2-(Diethylamino)ethanethiol, a new reagent for the odorless deprotection of aromatic methyl ethers

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SUPPORTING INFORMATION

- I. General Methods (page S1)
- II. Experimental procedure and analytical data for entries 2-19 (pages S2-S4)
- III. ¹H and ¹³C spectral data for entries 1-19 (pages S5-S42)

Total pages of supporting information: 42

I. General methods

All methyl aryl ethers, 2-(diethylamino)ethanethiol HCl, sodium *tert*-butoxide and anhydrous *N,N*-dimethylformamide were purchased from commercial sources and used as received. ¹H NMR spectra were recorded on a 400 MHz spectrometer in either CDCl₃ or d₆-DMSO as both solvent and internal standard. Infrared spectra were recorded and only the principal sharply defined bands are reported in cm⁻¹. Melting points are uncorrected.

II. Experimental procedure and spectral data

In a typical experimental procedure, the HCl salt of 2-(diethylamino)ethanethiol was suspended in dry *N,N*-dimethylformamide under a nitrogen atmosphere and the flask was cooled in an ice water bath.

NaOt-Bu was added in one portion and, after 5 minutes, the cooling bath was removed and the resulting milky suspension was stirred for 15 minutes. The methyl aryl ether was then added in one portion and the reaction was brought to reflux. When the reaction was complete, the flask was allowed to cool to ambient temperature and placed in an ice water bath. 1 N HCl was added dropwise to bring the pH to 1 and ethyl acetate was added. The two layers were separated and the aqueous layer was extracted with ethyl acetate twice more. The combined organic extracts were washed with water three times, saturated brine and dried over magnesium sulfate. After filtration, the solvent was removed to give a residue that was purified by flash chromatography or recrystallization.

3-Hydroxy-5-methoxybenzonitrile (entry 2): white solid. IR: 3339, 3082, 2999, 2951, 2844, 2237, 1597, 1506, 1451, 1436, 1351, 1340, 1309, 1202, 1171, 1061, 998, 850, 820, 672, 632 cm^{-1} ; MS m/z = 150 ($\text{M} + \text{H}$)⁺. $\text{C}_8\text{H}_7\text{NO}_2$: calcd.: C 64.42, H 4.73, N, 9.39; found: C 64.28, H, 4.74, N, 9.34. M.p. 156-158 °C.

2-Hydroxy-4-methoxybenzonitrile (entry 3): white solid. IR: 3215, 3023, 2226, 1609, 1594, 1512, 1448, 1431, 1378, 1321, 1276, 1211, 1104, 1026, 961, 830, 800, 672 cm^{-1} . MS m/z = 150 ($\text{M} + \text{H}$)⁺. $\text{C}_8\text{H}_7\text{NO}_2$: calcd.: C 64.42, H 4.73, N, 9.39; found: C 64.31, H, 4.74, N, 9.33. M.p. 169-171 °C.

3,5-Dimethoxy-4-hydroxybenzonitrile (entry 4): tan solid. IR: 3354, 2224, 1605, 1513, 1454, 1421, 1334, 1253, 1206, 1146, 1109, 853, 816, 792, 682 cm^{-1} . MS m/z = 180 ($\text{M} + \text{H}$)⁺. $\text{C}_9\text{H}_9\text{NO}_3$: calcd.: C 60.33, H 5.06, N, 7.82; found: C 60.23, H, 4.99, N, 7.76. M.p. 107-109 °C.

Ethyl 2-hydroxybenzoate (entry 5): pale yellow oil. IR: 3150, 2983, 1670, 1613, 1484, 1372, 1299, 1248, 1211, 1156, 1088, 754, 699, 665 cm^{-1} . MS m/z = 167 ($\text{M} + \text{H}$)⁺. $\text{C}_9\text{H}_{10}\text{O}_3$: calcd.: C 65.05, H 6.07; found: C 64.93, H, 6.16.

Ethyl 3-hydroxybenzoate (entry 6): white solid. IR: 3329, 3295, 1674, 1596, 1447, 1372, 1303, 1235, 1110, 1073, 1020, 754, 676, 655 cm^{-1} . MS m/z = 167 ($\text{M} + \text{H}$)⁺. $\text{C}_9\text{H}_{10}\text{O}_3$: calcd.: C 65.05, H 6.07;

found: C 64.96, H, 6.33. M.p. 70-72 °C.

Ethyl 4-hydroxybenzoate (entry 7): white solid. IR: 3190, 2977, 1667, 1605, 1589, 1443, 1315, 1288, 1234, 1167, 1134, 1106, 1016, 847, 768, 695, 620 cm^{-1} . MS $m/z = 167$ ($M + H$)⁺. $\text{C}_9\text{H}_{10}\text{O}_3$: calcd.: C 65.05, H 6.07; found: C 65.10, H, 5.93. M.p. 112-115 °C.

2-Bromophenol (entry 8): pale yellow oil. IR: 3498, 1595, 1577, 1472, 1446, 1333, 1289, 1246, 1176, 1115, 1022, 827, 743, 654 cm^{-1} . MS $m/z = 174$ ($M + H$)⁺. $\text{C}_6\text{H}_5\text{BrO}$: calcd.: C 41.65, H 2.91, Br 46.19; found: C 41.38, H, 2.90, Br 46.12.

3-Bromophenol (entry 9): pale yellow oil. IR: 3318, 1581, 1472, 1439, 1295, 1241, 1213, 1157, 1062, 995, 853, 766, 676 cm^{-1} . MS $m/z = 174$ ($M + H$)⁺. $\text{C}_6\text{H}_5\text{BrO}$: calcd.: C 41.65, H 2.91, Br 46.19; found: C 41.95, H, 3.10, Br 45.89.

4-Bromophenol (entry 10): tan solid. IR: 3336, 1882, 1589, 1487, 1433, 1240, 1217, 1173, 1068, 1005, 823, 808, 602 cm^{-1} . MS $m/z = 174$ ($M + H$)⁺. $\text{C}_6\text{H}_5\text{BrO}$: calcd.: C 41.65, H 2.91, Br 46.19; found: C 41.83, H, 2.82, Br 46.12. M.p. 54-64 °C.

4-Hydroxybenzaldehyde (entry 11): white solid. IR: 3158, 2879, 1905, 1663, 1647, 1588, 1518, 1449, 1385, 1314, 1282, 1215, 1155, 1112, 858, 831, 788, 703, 641 cm^{-1} . MS $m/z = 123$ ($M + H$)⁺. $\text{C}_7\text{H}_6\text{O}_2$: calcd.: C 68.85, H 4.95; found: C 68.86, H, 5.02. M. p. 115-118 °C.

4-Hydroxyacetophenone (entry 12): tan solid. IR: 3299, 2995, 1658, 1601, 1574, 1511, 1355, 1276, 1216, 1164, 1106, 961, 846, 814, 659 cm^{-1} . MS $m/z = 136$ ($M + H$)⁺. $\text{C}_8\text{H}_8\text{O}_2$: calcd.: C 70.58, H 5.92; found: C 70.42, H, 5.89. M. p. 106-108 °C.

4-Hydroxybenzophenone (entry 13): tan solid. IR: 3218, 1631, 1599, 1554, 1511, 1444, 1312, 1285, 1230, 1171, 1146, 939, 923, 847, 820, 738, 698, 680 cm^{-1} . MS $m/z = 199$ ($M + H$)⁺. $\text{C}_{13}\text{H}_{10}\text{O}_2$: calcd.: C 78.77, H 5.09; found: C 78.48, H, 5.39. M.p. 133-134 °C.

4,4'-dihydroxybenzophenone (entry 14): white solid. IR: 3334, 3144, 1626, 1592, 1584, 1571, 1445, 1316, 1240, 1162, 1151, 1115, 970, 929, 851, 769, 684, 633 cm^{-1} . MS $m/z = 215$ ($\text{M} + \text{H}$)⁺. $\text{C}_{13}\text{H}_{10}\text{O}_3$: calcd.: C 72.89, H 4.71; found: C 72.71, H, 4.57. M.p. 215-219 °C.

Cyclopropyl-4-hydroxyphenyl ketone (entry 15): tan solid. IR: 3141, 2817, 1640, 1604, 1582, 1562, 1514, 1386, 1292, 1226, 1167, 991, 847, 816, 748, 695 cm^{-1} . MS $m/z = 177$ ($\text{M} + \text{H}$)⁺. $\text{C}_{10}\text{H}_{10}\text{O}_2$: calcd.: C 74.06, H 6.21; found: C 73.70, H, 6.10. M.p. 105-107 °C.

1-(4-Hydroxyphenyl)-1H-imidazole (entry 16): tan solid. IR: 3115, 2575, 2478, 1595, 1527, 1506, 1468, 1394, 1251, 1120, 1063, 967, 923, 834, 801, 751, 658, 618 cm^{-1} . MS $m/z = 160$ ($\text{M} + \text{H}$)⁺. $\text{C}_9\text{H}_8\text{N}_2\text{O}_2$: calcd.: C 67.14, H 5.03, N 17.49; found: C 67.14, H, 5.02, N 17.28. M.p. 203-205 °C.

