

Advancing Endangered Species Act Consultations

Use of an Automated, Computational Pipeline to Extract Points of Departure from Public Data Sources

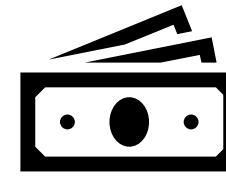


Monique Hazemi¹, Dan Villeneuve², Andrea LaTier³, Mark Jankowski³, Carlie LaLone², Christopher Schaupp¹, Manli Chan⁴, Derik Haggard⁴, Kali Mattingly⁵

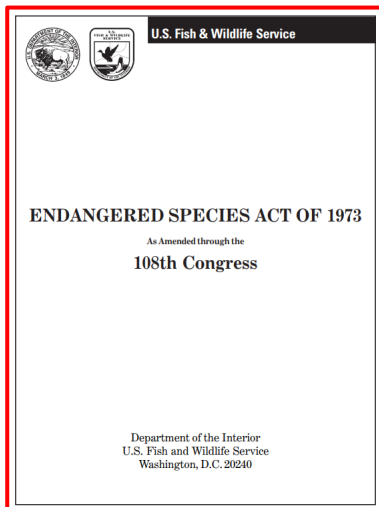
¹Oak Ridge Institute for Science and Education at USEPA GLTED, ²U.S. Environmental Protection Agency, Office of Research and Development (ORD), Great Lakes Toxicology and Ecology Division (GLTED), Duluth, MN, USA, ³U.S. Environmental Protection Agency, Region 10, Laboratory Services and Applied Science Division (LSASD), Seattle, WA, USA, ⁴U.S. Environmental Protection Agency, ORD, Scientific Computing and Data Curation Division (SCDCD), Research Triangle Park, NC, USA, ⁵SpecPro Professional Services, GLTED, Duluth, MN, USA

Summary: POD estimates derived from the automated pipeline tended to be at lower or approximately equal concentrations compared to manually derived results, providing evidence that the app can provide reasonable, and generally protective, PODs for ESA consultations.

Background



- Endangered Species Act (ESA) consultations are complicated and time and resource intensive
 - Species-specific toxicity analyses required for each chemical



Discharge

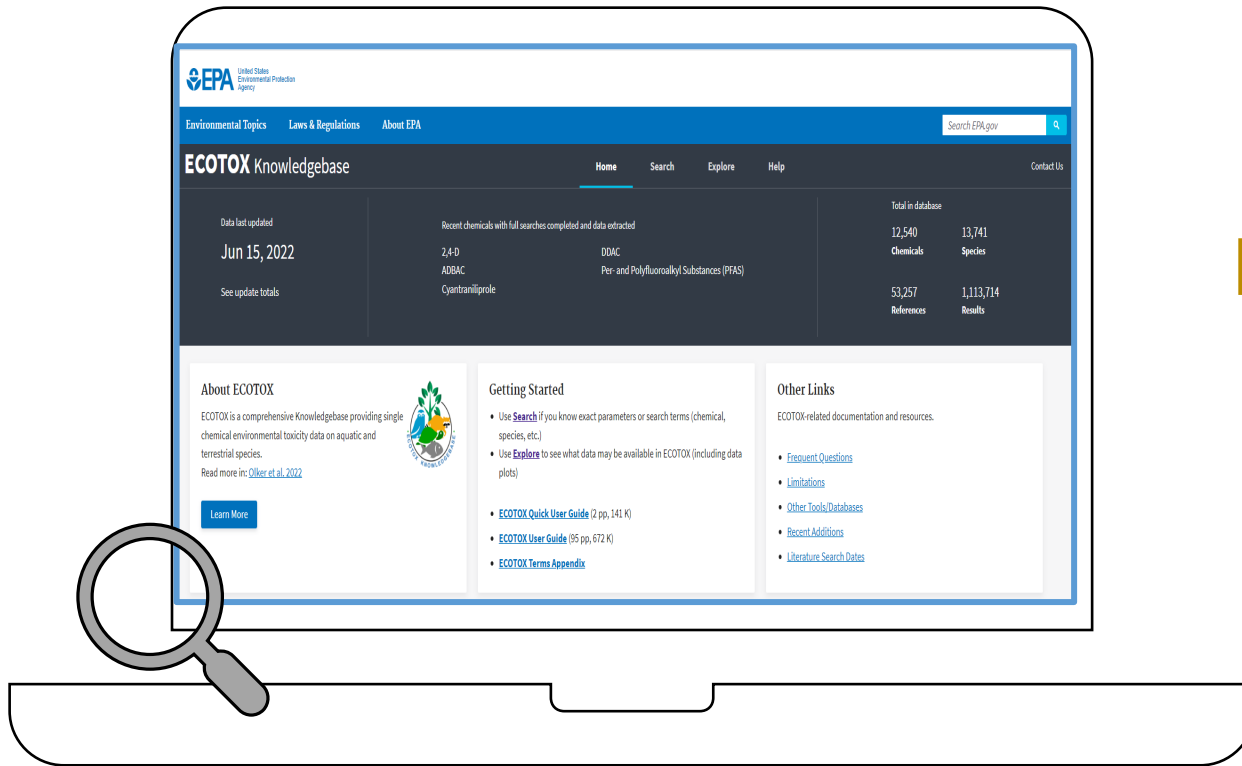


BDE-47
DTXSID3030056

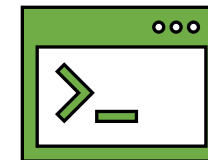


Coho salmon

Objective



*(For more info see next presentation by Dale Hoff:
5.01.T-03 - The ECOTOXicology Knowledgebase...)*



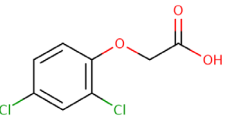
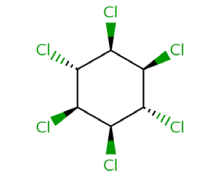
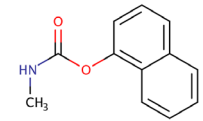
Coding

The App

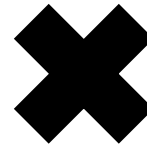


Point of departure (POD) < manually
derived toxicity benchmark value ???

