Agent Input/Output contract

Each lambda which calls a bedrock agent in the primary step function adheres to the following standardised contract. The summariser agent, which is the last stage of the step function is an outlier as it expects an array of agent outputs (ChatResponseModel).

Input Contract

```
{
  "question": string,
  "sessionId": string
}
```

example:

```
{
  "question": "Is there any data for Lansoprazole in the Ames test and what is the outcome?",
  "sessionId": "b744b736-0345-4add-86dc-cc3c829352d7"
}
```

Output Contract

```
export interface ChatResponseModel {
  question: string; // the input question
  response: string; // the output response of the agent
  metadata: AgentMetadataRecord[]; // metadata used to generate the response
  sessionId: string; // the chat session id
}

export interface LLMResponseModel extends ChatResponseModel {
  processDuration: ProcessDuration; // performance timing data for the lambda processing the invokeAgent or invokeModel bedrock call
}

export interface AgentResponseModel extends LLMResponseModel {
  agentId: string; // the id of the agent used
  agentAliasId: string; // the version of the agent used
}

// the types of metadata available
export enum AgentMetadataRecordType {
  VITIC = "vitic",
  KNOWLEDGEBASE = "knowledgeBase",
}

// vitic metadata structure
export type ViticMetadata = Record<string, any>;

```

```
// additional metadata from the bedrock kb
export interface KnowledgeBaseCitationMetadata {
  "x-amz-bedrock-kb-source-uri": string;
  "x-amz-bedrock-kb-document-page-number": number;
  "x-amz-bedrock-kb-chunk-id": string;
  "x-amz-bedrock-kb-data-source-id": string;
}

//knowledgebase metadata structure
export interface KnowledgeBaseCitation {
  text_excerpt: string;
  document_uri: string;
  page_number: number;
  reference_snippet: string;
  metadata: KnowledgeBaseCitationMetadata;
}

export type AgentMetadataRecord =
  | { type: AgentMetadataRecordType.VITIC; data: ViticMetadata }
  | {
      type: AgentMetadataRecordType.KNOWLEDGEBASE;
      data: KnowledgeBaseCitation;
    };

//timings in milliseconds for each phase of the agent processing
export interface ProcessDuration {
  total: number; // overall time taken
  process: number; //time between lambda start and agent request
  response: number; // time taken to make agent request
  parse: number; // time taken to stream agent response
}
```

example:

```
{
    "question": "Is beta-butyrolactone carcinogenic?",
    "response": "# Summary of Vitic Data\n\nThe Vitic data provides detailed information from various carcinogenicity studies on beta-butyrolactone. The key findings are:\n\n- Multiple studies conducted on rats and mice, including specific strains like Swiss, ICR/Ha, and Eastern Sprague-Dawley, found positive results for carcinogenicity.\n- The studies involved different routes of administration, including subcutaneous, dermal, gavage, and diet.\n- Doses varied, with some studies specifying exact amounts (e.g., 100 mg, 10%, 40.8 mg/kg/day) and others not providing details.\n- Exposure and experiment times were typically lifetime or chronic (e.g., 70 weeks), with one study involving a single dose.\n- The reliability of the studies ranged from reliable with restrictions to questionable reliability, based on Klimisch scores and Lhasa reliability grades.\n- Sources of the data included literature, the Carcinogenic Potency Database (CPDB), the International Agency for Research on Cancer (IARC) Monographs, and the EURL ECVAM Genotoxicity and Carcinogenicity Consolidated Database.\n- The IARC has classified beta-butyrolactone as a Group 2B carcinogen, possibly carcinogenic to humans.\n\n# Summary of Unstructured Data\n\nThe unstructured data provides information on the carcinogenicity and potential health risks of beta-butyrolactone, based on various studies and sources. The key findings are:\n\n- Beta-butyrolactone has been found to be carcinogenic in animal studies, producing tumors at the site of administration in mice and rats when applied to the skin, injected subcutaneously, or administered orally.\n- However, there is no direct evidence on the carcinogenicity of beta-butyrolactone in humans.\n- Beta-butyrolactone induced chromosomal aberrations in mammalian cells in vitro and was mutagenic to bacteria, suggesting it has genotoxic properties that could potentially lead to genetic mutations and associated health risks.\n- No specific safety precautions for handling beta-butyrolactone were provided, but general guidelines for working with hazardous chemicals were mentioned.\n- No non-carcinogenic alternatives to beta-butyrolactone for industrial or research applications were identified.\n\n# Combined Findings\n\nThe Vitic data and unstructured data consistently indicate that