N,N-Diphenyl-4-hydroxybenzamide (entry 17): tan solid. IR: 3316, 1641, 1606, 1586, 1509, 1486, 1338, 1304, 1275, 1215, 1165, 1100, 843, 756, 696, 661, 640, 605 cm^{-1} . MS $m/z = 160$ ($\text{M} + \text{H}$)⁺. $\text{C}_{19}\text{H}_{15}\text{NO}_2$: calcd.: C 78.87, H 5.23, N 4.84; found: C 78.50, H, 5.25, N 4.77. M.p. 190-193 °C.

4-Nitro-1-naphthol (entry 18): light green solid. IR: 3315, 1629, 1572, 1527, 1500, 1464, 1308, 1260, 1248, 1191, 1146, 1054, 985, 832, 758 cm^{-1} . MS $m/z = 190$ ($\text{M} - \text{H}$)⁺. $\text{C}_{10}\text{H}_7\text{NO}_3$: calcd.: C 63.49, H 3.73, N 7.40; found: C 63.74, H, 3.66, N 7.22. M.p. 158-163 °C.

3,5-Dimethoxyphenol (entry 19): light brown oil. IR: 3393, 2939, 2840, 1595, 1498, 1457, 1432, 1191, 1139, 1051, 994, 972, 924, 818, 678 cm^{-1} . MS $m/z = 154$ ($\text{M} - \text{H}$)⁺. HR-MS: calcd.: 154.0630; found: 154.0633.

III ¹H and ¹³C NMR spectra for entries 1-19

Entry 1: 4-hydroxy-1-naphthonitrile

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Frequency (MHz)	400.11	Nucleus	¹ H
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Receiver Gain	46.00	Solvent	DMSO-d6
Sweep Width (Hz)	6387.74	Temperature (degree C)	25.000
		Number of Transients	16
		Pulse Sequence	s2pul
		Spectrum Offset (Hz)	2400.6519

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	2.46	985.3	0.1303	14	7.70	3082.1	0.3092
2	2.47	987.0	0.1867	15	7.72	3087.7	0.2335
3	2.47	989.0	0.1333	16	7.72	3089.1	0.4970
4	6.94	2776.4	0.9346	17	7.72	3090.5	0.3576
5	6.96	2784.6	0.9224	18	7.74	3096.1	0.2689
6	7.56	3026.7	0.2255	19	7.74	3097.3	0.2601
7	7.57	3027.9	0.2373	20	7.92	3167.3	1.0000
8	7.58	3033.5	0.3066	21	7.94	3175.5	0.9123
9	7.59	3034.9	0.4198	22	7.95	3182.7	0.4345
10	7.59	3036.3	0.2630	23	7.97	3190.7	0.3547
11	7.60	3041.9	0.3121	24	8.22	3290.3	0.3617
12	7.61	3043.1	0.3046	25	8.24	3298.3	0.3455
13	7.70	3080.7	0.2847	26	11.46	4583.5	0.5854

No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	[6.91 .. 6.97]	1.027	1.15369e+10	1.027
2	[7.55 .. 7.62]	1.023	1.14872e+10	1.023
3	[7.69 .. 7.76]	1.043	1.17067e+10	1.043
4	[7.90 .. 7.99]	1.909	2.14400e+10	1.909
5	[8.20 .. 8.26]	1.000	1.12288e+10	1.000
6	[11.41 .. 11.49]	0.966	1.08481e+10	0.966

No.	Multiplet1	Shift1 (Hz)	(Hz)	J (Hz)	Type	H's
1	M00	2780.50	[2764.52 .. 2790.64]	8.19	d	1
2	M01	3034.90	[3022.23 .. 3048.35]	8.29	ddd	1
3	M01	3034.90	[3022.23 .. 3048.35]	6.92	ddd	1
4	M01	3034.90	[3022.23 .. 3048.35]	1.17	ddd	1
5	M02	3089.07	[3077.01 .. 3106.25]	8.33	ddd	1
6	M02	3089.07	[3077.01 .. 3106.25]	6.97	ddd	1
7	M02	3089.07	[3077.01 .. 3106.25]	1.27	ddd	1
8	M03	3179.02	[3162.79 .. 3198.27]	-	m	2
9	M04	3294.28	[3281.90 .. 3305.10]	7.99	d	1
10	M05	4583.54	[4563.65 .. 4598.16]	-	s	1

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Frequency (MHz)	100.62	Nucleus	13C	Number of Transients	512
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Receiver Gain	50.00	Solvent	DMSO-d6	Spectrum Offset (Hz)	10060.8252
Sweep Width (Hz)	24154.59	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	39.57	3981.1	0.1385	10	119.16	11989.6	0.1544
2	39.78	4002.5	0.4307	11	123.75	12451.1	0.3059
3	39.98	4023.1	0.8150	12	124.69	12546.2	0.2398
4	40.20	4044.5	1.0000	13	124.82	12558.7	0.1692
5	40.40	4065.1	0.8158	14	126.93	12771.0	0.2497
6	40.61	4086.5	0.4288	15	129.91	13071.8	0.2185
7	40.82	4107.1	0.1372	16	134.15	13497.8	0.0858
8	98.95	9956.5	0.1320	17	135.59	13643.1	0.2275
9	108.80	10947.3	0.2222	18	159.10	16007.9	0.1450

Entry 2: 3-Hydroxy-5-methoxybenzonitrile

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Original Points Count	32768	Points Count	32768
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Sweep Width (Hz)	6387.74	Temperature (degree C)	25.000
		Number of Transients	16
		Pulse Sequence	s2pul
		Spectrum Offset (Hz)	2400.6519

No.	(ppm)	(Hz)	Height
1	3.71	1485.1	1.0000
2	6.60	2640.3	0.0928
3	6.60	2642.7	0.1839
4	6.61	2644.8	0.1073
5	6.69	2676.4	0.1062
6	6.69	2677.8	0.1215
7	6.69	2678.5	0.1111
8	6.70	2679.9	0.1028
9	6.79	2716.8	0.0931
10	6.79	2717.9	0.0985
11	6.80	2718.9	0.0986
12	6.80	2720.3	0.0879
13	10.17	4068.9	0.1926

No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	[3.69 .. 3.76]	2.964	3.21714e+10	2.964
2	[6.58 .. 6.65]	0.980	1.06387e+10	0.980
3	[6.65 .. 6.72]	0.937	1.01701e+10	0.937
4	[6.74 .. 6.83]	0.955	1.03631e+10	0.955
5	[10.13 .. 10.22]	1.000	1.08544e+10	1.000

No.	Multiplet1	Shift1 (Hz)	(Hz)	J (Hz)	Type	H's
1	M00	1485.10	[1476.52 .. 1505.96]	-	s	3
2	M01	2642.61	[2631.56 .. 2659.25]	2.24	t	1
3	M01	2642.61	[2631.56 .. 2659.25]	2.24	t	1
4	M02	2678.15	[2662.36 .. 2687.71]	2.14	dd	1
5	M02	2678.15	[2662.36 .. 2687.71]	1.36	dd	1
6	M03	2718.46	[2698.23 .. 2732.15]	2.24	dd	1
7	M03	2718.46	[2698.23 .. 2732.15]	1.27	dd	1
8	M04	4068.89	[4055.05 .. 4089.55]	-	s	1

Acquisition Time (sec)	1.3566	Date	May 3 2006
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Frequency (MHz)	100.62	Nucleus	¹³ C
Original Points Count	32768	Points Count	32768
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		Number of Transients	512
		Pulse Sequence	s2pul
		Spectrum Offset (Hz)	10060.8252

No.	(ppm)	(Hz)	Height
1	39.53	3977.4	0.1114
2	39.74	3998.8	0.3640
3	39.95	4019.4	0.7276
4	40.16	4040.8	0.8422
5	40.36	4061.4	0.7218
6	40.58	4082.8	0.3604
7	40.78	4103.4	0.1077
8	56.19	5653.7	1.0000
9	107.33	10799.1	0.4418
10	108.90	10956.8	0.6888
11	111.97	11265.7	0.7841
12	113.01	11371.1	0.8704
13	119.42	12016.1	0.5070
14	159.76	16075.0	0.8473
15	161.47	16246.7	0.4190

Entry 3: 2-Hydroxy-4-methoxybenzonitrile

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Original Points Count	32768	Points Count	32768
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Sweep Width (Hz)	6387.74	Temperature (degree C)	25.000
		Number of Transients	16
		Pulse Sequence	s2pul
		Spectrum Offset (Hz)	2400.6519

No.	(ppm)	(Hz)	Height
1	3.72	1490.0	1.0000
2	6.46	2583.6	0.1457
3	6.46	2586.3	0.1811
4	6.47	2588.7	0.1990
5	6.47	2590.4	0.1711
6	7.44	2974.9	0.1629
7	7.46	2984.0	0.1588
8	10.98	4394.4	0.1884

No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	[3.70 .. 3.78]	3.084	4.99770e+10	3.084
2	[6.43 .. 6.51]	2.052	3.32524e+10	2.052
3	[7.41 .. 7.50]	1.000	1.62070e+10	1.000
4	[10.94 .. 11.03]	1.022	1.65567e+10	1.022