Methods – Query chemicals & species



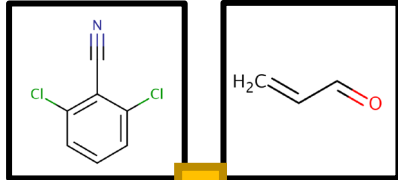
Chemical
2,4-Dichlorophenoxyacetic acid
4-Nonylphenol
Acrolein
Carbaryl
Diazinon
Dichlobenil
Dieldrin
Endrin
Heptachlor
Lindane
Pentachlorophenol



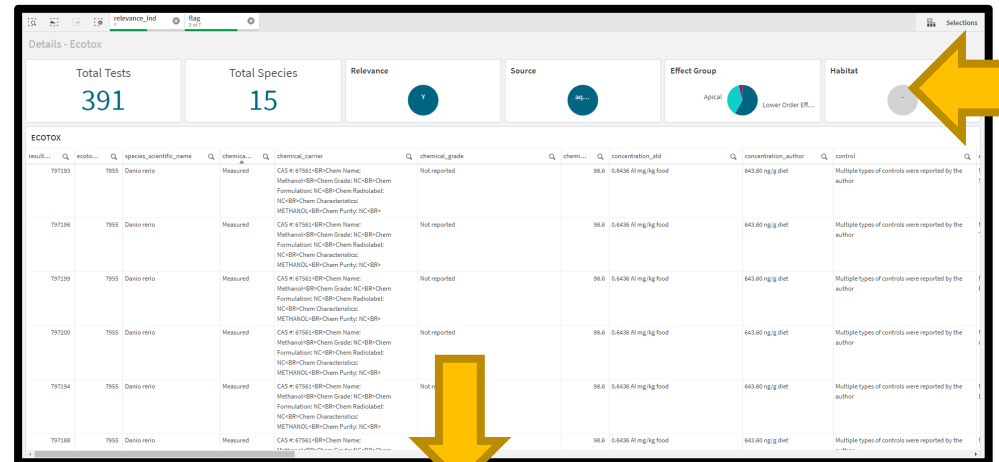
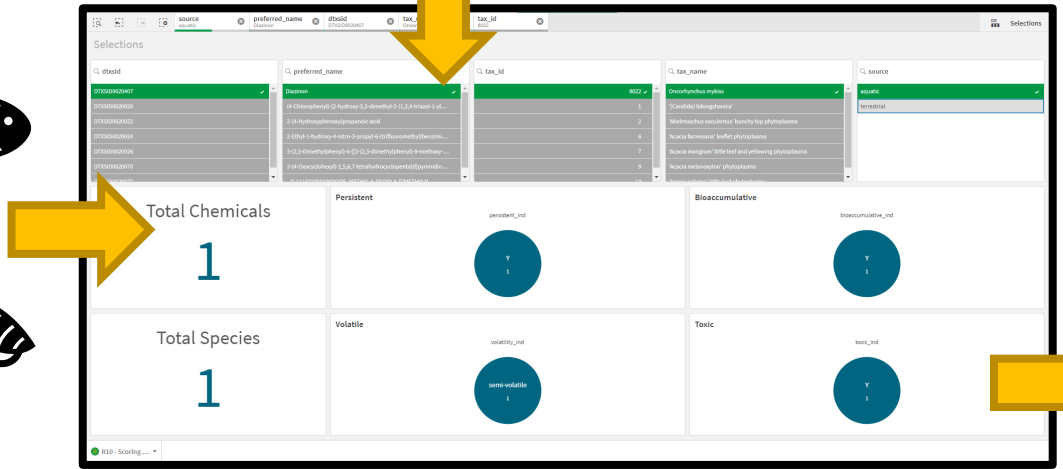
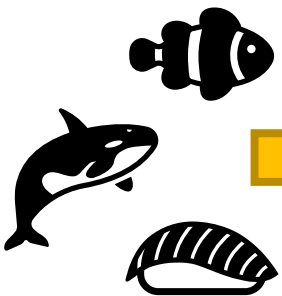
Broad range of taxa and mode of actions (herbicides, insecticides, fungicides, some have multiple uses)

Species	
Vernal pool fairy shrimp	<i>Branchinecta lynchi</i>
Steelhead	<i>Oncorhynchus mykiss</i>
Foskett speckled dace	<i>Rhinichthys osculus ssp.</i>
Bocaccio rockfish	<i>Sebastes paucispinis</i>





Methods



Calculated Summed Score

Rapid Tox			
ecotox_scientific_name	ecotox_common_name	concl...	Summed Score
Gadus morhua	Atlantic Cod	0.00023	4.4285714285714
Gadus morhua	Atlantic Cod	0.00023	4.4285714285714
Skeletonema costatum	Diatom	0.016	4.2619047619048
Gadus morhua	Atlantic Cod	0.00023	4.1904761904762
Gadus morhua	Atlantic Cod	0.00023	4.1904761904762
Gadus morhua	Atlantic Cod	0.00023	4.1904761904762
Gadus morhua	Atlantic Cod	0.00023	4.1904761904762
Danio rerio	Zebra Danio	0.01457385	4.1190476190476
Skeletonema costatum	Diatom	0.028	4.1190476190476

