

Strategies for Isotope-Loaded Liquid Scintillators

Physics Opportunities of Large Scale Liquid Scintillator Detectors (II)

Oct. 13 – Oct. 15, 2026

Michael Ford, Steven Dazeley

Prepared by LLNL under Contract DE-AC52-07NA27344.

Isotope loading routes for liquid scintillators

How do we maximize/optimize isotope (e.g., Te, Mo) loading while minimizing impact on liquid scintillator performance?

Isotope loading strategies:

- Direct dissolution using organic ligands
- Emulsion of metal-loaded water in scintillating oil (inverted WbLS)
- Dispersion of nanoparticles

Liquid scintillator formulating:

- Insensitive scintillating dyes/solvents

Table 1. Relative light yields of 0.5% Te-LS.

Samples	R. L. Y.
LS	100%
0.5%Te-LS (1,2-butanediol)	56% $\pm$ 3%
0.5%Te-LS (1,2-pentanediol)	59% $\pm$ 3%
0.5%Te-LS (1,2-hexanediol)	52% $\pm$ 3%
0.5%Te-LS (1,2-heptandiol)	56% $\pm$ 3%
0.5%Te-LS (1,2-octanediol)	56% $\pm$ 3%

Direct dissolution into LS (or dissolution with incorporation of an appropriate compatibilizer)

Many metals explored for scintillators:

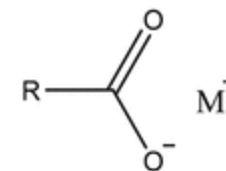
- Gd, Li, In, Te,...

Many coordinating compounds also explored:

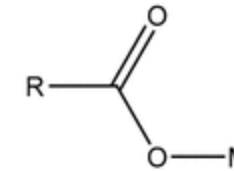
- Carboxylates, diketones, organophosphorus,...

Table 1. In solubility of various β -diketones in several solvents at room temperature

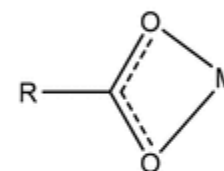
Solvent	β -diketone	In solubility, wt. %
Anisole	Hacac ($C_5H_8O_2$)	7.9 ± 0.1
Dichlorobenzene	Hacac	5.8 ± 0.1
PXE	Hacac	1.25 ± 0.05
PC	Hacac	1.20 ± 0.05
PC	Hdpm ($C_{11}H_{20}O_2$)	3.1 ± 0.1
PC	Hdbzm ($C_{15}H_{12}O_2$)	0.15 ± 0.03



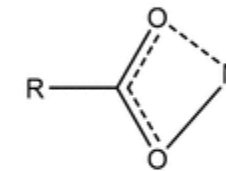
Ionic



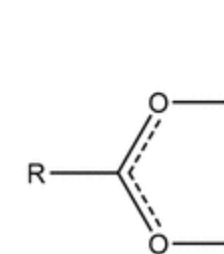
Unidentate



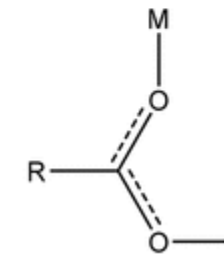
Chelating (sym)



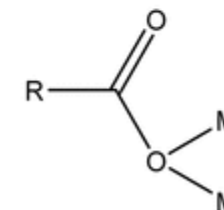
Chelating (anti)



Bridging (syn-syn)

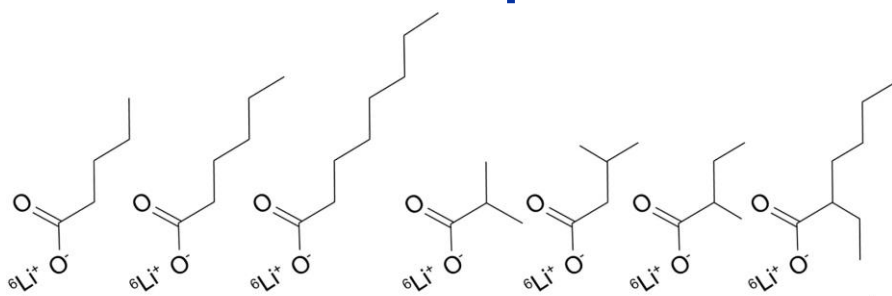


Bridging (anti-syn)



Bridging (Monoatomic)

These are not new strategies – but do we have new tools, compounds to explore, etc?