```

```
beta-butyrolactone has been found to be carcinogenic in animal studies, primarily in rodents. The Vitic data provides detailed information on the specific studies, including the species, routes of administration, doses, and reliability assessments. The unstructured data summarizes the overall findings and potential health risks, such as genotoxicity and the lack of direct evidence on carcinogenicity in humans.\n\nBoth datasets highlight the need for appropriate safety precautions when handling beta-butyrolactone due to its potential carcinogenic and genotoxic properties. The IARC classification of beta-butyrolactone as a Group 2B carcinogen, possibly carcinogenic to humans, further emphasizes the potential risks associated with exposure to this substance.",
    "metadata": [
      {
        "type": "knowledgeBase",
        "data": {
          "text_excerpt": "Based on the search results, there is evidence that beta-butyrolactone (β-butyrolactone) is carcinogenic in animals. Specifically, it was found to be carcinogenic in mice by skin application and subcutaneous injection, and in rats by oral administration and subcutaneous injection, producing tumors at the site of administration in both species.",
          "document_uri": "s3://lhasalimited-gen-ai-unstructured-data-store-transform/zotero-papers/unknown/Morita et al. - 1997 - Evaluation of the rodent micronucleus assay in the.pdf",
          "reference_snippet": "[ ]2B-10 b-Butyrolactone 3068-88-0 w xFig. 2B-10     Ž .IARC Mono., 11, 225–229 IARC, 1976b     ( )The 6th CSGMT MN assay Positize MMS Ž .Commun., 2, 109–116 1994     Significant, dose-dependent and reproducible pos- itive responses were obtained in bone marrow cells after double intraperitoneal treatments of 1500 mgrkg per treatment, although marginal or negative results were observed after double intraperitoneal or intravenous treatments.     Other genotoxicity data     b-Butyrolactone induced chromosomal aberra- Žtions in mammalian cells in vitro Loveday et al.,     .1989; Asanami et al., 1994 and was mutagenic to Ž .bacteria Zeiger et al., 1992; Asanami et al., 1994 .     ( )EÕidence for carcinogenicity to humans No data     EÕidence for carcinogenicity to animals ( )Sufficient     b-Butyrolactone was carcinogenic in mice by skin application and subcutaneous injection and in rats by oral administration and subcutaneous injection. It produced tumors at the site of administration in both species.",
          "metadata": {
            "x-amz-bedrock-kb-source-uri": "s3://lhasalimited-gen-ai-unstructured-data-store-transform/zotero-papers/unknown/Morita et al. - 1997 - Evaluation of the rodent micronucleus assay in the.pdf",
            "x-amz-bedrock-kb-document-page-number": 61,
            "x-amz-bedrock-kb-chunk-id": "1%3A0%3AapYI6JUBBXAqwfBUmZd2",
            "x-amz-bedrock-kb-data-source-id": "Q90PNFXDG3"
          },
          "year": null,
          "doi": null,
          "issue": null,
          "page_number": 61
        }
      },
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        "type": "knowledgeBase",
        "data": {
          "text_excerpt": "Based on the search results, beta-butyrolactone (BL-I) is not classified as a potential carcinogen by regulatory agencies. The results indicate that BL-I has been studied for its antitumor and cancer cell growth inhibitory activities against various cancer cell lines. One result states that the National Toxicology Program (NTP) concluded that there is a high likelihood that 1,4-butanediol, which is rapidly metabolized to gamma-hydroxybutyric acid like BL-I, would be negative for carcinogenicity in animal studies.",