Calculated Taxon Match Score

TRV & WQC from Biological Evaluations



1. Min POD

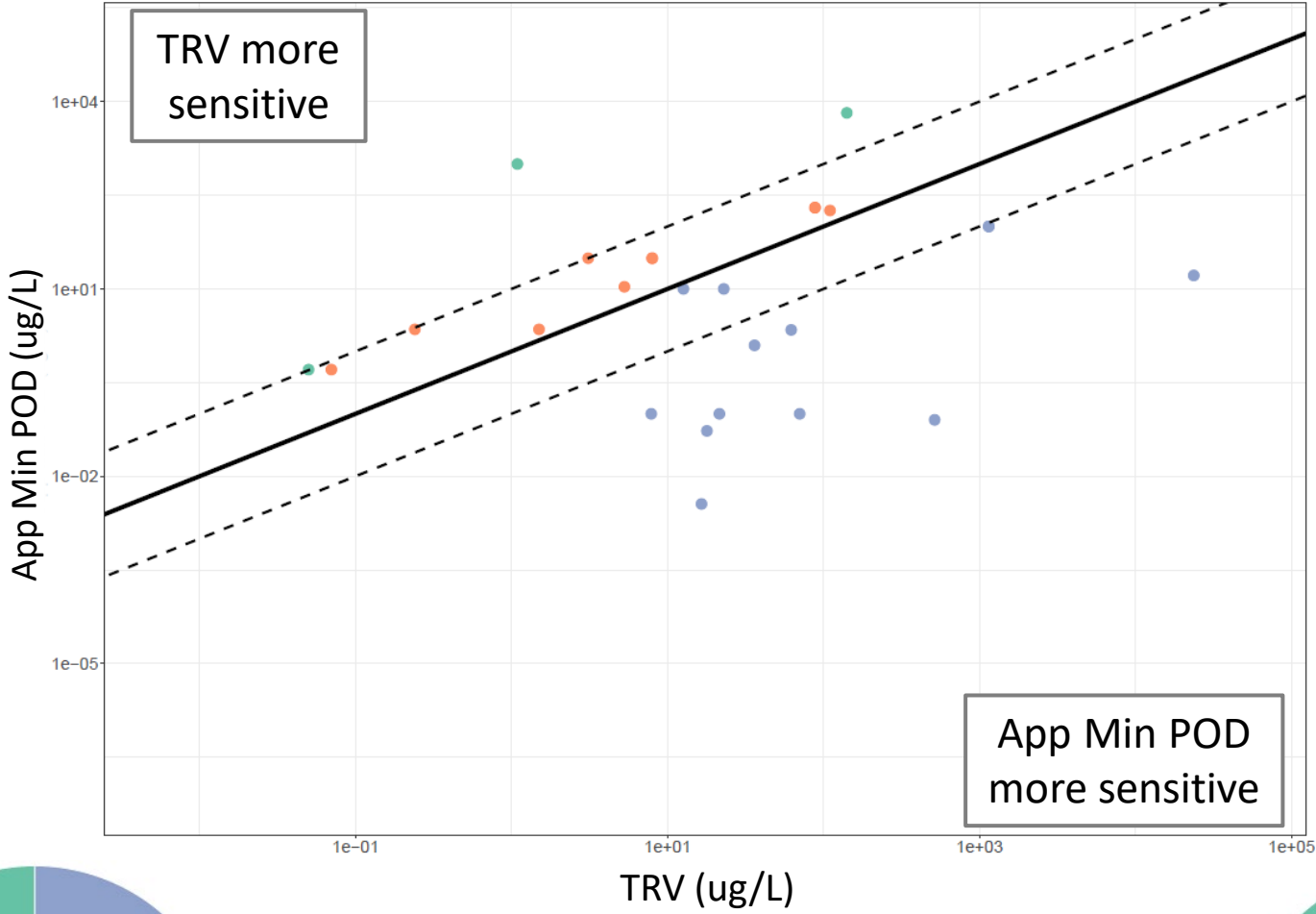
2. Min POD x highest taxon match

3. Min POD x highest sum score

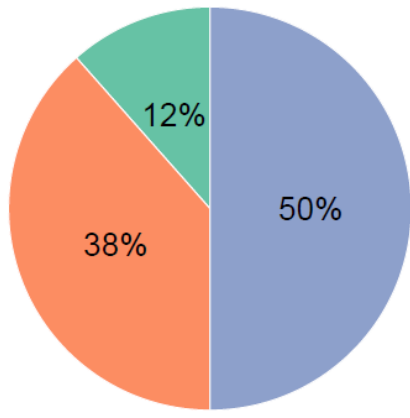
App-derived PODs < TRV or within 10x in majority of cases

Comparison category

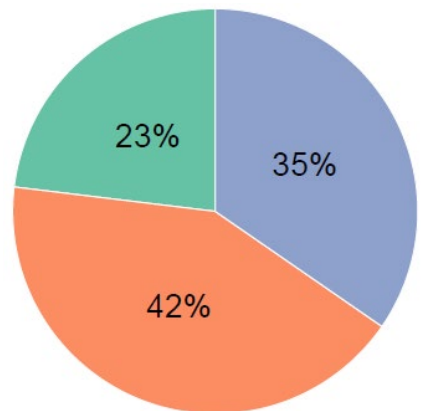
- App POD > manual value by more than a factor of 10
- App POD > manual value but within a factor of 10
- App POD < manual POD (i.e., protective)