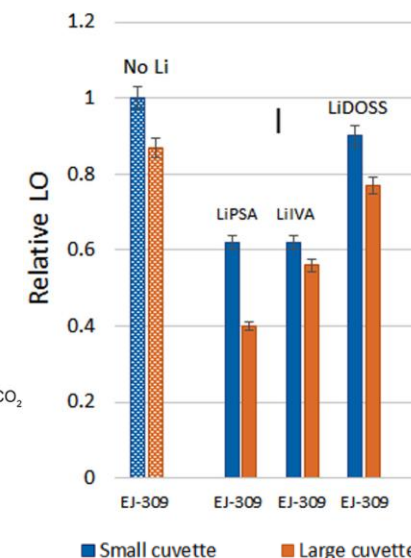
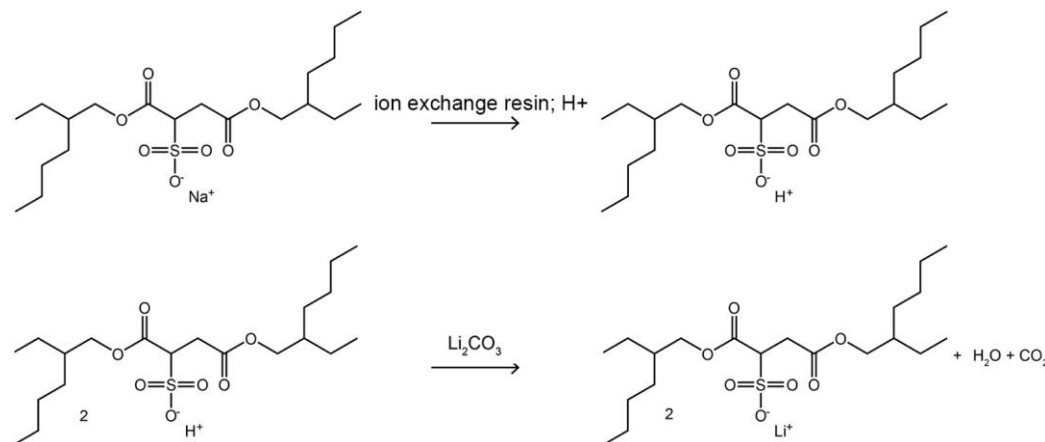
b) 23 °C; 85:15 styrene:MAA