          "document_uri": "s3://lhasalimited-gen-ai-unstructured-data-store-transform/zotero-papers/Xenobiotica/An et al. - 2017 - Isolation and identification of phase I metabolite.pdf",
          "reference_snippet": "BL-I and metabolites M-4 and M-5 exhibited potent cancer cell growth inhibitory activities against HL-60 (human leukemia) cell lines with the IC50 values of 13.2, 28.8 and 35.7mM, respectively.     4. On the basis of metabolites profile, a possible metabolism pathway for BL-I in rats has been proposed. This is the first systematic study on the phase I metabolites of BL-I.     Keywords
```

```
Butyrolactone I, cyclization, hydroxylation, metabolites     History     Received 17 February 2016 Revised 25 March 2016 Accepted 26 March 2016 Published online 7 September 2016     Introduction     Butyrolactone I (BL-I), a naturally occurring CDK (cyclin-     dependent kinase)-specific inhibitor isolated from Aspergillus terreus var. africanus IFO 8835, was first described in 1977     (Kiriyama et al., 1977). CDKs play a central role in the     regulation of the cell division cycle, which makes them a     promising target for the development of cancer therapeutic     agents. The CDK inhibitors block cell cycle progression and     display interesting antitumor activities (Huwe et al., 2003).",
          "metadata": {
            "x-amz-bedrock-kb-source-uri": "s3://lhasalimited-gen-ai-unstructured-data-store-transform/zotero-papers/Xenobiotica/An et al. - 2017 - Isolation and identification of phase I metabolite.pdf",
            "x-amz-bedrock-kb-document-page-number": 2,
            "x-amz-bedrock-kb-chunk-id": "1%3A0%3A7d9S6JUBUdEW4Xj0mK1v",
            "x-amz-bedrock-kb-data-source-id": "Q90PNFXDG3"
          },
          "year": null,
          "doi": null,
          "issue": null,
          "page_number": 2
        }
      },
      {
        "type": "knowledgeBase",
        "data": {
          "text_excerpt": "Based on the search results, beta-butyrolactone (BL-I) is not classified as a potential carcinogen by regulatory agencies. The results indicate that BL-I has been studied for its antitumor and cancer cell growth inhibitory activities against various cancer cell lines. One result states that the National Toxicology Program (NTP) concluded that there is a high likelihood that 1,4-butanediol, which is rapidly metabolized to gamma-hydroxybutyric acid like BL-I, would be negative for carcinogenicity in animal studies.",
          "document_uri": "s3://lhasalimited-gen-ai-unstructured-data-store-transform/pubmed/11803699.txt",
          "reference_snippet": "Because of the rapid and extensive conversion of gamma-butyrolactone to gamma-hydroxybutyric acid, the evaluation of gamma-butyrolactone was in fact an evaluation of gamma-hydroxybutyric acid. This summary report presents a review of the current literature which documents that both 1,4-butanediol and gamma-butyrolactone are rapidly metabolized to gamma-hydroxybutyric acid, and the pharmacologic and toxicologic responses to these chemicals are due to their metabolic conversion to gamma-hydroxybutyric acid. Because the toxicity and carcinogenicity of gamma-hydroxybutyric acid was fully evaluated in the NTP studies of gamma-butyrolactone, and a lack of organ-specific toxicity or carcinogenic potential was demonstrated, it is concluded that there is a high likelihood that 1,4-butanediol would be negative in a similar set of studies. For these reasons, it is the opinion of the NTP that 1,4-butanediol should be considered not carcinogenic in animals and no further evaluation of 1,4-butanediol is needed at this time.",
          "metadata": {
            "x-amz-bedrock-kb-source-uri": "s3://lhasalimited-gen-ai-unstructured-data-store-transform/pubmed/11803699.txt",
            "x-amz-bedrock-kb-document-page-number": null,
            "x-amz-bedrock-kb-chunk-id": "1%3A6%3Auqgf-ZUBBXAqwfBU_dD6",
            "x-amz-bedrock-kb-data-source-id": "Q90PNFXDG3"
          },
          "year": null,
          "doi": null,
          "issue": null,
          "page_number": "N/A"
        }
      },
      {
        "type": "knowledgeBase",
        "data": {
```

```
