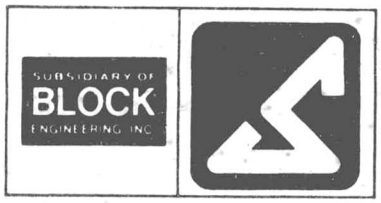
THE SADTLER STANDARD SPECTRA



SADTLER RESEARCH LABORATORIES, INC.

NMR
CHEMICAL SHIFT INDEX

SET 2

CREATIVE CHEMISTS SINCE 1874

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NMR NO.	ASSIGN-MENT	CHEM SHIFT -PPM-	PROTON GROUP	ENVIRONMENTAL GROUPS	S	SOLVENT
14098M	A	0.00	CH3	SI(CL/CH2/CH3)		CDCL3
3449M	A	0.01	CH3	SI(CH2/CH2/CH3)		CL2C=CCL2
9976M	A	0.01	HCHR	R3R5R6R6R5<C*-CH2/CH*-CH2>		CDCL3
9974M	A	0.01	HCHR	R3R5R6R6R5<C*-CH2/CH*-CH2>		CDCL3
9975M	A	0.02	HCHR	R3R5R6R6R5<C*-CH2/CH*-CH2>		CDCL3
8166M	A	0.02	HCHR	R3<CH(CH(CH3/CH3))-HCH>		CCL4
8168M	A	0.03	HCHR	R3<CH(CH2-R3)-HCH>		CCL4
8754M	A	0.04	CH3	SI(CH2/CH3/CH3)		CDCL3
6468M	A	0.04	CH3	SI(O/CH3/CH3)		CCL4
8760M	A	0.05	CH3	SI(CH2/CH3/CH3)		CDCL3
8759M	A	0.05	CH3	SI(CH2/CH3/CH3)		CDCL3
8752M	A	0.05	CH3	SI(CH2/CH3/CH3)		CDCL3
8753M	A	0.05	CH3	SI(CH2/CH3/CH3)		CDCL3
8750M	A	0.05	CH3	SI(CH2/CH3/CH3)		CDCL3
8183M	A	0.05	HCHR	R3<C(CH3/CH3)-CH(CH3)>		CCL4
8755M	A	0.06	CH3	SI(CH2/CH3/CH3)		CDCL3
8749M	A	0.06	CH3	SI(CH2/CH3/CH3)		CDCL3
8756M	A	0.06	CH3	SI(CH2/CH3/CH3)		CDCL3
8751M	A	0.06	CH3	SI(CH2/CH3/CH3)		CDCL3
6515M	A	0.06	CH3	SI(O/O/CH3)		CCL4
3450M	A	0.06	CH3	SI(Q3/CH3/CH3)		CL2C=CCL2
2561M	A	0.07- 0.68	CH2R	R3<CH(CH2-OH)-CH2>		CCL4
8758M	A	0.07	CH3	SI(CH2/CH3/CH3)		CDCL3
1364M	A	0.07	CH3	SI(O/CH3/CH3)		CDCL3
1364M	A	0.07	CH3	SI(O/O/CH3)		CDCL3
10789M	A	0.07	CH3	SI(R5AA/CH3/CH3)		CDCL3
4144M	A	0.08- 0.74	CH2R	R3<CH(CH2-A)-CH2>		CDCL3
6467M	A	0.08	CH3	R8OOOOSISISISI<SI(CH3)-O/G>		CCL4
8757M	A	0.08	CH3	SI(CH2/CH3/CH3)		CDCL3
2381M	A	0.09- 0.60	CH2R	R3<CH(CH(OH/A))-CH2>		CCL4
2562M	A	0.09- 0.64	CH2R	R3<CH(CH(OH/A))-CH2>		CCL4
1442M	A	0.09	CH3	R6N3SI3<SI(CH3)-NH/NH>		CCL4
12172M	A	0.09	CH3	SI(O/O/O)		CCL4
8163M	A	0.09	HCHR	R3<CH(CH2-CH3)-HCH>		CCL4
7686M	A	0.10- 0.70	CH2R	R3<CH(R5NN<C(R3)-NH/C(=O)>)-CH2>		DMSO-D6
1513M	A	0.10	CH3	R8N4SI4<SI(CH3)-NH/NH>		CCL4
10791M	A	0.10	CH3	SI(O/CH3/CH3)		CDCL3
6516M	A	0.10	CH3	SI(O/O/O)		CCL4
8165M	A	0.10- 0.70		UNSPECIFIED		CCL4
3703M	A	0.11	CH3	SI(N/CH3/CH3)		CCL4
8174M	A	0.11	HCHR	R3<CH(CH3)-CH(CH3)>		CCL4
2382M	A	0.12- 0.72	CH2R	R3<CH(CH(OH/R5S))-CH2>		CCL4
5183M	A	0.12	CH3	GE(CH3/CH3/CH3)		CDCL3
950M	A	0.12	CH3	SI(CH2/CH3/CH3)		CCL4
966M	A	0.12	CH3	SI(O/O/Q3)		CL2C=CCL2
1436M	A	0.13	CH3	SI(O/Q3/CH3)		CCL4
8462M	A	0.14	HCHR	R3<CH(CH2-R6NN)-HCH>		CDCL3
13244M	A	0.15	CH2R	R3R6(CH*-CH2/CH*-CH2)		CCL4
10787M	A	0.16	CH3	SI(C/CH3/CH3)		CDCL3
1443M	A	0.16	CH3	SI(O-CH2/Q3/CH3)		CCL4
3702M	A	0.17	CH3	SI(N/CH3/CH3)		CCL4
3703M	B	0.18	CH3	SI(N/CH3/CH3)		CCL4
7370M	A	0.18	CH3	SI(O/CH3/CH3)		CCL4
11616M	A	0.18	CH3	SI(QN/CHC/CH3)		CCL4
8163M	B	0.20- 0.80	CHR	R3<(CH2-CH3)/HCH-HCH>		CCL4
8894M	A	0.20	CH3	SI(O/Q3/CH3)		CDCL3
8163M	B	0.20- 0.80	HCHR	R3<CH(CH2-CH3)-HCH>		CCL4
7162M	A	0.20- 2.00		UNSPECIFIED		CDCL3
9522M	A	0.21	CH3	SN(CH3/CH3/CH3)		CCL4
5050M	A	0.21	HCHR	R3<C(C(OH/A/CH3)/CH3)-HCH>		CCL4
5050M	B	0.21	HCHR	R3<C(C(OH/A/CH3)/CH3)-HCH>		CCL4
8175M	A	0.23	CH2R	R3<C(CH3/CH3)-C(CH3/CH3)>		CCL4
947M	A	0.23	CH3	SI(O/CH2/CH3)		CCL4
10790M	A	0.25	CH3	SI(SI/CH3/CH3)		CDCL3
420BM	A	0.25- 2.82		UNSPECIFIED		CCL4
13026M	A	0.28	CH3	SI(A/CH3/CH3)		CDCL3
12976M	A	0.28	CH3	SI(N3/CH3/CH3)		CDCL3
11616M	B	0.28	CH3	SI(O/CH3/CH3)		CCL4
1713M	A	0.28	CH3	SI(O/O/A)		CCL4
1514M	A	0.29	CH3	SI(N/CH3/CH3)		CCL4
1627M	A	0.29	CH3	SI(O/A/CH3)		CCL4
13728M	A	0.29	CH3	SI(C/FERROCENE/CH3)		CDCL3
13729M	A	0.29	CH3	SI(O/FERROCENE/CH3)		CDCL3
8968M	A	0.30- 1.87	CHR	R6<(CH3)/CH2-CH(CH3)/CH2-CH(CH3)>		CCL4
3818M	A	0.30- 1.50	CH2	SN(CH2/CH2/CH2)/CH3		CCL4
3817M	A	0.30- 1.50	CH2	SN(CH2/CH2/CH2)/CH3		CCL4
8968M	A	0.30- 1.87	CH2R	R6<CH(CH3)-CH2/CH(CH3)-CH2>		CCL4
3818M	A	0.30- 1.50	CH3	CH2-SN		CCL4
3817M	A	0.30- 1.50	CH3	CH2-SN		CCL4
5478M	A	0.30	CH3	GE(O/CH3/CH3)		CCL4
8166M	B	0.31	CHR	R3<(CH(CH3/CH3))/HCH-HCH>		CCL4

: REPRESENTS TRIPLE BOND, → REPRESENTS AN ARROW AND < AND > REPRESENT BRACKETS.

NMR NO.	ASSIGN-MENT	CHEM SHIFT -PPM-	PROTON GROUP	ENVIRONMENTAL GROUPS	S	SOLVENT
8166M	B	0.31	HCHR	R3<CH(CH(CH3/CH3))-HCH>		CCL4
3766M	B	0.31	HCHR	R3<CH(C(OH/CH3))-HCH>		CCL4
3766M	A	0.31	HCHR	R3<CH(C(OH/CH3))-HCH>		CCL4
11851M	D	0.32	NH	C(=O)-O-NH/A		DMSO
11851M	D	0.32	NH	O-C(=O)-NH/C(=O)-A		DMSO
8183M	B	0.33- 0.97	CHR	R3<(CH3)/C(CH3/CH3)-HCH>		CCL4
3773M	A	0.33 APP.	CH2R	R3<CH(C(OH/R6/R3))-CH2>		CCL4
13755M	A	0.33	CH3	SI(NH/CH3/H)		CDCL3
8183M	B	0.33- 0.97	HCHR	R3<C(CH3/CH3)-CH(CH3)>		CCL4
5429M	A	0.33- 2.00		UNSPECIFIED		CCL4
9974M	B	0.34	HCHR	R3R5R6R6R5<C*-CH2/CH*-CH2>		CDCL3
2560M	A	0.35	CH2R	R3<CH(CH(OH/A))-CH2>		CCL4
340M	A	0.35	CH2R	R3(CH(C(OH/A/CH3))-CH2)		CCL4
9975M	B	0.35	HCHR	R3R5R6R6R5<C*-CH2/CH*-CH2>		CDCL3
9976M	B	0.36	HCHR	R3R5R6R6R5<C*-CH2/CH*-CH2>		CDCL3
3768M	A	0.37 APP.	CH2R	R3<CH(C(OH/A/CH3))-CH2>		CCL4
3914M	A	0.38	CH2R	R3<CH(C(OH/A/R3))-CH2>		CCL4
1872M	A	0.39	CH2R	R3<CH(CH(R6NO/R6NO))-CH2>		CDCL3
1872M	B	0.39	CH2R	R3<CH(CH(R6NO/R6NO))-CH2>		CDCL3
13730M	A	0.39	CH3	SI(FERROCENE/CH2/CH3)		CDCL3
12966M	A	0.39	NH	CH(CH2/CH3)/R6(CH-CH2/CH2)		CCL4
5453M	C	0.40- 1.90	CH2	CH2-OH/CH2-R5N		CDCL3
5453M	C	0.40- 1.90	CH2	R5N<CH-C(A/A)/CH2>/CH2-CH2		CDCL3
1413M	A	0.40- 0.98	CH3	CH2-CH		CCL4
1413M	A	0.40- 0.98	CH3	CH(O-C(=O)/CH2)		CCL4
3444M	A	0.40	CH3	SI(CL/CH3/CH3)		CL2C=CCL2
757M	D	0.40- 2.20		UNSPECIFIED		CDCL3
758M	D	0.40- 2.00		UNSPECIFIED		CCL4
13244M	B	0.40- 2.50		UNSPECIFIED		CCL4
3912M	A	0.41	CH2R	R3<CH(C(OH/A/R3))-CH2>		CCL4
8168M	B	0.41	HCHR	R3<CH(CH2-R3)-HCH>		CCL4
3905M	A	0.42	CH2R	R3<CH(C(OH/A/R3))-CH2>		CCL4
3913M	A	0.42	CH2R	R3<CH(C(OH/A/R3))-CH2>		CCL4
3949M	A	0.42- 2.10		UNSPECIFIED		CCL4
4774M	A	0.43- 2.26		UNSPECIFIED		CDCL3
1449M	A	0.44	CH2R	R3<CH(R5NN<C(R3)-NH/C(=O)>)-CH2>		CCL4
3448M	A	0.44	CH3	SI(CL/Q3/CH3)		CL2C=CCL2
3766M	B	0.44	HCHR	R3<CH(C(OH/CH3))-HCH>		CCL4
3766M	A	0.44	HCHR	R3<CH(C(OH/CH3))-HCH>		CCL4
8322M	A	0.45	HCHR	R5R5BI<CH*(CH=/CH2)/CH*(CH(CH2-O)/CH=)>		CDCL3
6640M	A	0.46	CH3	SN(N3/CH3/CH3)		DMSO-D6
12204M	A	0.47	CH3	CH(CH2/CH3)		CDCL3
4537M	A	0.48 APP.	CH2R	R3<CH(CH(OH/A))-CH2>		CDCL3
9483M	A	0.48	CH3	SI(R5NN/CH3/CH3)		CDCL3
10097M	A	0.48- 2.00		UNSPECIFIED		CDCL3
10184M	A	0.48- 1.95		UNSPECIFIED		CDCL3
12200M	A	0.49	CH3	CH(CH2/CH3)		CDCL3
7732M	A	0.49	CH3	CH(C/CH3)	S	D2O
3700M	A	0.50- 1.21	CH2R	R3<CH(C(=O)-NH2)-CH2>		CDCL3
3699M	A	0.50- 1.10	CH2R	R3<CH(C(=O)-NH)-CH2>		CDCL3
8167M	A	0.50	CH2R	R3<CH(Q2(CH3))-CH2>		CCL4
13937M	A	0.50- 1.60	CH2R	R3(CH(R5S(C=CH/CH=))-CH2)		CCL4
13938M	A	0.50- 1.60	CH2R	R3(CH(R5S(C=CH/S))-CH2)		CCL4
13939M	A	0.50- 1.20	CH2R	R3(CH(R5S(C=CH/S))-CH2)		CCL4
1571M	A	0.50- 2.20		UNSPECIFIED		CCL4
11683M	A	0.50- 2.10		UNSPECIFIED		CDCL3
9975M	E	0.50- 2.20		UNSPECIFIED		CDCL3
9976M	E	0.50- 2.20		UNSPECIFIED		CDCL3
12046M	A	0.50- 2.80		UNSPECIFIED		CCL4
14473M	A	0.50- 2.20		UNSPECIFIED		CDCL3
4143M	A	0.50- 2.75		UNSPECIFIED		CDCL3
9956M	E	0.50- 2.70		UNSPECIFIED		CDCL3
6376M	A	0.50- 2.00		UNSPECIFIED		CCL4
6377M	A	0.50- 2.10		UNSPECIFIED		CCL4
6378M	A	0.50- 2.00		UNSPECIFIED		CCL4
10272M	A	0.51- 2.10		UNSPECIFIED		CDCL3
8754M	B	0.52 APP.	CH2	SI(CH3/CH3/CH3)/CH2-CH2		CDCL3
8756M	B	0.52	CH2	SI(CH3/CH3/CH3)/CH2-CH2		CDCL3
3800M	A	0.52	NHR	R6N<C(CH3/CH3)-CH2/C(CH3/CH3)-CH2>		CCL4
2152M	A	0.52- 1.88		UNSPECIFIED		CCL4
8772M	A	0.53	NH	CH2-CH2/CH2-CH2		CCL4
13764M	A	0.54	CH3	SI(CL/CH2/CH3)		CDCL3
8753M	B	0.55	CH2	SI(CH3/CH3/CH3)/CH2-CH2		CDCL3
5479M	A	0.55	HCHR	R5R5BI<CH*(CH(NH-CH2)/CH2)/CH*(CH2/CH2)>		CCL4
5887M	C	0.56- 2.04	CH2.X	CH2.4	S	CDCL3
9224M	A	0.56	CH3	CH2-C		CDCL3
1085M	A	0.57	CH2	SI(O/O/O)/CH2-CH2		CCL4
10830M	A	0.57	CH3	CH(C/CH2)		CDCL3
9990M	A	0.57	CH3	R5R6R6R6<C*(CH(CH2-CH3)/CH2)>		CDCL3
8755M	B	0.58	CH2	SI(CH3/CH3/CH3)/CH2-CH2		CDCL3
1084M	A	0.58	CH2	SI(O/O/O)/CH2-CH2		CCL4