No.	Multiplet1	Shift1 (Hz)	(Hz)	J (Hz)	Type	H's
1	M00	1489.97	[1479.44 .. 1510.44]	-	s	3
2	M01	2587.26	[2573.47 .. 2603.49]	4.58	dd	2
3	M01	2587.26	[2573.47 .. 2603.49]	2.24	dd	2
4	M02	2979.44	[2964.53 .. 2999.81]	9.16	d	1
5	M03	4394.44	[4376.90 .. 4412.77]	-	s	1

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Sweep Width (Hz)	24154.59	Temperature (degree C)	25.000
		Number of Transients	512
		Pulse Sequence	s2pul
		Spectrum Offset (Hz)	10060.8252

No.	(ppm)	(Hz)	Height
1	39.72	3996.6	0.2418
2	39.93	4017.2	0.4695
3	40.14	4038.6	0.5703
4	40.34	4059.2	0.4812
5	40.56	4080.6	0.2480
6	40.77	4102.0	0.0826
7	56.09	5644.1	1.0000
8	91.88	9245.2	0.3847
9	101.69	10232.2	0.7342
10	107.28	10793.9	0.5347
11	118.01	11873.9	0.2758
12	134.96	13579.7	0.4409
13	162.47	16347.0	0.4865
14	164.66	16567.4	0.8889

Entry 4: 3,5-Dimethoxy-4-hydroxybenzonitrile

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Sweep Width (Hz)	6387.74	Temperature (degree C)	25.000
		Number of Transients	16
		Pulse Sequence	s2pul
		Spectrum Offset (Hz)	2400.6519

No.	(ppm)	(Hz)	Height
1	3.77	1509.5	1.0000
2	7.07	2830.8	0.4055
3	9.52	3810.2	0.0694

No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	[3.75 .. 3.80]	6.051	4.86409e+10	6.051
2	[7.03 .. 7.11]	2.000	1.60777e+10	2.000
3	[9.47 .. 9.57]	0.960	7.72053e+9	0.960

No.	Multiplet1	Shift1 (Hz)	(Hz)	Type	H's
1	M00	1509.46	[1500.30 .. 1522.14]	s	6
2	M01	2830.80	[2812.47 .. 2842.88]	s	2
3	M02	3810.20	[3789.34 .. 3828.72]	s	1

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Original Points Count	32768	Points Count	32768
Receiver Gain	50.00	Solvent	DMSO-d6
Sweep Width (Hz)	24154.59	Temperature (degree C)	25.000
		Number of Transients	512
		Pulse Sequence	s2pul
		Spectrum Offset (Hz)	10060.8252

No.	(ppm)	(Hz)	Height
1	39.76	4000.2	0.2400
2	39.96	4020.9	0.4674
3	40.17	4042.3	0.5601
4	40.38	4062.9	0.4732
5	40.59	4084.3	0.2364
6	40.80	4105.7	0.0886
7	57.01	5736.3	1.0000
8	100.51	10112.8	0.4148
9	110.49	11117.5	0.7581
10	120.36	12110.5	0.2385
11	141.34	14221.0	0.2542
12	148.76	14967.7	0.6718

Entry 5: Ethyl 2-hydroxybenzoate

5/5/2006 1:57 PM

Acquisition Time (sec)	5.1298	Date	May 5 2006
File Name	C:\Documents and Settings\maganoj.AMER\Desktop\publications\demethylation paper\H and C spectra\HAHN.CHEMISTRY.AA.WL.COM\SAMBA\20060505\2501		
Frequency (MHz)	400.11	Nucleus	¹ H
Original Points Count	32768	Points Count	32768
Receiver Gain	28.00	Pulse Sequence	s2pul
Spectrum Offset (Hz)	2400.6646	Solvent	CHLOROFORM-d
		Sweep Width (Hz)	6387.74
		Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	1.36	545.7	0.4920	16	6.94	2777.0	0.1108	1	[1.34 .. 1.41]	3.006	2.82617e+10	3.006
2	1.38	552.7	1.0000	17	6.96	2784.2	0.1329	2	[4.33 .. 4.40]	2.000	1.88017e+10	2.000
3	1.40	559.9	0.5479	18	6.96	2785.4	0.1182	3	[6.81 .. 6.87]	0.997	9.37098e+9	0.997
4	4.34	1738.0	0.1499	19	7.39	2955.2	0.0598	4	[6.91 .. 6.98]	0.944	8.87001e+9	0.944
5	4.36	1745.0	0.5170	20	7.39	2956.9	0.0585	5	[7.36 .. 7.44]	0.985	9.26371e+9	0.985
6	4.38	1752.2	0.4865	21	7.40	2962.4	0.0597	6	[7.77 .. 7.84]	0.974	9.15568e+9	0.974
7	4.40	1759.2	0.1398	22	7.41	2963.8	0.0871	7	[10.80 .. 10.88]	0.926	8.70311e+9	0.926
8	6.82	2727.5	0.0929	23	7.41	2964.9	0.0535					
9	6.82	2728.7	0.1004	24	7.42	2970.8	0.0506					
10	6.83	2734.7	0.1014	25	7.43	2972.5	0.0477					
11	6.84	2735.9	0.1299	26	7.81	3123.2	0.1181					
12	6.84	2736.7	0.1129	27	7.81	3124.6	0.1165					
13	6.85	2742.7	0.1051	28	7.83	3131.2	0.1209					
14	6.86	2743.9	0.1109	29	7.83	3132.6	0.1107					
15	6.94	2775.8	0.1197	30	10.85	4340.5	0.4310					

No.	Multiplet1	Shift1 (Hz)	(Hz)	J (Hz)	Type	H's	No.	Multiplet1	Shift1 (Hz)	(Hz)	J (Hz)	Type	H's
1	M00	552.76	[536.71 .. 563.41]	7.12	t	3	9	M03	2780.61	[2764.14 .. 2791.04]	8.38	dd	1
2	M00	552.76	[536.71 .. 563.41]	7.12	t	3	10	M03	2780.61	[2764.14 .. 2791.04]	1.17	dd	1
3	M01	1748.58	[1733.27 .. 1761.74]	7.02	q	2	11	M04	2963.79	[2944.46 .. 2977.80]	8.43	ddd	1
4	M01	1748.58	[1733.27 .. 1761.74]	7.02	q	2	12	M04	2963.79	[2944.46 .. 2977.80]	7.16	ddd	1
5	M01	1748.58	[1733.27 .. 1761.74]	7.02	q	2	13	M04	2963.79	[2944.46 .. 2977.80]	1.75	ddd	1
6	M02	2735.70	[2723.20 .. 2748.15]	8.09	ddd	1	14	M05	3127.90	[3108.02 .. 3138.04]	7.99	dd	1
7	M02	2735.70	[2723.20 .. 2748.15]	7.12	ddd	1	15	M05	3127.90	[3108.02 .. 3138.04]	1.36	dd	1
8	M02	2735.70	[2723.20 .. 2748.15]	1.17	ddd	1	16	M06	4340.46	[4320.18 .. 4351.37]	-	s	1

Acquisition Time (sec)	1.3566	Date	May 5 2006
File Name	C:\Documents and Settings\maganoj.AMER\Desktop\publications\demethylation paper\H and C spectra\HAHN.CHEMISTRY.AA.WL.COM\SAMBA\20060505\2502		
Frequency (MHz)	100.62	Nucleus	¹³ C
Original Points Count	32768	Points Count	32768
Receiver Gain	50.00	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	10060.7090	Sweep Width (Hz)	24154.59
		Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height
1	14.35	1443.7	0.9130
2	61.57	6195.4	0.6791
3	112.81	11350.4	0.4325
4	117.70	11842.8	1.0000
5	119.23	11996.1	0.6068
6	130.08	13088.6	0.6374
7	135.72	13656.2	0.8676
8	161.90	16290.1	0.4362
9	170.38	17143.0	0.3447

Entry 6: Ethyl 3-hydroxybenzoate

5/5/2006 10:32 AM

Acquisition Time (sec)	5.1298	Date	May 3 2006
File Name	C:\Documents and Settings\maganoj.AMER\Desktop\publications\demethylation paper\H and C spectra\AASUN702.RESEARCH.AA.WL.COM\NMR\HAHN\NHFILES\2006\20060503\8801		
Frequency (MHz)	400.11	Nucleus	1H
Original Points Count	32768	Points Count	32768
Receiver Gain	50.00	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	2400.6646	Sweep Width (Hz)	6387.74
		Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	1.36	542.7	0.5366	15	7.06	2825.7	0.0957	1	[1.35 .. 1.42]	2.989	2.63816e+10	2.989
2	1.37	550.0	1.0000	16	7.24	2898.1	0.1737	2	[4.33 .. 4.41]	2.000	1.76519e+10	2.000
3	1.39	557.0	0.5542	17	7.27	2910.5	0.1090	3	[7.00 .. 7.10]	1.012	8.93322e+9	1.012
4	4.34	1735.0	0.1698	18	7.29	2917.9	0.1928	4	[7.24 .. 7.33]	1.244	1.09804e+10	1.244
5	4.35	1742.2	0.5010	19	7.31	2925.4	0.0794	5	[7.53 .. 7.62]	1.934	1.70718e+10	1.934
6	4.37	1749.3	0.5107	20	7.31	2926.1	0.1031					
7	4.39	1756.5	0.1628	21	7.58	3032.0	0.0932					
8	7.03	2813.8	0.0902	22	7.58	3032.8	0.1528					
9	7.04	2815.0	0.0836	23	7.58	3034.5	0.2110					
10	7.04	2816.4	0.0789	24	7.59	3035.5	0.3195					
11	7.04	2817.6	0.0920	25	7.60	3041.9	0.1095					
12	7.05	2822.0	0.1009	26	7.61	3042.9	0.1130					
13	7.06	2823.0	0.1068	27	7.61	3044.5	0.0792					
14	7.06	2824.6	0.1094									