          "text_excerpt": "\nAnother result (source ba7b) provides general guidelines for working with hazardous chemicals, such as following procedures outlined in \"Prudent Practices in the Laboratory\", conducting risk assessments, using proper protective equipment, and properly disposing of chemical waste. While not specific to beta-butyrolactone, these would be prudent precautions when handling any potentially hazardous substance.",
          "document_uri": "s3://lhasalimited-gen-ai-unstructured-data-store-transform/zotero-papers/Organic Syntheses/Nottingham - 2018 - Trimethylsilyldiazo[13C]methane A Versatile 13C-L.pdf",
          "reference_snippet": "Replacing the balloons to ensure an excess of H2 is essential.      Working with Hazardous Chemicals     The procedures in Organic Syntheses are intended for use only by persons with proper training in experimental organic chemistry. All hazardous materials should be handled using the standard procedures for work with chemicals described in references such as \"Prudent Practices in the Laboratory\" (The National Academies Press, Washington, D.C., 2011; the full text can be accessed free of charge at http://www.nap.edu/catalog.php?record_id=12654). All chemical waste should be disposed of in accordance with local regulations. For general guidelines for the management of chemical waste, see Chapter 8 of Prudent Practices.     In some articles in Organic Syntheses, chemical-specific hazards are highlighted in red “Caution Notes” within a procedure. It is important to recognize that the absence of a caution note does not imply that no significant hazards are associated with the chemicals involved in that procedure. Prior to performing a reaction, a thorough risk assessment should be carried out that includes a review of the potential hazards associated with each chemical and experimental operation on the scale that is planned for the procedure. Guidelines for carrying out a risk assessment and for analyzing the hazards associated with chemicals can be found in Chapter 4 of Prudent Practices.     The procedures described in Organic Syntheses are provided as published and are conducted at one's own risk. Organic Syntheses, Inc., itsOrg.",
          "metadata": {
            "x-amz-bedrock-kb-source-uri": "s3://lhasalimited-gen-ai-unstructured-data-store-transform/zotero-papers/Organic Syntheses/Nottingham - 2018 - Trimethylsilyldiazo[13C]methane A Versatile 13C-L.pdf",
            "x-amz-bedrock-kb-document-page-number": 21,
            "x-amz-bedrock-kb-chunk-id": "1%3A0%3Aopb_55UBBXAqwfBUgF21",
            "x-amz-bedrock-kb-data-source-id": "Q90PNFXDG3"
          },
          "year": null,
          "doi": null,
          "issue": null,
          "page_number": 21
        }
      },
      {
        "type": "knowledgeBase",
        "data": {
          "text_excerpt": "Based on the search results, there is no direct mention of non-carcinogenic alternatives to beta-butyrolactone for industrial or research applications. However, some information suggests that beta-butyrolactone itself is carcinogenic and has been shown to induce tumors in animal studies.",
          "document_uri": "s3://lhasalimited-gen-ai-unstructured-data-store-transform/zotero-papers/Toxicologic Pathology/Cohen - 2001 - Alternative Models for Carcinogenicity Testing We.pdf",
          "reference_snippet": "However, those without a designation are con- sidered to be putative human noncarcinogens for a variety of reasons. Details regarding the results for various chem- icals in any given model are described in the publications from this workshop by the speci\ufffd c working group for those models.     NONGENOTOXIC NONCARCINOGENS     Ampicillin, D-mannitol, and sul\ufffd soxazole are accepted as nongenotoxic chemicals that are noncarcinogenic in animal models. Although they have not been evaluated by speci\ufffd c epidemiologic investigations, there has been no evidence of a carcinogenic hazard from these pharmaceutical chemicals after widespread clinical usage for many years. They were negative in all of the in vivo models in which they wereVol. 29(Suppl.), 2001 WEIGHT OF EVIDENCE EVALUATIONS ACROSS MODELS 185 TABLE 2.—Evaluation of the results in the various models as determined by the Assay Working Groups. Chemical Ratsa Micea Genotoxb p53 / RasH2 TgAC—dermal TgAC—oral XPA XPA/p53 Neonatal SHE Humanc Cyclophosphamide (G)d (G) Eq.e, f (G) Melphalan (IP) Eq.",