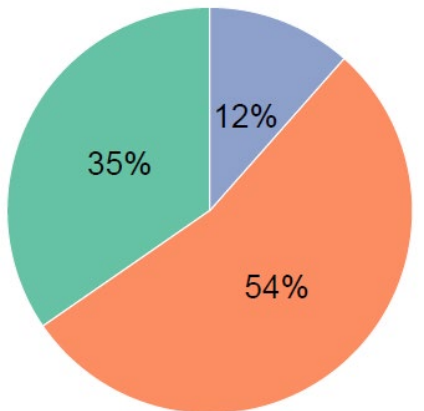
App Min POD vs. TRV



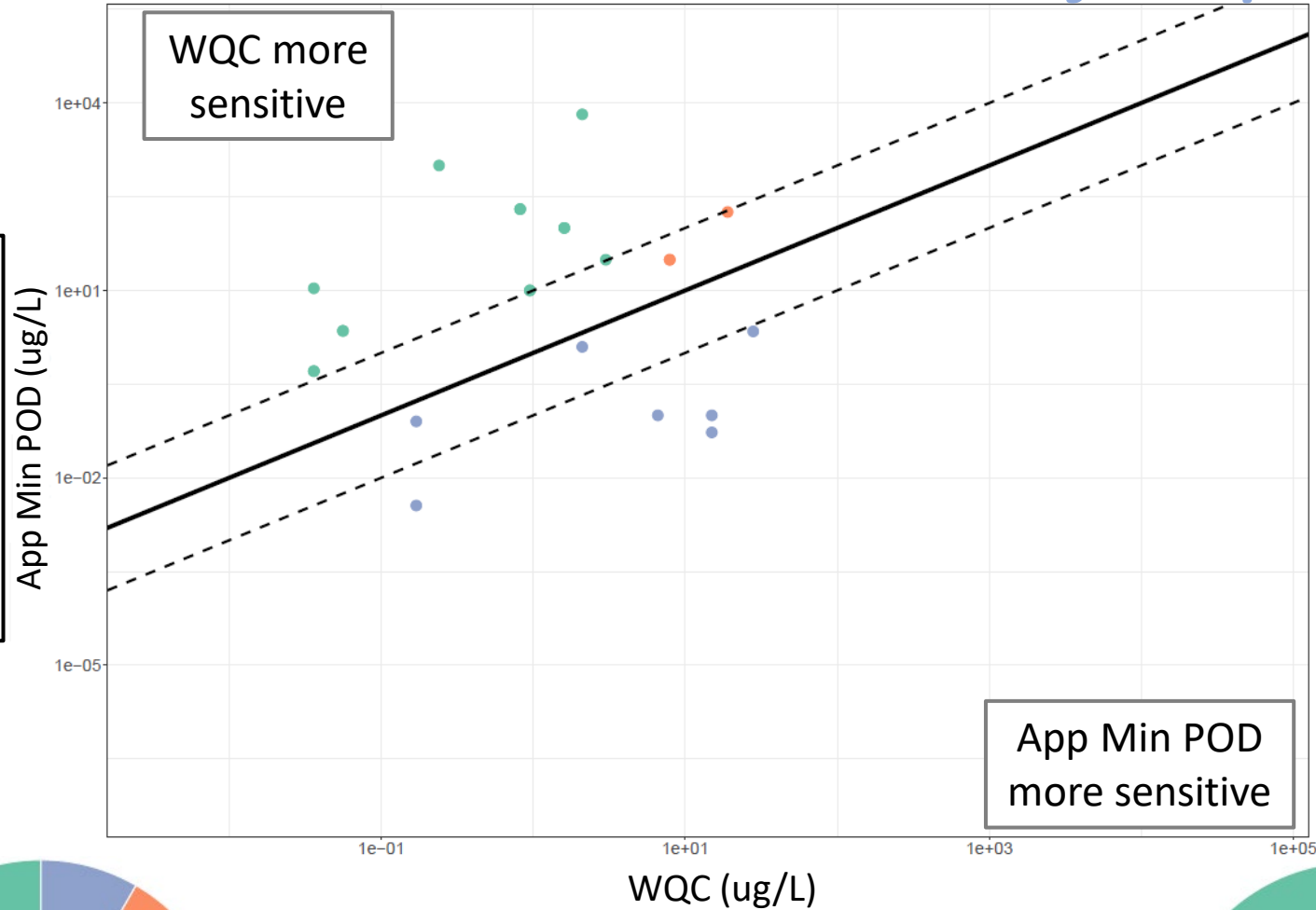
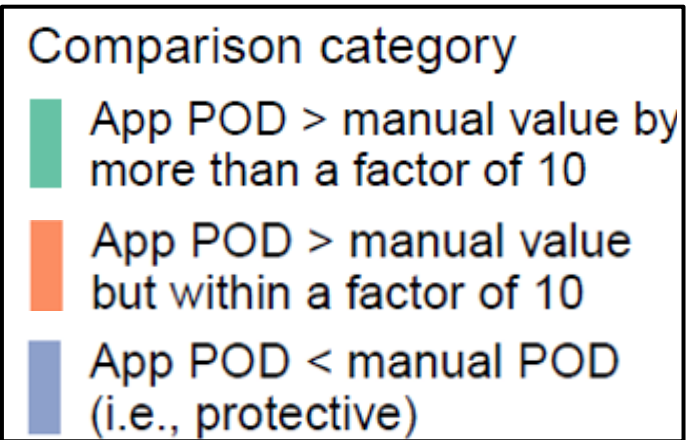
App Min POD Tax Match vs. TRV



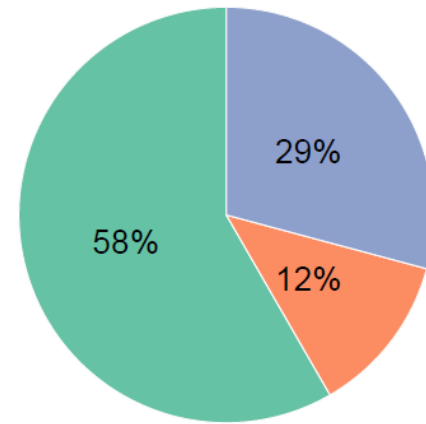
App Min POD Sum Score vs. TRV



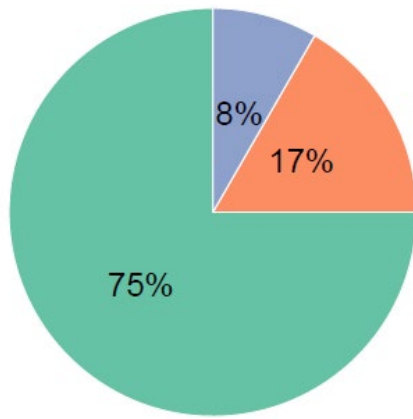
App-derived PODs > 10x **WQC** in majority of cases