No.	Multiplet1	Shift1 (Hz)	(Hz)	J (Hz)	Type	H's
1	M00	549.90	[538.85 .. 567.51]	7.12	t	3
2	M00	549.90	[538.85 .. 567.51]	7.12	t	3
3	M01	1745.75	[1731.32 .. 1763.10]	7.21	q	2
4	M01	1745.75	[1731.32 .. 1763.10]	7.21	q	2
5	M01	1745.75	[1731.32 .. 1763.10]	7.21	q	2
6	M02	2819.77	[2802.74 .. 2840.95]	8.14	ddd	1
7	M02	2819.77	[2802.74 .. 2840.95]	2.58	ddd	1
8	M02	2819.77	[2802.74 .. 2840.95]	1.17	ddd	1
9	M03	2915.61	[2895.14 .. 2932.18]	-	m	1
10	M04	3037.73	[3014.25 .. 3050.32]	-	m	2

Acquisition Time (sec)	1.3566	Date	May 3 2006		
File Name	C:\Documents and Settings\maganoj.AMER\Desktop\publications\demethylation paper\H and C spectra\AASUN702.RESEARCH.AA.WL.COM\NMR\HAHN\NHFILES\2006\20060503\8802				
Frequency (MHz)	100.62	Nucleus	13C	Number of Transients	512
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Receiver Gain	50.00	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	10060.7090	Sweep Width (Hz)	24154.59	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height
1	14.47	1455.4	0.5207
2	61.51	6188.8	0.2500
3	76.90	7737.5	0.8909
4	77.22	7770.0	0.8675
5	77.54	7801.7	0.9102
6	116.53	11724.9	0.3886
7	120.39	12113.3	0.4398
8	122.07	12282.1	1.0000
9	129.88	13068.7	0.4045
10	131.94	13275.1	0.3737
11	156.05	15701.8	0.4320
12	167.00	16803.2	0.1495

Entry 7: Ethyl 4-hydroxybenzoate

5/5/2006 10:36 AM

Acquisition Time (sec)	5.1298	Date	May 3 2006
File Name	C:\Documents and Settings\maganoj.AMER\Desktop\publications\demethylation paper\H and C spectra\AASUN702.RESEARCH.AA.WL.COM\NMR\HAHN\NHFILES\2006\20060503\8901		
Frequency (MHz)	400.11	Nucleus	¹ H
Original Points Count	32768	Points Count	32768
Receiver Gain	38.00	Solvent	DMSO-d6
Sweep Width (Hz)	6387.74	Temperature (degree C)	25.000
		Number of Transients	16
		Pulse Sequence	s2pul
		Spectrum Offset (Hz)	2400.6519

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	1.23	490.7	0.4231	9	6.81	2722.8	0.1227
2	1.24	497.7	1.0000	10	6.82	2727.5	0.1220
3	1.26	504.9	0.4237	11	6.82	2729.6	0.4821
4	4.18	1671.1	0.1293	12	7.76	3106.6	0.4288
5	4.19	1678.3	0.4135	13	7.77	3108.8	0.1212
6	4.21	1685.3	0.4179	14	7.78	3113.5	0.1173
7	4.23	1692.5	0.1230	15	7.79	3115.4	0.4434
8	6.80	2720.8	0.4054	16	10.26	4104.4	0.2680

No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	[1.19 .. 1.27]	2.932	2.93995e+10	2.932
2	[4.16 .. 4.24]	2.000	2.00523e+10	2.000
3	[6.77 .. 6.84]	2.014	2.01964e+10	2.014
4	[7.71 .. 7.80]	1.967	1.97166e+10	1.967
5	[10.21 .. 10.30]	1.015	1.01792e+10	1.015

No.	Multiplet1	Shift1 (Hz)	(Hz)	J (Hz)	Type	H's
1	M00	497.77	[478.02 .. 508.23]	7.12	t	3
2	M00	497.77	[478.02 .. 508.23]	7.12	t	3
3	M01	1681.80	[1665.22 .. 1696.03]	7.21	q	2
4	M01	1681.80	[1665.22 .. 1696.03]	7.21	q	2
5	M01	1681.80	[1665.22 .. 1696.03]	7.21	q	2
6	M02	2725.19	[2706.81 .. 2736.44]	-	m	2
7	M03	3111.08	[3084.42 .. 3120.48]	-	m	2
8	M04	4104.37	[4084.09 .. 4121.52]	-	s	1

Acquisition Time (sec)	1.3566	Date	May 3 2006
File Name	C:\Documents and Settings\maganoj.AMER\Desktop\publications\demethylation paper\H and C spectra\AASUN702.RESEARCH.AA.WL.COM\NMR\HAHN\NHFILES\2006\20060503\8902		
Frequency (MHz)	100.62	Nucleus	¹³ C
Original Points Count	32768	Points Count	32768
Receiver Gain	50.00	Solvent	DMSO-d6
Sweep Width (Hz)	24154.59	Temperature (degree C)	25.000
		Number of Transients	512
		Pulse Sequence	s2pul
		Spectrum Offset (Hz)	10060.8252

No.	(ppm)	(Hz)	Height
1	14.89	1498.3	0.4519
2	39.75	3999.5	0.2940
3	39.95	4020.2	0.5678
4	40.17	4041.5	0.6938
5	40.37	4062.2	0.5737
6	40.58	4083.5	0.2902
7	60.70	6107.1	0.3936
8	115.93	11664.5	1.0000
9	121.21	12196.0	0.2075
10	132.00	13281.1	0.8149
11	162.55	16355.1	0.2405
12	166.20	16722.9	0.2181

Entry 8: 2-Bromophenol

5/5/2006 10:40 AM

Acquisition Time (sec)	5.1298	Date	May 5 2006
File Name	C:\Documents and Settings\maganoj.AMER\Desktop\publications\demethylation paper\H and C spectra\HAHN.CHEMISTRY.AA.WL.COM\SAMBA\20060505\1101		
Frequency (MHz)	400.11	Nucleus	¹ H
Original Points Count	32768	Points Count	32768
Receiver Gain	32.00	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	2400.6646	Sweep Width (Hz)	6387.74
		Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height
1	5.64	2257.5	1.0000
2	6.79	2715.8	0.3461
3	6.79	2717.4	0.3676
4	6.81	2723.2	0.4090
5	6.81	2724.0	0.3761
6	6.81	2724.8	0.4370
7	6.83	2731.2	0.4235
8	6.83	2732.8	0.4403
9	7.03	2812.9	0.5128
10	7.03	2814.4	0.5057
11	7.05	2821.1	0.6241
12	7.05	2822.4	0.6000

No.	(ppm)	(Hz)	Height
13	7.20	2879.7	0.3164
14	7.20	2881.3	0.3302
15	7.22	2887.1	0.3116
16	7.22	2888.7	0.3340
17	7.22	2889.5	0.2889
18	7.24	2895.3	0.2460
19	7.24	2896.9	0.2425
20	7.45	2981.5	0.6316
21	7.46	2983.1	0.6174
22	7.47	2989.5	0.5944
23	7.48	2991.1	0.5837

No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	[5.60 .. 5.68]	0.919	1.49345e+10	0.919
2	[6.79 .. 6.87]	0.988	1.60573e+10	0.988
3	[7.00 .. 7.07]	0.944	1.53405e+10	0.944
4	[7.19 .. 7.28]	1.000	1.62562e+10	1.000
5	[7.42 .. 7.49]	0.940	1.52815e+10	0.940

No.	Multiplet	Shift1 (Hz)	(Hz)	J (Hz)	Type	H's
1	M00	2257.48	[2240.32 .. 2271.32]	-	s	1
2	M01	2724.15	[2715.40 .. 2750.10]	8.09	ddd	1
3	M01	2724.15	[2715.40 .. 2750.10]	7.31	ddd	1
4	M01	2724.15	[2715.40 .. 2750.10]	1.56	ddd	1
5	M02	2817.70	[2802.74 .. 2827.69]	8.09	dd	1
6	M02	2817.70	[2802.74 .. 2827.69]	1.46	dd	1
7	M03	2888.37	[2878.57 .. 2911.13]	8.38	ddd	1
8	M03	2888.37	[2878.57 .. 2911.13]	7.21	ddd	1
9	M03	2888.37	[2878.57 .. 2911.13]	1.56	ddd	1
10	M04	2986.28	[2968.44 .. 2996.71]	7.99	dd	1
11	M04	2986.28	[2968.44 .. 2996.71]	1.56	dd	1