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NMR NO.	ASSIGN-MENT	CHEM SHIFT -PPM-	PROTON GROUP	ENVIRONMENTAL GROUPS	S	SOLVENT
9278M	A	0.58- 1.07	CH3	CH(CH/CH3)		CCL4
9278M	A	0.58- 1.07	CH3	CH(CH/CH)		CCL4
9949M	A	0.58	CH3	R5R6R6R6<C*(CH(C(=O)-CH3)/CH2)>		CDCL3
10404M	A	0.58	NH	R6/R6		CCL4
4557M	A	0.58- 2.42		UNSPECIFIED		CCL4
5874M	C	0.59- 2.00	CH2.X	CH2.3		CCL4
1456M	A	0.59 APP.	CH2R	R3<CH(R5NN<C(R3)-NH/C(=O)>)-CH2>		TFA
1477M	A	0.59	CH3	R6<C(CH3)-HCH/HCH>		CDCL3
1477M	B	0.59	CH3	R6<C(CH3)-HCH/HCH>		CDCL3
14184M	A	0.59	HCHR	R5R5BI(CH*(C(CH2-OH/CH2-OH)/CH=)/CH*(CH=/CH2))		DMSO-D6
10773M	C	0.59- 2.40		UNSPECIFIED		CDCL3
2771M	B	0.59- 2.00		UNSPECIFIED		CCL4
5818M	B	0.59		UNSPECIFIED		CDCL3
1463M	A	0.60- 1.10	CH2	GE(R5NN/CH2/CH2)/CH2-CH2		CCL4
9915M	A	0.60- 1.30	CH2	R6OOPR6OBI<C(CH2/CH2/CH2)>/CH3		CDCL3
4431M	B	0.60- 1.97	CH2.X	CH2.6		DMSO-D6
1463M	A	0.60- 1.10	CH3	CH2-CH2		CCL4
9915M	A	0.60- 1.30	CH3	CH2-R6OOPR6OBI		CDCL3
9948M	A	0.60	CH3	R5R6R6R6<C*(CH(C(=O)-CH3)/CH2)>		CDCL3
13797M	A	0.60- 2.20		UNSPECIFIED		CDCL3
6765M	A	0.60- 2.00		UNSPECIFIED		CCL4
5093M	C	0.60- 1.62		UNSPECIFIED		CDCL3
13956M	B	0.60- 2.30		UNSPECIFIED		CDCL3
9974M	E	0.60- 2.50		UNSPECIFIED		CDCL3
3964M	C	0.60- 2.00		UNSPECIFIED		CCL4
11964M	A	0.60- 1.92		UNSPECIFIED		CCL4
3836M	A	0.60- 1.80		UNSPECIFIED		CCL4
12047M	A	0.60- 2.50		UNSPECIFIED		CDCL3
4560M	A	0.60- 2.20		UNSPECIFIED		CCL4
9299M	A	0.61	CH3	CH2-C		CCL4
9223M	A	0.61	CH3	CH2-C		CDCL3
9992M	A	0.61	CH3	R5R6R6R3OR6<C*(CH(CH(CH2/CH3))/CH2)>		CDCL3
9951M	A	0.61	CH3	R5R6R6R6<C*(CH(C(=O)-CH3)/CH2)>		CDCL3
9980M	A	0.61	CH3	R5R6R6R6<C*(CH(C(=O)-CH3)/CH2)>		CDCL3
6166M	A	0.61- 2.59		UNSPECIFIED		CDCL3
5890M	C	0.62- 2.08	CH2.X	CH2.3	S	CDCL3
9507M	A	0.62	CH2R	R3<CH(N(C(=O)-O/CH2))-CH2>		CCL4
3412M	A	0.62- 1.00	CH3	CH2-CH		CCL4
3412M	A	0.62- 1.00	CH3	CH(CH2/CH2)		CCL4
12081M	A	0.63	CH3	CH2-C		CDCL3
12081M	B	0.63	CH3	CH2-C		CDCL3
10815M	A	0.63	CH3	CH(CH2/CH3)		CDCL3
9993M	A	0.63	CH3	R5R6R6R6<C*(CH(CH(CH2/CH3))/CH2)>		CDCL3
9983M	A	0.63	CH3	R5R6R6R6<C*(CH(CH(O-C(=O)/CH3))/CH2)>		CDCL3
1472M	A	0.63	CH3	SI(CL/A/CH3)		CCL4
13765M	A	0.63	CH3	SI(O/CH/CH3)		CDCL3
5751M	A	0.63	NH	CH2-CH2/CH2-CH2		CCL4
4434M	B	0.64- 2.13	CH2	CH2-CH2/CH3		DMSO-D6
7159M	A	0.64- 1.36	CH2	CH2-C/CH3		CDCL3
4434M	B	0.64- 2.13	CH2	CH2-O/CH2-CH3		DMSO-D6
4212M	B	0.64- 2.11	CH2.X	CH2.3		CCL4
4375M	A	0.64- 2.57	CH2R	R5<CH2-C/CH2-CH2>		CDCL3
4375M	A	0.64- 2.57	CH2R	R5<C(OH/C(=O)-OH)-CH2/CH2-CH2>		CDCL3
10942M	A	0.64	CH3	CH2-C		CCL4
6159M	A	0.64	CH3	CH2-CH2		CCL4
7159M	A	0.64- 1.36	CH3	CH2-CH2		CDCL3
7079M	A	0.64	CH3	R5NOR6SPI<CH-N(CH3)/CH(A)>		CDCL3
9976M	C	0.64	CH3	R5R6R6R5R3<C*(CH(C(=O)-CH3)/CH2)>		CDCL3
9989M	A	0.64	CH3	R5R6R6R6<C*(CH(C(=O)-CH3)/CH2)>		CDCL3
11868M	A	0.64	CH3	R5R6R6R6(C*-CH(C(=O)-CH3)/CH2)		CDCL3
11870M	A	0.64	CH3	R5R6R6R6(C*-C(O-C(=O)-CH3/C(=O)-CH3)/CH2)		CDCL3
5391M	A	0.64- 1.68		UNSPECIFIED		CCL4
4023M	B	0.65- 1.90	CH2	CH2-CH2/CH3		CCL4
4023M	B	0.65- 1.90	CH2	CH2-O/CH2-CH3		CCL4
1461M	A	0.65- 1.10	CH2	GE(O-C(=O)/CH2/CH2)/CH2-CH2		CCL4
4417M	C	0.65- 1.55	CH2.X	CH2.3		CCL4
4580M	B	0.65- 2.08	CH2.X	CH2.4		CCL4
2242M	A	0.65	CH3	CH2-C		CDCL3
1418M	A	0.65	CH3	CH2-CH2		CCL4
1461M	A	0.65- 1.10	CH3	CH2-CH2		CCL4
9975M	C	0.65	CH3	R5R6R6R5R3<C*(C(O-C(=O)-CH3/C(=O)-CH3)/CH2)>		CDCL3
9950M	A	0.65	CH3	R5R6R6R6<C*(CH(C(=O)-CH3)/CH2)>		CDCL3
9943M	B	0.65	CH3	R5R6R6R6<C*(CH*/CH2)>		CDCL3
9943M	A	0.65	CH3	R5R6R6R6<C*(C(OH/C(=O))/CH2)>		CDCL3
1838M	A	0.65	CH3	R5R6R6R6<C*-CH(C(=O)-CH3)/CH2>		CDCL3
11866M	A	0.65	CH3	R5R6R6R6(C*-CH(C(=O)-CH3)/CH2)		CDCL3
11873M	A	0.65	CH3	R5R6R6R6(C*-C(O-C(=O)-CH3/C(=O)-CH3)/CH2)		CDCL3
5845M	A	0.65- 2.41		UNSPECIFIED		CCL4
3907M	B	0.65- 2.17		UNSPECIFIED		CCL4
7684M	C	0.65- 2.19		UNSPECIFIED		TFA
5433M	C	0.66- 1.84	CH2	CH2-CH/CH3		CCL4

: REPRESENTS TRIPLE BOND, ¬ REPRESENTS AN ARROW AND < AND > REPRESENT BRACKETS.