c) 65 °C; 85:15 styrene:MAA

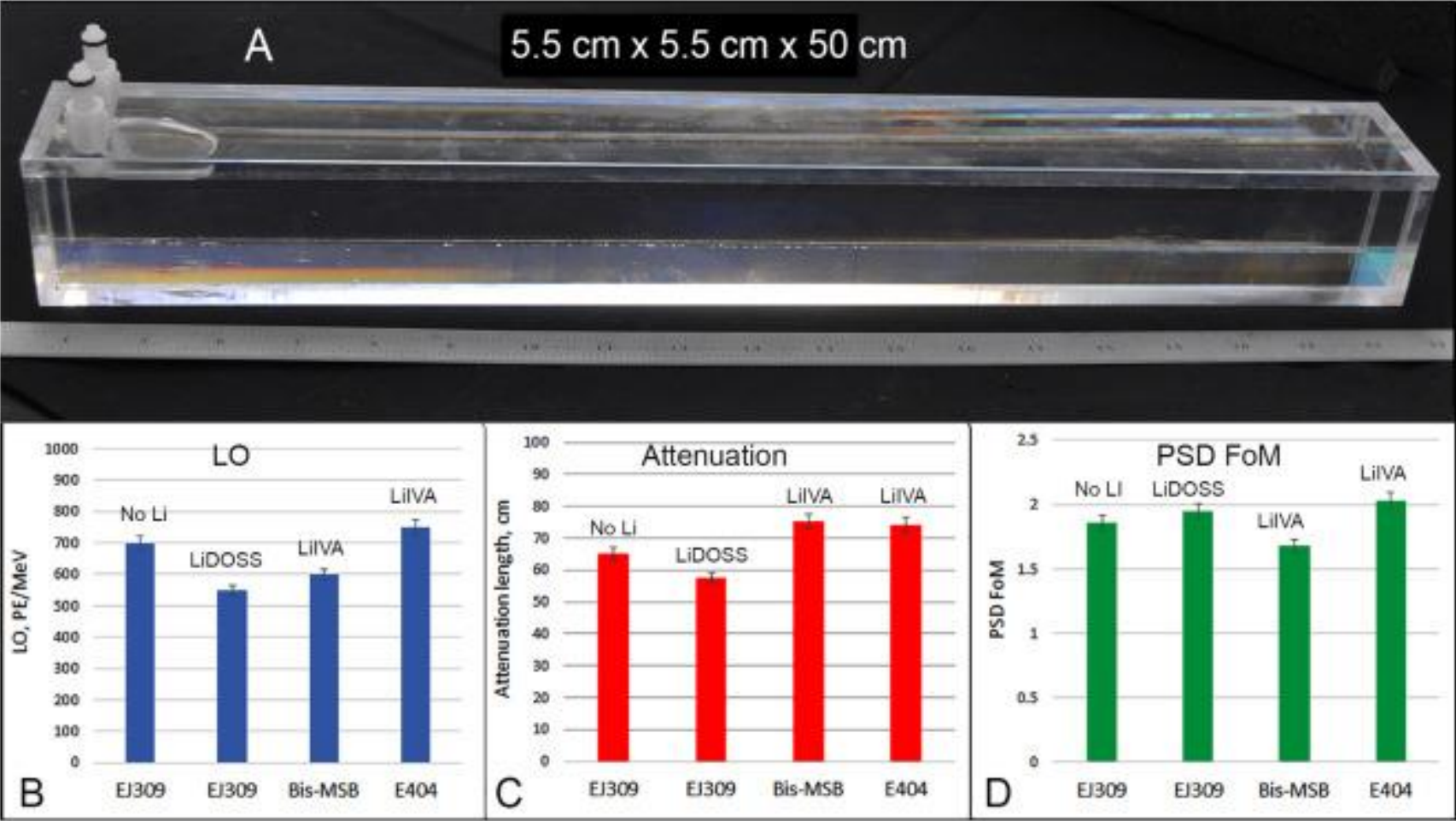


Sodium Docusate → Lithium Docusate – **directly soluble in organic liquids**

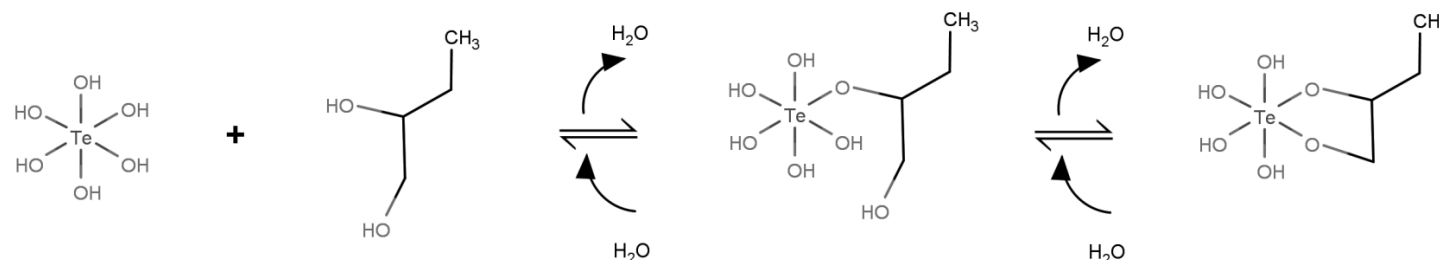


Li carboxylates require organic acid for solubility

These are not new strategies – but do we have new tools, compounds to explore, etc?



How can we extend this strategy to other isotopes?



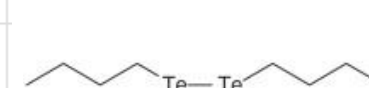
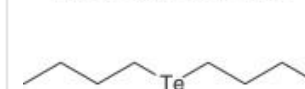
What could we leverage that's already available and underexplored for scintillators?