          "metadata": {
```

```
            "x-amz-bedrock-kb-source-uri": "s3://lhasalimited-gen-ai-unstructured-data-store-transform/zotero-papers/Toxicologic Pathology/Cohen - 2001 - Alternative Models for Carcinogenicity Testing We.pdf",
            "x-amz-bedrock-kb-document-page-number": 2,
            "x-amz-bedrock-kb-chunk-id": "1%3A1%3Aj5qI6JUBBXAqwfBU79Fx",
            "x-amz-bedrock-kb-data-source-id": "Q90PNFXDG3"
          },
          "year": null,
          "doi": null,
          "issue": null,
          "page_number": 2
        }
      },
      {
        "type": "vitic",
        "data": {
          "Result": "Positive",
          "Species": "Rat",
          "Strain": "Not specified",
          "Sex": "Not specified",
          "Test Type": "Lifetime study",
          "Guideline": "Not specified",
          "Year": null,
          "Route of Administration": "Subcutaneous",
          "Dose": "100 mg",
          "Vehicle": "Tricaprylin",
          "Exposure Time": "Lifetime",
          "Experiment Time": "Lifetime",
          "Frequency": "Not specified",
          "GLP": "Not specified",
          "Klimisch Score": "4- Not assignable",
          "Lhasa Reliability Grade": "B",
          "Lhasa Reliability": "Questionable reliability - some minor deviations from guidelines",
          "Source": "Literature"
        }
      },
      {
        "type": "vitic",
        "data": {
          "Result": "Positive",
          "Species": "Mouse",
          "Strain": "Swiss",
          "Sex": "Female",
          "Test Type": "Lifetime study",
          "Guideline": "Not specified",
          "Year": 1965,
          "Route of Administration": "Dermal",
          "Dose": "10%",
          "Vehicle": "Benzene",
          "Exposure Time": "Lifetime",
          "Experiment Time": "Lifetime",
          "Frequency": "3/week",
          "GLP": "Not specified",
          "Klimisch Score": "2- Reliable with restrictions",
          "Lhasa Reliability Grade": "B",
          "Lhasa Reliability": "Questionable reliability - some minor deviations from guidelines",
          "Source": "Literature"
        }
```

```
      },
      {
        "type": "vitic",
        "data": {
          "Result": "Positive",
          "Species": "Mouse",
          "Strain": "Not specified",
          "Sex": "Not specified",
          "Test Type": "Lifetime study",
          "Guideline": "Not specified",
          "Year": null,
          "Route of Administration": "Subcutaneous",
          "Dose": "10 mg",
          "Vehicle": "Tricaprylin",
          "Exposure Time": "Lifetime",
          "Experiment Time": "Lifetime",
          "Frequency": "Not specified",
          "GLP": "Not specified",
          "Klimisch Score": "4- Not assignable",
          "Lhasa Reliability Grade": "B",
          "Lhasa Reliability": "Questionable reliability - some minor deviations from guidelines",
          "Source": "Literature"
        }
      },
      {
        "type": "vitic",
        "data": {
          "Result": "Positive",
          "Species": "Rat",
          "Strain": "Eastern Sprague-Dawley",
          "Sex": "Female",
          "Test Type": "Chronic study",
          "Guideline": "Not specified",
          "Year": 1966,
          "Route of Administration": "Gavage",
          "Dose": "40.8 mg/kg/day",
          "Vehicle": "Not specified",
          "Exposure Time": "70 week(s)",
          "Experiment Time": "70 week(s)",
          "Frequency": "Not specified",
          "GLP": "Not specified",
          "Klimisch Score": "4- Not assignable",
          "Lhasa Reliability Grade": "C",
          "Lhasa Reliability": "Unreliable - Significant deviations from guidelines",
          "Source": "Carcinogenic Potency Database (CPDB)"
        }
      },
      {
        "type": "vitic",
        "data": {
          "Result": "Positive",
          "Species": "Rat",
          "Strain": "Not specified",
          "Sex": "Not specified",
          "Test Type": "Lifetime study",
