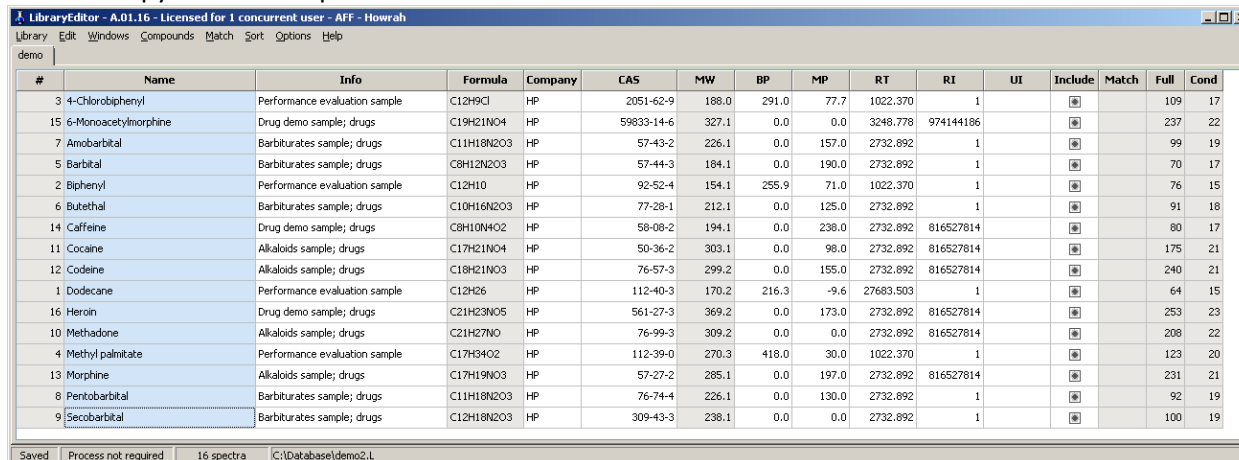


## Library editor

Load Agilent Demo library

Double click on 'Name' column to sort on compound name

Ctrl-C to copy names to clipboard



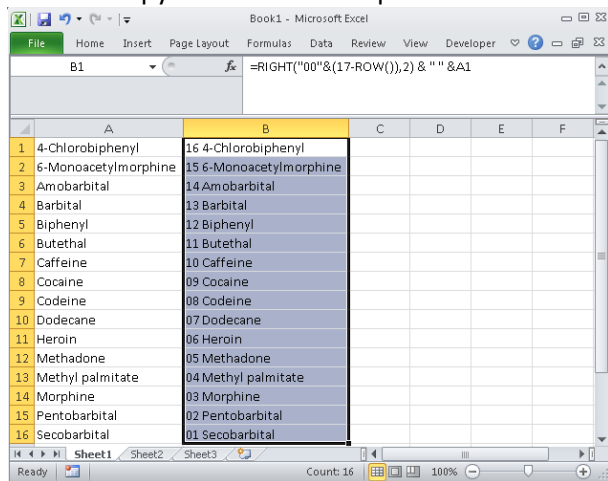
#	Name	Info	Formula	Company	CAS	MW	BP	MP	RT	RI	UI	Include	Match	Full	Cond
3	4-Chlorobiphenyl	Performance evaluation sample	C12H9Cl	HP	2051-62-9	188.0	291.0	77.7	1022.370	1		<input checked="" type="checkbox"/>		109	17
15	6-Monoacetylmorphine	Drug demo sample; drugs	C19H21NO4	HP	59833-14-6	327.1	0.0	0.0	3248.778	974144186		<input checked="" type="checkbox"/>		237	22
7	Amobarbital	Barbiturates sample; drugs	C11H18N2O3	HP	57-43-2	226.1	0.0	157.0	2732.892	1		<input checked="" type="checkbox"/>		99	19
5	Barbital	Barbiturates sample; drugs	C8H12N2O3	HP	57-44-3	184.1	0.0	190.0	2732.892	1		<input checked="" type="checkbox"/>		70	17
2	Biphenyl	Performance evaluation sample	C12H10	HP	92-52-4	154.1	255.9	71.0	1022.370	1		<input checked="" type="checkbox"/>		76	15
6	Butethal	Barbiturates sample; drugs	C10H16N2O3	HP	77-28-1	212.1	0.0	125.0	2732.892	1		<input checked="" type="checkbox"/>		91	18
14	Caffeine	Drug demo sample; drugs	C8H10N4O2	HP	58-08-2	194.1	0.0	238.0	2732.892	816527814		<input checked="" type="checkbox"/>		80	17
11	Cocaine	Alkaloids sample; drugs	C17H21NO4	HP	50-36-2	303.1	0.0	98.0	2732.892	816527814		<input checked="" type="checkbox"/>		175	21
12	Codeine	Alkaloids sample; drugs	C18H21NO3	HP	76-57-3	299.2	0.0	155.0	2732.892	816527814		<input checked="" type="checkbox"/>		240	21
1	Dodecane	Performance evaluation sample	C12H26	HP	112-40-3	170.2	216.3	-9.6	27683.503	1		<input checked="" type="checkbox"/>		64	15
16	Heroin	Drug demo sample; drugs	C21H23NO5	HP	561-27-3	369.2	0.0	173.0	2732.892	816527814		<input checked="" type="checkbox"/>		253	23
10	Methadone	Alkaloids sample; drugs	C21H27NO	HP	76-99-3	309.2	0.0	0.0	2732.892	816527814		<input checked="" type="checkbox"/>		208	22
4	Methyl palmitate	Performance evaluation sample	C17H34O2	HP	112-39-0	270.3	418.0	30.0	1022.370	1		<input checked="" type="checkbox"/>		123	20
13	Morphine	Alkaloids sample; drugs	C17H19NO3	HP	57-27-2	285.1	0.0	197.0	2732.892	816527814		<input checked="" type="checkbox"/>		231	21
8	Pentobarbital	Barbiturates sample; drugs	C11H18N2O3	HP	76-74-4	226.1	0.0	130.0	2732.892	1		<input checked="" type="checkbox"/>		92	19
9	Secobarbital	Barbiturates sample; drugs	C12H18N2O3	HP	309-43-3	238.1	0.0	0.0	2732.892	1		<input checked="" type="checkbox"/>		100	19