NMR NO.	ASSIGN-MENT	CHEM SHIFT -PPM-	PROTON GROUP	ENVIRONMENTAL GROUPS	S	SOLVENT
5433M	C	0.66- 1.84	CH2	CH(C(=O)-O/CH3)/CH2-CH3		CCL4
3145M	A	0.66	CH3	CH2-CH2		CCL4
4151M	A	0.66	CH3	CH2-CH2		CDCL3
1538M	A	0.66- 1.10	CH3	CH(R5/CH3/CH3)		CCL4
9953M	A	0.66	CH3	R5R6R6R6<C*(CH(CH(CH2/CH3))/CH2)>		CDCL3
9981M	A	0.66	CH3	R5R6R6R6<C*(CH(CH(CH2/CH3))/CH2)>		CDCL3
11890M	A	0.66	CH3	R5R6R6R6(C*-CH*(CH2-CH2)/CH2)		CDCL3
14046M	A	0.66	HCHR	R3(C(C(=O)-OH/CH2-CH3)-C(C(=O)-OH/CH2-CH3))		DMSO-D6
1420M	A	0.66	NH	CH2-CH2/CH2-CH2		CCL4
8447M	A	0.67- 1.15	CH2R	R3<CH(C(=O)-R6NN)-CH2>		CDCL3
12081M	B	0.67	CH3	CH2-C		CDCL3
12081M	A	0.67	CH3	CH2-C		CDCL3
10993M	A	0.67	CH3	CH2-C		CDCL3
10994M	A	0.67	CH3	CH2-C		CCL4
601M	A	0.67	CH3	CH2-C		CDCL3
2420M	A	0.67	CH3	CH(CH2/CH3)		CCL4
9965M	A	0.67	CH3	R5R6R6R6<C*(CH(C(=O)-CH3)/CH2)>		CDCL3
11891M	A	0.67	CH3	R5R6R6R6(C*-CH(CH(CH2/CH3))/CH2)		CDCL3
11886M	A	0.67	CH3	R5R6R6R6(C*-CH(CH(CH2/CH3))/CH2)		CDCL3
11859M	A	0.67	CH3	R5R6R6R6(C*-CH(C(=O)-CH3)/CH2)		CDCL3
8462M	B	0.67	HCHR	R3<CH(CH2-R6NN)-HCH>		CDCL3
7049M	A	0.67	NH	CH(CH3/CH3)/CH(CH3/CH3)		CCL4
2240M	A	0.67- 2.00		UNSPECIFIED		CDCL3
1872M	B	0.68	CH2R	R3<CH(CH(R6NO/R6NO))-CH2>		CDCL3
1872M	A	0.68	CH2R	R3<CH(CH(R6NO/R6NO))-CH2>		CDCL3
12722M	A	0.68- 1.30	CH2R	R3(CH(C(=O)-A)/CH2)		CCL4
256M	A	0.68	CH3	CH2-C		CCL4
2963M	A	0.68- 1.15	CH3	CH2-CH2		TFA
9970M	A	0.68	CH3	R5R6R6R6R500SPI<C*(CH(CH(CH2/CH3))/CH2)>		CDCL3
9957M	A	0.68	CH3	R5R6R6R6<C*(CH(CH(CH2/CH3))/CH2)>		CDCL3
9986M	A	0.68	CH3	R5R6R6R6<C*(CH(C(=O)-O-CH3)/CH2)>		CDCL3
11874M	A	0.68	CH3	R5R6R6R6(C*-C(O-C(=O)-CH3/C(=O)-CH3)/CH2)		CDCL3
8061M	A	0.68	CH3	SN(CL/CH3/CH3)		CDCL3
10898M	A	0.68	NH	R6/CH2-CH		CCL4
4353M	A	0.68- 2.17		UNSPECIFIED		DMSO-D6
3906M	A	0.68- 2.17		UNSPECIFIED		CCL4
11898M	C	0.68- 2.60		UNSPECIFIED		CDCL3
7300M	A	0.68- 2.15		UNSPECIFIED		CDCL3
3773M	B	0.69 APP.	CHR	R3<(C(OH/R6/R3))/CH2-CH2>		CCL4
14172M	B	0.69- 1.61	CH2	CH2-R6NN/CH3		CDCL3
9213M	A	0.69	CH3	CH2-C		CDCL3
13873M	A	0.69	CH3	CH2-C		DMSO-D6
2504M	A	0.69	CH3	CH2-C		CDCL3
10825M	A	0.69	CH3	CH2-C		CDCL3
7563M	A	0.69	CH3	CH2-C		CCL4
9296M	A	0.69	CH3	CH2-CH		CCL4
9978M	A	0.69	CH3	R5R6R6R6<C*(CH(CH(CH2/CH3))/CH2)>		CDCL3
9942M	A	0.69	CH3	R5R6R6R6<C*(CH(CH(CH2/CH3))/CH2)>		CDCL3
9962M	A	0.69	CH3	R5R6R6R6<C*(CH(CH(CH2/CH3))/CH2)>		CDCL3
9940M	A	0.69	CH3	R5R6R6R6<C*(CH(CH(CH2/CH3))/CH2)>		CDCL3
9941M	A	0.69	CH3	R5R6R6R6<C*(CH(CH(CH2/CH3))/CH2)>		CDCL3
9999M	A	0.69	CH3	R5R6R6R6<C*(CH(CH(CH2/CH3))/CH2)>		CDCL3
9982M	A	0.69	CH3	R5R6R6R6<C*(CH(CH(O-C(=O)/CH3))/CH2)>		CDCL3
10000M	A	0.69	CH3	R5R6R6R6<C*(CH(OH)/CH(CH(CH2/CH3)))>		CDCL3
11863M	A	0.69	CH3	R5R6R6R6(C*-CH(C(=O)-CH3)/CH2)		CDCL3
11860M	A	0.69	CH3	R5R6R6R6(C*-CH(C(=O)-CH3)/CH2)		CDCL3
11862M	A	0.69	CH3	R5R6R6R6(C*-CH(C(=O)-CH3/CH2)		CDCL3
11879M	A	0.69	CH3	R5R6R6R6(C*-C(O-C(=O)-CH3/C(=O)-CH3)/CH2)		CDCL3
1240M	A	0.69	NH	CH2-CH2/CH2-CH3		CCL4
1876M	A	0.69	NH	CH(CH2/CH3)/CH3		CCL4
5072M	A	0.69- 0.91		UNSPECIFIED		CCL4
6278M	D	0.70- 1.51	CH2	CH2-CH/CH3		CCL4
5456M	A	0.70- 2.10	CH2	CH2-C:N/CH2-R5N		CDCL3
13963M	A	0.70- 1.60	CH2	CH2-C/CH3		CDCL3
6278M	D	0.70- 1.51	CH2	CH(C-CH3)/CH2-CH3		CCL4
5456M	A	0.70	CH2	R5N<CH-C(A/A)/CH2>/CH2-CH2		CDCL3
12123M	A	0.70	CH2	SI(O/O/O)/CH3		CDCL3
10164M	A	0.70- 1.20	CH2	SN(O/CH2/CH2)/CH2-CH2		CDCL3
8266M	A	0.70- 1.21	CH2R	R3<CH(C(IO)-OH)-CH2>		CCL4
12723M	A	0.70- 1.30	CH2R	R3(CH(C(=O)-A)/CH2)		CCL4
12724M	A	0.70- 1.30	CH2R	R3(CH(C(=O)-A)/CH2)		CCL4
12727M	A	0.70- 1.40	CH2R	R3(CH(C(=O)-A)/CH2)		CCL4
13864M	A	0.70- 2.20	CH2R	R5(CH2-CH(CH(C(=O)-OH/A))/CH2-CH2)		CDCL3
13864M	A	0.70- 2.20	CH2R	R5(CH(CH(C(=O)-OH/A))-CH2/CH2-CH2)		CDCL3
6085M	A	0.70- 2.22	CH2R	R6<CH2-CH(OH)/CH2-CH2>		D2O
2513M	A	0.70- 2.00	CH2R	R6<CH(CH2-NH2)-CH2/CH2-CH(CH2-NH2)>		CDCL3
2530M	A	0.70- 1.80	CH2R	R6<CH(CH2-OH)-CH2/CH2-CH(CH2-OH)>		CDCL3
6085M	A	0.70- 2.22	CH2R	R6<CH(OH)-CH(OH)/CH2-CH2>		D2O
6922M	A	0.70	CH3	CH2-C		CDCL3
11262M	A	0.70	CH3	CH2-C		CDCL3
11086M	A	0.70- 1.12	CH3	CH2-CH		CCL4

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11086M	A	0.70- 1.12	CH3	CH2-CH2		CCL4
10164M	A	0.70- 1.20	CH3	CH2-CH2		CDCL3
13963M	A	0.70- 1.60	CH3	CH2-CH2		CDCL3
12959M	A	0.70- 1.00	CH3	CH2-CH2		CCL4
3682M	A	0.70	CH3	CH2-N		CDCL3
3682M	A	0.70	CH3	CH2-N		CDCL3
3682M	B	0.70	CH3	CH2-N		CDCL3
3682M	B	0.70	CH3	CH2-N		CDCL3
11001M	A	0.70	CH3	CH2-R6NN		CDCL3
12959M	A	0.70- 1.00	CH3	CH(CH2/CH2)		CCL4
2419M	A	0.70	CH3	CH(CH2/CH3)		CDCL3
9995M	A	0.70	CH3	R5R6R6R6<C*(CH2/CH2)>		CDCL3
9994M	A	0.70	CH3	R5R6R6R6<C*(CH2/CH2)>		CDCL3
9947M	A	0.70	CH3	R5R6R6R6<C*(CH(CH(CH2/CH3))/CH2)>		CDCL3
9979M	A	0.70	CH3	R5R6R6R6<C*(CH(C(=O)-CH3)/CH2)>		CDCL3
9987M	A	0.70	CH3	R5R6R6R6<C*(CH(C(=O)-HCH)/CH2)>		CDCL3
9988M	A	0.70	CH3	R5R6R6R6<C*(C(OH/C(=O)-HCH)/CH2)>		CDCL3
9997M	A	0.70	CH3	R5R6R6R6<C*(C(OH/C(=O)-HCH)/CH2)>		CDCL3
11887M	A	0.70	CH3	R5R6R6R6(C*-CH(CH(CH2/CH3))/CH2)		CDCL3
11892M	A	0.70	CH3	R5R6R6R6(C*-CH(CH(CH2/CH3))/CH2)		CDCL3
11888M	A	0.70	CH3	R5R6R6R6(C*-CH(CH(CH2/CH3))/CH2)		CDCL3
12335M	A	0.70	CH3	R5R6R6R6(C*-CH(CH(CH2/CH3))/CH2)		CDCL3
11889M	A	0.70	CH3	R5R6R6R6(C*-CH(C(=O)-CH3)/CH2)		CDCL3
9942M	D	0.70- 2.30		UNSPECIFIED		CDCL3
8165M	B	0.70- 1.50		UNSPECIFIED		CCL4
14327M	A	0.70- 1.90		UNSPECIFIED		DMSO-D6
8032M	A	0.70- 2.10		UNSPECIFIED		CDCL3
11897M	D	0.70- 2.58		UNSPECIFIED		CDCL3
13813M	A	0.70- 2.10		UNSPECIFIED		DMSO-D6
12527M	A	0.70- 1.90		UNSPECIFIED		D2O
12335M	D	0.70- 2.60		UNSPECIFIED		CDCL3
11044M	A	0.70- 2.40		UNSPECIFIED		CCL4
12558M	D	0.70- 2.30		UNSPECIFIED		CDCL3
13907M	A	0.70- 2.00		UNSPECIFIED		CDCL3
9978M	D	0.70- 2.70		UNSPECIFIED		CDCL3
3328M	A	0.70- 2.00		UNSPECIFIED		CDCL3
9541M	A	0.70- 2.15		UNSPECIFIED		CDCL3
12123M	B	0.70- 1.10		UNSPECIFIED		CDCL3
12963M	A	0.70- 1.10		UNSPECIFIED		CCL4
12965M	A	0.70- 1.00		UNSPECIFIED		CCL4
4356M	B	0.70- 2.30		UNSPECIFIED		CDCL3
5435M	A	0.70- 1.90		UNSPECIFIED		CDCL3
14555M	A	0.70- 2.20		UNSPECIFIED		CDCL3
14429M	A	0.70- 1.20		UNSPECIFIED		CCL4
5871M	B	0.71- 2.17	CH2	CH2-CH2/CH3		CDCL3
5871M	B	0.71- 2.17	CH2	CH2-N(+)/CH2-CH3		CDCL3
10294M	B	0.71- 1.89	CH2R	R6N(CH2-CH(CH3)/CH2-CH2)		CCL4
10294M	B	0.71- 1.89	CH2R	R6N(CH2-CH(CH3)/CH2-CH(CH3))		CCL4
12929M	A	0.71	CH3	CH2-C		DMSO-D6
10779M	A	0.71	CH3	CH2-C		CDCL3
1835M	A	0.71	CH3	CH2-CH2		CDCL3
13475M	A	0.71	CH3	CH2-R6N		DMSO-D6
9991M	A	0.71	CH3	R5R6R6R6<C*(CH(CH(CH2/CH3))/CH2)>		CDCL3
9939M	A	0.71	CH3	R5R6R6R6<C*(CH(CH(CH2/CH3))/CH2)>		CDCL3
12558M	A	0.71	CH3	R5R6R6R6(C*-CH(CH(CH2/CH3))/CH2)		CDCL3
11858M	A	0.71	CH3	R5R6R6R6(C*-CH(C(=O)-CH3)/CH2-CH2)		CDCL3
11869M	A	0.71	CH3	R5R6R6R6(C*-C(OH/C(=O)-CH3)/CH2)		CDCL3
5294M	A	0.71	CH3	R6N<CH-CH(OH)/CH(A<C-CH-CH-C(O-CH3)>)>		CDCL3
6570M	B	0.71	CH3	R6OOP<C(CH3)-HCH/HCH>		CCL4
6570M	A	0.71	CH3	R6OOP<C(CH3)-HCH/HCH>		CCL4
9051M	C	0.71- 1.13	NH	CH(CH2/CH3)/CH2-CH2		CDCL3
7437M	A	0.71	NH	R6<CH-CH2/CH2>/CH2-CH2		CCL4
6713M	A	0.71- 2.00		UNSPECIFIED		CCL4
1328M	A	0.72	CH3	CH2-CH2	S	CDCL3
10999M	A	0.72	CH3	CH2-R6NN		CDCL3
13100M	A	0.72	CH3	CH2-R6NO		DMSO-D6
11759M	A	0.72	CH3	CH(CH2/CH3)		CDCL3
14117M	A	0.72	CH3	C(CH2/CH3/CH3)		CDCL3
9998M	A	0.72	CH3	R5R6R6R6<C*(CH(C(=O)-CH3)/CH=>		CDCL3
11893M	A	0.72	CH3	R5R6R6R6(C*-CH(CH(CH2/CH3))/CH2)		CDCL3
11899M	A	0.72	CH3	R5R6R6R6(C*-CH(CH/CH2)/CH2)		CDCL3
11877M	A	0.72	CH3	R5R6R6R6(C*-CH(C(=O)-CH3)/CH2)		CDCL3
5053M	A	0.72- 2.30		UNSPECIFIED		CCL4
7587M	A	0.72- 2.26		UNSPECIFIED		DMSO-D6
568M	A	0.73	CH3	CH2-C		CCL4
3979M	A	0.73	CH3	CH2-C		CDCL3
2816M	A	0.73	CH3	CH2-CH2		CCL4
10226M	A	0.73	CH3	CH2-Q		DMSO-D6
10681M	A	0.73	CH3	C(CH2/CH3/CH3)		CDCL3
9968M	A	0.73	CH3	R5R6R6R6<C*(CH(CH(CH2/CH3))/CH2)>		CDCL3
9985M	A	0.73	CH3	R5R6R6R6<C*(CH(C(=O)-OH)/CH2)>		CDCL3