- Ionic surfactant derivative
- Catalysts
- Initiators
- Sol-gel precursors
- Semiconductors

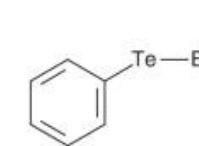
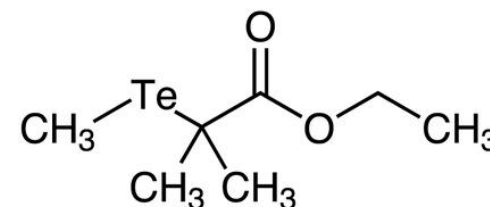
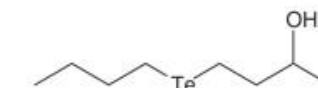
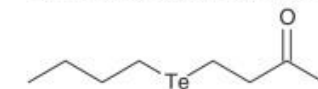
Size	Unit Price
100MG	\$32.00
1G	\$177.00

Must be considered:

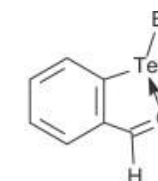
Bad-smelling compounds



Not bad-smelling compounds

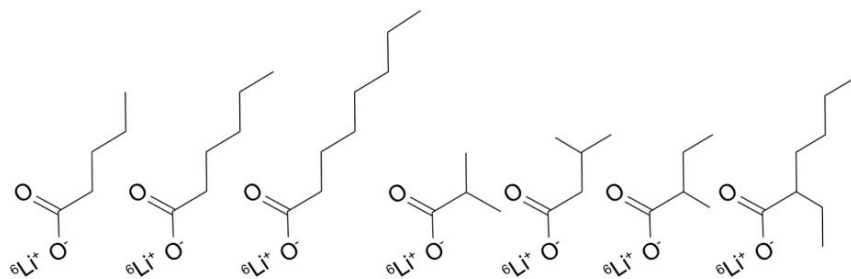


Unstable in solid state



Stable in solid state

These salts (and many metal salts) are directly soluble in water → which can then be dispersed into LS

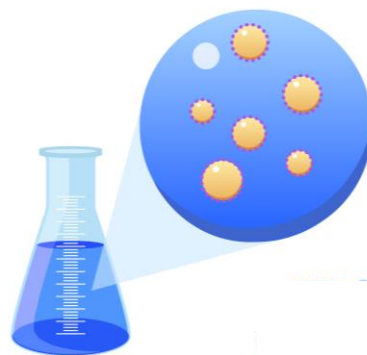
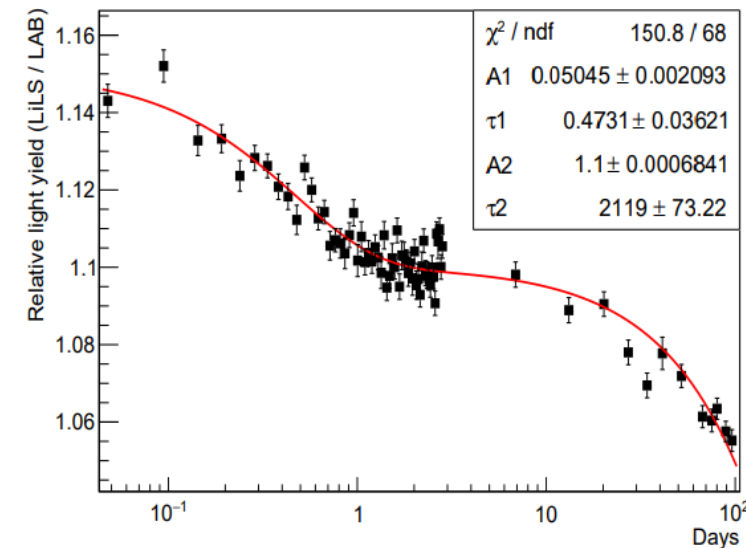