Acquisition Time (sec)	1.3566	Date	May 5 2006	
File Name	C:\Documents and Settings\maganoj.AMER\Desktop\publications\demethylation paper\H and C spectra\HAHN.CHEMISTRY.AA.WL.COM\SAMBA\20060505\1102			
Frequency (MHz)	100.62	Nucleus	13C	Number of Transients 512
Original Points Count	32768	Points Count	32768	Pulse Sequence s2pul
Receiver Gain	50.00	Solvent	CHLOROFORM-d	
Spectrum Offset (Hz)	10060.7090	Sweep Width (Hz)	24154.59	Temperature (degree C) 25.000

No.	(ppm)	(Hz)	Height
1	77.04	7751.5	0.1695
2	77.35	7783.2	0.1701
3	77.68	7815.7	0.1574
4	110.54	11121.9	0.3232
5	116.47	11719.0	0.8307
6	122.12	12287.3	0.6973
7	129.44	13023.7	1.0000
8	132.33	13314.9	0.8791
9	152.49	15343.6	0.4626

Entry 9: 3-Bromophenol

5/5/2006 10:57 AM

Acquisition Time (sec)	5.1298	Date	May 3 2006
File Name	C:\Documents and Settings\maganoj.AMER\Desktop\publications\demethylation paper\H and C spectra\AASUN702.RESEARCH.AA.WL.COM\NMR\HAHN\NHFILES\2006\20060503\9101		
Frequency (MHz)	400.11	Nucleus	¹ H
Original Points Count	32768	Points Count	32768
Receiver Gain	32.00	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	2400.6646	Sweep Width (Hz)	6387.74
		Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height
1	5.31	2126.1	0.0084
2	6.77	2709.0	0.1450
3	7.06	2825.0	0.0203

No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	[5.00 .. 5.69]	1.093	1.71315e+10	1.093
2	[6.73 .. 6.81]	1.000	1.56672e+10	1.000
3	[7.00 .. 7.04]	0.942	1.47633e+10	0.942
4	[7.06 .. 7.10]	1.830	2.86775e+10	1.830

No.	Multiplet1	Shift1 (Hz)	(Hz)	Type	H's
1	M00	2126.09	[2104.45 .. 2147.92]	s	1
2	M01	2708.97	[2691.62 .. 2726.51]	s	1
3	M02	2824.96	[2806.44 .. 2843.48]	s	3

Acquisition Time (sec)	1.3566	Date	May 3 2006		
File Name	C:\Documents and Settings\maganoj.AMER\Desktop\publications\demethylation paper\H and C spectra\AASUN702.RESEARCH.AA.WL.COM\NMR\HAHN\NHFILES\2006\20060503\9102				
Frequency (MHz)	100.62	Nucleus	13C	Number of Transients	512
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Receiver Gain	50.00	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	10060.7090	Sweep Width (Hz)	24154.59	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height
1	77.05	7753.0	0.1029
2	77.37	7784.7	0.1092
3	77.69	7817.2	0.0983
4	114.60	11531.0	0.7920
5	119.10	11983.6	1.0000
6	123.07	12383.1	0.2639
7	124.41	12518.0	0.6474
8	131.17	13197.7	0.8694
9	156.27	15724.0	0.3744

Entry 10: 4-Bromophenol

5/5/2006 11:04 AM

Acquisition Time (sec)	5.1298	Date	May 4 2006
File Name	C:\Documents and Settings\maganoj.AMER\Desktop\publications\demethylation paper\H and C spectra\AASUN702.RESEARCH.AA.WL.COM\NMR\HAHN\NHFILES\2006\20060504\1001		
Frequency (MHz)	400.11	Nucleus	¹ H
Original Points Count	32768	Points Count	32768
Receiver Gain	34.00	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	2400.6646	Sweep Width (Hz)	6387.74
		Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height
1	5.63	2253.6	0.1318
2	6.69	2676.0	0.0842
3	6.70	2679.3	0.8480
4	6.70	2681.7	0.2977
5	6.71	2686.2	0.2884
6	6.72	2688.3	1.0000
7	6.73	2691.6	0.1055
8	7.29	2918.7	0.0886
9	7.30	2922.0	0.8937
10	7.31	2924.2	0.2901
11	7.32	2928.7	0.2631
12	7.33	2931.0	0.8944
13	7.33	2934.3	0.0947

No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	[5.57 .. 5.68]	19.307	1.61215e+10	19.307
2	[6.67 .. 6.74]	40.808	3.40746e+10	40.808
3	[7.24 .. 7.34]	39.885	3.33035e+10	39.885

No.	Multiplet1	Shift1 (Hz)	(Hz)	Type	H's
1	M00	2253.58	[2229.60 .. 2273.46]	s	1
2	M01	2683.85	[2670.37 .. 2696.88]	m	2
3	M02	2926.49	[2897.87 .. 2936.08]	m	2

Acquisition Time (sec)	1.3566	Date	May 4 2006		
File Name	C:\Documents and Settings\maganoj.AMER\Desktop\publications\demethylation paper\H and C spectra\AASUN702.RESEARCH.AA.WL.COM\NMR\HAHN\NHFILES\2006\20060504\1002				
Frequency (MHz)	100.62	Nucleus	13C	Number of Transients	512
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Receiver Gain	50.00	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	10060.7090	Sweep Width (Hz)	24154.59	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height
1	77.03	7750.8	0.1003
2	77.35	7782.5	0.1041
3	77.66	7814.2	0.0927
4	113.43	11413.0	0.1556
5	117.51	11823.6	1.0000
6	132.82	13363.6	0.9564
7	154.46	15541.1	0.2950

Entry 11: 4-Hydroxybenzaldehyde

5/5/2006 11:10 AM

Acquisition Time (sec)	5.1298	Date	May 3 2006
File Name	C:\Documents and Settings\maganoj.AMER\Desktop\publications\demethylation paper\H and C spectra\AASUN702.RESEARCH.AA.WL.COM\NMR\HAHN\NHFILES\2006\20060503\9201		
Frequency (MHz)	400.11	Nucleus	¹ H
Original Points Count	32768	Points Count	32768
Receiver Gain	44.00	Solvent	DMSO-d6
Sweep Width (Hz)	6387.74	Temperature (degree C)	25.000
		Number of Transients	16
		Pulse Sequence	s2pul
		Spectrum Offset (Hz)	2400.6519

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	2.46	985.3	0.0523	10	7.71	3083.2	0.1078	1	[6.86 .. 6.92]	2.006	2.81707e+10	2.006
2	2.47	987.0	0.0756	11	7.71	3086.0	0.9445	2	[7.69 .. 7.75]	2.019	2.83633e+10	2.019
3	2.47	989.0	0.0544	12	7.72	3087.9	0.2859	3	[9.72 .. 9.78]	1.000	1.40453e+10	1.000
4	6.88	2752.0	0.0785	13	7.73	3092.6	0.2745	4	[10.50 .. 10.59]	1.005	1.41221e+10	1.005
5	6.88	2754.6	0.8109	14	7.73	3094.6	0.9443					
6	6.89	2756.5	0.2083	15	7.74	3097.3	0.1031					
7	6.90	2761.4	0.2171	16	9.75	3901.8	1.0000					
8	6.91	2763.0	0.7691	17	10.55	4221.1	0.3912					
9	6.91	2765.9	0.0829									

No.	Multiplet1	Shift1 (Hz)	(Hz)	J (Hz)	Type	H's
1	M00	2758.89	[2743.46 .. 2769.00]	-	m	1
2	M01	3090.27	[3078.38 .. 3100.40]	8.97	ddd	2
3	M01	3090.27	[3078.38 .. 3100.40]	2.73	ddd	2
4	M01	3090.27	[3078.38 .. 3100.40]	2.34	ddd	2
5	M02	3901.82	[3887.78 .. 3913.91]	-	s	1
6	M03	4221.14	[4202.23 .. 4238.68]	-	s	1

Acquisition Time (sec)	1.3566	Date	May 3 2006
File Name	C:\Documents and Settings\maganoj.AMER\Desktop\publications\demethylation paper\H and C spectra\AASUN702.RESEARCH.AA.WL.COM\NMR\HAHN\NHFILES\2006\20060503\9202		
Frequency (MHz)	100.62	Nucleus	¹³ C
Original Points Count	32768	Points Count	32768
Receiver Gain	50.00	Solvent	DMSO-d6
Sweep Width (Hz)	24154.59	Temperature (degree C)	25.000
		Number of Transients	512
		Pulse Sequence	s2pul
		Spectrum Offset (Hz)	10060.8252

No.	(ppm)	(Hz)	Height
1	39.76	4000.2	0.4004
2	39.97	4021.6	0.8321
3	40.17	4042.3	1.0000
4	40.39	4063.6	0.8707
5	40.59	4084.3	0.4264
6	116.49	11721.3	0.6888
7	129.10	12989.9	0.6796
8	132.75	13357.0	0.6866
9	163.96	16497.4	0.3672
10	191.58	19276.5	0.8705