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878M	A	0.73	CH3	SI(CL/CL/CH2)		CCL4
12792M	A	0.73	NH2	CH2-CH2		CCL4
10830M	B	0.73- 1.40		UNSPECIFIED		CDCL3
9953M	D	0.73- 2.25		UNSPECIFIED		CDCL3
13449M	A	0.74	CH3	C(CH2/CH3/CH3)		CDCL3
13060M	A	0.74	NH	C(CH3/CH3/CH3)/CH2-CH2		CDCL3
10404M	B	0.74- 2.09		UNSPECIFIED		CCL4
8168M	C	0.75 APP.	CHR	R3<(CH2-R3)/HCH-HCH>		CCL4
12728M	A	0.75- 1.30	CH2R	R3(CH(C(=O)-A)/CH2)		CCL4
12726M	A	0.75- 1.30	CH2R	R3(CH(C(=O)-A)/CH2)		CCL4
12725M	A	0.75- 1.30	CH2R	R3(CH(C(=O)-R5S)/CH2)		CCL4
7155M	A	0.75	CH3	CH2-C		CCL4
12942M	A	0.75	CH3	CH2-CH		DMSO-D6
2815M	A	0.75	CH3	CH2-CH2		CCL4
1124M	B	0.75	CH3	CH2-CH2		CDCL3
4145M	A	0.75	CH3	CH2-C(=O)		DMSO-D6
1124M	A	0.75	CH3	CH2-Q		CDCL3
1122M	A	0.75	CH3	CH2-Q(A<C-CH-CH-C(O-C(=O)-CH3)>/CH2-CH3/A<C-CH-CH-C(O-C(=O)-CH3)>)		CDCL3
1223M	A	0.75	CH3	CH2-R5NA		CDCL3
2473M	A	0.75	CH3	CH(CH2/CH2)		D2O
12957M	A	0.75	CH3	CH(CH2/CH3)		CDCL3
10999M	B	0.75	CH3	CH(CH2/CH3)		CDCL3
7732M	B	0.75	CH3	CH(C/CH3)	S	D2O
6460M	A	0.75	CH3	C(CH2/CH3/CH3)		CDCL3
8103M	B	0.75- 1.05	HCHR	R3R5O<CH*-C(=O)/CH*-C(A/A)>		CDCL3
8103M	A	0.75- 1.05	HCHR	R3R5O<CH*-C(=O)/CH*-C(A/A)>		CDCL3
8104M	A	0.75	HCHR	R3R5O<CH*-C(=O)/CH*-C(O/A)>		CDCL3
8174M	B	0.75	HCHR	R3<CH(CH3)-CH(CH3)>		CCL4
9942M	B	0.75- 1.10		UNSPECIFIED		CDCL3
9949M	C	0.75- 2.25		UNSPECIFIED		CDCL3
4140M	A	0.75- 2.10		UNSPECIFIED		CDCL3
5872M	A	0.75- 2.10		UNSPECIFIED		CDCL3
11039M	A	0.75- 2.12		UNSPECIFIED		DMSO-D6
2622M	A	0.75- 2.26		UNSPECIFIED		CDCL3
5479M	C	0.75- 1.90		UNSPECIFIED		CCL4
3951M	B	0.75- 2.16		UNSPECIFIED		CCL4
12992M	A	0.75- 2.67		UNSPECIFIED		CDCL3
8970M	A	0.75- 1.00		UNSPECIFIED		CCL4
13290M	A	0.75- 2.16		UNSPECIFIED		CDCL3
10823M	A	0.76	CH3	CH2-CH		CDCL3
2818M	A	0.76	CH3	CH2-CH2		CCL4
3758M	A	0.76	CH3	CH(CH2/CH3)		CDCL3
13266M	A	0.76	CH3	CH(CH2/CH3)		CDCL3
5074M	A	0.76	CH3	C(R6/CH/CH3)		CCL4
9944M	A	0.76	CH3	R5R6R6R6<C*(CH(OH)/CH2)>		CDCL3
9960M	A	0.76	CH3	R5R6R6R6<C*(C(OH/C(=O)-CH3)/CH2)>		CDCL3
11875M	A	0.76	CH3	R5R6R6R6(C*-C(OH/C(=O)-CH3)/CH2)		CDCL3
3822M	B	0.76- 2.17		UNSPECIFIED		CCL4
5143M	A	0.77	CH3	CH2-C		DMSO-D6
2147M	A	0.77	CH3	CH2-CH		CCL4
11713M	A	0.77	CH3	CH2-CH		CDCL3
11714M	A	0.77	CH3	CH2-CH2		CDCL3
4210M	A	0.77	CH3	CH2-Q		CDCL3
4918M	A	0.77	CH3	C(R6/CH/CH3)		CCL4
11883M	A	0.77	CH3	R5R6R6R6(C*-CH(OH)/CH2)		CDCL3
7886M	A	0.77	CH3	R6OO<C(CH3)-HCH/HCH>		CCL4
7886M	B	0.77	CH3	R6OO<C(CH3)-HCH/HCH>		CCL4
7207M	A	0.77	CH3	SI(A/A/A)		CDCL3
8626M	A	0.77- 2.11		UNSPECIFIED		CCL4
3145M	B	0.77 APP.		UNSPECIFIED		CCL4
8971M	D	0.77- 2.09		UNSPECIFIED		CDCL3
12711M	A	0.78- 1.32	CH2R	R3(CH(C(=O)-A)/CH2)		CDCL3
4416M	A	0.78	CH3	CH2-C		CCL4
5939M	A	0.78	CH3	CH2-C		CCL4
6663M	A	0.78	CH3	CH2-CH		CCL4
2360M	A	0.78	CH3	CH2-CH		CCL4
2371M	A	0.78	CH3	CH2-CH		CCL4
2417M	A	0.78	CH3	CH2-CH2		CDCL3
3825M	A	0.78	CH3	CH2-CH2		CDCL3
13101M	A	0.78	CH3	CH2-CH2		DMSO-D6
1226M	A	0.78	CH3	CH2-CH2		CDCL3
1226M	A	0.78	CH3	CH2-R5NA		CDCL3
7711M	A	0.78	CH3	CH2-R6NN	S	D2O
8873M	B	0.78	CH3	CH2-R6NN		CDCL3
8873M	A	0.78	CH3	CH2-R6NN		CDCL3
8785M	A	0.78	CH3	CH2-R6NN		DMSO-D6
10824M	A	0.78	CH3	CH(CH/CH3)		CDCL3
471M	A	0.78	CH3	C(CH2/CH2/CH2)		CCL4
8820M	A	0.78	CH3	C(CH2/CH3/CH3)		CDCL3
6461M	A	0.78	CH3	C(CH2/CH3/CH3)		CDCL3

: REPRESENTS TRIPLE BOND, ¬ REPRESENTS AN ARROW AND < AND > REPRESENT BRACKETS.

