**The Right Chemistry**
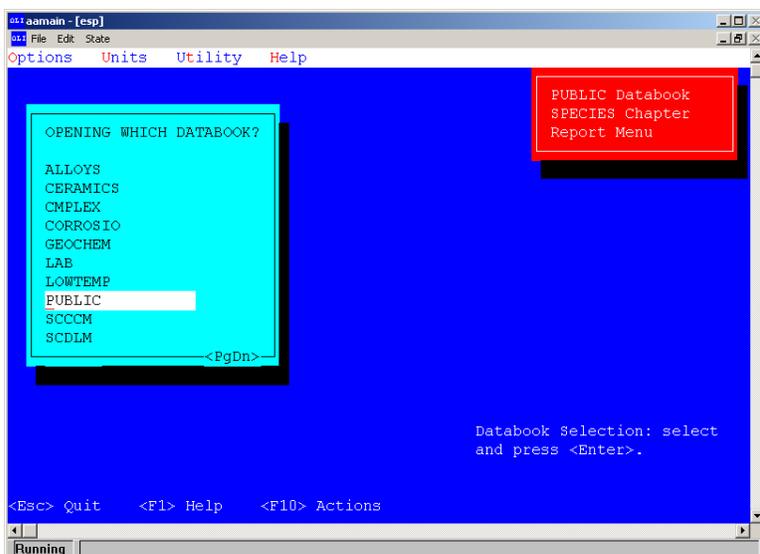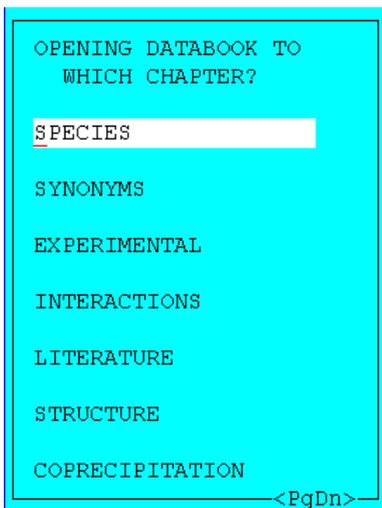
# OLI Tips #50
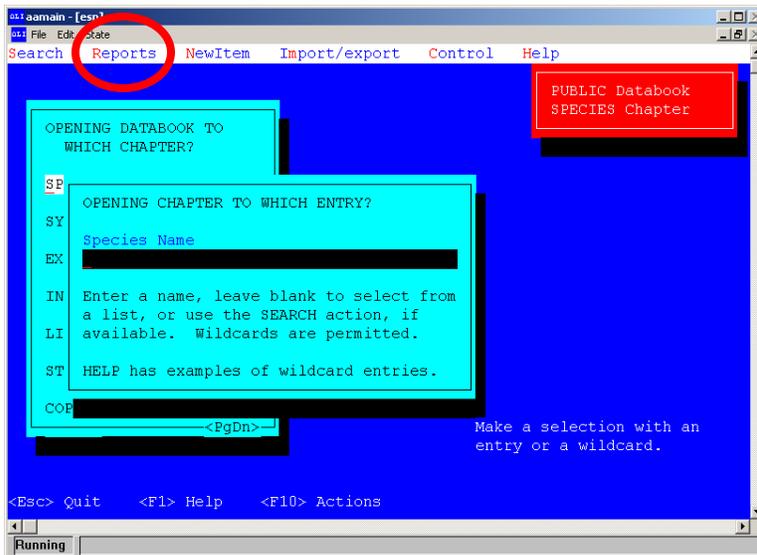### Generating a species listing report for the PUBLIC database