          "Guideline": "Not specified",
          "Year": null,
          "Route of Administration": "Diet",
```

```
          "Dose": "Not specified",
          "Vehicle": "Feed",
          "Exposure Time": "Lifetime",
          "Experiment Time": "Lifetime",
          "Frequency": "Not specified",
          "GLP": "Not specified",
          "Klimisch Score": "4- Not assignable",
          "Lhasa Reliability Grade": "A",
          "Lhasa Reliability": "Reliable - Conforms to guidelines",
          "Source": "Literature"
        }
      },
      {
        "type": "vitic",
        "data": {
          "Result": "Positive",
          "Species": "Mouse",
          "Strain": "ICR/Ha",
          "Sex": "Female",
          "Test Type": "Lifetime study",
          "Guideline": "Not specified",
          "Year": 1968,
          "Route of Administration": "Dermal",
          "Dose": "10 mg",
          "Vehicle": "Benzene",
          "Exposure Time": "Lifetime",
          "Experiment Time": "Lifetime",
          "Frequency": "3/week",
          "GLP": "Not specified",
          "Klimisch Score": "4- Not assignable",
          "Lhasa Reliability Grade": "B",
          "Lhasa Reliability": "Questionable reliability - some minor deviations from guidelines",
          "Source": "Literature"
        }
      },
      {
        "type": "vitic",
        "data": {
          "Result": "Positive",
          "Species": "Mouse",
          "Strain": "Swiss",
          "Sex": "Female",
          "Test Type": "Initiation-promotion assay",
          "Guideline": "Not specified",
          "Year": 1965,
          "Route of Administration": "Dermal",
          "Dose": "1 mg",
          "Vehicle": "Not specified",
          "Exposure Time": "Single dose",
          "Experiment Time": "Not specified",
          "Frequency": "Single dose",
          "GLP": "Not specified",
          "Klimisch Score": "2- Reliable with restrictions",
          "Lhasa Reliability Grade": "B",
          "Lhasa Reliability": "Questionable reliability - some minor deviations from guidelines",
          "Source": "Literature"
        }
      },
```

```
      {
        "type": "vitic",
        "data": {
          "Result": "Group 2B- Possibly carcinogenic to humans",
          "Species": "Not applicable",
          "Strain": "Not applicable",
          "Sex": "Not applicable",
          "Test Type": "Overall",
          "Guideline": "Not specified",
          "Year": 1999,
          "Route of Administration": "Not applicable",
          "Dose": "Not applicable",
          "Vehicle": "Not applicable",
          "Exposure Time": "Not applicable",
          "Experiment Time": "Not applicable",
          "Frequency": "Not applicable",
          "GLP": "Not applicable",
          "Klimisch Score": "1- Reliable without restriction",
          "Lhasa Reliability Grade": "B",
          "Lhasa Reliability": "Questionable reliability - some minor deviations from guidelines",
          "Source": "International Agency for Research on Cancer (IARC) Monographs"
        }
      },
      {
        "type": "vitic",
        "data": {
          "Result": "Positive",
          "Species": "Not applicable",
          "Strain": "Not applicable",
          "Sex": "Not applicable",
          "Test Type": "Overall",
          "Guideline": "Not specified",
          "Year": 2014,
          "Route of Administration": "Not applicable",
          "Dose": "Not applicable",
          "Vehicle": "Not applicable",
          "Exposure Time": "Not applicable",
          "Experiment Time": "Not applicable",
          "Frequency": "Not applicable",
          "GLP": "Not applicable",
          "Klimisch Score": "4- Not assignable",
          "Lhasa Reliability Grade": "B",
          "Lhasa Reliability": "Questionable reliability - some minor deviations from guidelines",
          "Source": "EURL ECVAM Genotoxicity and Carcinogenicity Consolidated Database"
        }
      }
    ],
    "sessionId": "35dbf53b-e57b-41a0-989a-f827b5a939ef",
    "processDuration": {
      "total": 19.1571,
      "process": 0.0006,
      "response": 0.1397,
      "parse": 19.0168
    },
    "agentId": "6NRUGQASJK",
    "agentAliasId": "KLK0CDMP0O"
  }
```