## Excel

Ctrl-V to paste in Excel

Change names

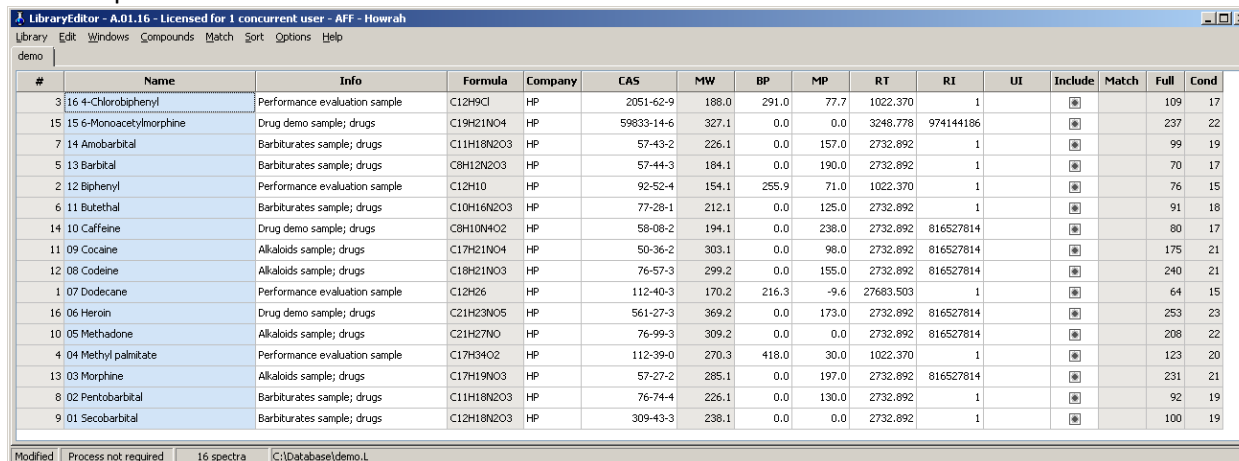
Ctrl-C to copy new names to clipboard



A	B
1 4-Chlorobiphenyl	16 4-Chlorobiphenyl
2 6-Monoacetylmorphine	15 6-Monoacetylmorphine
3 Amobarbital	14 Amobarbital
4 Barbital	13 Barbital
5 Biphenyl	12 Biphenyl
6 Butethal	11 Butethal
7 Caffeine	10 Caffeine
8 Cocaine	09 Cocaine
9 Codeine	08 Codeine
10 Dodecane	07 Dodecane
11 Heroin	06 Heroin
12 Methadone	05 Methadone
13 Methyl palmitate	04 Methyl palmitate
14 Morphine	03 Morphine
15 Pentobarbital	02 Pentobarbital
16 Secobarbital	01 Secobarbital