PROSPECT: aqueous solution of LiCl + nonionic surfactant

b) 23 °C; 85:15 styrene:MAA



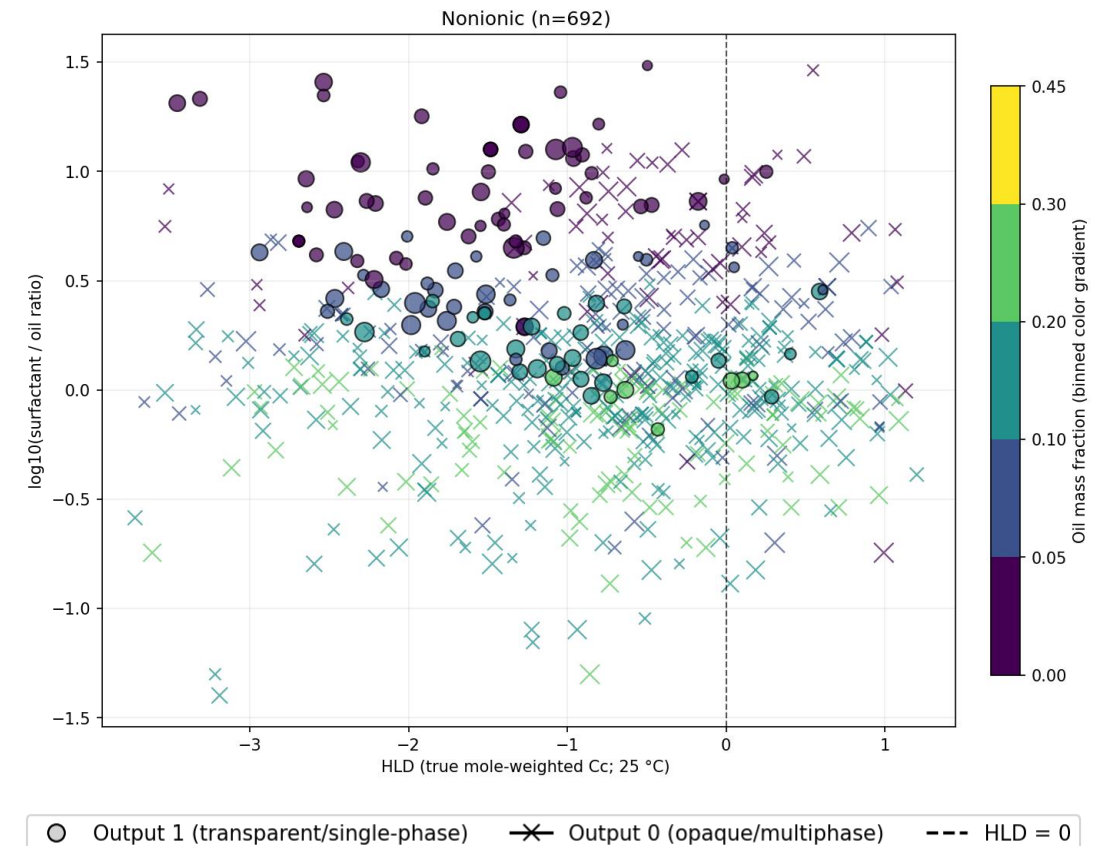
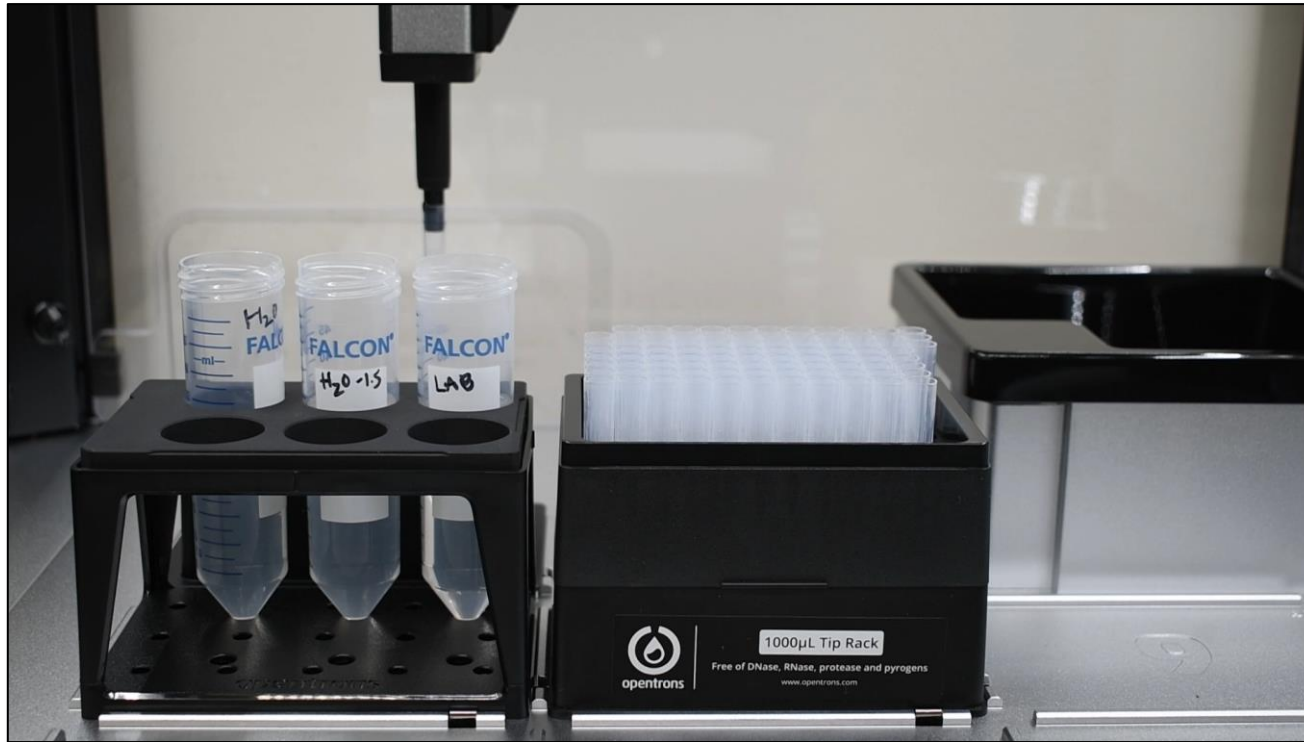
c) 65 °C; 85:15 styrene:MAA