Entry 12: 4-Hydroxyacetophenone

5/5/2006 11:14 AM

Acquisition Time (sec)	5.1298	Date	May 3 2006
File Name	C:\Documents and Settings\maganoj.AMER\Desktop\publications\demethylation paper\H and C spectral\AASUN702.RESEARCH.AA.WL.COM\NMR\HAHN\NHFILES\2006\20060503\9301		
Frequency (MHz)	400.11	Nucleus	¹ H
Original Points Count	32768	Points Count	32768
Receiver Gain	38.00	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	2400.6646	Sweep Width (Hz)	6387.74
		Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height
1	2.57	1030.1	1.0000
2	6.94	2778.8	0.2125
3	6.97	2787.5	0.2306
4	7.89	3155.8	0.2180
5	7.91	3164.6	0.2171
6	8.56	3426.0	0.0084

No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	[2.52 .. 2.63]	3.013	4.23951e+10	3.013
2	[6.89 .. 7.01]	2.035	2.86304e+10	2.035
3	[7.83 .. 7.97]	2.031	2.85754e+10	2.031
4	[8.36 .. 8.80]	1.026	1.44277e+10	1.026

No.	Multiplet1	Shift1 (Hz)	(Hz)	J (Hz)	Type	H's
1	M00	1030.11	[1015.88 .. 1046.10]	-	s	3
2	M01	2783.15	[2761.60 .. 2794.16]	8.77	d	2
3	M02	3160.17	[3138.63 .. 3171.57]	8.77	d	2
4	M03	3425.97	[3402.38 .. 3448.78]	-	s	1

Acquisition Time (sec)	1.3566	Date	May 3 2006
File Name	C:\Documents and Settings\maganoj.AMER\Desktop\publications\demethylation paper\H and C spectra\AASUN702.RESEARCH.AA.WL.COM\NMR\HAHN\NHFILES\2006\20060503\9302		
Frequency (MHz)	100.62	Nucleus	13C
Original Points Count	32768	Points Count	32768
Receiver Gain	50.00	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	10060.7090	Sweep Width (Hz)	24154.59
		Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height
1	26.50	2666.6	0.6225
2	76.97	7744.2	0.2466
3	77.28	7775.9	0.2616
4	77.60	7807.6	0.2389
5	115.88	11659.2	1.0000
6	129.48	13028.2	0.2131
7	131.57	13238.2	0.9491
8	162.05	16304.8	0.4350
9	199.44	20067.3	0.2504

Entry 13: 4-Hydroxybenzophenone

5/5/2006 11:18 AM

Acquisition Time (sec)	5.1298	Date	May 4 2006
File Name	C:\Documents and Settings\maganoj.AMER\Desktop\publications\demethylation paper\H and C spectra\AASUN702.RESEARCH.AA.WL.COM\NMR\SPIN\NSFILES\2006\20060504\0601		
Frequency (MHz)	399.90	Nucleus	1H
Original Points Count	32768	Points Count	32768
Receiver Gain	32.00	Solvent	DMSO-d6
Sweep Width (Hz)	6387.74	Temperature (degree C)	25.000
		Number of Transients	16
		Pulse Sequence	s2pul
		Spectrum Offset (Hz)	2399.4258

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	2.45	981.5	0.0424	13	7.47	2987.9	0.1410	25	7.59	3034.5	0.1339	1	[6.83 .. 6.92]	2.068	2.26274e+10	2.068
2	2.46	983.3	0.0618	14	7.48	2989.6	0.5688	26	7.59	3035.8	0.0742	2	[7.45 .. 7.51]	1.977	2.16334e+10	1.977
3	2.46	985.2	0.0441	15	7.49	2995.7	0.1704	27	7.61	3041.7	0.6706	3	[7.55 .. 7.64]	4.958	5.42569e+10	4.958
4	6.85	2738.1	0.0885	16	7.49	2997.2	0.4345	28	7.61	3043.2	0.6803	4	[10.34 .. 10.45]	1.000	1.09422e+10	1.000
5	6.85	2740.9	0.8909	17	7.50	2999.0	0.0977	29	7.61	3044.4	1.0000					
6	6.86	2743.0	0.2449	18	7.55	3018.3	0.1204	30	7.62	3046.3	0.2795					
7	6.87	2747.7	0.2445	19	7.55	3019.6	0.2515	31	7.62	3048.7	0.2207					
8	6.88	2749.6	0.8702	20	7.55	3021.2	0.1639	32	7.63	3050.1	0.5249					
9	6.88	2752.6	0.0964	21	7.56	3025.1	0.0949	33	7.63	3051.2	0.5242					
10	7.46	2981.4	0.1503	22	7.57	3027.0	0.2830	34	7.63	3053.2	0.9193					
11	7.46	2982.4	0.2448	23	7.58	3029.4	0.0989	35	7.64	3055.9	0.0972					
12	7.46	2984.0	0.1026	24	7.58	3033.1	0.0840	36	10.40	4157.5	0.1672					

No.	Multiplet1	Shift1 (Hz)	(Hz)	Type	H's
1	M00	2745.32	[2729.76 .. 2769.33]	m	2
2	M01	2989.64	[2980.07 .. 3001.32]	m	2
3	M02	3037.71	[3017.89 .. 3056.68]	m	5
4	M03	4157.53	[4135.89 .. 4179.17]	s	1

Acquisition Time (sec)	1.3566	Date	May 4 2006
File Name	C:\Documents and Settings\maganoj.AMER\Desktop\publications\demethylation paper\H and C spectra\AASUN702.RESEARCH.AA.WL.COM\NMR\SPIN\NSFILES\2006\20060504\0602		
Frequency (MHz)	100.57	Nucleus	¹³ C
Original Points Count	32768	Points Count	32768
Receiver Gain	50.00	Solvent	DMSO-d6
Sweep Width (Hz)	24154.59	Temperature (degree C)	25.000
		Number of Transients	512
		Pulse Sequence	s2pul
		Spectrum Offset (Hz)	10055.5898

No.	(ppm)	(Hz)	Height
1	39.54	3976.6	0.1295
2	39.75	3998.0	0.4230
3	39.96	4018.6	0.8715
4	40.17	4040.0	1.0000
5	40.38	4060.6	0.8630
6	40.58	4081.3	0.4116
7	40.80	4102.6	0.1392
8	115.92	11657.1	0.5448
9	128.56	12928.7	0.4935
10	128.99	12972.2	0.8090
11	129.77	13050.3	0.6093
12	132.42	13317.2	0.2722
13	133.16	13390.9	0.5885
14	138.77	13955.5	0.4982
15	162.65	16357.2	0.2861
16	194.95	19605.2	0.1835

Entry 14: 4,4'-dihydroxybenzophenone

5/5/2006 11:27 AM

Acquisition Time (sec)	5.1298	Date	May 3 2006		
File Name	C:\Documents and Settings\maganoj.AMER\Desktop\publications\demethylation paper\H and C spectra\AASUN702.RESEARCH.AA.WL.COM\NMR\HAHN\NHFILES\2006\20060503\9401				
Frequency (MHz)	400.11	Nucleus	1H	Number of Transients	16
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Receiver Gain	50.00	Solvent	DMSO-d6	Spectrum Offset (Hz)	2400.6519
Sweep Width (Hz)	6387.74	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height
1	6.83	2732.3	0.9307
2	6.85	2740.9	1.0000
3	7.56	3023.2	0.9897
4	7.58	3031.8	0.9387

No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	[6.80 .. 6.88]	4.005	3.24780e+10	4.005
2	[7.53 .. 7.60]	3.980	3.22755e+10	3.980
3	[10.18 .. 10.26]	2.000	1.62174e+10	2.000

No.	Multiplet1	Shift1 (Hz)	(Hz)	Type	H's
1	M01	2736.61	[2720.07 .. 2751.26]	m	4
2	M02	3027.46	[3011.31 .. 3041.34]	m	4
3	M03	4089.75	[4072.59 .. 4106.90]	s	2

Acquisition Time (sec)	1.3566	Date	May 3 2006
File Name	C:\Documents and Settings\maganoj.AMER\Desktop\publications\demethylation paper\H and C spectra\AASUN702.RESEARCH.AA.WL.COM\NMR\HAHN\NHFILES\2006\20060503\9402		
Frequency (MHz)	100.62	Nucleus	¹³ C
Original Points Count	32768	Points Count	32768
Receiver Gain	50.00	Solvent	DMSO-d6
Sweep Width (Hz)	24154.59	Temperature (degree C)	25.000
		Number of Transients	512
		Pulse Sequence	s2pul
		Spectrum Offset (Hz)	10060.8252

No.	(ppm)	(Hz)	Height
1	39.57	3981.1	0.1327
2	39.78	4002.5	0.4207
3	39.98	4023.1	0.8700
4	40.20	4044.5	1.0000
5	40.40	4065.1	0.8787
6	40.61	4085.8	0.4302
7	40.82	4107.1	0.1510
8	115.67	11638.7	0.3928
9	129.45	13025.3	0.1648
10	132.68	13349.7	0.4220
11	161.89	16289.5	0.1290
12	193.70	19489.5	0.0789