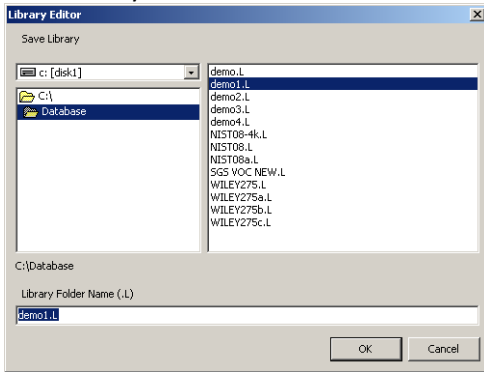
## Library editor

Ctrl-V to paste new names in 'Name' column

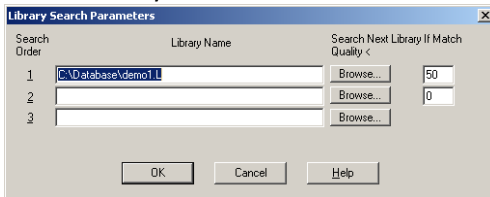


#	Name	Info	Formula	Company	CAS	MW	BP	MP	RT	RI	UI	Include	Match	Full	Cond
3	16 4-Chlorobiphenyl	Performance evaluation sample	C12H9Cl	HP	2051-62-9	188.0	291.0	77.7	1022.370	1		<input checked="" type="checkbox"/>		109	17
15	15 6-Monoacetylmorphine	Drug demo sample; drugs	C19H21NO4	HP	59833-14-6	327.1	0.0	0.0	3248.778	974144186		<input checked="" type="checkbox"/>		237	22
7	14 Amobarbital	Barbiturates sample; drugs	C11H18N2O3	HP	57-43-2	226.1	0.0	157.0	2732.892	1		<input checked="" type="checkbox"/>		99	19
5	13 Barbital	Barbiturates sample; drugs	C8H12N2O3	HP	57-44-3	184.1	0.0	190.0	2732.892	1		<input checked="" type="checkbox"/>		70	17
2	12 Biphenyl	Performance evaluation sample	C12H10	HP	92-52-4	154.1	255.9	71.0	1022.370	1		<input checked="" type="checkbox"/>		76	15
6	11 Butethal	Barbiturates sample; drugs	C10H16N2O3	HP	77-28-1	212.1	0.0	125.0	2732.892	1		<input checked="" type="checkbox"/>		91	18
14	10 Caffeine	Drug demo sample; drugs	C8H10N4O2	HP	58-08-2	194.1	0.0	238.0	2732.892	816527814		<input checked="" type="checkbox"/>		80	17
11	09 Cocaine	Alkaloids sample; drugs	C17H21NO4	HP	50-36-2	303.1	0.0	98.0	2732.892	816527814		<input checked="" type="checkbox"/>		175	21
12	08 Codeine	Alkaloids sample; drugs	C18H21NO3	HP	76-57-3	299.2	0.0	155.0	2732.892	816527814		<input checked="" type="checkbox"/>		240	21
1	07 Dodecane	Performance evaluation sample	C12H26	HP	112-40-3	170.2	216.3	-9.6	27683.503	1		<input checked="" type="checkbox"/>		64	15
16	06 Heroin	Drug demo sample; drugs	C21H23NO5	HP	561-27-3	369.2	0.0	173.0	2732.892	816527814		<input checked="" type="checkbox"/>		253	23
10	05 Methadone	Alkaloids sample; drugs	C21H27NO	HP	76-99-3	309.2	0.0	0.0	2732.892	816527814		<input checked="" type="checkbox"/>		208	22
4	04 Methyl palmitate	Performance evaluation sample	C17H34O2	HP	112-39-0	270.3	418.0	30.0	1022.370	1		<input checked="" type="checkbox"/>		123	20
13	03 Morphine	Alkaloids sample; drugs	C17H19NO3	HP	57-27-2	285.1	0.0	197.0	2732.892	816527814		<input checked="" type="checkbox"/>		231	21
8	02 Pentobarbital	Barbiturates sample; drugs	C11H18N2O3	HP	76-74-4	226.1	0.0	130.0	2732.892	1		<input checked="" type="checkbox"/>		92	19
9	01 Secobarbital	Barbiturates sample; drugs	C12H18N2O3	HP	309-43-3	238.1	0.0	0.0	2732.892	1		<input checked="" type="checkbox"/>		100	19

## Save library as demo1



## Agilent GCMS Chemstation DataAnalysis Select Library



## Chromatogram – Annotate chromatogram with PBM Results