1. Start the OLI/Engine or ESP program
2. Select OLI/Databook
3. Select PUBLIC Databook

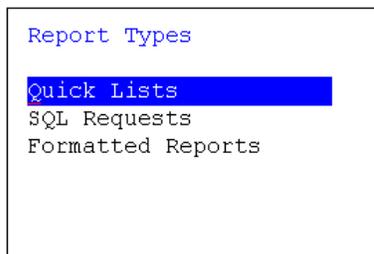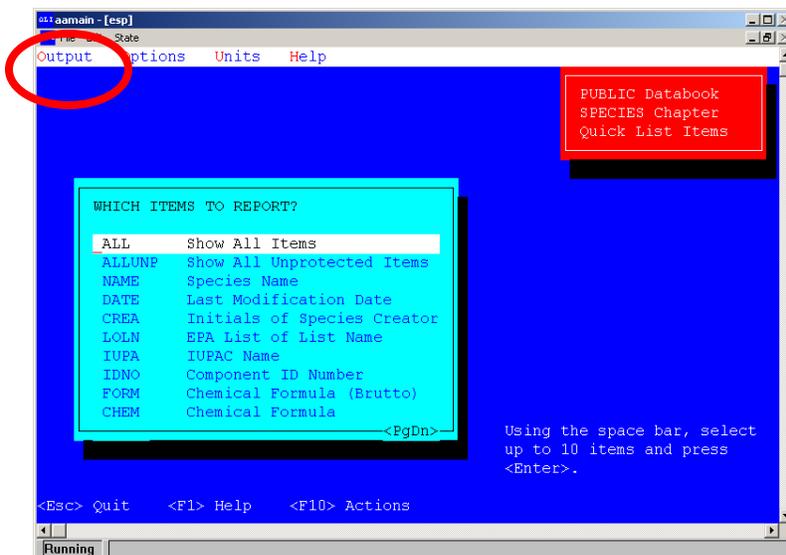

4. Select SPECIES chapter

5. Select REPORTS from the action line. Use the F10 key or ALT-R



6. Select Quick Lists

```
Report Types

Quick Lists
SQL Requests
Formatted Reports
```

7. Select OUTPUT from the action line. Use F10 or ALT-O

8.  Select DISK

```
Screen Only
Printer
Disk
```

9.  Enter a name. Maximum of 8 characters. This will be saved as a text file in the working folder.

```
File Name for report:
publist_
```

10. Press the <END> key or F3
11. Press the <END> key again to return to this menu

```
WHICH ITEMS TO REPORT?

 ALL       Show All Items
 ALLUNP    Show All Unprotected Items
 NAME      Species Name
 DATE      Last Modification Date
 CREA      Initials of Species Creator
 LOLN      EPA List of List Name
 IUPA      IUPAC Name
 IDNO      Component ID Number
 FORM      Chemical Formula (Brutto)
 CHEM      Chemical Formula
                              <PgDn>
```