Entry 15: Cyclopropyl-4-hydroxyphenyl ketone

5/5/2006 11:31 AM

Acquisition Time (sec)	5.1298	Date	May 3 2006
File Name	C:\Documents and Settings\maganoj.AMER\Desktop\publications\demethylation paper\H and C spectra\AASUN702.RESEARCH.AA.WL.COM\NMR\HAHN\NHFILES\2006\20060503\9501		
Frequency (MHz)	400.11	Nucleus	1H
Original Points Count	32768	Points Count	32768
Receiver Gain	38.00	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	2400.6646	Sweep Width (Hz)	6387.74
		Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height
1	1.01	406.1	0.1281
2	1.02	409.8	0.3612
3	1.03	413.3	0.4974
4	1.04	417.6	0.4077
5	1.05	421.1	0.4581
6	1.06	424.6	0.1700
7	1.22	487.4	0.1624
8	1.23	490.9	0.4656
9	1.24	495.2	0.5736
10	1.25	498.7	0.4249
11	1.26	502.8	0.1621
12	2.63	1053.1	0.1464
13	2.64	1056.4	0.1560

No.	(ppm)	(Hz)	Height
14	2.65	1060.9	0.2869
15	2.66	1065.4	0.1540
16	2.67	1068.7	0.1445
17	6.91	2765.1	0.9155
18	6.92	2767.1	0.2780
19	6.93	2771.9	0.2675
20	6.93	2773.9	1.0000
21	6.94	2776.8	0.1110
22	7.93	3174.7	0.9242
23	7.94	3176.6	0.2860
24	7.95	3181.5	0.2632
25	7.96	3183.5	0.9314

No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	[1.01 .. 1.10]	1.917	1.68959e+10	1.917
2	[1.18 .. 1.28]	2.018	1.77844e+10	2.018
3	[2.61 .. 2.70]	0.999	8.80507e+9	0.999
4	[6.88 .. 6.97]	1.946	1.71499e+10	1.946
5	[7.92 .. 8.00]	2.000	1.76254e+10	2.000

No.	Multiplet1	Shift1 (Hz)	(Hz)	J (Hz)	Type	H's
1	M00	415.42	[404.53 .. 439.62]	7.63	m	2
2	M00	415.42	[404.53 .. 439.62]	3.73	m	2
3	M00	415.42	[404.53 .. 439.62]	3.58	m	2
4	M00	415.42	[404.53 .. 439.62]	3.58	m	2
5	M01	494.99	[471.98 .. 510.78]	7.75	dt	2
6	M01	494.99	[471.98 .. 510.78]	3.83	dt	2
7	M01	494.99	[471.98 .. 510.78]	3.83	dt	2
8	M02	1060.91	[1044.54 .. 1079.24]	-	m	1
9	M03	2770.96	[2753.42 .. 2787.92]	-	m	2
10	M04	3179.08	[3167.67 .. 3200.23]	-	m	2

Acquisition Time (sec)	1.3566	Date	May 3 2006		
File Name	C:\Documents and Settings\maganoj.AMER\Desktop\publications\demethylation paper\H and C spectra\AASUN702.RESEARCH.AA.WL.COM\NMR\HAHN\NHFILES\2006\20060503\9502				
Frequency (MHz)	100.62	Nucleus	13C	Number of Transients	512
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Receiver Gain	50.00	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	10060.7090	Sweep Width (Hz)	24154.59	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height
1	12.14	1221.0	0.8856
2	17.21	1731.9	0.4262
3	76.94	7741.2	0.3327
4	77.26	7773.7	0.3144
5	77.57	7805.4	0.3328
6	115.76	11647.5	1.0000
7	130.40	13120.3	0.2922
8	131.03	13183.7	0.9806
9	161.50	16249.6	0.3192
10	201.45	20269.3	0.1659

Entry 16: 1-(4-Hydroxyphenyl)-1H-imidazole

5/5/2006 11:35 AM

Acquisition Time (sec)	5.1298	Date	May 3 2006
File Name	C:\Documents and Settings\maganoj.AMER\Desktop\publications\demethylation paper\H and C spectra\AASUN702.RESEARCH.AA.WL.COM\NMR\HAHN\NHFILES\2006\20060503\9601		
Frequency (MHz)	400.11	Nucleus	¹ H
Original Points Count	32768	Points Count	32768
Receiver Gain	44.00	Solvent	DMSO-d6
Sweep Width (Hz)	6387.74	Temperature (degree C)	25.000
		Number of Transients	16
		Pulse Sequence	s2pul
		Spectrum Offset (Hz)	2400.6519

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	Value	Absolute Value	Non-Negative Value	
1	2.46	985.3	0.0749	11	7.35	2939.8	0.1120	1	[6.78 .. 6.87]	2.015	2.83699e+10	2.015	
2	2.47	987.0	0.1031	12	7.36	2943.3	0.9819	2	[6.97 .. 7.07]	1.016	1.43035e+10	1.016	
3	2.47	989.0	0.0764	13	7.36	2945.4	0.2985	3	[7.30 .. 7.39]	2.000	2.81647e+10	2.000	
4	6.82	2729.4	0.0982	14	7.37	2949.9	0.2935	4	[7.48 .. 7.57]	0.965	1.35900e+10	0.965	
5	6.83	2732.9	0.9402	15	7.38	2952.1	0.8951	5	[7.97 .. 8.07]	0.953	1.34243e+10	0.953	
6	6.84	2735.1	0.2943	16	7.39	2955.6	0.0810	6	[9.67 .. 9.78]	0.845	1.18999e+10	0.845	
7	6.85	2739.6	0.3104	17	7.53	3013.5	0.2894						
8	6.85	2741.7	1.0000	18	8.03	3212.1	0.2603						
9	6.86	2745.2	0.0965	19	9.73	3894.2	0.1039						
10	7.03	2813.6	0.2683					No.	Multiplet1	Shift1 (Hz)	(Hz)	Type	H's
								1	M00	2737.32	[2711.10 .. 2748.14]	m	2
								2	M01	2813.64	[2788.49 .. 2830.80]	s	1
								3	M02	2947.67	[2922.81 .. 2957.70]	m	2
								4	M03	3013.46	[2992.01 .. 3030.42]	s	1
								5	M04	3212.11	[3186.96 .. 3227.70]	s	1
								6	M05	3894.22	[3868.68 .. 3913.52]	s	1

Acquisition Time (sec)	1.3566	Date	May 3 2006
File Name	C:\Documents and Settings\maganoj.AMER\Desktop\publications\demethylation paper\H and C spectra\AASUN702.RESEARCH.AA.WL.COM\NMR\HAHN\NHFILES\2006\20060503\9602		
Frequency (MHz)	100.62	Nucleus	¹³ C
Original Points Count	32768	Points Count	32768
Receiver Gain	50.00	Solvent	DMSO-d6
Sweep Width (Hz)	24154.59	Temperature (degree C)	25.000
		Number of Transients	512
		Pulse Sequence	s2pul
		Spectrum Offset (Hz)	10060.8252

No.	(ppm)	(Hz)	Height
1	39.55	3979.6	0.1362
2	39.76	4000.2	0.4126
3	39.97	4021.6	0.8624
4	40.17	4042.3	1.0000
5	40.39	4063.6	0.8640
6	40.59	4084.3	0.4401
7	40.80	4105.7	0.1507
8	99.99	10061.2	0.0382
9	116.72	11744.1	0.8534
10	119.14	11987.4	0.0450
11	122.93	12369.2	0.9441
12	129.64	13043.8	0.1451
13	130.00	13079.9	0.0917
14	157.09	15805.9	0.3798

Entry 17: *N,N*-Diphenyl-4-hydroxybenzamide

5/5/2006 11:42 AM

Acquisition Time (sec)	5.1298	Date	May 3 2006
File Name	C:\Documents and Settings\maganoj.AMER\Desktop\publications\demethylation paper\H and C spectra\AASUN702.RESEARCH.AA.WL.COM\NMR\HAHN\NHFILES\2006\20060503\9701		
Frequency (MHz)	400.11	Nucleus	¹ H
Original Points Count	32768	Points Count	32768
Receiver Gain	38.00	Solvent	DMSO-d6
Sweep Width (Hz)	6387.74	Temperature (degree C)	25.000
		Number of Transients	16
		Pulse Sequence	s2pul
		Spectrum Offset (Hz)	2400.6519

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	6.57	2628.6	0.6708	12	7.23	2894.0	0.6865	1	[6.55 .. 6.61]	2.000	1.24284e+10	2.000
2	6.57	2630.6	0.2132	13	7.24	2895.9	0.2141	2	[7.10 .. 7.18]	5.767	3.58381e+10	5.767
3	6.59	2635.3	0.2057	14	7.25	2900.8	0.2078	3	[7.23 .. 7.26]	1.999	1.24216e+10	1.999
4	6.59	2637.2	0.7002	15	7.25	2902.7	0.6619	4	[7.26 .. 7.31]	3.894	2.41969e+10	3.894
5	7.11	2843.1	0.8050	16	7.26	2906.4	0.7734	5	[9.82 .. 9.90]	1.035	6.43250e+9	1.035
6	7.12	2850.3	1.0000	17	7.27	2908.2	0.3049					
7	7.13	2851.7	0.8357	18	7.28	2914.4	0.9353					
8	7.13	2854.4	0.2735	19	7.30	2920.1	0.1848					
9	7.15	2862.0	0.5463	20	7.30	2922.0	0.4310					
10	7.17	2868.2	0.2485	21	9.87	3948.2	0.6533					
11	7.17	2869.4	0.3562									