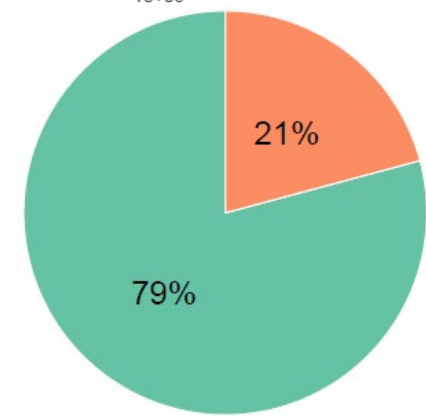
App Min POD vs. WQC



App Min POD Tax Match vs. WQC



App Min POD Sum Score vs. WQC



Concordance analysis: Paired t-test, Wilcoxon matched pairs signed rank test

Measure 1 (log10)	Measure 2 (log 10)	Paired t p-value	Paired t statistic	Wilcoxon p-value	Wilcoxon V statistic
TRV	Min POD	0.087	1.77		
TRV	Min POD SS			0.00011	33
TRV	Min POD TM	0.13	-1.57		
WQC	Min POD			0.089	108
WQC	Min POD SS			8.74E-06	0
WQC	Min POD TM	4.90E-05	-4.89		

4/6 cases where app-derived PODs were lower or \approx equal to manually-derived TRV or WQC

Agreement analysis: Intraclass correlation

2/6 cases where app-derived PODs and manually-derived TRV or WQC were concordant.

Poor and moderate degree of concordance.

Measure 1 (log10)	Measure 2 (log 10)	ICC p-value	ICC
TRV	Min POD	0.13	0.20
TRV	Min POD SS	0.027	0.40
TRV	Min POD TM	0.00015	0.61
WQC	Min POD	0.36	0.065
WQC	Min POD SS	0.26	0.056
WQC	Min POD TM	0.30	0.061

Conclusions

- Benefits of the app
 - Yields generally protective PODs for evaluated range of Endangered species and chemicals
 - ❖ App min POD is most conservative of 3 types, with min POD Taxon Match as runner-up
 - ❖ App min POD Taxon Match has highest degree of concordance with TRV
 - Helps standardize and track screening of chemicals for evaluation
 - Expedites assessment of toxicity data to prioritize BE development
 - 1 hr vs. 8 - 40 hrs, per chemical-species pair
- Looking ahead...
 - Calculated adjustment factors for ESA assessments
 - Considering weighted scoring function



Contributors

REGION 10 LSASD: Andrea LaTier, Mark Jankowski, Hunter Whitten, Rochelle Labiosa, Angela Adams, Rob Elleman

ORD SCDGD: Derik Haggard, Manli Chan, Bhaskar Sharma, Norman Adkins, Amar Singh, Saranagapani Addanki, James Renner

ORD CCTE GLTED: Carlie LaLone, Dan Villeneuve, Chris Schaupp, Jennifer Olker

ORISE FELLOWS: John Hoang

OMS CAB: Sherisse Marion, Bryan Chastain, Gregory Byrne, Samantha Arnette

SpecPro Professional Services: Kali Mattingly

This research was supported in part by an appointment to the Research Participation Program at the Great Lakes Toxicology & Ecology Division, U.S. Environmental Protection Agency, administered by the Oak Ridge Institute for Science and Education through an interagency agreement between the U.S. Department of Energy and EPA.

The authors have no conflicts of interest to declare.

The research presented here neither constitutes nor necessarily reflects official U.S. EPA policy.



References

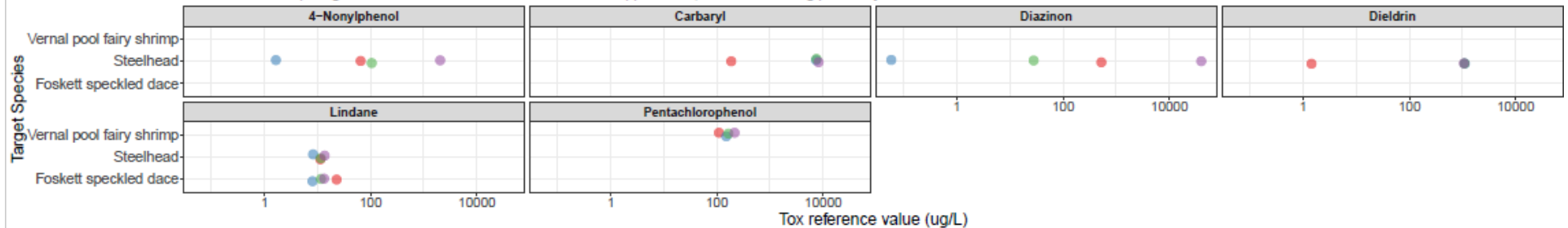
- United States. (1983). The Endangered Species Act as amended by Public Law 97-304 (the Endangered Species Act amendments of 1982). Washington: U.S. G.P.O.
- Olker, J. H., Elonen, C. M., Pilli, A., Anderson, A., Kinziger, B., Erickson, S., Skopinski, M., Pomplun, A., LaLone, C. A., Russom, C. L., & Hoff, D. (2022). The ECOTOXicology Knowledgebase: A Curated Database of Ecologically Relevant Toxicity Tests to Support Environmental Research and Risk Assessment. *Environmental Toxicology and Chemistry*, 41(6):1520-1539.
<https://doi.org/10.1002/etc.5324>
- Williams, A.J., Grulke, C.M., Edwards, J. et al. (2017). The CompTox Chemistry Dashboard: a community data resource for environmental chemistry. *Journal of Cheminformatics*, 9(61).
<https://doi.org/10.1186/s13321-017-0247-6>