NMR NO.	ASSIGN-MENT	CHEM SHIFT -PPM-	PROTON GROUP	ENVIRONMENTAL GROUPS	S	SOLVENT
7860M	A	0.78	CH3	R5R5BI<C(CH3)-CH*/CH(CH2-C(=O))>		CCL4
7861M	A	0.78	CH3	R5R5BI<C(CH3)-CH*/CH(CH2-C(=O))>		CCL4
7861M	C	0.78	CH3	R5R5BI<C(CH3)-CH*/CH(CH2-C(=O))>		CCL4
1351M	A	0.78	CH3	R5R6R6R6<C*-C(OH/CH3)/CH2>		CDCL3
9995M	B	0.78	CH3	R6R6R6R5<C*(CH*/CH2)>		CDCL3
9981M	B	0.78	CH3	R6R6R6R5<C*(CH*/CH2)>		CDCL3
1477M	B	0.78	CH3	R6<C(CH3)-HCH/HCH>		CDCL3
1477M	A	0.78	CH3	R6<C(CH3)-HCH/HCH>		CDCL3
10773M	A	0.78	CH3	R6(CH-CH2/CH2)		CDCL3
749M	A	0.78	CH3	R6(C(CH3)-CH2/CH2)		CDCL3
10788M	A	0.78	CH3	SI(A/A/A)		CDCL3
3900M	A	0.78	NHR	R6N<C(CH3/CH3)-HCH/C(CH3/CH3)-HCH>		CCL4
2543M	A	0.78	NH2	CH2-R6		CCL4
3900M	A	0.78 APP.	NH2	R6N<CH-HCH/HCH>		CCL4
5351M	A	0.78- 2.52		UNSPECIFIED		CCL4
5469M	C	0.78- 3.40		UNSPECIFIED		CDCL3
10185M	A	0.78- 2.40		UNSPECIFIED		CCL4
5861M	A	0.78- 2.28		UNSPECIFIED	S	D2O
8759M	B	0.79	CH2	SI(CH3/CH3/CH3)/CH2-NH		CDCL3
5156M	A	0.79	CH2	SN(CH2/CH2/CH2)/CH(CH3/CH3)		CCL4
8171M	A	0.79	CH3	CH2-C		CCL4
7217M	A	0.79	CH3	CH2-C		CDCL3
1879M	A	0.79	CH3	CH2-C		CCL4
10263M	A	0.79 APP.	CH3	CH2-C		CCL4
2374M	A	0.79	CH3	CH2-CH		CCL4
13569M	A	0.79	CH3	CH2-CH		CDCL3
11055M	A	0.79	CH3	CH2-CH		CCL4
9298M	A	0.79	CH3	CH2-CH2		CCL4
12925M	A	0.79	CH3	CH2-CH2		DMSO-D6
2418M	A	0.79	CH3	CH2-CH2		CCL4
7550M	A	0.79	CH3	CH2-CH2		CDCL3
7622M	A	0.79	CH3	CH2-CH2		CDCL3
1617M	A	0.79	CH3	CH2-CH2		CCL4
11711M	A	0.79	CH3	CH2-CH2		CDCL3
7656M	A	0.79	CH3	CH2-O-C(=O)		CDCL3
1222M	A	0.79	CH3	CH2-R5NA		CDCL3
7160M	B	0.79	CH3	CH(C/CH3)		CDCL3
7160M	A	0.79	CH3	CH(C/CH3)		CDCL3
10263M	A	0.79 APP.	CH3	C(CH/CH2/CH3)		CCL4
13956M	A	0.79	CH3	C(R6/CH2/CH3)		CDCL3
8171M	A	0.79	CH3	C(R6/CH2/CH3)		CCL4
9952M	A	0.79	CH3	R5R6R6R6<C*(CH(CH(OH/CH3))/CH2)>		CDCL3
4142M	A	0.79	CH3	R6<CH-CH2/CH2>		CDCL3
8114M	A	0.79	CH3	R6<CH-CH2/CH2>		CDCL3
136M	A	0.79	NH	CH2-CH/CH2-CH		CCL4
6775M	B	0.79- 2.10		UNSPECIFIED		CDCL3
6037M	A	0.79- 2.10		UNSPECIFIED		CCL4
9986M	C	0.79- 2.45		UNSPECIFIED		CDCL3
13266M	B	0.80- 1.75	CH	CH2-C/CH3/CH3		CDCL3
3821M	B	0.80- 2.00	CHR	R6N<(CH3)/CH2-CH2/CH2-CH2>		CCL4
8163M	C	0.80- 1.50	CH2	R3<CH-HCH/HCH>/CH3		CCL4
5234M	D	0.80- 2.10	CH2	R5N<CH-C(A/A)/CH2>/CH2-C(=O)		CDCL3
8752M	B	0.80	CH2-	SI(CH3/CH3/CH3)/CH2-NH		CDCL3
5155M	A	0.80 APP.	CH2	SN(Q3/Q3/CH2)/CH2-CH2		CCL4
12721M	A	0.80- 1.40	CH2R	R3(CH(C(=O)-A)/CH2)		CDCL3
12712M	A	0.80- 1.40	CH2R	R3(CH(C(=O)-A/CH2)		CDCL3
3821M	B	0.80- 2.00	CH2R	R6N<CH(CH3)-CH2/CH2-N(C(=O)-CH2)>		CCL4
9968M	D	0.80- 2.30	CH2R	R6R6R6R5<CH(OH)-CH2/CH2-C*(CH3)>		CDCL3
9968M	D	0.80- 2.30	CH2R	R6R6R6R5<C*(CH3)-CH*/CH2-CH(OH)>		CDCL3
8177M	B	0.80- 2.00	CH2R	R6<CH2-CH(CH3)/CH2-CH(CH3)>		CCL4
8177M	B	0.80- 2.00	CH2R	R6<CH(CH3)-C(=CH2)/CH2-CH2>		CCL4
11367M	A	0.80	CH3	CHI-CH		CDCL3
397M	A	0.80- 1.00	CH3	CH2-C		CCL4
10988M	A	0.80- 1.17	CH3	CH2-C		CCL4
8400M	B	0.80- 1.18	CH3	CH2-C		CDCL3
5075M	A	0.80	CH3	CH2-C		CCL4
5144M	A	0.80	CH3	CH2-C		DMSO-D6
11123M	A	0.80	CH3	CH2-CH		CCL4
31M	A	0.80	CH3	CH2-CH		CCL4
7773M	A	0.80	CH3	CH2-CH		CDCL3
12941M	A	0.80	CH3	CH2-CH		DMSO-D6
2572M	A	0.80	CH3	CH2-CH		CCL4
2330M	A	0.80	CH3	CH2-CH		CCL4
2475M	A	0.80	CH3	CH2-CH2		D2O
397M	A	0.80- 1.00	CH3	CH2-CH2		CCL4
10814M	A	0.80	CH3	CH2-CH2		CDCL3
827M	A	0.80	CH3	CH2-CH2		CDCL3
5682M	A	0.80	CH3	CH2-CH2		CCL4
14046M	B	0.80- 1.10	CH3	CH2-R3		DMSO-D6
8163M	C	0.80- 1.50	CH3	CH2-R3		CCL4
4382M	A	0.80	CH3	CH2-R5NN		CDCL3

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NMR NO.	ASSIGN-MENT	CHEM SHIFT -PPM-	PROTON GROUP	ENVIRONMENTAL GROUPS	S	SOLVENT
13477M	A	0.80	CH3	CH2-R6N		CDCL3
8910M	A	0.80	CH3	CH(CH2/CH3)		DMSO-D6
7157M	A	0.80	CH3	CH(C/CH3)		CDCL3
10988M	A	0.80- 1.17	CH3	CH(C/CH3)		CCL4
6784M	A	0.80- 1.20	CH3	CH(R6/CH3)		CCL4
11852M	A	0.80	CH3	C(CH2/CH2/CH2)		CDCL3
8628M	A	0.80	CH3	R4<C(CH3)-CH(QN(CH3/OH))/CH(CH2-C(=O)-O)>		DMSO-D6
9956M	A	0.80	CH3	R5R6R6R6<C*(CH(O-C(=O)-CH2)/CH2)>		CDCL3
9954M	A	0.80	CH3	R5R6R6R6<C*(C(=O)/CH2)>		CDCL3
11902M	A	0.80	CH3	R5R6R6R6(C*-CH*(CH(CH2/CH3)))		CDCL3
11867M	A	0.80	CH3	R5R6R6R6(C*-C(O-C(=O)-CH3/C(=O)-CH3)/CH2)		CDCL3
6457M	A	0.80	CH3	R5<C(C(=O)-OH)-C(CH3/CH3)/CH2>		DMSO-D6
4626M	A	0.80	CH3	R600<C(CH2-OH)-HCH/HCH>		CDCL3
13954M	A	0.80- 1.10	CH3	R6R600SPI(CH-CH2/CH2)		CDCL3
13954M	A	0.80- 1.10	CH3	R6R600SPI(C(CH3)-CH2/CH2)		CDCL3
9990M	B	0.80	CH3	R6R6R6R5<C*(CH*/CH2)>		CDCL3
9954M	B	0.80	CH3	R6R6R6R5<C*(CH*/CH2)>		CDCL3
9953M	B	0.80	CH3	R6R6R6R5<C*(CH*/CH2)>		CDCL3
11902M	D	0.80- 2.40	CH3	R6R6R6R5(C*-CH*/CH2)		CDCL3
6784M	A	0.80- 1.20	CH3	R6<CH-CH2/CH2>		CCL4
10329M	A	0.80	CH3	R6(CH-CH2/CH2)		CDCL3
2848M	A	0.80	CH3	SI(CL/CL/Q3)		CCL4
14046M	B	0.80- 1.10	HCHR	R3(C(C(=O)-OH/CH2-CH3)-C(C(=O)-OH/CH2-CH3))		DMSO-D6
3773M	C	0.80- 2.00	OH	C(R6/R3/R3)		CCL4
11893M	E	0.80- 2.10		UN		CDCL3
11900M	C	0.80- 2.10		UN		CDCL3
11888M	E	0.80- 2.20		UNSPECIFIED		CDCL3
11892M	E	0.80- 2.20		UNSPECIFIED		CDCL3
11890M	C	0.80- 2.05		UNSPECIFIED		CDCL3
11870M	C	0.80- 2.30		UNSPECIFIED		CDCL3
11878M	C	0.80- 2.50		UNSPECIFIED		CDCL3
11886M	E	0.80- 2.40		UNSPECIFIED		CDCL3
11868M	C	0.80- 2.20		UNSPECIFIED		CDCL3
11874M	C	0.80- 2.40		UNSPECIFIED		CDCL3
11881M	C	0.80- 2.70		UNSPECIFIED		CDCL3
11896M	C	0.80- 2.00		UNSPECIFIED		CDCL3
11877M	C	0.80- 2.20		UNSPECIFIED		CDCL3
11900M	C	0.80- 2.10		UNSPECIFIED		CDCL3
11865M	C	0.80- 2.40		UNSPECIFIED		CDCL3
11899M	E	0.80- 2.10		UNSPECIFIED		CDCL3
11893M	E	0.80- 2.10		UNSPECIFIED		CDCL3
11863M	D	0.80- 3.00		UNSPECIFIED		CDCL3
11871M	B	0.80- 2.30		UNSPECIFIED		CDCL3
11864M	C	0.80- 2.10		UNSPECIFIED		CDCL3
11883M	C	0.80- 2.20		UNSPECIFIED		CDCL3
11862M	D	0.80- 3.10		UNSPECIFIED		CDCL3
11889M	C	0.80- 2.30		UNSPECIFIED		CDCL3
11887M	E	0.80- 2.50		UNSPECIFIED		CDCL3
11885M	C	0.80- 2.70		UNSPECIFIED		CDCL3
11891M	D	0.80- 2.30		UNSPECIFIED		CDCL3
11884M	C	0.80- 2.10		UNSPECIFIED		CDCL3
11866M	C	0.80- 2.30		UNSPECIFIED		CDCL3
11869M	D	0.80- 2.10		UNSPECIFIED		CDCL3
11867M	D	0.80- 2.20		UNSPECIFIED		CDCL3
11880M	C	0.80- 2.20		UNSPECIFIED		CDCL3
11872M	D	0.80- 2.20		UNSPECIFIED		CDCL3
11875M	C	0.80- 2.20		UNSPECIFIED		CDCL3
8558M	A	0.80- 3.10		UNSPECIFIED		CCL4
2799M	C	0.80- 2.15		UNSPECIFIED		CDCL3
8008M	A	0.80- 1.90		UNSPECIFIED		CCL4
8025M	A	0.80- 3.70		UNSPECIFIED		CDCL3
7146M	A	0.80- 2.29		UNSPECIFIED		CDCL3
11611M	A	0.80- 2.00		UNSPECIFIED		DMSO-D6
14028M	A	0.80- 1.90		UNSPECIFIED		CDCL3
14521M	A	0.80- 2.10		UNSPECIFIED		DMSO-D6
7860M	C	0.80- 2.10		UNSPECIFIED		CCL4
13137M	A	0.80- 2.90		UNSPECIFIED		CDCL3
9940M	D	0.80- 2.20		UNSPECIFIED		CDCL3
9941M	E	0.80- 2.22		UNSPECIFIED		CDCL3
9939M	E	0.80- 2.10		UNSPECIFIED		CDCL3
9947M	E	0.80- 2.70		UNSPECIFIED		CDCL3
8180M	B	0.80- 2.30		UNSPECIFIED		CCL4
13954M	B	0.80- 2.40		UNSPECIFIED		CDCL3
13945M	A	0.80- 2.00		UNSPECIFIED		CDCL3
13998M	A	0.80- 2.60		UNSPECIFIED	S	CDCL3
5353M	A	0.80- 2.20		UNSPECIFIED		CCL4
3470M	A	0.80- 1.60		UNSPECIFIED		CDCL3
1838M	C	0.80- 2.50		UNSPECIFIED		CDCL3
13495M	C	0.80- 2.60		UNSPECIFIED		CDCL3
14092M	A	0.80- 2.10		UNSPECIFIED		CDCL3
8098M	B	0.80- 2.50		UNSPECIFIED		CCL4