No.	Multiplet1	Shift1 (Hz)	(Hz)	Type	H's
1	M00	2632.93	[2620.26 .. 2644.82]	m	2
2	M01	2857.00	[2839.96 .. 2870.95]	m	6
3	M02	2898.34	[2890.84 .. 2904.68]	m	2
4	M03	2914.23	[2904.68 .. 2924.37]	m	4
5	M04	3948.22	[3929.11 .. 3960.11]	s	1

Acquisition Time (sec)	1.3566	Date	May 3 2006
File Name	C:\Documents and Settings\maganoj.AMER\Desktop\publications\demethylation paper\H and C spectra\AASUN702.RESEARCH.AA.WL.COM\NMR\HAHN\NHFILES\2006\20060503\9702		
Frequency (MHz)	100.62	Nucleus	¹³ C
Original Points Count	32768	Points Count	32768
Receiver Gain	50.00	Solvent	DMSO-d6
Sweep Width (Hz)	24154.59	Temperature (degree C)	25.000
		Number of Transients	512
		Pulse Sequence	s2pul
		Spectrum Offset (Hz)	10060.8252

No.	(ppm)	(Hz)	Height
1	39.57	3981.8	0.0944
2	39.79	4003.2	0.3126
3	39.99	4023.8	0.6101
4	40.20	4045.2	0.7524
5	40.41	4065.9	0.6251
6	40.62	4087.2	0.3271
7	40.83	4107.9	0.1055
8	115.16	11587.1	0.4145
9	126.73	12751.1	0.3641
10	127.08	12786.5	0.1533
11	128.22	12901.5	0.8873
12	129.74	13054.1	1.0000
13	131.73	13254.6	0.4268
14	145.00	14589.6	0.3348
15	159.81	16080.1	0.2155
16	170.28	17132.8	0.1241

Entry 18: 4-Nitro-1-naphthol

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Acquisition Time (sec)	5.1298	Date	May 3 2006
File Name	C:\Documents and Settings\maganoj.AMER\Desktop\publications\demethylation paper\H and C spectra\AASUN702.RESEARCH.AA.WL.COM\NMR\HAHN\NHFILES\2006\20060503\9801		
Frequency (MHz)	400.11	Nucleus	¹ H
Original Points Count	32768	Points Count	32768
Receiver Gain	44.00	Solvent	DMSO-d ₆
Sweep Width (Hz)	6387.74	Temperature (degree C)	25.000
		Number of Transients	16
		Pulse Sequence	s2pul
		Spectrum Offset (Hz)	2400.6519

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	6.93	2774.1	0.9547	14	7.75	3101.4	0.3211	1	[6.90 .. 6.99]	1.047	1.45891e+10	1.047
2	6.95	2782.6	0.9494	15	7.76	3106.8	0.2626	2	[7.54 .. 7.64]	1.099	1.53053e+10	1.099
3	7.56	3025.9	0.2283	16	7.77	3108.2	0.2452	3	[7.69 .. 7.78]	1.077	1.50080e+10	1.077
4	7.57	3027.1	0.2422	17	8.27	3309.0	0.3344	4	[8.21 .. 8.30]	1.054	1.46840e+10	1.054
5	7.58	3033.0	0.2971	18	8.27	3309.8	0.3364	5	[8.33 .. 8.40]	0.986	1.37321e+10	0.986
6	7.58	3034.1	0.3795	19	8.29	3317.4	0.3242	6	[8.55 .. 8.64]	1.000	1.39287e+10	1.000
7	7.59	3035.7	0.2534	20	8.29	3318.2	0.3037	7	[11.70 .. 12.04]	0.989	1.37707e+10	0.989
8	7.60	3041.3	0.3082	21	8.35	3341.7	1.0000					
9	7.60	3042.5	0.2911	22	8.37	3350.3	0.9084					
10	7.73	3091.2	0.2777	23	8.61	3446.2	0.4189					
11	7.73	3092.6	0.3076	24	8.63	3454.6	0.4027					
12	7.74	3098.1	0.2505	25	11.88	4753.5	0.0475					
13	7.75	3099.8	0.3509									

No.	Multiplet1	Shift1 (Hz)	(Hz)	J (Hz)	Type	H's
1	M00	2778.36	[2762.37 .. 2795.32]	8.58	d	1
2	M01	3034.23	[3016.97 .. 3055.37]	8.38	ddd	1
3	M01	3034.23	[3016.97 .. 3055.37]	7.02	ddd	1
4	M01	3034.23	[3016.97 .. 3055.37]	1.17	ddd	1
5	M02	3099.74	[3075.45 .. 3113.85]	8.63	ddd	1
6	M02	3099.74	[3075.45 .. 3113.85]	6.97	ddd	1
7	M02	3099.74	[3075.45 .. 3113.85]	1.36	ddd	1
8	M03	3313.58	[3284.82 .. 3322.45]	8.38	dd	1
9	M03	3313.58	[3284.82 .. 3322.45]	0.78	dd	1
10	M04	3346.03	[3331.80 .. 3362.80]	8.58	d	1
11	M05	3450.43	[3420.70 .. 3458.91]	8.38	d	1
12	M06	4753.53	[4727.60 .. 4774.00]	-	s	1

Acquisition Time (sec)	1.3566	Date	May 3 2006
File Name	C:\Documents and Settings\maganoj.AMER\Desktop\publications\demethylation paper\H and C spectra\AASUN702.RESEARCH.AA.WL.COM\NMR\HAHN\NHFILES\2006\20060503\9802		
Frequency (MHz)	100.62	Nucleus	¹³ C
Original Points Count	32768	Points Count	32768
Receiver Gain	50.00	Solvent	DMSO-d6
Sweep Width (Hz)	24154.59	Temperature (degree C)	25.000
		Number of Transients	512
		Pulse Sequence	s2pul
		Spectrum Offset (Hz)	10060.8252

No.	(ppm)	(Hz)	Height
1	39.76	4001.0	0.4077
2	39.97	4021.6	0.8298
3	40.18	4043.0	1.0000
4	40.39	4063.6	0.8553
5	40.60	4085.0	0.4480
6	40.80	4105.7	0.1529
7	107.40	10806.5	0.4250
8	123.48	12424.5	0.4586
9	123.76	12452.5	0.5035
10	124.93	12569.8	0.2817
11	126.74	12752.6	0.3694
12	127.46	12824.8	0.4880
13	129.16	12995.8	0.4404
14	130.97	13177.9	0.4351
15	137.30	13814.8	0.2179
16	161.03	16202.5	0.4016

Entry 19: 3,5-Dimethoxyphenol

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Acquisition Time (sec)	5.1298	Date	May 5 2006
File Name	C:\Documents and Settings\maganoj.AMER\Desktop\publications\demethylation paper\H and C spectra\SPIN.CHEMISTRY_AA.WL.COM\SAMBA\20060505\0501		
Frequency (MHz)	399.90	Nucleus	1H
Original Points Count	32768	Points Count	32768
Receiver Gain	18.00	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	2399.3481	Sweep Width (Hz)	6387.74
		Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height
1	3.69	1477.4	0.4779
2	3.70	1480.5	1.0000
3	6.02	2407.2	0.0793
4	6.03	2410.0	0.2105
5	6.03	2412.3	0.2080
6	6.06	2424.2	0.0863
7	6.07	2426.2	0.0913
8	6.07	2428.5	0.0380
9	6.25	2497.7	0.0909

No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	[3.68 .. 3.75]	6.000	3.88579e+10	6.000
2	[6.01 .. 6.09]	2.934	1.90032e+10	2.934
3	[6.19 .. 6.30]	1.058	6.85134e+9	1.058

No.	Multiplet1	Shift1 (Hz)	(Hz)	J (Hz)	Type	H's
1	M00	1478.92	[1472.68 .. 1500.95]	-	m	6
2	M01	2418.06	[2403.34 .. 2434.34]	16.38	ddd	3
3	M01	2418.06	[2403.34 .. 2434.34]	2.53	ddd	3
4	M01	2418.06	[2403.34 .. 2434.34]	2.34	ddd	3
5	M02	2497.70	[2476.84 .. 2518.17]	-	s	1

Acquisition Time (sec)	1.3566	Date	May 5 2006	
File Name	C:\Documents and Settings\maganoj.AMER\Desktop\publications\demethylation paper\H and C spectra\SPIN.CHEMISTRY.AA.WL.COM\SAMBA\20060505\0502			
Frequency (MHz)	100.57	Nucleus	13C	Number of Transients 512
Original Points Count	32768	Points Count	32768	Pulse Sequence s2pul
Receiver Gain	50.00	Solvent	CHLOROFORM-d	
Spectrum Offset (Hz)	10055.5254	Sweep Width (Hz)	24154.59	Temperature (degree C) 25.000

No.	(ppm)	(Hz)	Height
1	55.58	5589.4	0.8514
2	93.51	9403.5	0.4239
3	94.68	9521.5	1.0000
4	157.63	15852.2	0.2507
5	161.71	16262.1	0.5190