Extra

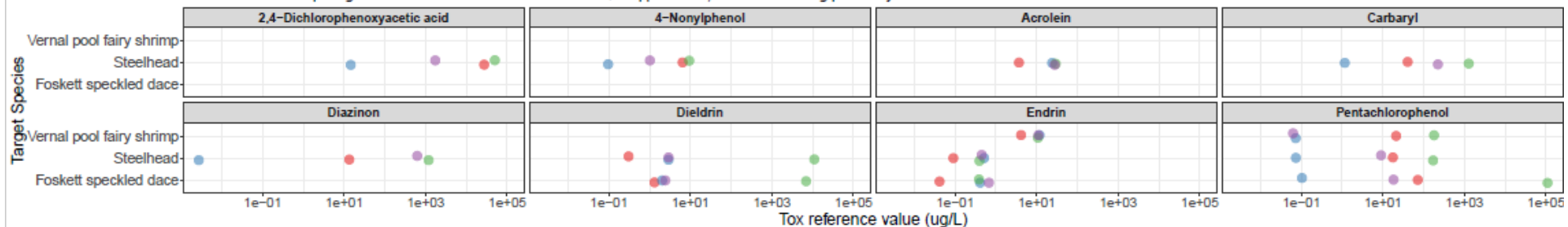
Summed Score Calculation

Scoring Categories	Examples [<i>high to low preference score</i>]
Taxonomic match	Species, genus, family, order, class.....
Effect type	Apical, neuro-endocrine-immune, lower order
POD type	More protective (e.g., LC10, vs. LC50) > score
Exposure type	Flow through, renewal, static.....
Control type	Multiple controls, concurrent control, historical control...
Exposure verification	Measured, nominal only
Summed Score	Sum of each scoring category (normalized to max score possible in category) – max. = 6

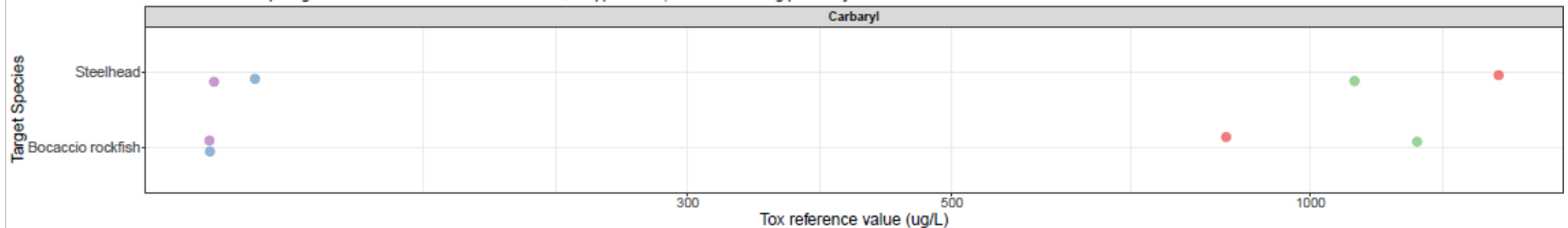
Fresh/Acute: Comparing 3 Min POD Calculation Methods from Qlik App vs. TRV, Subset-matching pairs only



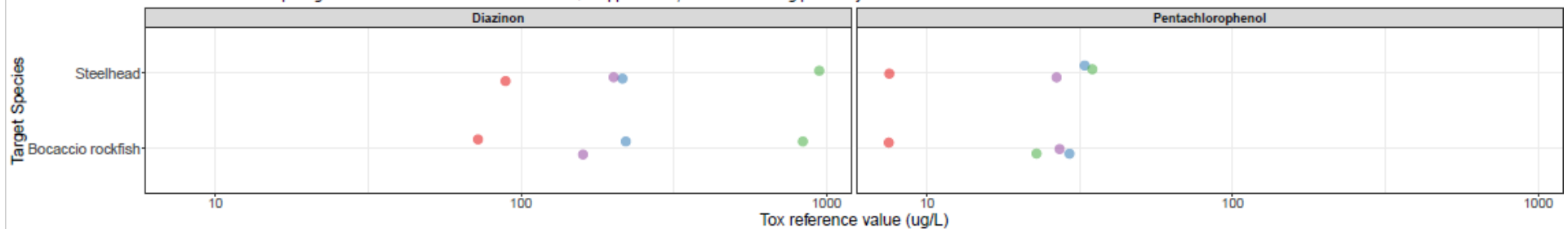
Fresh/Chronic: Comparing 3 Min POD Calculation Methods from Qlik App vs. TRV, Subset-matching pairs only



Marine/Acute: Comparing 3 Min POD Calculation Methods from Qlik App vs. TRV, Subset-matching pairs only



Marine/Chronic: Comparing 3 Min POD Calculation Methods from Qlik App vs. TRV, Subset-matching pairs only