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NMR NO.	ASSIGN-MENT	CHEM SHIFT -PPM-	PROTON GROUP	ENVIRONMENTAL GROUPS	S	SOLVENT
12955M	A	0.80- 1.10		UNSPECIFIED		CDCL3
12966M	B	0.80- 1.10		UNSPECIFIED		CCL4
12048M	A	0.80- 2.40		UNSPECIFIED		CDCL3
4440M	A	0.80- 2.28		UNSPECIFIED		DMSO-D6
811M	A	0.80- 2.00		UNSPECIFIED		CDCL3
5519M	B	0.80- 2.25		UNSPECIFIED		CDCL3
14143M	A	0.80- 2.20		UNSPECIFIED		CDCL3
9992M	D	0.80- 2.30		UNSPECIFIED		CDCL3
13747M	B	0.80- 2.10		UNSPECIFIED		CDCL3
11861M	D	0.80- 2.20		UNSPECIFIED		CDCL3
11858M	E	0.80- 2.20		UNSPECIFIED		CDCL3
11860M	D	0.80- 2.30		UNSPECIFIED		CDCL3
11859M	D	0.80- 2.30		UNSPECIFIED		CDCL3
6937M	A	0.80- 2.02		UNSPECIFIED		CCL4
11924M	B	0.80- 1.90		UNSPECIFIED		CCL4
11931M	A	0.80- 2.10		UNSPECIFIED		CDCL3
13197M	A	0.80- 1.90		UNSPECIFIED		DMSO-D6
2702M	A	0.80- 2.72		UNSPECIFIED		CDCL3
12759M	A	0.80- 2.60		UNSPECIFIED		CCL4
9008M	B	0.80- 2.20		UNSPECIFIED		CDCL3
9725M	C	0.80- 2.32		UNSPECIFIED		CDCL3
13015M	A	0.80- 2.00		UNSPECIFIED		DMSO-D6
12806M	B	0.80- 2.20		UNSPECIFIED		CCL4
13252M	A	0.80- 2.20		UNSPECIFIED		CCL4
12334M	A	0.80- 2.10		UNSPECIFIED		CDCL3
12283M	A	0.80- 2.30		UNSPECIFIED		CDCL3
291M	A	0.80- 2.10		UNSPECIFIED		CCL4
1313M	A	0.80- 2.15		UNSPECIFIED		CDCL3
11256M	A	0.80- 2.10		UNSPECIFIED		CCL4
9311M	B	0.81- 1.74	CHR	R6O<(CH3)/CH2-HCH/CH2-HCH		CCL4
9523M	A	0.81	CH2	SN(CH2/CH2/CH2)/CH2-CH3		CCL4
9311M	B	0.81- 1.74	CH2R	R6O<CH(CH3)-CH2/HCH-O>		CCL4
6159M	B	0.81	CH3	CH2-C		CCL4
11956M	A	0.81	CH3	CH2-C		DMSO-D6
3961M	A	0.81	CH3	CH2-C		CCL4
10828M	A	0.81	CH3	CH2-CH		CDCL3
6108M	A	0.81	CH3	CH2-CH		CCL4
7921M	A	0.81	CH3	CH2-CH		CCL4
2805M	A	0.81	CH3	CH2-CH		CCL4
3619M	A	0.81	CH3	CH2-CH2		CCL4
6869M	A	0.81	CH3	CH2-CH2		CCL4
777M	A	0.81	CH3	CH2-CH2		CDCL3
778M	A	0.81	CH3	CH2-CH2		CDCL3
10821M	A	0.81	CH3	CH2-CH2		CDCL3
3961M	A	0.81	CH3	CH2-CH2		CCL4
1221M	A	0.81	CH3	CH2-R5NA		CDCL3
8347M	A	0.81	CH3	CH2-R6A		CDCL3
13476M	A	0.81	CH3	CH2-R6N		CDCL3
13473M	A	0.81	CH3	CH2-R6N		CDCL3
10822M	A	0.81	CH3	CH(C/CH3)		CDCL3
10819M	A	0.81	CH3	CH(C/CH3)		CDCL3
10576M	A	0.81	CH3	R3R5RSTRI(C*-CH*/CH*/C(CH2-CH2/CH3))		CCL4
10576M	B	0.81	CH3	R5R5R3TRI(C(CH2-CH2)-C*(CH3)/CH*)		CCL4
11900M	A	0.81	CH3	R5R6R6R6(C*-CH(OH)/CH2)		CDCL3
11882M	A	0.81	CH3	R5R6R6R6(C*-CH(O-C(=O)-CH2)/CH2)		CDCL3
11896M	A	0.81	CH3	R5R6R6R6(C*-C(=O)/CH2)		CDCL3
9962M	B	0.81	CH3	R6R6R6R5<C*(CH*/CH2)>		CDCL3
9983M	B	0.81	CH3	R6R6R6R5<C*(CH*/CH2)>		CDCL3
11896M	B	0.81	CH3	R6R6R6R5(C*-CH*/CH2)		CDCL3
5050M	A	0.81	HCHR	R3<C(C(OH/A/CH3)/CH3)-HCH>		CCL4
5050M	B	0.81	HCHR	R3<C(C(OH/A/CH3)/CH3)-HCH>		CCL4
5680M	A	0.81 APP.		UNSPECIFIED		CCL4
1653M	A	0.81 APP.		UNSPECIFIED		CDCL3
3921M	A	0.81		UNSPECIFIED		CCL4
9159M	A	0.82- 1.49	CHR	R3<(C:N)/CH2-CH2>		CCL4
3137M	A	0.82	CH2	CH2-R5AA/CH2-C:C		DMSO-D6
8760M	B	0.82	CH2	SI(CH3/CH3/CH3)/CH2-NH		CDCL3
8751M	B	0.82	CH2	SI(CH3/CH3/CH3)/CH2-NH		CDCL3
9159M	A	0.82- 1.49	CH2R	R3<CH(C:N)-CH2>		CCL4
10614M	A	0.82	CH2R	R5R5BI(CH*(Q2/CH2))		CDCL3
11448M	A	0.82	CH3	CH2-C		CDCL3
7915M	A	0.82	CH3	CH2-C		CCL4
5145M	A	0.82	CH3	CH2-C		CDCL3
2750M	A	0.82	CH3	CH2-CH		CCL4
10953M	A	0.82	CH3	CH2-CH		CCL4
2687M	A	0.82	CH3	CH2-CH		CCL4
14144M	A	0.82	CH3	CH2-CH	S	CDCL3
11751M	A	0.82	CH3	CH2-CH		CDCL3
5257M	A	0.82	CH3	CH2-CH2		CCL4
1634M	A	0.82	CH3	CH2-CH2		CCL4
4853M	A	0.82	CH3	CH2-CH2		CDCL3

NMR NO.	ASSIGN-MENT	CHEM SHIFT -PPM-	PROTON GROUP	ENVIRONMENTAL GROUPS	S	SOLVENT
3877M	A	0.82	CH3	CH2-CH2		CCL4
5263M	A	0.82	CH3	CH2-CH2		CCL4
5448M	A	0.82 APP.	CH3	CH2-CH2		CDCL3
12051M	A	0.82	CH3	CH2-CH2		TFA
12944M	A	0.82	CH3	CH2-CH2		DMSO-D6
12946M	A	0.82	CH3	CH2-CH2		DMSO-D6
12406M	A	0.82	CH3	CH2-CH2		CDCL3
12933M	A	0.82	CH3	CH2-CH2		DMSO-D6
10565M	A	0.82	CH3	CH2-CH2		DMSO-D6
7156M	A	0.82	CH3	CH2-CH2		CDCL3
7711M	B	0.82	CH3	CH2-CH2	S	D2O
12957M	B	0.82	CH3	CH(CH2/CH3)		CDCL3
10263M	B	0.82	CH3	CH(C/CH3)		CCL4
5475M	A	0.82- 1.12	CH3	CH(R5N/CH3)		CCL4
4384M	A	0.82	CH3	C(CH/CH2/CH3)		CCL4
8672M	A	0.82	CH3	C(CH/CH3/CH3)		CCL4
2707M	A	0.82	CH3	R5R5BI<C(CH3)-C*(CH3)/CH*>		CDCL3
6395M	A	0.82	CH3	R5R5BI<C(CH3)-C*(CH3)/CH*>		CDCL3
6395M	C	0.82	CH3	R5R5BI<C(CH3)-C*(CH3)/CH*>		CDCL3
524M	A	0.82	CH3	R5R5BI(C(CH3)-C*(CH3)/CH*)		CCL4
30M	A	0.82	CH3	R5R5BI(C*-C(=O)/C/CH2)		CCL4
30M	B	0.82	CH3	R5R5BI(C-C*/CH*/CH3)		CCL4
30M	C	0.82	CH3	R5R5BI(C-C*/CH*/CH3)		CCL4
669M	B	0.82	CH3	R5R5BI(C-C*/CH*/CH3)		D2O
669M	A	0.82	CH3	R5R5BI(C-C*/CH*/CH3)		D2O
9994M	B	0.82	CH3	R6R6R6R5<C*(CH*/CH2)>		CDCL3
2909M	A	0.82	CH3	R6R6R6TRI<C*(CH2/CH2/CH2)>		CDCL3
2910M	A	0.82	CH3	R6R6R6TRI<C*-CH2/CH2/CH2>		CDCL3
9725M	A	0.82	CH3	R6<CH-CH2/CH2>		CDCL3
1270M	A	0.82	CH3	SN(=S/CH3)		CCL4
7435M	A	0.82	NH	R6<CH-CH2/CH2>/CH2-CH3		CCL4
5388M	A	0.82- 1.98		UNSPECIFIED		CDCL3
9705M	A	0.82- 2.29		UNSPECIFIED		CDCL3
13851M	A	0.82- 2.15		UNSPECIFIED		TFA
10444M	A	0.82- 2.07		UNSPECIFIED		CDCL3
6234M	A	0.82- 2.00		UNSPECIFIED		CCL4
10999M	C	0.83- 1.59	CH	CH2-CH2/CH3/CH3		CDCL3
3913M	B	0.83- 1.50	CHR	R3<(C(OH/A/R3))/CH2-CH2>		CCL4
2831M	A	0.83- 2.33	CH2R	R6<CH2-CH(OH)/CH2-CH2>		CDCL3
2831M	A	0.83- 2.33	CH2R	R6<CH(OH)-CH(OH)/CH2-CH2>		CDCL3
13282M	A	0.83- 2.20	CH2R	R6(CH2-CH2/CH2-CH2)		TFA
13282M	A	0.83- 2.20	CH2R	R6(CH2-CH(NH-SO3H)/CH2-CH2)		TFA
13269M	A	0.83	CH3	CH2-C		CCL4
7344M	A	0.83	CH3	CH2-C		C3D6O
9454M	A	0.83	CH3	CH2-C		CDCL3
10436M	A	0.83	CH3	CH2-C		CDCL3
4562M	A	0.83	CH3	CH2-CH		CCL4
11056M	A	0.83	CH3	CH2-CH		CCL4
7929M	A	0.83	CH3	CH2-CH		CCL4
4054M	A	0.83	CH3	CH2-CH2		CDCL3
12207M	A	0.83	CH3	CH2-CH2		CDCL3
10566M	A	0.83	CH3	CH2-CH2		DMSO-D6
5123M	A	0.83	CH3	CH2-CH2	S	CDCL3
1473M	A	0.83	CH3	CH2-CH2		CDCL3
11677M	A	0.83	CH3	CH2-CH2		CDCL3
2875M	A	0.83	CH3	CH2-CH2		CCL4
6480M	A	0.83	CH3	CH2-CH2		CDCL3
12932M	A	0.83	CH3	CH2-CH2		DMSO-D6
13596M	A	0.83	CH3	CH2-R4N		DMSO-D6
7681M	A	0.83	CH3	CH2-R5NN		DMSO-D6
11003M	A	0.83	CH3	CH2-R6NN		CDCL3
13097M	A	0.83	CH3	CH2-R6NO		DMSO-D6
5056M	A	0.83	CH3	CH(CH2/CH2)		CDCL3
8672M	B	0.83	CH3	CH(C/CH3)		CCL4
443M	A	0.83	CH3	HCH-CH		CCL4
6023M	B	0.83	CH3	R5R5BI<C(C*/CH*/CH3)>		CCL4
6023M	A	0.83	CH3	R5R5BI<C(C*/CH*/CH3)>		CCL4
6023M	C	0.83	CH3	R5R5BI<C*(C/CH/CH2)>		CCL4
10781M	A	0.83	CH3	R5R5BI(C(CH3)-C*(HCH-SO3H)/CH*)		D2O
12190M	A	0.83	HCHR	R5R5BIR3OR5R3O(CH*(CH*/CH*)/CH*(CH*/CH*))		CDCL3
4024M	A	0.83		CH2-R6A		CDCL3
2181M	A	0.83- 2.17		UNSPECIFIED		CDCL3
7M	A	0.83- 2.43		UNSPECIFIED		CCL4
1355M	B	0.83- 2.90		UNSPECIFIED		CCL4
9988M	C	0.83- 2.42		UNSPECIFIED		CDCL3
9979M	C	0.83- 2.67		UNSPECIFIED		CDCL3
9987M	C	0.83- 2.60		UNSPECIFIED		CDCL3
13908M	A	0.83- 1.90		UNSPECIFIED		DMSO-D6
5243M	A	0.83- 2.25		UNSPECIFIED	S	D2O
6080M	A	0.84	CH3	CH2-C		D2O
6277M	A	0.84	CH3	CH2-C		CCL4

: REPRESENTS TRIPLE BOND, → REPRESENTS AN ARROW AND < AND > REPRESENT BRACKETS.