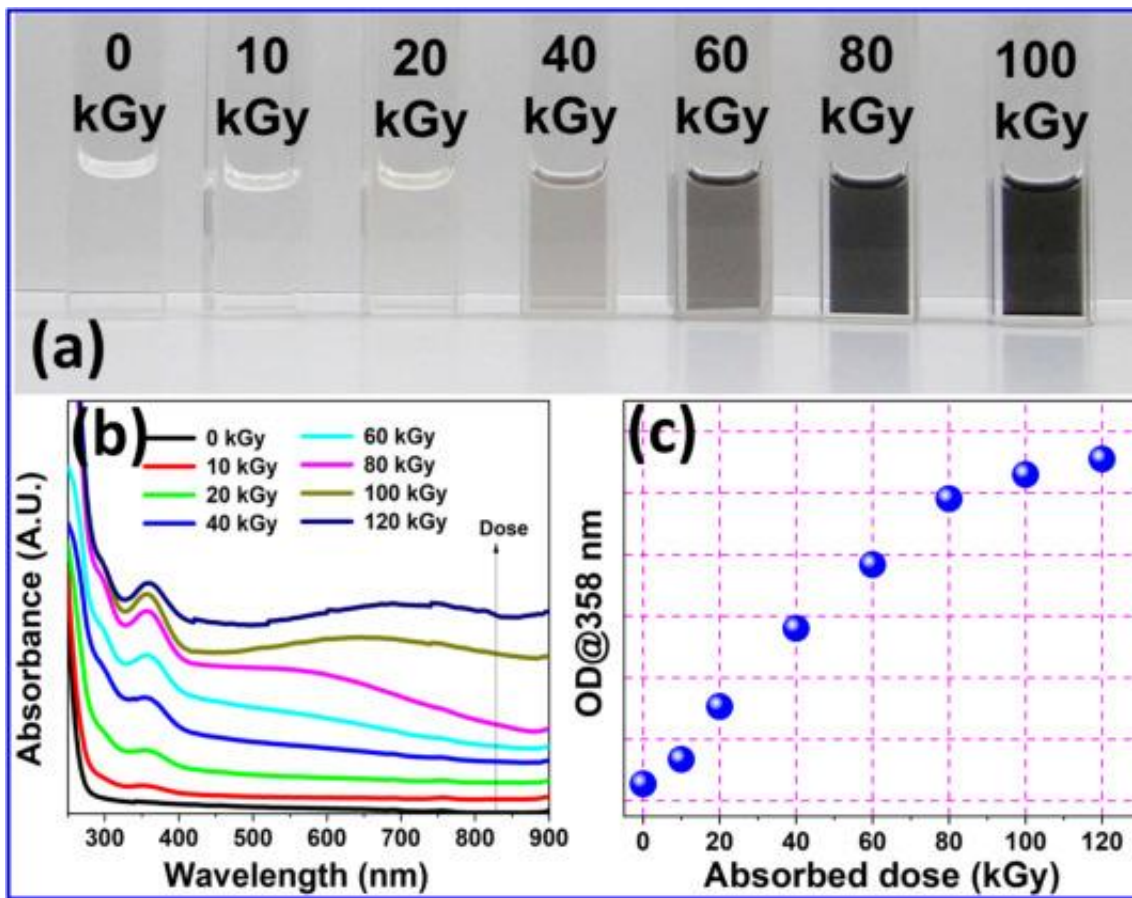
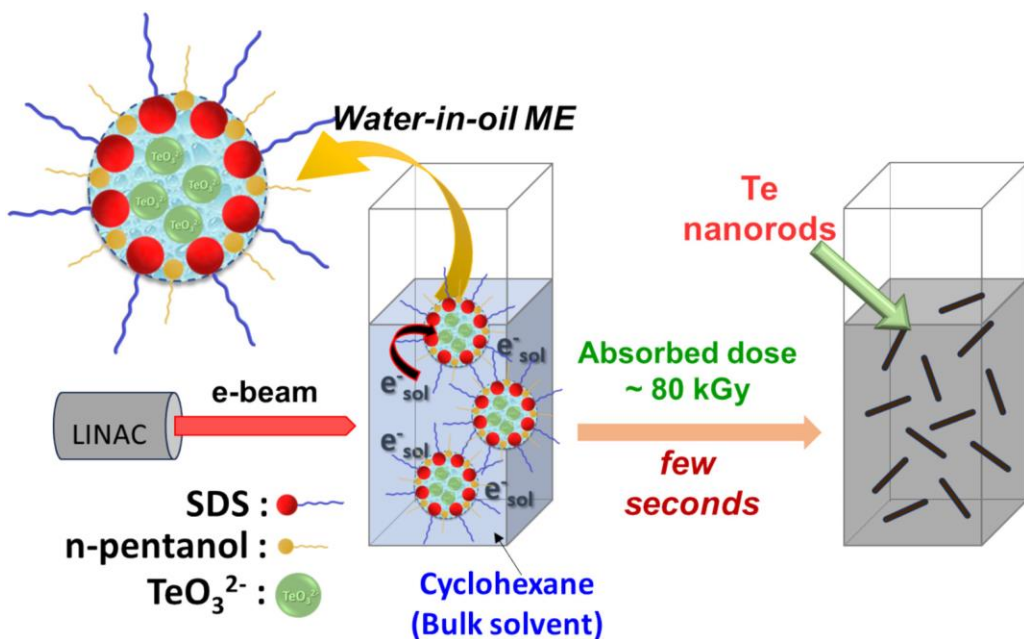
Inverted WbLS - water-in-oil emulsions