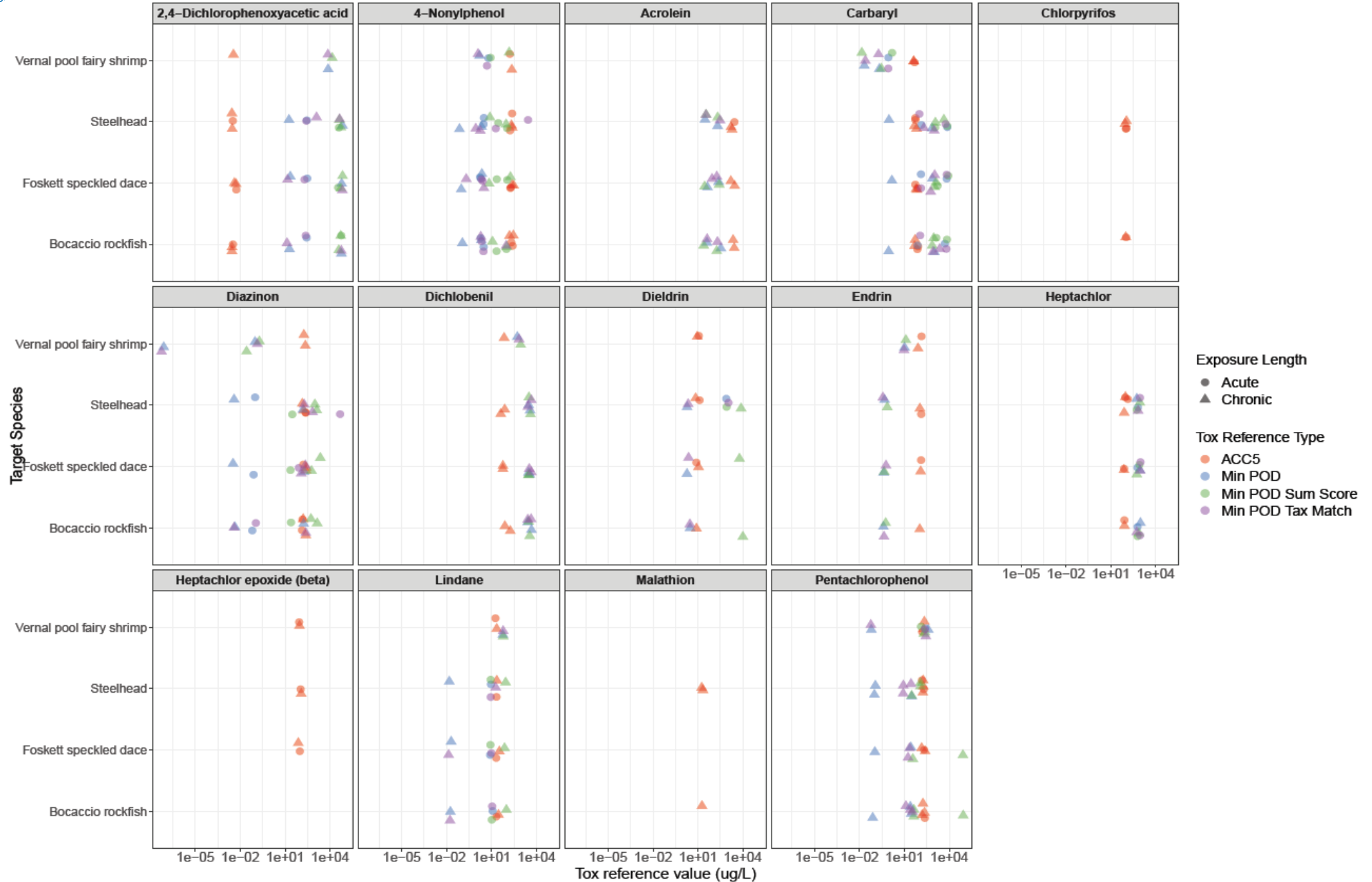
Tox Reference Type

- TRV
- Min POD
- Min POD Sum Score
- Min POD Tax Match



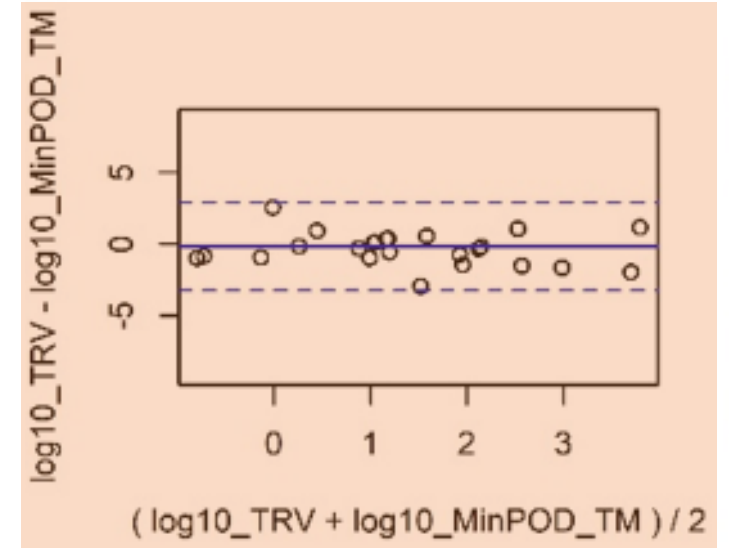
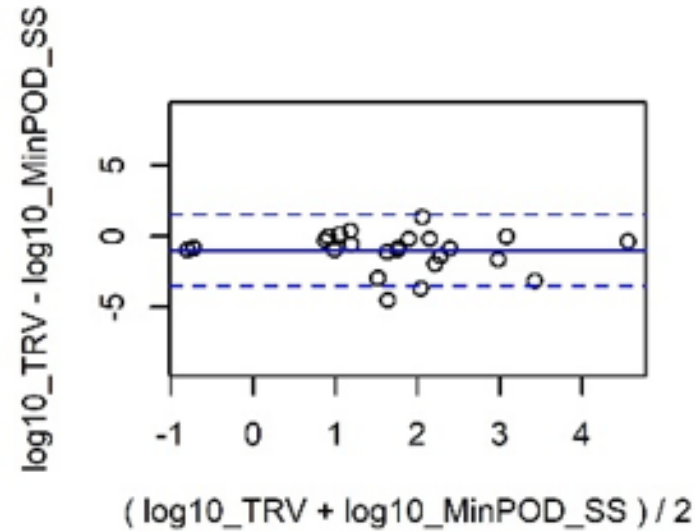
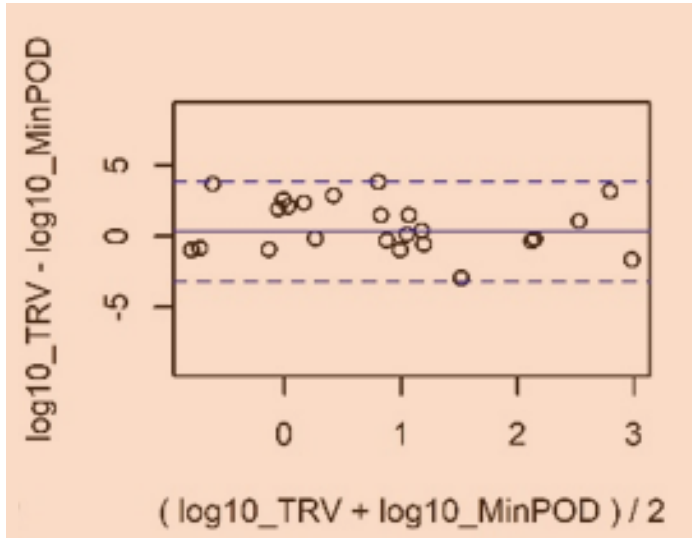
App-derived PODs vs. ToxCast ACC5