NMR NO.	ASSIGN-MENT	CHEM SHIFT -PPM-	PROTON GROUP	ENVIRONMENTAL GROUPS	S	SOLVENT
6277M	A	0.84	CH3	CH2-CH		CCL4
2572M	B	0.84	CH3	CH2-CH		CCL4
2578M	A	0.84	CH3	CH2-CH		CCL4
12229M	A	0.84	CH3	CH2-CH		CDCL3
955M	A	0.84	CH3	CH2-CH		CCL4
5681M	A	0.84 APP.	CH3	CH2-CH		CCL4
3616M	A	0.84	CH3	CH2-CH2		CCL4
5681M	A	0.84 APP.	CH3	CH2-CH2		CCL4
12049M	A	0.84	CH3	CH2-CH2	S	TFA
12021M	A	0.84	CH3	CH2-CH2		DMSO-D6
946M	A	0.84	CH3	CH2-CH2		CCL4
10987M	A	0.84	CH3	CH2-CH2		CCL4
12935M	A	0.84	CH3	CH2-CH2		DMSO-D6
12927M	A	0.84	CH3	CH2-CH2		DMSO-D6
12937M	A	0.84	CH3	CH2-CH2		DMSO-D6
14571M	A	0.84	CH3	CH2-CH2		DMSO-D6
5268M	A	0.84	CH3	CH2-CH2		CDCL3
4831M	A	0.84	CH3	CH2-CH2		CDCL3
3219M	A	0.84	CH3	CH2-CH2		CDCL3
13016M	A	0.84	CH3	CH2-CH2		DMSO-D6
876M	A	0.84 APP.	CH3	CH2-CH2		CCL4
9000M	A	0.84	CH3	CH2-R5NN		DMSO-D6
13474M	A	0.84	CH3	CH2-R6N		CDCL3
5048M	A	0.84	CH3	CH(CH2/CH2)		CDCL3
11886M	B	0.84	CH3	CH(CH2/CH3)		CDCL3
10679M	A	0.84	CH3	C(CH/CH2/CH3)		DMSO-D6
4236M	A	0.84	CH3	R5R5BI<C(C*/CH*/CH3>		CCL4
3407M	A	0.84	CH3	R6<CH-CH(CH3)/CH2>		CCL4
11689M	A	0.84	HCHR	R5R5BIR3O(CH*(CH*/CH2)/CH*(CH*(C(=O)-O-CH2)/CH*))		CCL4
2974M	A	0.84- 2.25		UNSPECIFIED		TFA
9951M	C	0.84- 3.00		UNSPECIFIED		CDCL3
4133M	A	0.85	CH3	CH2-C		CDCL3
6910M	A	0.85	CH3	CH2-C		CCL4
5938M	A	0.85	CH3	CH2-C		CCL4
3925M	A	0.85	CH3	CH2-C		CCL4
13538M	A	0.85	CH3	CH2-C	S	D2O
11464M	A	0.85	CH3	CH2-CH		CDCL3
848M	A	0.85	CH3	CH2-CH		CCL4
6293M	A	0.85	CH3	CH2-CH2		CDCL3
11362M	A	0.85	CH3	CH2-CH2		CDCL3
10171M	A	0.85	CH3	CH2-CH2		CDCL3
11030M	A	0.85	CH3	CH2-CH2		CCL4
3958M	A	0.85	CH3	CH2-CH2		CCL4
3955M	A	0.85	CH3	CH2-CH2		CCL4
3441M	A	0.85	CH3	CH2-CH2		CCL4
10882M	A	0.85	CH3	CH2-CH2		D2O
5261M	A	0.85	CH3	CH2-CH2		CCL4
5251M	A	0.85	CH3	CH2-CH2		CCL4
13161M	A	0.85	CH3	CH2-CH2		DMSO-D6
5191M	A	0.85	CH3	CH2-CH2		CDCL3
4123M	A	0.85	CH3	CH2-CH2		CDCL3
2766M	A	0.85	CH3	CH2-CH2		CCL4
2747M	A	0.85	CH3	CH2-CH2		CCL4
12938M	A	0.85	CH3	CH2-CH2		DMSO-D6
9744M	A	0.85	CH3	CH2-O-C(=O)		CDCL3
9744M	B	0.85	CH3	CH2-O-C(=O)		CDCL3
1923M	A	0.85	CH3	CH2-R6N		CDCL3
1121M	A	0.85	CH3	CH2-R6NN		CDCL3
1551M	A	0.85	CH3	CH2-R6R6NBI		CDCL3
1400M	A	0.85	CH3	CH2-R8OO		CCL4
7113M	A	0.85	CH3	CH(CH2/CH3)		CDCL3
9968M	B	0.85 APP.	CH3	CH(CH2/CH3)		CDCL3
3415M	A	0.85	CH3	CH(CH2/CH3)		CCL4
5074M	B	0.85	CH3	CH(C/CH3)		CCL4
10818M	A	0.85	CH3	CH(N/CH3)		CDCL3
13695M	A	0.85	CH3	CH(R5NN/CH3)		DMSO-D6
9968M	B	0.85 APP.	CH3	CH(R5R6R6R6/CH2)		CDCL3
11717M	A	0.85	CH3	C(CH2/CH2/CH3)		CDCL3
7915M	B	0.85	CH3	C(CH2/CH2/CH3)		CCL4
3413M	A	0.85	CH3	C(CH2/CH3/CH3)		CCL4
2766M	A	0.85	CH3	C(CH/CH3/CH3)		CCL4
2502M	A	0.85	CH3	C(CH/CH3/CH3)		CCL4
3955M	A	0.85	CH3	C(CH/CH3/CH3)		CCL4
3958M	A	0.85	CH3	C(CH/CH3/CH3)		CCL4
3406M	A	0.85 APP.	CH3	C(HCH/CH3/CH3)		CCL4
9008M	A	0.85	CH3	C(R6/CH3/CH3)		CDCL3
3406M	A	0.85 APP.	CH3	HCH-C		CCL4
5050M	C	0.85	CH3	R3<C(C(OH/A/CH3))-HCH/HCH>		CCL4
30M	A	0.85	CH3	R5R5BI(C*-C(=O)/C/CH2)		CCL4
30M	B	0.85	CH3	R5R5BI(C-C*/CH*/CH3)		CCL4
30M	C	0.85	CH3	R5R5BI(C-C*/CH*/CH3)		CCL4

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NMR NO.	ASSIGN-MENT	CHEM SHIFT -PPM-	PROTON GROUP	ENVIRONMENTAL GROUPS	S	SOLVENT
9977M	A	0.85	CH3	R5R6R6R6<C*(CH(O-C(=O)-R6)/CH2)>		CDCL3
9954M	A	0.85	CH3	R5R6R6R6<C*(C(=O)/CH2)>		CDCL3
11923M	A	0.85- 1.23	CH3	R6NN(C-NH/CH(CH3))		CDCL3
1690M	A	0.85	CH3	R6OOP<C(CH3)-CH2/CH2>		CCL4
1699M	C	0.85	CH3	R6OOP<C(CH3)-CH2/CH2>		CCL4
1699M	A	0.85	CH3	R6OOP<C(CH3)-CH2/CH2>		CCL4
1690M	B	0.85	CH3	R6OOP<C(CH3)-CH2/CH2>		CCL4
5153M	A	0.85	CH3	R6R6BI<C*-C(=O)/CH2/CH2>		CCL4
9954M	B	0.85	CH3	R6R6R6R5<C*(CH*/CH2)>		CDCL3
9982M	B	0.85	CH3	R6R6R6R5<C*(CH*/CH2)>		CDCL3
9986M	B	0.85	CH3	R6R6R6R5 C*(CH*/CH2)>		CDCL3
9985M	B	0.85	CH3	R6R6R6R5< *(CH*/CH2)>		CDCL3
9995M	C	0.85- 2.00		UNSPECIFIED		CDCL3
9970M	C	0.85- 2.51		UNSPECIFIED		CDCL3
9999M	D	0.85- 2.60		UNSPECIFIED		CDCL3
9819M	A	0.85- 2.11		UNSPECIFIED		CCL4
11368M	A	0.85- 2.00		UNSPECIFIED		CDCL3
12969M	D	0.85- 2.10		UNSPECIFIED		CDCL3
4132M	A	0.85- 2.25		UNSPECIFIED		CDCL3
725M	A	0.85- 2.00		UNSPECIFIED		CCL4
1047M	A	0.85- 2.30		UNSPECIFIED		CDCL3
7416M	A	0.86- 1.80	CHR	R6N<(CH2-A)/CH2-HCH/CH2-HCH>		CCL4
7416M	A	0.86- 1.80	CH2R	R6N<CH(CH2-A)-CH2/HCH-NH>		CCL4
4274M	A	0.86	CH3	CH2-C		CCL4
11492M	A	0.86	CH3	CH2-CH		CDCL3
4348M	A	0.86	CH3	CH2-CH		CCL4
12436M	A	0.86	CH3	CH2-CH		CCL4
12132M	A	0.86	CH3	CH2-CH		CDCL3
14300M	A	0.86	CH3	CH2-CH		CDCL3
14301M	A	0.86	CH3	CH2-CH		CDCL3
3416M	A	0.86	CH3	CH2-CH		CCL4
13111M	A	0.86	CH3	CH2-CH2		DMSO-D6
2857M	A	0.86	CH3	CH2-CH2		CDCL3
4431M	A	0.86	CH3	CH2-CH2		DMSO-D6
788M	A	0.86	CH3	CH2-CH2		CDCL3
3826M	A	0.86	CH3	CH2-CH2		CDCL3
5606M	A	0.86	CH3	CH2-CH2		CCL4
2336M	A	0.86	CH3	CH2-CH2		CDCL3
383M	A	0.86	CH3	CH2-CH2		CDCL3
6677M	A	0.86	CH3	CH2-CH2		CDCL3
10881M	A	0.86	CH3	CH2-CH2		D2O
4523M	A	0.86	CH3	CH2-CH2		CCL4
6292M	A	0.86	CH3	CH2-CH2		CDCL3
6263M	A	0.86	CH3	CH2-CH2		CDCL3
8544M	A	0.86	CH3	CH2-NH		CDCL3
8926M	A	0.86	CH3	CH2-O-C(=O)		CDCL3
2576M	A	0.86	CH3	CH2-R6		CCL4
5270M	A	0.86	CH3	CH(CH2/CH2)		CCL4
4233M	A	0.86	CH3	CH(CH2/CH2)		CCL4
5176M	A	0.86	CH3	CH(CH2/CH2)		CCL4
10746M	A	0.86	CH3	CH(CH2/CH3)		CCL4
52M	A	0.86	CH3	CH(CH2/CH3)		CCL4
5176M	A	0.86	CH3	CH(CH2/CH3)		CCL4
5682M	B	0.86	CH3	CH(CH2/CH3)		CCL4
4233M	A	0.86	CH3	CH(CH2/CH3)		CCL4
1645M	A	0.86	CH3	CH(CH2/CH3)		CDCL3
5620M	A	0.86	CH3	CH(CH2/CH3)		CDCL3
5425M	A	0.86	CH3	CH(CH2/CH3)		CDCL3
12299M	A	0.86	CH3	CH(CH2/CH3)		CDCL3
10260M	A	0.86	CH3	CH(CH/CH3)		CCL4
10828M	B	0.86	CH3	CH(C/CH2)		CDCL3
4274M	A	0.86	CH3	CH(C/CH3)		CCL4
381M	A	0.86	CH3	C(A/CH3/CH3)		CL2C=CCL2
8144M	A	0.86	CH3	C(CH2/CH2/CH2)		CDCL3
6022M	A	0.86	CH3	C(CH2/CH2/CH2)		DMSO-D6
9941M	B	0.86	CH3	C(CH2/CH3)		CDCL3
9276M	A	0.86	CH3	R4<C(CH3)-CH(OH)/CH(OH)>		DMSO-D6
1363M	A	0.86	CH3	R5R6R6R6R5NN<C*-C(OH/CH3)/CH2>		TFA
11897M	A	0.86	CH3	R5R6R6R6(C*-CH(O-C(=O)-CH2)/CH2)		CDCL3
367M	A	0.86	CH3	R6OOP(C(CH3)-CH2/CH2-O)		CDCL3
367M	C	0.86	CH3	R6OOP(C(CH3)-CH2/CH2-O)		CDCL3
2847M	A	0.86	CH3	SI(CL/CL/H)		CCL4
4263M	A	0.86	NH	CH2-Q2/CH2-CH3		CCL4
2507M	B	0.87- 2.24	CHR	R6N<(CH2-NH2)/CH2-CH2/CH2-CH2>		CDCL3
2507M	B	0.87- 2.24	CH2R	R6N<CH(CH2-NH2)-CH2/CH2-NH>		CDCL3
13955M	A	0.87 APP.	CH3	CH2-C		CDCL3
3875M	A	0.87 APP.	CH3	CH2-C		CCL4
3976M	A	0.87	CH3	CH2-C		CCL4
6867M	A	0.87	CH3	CH2-C		D2O
6278M	A	0.87	CH3	CH2-C		CCL4
3187M	A	0.87	CH3	CH2-CH		CCL4

