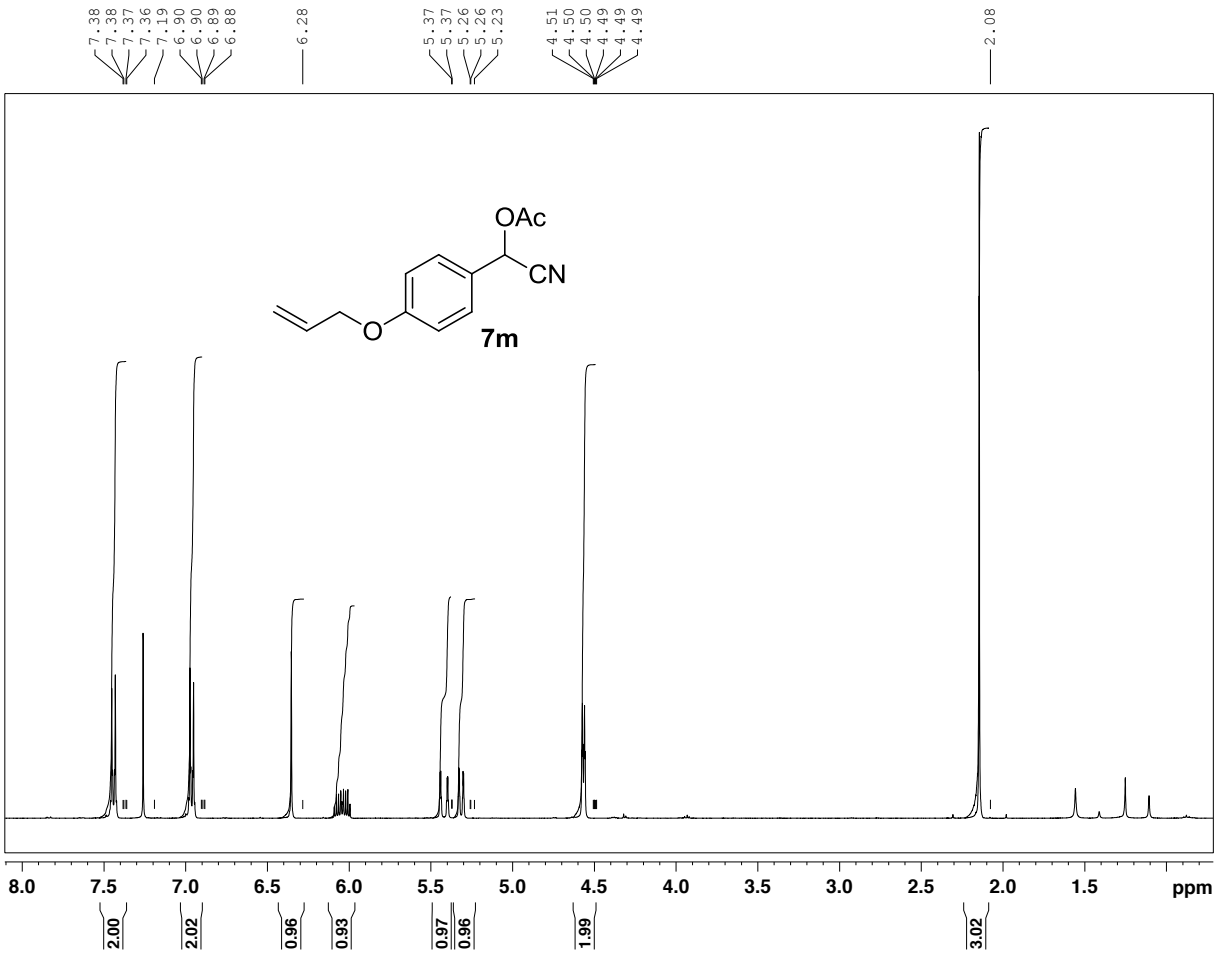
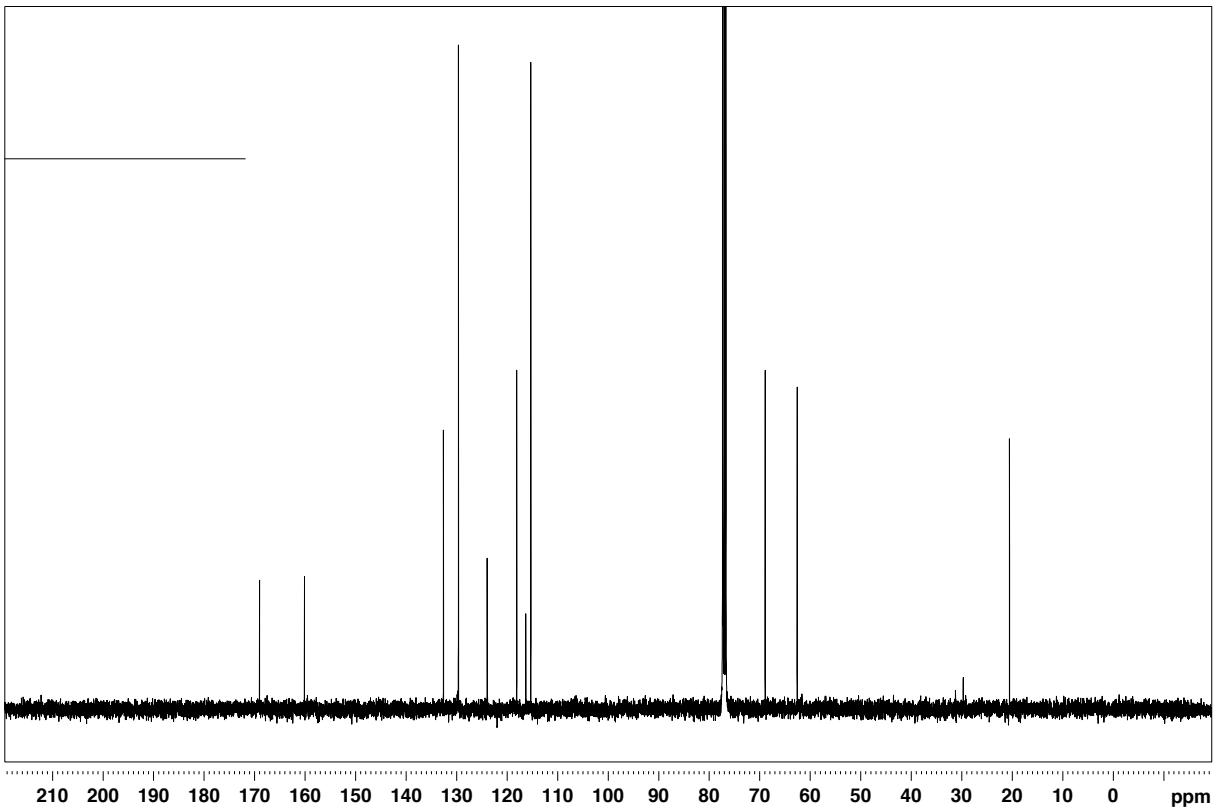
3.11
2.98


210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


7.38
7.38
7.37
7.36
7.19
6.90
6.90
6.89
6.88
6.28
5.37
5.37
5.26
5.26
5.23
4.51
4.50
4.50
4.49
4.49
4.49
2.08
OAc
CN
O
7m
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
ppm
2.00
2.02
0.96
0.93
0.97
0.96
1.99
3.02


210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

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