Comparing 3 Min POD Calculation Methods from Qlik App vs. ACC5

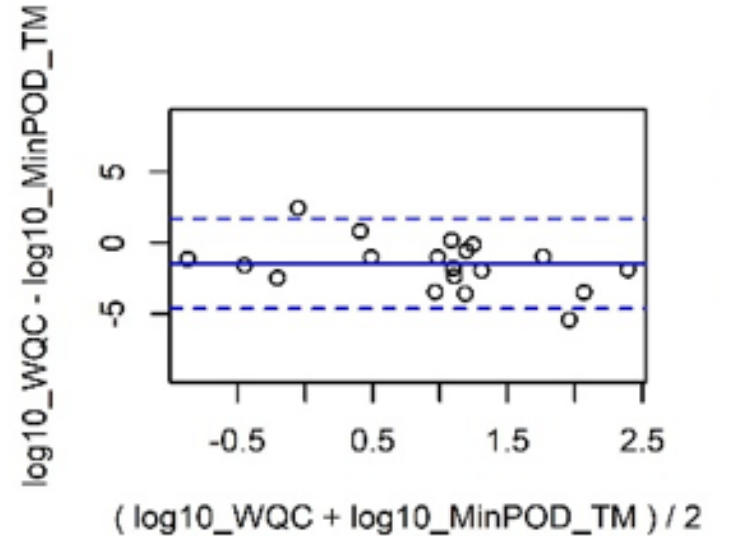
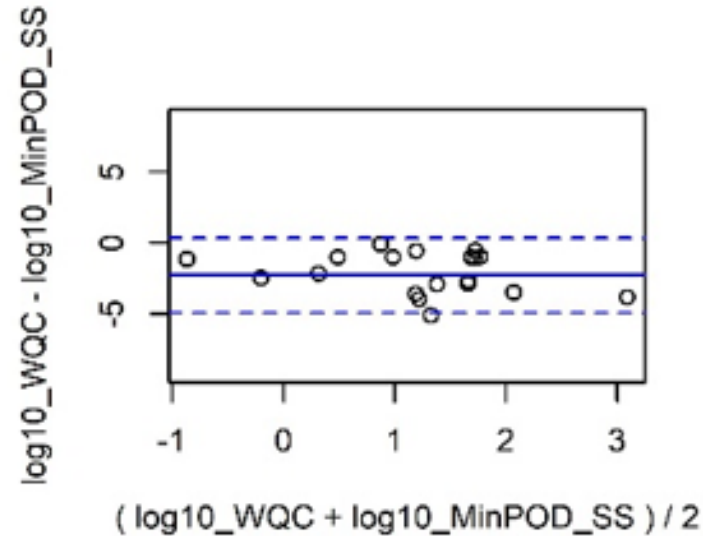
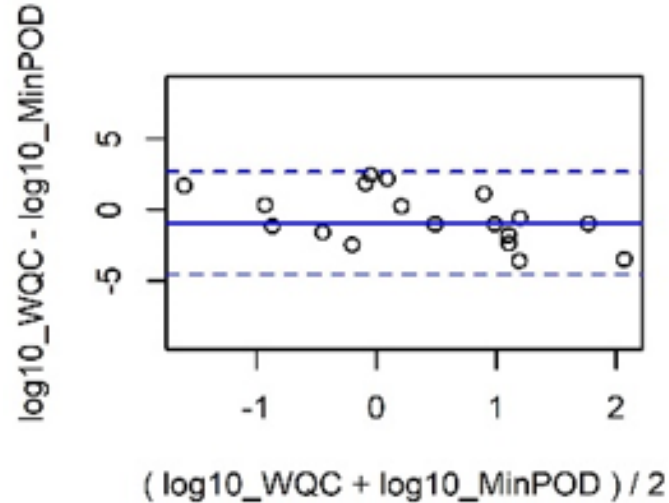


Agreement analysis: Bland-Altman

TRV
comparisons



WQC
comparisons



Min POD

Min POD SS

Min POD TM

Bland-Altman Agreement Analysis

meas_1	meas_2
log10_TRV	log10_MinPOD

BA_mean_difference	BA_SD	BA_LoA_lo_95CI	BA_LoA_up_95CI
0.326	1.759	-3.191	3.844

log10_TRV	log10_MinPOD_SS
log10_TRV	log10_MinPOD_TM

-1.021	1.248	-3.518	1.475
-0.190	1.528	-3.246	2.866

log10_WQC	log10_MinPOD
log10_WQC	log10_MinPOD_SS

-0.943	1.806	-4.556	2.669
-2.291	1.314	-4.920	0.337

log10_WQC	log10_MinPOD_TM
-----------	-----------------

-1.460	1.582	-4.625	1.704
--------	-------	--------	-------