12. Move the white bar down (the cursor) to the NAME field and press the
    <SpaceBar>

```
WHICH ITEMS TO REPORT?                              Report will contain:


 ALL       Show All Items                           NAME_
 ALLUNP    Show All Unprotected Items
>NAME      Species Name
 DATE      Last Modification Date
 CREA      Initials of Species Creator
 LOLN      EPA List of List Name
 IUPA      IUPAC Name
 IDNO      Component ID Number
 FORM      Chemical Formula (Brutto)
 CHEM      Chemical Formula
                              ─<PgDn>─              Report will be sent to a
                                                    disk file with extension .
                                                    QCK.
```
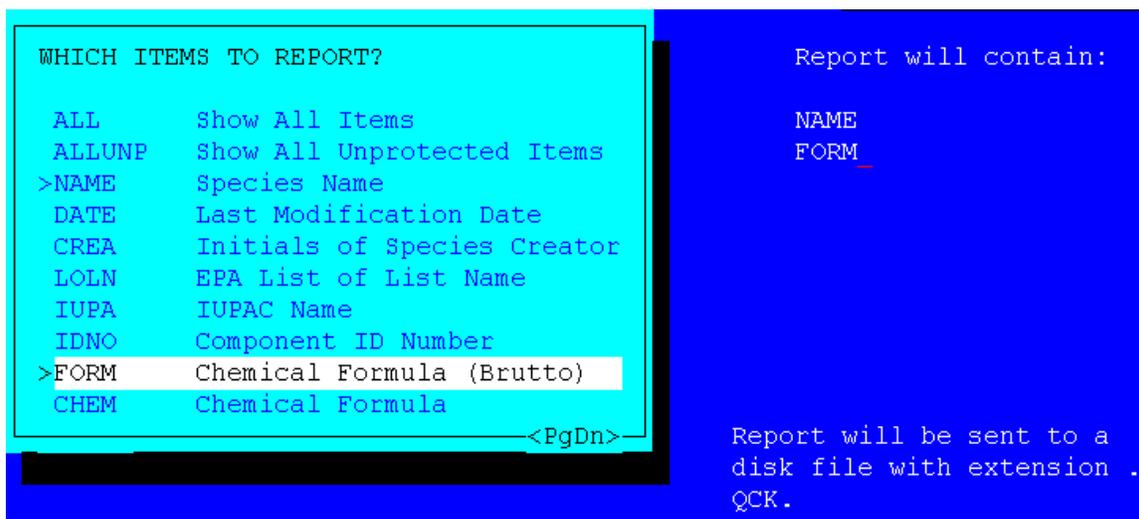
13. An arrow appears next to the name. The blue field updates with the selected item.
    It is recommended for a columnar list that only two items be selected.
14. Position the cursor on FORM to also include the chemical formula

```
WHICH ITEMS TO REPORT?                              Report will contain:


 ALL       Show All Items                           NAME
 ALLUNP    Show All Unprotected Items               FORM_
>NAME      Species Name
 DATE      Last Modification Date
 CREA      Initials of Species Creator
 LOLN      EPA List of List Name
 IUPA      IUPAC Name
 IDNO      Component ID Number
>FORM      Chemical Formula (Brutto)
 CHEM      Chemical Formula
                              ─<PgDn>─              Report will be sent to a
                                                    disk file with extension .
                                                    QCK.
```

15. Press the Enter key

```
WHICH SPECIES TO REPORT?

Species Name
_____
_

Enter a wildcard, a name, a list, or
use the SEARCH action.



Chemical formulas are case sensitive.
```

16. You may select only selected species. To see a full listing, leave this field blank.
17. Press the Enter Key

```
ANY SELECTION CRITERIA TO APPLY?

Criteria
_____
_

Enter criteria which will be applied
to the selection of species, in the
form "ITEM oper VALUE," e.g., ORG=IORG
A blank entry selects all.                En
HELP has examples of criteria.            pr
```

18. Additional search criteria may be added such as only species that contain a specific atom or grouping. To select all species leave this field blank.
19. Press the Enter key.
20. The screen will flicker as the file is created.
21. Press the END key to leave the file.
22. Repeatedly press the END key to leave the OLI Databook. Do not use the ESC key.
23. Locate the text file that you named in step 9 above. The file will have the extension QCK.
24. Open the file with NOTEPAD

```
NAME                FORM
ABIETICAC           C20H30O2
ACENAPHTHN          C12H10
ACENITRILE          C2H3N
ACET2               C4H8O4
ACETACID            C2H4O2
ACETAL              C6H14O2
ACETALDEHD          C2H4O
ACETAMIDE           C2H5NO
ACETANHYD           C4H6O3
ACETATEION          C2H3O2-1
ACETBR              C2H3BrO
ACETCL              C2H3ClO
ACETOIION           C4H7O2-1
ACETONE             C3H6O
ACETPHENON          C8H8O
ACETYLENE           C2H2
ACRIDINE            C13H9N
ACROLEIN2           C3H4O
ACRYLAMIDE          C3H5NO
```

This file contains the ESP name of the species (on the left) and the chemical formula on the right.