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NMR NO.	ASSIGN-MENT	CHEM SHIFT -PPM-	PROTON GROUP	ENVIRONMENTAL GROUPS	S	SOLVENT
2815M	B	0.87	CH3	CH2-CH		CCL4
8943M	A	0.87	CH3	CH2-CH		D2O
6641M	A	0.87	CH3	CH2-CH		CCL4
6104M	A	0.87	CH3	CH2-CH2		DMSO-D6
2875M	B	0.87	CH3	CH2-CH2		CCL4
2850M	A	0.87 APP.	CH3	CH2-CH2		CCL4
4426M	A	0.87	CH3	CH2-CH2		DMSO-D6
3135M	A	0.87	CH3	CH2-CH2		CCL4
793M	A	0.87	CH3	CH2-CH2		CDCL3
28M	A	0.87	CH3	CH2-CH2		CDCL3
5311M	A	0.87	CH3	CH2-CH2		CCL4
5263M	B	0.87	CH3	CH2-CH2		CCL4
2214M	A	0.87	CH3	CH2-CH2		CDCL3
13513M	A	0.87	CH3	CH2-CH2		DMSO-D6
10898M	B	0.87	CH3	CH2-CH2		CCL4
3875M	A	0.87 APP.	CH3	CH2-CH2		CCL4
3691M	A	0.87	CH3	CH2-CH2		CCL4
3691M	A	0.87	CH3	CH2-CH2		CCL4
2474M	A	0.87	CH3	CH2-CH2		D2O
5257M	B	0.87	CH3	CH2-CH2		CCL4
416M	A	0.87	CH3	CH2-CH2		CCL4
3753M	A	0.87	CH3	CH2-CH2		CDCL3
1417M	A	0.87	CH3	CH2-CH2		CCL4
5193M	A	0.87	CH3	CH2-CH2		CDCL3
5186M	A	0.87	CH3	CH2-CH2		CDCL3
13595M	A	0.87	CH3	CH2-CH2		CDCL3
13626M	A	0.87	CH3	CH2-CH2		CDCL3
2454M	A	0.87	CH3	CH2-CH2		CCL4
2458M	A	0.87	CH3	CH2-CH2		CCL4
2441M	A	0.87	CH3	CH2-CH2		CCL4
2456M	A	0.87	CH3	CH2-CH2		CCL4
2445M	A	0.87	CH3	CH2-CH2		CCL4
2455M	A	0.87	CH3	CH2-CH2		CCL4
2453M	A	0.87	CH3	CH2-CH2		CCL4
2457M	A	0.87	CH3	CH2-CH2		CCL4
640M	A	0.87	CH3	CH2-CH2		CDCL3
2816M	B	0.87	CH3	CH2-CH2		CCL4
2814M	A	0.87	CH3	CH2-CH2		CCL4
10708M	A	0.87	CH3	CH2-CH2		DMSO-D6
738M	A	0.87	CH3	CH2-CH2		CDCL3
106M	A	0.87	CH3	CH2-CH2		CDCL3
125M	A	0.87	CH3	CH2-CH2		CCL4
4217M	A	0.87	CH3	CH2-CH2		CDCL3
6278M	A	0.87	CH3	CH2-CH2		CCL4
260M	A	0.87	CH3	CH2-CH2		CDCL3
4601M	A	0.87	CH3	CH2-CH2		CCL4
4671M	A	0.87	CH3	CH2-CH2		DMSO-D6
315M	A	0.87	CH3	CH2-R6		CCL4
5647M	A	0.87	CH3	CH2-R6N		CDCL3
11712M	A	0.87	CH3	CH(CH2/CH3)		CDCL3
5265M	A	0.87	CH3	CH(CH2/CH3)		CCL4
5267M	A	0.87	CH3	CH(CH2/CH3)		CCL4
3156M	A	0.87	CH3	CH(CH2/CH3)		CCL4
2850M	A	0.87 APP.	CH3	CH(CH2/CH3)		CCL4
3416M	B	0.87	CH3	CH(CH2/CH3)		CCL4
3413M	B	0.87	CH3	CH(CH2/CH3)		CCL4
9940M	B	0.87 APP.	CH3	CH(CH/CH2)		CDCL3
875M	A	0.87	CH3	CH(CH/CH3)		CCL4
7160M	A	0.87	CH3	CH(C/CH3)		CDCL3
7160M	B	0.87	CH3	CH(C/CH3)		CDCL3
9953M	C	0.87 APP.	CH3	CH(R5R6R6R6/CH2)		CDCL3
4385M	A	0.87	CH3	C(CH2/CH2/CH3)		CCL4
9953M	C	0.87 APP.	CH3	C(CH2/CH3)		CDCL3
1897M	A	0.87	CH3	C(CH2/CH3/CH3)		CCL4
13955M	A	0.87 APP.	CH3	C(R6/CH2/CH3)		CDCL3
7953M	A	0.87	CH3	R4R6BI<C(CH3)-CH*/CH*>		CDCL3
4366M	B	0.87	CH3	R4<C(CH3)/CH/CH>		CDCL3
4366M	A	0.87	CH3	R4<C(CH3)/CH/CH>		CDCL3
9974M	D	0.87	CH3	R5R3R6R6R5<C*(CH*/CH2)>		CDCL3
6472M	A	0.87	CH3	R5R5BI<C(CH3)-C*(HCH-SO3-NA)/CH*>	S	D2O
6472M	B	0.87	CH3	R5R5BI<C(CH3)-C*(HCH-SO3-NA)/CH*>	S	D2O
9974M	C	0.87	CH3	R5R6R6R5R3<C*(C(OH/C:CH)/CH2)>		CDCL3
14196M	A	0.87	CH3	R6R6R6TRI(C*(CH2/CH2/CH2))		DMSO-D6
758M	A	0.87	CH3	R6(C(CH3)-CH2/CH2)		CCL4
758M	C	0.87	CH3	R6(C(CH3)-CH2/CH2)		CCL4
1576M	A	0.87	CH3	SI(CL/A/A)		CCL4
9990M	C	0.87- 2.00		UNSPECIFIED		CDCL3
3788M	B	0.87- 2.00		UNSPECIFIED		CDCL3
3234M	A	0.87 APP.		UNSPECIFIED		CCL4
7216M	B	0.88	CH2	C(OH/CH2/CH2)/CH3		CCL4
2313M	B	0.88- 1.83	CH2.X	CH2.3		CCL4

NMR NO.	ASSIGN-MENT	CHEM SHIFT -PPM-	PROTON GROUP	ENVIRONMENTAL GROUPS	S	SOLVENT
318M	A	0.88	CH3	CH2-C		CCL4
7216M	B	0.88	CH3	CH2-C		CCL4
11852M	B	0.88	CH3	CH2-C		CDCL3
302M	A	0.88	CH3	CH2-C		CDCL3
9049M	A	0.88	CH3	CH2-C		D2O
3302M	A	0.88	CH3	CH2-CH		CDCL3
4935M	A	0.88 APP.	CH3	CH2-CH		CCL4
5595M	A	0.88	CH3	CH2-CH		CCL4
12133M	A	0.88	CH3	CH2-CH		CDCL3
6447M	A	0.88	CH3	CH2-CH		CCL4
5268M	B	0.88	CH3	CH2-CH		CDCL3
11494M	A	0.88	CH3	CH2-CH		CDCL3
14M	A	0.88	CH3	CH2-CH		CDCL3
10560M	A	0.88	CH3	CH2-CH		DMSO-D6
10537M	A	0.88	CH3	CH2-CH		DMSO-D6
14306M	A	0.88	CH3	CH2-CH		CCL4
2621M	A	0.88	CH3	CH2-CH		CDCL3
2818M	B	0.88 APP.	CH3	CH2-CH		CCL4
4009M	A	0.88	CH3	CH2-CH2		CDCL3
4016M	A	0.88	CH3	CH2-CH2		CDCL3
3583M	A	0.88	CH3	CH2-CH2		CCL4
3612M	A	0.88	CH3	CH2-CH2		CCL4
2091M	A	0.88	CH3	CH2-CH2		CDCL3
5865M	A	0.88	CH3	CH2-CH2		CDCL3
5893M	A	0.88	CH3	CH2-CH2		CCL4
5868M	A	0.88	CH3	CH2-CH2		CDCL3
1557M	A	0.88	CH3	CH2-CH2		CCL4
1546M	A	0.88	CH3	CH2-CH2		CCL4
1560M	A	0.88	CH3	CH2-CH2		CCL4
2817M	A	0.88	CH3	CH2-CH2		CCL4
2776M	A	0.88	CH3	CH2-CH2		CCL4
2828M	A	0.88	CH3	CH2-CH2		CCL4
2743M	A	0.88	CH3	CH2-CH2		CCL4
2760M	A	0.88	CH3	CH2-CH2		CCL4
2752M	A	0.88	CH3	CH2-CH2		CDCL3
2594M	A	0.88	CH3	CH2-CH2		CDCL3
2596M	A	0.88	CH3	CH2-CH2		CCL4
2634M	A	0.88	CH3	CH2-CH2		CDCL3
10747M	A	0.88	CH3	CH2-CH2		DMSO-D6
641M	A	0.88	CH3	CH2-CH2		CCL4
644M	A	0.88	CH3	CH2-CH2		CDCL3
642M	A	0.88	CH3	CH2-CH2		CCL4
663M	A	0.88	CH3	CH2-CH2		CCL4
727M	A	0.88	CH3	CH2-CH2		CCL4
671M	A	0.88	CH3	CH2-CH2		CCL4
12184M	A	0.88	CH3	CH2-CH2		CDCL3
3414M	A	0.88	CH3	CH2-CH2		CCL4
3422M	A	0.88	CH3	CH2-CH2		CCL4
3391M	A	0.88	CH3	CH2-CH2		CDCL3
157M	A	0.88	CH3	CH2-CH2		CDCL3
202M	A	0.88	CH3	CH2-CH2		CCL4
167M	A	0.88	CH3	CH2-CH2		CDCL3
105M	A	0.88	CH3	CH2-CH2		CDCL3
151M	A	0.88	CH3	CH2-CH2		CDCL3
100M	A	0.88	CH3	CH2-CH2		CDCL3
203M	A	0.88	CH3	CH2-CH2		CDCL3
194M	A	0.88	CH3	CH2-CH2		CCL4
195M	A	0.88	CH3	CH2-CH2		CCL4
5197M	A	0.88	CH3	CH2-CH2		CDCL3
5194M	A	0.88	CH3	CH2-CH2		CDCL3
5125M	A	0.88	CH3	CH2-CH2	S	CDCL3
5137M	A	0.88	CH3	CH2-CH2		CDCL3
5056M	B	0.88	CH3	CH2-CH2		CDCL3
2452M	A	0.88	CH3	CH2-CH2		CCL4
2438M	A	0.88	CH3	CH2-CH2		CDCL3
2440M	A	0.88	CH3	CH2-CH2		CCL4
2459M	A	0.88	CH3	CH2-CH2		CCL4
2460M	A	0.88	CH3	CH2-CH2		CCL4
11126M	A	0.88	CH3	CH2-CH2		CDCL3
13098M	A	0.88	CH3	CH2-CH2		DMSO-D6
1464M	A	0.88	CH3	CH2-CH2		CCL4
1419M	A	0.88	CH3	CH2-CH2		CCL4
5684M	A	0.88	CH3	CH2-CH2		CCL4
1816M	A	0.88	CH3	CH2-CH2		CCL4
9M	A	0.88	CH3	CH2-CH2		CDCL3
2053M	A	0.88	CH3	CH2-CH2		CDCL3
11397M	A	0.88	CH3	CH2-CH2	S	D2O
5330M	A	0.88	CH3	CH2-CH2		CDCL3
2389M	A	0.88	CH3	CH2-CH2		CCL4
2416M	A	0.88	CH3	CH2-CH2		CDCL3
2241M	A	0.88	CH3	CH2-CH2		CCL4

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