Key questions: what surfactant to use? What metal salt? What loading?
How do we optimize performance?

Large parameter space can be explored using automation → synthesis of metal salt and formulation can be automated



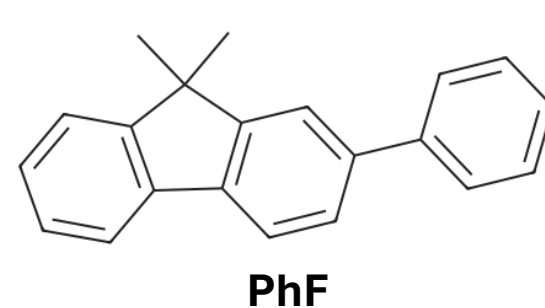
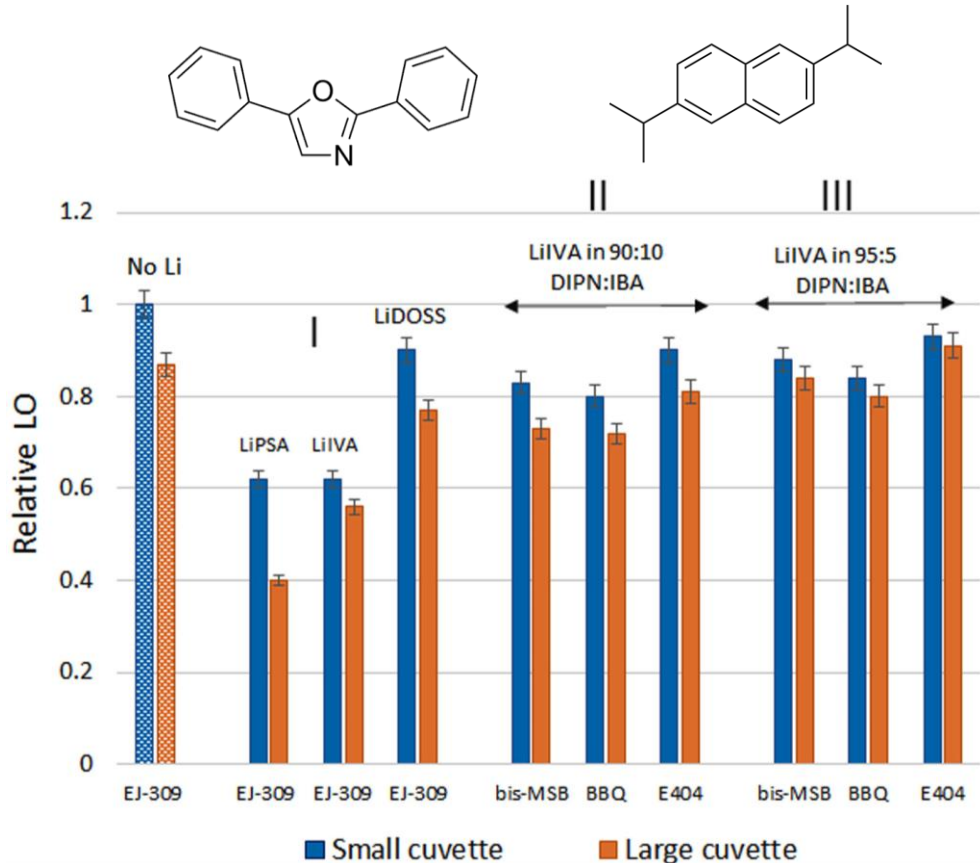
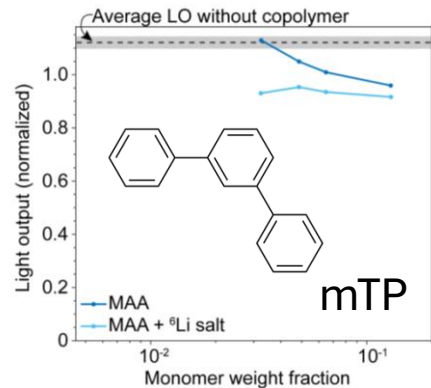
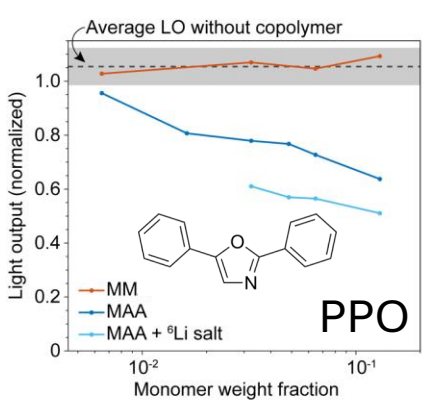
Water-in-oil emulsions can also be used to produce nanoparticles – may also be dispersed



Optical quality must be considered

Avoid deleterious effects of isotope loading – tune the liquid scintillator formulation

Some constituents of common scintillators (e.g., and especially, PPO) are sensitive to isotope loading strategies!



Composition	¹³⁷ Cs LO	PSD FoM	n _{th} ^o spot E, keV _{ee}	Hardness (Shore D)	Leaching
PPO					
30% PPO+0.2% bis-MSB in PVT	0.75	2.26	400	82	Slight
30% PPO+0.2% C460 in PVT	0.78	2.58	440	84	Slight
DIPN					
30% DIPN+0.5 %E404 in PS	1.15	3.55	570	75	No
30% DIPN+0.2% bis-MSB in PS	0.95	2.65	565	74	No
30% DIPN+0.2% C460 in PS	0.94	2.08	520	78	No
PhF					
30% PhF+0.2% bis-MSB in PVT	1.28	3.08	465	88	No
30% PhF+0.2% C460 in PVT	1.36	3.01	460	87	No
EJ-200	1.0	n/a	n/a	84	No

Isotope loading routes for liquid scintillators

How do we maximize/optimize isotope (e.g., Te, Mo) loading while minimizing impact on liquid scintillator performance?

Isotope loading strategies:

- Direct dissolution using organic ligands – **potential future strategies: alternative compatibilizers, drawing inspiration from other fields?**
- Emulsion of metal-loaded water in scintillating oil (inverted WbLS) – **potential future strategies: automated exploration and discovery of new compounds and formulations**
- Dispersion of nanoparticles – **potential future strategies: controlling size/shape/RI for stable, transparent dispersion**

Liquid scintillator formulating:

- Insensitive scintillating dyes/solvents – **potential future strategies: alternative dyes**